



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:39 AM UTC

PDB ID : 7W37 / pdb_00007w37
EMDB ID : EMD-32272
Title : Structure of USP14-bound human 26S proteasome in state EA1_UBL
Authors : Zhang, S.; Zou, S.; Yin, D.; Wu, Z.; Mao, Y.
Deposited on : 2021-11-25
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

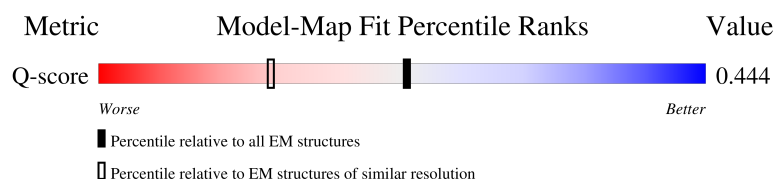
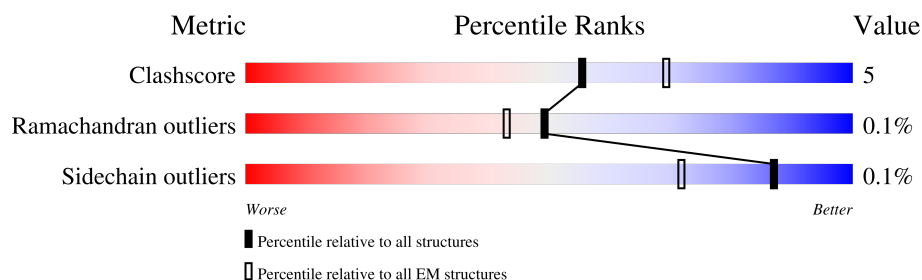
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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.



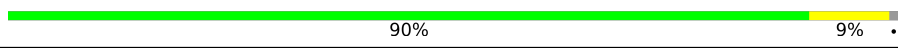
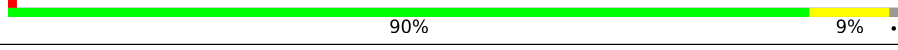
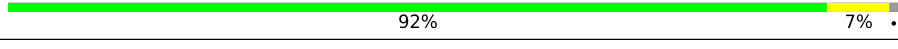
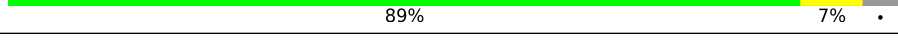
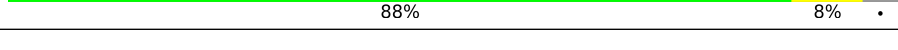
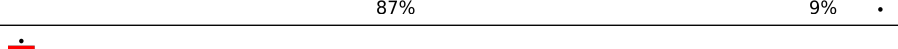
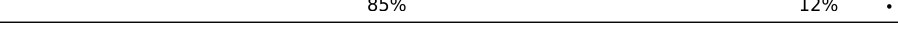
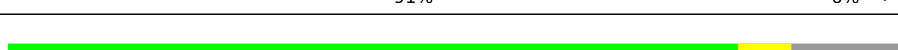
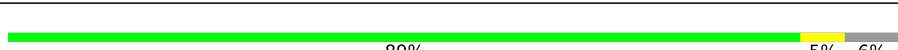
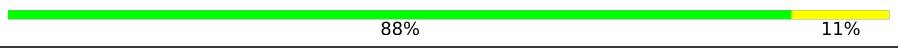
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	
2	B	440	
3	C	398	
4	D	418	

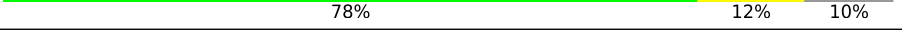
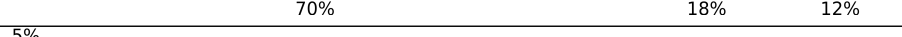
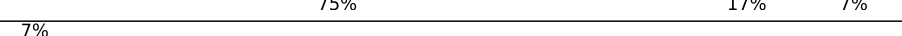
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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	269	
12	l	269	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	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	f	908	
32	x	494	
33	e	70	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 106025 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 protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	413	Total	C	N	O	S	0	0
			3240	2042	567	613	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	388	Total	C	N	O	S	0	0
			3042	1915	519	593	15		

- Molecule 3 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	379	Total	C	N	O	S	0	0
			2968	1867	534	551	16		

- Molecule 4 is a protein called 26S protease 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 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	376	Total	C	N	O	S	0	0
			2858	1802	496	545	15		

- 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	244	Total	C	N	O	S	0	0
			1880	1193	318	356	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
			1805	1154	307	338	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	250	Total	C	N	O	S	0	0
			1955	1234	336	375	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	1168	332	356	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	234	Total	C	N	O	S	0	0
			1782	1119	295	357	11		

- Molecule 12 is a protein called Isoform Long of 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	238	Total	C	N	O	S	0	0
			1861	1165	335	350	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	240	Total	C	N	O	S	0	0
			1881	1193	321	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	862	Total	C	N	O	S	0	0
			6748	4279	1147	1277	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	472	Total	C	N	O	S	0	0
			3754	2387	673	681	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	446	Total	C	N	O	S	0	0
			3635	2302	622	687	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- 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 non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	889	Total	C	N	O	S	0	0
			6866	4315	1174	1331	46		

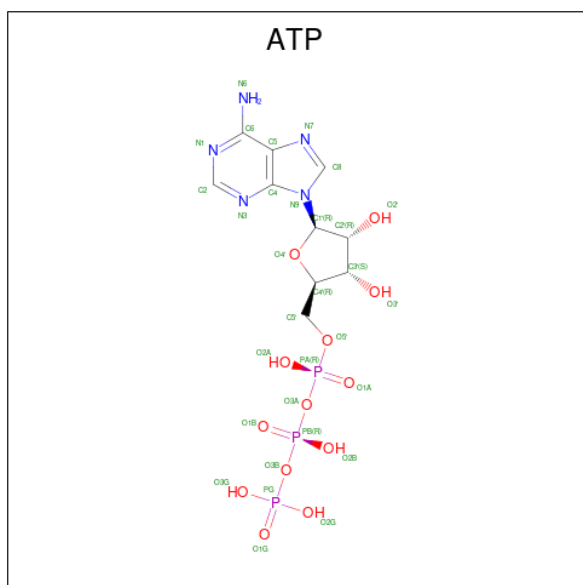
- Molecule 32 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	x	81	Total	C	N	O	S	0	0
			626	402	101	117	6		

- Molecule 33 is a protein called 26S proteasome complex subunit DSS1.

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

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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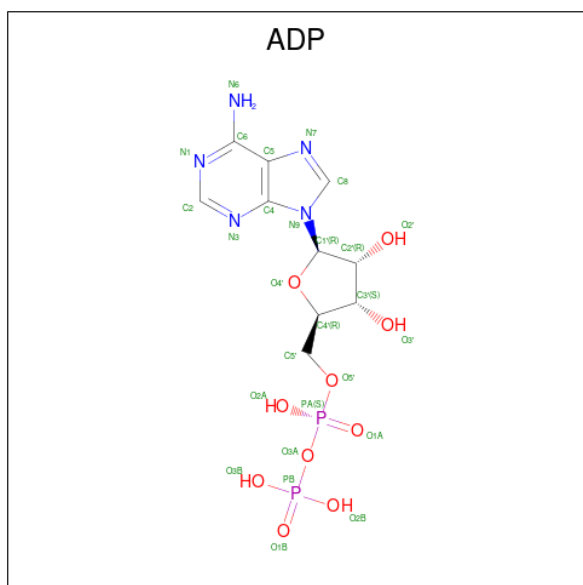
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Mol	Chain	Residues	Atoms					AltConf
34	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	Mg	0
			1	1	
35	B	1	Total	Mg	0
			1	1	
35	C	1	Total	Mg	0
			1	1	
35	D	1	Total	Mg	0
			1	1	
35	E	1	Total	Mg	0
			1	1	
35	F	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

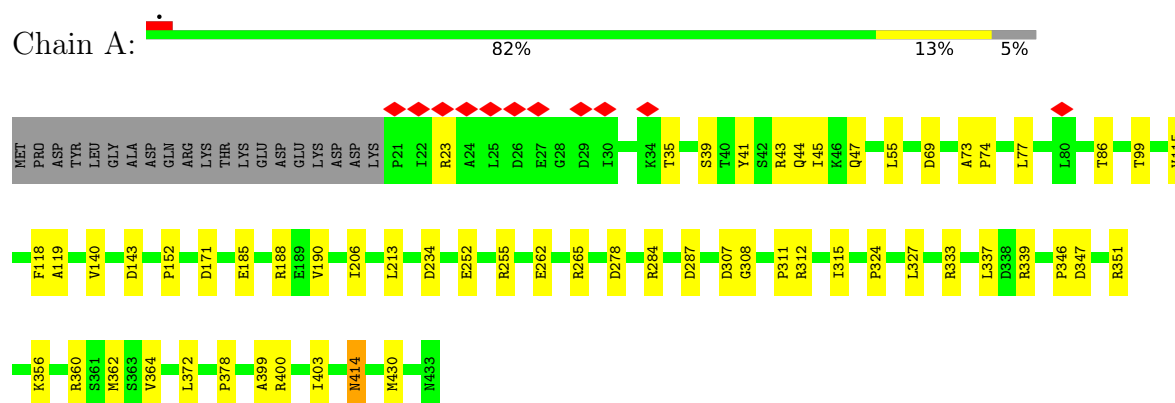
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

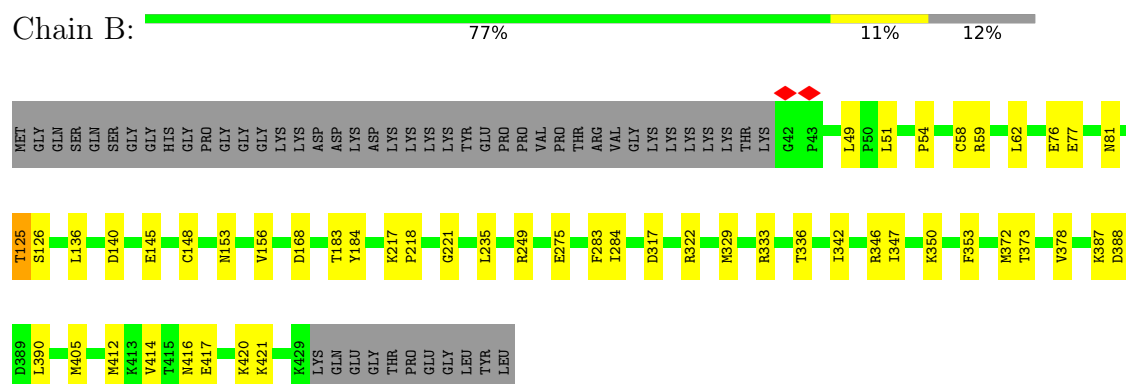
3 Residue-property plots [i](#)

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.

