



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 01:10 AM UTC

PDB ID : 9ZD8 / pdb_00009zd8
EMDB ID : EMD-74057
Title : The cryo-EM structure of Pakpunavirus P7-1 baseplate in extended status
Authors : Li, F.; Cingolani, G.
Deposited on : 2025-11-25
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

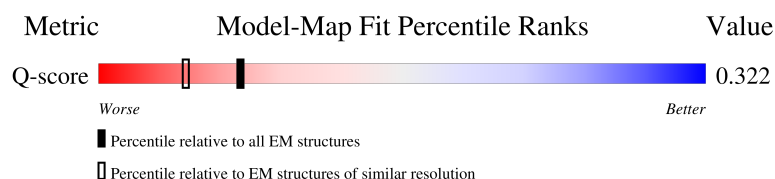
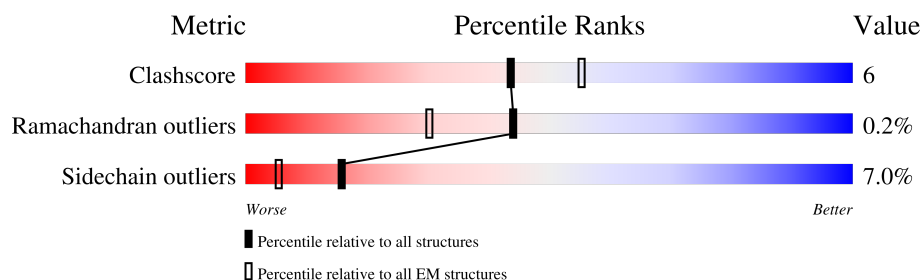
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	487	 6% 78% 19% .
1	L	487	 5% 78% 20% .
1	M	487	 0% 80% 17% .
1	N	487	 0% 80% 18% .


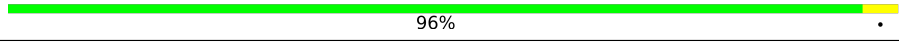
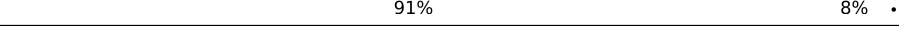
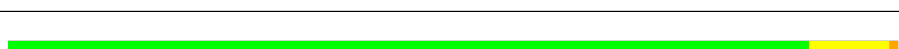
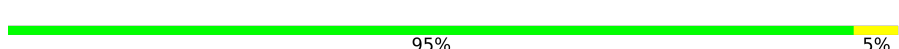
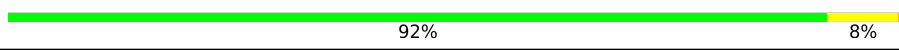

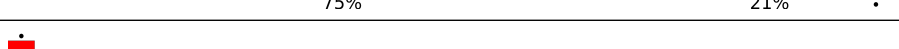



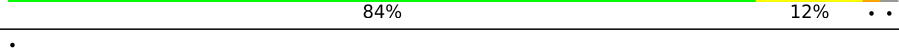

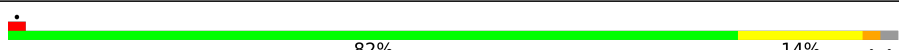


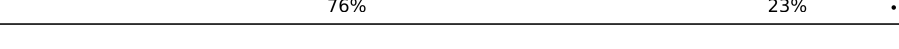







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Mol	Chain	Length	Quality of chain
1	V	487	
1	W	487	
1	X	487	
1	f	487	
1	g	487	
1	h	487	
1	o	487	
1	u	487	
2	l	243	
2	O	243	
2	Y	243	
2	i	243	
2	p	243	
2	v	243	
3	A	253	
3	B	253	
3	C	253	
3	D	253	
3	E	253	
3	F	253	
4	G	159	
4	Q	159	
4	a	159	
4	k	159	
4	q	159	

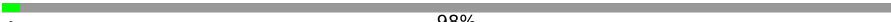
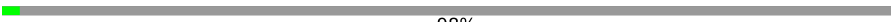







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Mol	Chain	Length	Quality of chain
4	w	159	
5	H	166	
5	R	166	
5	b	166	
5	l	166	
5	r	166	
5	x	166	
6	I	118	
6	S	118	
6	c	118	
6	m	118	
6	s	118	
6	y	118	
7	K	123	
7	U	123	
7	e	123	
7	n	123	
7	t	123	
7	z	123	
8	P	246	
8	Z	246	
8	j	246	
9	J	305	
9	T	305	
9	d	305	

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Mol	Chain	Length	Quality of chain
10	2	788	 98%
10	3	788	 98%
10	4	788	 98%
10	5	788	 98%
10	6	788	 98%
10	7	788	 98%
10	8	788	 96%
10	9	788	 96%
10	AA	788	 96%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 107757 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called gp88.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	486	Total 3681	C 2324	N 618	O 731	S 8	0	0
1	L	486	Total 3681	C 2324	N 618	O 731	S 8	0	0
1	M	486	Total 3681	C 2324	N 618	O 731	S 8	0	0
1	N	486	Total 3681	C 2324	N 618	O 731	S 8	0	0
1	V	486	Total 3681	C 2324	N 618	O 731	S 8	0	0
1	W	486	Total 3681	C 2324	N 618	O 731	S 8	0	0
1	X	486	Total 3681	C 2324	N 618	O 731	S 8	0	0
1	f	486	Total 3681	C 2324	N 618	O 731	S 8	0	0
1	g	486	Total 3681	C 2324	N 618	O 731	S 8	0	0
1	h	486	Total 3681	C 2324	N 618	O 731	S 8	0	0
1	o	486	Total 3681	C 2324	N 618	O 731	S 8	0	0
1	u	486	Total 3681	C 2324	N 618	O 731	S 8	0	0

- Molecule 2 is a protein called gp89.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	242	Total 1879	C 1201	N 315	O 362	S 1	0	0
2	O	242	Total 1879	C 1201	N 315	O 362	S 1	0	0
2	Y	242	Total 1879	C 1201	N 315	O 362	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	i	242	Total	C	N	O	S	0	0
			1879	1201	315	362	1		
2	p	242	Total	C	N	O	S	0	0
			1879	1201	315	362	1		
2	v	242	Total	C	N	O	S	0	0
			1879	1201	315	362	1		

- Molecule 3 is a protein called gp83.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	237	Total	C	N	O	S	0	0
			1876	1174	323	376	3		
3	B	237	Total	C	N	O	S	0	0
			1876	1174	323	376	3		
3	C	237	Total	C	N	O	S	0	0
			1876	1174	323	376	3		
3	D	237	Total	C	N	O	S	0	0
			1876	1174	323	376	3		
3	E	237	Total	C	N	O	S	0	0
			1876	1174	323	376	3		
3	F	237	Total	C	N	O	S	0	0
			1876	1174	323	376	3		

- Molecule 4 is a protein called gp79.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	158	Total	C	N	O	S	0	0
			1237	775	216	241	5		
4	Q	158	Total	C	N	O	S	0	0
			1237	775	216	241	5		
4	a	158	Total	C	N	O	S	0	0
			1237	775	216	241	5		
4	k	158	Total	C	N	O	S	0	0
			1237	775	216	241	5		
4	q	158	Total	C	N	O	S	0	0
			1237	775	216	241	5		
4	w	158	Total	C	N	O	S	0	0
			1237	775	216	241	5		

- Molecule 5 is a protein called gp78.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	166	Total	C	N	O	S	0	0
			1281	818	212	243	8		
5	R	166	Total	C	N	O	S	0	0
			1281	818	212	243	8		
5	b	166	Total	C	N	O	S	0	0
			1281	818	212	243	8		
5	l	166	Total	C	N	O	S	0	0
			1281	818	212	243	8		
5	r	166	Total	C	N	O	S	0	0
			1281	818	212	243	8		
5	x	166	Total	C	N	O	S	0	0
			1281	818	212	243	8		

- Molecule 6 is a protein called gp84.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	114	Total	C	N	O	S	0	0
			956	624	152	176	4		
6	S	114	Total	C	N	O	S	0	0
			956	624	152	176	4		
6	c	114	Total	C	N	O	S	0	0
			956	624	152	176	4		
6	m	114	Total	C	N	O	S	0	0
			956	624	152	176	4		
6	s	114	Total	C	N	O	S	0	0
			956	624	152	176	4		
6	y	114	Total	C	N	O	S	0	0
			956	624	152	176	4		

- Molecule 7 is a protein called gp87.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	120	Total	C	N	O	S	0	0
			979	628	163	183	5		
7	U	120	Total	C	N	O	S	0	0
			979	628	163	183	5		
7	e	120	Total	C	N	O	S	0	0
			979	628	163	183	5		
7	n	120	Total	C	N	O	S	0	0
			979	628	163	183	5		
7	t	120	Total	C	N	O	S	0	0
			979	628	163	183	5		
7	z	120	Total	C	N	O	S	0	0
			979	628	163	183	5		

- Molecule 8 is a protein called gp86.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	246	Total	C	N	O	S	0	0
			1874	1168	339	357	10		
8	Z	246	Total	C	N	O	S	0	0
			1874	1168	339	357	10		
8	j	246	Total	C	N	O	S	0	0
			1874	1168	339	357	10		

- Molecule 9 is a protein called gp85.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	304	Total	C	N	O	S	0	0
			2364	1463	415	475	11		
9	T	304	Total	C	N	O	S	0	0
			2364	1463	415	475	11		
9	d	304	Total	C	N	O	S	0	0
			2364	1463	415	475	11		

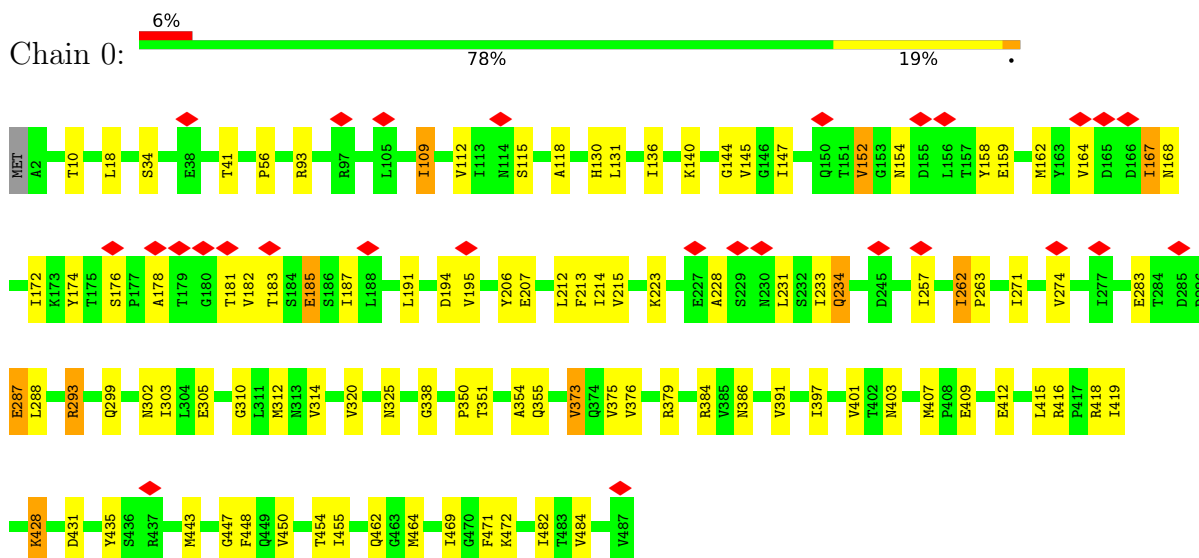
- Molecule 10 is a protein called gp88.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	19	Total	C	N	O		0	0
			143	85	27	31			
10	2	19	Total	C	N	O		0	0
			143	85	27	31			
10	3	19	Total	C	N	O		0	0
			143	85	27	31			
10	5	19	Total	C	N	O		0	0
			143	85	27	31			
10	6	19	Total	C	N	O		0	0
			143	85	27	31			
10	7	19	Total	C	N	O		0	0
			143	85	27	31			
10	8	32	Total	C	N	O	S	0	0
			255	152	45	57	1		
10	9	32	Total	C	N	O	S	0	0
			255	152	45	57	1		
10	AA	32	Total	C	N	O	S	0	0
			255	152	45	57	1		

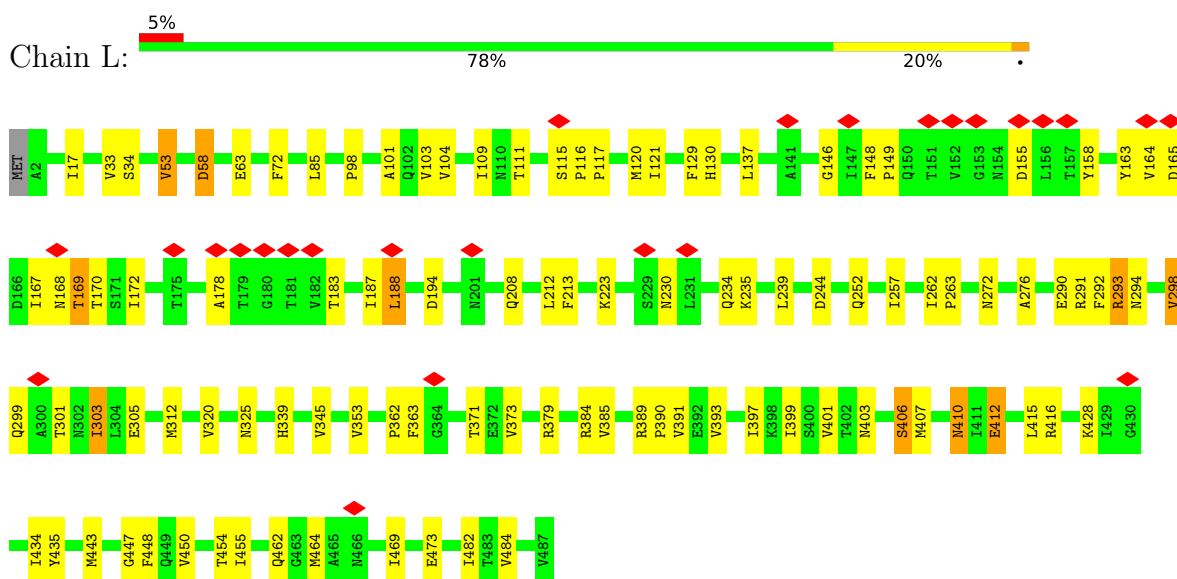
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

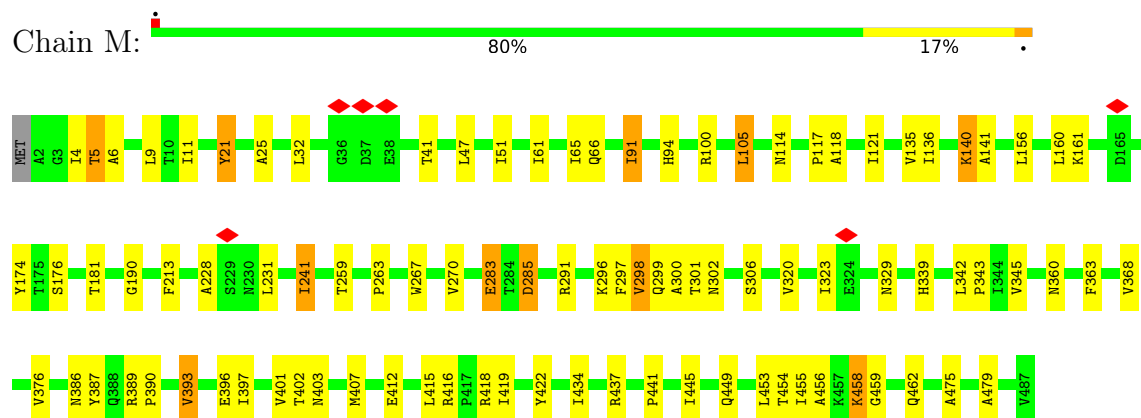
• Molecule 1: gp88



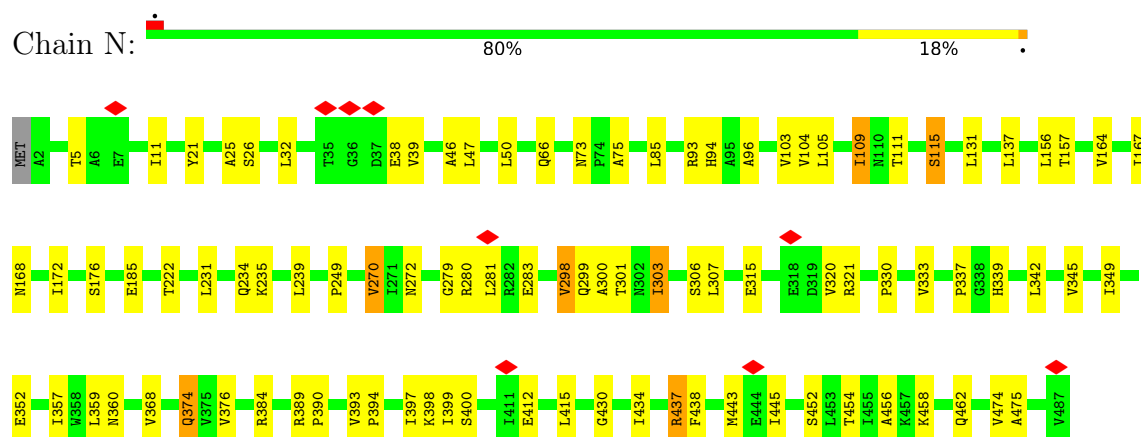
• Molecule 1: gp88



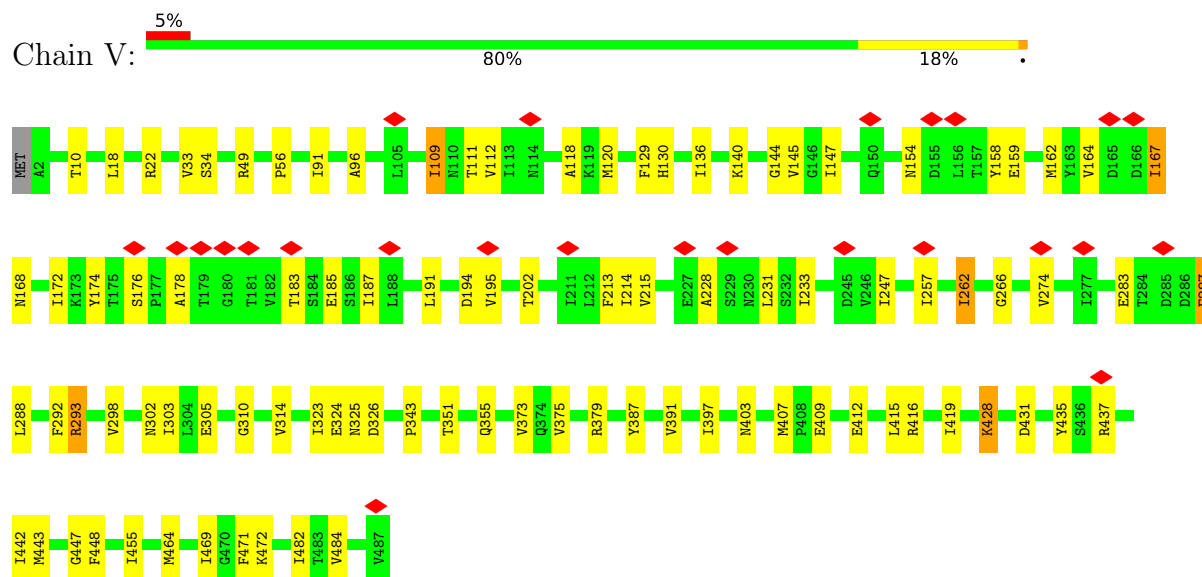
• Molecule 1: gp88



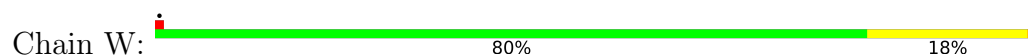
- Molecule 1: gp88

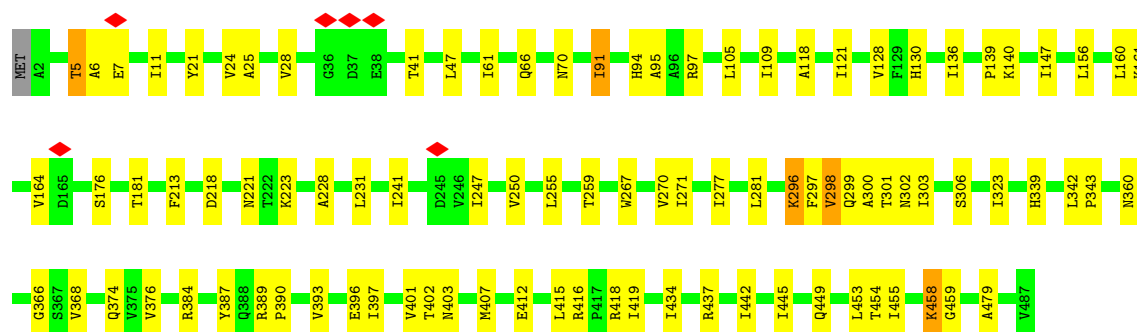


- Molecule 1: gp88

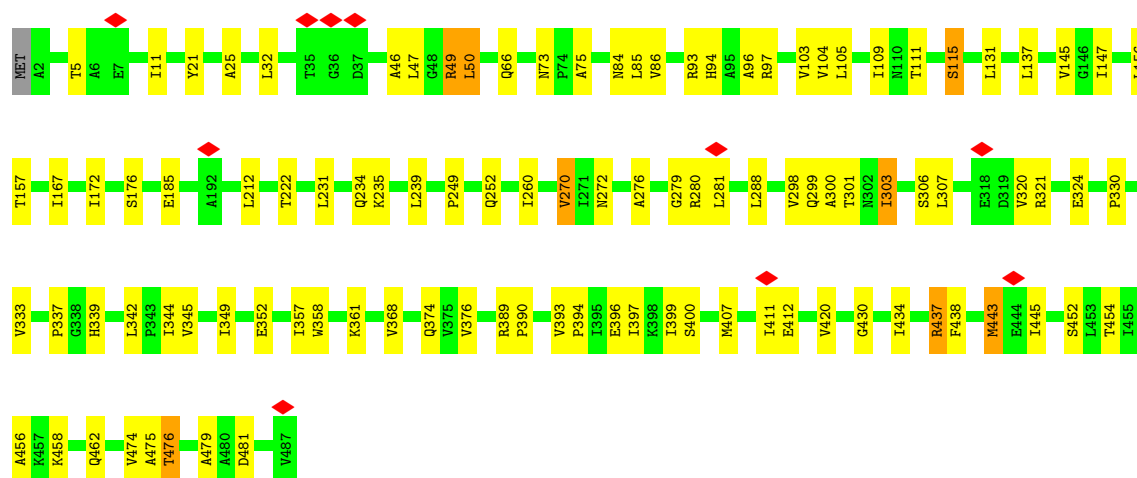
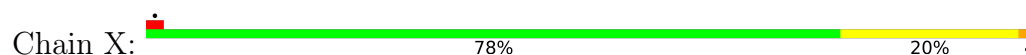


- Molecule 1: gp88

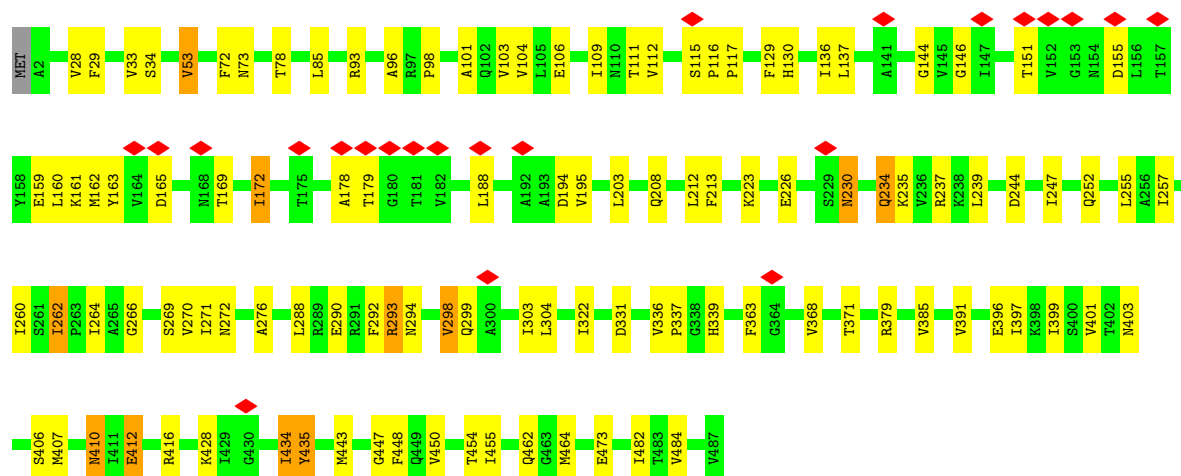
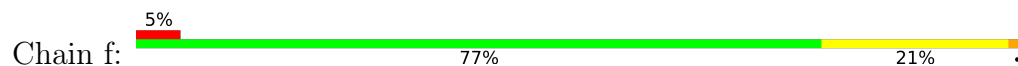




