



Full wwPDB EM Validation Report ⓘ

Apr 21, 2026 – 09:43 AM JST

PDB ID : 9K4R / pdb_00009k4r
EMDB ID : EMD-62067
Title : Structure of substrate-engaged human 26S proteasome RP-CP subcomplex in state EB.1
Authors : Wu, Z.; Chen, E.; Mao, Y.
Deposited on : 2024-10-21
Resolution : 3.10 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 : 1.8.5 (274361), CSD as541be (2020)
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

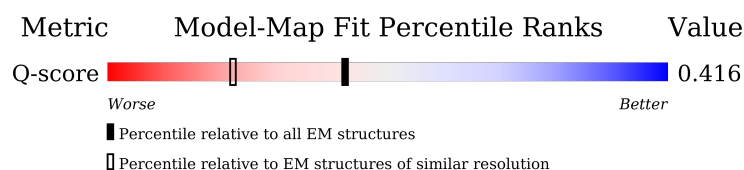
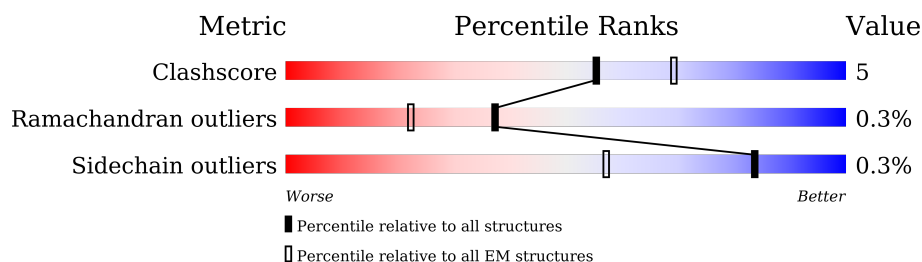
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	A	433	<div> <div>15%</div> <div>77%</div> <div>16%</div> <div>6%</div> </div>
2	B	440	<div> <div>16%</div> <div>79%</div> <div>11%</div> <div>10%</div> </div>
3	C	398	<div> <div>28%</div> <div>77%</div> <div>18%</div> <div>..</div> </div>
4	D	418	<div> <div>9%</div> <div>72%</div> <div>17%</div> <div>9%</div> </div>









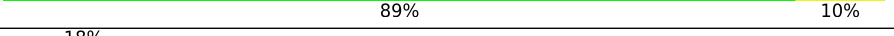


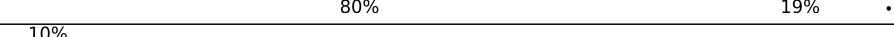
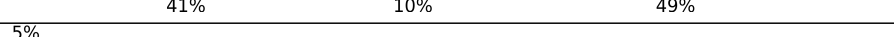
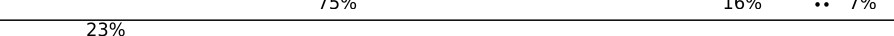


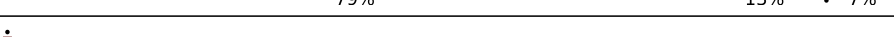

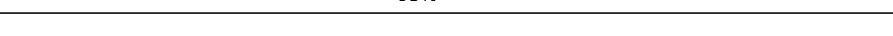
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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	

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Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	
21	U	953	
22	V	534	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	310	
30	d	350	
31	e	70	
32	f	908	
33	u	76	
34	v	28	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 106266 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 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	406	Total	C	N	O	S	0	0
			3164	1992	555	600	17		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	397	Total	C	N	O	S	0	0
			3099	1953	525	606	15		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	381	Total	C	N	O	S	0	0
			2978	1872	536	554	16		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

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

- Molecule 5 is a protein called Proteasome 26S subunit, ATPase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	389	Total	C	N	O	S	0	0
			3097	1947	552	581	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	415	Total	C	N	O	S	0	0
			3251	2038	561	634	18		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	244	Total	C	N	O	S	0	0
			1889	1198	316	362	13		
7	g	240	Total	C	N	O	S	0	0
			1867	1187	312	355	13		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1805	1152	305	342	6		
8	h	232	Total	C	N	O	S	0	0
			1801	1149	304	342	6		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	250	Total	C	N	O	S	1	0
			1958	1236	336	376	10		
9	i	248	Total	C	N	O	S	0	0
			1933	1222	330	371	10		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1880	1179	333	363	5		
10	j	239	Total	C	N	O	S	0	0
			1861	1166	327	363	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	234	Total	C	N	O	S	0	0
			1777	1117	295	354	11		
11	k	238	Total	C	N	O	S	0	0
			1813	1139	302	361	11		

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1866	1169	336	350	11		
12	l	240	Total	C	N	O	S	0	0
			1876	1175	338	352	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1876	1191	321	353	11		
13	m	242	Total	C	N	O	S	0	0
			1890	1200	323	356	11		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		
14	n	202	Total	C	N	O	S	0	0
			1510	947	258	293	12		

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1649	1038	279	320	12		
15	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1587	1010	264	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
18	r	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		
19	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

- Molecule 20 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	216	Total	C	N	O	S	0	0
			1683	1062	291	318	12		
20	t	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	818	Total	C	N	O	S	0	0
			6373	4047	1084	1197	45		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	444	Total	C	N	O	S	0	0
			3612	2301	645	653	13		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	441	Total	C	N	O	S	0	0
			3596	2277	613	682	24		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	422	Total	C	N	O	S	0	0
			3335	2116	567	639	13		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	389	Total	C	N	O	S	0	0
			3202	2041	545	598	18		

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 31 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	e	50	Total	C	N	O	0	0
			425	260	65	100		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	844	Total	C	N	O	S	0	0
			6529	4126	1108	1250	45		

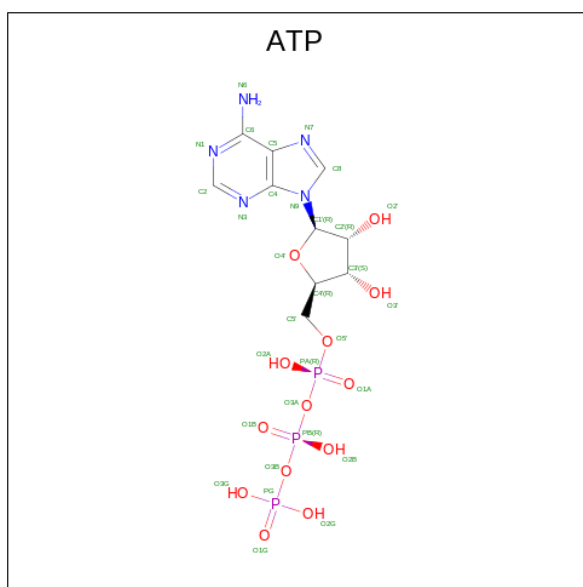
- Molecule 33 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 34 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	v	28	Total	C	N	O	0	0
			143	86	29	28		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

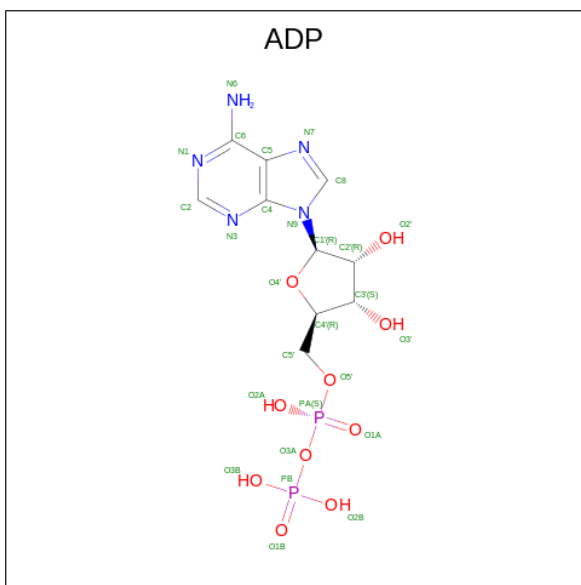


Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total	Mg	0
			1	1	
36	D	1	Total	Mg	0
			1	1	
36	F	1	Total	Mg	0
			1	1	

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
37	B	1	Total 27	C 10	N 5	O 10	P 2	0
37	E	1	Total 27	C 10	N 5	O 10	P 2	0

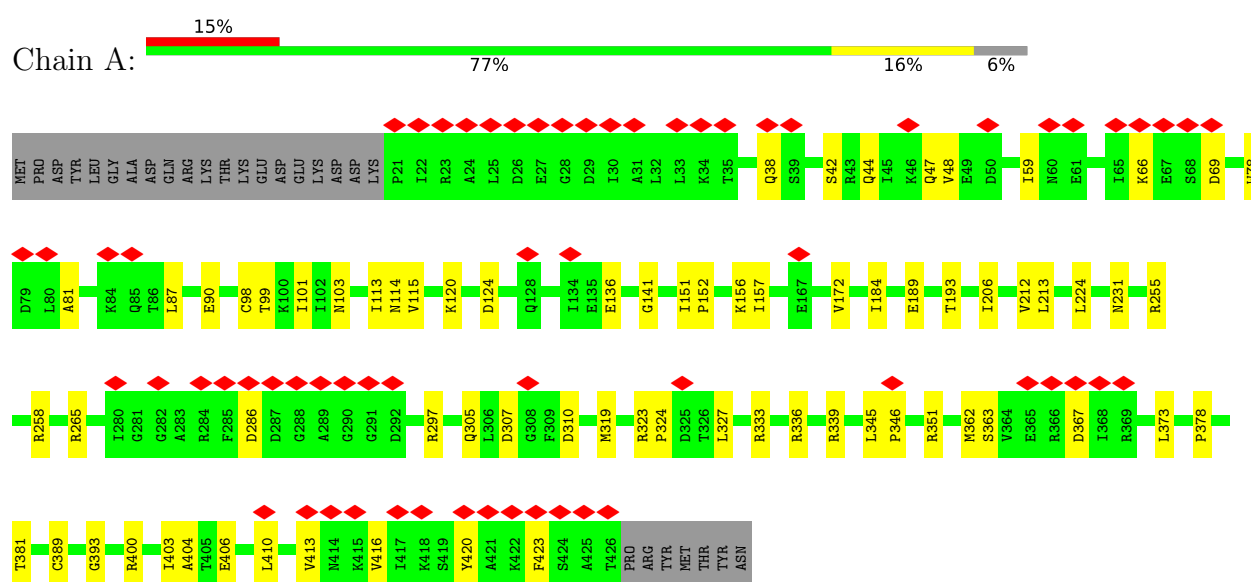
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

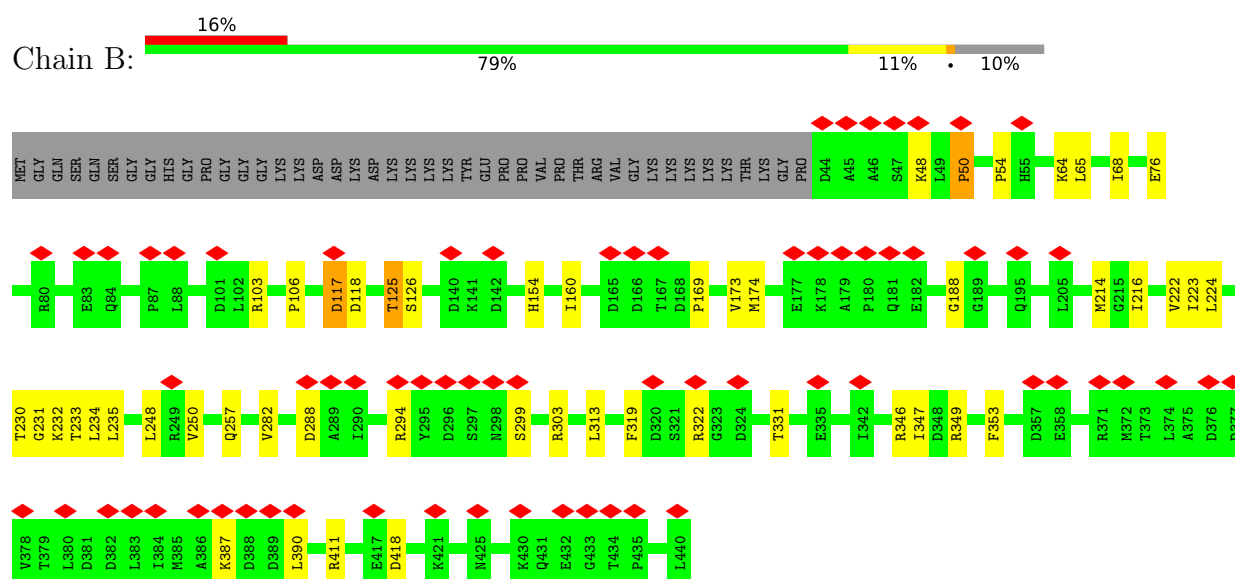
3 Residue-property plots

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

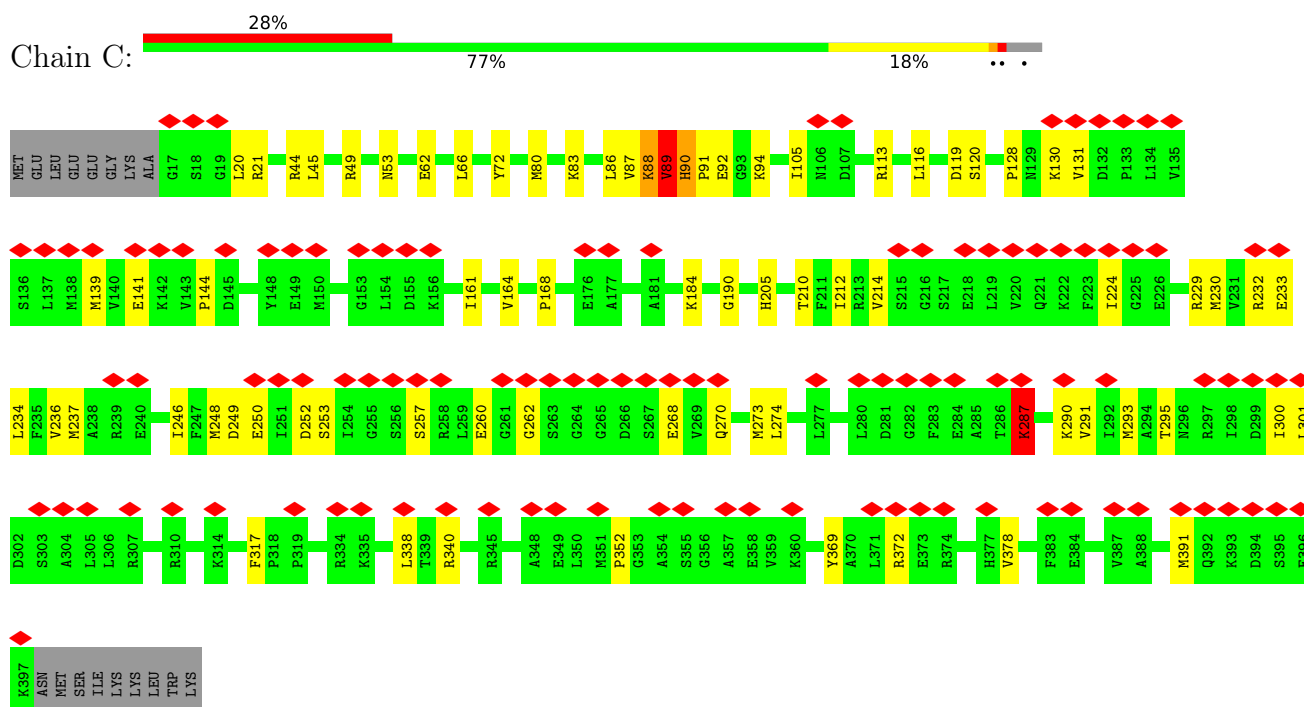
- Molecule 1: 26S proteasome regulatory subunit 7



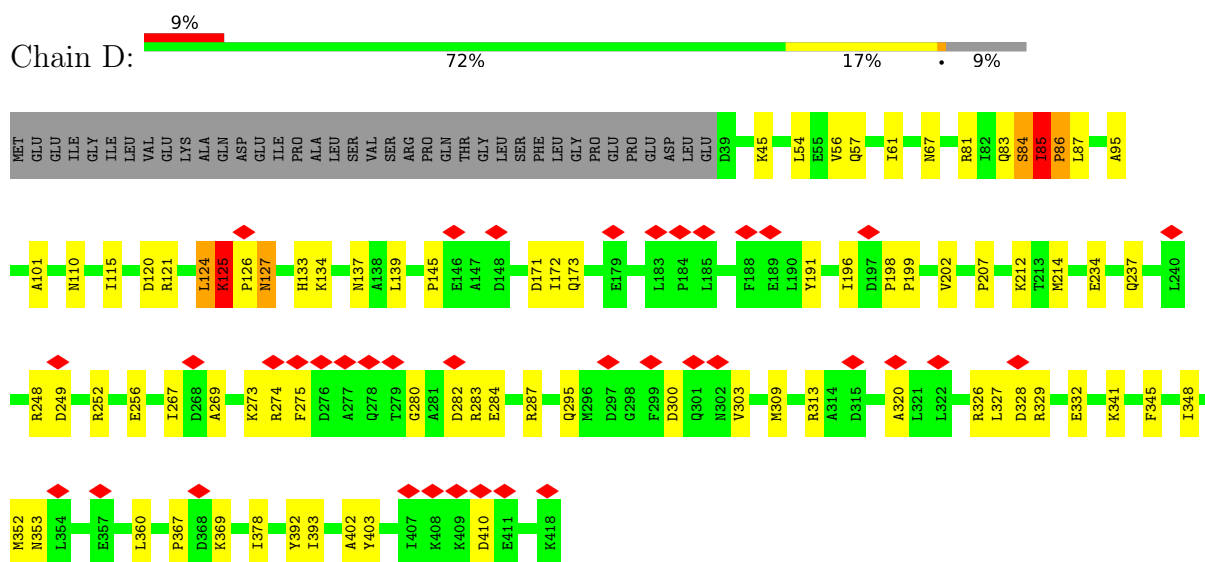
- Molecule 2: 26S proteasome regulatory subunit 4



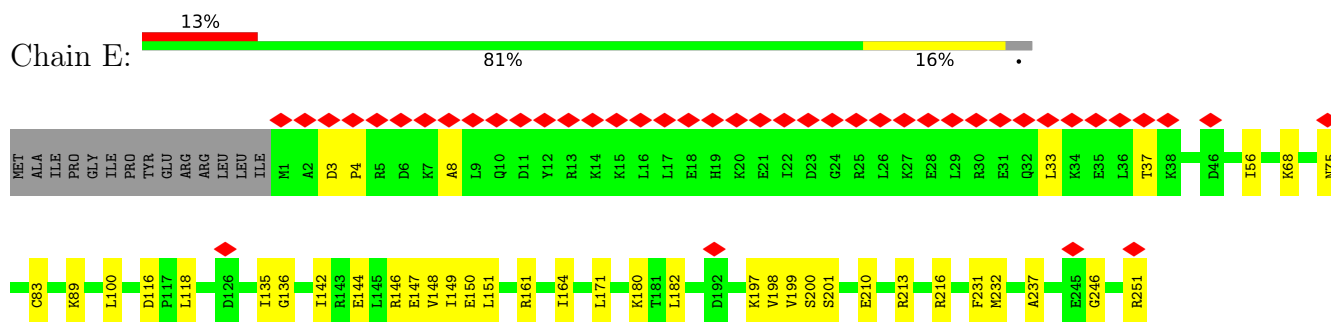
- Molecule 3: 26S proteasome regulatory subunit 8

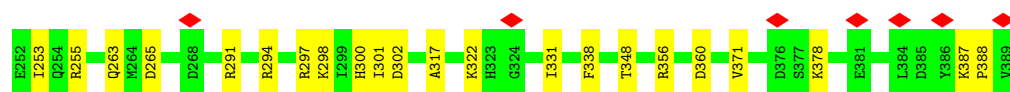


• Molecule 4: 26S proteasome regulatory subunit 6B

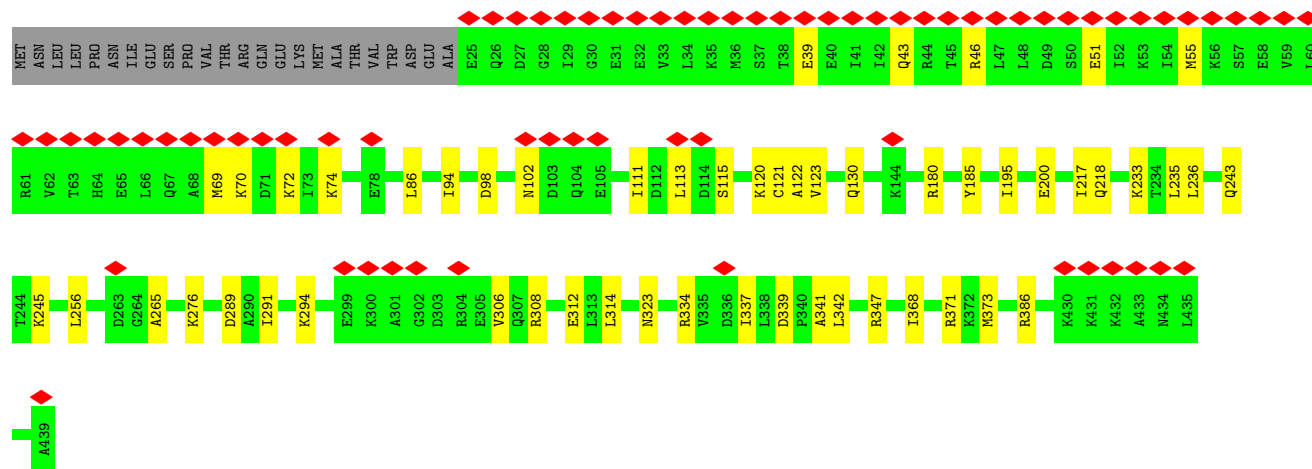
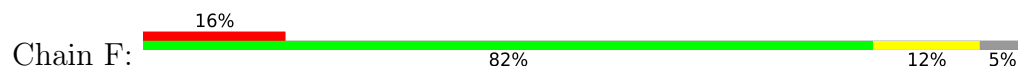


• Molecule 5: Proteasome 26S subunit, ATPase 6

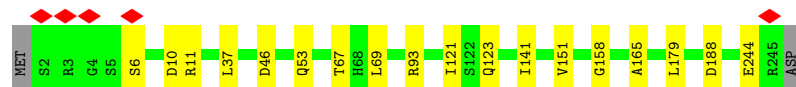




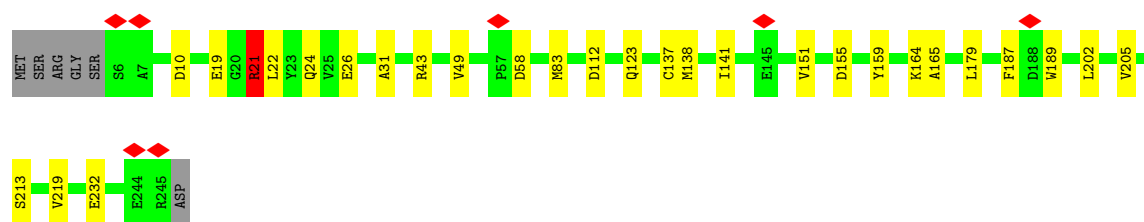
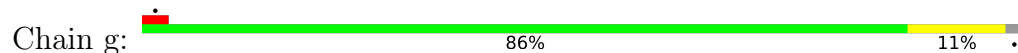
- Molecule 6: 26S proteasome regulatory subunit 6A



- Molecule 7: Proteasome subunit alpha type-6



- Molecule 7: Proteasome subunit alpha type-6

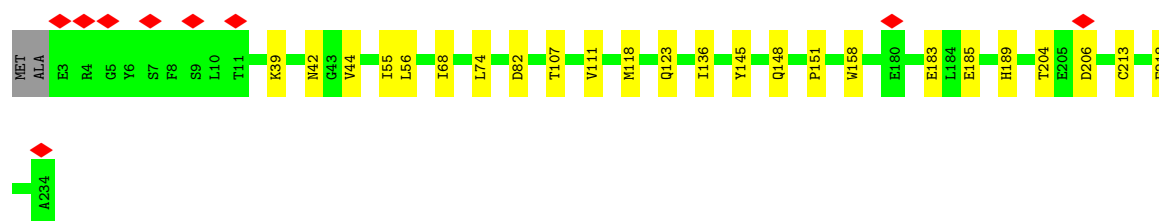


- Molecule 8: Proteasome subunit alpha type-2



- Molecule 8: Proteasome subunit alpha type-2

Chain h:  89% 10%




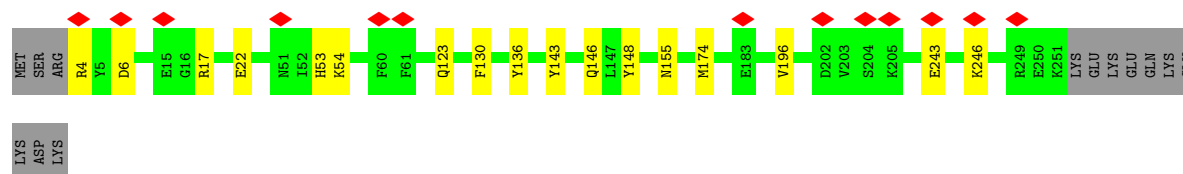
- Molecule 9: Proteasome subunit alpha type-4

Chain I:  89% 7%




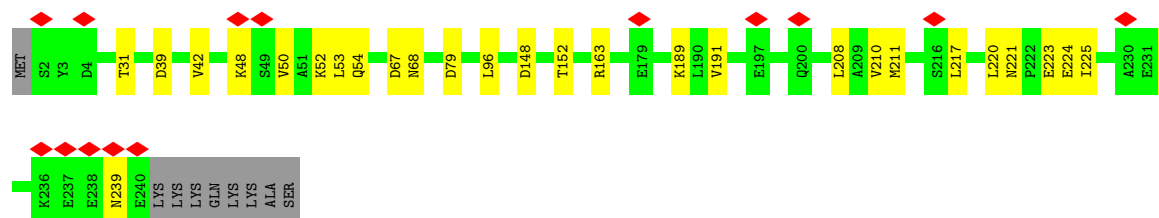
- Molecule 9: Proteasome subunit alpha type-4

Chain i:  89% 7% 5%




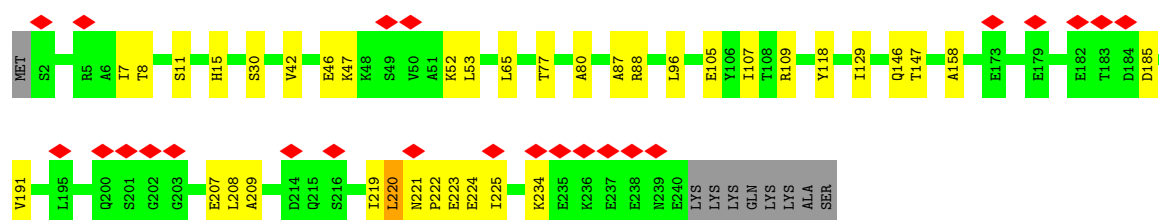
- Molecule 10: Proteasome subunit alpha type-7