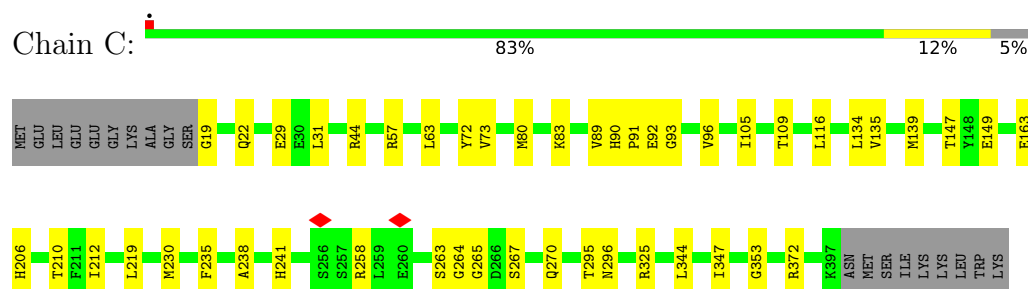
• Molecule 1: 26S protease regulatory subunit 7



• Molecule 2: 26S protease regulatory subunit 4

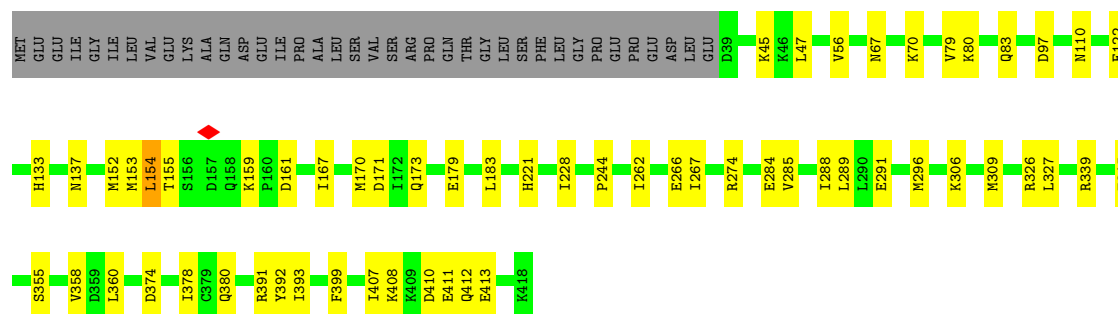


• Molecule 3: Isoform 2 of 26S proteasome regulatory subunit 8



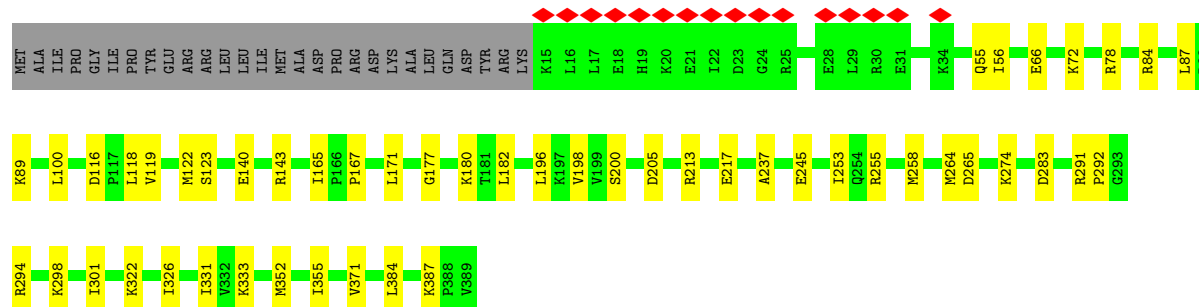
- Molecule 4: 26S protease regulatory subunit 6B

Chain D:  77% 14% 9%



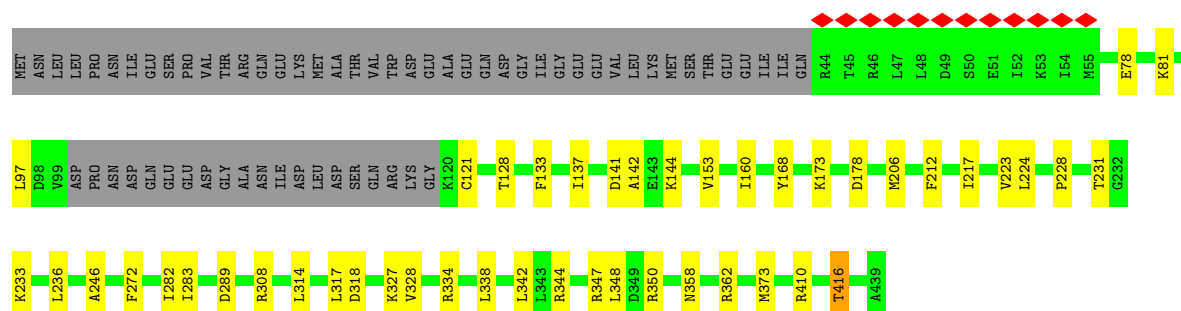
- Molecule 5: 26S proteasome regulatory subunit 10B

Chain E:  80% 13% 7%



- Molecule 6: 26S protease regulatory subunit 6A

Chain F:  75% 10% 14%



- Molecule 7: Proteasome subunit alpha type-6

Chain G:  90% 9% 1%

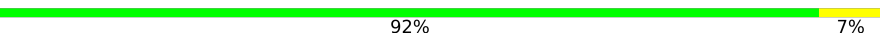


- Molecule 7: Proteasome subunit alpha type-6

Chain g:  90% 9%



- Molecule 8: Proteasome subunit alpha type-2

Chain H:  92% 7%



- Molecule 8: Proteasome subunit alpha type-2

Chain h:  87% 12%



- Molecule 9: Proteasome subunit alpha type-4

Chain I:  89% 7%



- Molecule 9: Proteasome subunit alpha type-4

Chain i:  88% 8%



- Molecule 10: Proteasome subunit alpha type-7

Chain J:  87% 9%

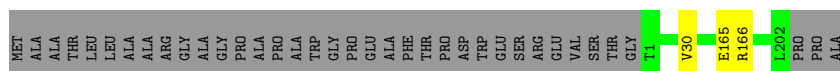


- Molecule 10: Proteasome subunit alpha type-7

Chain j:  85% 12%

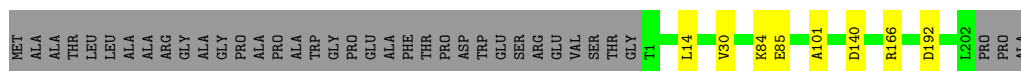


Chain N:  83% 15%



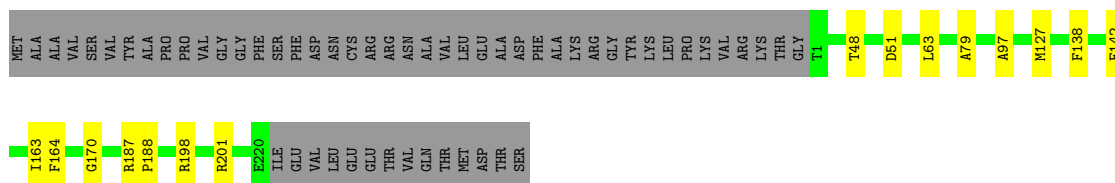
• Molecule 14: Proteasome subunit beta type-6

Chain n:  81% 15%



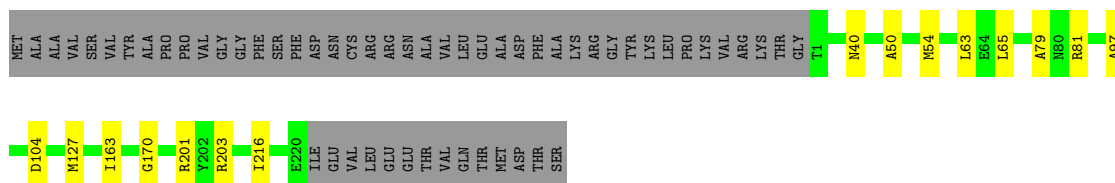
• Molecule 15: Proteasome subunit beta type-7

Chain O:  74% 5% 21%



• Molecule 15: Proteasome subunit beta type-7

Chain o:  74% 5% 21%



• Molecule 16: Proteasome subunit beta type-3

Chain P:  90% 10%



• Molecule 16: Proteasome subunit beta type-3

Chain p:  88% 11%



• Molecule 17: Proteasome subunit beta type-2

Chain Q:  88% 11%



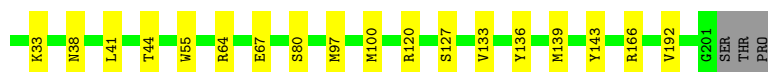
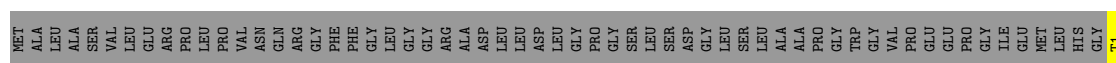
- Molecule 17: Proteasome subunit beta type-2

Chain q: 88% 11%



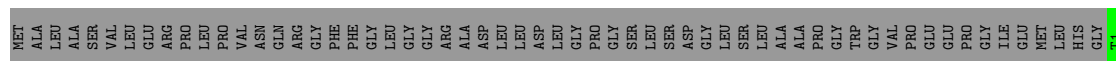
- Molecule 18: Proteasome subunit beta type-5

Chain R: 69% 7% 24%



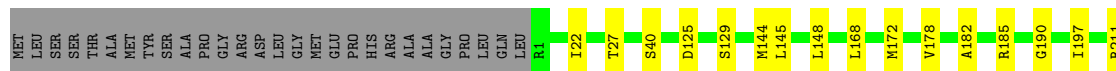
- Molecule 18: Proteasome subunit beta type-5

Chain r: 70% 7% 24%



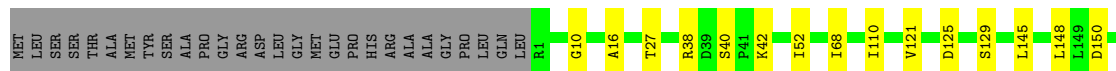
- Molecule 19: Proteasome subunit beta type-1

Chain S: 81% 7% 12%



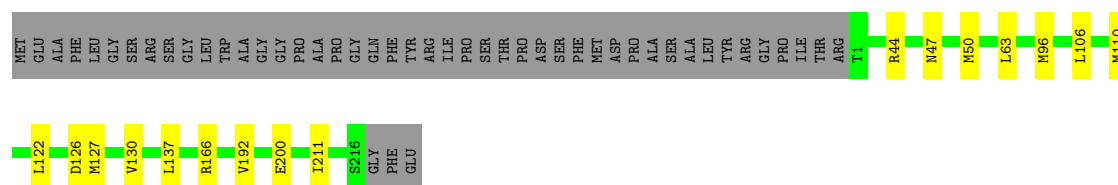
- Molecule 19: Proteasome subunit beta type-1

Chain s: 80% 8% 12%



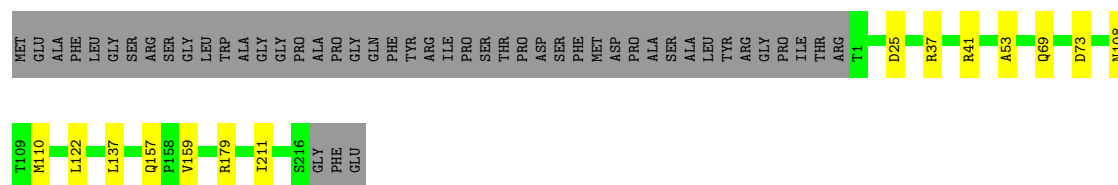
- Molecule 20: Proteasome subunit beta type-4

