



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 12:17 AM UTC

PDB ID : 9W39 / pdb_00009w39
EMDB ID : EMD-65595
Title : Structure of human 26S proteasome complexed with midnolin, 19S proteasome with Ubl bound
Authors : Zhu, C.; Qin, L.; Liang, L.
Deposited on : 2025-07-29
Resolution : 3.65 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

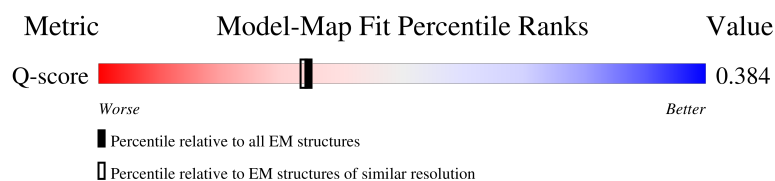
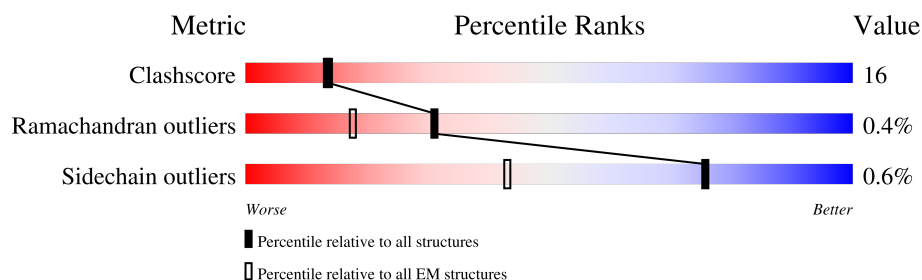
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.65 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	11564 (3.15 - 4.15)

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	f	856	<div> <div>7%</div> <div>90%</div> </div>
2	C	406	<div> <div>14%</div> <div>57%</div> <div>32%</div> <div>10%</div> </div>
3	D	418	<div> <div>62%</div> <div>28%</div> <div>9%</div> </div>
4	V	534	<div> <div>24%</div> <div>50%</div> <div>32%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
5	W	456	
6	X	422	
7	Y	389	
8	Z	324	
9	a	376	
10	b	377	
11	d	350	
12	e	70	
13	v	7	
14	U	953	
15	c	590	
16	A	433	
17	B	440	
18	E	389	
19	F	439	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 49219 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 Maltose/maltodextrin-binding periplasmic protein, Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	f	84	Total	C	N	O	S	0	0
			632	394	115	121	2		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	-387	MET	-	initiating methionine	UNP P0AEX9
f	-386	GLY	-	expression tag	UNP P0AEX9
f	-385	HIS	-	expression tag	UNP P0AEX9
f	-384	HIS	-	expression tag	UNP P0AEX9
f	-383	HIS	-	expression tag	UNP P0AEX9
f	-382	HIS	-	expression tag	UNP P0AEX9
f	-381	HIS	-	expression tag	UNP P0AEX9
f	-380	HIS	-	expression tag	UNP P0AEX9
f	-13	ASP	-	linker	UNP P0AEX9
f	-12	TYR	-	linker	UNP P0AEX9
f	-11	ASP	-	linker	UNP P0AEX9
f	-10	ILE	-	linker	UNP P0AEX9
f	-9	PRO	-	linker	UNP P0AEX9
f	-8	THR	-	linker	UNP P0AEX9
f	-7	THR	-	linker	UNP P0AEX9
f	-6	GLU	-	linker	UNP P0AEX9
f	-5	ASN	-	linker	UNP P0AEX9
f	-4	LEU	-	linker	UNP P0AEX9
f	-3	TYR	-	linker	UNP P0AEX9
f	-2	PHE	-	linker	UNP P0AEX9
f	-1	GLN	-	linker	UNP P0AEX9
f	0	GLY	-	linker	UNP P0AEX9

- Molecule 2 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	364	Total	C	N	O	S	0	0
			2870	1811	516	527	16		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	442	Total	C	N	O	S	0	0
			3592	2290	639	650	13		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	440	Total	C	N	O	S	0	0
			3582	2269	609	681	23		

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	384	Total	C	N	O	S	0	0
			3040	1935	513	580	12		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	376	Total	C	N	O	S	0	0
			3103	1979	531	576	17		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	270	Total	C	N	O	S	0	0
			2193	1417	360	407	9		

- Molecule 12 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	e	48	Total	C	N	O	0	0
			409	249	63	97		

- Molecule 13 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	v	7	Total	C	N	O	0	0
			35	21	7	7		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	818	Total	C	N	O	S	0	0
			6371	4046	1085	1196	44		

- Molecule 15 is a protein called Ubiquitin C-terminal hydrolase PSMD14, Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	293	Total	C	N	O	S	0	0
			2304	1457	396	432	19		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	311	GLU	-	linker	UNP O00487
c	312	ASN	-	linker	UNP O00487
c	313	LEU	-	linker	UNP O00487
c	314	TYR	-	linker	UNP O00487
c	315	PHE	-	linker	UNP O00487
c	316	GLN	-	linker	UNP O00487
c	317	GLY	-	linker	UNP O00487
c	318	ALA	-	linker	UNP O00487
c	555	HIS	-	expression tag	UNP A0A2U3DNX3
c	556	HIS	-	expression tag	UNP A0A2U3DNX3
c	557	HIS	-	expression tag	UNP A0A2U3DNX3
c	558	HIS	-	expression tag	UNP A0A2U3DNX3
c	559	HIS	-	expression tag	UNP A0A2U3DNX3
c	560	HIS	-	expression tag	UNP A0A2U3DNX3
c	561	SER	-	expression tag	UNP A0A2U3DNX3
c	562	ALA	-	expression tag	UNP A0A2U3DNX3
c	563	TRP	-	expression tag	UNP A0A2U3DNX3
c	564	SER	-	expression tag	UNP A0A2U3DNX3
c	565	HIS	-	expression tag	UNP A0A2U3DNX3
c	566	PRO	-	expression tag	UNP A0A2U3DNX3
c	567	GLN	-	expression tag	UNP A0A2U3DNX3
c	568	PHE	-	expression tag	UNP A0A2U3DNX3
c	569	GLU	-	expression tag	UNP A0A2U3DNX3
c	570	LYS	-	expression tag	UNP A0A2U3DNX3
c	571	GLY	-	expression tag	UNP A0A2U3DNX3
c	572	GLY	-	expression tag	UNP A0A2U3DNX3
c	573	GLY	-	expression tag	UNP A0A2U3DNX3
c	574	SER	-	expression tag	UNP A0A2U3DNX3
c	575	GLY	-	expression tag	UNP A0A2U3DNX3
c	576	GLY	-	expression tag	UNP A0A2U3DNX3
c	577	GLY	-	expression tag	UNP A0A2U3DNX3
c	578	SER	-	expression tag	UNP A0A2U3DNX3
c	579	GLY	-	expression tag	UNP A0A2U3DNX3
c	580	GLY	-	expression tag	UNP A0A2U3DNX3
c	581	SER	-	expression tag	UNP A0A2U3DNX3
c	582	ALA	-	expression tag	UNP A0A2U3DNX3
c	583	TRP	-	expression tag	UNP A0A2U3DNX3
c	584	SER	-	expression tag	UNP A0A2U3DNX3
c	585	HIS	-	expression tag	UNP A0A2U3DNX3
c	586	PRO	-	expression tag	UNP A0A2U3DNX3
c	587	GLN	-	expression tag	UNP A0A2U3DNX3
c	588	PHE	-	expression tag	UNP A0A2U3DNX3
c	589	GLU	-	expression tag	UNP A0A2U3DNX3

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Chain	Residue	Modelled	Actual	Comment	Reference
c	590	LYS	-	expression tag	UNP A0A2U3DNX3

- Molecule 16 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A	366	Total	C	N	O	S	0	0
			2863	1805	503	537	18		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B	340	Total	C	N	O	S	0	0
			2647	1663	451	521	12		

- Molecule 18 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	347	Total	C	N	O	S	0	0
			2721	1713	484	508	16		

- Molecule 19 is a protein called 26S proteasome regulatory subunit 6A.

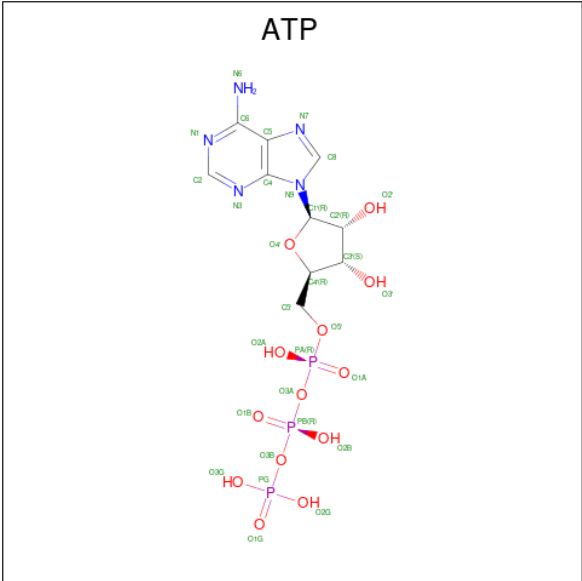
Mol	Chain	Residues	Atoms					AltConf	Trace
19	F	372	Total	C	N	O	S	0	0
			2902	1823	501	562	16		

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 21 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
21	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
21	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
22	c	1	Total	Zn	0
			1	1	

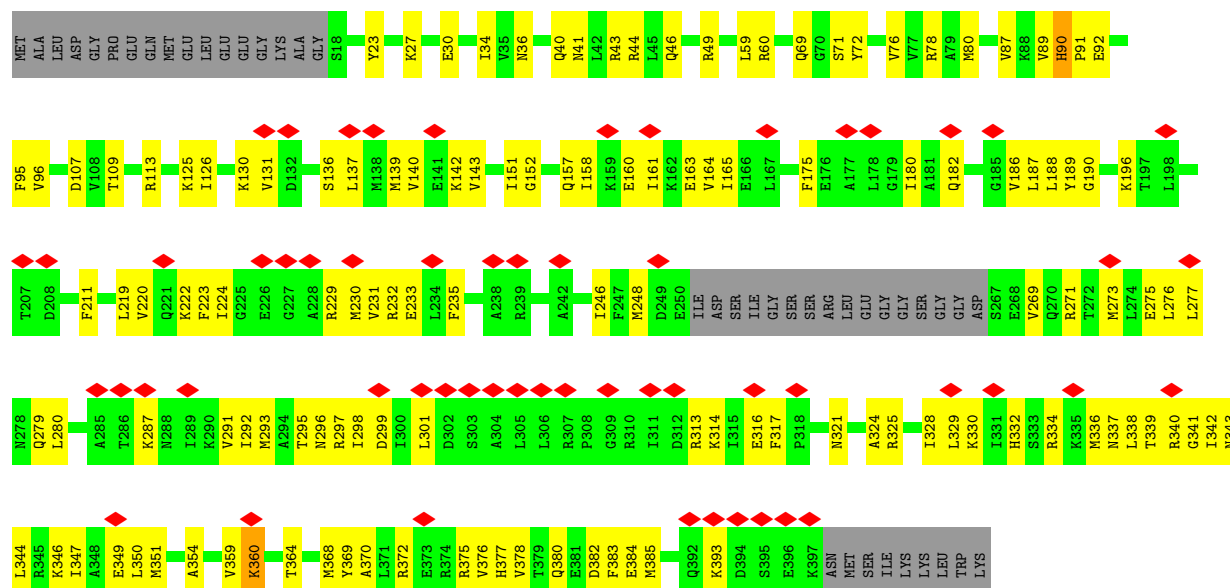
- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
23	B	1	Total	Mg	0
			1	1	
23	E	1	Total	Mg	0
			1	1	
23	F	1	Total	Mg	0
			1	1	

GLY SER PRO ASP GLY ALA SER GLY LEU LEU LEU ASP PHE GLU ASP SER VAL TRP LYS PRO VAL ASN PRO ASP TLE LYS SER SER PHE GLU VAL VAL ALA

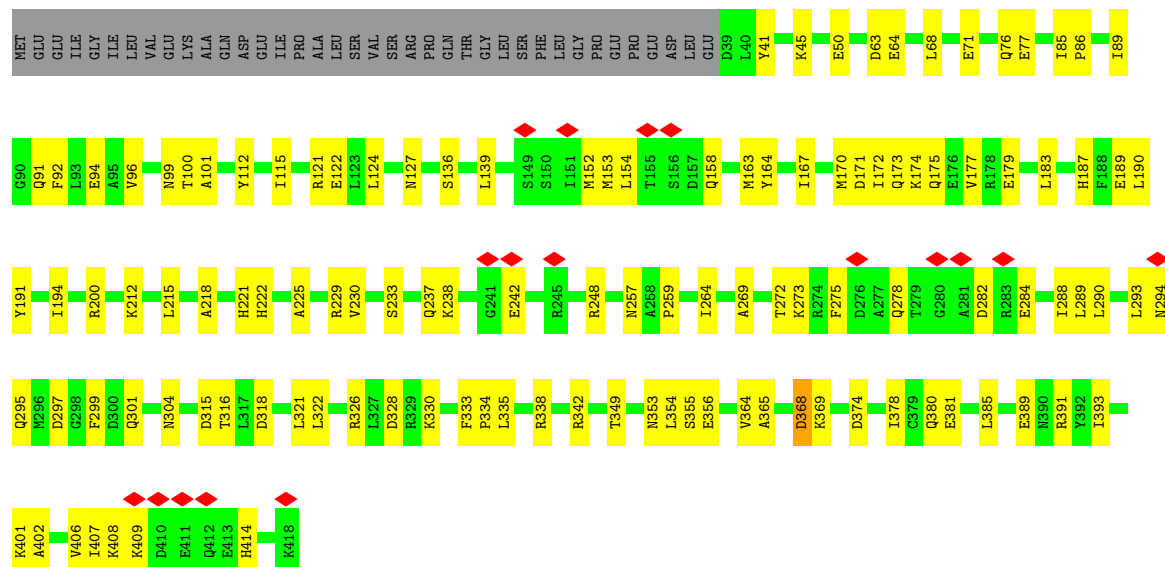
• Molecule 2: 26S proteasome regulatory subunit 8

Chain C: 



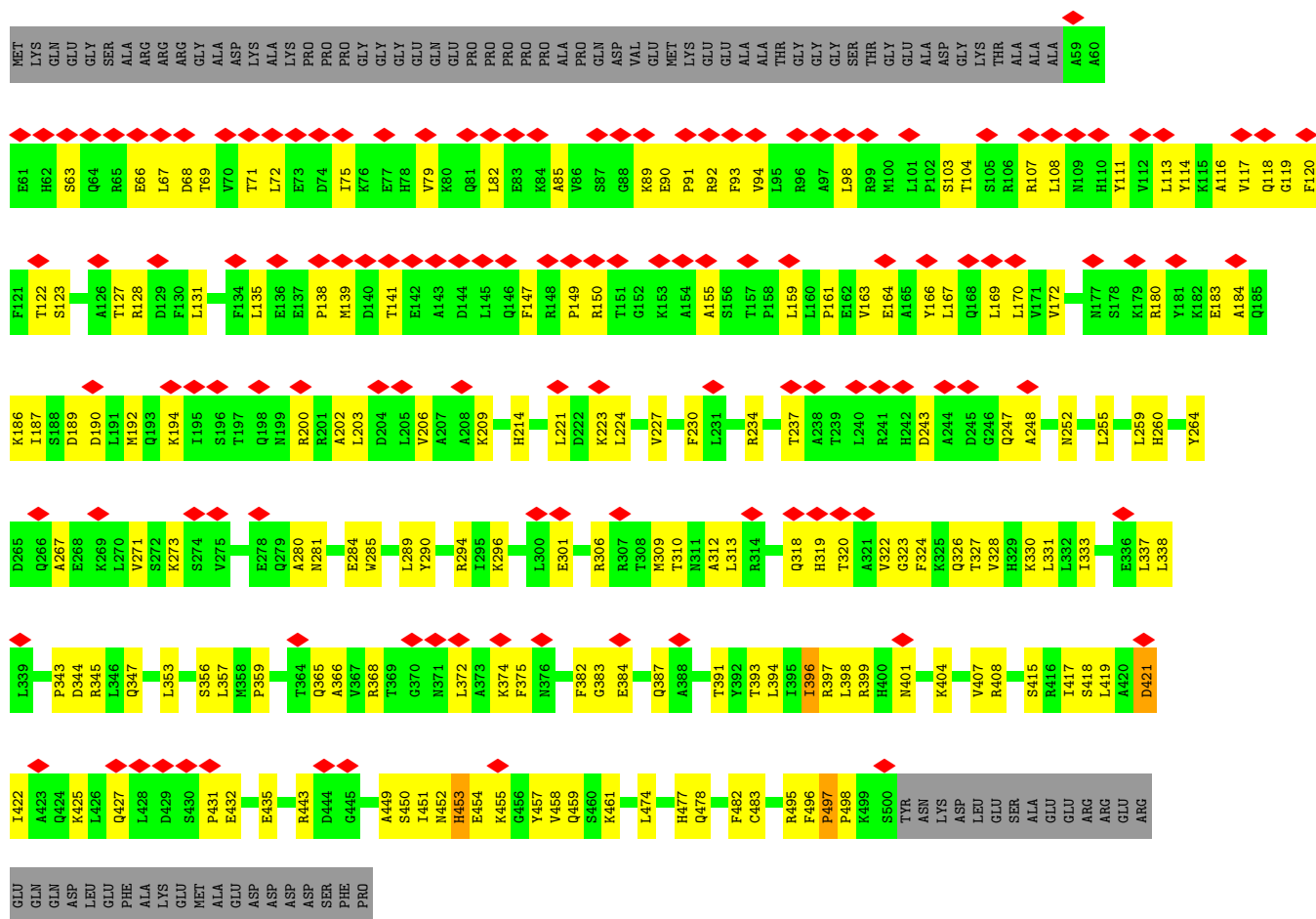
• Molecule 3: 26S proteasome regulatory subunit 6B

Chain D: 

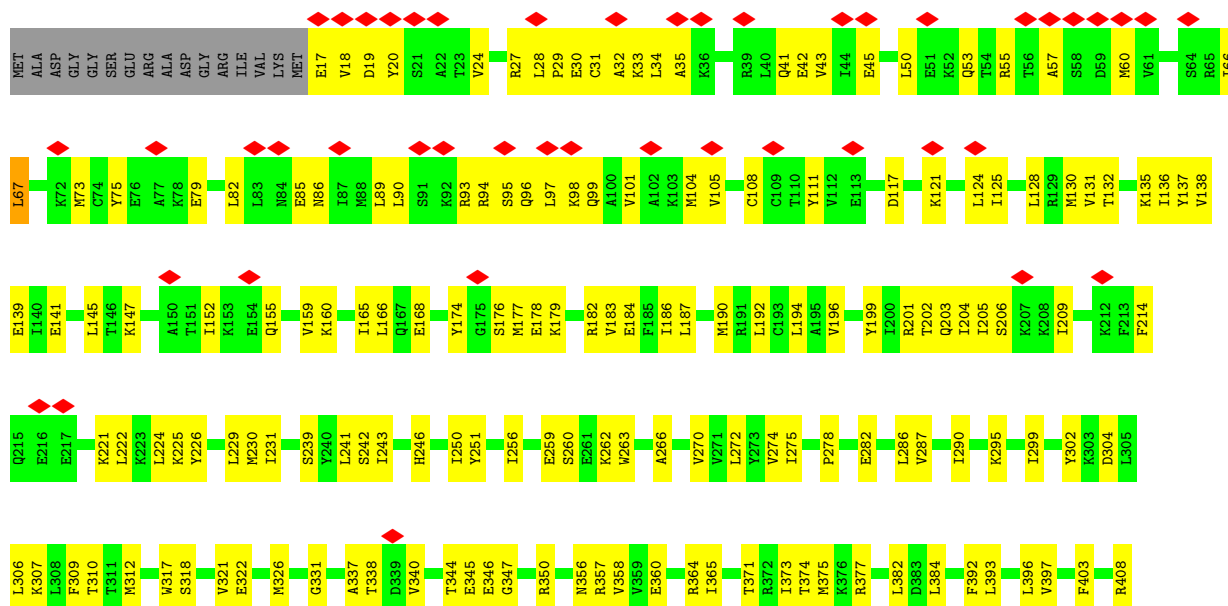


• Molecule 4: 26S proteasome non-ATPase regulatory subunit 3

Chain V: 

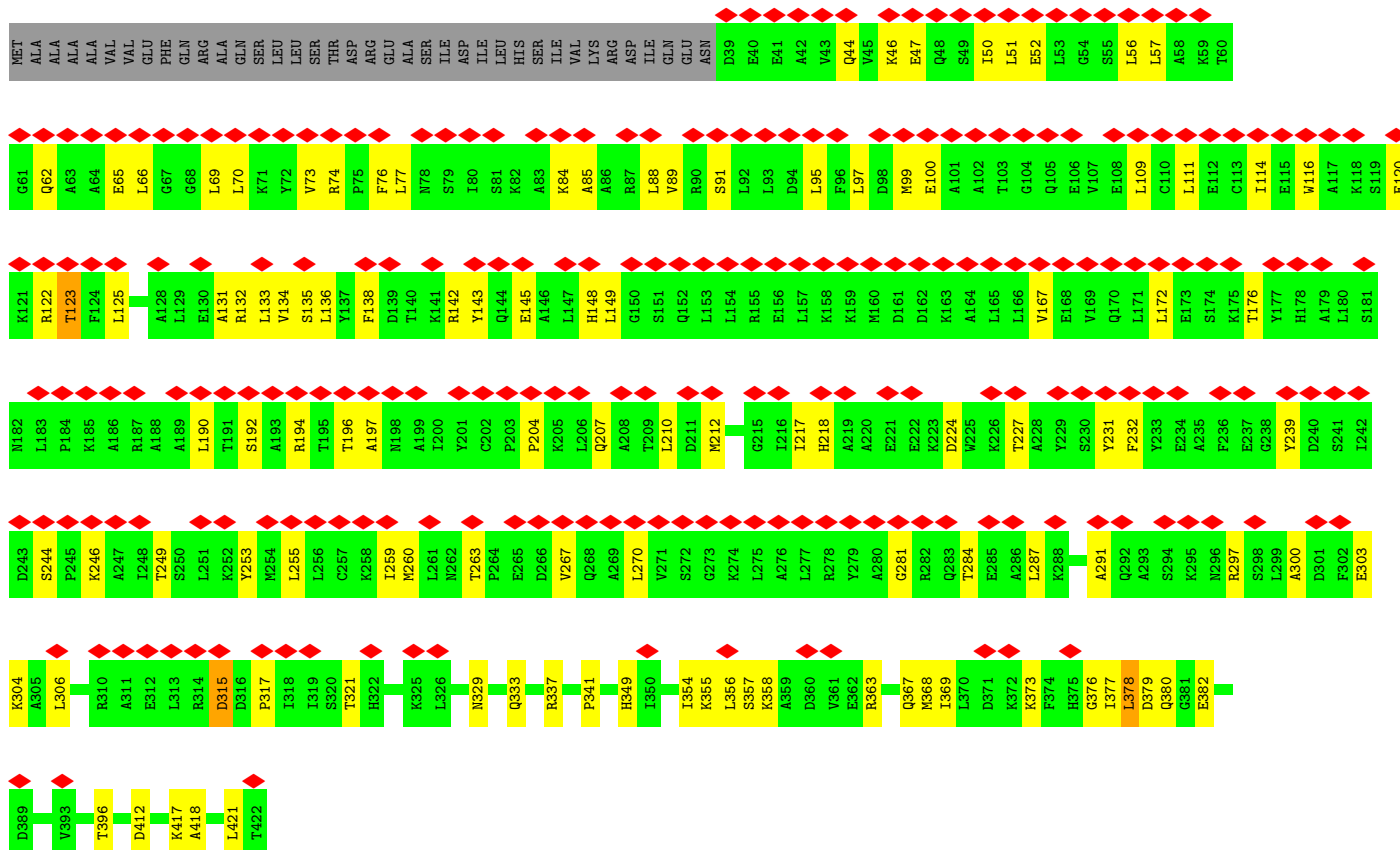


• Molecule 5: 26S proteasome non-ATPase regulatory subunit 12

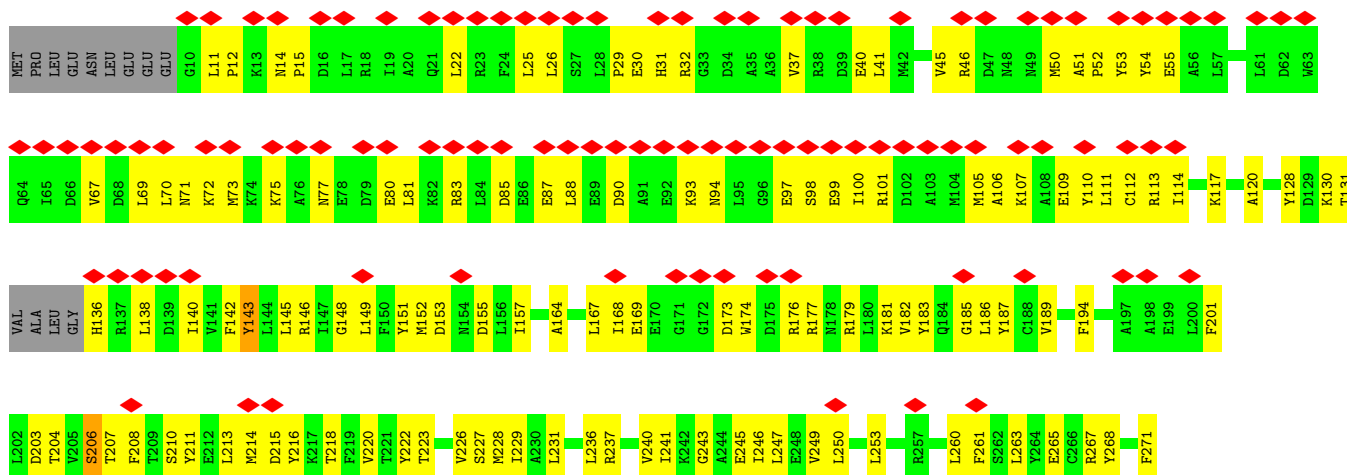


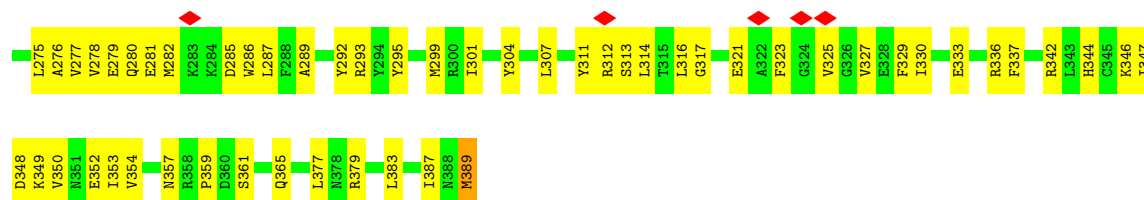


- Molecule 6: 26S proteasome non-ATPase regulatory subunit 11

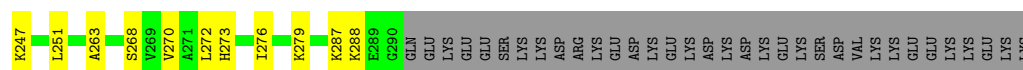
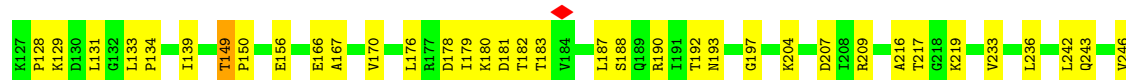
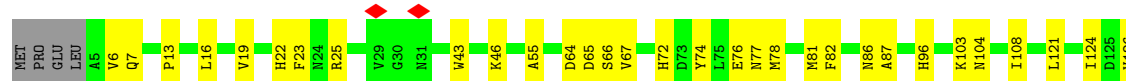


- Molecule 7: 26S proteasome non-ATPase regulatory subunit 6

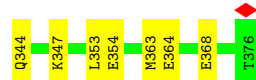




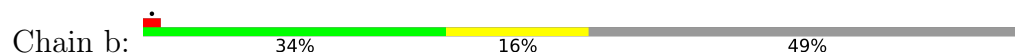
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 7



• Molecule 9: 26S proteasome non-ATPase regulatory subunit 13



• Molecule 10: 26S proteasome non-ATPase regulatory subunit 4

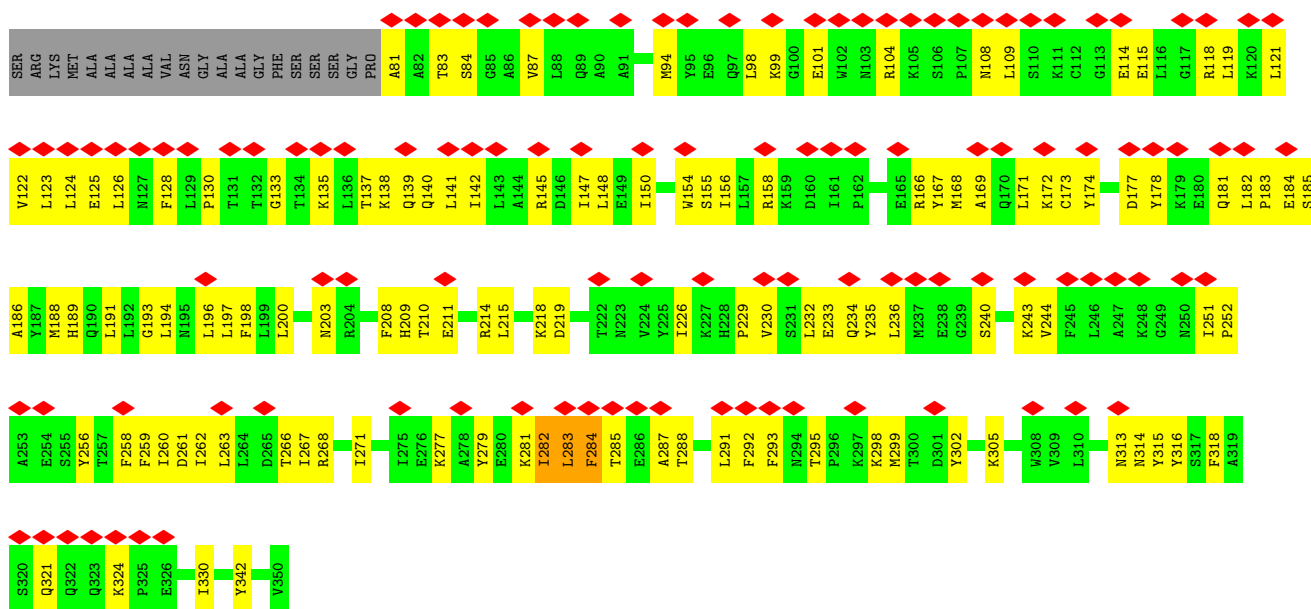


[illegible]

- Molecule 11: 26S proteasome non-ATPase regulatory subunit 8



MET	PHE	ILE	LYS	GLY	ARG	ALA	PRO	ARG	ALA	PRO	PRO	ARG	GLU	ARG	ARG	ARG	ALA	ALA	THR	ARG	GLY	GLY	LEU	ARG	GLN	VAL	VAL	ALA	PRO	PRO	ARG	ALA	ALA	LEU	GLY	SER	THR	SER	PRO	PRO	ARG	HIS	PHE	ARG	ARG	CYS	ARG	ARG	ARG	CYS	GLY	GLY	LEU	LEU	ALA	ALA
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- Molecule 12: 26S proteasome complex subunit SEM1



MET	SER	GLU	LYS	GLN	PRO	VAL	ASP	LEU	GLY	LEU	LEU	GLU	GLU	D16	E25	D26	W27	A28	G29	L30	D31	E32	D33	E34	D35	A36	H37	V38	V39	E40	D41	N42	W43	D44	D45	D46	D51	F52	S53	H63	GLY	TYR	LYS	MET	GLU	THR	SER
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- Molecule 13: Substrate



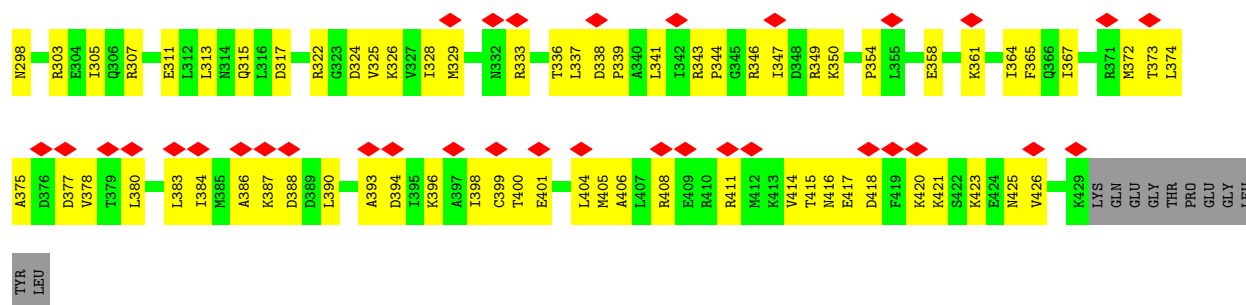
Diagram illustrating a sequence of nodes $x_1, x_2, x_3, x_4, x_5, x_6, x_7$. Nodes x_3 and x_5 are highlighted in red, and nodes x_4 and x_6 are highlighted in green. Red diamonds are placed above x_3 and x_5 , and green diamonds are placed above x_4 and x_6 .