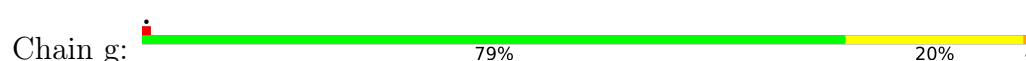
• Molecule 1: gp88

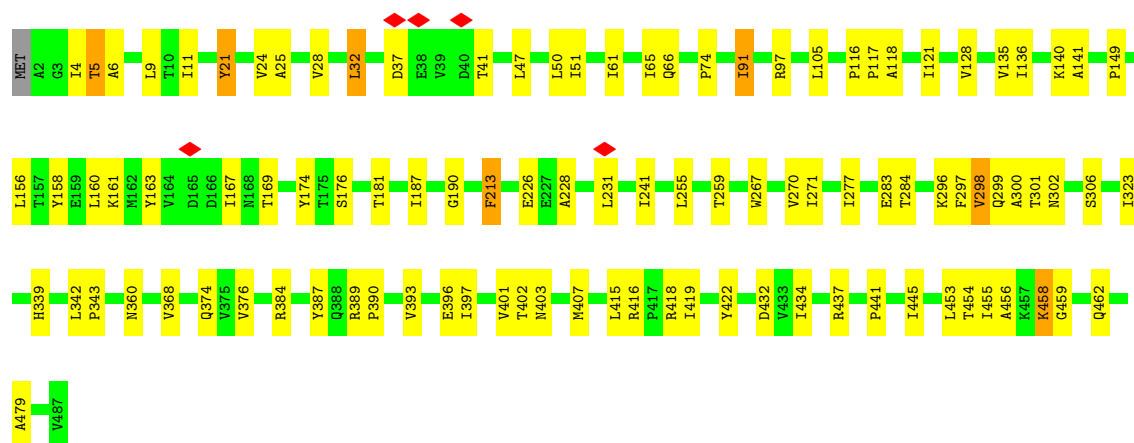


• Molecule 1: gp88



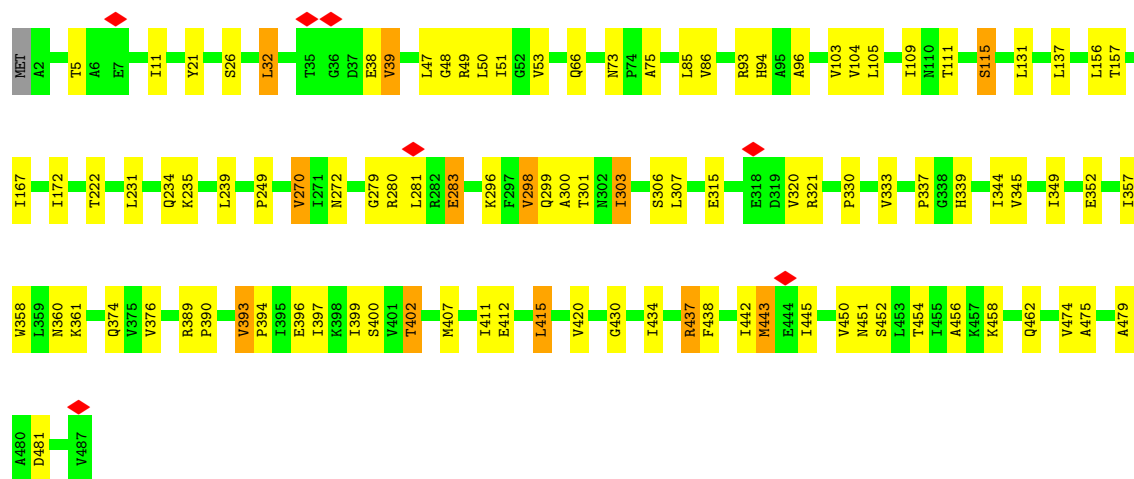
• Molecule 1: gp88





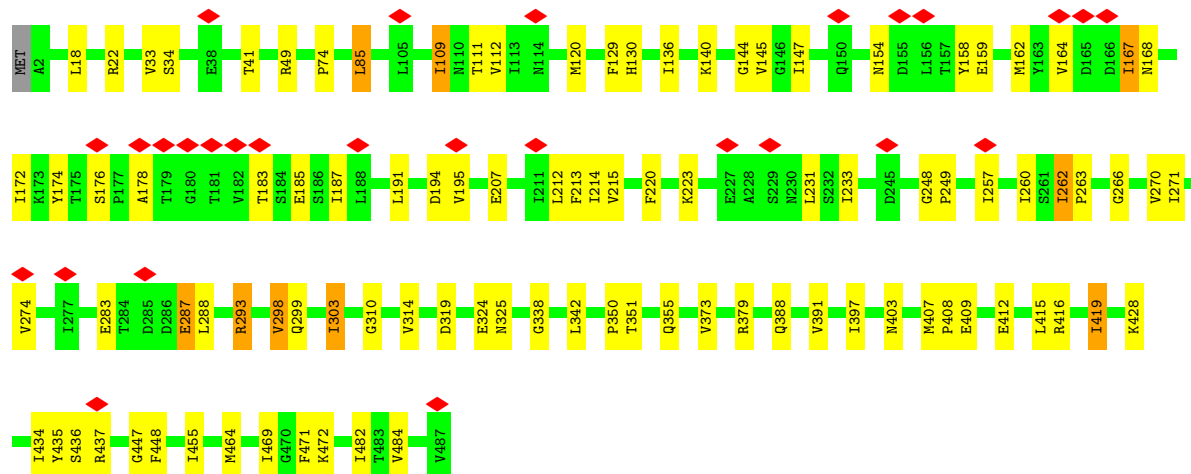
• Molecule 1: gp88

Chain h: 79% 18%

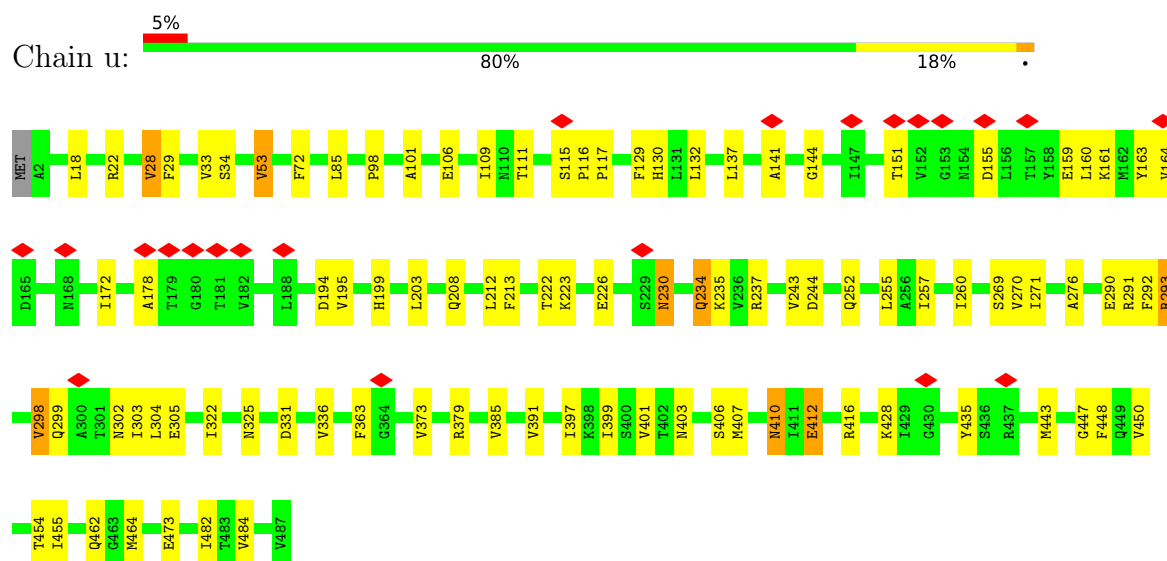


• Molecule 1: gp88

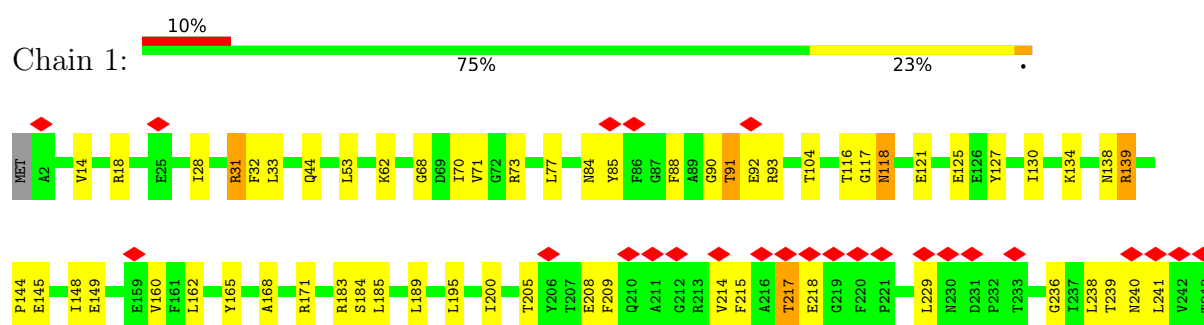
Chain o: 6% 79% 18%



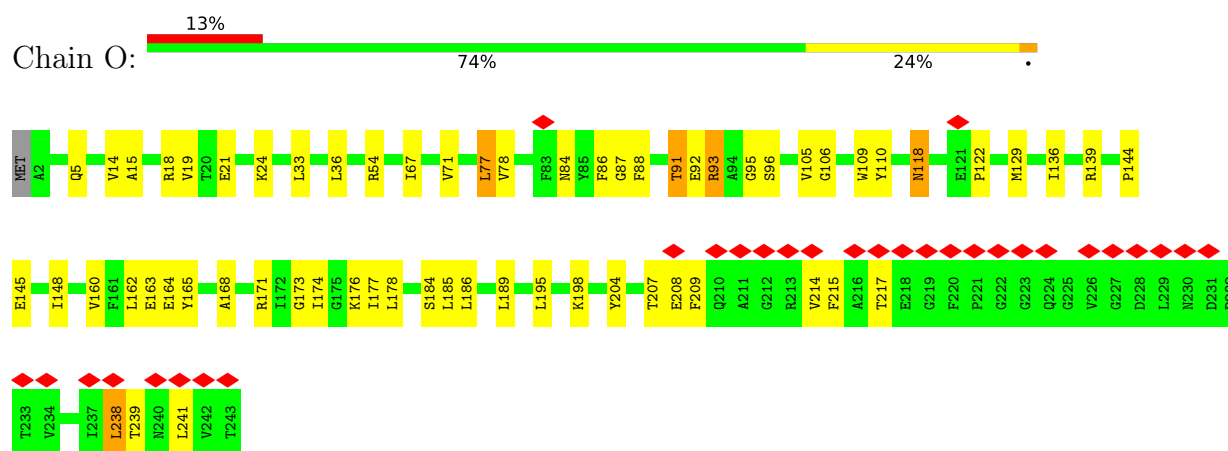
- Molecule 1: gp88



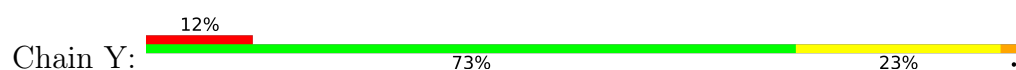
- Molecule 2: gp89

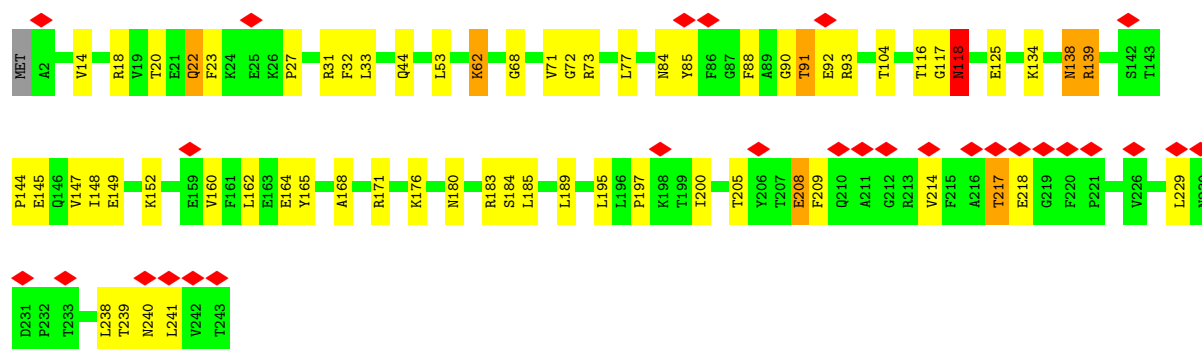


- Molecule 2: gp89

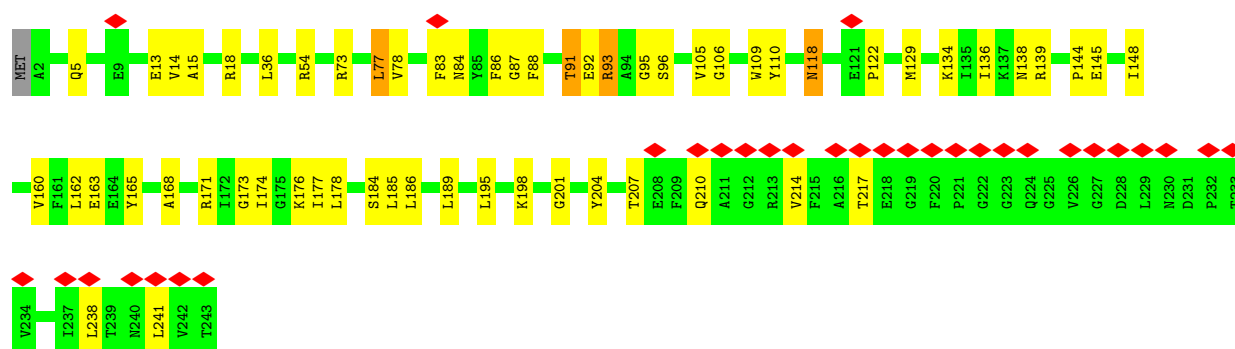
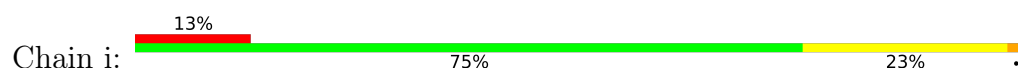


- Molecule 2: gp89

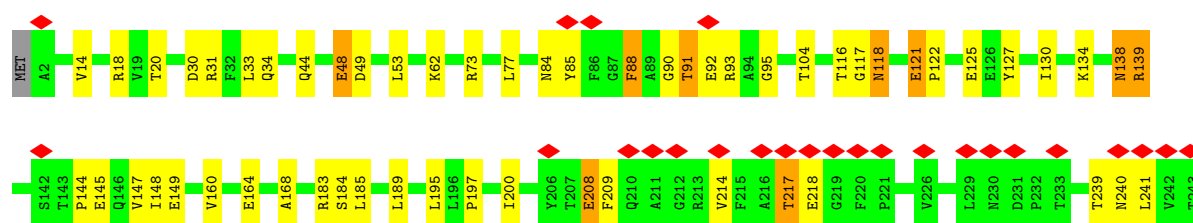
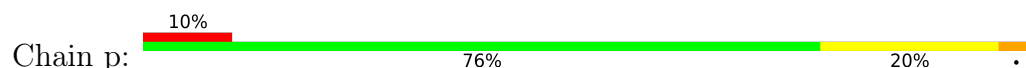




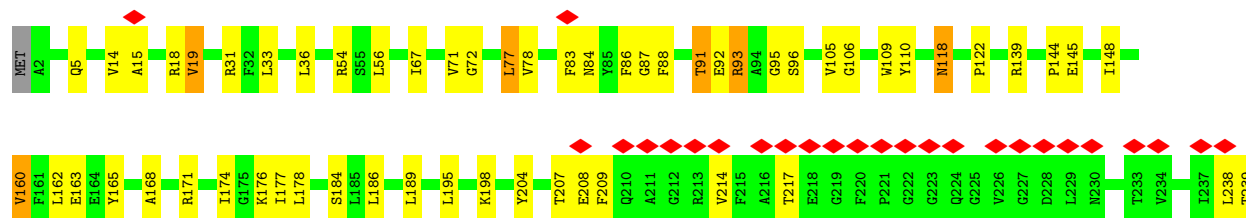
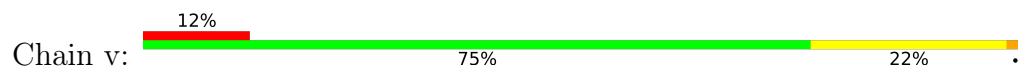
• Molecule 2: gp89

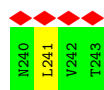


• Molecule 2: gp89



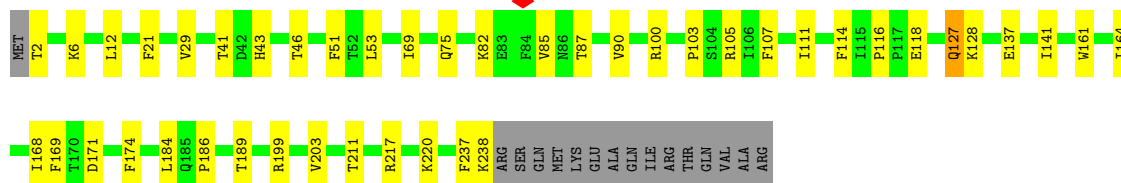
• Molecule 2: gp89





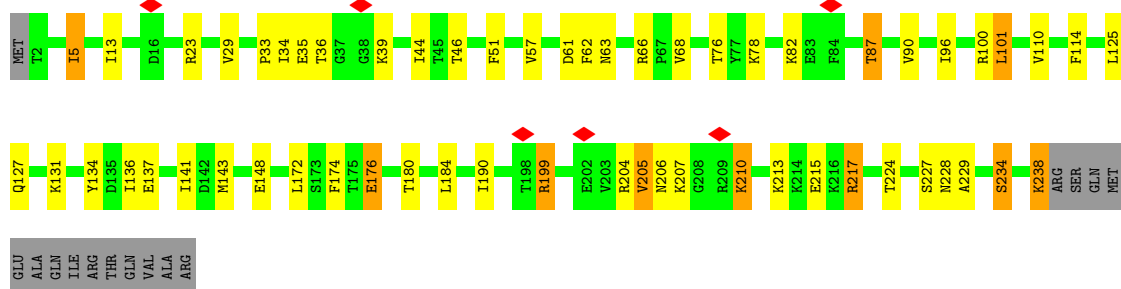
• Molecule 3: gp83

Chain A: 76% 17% 6%



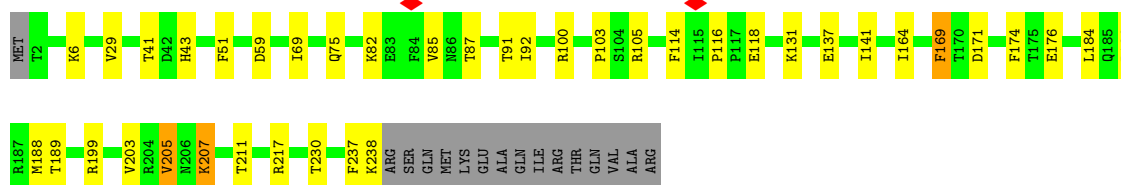
• Molecule 3: gp83

Chain B: 70% 19% 6%



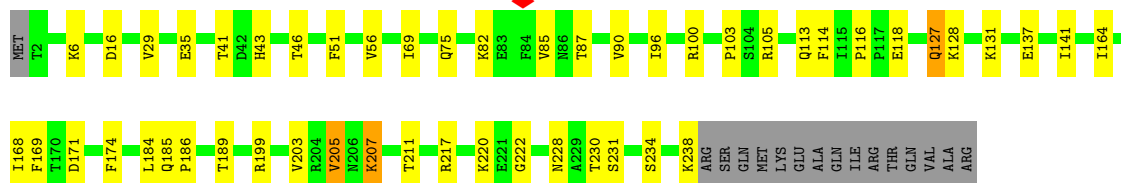
• Molecule 3: gp83

Chain C: 78% 15% 6%



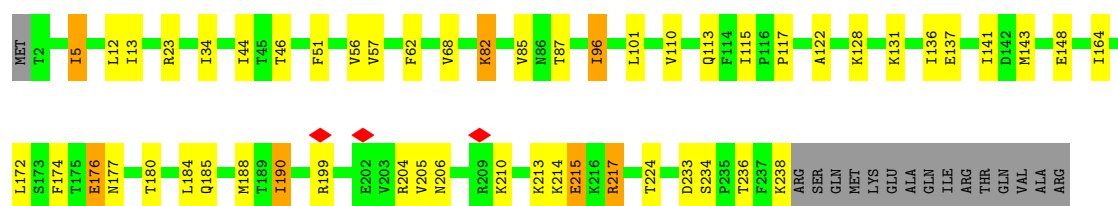
• Molecule 3: gp83

Chain D: 74% 19% 6%



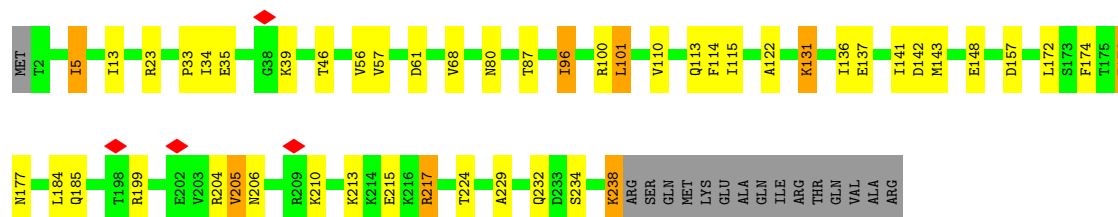
• Molecule 3: gp83

Chain E:  73% 18% 6%




- Molecule 3: gp83

Chain F:  74% 16% 6%




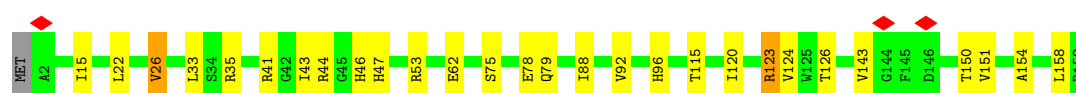
- Molecule 4: gp79

Chain G:  84% 14% ..




- Molecule 4: gp79

Chain Q:  82% 16% ..




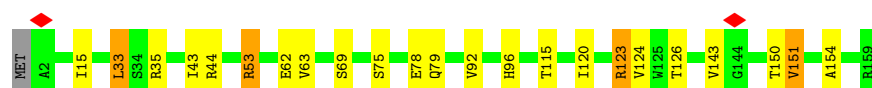
- Molecule 4: gp79

Chain a:  85% 13% ..




- Molecule 4: gp79


Chain k:  85% 12% ..



• Molecule 4: gp79

Chain q:  86% 11% ..

• Molecule 4: gp79

Chain w:  85% 11% ..


• Molecule 5: gp78

Chain H:  96% .


• Molecule 5: gp78

Chain R:  91% 8% .

• Molecule 5: gp78

Chain b:  90% 10%


• Molecule 5: gp78

Chain l:  90% 9% .


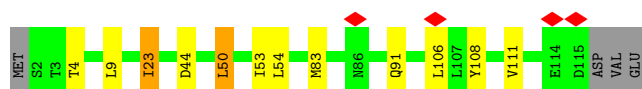
• Molecule 5: gp78

Chain r:  95% 5%

• Molecule 5: gp78

Chain x:  92% 8% .


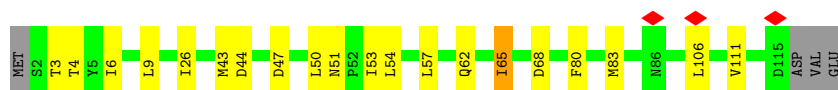
• Molecule 6: gp84

Chain I:  86% 8% ..


• Molecule 6: gp84

Chain S:  75% 21% .


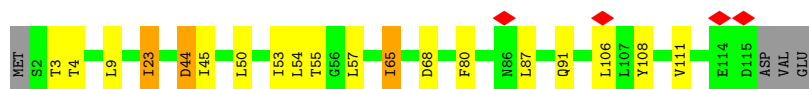
• Molecule 6: gp84

Chain c:  80% 16% ..

• Molecule 6: gp84

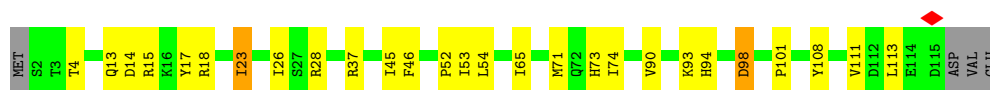
Chain m:  75% 20% ..

• Molecule 6: gp84

Chain s:  81% 14% ..

• Molecule 6: gp84

Chain y:  74% 21% ..



- Molecule 7: gp87

Chain K: 84% 12% ..



- Molecule 7: gp87

Chain U: 84% 14% .



- Molecule 7: gp87

Chain e: 81% 15% ..



- Molecule 7: gp87

Chain n: 82% 14% ..



- Molecule 7: gp87

Chain t: 85% 12% ..




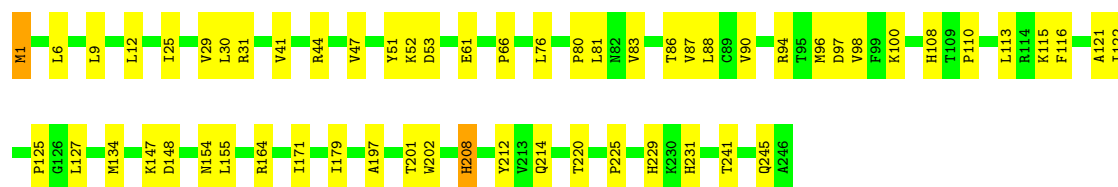
- Molecule 7: gp87

Chain z: 83% 15% .



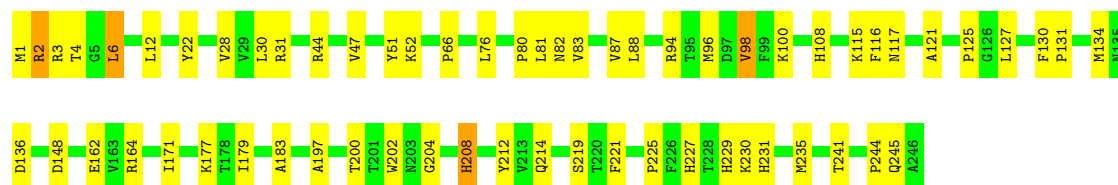
- Molecule 8: gp86

Chain P:  76% 23% .



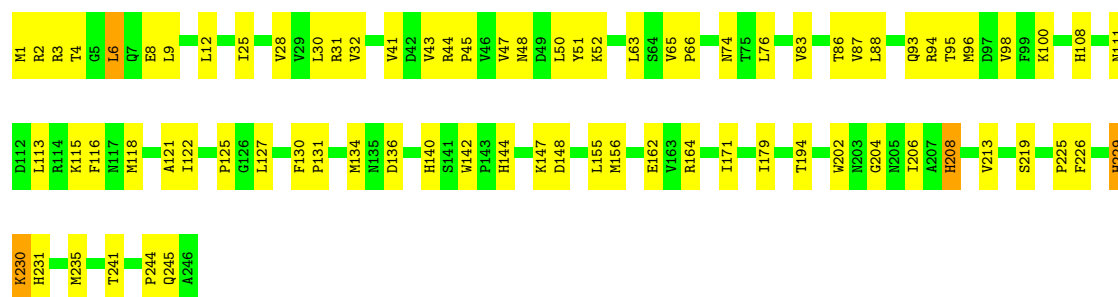
• Molecule 8: gp86

Chain Z:  75% 24% .



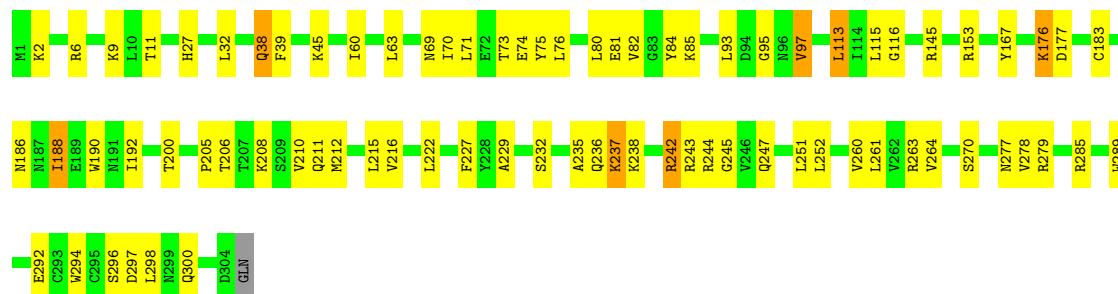
• Molecule 8: gp86

Chain j:  68% 30% .



• Molecule 9: gp85

Chain J:  74% 24% .



• Molecule 9: gp85

Chain T:  73% 24% .



GLN

- Molecule 10: gp88

Chain 2: 98%

LEU	LYS	LYS	SER	SER	ALA	ALA	ASP	ILE	ILE	SER	SER	PHE	ASN	LEU	LEU	VAL	ASN	VAL	SER	SER	GLY	GLY	ILE	ILE	ASP	ALA	ASP	GLN	GLN	GLY	GLY	ASN	ASN	VAL	VAL	GLU	THR	THR	GLU	GLU	ALA	GLN	GLU	GLU	ARG	VAL	VAL	ARG	ARG	GLU	GLU	ILE	ILE	VAL	VAL	SER	SER	ASN	ASN	VAL	LEU	GLU	GLU	GLU	GLU	ILE	ILE	SER	SER	ARG	ALA	ALA	ALA	ALA	TYR	LYS	GLU	GLU	SER	SER	GLN	GLN
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- Molecule 10: gp88

98%

- Molecule 10: gp88

98%

GLN	ASN	LEU	GLU	MET
GLN	GLY	GLN	LEU	ILE
MET	LEU	GLY	THR	ALA
GLY	ALA	THR	LYS	ALA
GLY	VAL	VAL	ALA	ILE
GLY	ALA	ASP	THR	ALA
ILE	THR	ASP	GLN	GLN
GLY	PRO	LEU	ARG	LEU
ILE	GLY	VAL	VAL	THR
GLU	ILE	VAL	VAL	GLY
LEU	ARG	GLU	VAL	GLY
ALA	LEU	LEU	LEU	GLU
GLY	SER	GLY	LYS	LEU
THR	VAL	LEU	ASN	LEU
GLY	ASP	ALA	ILE	PHE
ARG	ARG	GLN	ALA	THR
ALA	ALA	VAL	VAL	VAL
GLY	HIS	SER	ASP	ASP
PHE	LEU	ARG	ALA	SER
ILE	ARG	THR	ALA	ARG
PRO	LEU	THR	ALA	ARG
GLY	ARG	LEU	ALA	PRO
LEU	GLY	LEU	VAL	LEU
GLY	ILE	GLU	VAL	THR
GLY	GLN	TRP	LEU	ALA
ALA	ASP	LYS	ILE	PHE
PHE	VAL	LYS	SER	ASP
ALA	LEU	ARG	GLU	LYS
ALA	GLY	THR	LYS	LEU
ILE	ILE	GLU	GLN	ALA
MET	ILE	SER	GLN	ALA
GLN	ILE	ARG	GLU	GLY
LEU	ARG	PHE	ARG	VAL
ASN	ARG	ASN	ARG	GLU
ASN	GLY	ILE	ASN	ALA
GLN	VAL	HIS	ALA	ALA
GLN	ARG	LEU	THR	LEU
GLU	ILE	ASN	PRO	ARG
GLN	ILE	LYS	ILE	ARG
GLN	ASP	ASP	ARG	PHE
GLN	GLY	ILE	SER	LYS
GLN	GLY	SER	LYS	LYS
ARG	SER	ARG	SER	LEU
LEU	SER	SER	VAL	THR
ALA	ILE	LYS	ARG	ASN
LEU	GLY	ARG	LEU	LYS
MET	GLY	LEU	ASP	ARG
GLN	GLY	GLN	LEU	PHE
ALA	GLY	ASN	SER	GLY
VAL	VAL	ALA	LEU	GLY
GLY	ALA	ASN	GLY	VAL
GLY	GLY	ASN	ILE	GLY
GLY	GLY	ARG	ARG	LYS
GLN	GLY	THR	THR	THR
GLN	THR	ASP	LYS	ASP
ALA	ALA	VAL	ASN	THR
GLY	ALA	PHE	VAL	LYS
LEU	GLY	GLN	GLY	THR
LEU	HIS	GLY	LYS	THR
GLN	ILE	THR	THR	ALA
ALA	ARG	LEU	ALA	THR





THR	GLN	ASN	LEU	GLU	MET
ARG	GLY	LEU	GLN	ALA	ILE
ASP	MET	GLY	THR	LYS	ARG
ILE	MET	VAL	LYS	ALA	ARG
SER	GLY	ALA	VAL	ALA	ILE
GLN	ILE	THR	ASP	THR	ALA
ARG	GLY	PRO	LEU	GLN	ALA
LEU	SER	GLN	PRO	ARG	THR
GLY	GLU	ILE	GLU	VAL	THR
LEU	LEU	ARG	GLU	VAL	GLY
ASP	ALA	LEU	LEU	LEU	GLU
ASP	GLY	SER	GLY	LYS	LEU
ARG	TRP	VAL	LEU	ASN	LYS
ALA	GLY	ASP	ALA	ILE	PHI
ILE	ARG	ILE	GLN	THR	ALA
ILE	ARG	ALA	GLN	ALA	VAL
GLY	GLY	HIS	SER	ASP	VAL
SER	PHI	LEU	ARG	ASP	ASP
SER	ILE	LEU	ARG	ALA	SER
TYR	PRO	ARG	THR	ALA	ARG
VAL	LEU	ARG	LEU	ALA	PRO
LYS	LEU	GLY	TYR	VAL	LEU
MET	GLY	ILE	GLU	ARG	THR
MET	GLY	GLN	TRP	LEU	ALA
ALA	ALA	ASP	LYS	ILE	PHI
ALA	PHE	VAL	LYS	SER	ASP
GLY	ALA	LEU	ARG	GLU	LYS
GLN	ILE	GLN	THR	LEU	LYS
ALA	MET	GLN	GLU	LEU	LEU
SER	GLN	ILE	SER	GLN	ALA
ASN	LEU	ARG	ARG	GLY	GLY
THR	ASN	ALA	LYS	ASN	ALA
GLN	GLN	ILE	LEU	THR	LEU
VAL	GLU	ARG	ASN	PRO	ARG
ASP	LEU	ILE	ALA	ILE	GLU
GLY	GLN	ASP	ASP	ARG	PHE
PHE	ILE	LEU	ILE	LEU	SER
GLN	GLN	GLU	SER	LYS	LYS
ASN	ARG	SER	ARG	SER	LEU
SER	LEU	SER	SER	VAL	THR
MET	ALA	ILE	LYS	ARG	ASN
ALA	MET	ARG	LEU	LEU	LYS
GLU	GLN	GLY	LEU	ASP	ARG
TYR	ALA	GLY	GLN	LEU	PHE
GLY	VAL	GLY	ASN	SER	GLY
VAL	GLY	ALA	ASN	GLY	VAL
GLY	GLN	GLY	ARG	ILE	LYS
GLU	VAL	GLY	THR	ASP	THR
ASP	GLY	GLY	LEU	LYS	ASP
GLY	GLN	THR	ASP	ASN	THR
GLU	GLN	ALA	VAL	PHE	LYS
ALA	GLU	GLY	VAL	VAL	THR
MET	LEU	HIS	GLY	LYS	THR
LYS	GLN	ILE	ARG	THR	GLU
GLY	ALA	ARG	LEU	THR	THR

MET	GLN	ARG	GLY	GLN	VAL	ARG	ASN	GLU	MET	GLU	GLY	ALA	LEU	LYS	SER	ALA	ILE	ASP	ILE	SER	PHE	ASN	LEU	ASN	VAL	SER	GLY	ILE	ASP	ALA	GLN	GLY	ASN	VAL	M753	A757	V765	V768	L769	E772	A776	S783	Q784
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10400	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.045	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	697.344, 697.344, 697.344	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.362, 1.362, 1.362	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	O	0.12	0/3747	0.29	0/5117
1	L	0.12	0/3747	0.28	0/5117
1	M	0.12	0/3747	0.31	0/5117
1	N	0.11	0/3747	0.28	0/5117
1	V	0.12	0/3747	0.29	0/5117
1	W	0.12	0/3747	0.29	0/5117
1	X	0.11	0/3747	0.28	0/5117
1	f	0.12	0/3747	0.29	0/5117
1	g	0.12	0/3747	0.29	0/5117
1	h	0.11	0/3747	0.28	0/5117
1	o	0.12	0/3747	0.28	0/5117
1	u	0.12	0/3747	0.28	0/5117
2	1	0.13	0/1917	0.32	0/2598
2	O	0.12	0/1917	0.30	0/2598
2	Y	0.13	0/1917	0.31	0/2598
2	i	0.12	0/1917	0.30	0/2598
2	p	0.13	0/1917	0.31	0/2598
2	v	0.12	0/1917	0.30	0/2598
3	A	0.16	0/1910	0.31	0/2595
3	B	0.16	0/1910	0.31	0/2595
3	C	0.16	0/1910	0.32	0/2595
3	D	0.16	0/1910	0.31	0/2595
3	E	0.15	0/1910	0.31	0/2595
3	F	0.16	0/1910	0.31	0/2595
4	G	0.19	0/1261	0.29	0/1714
4	Q	0.19	0/1261	0.28	0/1714
4	a	0.19	0/1261	0.26	0/1714
4	k	0.19	0/1261	0.28	0/1714
4	q	0.19	0/1261	0.27	0/1714
4	w	0.19	0/1261	0.28	0/1714
5	H	0.19	0/1305	0.28	0/1767
5	R	0.20	0/1305	0.30	0/1767
5	b	0.19	0/1305	0.30	0/1767
5	l	0.20	0/1305	0.30	0/1767

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	r	0.19	0/1305	0.28	0/1767
5	x	0.19	0/1305	0.29	0/1767
6	I	0.13	0/984	0.27	0/1342
6	S	0.13	0/984	0.29	0/1342
6	c	0.13	0/984	0.29	0/1342
6	m	0.13	0/984	0.29	0/1342
6	s	0.13	0/984	0.27	0/1342
6	y	0.13	0/984	0.27	0/1342
7	K	0.15	0/1002	0.29	0/1360
7	U	0.15	0/1002	0.28	0/1360
7	e	0.15	0/1002	0.27	0/1360
7	n	0.14	0/1002	0.28	0/1360
7	t	0.15	0/1002	0.27	0/1360
7	z	0.14	0/1002	0.28	0/1360
8	P	0.11	0/1914	0.30	0/2606
8	Z	0.11	0/1914	0.28	0/2606
8	j	0.11	0/1914	0.31	0/2606
9	J	0.13	0/2397	0.32	0/3245
9	T	0.13	0/2397	0.33	0/3245
9	d	0.14	0/2397	0.33	0/3245
10	2	0.12	0/143	0.18	0/194
10	3	0.12	0/143	0.24	0/194
10	4	0.12	0/143	0.24	0/194
10	5	0.13	0/143	0.21	0/194
10	6	0.11	0/143	0.27	0/194
10	7	0.12	0/143	0.21	0/194
10	8	0.11	0/255	0.29	0/341
10	9	0.10	0/255	0.24	0/341
10	AA	0.10	0/255	0.28	0/341
All	All	0.14	0/109794	0.29	0/149400