Chain T:  76% 6% 18%



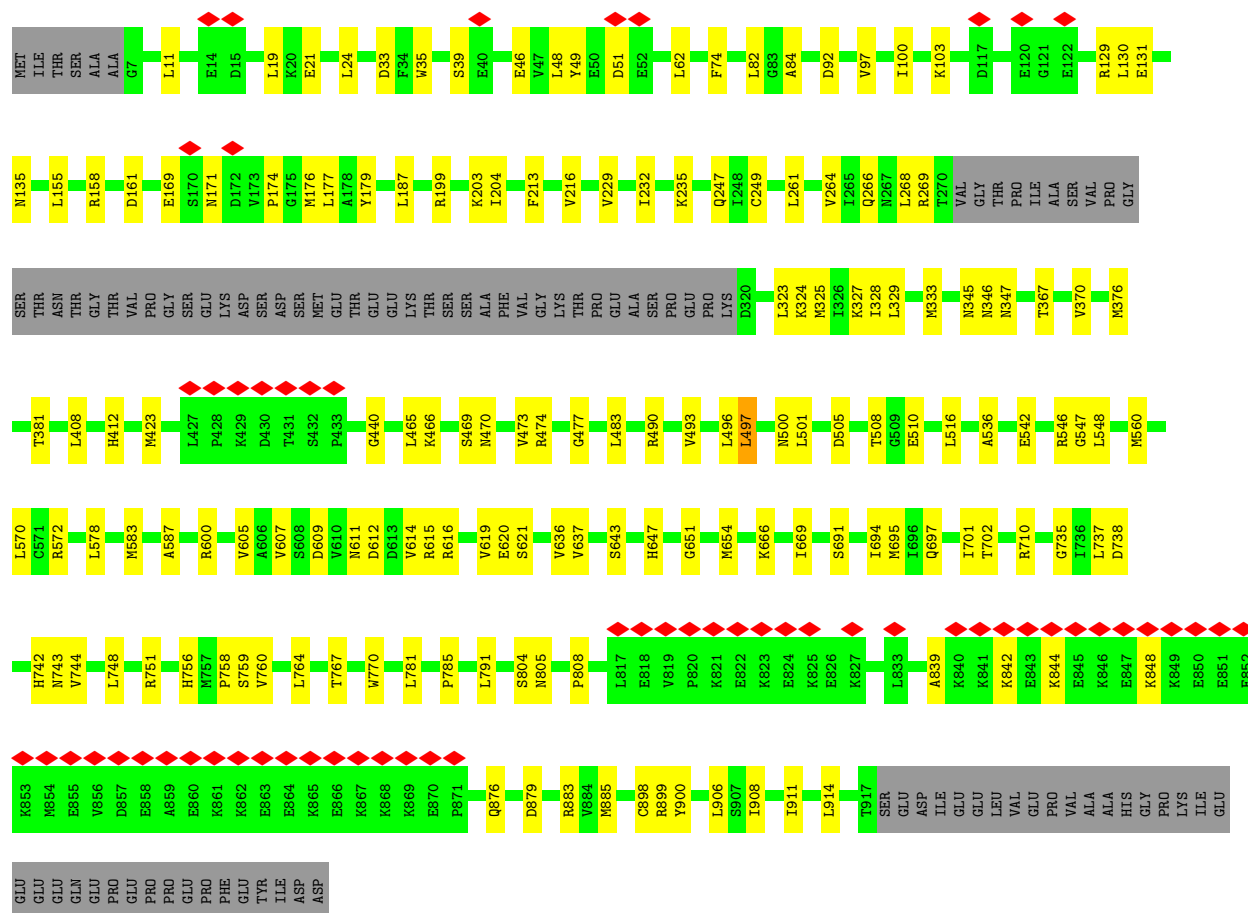
- Molecule 20: Proteasome subunit beta type-4

Chain t:  77% 5% 18%



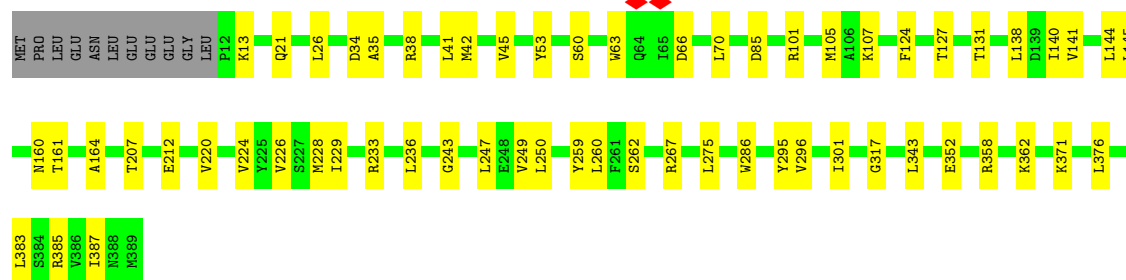
- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

Chain U:  6% 74% 16% 10%



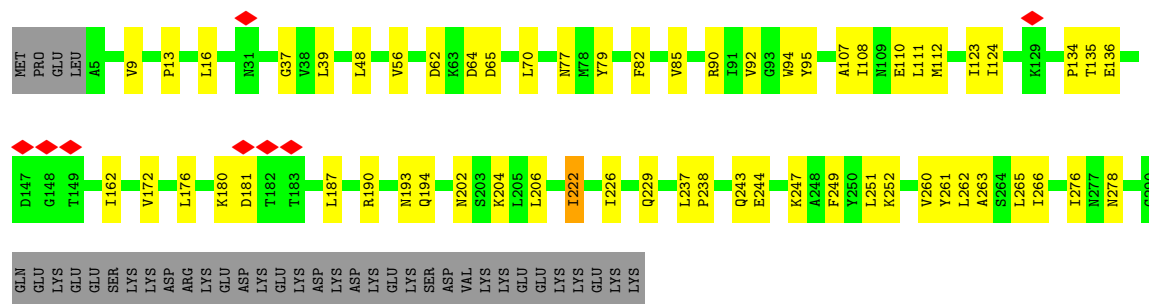
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

Chain Y:  81% 16%



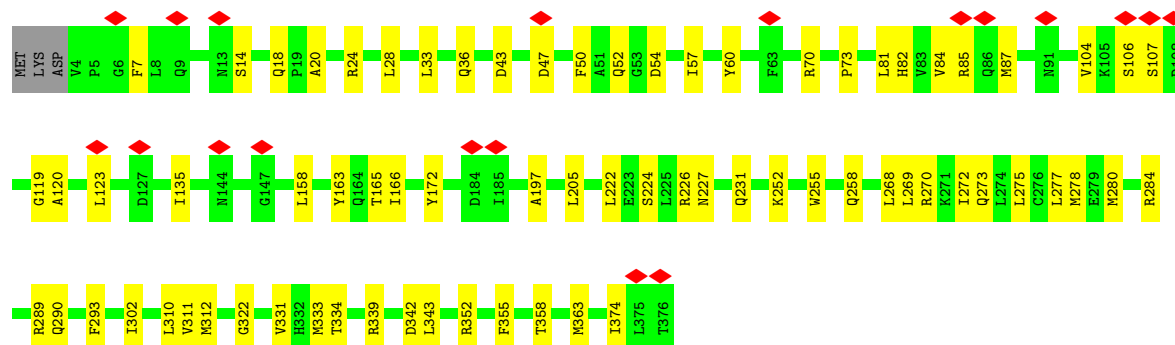
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

Chain Z:  70% 18% 12%



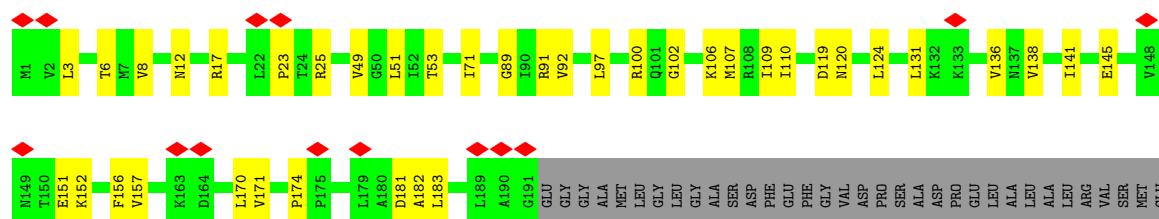
- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