Chain J:  85% 11% 6%

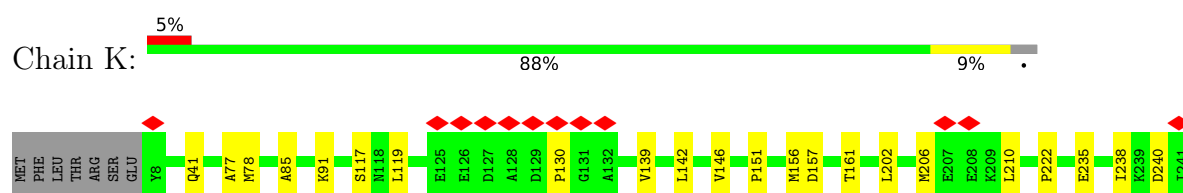


- Molecule 10: Proteasome subunit alpha type-7

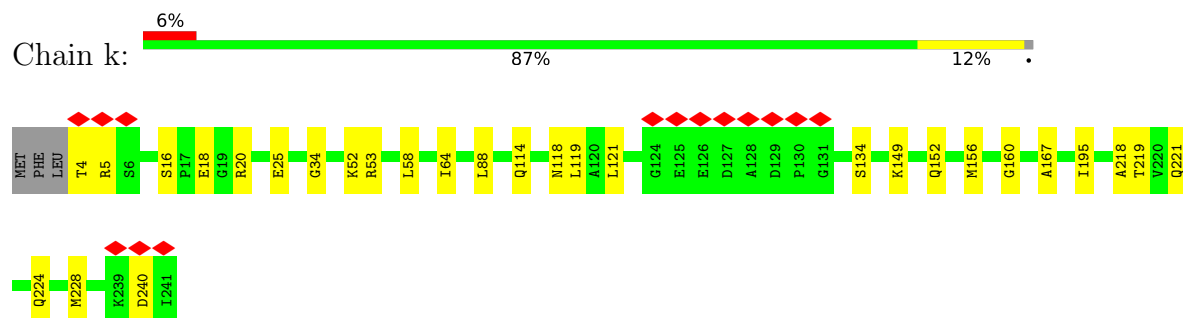
Chain j:  81% 15% 10%



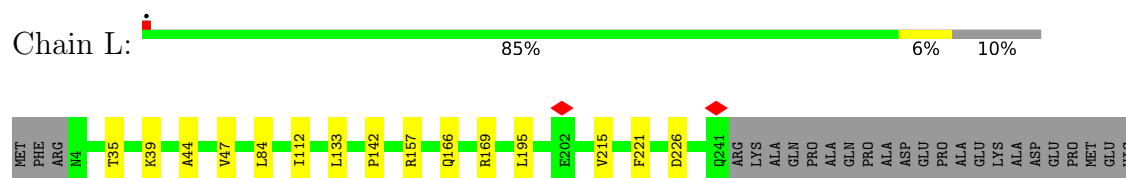
- Molecule 11: Proteasome subunit alpha type-5



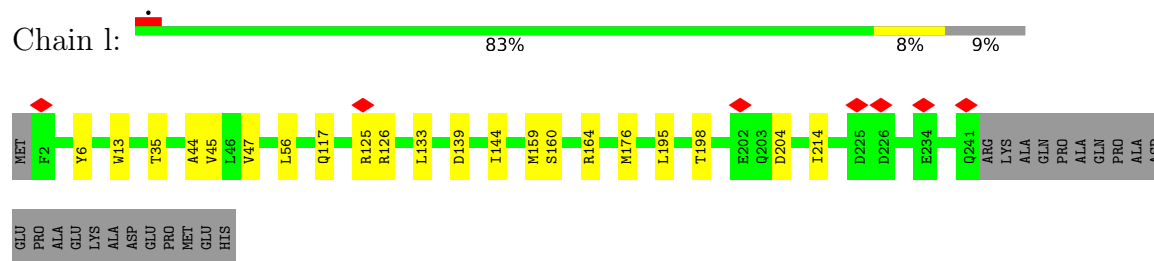
- Molecule 11: Proteasome subunit alpha type-5



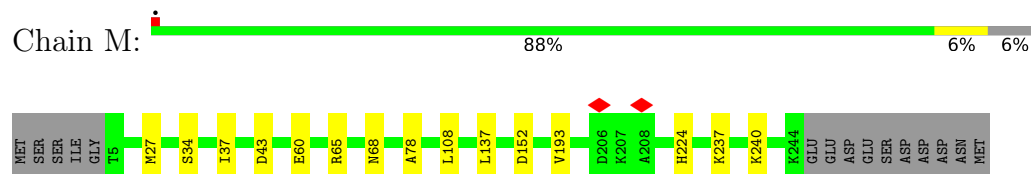
- Molecule 12: Proteasome subunit alpha type-1



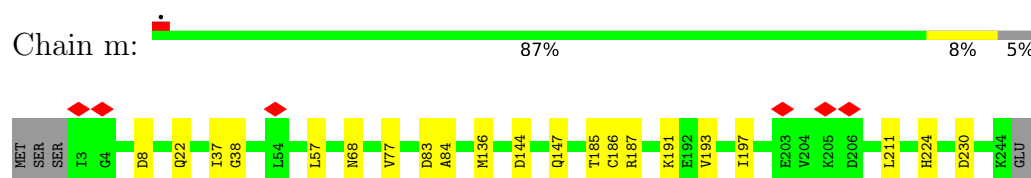
- Molecule 12: Proteasome subunit alpha type-1



- Molecule 13: Proteasome subunit alpha type-3




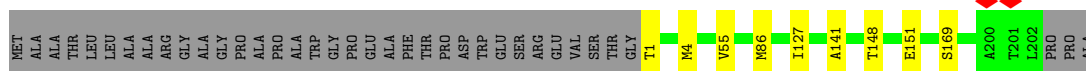
- Molecule 13: Proteasome subunit alpha type-3




ASN
MET

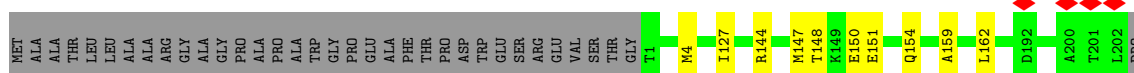
- Molecule 14: Proteasome subunit beta type-6

Chain N:  81% 15%



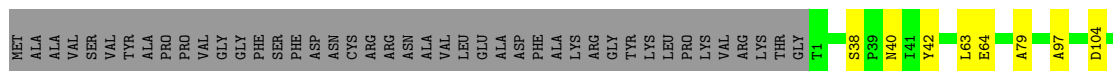
- Molecule 14: Proteasome subunit beta type-6

Chain n:  80% 15%

PRO
ALA

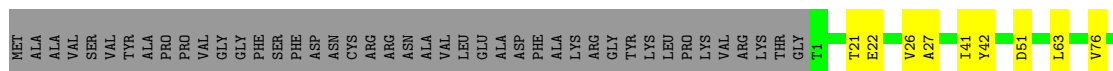
- Molecule 15: Proteasome subunit beta type-7

Chain O:  73% 6% 21%




- Molecule 15: Proteasome subunit beta type-7

Chain o:  73% 6% 21%




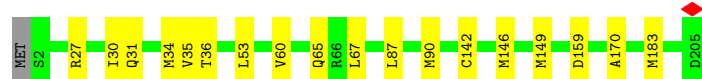
- Molecule 16: Proteasome subunit beta type-3

Chain P:  91% 8%




- Molecule 16: Proteasome subunit beta type-3

Chain p:  91% 9%




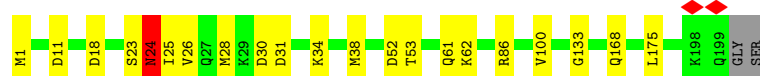
- Molecule 17: Proteasome subunit beta type-2

Chain Q:  89% 10%



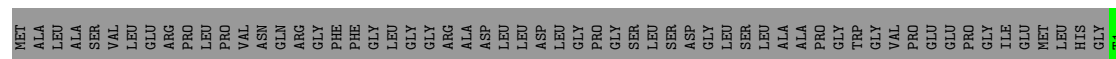
- Molecule 17: Proteasome subunit beta type-2

Chain q:  89% 10%



- Molecule 18: Proteasome subunit beta type-5

Chain R:  73% 24%




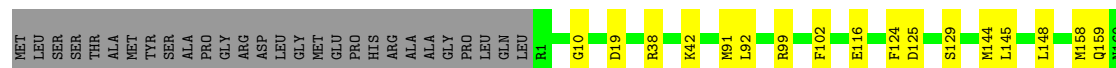
- Molecule 18: Proteasome subunit beta type-5

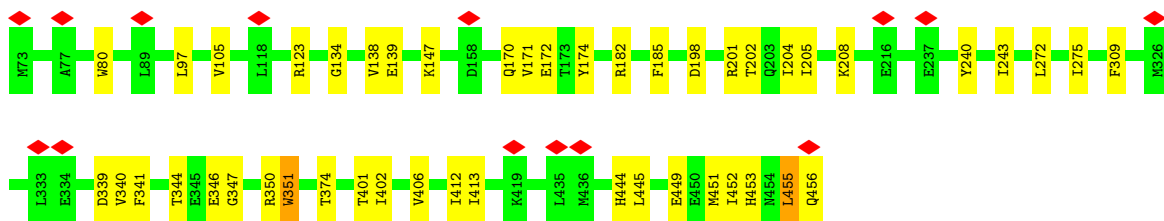
Chain r:  71% 5% 24%



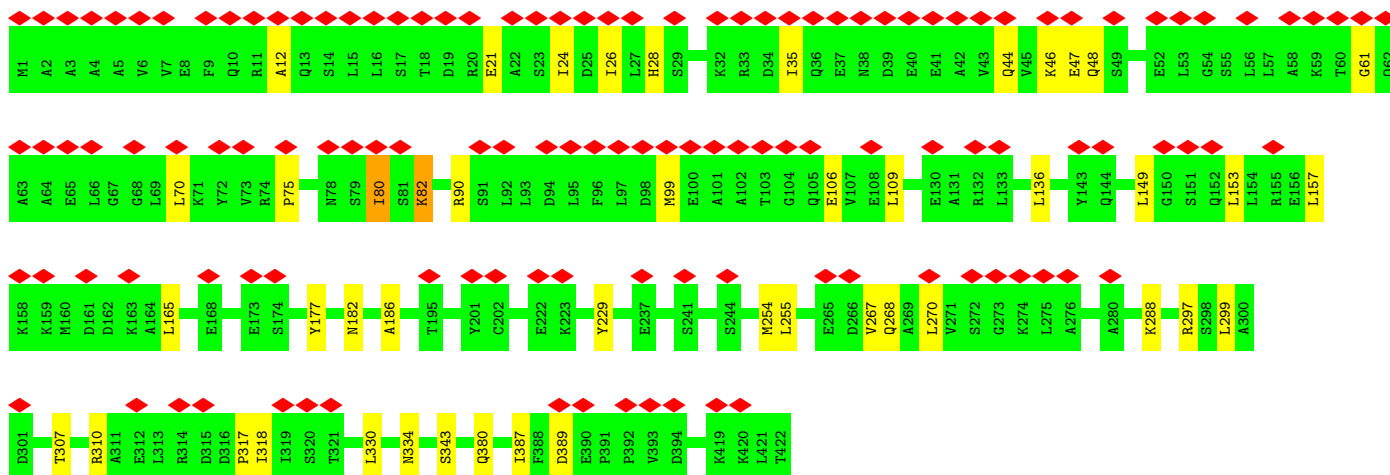
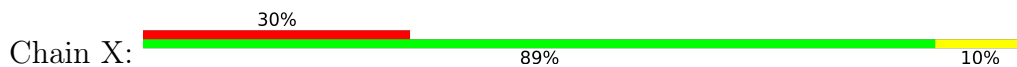
- Molecule 19: Proteasome subunit beta type-1

Chain S:  78% 10% 12%

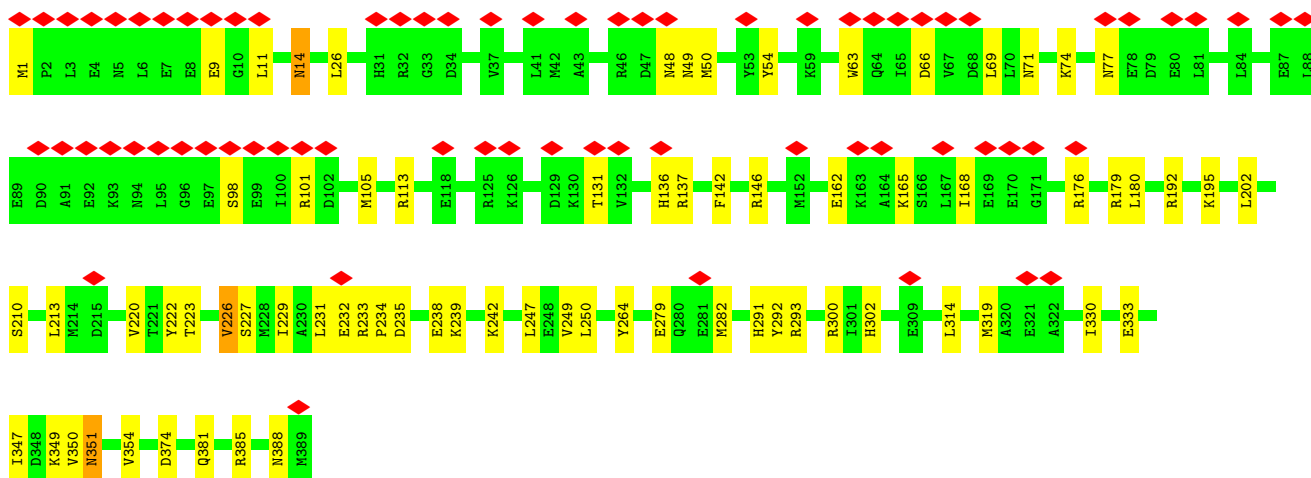
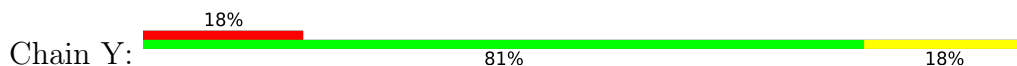




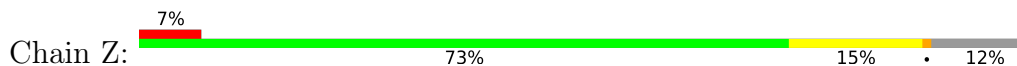
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

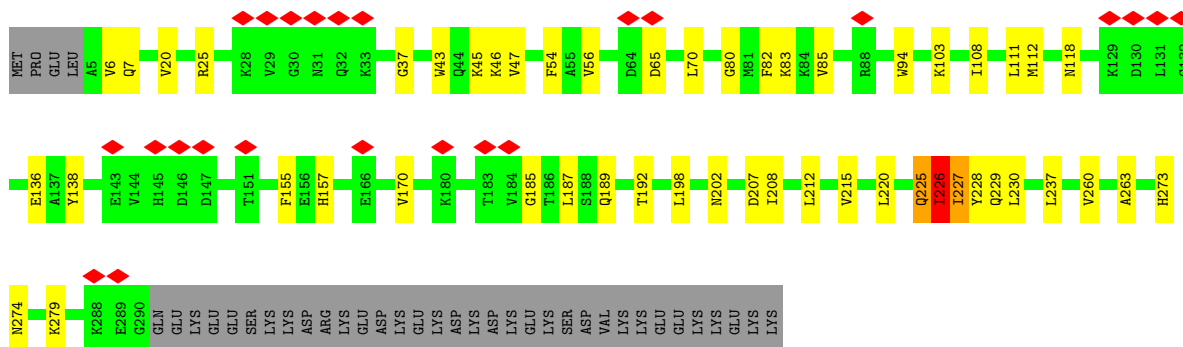


- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

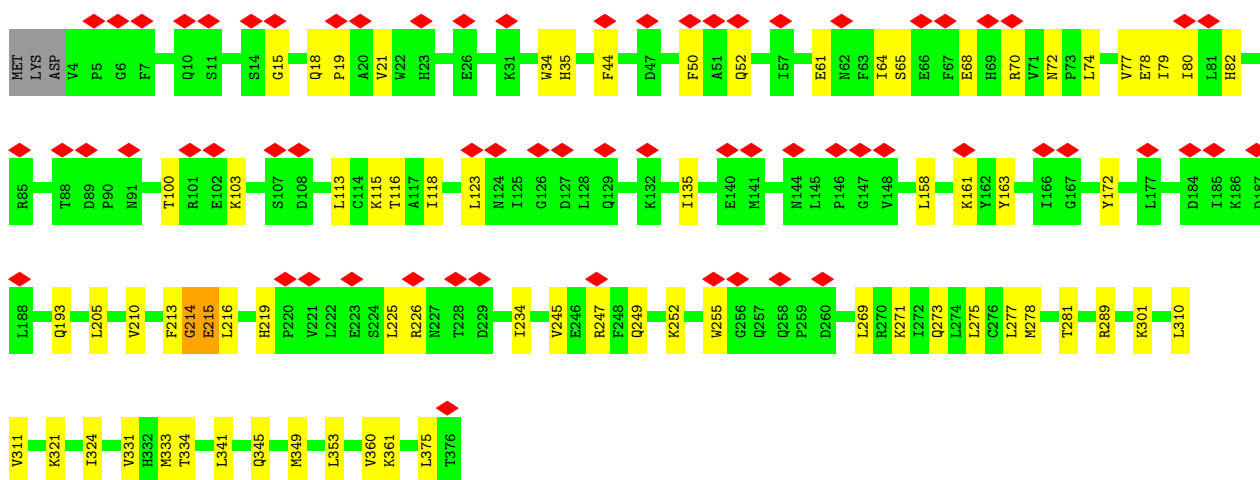


- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

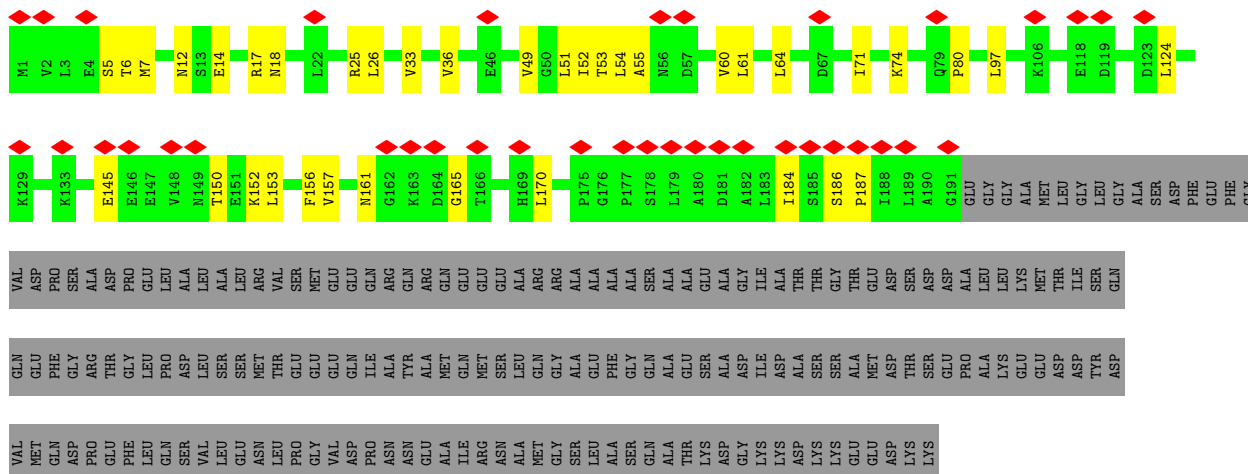




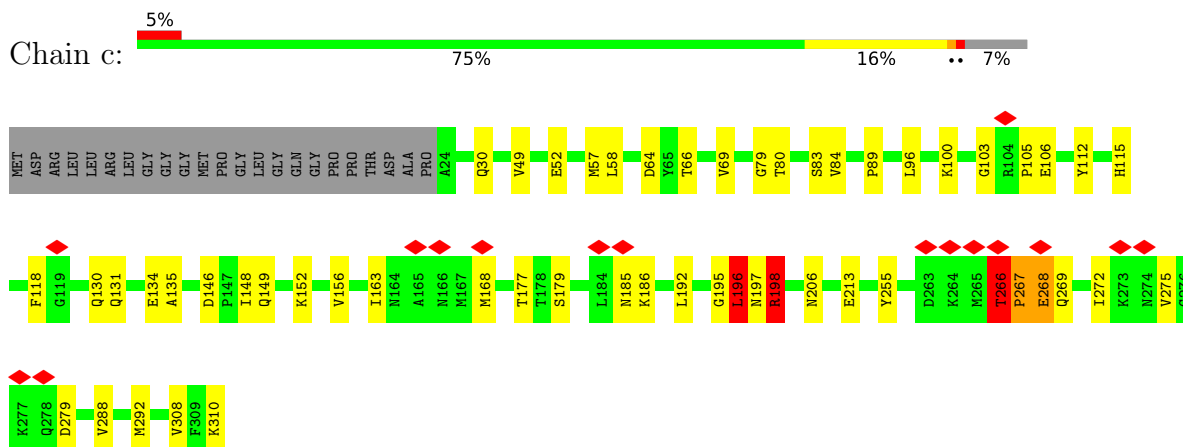
- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13



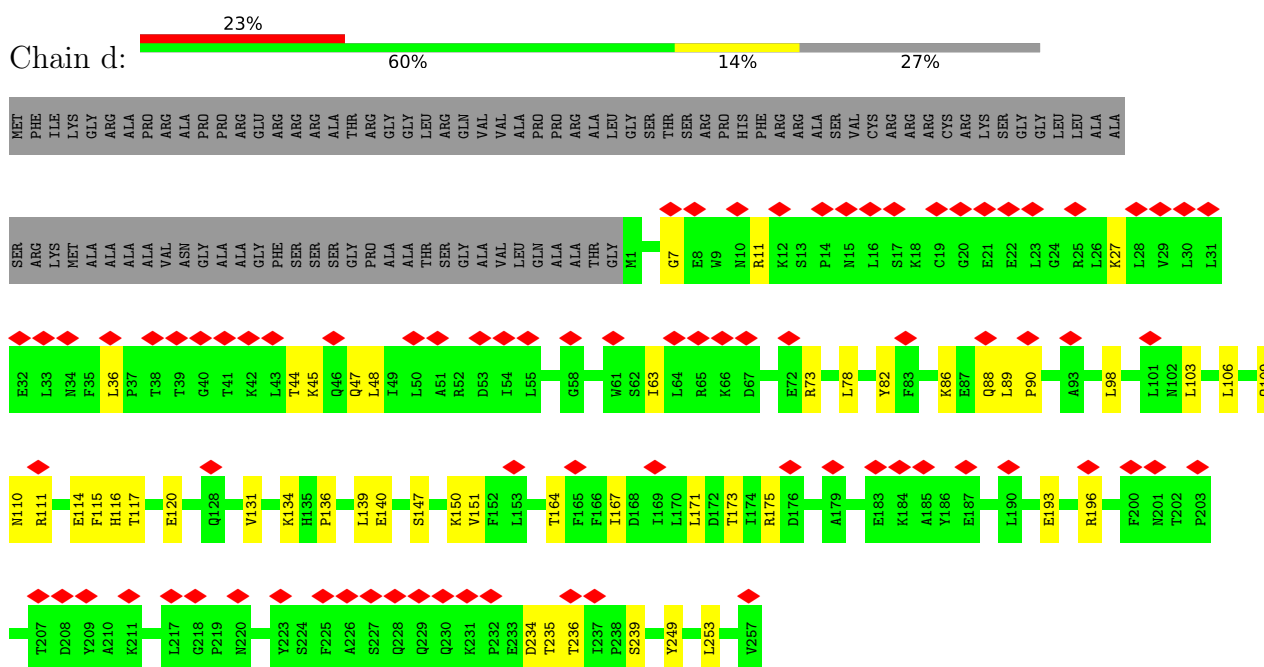
- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4



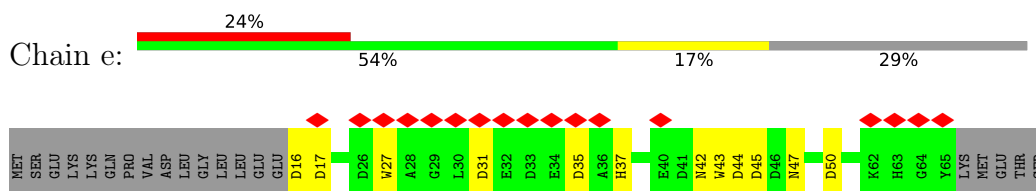
- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14



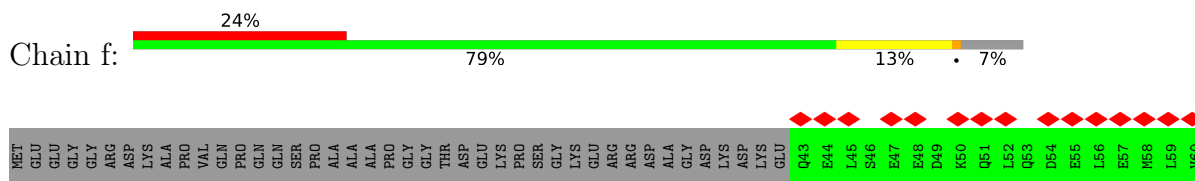
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



• Molecule 31: 26S proteasome complex subunit SEM1



• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	173931	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.024	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00582	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A	0.20	0/3215	0.51	0/4340
2	B	0.21	0/3144	0.47	0/4245
3	C	0.22	0/3017	0.48	0/4058
4	D	0.23	0/3089	0.49	0/4168
5	E	0.18	0/3145	0.47	0/4233
6	F	0.19	0/3292	0.44	0/4435
7	G	0.17	0/1923	0.42	0/2601
7	g	0.18	0/1901	0.39	0/2572
8	H	0.17	0/1844	0.39	0/2499
8	h	0.17	0/1840	0.41	0/2495
9	I	0.17	0/1991	0.43	0/2685
9	i	0.18	0/1963	0.47	0/2650
10	J	0.20	0/1906	0.45	0/2573
10	j	0.20	0/1887	0.41	0/2553
11	K	0.16	0/1804	0.38	0/2436
11	k	0.16	0/1841	0.41	2/2486 (0.1%)
12	L	0.16	0/1901	0.35	0/2570
12	l	0.16	0/1911	0.36	0/2584
13	M	0.15	0/1911	0.36	0/2573
13	m	0.17	0/1925	0.42	0/2592
14	N	0.16	0/1540	0.37	0/2085
14	n	0.18	0/1536	0.40	0/2080
15	O	0.16	0/1676	0.37	0/2271
15	o	0.16	0/1686	0.36	0/2282
16	P	0.18	0/1616	0.44	0/2180
16	p	0.16	0/1620	0.41	0/2184
17	Q	0.18	0/1621	0.41	2/2194 (0.1%)
17	q	0.19	0/1621	0.36	0/2194
18	R	0.17	0/1590	0.38	0/2147
18	r	0.17	0/1590	0.38	0/2147
19	S	0.17	0/1671	0.39	0/2252
19	s	0.18	0/1684	0.40	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.17	0/1716	0.34	0/2323
20	t	0.16	0/1720	0.36	0/2328
21	U	0.16	0/6488	0.42	0/8782
22	V	0.17	0/3681	0.41	0/4969
23	W	0.16	0/3644	0.41	0/4901
24	X	0.15	0/3381	0.42	1/4558 (0.0%)
25	Y	0.18	0/3261	0.45	0/4393
26	Z	0.23	0/2324	0.53	0/3150
27	a	0.21	0/3053	0.58	1/4133 (0.0%)
28	b	0.22	1/1478 (0.1%)	0.52	0/2001
29	c	0.24	0/2302	0.54	0/3110
30	d	0.19	0/2162	0.55	0/2919
31	e	0.19	0/437	0.54	0/595
32	f	0.23	0/6640	0.54	2/8988 (0.0%)
33	u	0.25	0/607	0.44	0/816
34	v	0.03	0/8	0.05	0/8
All	All	0.19	1/107803 (0.0%)	0.44	8/145606 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	186	SER	C-N	5.39	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	156	MET	CA-C-N	6.96	141.23	120.69
11	k	156	MET	C-N-CA	6.96	141.23	120.69
32	f	89	MET	CA-C-N	6.84	137.60	126.86
32	f	89	MET	C-N-CA	6.84	137.60	126.86
27	a	19	PRO	CA-N-CD	-5.48	104.33	112.00
24	X	75	PRO	CA-N-CD	-5.14	104.81	112.00
17	Q	23	SER	CA-C-N	5.04	131.16	121.54
17	Q	23	SER	C-N-CA	5.04	131.16	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3164	0	3201	44	0
2	B	3099	0	3143	33	0
3	C	2978	0	3075	50	0
4	D	3039	0	3075	63	0
5	E	3097	0	3174	39	0
6	F	3251	0	3318	39	0
7	G	1889	0	1885	13	0
7	g	1867	0	1867	20	0
8	H	1805	0	1784	13	0
8	h	1801	0	1773	14	0
9	I	1958	0	1960	10	0
9	i	1933	0	1923	12	0
10	J	1880	0	1892	22	0
10	j	1861	0	1846	27	0
11	K	1777	0	1762	12	0
11	k	1813	0	1796	16	0
12	L	1866	0	1852	10	0
12	l	1876	0	1856	14	0
13	M	1876	0	1861	9	0
13	m	1890	0	1880	13	0
14	N	1514	0	1487	5	0
14	n	1510	0	1483	6	0
15	O	1649	0	1659	11	0
15	o	1659	0	1681	10	0
16	P	1587	0	1598	11	0
16	p	1591	0	1609	12	0
17	Q	1588	0	1584	14	0
17	q	1588	0	1584	15	0
18	R	1559	0	1523	6	0
18	r	1559	0	1523	10	0
19	S	1641	0	1639	15	0
19	s	1654	0	1656	17	0
20	T	1683	0	1662	6	0
20	t	1687	0	1666	11	0
21	U	6373	0	6409	98	0
22	V	3612	0	3682	49	0
23	W	3596	0	3713	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	X	3335	0	3435	30	0
25	Y	3202	0	3204	47	0
26	Z	2281	0	2312	38	0
27	a	2995	0	3012	50	0
28	b	1458	0	1505	23	0
29	c	2260	0	2276	50	0
30	d	2116	0	2146	38	0
31	e	425	0	328	11	0
32	f	6529	0	6541	88	0
33	u	601	0	629	10	0
34	v	143	0	46	1	0
35	A	31	0	12	1	0
35	D	31	0	12	2	0
35	F	31	0	12	2	0
36	A	1	0	0	0	0
36	D	1	0	0	0	0
36	F	1	0	0	0	0
37	B	27	0	12	4	0
37	E	27	0	12	2	0
38	c	1	0	0	0	0
All	All	106266	0	106575	1058	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 5.