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	3681	0	3678	56	0
1	L	3681	0	3678	58	0
1	M	3681	0	3678	54	0
1	N	3681	0	3678	55	0
1	V	3681	0	3678	54	0
1	W	3681	0	3678	60	0
1	X	3681	0	3678	61	0
1	f	3681	0	3678	63	0
1	g	3681	0	3678	57	0
1	h	3681	0	3678	62	0
1	o	3681	0	3678	58	0
1	u	3681	0	3678	54	0
2	l	1879	0	1856	37	0
2	O	1879	0	1856	47	0
2	Y	1879	0	1856	42	0
2	i	1879	0	1856	43	0
2	p	1879	0	1856	34	0
2	v	1879	0	1856	45	0
3	A	1876	0	1849	23	0
3	B	1876	0	1849	36	0
3	C	1876	0	1849	17	0
3	D	1876	0	1849	22	0
3	E	1876	0	1849	33	0
3	F	1876	0	1849	29	0
4	G	1237	0	1203	11	0
4	Q	1237	0	1203	11	0
4	a	1237	0	1203	12	0
4	k	1237	0	1203	13	0
4	q	1237	0	1203	12	0
4	w	1237	0	1203	13	0
5	H	1281	0	1297	2	0
5	R	1281	0	1297	5	0
5	b	1281	0	1297	6	0
5	l	1281	0	1297	6	0
5	r	1281	0	1297	3	0
5	x	1281	0	1297	5	0
6	I	956	0	915	7	0
6	S	956	0	915	12	0
6	c	956	0	915	10	0
6	m	956	0	915	15	0
6	s	956	0	915	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	y	956	0	915	14	0
7	K	979	0	969	12	0
7	U	979	0	969	12	0
7	e	979	0	969	12	0
7	n	979	0	969	11	0
7	t	979	0	969	10	0
7	z	979	0	969	9	0
8	P	1874	0	1857	50	0
8	Z	1874	0	1857	46	0
8	j	1874	0	1857	59	0
9	J	2364	0	2343	42	0
9	T	2364	0	2343	42	0
9	d	2364	0	2343	38	0
10	2	143	0	133	0	0
10	3	143	0	133	0	0
10	4	143	0	133	1	0
10	5	143	0	133	0	0
10	6	143	0	133	1	0
10	7	143	0	133	0	0
10	8	255	0	247	10	0
10	9	255	0	247	8	0
10	AA	255	0	247	8	0
All	All	107757	0	106809	1384	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1384) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:299:GLN:H	2:Y:139:ARG:HH22	1.20	0.89
1:M:300:ALA:HB1	1:M:306:SER:HB2	1.63	0.81
2:1:139:ARG:HH22	1:g:299:GLN:H	1.26	0.81
1:M:437:ARG:HH21	1:f:443:MET:HE3	1.47	0.78
4:G:60:ARG:HG2	4:G:126:THR:HG22	1.65	0.77
2:v:84:ASN:HA	2:v:91:THR:H	1.49	0.77
1:g:300:ALA:HB1	1:g:306:SER:HB2	1.65	0.77
1:g:437:ARG:HH21	1:u:443:MET:HE3	1.51	0.76
1:g:458:LYS:HZ2	1:g:459:GLY:H	1.32	0.76
4:q:60:ARG:HG2	4:q:126:THR:HG22	1.65	0.76
1:L:412:GLU:HB3	1:L:484:VAL:HB	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:84:ASN:HA	2:O:91:THR:H	1.51	0.76
8:P:110:PRO:HD3	8:j:48:ASN:HB2	1.69	0.75
1:O:34:SER:H	7:z:1:MET:HE3	1.51	0.74
3:D:217:ARG:HE	3:D:238:LYS:HA	1.51	0.74
2:p:209:PHE:HB3	2:p:239:THR:HG23	1.69	0.73
2:1:209:PHE:HB3	2:1:239:THR:HG23	1.69	0.73
1:u:106:GLU:HB3	1:u:269:SER:HB3	1.69	0.73
1:f:412:GLU:HB3	1:f:484:VAL:HB	1.68	0.73
1:M:299:GLN:H	2:p:139:ARG:HH22	1.35	0.73
8:j:96:MET:HB3	8:j:100:LYS:HG3	1.69	0.72
1:N:249:PRO:HA	1:N:279:GLY:H	1.54	0.72
2:Y:73:ARG:HB2	2:Y:134:LYS:HG2	1.72	0.72
1:L:34:SER:H	7:U:1:MET:HE3	1.55	0.71
3:E:137:GLU:HB2	3:E:184:LEU:HD11	1.72	0.71
3:C:217:ARG:HE	3:C:238:LYS:HA	1.55	0.71
1:M:458:LYS:HZ2	1:M:459:GLY:H	1.36	0.71
1:h:303:ILE:HG22	1:h:306:SER:H	1.53	0.71
6:s:44:ASP:HB3	6:s:55:THR:HA	1.72	0.71
1:W:389:ARG:HD3	1:W:390:PRO:HD2	1.73	0.71
3:A:217:ARG:HE	3:A:238:LYS:HA	1.56	0.70
3:B:213:LYS:HE3	3:B:215:GLU:HB3	1.73	0.70
3:F:137:GLU:HB2	3:F:184:LEU:HD11	1.72	0.70
1:W:300:ALA:HB1	1:W:306:SER:HB2	1.72	0.70
2:p:239:THR:HG22	2:p:241:LEU:H	1.57	0.70
1:W:156:LEU:H	1:W:176:SER:HB3	1.57	0.70
1:u:412:GLU:HB3	1:u:484:VAL:HB	1.72	0.70
9:T:200:THR:HG21	9:T:206:THR:HG22	1.73	0.70
1:O:397:ILE:HB	1:O:482:ILE:HA	1.74	0.69
2:Y:209:PHE:HB3	2:Y:239:THR:HG23	1.74	0.69
2:1:239:THR:HG22	2:1:241:LEU:H	1.57	0.69
3:B:137:GLU:HB2	3:B:184:LEU:HD11	1.74	0.69
4:a:60:ARG:HG2	4:a:126:THR:HG22	1.72	0.69
9:d:38:GLN:HB2	9:d:285:ARG:HD2	1.75	0.69
1:f:391:VAL:HB	1:f:473:GLU:HG2	1.74	0.69
1:X:303:ILE:HG22	1:X:306:SER:H	1.57	0.69
8:P:9:LEU:HD12	10:8:773:ILE:HG13	1.74	0.68
1:X:11:ILE:HG21	1:X:66:GLN:HB2	1.73	0.68
9:J:6:ARG:HH21	9:J:289:TRP:HB2	1.58	0.68
1:N:46:ALA:HB2	7:U:19:ALA:HA	1.76	0.68
8:P:76:LEU:HB2	8:j:155:LEU:HD11	1.75	0.68
9:J:277:ASN:HB2	9:J:294:TRP:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:391:VAL:HB	1:u:473:GLU:HG2	1.74	0.68
1:L:391:VAL:HB	1:L:473:GLU:HG2	1.75	0.68
1:g:156:LEU:H	1:g:176:SER:HB3	1.57	0.68
7:n:1:MET:HG3	1:o:33:VAL:HG12	1.76	0.68
1:X:249:PRO:HA	1:X:279:GLY:H	1.57	0.68
4:a:53:ARG:HH22	4:k:44:ARG:HA	1.59	0.68
1:M:156:LEU:H	1:M:176:SER:HB3	1.59	0.67
1:V:397:ILE:HB	1:V:482:ILE:HA	1.75	0.67
2:1:73:ARG:HB2	2:1:134:LYS:HG2	1.77	0.67
1:o:397:ILE:HB	1:o:482:ILE:HA	1.75	0.67
7:n:1:MET:HE3	1:o:34:SER:H	1.59	0.67
1:o:319:ASP:HB2	1:o:428:LYS:HE2	1.77	0.67
1:X:46:ALA:HB2	7:e:19:ALA:HA	1.75	0.67
3:B:176:GLU:HB2	4:Q:43:ILE:HD11	1.75	0.67
1:f:106:GLU:HB3	1:f:269:SER:HB3	1.77	0.67
8:P:1:MET:HE2	9:J:229:ALA:HB3	1.77	0.66
1:g:389:ARG:HD3	1:g:390:PRO:HD2	1.77	0.66
1:W:434:ILE:HB	1:W:437:ARG:HB2	1.77	0.66
8:Z:229:HIS:HD2	8:j:244:PRO:HB3	1.60	0.66
8:P:202:TRP:HB3	8:Z:208:HIS:HB2	1.77	0.66
1:M:389:ARG:HD3	1:M:390:PRO:HD2	1.78	0.66
9:T:183:CYS:HG	9:T:190:TRP:CD1	2.13	0.66
3:C:176:GLU:HB3	4:q:43:ILE:HD11	1.78	0.66
2:i:86:PHE:HE2	2:i:110:TYR:H	1.42	0.65
1:u:401:VAL:HG12	1:u:450:VAL:HA	1.78	0.65
8:Z:2:ARG:HH12	9:d:51:LYS:HG3	1.61	0.65
1:h:249:PRO:HA	1:h:279:GLY:H	1.60	0.65
4:w:62:GLU:HG2	4:w:124:VAL:HG22	1.78	0.65
4:Q:62:GLU:HG2	4:Q:124:VAL:HG22	1.79	0.65
1:h:450:VAL:HG12	1:o:436:SER:HB2	1.77	0.65
7:K:1:MET:HE3	1:V:34:SER:H	1.63	0.64
6:c:54:LEU:HD23	6:c:57:LEU:HD11	1.79	0.64
1:g:418:ARG:HD2	1:g:445:ILE:HD11	1.79	0.64
2:1:104:THR:HG21	2:1:183:ARG:HD2	1.79	0.64
5:b:69:PRO:HG3	5:l:141:VAL:HG11	1.80	0.64
2:Y:104:THR:HG21	2:Y:183:ARG:HD2	1.79	0.64
6:m:54:LEU:HD11	6:m:71:MET:HE3	1.80	0.64
5:H:69:PRO:HG3	5:R:141:VAL:HG11	1.80	0.64
1:M:418:ARG:HD2	1:M:445:ILE:HD11	1.79	0.64
1:f:403:ASN:HB2	1:f:407:MET:HE2	1.80	0.64
1:h:103:VAL:HG12	1:h:272:ASN:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:k:151:VAL:HG13	4:k:154:ALA:HB2	1.80	0.64
1:L:403:ASN:HB2	1:L:407:MET:HE2	1.80	0.64
5:r:69:PRO:HG3	5:x:141:VAL:HG11	1.79	0.64
3:F:143:MET:HG3	3:F:148:GLU:HB3	1.80	0.63
1:W:458:LYS:HZ2	1:W:459:GLY:H	1.44	0.63
10:9:760:ARG:HD2	10:AA:753:MET:HB2	1.80	0.63
2:p:73:ARG:HB2	2:p:134:LYS:HG2	1.79	0.63
3:B:143:MET:HG3	3:B:148:GLU:HB3	1.81	0.63
8:Z:202:TRP:HB3	8:j:208:HIS:HB2	1.79	0.63
2:i:84:ASN:HA	2:i:91:THR:H	1.64	0.63
10:9:777:SER:HA	10:9:780:TYR:HD2	1.63	0.63
3:E:113:GLN:HG3	4:a:151:VAL:HG23	1.80	0.63
1:L:213:PHE:HE2	1:L:235:LYS:HG3	1.63	0.63
8:j:9:LEU:HD22	10:9:773:ILE:HG23	1.79	0.63
1:N:303:ILE:HG22	1:N:306:SER:H	1.64	0.63
1:X:115:SER:HB3	1:X:131:LEU:HB2	1.81	0.63
1:u:53:VAL:HG13	2:v:15:ALA:HB1	1.81	0.63
1:L:443:MET:HE3	1:W:437:ARG:HH21	1.63	0.63
1:X:103:VAL:HG12	1:X:272:ASN:HB3	1.81	0.63
9:J:183:CYS:HG	9:J:190:TRP:CD1	2.17	0.63
1:X:298:VAL:H	2:i:139:ARG:NH2	1.95	0.63
5:l:88:LYS:HB3	5:l:106:THR:HG23	1.80	0.63
1:g:396:GLU:HB2	1:g:458:LYS:HD2	1.81	0.62
6:S:26:ILE:HD12	6:S:28:ARG:HH21	1.63	0.62
1:V:49:ARG:HH11	2:Y:20:THR:HG21	1.65	0.62
1:u:213:PHE:HE2	1:u:235:LYS:HG3	1.64	0.62
3:F:176:GLU:HB2	4:w:43:ILE:HD11	1.82	0.62
2:Y:239:THR:HG22	2:Y:241:LEU:H	1.65	0.62
1:g:434:ILE:HB	1:g:437:ARG:HB2	1.80	0.62
2:i:88:PHE:HD2	2:i:95:GLY:H	1.47	0.62
1:o:112:VAL:HG13	1:o:136:ILE:HG12	1.82	0.62
1:u:406:SER:HB2	1:u:447:GLY:HA3	1.81	0.62
1:L:401:VAL:HG12	1:L:450:VAL:HA	1.81	0.62
1:u:403:ASN:HB2	1:u:407:MET:HE2	1.82	0.62
1:N:115:SER:HB3	1:N:131:LEU:HB2	1.82	0.62
9:T:6:ARG:HH21	9:T:289:TRP:HB2	1.65	0.62
7:t:1:MET:HE3	1:u:34:SER:H	1.65	0.62
1:g:343:PRO:HG2	1:g:387:TYR:HA	1.81	0.61
9:T:277:ASN:HB2	9:T:294:TRP:HB2	1.81	0.61
2:O:238:LEU:HD23	2:O:238:LEU:H	1.64	0.61
8:Z:212:TYR:HB3	8:j:219:SER:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:54:LEU:HD11	6:S:71:MET:HE3	1.81	0.61
4:a:151:VAL:HG13	4:a:154:ALA:HB2	1.82	0.61
1:g:118:ALA:HB1	1:g:267:TRP:HZ3	1.65	0.61
1:M:396:GLU:HB2	1:M:458:LYS:HD2	1.81	0.61
1:N:25:ALA:HB1	1:N:47:LEU:HD21	1.80	0.61
1:M:298:VAL:H	2:p:139:ARG:NH2	1.99	0.61
1:X:389:ARG:HD3	1:X:390:PRO:HD2	1.83	0.61
1:f:407:MET:HB2	1:f:448:PHE:HB3	1.80	0.61
1:h:11:ILE:HG21	1:h:66:GLN:HB2	1.82	0.61
1:g:416:ARG:HE	1:g:479:ALA:HB1	1.65	0.61
2:O:209:PHE:HB3	2:O:239:THR:HG23	1.81	0.61
1:V:162:MET:HE3	1:V:164:VAL:HG22	1.83	0.61
1:W:118:ALA:HB1	1:W:267:TRP:HZ3	1.66	0.61
4:k:62:GLU:HG2	4:k:124:VAL:HG22	1.82	0.61
1:N:96:ALA:HA	1:N:280:ARG:HB2	1.83	0.61
2:O:86:PHE:HE2	2:O:110:TYR:H	1.49	0.61
5:R:88:LYS:HB3	5:R:106:THR:HG23	1.81	0.61
1:V:447:GLY:H	1:X:437:ARG:HH12	1.49	0.61
2:v:207:THR:HG21	2:v:241:LEU:HD13	1.83	0.61
9:d:279:ARG:HB3	9:d:292:GLU:HB2	1.81	0.61
3:A:51:PHE:HE2	3:A:164:ILE:HG21	1.66	0.60
1:M:434:ILE:HB	1:M:437:ARG:HB2	1.83	0.60
8:P:171:ILE:HB	8:Z:179:ILE:HG12	1.82	0.60
1:V:154:ASN:HB3	1:V:178:ALA:HA	1.82	0.60
1:O:174:TYR:HB3	1:O:191:LEU:HD23	1.84	0.60
1:W:41:THR:HG22	1:W:47:LEU:HD23	1.83	0.60
3:F:213:LYS:HE3	3:F:215:GLU:HB3	1.82	0.60
1:L:17:ILE:HD13	1:L:58:ASP:HB3	1.83	0.60
1:M:11:ILE:HG21	1:M:66:GLN:HB2	1.82	0.60
1:N:389:ARG:HD3	1:N:390:PRO:HD2	1.83	0.60
1:h:115:SER:HB3	1:h:131:LEU:HB2	1.81	0.60
2:p:104:THR:HG21	2:p:183:ARG:HD2	1.82	0.60
1:M:323:ILE:HD12	1:M:342:LEU:HD23	1.83	0.60
7:n:41:LEU:HA	7:n:51:GLY:HA3	1.83	0.60
8:Z:47:VAL:HG11	8:j:94:ARG:HB3	1.84	0.60
1:o:162:MET:HE3	1:o:164:VAL:HG22	1.83	0.60
7:z:41:LEU:HA	7:z:51:GLY:HA3	1.82	0.60
1:O:154:ASN:HB3	1:O:178:ALA:HA	1.82	0.60
1:h:96:ALA:HA	1:h:280:ARG:HB2	1.84	0.60
1:h:330:PRO:HB3	1:h:337:PRO:HA	1.83	0.60
1:N:299:GLN:H	2:O:139:ARG:NH2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:32:LEU:HD21	9:T:85:LYS:HG3	1.84	0.60
2:i:176:LYS:HZ1	2:i:177:ILE:HG22	1.65	0.60
1:M:161:LYS:HG3	1:M:228:ALA:HB2	1.84	0.59
1:N:298:VAL:H	2:O:139:ARG:NH2	2.00	0.59
1:g:11:ILE:HG21	1:g:66:GLN:HB2	1.84	0.59
3:E:23:ARG:HB2	3:E:51:PHE:CD1	2.38	0.59
1:V:112:VAL:HG13	1:V:136:ILE:HG12	1.84	0.59
4:w:151:VAL:HG13	4:w:154:ALA:HB2	1.83	0.59
9:d:183:CYS:HG	9:d:190:TRP:CD1	2.20	0.59
7:K:41:LEU:HA	7:K:51:GLY:HA3	1.83	0.59
1:W:418:ARG:HD2	1:W:445:ILE:HD11	1.83	0.59
2:i:77:LEU:HA	2:i:122:PRO:HD3	1.84	0.59
4:k:63:VAL:HG21	4:k:69:SER:HB2	1.84	0.59
2:1:238:LEU:HD23	2:1:238:LEU:H	1.65	0.59
1:h:111:THR:HB	1:h:137:LEU:HD12	1.83	0.59
3:E:143:MET:HG3	3:E:148:GLU:HB3	1.83	0.59
1:M:416:ARG:HE	1:M:479:ALA:HB1	1.67	0.59
1:o:174:TYR:HB3	1:o:191:LEU:HD23	1.84	0.59
1:M:118:ALA:HB1	1:M:267:TRP:HZ3	1.67	0.59
1:h:400:SER:HB3	1:h:452:SER:HB3	1.85	0.59
1:o:154:ASN:HB3	1:o:178:ALA:HA	1.84	0.59
9:T:38:GLN:HB2	9:T:285:ARG:HD2	1.84	0.59
7:K:1:MET:HG3	1:V:33:VAL:HG12	1.84	0.59
1:M:41:THR:HG22	1:M:47:LEU:HD23	1.84	0.59
1:g:403:ASN:HA	1:g:407:MET:HE1	1.84	0.59
1:V:195:VAL:HG21	1:V:214:ILE:HD13	1.85	0.59
1:W:323:ILE:HD12	1:W:342:LEU:HD23	1.85	0.58
9:J:245:GLY:HA2	9:J:296:SER:HA	1.85	0.58
3:A:137:GLU:HG3	3:A:174:PHE:HE2	1.67	0.58
3:B:57:VAL:HG11	3:B:136:ILE:HD12	1.85	0.58
1:W:11:ILE:HG21	1:W:66:GLN:HB2	1.85	0.58
8:Z:212:TYR:HE1	8:Z:214:GLN:HB2	1.65	0.58
1:L:312:MET:HE2	1:L:320:VAL:HG12	1.86	0.58
1:O:162:MET:HE3	1:O:164:VAL:HG22	1.84	0.58
3:C:103:PRO:HD3	3:C:116:PRO:HG3	1.84	0.58
1:N:103:VAL:HG12	1:N:272:ASN:HB3	1.84	0.58
1:W:298:VAL:H	2:Y:139:ARG:NH2	2.01	0.58
1:O:112:VAL:HG13	1:O:136:ILE:HG12	1.86	0.58
1:W:396:GLU:HB2	1:W:458:LYS:HD2	1.85	0.58
9:d:6:ARG:HH21	9:d:289:TRP:HB2	1.67	0.58
1:h:49:ARG:HH21	1:h:50:LEU:HD12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:300:ALA:H	2:v:139:ARG:HH12	1.51	0.58
4:q:151:VAL:HG13	4:q:154:ALA:HB2	1.86	0.58
1:X:111:THR:HB	1:X:137:LEU:HD12	1.85	0.58
8:Z:229:HIS:CD2	8:j:244:PRO:HB3	2.38	0.58
2:1:139:ARG:NH2	1:g:298:VAL:H	2.02	0.58
6:m:26:ILE:HD12	6:m:28:ARG:HH21	1.69	0.58
7:z:52:ILE:HD11	7:z:75:GLU:HG2	1.84	0.58
2:O:88:PHE:HD2	2:O:95:GLY:H	1.51	0.57
1:L:454:THR:HB	1:L:462:GLN:HB3	1.85	0.57
1:N:330:PRO:HB3	1:N:337:PRO:HA	1.86	0.57
1:N:111:THR:HB	1:N:137:LEU:HD12	1.85	0.57
1:W:160:LEU:HB2	1:W:231:LEU:HD12	1.86	0.57
1:X:299:GLN:H	2:i:139:ARG:NH2	2.02	0.57
2:v:176:LYS:HZ1	2:v:177:ILE:HG22	1.68	0.57
3:E:176:GLU:HB2	4:k:43:ILE:HD11	1.86	0.57
1:h:437:ARG:HH12	1:o:447:GLY:H	1.51	0.57
1:h:298:VAL:H	2:v:139:ARG:NH2	2.03	0.57
1:X:330:PRO:HB3	1:X:337:PRO:HA	1.85	0.57
1:h:307:LEU:HD11	1:h:357:ILE:HD13	1.86	0.57
8:j:88:LEU:HB2	8:j:127:LEU:HD22	1.86	0.57
9:J:279:ARG:HB3	9:J:292:GLU:HB2	1.86	0.57
3:C:137:GLU:HG3	3:C:174:PHE:HE2	1.68	0.56
3:F:205:VAL:HG11	9:J:70:ILE:HD12	1.87	0.56
1:N:73:ASN:HD21	1:N:75:ALA:HB3	1.70	0.56
1:V:144:GLY:HA3	1:V:215:VAL:HG12	1.86	0.56
1:h:49:ARG:HH12	1:u:28:VAL:HG13	1.70	0.56
1:h:389:ARG:HD3	1:h:390:PRO:HD2	1.87	0.56
4:k:75:SER:O	4:k:79:GLN:HG2	2.05	0.56
7:t:1:MET:HG3	1:u:33:VAL:HG12	1.87	0.56
3:B:205:VAL:HG11	9:d:70:ILE:HD12	1.86	0.56
3:F:131:LYS:HD2	7:z:66:PRO:HB3	1.88	0.56
1:g:41:THR:HG22	1:g:47:LEU:HD23	1.87	0.56
2:i:207:THR:HG21	2:i:241:LEU:HD13	1.87	0.56
6:y:26:ILE:HD12	6:y:28:ARG:HH21	1.70	0.56
1:N:307:LEU:HD11	1:N:357:ILE:HD13	1.87	0.56
8:P:88:LEU:HB2	8:P:127:LEU:HD22	1.87	0.56
5:R:69:PRO:HG3	5:b:141:VAL:HG11	1.88	0.56
1:W:255:LEU:HD13	1:W:271:ILE:HG23	1.87	0.56
4:k:43:ILE:HG13	4:k:44:ARG:HG3	1.88	0.56
1:W:343:PRO:HG2	1:W:387:TYR:HA	1.85	0.56
3:E:204:ARG:CZ	6:S:14:ASP:HB3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:141:VAL:HG11	5:x:69:PRO:HG3	1.88	0.56
1:h:358:TRP:HA	1:h:361:LYS:HG2	1.86	0.56
2:v:86:PHE:HE2	2:v:110:TYR:H	1.53	0.56
1:M:25:ALA:HB1	1:M:47:LEU:HD21	1.87	0.56
1:u:331:ASP:HB3	1:u:336:VAL:HB	1.86	0.56
1:O:312:MET:HE2	1:O:320:VAL:HG12	1.87	0.56
3:C:51:PHE:HE2	3:C:164:ILE:HG21	1.70	0.56
4:G:53:ARG:HH22	4:Q:44:ARG:HA	1.70	0.56
1:L:168:ASN:HB3	1:L:170:THR:HG23	1.88	0.56
1:W:161:LYS:HG3	1:W:228:ALA:HB2	1.87	0.56
7:e:1:MET:HE3	1:f:34:SER:H	1.71	0.56
1:g:105:LEU:HD13	1:g:135:VAL:HG11	1.86	0.56
4:k:15:ILE:HG12	4:k:92:VAL:HG12	1.87	0.56
9:d:9:LYS:HB3	9:d:81:GLU:HB2	1.88	0.56
3:D:137:GLU:HG3	3:D:174:PHE:HE2	1.70	0.56
1:N:11:ILE:HG21	1:N:66:GLN:HB2	1.88	0.56
8:P:96:MET:HB3	8:P:100:LYS:HG3	1.88	0.56
2:p:84:ASN:HA	2:p:90:GLY:HA2	1.88	0.56
1:N:300:ALA:H	2:O:139:ARG:HH12	1.54	0.56
1:g:161:LYS:HG3	1:g:228:ALA:HB2	1.87	0.56
2:v:139:ARG:CZ	2:v:139:ARG:HA	2.36	0.56
1:W:458:LYS:HA	1:W:458:LYS:HZ3	1.71	0.55
1:f:401:VAL:HG12	1:f:450:VAL:HA	1.87	0.55
4:w:15:ILE:HG12	4:w:92:VAL:HG12	1.87	0.55
3:B:204:ARG:CZ	6:y:14:ASP:HB3	2.36	0.55
2:Y:84:ASN:HA	2:Y:90:GLY:HA2	1.87	0.55
1:o:158:TYR:HB3	1:o:231:LEU:HD21	1.88	0.55
3:F:57:VAL:HG11	3:F:136:ILE:HD12	1.88	0.55
1:N:400:SER:HB3	1:N:452:SER:HB3	1.87	0.55
4:G:151:VAL:HG13	4:G:154:ALA:HB2	1.88	0.55
1:W:24:VAL:O	1:W:28:VAL:HG23	2.07	0.55
1:V:183:THR:HG22	1:V:185:GLU:H	1.72	0.55
1:f:399:ILE:HB	1:f:484:VAL:HG22	1.88	0.55
1:O:144:GLY:HA3	1:O:215:VAL:HG12	1.89	0.55
1:O:447:GLY:H	1:N:437:ARG:HH12	1.55	0.55
6:I:50:LEU:HG	9:T:212:MET:HG2	1.87	0.55
9:T:245:GLY:HA2	9:T:296:SER:HA	1.89	0.55
1:L:98:PRO:HB2	1:L:244:ASP:HB3	1.88	0.55
1:u:454:THR:HB	1:u:462:GLN:HB3	1.88	0.55
9:d:235:ALA:HB3	9:d:242:ARG:HE	1.71	0.55
8:P:87:VAL:HG12	8:P:125:PRO:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:190:TRP:HZ3	9:T:192:ILE:HG13	1.72	0.55
1:f:260:ILE:HG13	1:f:270:VAL:HG12	1.89	0.55
2:i:174:ILE:HG21	2:i:178:LEU:HD21	1.88	0.55
1:o:144:GLY:HA3	1:o:215:VAL:HG12	1.89	0.55
3:E:213:LYS:HE2	3:E:215:GLU:HB3	1.87	0.55
1:N:397:ILE:HD11	1:N:399:ILE:HD11	1.88	0.55
1:o:195:VAL:HG21	1:o:214:ILE:HD13	1.88	0.55
2:v:88:PHE:HD2	2:v:95:GLY:H	1.54	0.55
2:O:176:LYS:HZ2	2:O:177:ILE:H	1.54	0.54
1:o:167:ILE:HD13	1:o:168:ASN:H	1.73	0.54
1:u:260:ILE:HG13	1:u:270:VAL:HG12	1.89	0.54
10:8:760:ARG:HD2	10:9:753:MET:HB2	1.90	0.54
3:D:51:PHE:HE2	3:D:164:ILE:HG21	1.72	0.54
1:g:25:ALA:HB1	1:g:47:LEU:HD21	1.89	0.54
2:v:77:LEU:HA	2:v:122:PRO:HD3	1.88	0.54
9:J:60:ILE:HD12	9:J:63:LEU:HD11	1.89	0.54
1:X:49:ARG:HH12	1:f:28:VAL:HG13	1.71	0.54
8:Z:200:THR:HB	8:j:206:ILE:HA	1.89	0.54
1:h:393:VAL:HG23	1:h:475:ALA:HA	1.90	0.54
1:M:343:PRO:HG2	1:M:387:TYR:HA	1.89	0.54
2:O:87:GLY:HA2	2:O:109:TRP:HE3	1.73	0.54
2:O:174:ILE:HG21	2:O:178:LEU:HD21	1.89	0.54
1:X:307:LEU:HD11	1:X:357:ILE:HD13	1.88	0.54
2:i:87:GLY:HA2	2:i:109:TRP:HE3	1.72	0.54
2:1:84:ASN:HA	2:1:90:GLY:HA2	1.90	0.54
1:N:394:PRO:HB2	1:N:458:LYS:HB2	1.90	0.54
4:Q:151:VAL:HG13	4:Q:154:ALA:HB2	1.90	0.54
1:X:358:TRP:HA	1:X:361:LYS:HG2	1.89	0.54
1:V:158:TYR:HE1	1:V:176:SER:HB3	1.71	0.54
2:1:185:LEU:HA	2:1:189:LEU:HD22	1.88	0.54
3:D:103:PRO:HD3	3:D:116:PRO:HG3	1.90	0.54
9:J:6:ARG:HA	9:J:84:TYR:HD1	1.73	0.54
1:f:397:ILE:HA	1:f:455:ILE:HG22	1.90	0.54
1:g:374:GLN:HE22	1:g:384:ARG:HG3	1.73	0.54
2:v:174:ILE:HG21	2:v:178:LEU:HD21	1.89	0.54
1:O:158:TYR:HE1	1:O:176:SER:HB3	1.72	0.54
3:B:131:LYS:HD2	7:K:66:PRO:HB3	1.90	0.54
1:V:111:THR:HG21	1:V:266:GLY:HA3	1.90	0.54
1:M:397:ILE:HG12	1:M:455:ILE:HG22	1.89	0.53
1:M:403:ASN:HA	1:M:407:MET:HE1	1.90	0.53
4:Q:15:ILE:HG12	4:Q:92:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:96:ALA:HA	1:X:280:ARG:HB2	1.88	0.53
1:g:323:ILE:HD12	1:g:342:LEU:HD23	1.89	0.53
1:h:402:THR:HB	1:h:451:ASN:HD21	1.73	0.53
10:8:758:GLN:O	10:8:762:ARG:HG3	2.08	0.53
1:L:208:GLN:HB3	1:L:213:PHE:HE1	1.72	0.53
1:X:298:VAL:H	2:i:139:ARG:HH21	1.56	0.53
1:h:299:GLN:H	2:v:139:ARG:NH2	2.06	0.53
8:j:51:TYR:HD2	10:9:783:SER:HB3	1.74	0.53
4:q:117:THR:HG23	4:q:119:GLY:H	1.74	0.53
1:u:53:VAL:HG21	2:v:19:VAL:HG23	1.89	0.53
9:T:235:ALA:HB3	9:T:242:ARG:HE	1.73	0.53
1:L:406:SER:HB2	1:L:447:GLY:HA3	1.89	0.53
8:P:212:TYR:CZ	8:P:214:GLN:HB2	2.42	0.53
8:P:220:THR:HB	8:j:213:VAL:HA	1.91	0.53
1:f:151:THR:HB	1:f:230:ASN:HB3	1.89	0.53
1:o:49:ARG:HH11	2:p:20:THR:HG21	1.74	0.53
10:8:753:MET:HE2	10:AA:757:ALA:HB1	1.90	0.53
3:C:184:LEU:HG	3:C:186:PRO:HD3	1.91	0.53
3:D:184:LEU:HG	3:D:186:PRO:HD3	1.90	0.53
1:g:160:LEU:HB2	1:g:231:LEU:HD12	1.90	0.53
2:i:139:ARG:CZ	2:i:139:ARG:HA	2.39	0.53
1:u:407:MET:HB2	1:u:448:PHE:HB3	1.90	0.53
2:1:184:SER:O	2:1:189:LEU:HB2	2.09	0.53
1:M:160:LEU:HB2	1:M:231:LEU:HD12	1.91	0.53
2:O:207:THR:HG21	2:O:241:LEU:HD13	1.90	0.53
1:W:415:LEU:HD11	1:W:442:ILE:HA	1.91	0.53
1:X:393:VAL:HG23	1:X:475:ALA:HA	1.91	0.53
8:j:140:HIS:CE1	8:j:162:GLU:HG2	2.44	0.53
5:l:69:PRO:HG3	5:r:141:VAL:HG11	1.90	0.53
1:0:409:GLU:OE1	2:O:118:ASN:HB2	2.09	0.53
3:B:206:ASN:C	9:d:69:ASN:HD21	2.16	0.53
2:O:139:ARG:CZ	2:O:139:ARG:HA	2.39	0.53
1:W:397:ILE:HG12	1:W:455:ILE:HG22	1.91	0.53
8:Z:225:PRO:O	8:Z:229:HIS:HB3	2.09	0.53
1:f:397:ILE:HB	1:f:482:ILE:HG23	1.90	0.53
1:0:207:GLU:HA	1:0:212:LEU:HA	1.90	0.53
1:u:399:ILE:HB	1:u:484:VAL:HG22	1.91	0.53
1:V:56:PRO:HG2	2:Y:18:ARG:HH12	1.74	0.53
1:W:296:LYS:HD2	2:Y:72:GLY:HA3	1.90	0.53
1:W:416:ARG:HE	1:W:479:ALA:HB1	1.74	0.53
1:o:409:GLU:OE1	2:v:118:ASN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:151:THR:HB	1:u:230:ASN:HB3	1.91	0.53
8:j:52:LYS:HD2	9:T:187:ASN:HD21	1.74	0.53
9:T:45:LYS:HB2	9:T:278:VAL:HB	1.90	0.53
1:0:109:ILE:HD12	1:0:233:ILE:HB	1.91	0.52
6:s:50:LEU:HG	9:d:212:MET:HG2	1.90	0.52
9:d:237:LYS:HG3	9:d:238:LYS:HD3	1.90	0.52
7:U:24:ARG:HA	7:U:110:ASN:HD21	1.74	0.52
1:V:167:ILE:HD13	1:V:168:ASN:H	1.74	0.52
1:X:394:PRO:HB2	1:X:458:LYS:HB2	1.91	0.52
4:a:33:LEU:HD13	4:a:57:ALA:HA	1.90	0.52
2:p:184:SER:O	2:p:189:LEU:HB2	2.09	0.52
2:O:176:LYS:HZ1	2:O:177:ILE:HG22	1.75	0.52
7:e:24:ARG:HA	7:e:110:ASN:HD21	1.74	0.52
3:F:204:ARG:CZ	6:m:14:ASP:HB3	2.39	0.52
1:X:25:ALA:HB1	1:X:47:LEU:HD21	1.91	0.52
1:X:397:ILE:HD11	1:X:399:ILE:HD11	1.91	0.52
1:f:111:THR:HB	1:f:137:LEU:HD12	1.91	0.52
6:s:54:LEU:HD23	6:s:57:LEU:HD11	1.92	0.52
9:d:60:ILE:HD12	9:d:63:LEU:HD11	1.90	0.52
1:f:144:GLY:HA3	1:f:237:ARG:HH11	1.74	0.52
1:h:299:GLN:O	1:h:301:THR:HG23	2.10	0.52
8:j:113:LEU:HD13	10:AA:784:GLN:HG3	1.91	0.52
1:u:129:PHE:HZ	1:u:252:GLN:HE22	1.55	0.52
4:w:53:ARG:H	4:w:53:ARG:CZ	2.23	0.52
8:P:208:HIS:HA	8:j:202:TRP:HB3	1.91	0.52
1:V:409:GLU:OE1	2:i:118:ASN:HB2	2.10	0.52
1:0:228:ALA:H	1:0:231:LEU:HD12	1.74	0.52
4:G:33:LEU:HD13	4:G:57:ALA:HA	1.92	0.52
7:K:52:ILE:HD11	7:K:75:GLU:HG2	1.91	0.52
1:0:354:ALA:HB1	1:0:375:VAL:HG22	1.91	0.52
2:Y:27:PRO:O	2:Y:31:ARG:HG2	2.10	0.52
2:O:77:LEU:HA	2:O:122:PRO:HD3	1.91	0.52
1:h:49:ARG:HH21	1:h:50:LEU:HA	1.75	0.52
3:A:103:PRO:HD3	3:A:116:PRO:HG3	1.90	0.51
1:o:183:THR:HG22	1:o:185:GLU:H	1.73	0.51
9:J:32:LEU:HD11	9:J:85:LYS:HD2	1.93	0.51
9:T:207:THR:HG23	9:T:261:LEU:HG	1.93	0.51
1:N:298:VAL:H	2:O:139:ARG:HH21	1.56	0.51
7:K:64:SER:HB2	7:K:66:PRO:HG2	1.91	0.51
1:L:407:MET:HB2	1:L:448:PHE:HB3	1.92	0.51
1:X:234:GLN:HG3	1:X:235:LYS:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:231:HIS:HD2	8:j:231:HIS:CE1	2.29	0.51
5:x:88:LYS:HB3	5:x:106:THR:HG23	1.92	0.51
7:z:63:ARG:HH11	7:z:63:ARG:HA	1.75	0.51
9:J:200:THR:HG21	9:J:206:THR:HG22	1.92	0.51
1:L:164:VAL:HA	1:L:223:LYS:HD3	1.91	0.51
1:V:302:ASN:HB3	1:V:305:GLU:HG3	1.93	0.51
2:Y:184:SER:O	2:Y:189:LEU:HB2	2.10	0.51
2:Y:185:LEU:HB3	2:Y:195:LEU:HD21	1.91	0.51
6:c:50:LEU:HG	9:J:212:MET:HG2	1.92	0.51
1:u:101:ALA:HB2	1:u:276:ALA:HB2	1.93	0.51
1:L:345:VAL:HG21	1:L:353:VAL:HG11	1.92	0.51
8:P:94:ARG:HB3	8:j:47:VAL:HG11	1.92	0.51
9:J:235:ALA:HB3	9:J:242:ARG:HE	1.75	0.51
1:O:158:TYR:HB3	1:O:231:LEU:HD21	1.92	0.51
3:B:51:PHE:HB2	3:B:190:ILE:HB	1.92	0.51
8:P:51:TYR:HD2	10:8:783:SER:HB3	1.75	0.51
7:n:64:SER:HB2	7:n:66:PRO:HG2	1.92	0.51
1:N:320:VAL:HG12	1:N:345:VAL:HG22	1.93	0.51
1:X:400:SER:HB3	1:X:452:SER:HB3	1.92	0.51
2:i:134:LYS:HZ3	2:i:138:ASN:HD22	1.59	0.51
5:l:135:MET:HE3	5:l:137:ILE:HG12	1.92	0.51
1:u:98:PRO:HB2	1:u:244:ASP:HB3	1.93	0.51
3:F:217:ARG:HH11	3:F:238:LYS:HA	1.75	0.51
2:O:239:THR:HG22	2:O:241:LEU:H	1.75	0.51
2:Y:238:LEU:HD23	2:Y:238:LEU:H	1.76	0.51
8:j:25:ILE:HD11	8:j:47:VAL:HB	1.91	0.51
1:u:144:GLY:HA3	1:u:237:ARG:HH11	1.76	0.51
2:1:117:GLY:O	2:1:118:ASN:HB2	2.11	0.51
1:N:234:GLN:HG3	1:N:235:LYS:HG3	1.92	0.51
2:Y:117:GLY:O	2:Y:118:ASN:HB2	2.11	0.51
2:Y:185:LEU:HA	2:Y:189:LEU:HD22	1.93	0.51
1:h:412:GLU:CD	1:h:412:GLU:H	2.19	0.51
8:j:30:LEU:HD21	8:j:44:ARG:HB3	1.93	0.51
2:p:14:VAL:O	2:p:18:ARG:HG2	2.11	0.51
9:J:45:LYS:HB2	9:J:278:VAL:HB	1.93	0.51
8:P:1:MET:HE3	9:J:245:GLY:HA3	1.92	0.50
1:f:213:PHE:HE2	1:f:235:LYS:HG3	1.76	0.50
4:q:33:LEU:HD13	4:q:57:ALA:HA	1.93	0.50
9:d:245:GLY:HA2	9:d:296:SER:HA	1.91	0.50