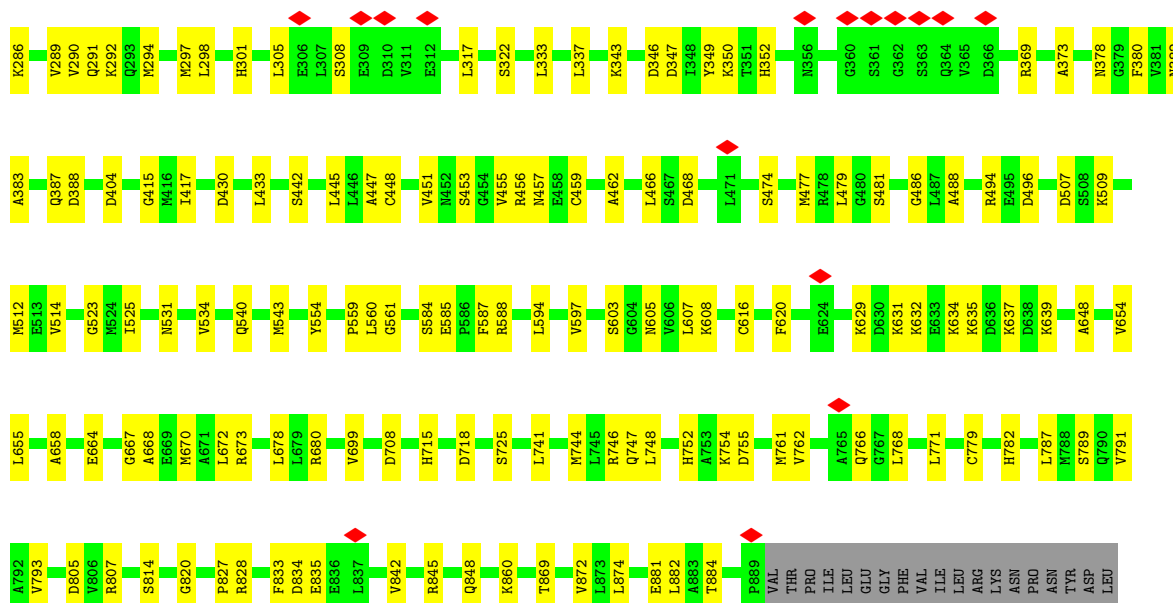
Chain a:  5% 80% 19%



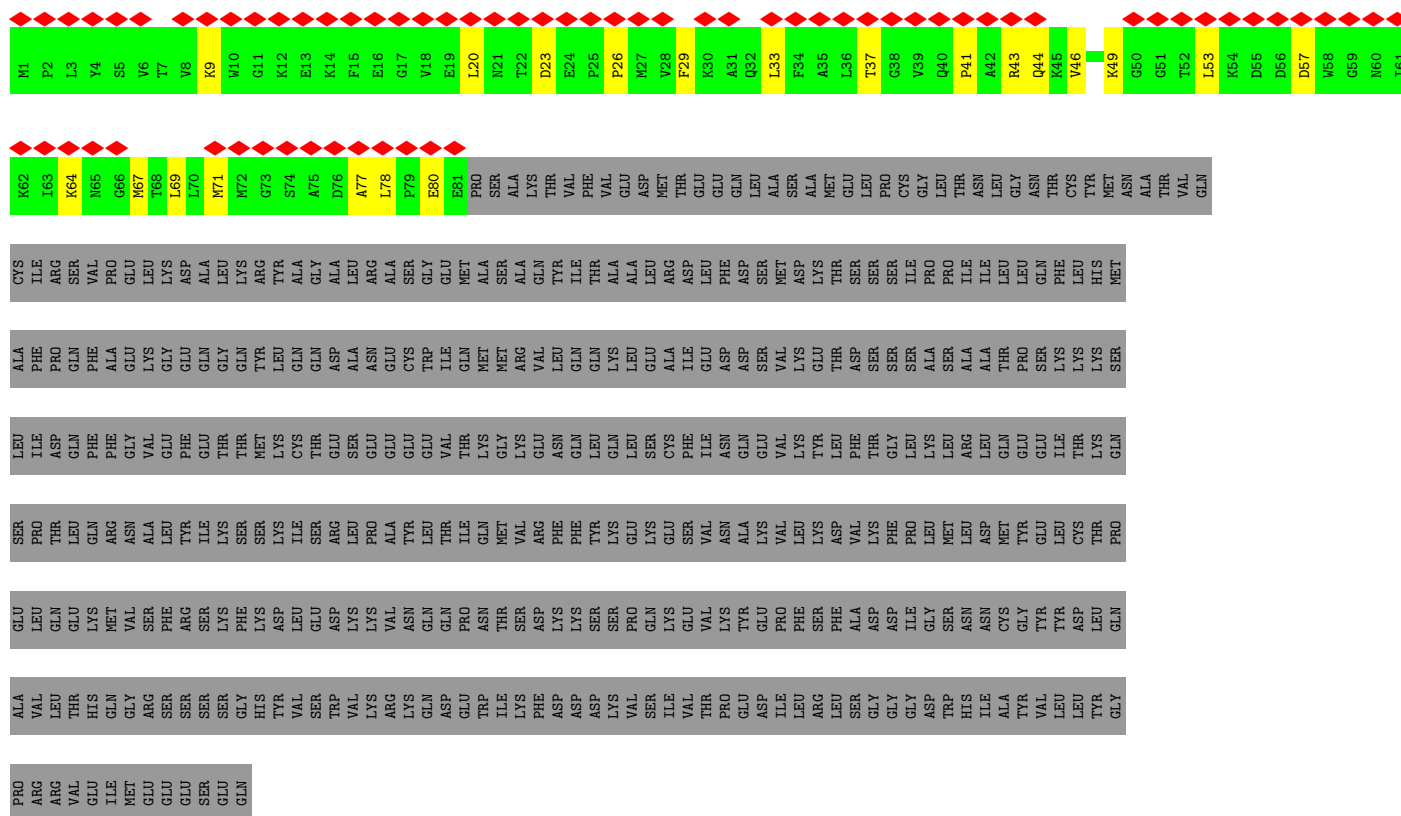
- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