All (1058) 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)
32:f:585:GLU:HB2	32:f:586:PRO:HD2	1.41	1.03
25:Y:222:TYR:O	25:Y:226:VAL:HG12	1.77	0.84
3:C:44:ARG:HG3	22:V:496:PHE:HE2	1.45	0.81
10:J:221:ASN:HD21	10:J:223:GLU:HB3	1.46	0.79
29:c:192:LEU:HA	29:c:196:LEU:HB2	1.63	0.79
2:B:173:VAL:HG22	3:C:274:LEU:HD11	1.65	0.77
10:J:208:LEU:HD22	10:J:220:LEU:HD22	1.66	0.77
32:f:550:LEU:HD21	32:f:586:PRO:HB2	1.68	0.74
10:j:221:ASN:HD21	10:j:223:GLU:HB3	1.52	0.74
4:D:124:LEU:O	4:D:125:LYS:HB2	1.86	0.74
9:i:143:TYR:HB2	9:i:146:GLN:HE21	1.52	0.74
29:c:267:PRO:O	29:c:269:GLN:N	2.22	0.72
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:267:PRO:C	29:c:269:GLN:H	1.98	0.72
22:V:85:ALA:HB2	22:V:93:PHE:HB2	1.70	0.72
10:j:208:LEU:HD22	10:j:220:LEU:HG	1.71	0.71
22:V:354:LYS:HG3	22:V:358:MET:HE3	1.72	0.70
32:f:348:ILE:HG23	32:f:352:HIS:ND1	2.07	0.70
10:J:221:ASN:HD22	10:J:224:GLU:HG3	1.57	0.70
21:U:18:GLN:HB3	30:d:27:LYS:NZ	2.07	0.69
3:C:44:ARG:HG3	22:V:496:PHE:CE2	2.27	0.69
31:e:35:ASP:HB3	31:e:37:HIS:HD1	1.58	0.68
2:B:68:ILE:HA	32:f:670:MET:HE1	1.76	0.68
3:C:229:ARG:HE	3:C:232:ARG:HG3	1.60	0.67
3:C:352:PRO:HD2	3:C:391:MET:HE1	1.77	0.67
26:Z:260:VAL:HA	29:c:292:MET:HE1	1.77	0.67
4:D:269:ALA:HB1	5:E:255:ARG:HG2	1.78	0.66
5:E:198:VAL:HG12	5:E:200:SER:H	1.59	0.66
10:j:209:ALA:HB2	10:j:219:ILE:HD12	1.77	0.66
4:D:85:ILE:HB	4:D:86:PRO:HD3	1.78	0.66
21:U:208:LEU:HD23	21:U:210:LYS:H	1.60	0.66
6:F:276:LYS:HD3	6:F:323:ASN:HD22	1.61	0.66
29:c:267:PRO:C	29:c:269:GLN:N	2.54	0.65
10:J:221:ASN:ND2	10:J:223:GLU:HB3	2.11	0.65
3:C:90:HIS:HB3	3:C:91:PRO:HD3	1.78	0.65
23:W:453:HIS:HA	26:Z:103:LYS:HE3	1.79	0.65
27:a:289:ARG:HB3	27:a:333:MET:HB2	1.79	0.65
30:d:86:LYS:HG2	30:d:89:LEU:HD13	1.79	0.65
17:Q:25:ILE:HG23	17:Q:26:VAL:HG13	1.77	0.65
29:c:96:LEU:HD12	33:u:8:LEU:HD22	1.79	0.65
20:T:61:GLN:HA	20:T:64:LYS:HZ3	1.61	0.64
30:d:88:GLN:HG2	30:d:89:LEU:H	1.61	0.64
2:B:188:GLY:H	37:B:501:ADP:HN62	1.44	0.64
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.79	0.64
2:B:234:LEU:HD11	37:B:501:ADP:H2'	1.79	0.64
32:f:520:LEU:HD11	32:f:798:THR:HG22	1.79	0.64
25:Y:347:ILE:HG13	25:Y:354:VAL:HG22	1.80	0.64
32:f:842:VAL:H	32:f:870:THR:HG22	1.63	0.64
32:f:348:ILE:O	32:f:352:HIS:N	2.31	0.64
32:f:861:THR:HB	32:f:879:ARG:HH11	1.62	0.63
29:c:89:PRO:HG2	33:u:44:ILE:HD11	1.80	0.63
30:d:82:TYR:HA	30:d:86:LYS:HE3	1.80	0.63
32:f:585:GLU:O	32:f:587:PHE:N	2.31	0.62
26:Z:226:ILE:HG22	26:Z:230:LEU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:199:PRO:HB3	4:D:328:ASP:HB2	1.80	0.62
3:C:83:LYS:HG2	3:C:105:ILE:HD11	1.82	0.62
4:D:121:ARG:HA	4:D:124:LEU:HD23	1.81	0.62
17:Q:5:ILE:HD11	17:Q:143:LEU:HD11	1.82	0.62
32:f:692:LEU:HB3	32:f:800:LEU:HD22	1.81	0.62
8:H:95:GLN:NE2	15:O:64:GLU:OE2	2.34	0.61
16:P:149:MET:HE1	16:P:173:ASN:HD22	1.65	0.61
19:S:159:GLN:NE2	15:o:207:GLY:O	2.34	0.61
3:C:80:MET:HE1	3:C:86:LEU:HB2	1.83	0.61
4:D:173:GLN:NE2	4:D:332:GLU:O	2.34	0.61
4:D:280:GLY:HA2	4:D:283:ARG:HH21	1.66	0.61
21:U:18:GLN:CB	30:d:27:LYS:NZ	2.63	0.60
6:F:69:MET:HA	6:F:72:LYS:HB2	1.83	0.60
1:A:323:ARG:HD3	2:B:294:ARG:HE	1.66	0.60
3:C:262:GLY:HA2	3:C:270:GLN:HE22	1.66	0.60
32:f:320:ILE:HA	32:f:325:GLN:HE22	1.65	0.60
25:Y:48:ASN:HB3	25:Y:50:MET:HE3	1.83	0.60
21:U:808:PRO:HD3	21:U:874:ASN:HA	1.83	0.60
5:E:4:PRO:HG2	5:E:8:ALA:H	1.67	0.60
30:d:193:GLU:HA	30:d:196:ARG:HD3	1.84	0.60
19:S:148:LEU:HD23	19:S:178:VAL:HG12	1.83	0.60
4:D:353:ASN:ND2	4:D:392:TYR:O	2.34	0.60
24:X:106:GLU:HB3	24:X:136:LEU:HD21	1.83	0.60
10:j:7:ILE:HG13	10:j:8:THR:HG23	1.84	0.60
7:g:137:CYS:SG	7:g:138:MET:N	2.75	0.59
17:q:168:GLN:NE2	17:q:175:LEU:O	2.36	0.59
5:E:253:ILE:HG13	6:F:308:ARG:HH22	1.68	0.59
22:V:108:LEU:HD23	22:V:174:PHE:HB2	1.84	0.59
2:B:173:VAL:CG2	3:C:274:LEU:HD11	2.32	0.59
21:U:802:TYR:HB2	21:U:878:LEU:HB2	1.83	0.59
19:s:144:MET:HE1	19:s:186:ASP:HB2	1.84	0.59
1:A:38:GLN:HB3	1:A:42:SER:HB3	1.84	0.59
15:O:63:LEU:HD11	15:O:79:ALA:HB2	1.83	0.59
24:X:380:GLN:HB2	25:Y:314:LEU:HA	1.83	0.59
6:F:94:ILE:HD12	6:F:123:VAL:HG12	1.85	0.59
30:d:171:LEU:HD22	30:d:175:ARG:HH12	1.68	0.59
23:W:171:VAL:HG12	23:W:182:ARG:HG3	1.85	0.58
13:m:68:ASN:OD1	13:m:224:HIS:ND1	2.37	0.58
14:N:148:THR:OG1	14:N:151:GLU:OE1	2.20	0.58
5:E:317:ALA:O	5:E:322:LYS:NZ	2.36	0.58
27:a:135:ILE:HG12	27:a:158:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HG22	6:F:373:MET:HE1	1.85	0.58
1:A:258:ARG:HA	1:A:305:GLN:HE22	1.67	0.58
1:A:393:GLY:HA3	2:B:216:ILE:HD13	1.85	0.58
2:B:174:MET:HE2	2:B:250:VAL:HG22	1.85	0.58
21:U:383:ASP:HB3	21:U:386:LEU:HB3	1.84	0.58
32:f:345:PRO:HG3	32:f:378:ASN:HB2	1.85	0.58
10:J:221:ASN:ND2	10:J:224:GLU:HG3	2.19	0.58
17:Q:68:LYS:HD3	17:Q:74:GLU:HG3	1.84	0.58
25:Y:231:LEU:HD12	25:Y:234:PRO:HG2	1.85	0.58
9:i:243:GLU:HA	9:i:246:LYS:HZ3	1.68	0.58
10:J:211:MET:HB2	10:J:217:LEU:HD13	1.86	0.58
25:Y:168:ILE:HD12	25:Y:180:LEU:HD13	1.85	0.58
32:f:894:LEU:HA	32:f:898:VAL:HG21	1.86	0.58
23:W:451:MET:O	23:W:455:LEU:HG	2.04	0.58
5:E:148:VAL:HG13	5:E:149:ILE:HG13	1.85	0.58
23:W:406:VAL:HA	23:W:413:ILE:HG22	1.86	0.58
28:b:12:ASN:HB2	28:b:80:PRO:HA	1.85	0.58
10:J:96:LEU:HD13	17:Q:62:LYS:HD2	1.85	0.57
29:c:115:HIS:HB3	29:c:118:PHE:HB2	1.85	0.57
6:F:294:LYS:HA	6:F:339:ASP:HB3	1.86	0.57
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.36	0.57
21:U:18:GLN:HB3	30:d:27:LYS:HZ1	1.66	0.57
21:U:191:LYS:HD2	21:U:194:ARG:HH21	1.69	0.57
27:a:70:ARG:O	28:b:17:ARG:NH2	2.37	0.57
7:g:165:ALA:HB3	8:h:56:LEU:HD22	1.86	0.57
3:C:168:PRO:HB2	3:C:290:LYS:HZ1	1.70	0.57
21:U:18:GLN:HG3	30:d:27:LYS:NZ	2.19	0.57
18:R:100:MET:HE3	18:R:126:PHE:HB2	1.85	0.57
22:V:228:ARG:HH22	22:V:261:TYR:HB2	1.70	0.57
32:f:585:GLU:HB2	32:f:586:PRO:CD	2.22	0.57
13:m:37:ILE:HD11	13:m:193:VAL:HG13	1.86	0.57
6:F:233:LYS:NZ	35:F:501:ATP:O1B	2.37	0.57
21:U:798:PRO:O	21:U:880:ASN:ND2	2.37	0.57
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	1.86	0.57
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.85	0.57
9:i:53:HIS:CG	9:i:54:LYS:H	2.22	0.57
13:m:187:ARG:O	13:m:191:LYS:NZ	2.37	0.57
27:a:214:GLY:O	27:a:216:LEU:N	2.37	0.57
28:b:25:ARG:NH2	28:b:145:GLU:OE1	2.37	0.57
33:u:4:PHE:HE2	33:u:64:GLU:HG2	1.69	0.57
17:Q:144:ASP:OD2	18:r:166:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:449:GLU:HA	23:W:452:ILE:HD12	1.85	0.57
5:E:161:ARG:NH2	23:W:139:GLU:OE2	2.38	0.57
22:V:82:LEU:HD23	22:V:94:VAL:HG12	1.87	0.57
23:W:351:TRP:HA	23:W:351:TRP:CE3	2.39	0.57
11:k:52:LYS:NZ	11:k:64:ILE:O	2.38	0.57
3:C:144:PRO:O	3:C:205:HIS:ND1	2.38	0.57
3:C:224:ILE:HG12	3:C:268:GLU:HG2	1.86	0.57
19:S:38:ARG:NH2	15:o:164:PHE:O	2.38	0.56
2:B:299:SER:HA	2:B:303:ARG:HB2	1.87	0.56
27:a:210:VAL:HA	27:a:213:PHE:CE1	2.40	0.56
12:l:159:MET:HE3	12:l:160:SER:H	1.70	0.56
15:O:104:ASP:O	15:O:180:LYS:NZ	2.39	0.56
21:U:30:VAL:HA	21:U:33:ASP:HB2	1.88	0.56
23:W:374:THR:HG22	23:W:412:ILE:HG13	1.87	0.56
5:E:356:ARG:NH1	6:F:200:GLU:OE2	2.38	0.56
23:W:346:GLU:HG3	23:W:350:ARG:CZ	2.35	0.56
28:b:61:LEU:HD23	28:b:74:LYS:HD2	1.87	0.56
1:A:101:ILE:HA	1:A:113:ILE:HG12	1.87	0.56
21:U:18:GLN:O	21:U:18:GLN:NE2	2.39	0.56
16:p:65:GLN:OE1	17:q:86:ARG:NH2	2.38	0.56
22:V:264:TYR:HE2	30:d:120:GLU:HG2	1.69	0.56
13:m:197:ILE:HG21	13:m:211:LEU:HD13	1.88	0.56
3:C:248:MET:HB2	3:C:293:MET:HG3	1.87	0.56
5:E:198:VAL:HB	5:E:232:MET:HG2	1.88	0.56
25:Y:279:GLU:HA	25:Y:282:MET:HE2	1.86	0.56
29:c:195:GLY:O	29:c:198:ARG:HB2	2.06	0.56
18:R:166:ARG:NH1	16:p:34:MET:O	2.38	0.56
21:U:415:HIS:O	21:U:450:HIS:NE2	2.39	0.56
32:f:140:LEU:HD23	32:f:165:GLU:HB3	1.88	0.56
23:W:60:MET:HE2	23:W:97:LEU:HD11	1.87	0.56
9:i:155:ASN:OD1	10:j:77:THR:OG1	2.24	0.56
1:A:404:ALA:HB2	2:B:214:MET:HE1	1.89	0.55
10:j:221:ASN:HB3	10:j:224:GLU:HG2	1.88	0.55
1:A:362:MET:HE1	1:A:389:CYS:HB3	1.87	0.55
3:C:20:LEU:HD12	3:C:21:ARG:HG3	1.88	0.55
21:U:398:ASN:H	21:U:401:LYS:HE2	1.71	0.55
22:V:477:HIS:ND1	30:d:249:TYR:OH	2.39	0.55
25:Y:300:ARG:NH1	25:Y:333:GLU:OE2	2.39	0.55
32:f:668:ALA:HA	32:f:697:ILE:HD11	1.88	0.55
11:k:114:GLN:O	11:k:118:ASN:ND2	2.39	0.55
6:F:217:ILE:HG13	6:F:218:GLN:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:198:VAL:HG22	19:S:203:ILE:HG12	1.87	0.55
27:a:15:GLY:O	27:a:18:GLN:NE2	2.38	0.55
3:C:49:ARG:HD2	21:U:639:LEU:HD21	1.89	0.55
3:C:90:HIS:HB3	3:C:91:PRO:CD	2.35	0.55
11:K:117:SER:HB3	11:K:156:MET:HE2	1.88	0.55
22:V:177:ASN:O	22:V:179:LYS:NZ	2.39	0.55
26:Z:138:TYR:HB3	26:Z:155:PHE:HB3	1.88	0.55
14:n:148:THR:OG1	14:n:151:GLU:OE1	2.24	0.55
23:W:174:TYR:O	23:W:182:ARG:NH2	2.36	0.55
14:N:4:MET:HG3	14:N:127:ILE:HG22	1.88	0.55
21:U:653:ALA:HB2	21:U:675:MET:HE2	1.87	0.55
25:Y:235:ASP:O	25:Y:239:LYS:NZ	2.39	0.55
19:s:204:ARG:NH1	19:s:206:GLU:OE2	2.40	0.55
2:B:222:VAL:HG12	2:B:349:ARG:HB2	1.89	0.55
2:B:313:LEU:O	2:B:346:ARG:NH1	2.40	0.55
16:P:203:ARG:NH2	16:P:205:ASP:OD2	2.38	0.55
23:W:444:HIS:NE2	26:Z:207:ASP:OD1	2.40	0.55
1:A:99:THR:HG22	1:A:115:VAL:HA	1.87	0.54
32:f:96:LEU:HD11	32:f:128:VAL:HG12	1.89	0.54
22:V:461:LYS:NZ	22:V:462:GLU:O	2.40	0.54
25:Y:50:MET:O	25:Y:54:TYR:N	2.39	0.54
25:Y:388:ASN:HB2	26:Z:279:LYS:HE3	1.88	0.54
10:j:105:GLU:OE2	10:j:109:ARG:NH1	2.39	0.54
33:u:22:THR:OG1	33:u:25:ASN:OD1	2.25	0.54
4:D:85:ILE:HB	4:D:86:PRO:CD	2.36	0.54
6:F:235:LEU:HD21	35:F:501:ATP:H2'	1.90	0.54
23:W:201:ARG:HD3	23:W:204:ILE:HD11	1.89	0.54
32:f:616:CYS:O	32:f:650:GLN:NE2	2.40	0.54
5:E:265:ASP:OD2	5:E:291:ARG:NH2	2.36	0.54
25:Y:292:TYR:OH	25:Y:293:ARG:NH2	2.41	0.54
26:Z:273:HIS:HD1	29:c:255:TYR:HH	1.54	0.54
1:A:286:ASP:OD2	6:F:334:ARG:NH1	2.41	0.54
11:K:91:LYS:HG2	11:K:119:LEU:HD11	1.90	0.54
20:T:25:ASP:OD1	20:T:41:ARG:NH2	2.39	0.54
27:a:324:ILE:HG13	27:a:331:VAL:HG13	1.90	0.54
10:j:146:GLN:NE2	10:j:147:THR:O	2.40	0.54
22:V:350:GLN:HB2	22:V:353:LEU:HB3	1.90	0.54
19:S:144:MET:HE1	19:S:185:ARG:HB2	1.90	0.54
1:A:351:ARG:NH1	1:A:378:PRO:O	2.41	0.54
3:C:119:ASP:OD1	3:C:120:SER:N	2.40	0.54
32:f:348:ILE:O	32:f:350:LYS:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:549:GLU:HG3	32:f:587:PHE:CG	2.43	0.54
1:A:44:GLN:OE1	1:A:47:GLN:NE2	2.40	0.53
3:C:141:GLU:HG3	3:C:212:ILE:HG12	1.89	0.53
13:M:108:LEU:HD11	13:M:137:LEU:HB3	1.89	0.53
32:f:418:LEU:HD13	32:f:425:GLY:HA2	1.90	0.53
7:g:10:ASP:O	7:g:24:GLN:NE2	2.41	0.53
8:h:111:VAL:HG22	8:h:136:ILE:HD12	1.89	0.53
10:j:221:ASN:ND2	10:j:223:GLU:HB3	2.20	0.53
12:l:117:GLN:NE2	13:m:83:ASP:OD1	2.41	0.53
1:A:98:CYS:HA	1:A:141:GLY:HA2	1.90	0.53
2:B:230:THR:HG21	2:B:353:PHE:HB3	1.90	0.53
19:S:209:SER:OG	19:S:212:LYS:NZ	2.41	0.53
27:a:193:GLN:HB3	27:a:225:LEU:HD13	1.90	0.53
20:t:25:ASP:OD1	20:t:41:ARG:NH2	2.39	0.53
2:B:224:LEU:HD21	2:B:235:LEU:HD22	1.89	0.53
5:E:182:LEU:HD22	37:E:401:ADP:H2'	1.91	0.53
16:P:149:MET:HE2	16:P:153:LEU:HD11	1.90	0.53
21:U:678:ASP:O	21:U:684:ARG:NH1	2.36	0.53
23:W:240:TYR:HA	23:W:243:ILE:HD12	1.89	0.53
23:W:401:THR:HG23	23:W:402:ILE:HD12	1.89	0.53
25:Y:26:LEU:HD13	25:Y:63:TRP:HH2	1.73	0.53
7:G:123:GLN:NE2	8:H:82:ASP:OD1	2.41	0.53
32:f:470:VAL:HG13	32:f:471:LEU:HG	1.89	0.53
14:n:4:MET:HE1	14:n:159:ALA:HB3	1.91	0.53
14:n:144:ARG:H	14:n:147:MET:HE3	1.74	0.53
4:D:145:PRO:HB2	4:D:256:GLU:HG3	1.90	0.53
9:I:119:GLN:NE2	10:J:79:ASP:OD1	2.40	0.53
24:X:35:ILE:HD12	24:X:46:LYS:HD2	1.90	0.53
27:a:226:ARG:HB3	27:a:234:ILE:HD11	1.89	0.53
24:X:307:THR:HA	24:X:310:ARG:HE	1.74	0.53
30:d:147:SER:OG	30:d:150:LYS:NZ	2.42	0.53
10:j:42:VAL:HG11	10:j:191:VAL:HG21	1.90	0.53
12:l:6:TYR:OH	13:m:8:ASP:OD2	2.27	0.53
4:D:345:PHE:HB3	4:D:360:LEU:HD21	1.89	0.53
21:U:10:SER:HB2	30:d:73:ARG:HG3	1.89	0.53
4:D:249:ASP:OD1	4:D:252:ARG:NH2	2.41	0.53
10:J:68:ASN:HA	10:J:211:MET:HE1	1.91	0.53
15:O:174:ASP:OD2	15:O:187:ARG:NH1	2.42	0.53
19:S:125:ASP:OD1	19:S:129:SER:N	2.42	0.53
29:c:52:GLU:OE2	33:u:76:GLY:HA2	2.08	0.53
30:d:44:THR:OG1	30:d:47:GLN:NE2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:21:ARG:NH1	7:g:26:GLU:HB3	2.23	0.53
1:A:78:TRP:HA	1:A:81:ALA:HB3	1.91	0.53
3:C:87:VAL:HG12	3:C:89:VAL:H	1.74	0.53
30:d:110:ASN:ND2	30:d:173:THR:OG1	2.40	0.53
11:k:121:LEU:HD23	11:k:160:GLY:HA3	1.91	0.53
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.90	0.52
7:G:158:GLY:O	8:H:84:ARG:NH2	2.42	0.52
22:V:463:MET:HE3	22:V:465:ASP:H	1.74	0.52
7:g:43:ARG:HH21	7:g:164:LYS:HG2	1.73	0.52
2:B:319:PHE:HB3	2:B:322:ARG:HH12	1.74	0.52
3:C:257:SER:HB2	3:C:301:LEU:HA	1.90	0.52
15:O:164:PHE:O	19:s:38:ARG:NH2	2.42	0.52
22:V:311:ASN:OD1	22:V:314:ARG:NH1	2.39	0.52
7:g:187:PHE:HD1	7:g:189:TRP:HE1	1.56	0.52
8:H:93:LEU:HD13	8:H:113:ARG:HB3	1.90	0.52
25:Y:226:VAL:O	25:Y:229:ILE:HG22	2.08	0.52
4:D:341:LYS:NZ	4:D:367:PRO:O	2.42	0.52
11:K:210:LEU:HG	11:K:238:ILE:HD11	1.92	0.52
16:P:35:VAL:HG12	16:P:36:THR:HG23	1.92	0.52
6:F:314:LEU:HD21	6:F:342:LEU:HA	1.92	0.52
12:L:157:ARG:NH2	13:M:60:GLU:OE1	2.43	0.52
23:W:275:ILE:HG23	23:W:309:PHE:HE2	1.75	0.52
30:d:7:GLY:O	30:d:11:ARG:NH2	2.42	0.52
21:U:155:LEU:O	21:U:158:ARG:NH1	2.43	0.52
21:U:167:ILE:HB	21:U:177:LEU:HD11	1.91	0.52
32:f:474:SER:HB3	32:f:477:MET:HB2	1.92	0.52
16:p:159:ASP:OD1	16:p:159:ASP:N	2.41	0.52
26:Z:237:LEU:HD12	29:c:310:LYS:HB2	1.91	0.52
7:g:49:VAL:HG22	7:g:219:VAL:HG12	1.92	0.52
4:D:56:VAL:HG21	21:U:599:ILE:HG23	1.92	0.52
6:F:334:ARG:HH11	6:F:337:ILE:HD11	1.74	0.52
4:D:115:ILE:HG22	4:D:139:LEU:HD12	1.92	0.52
13:M:68:ASN:OD1	13:M:224:HIS:ND1	2.43	0.52
13:M:237:LYS:HA	13:M:240:LYS:HE3	1.92	0.52
22:V:343:PRO:O	31:e:43:TRP:NE1	2.43	0.52
24:X:47:GLU:OE2	24:X:80:ILE:HG21	2.10	0.52
32:f:384:ALA:HA	32:f:419:LEU:HB3	1.92	0.52
15:o:112:SER:HB2	15:o:127:MET:HE3	1.92	0.52
17:q:25:ILE:HG22	17:q:26:VAL:HG13	1.92	0.52
4:D:67:ASN:HD22	21:U:607:VAL:HG12	1.74	0.51
19:S:10:GLY:HA3	19:S:42:LYS:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:196:LEU:C	29:c:198:ARG:H	2.17	0.51
1:A:410:LEU:HA	1:A:413:VAL:HG22	1.92	0.51
21:U:160:LEU:HD21	21:U:196:LYS:HB3	1.92	0.51
27:a:34:TRP:HZ3	27:a:64:ILE:HG23	1.75	0.51
32:f:75:LEU:HD11	32:f:113:MET:HE1	1.91	0.51
12:l:139:ASP:N	12:l:139:ASP:OD1	2.41	0.51
6:F:368:ILE:HG23	6:F:371:ARG:HH22	1.76	0.51
10:J:50:VAL:HB	10:J:54:GLN:HB2	1.91	0.51
21:U:483:LEU:HD11	21:U:781:LEU:HD11	1.93	0.51
24:X:157:LEU:HD21	24:X:165:LEU:HD23	1.92	0.51
32:f:178:LYS:HA	32:f:181:ARG:HG2	1.91	0.51
32:f:795:GLY:O	32:f:798:THR:OG1	2.27	0.51
4:D:126:PRO:O	4:D:127:ASN:C	2.53	0.51
8:H:204:THR:OG1	8:H:206:ASP:OD1	2.27	0.51
25:Y:66:ASP:HB3	25:Y:69:LEU:HB3	1.91	0.51
28:b:124:LEU:HD13	28:b:156:PHE:HB2	1.93	0.51
2:B:103:ARG:HB2	2:B:160:ILE:HD13	1.93	0.51
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.92	0.51
8:H:111:VAL:HG22	8:H:136:ILE:HD12	1.92	0.51
21:U:133:ILE:HG22	21:U:136:LYS:HE2	1.92	0.51
22:V:496:PHE:HB2	22:V:497:PRO:HD3	1.93	0.51
27:a:77:VAL:HA	27:a:80:ILE:HG12	1.93	0.51
27:a:210:VAL:HG12	27:a:213:PHE:CE2	2.45	0.51
30:d:103:LEU:HD23	30:d:136:PRO:HB2	1.92	0.51
32:f:586:PRO:O	32:f:589:SER:N	2.44	0.51
4:D:45:LYS:HE2	21:U:187:LEU:HB2	1.92	0.51
4:D:234:GLU:O	4:D:237:GLN:NE2	2.43	0.51
21:U:334:ALA:O	21:U:338:HIS:ND1	2.43	0.51
21:U:890:LYS:HG3	21:U:891:VAL:HG13	1.92	0.51
15:o:63:LEU:HD11	15:o:79:ALA:HB2	1.92	0.51
1:A:297:ARG:HH22	6:F:306:VAL:HG21	1.76	0.51
1:A:307:ASP:OD2	1:A:333:ARG:NH2	2.40	0.51
12:L:44:ALA:HB2	12:L:142:PRO:HB3	1.92	0.51
24:X:229:TYR:HE1	24:X:254:MET:HE2	1.75	0.51
24:X:255:LEU:HD22	24:X:267:VAL:HG13	1.92	0.51
24:X:317:PRO:HG2	24:X:318:ILE:HD12	1.93	0.51
25:Y:71:ASN:HA	25:Y:74:LYS:HG2	1.92	0.51
27:a:72:ASN:HD21	27:a:74:LEU:HD12	1.76	0.51
11:k:167:ALA:HB3	12:l:56:LEU:HD21	1.92	0.51
2:B:125:THR:OG1	2:B:126:SER:N	2.44	0.51
7:G:6:SER:OG	7:G:11:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:299:LEU:HD12	24:X:330:LEU:HD23	1.92	0.51
26:Z:136:GLU:OE2	26:Z:157:HIS:ND1	2.44	0.51
29:c:57:MET:HE3	29:c:112:TYR:HB3	1.93	0.51
29:c:177:THR:HG23	29:c:179:SER:H	1.75	0.51
5:E:83:CYS:HB2	5:E:89:LYS:HE2	1.92	0.51
23:W:340:VAL:O	23:W:350:ARG:HD3	2.11	0.51
25:Y:98:SER:OG	25:Y:101:ARG:NH2	2.44	0.51
3:C:233:GLU:HA	3:C:236:VAL:HB	1.92	0.50
21:U:346:ASN:ND2	21:U:380:THR:OG1	2.45	0.50
25:Y:314:LEU:O	25:Y:354:VAL:N	2.43	0.50
27:a:360:VAL:HG22	29:c:308:VAL:HG13	1.93	0.50
29:c:192:LEU:CA	29:c:196:LEU:HB2	2.37	0.50
29:c:196:LEU:O	29:c:198:ARG:N	2.37	0.50
30:d:139:LEU:HD11	30:d:151:VAL:HG13	1.92	0.50
8:h:68:ILE:HD11	8:h:74:LEU:HD12	1.92	0.50
11:K:41:GLN:NE2	11:K:151:PRO:O	2.44	0.50
27:a:35:HIS:NE2	28:b:14:GLU:O	2.44	0.50
27:a:341:LEU:HD13	27:a:345:GLN:HB2	1.94	0.50
11:k:20:ARG:NH2	11:k:25:GLU:OE2	2.40	0.50
10:J:148:ASP:OD1	10:J:152:THR:N	2.38	0.50
9:i:174:MET:HE2	9:i:196:VAL:HG22	1.92	0.50
19:s:27:THR:HB	19:s:40:SER:H	1.75	0.50
3:C:340:ARG:NH1	25:Y:9:GLU:OE2	2.45	0.50
22:V:280:ALA:O	25:Y:385:ARG:NH2	2.44	0.50
26:Z:185:GLY:O	26:Z:189:GLN:NE2	2.44	0.50
29:c:30:GLN:HB3	29:c:66:THR:HG22	1.93	0.50
32:f:585:GLU:CB	32:f:586:PRO:HD2	2.25	0.50
10:j:185:ASP:OD1	10:j:185:ASP:N	2.44	0.50