2:1:208:GLU:H	2:1:240:ASN:HB3	1.76	0.50
6:y:54:LEU:HD11	6:y:71:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:63:ARG:NH1	7:K:63:ARG:HA	2.27	0.50
4:a:117:THR:HG23	4:a:119:GLY:H	1.75	0.50
7:t:24:ARG:HA	7:t:110:ASN:HD21	1.77	0.50
3:B:61:ASP:HB2	4:G:48:THR:HG23	1.93	0.50
3:E:57:VAL:HG11	3:E:136:ILE:HD12	1.92	0.50
1:N:393:VAL:HG23	1:N:475:ALA:HA	1.94	0.50
1:X:412:GLU:H	1:X:412:GLU:CD	2.20	0.50
1:O:195:VAL:HG21	1:O:214:ILE:HD13	1.92	0.50
2:1:144:PRO:O	2:1:148:ILE:HG12	2.12	0.50
8:P:47:VAL:HG11	8:Z:94:ARG:HB3	1.92	0.50
1:f:435:TYR:HB2	1:f:455:ILE:HD11	1.94	0.50
3:C:237:PHE:HB2	6:c:83:MET:HE1	1.93	0.50
8:Z:148:ASP:HB2	8:Z:164:ARG:HH11	1.76	0.50
1:h:320:VAL:HG12	1:h:345:VAL:HG22	1.94	0.50
2:p:145:GLU:O	2:p:149:GLU:HG2	2.12	0.50
7:e:53:PRO:HB2	7:e:56:GLU:HB2	1.94	0.50
8:j:87:VAL:HG12	8:j:125:PRO:HA	1.94	0.50
8:j:115:LYS:HB3	8:j:116:PHE:HD1	1.77	0.50
1:u:397:ILE:HB	1:u:482:ILE:HG23	1.94	0.50
2:v:96:SER:O	2:v:106:GLY:HA3	2.12	0.50
9:J:9:LYS:HB3	9:J:81:GLU:HB2	1.92	0.50
2:1:145:GLU:O	2:1:149:GLU:HG2	2.12	0.50
3:A:184:LEU:HG	3:A:186:PRO:HD3	1.94	0.50
3:F:113:GLN:HG3	4:q:151:VAL:HG23	1.94	0.50
1:M:100:ARG:HH21	1:M:241:ILE:HD11	1.75	0.50
4:q:109:ASN:HD21	4:w:35:ARG:HD3	1.77	0.50
2:1:91:THR:HG22	2:1:92:GLU:H	1.77	0.49
3:E:56:VAL:HG12	3:E:185:GLN:HG2	1.94	0.49
1:L:149:PRO:HD3	1:L:188:LEU:HG	1.94	0.49
8:P:113:LEU:HD21	8:j:50:LEU:HB3	1.93	0.49
1:o:158:TYR:HE1	1:o:176:SER:HB3	1.77	0.49
1:O:443:MET:HG3	1:N:437:ARG:HE	1.77	0.49
4:G:75:SER:O	4:G:79:GLN:HG2	2.12	0.49
1:L:33:VAL:HG12	7:U:1:MET:HG3	1.94	0.49
1:W:403:ASN:HA	1:W:407:MET:HE1	1.94	0.49
1:X:49:ARG:HH21	1:X:50:LEU:HA	1.77	0.49
7:n:63:ARG:HA	7:n:63:ARG:NH1	2.26	0.49
3:C:207:LYS:H	3:C:207:LYS:HD2	1.77	0.49
2:Y:208:GLU:H	2:Y:240:ASN:HB3	1.77	0.49
8:Z:88:LEU:HB2	8:Z:127:LEU:HD22	1.95	0.49
1:g:4:ILE:HD12	1:g:9:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:456:ALA:HB2	1:g:462:GLN:HA	1.94	0.49
8:j:148:ASP:HB2	8:j:164:ARG:HH11	1.76	0.49
2:Y:145:GLU:O	2:Y:149:GLU:HG2	2.13	0.49
1:f:298:VAL:HG23	1:f:299:GLN:H	1.77	0.49
1:h:394:PRO:HB2	1:h:458:LYS:HB2	1.94	0.49
1:o:111:THR:HG21	1:o:266:GLY:HA3	1.93	0.49
2:p:117:GLY:O	2:p:118:ASN:HB2	2.12	0.49
1:u:208:GLN:HB3	1:u:213:PHE:HE1	1.76	0.49
9:T:80:LEU:HB3	9:T:93:LEU:HB3	1.94	0.49
9:d:45:LYS:HB2	9:d:278:VAL:HB	1.93	0.49
9:d:200:THR:HG21	9:d:206:THR:HG22	1.93	0.49
3:B:207:LYS:HG3	3:B:210:LYS:HE3	1.94	0.49
1:V:109:ILE:HD12	1:V:233:ILE:HB	1.95	0.49
1:V:158:TYR:HB3	1:V:231:LEU:HD21	1.93	0.49
1:W:28:VAL:C	2:Y:31:ARG:HH22	2.21	0.49
1:W:374:GLN:HE22	1:W:384:ARG:HG3	1.77	0.49
1:f:101:ALA:HB2	1:f:276:ALA:HB2	1.93	0.49
1:g:24:VAL:O	1:g:28:VAL:HG23	2.13	0.49
1:u:298:VAL:HG23	1:u:299:GLN:H	1.78	0.49
1:0:56:PRO:HG2	2:1:18:ARG:HH12	1.77	0.49
8:P:201:THR:HB	8:j:194:THR:HA	1.95	0.49
8:P:225:PRO:O	8:P:229:HIS:HB3	2.12	0.49
8:j:140:HIS:HE1	8:j:142:TRP:HE3	1.60	0.49
9:d:190:TRP:HZ3	9:d:192:ILE:HG13	1.78	0.49
2:1:168:ALA:HB3	1:g:339:HIS:CE1	2.47	0.49
3:F:204:ARG:CZ	6:m:17:TYR:HB3	2.43	0.49
1:N:390:PRO:HB2	1:N:474:VAL:HG12	1.95	0.49
1:W:25:ALA:HB1	1:W:47:LEU:HD21	1.94	0.49
8:Z:30:LEU:HD21	8:Z:44:ARG:HB3	1.95	0.49
8:Z:66:PRO:HD2	8:Z:121:ALA:O	2.13	0.49
1:f:129:PHE:HZ	1:f:252:GLN:HE22	1.60	0.49
1:h:397:ILE:HD11	1:h:399:ILE:HD11	1.94	0.49
2:i:96:SER:O	2:i:106:GLY:HA3	2.13	0.49
1:0:18:LEU:HD11	7:z:46:LEU:HD11	1.94	0.49
1:0:379:ARG:NH2	2:1:160:VAL:HG12	2.28	0.49
6:I:9:LEU:HB2	6:I:106:LEU:HD23	1.94	0.49
2:i:144:PRO:O	2:i:148:ILE:HG12	2.13	0.49
1:o:109:ILE:HD12	1:o:233:ILE:HB	1.94	0.49
1:u:172:ILE:HG21	1:u:195:VAL:HG22	1.95	0.49
3:B:5:ILE:HG23	3:B:13:ILE:HB	1.95	0.48
3:B:90:VAL:HG13	3:B:127:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:443:MET:HE3	1:W:437:ARG:NH2	2.27	0.48
2:Y:31:ARG:HB2	2:Y:31:ARG:CZ	2.43	0.48
1:f:406:SER:HB2	1:f:447:GLY:HA3	1.95	0.48
1:u:18:LEU:HD22	1:u:22:ARG:HH12	1.77	0.48
9:d:277:ASN:O	9:d:293:CYS:HA	2.13	0.48
4:G:53:ARG:HH12	4:Q:44:ARG:C	2.20	0.48
1:V:437:ARG:HG2	1:X:443:MET:HE1	1.94	0.48
1:h:434:ILE:HG22	1:h:437:ARG:H	1.78	0.48
1:u:155:ASP:HB2	1:u:178:ALA:HA	1.95	0.48
3:D:113:GLN:HB2	4:w:151:VAL:HG23	1.94	0.48
2:O:14:VAL:O	2:O:18:ARG:HG2	2.12	0.48
2:O:144:PRO:O	2:O:148:ILE:HG12	2.13	0.48
8:P:66:PRO:HD2	8:P:121:ALA:O	2.13	0.48
2:Y:91:THR:HG22	2:Y:92:GLU:H	1.78	0.48
1:g:397:ILE:HG12	1:g:455:ILE:HG22	1.94	0.48
1:h:48:GLY:HA2	1:h:51:ILE:HD12	1.95	0.48
1:o:471:PHE:CE2	1:o:472:LYS:HG3	2.47	0.48
1:V:412:GLU:HB3	1:V:484:VAL:HB	1.95	0.48
1:g:121:ILE:HG23	1:g:259:THR:HB	1.96	0.48
2:p:185:LEU:HA	2:p:189:LEU:HD22	1.95	0.48
7:t:40:PHE:HB2	7:t:43:GLU:CD	2.37	0.48
9:J:145:ARG:CZ	9:J:153:ARG:HB2	2.43	0.48
1:O:183:THR:HG22	1:O:185:GLU:H	1.77	0.48
2:Y:85:TYR:HA	2:Y:117:GLY:N	2.28	0.48
1:O:397:ILE:HG21	1:O:482:ILE:HG23	1.96	0.48
8:Z:31:ARG:HA	8:Z:83:VAL:HG22	1.95	0.48
2:p:185:LEU:HB3	2:p:195:LEU:HD21	1.95	0.48
7:t:63:ARG:HA	7:t:63:ARG:NH1	2.28	0.48
3:D:207:LYS:H	3:D:207:LYS:HD2	1.78	0.48
7:U:12:LEU:HD12	7:U:12:LEU:H	1.79	0.48
1:h:298:VAL:H	2:v:139:ARG:HH21	1.61	0.48
1:h:349:ILE:HB	1:h:352:GLU:HG2	1.96	0.48
1:o:407:MET:CG	1:o:448:PHE:HB3	2.44	0.48
4:Q:75:SER:O	4:Q:79:GLN:HG2	2.13	0.48
1:X:73:ASN:HD21	1:X:75:ALA:HB3	1.77	0.48
2:Y:165:TYR:HD2	2:Y:171:ARG:HD3	1.78	0.48
3:E:23:ARG:HB2	3:E:51:PHE:HD1	1.77	0.48
3:F:210:LYS:HD3	3:F:210:LYS:H	1.78	0.48
1:L:410:ASN:OD1	2:Y:116:THR:HG21	2.14	0.48
7:U:63:ARG:HA	7:U:63:ARG:NH1	2.29	0.48
1:X:300:ALA:H	2:i:139:ARG:HH12	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:299:GLN:O	1:g:301:THR:HG23	2.14	0.48
8:j:43:VAL:HG22	8:j:65:VAL:HG21	1.96	0.48
2:v:91:THR:HG22	2:v:92:GLU:H	1.79	0.48
2:v:144:PRO:O	2:v:148:ILE:HG12	2.14	0.48
10:8:762:ARG:HE	10:AA:768:VAL:HG22	1.78	0.48
1:0:152:VAL:HG12	1:0:182:VAL:HG23	1.96	0.48
8:P:31:ARG:HA	8:P:83:VAL:HG22	1.96	0.48
8:P:147:LYS:HA	8:Z:80:PRO:HB3	1.94	0.48
8:P:231:HIS:O	8:j:241:THR:HG23	2.14	0.48
5:R:28:PHE:HD1	5:R:29:ILE:HG13	1.79	0.48
8:j:2:ARG:H	8:j:2:ARG:HD2	1.78	0.48
9:T:60:ILE:HD12	9:T:63:LEU:HD11	1.95	0.48
3:D:137:GLU:HB2	3:D:184:LEU:HD22	1.96	0.47
3:E:82:LYS:HE3	3:E:85:VAL:HG21	1.95	0.47
1:M:456:ALA:HB2	1:M:462:GLN:HA	1.96	0.47
1:X:299:GLN:HB3	2:i:139:ARG:HH12	1.79	0.47
8:Z:98:VAL:HB	8:Z:108:HIS:CD2	2.49	0.47
7:e:63:ARG:HA	7:e:63:ARG:NH1	2.28	0.47
1:f:72:PHE:HA	1:f:85:LEU:HD11	1.96	0.47
7:t:40:PHE:O	7:t:51:GLY:HA3	2.14	0.47
4:Q:115:THR:H	4:Q:123:ARG:NH2	2.12	0.47
1:h:234:GLN:HG3	1:h:235:LYS:HG3	1.95	0.47
8:j:140:HIS:HE1	8:j:162:GLU:HG2	1.78	0.47
1:o:298:VAL:HG23	1:o:299:GLN:H	1.79	0.47
9:d:80:LEU:HB3	9:d:93:LEU:HB3	1.95	0.47
2:1:116:THR:HG21	1:u:410:ASN:OD1	2.15	0.47
2:p:88:PHE:HB3	2:p:95:GLY:H	1.78	0.47
2:p:91:THR:HG22	2:p:92:GLU:H	1.79	0.47
3:C:91:THR:HG23	3:C:92:ILE:HG13	1.96	0.47
8:P:97:ASP:HA	9:T:167:TYR:HE2	1.79	0.47
1:V:443:MET:HG3	1:X:437:ARG:HE	1.79	0.47
3:D:171:ASP:HB3	3:D:189:THR:HB	1.95	0.47
1:L:101:ALA:HB2	1:L:276:ALA:HB2	1.96	0.47
1:M:302:ASN:HD21	1:o:303:ILE:HG12	1.80	0.47
1:N:456:ALA:HB2	1:N:462:GLN:HA	1.97	0.47
1:f:112:VAL:HG22	1:f:136:ILE:HG23	1.96	0.47
8:j:115:LYS:HB3	8:j:116:PHE:CD1	2.49	0.47
1:o:397:ILE:HG21	1:o:482:ILE:HG23	1.96	0.47
6:y:93:LYS:HG3	6:y:94:HIS:CD2	2.49	0.47
9:T:261:LEU:HD22	9:T:298:LEU:HD11	1.97	0.47
2:1:14:VAL:O	2:1:18:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:63:GLU:OE1	6:y:37:ARG:HG3	2.14	0.47
2:O:184:SER:O	2:O:189:LEU:HB2	2.14	0.47
6:c:65:ILE:HG23	6:c:80:PHE:HB2	1.96	0.47
1:f:331:ASP:HB3	1:f:336:VAL:HB	1.96	0.47
1:u:111:THR:HB	1:u:137:LEU:HD12	1.96	0.47
9:d:249:LYS:HD2	9:d:292:GLU:HG2	1.97	0.47
3:E:204:ARG:CZ	6:S:17:TYR:HB3	2.44	0.47
1:L:53:VAL:HG21	2:O:19:VAL:HG23	1.97	0.47
1:L:158:TYR:CZ	1:L:187:ILE:HD13	2.50	0.47
1:L:399:ILE:HB	1:L:484:VAL:HG22	1.96	0.47
1:N:339:HIS:CE1	2:O:168:ALA:HB3	2.50	0.47
2:O:215:PHE:HB3	2:O:238:LEU:HB3	1.96	0.47
1:W:164:VAL:HG11	1:W:223:LYS:HE2	1.96	0.47
7:e:12:LEU:H	7:e:12:LEU:HD12	1.80	0.47
1:f:203:LEU:HD21	1:f:223:LYS:HE3	1.97	0.47
2:i:14:VAL:O	2:i:18:ARG:HG2	2.14	0.47
8:j:45:PRO:HG2	8:j:118:MET:HE3	1.97	0.47
1:o:412:GLU:HB3	1:o:484:VAL:HB	1.97	0.47
2:v:84:ASN:HA	2:v:91:THR:N	2.24	0.47
9:J:113:LEU:HD12	9:J:115:LEU:HD21	1.97	0.47
9:J:216:VAL:HG12	9:J:222:LEU:HD22	1.97	0.47
1:M:299:GLN:O	1:M:301:THR:HG23	2.15	0.47
2:O:87:GLY:HA2	2:O:109:TRP:CE3	2.50	0.47
6:S:53:ILE:HG22	6:S:54:LEU:HD12	1.95	0.47
6:m:53:ILE:HG22	6:m:54:LEU:HD12	1.95	0.47
4:w:115:THR:H	4:w:123:ARG:NH2	2.12	0.47
9:d:10:LEU:HD13	9:d:80:LEU:HD13	1.97	0.47
1:L:116:PRO:HB2	1:L:117:PRO:HD3	1.97	0.47
1:V:407:MET:CG	1:V:448:PHE:HB3	2.44	0.47
1:W:299:GLN:O	1:W:301:THR:HG23	2.15	0.47
1:W:339:HIS:CE1	2:Y:168:ALA:HB3	2.50	0.47
5:l:28:PHE:HD1	5:l:29:ILE:HG13	1.80	0.47
1:o:120:MET:HG3	1:o:129:PHE:HB2	1.97	0.47
1:o:207:GLU:HB2	1:o:212:LEU:HD12	1.97	0.47
1:o:293:ARG:O	1:o:293:ARG:HG2	2.15	0.47
3:F:131:LYS:HB2	3:F:131:LYS:HE2	1.65	0.47
1:L:163:TYR:CE2	1:L:169:THR:HA	2.50	0.47
1:h:26:SER:HA	1:h:39:VAL:HG21	1.97	0.47
2:p:144:PRO:O	2:p:148:ILE:HG12	2.15	0.47
9:J:244:ARG:O	9:J:297:ASP:HB2	2.15	0.47
9:T:145:ARG:CZ	9:T:153:ARG:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:205:VAL:HG12	3:C:207:LYS:HE2	1.97	0.46
3:E:117:PRO:HB2	4:a:141:GLN:NE2	2.30	0.46
3:E:210:LYS:NZ	6:S:21:VAL:HB	2.30	0.46
1:L:262:ILE:HD12	1:L:263:PRO:HD2	1.97	0.46
1:V:303:ILE:H	1:V:303:ILE:HD12	1.79	0.46
1:W:412:GLU:O	1:W:416:ARG:HG2	2.14	0.46
2:Y:171:ARG:HG3	2:Y:205:THR:HB	1.97	0.46
8:Z:241:THR:HG23	8:j:231:HIS:O	2.15	0.46
7:e:1:MET:HG3	1:f:33:VAL:HG12	1.97	0.46
1:f:208:GLN:HB3	1:f:213:PHE:HE1	1.80	0.46
1:f:379:ARG:HH22	2:i:160:VAL:HG12	1.81	0.46
1:h:47:LEU:O	1:h:51:ILE:HG13	2.15	0.46
8:j:66:PRO:HD2	8:j:121:ALA:O	2.15	0.46
4:q:53:ARG:HH12	4:w:44:ARG:C	2.23	0.46
9:J:261:LEU:HD22	9:J:298:LEU:HD11	1.97	0.46
1:0:167:ILE:HD13	1:0:168:ASN:H	1.80	0.46
1:M:320:VAL:HG23	1:M:345:VAL:HG12	1.97	0.46
8:P:134:MET:HB3	8:Z:76:LEU:HD22	1.97	0.46
1:g:415:LEU:HD12	1:g:419:ILE:HD11	1.97	0.46
1:o:164:VAL:HG13	1:o:223:LYS:HZ2	1.81	0.46
9:T:138:LYS:HE3	9:T:156:TYR:HB2	1.96	0.46
1:0:303:ILE:HD12	1:0:303:ILE:H	1.81	0.46
3:F:210:LYS:NZ	6:m:21:VAL:HB	2.30	0.46
8:Z:3:ARG:HH22	9:d:279:ARG:HD2	1.80	0.46
1:f:454:THR:HB	1:f:462:GLN:HB3	1.97	0.46
1:h:104:VAL:HG12	1:h:239:LEU:HD23	1.97	0.46
1:h:420:VAL:HG21	1:h:479:ALA:HB2	1.97	0.46
4:k:115:THR:H	4:k:123:ARG:NH2	2.13	0.46
1:W:140:LYS:HE3	1:W:140:LYS:HB3	1.76	0.46
2:v:83:PHE:O	2:v:91:THR:HA	2.16	0.46
8:P:115:LYS:HB3	8:P:116:PHE:HD2	1.80	0.46
4:Q:26:VAL:HG12	4:Q:62:GLU:HB2	1.96	0.46
7:U:52:ILE:HD11	7:U:75:GLU:HG2	1.97	0.46
1:X:342:LEU:HD13	1:X:368:VAL:HG23	1.96	0.46
1:o:342:LEU:HD21	1:o:388:GLN:HE21	1.79	0.46
2:p:85:TYR:HA	2:p:117:GLY:N	2.31	0.46
2:v:14:VAL:O	2:v:18:ARG:HG2	2.16	0.46
1:L:103:VAL:HG12	1:L:272:ASN:HB3	1.98	0.46
9:d:145:ARG:CZ	9:d:153:ARG:HB2	2.46	0.46
3:B:125:LEU:HD13	3:B:126:PRO:HD2	1.98	0.46
1:M:339:HIS:CE1	2:p:168:ALA:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:86:PHE:HE2	2:O:110:TYR:N	2.12	0.46
2:O:91:THR:HG22	2:O:92:GLU:H	1.80	0.46
8:P:30:LEU:HD21	8:P:44:ARG:HB3	1.98	0.46
1:V:407:MET:HG3	1:V:448:PHE:HB3	1.98	0.46
1:W:121:ILE:HG23	1:W:259:THR:HB	1.96	0.46
8:Z:134:MET:HB3	8:j:76:LEU:HD22	1.97	0.46
1:f:363:PHE:HD1	2:i:144:PRO:HG3	1.80	0.46
1:g:97:ARG:HH12	1:g:277:ILE:HG21	1.81	0.46
1:O:325:ASN:HD21	1:O:338:GLY:HA2	1.81	0.46
3:F:137:GLU:O	3:F:141:ILE:HG12	2.16	0.46
8:P:1:MET:HA	9:J:232:SER:HB3	1.98	0.46
1:X:156:LEU:H	1:X:176:SER:HB3	1.80	0.46
1:X:339:HIS:HB2	1:f:339:HIS:CE1	2.51	0.46
8:j:32:VAL:HA	8:j:41:VAL:HG12	1.97	0.46
1:o:379:ARG:NH2	2:p:160:VAL:HG12	2.30	0.46
4:w:123:ARG:HD2	4:w:123:ARG:N	2.31	0.46
9:J:205:PRO:HB3	9:J:261:LEU:HD21	1.98	0.46
9:T:9:LYS:HB3	9:T:81:GLU:HB2	1.98	0.46
3:F:34:ILE:HG22	3:F:35:GLU:H	1.81	0.46
1:L:155:ASP:HB2	1:L:178:ALA:HA	1.98	0.46
1:L:397:ILE:HA	1:L:455:ILE:HG22	1.96	0.46
2:O:84:ASN:HA	2:O:91:THR:N	2.25	0.46
8:P:241:THR:HG23	8:Z:231:HIS:O	2.15	0.46
1:h:339:HIS:CE1	2:v:168:ALA:HB3	2.51	0.46
2:v:86:PHE:HE2	2:v:110:TYR:N	2.13	0.46
2:1:171:ARG:HG3	2:1:205:THR:HB	1.98	0.46
3:B:234:SER:O	3:B:238:LYS:HG2	2.16	0.46
3:E:210:LYS:H	3:E:210:LYS:HD3	1.81	0.46
7:K:46:LEU:HD11	1:V:18:LEU:HD11	1.98	0.46
7:K:85:ILE:HG12	7:K:105:VAL:HG12	1.97	0.46
1:N:104:VAL:HG12	1:N:239:LEU:HD23	1.98	0.46
1:V:293:ARG:O	1:V:293:ARG:HG2	2.15	0.46
1:g:422:TYR:CG	1:g:441:PRO:HG3	2.51	0.46
7:n:52:ILE:HD11	7:n:75:GLU:HG2	1.98	0.46
7:t:53:PRO:HB2	7:t:56:GLU:HB2	1.98	0.46
2:v:186:LEU:HD23	2:v:195:LEU:HD23	1.98	0.46
1:O:293:ARG:O	1:O:293:ARG:HG2	2.16	0.45
1:L:339:HIS:CE1	1:N:339:HIS:HB2	2.51	0.45
1:g:158:TYR:CZ	1:g:187:ILE:HD13	2.51	0.45
2:i:184:SER:O	2:i:189:LEU:HB2	2.15	0.45
6:y:45:ILE:HG22	6:y:53:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:8:777:SER:HA	10:8:780:TYR:HD2	1.81	0.45
1:0:350:PRO:HB3	1:0:373:VAL:HG11	1.99	0.45
3:E:5:ILE:HG23	3:E:13:ILE:HB	1.98	0.45
3:E:233:ASP:H	3:E:236:THR:HB	1.80	0.45
3:F:206:ASN:C	9:J:69:ASN:HD21	2.24	0.45
1:L:72:PHE:HA	1:L:85:LEU:HD11	1.98	0.45
1:L:146:GLY:HA2	1:L:213:PHE:HA	1.98	0.45
1:V:471:PHE:HE2	1:V:472:LYS:HE3	1.81	0.45
1:X:260:ILE:HD11	1:X:270:VAL:HG12	1.99	0.45
8:Z:87:VAL:HG12	8:Z:125:PRO:HA	1.98	0.45
2:i:91:THR:HG22	2:i:92:GLU:H	1.81	0.45
4:k:53:ARG:H	4:k:53:ARG:CZ	2.29	0.45
9:T:237:LYS:HD2	9:d:124:GLU:HG3	1.98	0.45
9:T:279:ARG:HB3	9:T:292:GLU:HB2	1.98	0.45
2:1:184:SER:HB3	2:1:189:LEU:HD13	1.98	0.45
3:B:227:SER:H	1:L:294:ASN:CG	2.24	0.45
6:I:4:THR:HG22	6:I:111:VAL:HG22	1.99	0.45
8:P:6:LEU:HD23	10:AA:776:ALA:HB2	1.98	0.45
1:W:66:GLN:HE21	1:W:70:ASN:ND2	2.15	0.45
1:X:299:GLN:O	1:X:301:THR:HG23	2.16	0.45
1:X:349:ILE:HB	1:X:352:GLU:HG2	1.98	0.45
8:Z:197:ALA:O	8:j:204:GLY:HA3	2.16	0.45
3:A:217:ARG:NE	3:A:238:LYS:HA	2.29	0.45
1:M:415:LEU:HD12	1:M:419:ILE:HD11	1.98	0.45
1:X:93:ARG:HG3	1:X:288:LEU:HD22	1.99	0.45
1:f:172:ILE:HG21	1:f:195:VAL:HG22	1.99	0.45
1:o:407:MET:HG3	1:o:448:PHE:HB3	1.99	0.45
4:q:146:ASP:OD1	5:r:88:LYS:HE3	2.16	0.45
1:u:213:PHE:CE2	1:u:235:LYS:HG3	2.48	0.45
9:J:80:LEU:HB3	9:J:93:LEU:HB3	1.99	0.45
9:d:32:LEU:HD11	9:d:85:LYS:HD2	1.97	0.45
2:1:185:LEU:HB3	2:1:195:LEU:HD21	1.98	0.45
3:F:5:ILE:HG23	3:F:13:ILE:HB	1.98	0.45
1:X:320:VAL:HG12	1:X:345:VAL:HG22	1.98	0.45
6:c:47:ASP:HB3	6:c:53:ILE:HD11	1.97	0.45
8:j:140:HIS:CE1	8:j:142:TRP:HE3	2.35	0.45
6:s:4:THR:HG22	6:s:111:VAL:HG22	1.98	0.45
3:D:205:VAL:HG12	3:D:207:LYS:HE2	1.98	0.45
3:E:217:ARG:HH11	3:E:238:LYS:HA	1.81	0.45
1:N:307:LEU:HD13	1:N:360:ASN:HB2	1.99	0.45
8:P:179:ILE:HG12	8:Z:183:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:97:ARG:HB3	1:X:279:GLY:HA2	1.98	0.45
1:X:104:VAL:HG12	1:X:239:LEU:HD23	1.99	0.45
6:m:8:THR:HG22	6:m:107:LEU:HG	1.99	0.45
3:B:100:ARG:O	3:B:101:LEU:HB3	2.16	0.45
3:F:56:VAL:HG12	3:F:185:GLN:HG2	1.99	0.45
1:N:303:ILE:CG2	1:N:306:SER:H	2.30	0.45
1:N:412:GLU:H	1:N:412:GLU:CD	2.25	0.45
7:U:114:LEU:HD12	7:U:114:LEU:H	1.82	0.45
1:X:321:ARG:NH1	1:X:430:GLY:HA3	2.32	0.45
1:f:363:PHE:CD1	2:i:144:PRO:HG3	2.51	0.45
1:g:255:LEU:HD13	1:g:271:ILE:HG23	1.98	0.45
7:n:38:TYR:HD1	7:n:38:TYR:HA	1.68	0.45
9:T:208:LYS:HE2	9:T:303:ILE:HA	1.98	0.45
1:O:428:LYS:HG2	1:O:431:ASP:OD2	2.17	0.45
1:L:301:THR:HB	1:L:305:GLU:HB2	1.99	0.45
1:L:379:ARG:HH12	2:O:160:VAL:HG12	1.82	0.45
1:M:91:ILE:HD12	1:M:291:ARG:HH22	1.82	0.45
8:P:90:VAL:HG23	8:P:122:ILE:HB	1.98	0.45
1:W:28:VAL:HG12	2:Y:31:ARG:NH1	2.31	0.45
1:f:98:PRO:HB2	1:f:244:ASP:HB3	1.99	0.45
1:g:61:ILE:O	1:g:65:ILE:HG12	2.17	0.45
1:h:299:GLN:HB3	2:v:139:ARG:HH12	1.81	0.45
8:j:63:LEU:HD12	9:d:168:GLY:HA3	1.98	0.45
1:u:72:PHE:HA	1:u:85:LEU:HD11	1.98	0.45
1:O:303:ILE:HG12	1:g:302:ASN:HD21	1.81	0.45
1:O:454:THR:HB	1:O:462:GLN:HB3	1.99	0.45
3:B:34:ILE:HG22	3:B:35:GLU:H	1.81	0.45
3:B:217:ARG:HH11	3:B:238:LYS:HA	1.82	0.45
1:W:97:ARG:HH12	1:W:277:ILE:HG21	1.81	0.45
8:Z:171:ILE:HB	8:j:179:ILE:HD13	1.98	0.45
4:a:53:ARG:HH12	4:k:44:ARG:C	2.25	0.45
7:n:115:PRO:HD3	1:o:34:SER:HA	1.98	0.45
10:8:765:VAL:HG22	10:9:765:VAL:HG22	1.99	0.45
3:B:36:THR:HB	9:d:218:ARG:CZ	2.47	0.45
1:L:104:VAL:HG22	1:L:239:LEU:HD23	1.99	0.45
1:M:114:ASN:O	1:M:117:PRO:HD2	2.17	0.45
1:M:422:TYR:CG	1:M:441:PRO:HG3	2.53	0.45
1:N:11:ILE:HD13	1:N:66:GLN:HB2	1.99	0.45
7:e:114:LEU:HD12	7:e:114:LEU:H	1.82	0.45
1:f:304:LEU:HD11	1:f:322:ILE:HG21	1.99	0.45
1:g:149:PRO:HB3	1:g:158:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:281:LEU:HD23	1:h:281:LEU:HA	1.87	0.45
2:i:86:PHE:HE2	2:i:110:TYR:N	2.14	0.45
9:J:190:TRP:HZ3	9:J:192:ILE:HG13	1.82	0.45
9:d:43:ILE:HG23	9:d:56:ALA:HB2	1.99	0.45
9:d:63:LEU:HD23	9:d:63:LEU:HA	1.85	0.45
2:1:217:THR:HG22	2:1:218:GLU:H	1.81	0.44
3:B:137:GLU:O	3:B:141:ILE:HG12	2.17	0.44
3:D:231:SER:HB2	6:s:87:LEU:HD13	2.00	0.44
1:M:118:ALA:HB1	1:M:267:TRP:CZ3	2.49	0.44
6:S:84:PRO:HB3	6:S:104:PHE:CE2	2.52	0.44
1:f:104:VAL:HG22	1:f:239:LEU:HD23	1.99	0.44
1:o:220:PHE:HD2	1:o:350:PRO:HB2	1.82	0.44
1:o:262:ILE:HA	1:o:263:PRO:HD3	1.85	0.44
1:o:283:GLU:HG3	1:o:287:GLU:HB3	1.99	0.44
3:A:237:PHE:HB2	6:I:83:MET:HE1	1.98	0.44
3:B:131:LYS:HE2	3:B:131:LYS:HB2	1.75	0.44
3:E:117:PRO:HB2	4:a:141:GLN:HE22	1.83	0.44
1:L:298:VAL:HG23	1:L:299:GLN:H	1.82	0.44
1:V:174:TYR:HB3	1:V:191:LEU:HD23	1.98	0.44
1:V:428:LYS:HG2	1:V:431:ASP:OD2	2.18	0.44
1:f:116:PRO:HB2	1:f:117:PRO:HD3	1.98	0.44
1:g:140:LYS:HD2	1:g:141:ALA:N	2.31	0.44
6:y:46:PHE:HD1	6:y:52:PRO:HA	1.82	0.44
9:d:244:ARG:O	9:d:297:ASP:HB2	2.16	0.44
2:1:165:TYR:HD2	2:1:171:ARG:HD3	1.81	0.44
3:E:137:GLU:O	3:E:141:ILE:HG12	2.17	0.44
1:N:342:LEU:HD13	1:N:368:VAL:HG23	1.99	0.44
1:N:374:GLN:HB3	1:N:384:ARG:HH11	1.82	0.44
1:V:91:ILE:HD12	1:V:292:PHE:HD1	1.81	0.44
4:k:33:LEU:HD12	4:k:33:LEU:HA	1.82	0.44
1:o:325:ASN:HD21	1:o:338:GLY:HA2	1.81	0.44
1:u:203:LEU:HD21	1:u:223:LYS:HE3	1.98	0.44
1:M:91:ILE:HD13	1:M:91:ILE:HA	1.83	0.44
6:m:13:GLN:HE22	6:m:101:PRO:HG2	1.81	0.44
1:u:363:PHE:CD1	2:v:144:PRO:HG3	2.53	0.44
1:u:397:ILE:HA	1:u:455:ILE:HG22	1.99	0.44
1:0:262:ILE:HA	1:0:263:PRO:HD3	1.85	0.44
1:0:407:MET:HB2	1:0:448:PHE:HB3	1.99	0.44
8:P:6:LEU:HD22	10:AA:772:GLU:HG3	2.00	0.44
1:W:121:ILE:HD13	1:W:128:VAL:HG12	1.99	0.44
1:g:118:ALA:HB1	1:g:267:TRP:CZ3	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:407:MET:HB3	1:g:407:MET:HE2	1.71	0.44
8:j:225:PRO:O	8:j:229:HIS:HB3	2.17	0.44
6:m:61:PRO:HA	6:m:82:LEU:HB3	1.99	0.44
1:o:409:GLU:CD	2:v:118:ASN:HD22	2.26	0.44
7:t:114:LEU:H	7:t:114:LEU:HD12	1.82	0.44
2:v:87:GLY:HA2	2:v:109:TRP:HE3	1.83	0.44
5:x:28:PHE:HD1	5:x:29:ILE:HG13	1.82	0.44
9:d:228:TYR:HE1	9:d:244:ARG:HB3	1.83	0.44
1:0:234:GLN:HE21	1:0:234:GLN:N	2.16	0.44
1:0:407:MET:CG	1:0:448:PHE:HB3	2.47	0.44
3:D:90:VAL:HG13	3:D:127:GLN:HG2	1.99	0.44
1:N:26:SER:HA	1:N:39:VAL:HG21	1.99	0.44
2:O:198:LYS:HG3	2:O:204:TYR:CE1	2.52	0.44
2:Y:144:PRO:O	2:Y:148:ILE:HG12	2.18	0.44
4:a:115:THR:HB	4:a:121:GLU:CD	2.43	0.44
2:i:83:PHE:O	2:i:91:THR:HA	2.17	0.44
2:i:93:ARG:HA	2:i:93:ARG:HH11	1.83	0.44
2:p:217:THR:HG22	2:p:218:GLU:H	1.82	0.44
1:u:379:ARG:HH12	2:v:160:VAL:HG12	1.83	0.44
1:0:118:ALA:HA	1:0:262:ILE:HG12	1.99	0.44
1:0:164:VAL:HG13	1:0:223:LYS:HZ2	1.83	0.44
1:0:471:PHE:CE2	1:0:472:LYS:HG3	2.53	0.44
1:X:231:LEU:HD23	1:X:231:LEU:HA	1.85	0.44
1:X:339:HIS:CE1	2:i:168:ALA:HB3	2.52	0.44
1:f:292:PHE:O	1:f:293:ARG:HB3	2.17	0.44
1:h:47:LEU:HD11	7:t:14:PHE:HE1	1.83	0.44
1:o:303:ILE:HD12	1:o:303:ILE:H	1.83	0.44
2:p:121:GLU:HG3	2:p:122:PRO:HD2	2.00	0.44
9:J:243:ARG:HA	9:J:243:ARG:HD3	1.83	0.44
9:d:205:PRO:HB3	9:d:261:LEU:HD21	1.99	0.44
1:0:412:GLU:O	1:0:416:ARG:HG3	2.18	0.44
3:A:107:PHE:HD2	3:A:111:ILE:HG13	1.83	0.44
4:G:15:ILE:HG12	4:G:92:VAL:HG12	1.99	0.44
1:N:454:THR:OG1	1:N:462:GLN:HB3	2.17	0.44
8:P:179:ILE:HD13	8:j:171:ILE:HB	2.00	0.44
2:Y:217:THR:HG22	2:Y:218:GLU:H	1.83	0.44
1:f:410:ASN:OD1	2:p:116:THR:HG21	2.17	0.44
1:g:387:TYR:HE2	1:g:389:ARG:HH12	1.64	0.44
1:h:407:MET:SD	1:h:411:ILE:HG21	2.58	0.44
2:i:198:LYS:HG3	2:i:204:TYR:CE1	2.53	0.44
2:p:208:GLU:HG3	2:p:240:ASN:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:76:LEU:O	9:J:97:VAL:HG23	2.18	0.44
3:A:141:ILE:HD11	3:E:23:ARG:HH21	1.83	0.44
3:F:100:ARG:O	3:F:101:LEU:HB3	2.18	0.44
1:V:397:ILE:HG21	1:V:482:ILE:HG23	1.99	0.44
1:g:213:PHE:HD1	1:g:213:PHE:HA	1.75	0.44
1:h:321:ARG:NH1	1:h:430:GLY:HA3	2.33	0.44
4:k:123:ARG:HD2	4:k:123:ARG:N	2.32	0.44
1:u:164:VAL:HA	1:u:223:LYS:HG2	1.99	0.44
7:z:63:ARG:HA	7:z:63:ARG:NH1	2.32	0.44
9:T:237:LYS:HG3	9:T:238:LYS:HD3	1.99	0.44
3:F:33:PRO:HA	3:F:39:LYS:HD2	2.00	0.43
1:M:5:THR:HG22	1:M:6:ALA:H	1.83	0.43
1:V:283:GLU:HG3	1:V:287:GLU:HB3	2.00	0.43
1:W:415:LEU:HD12	1:W:419:ILE:HD11	1.99	0.43
1:f:293:ARG:HE	1:f:294:ASN:ND2	2.15	0.43
1:h:299:GLN:HB3	2:v:139:ARG:NH1	2.32	0.43
2:v:162:LEU:HD12	2:v:162:LEU:HA	1.84	0.43
2:v:184:SER:O	2:v:189:LEU:HB2	2.18	0.43
1:O:401:VAL:HG12	1:O:450:VAL:HG22	2.00	0.43
2:1:138:ASN:HA	1:g:297:PHE:CE1	2.53	0.43
3:B:176:GLU:HA	3:B:180:THR:HG21	1.99	0.43
6:I:23:ILE:HD11	6:I:108:TYR:CZ	2.53	0.43
1:M:363:PHE:HE1	1:o:324:GLU:HG2	1.83	0.43
1:X:147:ILE:HB	1:X:212:LEU:HB3	1.98	0.43
2:i:173:GLY:HA2	2:i:207:THR:O	2.18	0.43
8:j:31:ARG:HA	8:j:83:VAL:HG22	2.00	0.43
8:j:144:HIS:CG	8:j:164:ARG:HH22	2.36	0.43
1:u:292:PHE:O	1:u:293:ARG:HB3	2.17	0.43
9:J:210:VAL:O	9:J:263:ARG:HD2	2.19	0.43
9:T:277:ASN:O	9:T:293:CYS:HA	2.18	0.43
10:9:758:GLN:O	10:9:762:ARG:HG3	2.17	0.43
2:1:85:TYR:HA	2:1:117:GLY:N	2.33	0.43
3:C:137:GLU:HB2	3:C:184:LEU:HD22	2.01	0.43
3:E:131:LYS:HD2	7:n:66:PRO:HB3	2.00	0.43
1:L:53:VAL:HG13	2:O:15:ALA:HB1	1.99	0.43
8:P:197:ALA:O	8:Z:204:GLY:HA3	2.17	0.43
1:V:379:ARG:NH2	2:Y:160:VAL:HG12	2.33	0.43
1:u:116:PRO:HB2	1:u:117:PRO:HD3	1.98	0.43
9:J:74:GLU:HB3	9:J:75:TYR:CE2	2.54	0.43
9:d:74:GLU:HB3	9:d:75:TYR:CE2	2.53	0.43
9:d:277:ASN:HB2	9:d:294:TRP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:9:765:VAL:HG22	10:AA:765:VAL:HG22	2.00	0.43
3:A:217:ARG:NH1	3:A:220:LYS:HB2	2.34	0.43
1:L:434:ILE:HG21	1:W:449:GLN:HG3	2.00	0.43
1:M:94:HIS:HB2	1:M:283:GLU:OE1	2.18	0.43