Chain b:  40% 10% 49%





• Molecule 32: Ubiquitin carboxyl-terminal hydrolase 14



• Molecule 33: 26S proteasome complex subunit DSS1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	367235	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.003	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.18	0/3294	0.50	0/4447
2	B	0.17	0/3086	0.46	0/4164
3	C	0.18	0/3007	0.48	2/4045 (0.0%)
4	D	0.19	0/3089	0.49	0/4168
5	E	0.18	0/2904	0.46	0/3924
6	F	0.17	0/2896	0.43	0/3912
7	G	0.16	0/1923	0.39	0/2601
7	g	0.15	0/1914	0.41	0/2590
8	H	0.16	0/1844	0.38	0/2499
8	h	0.14	0/1844	0.35	0/2497
9	I	0.15	0/1991	0.38	0/2685
9	i	0.16	0/1985	0.40	0/2677
10	J	0.17	0/1906	0.44	0/2573
10	j	0.15	0/1887	0.40	0/2549
11	K	0.15	0/1804	0.37	0/2436
11	k	0.13	0/1809	0.33	0/2444
12	L	0.14	0/1901	0.35	0/2570
12	l	0.14	0/1896	0.37	0/2565
13	M	0.14	0/1911	0.36	0/2573
13	m	0.13	0/1916	0.31	0/2580
14	N	0.13	0/1540	0.31	0/2085
14	n	0.13	0/1536	0.30	0/2080
15	O	0.14	0/1676	0.37	0/2271
15	o	0.13	0/1686	0.34	0/2282
16	P	0.15	0/1616	0.40	0/2180
16	p	0.15	0/1620	0.40	0/2184
17	Q	0.13	0/1621	0.34	0/2194
17	q	0.13	0/1621	0.33	0/2194
18	R	0.14	0/1590	0.33	0/2147
18	r	0.13	0/1590	0.31	0/2147
19	S	0.16	0/1671	0.40	2/2252 (0.1%)
19	s	0.17	0/1684	0.44	2/2268 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.13	0/1716	0.35	0/2323
20	t	0.14	0/1720	0.34	0/2328
21	U	0.18	0/6864	0.48	0/9271
22	V	0.17	0/3824	0.42	0/5170
23	W	0.23	1/3683 (0.0%)	0.59	2/4952 (0.0%)
24	X	0.18	0/3053	0.44	0/4115
25	Y	0.20	0/3173	0.52	0/4273
26	Z	0.18	0/2324	0.50	1/3150 (0.0%)
27	a	0.19	0/3053	0.51	0/4133
28	b	0.21	0/1478	0.54	0/2001
29	c	0.22	0/2302	0.58	0/3110
30	d	0.22	0/2162	0.52	0/2919
31	f	0.21	0/6980	0.56	2/9433 (0.0%)
32	x	0.20	0/638	0.55	0/859
33	e	0.22	0/437	0.61	0/595
All	All	0.17	1/107665 (0.0%)	0.45	11/145415 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	307	LYS	CA-C	5.35	1.59	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	f	872	VAL	N-CA-C	-6.81	106.86	113.53
3	C	241	HIS	CA-C-N	5.64	130.47	121.62
3	C	241	HIS	C-N-CA	5.64	130.47	121.62
23	W	116	THR	CA-C-N	5.57	132.18	121.54
23	W	116	THR	C-N-CA	5.57	132.18	121.54
31	f	699	VAL	N-CA-C	-5.43	106.55	112.80
26	Z	92	VAL	N-CA-C	-5.27	108.37	113.53
19	s	190	GLY	CA-C-N	5.18	131.44	121.54
19	s	190	GLY	C-N-CA	5.18	131.44	121.54
19	S	190	GLY	CA-C-N	5.07	131.22	121.54
19	S	190	GLY	C-N-CA	5.07	131.22	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	3240	0	3286	41	0
2	B	3042	0	3100	32	0
3	C	2968	0	3067	31	0
4	D	3039	0	3075	48	0
5	E	2860	0	2827	36	0
6	F	2858	0	2853	37	0
7	G	1889	0	1885	16	0
7	g	1880	0	1875	15	0
8	H	1805	0	1784	12	0
8	h	1805	0	1798	20	0
9	I	1958	0	1960	10	0
9	i	1955	0	1955	13	0
10	J	1880	0	1892	17	0
10	j	1861	0	1865	19	0
11	K	1777	0	1762	12	0
11	k	1782	0	1766	10	0
12	L	1866	0	1852	11	0
12	l	1861	0	1839	8	0
13	M	1876	0	1861	15	0
13	m	1881	0	1868	8	0
14	N	1514	0	1487	3	0
14	n	1510	0	1483	6	0
15	O	1649	0	1659	8	0
15	o	1659	0	1681	11	0
16	P	1587	0	1598	14	0
16	p	1591	0	1609	15	0
17	Q	1588	0	1584	18	0
17	q	1588	0	1584	16	0
18	R	1559	0	1523	12	0
18	r	1559	0	1523	14	0
19	S	1641	0	1639	10	0
19	s	1654	0	1656	12	0
20	T	1683	0	1662	10	0
20	t	1687	0	1666	9	0
21	U	6748	0	6813	96	0
22	V	3754	0	3749	40	0
23	W	3635	0	3762	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	X	3009	0	3113	34	0
25	Y	3115	0	3120	37	0
26	Z	2281	0	2312	43	0
27	a	2995	0	3012	48	0
28	b	1458	0	1505	23	0
29	c	2260	0	2276	43	0
30	d	2116	0	2146	37	0
31	f	6866	0	6866	139	0
32	x	626	0	642	12	0
33	e	425	0	328	3	0
34	A	31	0	12	0	0
34	B	31	0	12	0	0
34	D	31	0	12	0	0
34	E	31	0	12	1	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	E	1	0	0	0	0
35	F	1	0	0	0	0
36	C	27	0	12	1	0
36	F	27	0	12	0	0
37	c	1	0	0	0	0
All	All	106025	0	106240	1069	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 (1069) 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)
21:U:35:TRP:O	21:U:39:SER:HB2	1.82	0.79
31:f:462:ALA:O	31:f:466:LEU:HB2	1.85	0.75
5:E:198:VAL:HG12	5:E:200:SER:H	1.54	0.72
29:c:75:MET:SD	29:c:92:GLN:NE2	2.64	0.70
20:T:96:MET:HE2	20:T:110:MET:HE1	1.75	0.68
31:f:654:VAL:O	31:f:658:ALA:HB3	1.92	0.68
31:f:746:ARG:NH1	31:f:747:GLN:OE1	2.28	0.66
19:S:148:LEU:HD23	19:S:178:VAL:HG12	1.77	0.65
7:g:181:LYS:HA	7:g:184:LYS:HE3	1.78	0.65
13:M:227:VAL:O	13:M:232:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:275:MET:SD	31:f:286:LYS:NZ	2.69	0.64
27:a:278:MET:HB3	27:a:339:ARG:HH22	1.63	0.64
10:J:96:LEU:HD11	17:Q:58:GLU:HB3	1.80	0.63
5:E:237:ALA:HB1	6:F:308:ARG:HG3	1.81	0.63
23:W:315:MET:HB3	23:W:320:LEU:HD11	1.81	0.63
12:l:41:LYS:HG3	12:l:42:THR:HG23	1.79	0.63
31:f:298:LEU:HB3	31:f:456:ARG:HH22	1.65	0.62
23:W:363:ILE:HD11	23:W:382:LEU:HD11	1.81	0.62
27:a:33:LEU:HD13	27:a:36:GLN:HB2	1.80	0.62
23:W:363:ILE:HD13	23:W:366:MET:HE3	1.79	0.62
31:f:453:SER:HA	31:f:488:ALA:HA	1.81	0.62
25:Y:301:ILE:HG13	25:Y:343:LEU:HD12	1.82	0.62
10:j:116:GLN:NE2	10:j:120:GLN:OE1	2.33	0.62
1:A:55:LEU:HD11	2:B:76:GLU:HG2	1.82	0.62
17:Q:68:LYS:HG3	17:Q:74:GLU:HG2	1.82	0.62
16:P:205:ASP:HB3	18:r:192:VAL:HG11	1.82	0.61
4:D:67:ASN:ND2	21:U:607:VAL:O	2.33	0.61
2:B:54:PRO:HA	31:f:835:GLU:HB3	1.81	0.61
31:f:789:SER:H	31:f:793:VAL:HB	1.64	0.61
21:U:440:GLY:HA2	21:U:473:VAL:HG13	1.83	0.61
3:C:135:VAL:HG12	3:C:139:MET:HE2	1.83	0.61
22:V:85:ALA:HB2	22:V:93:PHE:HB2	1.80	0.61
28:b:157:VAL:HG11	28:b:170:LEU:HB2	1.82	0.61
21:U:381:THR:HG22	21:U:412:HIS:HA	1.83	0.61
25:Y:101:ARG:HE	25:Y:131:THR:HG22	1.66	0.61
21:U:247:GLN:NE2	21:U:911:ILE:O	2.34	0.61
21:U:751:ARG:HE	21:U:908:ILE:HA	1.65	0.61
31:f:369:ARG:HH21	31:f:744:MET:HE3	1.65	0.61
2:B:49:LEU:HG	2:B:51:LEU:HD23	1.82	0.61
31:f:229:VAL:HG13	31:f:605:ASN:HD22	1.66	0.61
1:A:284:ARG:HH21	6:F:334:ARG:HG3	1.66	0.60
21:U:748:LEU:HD23	21:U:760:VAL:HG22	1.83	0.60
25:Y:226:VAL:HA	25:Y:229:ILE:HD12	1.83	0.60
9:i:106:PRO:HB2	9:i:109:GLN:HG3	1.83	0.60
31:f:828:ARG:HG2	31:f:845:ARG:H	1.65	0.60
4:D:339:ARG:NH2	24:X:202:CYS:SG	2.74	0.60
11:K:20:ARG:NH1	11:K:25:GLU:OE1	2.34	0.60
21:U:694:ILE:HG23	21:U:695:MET:HG2	1.84	0.60
4:D:392:TYR:H	23:W:136:ILE:HD11	1.65	0.60
13:M:108:LEU:HD11	13:M:137:LEU:HB3	1.84	0.59
12:l:137:TYR:OH	12:l:217:LYS:NZ	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:43:ARG:HH21	7:g:164:LYS:HG2	1.66	0.59
9:i:174:MET:SD	9:i:195:LYS:NZ	2.75	0.59
13:m:34:SER:OG	13:m:65:ARG:NH1	2.35	0.59
1:A:324:PRO:HA	1:A:327:LEU:HD13	1.84	0.59
13:M:34:SER:OG	13:M:65:ARG:NH1	2.34	0.59
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.84	0.59
31:f:631:LYS:HA	31:f:634:LYS:HE2	1.83	0.59
15:O:138:PHE:O	15:O:142:PHE:HB2	2.01	0.59
2:B:284:ILE:HB	2:B:329:MET:HG2	1.84	0.59
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.85	0.59
31:f:125:ILE:HG23	31:f:131:MET:HE1	1.84	0.59
21:U:346:ASN:HD22	21:U:347:ASN:N	2.00	0.59
2:B:372:MET:HE3	2:B:414:VAL:HG21	1.85	0.58
23:W:132:THR:HG23	23:W:134:GLY:H	1.68	0.58
25:Y:233:ARG:HA	25:Y:236:LEU:HD12	1.84	0.58
21:U:605:VAL:O	21:U:609:ASP:HB2	2.02	0.58
8:h:59:GLU:HG2	8:h:60:ARG:HD3	1.85	0.58
31:f:672:LEU:HD13	31:f:708:ASP:HB3	1.84	0.58
1:A:252:GLU:OE1	1:A:255:ARG:NH1	2.37	0.58
23:W:230:MET:HE3	23:W:246:HIS:HE1	1.69	0.58
3:C:44:ARG:NH2	22:V:492:LYS:O	2.36	0.58
6:F:282:ILE:HG22	6:F:327:LYS:HB2	1.84	0.58
25:Y:21:GLN:HE22	25:Y:286:TRP:H	1.51	0.58
21:U:213:PHE:HA	21:U:216:VAL:HG12	1.86	0.58