- Molecule 14: 26S proteasome non-ATPase regulatory subunit 1



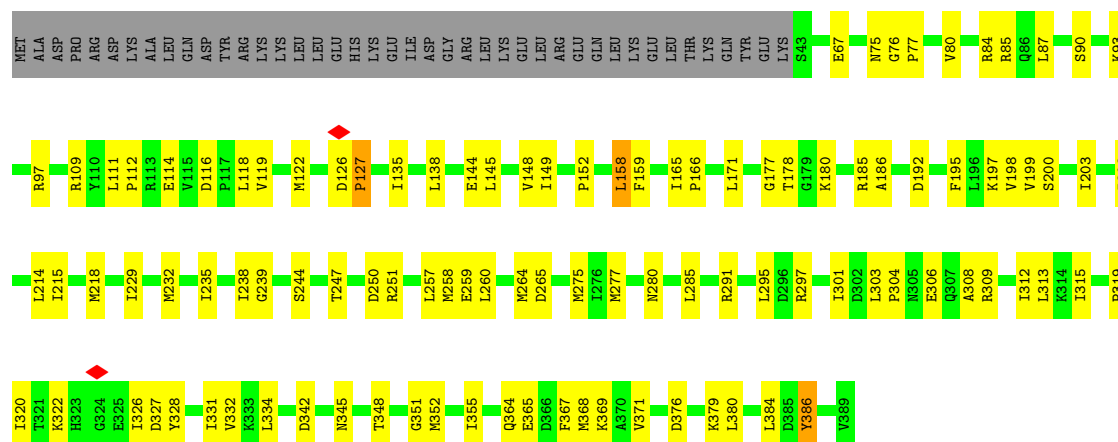






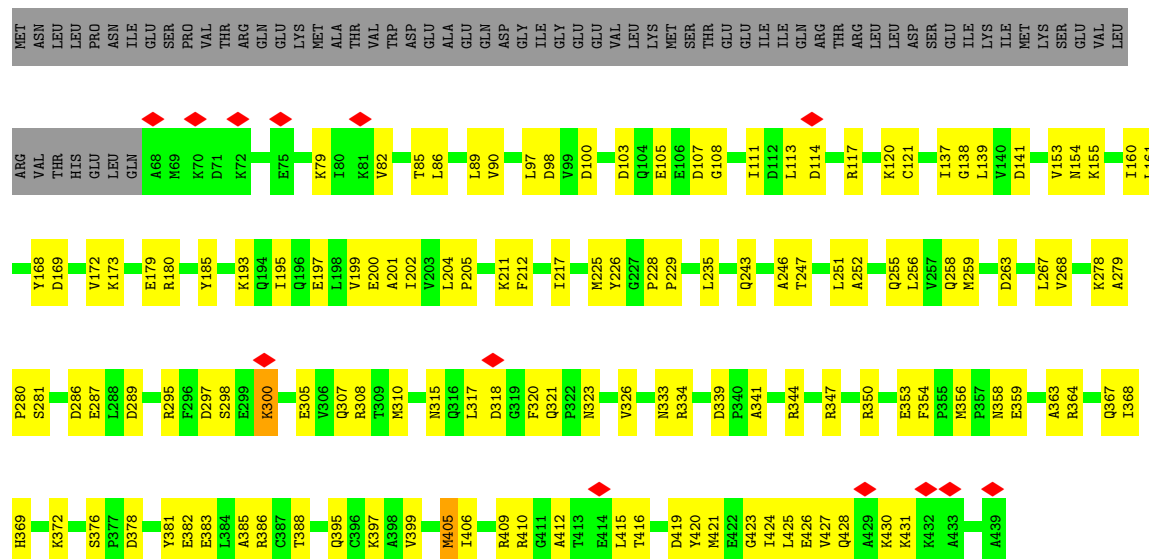
• Molecule 18: 26S proteasome regulatory subunit 10B

Chain E: 62% 26% 11%



• Molecule 19: 26S proteasome regulatory subunit 6A

Chain F: 54% 30% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22385	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.571	Depositor
Minimum map value	-0.306	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.081	Depositor
Map size (Å)	340.0, 340.0, 340.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, ADP, ATP

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	f	0.19	0/640	0.49	0/863
2	C	0.23	0/2908	0.51	0/3912
3	D	0.25	0/3089	0.50	0/4168
4	V	0.20	0/3662	0.46	0/4946
5	W	0.26	0/3630	0.55	0/4884
6	X	0.16	0/3084	0.41	0/4157
7	Y	0.24	0/3160	0.54	0/4254
8	Z	0.21	0/2324	0.44	0/3150
9	a	0.20	0/3053	0.50	0/4133
10	b	0.19	0/1478	0.47	0/2001
11	d	0.20	0/2239	0.51	0/3025
12	e	0.22	0/420	0.52	0/572
14	U	0.21	0/6486	0.43	0/8777
15	c	0.20	0/2347	0.39	0/3174
16	A	0.19	0/2914	0.48	0/3937
17	B	0.22	0/2684	0.53	0/3623
18	E	0.20	0/2765	0.46	0/3730
19	F	0.19	0/2942	0.43	0/3967
All	All	0.21	0/49825	0.48	0/67273

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 [i](#)

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	f	632	0	663	16	0
2	C	2870	0	2976	116	0
3	D	3039	0	3076	93	0
4	V	3592	0	3647	158	0
5	W	3582	0	3693	133	0
6	X	3040	0	3134	84	0
7	Y	3103	0	3104	163	0
8	Z	2281	0	2312	66	0
9	a	2995	0	3012	90	0
10	b	1458	0	1505	49	0
11	d	2193	0	2221	122	0
12	e	409	0	316	12	0
13	v	35	0	10	0	0
14	U	6371	0	6409	178	0
15	c	2304	0	2315	60	0
16	A	2863	0	2895	92	0
17	B	2647	0	2684	106	0
18	E	2721	0	2770	87	0
19	F	2902	0	2956	100	0
20	C	27	0	12	1	0
20	F	27	0	12	1	0
21	A	31	0	12	2	0
21	B	31	0	12	3	0
21	D	31	0	12	0	0
21	E	31	0	12	3	0
22	c	1	0	0	0	0
23	B	1	0	0	0	0
23	E	1	0	0	0	0
23	F	1	0	0	0	0
All	All	49219	0	49770	1574	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 16.