8:P:80:PRO:HB3	8:j:147:LYS:HA	2.00	0.43
8:P:231:HIS:HD2	8:Z:231:HIS:CE1	2.36	0.43
1:V:18:LEU:HD22	1:V:22:ARG:HH12	1.84	0.43
1:W:109:ILE:HD11	1:W:139:PRO:HD3	2.00	0.43
1:f:162:MET:SD	1:f:203:LEU:HG	2.59	0.43
1:h:390:PRO:HB2	1:h:474:VAL:HG12	2.01	0.43
1:h:454:THR:OG1	1:h:462:GLN:HB3	2.19	0.43
2:i:73:ARG:HB2	2:i:134:LYS:HG2	2.01	0.43
8:j:2:ARG:NH1	9:T:51:LYS:HG3	2.34	0.43
7:n:85:ILE:HG13	7:n:105:VAL:HG12	1.99	0.43
1:u:304:LEU:HD11	1:u:322:ILE:HG21	1.99	0.43
10:4:693:VAL:O	10:4:697:ILE:HG12	2.19	0.43
3:F:204:ARG:HH11	6:m:16:LYS:N	2.16	0.43
1:L:363:PHE:CD1	2:O:144:PRO:HG3	2.53	0.43
2:O:96:SER:O	2:O:106:GLY:HA3	2.17	0.43
2:O:173:GLY:HA2	2:O:207:THR:O	2.18	0.43
1:V:112:VAL:HG22	1:V:136:ILE:HG23	1.99	0.43
1:X:394:PRO:HA	1:X:476:THR:HG22	2.00	0.43
2:Y:184:SER:HB3	2:Y:189:LEU:HD13	1.98	0.43
8:Z:235:MET:HB3	8:j:235:MET:HB3	2.00	0.43
1:g:453:LEU:HD23	1:g:454:THR:N	2.34	0.43
8:j:98:VAL:HB	8:j:108:HIS:ND1	2.34	0.43
5:x:153:GLY:O	5:x:157:LEU:HB2	2.18	0.43
9:d:261:LEU:HD22	9:d:298:LEU:HD11	2.01	0.43
2:1:215:PHE:HD1	2:1:236:GLY:HA3	1.84	0.43
1:L:393:VAL:HG21	1:L:469:ILE:HD11	2.00	0.43
1:W:5:THR:HG22	1:W:6:ALA:H	1.84	0.43
8:Z:94:ARG:NH1	9:T:172:ARG:HH22	2.16	0.43
1:f:213:PHE:CE2	1:f:235:LYS:HG3	2.52	0.43
1:h:456:ALA:HB2	1:h:462:GLN:HA	2.01	0.43
1:0:310:GLY:O	1:0:314:VAL:HG23	2.19	0.43
1:0:412:GLU:HB3	1:0:484:VAL:HB	2.00	0.43
1:M:140:LYS:HD2	1:M:141:ALA:H	1.83	0.43
6:S:13:GLN:HE22	6:S:101:PRO:HG2	1.82	0.43
1:V:118:ALA:HA	1:V:262:ILE:HG12	2.01	0.43
2:Y:147:VAL:HG22	2:Y:197:PRO:HG2	2.01	0.43
2:Y:152:LYS:HE2	2:Y:152:LYS:HB3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:156:LEU:HD23	1:h:156:LEU:HA	1.93	0.43
2:i:186:LEU:HD23	2:i:195:LEU:HD23	2.01	0.43
6:s:45:ILE:HD11	6:s:80:PHE:HE2	1.84	0.43
9:T:210:VAL:O	9:T:263:ARG:HD2	2.19	0.43
1:0:112:VAL:HG22	1:0:136:ILE:HG23	2.01	0.43
3:A:171:ASP:HB3	3:A:189:THR:HB	2.00	0.43
3:B:204:ARG:CZ	6:y:17:TYR:HB3	2.49	0.43
3:C:41:THR:C	3:C:43:HIS:H	2.27	0.43
3:C:169:PHE:HE1	3:C:188:MET:HB3	1.84	0.43
3:D:127:GLN:HB3	3:D:128:LYS:H	1.52	0.43
3:E:96:ILE:HA	3:E:122:ALA:HA	2.01	0.43
7:K:115:PRO:HD3	1:V:34:SER:HA	2.00	0.43
1:X:252:GLN:HB2	1:X:276:ALA:HB3	2.00	0.43
1:X:454:THR:OG1	1:X:462:GLN:HB3	2.19	0.43
1:X:456:ALA:HB2	1:X:462:GLN:HA	1.99	0.43
2:Y:164:GLU:H	2:Y:164:GLU:CD	2.26	0.43
8:Z:88:LEU:HD22	8:j:122:ILE:HG21	2.01	0.43
1:f:111:THR:HG21	1:f:266:GLY:HA3	2.00	0.43
1:g:116:PRO:HB2	1:g:117:PRO:HD3	2.01	0.43
1:h:93:ARG:O	1:h:94:HIS:HB2	2.19	0.43
1:h:396:GLU:HG2	1:h:481:ASP:HB3	2.01	0.43
1:o:112:VAL:HG22	1:o:136:ILE:HG23	2.01	0.43
6:s:65:ILE:HG23	6:s:80:PHE:HB2	2.00	0.43
6:y:4:THR:HG22	6:y:111:VAL:HG13	2.01	0.43
9:J:244:ARG:N	9:J:244:ARG:HE	2.15	0.43
9:T:244:ARG:N	9:T:244:ARG:HE	2.17	0.43
1:0:183:THR:O	1:0:187:ILE:HG13	2.19	0.43
2:1:68:GLY:HA2	2:1:71:VAL:HG22	2.00	0.43
3:A:127:GLN:HB3	3:A:128:LYS:H	1.51	0.43
3:E:214:LYS:HE3	3:E:214:LYS:HB3	1.88	0.43
1:u:132:LEU:HD13	1:u:243:VAL:HG21	1.99	0.43
7:z:85:ILE:HG12	7:z:105:VAL:HG12	2.00	0.43
3:B:44:ILE:HG12	3:D:168:ILE:HD12	2.01	0.43
1:L:111:THR:HB	1:L:137:LEU:HD12	2.00	0.43
1:M:21:TYR:HB3	1:M:51:ILE:HD12	2.01	0.43
1:N:109:ILE:HG23	1:W:250:VAL:HG22	2.01	0.43
1:V:96:ALA:HB1	1:V:247:ILE:HG21	2.01	0.43
1:W:453:LEU:HD23	1:W:454:THR:N	2.34	0.43
1:X:407:MET:SD	1:X:411:ILE:HG21	2.58	0.43
8:Z:130:PHE:HB2	8:Z:131:PRO:HD3	2.01	0.43
1:f:146:GLY:HA2	1:f:213:PHE:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:296:LYS:HB2	1:g:296:LYS:HE2	1.77	0.43
2:i:129:MET:HG2	2:i:185:LEU:HD13	1.99	0.43
2:i:134:LYS:NZ	2:i:138:ASN:HD22	2.16	0.43
2:i:165:TYR:CE1	2:i:171:ARG:HD3	2.54	0.43
6:m:4:THR:HG22	6:m:111:VAL:HG13	2.01	0.43
9:J:176:LYS:HE2	9:J:176:LYS:HB3	1.86	0.43
1:0:283:GLU:HG3	1:0:287:GLU:HB3	2.01	0.42
3:A:174:PHE:CE1	3:A:186:PRO:HB3	2.54	0.42
3:C:141:ILE:HD11	3:F:23:ARG:HH21	1.84	0.42
3:D:56:VAL:HG12	3:D:185:GLN:HG2	2.01	0.42
3:E:131:LYS:HE2	3:E:131:LYS:HB2	1.82	0.42
1:L:303:ILE:HD13	1:L:362:PRO:HG3	2.01	0.42
2:O:186:LEU:HD23	2:O:195:LEU:HD23	2.01	0.42
8:P:98:VAL:HB	8:P:108:HIS:ND1	2.34	0.42
1:X:281:LEU:HD23	1:X:281:LEU:HA	1.85	0.42
1:f:93:ARG:HB3	1:f:288:LEU:HD12	2.00	0.42
1:f:115:SER:HB3	1:f:116:PRO:HD3	2.01	0.42
6:s:91:GLN:H	6:s:91:GLN:HG2	1.62	0.42
2:v:198:LYS:HG3	2:v:204:TYR:CE1	2.54	0.42
4:w:88:ILE:HD12	4:w:88:ILE:HA	1.85	0.42
6:y:13:GLN:HE22	6:y:101:PRO:HG2	1.84	0.42
2:1:31:ARG:NH1	1:g:28:VAL:HG12	2.34	0.42
3:E:12:LEU:HD12	3:E:12:LEU:HA	1.88	0.42
1:M:387:TYR:HE2	1:M:389:ARG:HH12	1.66	0.42
2:O:129:MET:HG2	2:O:185:LEU:HD13	2.00	0.42
8:P:25:ILE:HD11	8:P:47:VAL:HB	1.99	0.42
8:P:148:ASP:HB2	8:P:164:ARG:HH11	1.83	0.42
1:W:91:ILE:HD13	1:W:91:ILE:HA	1.89	0.42
1:h:73:ASN:HD21	1:h:75:ALA:HB3	1.84	0.42
2:v:93:ARG:HA	2:v:93:ARG:HH11	1.84	0.42
9:J:38:GLN:HB2	9:J:285:ARG:HD2	1.99	0.42
9:T:227:PHE:CE1	9:T:247:GLN:HB2	2.54	0.42
10:6:693:VAL:O	10:6:697:ILE:HG12	2.19	0.42
1:0:471:PHE:HE2	1:0:472:LYS:HE3	1.84	0.42
3:B:33:PRO:HA	3:B:39:LYS:HD2	2.01	0.42
1:L:397:ILE:HB	1:L:482:ILE:HG23	2.01	0.42
1:M:263:PRO:HG3	8:Z:31:ARG:HD3	2.01	0.42
1:M:407:MET:HE2	1:M:407:MET:HB3	1.72	0.42
1:N:168:ASN:HD21	1:W:418:ARG:CZ	2.32	0.42
7:U:40:PHE:O	7:U:51:GLY:HA3	2.19	0.42
1:X:434:ILE:HG22	1:X:437:ARG:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:68:GLY:HA2	2:Y:71:VAL:HG22	2.00	0.42
1:f:262:ILE:HG23	1:f:264:ILE:HG13	2.00	0.42
1:g:5:THR:HG22	1:g:6:ALA:H	1.83	0.42
1:h:437:ARG:NH1	1:o:447:GLY:H	2.16	0.42
1:o:174:TYR:HE2	1:o:187:ILE:HA	1.85	0.42
1:o:419:ILE:HD13	1:o:419:ILE:HA	1.76	0.42
2:p:30:ASP:O	2:p:34:GLN:HG3	2.19	0.42
1:u:141:ALA:HA	1:u:222:THR:HB	2.02	0.42
9:d:244:ARG:HE	9:d:244:ARG:N	2.17	0.42
3:D:90:VAL:HA	3:D:127:GLN:HG2	2.01	0.42
1:L:129:PHE:HZ	1:L:252:GLN:HE22	1.66	0.42
1:M:412:GLU:O	1:M:416:ARG:HG2	2.19	0.42
1:V:343:PRO:HG2	1:V:387:TYR:HA	2.02	0.42
1:V:471:PHE:CE2	1:V:472:LYS:HG3	2.55	0.42
1:W:94:HIS:HB3	1:W:95:ALA:H	1.55	0.42
8:Z:244:PRO:HG3	8:j:226:PHE:O	2.19	0.42
4:a:41:ARG:HA	4:a:47:HIS:ND1	2.33	0.42
1:f:293:ARG:O	1:f:293:ARG:HG2	2.18	0.42
1:g:21:TYR:HB3	1:g:51:ILE:HD12	2.02	0.42
1:g:163:TYR:CZ	1:g:169:THR:HG22	2.55	0.42
2:i:136:ILE:HD13	2:i:136:ILE:HA	1.90	0.42
2:v:165:TYR:CE1	2:v:171:ARG:HD3	2.55	0.42
1:0:34:SER:HA	7:z:115:PRO:HD3	2.02	0.42
3:D:222:GLY:O	3:D:228:ASN:HB2	2.20	0.42
6:I:53:ILE:O	6:I:54:LEU:HD12	2.19	0.42
8:P:115:LYS:HB3	8:P:116:PHE:CD2	2.55	0.42
1:h:415:LEU:HD21	1:h:442:ILE:HG23	2.01	0.42
1:o:183:THR:O	1:o:187:ILE:HG13	2.20	0.42
6:s:9:LEU:HB2	6:s:106:LEU:HD23	2.00	0.42
1:u:160:LEU:HD12	1:u:226:GLU:O	2.19	0.42
3:A:141:ILE:HD13	3:A:141:ILE:HA	1.87	0.42
4:G:123:ARG:N	4:G:123:ARG:HD2	2.34	0.42
1:N:105:LEU:HG	1:N:270:VAL:HB	2.01	0.42
1:N:280:ARG:HH21	1:N:283:GLU:HG3	1.84	0.42
2:O:165:TYR:CE1	2:O:171:ARG:HD3	2.54	0.42
8:j:2:ARG:HH12	9:T:51:LYS:HG3	1.84	0.42
1:o:403:ASN:HB2	1:o:407:MET:HE2	2.02	0.42
9:T:74:GLU:HB3	9:T:75:TYR:CE1	2.54	0.42
2:1:70:ILE:HG12	1:g:74:PRO:HG2	2.02	0.42
3:B:23:ARG:HH21	3:D:141:ILE:HD11	1.85	0.42
3:B:199:ARG:HH11	3:B:199:ARG:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:165:ASP:O	1:L:167:ILE:HG12	2.20	0.42
1:N:164:VAL:O	1:N:168:ASN:HB2	2.20	0.42
2:O:198:LYS:HA	2:O:204:TYR:CZ	2.54	0.42
6:S:93:LYS:HG3	6:S:94:HIS:ND1	2.34	0.42
1:W:218:ASP:HB3	1:W:221:ASN:HB2	2.02	0.42
1:X:390:PRO:HB2	1:X:474:VAL:HG12	2.01	0.42
6:c:47:ASP:OD2	6:c:51:ASN:HB2	2.19	0.42
7:e:40:PHE:HB2	7:e:43:GLU:CD	2.44	0.42
1:h:315:GLU:CD	1:h:315:GLU:H	2.28	0.42
1:u:115:SER:HB3	1:u:116:PRO:HD3	2.01	0.42
1:u:234:GLN:HE21	1:u:234:GLN:HB3	1.68	0.42
1:u:293:ARG:O	1:u:293:ARG:HG2	2.20	0.42
9:T:176:LYS:HB3	9:T:176:LYS:HE2	1.76	0.42
3:A:41:THR:C	3:A:43:HIS:H	2.27	0.42
3:A:168:ILE:HD12	3:E:44:ILE:HG12	2.02	0.42
3:B:76:THR:HG21	7:U:56:GLU:HB3	2.02	0.42
7:K:38:TYR:HB3	2:Y:22:GLN:HG2	2.01	0.42
1:M:174:TYR:CE1	1:M:190:GLY:HA3	2.55	0.42
2:O:93:ARG:NH1	2:O:93:ARG:HA	2.34	0.42
1:X:84:ASN:CG	1:f:73:ASN:HD21	2.28	0.42
6:c:9:LEU:HB2	6:c:106:LEU:HD23	2.02	0.42
7:e:38:TYR:HD1	7:e:38:TYR:HA	1.70	0.42
1:f:103:VAL:HG12	1:f:272:ASN:HB3	2.02	0.42
1:f:155:ASP:HB2	1:f:178:ALA:HA	2.01	0.42
2:p:127:TYR:HA	2:p:130:ILE:HG22	2.01	0.42
1:L:115:SER:HB3	1:L:116:PRO:HD3	2.01	0.42
1:L:188:LEU:HD22	1:L:212:LEU:HB3	2.01	0.42
1:N:156:LEU:H	1:N:176:SER:HB3	1.85	0.42
2:O:162:LEU:HD12	2:O:162:LEU:HA	1.87	0.42
1:X:93:ARG:O	1:X:94:HIS:HB2	2.20	0.42
8:Z:22:TYR:HA	8:j:93:GLN:NE2	2.34	0.42
1:u:161:LYS:HB3	1:u:163:TYR:HE1	1.84	0.42
9:d:192:ILE:HG22	9:d:193:SER:O	2.20	0.42
3:A:21:PHE:HD1	3:A:53:LEU:HD13	1.85	0.42
3:A:161:TRP:CZ2	3:B:134:TYR:HB3	2.55	0.42
1:N:299:GLN:H	2:O:139:ARG:HH22	1.66	0.42
1:N:321:ARG:NH1	1:N:430:GLY:HA3	2.35	0.42
6:S:13:GLN:NE2	6:S:101:PRO:HG2	2.35	0.42
1:X:396:GLU:HG2	1:X:481:ASP:HB3	2.02	0.42
1:f:163:TYR:CE2	1:f:169:THR:HG23	2.55	0.42
1:f:379:ARG:NH2	2:i:160:VAL:HG12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:174:TYR:CE2	1:o:187:ILE:HA	2.54	0.42
1:o:350:PRO:HB3	1:o:373:VAL:HG21	2.01	0.42
9:T:213:ALA:HB1	9:T:261:LEU:O	2.19	0.42
3:D:41:THR:C	3:D:43:HIS:H	2.27	0.41
1:L:412:GLU:HB2	1:L:416:ARG:CZ	2.50	0.41
8:P:231:HIS:CE1	8:j:231:HIS:HD2	2.38	0.41
1:V:174:TYR:CE2	1:V:187:ILE:HA	2.54	0.41
1:X:105:LEU:HG	1:X:270:VAL:HB	2.01	0.41
8:Z:100:LYS:HB2	9:J:167:TYR:CZ	2.55	0.41
1:f:337:PRO:HD2	1:f:368:VAL:HG11	2.02	0.41
1:h:47:LEU:HD12	1:h:47:LEU:H	1.85	0.41
1:h:105:LEU:HG	1:h:270:VAL:HB	2.02	0.41
1:h:320:VAL:HA	1:h:344:ILE:O	2.21	0.41
2:p:147:VAL:HG22	2:p:197:PRO:HG2	2.02	0.41
9:J:186:ASN:HB2	9:J:188:ILE:HD11	2.02	0.41
9:T:190:TRP:CZ3	9:T:192:ILE:HG13	2.53	0.41
1:0:115:SER:HB2	1:0:131:LEU:HB2	2.02	0.41
1:0:174:TYR:CE2	1:0:187:ILE:HA	2.54	0.41
1:0:447:GLY:H	1:N:437:ARG:NH1	2.17	0.41
1:M:297:PHE:CE1	2:p:138:ASN:HA	2.55	0.41
1:N:231:LEU:HD23	1:N:231:LEU:HA	1.86	0.41
1:V:49:ARG:HD2	2:Y:23:PHE:HE2	1.85	0.41
5:b:88:LYS:HB3	5:b:106:THR:HG23	2.01	0.41
1:h:307:LEU:HD13	1:h:360:ASN:HB2	2.02	0.41
2:p:184:SER:HB3	2:p:189:LEU:HD13	2.01	0.41
2:1:139:ARG:HH21	1:g:298:VAL:H	1.68	0.41
3:B:82:LYS:HE2	3:B:82:LYS:HA	2.01	0.41
1:M:32:LEU:HB2	2:p:31:ARG:NH2	2.35	0.41
8:P:245:GLN:NE2	8:j:230:LYS:HB2	2.35	0.41
8:Z:52:LYS:HE3	9:d:187:ASN:CG	2.45	0.41
6:c:4:THR:HG22	6:c:111:VAL:HG22	2.03	0.41
6:c:43:MET:HE3	6:c:43:MET:HB3	1.86	0.41
1:f:161:LYS:HB2	1:f:226:GLU:HB2	2.02	0.41
1:g:121:ILE:HD13	1:g:128:VAL:HG12	2.02	0.41
1:o:18:LEU:HB3	1:o:22:ARG:NH1	2.34	0.41
1:u:363:PHE:HD1	2:v:144:PRO:HG3	1.84	0.41
2:v:88:PHE:HB2	2:v:95:GLY:H	1.85	0.41
9:J:82:VAL:HG23	9:J:252:LEU:HD21	2.02	0.41
9:J:176:LYS:HG2	9:J:177:ASP:N	2.35	0.41
3:F:23:ARG:C	3:F:23:ARG:HH11	2.29	0.41
1:W:281:LEU:HD23	1:W:281:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:176:LYS:HD2	2:Y:176:LYS:HA	1.87	0.41
8:Z:115:LYS:HB3	8:Z:116:PHE:CD2	2.55	0.41
4:a:123:ARG:HD2	4:a:123:ARG:N	2.35	0.41
1:f:53:VAL:HG13	2:i:15:ALA:HB1	2.01	0.41
1:f:234:GLN:HE21	1:f:234:GLN:HB3	1.69	0.41
1:f:412:GLU:O	1:f:416:ARG:HG3	2.20	0.41
1:g:149:PRO:HB3	1:g:158:TYR:HE2	1.86	0.41
1:h:231:LEU:HD23	1:h:231:LEU:HA	1.84	0.41
1:o:310:GLY:O	1:o:314:VAL:HG23	2.20	0.41
6:y:13:GLN:OE1	6:y:98:ASP:HA	2.20	0.41
9:J:9:LYS:HD3	9:J:81:GLU:OE1	2.20	0.41
9:J:227:PHE:CE1	9:J:247:GLN:HB2	2.55	0.41
9:d:82:VAL:HG23	9:d:252:LEU:HD21	2.01	0.41
4:G:117:THR:HG23	4:G:119:GLY:H	1.85	0.41
1:M:105:LEU:HD11	1:M:135:VAL:HG11	2.01	0.41
1:W:7:GLU:O	2:Y:62:LYS:HD2	2.21	0.41
1:W:97:ARG:O	1:W:247:ILE:HG23	2.20	0.41
1:W:407:MET:HE2	1:W:407:MET:HB3	1.80	0.41
5:b:121:LEU:HD12	5:b:121:LEU:HA	1.91	0.41
2:i:84:ASN:HA	2:i:91:THR:N	2.31	0.41
6:m:13:GLN:NE2	6:m:101:PRO:HG2	2.35	0.41
6:m:93:LYS:HE3	6:m:94:HIS:HE1	1.86	0.41
1:o:74:PRO:HA	1:o:85:LEU:HD13	2.02	0.41
3:F:204:ARG:NE	6:m:14:ASP:HB3	2.35	0.41
1:L:293:ARG:O	1:L:293:ARG:HG2	2.21	0.41
1:M:449:GLN:HG3	1:f:434:ILE:HG21	2.02	0.41
1:N:299:GLN:O	1:N:301:THR:HG23	2.21	0.41
8:P:76:LEU:HD22	8:j:134:MET:HB3	2.02	0.41
1:V:326:ASP:HB2	1:W:366:GLY:N	2.35	0.41
1:V:471:PHE:CD2	1:V:472:LYS:HG3	2.56	0.41
1:W:147:ILE:HB	1:W:231:LEU:HD22	2.01	0.41
2:Y:104:THR:HG23	2:Y:180:ASN:HA	2.03	0.41
7:e:61:LYS:HD3	7:e:61:LYS:HA	1.79	0.41
4:q:123:ARG:N	4:q:123:ARG:HD2	2.35	0.41
7:t:79:ASP:HB3	7:t:82:VAL:HG12	2.02	0.41
6:y:23:ILE:HD11	6:y:108:TYR:CZ	2.56	0.41
9:J:95:GLY:HA3	9:J:116:GLY:O	2.21	0.41
9:J:237:LYS:HG2	9:J:238:LYS:N	2.35	0.41
1:O:302:ASN:HB3	1:O:305:GLU:HG3	2.02	0.41
2:1:127:TYR:HA	2:1:130:ILE:HG22	2.02	0.41
3:A:90:VAL:HA	3:A:127:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:140:LYS:HD2	1:M:141:ALA:N	2.35	0.41
2:O:67:ILE:O	2:O:71:VAL:HG22	2.20	0.41
6:S:61:PRO:HA	6:S:82:LEU:HB3	2.02	0.41
1:h:280:ARG:HH21	1:h:283:GLU:HG3	1.86	0.41
5:l:37:PRO:HB2	5:l:38:PHE:CD2	2.56	0.41
1:u:302:ASN:HB3	1:u:305:GLU:HG3	2.03	0.41
1:u:412:GLU:O	1:u:416:ARG:HG3	2.21	0.41
2:v:87:GLY:HA2	2:v:109:TRP:CE3	2.56	0.41
9:J:264:VAL:O	9:J:270:SER:HA	2.20	0.41
3:A:2:THR:HG23	4:Q:46:HIS:CD2	2.56	0.41
3:A:141:ILE:HD11	3:E:23:ARG:NH2	2.35	0.41
3:B:172:LEU:HD21	3:B:174:PHE:CZ	2.56	0.41
3:C:137:GLU:O	3:C:141:ILE:HG12	2.21	0.41
3:E:51:PHE:HE2	3:E:164:ILE:HG21	1.85	0.41
3:E:188:MET:HG3	3:E:190:ILE:HD11	2.03	0.41
6:I:91:GLN:H	6:I:91:GLN:HG2	1.66	0.41
2:O:88:PHE:HB2	2:O:95:GLY:N	2.36	0.41
8:P:6:LEU:HD12	8:P:6:LEU:HA	1.93	0.41
8:P:155:LEU:HD11	8:Z:76:LEU:HB2	2.01	0.41
4:Q:41:ARG:HA	4:Q:47:HIS:CD2	2.56	0.41
6:S:4:THR:HG22	6:S:111:VAL:HG22	2.03	0.41
7:U:59:LEU:HD13	7:U:59:LEU:HA	1.93	0.41
1:V:403:ASN:HB2	1:V:407:MET:HE2	2.02	0.41
5:b:9:ASP:HB3	5:b:96:THR:OG1	2.21	0.41
1:h:296:LYS:NZ	2:v:72:GLY:HA3	2.36	0.41
8:j:130:PHE:HB2	8:j:131:PRO:HD3	2.03	0.41
4:q:88:ILE:HD12	4:q:88:ILE:HA	1.79	0.41
6:s:45:ILE:HD11	6:s:80:PHE:CE2	2.55	0.41
1:u:164:VAL:O	1:u:223:LYS:HA	2.21	0.41
2:l:28:ILE:HG12	1:g:32:LEU:HD21	2.02	0.41
3:A:12:LEU:HD23	3:A:12:LEU:HA	1.92	0.41
3:C:171:ASP:HB3	3:C:189:THR:HB	2.03	0.41
3:C:217:ARG:HH21	6:c:6:ILE:HD11	1.86	0.41
3:D:131:LYS:HA	3:D:131:LYS:HD2	1.87	0.41
1:L:469:ILE:HD12	1:L:469:ILE:HA	1.95	0.41
1:N:398:LYS:HD2	1:N:462:GLN:HG3	2.02	0.41
1:V:120:MET:HG3	1:V:129:PHE:HB2	2.03	0.41
1:V:310:GLY:O	1:V:314:VAL:HG23	2.21	0.41
1:V:447:GLY:H	1:X:437:ARG:NH1	2.16	0.41
1:W:297:PHE:CE1	2:Y:138:ASN:HA	2.55	0.41
1:W:303:ILE:HG22	1:W:306:SER:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:97:ARG:O	1:X:279:GLY:HA3	2.21	0.41
7:e:52:ILE:HD11	7:e:75:GLU:HG2	2.02	0.41
1:f:96:ALA:HB1	1:f:247:ILE:HG21	2.03	0.41
1:f:160:LEU:HD12	1:f:226:GLU:O	2.19	0.41
2:i:84:ASN:HA	2:i:91:THR:HA	2.03	0.41
1:o:260:ILE:HD11	1:o:270:VAL:HG12	2.02	0.41
2:p:85:TYR:CD2	2:p:92:GLU:HG3	2.56	0.41
2:p:164:GLU:CD	2:p:164:GLU:H	2.28	0.41
2:p:239:THR:HG22	2:p:241:LEU:N	2.31	0.41
6:s:23:ILE:HD11	6:s:108:TYR:CZ	2.55	0.41
4:w:33:LEU:HD12	4:w:33:LEU:HA	1.85	0.41
6:y:53:ILE:HG22	6:y:54:LEU:HD12	2.02	0.41
9:T:203:ASN:HA	9:T:274:ARG:NH1	2.36	0.41
1:O:418:ARG:HE	1:O:418:ARG:HB2	1.74	0.41
3:A:174:PHE:CD2	3:A:184:LEU:HD11	2.56	0.41
3:E:176:GLU:HA	3:E:180:THR:HG21	2.03	0.41
3:F:61:ASP:HB2	4:q:48:THR:HG23	2.03	0.41
3:F:172:LEU:HD21	3:F:174:PHE:CZ	2.56	0.41
7:K:63:ARG:HA	7:K:63:ARG:HH11	1.86	0.41
1:L:379:ARG:NH1	2:O:160:VAL:HG12	2.36	0.41
1:M:61:ILE:O	1:M:65:ILE:HG12	2.21	0.41
7:U:53:PRO:HB2	7:U:56:GLU:HB2	2.02	0.41
1:W:61:ILE:HD13	1:W:61:ILE:HA	1.96	0.41
8:Z:96:MET:HB3	8:Z:100:LYS:HG3	2.03	0.41
9:T:50:LYS:NZ	9:T:50:LYS:HB2	2.36	0.41
9:T:243:ARG:HD3	9:T:243:ARG:HA	1.87	0.41
3:B:78:LYS:HE2	3:B:78:LYS:HB2	1.93	0.40
3:E:172:LEU:HD21	3:E:174:PHE:CZ	2.56	0.40
3:F:229:ALA:HB1	3:F:232:GLN:HG3	2.03	0.40
2:O:33:LEU:HD23	2:O:33:LEU:HA	1.85	0.40
1:X:320:VAL:HA	1:X:344:ILE:O	2.21	0.40
1:X:324:GLU:OE2	2:i:201:GLY:HA2	2.20	0.40
2:Y:14:VAL:O	2:Y:18:ARG:HG2	2.21	0.40
8:Z:6:LEU:HD12	8:Z:6:LEU:H	1.87	0.40
5:b:74:LEU:HD23	5:b:74:LEU:HA	1.94	0.40
1:h:443:MET:HE1	1:o:437:ARG:HG2	2.03	0.40
7:n:79:ASP:HB3	7:n:82:VAL:HG12	2.02	0.40
1:o:412:GLU:O	1:o:416:ARG:HG3	2.20	0.40
6:s:53:ILE:O	6:s:54:LEU:HD12	2.19	0.40
1:u:85:LEU:HD23	1:u:85:LEU:HA	1.90	0.40
1:u:379:ARG:NH1	2:v:160:VAL:HG12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:y:73:HIS:CD2	6:y:74:ILE:HG12	2.56	0.40
1:0:174:TYR:HE2	1:0:187:ILE:HA	1.87	0.40
2:1:28:ILE:O	2:1:31:ARG:HG3	2.21	0.40
3:B:228:ASN:ND2	3:B:229:ALA:H	2.18	0.40
3:E:206:ASN:C	9:T:69:ASN:HD21	2.29	0.40
4:G:88:ILE:HD12	4:G:88:ILE:HA	1.82	0.40
1:M:4:ILE:HD12	1:M:9:LEU:HD13	2.03	0.40
1:M:453:LEU:HD23	1:M:454:THR:N	2.35	0.40
1:N:315:GLU:CD	1:N:315:GLU:H	2.29	0.40
1:N:434:ILE:HG22	1:N:437:ARG:H	1.85	0.40
2:O:21:GLU:HA	2:O:24:LYS:HG2	2.03	0.40
2:O:136:ILE:HD13	2:O:136:ILE:HA	1.88	0.40
1:V:228:ALA:H	1:V:231:LEU:HD12	1.85	0.40
1:V:303:ILE:HG12	1:W:302:ASN:HD21	1.86	0.40
1:V:442:ILE:H	1:V:442:ILE:HG13	1.72	0.40
1:W:403:ASN:HA	1:W:407:MET:CE	2.51	0.40
8:Z:51:TYR:HD2	10:AA:783:SER:HB3	1.86	0.40
1:f:188:LEU:HD22	1:f:212:LEU:HB3	2.02	0.40
8:j:140:HIS:HD2	8:j:144:HIS:CD2	2.39	0.40
1:o:248:GLY:HA2	1:o:249:PRO:HD3	1.97	0.40
2:p:48:GLU:HG3	2:p:49:ASP:N	2.35	0.40
9:T:9:LYS:HD3	9:T:81:GLU:OE1	2.21	0.40
9:T:43:ILE:HG23	9:T:56:ALA:HB2	2.04	0.40
1:0:379:ARG:HH22	2:1:160:VAL:HG12	1.86	0.40
1:0:403:ASN:HB2	1:0:407:MET:HE2	2.03	0.40
3:D:217:ARG:NH1	3:D:220:LYS:HB2	2.37	0.40
3:F:96:ILE:HA	3:F:122:ALA:HA	2.04	0.40
1:L:292:PHE:C	1:L:294:ASN:H	2.28	0.40
1:L:389:ARG:HG2	1:L:390:PRO:HD2	2.04	0.40
1:M:363:PHE:CE1	1:o:324:GLU:HG2	2.56	0.40
8:P:52:LYS:HD2	10:8:782:GLU:OE1	2.21	0.40
1:X:420:VAL:HG21	1:X:479:ALA:HB2	2.03	0.40
1:g:91:ILE:HD13	1:g:91:ILE:HA	1.88	0.40
1:g:174:TYR:CE1	1:g:190:GLY:HA3	2.57	0.40
2:v:33:LEU:HD23	2:v:33:LEU:HA	1.90	0.40
10:8:781:LYS:HA	10:8:781:LYS:HD3	1.89	0.40
3:D:16:ASP:HB3	4:w:48:THR:OG1	2.21	0.40
1:M:121:ILE:HG23	1:M:259:THR:HB	2.03	0.40
1:M:393:VAL:HG13	1:M:475:ALA:HA	2.03	0.40
8:P:29:VAL:HG13	8:P:41:VAL:HB	2.02	0.40
5:R:35:ILE:HD12	5:R:35:ILE:HA	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:32:LEU:HD23	2:v:31:ARG:NE	2.37	0.40
8:j:66:PRO:HD3	8:j:100:LYS:HE3	2.02	0.40
2:v:67:ILE:O	2:v:71:VAL:HG22	2.21	0.40
9:T:100:THR:HA	9:T:112:GLN:O	2.21	0.40
2:1:85:TYR:CD2	2:1:92:GLU:HG3	2.56	0.40
3:B:66:ARG:NH1	3:B:87:THR:HB	2.36	0.40
1:L:415:LEU:HD23	1:L:415:LEU:HA	1.94	0.40
1:N:93:ARG:O	1:N:94:HIS:HB2	2.21	0.40
1:N:281:LEU:HD23	1:N:281:LEU:HA	1.85	0.40
1:N:349:ILE:HB	1:N:352:GLU:HG2	2.04	0.40
8:P:44:ARG:HE	8:P:61:GLU:HG2	1.86	0.40
8:P:212:TYR:HB3	8:Z:219:SER:HA	2.02	0.40
1:V:183:THR:O	1:V:187:ILE:HG13	2.21	0.40
1:V:412:GLU:O	1:V:416:ARG:HG3	2.20	0.40
2:i:162:LEU:HD12	2:i:162:LEU:HA	1.85	0.40
2:i:177:ILE:HD13	2:i:210:GLN:HE21	1.87	0.40
6:m:13:GLN:OE1	6:m:98:ASP:HA	2.21	0.40
1:o:407:MET:HG2	1:o:408:PRO:O	2.21	0.40
2:v:165:TYR:CD1	2:v:171:ARG:HD3	2.56	0.40
2:v:209:PHE:HB3	2:v:239:THR:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	484/487 (99%)	462 (96%)	22 (4%)	0	100	100
1	L	484/487 (99%)	465 (96%)	19 (4%)	0	100	100
1	M	484/487 (99%)	454 (94%)	29 (6%)	1 (0%)	43	72
1	N	484/487 (99%)	462 (96%)	20 (4%)	2 (0%)	30	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	484/487 (99%)	466 (96%)	18 (4%)	0	100	100
1	W	484/487 (99%)	461 (95%)	23 (5%)	0	100	100
1	X	484/487 (99%)	460 (95%)	23 (5%)	1 (0%)	43	72
1	f	484/487 (99%)	466 (96%)	18 (4%)	0	100	100
1	g	484/487 (99%)	463 (96%)	20 (4%)	1 (0%)	43	72
1	h	484/487 (99%)	463 (96%)	19 (4%)	2 (0%)	30	61
1	o	484/487 (99%)	466 (96%)	18 (4%)	0	100	100
1	u	484/487 (99%)	464 (96%)	20 (4%)	0	100	100
2	l	240/243 (99%)	218 (91%)	21 (9%)	1 (0%)	30	61
2	O	240/243 (99%)	217 (90%)	21 (9%)	2 (1%)	16	49
2	Y	240/243 (99%)	217 (90%)	22 (9%)	1 (0%)	30	61
2	i	240/243 (99%)	218 (91%)	20 (8%)	2 (1%)	16	49
2	p	240/243 (99%)	218 (91%)	21 (9%)	1 (0%)	30	61
2	v	240/243 (99%)	219 (91%)	19 (8%)	2 (1%)	16	49
3	A	235/253 (93%)	216 (92%)	19 (8%)	0	100	100
3	B	235/253 (93%)	212 (90%)	22 (9%)	1 (0%)	30	61
3	C	235/253 (93%)	212 (90%)	23 (10%)	0	100	100
3	D	235/253 (93%)	215 (92%)	20 (8%)	0	100	100
3	E	235/253 (93%)	211 (90%)	23 (10%)	1 (0%)	30	61
3	F	235/253 (93%)	214 (91%)	20 (8%)	1 (0%)	30	61
4	G	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
4	Q	156/159 (98%)	148 (95%)	8 (5%)	0	100	100
4	a	156/159 (98%)	149 (96%)	7 (4%)	0	100	100
4	k	156/159 (98%)	146 (94%)	10 (6%)	0	100	100
4	q	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
4	w	156/159 (98%)	147 (94%)	9 (6%)	0	100	100
5	H	164/166 (99%)	158 (96%)	6 (4%)	0	100	100
5	R	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
5	b	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
5	l	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
5	r	164/166 (99%)	159 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	x	164/166 (99%)	160 (98%)	4 (2%)	0	100	100
6	I	112/118 (95%)	107 (96%)	5 (4%)	0	100	100
6	S	112/118 (95%)	105 (94%)	7 (6%)	0	100	100
6	c	112/118 (95%)	107 (96%)	5 (4%)	0	100	100
6	m	112/118 (95%)	104 (93%)	8 (7%)	0	100	100
6	s	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
6	y	112/118 (95%)	105 (94%)	7 (6%)	0	100	100
7	K	118/123 (96%)	109 (92%)	9 (8%)	0	100	100
7	U	118/123 (96%)	112 (95%)	6 (5%)	0	100	100
7	e	118/123 (96%)	110 (93%)	8 (7%)	0	100	100
7	n	118/123 (96%)	110 (93%)	8 (7%)	0	100	100
7	t	118/123 (96%)	112 (95%)	6 (5%)	0	100	100
7	z	118/123 (96%)	111 (94%)	7 (6%)	0	100	100
8	P	244/246 (99%)	226 (93%)	18 (7%)	0	100	100
8	Z	244/246 (99%)	224 (92%)	19 (8%)	1 (0%)	30	61
8	j	244/246 (99%)	226 (93%)	17 (7%)	1 (0%)	30	61
9	J	302/305 (99%)	270 (89%)	32 (11%)	0	100	100
9	T	302/305 (99%)	272 (90%)	30 (10%)	0	100	100
9	d	302/305 (99%)	270 (89%)	32 (11%)	0	100	100
10	2	17/788 (2%)	17 (100%)	0	0	100	100
10	3	17/788 (2%)	17 (100%)	0	0	100	100
10	4	17/788 (2%)	17 (100%)	0	0	100	100
10	5	17/788 (2%)	17 (100%)	0	0	100	100
10	6	17/788 (2%)	17 (100%)	0	0	100	100
10	7	17/788 (2%)	17 (100%)	0	0	100	100
10	8	30/788 (4%)	29 (97%)	1 (3%)	0	100	100
10	9	30/788 (4%)	30 (100%)	0	0	100	100
10	AA	30/788 (4%)	30 (100%)	0	0	100	100
All	All	13788/20961 (66%)	12962 (94%)	805 (6%)	21 (0%)	44	72