22:V:176:MET:HE3	22:V:217:VAL:HG22	1.85	0.58
22:V:497:PRO:HG3	26:Z:278:ASN:HB3	1.86	0.58
17:q:1:MET:HE3	17:q:133:GLY:HA2	1.86	0.58
2:B:58:CYS:SG	2:B:59:ARG:N	2.76	0.58
24:X:374:PHE:HZ	24:X:387:ILE:HG12	1.69	0.58
6:F:318:ASP:HB3	6:F:347:ARG:HG2	1.86	0.57
20:t:41:ARG:NH1	20:t:53:ALA:O	2.38	0.57
21:U:92:ASP:HA	21:U:97:VAL:HG21	1.85	0.57
21:U:345:ASN:O	21:U:743:ASN:ND2	2.37	0.57
24:X:255:LEU:HD22	24:X:267:VAL:HG13	1.86	0.57
28:b:97:LEU:HA	28:b:100:ARG:HG3	1.85	0.57
20:t:157:GLN:NE2	20:t:159:VAL:O	2.38	0.57
23:W:274:VAL:O	23:W:283:GLN:NE2	2.37	0.57
26:Z:135:THR:HG21	26:Z:162:ILE:HD11	1.85	0.57
3:C:29:GLU:HB2	22:V:201:ARG:HE	1.69	0.57
6:F:358:ASN:O	6:F:362:ARG:NH1	2.37	0.57
22:V:467:TYR:OH	24:X:397:TYR:OH	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:244:GLU:OE1	31:f:244:GLU:N	2.37	0.57
5:E:265:ASP:OD2	5:E:291:ARG:NH2	2.37	0.57
7:G:190:THR:OG1	7:G:193:GLN:OE1	2.22	0.57
21:U:155:LEU:O	21:U:158:ARG:NH1	2.37	0.57
23:W:90:LEU:O	23:W:96:GLN:NE2	2.36	0.57
21:U:328:ILE:HG13	21:U:329:LEU:HG	1.85	0.57
30:d:61:TRP:HZ3	30:d:65:ARG:HD2	1.68	0.57
24:X:221:GLU:HB3	24:X:223:LYS:HG2	1.87	0.57
31:f:369:ARG:HH22	31:f:741:LEU:HA	1.70	0.57
6:F:231:THR:HG1	6:F:233:LYS:HZ3	1.50	0.56
22:V:371:ASN:OD1	22:V:427:GLN:NE2	2.38	0.56
29:c:27:THR:HB	29:c:175:ARG:HB3	1.86	0.56
17:q:168:GLN:NE2	17:q:175:LEU:O	2.37	0.56
4:D:244:PRO:HB3	4:D:291:GLU:HG3	1.87	0.56
23:W:175:GLY:O	23:W:182:ARG:NH2	2.39	0.56
21:U:131:GLU:O	21:U:135:ASN:ND2	2.39	0.56
24:X:258:LYS:HD3	24:X:266:ASP:HB2	1.87	0.56
7:G:158:GLY:O	8:H:84:ARG:NH2	2.37	0.56
20:T:44:ARG:NH2	20:T:47:ASN:OD1	2.38	0.56
12:l:117:GLN:NE2	13:m:83:ASP:OD1	2.39	0.56
6:F:224:LEU:HB2	6:F:348:LEU:HD13	1.88	0.56
22:V:243:ASP:O	22:V:247:GLN:NE2	2.38	0.56
11:k:210:LEU:HA	11:k:214:ASN:HD21	1.71	0.56
31:f:670:MET:O	31:f:673:ARG:NH1	2.39	0.56
5:E:72:LYS:HB2	5:E:78:ARG:HG2	1.88	0.56
5:E:84:ARG:HB2	5:E:87:LEU:HD23	1.87	0.56
8:H:143:ARG:NH1	8:H:144:PRO:O	2.39	0.56
26:Z:249:PHE:HZ	29:c:303:MET:HG2	1.70	0.56
7:g:158:GLY:O	8:h:84:ARG:NH2	2.36	0.56
31:f:172:GLU:HB3	31:f:208:LEU:HD11	1.87	0.56
1:A:99:THR:HG22	1:A:115:VAL:HG12	1.88	0.56
2:B:405:MET:HE1	2:B:421:LYS:HD2	1.87	0.56
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.39	0.56
18:R:64:ARG:NH1	18:R:67:GLU:OE1	2.39	0.56
16:p:65:GLN:OE1	17:q:86:ARG:NH2	2.38	0.56
3:C:258:ARG:HG2	3:C:265:GLY:H	1.69	0.56
4:D:411:GLU:HG2	4:D:413:GLU:H	1.70	0.56
27:a:20:ALA:HB1	27:a:24:ARG:HH12	1.71	0.56
29:c:31:VAL:HB	29:c:205:ILE:HG22	1.88	0.56
11:k:52:LYS:NZ	11:k:61:PRO:O	2.39	0.56
23:W:299:ILE:HG22	23:W:301:LYS:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:119:GLN:HG3	9:i:81:SER:HB2	1.88	0.56
32:x:49:LYS:HE2	32:x:67:MET:HB2	1.88	0.56
31:f:180:GLN:HE21	31:f:215:ASP:HB2	1.71	0.55
31:f:869:THR:HA	31:f:884:THR:HA	1.87	0.55
11:k:13:ASN:HB2	12:l:126:ARG:HG2	1.87	0.55
16:p:58:THR:O	17:q:85:ARG:NH2	2.39	0.55
1:A:234:ASP:O	31:f:352:HIS:NE2	2.39	0.55
21:U:609:ASP:O	21:U:615:ARG:NH1	2.36	0.55
27:a:43:ASP:O	27:a:47:ASP:HB2	2.06	0.55
1:A:23:ARG:NH2	31:f:4:GLY:O	2.38	0.55
6:F:168:TYR:HB2	6:F:173:LYS:HE2	1.88	0.55
21:U:611:ASN:HB3	21:U:614:VAL:HG12	1.89	0.55
32:x:78:LEU:HG	32:x:80:GLU:HG3	1.88	0.55
1:A:347:ASP:O	1:A:351:ARG:NH1	2.40	0.55
21:U:469:SER:OG	21:U:470:ASN:N	2.37	0.55
21:U:497:LEU:HB3	21:U:516:LEU:HD13	1.88	0.55
16:P:27:ARG:HB2	16:P:183:MET:HB2	1.89	0.55
16:P:35:VAL:HG12	16:P:36:THR:HG23	1.88	0.55
26:Z:263:ALA:HB3	29:c:292:MET:HE3	1.89	0.55
30:d:45:LYS:HA	30:d:48:LEU:HD12	1.88	0.55
31:f:333:LEU:HA	31:f:337:LEU:HB2	1.88	0.55
3:C:83:LYS:HG2	3:C:105:ILE:HD11	1.89	0.55
5:E:213:ARG:NH1	5:E:217:GLU:OE2	2.40	0.55
6:F:410:ARG:NH2	6:F:416:THR:OG1	2.39	0.55
22:V:150:ARG:NH1	22:V:157:THR:O	2.40	0.55
3:C:31:LEU:HD22	4:D:47:LEU:HB3	1.88	0.55
24:X:106:GLU:HB3	24:X:136:LEU:HD21	1.89	0.55
29:c:224:SER:HB3	29:c:227:GLU:HB3	1.89	0.55
8:h:14:SER:HB3	8:h:18:LYS:H	1.72	0.55
1:A:35:THR:O	1:A:39:SER:OG	2.25	0.54
5:E:180:LYS:HG2	5:E:301:ILE:HD12	1.89	0.54
10:J:96:LEU:HD22	17:Q:62:LYS:HD3	1.88	0.54
21:U:791:LEU:HD22	21:U:911:ILE:HD11	1.88	0.54
23:W:221:LYS:HD3	23:W:225:LYS:HD3	1.88	0.54
24:X:194:ARG:HG2	24:X:210:LEU:HD21	1.87	0.54
26:Z:172:VAL:HG13	29:c:217:LEU:HD21	1.90	0.54
15:o:216:ILE:HD11	16:p:194:LYS:HD2	1.90	0.54
31:f:229:VAL:HG21	31:f:607:LEU:HD23	1.89	0.54
3:C:63:LEU:HD12	4:D:79:VAL:HA	1.87	0.54
13:M:8:ASP:O	13:M:22:GLN:NE2	2.40	0.54
24:X:170:GLN:NE2	24:X:173:GLU:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:241:ALA:O	7:g:245:ARG:NH1	2.40	0.54
1:A:39:SER:O	1:A:43:ARG:NH1	2.40	0.54
25:Y:26:LEU:HD21	25:Y:60:SER:HB2	1.88	0.54
31:f:415:GLY:H	31:f:447:ALA:HB1	1.71	0.54
4:D:70:LYS:NZ	26:Z:180:LYS:O	2.40	0.54
21:U:176:MET:HG2	21:U:179:TYR:HE1	1.73	0.54
7:g:155:ASP:OD1	7:g:159:TYR:N	2.39	0.54
31:f:72:ARG:HA	31:f:83:ARG:HH22	1.73	0.54
31:f:664:GLU:OE1	31:f:667:GLY:N	2.37	0.54
8:H:93:LEU:HD13	8:H:113:ARG:HB3	1.90	0.54
8:h:143:ARG:NH1	8:h:144:PRO:O	2.41	0.54
31:f:168:LYS:HG2	31:f:204:ALA:HB2	1.90	0.54
2:B:373:THR:OG1	2:B:412:MET:O	2.25	0.54
25:Y:243:GLY:O	25:Y:247:LEU:HB2	2.08	0.54
27:a:277:LEU:HD11	27:a:311:VAL:HG12	1.90	0.54
18:r:64:ARG:NH1	18:r:67:GLU:OE1	2.40	0.54
21:U:21:GLU:HA	21:U:24:LEU:HG	1.89	0.54
4:D:410:ASP:OD1	4:D:412:GLN:NE2	2.38	0.53
23:W:344:THR:O	23:W:348:GLU:HB2	2.08	0.53
31:f:291:GLN:NE2	31:f:881:GLU:OE2	2.41	0.53
3:C:263:SER:OG	3:C:264:GLY:N	2.41	0.53
23:W:443:THR:HG21	26:Z:204:LYS:HG3	1.90	0.53
21:U:48:LEU:HA	21:U:51:ASP:HB2	1.89	0.53
22:V:450:SER:OG	22:V:451:ILE:N	2.42	0.53
31:f:93:PRO:O	31:f:97:LYS:N	2.39	0.53
6:F:272:PHE:HE1	6:F:283:ILE:HG12	1.73	0.53
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.89	0.53
21:U:883:ARG:NH2	21:U:885:MET:SD	2.82	0.53
22:V:443:ARG:HH21	30:d:181:CYS:HA	1.74	0.53
23:W:220:GLU:HG3	23:W:221:LYS:HG2	1.91	0.53
29:c:273:LYS:O	29:c:277:LYS:NZ	2.42	0.53
11:K:235:GLU:HA	11:K:238:ILE:HG22	1.90	0.53
12:L:176:MET:HE1	13:M:56:LYS:HB3	1.90	0.53
23:W:149:LEU:HB2	23:W:185:PHE:HE2	1.73	0.53
25:Y:247:LEU:HD12	25:Y:250:LEU:HD11	1.91	0.53
26:Z:37:GLY:HA2	26:Z:56:VAL:HG12	1.89	0.53
31:f:15:GLN:O	31:f:19:ALA:N	2.41	0.53
31:f:350:LYS:HG2	31:f:747:GLN:HE21	1.74	0.53
10:J:116:GLN:NE2	11:K:84:ASP:OD1	2.42	0.53
17:Q:137:PHE:HB3	18:r:133:VAL:HG21	1.90	0.53
21:U:701:ILE:HG23	21:U:702:THR:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:215:TRP:HE3	30:d:222:TYR:HB3	1.74	0.53
21:U:82:LEU:O	21:U:129:ARG:NE	2.41	0.53
8:H:109:GLN:OE1	16:P:77:LYS:NZ	2.39	0.53
28:b:100:ARG:NH1	28:b:102:GLY:O	2.42	0.53
31:f:176:ALA:HB3	31:f:178:LYS:HE3	1.91	0.53
11:K:146:VAL:HG11	11:K:222:PRO:HA	1.90	0.53
19:S:125:ASP:OD1	19:S:129:SER:N	2.42	0.53
21:U:100:ILE:HA	21:U:103:LYS:HE2	1.90	0.53
22:V:86:VAL:HG13	22:V:200:ARG:HH22	1.74	0.53
27:a:73:PRO:HG3	27:a:104:VAL:HG11	1.91	0.53
31:f:869:THR:HG22	31:f:882:LEU:HB3	1.91	0.53
22:V:289:LEU:HB3	22:V:312:ALA:HB2	1.90	0.52
22:V:355:ARG:NE	33:e:27:TRP:O	2.41	0.52
26:Z:39:LEU:HD13	26:Z:95:TYR:HB3	1.90	0.52
8:H:166:ASN:OD1	8:H:169:ASN:ND2	2.41	0.52
31:f:648:ALA:HB1	31:f:678:LEU:HD21	1.91	0.52
4:D:393:ILE:HD12	23:W:133:GLU:HB2	1.92	0.52
11:K:91:LYS:HG2	11:K:119:LEU:HD11	1.92	0.52
17:q:26:VAL:HG21	18:r:136:TYR:HE2	1.73	0.52
18:r:182:ASP:OD1	18:r:182:ASP:N	2.42	0.52
7:G:112:ASP:N	7:G:112:ASP:OD1	2.41	0.52
20:T:50:MET:HE2	20:T:192:VAL:HG12	1.90	0.52
23:W:98:LYS:HA	23:W:135:LYS:HZ1	1.74	0.52