3:C:62:GLU:HG2	3:C:66:LEU:HD13	1.94	0.50
17:Q:137:PHE:HB3	18:r:133:VAL:HG21	1.94	0.50
21:U:432:SER:OG	21:U:435:SER:O	2.29	0.50
10:J:208:LEU:HD22	10:J:220:LEU:CD2	2.41	0.50
22:V:321:ALA:HB1	22:V:324:PHE:HB3	1.93	0.50
16:p:67:LEU:HD21	16:p:87:LEU:HD11	1.94	0.50
11:K:85:ALA:HB2	11:K:139:VAL:HG11	1.93	0.50
21:U:214:ILE:HB	21:U:904:LYS:HZ1	1.76	0.50
19:s:125:ASP:OD1	19:s:129:SER:N	2.45	0.50
25:Y:105:MET:SD	25:Y:136:HIS:NE2	2.85	0.50
25:Y:210:SER:HB3	25:Y:213:LEU:HD23	1.94	0.50
32:f:237:VAL:HB	32:f:248:LEU:HD11	1.93	0.50
10:j:222:PRO:HA	10:j:225:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:PRO:HA	1:A:327:LEU:HD23	1.94	0.50
25:Y:220:VAL:HG21	25:Y:249:VAL:HG21	1.92	0.50
33:u:23:ILE:HB	33:u:52:ASP:HA	1.92	0.50
1:A:103:ASN:HA	1:A:136:GLU:HG2	1.94	0.49
27:a:273:GLN:HB3	27:a:310:LEU:HD11	1.94	0.49
29:c:146:ASP:OD2	29:c:149:GLN:N	2.37	0.49
15:o:22:GLU:HG2	15:o:27:ALA:HB2	1.93	0.49
1:A:156:LYS:NZ	1:A:157:ILE:O	2.45	0.49
21:U:8:ILE:HD11	30:d:36:LEU:HD11	1.93	0.49
21:U:772:TRP:HD1	21:U:775:LEU:HB2	1.78	0.49
27:a:65:SER:HA	27:a:68:GLU:HB2	1.95	0.49
27:a:214:GLY:O	27:a:215:GLU:C	2.55	0.49
16:p:27:ARG:HB2	16:p:183:MET:HB2	1.94	0.49
5:E:136:GLY:O	37:E:401:ADP:N6	2.38	0.49
5:E:146:ARG:NH1	5:E:150:GLU:OE1	2.45	0.49
32:f:583:VAL:HG12	32:f:584:SER:H	1.78	0.49
5:E:144:GLU:O	5:E:297:ARG:NH2	2.43	0.49
21:U:611:ASN:HB3	21:U:614:VAL:HG12	1.94	0.49
30:d:109:GLN:OE1	30:d:111:ARG:NH2	2.46	0.49
8:H:16:SER:OG	8:H:18:LYS:NZ	2.41	0.49
24:X:12:ALA:HB2	24:X:26:ILE:HG21	1.93	0.49
24:X:389:ASP:OD1	24:X:389:ASP:N	2.41	0.49
7:g:21:ARG:HH11	7:g:26:GLU:HB3	1.77	0.49
8:h:148:GLN:OE1	8:h:158:TRP:NE1	2.45	0.49
6:F:43:GLN:HA	6:F:46:ARG:HG2	1.95	0.49
22:V:337:LEU:HD21	22:V:364:THR:HG23	1.94	0.49
23:W:445:LEU:HD22	26:Z:157:HIS:HB2	1.94	0.49
27:a:321:LYS:O	27:a:334:THR:OG1	2.27	0.49
32:f:654:VAL:HA	32:f:657:ILE:HD12	1.95	0.49
1:A:66:LYS:NZ	1:A:69:ASP:OD1	2.38	0.49
4:D:85:ILE:O	4:D:87:LEU:HG	2.11	0.49
7:G:10:ASP:OD1	7:G:10:ASP:N	2.45	0.49
29:c:279:ASP:OD1	29:c:279:ASP:N	2.44	0.49
12:l:164:ARG:NH1	12:l:198:THR:O	2.45	0.49
1:A:367:ASP:HB2	1:A:406:GLU:HG3	1.93	0.49
21:U:34:PHE:O	21:U:38:ILE:HG12	2.13	0.49
21:U:766:PHE:O	21:U:776:SER:OG	2.28	0.49
22:V:287:ARG:NH2	31:e:17:ASP:OD2	2.43	0.49
27:a:247:ARG:HH22	27:a:269:LEU:HD22	1.76	0.49
32:f:470:VAL:HG11	32:f:500:LEU:HD21	1.95	0.49
4:D:124:LEU:C	4:D:126:PRO:HD2	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:49:ASN:OD1	25:Y:77:ASN:ND2	2.45	0.49
32:f:550:LEU:CD2	32:f:586:PRO:HB2	2.40	0.49
3:C:246:ILE:HB	3:C:291:VAL:HG12	1.94	0.49
29:c:269:GLN:HA	29:c:272:ILE:HG22	1.95	0.49
16:p:35:VAL:HG12	16:p:36:THR:HG23	1.95	0.49
1:A:265:ARG:NH2	1:A:310:ASP:O	2.46	0.48
18:R:35:ILE:HD11	18:R:45:MET:HG3	1.95	0.48
21:U:18:GLN:HG3	30:d:27:LYS:HZ2	1.77	0.48
24:X:149:LEU:HG	24:X:153:LEU:HB2	1.94	0.48
26:Z:37:GLY:HA2	26:Z:56:VAL:HG12	1.95	0.48
5:E:75:ASN:HD22	6:F:130:GLN:HG2	1.77	0.48
24:X:70:LEU:HD13	24:X:109:LEU:HD23	1.95	0.48
27:a:216:LEU:HA	27:a:219:HIS:HB2	1.94	0.48
28:b:157:VAL:HG21	28:b:170:LEU:HB2	1.96	0.48
4:D:274:ARG:NH2	4:D:282:ASP:OD2	2.47	0.48
9:I:86:LEU:HD22	9:I:114:LEU:HD11	1.94	0.48
11:K:235:GLU:HA	11:K:238:ILE:HG22	1.95	0.48
21:U:18:GLN:CG	30:d:27:LYS:NZ	2.76	0.48
10:j:158:ALA:HB3	11:k:58:LEU:HD21	1.94	0.48
5:E:216:ARG:HG3	5:E:263:GLN:HE22	1.78	0.48
21:U:632:GLN:O	21:U:635:SER:OG	2.32	0.48
26:Z:198:LEU:HD11	29:c:308:VAL:HG21	1.94	0.48
29:c:80:THR:OG1	29:c:83:SER:O	2.27	0.48
30:d:114:GLU:HA	30:d:117:THR:HG22	1.95	0.48
32:f:211:ILE:HG23	32:f:213:GLN:H	1.78	0.48
7:g:112:ASP:OD1	7:g:112:ASP:N	2.43	0.48
11:k:34:GLY:O	11:k:53:ARG:NH1	2.46	0.48
18:r:35:ILE:N	18:r:43:GLY:O	2.46	0.48
22:V:496:PHE:H	22:V:497:PRO:HD2	1.78	0.48
25:Y:162:GLU:HA	25:Y:165:LYS:HG2	1.95	0.48
27:a:70:ARG:HH21	28:b:80:PRO:HD2	1.78	0.48
32:f:93:PRO:HB2	32:f:96:LEU:HB2	1.94	0.48
17:q:26:VAL:HG21	18:r:136:TYR:HE2	1.79	0.48
21:U:30:VAL:HG12	21:U:34:PHE:HE2	1.78	0.48
24:X:44:GLN:HG3	24:X:48:GLN:HE22	1.79	0.48
26:Z:20:VAL:HG11	29:c:213:GLU:HB3	1.94	0.48
32:f:65:GLU:O	32:f:66:LYS:C	2.57	0.48
11:k:88:LEU:HD23	11:k:119:LEU:HD23	1.96	0.48
14:n:4:MET:HG3	14:n:127:ILE:HG22	1.95	0.48
16:p:30:ILE:HG22	16:p:31:GLN:H	1.77	0.48
3:C:53:ASN:HD21	21:U:643:SER:HA	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:39:LYS:HE2	12:L:157:ARG:HG3	1.95	0.48
21:U:422:LEU:HD21	21:U:446:LEU:HD11	1.96	0.48
32:f:398:TRP:HA	32:f:401:LYS:HD3	1.95	0.48
20:t:25:ASP:HA	20:t:187:PHE:HA	1.94	0.48
2:B:248:LEU:HD12	2:B:282:VAL:HG22	1.96	0.48
3:C:113:ARG:NH2	3:C:128:PRO:O	2.47	0.48
3:C:338:LEU:HA	3:C:378:VAL:HB	1.95	0.48
4:D:84:SER:O	4:D:85:ILE:C	2.57	0.48
4:D:378:ILE:HG23	4:D:402:ALA:HB1	1.96	0.48
10:J:96:LEU:HD11	17:Q:58:GLU:HB3	1.96	0.48
21:U:167:ILE:HG22	21:U:176:MET:HE2	1.95	0.48
29:c:266:THR:O	29:c:267:PRO:C	2.57	0.48
31:e:16:ASP:OD1	31:e:16:ASP:N	2.47	0.48
32:f:288:VAL:HG12	32:f:292:LYS:HZ1	1.78	0.48
26:Z:263:ALA:HB1	29:c:288:VAL:HG13	1.95	0.48
3:C:234:LEU:HA	3:C:237:MET:HE2	1.94	0.48
6:F:102:ASN:H	6:F:115:SER:HB2	1.78	0.48
21:U:45:ILE:HG21	21:U:64:ALA:HB2	1.95	0.48
22:V:417:ILE:HD12	22:V:422:ILE:HB	1.95	0.48
27:a:100:THR:HA	27:a:103:LYS:HG2	1.95	0.48
7:g:165:ALA:HB1	7:g:179:LEU:HD13	1.95	0.48
7:g:202:LEU:HA	7:g:205:VAL:HG12	1.96	0.48
21:U:623:GLY:HA3	21:U:658:ILE:HG13	1.96	0.47
27:a:34:TRP:HD1	28:b:18:ASN:HA	1.79	0.47
12:L:226:ASP:OD1	12:L:226:ASP:N	2.48	0.47
30:d:86:LYS:HD3	30:d:89:LEU:HD22	1.96	0.47
7:g:31:ALA:HB1	7:g:83:MET:HE3	1.95	0.47
12:l:13:TRP:H	13:m:22:GLN:HE22	1.62	0.47
1:A:345:LEU:HD21	1:A:381:THR:HG22	1.95	0.47
12:L:47:VAL:HG12	12:L:195:LEU:HD22	1.95	0.47
12:L:166:GLN:OE1	12:L:169:ARG:NH2	2.47	0.47
24:X:268:GLN:OE1	24:X:288:LYS:NZ	2.47	0.47
20:t:50:MET:HE3	20:t:192:VAL:HB	1.96	0.47
4:D:125:LYS:HA	4:D:125:LYS:HD2	1.39	0.47
23:W:147:LYS:HD2	23:W:185:PHE:HE1	1.79	0.47
27:a:213:PHE:O	27:a:214:GLY:C	2.57	0.47
28:b:26:LEU:HD11	28:b:80:PRO:HG3	1.96	0.47
32:f:678:LEU:HD22	32:f:686:LEU:HD21	1.96	0.47
20:t:193:THR:HG23	20:t:195:LYS:H	1.80	0.47
19:S:99:ARG:HH21	19:S:102:PHE:HD2	1.63	0.47
10:j:30:SER:HB3	10:j:46:GLU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:482:PHE:HZ	25:Y:381:GLN:HG3	1.79	0.47
29:c:49:VAL:HG23	29:c:148:ILE:HD11	1.97	0.47
32:f:231:LEU:HG	32:f:853:VAL:HG22	1.97	0.47
19:s:72:LEU:HG	19:s:83:MET:SD	2.55	0.47
13:M:34:SER:HB3	13:M:65:ARG:HH12	1.78	0.47
21:U:699:THR:OG1	21:U:810:THR:O	2.32	0.47
32:f:344:VAL:HG23	32:f:346:ASP:H	1.79	0.47
10:j:87:ALA:HB1	10:j:107:ILE:HD11	1.97	0.47
20:t:126:ASP:OD1	20:t:130:VAL:N	2.46	0.47
4:D:267:ILE:HD13	4:D:309:MET:HG2	1.96	0.47
21:U:788:VAL:HG13	21:U:884:VAL:HG11	1.97	0.47
32:f:65:GLU:C	32:f:66:LYS:HE3	2.40	0.47
32:f:557:TRP:HA	32:f:560:LEU:HD12	1.97	0.47
7:g:58:ASP:OD1	7:g:58:ASP:N	2.45	0.47
11:k:4:THR:OG1	11:k:5:ARG:N	2.45	0.47
10:J:42:VAL:HG22	10:J:210:VAL:HG12	1.96	0.47
21:U:18:GLN:NE2	21:U:18:GLN:C	2.73	0.47
21:U:33:ASP:O	21:U:35:TRP:N	2.48	0.47
24:X:24:ILE:HG22	24:X:28:HIS:CE1	2.49	0.47
3:C:45:LEU:HB3	4:D:61:ILE:HG21	1.96	0.47
4:D:248:ARG:HG2	4:D:295:GLN:HE22	1.79	0.47
5:E:360:ASP:N	5:E:360:ASP:OD1	2.48	0.47
7:G:37:LEU:HD22	7:G:53:GLN:HG3	1.97	0.47
11:K:77:ALA:HB3	11:K:142:LEU:HB2	1.97	0.47
24:X:297:ARG:O	24:X:334:ASN:ND2	2.48	0.47
32:f:586:PRO:O	32:f:587:PHE:C	2.58	0.47
13:m:38:GLY:HA3	13:m:136:MET:HE1	1.96	0.47
17:q:38:MET:HE1	17:q:61:GLN:HA	1.97	0.47
8:H:175:GLU:O	9:I:54:LYS:NZ	2.43	0.46
25:Y:319:MET:HG3	25:Y:330:ILE:HG21	1.97	0.46
26:Z:94:TRP:HB3	26:Z:112:MET:HE3	1.97	0.46
29:c:57:MET:HB3	29:c:69:VAL:HG21	1.97	0.46
32:f:151:LEU:HB3	32:f:159:VAL:HG22	1.96	0.46
32:f:313:GLU:HG3	32:f:316:ASP:HB2	1.98	0.46
9:i:136:TYR:HB2	9:i:148:TYR:HB2	1.96	0.46
12:l:35:THR:HG23	12:l:133:LEU:HD12	1.98	0.46
20:t:27:LEU:HD22	20:t:184:TYR:HB2	1.97	0.46
1:A:172:VAL:O	1:A:231:ASN:ND2	2.48	0.46
6:F:265:ALA:HA	6:F:312:GLU:HG2	1.96	0.46
26:Z:226:ILE:HA	26:Z:229:GLN:CD	2.39	0.46
27:a:50:PHE:HD2	27:a:52:GLN:HB3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:135:ALA:HB3	33:u:36:ILE:HD11	1.96	0.46
7:G:244:GLU:O	23:W:52:LYS:NZ	2.48	0.46
17:Q:31:ASP:OD1	17:Q:31:ASP:N	2.48	0.46
20:T:27:LEU:HD22	20:T:184:TYR:HB2	1.96	0.46
21:U:886:PRO:HA	21:U:889:LEU:HD23	1.98	0.46
26:Z:215:VAL:HA	26:Z:220:LEU:HB2	1.97	0.46
27:a:77:VAL:HG21	27:a:113:LEU:HD11	1.96	0.46
32:f:726:ILE:HG12	32:f:748:LEU:HD21	1.98	0.46
8:h:213:CYS:HB2	8:h:218:PHE:HD1	1.79	0.46
33:u:63:LYS:HD3	33:u:64:GLU:HB2	1.98	0.46
6:F:70:LYS:HE3	6:F:74:LYS:NZ	2.31	0.46
13:M:27:MET:HE1	13:M:152:ASP:HB2	1.98	0.46
14:N:141:ALA:HB2	14:n:162:LEU:HD11	1.97	0.46
10:j:80:ALA:HA	10:j:129:ILE:HD13	1.96	0.46
1:A:151:ILE:HD12	1:A:152:PRO:HD2	1.98	0.46
2:B:411:ARG:NH2	2:B:418:ASP:OD1	2.41	0.46
3:C:72:TYR:N	3:C:116:LEU:O	2.46	0.46
3:C:230:MET:SD	3:C:230:MET:N	2.89	0.46
4:D:352:MET:HE3	5:E:164:ILE:HD11	1.97	0.46
17:Q:52:ASP:OD1	18:R:88:TYR:OH	2.31	0.46
25:Y:142:PHE:HE2	25:Y:176:ARG:HD2	1.78	0.46
25:Y:349:LYS:O	25:Y:351:ASN:N	2.49	0.46
30:d:78:LEU:HD13	30:d:98:LEU:HD21	1.97	0.46
3:C:130:LYS:HG3	3:C:131:VAL:H	1.80	0.46
4:D:133:HIS:HB3	4:D:137:ASN:H	1.80	0.46
12:L:84:LEU:HD11	12:L:112:ILE:HD12	1.97	0.46
21:U:119:PRO:HA	21:U:123:LYS:HD3	1.97	0.46
24:X:24:ILE:CG2	24:X:28:HIS:HE1	2.29	0.46
27:a:252:LYS:HA	27:a:255:TRP:HE3	1.80	0.46
27:a:345:GLN:O	27:a:349:MET:HG3	2.16	0.46
3:C:250:GLU:HG3	3:C:295:THR:HA	1.98	0.46
6:F:98:ASP:N	6:F:98:ASP:OD1	2.48	0.46
16:P:70:ARG:HD2	16:P:94:LEU:HD12	1.98	0.46
21:U:16:GLU:HB2	21:U:20:LYS:HB2	1.97	0.46
22:V:259:LEU:HD11	22:V:294:ARG:HD3	1.96	0.46
23:W:105:VAL:HG21	23:W:138:VAL:HG12	1.97	0.46
25:Y:14:ASN:C	25:Y:14:ASN:HD22	2.23	0.46
29:c:196:LEU:C	29:c:198:ARG:N	2.74	0.46
19:s:10:GLY:HA3	19:s:42:LYS:HE2	1.97	0.46
16:P:143:ALA:HA	16:P:146:MET:HE3	1.97	0.46
16:P:193:ASP:OD1	16:P:193:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:e:50:ASP:OD1	31:e:50:ASP:N	2.49	0.46
32:f:348:ILE:O	32:f:349:TYR:C	2.58	0.46
5:E:348:THR:HA	6:F:217:ILE:HD12	1.97	0.46
11:K:146:VAL:HG11	11:K:222:PRO:HA	1.97	0.46
21:U:579:ARG:NH1	21:U:609:ASP:OD1	2.49	0.46
26:Z:65:ASP:OD1	26:Z:65:ASP:N	2.49	0.46
29:c:149:GLN:HB2	29:c:156:VAL:HG21	1.98	0.46
19:s:91:MET:HE2	19:s:91:MET:HB3	1.77	0.46
1:A:363:SER:HB2	2:B:214:MET:HE3	1.97	0.46
2:B:232:LYS:NZ	2:B:331:THR:O	2.41	0.46
21:U:794:ASP:OD1	21:U:794:ASP:N	2.48	0.46
22:V:494:MET:HE1	26:Z:274:ASN:HB3	1.97	0.46
31:e:44:ASP:OD1	31:e:47:ASN:ND2	2.39	0.46
18:r:83:LEU:HA	18:r:86:MET:HE3	1.98	0.46
19:s:166:LEU:HD21	19:s:171:ALA:HB2	1.98	0.46
4:D:348:ILE:HD11	35:D:501:ATP:H2	1.81	0.45
10:J:48:LYS:HD2	10:J:163:ARG:HH22	1.81	0.45
15:O:38:SER:OG	15:O:40:ASN:OD1	2.30	0.45
25:Y:202:LEU:HD13	25:Y:239:LYS:HD2	1.98	0.45
19:s:16:ALA:HB2	19:s:121:VAL:HG23	1.99	0.45
3:C:287:LYS:HE3	3:C:287:LYS:HB2	1.56	0.45
4:D:57:GLN:O	4:D:61:ILE:HG12	2.16	0.45
5:E:210:GLU:OE2	5:E:213:ARG:NH2	2.41	0.45
21:U:541:HIS:HB2	21:U:544:ILE:HG22	1.98	0.45
23:W:344:THR:HG23	23:W:347:GLY:H	1.82	0.45
25:Y:238:GLU:HG3	25:Y:239:LYS:HG3	1.97	0.45
27:a:123:LEU:HD21	27:a:161:LYS:HG3	1.98	0.45
30:d:234:ASP:OD1	30:d:235:THR:N	2.49	0.45
32:f:156:HIS:O	32:f:160:ARG:HG2	2.16	0.45
10:j:96:LEU:HB2	17:q:62:LYS:HD2	1.98	0.45
13:m:144:ASP:OD2	13:m:147:GLN:NE2	2.48	0.45
1:A:59:ILE:HD11	2:B:76:GLU:HB3	1.97	0.45
4:D:393:ILE:HD12	23:W:134:GLY:HA2	1.99	0.45
6:F:39:GLU:HB3	6:F:43:GLN:HB2	1.98	0.45
21:U:30:VAL:HG12	21:U:34:PHE:CE2	2.51	0.45
25:Y:233:ARG:HH21	25:Y:264:TYR:HA	1.81	0.45
9:i:17:ARG:NH1	9:i:22:GLU:OE2	2.49	0.45
1:A:413:VAL:HA	1:A:416:VAL:HG22	1.98	0.45
2:B:64:LYS:O	2:B:68:ILE:HG12	2.17	0.45
14:N:1:THR:N	14:N:169:SER:O	2.49	0.45
19:S:158:MET:HE2	19:S:161:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:146:LYS:HE2	21:U:148:LYS:HB2	1.98	0.45
21:U:265:ILE:HA	21:U:268:LEU:HD12	1.98	0.45
22:V:419:LEU:HA	22:V:422:ILE:HG22	1.98	0.45
32:f:389:LYS:HD2	32:f:392:THR:HB	1.97	0.45
8:h:55:ILE:HD12	8:h:55:ILE:H	1.81	0.45
12:l:47:VAL:HG12	12:l:195:LEU:HD22	1.98	0.45
2:B:223:ILE:HD11	2:B:347:ILE:HD13	1.99	0.45
22:V:345:ARG:NH2	31:e:45:ASP:OD1	2.50	0.45
5:E:33:LEU:O	5:E:37:THR:OG1	2.28	0.45
6:F:289:ASP:OD1	6:F:289:ASP:N	2.48	0.45
11:K:240:ASP:OD1	11:K:240:ASP:N	2.49	0.45
15:O:140:ASP:OD2	20:t:171:ARG:NH2	2.46	0.45
21:U:367:THR:HG22	21:U:400:ALA:HB2	1.99	0.45
25:Y:247:LEU:HD23	25:Y:250:LEU:HD21	1.99	0.45
26:Z:45:LYS:HG3	26:Z:46:LYS:H	1.82	0.45
27:a:100:THR:HG22	27:a:103:LYS:HE2	1.99	0.45
10:j:11:SER:OG	10:j:15:HIS:N	2.50	0.45
11:k:16:SER:OG	11:k:18:GLU:OE1	2.35	0.45
13:m:185:THR:OG1	13:m:186:CYS:N	2.49	0.45
19:s:8:ASN:HD22	19:s:58:HIS:HB2	1.81	0.45
19:s:52:ILE:HG13	19:s:110:ILE:HG12	1.99	0.45
8:H:150:ASP:OD1	8:H:154:ALA:N	2.47	0.45
21:U:18:GLN:HE21	21:U:18:GLN:HA	1.82	0.45
30:d:45:LYS:HA	30:d:48:LEU:HB2	1.98	0.45
32:f:240:VAL:O	32:f:245:ASN:ND2	2.41	0.45
1:A:124:ASP:HB2	6:F:86:LEU:HD22	1.97	0.45
4:D:300:ASP:OD1	4:D:303:VAL:N	2.43	0.45
6:F:195:ILE:HG12	6:F:236:LEU:HD21	1.99	0.45
20:T:25:ASP:HA	20:T:187:PHE:HA	1.99	0.45
21:U:710:ARG:HE	21:U:737:LEU:HD23	1.81	0.45
23:W:47:LEU:HD22	23:W:66:ILE:HD11	1.98	0.45
26:Z:226:ILE:O	26:Z:228:TYR:N	2.50	0.45
27:a:115:LYS:HA	27:a:118:ILE:HD12	1.98	0.45
32:f:549:GLU:HG3	32:f:587:PHE:CD2	2.52	0.45
20:t:27:LEU:HD11	20:t:34:ALA:HB1	1.99	0.45
1:A:87:LEU:HA	1:A:90:GLU:HB2	1.98	0.45
19:S:19:ASP:OD1	19:S:19:ASP:N	2.48	0.45
4:D:67:ASN:ND2	21:U:607:VAL:O	2.49	0.45
11:K:202:LEU:O	11:K:206:MET:HG2	2.17	0.45
21:U:469:SER:OG	21:U:470:ASN:N	2.50	0.45
25:Y:11:LEU:HG	25:Y:179:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:51:LEU:HD23	28:b:71:ILE:HG23	1.99	0.45
15:O:97:ALA:HB1	15:O:127:MET:HE3	1.99	0.44
15:O:112:SER:HB3	15:O:125:VAL:HG11	1.99	0.44
21:U:428:PRO:HG3	21:U:439:GLU:HB3	1.98	0.44
26:Z:208:ILE:HG23	27:a:353:LEU:HD21	2.00	0.44
27:a:163:TYR:CE1	27:a:172:TYR:HB2	2.51	0.44
29:c:64:ASP:OD2	29:c:64:ASP:N	2.50	0.44
32:f:66:LYS:HB2	32:f:67:ASP:H	1.70	0.44
8:h:118:MET:HE2	8:h:151:PRO:HA	1.98	0.44
4:D:83:GLN:O	4:D:84:SER:C	2.59	0.44
4:D:410:ASP:OD1	4:D:410:ASP:N	2.50	0.44
5:E:135:ILE:HD11	5:E:142:ILE:HD11	1.98	0.44
8:H:203:MET:HA	8:H:207:ASN:HD21	1.82	0.44
24:X:24:ILE:CG2	24:X:28:HIS:CE1	3.00	0.44
26:Z:70:LEU:HD12	26:Z:111:LEU:HD22	1.98	0.44
27:a:78:GLU:O	27:a:82:HIS:ND1	2.37	0.44
27:a:249:GLN:HA	27:a:252:LYS:HB2	1.99	0.44
32:f:385:PHE:HE2	32:f:773:LYS:HD2	1.83	0.44
11:k:195:ILE:HD11	11:k:219:THR:HG21	2.00	0.44
1:A:114:ASN:HB3	1:A:120:LYS:HG2	1.98	0.44
10:J:42:VAL:HG11	10:J:191:VAL:HG21	1.99	0.44
17:Q:4:LEU:HD22	17:Q:45:LEU:HD23	1.99	0.44
19:S:116:GLU:N	19:S:116:GLU:OE2	2.50	0.44
29:c:100:LYS:HG2	29:c:105:PRO:HB3	1.98	0.44
11:k:221:GLN:HB2	11:k:224:GLN:HG2	1.98	0.44
16:p:53:LEU:HB3	16:p:60:VAL:HG22	1.99	0.44
17:q:23:SER:HB2	17:q:28:MET:HE2	1.99	0.44
1:A:400:ARG:HB3	32:f:89:MET:HG3	1.99	0.44
4:D:81:ARG:HH21	29:c:156:VAL:HG11	1.82	0.44
4:D:85:ILE:O	4:D:86:PRO:C	2.61	0.44
7:G:188:ASP:OD1	7:G:188:ASP:N	2.48	0.44
21:U:18:GLN:CB	30:d:27:LYS:HZ1	2.28	0.44
26:Z:54:PHE:HB3	26:Z:82:PHE:HE2	1.83	0.44
26:Z:202:ASN:ND2	27:a:361:LYS:HD3	2.32	0.44
28:b:53:THR:OG1	28:b:54:LEU:N	2.50	0.44
7:g:155:ASP:OD1	7:g:159:TYR:N	2.44	0.44
8:h:107:THR:HB	8:h:145:TYR:HD2	1.82	0.44
9:i:4:ARG:HG3	9:i:6:ASP:H	1.83	0.44
17:q:11:ASP:N	17:q:11:ASP:OD1	2.49	0.44
5:E:197:LYS:HG3	5:E:231:PHE:HD2	1.82	0.44
21:U:505:ASP:HB3	21:U:508:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:524:LYS:HD2	21:U:556:MET:HE3	2.00	0.44
21:U:327:LYS:HB3	21:U:333:MET:HE1	1.98	0.44
24:X:177:TYR:O	24:X:182:ASN:N	2.50	0.44
13:m:230:ASP:OD1	13:m:230:ASP:N	2.51	0.44
17:q:52:ASP:OD1	18:r:88:TYR:OH	2.29	0.44
2:B:106:PRO:HB2	2:B:154:HIS:CD2	2.52	0.44
8:H:74:LEU:HD12	8:H:87:VAL:HG22	1.99	0.44
26:Z:70:LEU:HD11	26:Z:108:ILE:HG23	2.00	0.44
28:b:5:SER:HB3	28:b:64:LEU:HD21	2.00	0.44
30:d:106:LEU:HD21	30:d:114:GLU:HB2	1.99	0.44
8:h:204:THR:OG1	8:h:206:ASP:OD1	2.32	0.44
2:B:387:LYS:HB3	2:B:390:LEU:HD23	1.99	0.44
4:D:171:ASP:OD1	4:D:172:ILE:N	2.49	0.44
6:F:341:ALA:O	6:F:347:ARG:NH1	2.51	0.44
21:U:443:LEU:HA	21:U:446:LEU:HD13	1.99	0.44
28:b:124:LEU:HD21	28:b:152:LYS:HB3	2.00	0.44
10:j:220:LEU:HD12	10:j:225:ILE:CG1	2.47	0.44
2:B:169:PRO:O	2:B:173:VAL:HG23	2.18	0.44
4:D:320:ALA:O	4:D:326:ARG:NH1	2.50	0.44
19:S:91:MET:HE2	19:S:91:MET:HB3	1.79	0.44
21:U:602:LEU:HD21	21:U:621:SER:HB2	2.00	0.44
22:V:245:ASP:OD1	22:V:246:GLY:N	2.50	0.44
22:V:337:LEU:HB3	22:V:398:LEU:HD11	2.00	0.44
22:V:410:ILE:HG21	22:V:422:ILE:HG13	2.00	0.44
23:W:80:TRP:HB2	23:W:123:ARG:HH22	1.83	0.44
24:X:177:TYR:HB2	24:X:186:ALA:HB2	2.00	0.44
30:d:164:THR:HA	30:d:167:ILE:HG12	2.00	0.44
32:f:151:LEU:HD23	32:f:159:VAL:HG22	2.00	0.44
32:f:794:ALA:O	32:f:798:THR:HG23	2.17	0.44
19:s:8:ASN:ND2	19:s:58:HIS:HB2	2.32	0.44
3:C:252:ASP:OD1	3:C:252:ASP:N	2.50	0.43
14:N:55:VAL:HA	14:N:86:MET:HE1	2.00	0.43
7:g:21:ARG:HE	7:g:21:ARG:HB2	1.31	0.43
4:D:120:ASP:N	4:D:120:ASP:OD1	2.51	0.43