All (1574) 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)
4:V:189:ASP:HA	4:V:192:MET:HE2	1.45	0.98
7:Y:14:ASN:HB2	7:Y:113:ARG:HH21	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:GLU:HB2	2:C:313:ARG:HH12	1.42	0.84
4:V:443:ARG:HA	11:d:277:LYS:HD2	1.58	0.84
18:E:322:LYS:HD2	18:E:326:ILE:HD11	1.60	0.83
7:Y:313:SER:HB3	7:Y:353:ILE:HD11	1.60	0.83
6:X:363:ARG:HH12	6:X:367:GLN:HB2	1.42	0.82
18:E:348:THR:HA	19:F:217:ILE:HD11	1.61	0.81
9:a:363:MET:HE3	15:c:307:VAL:HG11	1.62	0.81
8:Z:263:ALA:HB1	15:c:288:VAL:HG23	1.62	0.80
17:B:420:LYS:HA	17:B:423:LYS:HD3	1.64	0.80
8:Z:182:THR:HG22	8:Z:183:THR:H	1.44	0.79
7:Y:52:PRO:HG2	7:Y:114:ILE:HD12	1.65	0.79
16:A:220:THR:HG21	16:A:343:PHE:HB3	1.65	0.78
14:U:74:PHE:HB3	14:U:103:LYS:HG2	1.65	0.78
6:X:97:LEU:HD11	6:X:136:LEU:HD23	1.65	0.78
6:X:363:ARG:O	6:X:363:ARG:NH1	2.15	0.78
5:W:117:ASP:O	5:W:121:LYS:HB2	1.83	0.78
7:Y:176:ARG:HD2	7:Y:179:ARG:HH21	1.47	0.78
6:X:396:THR:HG22	15:c:242:GLU:HG3	1.66	0.77
7:Y:46:ARG:HG3	7:Y:69:LEU:HD13	1.67	0.77
14:U:9:ILE:HG21	14:U:41:SER:HB2	1.65	0.77
5:W:375:MET:HE3	5:W:411:GLY:HA2	1.67	0.76
4:V:122:THR:HG21	4:V:155:ALA:HA	1.67	0.76
9:a:70:ARG:HG3	9:a:73:PRO:HD3	1.67	0.75
16:A:212:VAL:HG12	16:A:339:ARG:HB2	1.66	0.75
17:B:281:ILE:HD12	17:B:328:ILE:HD11	1.66	0.75
5:W:177:MET:SD	5:W:178:GLU:N	2.59	0.75
11:d:200:LEU:HD21	11:d:233:GLU:HB2	1.69	0.75
14:U:218:GLN:HG2	14:U:752:THR:HG21	1.68	0.74
1:f:71:LEU:HD22	1:f:98:LEU:HD11	1.70	0.74
6:X:232:PHE:CE2	6:X:253:TYR:HB2	2.22	0.74
1:f:90:VAL:HG23	1:f:94:SER:HB2	1.69	0.74
18:E:352:MET:HE1	19:F:350:ARG:HH12	1.52	0.74
7:Y:67:VAL:HA	7:Y:70:LEU:HB3	1.69	0.74
11:d:101:GLU:HA	11:d:104:ARG:HE	1.52	0.74
3:D:127:ASN:HD22	3:D:248:ARG:HD3	1.53	0.73
3:D:342:ARG:HB3	3:D:364:VAL:HG11	1.68	0.73
5:W:326:MET:HE2	5:W:326:MET:H	1.52	0.73
5:W:55:ARG:NH1	5:W:94:ARG:O	2.21	0.73
4:V:98:LEU:HD11	4:V:209:LYS:HG3	1.71	0.73
4:V:264:TYR:CE2	11:d:210:THR:HB	2.23	0.73
4:V:120:PHE:HB3	4:V:167:LEU:HD13	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:451:ILE:HG13	4:V:458:VAL:HG22	1.70	0.72
4:V:116:ALA:O	4:V:120:PHE:HB2	1.89	0.72
11:d:167:TYR:O	11:d:171:LEU:HB3	1.90	0.72
8:Z:149:THR:HB	8:Z:150:PRO:HD3	1.72	0.72
7:Y:301:ILE:HG21	7:Y:342:ARG:HD2	1.71	0.72
11:d:232:LEU:HD11	11:d:263:LEU:HD21	1.72	0.72
16:A:365:GLU:HG2	16:A:368:ILE:HG13	1.71	0.71
9:a:11:SER:HA	9:a:14:SER:HB2	1.71	0.71
3:D:378:ILE:HG12	3:D:406:VAL:HG11	1.70	0.71
6:X:99:MET:SD	6:X:100:GLU:N	2.64	0.71
2:C:190:GLY:HA3	2:C:317:PHE:HB2	1.72	0.71
7:Y:278:VAL:HG22	7:Y:282:MET:HE2	1.72	0.70
6:X:74:ARG:O	6:X:74:ARG:NH1	2.23	0.70
9:a:72:ASN:O	9:a:74:LEU:N	2.24	0.70
5:W:179:LYS:HA	5:W:182:ARG:HD3	1.73	0.70
16:A:307:ASP:OD1	16:A:333:ARG:NH2	2.25	0.69
17:B:120:HIS:HA	17:B:135:ILE:HG13	1.74	0.69
19:F:185:TYR:H	19:F:243:GLN:HE21	1.38	0.69
6:X:418:ALA:HB1	7:Y:387:ILE:HD11	1.74	0.69
4:V:163:VAL:O	4:V:167:LEU:HG	1.92	0.69
11:d:279:TYR:CD2	11:d:283:LEU:HD23	2.26	0.69
18:E:84:ARG:NH2	19:F:105:GLU:OE1	2.25	0.69
11:d:138:LYS:O	11:d:142:ILE:HG12	1.93	0.69
11:d:123:LEU:HA	11:d:126:LEU:HG	1.75	0.69
2:C:360:LYS:O	2:C:364:THR:HG23	1.92	0.69
3:D:237:GLN:HG3	3:D:242:GLU:HB2	1.74	0.69
2:C:40:GLN:OE1	4:V:495:ARG:NH1	2.26	0.69
16:A:74:PRO:O	16:A:78:TRP:HB2	1.92	0.68
4:V:383:GLY:O	4:V:387:GLN:HG2	1.94	0.68
4:V:111:TYR:HD2	4:V:138:PRO:HB3	1.57	0.68
3:D:187:HIS:HB3	3:D:190:LEU:HB3	1.73	0.68
9:a:44:PHE:O	9:a:48:PRO:HD3	1.94	0.68
7:Y:293:ARG:NH2	12:e:51:ASP:OD1	2.27	0.68
18:E:355:ILE:HG23	19:F:211:LYS:HZ2	1.58	0.68
2:C:369:TYR:HA	2:C:372:ARG:HD2	1.75	0.68
5:W:224:LEU:HD11	5:W:256:ILE:HD11	1.76	0.68
17:B:149:SER:HB2	17:B:163:LEU:HB3	1.76	0.68
4:V:417:ILE:HD11	4:V:421:ASP:HB2	1.76	0.67
19:F:363:ALA:HB2	19:F:385:ALA:HB2	1.75	0.67
7:Y:265:GLU:OE2	7:Y:267:ARG:NH1	2.28	0.67
4:V:345:ARG:NH1	12:e:46:ASP:OD2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:184:GLU:HB2	11:d:188:MET:HG2	1.74	0.67
17:B:234:LEU:HD22	21:B:501:ATP:H2'	1.77	0.67
5:W:79:GLU:HB3	5:W:82:LEU:HB2	1.76	0.67
11:d:282:ILE:HB	11:d:315:TYR:HA	1.77	0.67
14:U:374:SER:HB2	14:U:407:SER:HB2	1.75	0.67
9:a:280:MET:HE1	9:a:296:ILE:HG12	1.77	0.67
19:F:255:GLN:O	19:F:258:GLN:NE2	2.28	0.67
18:E:144:GLU:OE2	18:E:297:ARG:NH1	2.28	0.67
18:E:327:ASP:OD2	18:E:364:GLN:NE2	2.26	0.66
17:B:284:ILE:HB	17:B:329:MET:HG2	1.77	0.66
5:W:221:LYS:O	5:W:221:LYS:NZ	2.29	0.66
7:Y:344:HIS:HB3	7:Y:357:ASN:HB3	1.76	0.66
4:V:450:SER:HB3	4:V:461:LYS:HE3	1.78	0.66
7:Y:26:LEU:HD13	7:Y:32:ARG:HA	1.78	0.66
11:d:282:ILE:HG23	11:d:283:LEU:H	1.59	0.66
3:D:167:ILE:HG21	3:D:174:LYS:HD2	1.77	0.66
5:W:105:VAL:HG11	5:W:138:VAL:HG11	1.78	0.66
14:U:448:LEU:HD12	14:U:483:LEU:HD21	1.78	0.66
18:E:198:VAL:HG12	18:E:200:SER:H	1.60	0.66
5:W:326:MET:HE2	5:W:326:MET:N	2.11	0.66
7:Y:293:ARG:HH22	12:e:51:ASP:HA	1.59	0.66
3:D:353:ASN:HB3	3:D:393:ILE:HD12	1.78	0.66
16:A:410:LEU:O	16:A:414:ASN:ND2	2.28	0.66
4:V:419:LEU:HD11	4:V:451:ILE:HD11	1.78	0.66
8:Z:246:VAL:HG12	11:d:330:ILE:HD11	1.77	0.65
17:B:103:ARG:HG2	17:B:160:ILE:HG21	1.78	0.65
4:V:273:LYS:HE2	14:U:71:LEU:HD22	1.78	0.65
5:W:299:ILE:HG22	5:W:302:TYR:HB2	1.78	0.65
3:D:153:MET:HE1	3:D:229:ARG:HG2	1.77	0.65
14:U:101:ILE:HD12	14:U:137:MET:HE1	1.78	0.65
19:F:318:ASP:HB3	19:F:347:ARG:HG2	1.78	0.65
17:B:411:ARG:NH1	17:B:417:GLU:OE1	2.28	0.65
18:E:352:MET:HE1	19:F:350:ARG:NH1	2.12	0.65
7:Y:227:SER:O	7:Y:231:LEU:HB2	1.96	0.65
14:U:410:VAL:HG23	14:U:448:LEU:HD21	1.79	0.65
2:C:143:VAL:HG21	2:C:211:PHE:HD2	1.61	0.65
2:C:339:THR:N	2:C:378:VAL:H	1.94	0.65
4:V:72:LEU:HD13	4:V:147:PHE:HB2	1.77	0.65
4:V:477:HIS:ND1	11:d:342:TYR:OH	2.21	0.65
5:W:17:GLU:N	5:W:57:ALA:O	2.29	0.65
5:W:125:ILE:HG23	5:W:145:LEU:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:108:ASP:O	9:a:110:ALA:N	2.30	0.64
16:A:183:GLN:N	16:A:183:GLN:OE1	2.31	0.64
4:V:419:LEU:HA	4:V:422:ILE:HD12	1.80	0.64
5:W:382:LEU:HD23	5:W:384:LEU:HB2	1.79	0.64
7:Y:237:ARG:HA	7:Y:241:ILE:HD13	1.80	0.64
19:F:98:ASP:HB3	19:F:120:LYS:HG2	1.79	0.64
4:V:82:LEU:HD22	4:V:94:VAL:HG12	1.80	0.64
2:C:152:GLY:O	20:C:501:ADP:N6	2.28	0.64
3:D:284:GLU:O	3:D:288:ILE:HG12	1.98	0.64
10:b:169:HIS:HB2	10:b:187:PRO:HB3	1.80	0.64
11:d:281:LYS:HG3	11:d:315:TYR:HD2	1.63	0.64
16:A:346:PRO:O	16:A:351:ARG:NH2	2.31	0.64
4:V:92:ARG:NH2	7:Y:389:MET:SD	2.71	0.63
5:W:128:LEU:HA	5:W:131:VAL:HG12	1.80	0.63
9:a:52:GLN:O	9:a:86:GLN:NE2	2.31	0.63
14:U:406:ALA:HA	14:U:445:ALA:HB2	1.78	0.63
18:E:126:ASP:HB2	18:E:197:LYS:HZ1	1.62	0.63
6:X:380:GLN:HB2	7:Y:311:TYR:HD2	1.62	0.63
3:D:171:ASP:OD1	3:D:172:ILE:N	2.32	0.63
5:W:331:GLY:HA3	5:W:337:ALA:HB2	1.80	0.63
15:c:26:ASP:OD1	15:c:27:THR:N	2.31	0.63
18:E:109:ARG:NH2	19:F:114:ASP:O	2.31	0.63
2:C:340:ARG:C	7:Y:207:THR:HG23	2.23	0.63
4:V:161:PRO:HB2	4:V:203:LEU:HD11	1.80	0.63
5:W:346:GLU:HG3	5:W:350:ARG:HH12	1.64	0.63
14:U:723:ASP:OD1	14:U:724:VAL:N	2.31	0.63
6:X:190:LEU:HD22	6:X:217:ILE:HG21	1.80	0.63
9:a:364:GLU:O	9:a:368:GLU:HG2	1.99	0.63
17:B:279:PRO:HA	17:B:324:ASP:HB3	1.81	0.63
4:V:108:LEU:HD11	4:V:170:LEU:HD12	1.79	0.63
16:A:293:ASN:HA	16:A:296:GLN:HE21	1.64	0.63
10:b:166:THR:O	10:b:169:HIS:NE2	2.32	0.62
4:V:71:THR:O	4:V:75:ILE:HG13	1.99	0.62
4:V:192:MET:HB2	4:V:230:PHE:CZ	2.34	0.62
5:W:338:THR:HB	5:W:340:VAL:HG22	1.81	0.62
7:Y:70:LEU:HA	7:Y:73:MET:HG2	1.81	0.62
17:B:405:MET:HA	17:B:408:ARG:HB2	1.80	0.62
4:V:417:ILE:HD13	7:Y:349:LYS:HG3	1.80	0.62
18:E:235:ILE:HG12	18:E:277:MET:HE3	1.81	0.62
2:C:229:ARG:HH22	17:B:265:LYS:HE3	1.65	0.62
2:C:36:ASN:HB3	4:V:89:LYS:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:78:ARG:NH1	2:C:80:MET:SD	2.72	0.62
1:f:39:THR:HG21	15:c:137:SER:HB2	1.82	0.62
3:D:96:VAL:HG11	3:D:112:TYR:HE1	1.64	0.62
7:Y:186:LEU:HD21	7:Y:214:MET:HE1	1.82	0.62
14:U:322:THR:HA	14:U:325:MET:HE3	1.82	0.62
9:a:77:VAL:HG21	9:a:110:ALA:HB1	1.80	0.62
11:d:156:ILE:HD11	11:d:194:LEU:HD21	1.81	0.62
18:E:90:SER:O	18:E:93:LYS:NZ	2.32	0.62
18:E:198:VAL:HB	18:E:232:MET:HG2	1.82	0.62
6:X:412:ASP:OD1	7:Y:379:ARG:NH2	2.32	0.61
7:Y:52:PRO:HD2	7:Y:114:ILE:HB	1.81	0.61
18:E:264:MET:HG2	18:E:275:MET:HE1	1.82	0.61
4:V:333:ILE:HG12	4:V:347:GLN:HE22	1.64	0.61
14:U:132:GLY:O	14:U:136:LYS:HG2	1.99	0.61
6:X:377:ILE:HG23	7:Y:312:ARG:HH12	1.66	0.61
3:D:275:PHE:HD1	3:D:282:ASP:HB3	1.66	0.61
17:B:190:LEU:HB3	17:B:193:GLN:HB2	1.82	0.61
7:Y:268:TYR:HE2	7:Y:307:LEU:HD13	1.65	0.61
16:A:277:ILE:HG21	16:A:319:MET:HG2	1.82	0.61
19:F:107:ASP:OD1	19:F:108:GLY:N	2.31	0.61
19:F:195:ILE:O	19:F:199:VAL:HG23	2.01	0.61
2:C:151:ILE:HG21	2:C:158:ILE:HD11	1.81	0.61
7:Y:25:LEU:HD13	7:Y:31:HIS:ND1	2.14	0.61
6:X:116:TRP:NE1	6:X:120:GLU:OE2	2.33	0.61
2:C:332:HIS:HD2	2:C:359:VAL:HG12	1.65	0.61
4:V:496:PHE:C	4:V:498:PRO:HD3	2.26	0.61
5:W:435:LEU:HD11	8:Z:233:VAL:HG13	1.82	0.61
3:D:115:ILE:HG22	3:D:139:LEU:HB2	1.81	0.60
10:b:97:LEU:HD23	10:b:107:MET:HB3	1.81	0.60
19:F:247:THR:HG21	19:F:278:LYS:HG3	1.83	0.60
4:V:200:ARG:HB2	4:V:203:LEU:HD12	1.83	0.60
7:Y:80:GLU:OE2	7:Y:83:ARG:NH2	2.32	0.60
17:B:187:ILE:HG21	17:B:190:LEU:HG	1.83	0.60
4:V:255:LEU:O	4:V:259:LEU:HG	2.01	0.60
3:D:389:GLU:OE1	3:D:391:ARG:NH1	2.34	0.60
4:V:419:LEU:HD13	4:V:435:GLU:HG2	1.84	0.60
10:b:140:ILE:HG21	10:b:153:LEU:HD11	1.83	0.60
14:U:345:ASN:O	14:U:743:ASN:ND2	2.34	0.60
17:B:141:LYS:HA	17:B:144:LEU:HD23	1.83	0.60
18:E:351:GLY:HA3	19:F:217:ILE:HD13	1.81	0.60
4:V:68:ASP:O	4:V:72:LEU:HG	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:168:MET:SD	11:d:168:MET:N	2.75	0.60
16:A:113:ILE:HG22	16:A:121:PHE:H	1.66	0.60
6:X:417:LYS:NZ	15:c:262:GLU:OE1	2.31	0.60
11:d:267:ILE:O	11:d:271:ILE:HG23	2.01	0.60
14:U:756:HIS:HB3	14:U:759:SER:HB2	1.83	0.60
6:X:52:GLU:O	6:X:56:LEU:HG	2.02	0.60
14:U:138:PHE:CE1	14:U:162:VAL:HG11	2.37	0.60
5:W:260:SER:HA	5:W:263:TRP:CD1	2.37	0.60
7:Y:186:LEU:HD23	7:Y:222:TYR:OH	2.01	0.60
18:E:327:ASP:H	18:E:364:GLN:NE2	2.00	0.60
6:X:255:LEU:HD22	6:X:267:VAL:HG23	1.83	0.60
5:W:85:GLU:O	5:W:89:LEU:HG	2.02	0.60
5:W:201:ARG:HA	5:W:204:ILE:HD12	1.84	0.60
7:Y:194:PHE:HD1	7:Y:226:VAL:HG23	1.67	0.60
9:a:126:GLY:HA3	9:a:129:GLN:HE22	1.67	0.60
16:A:206:ILE:HD13	19:F:405:MET:HE3	1.84	0.60
16:A:272:ILE:HD12	16:A:315:ILE:HG21	1.84	0.60
17:B:120:HIS:HB2	17:B:134:SER:HA	1.84	0.60
19:F:423:GLY:O	19:F:427:VAL:HG23	2.02	0.60
6:X:70:LEU:HD23	6:X:109:LEU:HD22	1.83	0.59
6:X:255:LEU:HD23	6:X:270:LEU:HD23	1.84	0.59
14:U:78:LEU:HD11	14:U:104:CYS:HB2	1.82	0.59
3:D:152:MET:SD	3:D:257:ASN:ND2	2.75	0.59
3:D:328:ASP:OD1	3:D:328:ASP:N	2.32	0.59
16:A:71:GLY:HA3	17:B:162:VAL:HG12	1.84	0.59
7:Y:220:VAL:HG21	7:Y:249:VAL:HG21	1.82	0.59
17:B:190:LEU:O	17:B:192:ASN:N	2.36	0.59
2:C:49:ARG:NE	3:D:64:GLU:OE2	2.34	0.59
8:Z:81:MET:HE2	15:c:94:LYS:HG2	1.84	0.59
17:B:380:LEU:HD13	17:B:383:LEU:HD12	1.85	0.59
6:X:145:GLU:O	6:X:148:HIS:ND1	2.35	0.59
14:U:463:ASN:HA	14:U:466:LYS:HE3	1.85	0.59
18:E:309:ARG:HE	18:E:332:VAL:HG13	1.66	0.59
7:Y:201:PHE:CE2	7:Y:222:TYR:HE1	2.20	0.59
11:d:166:ARG:NH1	14:U:13:ASP:OD1	2.36	0.59
19:F:193:LYS:O	19:F:197:GLU:HG3	2.02	0.59
3:D:269:ALA:HB2	18:E:258:MET:SD	2.43	0.59
19:F:235:LEU:HD22	20:F:501:ADP:H2'	1.84	0.59
5:W:159:VAL:HG23	5:W:160:LYS:HD3	1.83	0.59
6:X:379:ASP:HB2	7:Y:312:ARG:HH21	1.67	0.59
14:U:31:VAL:HG23	14:U:38:ILE:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:103:SER:O	4:V:107:ARG:HB2	2.03	0.59
4:V:353:LEU:HD12	4:V:357:LEU:HD11	1.84	0.59
4:V:333:ILE:O	4:V:337:LEU:HG	2.02	0.58
4:V:451:ILE:HA	4:V:458:VAL:HA	1.84	0.58
10:b:11:ASP:H	10:b:29:GLN:HE22	1.51	0.58
14:U:141:CYS:HB3	14:U:150:ALA:HB2	1.85	0.58
1:f:69:GLU:OE1	1:f:69:GLU:N	2.27	0.58
2:C:230:MET:HG2	17:B:173:VAL:HG11	1.85	0.58
19:F:359:GLU:N	19:F:359:GLU:OE1	2.35	0.58
7:Y:387:ILE:HD13	8:Z:276:ILE:HD12	1.85	0.58
2:C:80:MET:HE3	2:C:80:MET:HA	1.84	0.58
7:Y:52:PRO:O	7:Y:55:GLU:HG2	2.04	0.58
14:U:321:GLN:O	14:U:325:MET:HG3	2.03	0.58
14:U:786:THR:HG23	14:U:786:THR:O	2.02	0.58
15:c:138:GLU:HG2	15:c:139:ARG:HG2	1.86	0.58
17:B:123:VAL:HG21	17:B:152:LEU:HD21	1.85	0.58
3:D:233:SER:OG	18:E:259:GLU:OE1	2.20	0.58
7:Y:97:GLU:O	7:Y:99:GLU:N	2.36	0.58
11:d:193:GLY:O	11:d:197:LEU:HD12	2.03	0.58
4:V:344:ASP:OD2	4:V:344:ASP:N	2.34	0.58
8:Z:180:LYS:NZ	8:Z:181:ASP:O	2.36	0.58
16:A:365:GLU:HG3	16:A:367:ASP:H	1.69	0.58
18:E:138:LEU:H	18:E:138:LEU:HD12	1.69	0.58
3:D:173:GLN:HE22	3:D:334:PRO:HD2	1.66	0.58
8:Z:243:GLN:OE1	8:Z:247:LYS:NZ	2.36	0.58
14:U:103:LYS:HD2	14:U:103:LYS:O	2.04	0.58
18:E:75:ASN:OD1	18:E:77:PRO:HD2	2.04	0.58
2:C:324:ALA:O	2:C:328:ILE:HG13	2.04	0.58
2:C:368:MET:HE3	2:C:368:MET:HA	1.86	0.58
7:Y:383:LEU:HD23	8:Z:272:LEU:HD13	1.85	0.58
17:B:343:ARG:HG2	17:B:346:ARG:HB2	1.85	0.58
19:F:367:GLN:HG2	19:F:381:TYR:CD2	2.38	0.58
6:X:354:ILE:HG23	6:X:356:LEU:HG	1.85	0.58
7:Y:246:ILE:O	7:Y:250:LEU:HG	2.03	0.58
11:d:219:ASP:HB2	11:d:226:ILE:HD13	1.85	0.58
14:U:46:GLU:O	14:U:50:GLU:HG2	2.03	0.58
14:U:213:PHE:HA	14:U:216:VAL:HG12	1.85	0.58
14:U:423:MET:HE3	14:U:423:MET:HA	1.86	0.58
2:C:142:LYS:HG3	2:C:142:LYS:O	2.04	0.58
10:b:165:GLY:O	10:b:167:GLY:N	2.34	0.58
2:C:325:ARG:O	2:C:329:LEU:HG	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:408:ARG:HH11	4:V:408:ARG:HA	1.69	0.57
2:C:222:LYS:HG3	2:C:223:PHE:CD2	2.38	0.57
4:V:296:LYS:HB3	4:V:301:GLU:HB2	1.86	0.57
11:d:208:PHE:HE2	11:d:229:PRO:HB2	1.68	0.57
14:U:567:ILE:HD12	14:U:586:VAL:HG23	1.86	0.57
15:c:25:VAL:HG23	15:c:175:ARG:HG2	1.86	0.57
17:B:112:LEU:HD22	17:B:144:LEU:HD12	1.86	0.57
5:W:214:PHE:HE1	5:W:222:LEU:HB2	1.69	0.57
14:U:218:GLN:O	14:U:222:PHE:HD1	1.87	0.57
19:F:289:ASP:OD1	19:F:289:ASP:N	2.35	0.57
2:C:340:ARG:HD2	7:Y:204:THR:HA	1.86	0.57
2:C:372:ARG:NH2	3:D:175:GLN:OE1	2.38	0.57
3:D:179:GLU:HA	3:D:183:LEU:HB3	1.86	0.57
5:W:199:TYR:O	5:W:203:GLN:HG2	2.04	0.57
17:B:197:ILE:HG21	17:B:235:LEU:HD11	1.85	0.57
2:C:189:TYR:CZ	2:C:316:GLU:HB2	2.40	0.57
4:V:366:ALA:HB2	4:V:374:LYS:HZ2	1.70	0.57
4:V:457:TYR:CD2	7:Y:350:VAL:HG21	2.39	0.57
5:W:259:GLU:HB3	5:W:262:LYS:HG2	1.86	0.57
7:Y:279:GLU:OE2	12:e:53:SER:OG	2.22	0.57
9:a:219:HIS:CD2	9:a:222:LEU:HD12	2.39	0.57
14:U:603:LEU:O	14:U:607:VAL:HG22	2.04	0.57
17:B:200:SER:HB3	17:B:349:ARG:NH1	2.19	0.57
19:F:410:ARG:HD2	19:F:412:ALA:H	1.70	0.57
2:C:369:TYR:HE2	2:C:385:MET:HB3	1.69	0.57
6:X:85:ALA:O	6:X:89:VAL:HG12	2.05	0.57
9:a:21:VAL:HA	9:a:24:ARG:HG3	1.87	0.57
16:A:178:GLY:O	21:A:501:ATP:N6	2.38	0.57
11:d:282:ILE:HG23	11:d:283:LEU:N	2.20	0.57
17:B:232:LYS:NZ	21:B:501:ATP:O2B	2.28	0.57
18:E:376:ASP:HA	18:E:379:LYS:HE2	1.85	0.57
6:X:377:ILE:HG23	7:Y:312:ARG:NH1	2.19	0.57
17:B:380:LEU:HA	17:B:383:LEU:HD12	1.86	0.57
19:F:286:ASP:OD2	19:F:287:GLU:N	2.38	0.57
17:B:196:GLU:HG3	17:B:349:ARG:NH1	2.19	0.57
2:C:90:HIS:CE1	2:C:92:GLU:HB2	2.40	0.56
9:a:71:VAL:O	9:a:71:VAL:HG12	2.05	0.56
11:d:268:ARG:HH21	11:d:292:PHE:HB3	1.69	0.56
2:C:219:LEU:HD11	3:D:289:LEU:HD23	1.86	0.56
3:D:225:ALA:HB1	3:D:259:PRO:O	2.05	0.56
5:W:121:LYS:O	5:W:125:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:287:ALA:O	11:d:291:LEU:HG	2.04	0.56
16:A:182:GLU:O	16:A:186:LYS:HG3	2.05	0.56
16:A:354:ILE:HG23	16:A:385:ILE:HG21	1.87	0.56
5:W:35:ALA:HB2	5:W:43:VAL:HG21	1.86	0.56
5:W:312:MET:HE3	5:W:365:ILE:HD13	1.86	0.56
6:X:260:MET:HE3	6:X:260:MET:O	2.05	0.56
7:Y:81:LEU:HD12	7:Y:110:TYR:HE2	1.69	0.56
18:E:203:ILE:HD11	18:E:238:ILE:HG13	1.87	0.56
18:E:215:ILE:HD13	18:E:260:LEU:HB2	1.87	0.56
19:F:410:ARG:NH2	19:F:419:ASP:OD2	2.38	0.56
3:D:189:GLU:N	3:D:189:GLU:OE1	2.37	0.56
5:W:130:MET:SD	5:W:131:VAL:N	2.79	0.56
7:Y:336:ARG:HH22	12:e:44:ASP:HB3	1.70	0.56
10:b:125:VAL:O	10:b:129:LYS:HG2	2.05	0.56
14:U:325:MET:O	14:U:329:LEU:HG	2.06	0.56
8:Z:190:ARG:HG2	8:Z:190:ARG:HH11	1.71	0.56
11:d:94:MET:HG2	11:d:119:LEU:HD13	1.87	0.56
14:U:54:PHE:HD1	14:U:56:SER:H	1.53	0.56
18:E:165:ILE:HD12	18:E:166:PRO:HD2	1.86	0.56
14:U:15:ASP:OD1	14:U:15:ASP:N	2.37	0.56
14:U:208:LEU:HD23	14:U:210:LYS:H	1.70	0.56
14:U:69:TYR:CD1	14:U:99:THR:HG21	2.40	0.56
18:E:97:ARG:HH12	18:E:114:GLU:HB3	1.71	0.56
19:F:341:ALA:O	19:F:347:ARG:NH1	2.38	0.56
3:D:71:GLU:HG2	14:U:644:TYR:CZ	2.40	0.56
4:V:289:LEU:HB3	4:V:312:ALA:HB2	1.88	0.56
4:V:482:PHE:CE2	7:Y:377:LEU:HD22	2.41	0.56
4:V:63:SER:O	4:V:66:GLU:HG3	2.05	0.56
5:W:270:VAL:HG12	5:W:290:ILE:HD12	1.88	0.56
7:Y:29:PRO:HA	7:Y:32:ARG:HH21	1.71	0.56
7:Y:208:PHE:CE2	7:Y:210:SER:O	2.59	0.56
14:U:713:TYR:O	14:U:717:ILE:HG22	2.06	0.56
19:F:141:ASP:OD1	19:F:141:ASP:N	2.38	0.56
2:C:71:SER:OG	2:C:72:TYR:N	2.39	0.56
4:V:119:GLY:HA3	4:V:149:PRO:HD2	1.88	0.56
14:U:596:ASN:OD1	14:U:597:LYS:N	2.39	0.56
16:A:85:GLN:HG3	17:B:136:LEU:HD22	1.87	0.56
16:A:387:SER:O	16:A:391:GLU:HG2	2.06	0.56
3:D:163:MET:HA	3:D:222:HIS:HE1	1.71	0.55
3:D:183:LEU:HG	3:D:191:TYR:HE2	1.71	0.55
4:V:114:TYR:CD1	4:V:138:PRO:HD3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:84:LYS:O	6:X:88:LEU:HD12	2.06	0.55
5:W:306:LEU:O	5:W:310:THR:HG22	2.07	0.55
5:W:29:PRO:O	5:W:33:LYS:HG2	2.05	0.55
5:W:373:ILE:HD11	5:W:377:ARG:HB2	1.87	0.55
7:Y:41:LEU:O	7:Y:45:VAL:HG22	2.07	0.55
11:d:203:ASN:HB2	11:d:266:THR:HG21	1.89	0.55
11:d:293:PHE:HA	11:d:298:LYS:HE2	1.88	0.55
14:U:62:LEU:HD22	14:U:87:LEU:HB3	1.86	0.55
2:C:296:ASN:OD1	2:C:297:ARG:HG3	2.06	0.55
3:D:374:ASP:O	3:D:378:ILE:HG13	2.06	0.55
4:V:425:LYS:O	4:V:427:GLN:NE2	2.40	0.55
8:Z:96:HIS:HD2	8:Z:121:LEU:HD11	1.72	0.55
9:a:77:VAL:O	9:a:81:LEU:HG	2.05	0.55
7:Y:11:LEU:HD21	7:Y:142:PHE:HD2	1.71	0.55
7:Y:22:LEU:HD13	7:Y:41:LEU:HB2	1.88	0.55
7:Y:261:PHE:O	7:Y:265:GLU:HG2	2.06	0.55
11:d:130:PRO:HD2	11:d:178:TYR:CZ	2.40	0.55
14:U:164:GLU:OE2	14:U:204:ILE:HD11	2.06	0.55
14:U:166:THR:O	14:U:170:SER:OG	2.22	0.55
2:C:329:LEU:HD23	2:C:359:VAL:HG13	1.89	0.55
3:D:259:PRO:HB3	3:D:304:ASN:HB2	1.89	0.55
3:D:368:ASP:OD1	3:D:409:LYS:NZ	2.29	0.55
4:V:108:LEU:HD13	4:V:113:LEU:HD11	1.87	0.55
7:Y:101:ARG:O	7:Y:105:MET:HG3	2.07	0.55
16:A:198:PRO:O	16:A:202:VAL:HG23	2.06	0.55
6:X:133:LEU:HD12	6:X:136:LEU:HD11	1.87	0.55
6:X:194:ARG:HE	6:X:210:LEU:HD21	1.70	0.55
14:U:169:GLU:N	14:U:169:GLU:OE2	2.39	0.55
16:A:351:ARG:O	16:A:354:ILE:HG22	2.07	0.55
19:F:279:ALA:HB3	19:F:280:PRO:HD3	1.89	0.55
19:F:369:HIS:ND1	19:F:397:LYS:HB2	2.22	0.55
5:W:135:LYS:HG2	5:W:137:TYR:CZ	2.42	0.55
9:a:287:ASN:OD1	9:a:288:HIS:N	2.39	0.55
11:d:115:GLU:HA	11:d:118:ARG:HG2	1.89	0.55
1:f:58:LYS:HE2	1:f:62:GLN:HE21	1.71	0.55
2:C:248:MET:HE3	2:C:248:MET:HA	1.89	0.55
11:d:252:PRO:HG2	11:d:256:TYR:HE1	1.72	0.55
17:B:281:ILE:HG13	17:B:281:ILE:O	2.06	0.55
18:E:247:THR:O	18:E:251:ARG:HG3	2.07	0.55
4:V:120:PHE:O	4:V:150:ARG:NE	2.38	0.55
7:Y:275:LEU:HA	7:Y:278:VAL:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:248:LYS:HA	17:B:260:LEU:HD12	1.88	0.55
19:F:405:MET:HE2	19:F:405:MET:HA	1.88	0.55
7:Y:50:MET:HB3	7:Y:53:TYR:HB3	1.89	0.54
14:U:764:LEU:O	14:U:767:THR:OG1	2.24	0.54
15:c:225:TRP:H	15:c:225:TRP:CD1	2.24	0.54
4:V:117:VAL:O	4:V:128:ARG:NH2	2.39	0.54
5:W:141:GLU:OE1	5:W:141:GLU:N	2.39	0.54
7:Y:90:ASP:HA	7:Y:93:LYS:HD2	1.88	0.54
9:a:16:PRO:C	9:a:18:GLN:H	2.15	0.54
17:B:405:MET:SD	17:B:421:LYS:HD2	2.47	0.54
18:E:116:ASP:HB3	18:E:119:VAL:HG22	1.90	0.54
16:A:243:SER:HB2	17:B:311:GLU:OE2	2.07	0.54
18:E:380:LEU:HD12	18:E:380:LEU:H	1.71	0.54
2:C:341:GLY:N	7:Y:207:THR:HG23	2.22	0.54
4:V:190:ASP:O	4:V:194:LYS:HG2	2.08	0.54
6:X:281:GLY:H	6:X:284:THR:HB	1.72	0.54
7:Y:282:MET:HE1	7:Y:295:TYR:CD2	2.42	0.54
14:U:391:GLU:OE2	14:U:391:GLU:N	2.40	0.54
14:U:564:ASP:O	14:U:568:GLU:HG2	2.07	0.54
4:V:345:ARG:HD3	12:e:43:TRP:CZ3	2.42	0.54
19:F:258:GLN:HB2	19:F:263:ASP:HB3	1.88	0.54
5:W:270:VAL:O	5:W:274:VAL:HG12	2.07	0.54
6:X:47:GLU:HA	6:X:50:ILE:HG22	1.89	0.54
6:X:142:ARG:NH1	6:X:143:TYR:H	2.06	0.54
8:Z:131:LEU:HG	15:c:222:LYS:NZ	2.22	0.54
2:C:96:VAL:HG11	17:B:107:MET:HE2	1.89	0.54
9:a:226:ARG:HH22	9:a:230:ARG:NE	2.06	0.54
9:a:235:ASP:HB3	9:a:251:LEU:HD21	1.90	0.54
14:U:446:LEU:HD21	14:U:457:ILE:HD12	1.88	0.54
19:F:111:ILE:HG12	19:F:114:ASP:H	1.72	0.54
19:F:256:LEU:HD13	19:F:268:VAL:HG22	1.88	0.54
2:C:186:VAL:HB	2:C:292:ILE:HG12	1.90	0.54
3:D:163:MET:HE1	3:D:221:HIS:HE1	1.73	0.54
5:W:374:THR:HG23	9:a:327:VAL:HG22	1.90	0.54
6:X:421:LEU:HD11	8:Z:279:LYS:HB3	1.89	0.54
14:U:172:ASP:O	14:U:176:MET:HG2	2.08	0.54
14:U:900:TYR:HB3	14:U:914:LEU:HD21	1.87	0.54
16:A:307:ASP:HB3	16:A:336:ARG:HE	1.73	0.54
19:F:281:SER:HB2	19:F:326:VAL:HG12	1.90	0.54
4:V:248:ALA:O	4:V:252:ASN:ND2	2.37	0.54
7:Y:85:ASP:OD2	7:Y:107:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:245:GLU:O	7:Y:249:VAL:HG22	2.07	0.54
14:U:757:MET:HA	14:U:760:VAL:HG22	1.90	0.54
2:C:161:ILE:HD13	2:C:188:LEU:HD21	1.90	0.54
7:Y:153:ASP:O	7:Y:157:ILE:HG12	2.07	0.54
14:U:458:ILE:HG12	14:U:485:ALA:HB2	1.90	0.54
4:V:118:GLN:HA	4:V:128:ARG:HH22	1.73	0.53
11:d:169:ALA:HB1	14:U:7:GLY:HA3	1.89	0.53
11:d:282:ILE:O	11:d:283:LEU:CB	2.55	0.53
11:d:302:TYR:HA	11:d:305:LYS:HZ3	1.73	0.53
14:U:66:LYS:HA	14:U:96:TYR:CE2	2.43	0.53
14:U:596:ASN:O	14:U:600:ARG:HG3	2.08	0.53
17:B:374:LEU:HD22	17:B:378:VAL:HG11	1.91	0.53
18:E:76:GLY:H	18:E:77:PRO:HD2	1.72	0.53
2:C:143:VAL:HG21	2:C:211:PHE:CD2	2.41	0.53
3:D:335:LEU:HD23	3:D:369:LYS:HB3	1.91	0.53
17:B:115:ILE:HD11	17:B:144:LEU:HB3	1.90	0.53
17:B:337:LEU:HD12	17:B:341:LEU:HD23	1.91	0.53
4:V:264:TYR:CZ	11:d:210:THR:HB	2.43	0.53
6:X:363:ARG:NH1	6:X:367:GLN:HB2	2.20	0.53
11:d:133:GLY:HA2	11:d:178:TYR:HD1	1.73	0.53
11:d:288:THR:OG1	11:d:293:PHE:O	2.26	0.53
16:A:398:ARG:NH2	17:B:196:GLU:OE1	2.37	0.53
17:B:338:ASP:OD1	17:B:339:PRO:HD2	2.09	0.53
2:C:90:HIS:HB2	2:C:91:PRO:CD	2.38	0.53
3:D:41:TYR:OH	14:U:156:GLU:OE2	2.21	0.53
8:Z:149:THR:HG23	9:a:178:ARG:HA	1.91	0.53
5:W:241:LEU:HD11	5:W:282:GLU:HG2	1.90	0.53
5:W:392:PHE:O	5:W:396:LEU:HG	2.08	0.53
6:X:167:VAL:HG21	6:X:197:ALA:HB2	1.91	0.53
7:Y:208:PHE:CD2	7:Y:211:TYR:HA	2.44	0.53
14:U:21:GLU:OE1	14:U:21:GLU:N	2.39	0.53
14:U:742:HIS:HB3	14:U:883:ARG:HH21	1.74	0.53
14:U:878:LEU:HD12	14:U:882:ALA:HB1	1.90	0.53
2:C:175:PHE:HB3	2:C:180:ILE:HB	1.91	0.53
3:D:315:ASP:OD2	3:D:316:THR:N	2.41	0.53
14:U:64:ALA:O	14:U:67:VAL:HG22	2.08	0.53
9:a:194:GLN:HB2	9:a:225:LEU:HD12	1.91	0.53
11:d:177:ASP:HB2	14:U:2:ILE:HG22	1.91	0.53
11:d:188:MET:HG3	11:d:189:HIS:CD2	2.43	0.53
2:C:346:LYS:O	2:C:349:GLU:HG2	2.09	0.53
6:X:212:MET:HE2	6:X:246:LYS:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:186:LEU:HA	7:Y:222:TYR:OH	2.09	0.53
10:b:115:SER:OG	10:b:116:PRO:HD2	2.09	0.53
11:d:83:THR:O	11:d:87:VAL:HG13	2.07	0.53
14:U:185:MET:HE2	14:U:185:MET:HA	1.91	0.53
6:X:74:ARG:HH12	6:X:77:LEU:HD22	1.74	0.53
7:Y:138:LEU:HD12	7:Y:176:ARG:HG2	1.91	0.53
16:A:248:LYS:HE2	16:A:249:TYR:CZ	2.44	0.53
17:B:292:THR:HG21	17:B:333:ARG:HH22	1.73	0.53
19:F:399:VAL:HA	19:F:427:VAL:HG21	1.91	0.53
4:V:90:GLU:HG2	4:V:93:PHE:CZ	2.44	0.53
6:X:91:SER:O	6:X:95:LEU:HG	2.09	0.53
16:A:190:VAL:HG11	16:A:212:VAL:HG13	1.91	0.53
17:B:380:LEU:O	17:B:384:ILE:HG23	2.09	0.53
18:E:306:GLU:HG3	18:E:332:VAL:HG11	1.90	0.53
4:V:67:LEU:O	4:V:71:THR:HG23	2.10	0.52
7:Y:208:PHE:CZ	7:Y:210:SER:O	2.61	0.52
14:U:788:VAL:HG12	14:U:884:VAL:HG21	1.91	0.52
16:A:143:ASP:OD2	16:A:148:GLN:N	2.41	0.52
19:F:201:ALA:HB2	19:F:350:ARG:HH21	1.74	0.52
19:F:205:PRO:HA	19:F:212:PHE:CE1	2.44	0.52
1:f:43:TYR:CE1	1:f:64:LEU:HD21	2.44	0.52
4:V:454:GLU:OE1	11:d:283:LEU:HA	2.09	0.52
5:W:178:GLU:O	5:W:182:ARG:HG3	2.09	0.52
9:a:65:SER:C	9:a:69:HIS:HB3	2.34	0.52
9:a:89:ASP:HB2	9:a:92:VAL:HG12	1.91	0.52
14:U:563:ALA:O	14:U:567:ILE:HG12	2.09	0.52
14:U:793:LYS:NZ	14:U:914:LEU:O	2.37	0.52
4:V:306:ARG:O	4:V:310:THR:HG23	2.08	0.52
5:W:29:PRO:O	5:W:33:LYS:NZ	2.38	0.52
7:Y:174:TRP:CG	7:Y:177:ARG:HD2	2.43	0.52
9:a:80:ILE:HG21	9:a:100:THR:HG21	1.91	0.52
9:a:245:VAL:O	9:a:249:GLN:HG2	2.09	0.52
4:V:326:GLN:O	4:V:330:LYS:HG2	2.09	0.52
5:W:408:ARG:HH12	6:X:349:HIS:CG	2.27	0.52
15:c:206:ASN:OD1	15:c:207:TYR:N	2.42	0.52
5:W:179:LYS:O	5:W:183:VAL:HG13	2.08	0.52
9:a:127:ASP:O	9:a:131:THR:OG1	2.26	0.52
11:d:256:TYR:O	11:d:260:ILE:HG12	2.09	0.52
14:U:246:TYR:CD2	14:U:795:LEU:HD21	2.44	0.52
16:A:346:PRO:HD2	16:A:351:ARG:HH12	1.74	0.52
19:F:79:LYS:HA	19:F:82:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:105:MET:HE1	7:Y:136:HIS:HB3	1.90	0.52
10:b:22:LEU:HD11	10:b:179:LEU:HA	1.91	0.52
11:d:142:ILE:HG23	11:d:182:LEU:HD11	1.91	0.52
17:B:255:LEU:HB2	17:B:290:ILE:HD12	1.90	0.52
2:C:113:ARG:NH1	3:D:94:GLU:OE2	2.43	0.52
2:C:231:VAL:HG13	2:C:232:ARG:HG3	1.92	0.52
2:C:347:ILE:HD12	2:C:383:PHE:HB3	1.91	0.52
4:V:449:ALA:HA	4:V:461:LYS:H	1.75	0.52
11:d:155:SER:HA	11:d:158:ARG:HB2	1.92	0.52
3:D:154:LEU:HD23	3:D:158:GLN:HB2	1.92	0.52
5:W:346:GLU:HG3	5:W:350:ARG:NH1	2.24	0.52
10:b:116:PRO:HD3	10:b:146:GLU:HG2	1.91	0.52
10:b:101:GLN:HE22	15:c:101:GLN:CD	2.18	0.52
17:B:372:MET:HE1	17:B:399:CYS:O	2.09	0.52
3:D:385:LEU:HD11	3:D:401:LYS:HG2	1.92	0.52
6:X:116:TRP:O	6:X:120:GLU:HG2	2.10	0.52
6:X:172:LEU:O	6:X:176:THR:HG23	2.09	0.52
7:Y:145:LEU:O	7:Y:149:LEU:HG	2.10	0.51
8:Z:19:VAL:HG21	8:Z:124:ILE:HD12	1.92	0.51
8:Z:272:LEU:O	8:Z:276:ILE:HG12	2.09	0.51
10:b:128:ALA:HB2	10:b:156:PHE:CD1	2.45	0.51
10:b:147:GLU:O	10:b:149:ASN:N	2.43	0.51
11:d:295:THR:HB	11:d:298:LYS:HB3	1.92	0.51
14:U:27:LEU:HA	14:U:30:VAL:HG12	1.92	0.51
17:B:222:VAL:HA	17:B:349:ARG:HB2	1.91	0.51
2:C:125:LYS:NZ	2:C:126:ILE:O	2.43	0.51
3:D:122:GLU:OE2	15:c:282:ARG:NH2	2.26	0.51
4:V:356:SER:HB2	12:e:25:GLU:HB3	1.91	0.51
8:Z:104:ASN:O	8:Z:108:ILE:HG12	2.09	0.51
9:a:184:ASP:OD1	9:a:184:ASP:N	2.43	0.51
2:C:340:ARG:C	7:Y:207:THR:CG2	2.83	0.51
2:C:340:ARG:NH1	7:Y:203:ASP:OD2	2.44	0.51
5:W:230:MET:HE3	5:W:230:MET:HA	1.92	0.51
7:Y:185:GLY:HA3	7:Y:201:PHE:CZ	2.45	0.51
16:A:192:GLU:OE2	16:A:232:ARG:HG2	2.10	0.51
5:W:443:THR:HG21	8:Z:204:LYS:HD2	1.93	0.51
11:d:137:THR:HG22	11:d:139:GLN:HB2	1.91	0.51
5:W:260:SER:HA	5:W:263:TRP:NE1	2.26	0.51
7:Y:112:CYS:HG	7:Y:143:TYR:HE1	1.58	0.51
8:Z:81:MET:HE1	15:c:98:MET:HG3	1.91	0.51
11:d:209:HIS:NE2	11:d:233:GLU:OE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:376:MET:HG3	14:U:738:ASP:O	2.10	0.51
14:U:421:GLN:N	14:U:421:GLN:OE1	2.43	0.51
14:U:516:LEU:HD13	14:U:532:MET:HE1	1.92	0.51
7:Y:304:TYR:HA	7:Y:323:PHE:CZ	2.45	0.51
11:d:124:LEU:HD21	14:U:19:LEU:HD23	1.93	0.51
11:d:124:LEU:HD11	14:U:19:LEU:HG	1.91	0.51
11:d:240:SER:HB2	11:d:243:LYS:HZ3	1.76	0.51
17:B:182:GLU:OE1	17:B:237:LYS:HB3	2.10	0.51
19:F:226:TYR:CZ	19:F:353:GLU:HB2	2.45	0.51
2:C:368:MET:O	2:C:372:ARG:HG3	2.10	0.51
6:X:357:SER:OG	6:X:358:LYS:N	2.42	0.51
9:a:20:ALA:O	9:a:24:ARG:HG2	2.11	0.51
11:d:279:TYR:HD1	11:d:284:PHE:HD2	1.58	0.51
14:U:109:THR:O	14:U:113:VAL:HG23	2.11	0.51
15:c:255:TYR:O	15:c:259:VAL:HG12	2.10	0.51
16:A:383:ALA:HB1	17:B:344:PRO:HB2	1.93	0.51
2:C:232:ARG:HB3	2:C:235:PHE:HB2	1.93	0.51
2:C:273:MET:HE1	2:C:291:VAL:HG23	1.93	0.51
4:V:127:THR:O	4:V:131:LEU:HG	2.11	0.51
8:Z:13:PRO:HB3	15:c:220:LEU:HD11	1.92	0.51
3:D:179:GLU:O	3:D:191:TYR:OH	2.28	0.51
7:Y:348:ASP:O	7:Y:352:GLU:N	2.42	0.51
15:c:36:LEU:HD11	15:c:40:LYS:HE3	1.93	0.51
15:c:251:LEU:HD21	15:c:283:HIS:HB3	1.93	0.51
17:B:204:PRO:HD3	17:B:211:TYR:CZ	2.45	0.51
2:C:246:ILE:HB	2:C:291:VAL:HG12	1.93	0.51
5:W:202:THR:HA	5:W:205:ILE:HG22	1.92	0.51
7:Y:101:ARG:HG3	7:Y:105:MET:HE3	1.91	0.51
7:Y:157:ILE:HG13	7:Y:187:TYR:CE1	2.46	0.51
7:Y:177:ARG:O	7:Y:181:LYS:HG2	2.11	0.51
8:Z:192:THR:HG23	8:Z:193:ASN:OD1	2.11	0.51
11:d:172:LYS:NZ	11:d:211:GLU:OE1	2.43	0.51
11:d:208:PHE:CE2	11:d:229:PRO:HB2	2.46	0.51
14:U:456:ASP:N	14:U:456:ASP:OD1	2.44	0.51
1:f:51:GLU:O	1:f:85:LEU:N	2.44	0.50
6:X:51:LEU:HD21	6:X:88:LEU:HG	1.93	0.50
7:Y:138:LEU:HD22	7:Y:167:LEU:HD23	1.93	0.50
7:Y:215:ASP:OD1	7:Y:216:TYR:N	2.45	0.50
8:Z:178:ASP:OD1	8:Z:179:ILE:N	2.43	0.50
14:U:320:ASP:OD1	14:U:321:GLN:N	2.44	0.50
17:B:235:LEU:O	17:B:239:VAL:HG23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:E:148:VAL:HG13	18:E:149:ILE:HG23	1.93	0.50
2:C:60:ARG:NH2	3:D:71:GLU:OE2	2.44	0.50
14:U:807:LYS:HD2	14:U:872:GLU:HB3	1.91	0.50
4:V:139:MET:HE3	4:V:139:MET:HA	1.93	0.50
10:b:19:GLY:HA2	10:b:24:THR:HA	1.94	0.50
3:D:115:ILE:HG22	3:D:139:LEU:HD12	1.91	0.50
4:V:159:LEU:HD23	4:V:159:LEU:H	1.76	0.50
9:a:226:ARG:HH12	9:a:230:ARG:CZ	2.24	0.50
11:d:279:TYR:CD1	11:d:284:PHE:HB3	2.46	0.50
17:B:373:THR:HG23	17:B:414:VAL:HG12	1.92	0.50
9:a:79:ILE:O	9:a:83:VAL:HG13	2.12	0.50
10:b:4:GLU:N	10:b:47:ASN:OD1	2.41	0.50
16:A:368:ILE:HG12	16:A:406:GLU:CD	2.37	0.50
17:B:406:ALA:HB2	17:B:414:VAL:HG23	1.94	0.50
19:F:251:LEU:HD23	19:F:252:ALA:N	2.27	0.50
5:W:456:GLN:OE1	5:W:456:GLN:N	2.44	0.50
7:Y:29:PRO:HA	7:Y:32:ARG:HE	1.76	0.50
17:B:358:GLU:HA	17:B:361:LYS:HD2	1.94	0.50
6:X:62:GLN:HB3	6:X:65:GLU:HB2	1.94	0.50
2:C:271:ARG:O	2:C:275:GLU:HG3	2.12	0.50
18:E:244:SER:HB3	19:F:300:LYS:HA	1.93	0.50
3:D:381:GLU:OE2	18:E:297:ARG:NH1	2.43	0.50
16:A:371:GLU:H	16:A:371:GLU:CD	2.19	0.50
17:B:394:ASP:O	17:B:398:ILE:HG12	2.12	0.50
2:C:36:ASN:HB3	4:V:89:LYS:CD	2.42	0.49
4:V:267:ALA:O	4:V:271:VAL:HG13	2.12	0.49
5:W:42:GLU:H	5:W:42:GLU:CD	2.20	0.49
6:X:132:ARG:HD2	6:X:135:SER:OG	2.12	0.49
14:U:49:TYR:CD1	14:U:61:ALA:HB2	2.47	0.49
14:U:427:LEU:HD22	14:U:442:GLY:HA3	1.94	0.49
16:A:215:PHE:CE2	19:F:431:LYS:HE2	2.47	0.49
18:E:178:THR:N	21:E:401:ATP:O2B	2.45	0.49
3:D:230:VAL:HG23	3:D:264:ILE:HG23	1.94	0.49
3:D:380:GLN:NE2	18:E:165:ILE:O	2.45	0.49
4:V:180:ARG:NH2	4:V:183:GLU:OE1	2.45	0.49
4:V:394:LEU:HD23	4:V:397:ARG:NH2	2.27	0.49
5:W:182:ARG:HG2	5:W:182:ARG:HH11	1.77	0.49
7:Y:117:LYS:HD3	7:Y:151:TYR:CE2	2.47	0.49
14:U:901:GLN:NE2	14:U:902:PRO:HD2	2.27	0.49
18:E:313:LEU:HD22	18:E:328:TYR:HD1	1.78	0.49
2:C:330:LYS:O	2:C:334:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:182:ARG:O	5:W:186:ILE:HG12	2.12	0.49
10:b:181:ASP:OD1	10:b:182:ALA:N	2.46	0.49
16:A:73:ALA:HB3	16:A:78:TRP:CD1	2.47	0.49
17:B:103:ARG:HE	17:B:160:ILE:HG22	1.78	0.49
8:Z:23:PHE:CD2	8:Z:126:VAL:HG11	2.47	0.49
2:C:136:SER:O	2:C:140:VAL:HG23	2.11	0.49
4:V:393:THR:O	4:V:397:ARG:HG3	2.12	0.49
4:V:451:ILE:HG23	11:d:279:TYR:CD2	2.47	0.49
9:a:255:TRP:CD1	9:a:255:TRP:C	2.90	0.49
11:d:126:LEU:HD13	11:d:140:GLN:HB3	1.94	0.49
14:U:62:LEU:O	14:U:66:LYS:HG3	2.13	0.49
17:B:245:ALA:HB1	17:B:279:PRO:O	2.12	0.49
18:E:313:LEU:HD22	18:E:328:TYR:CD1	2.47	0.49
5:W:278:PRO:HG3	5:W:357:ARG:NH2	2.26	0.49
7:Y:12:PRO:HG2	7:Y:143:TYR:HE2	1.77	0.49
10:b:184:ILE:HD12	10:b:188:ILE:HG21	1.95	0.49
14:U:789:ILE:HG12	14:U:881:PRO:HB3	1.94	0.49
8:Z:131:LEU:HG	15:c:222:LYS:HZ2	1.75	0.49
9:a:34:TRP:CZ3	9:a:67:PHE:HB2	2.47	0.49
9:a:188:LEU:O	9:a:193:GLN:NE2	2.46	0.49
16:A:154:PRO:HG3	17:B:116:ILE:HD13	1.94	0.49
16:A:401:ARG:NH2	16:A:408:ASP:OD2	2.45	0.49
4:V:417:ILE:HG23	4:V:422:ILE:HD11	1.94	0.49
5:W:55:ARG:HD2	5:W:94:ARG:O	2.12	0.49
6:X:317:PRO:O	6:X:321:THR:HG23	2.13	0.49
11:d:281:LYS:O	11:d:282:ILE:HG22	2.13	0.49
17:B:99:VAL:HG22	17:B:138:PHE:CE2	2.48	0.49
4:V:323:GLY:O	4:V:327:THR:HG22	2.12	0.49
5:W:125:ILE:HG23	5:W:145:LEU:CD1	2.43	0.49
7:Y:110:TYR:HA	7:Y:113:ARG:HB3	1.94	0.49
7:Y:285:ASP:OD1	7:Y:286:TRP:N	2.45	0.49
14:U:2:ILE:HG12	14:U:3:THR:H	1.78	0.49
14:U:115:ASN:ND2	14:U:123:LYS:HD2	2.28	0.49
15:c:189:ILE:HD12	15:c:189:ILE:H	1.78	0.49
17:B:233:THR:HG22	17:B:237:LYS:NZ	2.27	0.49
2:C:69:GLN:HA	3:D:136:SER:HB3	1.93	0.49
6:X:300:ALA:O	6:X:304:LYS:HG2	2.13	0.49
7:Y:208:PHE:CZ	7:Y:214:MET:HG2	2.48	0.49
8:Z:55:ALA:HB3	15:c:102:THR:HG21	1.94	0.49
8:Z:72:HIS:O	8:Z:76:GLU:HG3	2.13	0.49
9:a:141:MET:SD	9:a:141:MET:N	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:212:ASN:HD21	9:a:215:GLU:HG3	1.78	0.49
11:d:104:ARG:HH22	11:d:108:ASN:H	1.60	0.49
11:d:137:THR:HB	11:d:140:GLN:HG3	1.94	0.49
2:C:339:THR:H	2:C:378:VAL:H	1.59	0.48
5:W:131:VAL:HG13	5:W:132:THR:HG23	1.95	0.48
7:Y:148:GLY:O	7:Y:152:MET:N	2.46	0.48
9:a:257:GLN:OE1	9:a:257:GLN:N	2.45	0.48
14:U:798:PRO:O	14:U:880:ASN:ND2	2.46	0.48
14:U:798:PRO:HD2	14:U:880:ASN:HD21	1.78	0.48
18:E:67:GLU:OE2	18:E:85:ARG:NH2	2.42	0.48
4:V:482:PHE:HE2	7:Y:377:LEU:HD22	1.77	0.48
11:d:298:LYS:HG2	11:d:302:TYR:HE2	1.78	0.48
14:U:247:GLN:OE1	14:U:912:ILE:HD12	2.13	0.48
17:B:95:GLU:O	17:B:99:VAL:HG23	2.13	0.48
18:E:331:ILE:HG23	18:E:371:VAL:HG11	1.94	0.48
4:V:264:TYR:HE1	11:d:214:ARG:HE	1.60	0.48
4:V:432:GLU:OE1	4:V:432:GLU:N	2.45	0.48
7:Y:250:LEU:HA	7:Y:253:LEU:HB2	1.95	0.48
14:U:131:GLU:O	14:U:134:VAL:HG12	2.12	0.48
14:U:633:CYS:HB3	14:U:634:PRO:HD3	1.95	0.48
2:C:160:GLU:O	2:C:164:VAL:HG23	2.13	0.48
3:D:85:ILE:HG22	3:D:86:PRO:HD3	1.96	0.48
12:e:41:ASP:O	12:e:42:ASN:HB2	2.13	0.48
19:F:172:VAL:HG23	19:F:267:LEU:HD23	1.95	0.48
4:V:202:ALA:O	4:V:206:VAL:HG22	2.14	0.48
4:V:290:TYR:CD2	4:V:328:VAL:HG22	2.48	0.48
5:W:28:LEU:HD21	5:W:66:ILE:HG22	1.96	0.48
6:X:111:LEU:HA	6:X:114:ILE:HG22	1.95	0.48
7:Y:304:TYR:HA	7:Y:323:PHE:HZ	1.79	0.48
4:V:322:VAL:O	4:V:326:GLN:HG3	2.12	0.48
5:W:159:VAL:HB	5:W:196:VAL:HG12	1.96	0.48
5:W:448:LYS:O	5:W:452:ILE:HG22	2.12	0.48
9:a:180:LEU:HD13	9:a:222:LEU:HD11	1.94	0.48
11:d:167:TYR:O	11:d:171:LEU:CB	2.59	0.48
14:U:24:LEU:HD11	14:U:60:ALA:HA	1.96	0.48
14:U:229:VAL:HA	14:U:232:ILE:HG22	1.94	0.48
1:f:109:GLN:NE2	15:c:125:VAL:HG23	2.28	0.48
2:C:41:ASN:OD1	2:C:44:ARG:NH2	2.44	0.48
3:D:408:LYS:HE2	3:D:408:LYS:HB2	1.76	0.48
17:B:256:ILE:HG23	17:B:298:ASN:HD22	1.79	0.48
7:Y:186:LEU:HD23	7:Y:222:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:173:CYS:SG	14:U:5:ALA:HA	2.54	0.48
15:c:122:LEU:HB2	15:c:200:TYR:CE1	2.49	0.48
18:E:334:LEU:HD23	18:E:334:LEU:HA	1.74	0.48
2:C:76:VAL:HA	2:C:87:VAL:HG12	1.96	0.48
7:Y:70:LEU:HA	7:Y:73:MET:SD	2.54	0.48
11:d:321:GLN:HG3	11:d:324:LYS:HG3	1.95	0.48
16:A:358:HIS:CE1	16:A:386:ARG:HB2	2.49	0.48
17:B:425:ASN:OD1	17:B:426:VAL:HG23	2.13	0.48
1:f:84:LYS:O	1:f:87:GLU:HG3	2.13	0.48
6:X:287:LEU:HA	6:X:287:LEU:HD23	1.65	0.48
7:Y:304:TYR:CD2	7:Y:337:PHE:HE2	2.31	0.48
9:a:122:LYS:HD2	9:a:130:VAL:HB	1.94	0.48
9:a:132:LYS:O	9:a:136:GLU:HG3	2.14	0.48
17:B:313:LEU:HD12	17:B:341:LEU:HD13	1.95	0.48
19:F:180:ARG:HH12	19:F:246:ALA:H	1.62	0.48
2:C:298:ILE:HB	2:C:301:LEU:HD23	1.97	0.47
5:W:304:ASP:O	5:W:307:LYS:HG3	2.13	0.47
6:X:44:GLN:O	6:X:47:GLU:HG3	2.14	0.47
8:Z:74:TYR:OH	15:c:102:THR:OG1	2.31	0.47
8:Z:197:GLY:HA2	15:c:225:TRP:CB	2.44	0.47
15:c:265:MET:HE3	15:c:266:THR:H	1.79	0.47
15:c:291:LEU:O	15:c:295:ASN:ND2	2.47	0.47
19:F:305:GLU:OE2	19:F:308:ARG:NH2	2.42	0.47
19:F:363:ALA:O	19:F:367:GLN:HG3	2.13	0.47
19:F:420:TYR:O	19:F:424:ILE:HG23	2.14	0.47
4:V:221:LEU:HB3	4:V:223:LYS:HE3	1.96	0.47
4:V:431:PRO:O	4:V:435:GLU:HG3	2.13	0.47
6:X:329:ASN:O	6:X:333:GLN:HG3	2.15	0.47
8:Z:16:LEU:HB3	15:c:216:MET:SD	2.54	0.47
10:b:24:THR:HG22	10:b:26:LEU:H	1.79	0.47
11:d:147:ILE:O	11:d:150:ILE:HG13	2.13	0.47
19:F:139:LEU:HD12	19:F:161:LEU:HD23	1.95	0.47
1:f:86:GLN:HA	1:f:90:VAL:HG13	1.96	0.47
11:d:198:PHE:HB2	11:d:259:PHE:CZ	2.49	0.47
16:A:333:ARG:HE	16:A:336:ARG:NH1	2.12	0.47
17:B:223:ILE:HD11	17:B:329:MET:HE3	1.96	0.47
18:E:239:GLY:HA2	18:E:257:LEU:HD12	1.96	0.47
18:E:351:GLY:O	18:E:355:ILE:HG12	2.13	0.47
2:C:351:MET:HE3	2:C:354:ALA:HB3	1.96	0.47
4:V:417:ILE:HG13	4:V:422:ILE:HG13	1.95	0.47
4:V:451:ILE:HG12	11:d:279:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:225:LYS:HD2	5:W:229:LEU:HD23	1.96	0.47
7:Y:30:GLU:OE2	7:Y:31:HIS:HD2	1.97	0.47
7:Y:333:GLU:HG3	7:Y:337:PHE:CZ	2.50	0.47
9:a:217:LEU:HD22	9:a:238:TYR:CE1	2.49	0.47
11:d:188:MET:HA	11:d:188:MET:HE2	1.96	0.47
19:F:97:LEU:O	19:F:121:CYS:N	2.44	0.47
2:C:23:TYR:O	2:C:27:LYS:HG2	2.14	0.47
4:V:138:PRO:HB2	4:V:141:THR:HB	1.97	0.47
4:V:396:ILE:O	4:V:399:ARG:HB3	2.13	0.47
8:Z:6:VAL:HG12	8:Z:43:TRP:CH2	2.50	0.47
14:U:320:ASP:O	14:U:324:LYS:HG3	2.14	0.47
15:c:210:ASN:HB2	15:c:213:GLU:HG3	1.96	0.47
18:E:135:ILE:HD11	18:E:186:ALA:HB2	1.97	0.47
4:V:330:LYS:HE2	4:V:330:LYS:HB3	1.71	0.47
5:W:287:VAL:HA	5:W:290:ILE:HG22	1.97	0.47