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	118	ASN
1	M	285	ASP
2	O	118	ASN
2	Y	118	ASN
2	i	118	ASN
2	p	118	ASN
2	v	118	ASN
8	j	6	LEU
1	N	38	GLU
1	h	38	GLU
8	Z	4	THR
3	B	101	LEU
3	E	101	LEU
3	F	101	LEU
1	N	167	ILE
1	X	167	ILE
1	h	167	ILE
2	O	105	VAL
1	g	167	ILE
2	i	105	VAL
2	v	105	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	410/411 (100%)	370 (90%)	40 (10%)	7	31
1	L	410/411 (100%)	379 (92%)	31 (8%)	12	39
1	M	410/411 (100%)	387 (94%)	23 (6%)	19	47
1	N	410/411 (100%)	387 (94%)	23 (6%)	19	47
1	V	410/411 (100%)	376 (92%)	34 (8%)	10	35
1	W	410/411 (100%)	391 (95%)	19 (5%)	24	51
1	X	410/411 (100%)	386 (94%)	24 (6%)	18	45
1	f	410/411 (100%)	381 (93%)	29 (7%)	13	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	g	410/411 (100%)	387 (94%)	23 (6%)	19	47
1	h	410/411 (100%)	384 (94%)	26 (6%)	16	44
1	o	410/411 (100%)	379 (92%)	31 (8%)	12	39
1	u	410/411 (100%)	383 (93%)	27 (7%)	15	43
2	l	197/198 (100%)	179 (91%)	18 (9%)	9	33
2	O	197/198 (100%)	183 (93%)	14 (7%)	13	40
2	Y	197/198 (100%)	177 (90%)	20 (10%)	7	30
2	i	197/198 (100%)	184 (93%)	13 (7%)	15	43
2	p	197/198 (100%)	180 (91%)	17 (9%)	10	34
2	v	197/198 (100%)	181 (92%)	16 (8%)	11	36
3	A	212/226 (94%)	195 (92%)	17 (8%)	11	37
3	B	212/226 (94%)	194 (92%)	18 (8%)	10	35
3	C	212/226 (94%)	192 (91%)	20 (9%)	8	32
3	D	212/226 (94%)	189 (89%)	23 (11%)	6	28
3	E	212/226 (94%)	192 (91%)	20 (9%)	8	32
3	F	212/226 (94%)	192 (91%)	20 (9%)	8	32
4	G	138/139 (99%)	129 (94%)	9 (6%)	15	43
4	Q	138/139 (99%)	124 (90%)	14 (10%)	7	30
4	a	138/139 (99%)	128 (93%)	10 (7%)	13	40
4	k	138/139 (99%)	127 (92%)	11 (8%)	11	37
4	q	138/139 (99%)	129 (94%)	9 (6%)	15	43
4	w	138/139 (99%)	125 (91%)	13 (9%)	8	32
5	H	142/142 (100%)	137 (96%)	5 (4%)	32	57
5	R	142/142 (100%)	133 (94%)	9 (6%)	16	44
5	b	142/142 (100%)	134 (94%)	8 (6%)	19	47
5	l	142/142 (100%)	135 (95%)	7 (5%)	22	49
5	r	142/142 (100%)	136 (96%)	6 (4%)	26	53
5	x	142/142 (100%)	135 (95%)	7 (5%)	22	49
6	I	104/108 (96%)	101 (97%)	3 (3%)	37	60
6	S	104/108 (96%)	97 (93%)	7 (7%)	15	42
6	c	104/108 (96%)	98 (94%)	6 (6%)	18	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	m	104/108 (96%)	98 (94%)	6 (6%)	18	46
6	s	104/108 (96%)	99 (95%)	5 (5%)	23	50
6	y	104/108 (96%)	97 (93%)	7 (7%)	15	42
7	K	110/112 (98%)	104 (94%)	6 (6%)	19	47
7	U	110/112 (98%)	107 (97%)	3 (3%)	39	61
7	e	110/112 (98%)	104 (94%)	6 (6%)	19	47
7	n	110/112 (98%)	103 (94%)	7 (6%)	16	43
7	t	110/112 (98%)	106 (96%)	4 (4%)	31	56
7	z	110/112 (98%)	103 (94%)	7 (6%)	16	43
8	P	209/209 (100%)	202 (97%)	7 (3%)	33	58
8	Z	209/209 (100%)	192 (92%)	17 (8%)	11	36
8	j	209/209 (100%)	192 (92%)	17 (8%)	11	36
9	J	265/266 (100%)	245 (92%)	20 (8%)	12	39
9	T	265/266 (100%)	237 (89%)	28 (11%)	6	28
9	d	265/266 (100%)	246 (93%)	19 (7%)	13	40
10	2	15/620 (2%)	14 (93%)	1 (7%)	15	42
10	3	15/620 (2%)	14 (93%)	1 (7%)	15	42
10	4	15/620 (2%)	14 (93%)	1 (7%)	15	42
10	5	15/620 (2%)	14 (93%)	1 (7%)	15	42
10	6	15/620 (2%)	14 (93%)	1 (7%)	15	42
10	7	15/620 (2%)	14 (93%)	1 (7%)	15	42
10	8	29/620 (5%)	28 (97%)	1 (3%)	32	57
10	9	29/620 (5%)	28 (97%)	1 (3%)	32	57
10	AA	29/620 (5%)	27 (93%)	2 (7%)	14	41
All	All	11937/17487 (68%)	11098 (93%)	839 (7%)	16	41