19:s:145:LEU:HD22	19:s:178:VAL:HB	1.91	0.52
31:f:257:ARG:HD2	31:f:289:VAL:HG11	1.92	0.52
32:x:46:VAL:HG23	32:x:71:MET:HE1	1.91	0.52
9:I:106:PRO:HB2	9:I:109:GLN:HG3	1.91	0.52
17:Q:26:VAL:HG21	18:R:136:TYR:HE2	1.75	0.52
22:V:119:GLY:HA2	22:V:148:ARG:HD3	1.92	0.52
22:V:265:ASP:OD1	22:V:265:ASP:N	2.41	0.52
22:V:468:SER:HB3	26:Z:247:LYS:HD3	1.90	0.52
31:f:24:THR:HA	31:f:31:LYS:HD3	1.91	0.52
31:f:101:PRO:O	31:f:105:LYS:NZ	2.43	0.52
15:O:198:ARG:HD2	15:O:201:ARG:HH22	1.74	0.52
18:R:166:ARG:NH1	16:p:34:MET:O	2.42	0.52
21:U:619:VAL:HG23	21:U:651:GLY:HA3	1.92	0.52
24:X:414:LEU:HA	24:X:417:LYS:HG2	1.92	0.52
26:Z:222:ILE:HG23	26:Z:226:ILE:HB	1.92	0.52
27:a:269:LEU:HD12	27:a:272:ILE:HD11	1.90	0.52
10:j:211:MET:HG3	10:j:217:LEU:HD12	1.92	0.52
1:A:308:GLY:H	1:A:311:PRO:HG3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:770:TRP:HA	29:c:180:ASN:HB3	1.91	0.52
22:V:443:ARG:NH2	30:d:180:GLY:O	2.43	0.52
5:E:253:ILE:HG13	6:F:308:ARG:HH22	1.74	0.52
15:O:63:LEU:HD11	15:O:79:ALA:HB2	1.91	0.52
18:R:133:VAL:HG21	17:q:137:PHE:HB3	1.92	0.52
20:T:63:LEU:HD21	20:T:106:LEU:HD13	1.92	0.52
21:U:376:MET:HE3	21:U:735:GLY:HA2	1.92	0.52
21:U:483:LEU:HD11	21:U:781:LEU:HD11	1.92	0.52
22:V:225:ASP:OD1	22:V:228:ARG:NH1	2.43	0.52
31:f:199:ASN:HA	31:f:202:HIS:CD2	2.44	0.52
2:B:217:LYS:HD3	2:B:218:PRO:HD2	1.91	0.52
23:W:220:GLU:OE1	23:W:257:GLN:NE2	2.43	0.52
25:Y:85:ASP:OD1	25:Y:107:LYS:NZ	2.40	0.52
27:a:120:ALA:HA	27:a:123:LEU:HD13	1.92	0.52
31:f:245:ASN:HB3	31:f:256:PHE:HB2	1.91	0.52
1:A:307:ASP:OD2	1:A:333:ARG:NH2	2.36	0.51
23:W:169:LEU:O	23:W:173:THR:OG1	2.27	0.51
23:W:366:MET:O	23:W:370:TYR:HB2	2.09	0.51
23:W:275:ILE:HG13	23:W:308:LEU:HD11	1.92	0.51
28:b:51:LEU:HD23	28:b:71:ILE:HG23	1.91	0.51
9:i:174:MET:HE1	9:i:196:VAL:HA	1.92	0.51
17:q:35:MET:HE2	17:q:45:LEU:HD21	1.92	0.51
31:f:654:VAL:O	31:f:658:ALA:CB	2.57	0.51
5:E:140:GLU:OE1	5:E:143:ARG:NH2	2.43	0.51
25:Y:220:VAL:HG21	25:Y:249:VAL:HG21	1.92	0.51
27:a:82:HIS:HD2	27:a:85:ARG:HH12	1.58	0.51
27:a:275:LEU:HD13	27:a:278:MET:HG3	1.92	0.51
10:j:39:ASP:HA	10:j:213:ARG:HH22	1.75	0.51
31:f:585:GLU:HG2	31:f:587:PHE:H	1.75	0.51
29:c:244:VAL:HG12	29:c:248:MET:HE2	1.92	0.51
19:s:27:THR:HB	19:s:40:SER:H	1.76	0.51
19:s:125:ASP:OD1	19:s:129:SER:N	2.44	0.51
31:f:383:ALA:HA	31:f:417:ILE:HA	1.93	0.51
3:C:219:LEU:HD11	4:D:289:LEU:HD22	1.91	0.51
6:F:97:LEU:N	6:F:121:CYS:O	2.43	0.51
21:U:199:ARG:O	21:U:203:LYS:NZ	2.41	0.51
28:b:141:ILE:HG23	28:b:171:VAL:HB	1.93	0.51
4:D:380:GLN:NE2	5:E:165:ILE:O	2.40	0.51
26:Z:107:ALA:HA	26:Z:110:GLU:HG2	1.93	0.51
18:R:38:ASN:HD21	18:R:41:LEU:HD12	1.76	0.51
24:X:221:GLU:O	24:X:223:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:123:ILE:HB	26:Z:136:GLU:HB3	1.93	0.51
27:a:289:ARG:NH1	27:a:334:THR:O	2.44	0.51
16:p:27:ARG:HB2	16:p:183:MET:HB2	1.92	0.51
20:t:122:LEU:HG	20:t:137:LEU:HD12	1.93	0.51
22:V:404:LYS:HD2	22:V:446:VAL:HG21	1.93	0.51
7:g:120:ASP:OD1	8:h:84:ARG:NH1	2.43	0.51
4:D:345:PHE:HB3	4:D:360:LEU:HD23	1.92	0.51
14:N:165:GLU:OE2	20:t:37:ARG:NH1	2.39	0.51
30:d:198:LEU:HD12	30:d:200:PHE:HE1	1.76	0.51
1:A:430:MET:HE3	10:J:12:PRO:HB2	1.92	0.50
3:C:372:ARG:NH1	4:D:179:GLU:OE2	2.44	0.50
17:Q:31:ASP:OD1	17:Q:31:ASP:N	2.42	0.50
23:W:160:LYS:NZ	23:W:161:GLU:OE2	2.44	0.50
23:W:120:ILE:O	23:W:123:ARG:NH1	2.44	0.50
26:Z:124:ILE:HG22	26:Z:135:THR:HA	1.93	0.50
2:B:333:ARG:HD3	2:B:336:THR:HG21	1.92	0.50
28:b:107:MET:HB3	28:b:136:VAL:HG13	1.93	0.50
31:f:206:ASP:OD1	31:f:207:LEU:N	2.43	0.50
32:x:26:PRO:HA	32:x:29:PHE:HB2	1.93	0.50
4:D:274:ARG:N	5:E:245:GLU:OE2	2.42	0.50
17:Q:144:ASP:OD2	18:r:166:ARG:NH2	2.44	0.50
19:S:145:LEU:HD22	19:S:178:VAL:HB	1.93	0.50
21:U:346:ASN:HD22	21:U:347:ASN:H	1.57	0.50
22:V:449:ALA:HB3	22:V:460:SER:HA	1.93	0.50
31:f:479:LEU:HD22	31:f:514:VAL:HG22	1.93	0.50
2:B:387:LYS:HB3	2:B:390:LEU:HD23	1.92	0.50
21:U:710:ARG:HE	21:U:737:LEU:HD23	1.76	0.50
1:A:346:PRO:HB2	1:A:351:ARG:HG2	1.94	0.50
4:D:374:ASP:HB3	5:E:292:PRO:HG2	1.92	0.50
11:K:202:LEU:O	11:K:206:MET:HB2	2.11	0.50
18:R:139:MET:O	18:R:143:TYR:HB2	2.12	0.50
22:V:338:LEU:HD21	22:V:397:ARG:HG3	1.93	0.50
23:W:208:LYS:O	23:W:211:THR:OG1	2.29	0.50
25:Y:34:ASP:O	25:Y:38:ARG:NH1	2.44	0.50
5:E:119:VAL:O	5:E:123:SER:OG	2.28	0.50
11:K:240:ASP:OD1	11:K:241:ILE:N	2.44	0.50
12:L:226:ASP:OD1	12:L:226:ASP:N	2.44	0.50
4:D:45:LYS:HG3	21:U:187:LEU:HD13	1.93	0.50
21:U:636:VAL:HG23	21:U:637:VAL:HG23	1.94	0.50
24:X:377:ILE:HG22	24:X:386:ILE:HB	1.93	0.50
28:b:174:PRO:HD3	28:b:183:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:111:TRP:HE1	29:c:130:GLN:HG2	1.76	0.50
31:f:117:GLU:H	31:f:120:ARG:HH21	1.59	0.50
3:C:57:ARG:NH2	21:U:643:SER:O	2.42	0.50
8:H:222:THR:OG1	8:H:225:GLU:OE1	2.24	0.50
17:Q:37:LYS:O	17:Q:61:GLN:NE2	2.45	0.50
18:R:80:SER:OG	18:R:120:ARG:NH1	2.43	0.50
19:S:27:THR:HB	19:S:40:SER:H	1.77	0.50
22:V:175:MET:HE3	22:V:180:ARG:HE	1.75	0.49
22:V:258:TYR:HE2	22:V:270:LEU:HD12	1.77	0.49
23:W:254:PRO:HG3	23:W:262:LYS:HE3	1.94	0.49
27:a:165:THR:HG22	27:a:166:ILE:H	1.76	0.49
30:d:44:THR:OG1	30:d:47:GLN:NE2	2.44	0.49
8:h:204:THR:OG1	8:h:206:ASP:OD1	2.28	0.49
16:p:35:VAL:HG12	16:p:36:THR:HG23	1.94	0.49
31:f:289:VAL:HA	31:f:292:LYS:HG2	1.94	0.49
25:Y:387:ILE:HG21	26:Z:276:ILE:HD11	1.95	0.49
30:d:212:LYS:HD2	30:d:213:ARG:HG2	1.95	0.49
2:B:275:GLU:OE1	2:B:322:ARG:NH2	2.45	0.49
10:J:196:LEU:HA	10:J:199:VAL:HG12	1.93	0.49
23:W:396:LEU:HD13	23:W:402:ILE:HD13	1.94	0.49
27:a:355:PHE:HA	27:a:358:THR:HG22	1.95	0.49
31:f:457:ASN:ND2	31:f:459:CYS:SG	2.85	0.49
7:G:6:SER:OG	7:G:11:ARG:NH1	2.45	0.49
27:a:197:ALA:HB2	27:a:222:LEU:HD22	1.93	0.49
11:k:52:LYS:NZ	11:k:64:ILE:O	2.46	0.49
31:f:787:LEU:HD23	31:f:791:VAL:HB	1.95	0.49
11:K:41:GLN:NE2	11:K:151:PRO:O	2.45	0.49
21:U:62:LEU:HD12	21:U:84:ALA:HB1	1.94	0.49
28:b:25:ARG:NH2	28:b:145:GLU:OE1	2.45	0.49
7:g:165:ALA:HB1	7:g:179:LEU:HD13	1.94	0.49
31:f:46:SER:OG	31:f:57:GLU:OE2	2.30	0.49
31:f:664:GLU:HB3	31:f:668:ALA:H	1.78	0.49
21:U:542:GLU:OE2	21:U:546:ARG:NH2	2.46	0.49
21:U:900:TYR:HB3	21:U:914:LEU:HG	1.95	0.49
23:W:316:ARG:NH1	23:W:383:ASP:OD1	2.41	0.49
25:Y:13:LYS:HB3	25:Y:212:GLU:HB2	1.93	0.49
17:q:52:ASP:OD1	18:r:88:TYR:OH	2.28	0.49
3:C:325:ARG:HD3	3:C:353:GLY:HA2	1.95	0.49
8:H:106:PRO:HB2	8:H:109:GLN:HG2	1.95	0.49
24:X:70:LEU:HD11	24:X:92:LEU:HB3	1.95	0.49
6:F:141:ASP:OD1	6:F:141:ASP:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:212:PHE:HD1	6:F:217:ILE:HD11	1.78	0.49
22:V:223:LYS:O	22:V:225:ASP:N	2.46	0.49
22:V:428:LEU:HD21	22:V:437:ILE:HG13	1.95	0.49
24:X:214:SER:O	24:X:218:HIS:ND1	2.35	0.49
27:a:50:PHE:HD2	27:a:52:GLN:HB3	1.77	0.49
29:c:157:ILE:HG23	29:c:205:ILE:HD11	1.94	0.49
9:i:161:ALA:HB3	10:j:53:LEU:HD23	1.95	0.49
12:l:172:LEU:O	12:l:176:MET:HB3	2.13	0.49
16:p:67:LEU:HD11	16:p:91:VAL:HG22	1.94	0.49
6:F:318:ASP:O	6:F:347:ARG:NH1	2.46	0.49
21:U:501:LEU:HD11	21:U:548:LEU:HD11	1.95	0.49
10:j:42:VAL:HG22	10:j:210:VAL:HG22	1.93	0.49
31:f:369:ARG:HH22	31:f:741:LEU:HD13	1.78	0.49
31:f:531:ASN:HA	31:f:534:VAL:HG22	1.94	0.49
1:A:287:ASP:OD1	1:A:287:ASP:N	2.44	0.49
3:C:134:LEU:HD11	3:C:212:ILE:HG12	1.95	0.49
21:U:161:ASP:OD1	21:U:161:ASP:N	2.45	0.49
8:h:3:GLU:HG2	8:h:4:ARG:HE	1.77	0.49
17:q:11:ASP:N	17:q:11:ASP:OD1	2.46	0.49
32:x:43:ARG:HH22	32:x:77:ALA:HB2	1.77	0.49
5:E:84:ARG:HG2	29:c:50:PRO:HG3	1.95	0.48