6:X:369:ILE:HD12	6:X:376:GLY:O	2.15	0.47
18:E:158:LEU:HD12	18:E:159:PHE:H	1.79	0.47
19:F:383:GLU:OE2	19:F:386:ARG:NH2	2.47	0.47
2:C:157:GLN:HG2	2:C:317:PHE:CE1	2.49	0.47
2:C:196:LYS:HG2	2:C:317:PHE:HD2	1.79	0.47
2:C:232:ARG:HD3	2:C:279:GLN:HG3	1.96	0.47
5:W:139:GLU:OE2	5:W:176:SER:OG	2.23	0.47
5:W:318:SER:O	5:W:322:GLU:HG2	2.14	0.47
5:W:360:GLU:O	5:W:364:ARG:HG3	2.14	0.47
6:X:142:ARG:HH11	6:X:143:TYR:H	1.63	0.47
8:Z:65:ASP:OD1	8:Z:66:SER:N	2.48	0.47
9:a:226:ARG:HH22	9:a:230:ARG:HE	1.63	0.47
14:U:78:LEU:HD22	14:U:103:LYS:HG3	1.96	0.47
14:U:770:TRP:O	15:c:179:SER:HB2	2.14	0.47
15:c:54:MET:HB2	15:c:77:GLN:OE1	2.15	0.47
17:B:153:ASN:O	17:B:157:HIS:N	2.39	0.47
17:B:317:ASP:HB3	17:B:346:ARG:HG3	1.96	0.47
18:E:97:ARG:NH2	18:E:112:PRO:O	2.47	0.47
18:E:152:PRO:HB3	18:E:166:PRO:HG3	1.97	0.47
2:C:340:ARG:NE	7:Y:204:THR:HG23	2.29	0.47
2:C:347:ILE:CD1	2:C:383:PHE:HB3	2.45	0.47
2:C:376:VAL:HG12	2:C:377:HIS:ND1	2.30	0.47
3:D:177:VAL:HG11	3:D:215:LEU:HD21	1.97	0.47
8:Z:166:GLU:O	8:Z:170:VAL:HG13	2.13	0.47
10:b:7:MET:HB2	10:b:97:LEU:HD11	1.96	0.47
14:U:115:ASN:HD21	14:U:123:LYS:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:676:THR:HG21	14:U:712:LEU:HD21	1.97	0.47
16:A:325:ASP:OD1	16:A:326:THR:HG23	2.15	0.47
4:V:474:LEU:O	4:V:478:GLN:HG3	2.14	0.47
5:W:190:MET:HE3	5:W:205:ILE:HG23	1.96	0.47
9:a:18:GLN:HB3	9:a:22:TRP:NE1	2.30	0.47
11:d:218:LYS:HG3	11:d:219:ASP:N	2.30	0.47
14:U:587:ALA:HB2	14:U:621:SER:OG	2.15	0.47
16:A:223:THR:O	16:A:227:ARG:HG3	2.15	0.47
16:A:410:LEU:HA	16:A:413:VAL:HG12	1.96	0.47
18:E:250:ASP:OD1	18:E:250:ASP:N	2.47	0.47
18:E:319:PRO:C	18:E:320:ILE:HD13	2.40	0.47
3:D:45:LYS:HA	3:D:45:LYS:HD3	1.72	0.47
3:D:85:ILE:CG2	3:D:86:PRO:HD3	2.44	0.47
3:D:170:MET:HG2	3:D:173:GLN:HB2	1.96	0.47
4:V:72:LEU:HD22	4:V:147:PHE:CD2	2.50	0.47
5:W:104:MET:HE2	5:W:104:MET:HA	1.96	0.47
7:Y:208:PHE:CE2	7:Y:211:TYR:HA	2.50	0.47
7:Y:231:LEU:HD23	7:Y:236:LEU:HA	1.97	0.47
7:Y:243:GLY:O	7:Y:247:LEU:HD22	2.15	0.47
14:U:45:ILE:HD11	14:U:63:VAL:HB	1.97	0.47
14:U:58:GLN:HB2	14:U:87:LEU:HD23	1.95	0.47
14:U:208:LEU:CD2	14:U:210:LYS:H	2.28	0.47
16:A:173:THR:HG22	16:A:175:SER:H	1.80	0.47
19:F:382:GLU:HG2	19:F:386:ARG:HD3	1.97	0.47
2:C:189:TYR:HA	2:C:295:THR:O	2.15	0.46
5:W:17:GLU:HG2	5:W:18:VAL:HG13	1.97	0.46
5:W:209:ILE:HG21	5:W:226:TYR:CE2	2.50	0.46
10:b:20:ASP:OD1	10:b:25:ARG:NH2	2.44	0.46
14:U:24:LEU:HG	14:U:59:PHE:HD2	1.80	0.46
14:U:549:ALA:O	14:U:581:SER:OG	2.25	0.46
16:A:175:SER:O	16:A:357:ILE:HD11	2.15	0.46
18:E:75:ASN:OD1	18:E:76:GLY:N	2.43	0.46
19:F:137:ILE:O	19:F:160:ILE:HG12	2.15	0.46
19:F:421:MET:O	19:F:424:ILE:HG12	2.15	0.46
3:D:89:ILE:HD11	18:E:80:VAL:HG23	1.97	0.46
3:D:278:GLN:N	3:D:278:GLN:OE1	2.46	0.46
4:V:234:ARG:HA	4:V:237:THR:HG22	1.97	0.46
4:V:453:HIS:HB3	11:d:283:LEU:HG	1.97	0.46
5:W:152:ILE:O	5:W:155:GLN:HG3	2.15	0.46
5:W:275:ILE:HG23	5:W:309:PHE:CE2	2.50	0.46
14:U:251:ASP:OD1	14:U:252:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:180:CYS:SG	16:A:181:LYS:N	2.87	0.46
16:A:206:ILE:HA	19:F:372:LYS:NZ	2.30	0.46
16:A:336:ARG:O	16:A:337:LEU:HD23	2.14	0.46
18:E:384:LEU:HB3	18:E:386:TYR:CE1	2.51	0.46
4:V:375:PHE:CE1	4:V:399:ARG:HB2	2.50	0.46
5:W:89:LEU:O	5:W:93:ARG:HG2	2.15	0.46
11:d:115:GLU:HG3	11:d:118:ARG:HH11	1.81	0.46
18:E:199:VAL:HG21	19:F:315:ASN:ND2	2.30	0.46
3:D:293:LEU:HG	3:D:326:ARG:NH1	2.31	0.46
3:D:349:THR:HB	3:D:354:LEU:HD22	1.97	0.46
4:V:150:ARG:CZ	4:V:159:LEU:HB3	2.45	0.46
6:X:249:THR:HB	6:X:253:TYR:HE1	1.81	0.46
7:Y:70:LEU:HA	7:Y:73:MET:CG	2.44	0.46
7:Y:112:CYS:SG	7:Y:143:TYR:HE1	2.39	0.46
8:Z:149:THR:HB	8:Z:150:PRO:CD	2.43	0.46
10:b:129:LYS:O	10:b:133:LYS:HG3	2.16	0.46
16:A:158:ASP:O	16:A:161:VAL:N	2.48	0.46
18:E:171:LEU:HB2	18:E:295:LEU:HD13	1.97	0.46
2:C:235:PHE:CE2	2:C:276:LEU:HD22	2.51	0.46
2:C:299:ASP:OD1	2:C:299:ASP:N	2.49	0.46
3:D:290:LEU:HD23	3:D:294:ASN:ND2	2.30	0.46
7:Y:182:VAL:O	7:Y:186:LEU:HG	2.15	0.46
9:a:50:PHE:CD2	9:a:52:GLN:HB2	2.51	0.46
10:b:122:LYS:O	10:b:126:LYS:HG2	2.16	0.46
11:d:279:TYR:CE1	11:d:284:PHE:HB3	2.51	0.46
14:U:719:ASP:OD1	14:U:720:LYS:N	2.48	0.46
17:B:364:ILE:HA	17:B:367:ILE:HD12	1.98	0.46
19:F:350:ARG:HG3	19:F:350:ARG:HH11	1.81	0.46
2:C:137:LEU:HD12	2:C:220:VAL:HB	1.97	0.46
2:C:224:ILE:HD11	2:C:233:GLU:O	2.16	0.46
3:D:200:ARG:HH21	3:D:301:GLN:NE2	2.13	0.46
4:V:183:GLU:HG3	4:V:184:ALA:N	2.30	0.46
4:V:224:LEU:HA	4:V:227:VAL:HG12	1.98	0.46
11:d:174:TYR:HA	11:d:178:TYR:HD2	1.79	0.46
11:d:252:PRO:HG2	11:d:256:TYR:CE1	2.51	0.46
15:c:272:ILE:HG22	15:c:272:ILE:O	2.16	0.46
16:A:326:THR:O	16:A:326:THR:OG1	2.32	0.46
4:V:281:ASN:ND2	4:V:284:GLU:OE2	2.41	0.46
14:U:173:VAL:O	14:U:177:LEU:HD23	2.16	0.46
15:c:243:SER:O	15:c:247:GLU:HG2	2.15	0.46
17:B:338:ASP:HB3	17:B:341:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:272:THR:HG22	3:D:273:LYS:H	1.80	0.46
6:X:297:ARG:HG3	6:X:337:ARG:HD3	1.98	0.46
7:Y:183:TYR:CE1	7:Y:213:LEU:HD21	2.51	0.46
9:a:261:LEU:HD22	9:a:268:LEU:HD11	1.97	0.46
10:b:116:PRO:HA	10:b:151:GLU:OE2	2.16	0.46
11:d:156:ILE:HG12	11:d:258:PHE:CD2	2.51	0.46
15:c:284:LEU:O	15:c:288:VAL:HG12	2.16	0.46
17:B:315:GLN:O	17:B:322:ARG:NH1	2.49	0.46
17:B:364:ILE:HG12	21:B:501:ATP:N1	2.30	0.46
19:F:202:ILE:C	19:F:205:PRO:HD2	2.41	0.46
19:F:307:GLN:HA	19:F:310:MET:HE2	1.98	0.46
1:f:103:GLU:O	15:c:129:THR:OG1	2.26	0.46
1:f:109:GLN:HE22	15:c:125:VAL:HG23	1.80	0.46
2:C:182:GLN:HE21	2:C:287:LYS:HG2	1.81	0.46
2:C:344:LEU:HA	2:C:347:ILE:HG22	1.98	0.46
4:V:85:ALA:HA	4:V:90:GLU:HB2	1.96	0.46
4:V:89:LYS:HG3	4:V:91:PRO:HD3	1.97	0.46
4:V:243:ASP:O	4:V:247:GLN:HG3	2.16	0.46
5:W:32:ALA:HB3	5:W:33:LYS:NZ	2.31	0.46
7:Y:325:VAL:HB	7:Y:329:PHE:HD2	1.81	0.46
8:Z:25:ARG:NH2	15:c:102:THR:HG22	2.31	0.46
9:a:140:GLU:OE1	9:a:140:GLU:N	2.44	0.46
11:d:119:LEU:O	11:d:123:LEU:HG	2.16	0.46
11:d:182:LEU:HD12	11:d:183:PRO:HD2	1.97	0.46
16:A:333:ARG:HH21	16:A:336:ARG:CZ	2.29	0.46
5:W:60:MET:CE	5:W:99:GLN:HB3	2.45	0.45
6:X:377:ILE:O	7:Y:312:ARG:NH2	2.40	0.45
10:b:180:ALA:O	10:b:184:ILE:HG12	2.15	0.45
14:U:66:LYS:HA	14:U:96:TYR:HE2	1.81	0.45
2:C:36:ASN:HB3	4:V:89:LYS:CE	2.46	0.45
5:W:124:LEU:O	5:W:128:LEU:HG	2.16	0.45
8:Z:78:MET:HE3	8:Z:82:PHE:HE1	1.81	0.45
16:A:172:VAL:HG12	16:A:228:ALA:HB2	1.98	0.45
17:B:174:MET:HE2	17:B:174:MET:HB3	1.83	0.45
17:B:387:LYS:HG2	17:B:388:ASP:H	1.81	0.45
19:F:204:LEU:HB3	19:F:205:PRO:HD3	1.97	0.45
3:D:355:SER:HA	3:D:393:ILE:HD11	1.98	0.45
5:W:299:ILE:CG2	5:W:302:TYR:HB2	2.45	0.45
8:Z:188:SER:O	8:Z:192:THR:HG22	2.16	0.45
9:a:188:LEU:HD11	9:a:193:GLN:HB3	1.98	0.45
11:d:99:LYS:HE3	11:d:99:LYS:HB3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:166:ARG:HD2	14:U:11:LEU:HA	1.98	0.45
11:d:261:ASP:OD1	11:d:262:ILE:N	2.48	0.45
11:d:284:PHE:HE2	11:d:318:PHE:HZ	1.64	0.45
14:U:59:PHE:O	14:U:63:VAL:HG23	2.16	0.45
14:U:208:LEU:HD23	14:U:209:GLU:N	2.31	0.45
15:c:150:SER:HB3	15:c:155:VAL:HG12	1.98	0.45
16:A:81:ALA:HB2	17:B:137:SER:HB2	1.97	0.45
2:C:90:HIS:CB	2:C:91:PRO:CD	2.94	0.45
2:C:187:LEU:HB3	2:C:314:LYS:HG2	1.98	0.45
2:C:332:HIS:CG	2:C:360:LYS:HD2	2.51	0.45
3:D:163:MET:HE1	3:D:221:HIS:CE1	2.51	0.45
3:D:248:ARG:HA	3:D:295:GLN:OE1	2.17	0.45
5:W:373:ILE:HD11	5:W:377:ARG:CB	2.46	0.45
7:Y:208:PHE:CZ	7:Y:214:MET:HE3	2.51	0.45
11:d:282:ILE:HD12	11:d:313:ASN:O	2.17	0.45
14:U:345:ASN:HB2	14:U:743:ASN:ND2	2.30	0.45
16:A:397:ILE:HD11	17:B:214:MET:HG2	1.99	0.45
19:F:323:ASN:OD1	19:F:323:ASN:N	2.50	0.45
2:C:30:GLU:O	2:C:34:ILE:HG13	2.16	0.45
3:D:355:SER:OG	3:D:356:GLU:N	2.46	0.45
5:W:86:ASN:O	5:W:90:LEU:HG	2.16	0.45
6:X:368:MET:HB3	6:X:373:LYS:HB2	1.99	0.45
7:Y:112:CYS:HB3	7:Y:120:ALA:HB1	1.97	0.45
10:b:21:PHE:HA	10:b:177:PRO:HB3	1.97	0.45
14:U:63:VAL:O	14:U:67:VAL:HG13	2.16	0.45
14:U:97:VAL:O	14:U:101:ILE:HG12	2.17	0.45
16:A:371:GLU:OE1	16:A:371:GLU:N	2.34	0.45
17:B:405:MET:HA	17:B:408:ARG:CB	2.46	0.45
19:F:113:LEU:HD12	19:F:117:ARG:NH2	2.31	0.45
19:F:154:ASN:OD1	19:F:155:LYS:N	2.49	0.45
19:F:423:GLY:HA2	19:F:426:GLU:OE2	2.16	0.45
2:C:46:GLN:NE2	14:U:639:LEU:HD11	2.32	0.45
2:C:139:MET:HE2	3:D:294:ASN:OD1	2.16	0.45
4:V:452:ASN:N	4:V:457:TYR:O	2.47	0.45
8:Z:183:THR:OG1	8:Z:187:LEU:HD13	2.16	0.45
8:Z:217:THR:HG23	8:Z:219:LYS:HG3	1.98	0.45
9:a:58:LYS:HD2	9:a:96:PHE:CE2	2.51	0.45
9:a:194:GLN:NE2	9:a:229:ASP:OD2	2.50	0.45
11:d:232:LEU:HD21	11:d:263:LEU:CD2	2.47	0.45
14:U:247:GLN:OE1	14:U:913:ILE:HG22	2.15	0.45
15:c:136:LEU:HD23	15:c:136:LEU:HA	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:E:313:LEU:HD11	18:E:331:ILE:HG21	1.99	0.45
19:F:376:SER:OG	19:F:378:ASP:OD1	2.31	0.45
2:C:92:GLU:HG2	2:C:95:PHE:HZ	1.82	0.45
5:W:344:THR:HG23	5:W:347:GLY:H	1.82	0.45
7:Y:94:ASN:OD1	7:Y:94:ASN:N	2.49	0.45
9:a:189:PRO:HG2	9:a:192:GLU:HG3	1.98	0.45
14:U:243:LEU:HD11	14:U:793:LYS:HD2	1.98	0.45
16:A:81:ALA:O	16:A:84:LYS:HG2	2.17	0.45
16:A:284:ARG:HA	16:A:296:GLN:OE1	2.17	0.45
16:A:405:THR:OG1	16:A:406:GLU:N	2.50	0.45
3:D:290:LEU:HD23	3:D:294:ASN:HD21	1.81	0.45
3:D:381:GLU:HB3	3:D:402:ALA:HB1	1.99	0.45
4:V:69:THR:HA	4:V:72:LEU:HD12	1.99	0.45
4:V:353:LEU:HD23	4:V:353:LEU:H	1.81	0.45
5:W:251:TYR:HB2	5:W:266:ALA:HB1	1.97	0.45
7:Y:110:TYR:O	7:Y:114:ILE:HG12	2.17	0.45
7:Y:263:LEU:HB2	7:Y:271:PHE:CD1	2.52	0.45
14:U:680:VAL:HG12	14:U:683:VAL:HG12	1.99	0.45
14:U:900:TYR:CG	14:U:914:LEU:HD21	2.52	0.45
15:c:103:GLY:O	15:c:105:PRO:HD3	2.16	0.45
16:A:80:LEU:HD23	16:A:80:LEU:HA	1.83	0.45
18:E:84:ARG:HB2	18:E:87:LEU:HD13	1.98	0.45
18:E:365:GLU:O	18:E:369:LYS:HG3	2.16	0.45
2:C:321:ASN:O	2:C:325:ARG:HG3	2.17	0.45
3:D:190:LEU:O	3:D:194:ILE:HG22	2.17	0.45
3:D:322:LEU:HD12	3:D:330:LYS:NZ	2.32	0.45
5:W:287:VAL:HG23	5:W:306:LEU:HD11	1.99	0.45
9:a:363:MET:HE2	9:a:363:MET:HA	1.98	0.45
10:b:3:LEU:HD22	10:b:105:HIS:CE1	2.52	0.45
15:c:57:MET:HG2	15:c:72:VAL:HG12	1.99	0.45
19:F:358:ASN:ND2	19:F:359:GLU:OE1	2.50	0.45
5:W:128:LEU:HA	5:W:131:VAL:CG1	2.46	0.45
5:W:272:LEU:HD23	5:W:272:LEU:HA	1.68	0.45
8:Z:22:HIS:CE1	8:Z:55:ALA:HB1	2.52	0.45
8:Z:64:ASP:HB2	8:Z:67:VAL:HG23	1.98	0.45
11:d:109:LEU:HD22	11:d:154:TRP:CD1	2.52	0.45
14:U:254:GLU:OE2	14:U:751:ARG:NH1	2.50	0.45
16:A:72:LEU:HG	16:A:78:TRP:HE1	1.82	0.45
16:A:101:ILE:HG23	16:A:137:GLY:H	1.82	0.45
1:f:85:LEU:HD12	1:f:90:VAL:HG11	1.98	0.44
2:C:338:LEU:HA	2:C:378:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:309:MET:HA	4:V:309:MET:HE2	1.98	0.44
6:X:46:LYS:HE2	6:X:76:PHE:HZ	1.82	0.44
6:X:315:ASP:N	6:X:315:ASP:OD1	2.50	0.44
6:X:382:GLU:N	6:X:382:GLU:OE1	2.50	0.44
10:b:184:ILE:HB	10:b:188:ILE:HG13	1.99	0.44
11:d:281:LYS:HG3	11:d:315:TYR:CD2	2.47	0.44
16:A:159:PRO:O	16:A:163:MET:HG3	2.17	0.44
17:B:233:THR:O	17:B:237:LYS:HG3	2.16	0.44
4:V:91:PRO:O	4:V:94:VAL:HG22	2.17	0.44
4:V:159:LEU:HG	4:V:164:GLU:HB3	1.99	0.44
5:W:382:LEU:CD2	5:W:384:LEU:HB2	2.46	0.44
9:a:54:ASP:HA	9:a:57:ILE:HB	1.99	0.44
9:a:60:TYR:HA	9:a:63:PHE:CD2	2.52	0.44
10:b:38:HIS:HB3	10:b:42:ARG:NH2	2.32	0.44
16:A:249:TYR:CE2	19:F:259:MET:HE1	2.51	0.44
19:F:169:ASP:O	19:F:173:LYS:HG2	2.18	0.44
4:V:290:TYR:HD2	4:V:328:VAL:HG22	1.81	0.44
6:X:125:LEU:HD12	6:X:125:LEU:H	1.83	0.44
6:X:218:HIS:CD2	6:X:231:TYR:HE2	2.36	0.44
7:Y:276:ALA:O	7:Y:280:GLN:HG2	2.18	0.44
9:a:112:ILE:O	9:a:116:THR:HG23	2.18	0.44
9:a:353:LEU:HD23	9:a:353:LEU:HA	1.83	0.44
11:d:268:ARG:O	11:d:271:ILE:HG12	2.17	0.44
11:d:279:TYR:CD2	11:d:283:LEU:CD2	2.98	0.44
14:U:39:SER:CB	14:U:71:LEU:HD21	2.48	0.44
14:U:188:MET:HE2	14:U:194:ARG:HA	2.00	0.44
18:E:122:MET:HE1	18:E:218:MET:HG2	1.98	0.44
18:E:192:ASP:OD2	18:E:192:ASP:N	2.45	0.44
2:C:89:VAL:HG12	2:C:90:HIS:CD2	2.52	0.44
2:C:347:ILE:HA	2:C:350:LEU:HG	2.00	0.44
4:V:294:ARG:HD3	4:V:331:LEU:HD22	2.00	0.44
4:V:384:GLU:H	4:V:384:GLU:HG3	1.63	0.44
5:W:214:PHE:CE1	5:W:222:LEU:HB2	2.50	0.44
6:X:131:ALA:O	6:X:134:VAL:HG12	2.17	0.44
7:Y:136:HIS:O	7:Y:140:ILE:HG12	2.18	0.44
7:Y:316:LEU:HD11	7:Y:347:ILE:HD11	1.98	0.44
9:a:27:GLU:HA	9:a:30:THR:HG1	1.82	0.44
9:a:142:LEU:HD23	9:a:142:LEU:HA	1.60	0.44
14:U:159:ARG:HB3	14:U:162:VAL:HG12	1.99	0.44
14:U:665:ASN:O	14:U:669:ILE:HG12	2.17	0.44
16:A:234:ASP:OD2	16:A:234:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:334:PRO:HG3	19:F:395:GLN:HG3	2.00	0.44
17:B:184:TYR:OH	17:B:239:VAL:HG22	2.18	0.44
19:F:197:GLU:HA	19:F:200:GLU:HG2	1.98	0.44
4:V:318:GLN:O	4:V:320:THR:N	2.50	0.44
4:V:401:ASN:O	4:V:401:ASN:OD1	2.35	0.44
7:Y:240:VAL:HG12	7:Y:260:LEU:HD21	2.00	0.44
8:Z:103:LYS:HB2	8:Z:103:LYS:HE3	1.68	0.44
9:a:70:ARG:O	9:a:73:PRO:HA	2.17	0.44
11:d:230:VAL:O	11:d:234:GLN:HG3	2.17	0.44
14:U:557:TYR:CD2	14:U:588:MET:HG3	2.52	0.44
16:A:293:ASN:O	16:A:297:ARG:HG3	2.17	0.44
16:A:351:ARG:NH1	16:A:380:SER:O	2.51	0.44
3:D:407:ILE:HD13	3:D:407:ILE:HA	1.84	0.44
11:d:154:TRP:O	11:d:158:ARG:HG2	2.18	0.44
11:d:314:ASN:HA	11:d:316:TYR:CZ	2.52	0.44
15:c:62:VAL:HB	15:c:66:THR:OG1	2.18	0.44
18:E:280:ASN:ND2	21:E:401:ATP:O2G	2.45	0.44
2:C:230:MET:HE2	2:C:230:MET:HA	1.99	0.44
2:C:393:LYS:HA	2:C:393:LYS:HD3	1.88	0.44
7:Y:128:TYR:HA	7:Y:131:THR:HB	2.00	0.44
9:a:132:LYS:HD2	9:a:132:LYS:C	2.43	0.44
14:U:148:LYS:H	14:U:148:LYS:HD3	1.83	0.44
14:U:411:ILE:HG22	14:U:412:HIS:HD2	1.83	0.44
19:F:85:THR:OG1	19:F:86:LEU:N	2.51	0.44
2:C:334:ARG:HD3	2:C:334:ARG:HA	1.90	0.44
5:W:50:LEU:HA	5:W:53:GLN:OE1	2.17	0.44
5:W:66:ILE:HG13	5:W:67:LEU:HD23	2.00	0.44
5:W:414:ASN:OD1	5:W:416:GLN:HG2	2.17	0.44
8:Z:247:LYS:O	8:Z:251:LEU:HD23	2.18	0.44
9:a:52:GLN:OE1	9:a:86:GLN:NE2	2.51	0.44
9:a:252:LYS:HA	9:a:255:TRP:CD2	2.53	0.44
11:d:172:LYS:HB3	11:d:172:LYS:HE2	1.73	0.44
11:d:197:LEU:HG	11:d:229:PRO:HB3	2.00	0.44
15:c:42:LEU:HD11	15:c:155:VAL:HG11	2.00	0.44
16:A:215:PHE:HE2	19:F:431:LYS:HE2	1.81	0.44
18:E:118:LEU:HD12	18:E:214:LEU:HD21	1.98	0.44
4:V:318:GLN:HE21	4:V:319:HIS:CD2	2.35	0.44
4:V:450:SER:N	4:V:459:GLN:O	2.38	0.44
4:V:497:PRO:N	4:V:498:PRO:HD3	2.32	0.44
7:Y:327:VAL:O	7:Y:330:ILE:HG22	2.18	0.44
8:Z:288:LYS:HB2	8:Z:288:LYS:HE2	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:70:ARG:HG3	9:a:73:PRO:CD	2.41	0.44
9:a:244:ASN:ND2	9:a:247:ARG:HG2	2.32	0.44
14:U:450:HIS:CE1	14:U:457:ILE:HG13	2.53	0.44
17:B:293:LYS:HE3	17:B:295:TYR:CE2	2.53	0.44
17:B:411:ARG:NE	17:B:418:ASP:OD2	2.51	0.44
19:F:364:ARG:O	19:F:368:ILE:HG12	2.17	0.44
2:C:59:LEU:HD21	3:D:76:GLN:HG2	1.99	0.43
2:C:130:LYS:NZ	2:C:131:VAL:O	2.51	0.43
2:C:343:ASN:O	2:C:346:LYS:HG2	2.18	0.43
5:W:187:LEU:HA	5:W:190:MET:HG3	2.00	0.43
5:W:356:ASN:O	5:W:360:GLU:HG3	2.18	0.43
9:a:18:GLN:O	9:a:19:PRO:C	2.60	0.43
9:a:87:MET:HB3	9:a:92:VAL:HG13	1.99	0.43
10:b:4:GLU:HB3	10:b:47:ASN:ND2	2.33	0.43
10:b:125:VAL:HG13	10:b:129:LYS:HE3	2.00	0.43
14:U:420:LEU:HD12	14:U:420:LEU:H	1.83	0.43
14:U:448:LEU:HA	14:U:483:LEU:HD21	1.99	0.43
11:d:109:LEU:HD22	11:d:154:TRP:HD1	1.82	0.43
19:F:103:ASP:OD1	19:F:103:ASP:N	2.49	0.43
19:F:153:VAL:HG12	19:F:160:ILE:HG22	1.99	0.43
2:C:338:LEU:C	2:C:378:VAL:H	2.26	0.43
4:V:345:ARG:HD2	4:V:345:ARG:HA	1.51	0.43
4:V:359:PRO:HG3	4:V:382:PHE:CE2	2.53	0.43
7:Y:317:GLY:O	7:Y:321:GLU:HG2	2.18	0.43
7:Y:336:ARG:NH1	12:e:44:ASP:OD1	2.48	0.43
9:a:68:GLU:O	9:a:70:ARG:N	2.51	0.43
10:b:26:LEU:HD12	10:b:26:LEU:HA	1.82	0.43
14:U:69:TYR:CE1	14:U:99:THR:HG21	2.52	0.43
14:U:410:VAL:HG23	14:U:448:LEU:CD2	2.45	0.43
17:B:252:GLY:HA3	17:B:287:ILE:HA	2.00	0.43
18:E:265:ASP:OD2	18:E:291:ARG:NH2	2.49	0.43
18:E:327:ASP:H	18:E:364:GLN:HE22	1.66	0.43
19:F:385:ALA:HA	19:F:388:THR:HG22	2.00	0.43
3:D:71:GLU:HA	3:D:71:GLU:OE1	2.18	0.43
3:D:139:LEU:HA	3:D:139:LEU:HD23	1.80	0.43
4:V:114:TYR:O	4:V:117:VAL:HG12	2.18	0.43
5:W:160:LYS:HE2	5:W:160:LYS:HB2	1.64	0.43
8:Z:133:LEU:HD13	8:Z:134:PRO:HD2	2.01	0.43
11:d:283:LEU:HA	11:d:283:LEU:HD12	1.87	0.43
14:U:579:ARG:NH1	14:U:609:ASP:OD1	2.50	0.43
15:c:125:VAL:HA	15:c:128:ASN:HD22	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:221:GLY:HA2	21:A:501:ATP:O1A	2.18	0.43
17:B:375:ALA:HB2	17:B:415:THR:HG22	2.00	0.43
19:F:225:MET:HB3	19:F:354:PHE:CE1	2.54	0.43
4:V:161:PRO:HA	4:V:164:GLU:HG2	2.01	0.43
4:V:453:HIS:CE1	11:d:285:THR:HA	2.54	0.43
5:W:75:TYR:CZ	5:W:111:TYR:HB3	2.53	0.43
5:W:344:THR:OG1	5:W:345:GLU:N	2.51	0.43
7:Y:15:PRO:CD	7:Y:146:ARG:HB3	2.47	0.43
7:Y:109:GLU:O	7:Y:113:ARG:HB2	2.18	0.43
8:Z:287:LYS:HE3	8:Z:287:LYS:HB3	1.93	0.43
9:a:186:LYS:NZ	9:a:221:VAL:HB	2.33	0.43
14:U:615:ARG:O	14:U:619:VAL:HG23	2.19	0.43
14:U:660:CYS:O	14:U:694:ILE:HG12	2.17	0.43
14:U:794:ASP:O	14:U:796:LYS:NZ	2.52	0.43
16:A:353:HIS:O	16:A:357:ILE:HB	2.18	0.43
17:B:280:SER:O	17:B:325:VAL:HA	2.18	0.43
18:E:126:ASP:HB2	18:E:197:LYS:NZ	2.30	0.43
2:C:332:HIS:CD2	2:C:360:LYS:HD2	2.54	0.43
3:D:92:PHE:HE1	3:D:101:ALA:HB1	1.84	0.43
4:V:280:ALA:HB3	4:V:285:TRP:NE1	2.33	0.43
5:W:98:LYS:HB2	5:W:137:TYR:CD2	2.54	0.43
6:X:239:TYR:HD1	6:X:244:SER:HB3	1.83	0.43
7:Y:75:LYS:HE2	7:Y:75:LYS:HB3	1.82	0.43
8:Z:207:ASP:OD1	8:Z:207:ASP:C	2.61	0.43
9:a:112:ILE:HG13	9:a:138:VAL:HG23	2.00	0.43
9:a:286:ALA:HA	9:a:289:ARG:HE	1.84	0.43
11:d:145:ARG:HH22	11:d:184:GLU:HA	1.83	0.43
14:U:678:ASP:OD1	14:U:679:PRO:HD2	2.17	0.43
18:E:145:LEU:HD12	18:E:145:LEU:HA	1.84	0.43
18:E:180:LYS:N	21:E:401:ATP:O1B	2.52	0.43
2:C:90:HIS:HB2	2:C:91:PRO:HD2	2.00	0.43
4:V:63:SER:O	4:V:67:LEU:HG	2.19	0.43
4:V:343:PRO:O	12:e:43:TRP:HZ2	2.02	0.43
5:W:19:ASP:OD1	5:W:20:TYR:N	2.52	0.43
5:W:174:TYR:O	5:W:182:ARG:NH1	2.52	0.43
7:Y:51:ALA:HB3	7:Y:52:PRO:HD3	2.01	0.43
10:b:32:ALA:O	10:b:35:ILE:HG22	2.19	0.43
10:b:124:LEU:HD23	10:b:124:LEU:HA	1.87	0.43
14:U:725:MET:HE3	15:c:183:HIS:CD2	2.54	0.43
14:U:901:GLN:O	14:U:915:LYS:N	2.49	0.43
16:A:85:GLN:CD	16:A:89:SER:HB3	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:120:LYS:HB2	19:F:90:VAL:HG21	2.01	0.43
17:B:272:ARG:HH12	17:B:276:GLU:HB2	1.83	0.43
18:E:195:PHE:CD1	18:E:229:ILE:HB	2.54	0.43
18:E:313:LEU:HD11	18:E:331:ILE:CG2	2.48	0.43
2:C:336:MET:HE2	2:C:336:MET:HB2	1.92	0.43
4:V:166:TYR:CZ	4:V:170:LEU:HD21	2.54	0.43
4:V:313:LEU:HD23	4:V:313:LEU:HA	1.81	0.43
7:Y:277:VAL:O	7:Y:281:GLU:HG2	2.18	0.43
9:a:140:GLU:HA	9:a:143:ASN:HD21	1.83	0.43
10:b:21:PHE:HE1	10:b:28:ALA:HB1	1.84	0.43
10:b:120:ASN:H	10:b:120:ASN:HD22	1.66	0.43
11:d:81:ALA:HB3	11:d:84:SER:HB3	2.00	0.43
11:d:185:SER:OG	11:d:186:ALA:N	2.52	0.43
14:U:357:LYS:HD3	14:U:385:PHE:CZ	2.54	0.43
14:U:376:MET:HE2	14:U:376:MET:HB2	1.88	0.43
14:U:553:ALA:HA	14:U:585:THR:OG1	2.19	0.43
15:c:251:LEU:HG	15:c:284:LEU:HG	2.01	0.43
16:A:278:ASP:OD2	16:A:323:ARG:HG3	2.18	0.43
2:C:340:ARG:O	2:C:342:ILE:HD12	2.18	0.43
3:D:91:GLN:HE22	3:D:248:ARG:NH1	2.17	0.43
4:V:71:THR:HG22	4:V:107:ARG:HG3	2.00	0.43
4:V:290:TYR:HA	4:V:309:MET:HE1	2.01	0.43
4:V:455:LYS:HB3	4:V:457:TYR:CE2	2.54	0.43
14:U:67:VAL:O	14:U:71:LEU:HG	2.19	0.43
14:U:324:LYS:HA	14:U:327:LYS:HZ2	1.84	0.43
14:U:368:ALA:HB2	14:U:728:PHE:CD2	2.54	0.43
17:B:175:LYS:HZ2	17:B:177:GLU:HG2	1.84	0.43
19:F:320:PHE:O	19:F:321:GLN:HB2	2.18	0.43
2:C:90:HIS:HE1	2:C:92:GLU:HB2	1.82	0.43
3:D:171:ASP:OD1	3:D:171:ASP:C	2.62	0.43
5:W:24:VAL:HB	5:W:28:LEU:HD11	2.01	0.43
5:W:259:GLU:OE2	5:W:260:SER:N	2.47	0.43
7:Y:83:ARG:O	7:Y:87:GLU:HG2	2.19	0.43
7:Y:201:PHE:HB3	7:Y:223:THR:HG23	2.00	0.43
11:d:122:VAL:HA	11:d:125:GLU:HG2	2.01	0.43
11:d:233:GLU:HA	11:d:236:LEU:HG	2.00	0.43
14:U:62:LEU:O	14:U:65:SER:OG	2.30	0.43
14:U:490:ARG:HB2	14:U:493:VAL:HG22	2.00	0.43
15:c:239:LYS:HD3	15:c:239:LYS:HA	1.78	0.43
16:A:84:LYS:HB3	16:A:84:LYS:HE2	1.87	0.43
2:C:157:GLN:HG2	2:C:317:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:183:GLU:O	4:V:187:ILE:HG13	2.19	0.42
5:W:403:PHE:C	5:W:403:PHE:CD2	2.96	0.42
6:X:270:LEU:HD12	6:X:270:LEU:HA	1.87	0.42
6:X:304:LYS:HA	6:X:304:LYS:HD3	1.78	0.42
7:Y:201:PHE:CE2	7:Y:222:TYR:CE1	3.06	0.42
14:U:108:TYR:CE2	14:U:134:VAL:HG11	2.54	0.42
17:B:343:ARG:HD2	17:B:346:ARG:HH11	1.84	0.42
17:B:418:ASP:OD1	17:B:418:ASP:N	2.52	0.42
19:F:428:GLN:HE22	19:F:430:LYS:HB2	1.84	0.42
2:C:340:ARG:CB	7:Y:207:THR:HG23	2.48	0.42
2:C:340:ARG:HB2	7:Y:206:SER:CB	2.49	0.42
3:D:318:ASP:HB3	3:D:321:LEU:HG	2.00	0.42
4:V:104:THR:O	4:V:108:LEU:HG	2.19	0.42
5:W:128:LEU:HB2	5:W:145:LEU:CD2	2.49	0.42
5:W:393:LEU:O	5:W:397:VAL:HG23	2.19	0.42
6:X:138:PHE:HD2	6:X:176:THR:HG22	1.84	0.42
7:Y:164:ALA:O	7:Y:168:ILE:HG12	2.18	0.42
7:Y:229:ILE:HA	7:Y:299:MET:HE1	2.00	0.42
14:U:201:LEU:HD12	14:U:201:LEU:HA	1.82	0.42
14:U:786:THR:O	14:U:786:THR:CG2	2.67	0.42
17:B:377:ASP:OD1	17:B:416:ASN:HB2	2.19	0.42
18:E:197:LYS:HD3	19:F:320:PHE:CE2	2.53	0.42
3:D:91:GLN:HE22	3:D:248:ARG:HH12	1.67	0.42
5:W:41:GLN:O	5:W:45:GLU:HG2	2.18	0.42
6:X:138:PHE:CD2	6:X:176:THR:HG22	2.55	0.42
7:Y:101:ARG:HH22	7:Y:130:LYS:HB3	1.83	0.42
7:Y:189:VAL:HG13	7:Y:287:LEU:HD21	2.01	0.42
9:a:21:VAL:O	9:a:25:LEU:HG	2.20	0.42
9:a:130:VAL:O	9:a:133:GLU:HG3	2.19	0.42
9:a:284:ARG:NH2	9:a:295:GLU:OE1	2.52	0.42
14:U:2:ILE:HG23	14:U:3:THR:HG23	2.01	0.42
16:A:77:LEU:HA	16:A:80:LEU:HG	2.00	0.42
17:B:264:PRO:HB3	17:B:311:GLU:OE2	2.18	0.42
17:B:265:LYS:HG3	17:B:268:ARG:HH21	1.84	0.42
19:F:228:PRO:HG2	19:F:356:MET:HG2	2.01	0.42
6:X:218:HIS:NE2	6:X:227:THR:OG1	2.35	0.42
6:X:249:THR:O	6:X:253:TYR:CD1	2.72	0.42
6:X:355:LYS:O	6:X:356:LEU:HD23	2.20	0.42
7:Y:14:ASN:HB2	7:Y:113:ARG:NH2	2.20	0.42
8:Z:139:ILE:HG22	8:Z:156:GLU:HB3	2.01	0.42
9:a:344:GLN:HA	9:a:347:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:120:ASN:H	10:b:120:ASN:ND2	2.17	0.42
11:d:235:TYR:CE2	11:d:243:LYS:HD2	2.53	0.42
11:d:235:TYR:HB3	11:d:244:VAL:HG13	2.01	0.42
14:U:658:ILE:HD11	14:U:767:THR:HG21	2.01	0.42
15:c:166:ASN:HB2	15:c:167:MET:HE2	2.00	0.42
17:B:393:ALA:O	17:B:396:LYS:HG3	2.19	0.42
18:E:352:MET:HE3	18:E:352:MET:HB3	1.67	0.42
2:C:248:MET:HE2	2:C:269:VAL:HG13	2.00	0.42
4:V:120:PHE:HB3	4:V:167:LEU:CD1	2.43	0.42
4:V:122:THR:CG2	4:V:155:ALA:HA	2.45	0.42
4:V:415:SER:HB2	7:Y:346:LYS:HB3	2.01	0.42
4:V:453:HIS:CG	11:d:285:THR:H	2.37	0.42
8:Z:182:THR:O	8:Z:183:THR:OG1	2.30	0.42
11:d:284:PHE:CE2	11:d:318:PHE:HZ	2.37	0.42
14:U:323:LEU:O	14:U:327:LYS:HG3	2.19	0.42
16:A:284:ARG:HH11	16:A:300:LEU:HD21	1.84	0.42
17:B:401:GLU:O	17:B:405:MET:HG3	2.20	0.42
1:f:86:GLN:HA	1:f:90:VAL:CG1	2.50	0.42
3:D:124:LEU:H	3:D:124:LEU:HD12	1.84	0.42
5:W:166:LEU:HD23	5:W:166:LEU:HA	1.87	0.42
5:W:201:ARG:NH1	5:W:201:ARG:HB2	2.35	0.42
7:Y:155:ASP:OD1	7:Y:155:ASP:N	2.52	0.42
7:Y:189:VAL:HG11	7:Y:222:TYR:OH	2.20	0.42
8:Z:180:LYS:HD2	8:Z:180:LYS:HA	1.85	0.42
8:Z:182:THR:HG22	8:Z:183:THR:N	2.22	0.42
9:a:87:MET:SD	9:a:87:MET:N	2.93	0.42
14:U:2:ILE:HG23	14:U:3:THR:N	2.35	0.42
15:c:80:THR:HB	19:F:113:LEU:HD22	2.01	0.42
16:A:151:ILE:HD12	16:A:152:PRO:HD2	1.99	0.42
16:A:166:VAL:HG11	16:A:237:PHE:HB3	2.00	0.42
16:A:184:ILE:O	16:A:188:ARG:HG3	2.20	0.42
16:A:218:PRO:HB2	17:B:343:ARG:HH21	1.84	0.42
17:B:120:HIS:CB	17:B:134:SER:HA	2.50	0.42
2:C:248:MET:HB2	2:C:293:MET:HB2	2.01	0.42
2:C:337:ASN:O	2:C:377:HIS:HA	2.19	0.42
2:C:380:GLN:HE22	2:C:384:GLU:HB2	1.83	0.42
5:W:165:ILE:O	5:W:168:GLU:HG2	2.20	0.42
5:W:231:ILE:HD12	5:W:243:ILE:HG23	2.01	0.42
6:X:57:LEU:HB3	6:X:66:LEU:HG	2.02	0.42
7:Y:314:LEU:O	7:Y:354:VAL:HG23	2.20	0.42
11:d:108:ASN:OD1	11:d:109:LEU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:128:PHE:O	11:d:174:TYR:OH	2.24	0.42
16:A:284:ARG:O	19:F:334:ARG:NH1	2.52	0.42
2:C:230:MET:SD	2:C:232:ARG:NH2	2.88	0.42
3:D:63:ASP:OD2	3:D:63:ASP:C	2.62	0.42
4:V:425:LYS:O	4:V:425:LYS:HD2	2.19	0.42
5:W:27:ARG:HG3	5:W:31:CYS:SG	2.60	0.42
5:W:30:GLU:HG2	5:W:34:LEU:HD13	2.01	0.42
5:W:286:LEU:O	5:W:290:ILE:HG22	2.19	0.42
6:X:218:HIS:NE2	6:X:224:ASP:OD1	2.53	0.42
8:Z:126:VAL:O	8:Z:128:PRO:HD3	2.20	0.42
8:Z:236:LEU:HD23	8:Z:236:LEU:HA	1.82	0.42
8:Z:273:HIS:ND1	15:c:255:TYR:OH	2.50	0.42
9:a:140:GLU:HA	9:a:143:ASN:ND2	2.34	0.42
9:a:186:LYS:HG3	9:a:221:VAL:HG11	2.02	0.42
15:c:163:ILE:HG22	15:c:199:HIS:C	2.45	0.42
16:A:108:ASP:CG	16:A:109:PRO:HD2	2.45	0.42
17:B:386:ALA:HB3	17:B:390:LEU:HD11	2.01	0.42
18:E:97:ARG:HE	18:E:111:LEU:HB2	1.85	0.42
1:f:54:GLU:OE1	1:f:58:LYS:HG2	2.20	0.42
2:C:277:LEU:HA	2:C:280:LEU:HD12	2.02	0.42
3:D:170:MET:HG2	3:D:170:MET:O	2.20	0.42
4:V:391:THR:HA	4:V:394:LEU:CD1	2.50	0.42
5:W:317:TRP:O	5:W:321:VAL:HG12	2.19	0.42
9:a:18:GLN:CB	9:a:22:TRP:HE1	2.32	0.42
10:b:114:GLY:HA2	10:b:143:PHE:O	2.20	0.42
14:U:423:MET:O	14:U:427:LEU:HB3	2.20	0.42
17:B:347:ILE:HG22	17:B:350:LYS:HG2	2.01	0.42
3:D:121:ARG:HB2	15:c:274:ASN:ND2	2.35	0.42
4:V:186:LYS:HA	4:V:189:ASP:OD2	2.20	0.42
5:W:295:LYS:HB2	5:W:295:LYS:HE2	1.81	0.42
6:X:303:GLU:HA	6:X:306:LEU:HG	2.02	0.42
7:Y:316:LEU:HB2	7:Y:352:GLU:HB3	2.02	0.42
8:Z:6:VAL:HG12	8:Z:43:TRP:HH2	1.84	0.42
11:d:218:LYS:HB2	11:d:218:LYS:HE3	1.72	0.42
14:U:322:THR:O	14:U:326:ILE:HG13	2.19	0.42
14:U:357:LYS:HE2	14:U:389:ASN:CG	2.45	0.42
19:F:317:LEU:HD23	19:F:317:LEU:HA	1.91	0.42
3:D:164:TYR:CD1	3:D:218:ALA:HB1	2.54	0.41
3:D:200:ARG:HD2	3:D:299:PHE:HD2	1.84	0.41
3:D:212:LYS:HG2	3:D:333:PHE:CG	2.54	0.41
4:V:123:SER:H	4:V:150:ARG:NH2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:418:SER:HA	4:V:457:TYR:HA	2.02	0.41
5:W:147:LYS:NZ	5:W:184:GLU:OE1	2.52	0.41
7:Y:37:VAL:HA	7:Y:40:GLU:OE1	2.20	0.41
7:Y:88:LEU:HD23	7:Y:88:LEU:HA	1.92	0.41
7:Y:287:LEU:HD23	7:Y:287:LEU:O	2.20	0.41
9:a:132:LYS:O	9:a:132:LYS:HD2	2.20	0.41
14:U:199:ARG:HH11	14:U:223:LEU:HD22	1.84	0.41
3:D:99:ASN:O	3:D:100:THR:OG1	2.29	0.41
4:V:200:ARG:HB2	4:V:203:LEU:HB2	2.02	0.41
5:W:250:ILE:HG23	5:W:256:ILE:HD13	2.01	0.41
7:Y:194:PHE:CD2	7:Y:229:ILE:HD13	2.55	0.41
10:b:18:ASN:O	10:b:25:ARG:HG3	2.20	0.41
14:U:217:CYS:O	14:U:221:ILE:HG12	2.20	0.41
14:U:336:GLU:OE2	14:U:337:LEU:HD22	2.20	0.41
14:U:567:ILE:HD11	14:U:585:THR:HG22	2.02	0.41
14:U:633:CYS:O	14:U:637:VAL:HG22	2.20	0.41
14:U:641:SER:OG	14:U:675:MET:SD	2.77	0.41
15:c:121:TRP:HZ3	15:c:123:SER:HB3	1.85	0.41
19:F:168:TYR:HB2	19:F:173:LYS:HE2	2.01	0.41
2:C:40:GLN:HG2	2:C:43:ARG:NH1	2.35	0.41
7:Y:100:ILE:HG13	7:Y:101:ARG:N	2.35	0.41
7:Y:275:LEU:HA	7:Y:278:VAL:CG1	2.50	0.41
8:Z:270:VAL:HG13	15:c:281:LYS:HE2	2.02	0.41
14:U:557:TYR:HD2	14:U:588:MET:HG3	1.85	0.41
19:F:137:ILE:HG13	19:F:138:GLY:N	2.35	0.41
19:F:406:ILE:HA	19:F:409:ARG:HD3	2.02	0.41
1:f:75:HIS:HB2	1:f:96:LEU:HD22	2.01	0.41
2:C:334:ARG:NH1	7:Y:173:ASP:HA	2.35	0.41
3:D:338:ARG:HD2	3:D:365:ALA:HA	2.02	0.41
4:V:365:GLN:HA	4:V:368:ARG:NH1	2.36	0.41
8:Z:7:GLN:HG2	8:Z:46:LYS:HB3	2.01	0.41
8:Z:209:ARG:NH1	9:a:354:GLU:OE1	2.53	0.41
9:a:210:VAL:HG23	9:a:210:VAL:O	2.20	0.41
11:d:268:ARG:NH2	11:d:292:PHE:HB3	2.33	0.41
14:U:127:ASP:HB3	14:U:130:LEU:HD12	2.02	0.41
14:U:138:PHE:CD1	14:U:162:VAL:HG21	2.56	0.41
16:A:72:LEU:HG	16:A:78:TRP:NE1	2.35	0.41
17:B:396:LYS:O	17:B:400:THR:HG22	2.20	0.41
18:E:177:GLY:N	19:F:344:ARG:HD2	2.35	0.41
3:D:85:ILE:N	3:D:86:PRO:HD3	2.36	0.41
5:W:108:CYS:HA	5:W:111:TYR:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:173:ASP:CG	7:Y:176:ARG:HB2	2.45	0.41
7:Y:245:GLU:OE2	7:Y:245:GLU:N	2.49	0.41
8:Z:176:LEU:HD23	8:Z:176:LEU:HA	1.91	0.41
9:a:212:ASN:ND2	9:a:215:GLU:HG3	2.35	0.41
10:b:10:VAL:HG13	10:b:29:GLN:NE2	2.35	0.41
10:b:117:VAL:HG13	10:b:151:GLU:OE2	2.20	0.41
15:c:181:LEU:HD23	15:c:181:LEU:HA	1.87	0.41
18:E:118:LEU:HD23	18:E:118:LEU:HA	1.84	0.41
19:F:295:ARG:NH2	19:F:339:ASP:OD2	2.47	0.41
4:V:159:LEU:H	4:V:159:LEU:CD2	2.33	0.41
4:V:324:PHE:O	4:V:328:VAL:HG23	2.20	0.41
4:V:345:ARG:HD3	12:e:43:TRP:CE3	2.55	0.41
5:W:231:ILE:HD11	5:W:246:HIS:HB2	2.01	0.41
5:W:397:VAL:HB	6:X:341:PRO:HB3	2.03	0.41
7:Y:359:PRO:C	7:Y:361:SER:H	2.29	0.41
8:Z:86:ASN:OD1	8:Z:87:ALA:N	2.53	0.41
8:Z:242:LEU:O	8:Z:246:VAL:HG13	2.21	0.41
10:b:116:PRO:HD3	10:b:146:GLU:CG	2.51	0.41
11:d:114:GLU:HG3	11:d:118:ARG:NH1	2.35	0.41
15:c:46:ARG:HD2	15:c:46:ARG:HA	1.80	0.41
15:c:161:ARG:HD2	15:c:201:TYR:OH	2.21	0.41
16:A:214:LEU:HG	16:A:343:PHE:CE1	2.55	0.41
16:A:352:THR:O	16:A:356:LYS:HG2	2.20	0.41
16:A:363:SER:HB3	17:B:214:MET:HE3	2.01	0.41
17:B:298:ASN:OD1	17:B:298:ASN:C	2.62	0.41
4:V:114:TYR:HA	4:V:135:LEU:HD11	2.01	0.41
5:W:239:SER:O	5:W:242:SER:OG	2.38	0.41
6:X:111:LEU:HA	6:X:111:LEU:HD23	1.88	0.41
11:d:171:LEU:HD21	11:d:191:LEU:CD2	2.50	0.41
11:d:215:LEU:HA	11:d:215:LEU:HD23	1.80	0.41
14:U:35:TRP:HA	14:U:38:ILE:HG22	2.02	0.41
14:U:103:LYS:HD2	14:U:103:LYS:C	2.46	0.41
17:B:180:PRO:O	17:B:241:ASN:HB2	2.20	0.41
17:B:365:PHE:CZ	17:B:383:LEU:HB3	2.55	0.41
19:F:367:GLN:HG2	19:F:381:TYR:CE2	2.55	0.41
19:F:376:SER:HB2	19:F:415:LEU:O	2.21	0.41
2:C:370:ALA:CB	2:C:378:VAL:HG22	2.51	0.41
4:V:79:VAL:HA	4:V:82:LEU:HG	2.02	0.41
4:V:180:ARG:HB2	4:V:183:GLU:OE2	2.20	0.41
4:V:372:LEU:H	4:V:372:LEU:HD22	1.86	0.41
4:V:483:CYS:SG	8:Z:268:SER:HB3	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:93:ARG:HB2	5:W:96:GLN:HG2	2.03	0.41
5:W:317:TRP:CD1	5:W:358:VAL:HG11	2.55	0.41
6:X:122:ARG:O	6:X:123:THR:OG1	2.39	0.41
7:Y:106:ALA:O	7:Y:109:GLU:HG3	2.20	0.41
7:Y:223:THR:HA	7:Y:226:VAL:HG12	2.03	0.41
9:a:70:ARG:O	9:a:71:VAL:C	2.64	0.41
11:d:121:LEU:HD13	11:d:121:LEU:HA	1.92	0.41
11:d:137:THR:O	11:d:141:LEU:HG	2.20	0.41
14:U:155:LEU:HD12	14:U:183:LEU:HD23	2.02	0.41
14:U:411:ILE:HG22	14:U:412:HIS:CD2	2.56	0.41
18:E:303:LEU:HA	18:E:304:PRO:HD3	1.95	0.41
19:F:89:LEU:O	19:F:153:VAL:HG22	2.21	0.41
19:F:229:PRO:HA	19:F:333:ASN:HD21	1.86	0.41
3:D:77:GLU:OE1	3:D:77:GLU:C	2.64	0.41
3:D:284:GLU:HA	3:D:284:GLU:OE1	2.21	0.41
4:V:200:ARG:HD3	4:V:203:LEU:HD12	2.03	0.41
4:V:338:LEU:CA	4:V:398:LEU:HD12	2.51	0.41
4:V:404:LYS:O	4:V:407:VAL:HG22	2.20	0.41
5:W:377:ARG:HA	5:W:377:ARG:HD2	1.68	0.41
6:X:47:GLU:O	6:X:51:LEU:HG	2.20	0.41
6:X:263:THR:O	6:X:263:THR:OG1	2.35	0.41
7:Y:107:LYS:O	7:Y:111:LEU:HG	2.20	0.41
7:Y:237:ARG:O	7:Y:241:ILE:HB	2.20	0.41
7:Y:293:ARG:HD3	7:Y:293:ARG:HA	1.76	0.41
8:Z:167:ALA:O	8:Z:170:VAL:HG22	2.21	0.41
9:a:23:HIS:CE1	9:a:27:GLU:OE1	2.74	0.41
9:a:41:VAL:O	9:a:45:VAL:HG23	2.21	0.41
9:a:130:VAL:HG13	9:a:131:THR:N	2.35	0.41
10:b:3:LEU:HB3	10:b:105:HIS:HA	2.02	0.41
10:b:81:LYS:HE3	10:b:81:LYS:HB2	1.77	0.41
10:b:131:LEU:HD22	10:b:136:VAL:HB	2.02	0.41
11:d:148:LEU:HD22	11:d:167:TYR:CD1	2.56	0.41
11:d:196:LEU:HB3	11:d:208:PHE:HE2	1.86	0.41
11:d:197:LEU:HD13	11:d:256:TYR:CD2	2.56	0.41
14:U:52:GLU:HA	14:U:57:ARG:HD3	2.03	0.41
14:U:412:HIS:ND1	14:U:422:LEU:HD21	2.36	0.41
14:U:457:ILE:HA	14:U:457:ILE:HD13	1.83	0.41
14:U:588:MET:CE	14:U:764:LEU:HD22	2.51	0.41
16:A:206:ILE:HD13	19:F:405:MET:CE	2.50	0.41
17:B:303:ARG:HB3	17:B:307:ARG:NH1	2.35	0.41
18:E:185:ARG:HG2	19:F:320:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:E:352:MET:HE1	19:F:350:ARG:HH22	1.86	0.41
19:F:297:ASP:O	19:F:298:SER:OG	2.36	0.41
19:F:424:ILE:HG13	19:F:425:LEU:N	2.36	0.41
2:C:313:ARG:HH21	17:B:404:LEU:HD13	1.85	0.41
4:V:166:TYR:O	4:V:169:LEU:HB3	2.21	0.41
5:W:136:ILE:O	5:W:139:GLU:HG2	2.20	0.41
7:Y:14:ASN:HA	7:Y:15:PRO:HA	1.84	0.41
7:Y:71:ASN:OD1	7:Y:72:LYS:N	2.54	0.41
7:Y:218:THR:O	7:Y:222:TYR:HB2	2.21	0.41
11:d:281:LYS:HE3	11:d:315:TYR:HB3	2.02	0.41
11:d:313:ASN:O	11:d:315:TYR:HD1	2.03	0.41
14:U:208:LEU:O	14:U:211:PRO:HD3	2.20	0.41
14:U:452:ASN:HD21	14:U:757:MET:HE1	1.86	0.41
16:A:86:THR:HG22	17:B:102:LEU:HD13	2.02	0.41
17:B:290:ILE:HG12	17:B:305:ILE:HD12	2.03	0.41
18:E:342:ASP:HA	18:E:345:ASN:HB3	2.03	0.41
4:V:421:ASP:OD1	4:V:421:ASP:N	2.53	0.40
5:W:97:LEU:O	5:W:101:VAL:HG23	2.20	0.40
5:W:203:GLN:O	5:W:206:SER:OG	2.39	0.40
6:X:204:PRO:O	6:X:207:GLN:HG2	2.21	0.40
7:Y:77:ASN:HD21	7:Y:114:ILE:HG22	1.86	0.40
7:Y:169:GLU:OE2	7:Y:169:GLU:HA	2.21	0.40
7:Y:361:SER:O	7:Y:365:GLN:HG3	2.21	0.40
8:Z:216:ALA:HA	9:a:343:LEU:HD11	2.03	0.40
14:U:42:VAL:HG22	14:U:46:GLU:HG3	2.03	0.40
14:U:236:LEU:HG	14:U:245:ALA:HB2	2.02	0.40
14:U:351:MET:HE3	14:U:351:MET:HB3	1.89	0.40
14:U:892:LEU:HD23	14:U:906:LEU:HB3	2.03	0.40
17:B:162:VAL:HG22	17:B:163:LEU:H	1.86	0.40
17:B:273:VAL:HG22	17:B:277:HIS:NE2	2.36	0.40
18:E:285:LEU:HD23	18:E:285:LEU:HA	1.88	0.40
18:E:312:ILE:O	18:E:315:ILE:HG22	2.20	0.40
2:C:161:ILE:HG13	2:C:165:ILE:HD12	2.03	0.40
4:V:260:HIS:C	4:V:260:HIS:CD2	2.99	0.40
5:W:307:LYS:HA	5:W:310:THR:HG22	2.02	0.40
6:X:148:HIS:CE1	6:X:149:LEU:HG	2.57	0.40
9:a:292:THR:HG23	9:a:295:GLU:HB3	2.03	0.40
11:d:98:LEU:HG	11:d:115:GLU:HB3	2.03	0.40
11:d:135:LYS:HB2	11:d:181:GLN:HB3	2.02	0.40
16:A:85:GLN:OE1	16:A:89:SER:HB3	2.20	0.40
16:A:271:LEU:HD12	16:A:316:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:404:LEU:HA	17:B:404:LEU:HD23	1.82	0.40
18:E:214:LEU:HD23	18:E:214:LEU:HA	1.94	0.40
3:D:167:ILE:CG2	3:D:174:LYS:HD2	2.49	0.40
4:V:169:LEU:HA	4:V:172:VAL:HG12	2.02	0.40
5:W:35:ALA:HB3	5:W:73:MET:HE3	2.03	0.40
6:X:259:ILE:HG12	6:X:291:ALA:HB2	2.04	0.40
9:a:111:VAL:O	9:a:115:LYS:HG3	2.22	0.40
9:a:284:ARG:HG3	9:a:285:PRO:HD2	2.03	0.40
10:b:147:GLU:HG3	10:b:149:ASN:OD1	2.22	0.40
14:U:346:ASN:ND2	14:U:380:THR:OG1	2.54	0.40
16:A:393:GLY:O	16:A:397:ILE:HG12	2.21	0.40
18:E:308:ALA:O	18:E:312:ILE:HG13	2.22	0.40
2:C:375:ARG:NH2	2:C:382:ASP:OD2	2.55	0.40
4:V:391:THR:HA	4:V:394:LEU:HD12	2.02	0.40
5:W:95:SER:O	5:W:95:SER:OG	2.32	0.40
5:W:117:ASP:O	5:W:121:LYS:CB	2.63	0.40
5:W:371:THR:OG1	5:W:416:GLN:OE1	2.39	0.40
6:X:69:LEU:O	6:X:73:VAL:HG13	2.22	0.40
6:X:192:SER:O	6:X:196:THR:HG23	2.21	0.40
6:X:300:ALA:O	6:X:303:GLU:HG2	2.21	0.40
6:X:378:LEU:C	7:Y:312:ARG:NH2	2.79	0.40
7:Y:73:MET:O	7:Y:77:ASN:HB2	2.22	0.40
7:Y:295:TYR:CZ	7:Y:299:MET:HE3	2.57	0.40
8:Z:77:ASN:HB2	15:c:98:MET:HE1	2.03	0.40
8:Z:129:LYS:HE3	8:Z:129:LYS:HB3	1.94	0.40
10:b:122:LYS:HZ3	10:b:122:LYS:H	1.68	0.40
12:e:27:TRP:HB3	12:e:30:LEU:HD13	2.03	0.40
14:U:573:ASP:OD1	14:U:574:LYS:N	2.54	0.40
16:A:74:PRO:O	16:A:78:TRP:CB	2.67	0.40
18:E:295:LEU:HD23	18:E:295:LEU:HA	1.85	0.40
18:E:367:PHE:O	18:E:371:VAL:HG13	2.21	0.40
2:C:107:ASP:OD1	2:C:107:ASP:N	2.53	0.40
3:D:68:LEU:HD23	3:D:68:LEU:HA	1.89	0.40
3:D:238:LYS:HA	18:E:208:ILE:HG13	2.03	0.40
3:D:297:ASP:OD1	3:D:297:ASP:N	2.54	0.40
4:V:192:MET:SD	4:V:214:HIS:CE1	3.15	0.40
5:W:60:MET:HA	5:W:97:LEU:HD12	2.03	0.40
5:W:374:THR:HG22	5:W:411:GLY:O	2.21	0.40
5:W:440:ASN:O	5:W:443:THR:OG1	2.34	0.40
7:Y:50:MET:O	7:Y:54:TYR:HB2	2.21	0.40
7:Y:228:MET:HE3	7:Y:228:MET:HB2	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:289:ALA:O	7:Y:292:TYR:HD2	2.05	0.40
10:b:16:MET:HE2	10:b:16:MET:HA	2.03	0.40
10:b:22:LEU:HD12	10:b:28:ALA:HB2	2.04	0.40
10:b:184:ILE:HG13	10:b:184:ILE:O	2.21	0.40
11:d:196:LEU:HB3	11:d:208:PHE:CE2	2.56	0.40
11:d:293:PHE:HD2	11:d:299:MET:SD	2.45	0.40
14:U:692:ALA:HB2	14:U:733:ALA:HB1	2.03	0.40
15:c:145:VAL:HG22	15:c:157:ILE:HD12	2.02	0.40
17:B:201:VAL:HB	17:B:326:LYS:HG3	2.03	0.40
17:B:336:THR:C	17:B:337:LEU:HD22	2.47	0.40
18:E:178:THR:HB	18:E:301:ILE:HG22	2.04	0.40
18:E:364:GLN:O	18:E:368:MET:HG2	2.21	0.40
19:F:100:ASP:N	19:F:100:ASP:OD1	2.54	0.40
19:F:430:LYS:HG2	19:F:431:LYS:N	2.36	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	f	82/856 (10%)	81 (99%)	1 (1%)	0	100	100
2	C	360/406 (89%)	325 (90%)	34 (9%)	1 (0%)	36	64
3	D	378/418 (90%)	351 (93%)	26 (7%)	1 (0%)	36	64
4	V	440/534 (82%)	418 (95%)	21 (5%)	1 (0%)	43	70
5	W	438/456 (96%)	411 (94%)	27 (6%)	0	100	100
6	X	382/422 (90%)	370 (97%)	11 (3%)	1 (0%)	36	64
7	Y	372/389 (96%)	349 (94%)	22 (6%)	1 (0%)	36	64
8	Z	284/324 (88%)	274 (96%)	9 (3%)	1 (0%)	30	58
9	a	371/376 (99%)	336 (91%)	31 (8%)	4 (1%)	11	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	b	189/377 (50%)	169 (89%)	18 (10%)	2 (1%)	11	39
11	d	268/350 (77%)	247 (92%)	18 (7%)	3 (1%)	11	39
12	e	46/70 (66%)	34 (74%)	10 (22%)	2 (4%)	2	16
14	U	812/953 (85%)	780 (96%)	32 (4%)	0	100	100
15	c	291/590 (49%)	278 (96%)	12 (4%)	1 (0%)	36	64
16	A	364/433 (84%)	324 (89%)	39 (11%)	1 (0%)	36	64
17	B	338/440 (77%)	303 (90%)	32 (10%)	3 (1%)	14	43
18	E	345/389 (89%)	326 (94%)	17 (5%)	2 (1%)	21	51
19	F	370/439 (84%)	337 (91%)	31 (8%)	2 (0%)	24	55
All	All	6130/8222 (75%)	5713 (93%)	391 (6%)	26 (0%)	31	58