All (839) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	THR
1	0	41	THR
1	0	93	ARG
1	0	109	ILE
1	0	130	HIS

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Mol	Chain	Res	Type
1	0	140	LYS
1	0	145	VAL
1	0	147	ILE
1	0	152	VAL
1	0	159	GLU
1	0	167	ILE
1	0	172	ILE
1	0	181	THR
1	0	185	GLU
1	0	194	ASP
1	0	206	TYR
1	0	213	PHE
1	0	234	GLN
1	0	257	ILE
1	0	262	ILE
1	0	271	ILE
1	0	274	VAL
1	0	287	GLU
1	0	288	LEU
1	0	293	ARG
1	0	299	GLN
1	0	351	THR
1	0	355	GLN
1	0	373	VAL
1	0	376	VAL
1	0	384	ARG
1	0	386	ASN
1	0	391	VAL
1	0	415	LEU
1	0	419	ILE
1	0	428	LYS
1	0	435	TYR
1	0	455	ILE
1	0	464	MET
1	0	469	ILE
2	1	31	ARG
2	1	32	PHE
2	1	33	LEU
2	1	44	GLN
2	1	53	LEU
2	1	62	LYS
2	1	77	LEU

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Mol	Chain	Res	Type
2	1	88	PHE
2	1	91	THR
2	1	93	ARG
2	1	121	GLU
2	1	125	GLU
2	1	139	ARG
2	1	162	LEU
2	1	200	ILE
2	1	214	VAL
2	1	217	THR
2	1	229	LEU
3	A	6	LYS
3	A	29	VAL
3	A	46	THR
3	A	69	ILE
3	A	75	GLN
3	A	82	LYS
3	A	85	VAL
3	A	87	THR
3	A	100	ARG
3	A	105	ARG
3	A	114	PHE
3	A	118	GLU
3	A	127	GLN
3	A	169	PHE
3	A	199	ARG
3	A	203	VAL
3	A	211	THR
3	B	5	ILE
3	B	29	VAL
3	B	46	THR
3	B	62	PHE
3	B	63	ASN
3	B	68	VAL
3	B	87	THR
3	B	96	ILE
3	B	110	VAL
3	B	114	PHE
3	B	176	GLU
3	B	199	ARG
3	B	205	VAL
3	B	210	LYS

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Mol	Chain	Res	Type
3	B	217	ARG
3	B	224	THR
3	B	234	SER
3	B	238	LYS
3	C	6	LYS
3	C	29	VAL
3	C	59	ASP
3	C	69	ILE
3	C	75	GLN
3	C	82	LYS
3	C	85	VAL
3	C	87	THR
3	C	100	ARG
3	C	105	ARG
3	C	114	PHE
3	C	118	GLU
3	C	131	LYS
3	C	169	PHE
3	C	199	ARG
3	C	203	VAL
3	C	205	VAL
3	C	207	LYS
3	C	211	THR
3	C	230	THR
3	D	6	LYS
3	D	29	VAL
3	D	35	GLU
3	D	46	THR
3	D	69	ILE
3	D	75	GLN
3	D	82	LYS
3	D	85	VAL
3	D	87	THR
3	D	96	ILE
3	D	100	ARG
3	D	105	ARG
3	D	114	PHE
3	D	118	GLU
3	D	127	GLN
3	D	169	PHE
3	D	199	ARG
3	D	203	VAL

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Mol	Chain	Res	Type
3	D	205	VAL
3	D	207	LYS
3	D	211	THR
3	D	230	THR
3	D	234	SER
3	E	5	ILE
3	E	34	ILE
3	E	46	THR
3	E	62	PHE
3	E	68	VAL
3	E	82	LYS
3	E	87	THR
3	E	96	ILE
3	E	110	VAL
3	E	115	ILE
3	E	128	LYS
3	E	176	GLU
3	E	177	ASN
3	E	190	ILE
3	E	199	ARG
3	E	205	VAL
3	E	215	GLU
3	E	217	ARG
3	E	224	THR
3	E	234	SER
3	F	5	ILE
3	F	46	THR
3	F	68	VAL
3	F	80	ASN
3	F	87	THR
3	F	96	ILE
3	F	110	VAL
3	F	114	PHE
3	F	115	ILE
3	F	131	LYS
3	F	142	ASP
3	F	157	ASP
3	F	176	GLU
3	F	177	ASN
3	F	199	ARG
3	F	205	VAL
3	F	217	ARG

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Mol	Chain	Res	Type
3	F	224	THR
3	F	234	SER
3	F	238	LYS
4	G	22	LEU
4	G	26	VAL
4	G	35	ARG
4	G	111	TYR
4	G	120	ILE
4	G	143	VAL
4	G	150	THR
4	G	151	VAL
4	G	158	LEU
5	H	8	ARG
5	H	51	VAL
5	H	77	LEU
5	H	82	ILE
5	H	125	THR
6	I	23	ILE
6	I	44	ASP
6	I	50	LEU
7	K	26	VAL
7	K	38	TYR
7	K	52	ILE
7	K	82	VAL
7	K	92	ILE
7	K	99	TYR
1	L	53	VAL
1	L	58	ASP
1	L	109	ILE
1	L	120	MET
1	L	121	ILE
1	L	130	HIS
1	L	148	PHE
1	L	169	THR
1	L	172	ILE
1	L	183	THR
1	L	188	LEU
1	L	194	ASP
1	L	230	ASN
1	L	234	GLN
1	L	257	ILE
1	L	290	GLU

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Mol	Chain	Res	Type
1	L	291	ARG
1	L	293	ARG
1	L	298	VAL
1	L	303	ILE
1	L	325	ASN
1	L	371	THR
1	L	373	VAL
1	L	384	ARG
1	L	385	VAL
1	L	406	SER
1	L	410	ASN
1	L	412	GLU
1	L	428	LYS
1	L	435	TYR
1	L	464	MET
1	M	5	THR
1	M	21	TYR
1	M	91	ILE
1	M	105	LEU
1	M	136	ILE
1	M	140	LYS
1	M	181	THR
1	M	213	PHE
1	M	241	ILE
1	M	270	VAL
1	M	283	GLU
1	M	285	ASP
1	M	296	LYS
1	M	298	VAL
1	M	329	ASN
1	M	360	ASN
1	M	368	VAL
1	M	376	VAL
1	M	386	ASN
1	M	393	VAL
1	M	401	VAL
1	M	402	THR
1	M	458	LYS
1	N	5	THR
1	N	21	TYR
1	N	32	LEU
1	N	50	LEU

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Mol	Chain	Res	Type
1	N	85	LEU
1	N	109	ILE
1	N	115	SER
1	N	157	THR
1	N	172	ILE
1	N	185	GLU
1	N	222	THR
1	N	270	VAL
1	N	298	VAL
1	N	303	ILE
1	N	333	VAL
1	N	359	LEU
1	N	374	GLN
1	N	376	VAL
1	N	415	LEU
1	N	437	ARG
1	N	438	PHE
1	N	443	MET
1	N	445	ILE
2	O	5	GLN
2	O	36	LEU
2	O	54	ARG
2	O	77	LEU
2	O	78	VAL
2	O	91	THR
2	O	93	ARG
2	O	145	GLU
2	O	163	GLU
2	O	164	GLU
2	O	208	GLU
2	O	214	VAL
2	O	217	THR
2	O	238	LEU
8	P	1	MET
8	P	12	LEU
8	P	53	ASP
8	P	81	LEU
8	P	86	THR
8	P	154	ASN
8	P	208	HIS
4	Q	22	LEU
4	Q	26	VAL

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Mol	Chain	Res	Type
4	Q	33	LEU
4	Q	35	ARG
4	Q	53	ARG
4	Q	78	GLU
4	Q	88	ILE
4	Q	96	HIS
4	Q	120	ILE
4	Q	123	ARG
4	Q	126	THR
4	Q	143	VAL
4	Q	150	THR
4	Q	158	LEU
5	R	8	ARG
5	R	25	GLU
5	R	47	GLU
5	R	51	VAL
5	R	64	ILE
5	R	82	ILE
5	R	103	LEU
5	R	105	LEU
5	R	141	VAL
6	S	15	ARG
6	S	18	ARG
6	S	19	TYR
6	S	65	ILE
6	S	90	VAL
6	S	98	ASP
6	S	113	LEU
7	U	26	VAL
7	U	38	TYR
7	U	82	VAL
1	V	10	THR
1	V	109	ILE
1	V	130	HIS
1	V	140	LYS
1	V	145	VAL
1	V	147	ILE
1	V	159	GLU
1	V	167	ILE
1	V	172	ILE
1	V	194	ASP
1	V	202	THR

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Mol	Chain	Res	Type
1	V	213	PHE
1	V	257	ILE
1	V	262	ILE
1	V	274	VAL
1	V	287	GLU
1	V	288	LEU
1	V	293	ARG
1	V	298	VAL
1	V	323	ILE
1	V	324	GLU
1	V	325	ASN
1	V	351	THR
1	V	355	GLN
1	V	373	VAL
1	V	375	VAL
1	V	391	VAL
1	V	415	LEU
1	V	419	ILE
1	V	428	LYS
1	V	435	TYR
1	V	455	ILE
1	V	464	MET
1	V	469	ILE
1	W	5	THR
1	W	21	TYR
1	W	91	ILE
1	W	105	LEU
1	W	130	HIS
1	W	136	ILE
1	W	181	THR
1	W	213	PHE
1	W	241	ILE
1	W	270	VAL
1	W	296	LYS
1	W	298	VAL
1	W	360	ASN
1	W	368	VAL
1	W	376	VAL
1	W	393	VAL
1	W	401	VAL
1	W	402	THR
1	W	458	LYS

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Mol	Chain	Res	Type
1	X	5	THR
1	X	21	TYR
1	X	32	LEU
1	X	49	ARG
1	X	50	LEU
1	X	85	LEU
1	X	86	VAL
1	X	109	ILE
1	X	115	SER
1	X	145	VAL
1	X	157	THR
1	X	172	ILE
1	X	185	GLU
1	X	222	THR
1	X	270	VAL
1	X	303	ILE
1	X	333	VAL
1	X	374	GLN
1	X	376	VAL
1	X	437	ARG
1	X	438	PHE
1	X	443	MET
1	X	445	ILE
1	X	476	THR
2	Y	22	GLN
2	Y	32	PHE
2	Y	33	LEU
2	Y	44	GLN
2	Y	53	LEU
2	Y	62	LYS
2	Y	77	LEU
2	Y	88	PHE
2	Y	91	THR
2	Y	93	ARG
2	Y	118	ASN
2	Y	125	GLU
2	Y	138	ASN
2	Y	139	ARG
2	Y	162	LEU
2	Y	200	ILE
2	Y	208	GLU
2	Y	214	VAL

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Mol	Chain	Res	Type
2	Y	217	THR
2	Y	229	LEU
8	Z	1	MET
8	Z	2	ARG
8	Z	6	LEU
8	Z	12	LEU
8	Z	28	VAL
8	Z	81	LEU
8	Z	82	ASN
8	Z	98	VAL
8	Z	117	ASN
8	Z	136	ASP
8	Z	162	GLU
8	Z	177	LYS
8	Z	208	HIS
8	Z	221	PHE
8	Z	227	HIS
8	Z	230	LYS
8	Z	245	GLN
4	a	22	LEU
4	a	26	VAL
4	a	35	ARG
4	a	111	TYR
4	a	120	ILE
4	a	123	ARG
4	a	143	VAL
4	a	150	THR
4	a	151	VAL
4	a	158	LEU
5	b	8	ARG
5	b	27	GLU
5	b	51	VAL
5	b	77	LEU
5	b	82	ILE
5	b	125	THR
5	b	128	LEU
5	b	148	GLN
6	c	3	THR
6	c	26	ILE
6	c	44	ASP
6	c	62	GLN
6	c	65	ILE

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Mol	Chain	Res	Type
6	c	68	ASP
7	e	26	VAL
7	e	38	TYR
7	e	46	LEU
7	e	82	VAL
7	e	92	ILE
7	e	97	ARG
1	f	29	PHE
1	f	53	VAL
1	f	78	THR
1	f	109	ILE
1	f	130	HIS
1	f	159	GLU
1	f	165	ASP
1	f	172	ILE
1	f	179	THR
1	f	194	ASP
1	f	230	ASN
1	f	234	GLN
1	f	255	LEU
1	f	257	ILE
1	f	262	ILE
1	f	271	ILE
1	f	290	GLU
1	f	293	ARG
1	f	298	VAL
1	f	303	ILE
1	f	371	THR
1	f	385	VAL
1	f	396	GLU
1	f	410	ASN
1	f	412	GLU
1	f	428	LYS
1	f	434	ILE
1	f	435	TYR
1	f	464	MET
1	g	5	THR
1	g	21	TYR
1	g	32	LEU
1	g	37	ASP
1	g	50	LEU
1	g	91	ILE

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Mol	Chain	Res	Type
1	g	136	ILE
1	g	181	THR
1	g	213	PHE
1	g	226	GLU
1	g	241	ILE
1	g	270	VAL
1	g	283	GLU
1	g	284	THR
1	g	298	VAL
1	g	360	ASN
1	g	368	VAL
1	g	376	VAL
1	g	393	VAL
1	g	401	VAL
1	g	402	THR
1	g	432	ASP
1	g	458	LYS
1	h	5	THR
1	h	21	TYR
1	h	32	LEU
1	h	39	VAL
1	h	53	VAL
1	h	85	LEU
1	h	86	VAL
1	h	109	ILE
1	h	115	SER
1	h	157	THR
1	h	172	ILE
1	h	222	THR
1	h	270	VAL
1	h	283	GLU
1	h	298	VAL
1	h	303	ILE
1	h	333	VAL
1	h	374	GLN
1	h	376	VAL
1	h	393	VAL
1	h	402	THR
1	h	415	LEU
1	h	437	ARG
1	h	438	PHE
1	h	443	MET

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Mol	Chain	Res	Type
1	h	445	ILE
2	i	5	GLN
2	i	13	GLU
2	i	36	LEU
2	i	54	ARG
2	i	77	LEU
2	i	78	VAL
2	i	91	THR
2	i	93	ARG
2	i	145	GLU
2	i	163	GLU
2	i	214	VAL
2	i	217	THR
2	i	238	LEU
8	j	1	MET
8	j	3	ARG
8	j	4	THR
8	j	6	LEU
8	j	8	GLU
8	j	12	LEU
8	j	28	VAL
8	j	74	ASN
8	j	86	THR
8	j	95	THR
8	j	111	ASN
8	j	136	ASP
8	j	156	MET
8	j	208	HIS
8	j	229	HIS
8	j	230	LYS
8	j	245	GLN
4	k	33	LEU
4	k	35	ARG
4	k	53	ARG
4	k	78	GLU
4	k	96	HIS
4	k	120	ILE
4	k	123	ARG
4	k	126	THR
4	k	143	VAL
4	k	150	THR
4	k	151	VAL

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Mol	Chain	Res	Type
5	l	25	GLU
5	l	47	GLU
5	l	51	VAL
5	l	82	ILE
5	l	103	LEU
5	l	105	LEU
5	l	141	VAL
6	m	15	ARG
6	m	18	ARG
6	m	19	TYR
6	m	90	VAL
6	m	98	ASP
6	m	113	LEU
7	n	22	THR
7	n	26	VAL
7	n	38	TYR
7	n	82	VAL
7	n	92	ILE
7	n	99	TYR
7	n	108	THR
1	o	41	THR
1	o	85	LEU
1	o	109	ILE
1	o	130	HIS
1	o	140	LYS
1	o	145	VAL
1	o	147	ILE
1	o	159	GLU
1	o	167	ILE
1	o	172	ILE
1	o	194	ASP
1	o	213	PHE
1	o	257	ILE
1	o	262	ILE
1	o	271	ILE
1	o	274	VAL
1	o	287	GLU
1	o	288	LEU
1	o	293	ARG
1	o	298	VAL
1	o	303	ILE
1	o	351	THR

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Mol	Chain	Res	Type
1	o	355	GLN
1	o	391	VAL
1	o	415	LEU
1	o	419	ILE
1	o	434	ILE
1	o	435	TYR
1	o	455	ILE
1	o	464	MET
1	o	469	ILE
2	p	33	LEU
2	p	44	GLN
2	p	48	GLU
2	p	53	LEU
2	p	62	LYS
2	p	77	LEU
2	p	88	PHE
2	p	91	THR
2	p	93	ARG
2	p	121	GLU
2	p	125	GLU
2	p	138	ASN
2	p	139	ARG
2	p	200	ILE
2	p	208	GLU
2	p	214	VAL
2	p	217	THR
4	q	22	LEU
4	q	26	VAL
4	q	35	ARG
4	q	88	ILE
4	q	120	ILE
4	q	123	ARG
4	q	143	VAL
4	q	151	VAL
4	q	158	LEU
5	r	13	THR
5	r	27	GLU
5	r	51	VAL
5	r	77	LEU
5	r	82	ILE
5	r	125	THR
6	s	3	THR

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Mol	Chain	Res	Type
6	s	23	ILE
6	s	44	ASP
6	s	65	ILE
6	s	68	ASP
7	t	26	VAL
7	t	38	TYR
7	t	82	VAL
7	t	97	ARG
1	u	28	VAL
1	u	29	PHE
1	u	53	VAL
1	u	109	ILE
1	u	130	HIS
1	u	159	GLU
1	u	194	ASP
1	u	199	HIS
1	u	212	LEU
1	u	230	ASN
1	u	234	GLN
1	u	255	LEU
1	u	257	ILE
1	u	271	ILE
1	u	290	GLU
1	u	291	ARG
1	u	293	ARG
1	u	298	VAL
1	u	303	ILE
1	u	325	ASN
1	u	373	VAL
1	u	385	VAL
1	u	410	ASN
1	u	412	GLU
1	u	428	LYS
1	u	435	TYR
1	u	464	MET
2	v	5	GLN
2	v	19	VAL
2	v	36	LEU
2	v	54	ARG
2	v	56	LEU
2	v	77	LEU
2	v	78	VAL

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Mol	Chain	Res	Type
2	v	91	THR
2	v	93	ARG
2	v	145	GLU
2	v	160	VAL
2	v	163	GLU
2	v	208	GLU
2	v	214	VAL
2	v	217	THR
2	v	238	LEU
4	w	33	LEU
4	w	35	ARG
4	w	48	THR
4	w	53	ARG
4	w	63	VAL
4	w	78	GLU
4	w	96	HIS
4	w	120	ILE
4	w	123	ARG
4	w	126	THR
4	w	143	VAL
4	w	150	THR
4	w	158	LEU
5	x	25	GLU
5	x	47	GLU
5	x	51	VAL
5	x	64	ILE
5	x	82	ILE
5	x	105	LEU
5	x	141	VAL
6	y	15	ARG
6	y	18	ARG
6	y	23	ILE
6	y	65	ILE
6	y	90	VAL
6	y	98	ASP
6	y	113	LEU
7	z	11	ASP
7	z	26	VAL
7	z	38	TYR
7	z	82	VAL
7	z	92	ILE
7	z	95	HIS

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Mol	Chain	Res	Type
7	z	99	TYR
9	J	2	LYS
9	J	11	THR
9	J	27	HIS
9	J	38	GLN
9	J	39	PHE
9	J	71	LEU
9	J	73	THR
9	J	97	VAL
9	J	113	LEU
9	J	176	LYS
9	J	188	ILE
9	J	208	LYS
9	J	211	GLN
9	J	215	LEU
9	J	236	GLN
9	J	237	LYS
9	J	242	ARG
9	J	251	LEU
9	J	260	VAL
9	J	300	GLN
9	T	2	LYS
9	T	11	THR
9	T	27	HIS
9	T	38	GLN
9	T	39	PHE
9	T	50	LYS
9	T	71	LEU
9	T	73	THR
9	T	75	TYR
9	T	77	THR
9	T	78	CYS
9	T	85	LYS
9	T	97	VAL
9	T	113	LEU
9	T	170	GLN
9	T	176	LYS
9	T	188	ILE
9	T	201	ASP
9	T	206	THR
9	T	207	THR
9	T	211	GLN

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Mol	Chain	Res	Type
9	T	215	LEU
9	T	236	GLN
9	T	237	LYS
9	T	241	ARG
9	T	252	LEU
9	T	260	VAL
9	T	300	GLN
9	d	11	THR
9	d	27	HIS
9	d	38	GLN
9	d	39	PHE
9	d	73	THR
9	d	77	THR
9	d	78	CYS
9	d	97	VAL
9	d	113	LEU
9	d	176	LYS
9	d	188	ILE
9	d	208	LYS
9	d	210	VAL
9	d	211	GLN
9	d	236	GLN
9	d	237	LYS
9	d	241	ARG
9	d	251	LEU
9	d	260	VAL
10	4	702	THR
10	2	690	ASP
10	3	702	THR
10	5	690	ASP
10	6	702	THR
10	7	690	ASP
10	8	773	ILE
10	9	769	LEU
10	AA	753	MET
10	AA	769	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	44	ASN
1	0	383	HIS

Continued on next page...

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Mol	Chain	Res	Type
1	0	451	ASN
2	1	210	GLN
3	A	163	GLN
3	B	80	ASN
3	B	177	ASN
3	C	43	HIS
3	D	24	GLN
3	D	177	ASN
3	D	228	ASN
3	E	177	ASN
4	G	70	ASN
5	H	53	ASN
6	I	51	ASN
6	I	77	ASN
7	K	95	HIS
1	L	44	ASN
1	L	73	ASN
1	L	339	HIS
1	M	66	GLN
1	M	70	ASN
1	M	329	ASN
1	M	462	GLN
1	N	84	ASN
1	N	198	ASN
1	N	386	ASN
2	O	22	GLN
8	P	154	ASN
8	P	203	ASN
4	Q	46	HIS
1	V	44	ASN
1	V	339	HIS
1	V	451	ASN
1	W	66	GLN
1	W	329	ASN
1	W	339	HIS
8	Z	108	HIS
8	Z	205	ASN
8	Z	222	ASN
8	Z	231	HIS
4	a	3	ASN
4	a	122	ASN
6	c	51	ASN

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Mol	Chain	Res	Type
6	c	77	ASN
1	f	44	ASN
1	f	73	ASN
1	g	329	ASN
1	g	339	HIS
1	h	154	ASN
2	i	22	GLN
2	i	138	ASN
2	i	203	ASN
8	j	140	HIS
8	j	154	ASN
4	k	152	GLN
6	m	13	GLN
7	n	31	GLN
1	o	66	GLN
1	o	329	ASN
1	o	451	ASN
2	p	210	GLN
4	q	70	ASN
4	q	122	ASN
5	r	53	ASN
6	s	51	ASN
6	s	77	ASN
7	t	31	GLN
1	u	44	ASN
1	u	388	GLN
2	v	22	GLN
4	w	152	GLN
6	y	62	GLN
7	z	31	GLN
9	J	19	GLN
9	J	62	ASN
9	J	186	ASN
9	T	14	ASN
9	T	62	ASN
9	T	107	ASN
9	d	62	ASN
10	AA	784	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

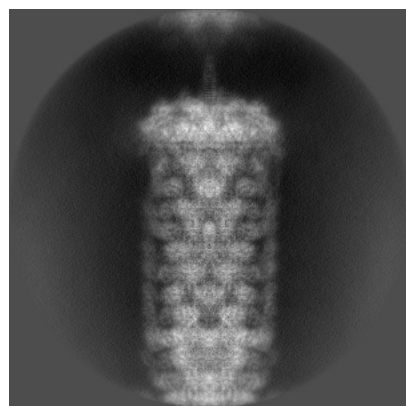
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74057. These allow visual inspection of the internal detail of the map and identification of artifacts.

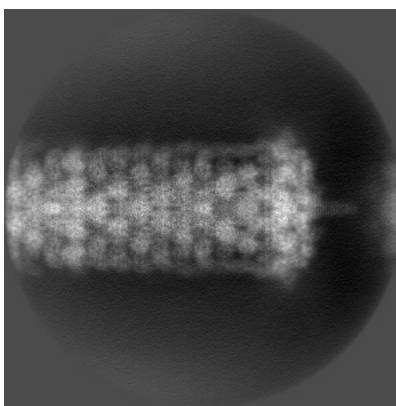
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

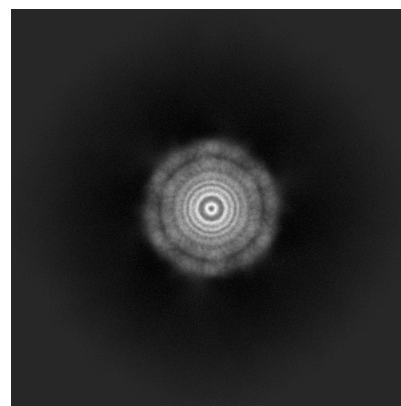
6.1.1 Primary map



X

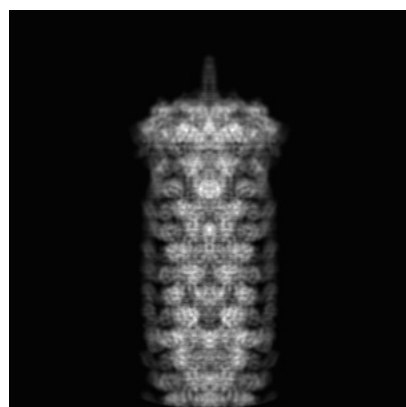


Y

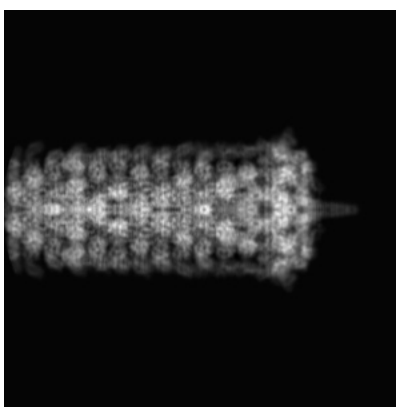


Z

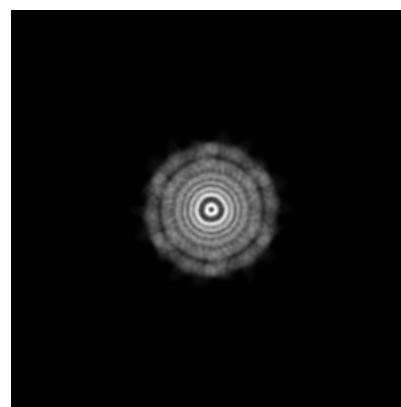
6.1.2 Raw map



X



Y

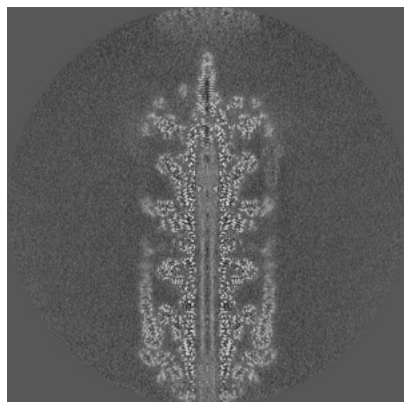


Z

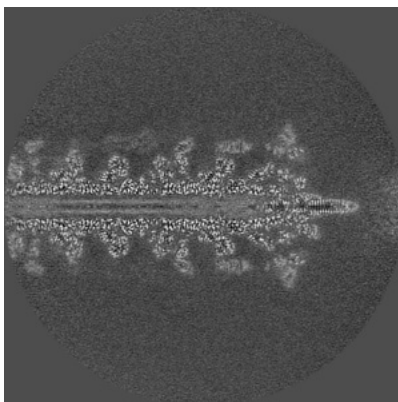
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

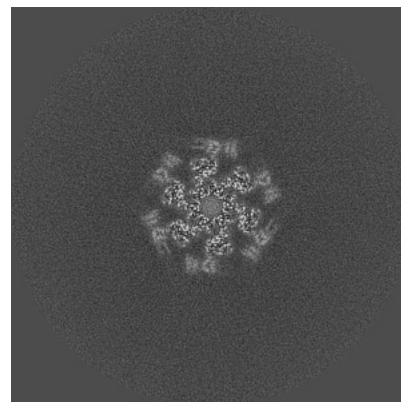
6.2.1 Primary map



X Index: 256

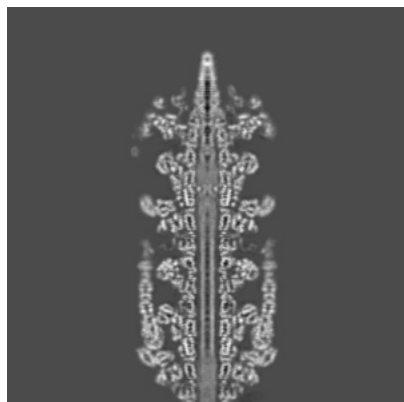


Y Index: 256

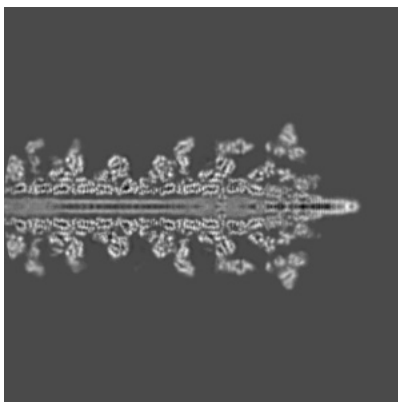


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

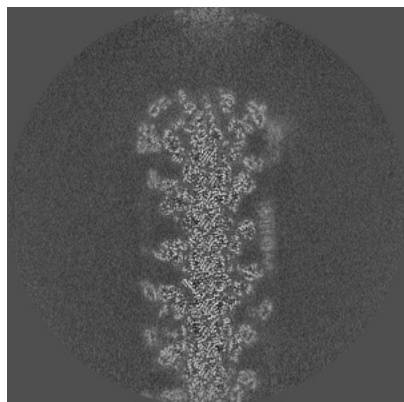


Z Index: 256

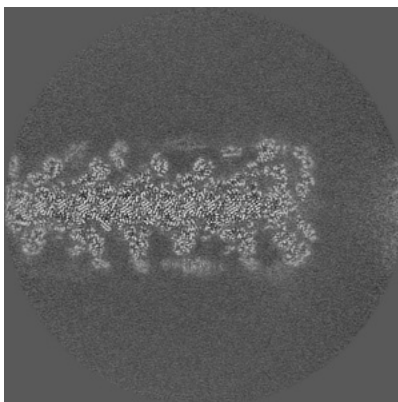
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

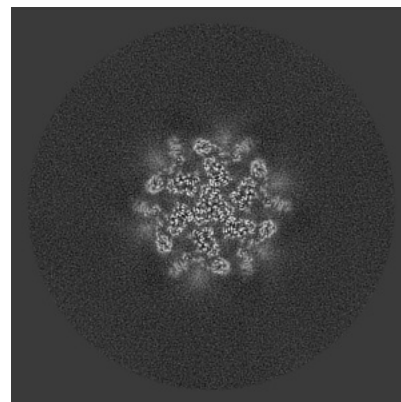
6.3.1 Primary map



X Index: 273

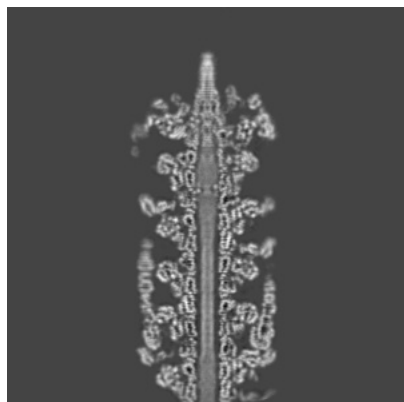


Y Index: 238

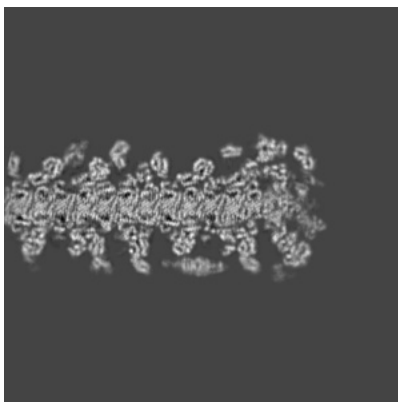


Z Index: 358

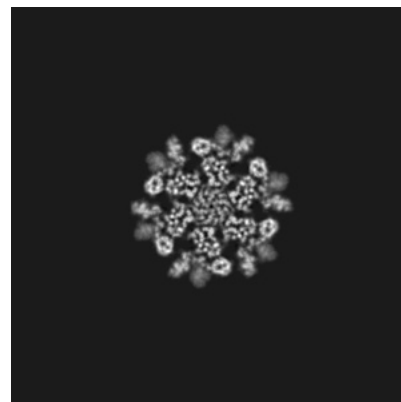
6.3.2 Raw map



X Index: 252



Y Index: 238

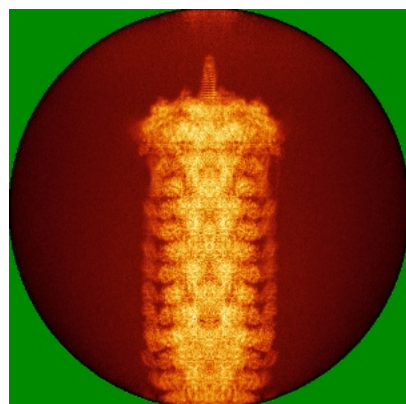


Z Index: 358

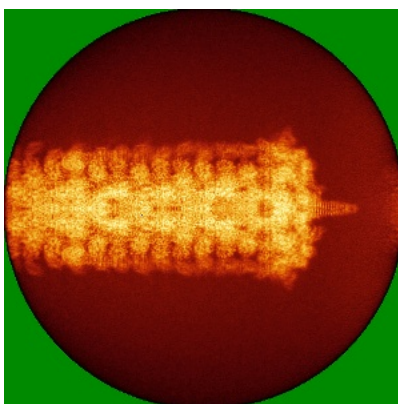
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