12:L:35:THR:HG23	12:L:133:LEU:HD12	2.00	0.43
21:U:607:VAL:O	21:U:615:ARG:NH1	2.45	0.43
22:V:397:ARG:HE	30:d:116:HIS:CD2	2.36	0.43
1:A:255:ARG:HA	1:A:258:ARG:HD3	1.99	0.43
4:D:95:ALA:HA	4:D:101:ALA:HA	2.00	0.43
20:T:122:LEU:HG	20:T:137:LEU:HD12	2.00	0.43
27:a:61:GLU:HG3	27:a:79:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:281:THR:O	27:a:289:ARG:NH1	2.48	0.43
32:f:755:ASP:OD2	32:f:758:ASN:ND2	2.51	0.43
12:l:176:MET:HE2	13:m:57:LEU:HD23	2.00	0.43
5:E:3:ASP:OD1	5:E:3:ASP:N	2.50	0.43
13:M:65:ARG:HH21	13:M:78:ALA:HA	1.83	0.43
23:W:346:GLU:O	23:W:350:ARG:HD2	2.18	0.43
25:Y:220:VAL:HA	25:Y:223:THR:HG22	2.00	0.43
32:f:405:HIS:CE1	32:f:813:LYS:HB3	2.53	0.43
32:f:658:ALA:HB2	32:f:693:ALA:HB1	1.99	0.43
32:f:752:HIS:CD2	32:f:758:ASN:HB3	2.53	0.43
11:k:240:ASP:N	11:k:240:ASP:OD1	2.45	0.43
4:D:85:ILE:HD13	5:E:68:LYS:HG2	2.01	0.43
9:I:161:ALA:HB1	9:I:175:LEU:HD13	1.99	0.43
26:Z:192:THR:HG22	27:a:375:LEU:HG	2.00	0.43
4:D:191:TYR:HB3	4:D:198:PRO:HG3	2.01	0.43
4:D:273:LYS:HE3	4:D:273:LYS:HB3	1.84	0.43
5:E:171:LEU:HD23	5:E:298:LYS:HG3	1.99	0.43
10:j:65:LEU:HD13	10:j:88:ARG:HG3	2.01	0.43
2:B:288:ASP:N	2:B:288:ASP:OD1	2.51	0.43
3:C:91:PRO:HG2	3:C:92:GLU:HG3	2.01	0.43
10:J:67:ASP:OD1	10:J:67:ASP:N	2.52	0.43
21:U:329:LEU:HD23	21:U:329:LEU:HA	1.89	0.43
21:U:664:GLY:N	21:U:698:GLN:HE22	2.17	0.43
22:V:99:ARG:O	31:e:16:ASP:N	2.51	0.43
22:V:355:ARG:HD2	31:e:27:TRP:HB2	2.01	0.43
31:e:31:ASP:OD1	31:e:31:ASP:N	2.49	0.43
32:f:279:GLU:O	32:f:283:THR:OG1	2.27	0.43
8:h:185:GLU:O	8:h:189:HIS:ND1	2.47	0.43
10:j:220:LEU:HD12	10:j:225:ILE:HG12	2.00	0.43
34:v:25:LYS:O	34:v:27:UNK:N	2.51	0.43
1:A:48:VAL:HG11	2:B:65:LEU:HB3	2.00	0.43
4:D:202:VAL:HG23	4:D:329:ARG:HB2	2.01	0.43
4:D:313:ARG:HA	4:D:313:ARG:HH11	1.84	0.43
6:F:121:CYS:SG	6:F:122:ALA:N	2.92	0.43
19:S:92:LEU:HD23	19:S:124:PHE:HE2	1.84	0.43
27:a:277:LEU:HD11	27:a:311:VAL:HG12	2.00	0.43
16:p:149:MET:HE3	16:p:149:MET:HB3	1.89	0.43
6:F:51:GLU:HG2	6:F:55:MET:HE2	1.99	0.43
11:K:157:ASP:OD1	11:K:161:THR:N	2.51	0.43
21:U:18:GLN:HB3	30:d:27:LYS:HZ3	1.83	0.43
21:U:780:SER:HA	21:U:783:TYR:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:201:ARG:HH12	22:V:241:ARG:HD3	1.83	0.43
26:Z:43:TRP:HH2	26:Z:118:ASN:HD21	1.67	0.43
28:b:18:ASN:HD21	28:b:25:ARG:NH2	2.17	0.43
32:f:686:LEU:O	32:f:690:VAL:HG23	2.19	0.43
3:C:86:LEU:HD21	3:C:94:LYS:HD2	2.01	0.43
5:E:147:GLU:HG3	5:E:151:LEU:HD12	2.01	0.43
28:b:150:THR:HB	28:b:153:LEU:HB2	2.01	0.43
28:b:184:ILE:HA	28:b:187:PRO:HD2	2.01	0.43
4:D:207:PRO:O	4:D:212:LYS:NZ	2.52	0.42
6:F:111:ILE:HG12	6:F:113:LEU:H	1.82	0.42
27:a:21:VAL:HB	27:a:44:PHE:HE1	1.84	0.42
28:b:33:VAL:HA	28:b:36:VAL:HG22	2.01	0.42
29:c:163:ILE:HD12	29:c:163:ILE:HA	1.91	0.42
32:f:852:VAL:HG13	32:f:859:PRO:HG2	2.00	0.42
16:p:90:MET:HE2	16:p:90:MET:HB3	1.95	0.42
3:C:249:ASP:OD1	3:C:249:ASP:N	2.52	0.42
4:D:45:LYS:HG2	21:U:187:LEU:HD22	2.01	0.42
7:G:46:ASP:OD1	7:G:46:ASP:N	2.49	0.42
10:J:220:LEU:HD23	10:J:225:ILE:HG12	2.01	0.42
19:S:145:LEU:HD22	19:S:178:VAL:HB	2.01	0.42
21:U:898:CYS:SG	21:U:899:ARG:N	2.93	0.42
22:V:309:MET:HE3	22:V:331:LEU:HD22	2.01	0.42
29:c:130:GLN:NE2	29:c:134:GLU:OE2	2.50	0.42
31:e:42:ASN:OD1	31:e:43:TRP:N	2.52	0.42
32:f:688:ARG:O	32:f:724:ASN:ND2	2.38	0.42
9:i:123:GLN:HE22	10:j:118:TYR:HD2	1.67	0.42
33:u:1:MET:N	33:u:17:VAL:O	2.46	0.42
3:C:253:SER:HB3	3:C:300:ILE:HD11	2.01	0.42
6:F:386:ARG:HE	12:L:166:GLN:NE2	2.17	0.42
12:L:215:VAL:HB	12:L:221:PHE:HD1	1.83	0.42
22:V:465:ASP:HB3	22:V:468:SER:HB3	2.00	0.42
24:X:61:GLY:HA2	24:X:99:MET:HE1	2.00	0.42
26:Z:80:GLY:HA2	26:Z:83:LYS:HE2	2.01	0.42
29:c:168:MET:HE2	29:c:198:ARG:NH2	2.34	0.42
32:f:501:LEU:HD23	32:f:501:LEU:HA	1.91	0.42
32:f:694:LEU:HA	32:f:697:ILE:HG22	2.02	0.42
16:p:149:MET:HE2	16:p:170:ALA:HA	2.01	0.42
1:A:420:TYR:HA	1:A:423:PHE:HB2	2.00	0.42
2:B:257:GLN:HE22	3:C:260:GLU:HA	1.85	0.42
4:D:121:ARG:HB3	29:c:275:VAL:HG23	2.00	0.42
5:E:116:ASP:O	5:E:118:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:49:TYR:O	21:U:57:ARG:NH2	2.52	0.42
21:U:519:VAL:HG23	21:U:520:MET:SD	2.59	0.42
32:f:289:VAL:HA	32:f:292:LYS:HG2	2.02	0.42
7:g:213:SER:OG	7:g:232:GLU:OE2	2.33	0.42
8:h:39:LYS:HG3	8:h:44:VAL:HG22	2.02	0.42
18:r:182:ASP:OD1	18:r:182:ASP:N	2.47	0.42
5:E:331:ILE:HG23	5:E:371:VAL:HG21	2.01	0.42
9:I:38:LEU:HD23	9:I:160:LYS:HG2	2.01	0.42
23:W:201:ARG:HA	23:W:204:ILE:HG12	2.00	0.42
32:f:791:VAL:HG12	32:f:823:ALA:HB1	2.00	0.42
1:A:114:ASN:HA	1:A:120:LYS:HA	2.01	0.42
3:C:53:ASN:ND2	21:U:642:GLU:O	2.53	0.42
3:C:161:ILE:HA	3:C:164:VAL:HG12	2.01	0.42
4:D:284:GLU:HA	4:D:287:ARG:HG2	2.01	0.42
4:D:378:ILE:HD13	4:D:403:TYR:HE1	1.85	0.42
6:F:180:ARG:HH12	6:F:245:LYS:HA	1.84	0.42
10:J:52:LYS:HG3	10:J:53:LEU:HD12	2.01	0.42
16:P:30:ILE:HG22	16:P:31:GLN:H	1.84	0.42
17:Q:13:VAL:HG11	17:Q:105:ALA:HB1	2.01	0.42
24:X:70:LEU:HD22	24:X:109:LEU:HG	2.02	0.42
24:X:254:MET:HE1	24:X:270:LEU:HD13	2.02	0.42
25:Y:195:LYS:HD3	25:Y:195:LYS:HA	1.91	0.42
25:Y:232:GLU:OE2	25:Y:302:HIS:ND1	2.53	0.42
25:Y:238:GLU:HA	25:Y:242:LYS:HB2	2.01	0.42
26:Z:225:GLN:O	26:Z:227:ILE:N	2.52	0.42
28:b:12:ASN:HD21	28:b:55:ALA:HB2	1.85	0.42
28:b:161:ASN:HB2	28:b:165:GLY:HA3	2.01	0.42
29:c:266:THR:O	29:c:268:GLU:N	2.52	0.42
32:f:379:GLY:HA2	32:f:417:ILE:HD11	2.01	0.42
20:t:127:MET:HE3	20:t:127:MET:HB2	1.93	0.42
7:G:67:THR:HG22	7:G:69:LEU:H	1.84	0.42
16:P:115:LYS:HA	16:P:115:LYS:HD3	1.83	0.42
21:U:82:LEU:HB3	21:U:129:ARG:HG3	2.00	0.42
21:U:475:HIS:HA	21:U:511:ALA:HB2	2.01	0.42
23:W:339:ASP:N	23:W:339:ASP:OD1	2.52	0.42
25:Y:131:THR:HG23	25:Y:137:ARG:HE	1.85	0.42
30:d:63:ILE:HD12	30:d:63:ILE:HA	1.95	0.42
32:f:513:GLU:HA	32:f:554:TYR:HE2	1.85	0.42
8:h:42:ASN:ND2	8:h:183:GLU:OE2	2.53	0.42
16:p:142:CYS:O	16:p:146:MET:HG3	2.20	0.42
3:C:184:LYS:HA	3:C:290:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:256:LEU:HD12	6:F:291:ILE:HD13	2.01	0.42
21:U:99:THR:HG21	22:V:240:LEU:HD21	2.01	0.42
22:V:122:THR:H	22:V:150:ARG:HH21	1.67	0.42
22:V:479:ARG:NH2	25:Y:374:ASP:OD1	2.52	0.42
32:f:346:ASP:HA	32:f:350:LYS:HG3	2.02	0.42
32:f:735:GLY:O	32:f:828:ARG:NH1	2.53	0.42
32:f:822:VAL:HA	32:f:825:MET:HE2	2.02	0.42
8:h:123:GLN:HE22	9:i:130:PHE:HE1	1.68	0.42
17:q:23:SER:O	17:q:24:ASN:HB3	2.19	0.42
19:s:99:ARG:HH21	19:s:102:PHE:HD2	1.67	0.42
1:A:212:VAL:HG22	1:A:339:ARG:HB2	2.02	0.42
5:E:180:LYS:HG2	5:E:301:ILE:HD12	2.02	0.42
18:R:97:MET:HB3	18:R:116:SER:HB3	2.02	0.42
21:U:495:ASP:OD1	21:U:498:LYS:NZ	2.51	0.42
25:Y:142:PHE:HB3	25:Y:146:ARG:HH21	1.85	0.42
26:Z:25:ARG:HB3	29:c:103:GLY:HA2	2.02	0.42
32:f:96:LEU:HD13	32:f:129:LEU:HD13	2.02	0.42
32:f:342:PRO:HB3	32:f:390:LEU:HB2	2.01	0.42
7:g:187:PHE:HB2	7:g:189:TRP:CD1	2.55	0.42
10:j:234:LYS:HA	10:j:234:LYS:HD2	1.87	0.42
17:q:1:MET:HE2	17:q:133:GLY:HA2	2.01	0.42
1:A:156:LYS:HA	1:A:156:LYS:HD2	1.78	0.42
5:E:199:VAL:HG23	5:E:201:SER:H	1.84	0.42
5:E:237:ALA:O	6:F:308:ARG:NE	2.53	0.42
32:f:288:VAL:HG12	32:f:292:LYS:NZ	2.35	0.42
9:i:53:HIS:CD2	9:i:54:LYS:H	2.37	0.42
17:q:30:ASP:OD1	17:q:30:ASP:N	2.51	0.42
3:C:88:LYS:HB3	3:C:88:LYS:HE3	1.34	0.41
8:H:232:ALA:HB1	24:X:90:ARG:HH11	1.85	0.41
17:Q:19:ARG:NH1	17:Q:179:SER:OG	2.44	0.41
21:U:265:ILE:HD11	21:U:326:ILE:HG23	2.01	0.41
24:X:47:GLU:OE2	24:X:80:ILE:HD13	2.20	0.41
25:Y:192:ARG:HG3	25:Y:291:HIS:CE1	2.55	0.41
26:Z:170:VAL:HG22	29:c:152:LYS:HA	2.01	0.41
29:c:58:LEU:HG	29:c:106:GLU:HG2	2.02	0.41
30:d:131:VAL:HA	30:d:134:LYS:HB3	2.01	0.41
32:f:99:LEU:HA	32:f:102:HIS:HB2	2.02	0.41
32:f:151:LEU:HD23	32:f:159:VAL:HA	2.02	0.41
20:t:97:TYR:HA	20:t:100:ARG:HG2	2.01	0.41
4:D:54:LEU:HD23	4:D:54:LEU:HA	1.92	0.41
4:D:274:ARG:HG2	4:D:275:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:189:LYS:HA	10:J:232:ILE:HD11	2.01	0.41
22:V:98:LEU:HD22	22:V:209:LYS:HD2	2.01	0.41
22:V:396:ILE:HD13	22:V:396:ILE:HA	1.95	0.41
29:c:206:ASN:OD1	29:c:206:ASN:N	2.51	0.41
11:k:149:LYS:HE2	11:k:152:GLN:HE22	1.85	0.41
15:o:51:ASP:HB3	15:o:94:ILE:HG23	2.02	0.41
17:q:53:THR:HG22	17:q:100:VAL:HG12	2.02	0.41
3:C:369:TYR:HA	3:C:372:ARG:HG2	2.01	0.41
4:D:133:HIS:CD2	4:D:134:LYS:H	2.38	0.41
4:D:248:ARG:HG2	4:D:295:GLN:NE2	2.35	0.41
24:X:21:GLU:HA	24:X:24:ILE:HD12	2.01	0.41
27:a:278:MET:HA	27:a:281:THR:HG22	2.01	0.41
29:c:84:VAL:O	33:u:74:ARG:HG2	2.21	0.41
32:f:66:LYS:O	32:f:67:ASP:C	2.63	0.41
12:l:44:ALA:HB1	12:l:144:ILE:HD11	2.02	0.41
18:r:21:THR:HG22	18:r:26:ILE:HG12	2.02	0.41
1:A:213:LEU:HA	1:A:319:MET:HB2	2.02	0.41
2:B:231:GLY:N	37:B:501:ADP:O1A	2.47	0.41
6:F:236:LEU:HD23	6:F:236:LEU:HA	1.87	0.41
21:U:2:ILE:HD12	30:d:36:LEU:HD13	2.01	0.41
22:V:80:LYS:HE2	22:V:84:LYS:NZ	2.36	0.41
17:q:31:ASP:OD1	17:q:31:ASP:N	2.52	0.41
5:E:56:ILE:N	5:E:100:LEU:O	2.49	0.41
5:E:291:ARG:HE	5:E:294:ARG:NH1	2.18	0.41
5:E:387:LYS:HD2	5:E:388:PRO:HD2	2.02	0.41
11:K:78:MET:HE3	11:K:85:ALA:HB3	2.02	0.41
13:M:43:ASP:OD1	13:M:43:ASP:N	2.53	0.41
21:U:358:ASP:OD1	21:U:358:ASP:N	2.54	0.41
21:U:422:LEU:HD23	21:U:427:LEU:HD12	2.01	0.41
23:W:272:LEU:HD22	23:W:341:PHE:HE2	1.86	0.41
25:Y:223:THR:O	25:Y:227:SER:HB3	2.20	0.41
26:Z:212:LEU:HA	26:Z:215:VAL:HG12	2.02	0.41
28:b:52:ILE:HD13	28:b:60:VAL:HG22	2.03	0.41
29:c:79:GLY:HA2	29:c:84:VAL:HG23	2.02	0.41
32:f:266:LEU:HD12	32:f:266:LEU:HA	1.95	0.41
19:s:18:GLU:OE1	19:s:18:GLU:N	2.51	0.41
6:F:98:ASP:HB3	6:F:120:LYS:HD2	2.02	0.41
7:G:165:ALA:HB1	7:G:179:LEU:HD13	2.03	0.41
23:W:198:ASP:O	23:W:202:THR:OG1	2.30	0.41
23:W:205:ILE:HA	23:W:208:LYS:HE3	2.03	0.41
23:W:272:LEU:HD23	23:W:272:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:455:LEU:HB2	23:W:456:GLN:NE2	2.36	0.41
30:d:236:THR:O	30:d:239:SER:OG	2.25	0.41
32:f:580:LEU:HD21	32:f:591:ALA:HB3	2.02	0.41
12:l:204:ASP:OD1	12:l:204:ASP:N	2.54	0.41
15:o:21:THR:HG22	15:o:26:VAL:HA	2.01	0.41
15:o:163:ILE:HG12	15:o:170:GLY:HA2	2.03	0.41
6:F:245:LYS:HE2	6:F:245:LYS:HB2	1.80	0.41
9:I:58:GLU:HG3	9:I:60:PHE:CE1	2.56	0.41
21:U:14:GLU:O	21:U:20:LYS:NZ	2.53	0.41
24:X:343:SER:HA	24:X:387:ILE:HB	2.01	0.41
27:a:271:LYS:O	27:a:275:LEU:HB2	2.20	0.41
29:c:266:THR:O	29:c:268:GLU:HG2	2.21	0.41
2:B:233:THR:OG1	37:B:501:ADP:O3B	2.37	0.41
9:I:136:TYR:HB2	9:I:148:TYR:HB2	2.03	0.41
9:I:246:LYS:HG3	9:I:249:ARG:HH21	1.85	0.41
21:U:791:LEU:HD22	21:U:911:ILE:HD11	2.01	0.41
21:U:879:ASP:N	21:U:879:ASP:OD1	2.52	0.41
23:W:50:LEU:O	23:W:54:THR:HG23	2.20	0.41
23:W:170:GLN:NE2	23:W:172:GLU:OE1	2.54	0.41
10:j:8:THR:HG21	11:k:134:SER:HB3	2.03	0.41
14:n:150:GLU:O	14:n:154:GLN:HG2	2.21	0.41
15:o:42:TYR:HE2	15:o:183:LEU:HD21	1.85	0.41
1:A:189:GLU:O	1:A:193:THR:OG1	2.38	0.41
3:C:90:HIS:CE1	4:D:110:ASN:HB2	2.56	0.41
3:C:139:MET:HG3	3:C:214:VAL:HG22	2.03	0.41
3:C:190:GLY:HA3	3:C:317:PHE:HB2	2.02	0.41
5:E:246:GLY:O	5:E:251:ARG:NH1	2.48	0.41
15:O:42:TYR:HB2	15:O:178:ILE:HD11	2.03	0.41
18:R:182:ASP:OD1	18:R:182:ASP:N	2.54	0.41
25:Y:349:LYS:HD3	25:Y:349:LYS:HA	1.83	0.41
26:Z:45:LYS:HB3	26:Z:47:VAL:HG12	2.02	0.41
28:b:6:THR:HB	28:b:49:VAL:HG22	2.03	0.41
28:b:7:MET:HB2	28:b:97:LEU:HD11	2.02	0.41
32:f:402:ASN:HB3	32:f:406:GLY:HA3	2.02	0.41
32:f:585:GLU:O	32:f:586:PRO:C	2.63	0.41
32:f:800:LEU:HD23	32:f:800:LEU:HA	1.84	0.41
7:g:21:ARG:NE	7:g:22:LEU:H	2.19	0.41
7:g:123:GLN:NE2	8:h:82:ASP:OD1	2.54	0.41
10:j:52:LYS:HG3	10:j:53:LEU:HG	2.01	0.41
12:l:45:VAL:HG12	12:l:214:ILE:HG12	2.02	0.41
17:q:18:ASP:O	17:q:34:LYS:NZ	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:r:51:ASP:OD1	19:s:97:TYR:OH	2.32	0.41
18:r:115:ASP:N	18:r:115:ASP:OD1	2.53	0.41
20:t:63:LEU:HD23	20:t:63:LEU:HA	1.93	0.41
3:C:273:MET:HE2	3:C:273:MET:HB3	1.98	0.41
5:E:338:PHE:HD1	5:E:378:LYS:HZ1	1.69	0.41
13:M:37:ILE:HD11	13:M:193:VAL:HG13	2.01	0.41
21:U:70:HIS:O	22:V:236:ARG:NH2	2.54	0.41
27:a:205:LEU:HD12	27:a:205:LEU:HA	1.94	0.41
27:a:275:LEU:HD12	27:a:275:LEU:HA	1.88	0.41
29:c:131:GLN:HA	29:c:134:GLU:HB2	2.03	0.41
9:i:53:HIS:CG	9:i:54:LYS:N	2.86	0.41
4:D:309:MET:HE1	4:D:327:LEU:HD21	2.03	0.40
7:G:93:ARG:HE	7:G:121:ILE:HD13	1.86	0.40
20:T:53:ALA:HB2	20:T:110:MET:HG3	2.02	0.40
21:U:52:GLU:OE1	21:U:57:ARG:NH1	2.54	0.40
23:W:172:GLU:HA	23:W:182:ARG:HD3	2.02	0.40
25:Y:113:ARG:HD2	25:Y:113:ARG:HA	1.86	0.40
29:c:267:PRO:O	29:c:268:GLU:C	2.65	0.40
30:d:115:PHE:CE2	30:d:140:GLU:HG2	2.56	0.40
32:f:550:LEU:HD21	32:f:587:PHE:H	1.86	0.40
15:o:41:ILE:HG12	15:o:76:VAL:HG22	2.03	0.40
1:A:184:ILE:HD12	1:A:184:ILE:HA	2.00	0.40
9:I:76:VAL:HG12	9:I:134:LEU:HG	2.03	0.40
10:J:39:ASP:OD1	10:J:39:ASP:N	2.54	0.40
15:O:63:LEU:HD23	15:O:63:LEU:HA	1.93	0.40
22:V:447:ILE:HD12	22:V:447:ILE:HA	1.94	0.40
26:Z:187:LEU:HD21	30:d:253:LEU:HD22	2.04	0.40
13:m:77:VAL:HG11	13:m:84:ALA:HB1	2.03	0.40
4:D:85:ILE:H	4:D:85:ILE:HG12	1.74	0.40
4:D:369:LYS:HE3	4:D:369:LYS:HA	2.04	0.40
5:E:300:HIS:NE2	5:E:302:ASP:OD1	2.53	0.40
6:F:185:TYR:CE2	6:F:243:GLN:HG3	2.56	0.40
21:U:33:ASP:HB3	21:U:34:PHE:H	1.58	0.40
21:U:628:ARG:NH1	21:U:749:GLN:OE1	2.54	0.40
22:V:176:MET:HE2	22:V:217:VAL:HG23	2.03	0.40
22:V:403:ILE:HD11	22:V:426:LEU:HD23	2.04	0.40
1:A:224:LEU:HD11	35:A:501:ATP:H2'	2.03	0.40
1:A:333:ARG:HH21	1:A:336:ARG:CZ	2.35	0.40
10:J:31:THR:OG1	10:J:163:ARG:O	2.36	0.40
21:U:167:ILE:HD12	21:U:177:LEU:HD21	2.01	0.40
21:U:198:LEU:HD21	21:U:219:CYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:682:TYR:HB3	21:U:725:MET:HE3	2.03	0.40
22:V:189:ASP:HA	22:V:192:MET:HE2	2.03	0.40
25:Y:1:MET:HE2	25:Y:1:MET:HB3	1.99	0.40
26:Z:6:VAL:O	26:Z:7:GLN:HG3	2.22	0.40
27:a:113:LEU:HA	27:a:116:THR:HG23	2.02	0.40
27:a:210:VAL:HG12	27:a:213:PHE:CZ	2.57	0.40
27:a:245:VAL:HG11	27:a:301:LYS:HD3	2.03	0.40
32:f:404:ASP:OD1	32:f:404:ASP:N	2.55	0.40
10:j:207:GLU:HG2	10:j:219:ILE:HD11	2.02	0.40
12:l:125:ARG:NH1	12:l:126:ARG:O	2.55	0.40
2:B:48:LYS:C	2:B:50:PRO:HD3	2.47	0.40
4:D:191:TYR:HA	4:D:196:ILE:HD12	2.03	0.40
4:D:214:MET:HE1	35:D:501:ATP:H2'	2.04	0.40
6:F:113:LEU:HD23	29:c:80:THR:HA	2.03	0.40
16:P:58:THR:O	17:Q:85:ARG:NH2	2.55	0.40
22:V:80:LYS:HB3	22:V:84:LYS:NZ	2.36	0.40
22:V:175:MET:HE3	22:V:175:MET:HB3	1.92	0.40
24:X:82:LYS:HD2	24:X:82:LYS:HA	1.32	0.40
10:j:47:LYS:HB3	10:j:47:LYS:HE3	1.75	0.40
11:k:218:ALA:HB2	11:k:228:MET:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	A	404/433 (93%)	354 (88%)	49 (12%)	1 (0%)	43	73
2	B	395/440 (90%)	347 (88%)	45 (11%)	3 (1%)	16	47
3	C	379/398 (95%)	334 (88%)	42 (11%)	3 (1%)	16	47
4	D	378/418 (90%)	325 (86%)	48 (13%)	5 (1%)	9	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	387/403 (96%)	356 (92%)	31 (8%)	0	100	100
6	F	413/439 (94%)	387 (94%)	26 (6%)	0	100	100
7	G	242/246 (98%)	233 (96%)	9 (4%)	0	100	100
7	g	238/246 (97%)	221 (93%)	16 (7%)	1 (0%)	30	61
8	H	230/234 (98%)	221 (96%)	9 (4%)	0	100	100
8	h	230/234 (98%)	217 (94%)	13 (6%)	0	100	100
9	I	249/261 (95%)	240 (96%)	9 (4%)	0	100	100
9	i	246/261 (94%)	234 (95%)	12 (5%)	0	100	100
10	J	237/248 (96%)	227 (96%)	10 (4%)	0	100	100
10	j	237/248 (96%)	228 (96%)	9 (4%)	0	100	100
11	K	232/241 (96%)	220 (95%)	11 (5%)	1 (0%)	30	61
11	k	236/241 (98%)	224 (95%)	12 (5%)	0	100	100
12	L	236/263 (90%)	229 (97%)	7 (3%)	0	100	100
12	l	238/263 (90%)	229 (96%)	9 (4%)	0	100	100
13	M	238/255 (93%)	233 (98%)	5 (2%)	0	100	100
13	m	240/255 (94%)	231 (96%)	9 (4%)	0	100	100
14	N	200/239 (84%)	193 (96%)	7 (4%)	0	100	100
14	n	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
15	O	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
15	o	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
16	P	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
16	p	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
17	Q	197/201 (98%)	190 (96%)	7 (4%)	0	100	100
17	q	197/201 (98%)	193 (98%)	3 (2%)	1 (0%)	24	57
18	R	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
18	r	199/263 (76%)	191 (96%)	8 (4%)	0	100	100
19	S	211/241 (88%)	206 (98%)	5 (2%)	0	100	100
19	s	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
20	T	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
20	t	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
21	U	812/953 (85%)	765 (94%)	46 (6%)	1 (0%)	48	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	V	442/534 (83%)	431 (98%)	10 (2%)	1 (0%)	43	73
23	W	439/456 (96%)	430 (98%)	9 (2%)	0	100	100
24	X	420/422 (100%)	395 (94%)	24 (6%)	1 (0%)	43	73
25	Y	387/389 (100%)	358 (92%)	28 (7%)	1 (0%)	36	67
26	Z	284/324 (88%)	255 (90%)	27 (10%)	2 (1%)	18	49
27	a	371/376 (99%)	335 (90%)	34 (9%)	2 (0%)	24	57
28	b	189/377 (50%)	166 (88%)	23 (12%)	0	100	100
29	c	285/310 (92%)	256 (90%)	23 (8%)	6 (2%)	5	25
30	d	255/350 (73%)	219 (86%)	35 (14%)	1 (0%)	30	61
31	e	48/70 (69%)	41 (85%)	7 (15%)	0	100	100
32	f	840/908 (92%)	790 (94%)	45 (5%)	5 (1%)	21	52
33	u	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
34	v	1/28 (4%)	1 (100%)	0	0	100	100
All	All	13414/14980 (90%)	12589 (94%)	790 (6%)	35 (0%)	37	67