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	Y	98	SER
8	Z	149	THR
11	d	283	LEU
15	c	262	GLU
16	A	82	ALA
17	B	117	ASP
19	F	179	GLU
2	C	90	HIS
9	a	69	HIS
17	B	191	ASP
3	D	368	ASP
9	a	222	LEU
18	E	386	TYR
11	d	282	ILE
6	X	123	THR
9	a	73	PRO
10	b	22	LEU
11	d	284	PHE
12	e	39	TRP
12	e	42	ASN
19	F	300	LYS
4	V	497	PRO
18	E	127	PRO
9	a	71	VAL
17	B	354	PRO

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Mol	Chain	Res	Type
10	b	148	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	f	70/690 (10%)	69 (99%)	1 (1%)	59	68
2	C	315/352 (90%)	313 (99%)	2 (1%)	78	78
3	D	333/366 (91%)	331 (99%)	2 (1%)	78	78
4	V	388/460 (84%)	385 (99%)	3 (1%)	73	74
5	W	404/416 (97%)	401 (99%)	3 (1%)	76	76
6	X	330/362 (91%)	328 (99%)	2 (1%)	78	78
7	Y	333/344 (97%)	330 (99%)	3 (1%)	70	73
8	Z	257/295 (87%)	257 (100%)	0	100	100
9	a	333/336 (99%)	332 (100%)	1 (0%)	86	81
10	b	167/312 (54%)	166 (99%)	1 (1%)	78	78
11	d	237/294 (81%)	236 (100%)	1 (0%)	84	79
12	e	43/63 (68%)	43 (100%)	0	100	100
14	U	695/816 (85%)	690 (99%)	5 (1%)	76	76
15	c	257/500 (51%)	257 (100%)	0	100	100
16	A	310/372 (83%)	307 (99%)	3 (1%)	68	72
17	B	296/385 (77%)	294 (99%)	2 (1%)	76	76
18	E	298/341 (87%)	296 (99%)	2 (1%)	76	76
19	F	316/379 (83%)	314 (99%)	2 (1%)	78	78
All	All	5382/7083 (76%)	5349 (99%)	33 (1%)	76	78