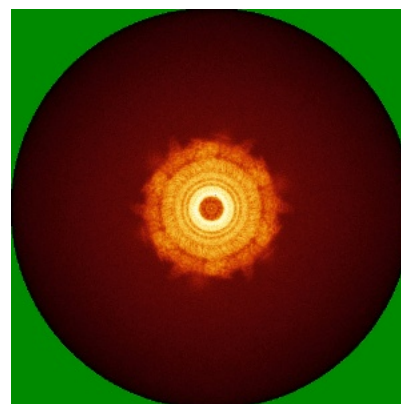
6.4.1 Primary map



X

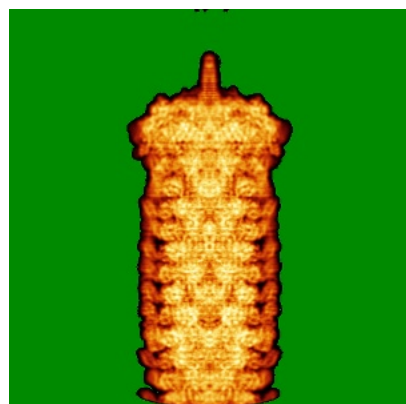


Y

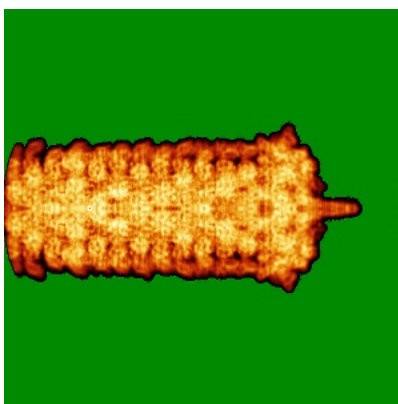


Z

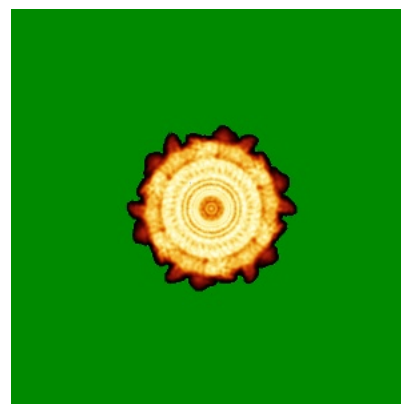
6.4.2 Raw map



X



Y

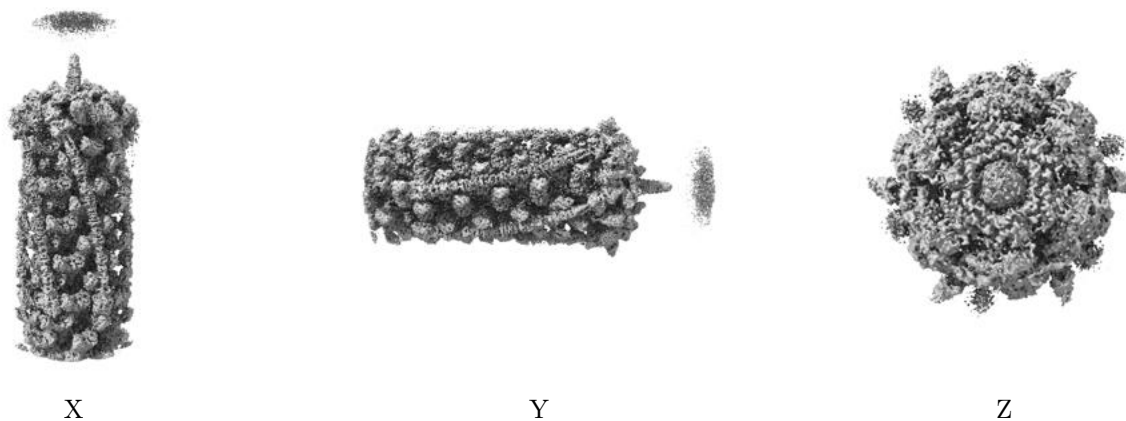


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

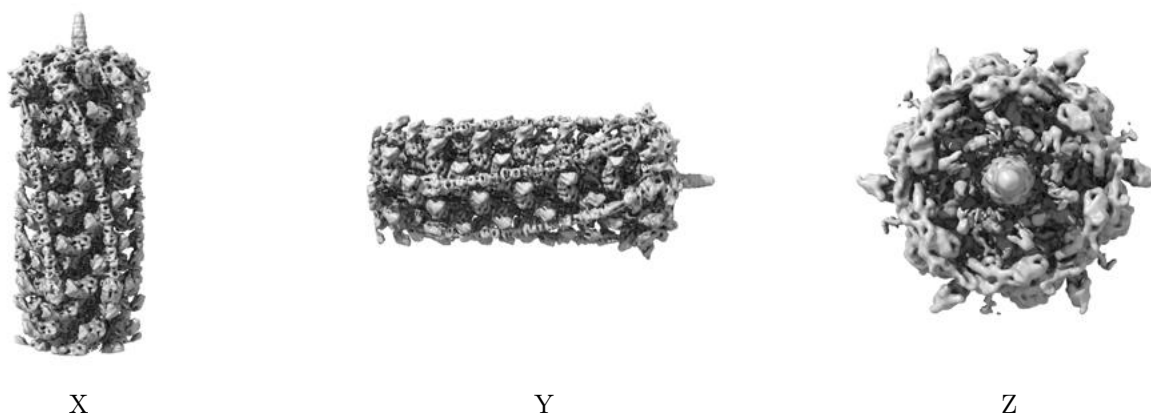
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

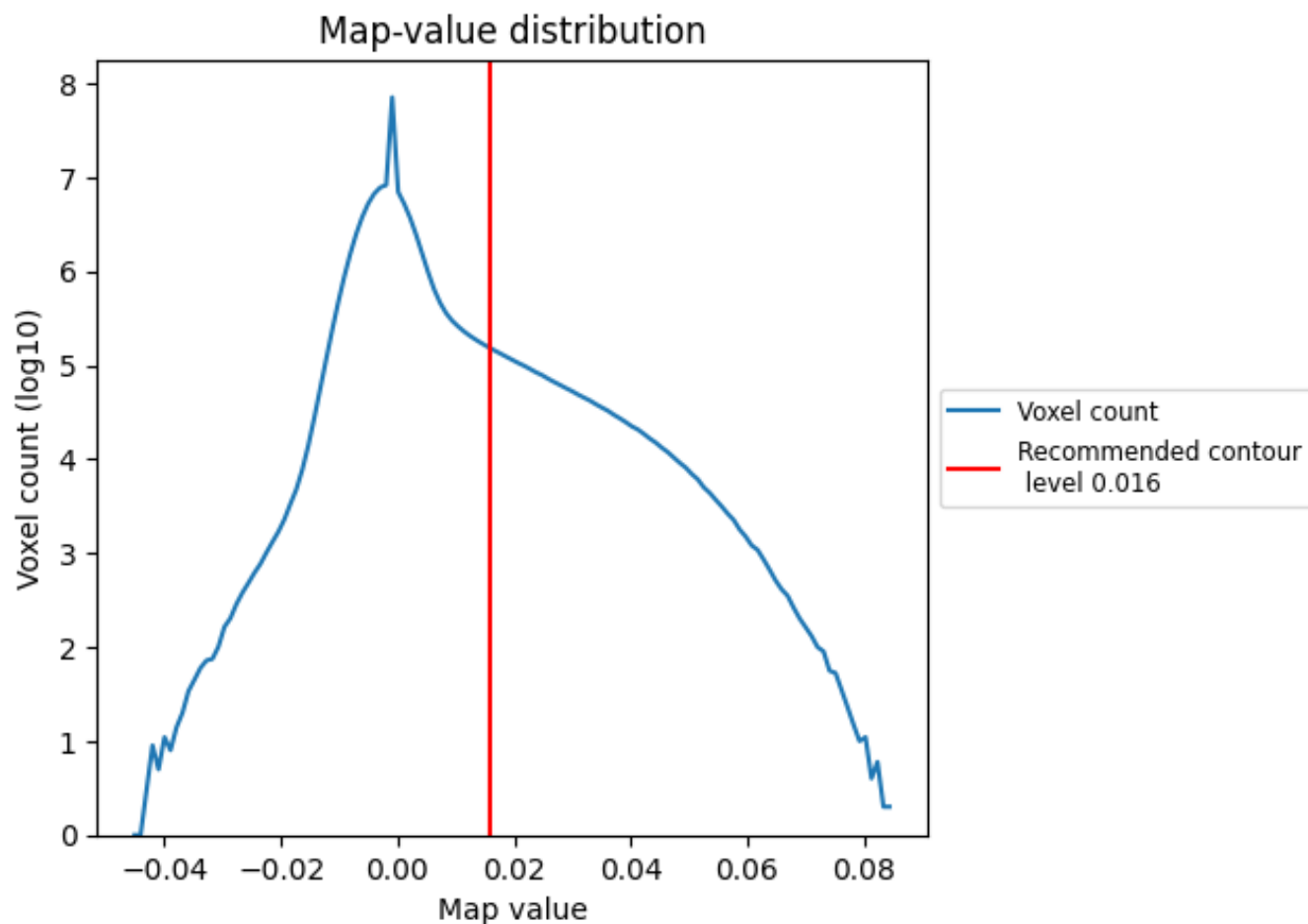
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

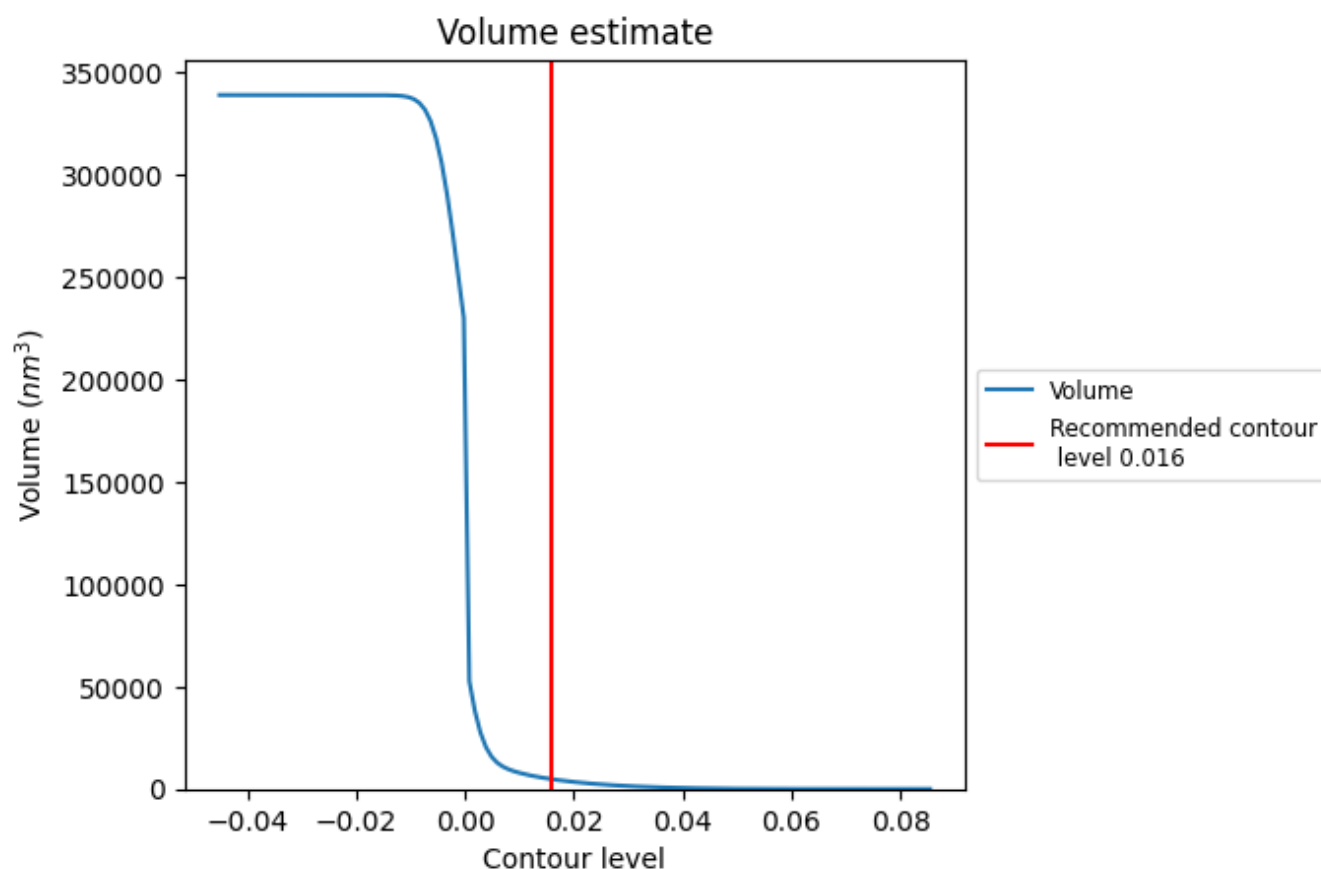
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

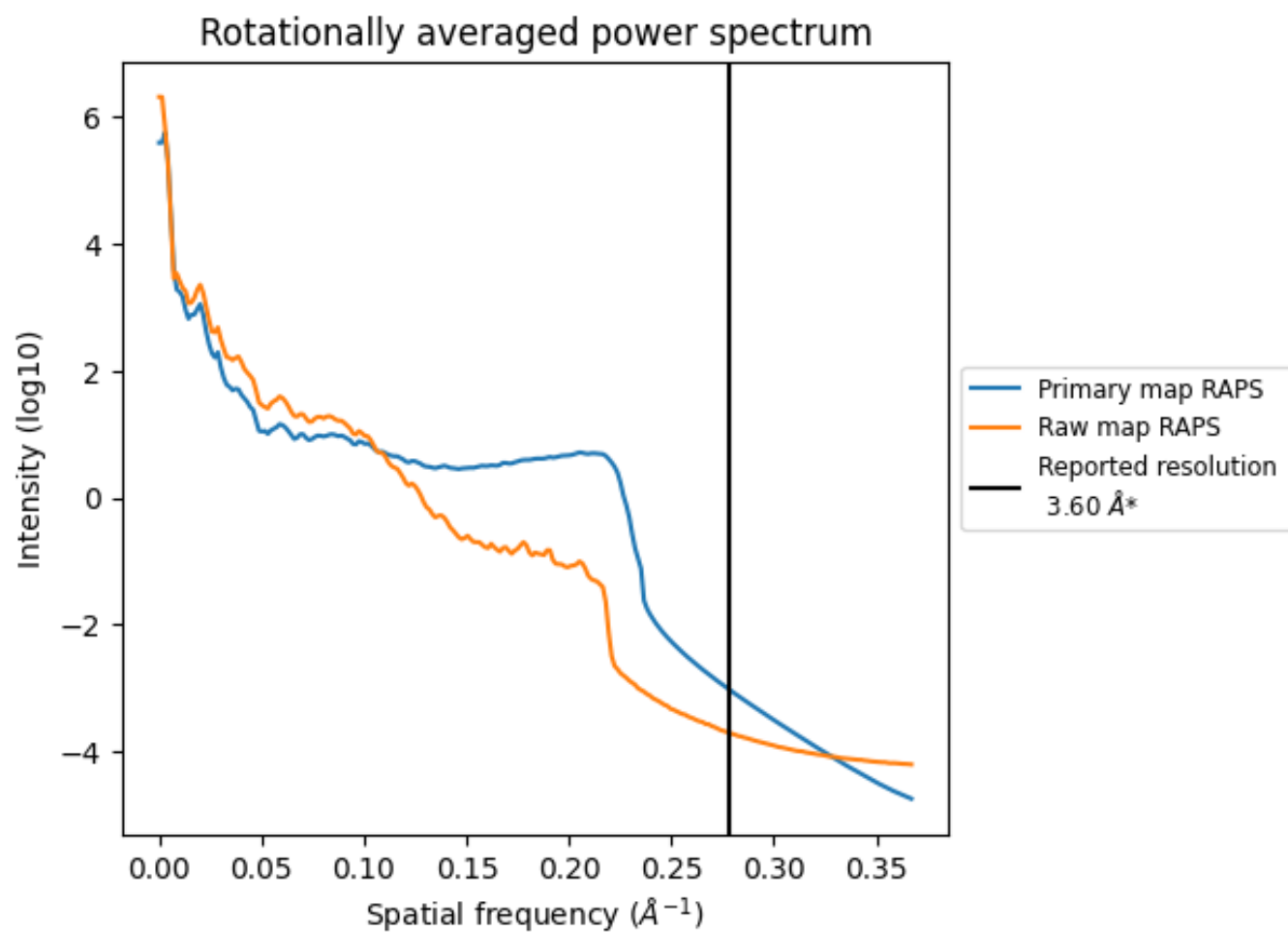
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4755 nm^3 ; this corresponds to an approximate mass of 4295 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

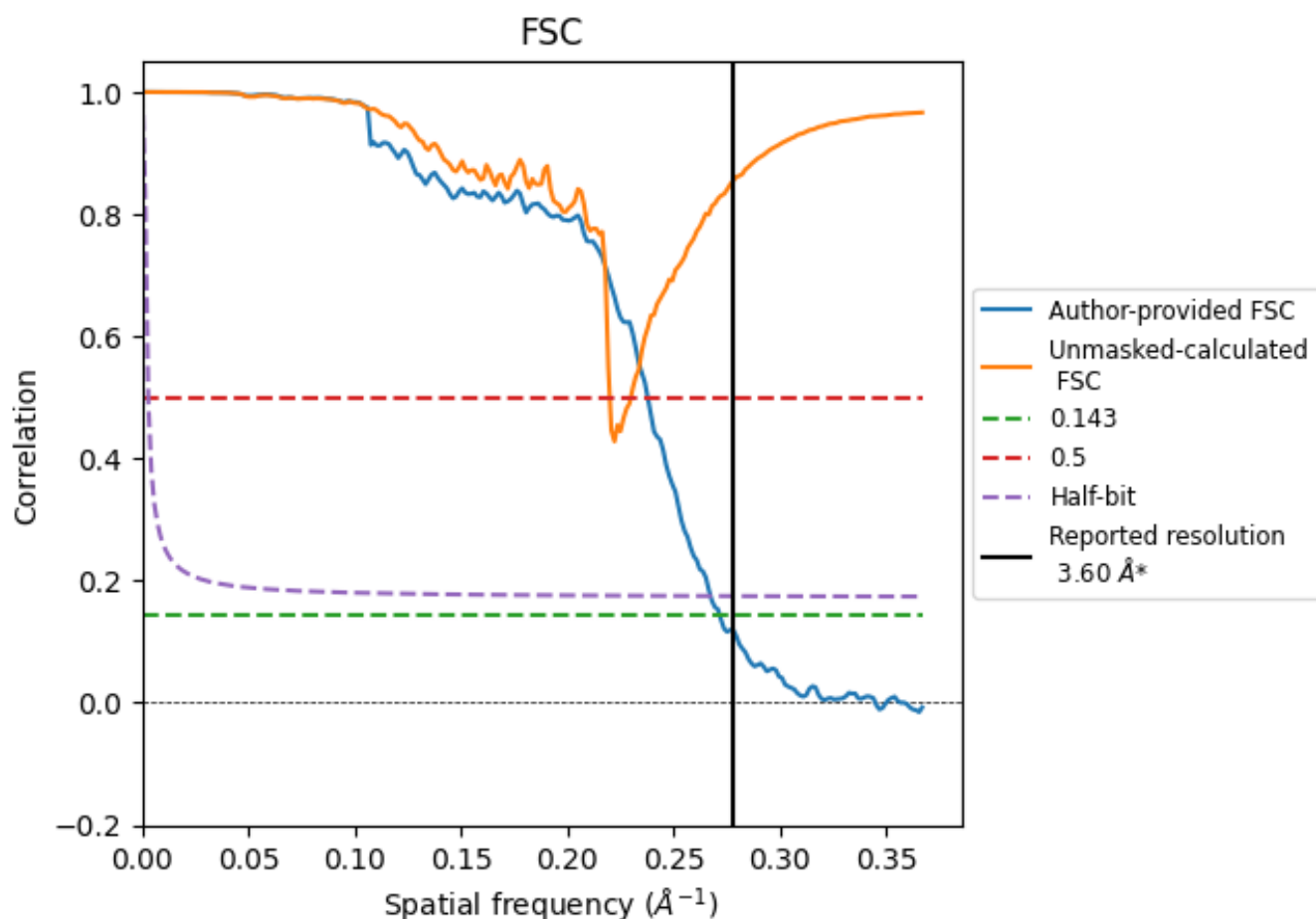


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

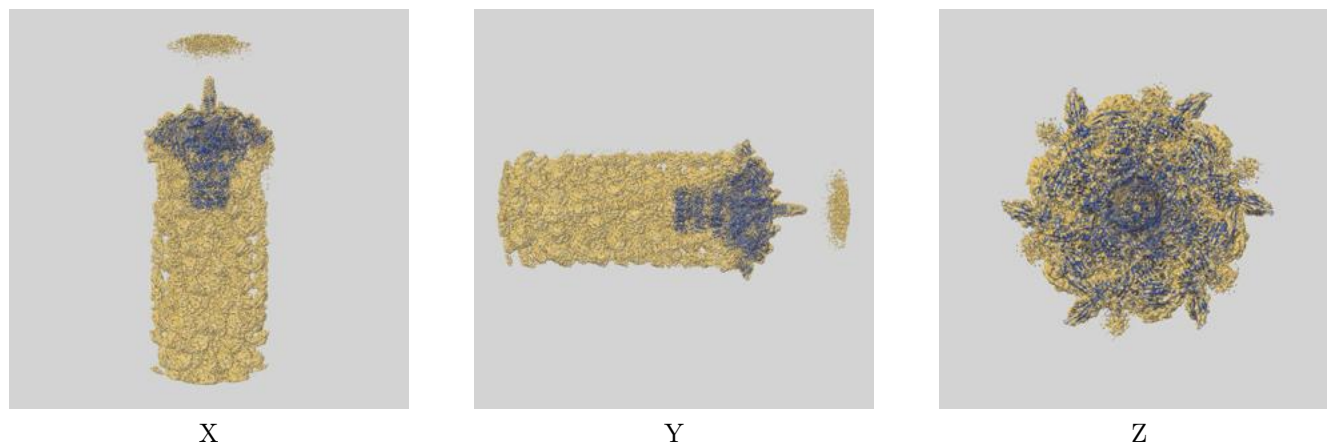
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.68	4.20	3.74
Unmasked-calculated*	-	4.54	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

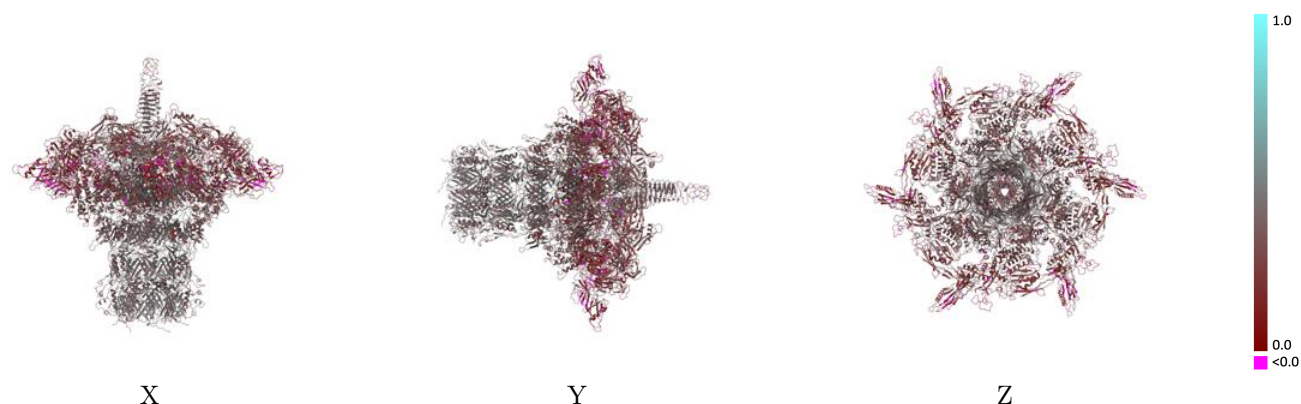
This section contains information regarding the fit between EMDB map EMD-74057 and PDB model 9ZD8. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



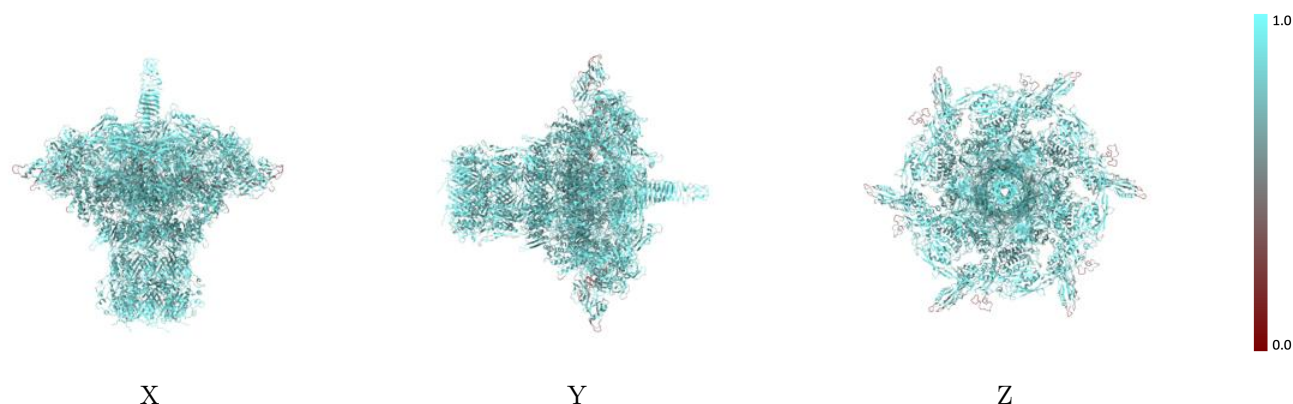
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



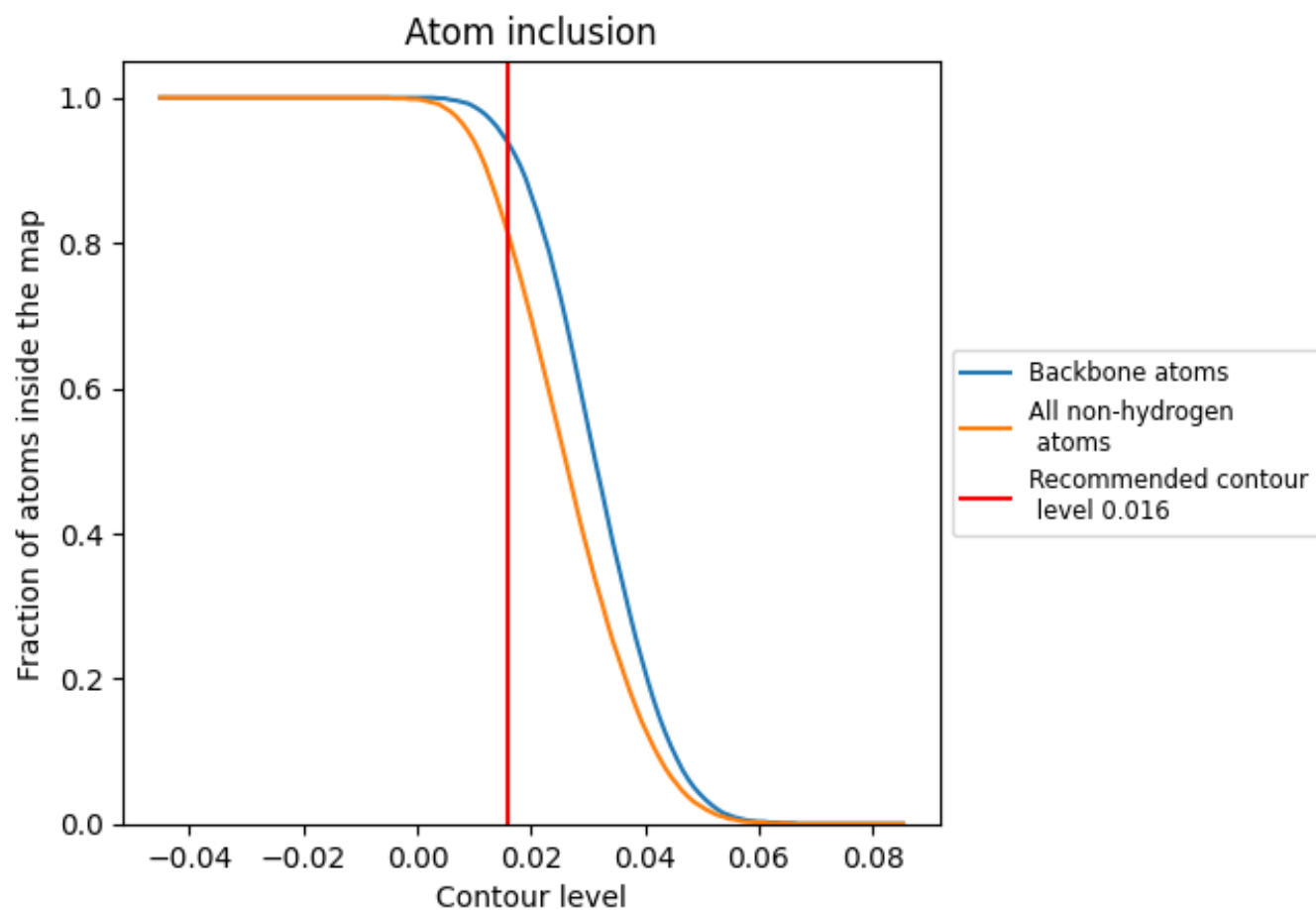
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



























































The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8130	 0.3220
0	 0.7610	 0.2330
1	 0.7380	 0.2310
2	 0.7090	 0.3730
3	 0.7450	 0.3620
4	 0.7380	 0.3590
5	 0.7090	 0.3620
6	 0.7230	 0.3570
7	 0.7310	 0.3670
8	 0.8190	 0.3650
9	 0.8150	 0.3550
A	 0.8300	 0.3840
AA	 0.8100	 0.3660
B	 0.8170	 0.3790
C	 0.8260	 0.3800
D	 0.8280	 0.3830
E	 0.8190	 0.3810
F	 0.8170	 0.3770
G	 0.8480	 0.4170
H	 0.8600	 0.4240
I	 0.7820	 0.2820
J	 0.8620	 0.3740
K	 0.8190	 0.3660
L	 0.7720	 0.2330
M	 0.8560	 0.3400
N	 0.8240	 0.3080
O	 0.7150	 0.2290
P	 0.8880	 0.3600
Q	 0.8470	 0.4220
R	 0.8600	 0.4310
S	 0.8030	 0.3160
T	 0.8630	 0.3740
U	 0.8230	 0.3570
V	 0.7620	 0.2330
W	 0.8570	 0.3430



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Chain	Atom inclusion	Q-score
X	 0.8230	 0.3060
Y	 0.7320	 0.2290
Z	 0.8830	 0.3640
a	 0.8400	 0.4120
b	 0.8550	 0.4270
c	 0.7900	 0.2810
d	 0.8610	 0.3750
e	 0.8260	 0.3590
f	 0.7770	 0.2420
g	 0.8570	 0.3400
h	 0.8240	 0.3020
i	 0.7150	 0.2340
j	 0.8830	 0.3650
k	 0.8540	 0.4230
l	 0.8600	 0.4290
m	 0.8070	 0.3140
n	 0.8160	 0.3640
o	 0.7630	 0.2310
p	 0.7340	 0.2290
q	 0.8440	 0.4170
r	 0.8600	 0.4250
s	 0.7880	 0.2840
t	 0.8210	 0.3550
u	 0.7760	 0.2360
v	 0.7150	 0.2320
w	 0.8500	 0.4230
x	 0.8530	 0.4300
y	 0.8160	 0.3150
z	 0.8180	 0.3650