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	85	ILE
4	D	125	LYS
21	U	34	PHE
27	a	215	GLU
29	c	268	GLU
32	f	586	PRO
7	g	21	ARG
2	B	54	PRO
3	C	90	HIS
4	D	127	ASN
25	Y	350	VAL
27	a	214	GLY
29	c	196	LEU
29	c	198	ARG
32	f	66	LYS
32	f	585	GLU
17	q	24	ASN
2	B	50	PRO
4	D	84	SER

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Mol	Chain	Res	Type
22	V	496	PHE
26	Z	226	ILE
26	Z	227	ILE
32	f	348	ILE
32	f	349	TYR
2	B	117	ASP
3	C	89	VAL
3	C	287	LYS
4	D	86	PRO
29	c	267	PRO
30	d	90	PRO
29	c	185	ASN
29	c	266	THR
11	K	130	PRO
1	A	346	PRO
24	X	80	ILE

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	A	342/372 (92%)	340 (99%)	2 (1%)	78	83
2	B	345/385 (90%)	342 (99%)	3 (1%)	70	80
3	C	326/346 (94%)	322 (99%)	4 (1%)	63	78
4	D	333/366 (91%)	330 (99%)	3 (1%)	70	80
5	E	341/353 (97%)	341 (100%)	0	100	100
6	F	357/379 (94%)	357 (100%)	0	100	100
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	200 (99%)	2 (1%)	68	79
8	H	188/191 (98%)	187 (100%)	1 (0%)	81	85
8	h	187/191 (98%)	187 (100%)	0	100	100
9	I	207/221 (94%)	207 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	i	202/221 (91%)	202 (100%)	0	100	100
10	J	201/211 (95%)	200 (100%)	1 (0%)	81	85
10	j	197/211 (93%)	196 (100%)	1 (0%)	81	85
11	K	193/203 (95%)	193 (100%)	0	100	100
11	k	197/203 (97%)	197 (100%)	0	100	100
12	L	202/224 (90%)	202 (100%)	0	100	100
12	l	202/224 (90%)	202 (100%)	0	100	100
13	M	196/212 (92%)	196 (100%)	0	100	100
13	m	198/212 (93%)	198 (100%)	0	100	100
14	N	157/181 (87%)	157 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	179/228 (78%)	179 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	168/171 (98%)	168 (100%)	0	100	100
17	q	168/171 (98%)	167 (99%)	1 (1%)	78	83
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	156/202 (77%)	156 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	178/199 (89%)	178 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	696/816 (85%)	693 (100%)	3 (0%)	84	86
22	V	390/460 (85%)	390 (100%)	0	100	100
23	W	406/416 (98%)	404 (100%)	2 (0%)	81	85
24	X	362/362 (100%)	361 (100%)	1 (0%)	86	87
25	Y	344/344 (100%)	341 (99%)	3 (1%)	70	80
26	Z	257/295 (87%)	255 (99%)	2 (1%)	73	81
27	a	333/336 (99%)	333 (100%)	0	100	100
28	b	167/312 (54%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	c	252/268 (94%)	247 (98%)	5 (2%)	48	72
30	d	231/294 (79%)	231 (100%)	0	100	100
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	711/763 (93%)	710 (100%)	1 (0%)	88	90
33	u	68/68 (100%)	68 (100%)	0	100	100
34	v	1/1 (100%)	0	1 (100%)	0	0
All	All	11459/12683 (90%)	11423 (100%)	36 (0%)	84	87

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	LEU
1	A	403	ILE
2	B	117	ASP
2	B	118	ASP
2	B	125	THR
3	C	88	LYS
3	C	89	VAL
3	C	210	THR
3	C	287	LYS
4	D	85	ILE
4	D	124	LEU
4	D	125	LYS
8	H	140	ASN
10	J	239	ASN
21	U	18	GLN
21	U	19	LEU
21	U	34	PHE
23	W	351	TRP
23	W	455	LEU
24	X	82	LYS
25	Y	14	ASN
25	Y	226	VAL
25	Y	351	ASN
26	Z	225	GLN
26	Z	226	ILE
29	c	186	LYS
29	c	196	LEU
29	c	197	ASN
29	c	198	ARG

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Mol	Chain	Res	Type
29	c	266	THR
32	f	66	LYS
7	g	19	GLU
7	g	21	ARG
10	j	220	LEU
17	q	24	ASN
34	v	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	197	HIS
1	A	305	GLN
1	A	353	HIS
2	B	181	GLN
2	B	306	GLN
3	C	50	ASN
3	C	53	ASN
3	C	67	GLN
3	C	69	GLN
4	D	133	HIS
4	D	257	ASN
5	E	45	ASN
5	E	220	ASN
5	E	254	GLN
5	E	271	HIS
6	F	92	ASN
7	G	128	ASN
8	H	88	HIS
8	H	95	GLN
8	H	109	GLN
8	H	140	ASN
8	H	179	ASN
9	I	53	HIS
9	I	142	HIS
10	J	23	GLN
10	J	54	GLN
11	K	204	GLN
12	L	16	GLN
12	L	86	ASN
12	L	143	HIS

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Mol	Chain	Res	Type
13	M	143	ASN
14	N	154	GLN
14	N	158	ASN
15	O	66	HIS
15	O	165	ASN
16	P	7	ASN
16	P	33	GLN
16	P	93	ASN
17	Q	8	GLN
17	Q	101	ASN
18	R	151	GLN
20	T	213	HIS
21	U	18	GLN
21	U	28	ASN
21	U	32	ASN
21	U	111	GLN
21	U	115	ASN
21	U	207	ASN
21	U	340	GLN
21	U	346	ASN
21	U	384	GLN
21	U	389	ASN
21	U	412	HIS
21	U	438	GLN
21	U	491	GLN
21	U	718	ASN
21	U	901	GLN
22	V	146	GLN
22	V	168	GLN
22	V	177	ASN
22	V	257	ASN
23	W	236	HIS
24	X	28	HIS
24	X	44	GLN
24	X	48	GLN
24	X	322	HIS
24	X	349	HIS
25	Y	14	ASN
25	Y	258	GLN
26	Z	77	ASN
26	Z	109	ASN
26	Z	202	ASN

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Mol	Chain	Res	Type
26	Z	224	HIS
26	Z	243	GLN
27	a	9	GLN
27	a	249	GLN
27	a	257	GLN
28	b	142	ASN
29	c	101	GLN
29	c	115	HIS
29	c	128	ASN
29	c	164	ASN
29	c	269	GLN
32	f	171	GLN
32	f	273	ASN
32	f	301	HIS
32	f	325	GLN
32	f	452	ASN
32	f	650	GLN
32	f	782	HIS
32	f	786	GLN
7	g	33	ASN
7	g	193	GLN
8	h	88	HIS
8	h	95	GLN
9	i	20	GLN
9	i	95	GLN
9	i	166	ASN
10	j	15	HIS
10	j	239	ASN
11	k	73	HIS
11	k	98	ASN
13	m	22	GLN
13	m	147	GLN
14	n	158	ASN
16	p	31	GLN
17	q	82	ASN
17	q	99	HIS
17	q	101	ASN
17	q	132	HIS
18	r	119	ASN
18	r	151	GLN
18	r	196	HIS
19	s	8	ASN

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Mol	Chain	Res	Type
20	t	157	GLN
33	u	49	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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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$
37	ADP	E	401	-	27,29,29	1.35	4 (14%)	42,45,45	1.98	10 (23%)
35	ATP	F	501	36	29,33,33	0.31	0	44,52,52	0.54	1 (2%)
35	ATP	A	501	36	29,33,33	0.30	0	44,52,52	0.46	1 (2%)
35	ATP	D	501	36	29,33,33	0.31	0	44,52,52	0.50	0
37	ADP	B	501	-	27,29,29	1.36	4 (14%)	42,45,45	1.98	9 (21%)

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
37	ADP	E	401	-	-	2/16/32/32	0/3/3/3
35	ATP	F	501	36	-	2/22/38/38	0/3/3/3
35	ATP	A	501	36	-	4/22/38/38	0/3/3/3
35	ATP	D	501	36	-	5/22/38/38	0/3/3/3
37	ADP	B	501	-	-	4/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B	501	ADP	C5-C4	4.55	1.47	1.39
37	E	401	ADP	C5-C4	4.49	1.47	1.39
37	B	501	ADP	C5-C6	2.60	1.48	1.41
37	E	401	ADP	C5-C6	2.55	1.48	1.41
37	E	401	ADP	C5-N7	-2.34	1.34	1.39
37	E	401	ADP	C8-N7	2.31	1.36	1.31
37	B	501	ADP	C5-N7	-2.30	1.34	1.39
37	B	501	ADP	C8-N7	2.25	1.35	1.31

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B	501	ADP	C5-C4-N3	-6.39	118.42	126.75
37	E	401	ADP	C5-C4-N3	-6.15	118.72	126.75
37	B	501	ADP	N3-C4-N9	5.06	135.41	127.08
37	E	401	ADP	N3-C4-N9	4.90	135.16	127.08
37	E	401	ADP	C2-N3-C4	3.83	120.79	111.75
37	E	401	ADP	PA-O3A-PB	-3.82	119.71	132.83
37	B	501	ADP	C2-N3-C4	3.82	120.78	111.75
37	B	501	ADP	PA-O3A-PB	-3.46	120.94	132.83
37	E	401	ADP	N3-C2-N1	-3.11	123.74	128.60
37	B	501	ADP	C4-C5-N7	-3.09	106.85	110.62
37	B	501	ADP	N3-C2-N1	-2.99	123.92	128.60
37	E	401	ADP	C4-C5-N7	-2.97	107.00	110.62
37	B	501	ADP	C3'-C2'-C1'	2.76	106.66	101.43
37	E	401	ADP	C3'-C2'-C1'	2.73	106.60	101.43
37	B	501	ADP	C5-N7-C8	2.59	107.19	103.51
37	E	401	ADP	C5-N7-C8	2.50	107.07	103.51
37	E	401	ADP	C4-N9-C8	2.42	108.36	105.73
37	B	501	ADP	C4-N9-C8	2.37	108.30	105.73
35	F	501	ATP	PB-O3B-PG	2.04	139.81	132.83
35	A	501	ATP	PB-O3B-PG	2.03	139.78	132.83
37	E	401	ADP	C6-C5-N7	2.02	135.78	132.02

There are no chirality outliers.

All (17) torsion outliers are listed below:

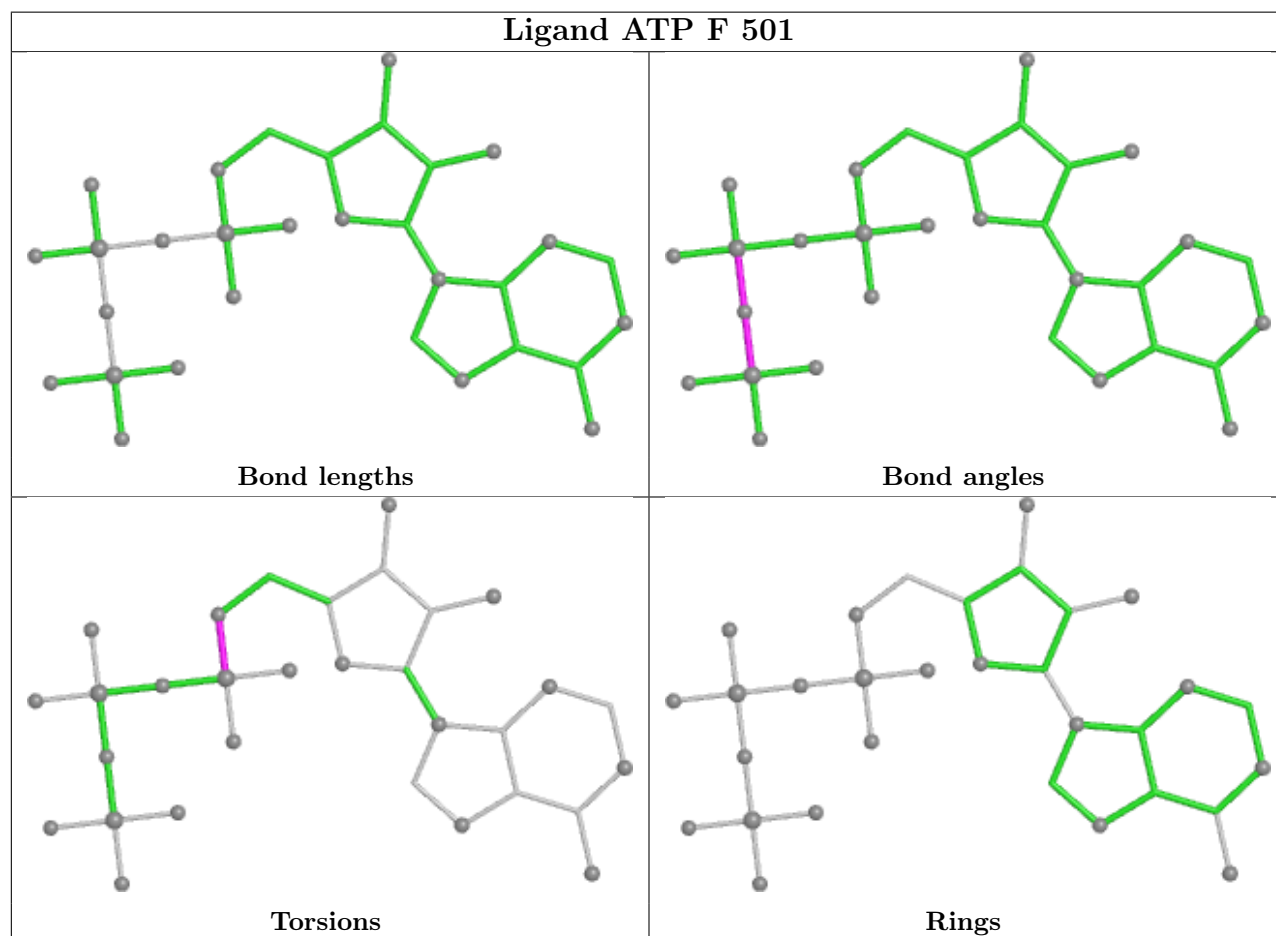
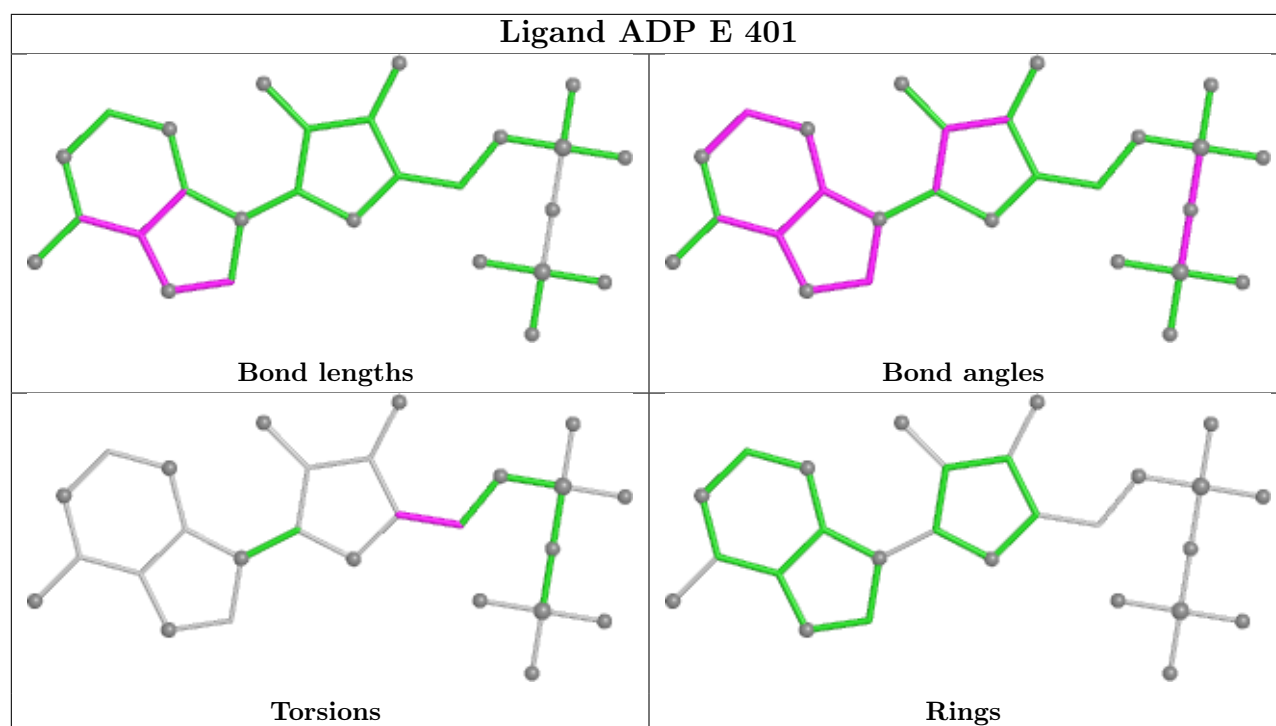
Mol	Chain	Res	Type	Atoms
35	A	501	ATP	C5'-O5'-PA-O1A
35	A	501	ATP	C5'-O5'-PA-O2A
35	D	501	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	C4'-C5'-O5'-PA
35	D	501	ATP	C3'-C4'-C5'-O5'
35	F	501	ATP	C5'-O5'-PA-O1A
37	B	501	ADP	O4'-C4'-C5'-O5'
37	E	401	ADP	O4'-C4'-C5'-O5'
35	D	501	ATP	O4'-C4'-C5'-O5'
37	B	501	ADP	C3'-C4'-C5'-O5'
37	E	401	ADP	C3'-C4'-C5'-O5'
35	A	501	ATP	C5'-O5'-PA-O3A
35	F	501	ATP	C5'-O5'-PA-O3A
35	A	501	ATP	PA-O3A-PB-O2B
35	D	501	ATP	C5'-O5'-PA-O1A
37	B	501	ADP	C5'-O5'-PA-O3A
37	B	501	ADP	C5'-O5'-PA-O2A