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	f	88	PHE

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Mol	Chain	Res	Type
2	C	109	THR
2	C	360	LYS
3	D	50	GLU
3	D	414	HIS
4	V	396	ILE
4	V	421	ASP
4	V	453	HIS
5	W	67	LEU
5	W	192	LEU
5	W	194	LEU
6	X	315	ASP
6	X	378	LEU
7	Y	143	TYR
7	Y	206	SER
7	Y	389	MET
9	a	125	ILE
10	b	41	THR
11	d	251	ILE
14	U	252	LEU
14	U	326	ILE
14	U	386	LEU
14	U	788	VAL
14	U	897	THR
16	A	83	ASP
16	A	101	ILE
16	A	403	ILE
17	B	125	THR
17	B	144	LEU
18	E	127	PRO
18	E	158	LEU
19	F	405	MET
19	F	416	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	f	36	HIS
1	f	62	GLN
2	C	46	GLN
2	C	53	ASN
2	C	64	GLN
2	C	171	HIS

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Mol	Chain	Res	Type
2	C	380	GLN
3	D	57	GLN
3	D	67	ASN
3	D	127	ASN
3	D	135	HIS
3	D	137	ASN
3	D	173	GLN
3	D	187	HIS
3	D	222	HIS
3	D	294	ASN
3	D	301	GLN
3	D	353	ASN
3	D	380	GLN
4	V	125	ASN
4	V	198	GLN
4	V	214	HIS
4	V	247	GLN
4	V	260	HIS
4	V	299	GLN
4	V	319	HIS
4	V	329	HIS
4	V	347	GLN
4	V	377	GLN
4	V	401	ASN
4	V	487	HIS
4	V	488	ASN
5	W	26	GLN
5	W	84	ASN
5	W	86	ASN
5	W	236	HIS
5	W	246	HIS
5	W	257	GLN
5	W	395	ASN
5	W	454	ASN
6	X	105	GLN
6	X	144	GLN
6	X	329	ASN
6	X	334	ASN
6	X	346	GLN
7	Y	31	HIS
7	Y	154	ASN
7	Y	160	ASN

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Mol	Chain	Res	Type
7	Y	196	GLN
7	Y	306	GLN
7	Y	367	GLN
8	Z	157	HIS
8	Z	194	GLN
9	a	62	ASN
9	a	69	HIS
9	a	164	GLN
9	a	193	GLN
9	a	194	GLN
9	a	231	GLN
9	a	244	ASN
9	a	290	GLN
10	b	29	GLN
10	b	44	ASN
10	b	76	HIS
10	b	101	GLN
10	b	105	HIS
10	b	137	ASN
11	d	189	HIS
11	d	195	ASN
11	d	314	ASN
14	U	28	ASN
14	U	58	GLN
14	U	149	GLN
14	U	195	ASN
14	U	267	ASN
14	U	346	ASN
14	U	347	ASN
14	U	389	ASN
14	U	452	ASN
14	U	527	GLN
14	U	665	ASN
14	U	685	GLN
14	U	698	GLN
14	U	718	ASN
14	U	749	GLN
14	U	901	GLN
15	c	128	ASN
15	c	183	HIS
15	c	241	ASN
15	c	274	ASN

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Mol	Chain	Res	Type
15	c	283	HIS
15	c	287	HIS
15	c	295	ASN
15	c	312	ASN
16	A	296	GLN
17	B	131	HIS
17	B	207	HIS
18	E	225	HIS
19	F	243	GLN
19	F	367	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
21	ATP	E	401	23	32,33,33	0.40	0	48,52,52	0.28	0
21	ATP	A	501	-	32,33,33	0.29	0	48,52,52	0.35	0
20	ADP	C	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.82	7 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	ADP	F	501	23	28,29,29	1.38	4 (14%)	43,45,45	1.87	9 (20%)
21	ATP	B	501	23	32,33,33	0.30	0	48,52,52	0.28	0
21	ATP	D	501	-	32,33,33	0.42	0	48,52,52	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	ATP	E	401	23	-	3/22/38/38	0/3/3/3
21	ATP	A	501	-	-	7/22/38/38	0/3/3/3
20	ADP	C	501	-	-	2/16/32/32	0/3/3/3
20	ADP	F	501	23	-	3/16/32/32	0/3/3/3
21	ATP	B	501	23	-	3/22/38/38	0/3/3/3
21	ATP	D	501	-	-	3/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	501	ADP	C5-C4	4.65	1.47	1.39
20	F	501	ADP	C5-C4	4.55	1.47	1.39
20	C	501	ADP	C5-C6	2.59	1.48	1.41
20	F	501	ADP	C5-C6	2.55	1.48	1.41
20	C	501	ADP	C5-N7	-2.42	1.34	1.39
20	F	501	ADP	C5-N7	-2.37	1.34	1.39
20	F	501	ADP	C8-N7	2.18	1.35	1.31
20	C	501	ADP	C8-N7	2.13	1.35	1.31

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	501	ADP	C5-C4-N3	-6.13	118.28	126.72
20	F	501	ADP	C5-C4-N3	-5.94	118.54	126.72
20	C	501	ADP	N3-C4-N9	5.05	135.75	127.17
20	F	501	ADP	N3-C4-N9	4.86	135.44	127.17
20	F	501	ADP	C2-N3-C4	3.83	121.19	111.83
20	C	501	ADP	C2-N3-C4	3.76	121.02	111.83
20	F	501	ADP	N3-C2-N1	-3.45	123.36	128.58
20	F	501	ADP	C4-C5-N7	-3.23	106.88	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	501	ADP	C4-C5-N7	-3.22	106.90	110.58
20	C	501	ADP	N3-C2-N1	-3.15	123.81	128.58
20	F	501	ADP	C4-N9-C8	2.73	108.60	105.74
20	C	501	ADP	C4-N9-C8	2.58	108.45	105.74
20	F	501	ADP	C5-N7-C8	2.48	107.34	103.45
20	C	501	ADP	C5-N7-C8	2.33	107.11	103.45
20	F	501	ADP	C5'-C4'-C3'	-2.06	107.79	115.21
20	F	501	ADP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	F	501	ADP	C5'-O5'-PA-O1A
20	F	501	ADP	C5'-O5'-PA-O2A
20	F	501	ADP	C5'-O5'-PA-O3A
21	D	501	ATP	C5'-O5'-PA-O1A
21	A	501	ATP	C5'-O5'-PA-O2A
21	A	501	ATP	C5'-O5'-PA-O3A
21	B	501	ATP	C5'-O5'-PA-O1A
21	B	501	ATP	C5'-O5'-PA-O2A
21	B	501	ATP	C5'-O5'-PA-O3A
20	C	501	ADP	C3'-C4'-C5'-O5'
21	E	401	ATP	C3'-C4'-C5'-O5'
20	C	501	ADP	O4'-C4'-C5'-O5'
21	E	401	ATP	O4'-C4'-C5'-O5'
21	D	501	ATP	C5'-O5'-PA-O2A
21	D	501	ATP	C5'-O5'-PA-O3A
21	A	501	ATP	PA-O3A-PB-O2B
21	A	501	ATP	C2'-C1'-N9-C8
21	A	501	ATP	C2'-C1'-N9-C4
21	E	401	ATP	PB-O3B-PG-O1G
21	A	501	ATP	C3'-C4'-C5'-O5'
21	A	501	ATP	PA-O3A-PB-O1B

There are no ring outliers.

5 monomers are involved in 10 short contacts:

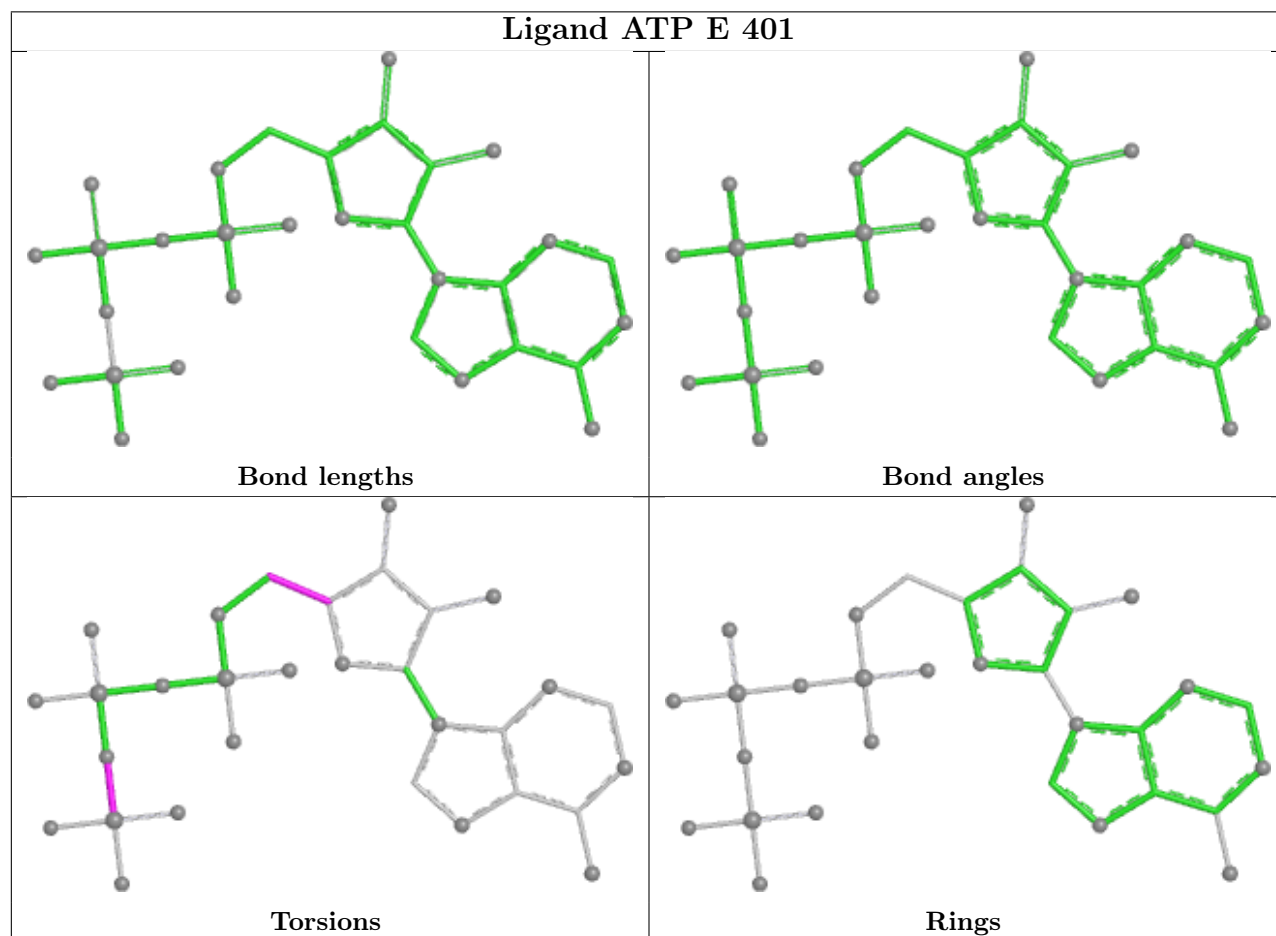
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	E	401	ATP	3	0
21	A	501	ATP	2	0

Continued on next page...

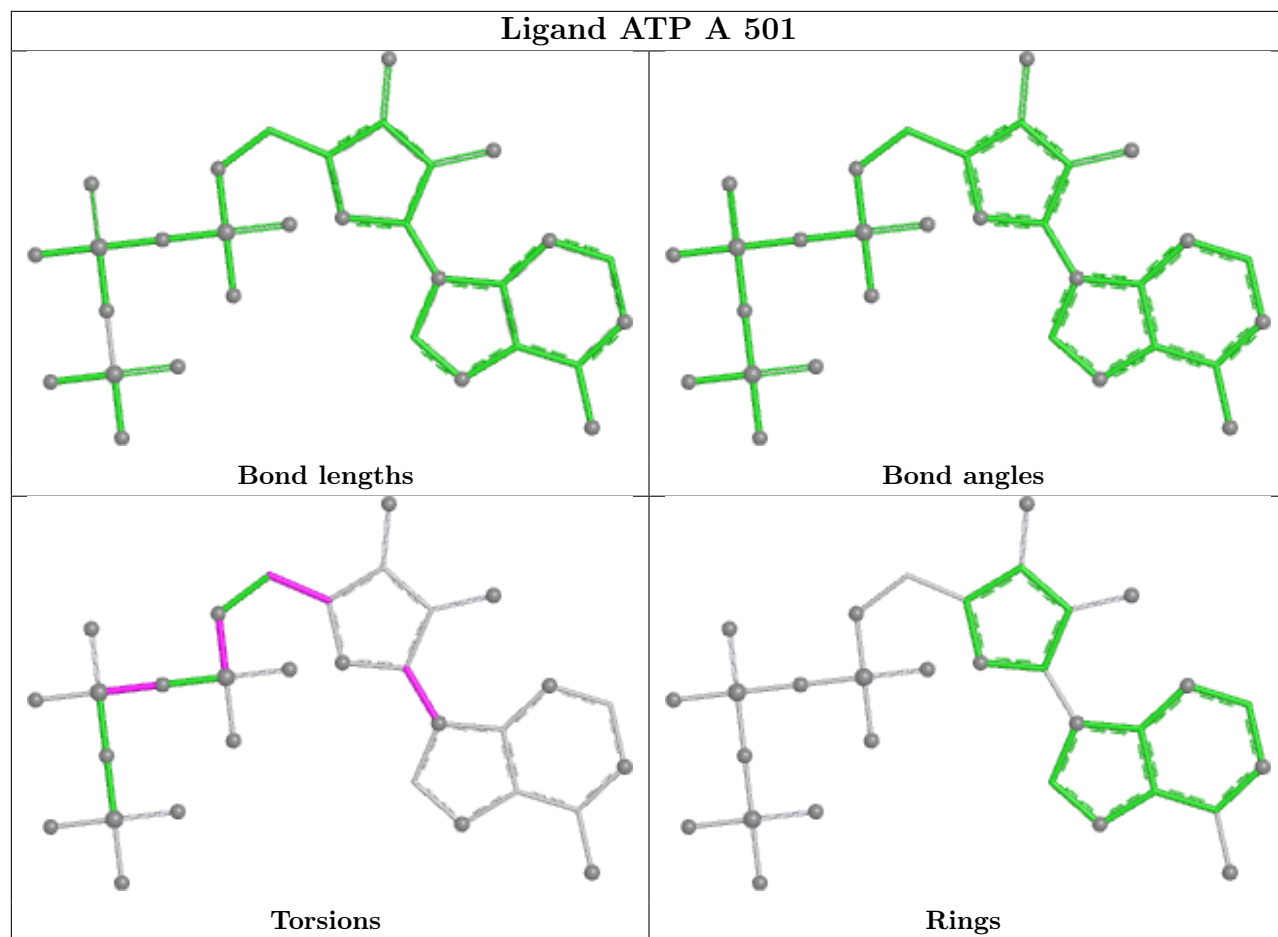
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	501	ADP	1	0
20	F	501	ADP	1	0
21	B	501	ATP	3	0

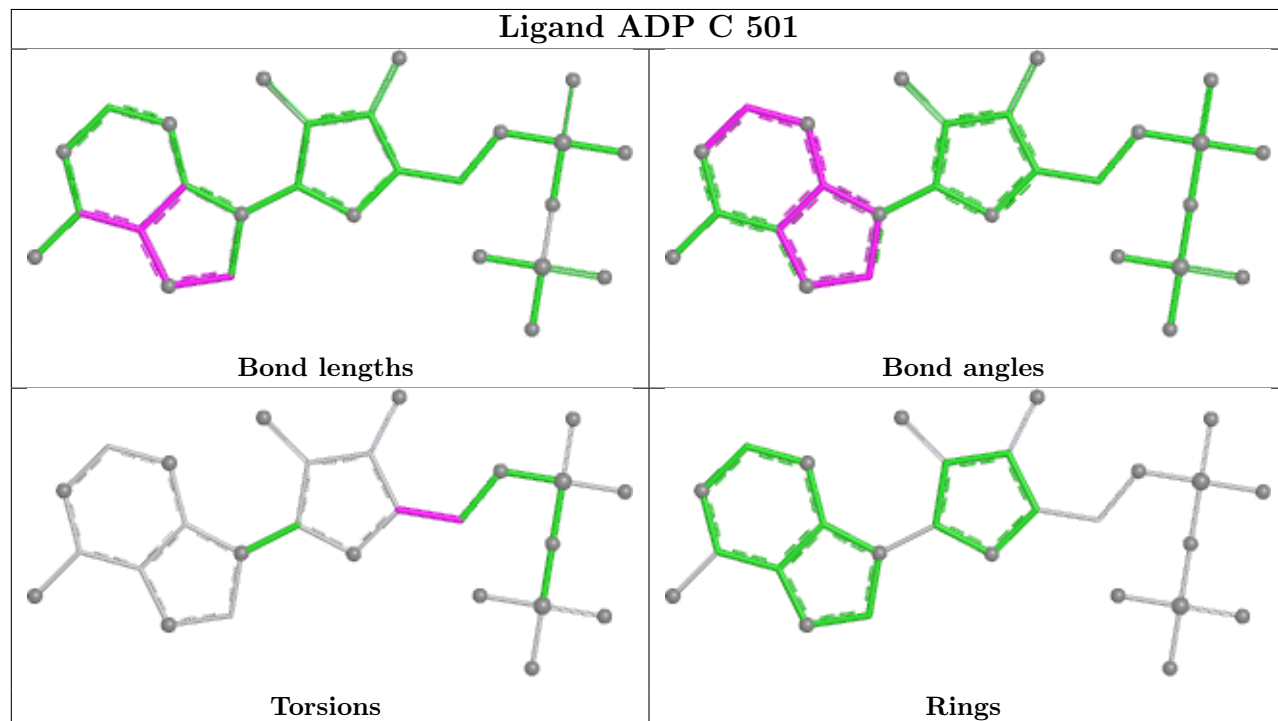
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

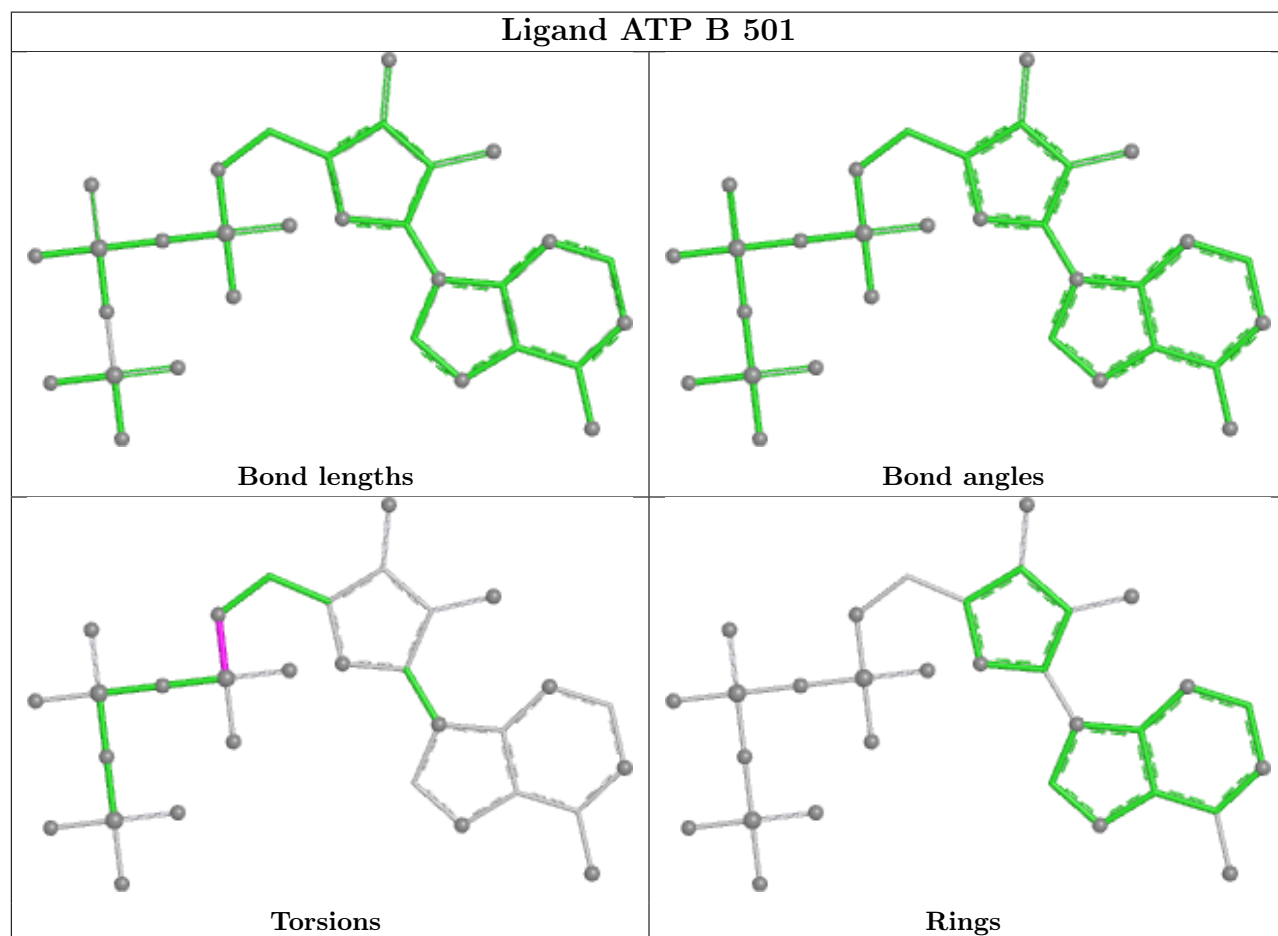
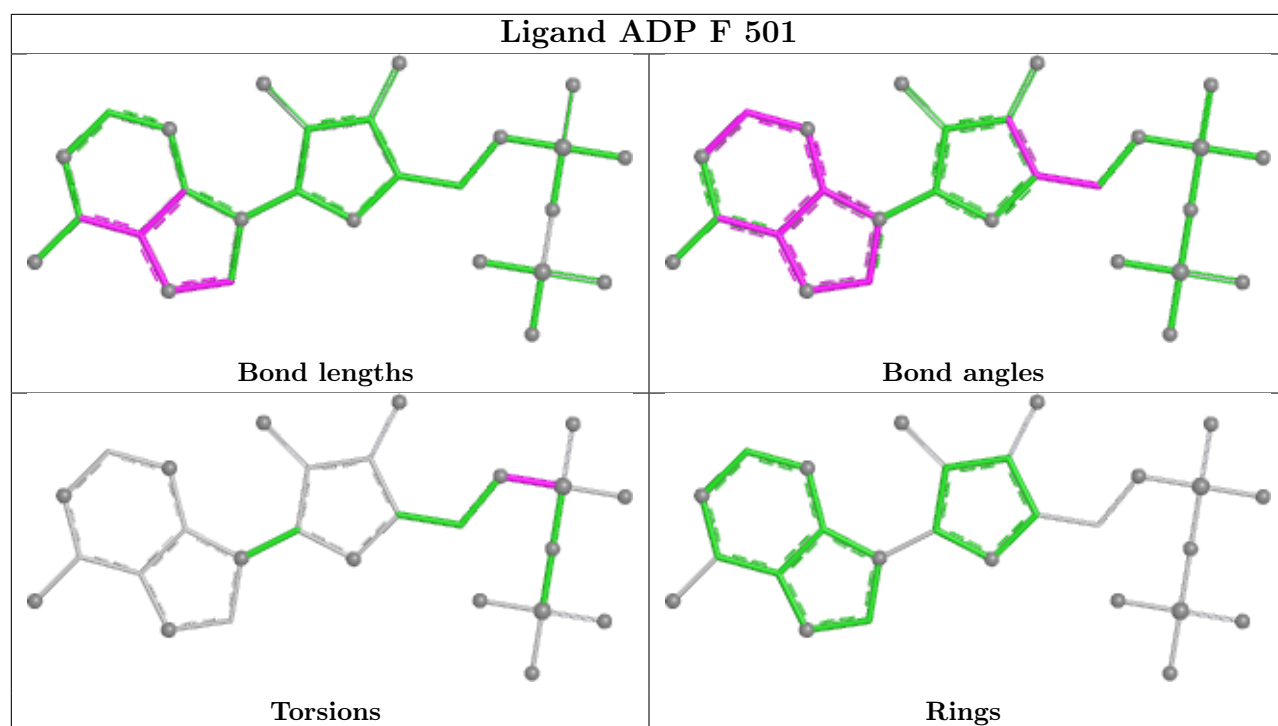


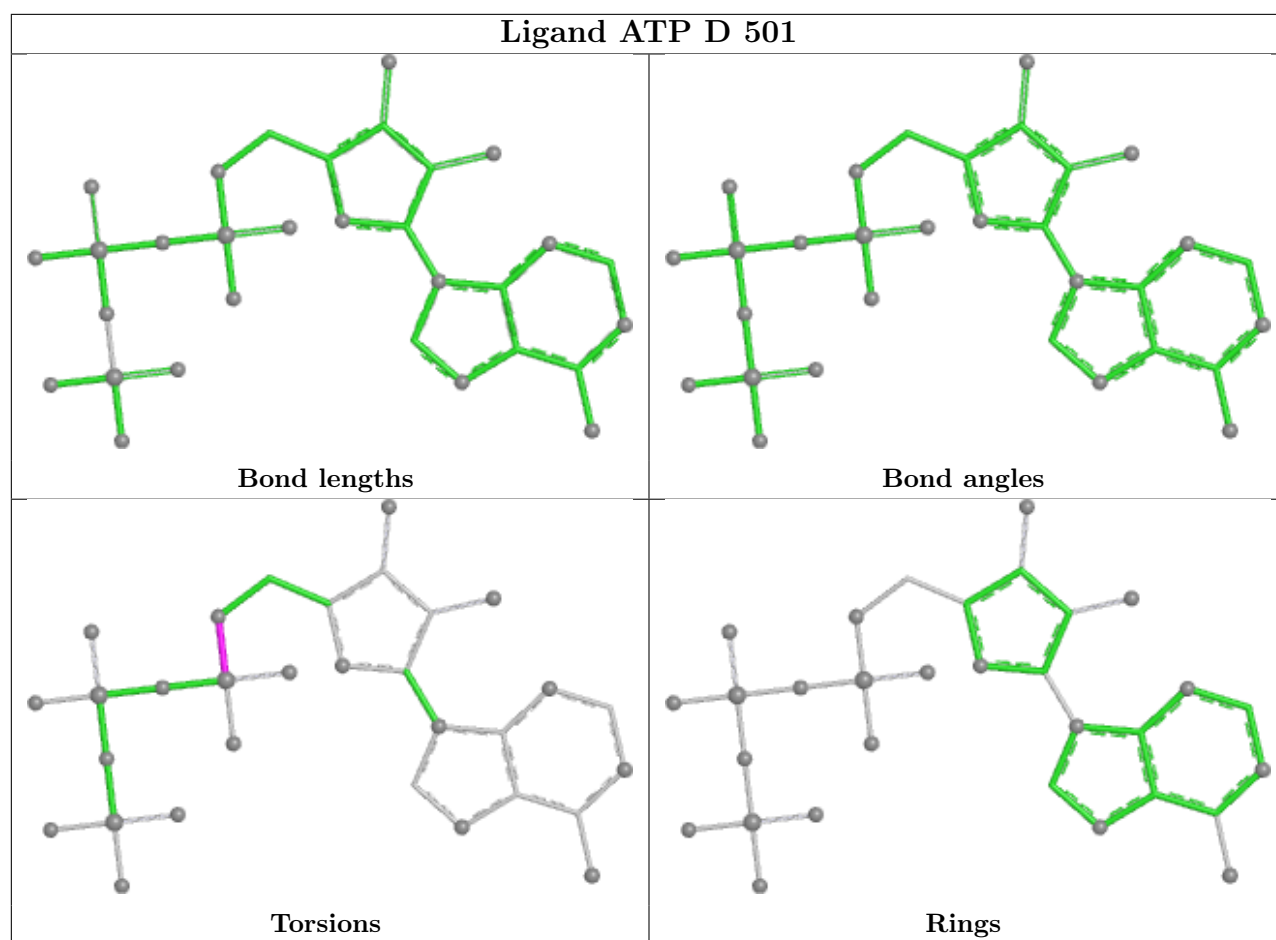
Ligand ATP A 501



Ligand ADP C 501







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.

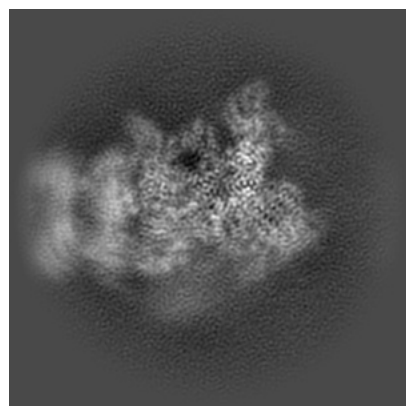
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65595. These allow visual inspection of the internal detail of the map and identification of artifacts.

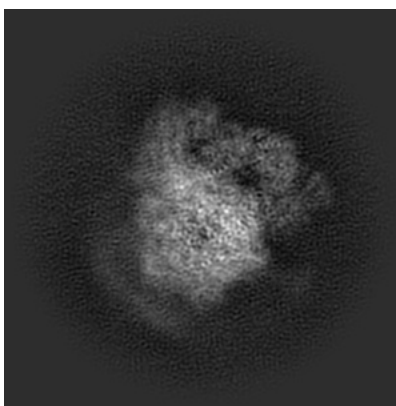
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

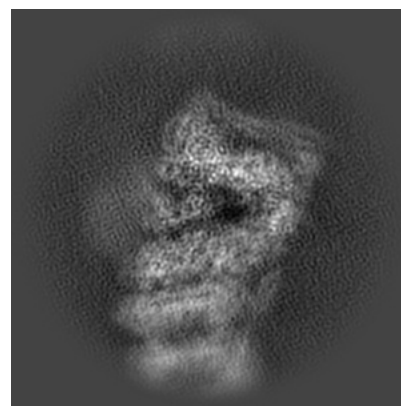
6.1.1 Primary map



X

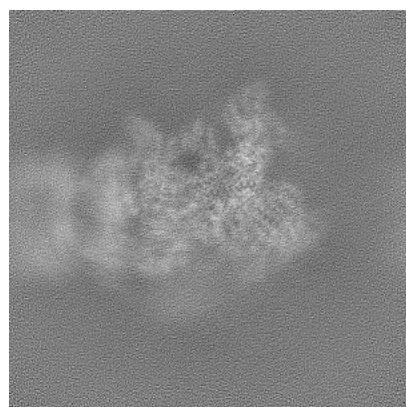


Y

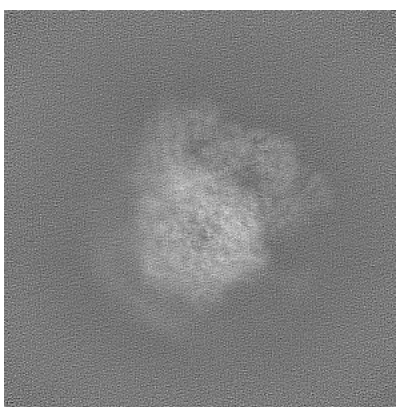


Z

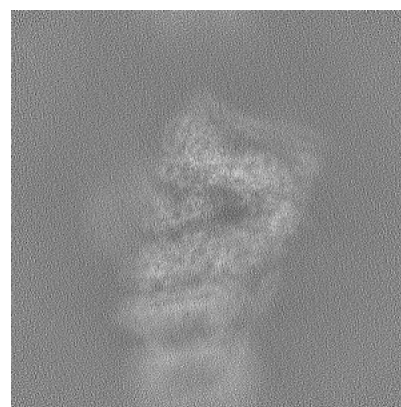
6.1.2 Raw map



X



Y

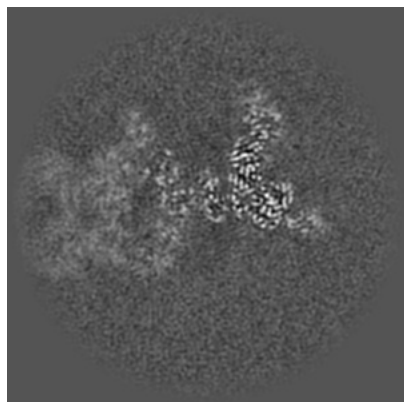


Z

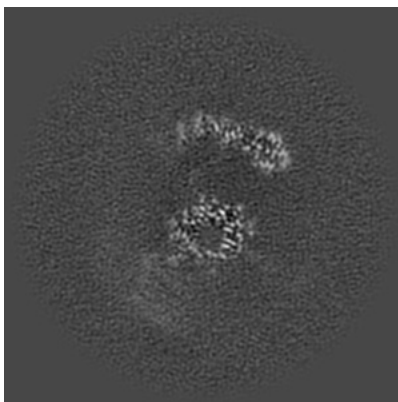
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

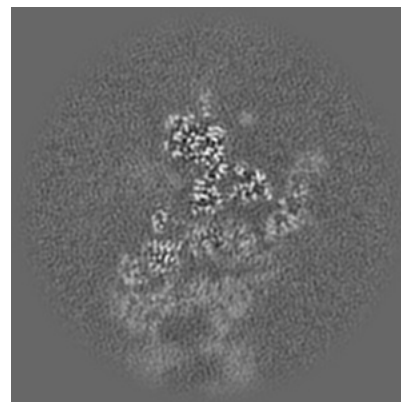
6.2.1 Primary map



X Index: 200

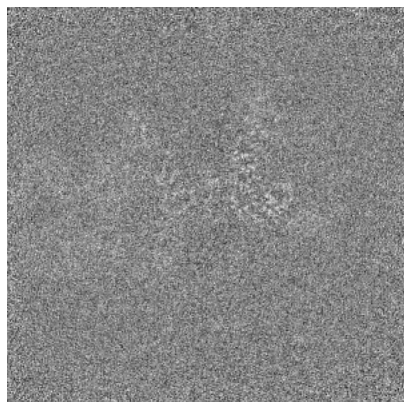


Y Index: 200

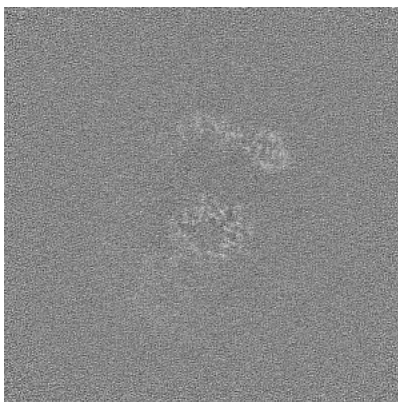


Z Index: 200

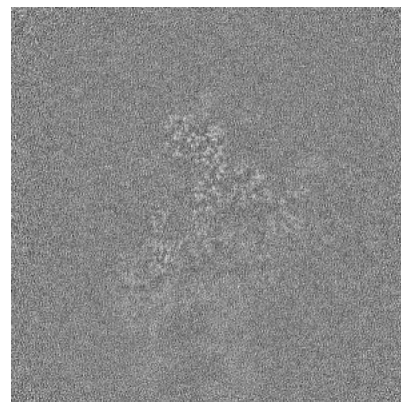
6.2.2 Raw map



X Index: 200



Y Index: 200

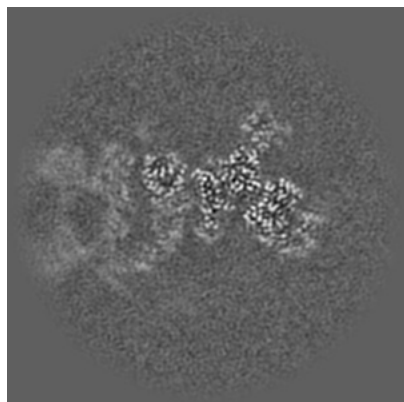


Z Index: 200

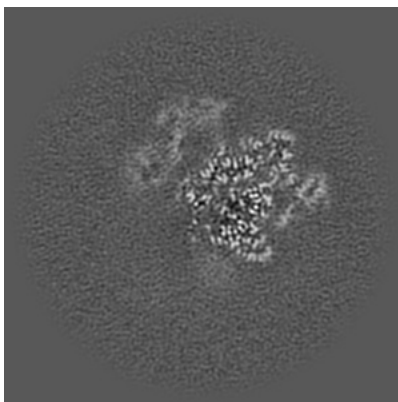
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

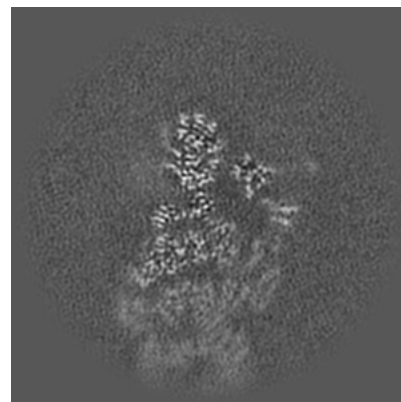
6.3.1 Primary map



X Index: 185

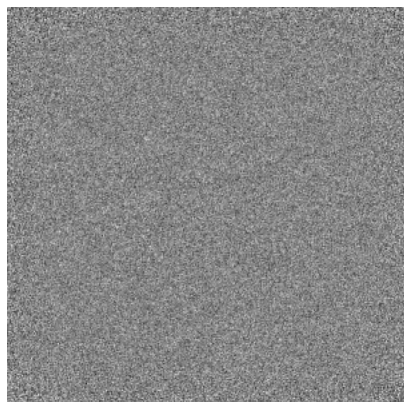


Y Index: 237

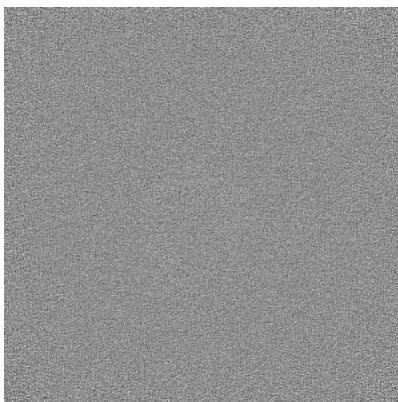


Z Index: 217

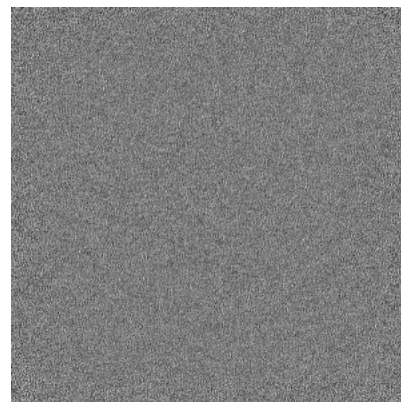
6.3.2 Raw map



X Index: 0



Y Index: 0

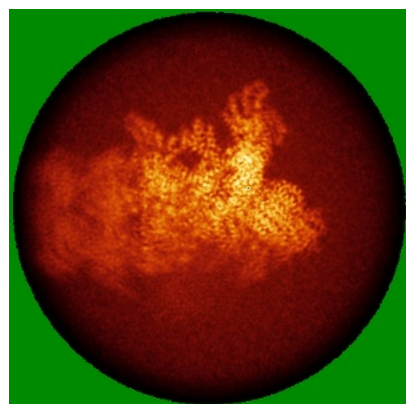


Z Index: 0

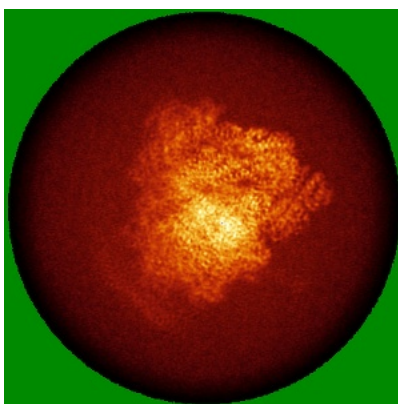
The images above show the largest variance slices of the map in three orthogonal directions.