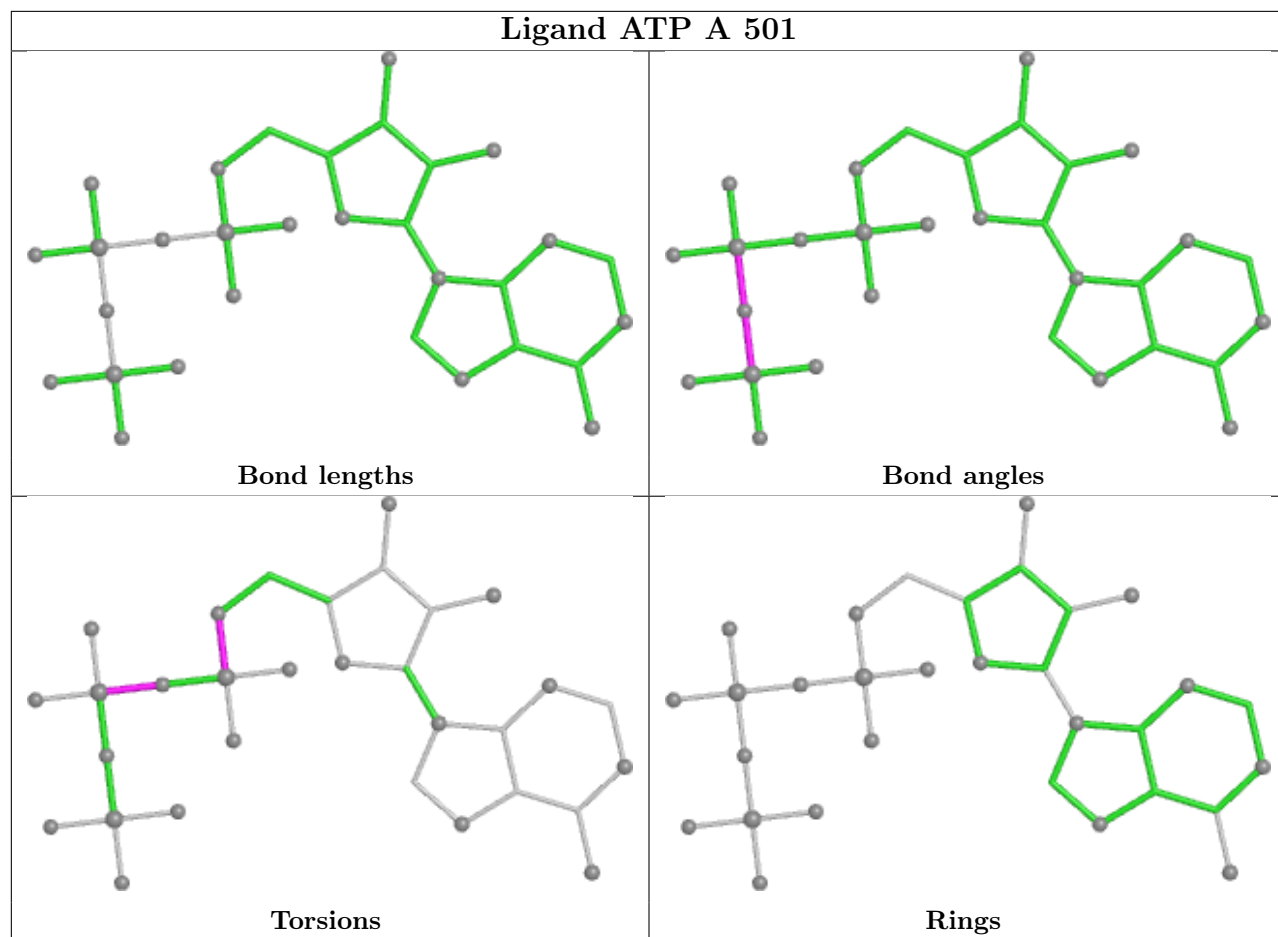
There are no ring outliers.

5 monomers are involved in 11 short contacts:

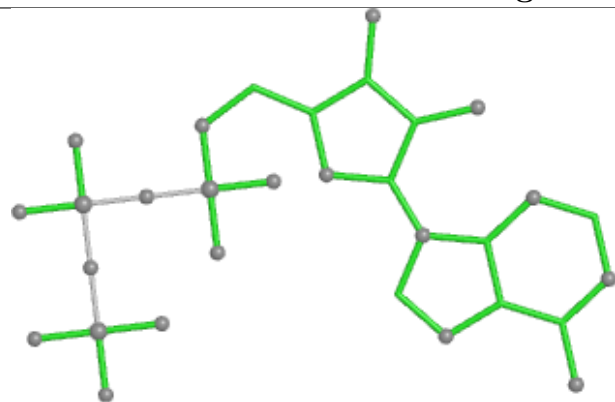
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	E	401	ADP	2	0
35	F	501	ATP	2	0
35	A	501	ATP	1	0
35	D	501	ATP	2	0
37	B	501	ADP	4	0

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.

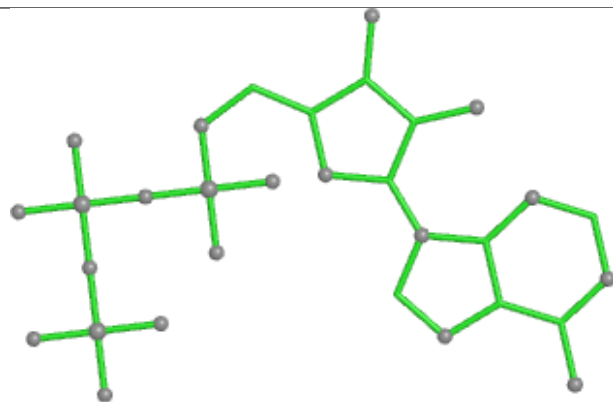




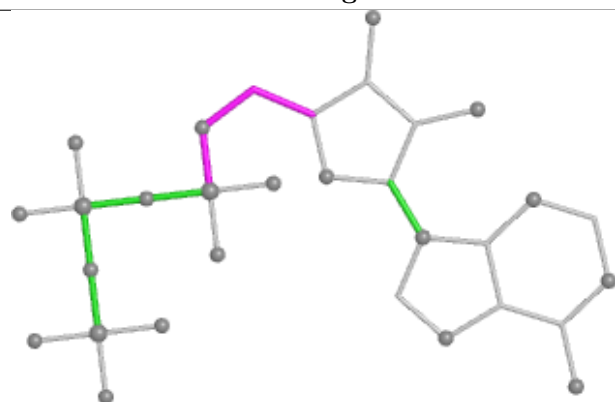
Ligand ATP D 501



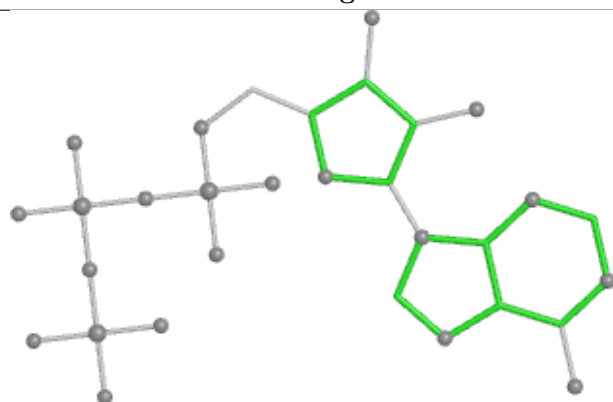
Bond lengths



Bond angles

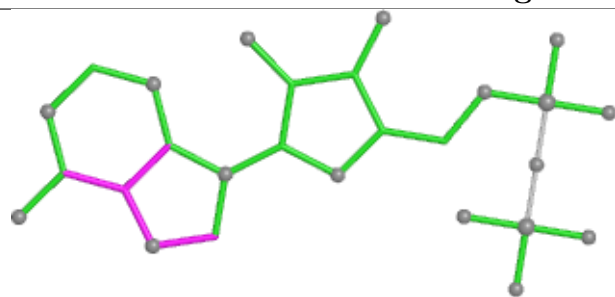


Torsions

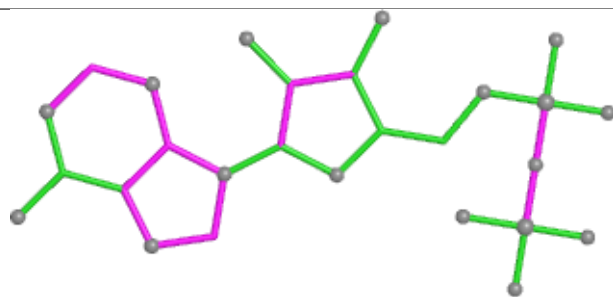


Rings

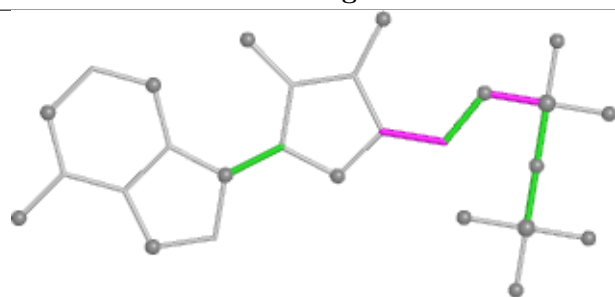
Ligand ADP B 501



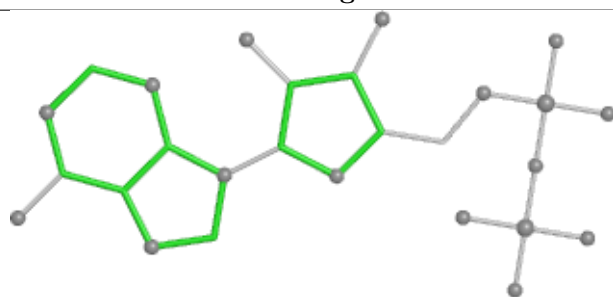
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

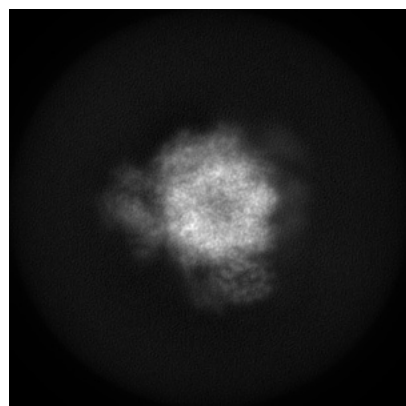
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62067. 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](#)

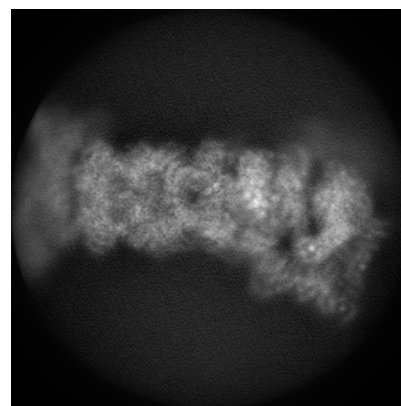
6.1.1 Primary map



X

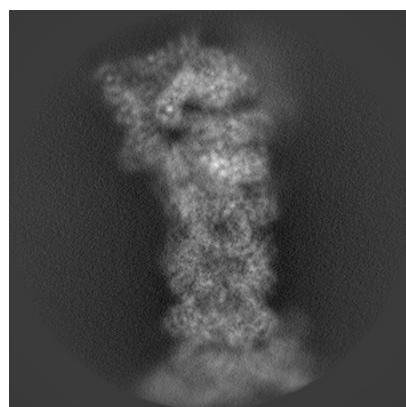


Y

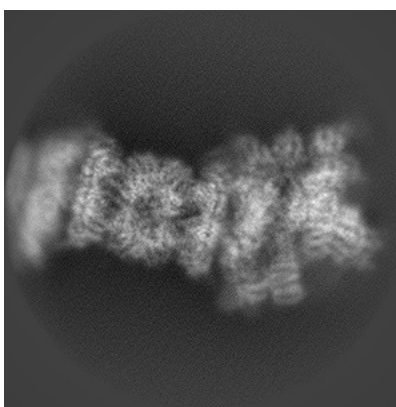


Z

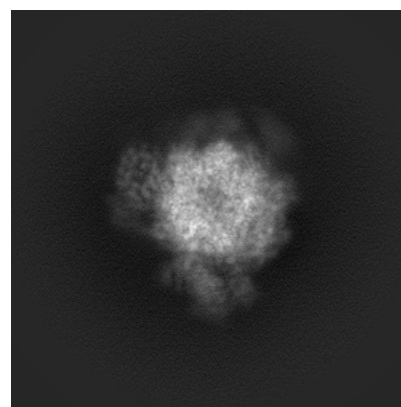
6.1.2 Raw map



X



Y

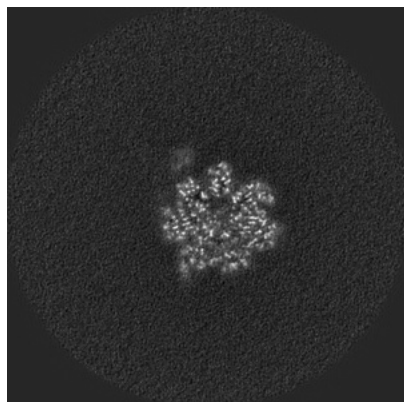


Z

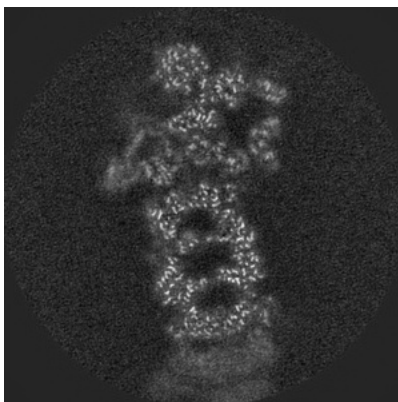
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

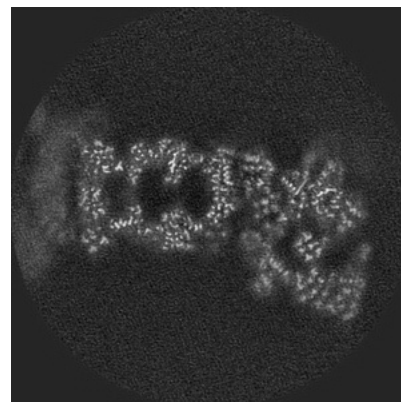
6.2.1 Primary map



X Index: 300

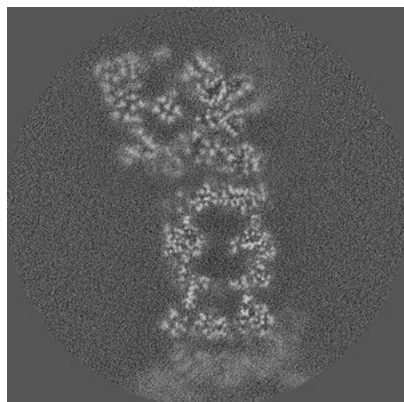


Y Index: 300

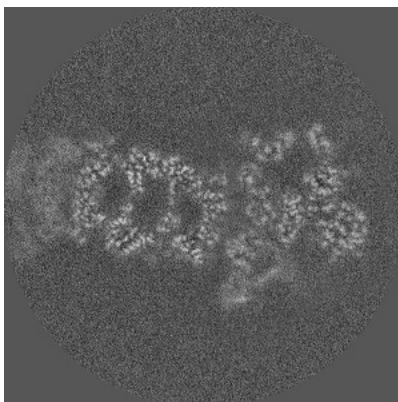


Z Index: 300

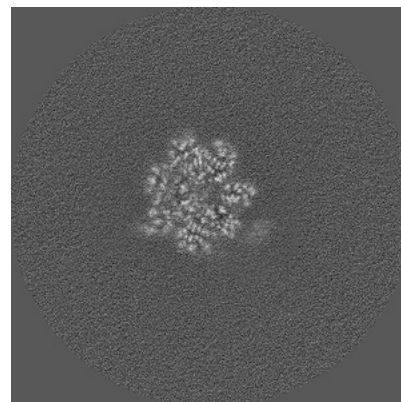
6.2.2 Raw map



X Index: 300



Y Index: 300

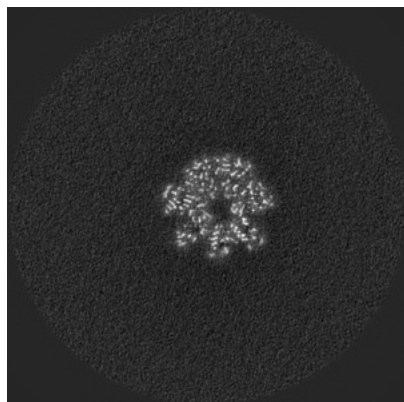


Z Index: 300

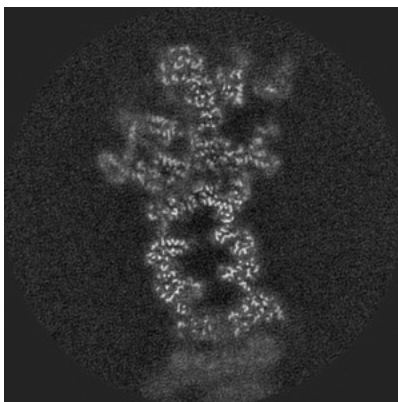
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

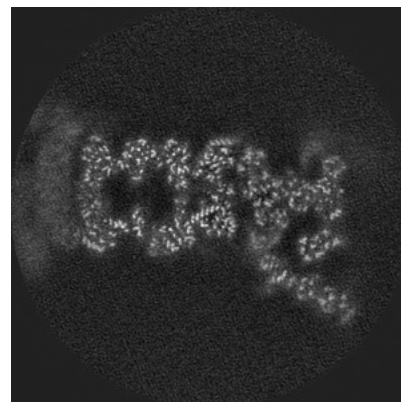
6.3.1 Primary map



X Index: 248

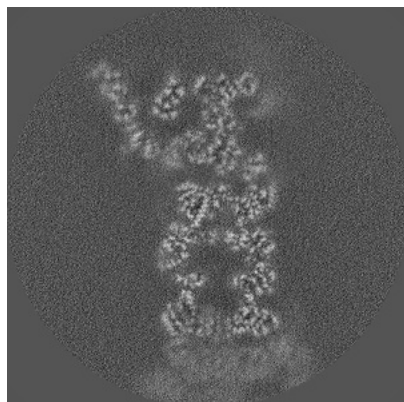


Y Index: 312

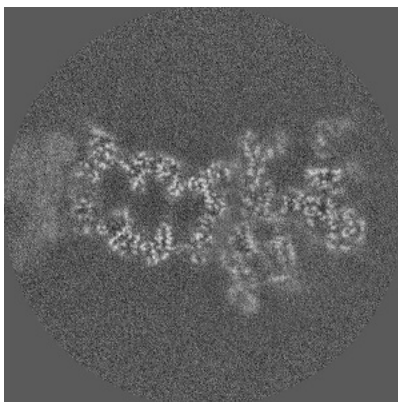


Z Index: 315

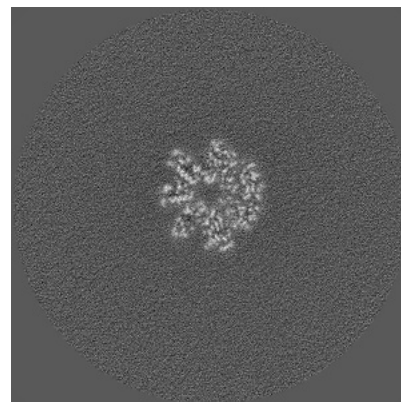
6.3.2 Raw map



X Index: 316



Y Index: 312

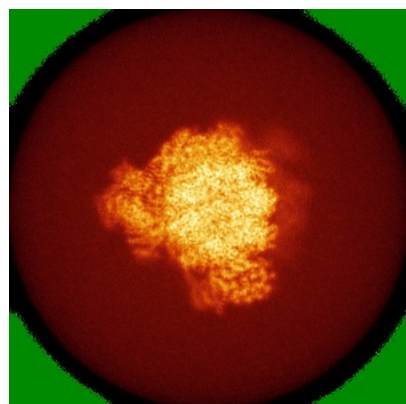


Z Index: 247

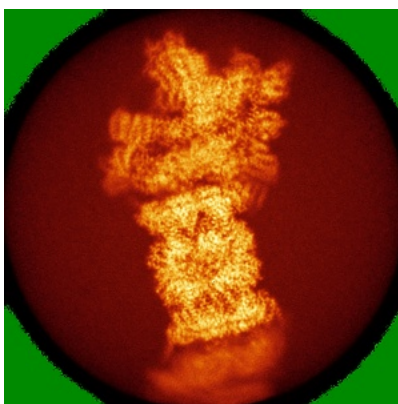
The images above show the largest variance slices of the map in three orthogonal directions.

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

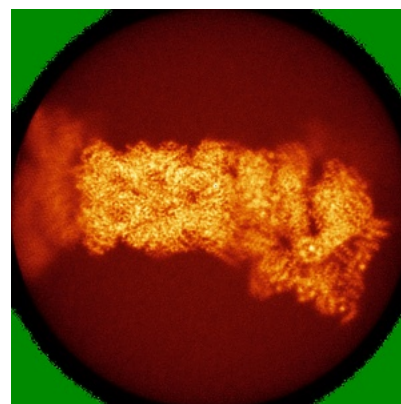
6.4.1 Primary map



X

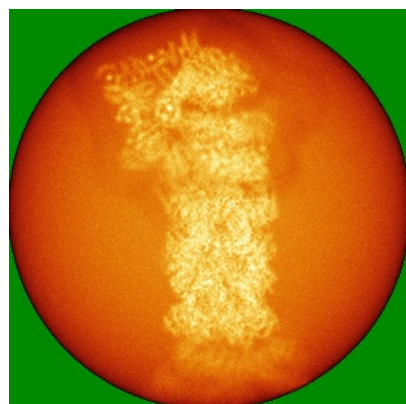


Y

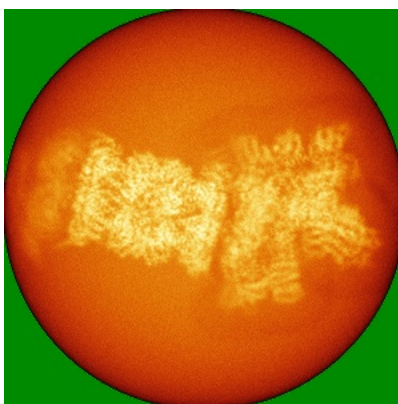


Z

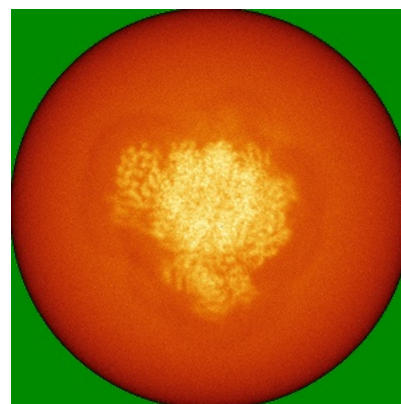
6.4.2 Raw map



X



Y

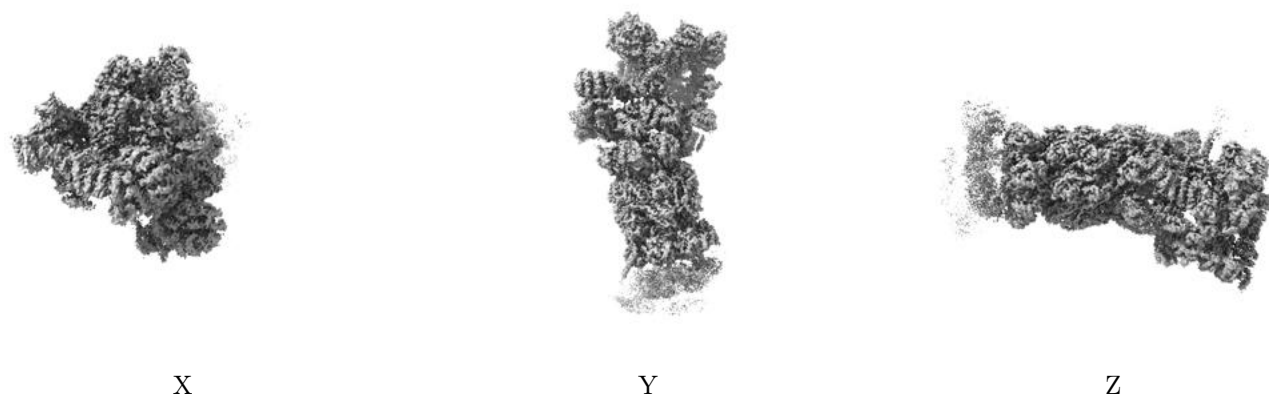


Z

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.