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

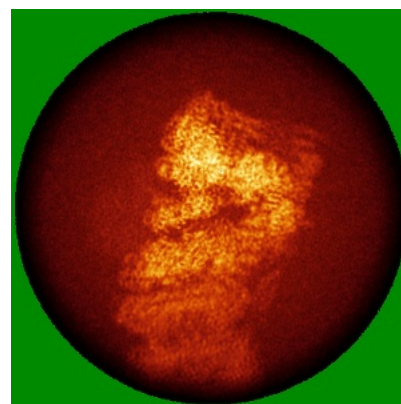
6.4.1 Primary map



X

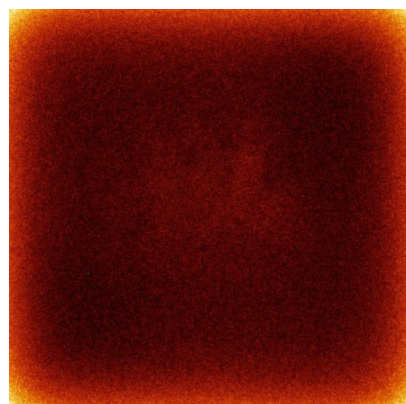


Y

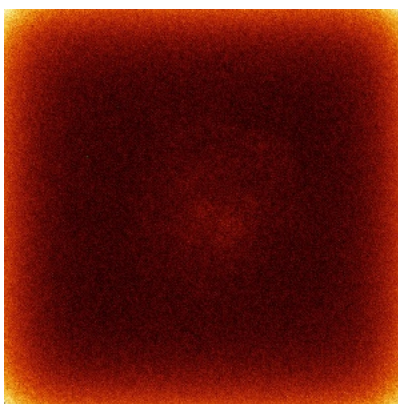


Z

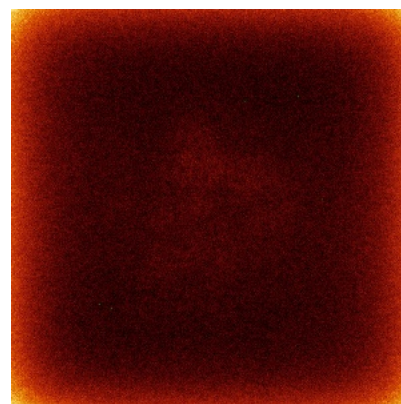
6.4.2 Raw map



X



Y

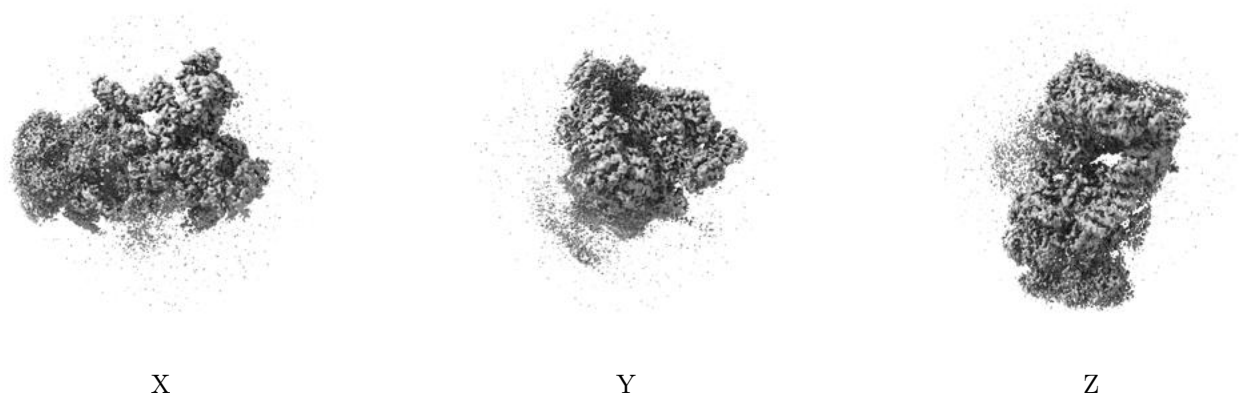


Z

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.

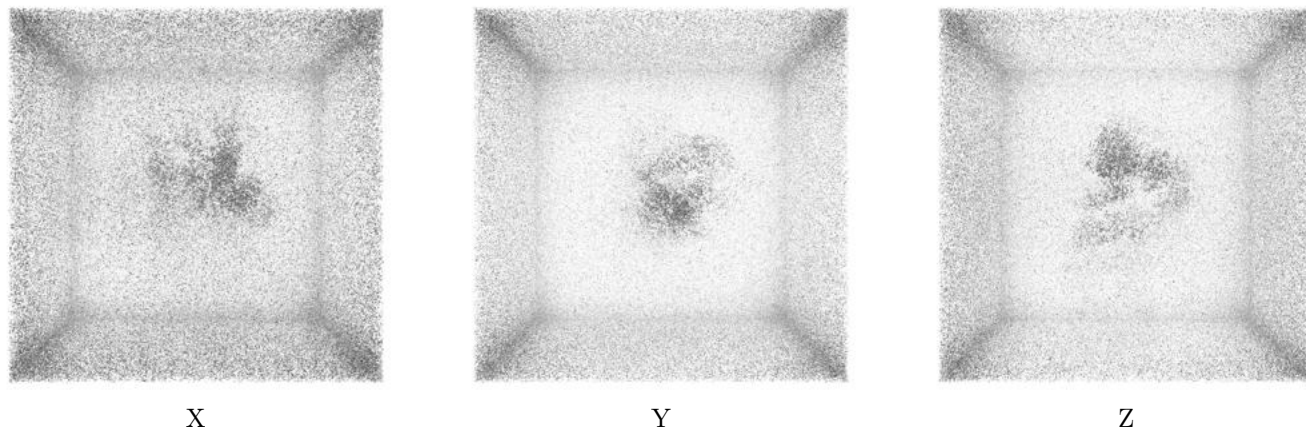
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.081. 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.

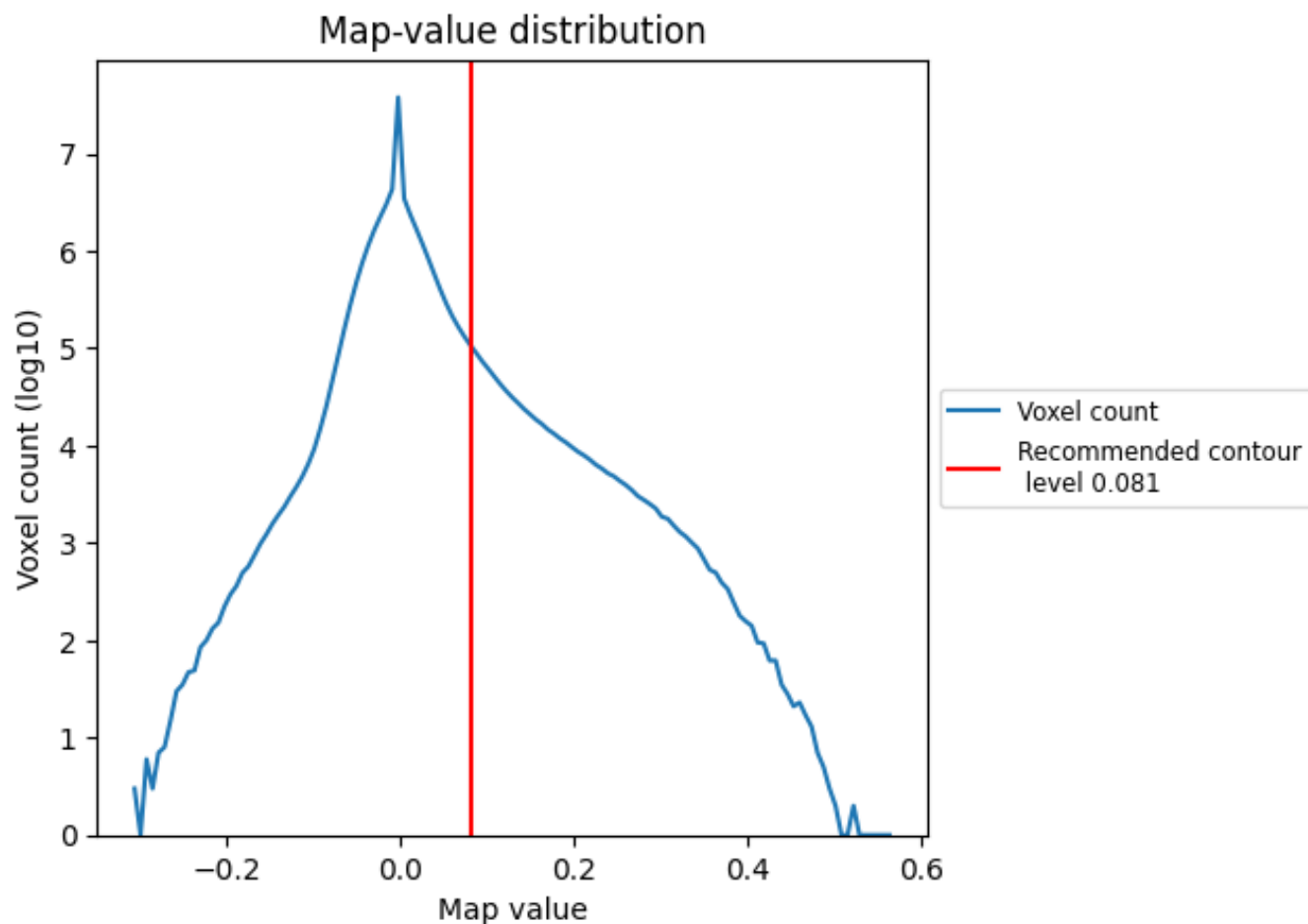
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

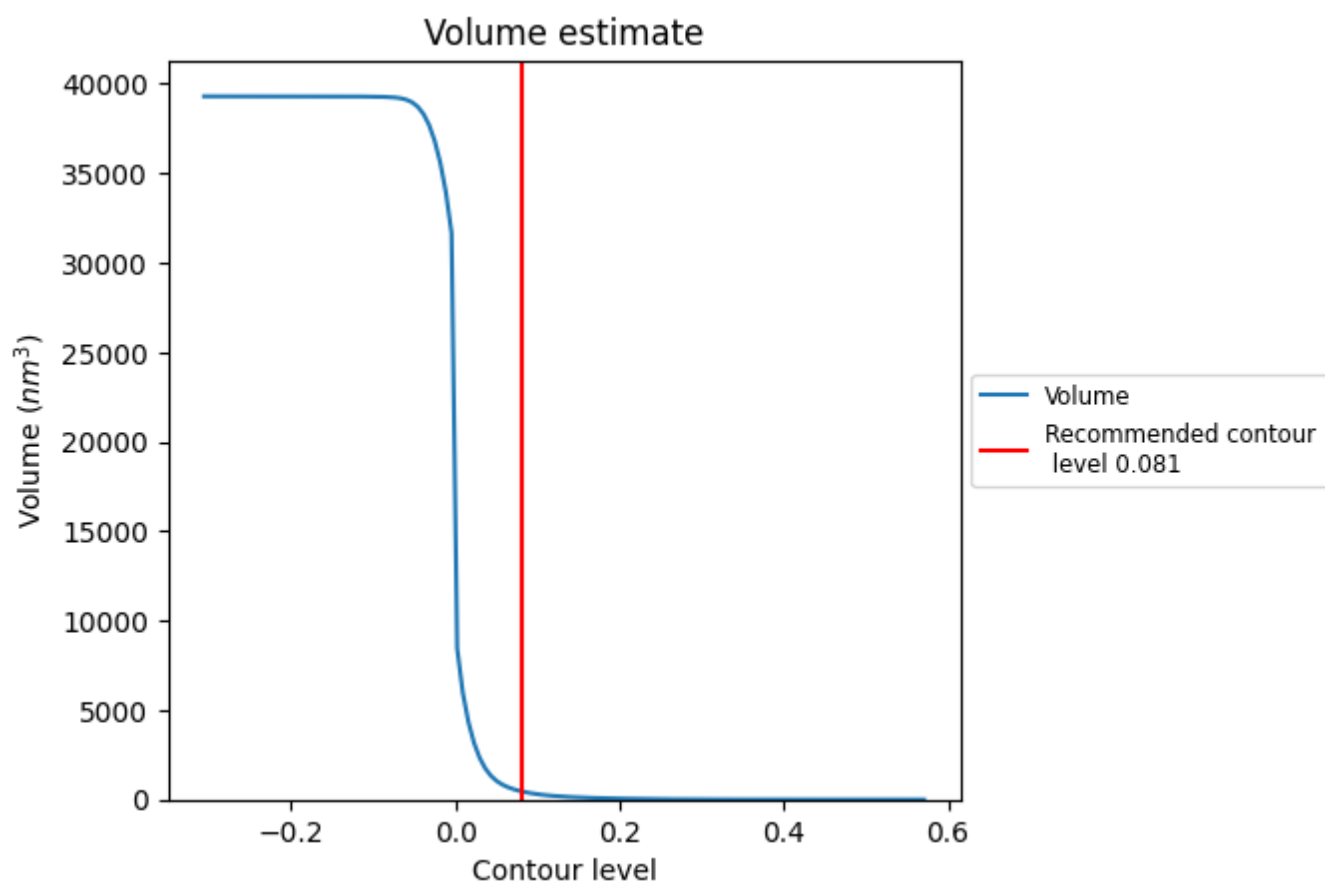
This section contains the results of statistical analysis of the map.

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.

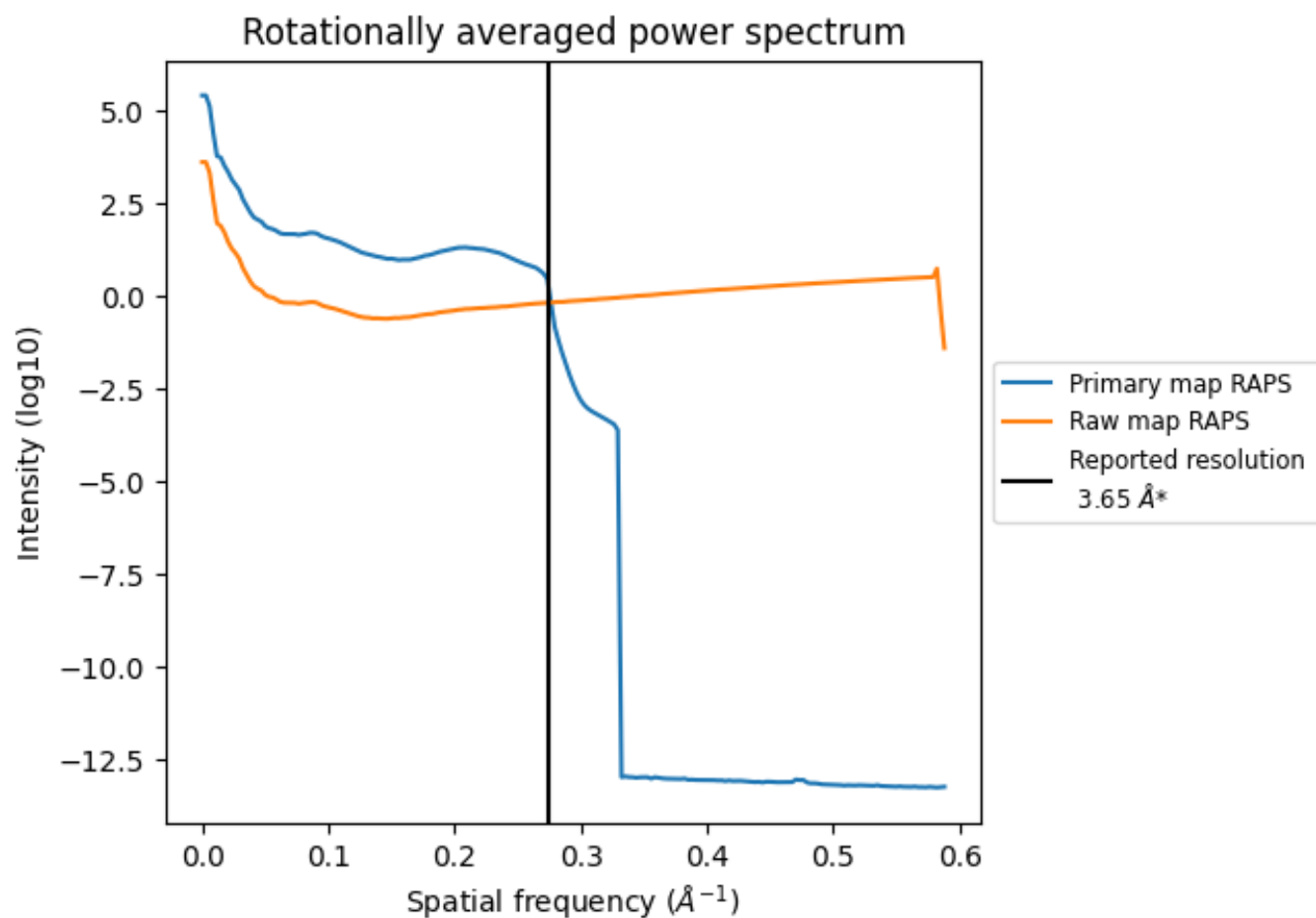
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 455 nm³; this corresponds to an approximate mass of 411 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 ⓘ

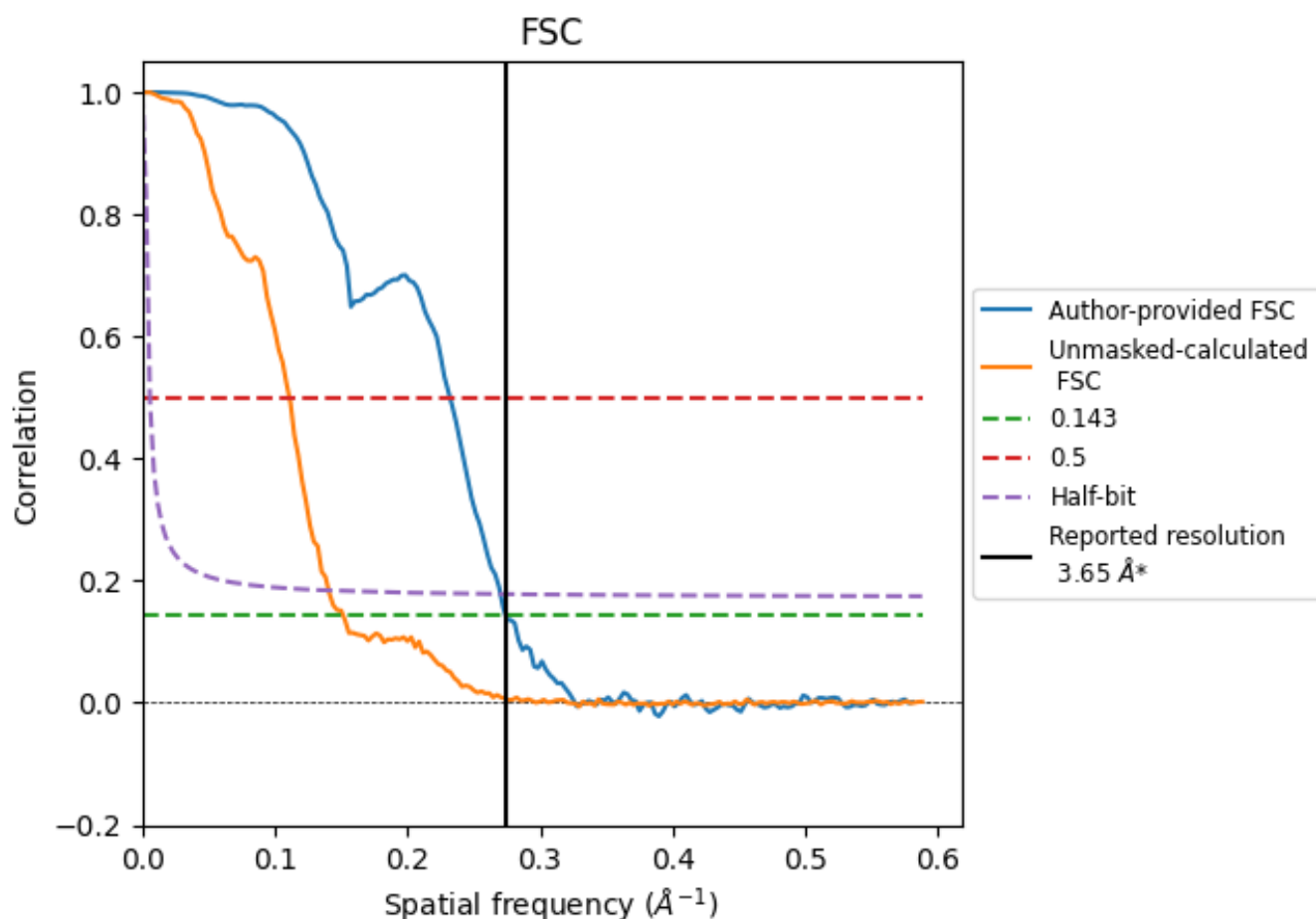


*Reported resolution corresponds to spatial frequency of 0.274 Å⁻¹

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 0.274 \AA^{-1}

8.2 Resolution estimates [i](#)

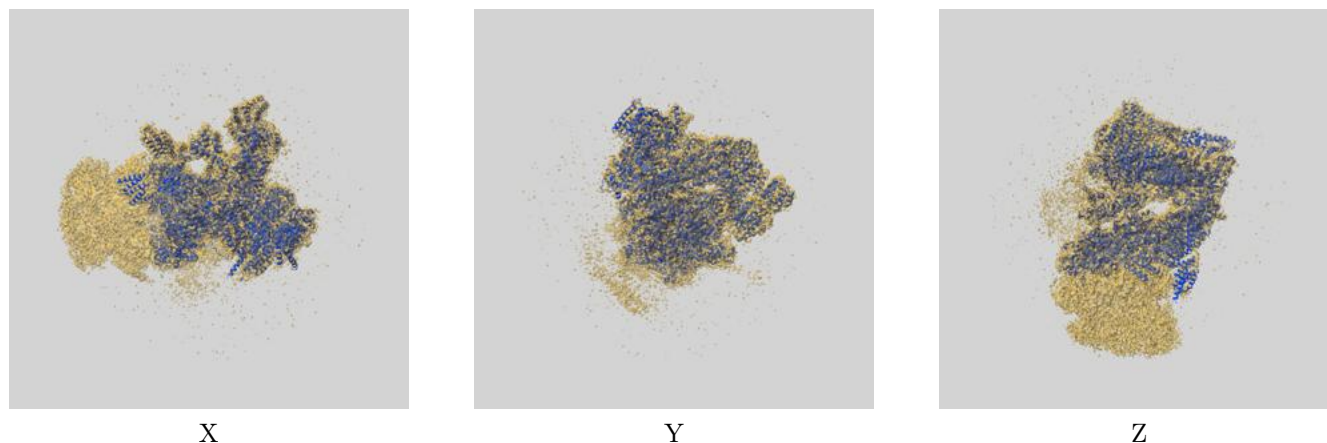
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.65	4.31	3.70
Unmasked-calculated*	6.60	9.01	7.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.60 differs from the reported value 3.65 by more than 10 %

9 Map-model fit [i](#)

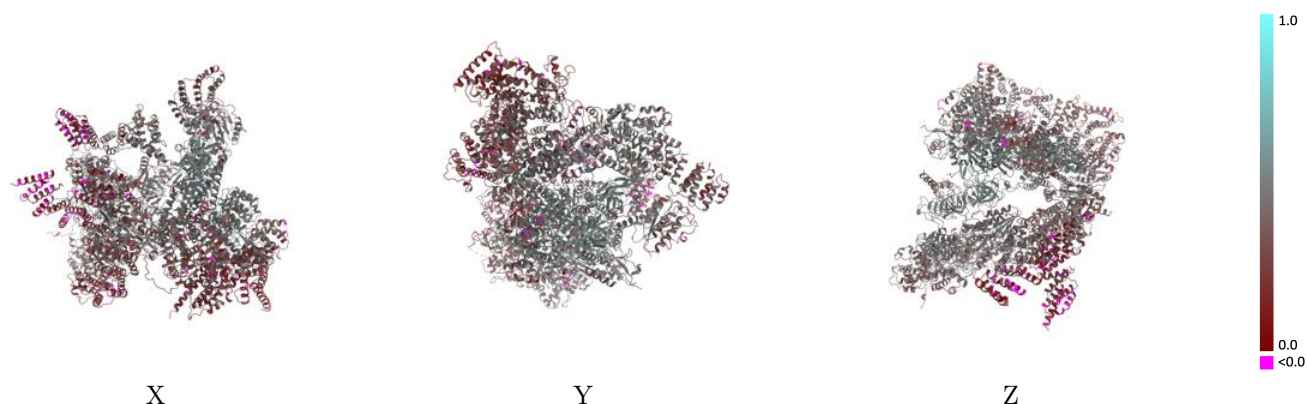
This section contains information regarding the fit between EMDB map EMD-65595 and PDB model 9W39. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



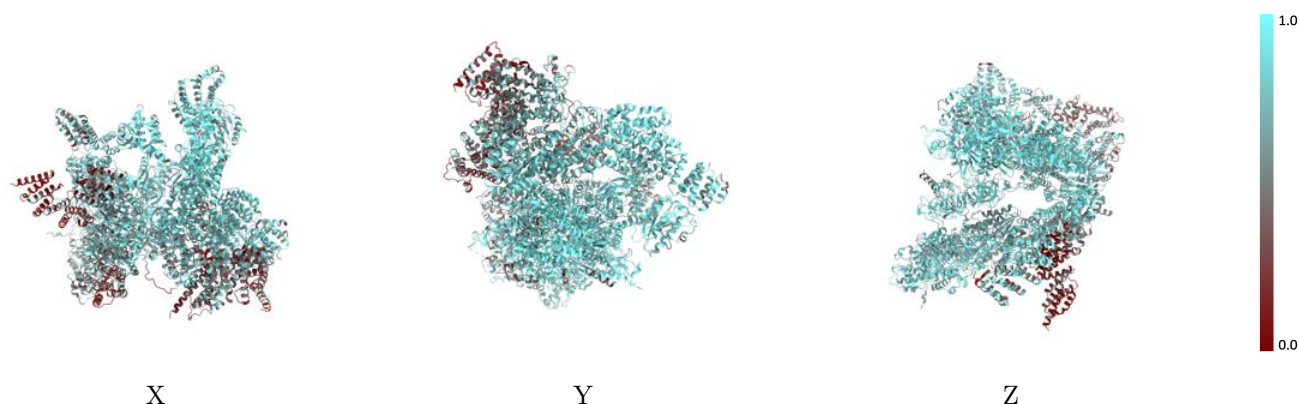
The images above show the 3D surface view of the map at the recommended contour level 0.081 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



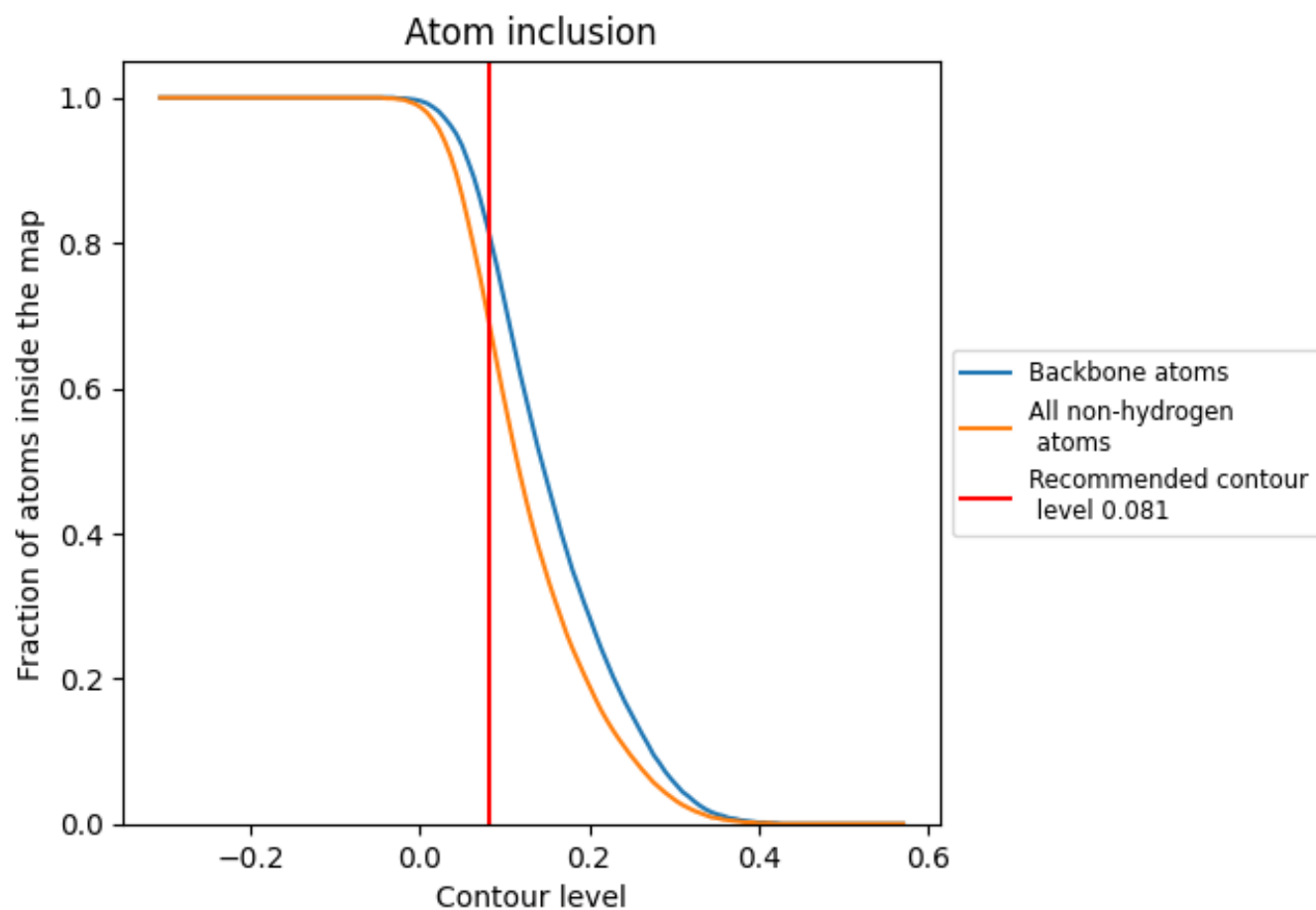
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.081).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 70% 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 (0.081) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6970	 0.3840
A	 0.7230	 0.4080
B	 0.5980	 0.3530
C	 0.6540	 0.3800
D	 0.7710	 0.4400
E	 0.8330	 0.4630
F	 0.7810	 0.4430
U	 0.7740	 0.4140
V	 0.5700	 0.3260
W	 0.7430	 0.3300
X	 0.3470	 0.2140
Y	 0.5700	 0.3180
Z	 0.8500	 0.4820
a	 0.8210	 0.4100
b	 0.7720	 0.4050
c	 0.8620	 0.5010
d	 0.4580	 0.2700
e	 0.5740	 0.3340
f	 0.8530	 0.4610
v	 0.5430	 0.3770