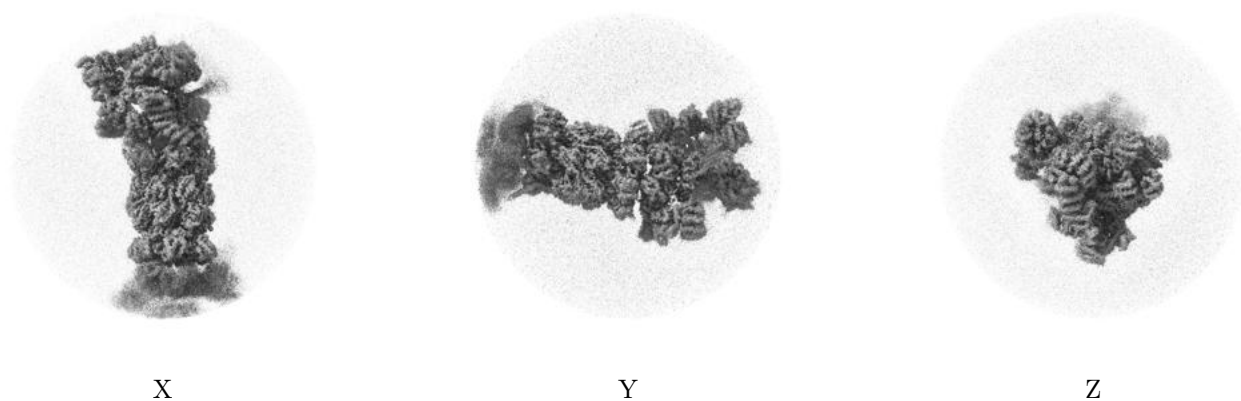
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00582. 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.

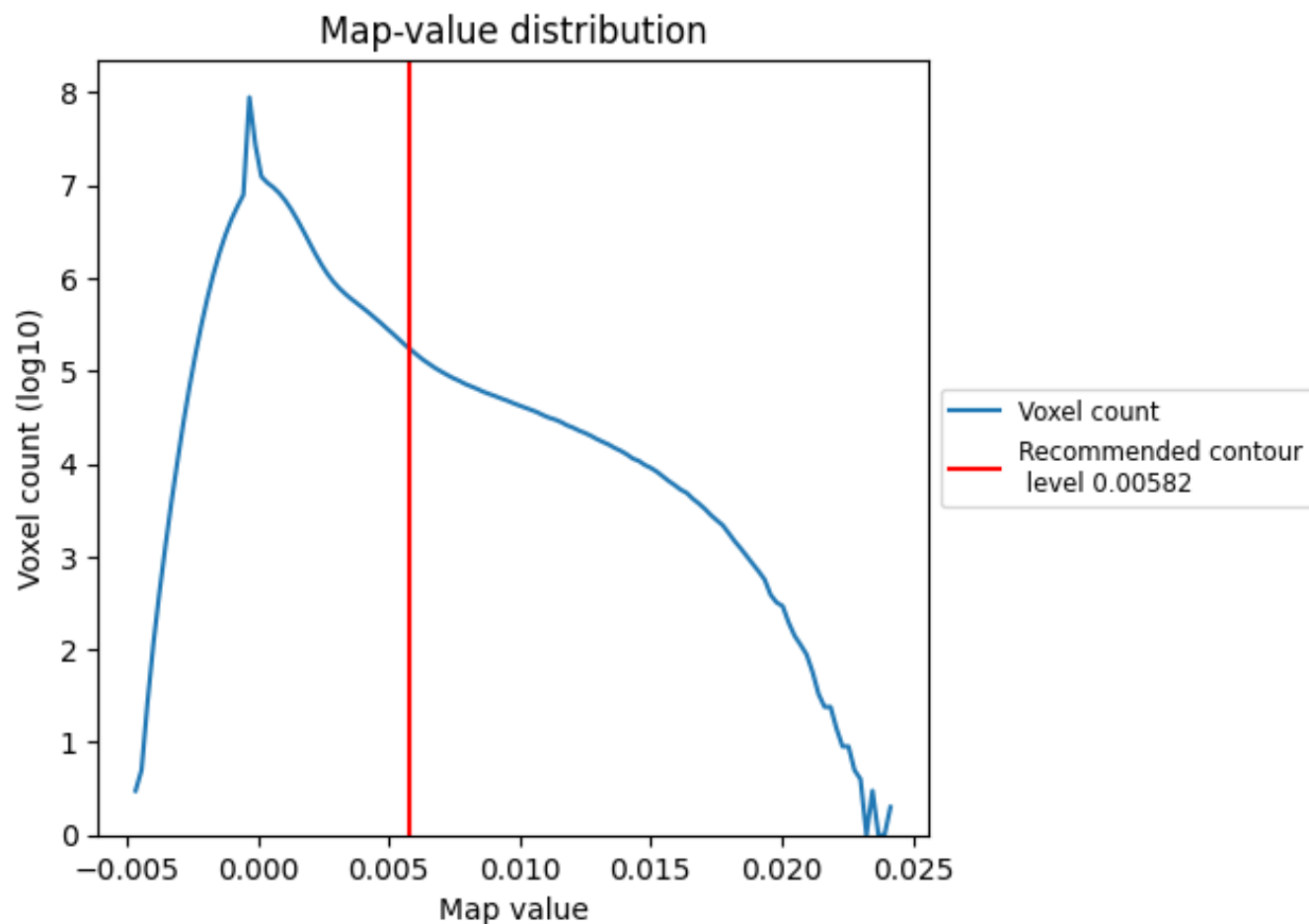
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

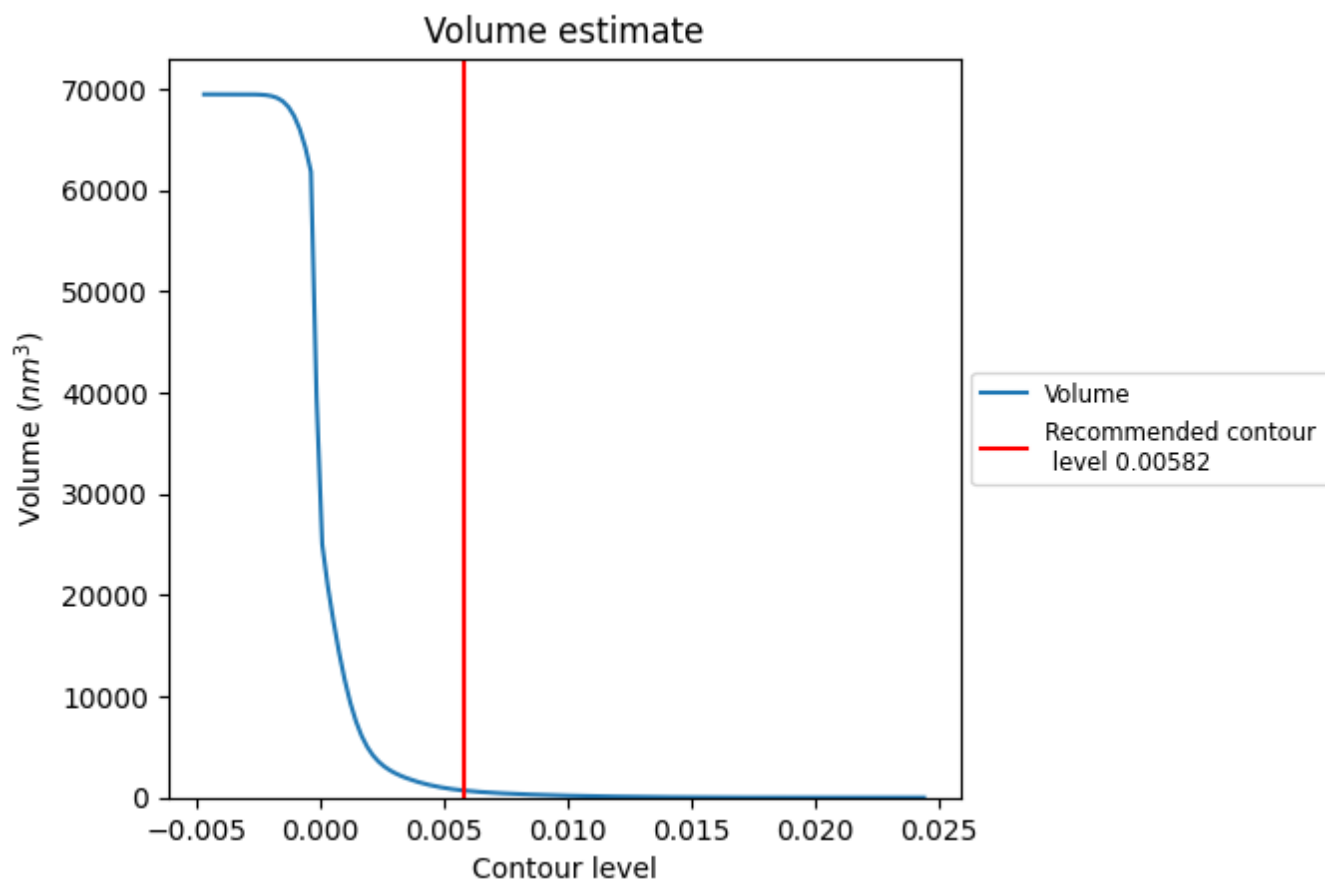
This section contains the results of statistical analysis of the map.

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.

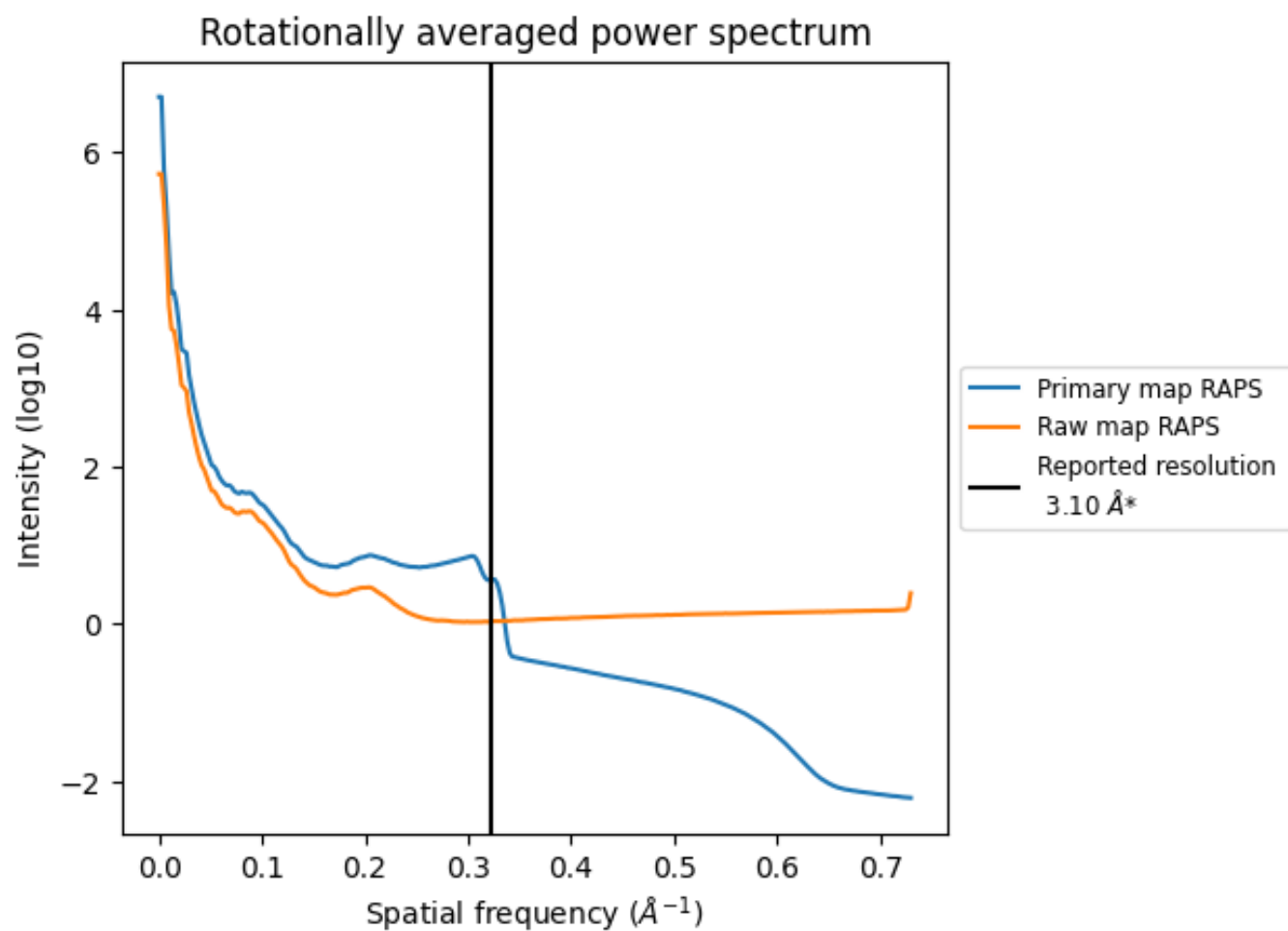
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 697 nm³; this corresponds to an approximate mass of 629 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 [i](#)

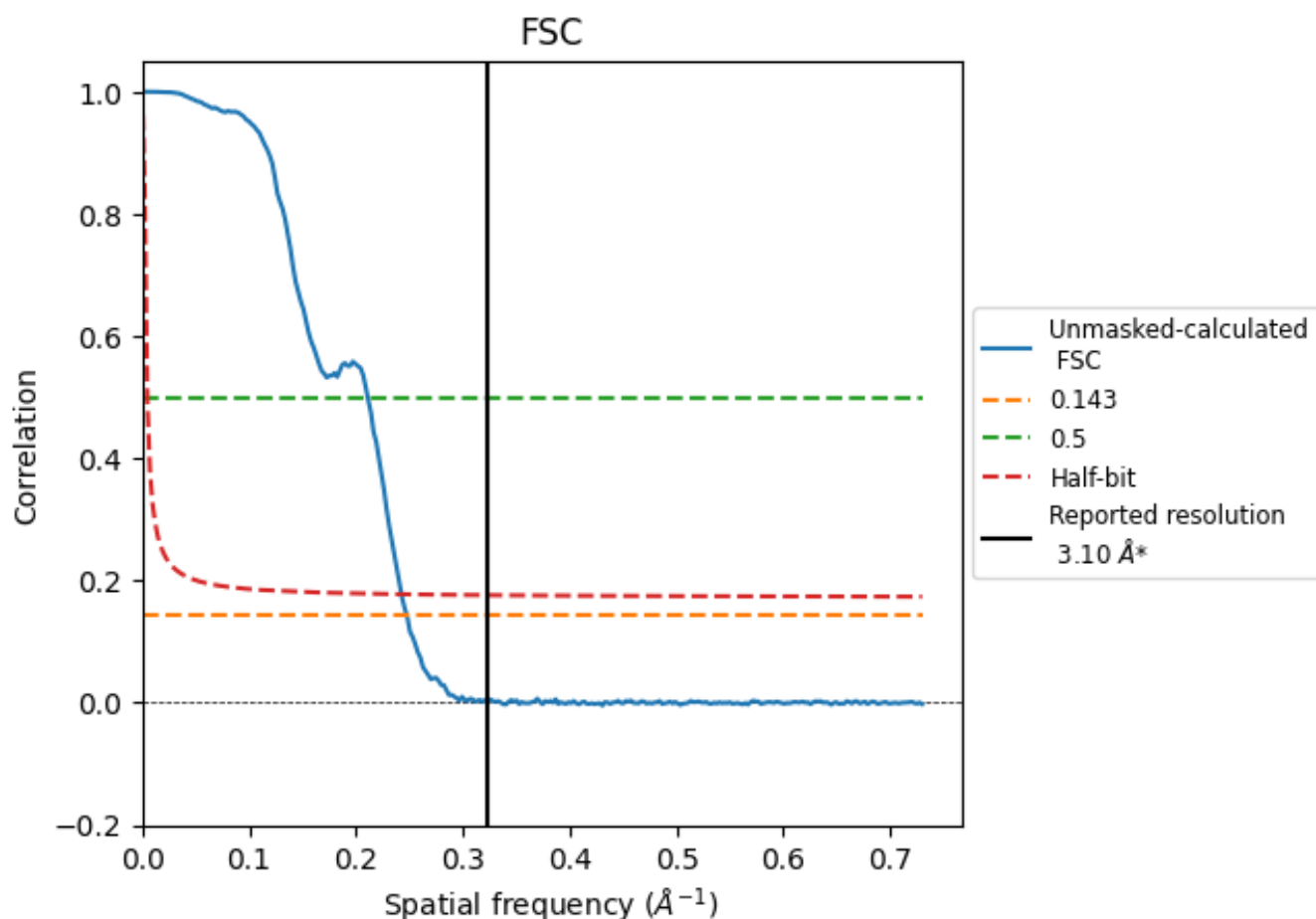


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

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 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

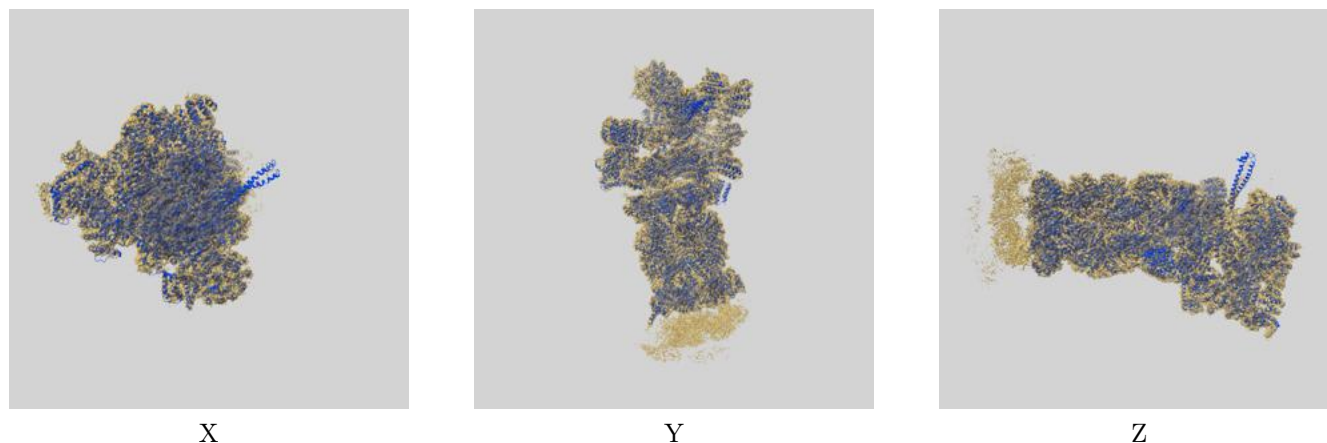
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.04	4.74	4.12

*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 4.04 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

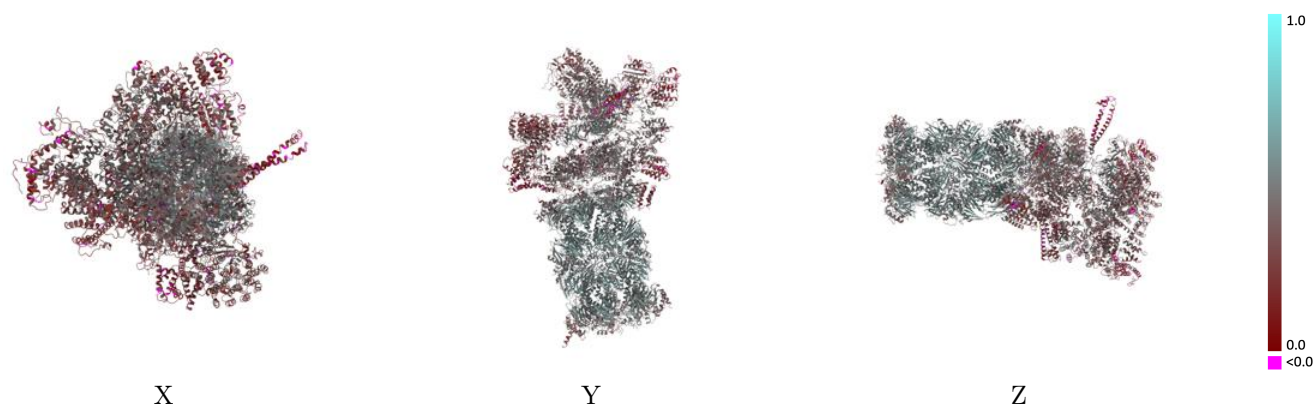
This section contains information regarding the fit between EMDB map EMD-62067 and PDB model 9K4R. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



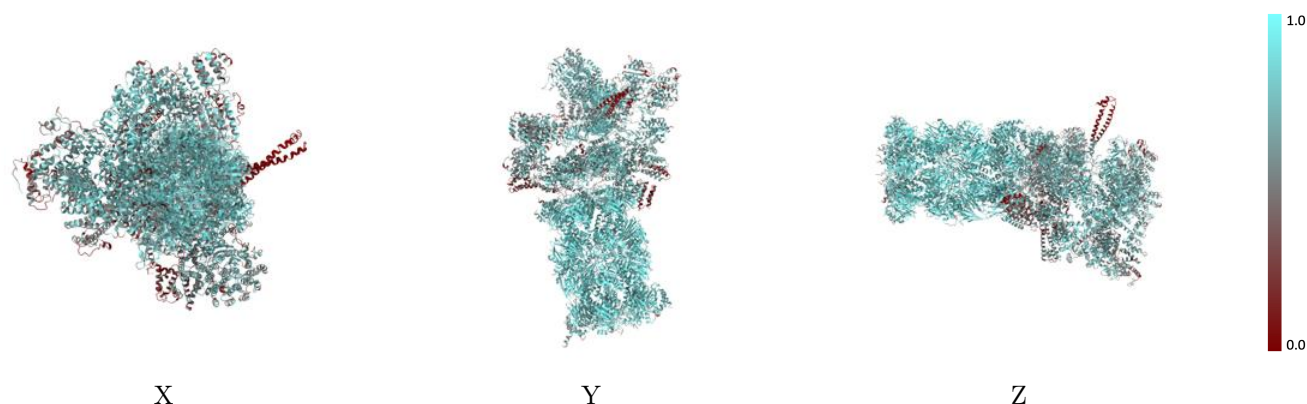
The images above show the 3D surface view of the map at the recommended contour level 0.00582 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



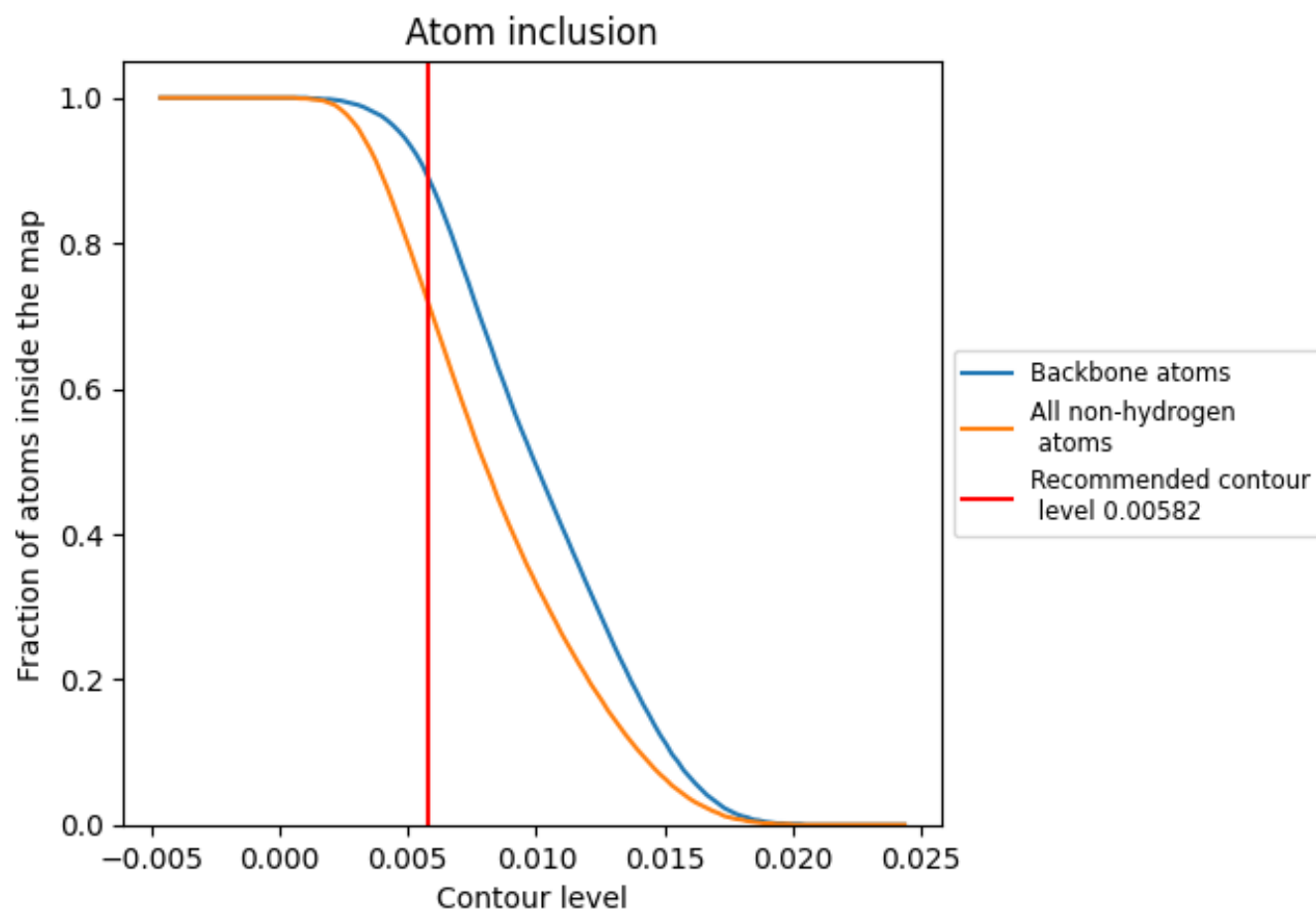
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00582).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 72% 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 (0.00582) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7150	 0.4160
A	 0.6400	 0.3650
B	 0.6070	 0.3560
C	 0.5510	 0.3250
D	 0.6760	 0.4050
E	 0.6730	 0.4010
F	 0.6380	 0.3900
G	 0.8140	 0.5000
H	 0.8290	 0.5020
I	 0.7930	 0.4750
J	 0.7660	 0.4450
K	 0.7730	 0.4880
L	 0.8480	 0.5160
M	 0.8310	 0.4960
N	 0.8780	 0.5320
O	 0.8710	 0.5220
P	 0.8750	 0.5290
Q	 0.8650	 0.5240
R	 0.8790	 0.5170
S	 0.8490	 0.5200
T	 0.8810	 0.5390
U	 0.6820	 0.3670
V	 0.6230	 0.3370
W	 0.6550	 0.3570
X	 0.5240	 0.3290
Y	 0.6310	 0.3110
Z	 0.7130	 0.3990
a	 0.6200	 0.2940
b	 0.5670	 0.3280
c	 0.7320	 0.4200
d	 0.5000	 0.2670
e	 0.4990	 0.2920
f	 0.5440	 0.2800
g	 0.7860	 0.4800
h	 0.8070	 0.4840



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Chain	Atom inclusion	Q-score
i	 0.7500	 0.4520
j	 0.6980	 0.4230
k	 0.7440	 0.4600
l	 0.8160	 0.4900
m	 0.7940	 0.4780
n	 0.8720	 0.5290
o	 0.8560	 0.5210
p	 0.8680	 0.5240
q	 0.8590	 0.5140
r	 0.8750	 0.5230
s	 0.8480	 0.5160
t	 0.8750	 0.5200
u	 0.7260	 0.4090
v	 0.4550	 0.3990