17:Q:83:PHE:O	17:Q:87:ASN:ND2	2.37	0.48
21:U:268:LEU:HB3	21:U:325:MET:HE1	1.95	0.48
21:U:490:ARG:HB2	21:U:493:VAL:HG12	1.94	0.48
15:o:50:ALA:HB2	16:p:129:CYS:HB2	1.95	0.48
17:q:22:ALA:HA	17:q:27:GLN:HA	1.95	0.48
2:B:183:THR:OG1	2:B:184:TYR:N	2.46	0.48
6:F:358:ASN:HD21	13:M:205:LYS:HD2	1.78	0.48
23:W:215:GLN:HG2	23:W:223:LYS:HE2	1.94	0.48
2:B:342:ILE:HG22	2:B:350:LYS:HE3	1.94	0.48
3:C:196:LYS:N	36:C:501:ADP:O1B	2.43	0.48
21:U:323:LEU:HB3	21:U:327:LYS:HE2	1.94	0.48
22:V:76:LYS:HE3	22:V:149:PRO:HB3	1.95	0.48
27:a:84:VAL:HA	27:a:87:MET:HG2	1.95	0.48
31:f:512:MET:HE1	31:f:554:TYR:HB2	1.95	0.48
5:E:205:ASP:OD1	5:E:205:ASP:N	2.45	0.48
19:S:145:LEU:HD21	19:S:182:ALA:HB2	1.95	0.48
22:V:121:PHE:O	22:V:128:ARG:NH1	2.46	0.48
25:Y:53:TYR:CE2	25:Y:70:LEU:HD21	2.48	0.48
7:g:103:TYR:O	15:o:81:ARG:NH2	2.46	0.48
10:j:148:ASP:OD1	10:j:152:THR:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:p:30:ILE:HG22	16:p:31:GLN:H	1.78	0.48
20:t:108:ASN:HB3	20:t:110:MET:HE3	1.94	0.48
21:U:232:ILE:HA	21:U:235:LYS:HD2	1.95	0.48
27:a:284:ARG:NH1	27:a:290:GLN:O	2.46	0.48
30:d:11:ARG:HE	30:d:12:LYS:HG2	1.79	0.48
17:q:31:ASP:OD1	17:q:31:ASP:N	2.46	0.48
31:f:634:LYS:HD3	31:f:673:ARG:HH21	1.77	0.48
16:P:177:ARG:NH2	19:s:150:ASP:OD2	2.37	0.48
23:W:112:VAL:HG12	23:W:123:ARG:HH22	1.78	0.48
27:a:14:SER:HB2	27:a:18:GLN:HG2	1.94	0.48
27:a:54:ASP:HA	27:a:57:ILE:HG22	1.94	0.48
30:d:164:THR:HA	30:d:167:ILE:HG12	1.95	0.48
31:f:456:ARG:HH21	31:f:494:ARG:HH21	1.62	0.48
2:B:77:GLU:OE2	2:B:81:ASN:ND2	2.46	0.48
4:D:355:SER:HB3	4:D:393:ILE:HD13	1.94	0.48
19:S:144:MET:HE1	19:S:185:ARG:HB2	1.94	0.48
22:V:131:LEU:HD13	22:V:171:VAL:HG21	1.96	0.48
29:c:269:GLN:HA	29:c:272:ILE:HG22	1.96	0.48
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.95	0.48
10:j:204:LYS:NZ	10:j:222:PRO:O	2.46	0.48
11:k:221:GLN:HB2	11:k:224:GLN:HG2	1.96	0.48
31:f:637:LYS:HD2	31:f:678:LEU:HD22	1.96	0.48
2:B:221:GLY:HA3	2:B:347:ILE:HA	1.96	0.48
21:U:82:LEU:HD11	21:U:130:LEU:HD13	1.96	0.48
21:U:804:SER:OG	21:U:805:ASN:N	2.47	0.48
30:d:35:PHE:O	30:d:81:TYR:OH	2.29	0.48
10:j:192:ILE:HD12	10:j:206:ILE:HD12	1.96	0.48
21:U:74:PHE:HB3	21:U:103:LYS:HD2	1.95	0.48
21:U:327:LYS:HG2	21:U:333:MET:SD	2.54	0.48
23:W:247:TYR:HA	23:W:250:ILE:HG12	1.95	0.48
30:d:234:ASP:OD1	30:d:234:ASP:N	2.47	0.48
8:h:175:GLU:OE2	9:i:53:HIS:NE2	2.46	0.48
4:D:170:MET:HG2	4:D:173:GLN:HB2	1.96	0.48
17:Q:44:LEU:HD11	17:Q:102:LEU:HD22	1.96	0.48
21:U:583:MET:SD	21:U:605:VAL:HG11	2.54	0.48
22:V:296:LYS:HB3	22:V:301:GLU:HB3	1.94	0.48
1:A:278:ASP:N	1:A:278:ASP:OD1	2.44	0.47
2:B:59:ARG:NH1	31:f:223:GLU:OE2	2.47	0.47
25:Y:42:MET:HA	25:Y:45:VAL:HG22	1.95	0.47
26:Z:263:ALA:HB1	29:c:288:VAL:HG13	1.95	0.47
4:D:309:MET:HG3	4:D:327:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:204:VAL:HG13	13:M:205:LYS:HG3	1.94	0.47
16:P:53:LEU:HB3	16:P:60:VAL:HG22	1.96	0.47
17:Q:11:ASP:N	17:Q:11:ASP:OD1	2.46	0.47
1:A:69:ASP:OD1	1:A:69:ASP:N	2.45	0.47
2:B:145:GLU:HG2	2:B:148:CYS:HB2	1.97	0.47
6:F:153:VAL:HG22	6:F:160:ILE:HG22	1.96	0.47
23:W:401:THR:HG23	23:W:402:ILE:HD12	1.95	0.47
32:x:9:LYS:N	32:x:69:LEU:O	2.43	0.47
3:C:163:GLU:HA	3:C:167:LEU:HD13	1.96	0.47
4:D:80:LYS:O	4:D:83:GLN:NE2	2.48	0.47
4:D:267:ILE:HD12	4:D:267:ILE:H	1.78	0.47
5:E:352:MET:HA	5:E:355:ILE:HG22	1.95	0.47
6:F:178:ASP:N	6:F:178:ASP:OD1	2.48	0.47
6:F:289:ASP:OD1	6:F:289:ASP:N	2.47	0.47
10:J:50:VAL:HB	10:J:54:GLN:HB2	1.95	0.47
21:U:691:SER:HA	21:U:694:ILE:HG22	1.96	0.47
21:U:770:TRP:O	29:c:179:SER:OG	2.31	0.47
27:a:119:GLY:HA3	27:a:158:LEU:HD11	1.96	0.47
30:d:70:SER:HA	30:d:73:ARG:HH21	1.79	0.47
19:s:52:ILE:HG13	19:s:110:ILE:HG12	1.97	0.47
7:G:67:THR:HG22	7:G:69:LEU:H	1.79	0.47
26:Z:202:ASN:ND2	26:Z:206:LEU:HD13	2.30	0.47
31:f:178:LYS:HA	31:f:181:ARG:HB2	1.95	0.47
1:A:171:ASP:OD1	1:A:171:ASP:N	2.41	0.47
9:I:119:GLN:NE2	10:J:79:ASP:OD1	2.43	0.47
13:M:152:ASP:OD2	13:M:154:SER:OG	2.32	0.47
14:N:166:ARG:NH2	14:n:140:ASP:OD2	2.43	0.47
21:U:879:ASP:OD1	21:U:879:ASP:N	2.46	0.47
23:W:235:GLN:O	23:W:235:GLN:NE2	2.47	0.47
25:Y:385:ARG:HA	25:Y:385:ARG:HD3	1.77	0.47
26:Z:62:ASP:N	26:Z:62:ASP:OD1	2.45	0.47
7:g:180:GLU:HG2	8:h:55:ILE:HG22	1.96	0.47
2:B:153:ASN:HD22	2:B:156:VAL:HG22	1.79	0.47
4:D:391:ARG:HG2	4:D:393:ILE:H	1.79	0.47
7:G:188:ASP:OD1	7:G:188:ASP:N	2.46	0.47
9:I:38:LEU:HD23	9:I:160:LYS:HG2	1.96	0.47
12:L:41:LYS:HG2	12:L:180:MET:HE3	1.96	0.47
16:P:189:ILE:HB	16:P:196:THR:HB	1.96	0.47
18:R:55:TRP:HB2	18:R:97:MET:HE1	1.96	0.47
21:U:756:HIS:HB3	21:U:759:SER:HB3	1.97	0.47
26:Z:70:LEU:HD11	26:Z:108:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:131:LEU:HD22	28:b:136:VAL:HB	1.97	0.47
9:i:234:GLU:HA	9:i:237:ILE:HG12	1.95	0.47
15:o:201:ARG:HB3	15:o:203:ARG:HH22	1.78	0.47
31:f:486:GLY:HA2	31:f:525:ILE:HD11	1.95	0.47
5:E:119:VAL:HA	5:E:122:MET:HG2	1.97	0.47
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.97	0.47
30:d:178:ILE:HG21	30:d:198:LEU:HD21	1.96	0.47
13:m:8:ASP:O	13:m:22:GLN:NE2	2.48	0.47
31:f:507:ASP:OD2	31:f:509:LYS:NZ	2.48	0.47
32:x:20:LEU:HD12	32:x:29:PHE:HE1	1.78	0.47
3:C:80:MET:HE1	3:C:96:VAL:HG13	1.96	0.47
3:C:295:THR:OG1	3:C:296:ASN:N	2.48	0.47
10:J:66:ASP:HA	17:Q:69:MET:HE3	1.96	0.47
21:U:666:LYS:HA	21:U:669:ILE:HD12	1.96	0.47
22:V:480:ILE:HD11	26:Z:261:TYR:HA	1.96	0.47
27:a:224:SER:HA	27:a:227:ASN:HB2	1.97	0.47
28:b:151:GLU:OE1	28:b:152:LYS:NZ	2.35	0.47
10:j:185:ASP:OD1	10:j:185:ASP:N	2.48	0.47
24:X:393:VAL:HB	25:Y:362:LYS:HD3	1.97	0.47
25:Y:34:ASP:OD1	25:Y:35:ALA:N	2.47	0.47
10:j:36:ARG:HH21	10:j:157:LYS:HG2	1.78	0.47
1:A:190:VAL:HG21	1:A:339:ARG:HG3	1.97	0.46
5:E:200:SER:O	5:E:200:SER:OG	2.32	0.46
23:W:123:ARG:HA	23:W:126:ASP:HB2	1.96	0.46
23:W:216:GLU:OE1	23:W:223:LYS:NZ	2.38	0.46
23:W:328:LEU:HD11	23:W:351:TRP:HZ2	1.80	0.46
27:a:205:LEU:HG	27:a:268:LEU:HD11	1.96	0.46
29:c:303:MET:HE1	30:d:242:LEU:HB2	1.96	0.46
10:j:135:GLY:HA2	10:j:211:MET:HE1	1.96	0.46
31:f:597:VAL:HG11	31:f:635:LYS:HB3	1.97	0.46
2:B:378:VAL:HG12	2:B:416:ASN:HA	1.96	0.46
5:E:171:LEU:HD21	5:E:298:LYS:HG2	1.96	0.46
14:N:30:VAL:HG11	20:t:211:ILE:HG23	1.96	0.46
29:c:265:MET:SD	29:c:265:MET:N	2.87	0.46
30:d:6:LYS:HA	30:d:6:LYS:HD3	1.78	0.46
18:r:83:LEU:HA	18:r:86:MET:HE2	1.97	0.46
31:f:229:VAL:HG11	31:f:607:LEU:HB2	1.97	0.46
31:f:261:ARG:HG3	31:f:267:ARG:HH12	1.80	0.46
4:D:122:GLU:OE2	29:c:282:ARG:NH2	2.44	0.46
4:D:267:ILE:HG12	4:D:309:MET:HE2	1.97	0.46
11:K:167:ALA:HB3	12:L:56:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:65:ASP:OD1	26:Z:65:ASP:N	2.46	0.46
29:c:245:VAL:HA	29:c:248:MET:HE3	1.96	0.46
8:h:9:SER:HA	8:h:125:GLY:HA2	1.96	0.46
9:i:21:VAL:O	9:i:25:MET:HG2	2.16	0.46
6:F:141:ASP:OD1	6:F:144:LYS:NZ	2.40	0.46
23:W:272:LEU:HD21	23:W:301:LYS:HE3	1.97	0.46
25:Y:376:LEU:HD22	26:Z:265:LEU:HD21	1.96	0.46
28:b:12:ASN:OD1	28:b:53:THR:OG1	2.32	0.46
31:f:827:PRO:HG2	31:f:848:GLN:HB3	1.95	0.46
16:P:136:PHE:HZ	16:P:151:GLU:HG2	1.79	0.46
24:X:281:GLY:H	24:X:284:THR:HG22	1.81	0.46
12:l:80:ASP:OD2	12:l:126:ARG:NH1	2.46	0.46
1:A:399:ALA:O	1:A:400:ARG:NE	2.45	0.46
12:L:104:PRO:HB2	12:L:107:ARG:HG3	1.96	0.46
18:R:44:THR:HG1	18:R:100:MET:H	1.63	0.46
30:d:58:GLY:HA2	30:d:61:TRP:CD1	2.51	0.46
9:i:178:ASP:OD2	9:i:195:LYS:NZ	2.43	0.46
31:f:298:LEU:HA	31:f:301:HIS:CE1	2.51	0.46
15:O:97:ALA:HB1	15:O:127:MET:HE2	1.96	0.46
27:a:252:LYS:HA	27:a:255:TRP:CE2	2.51	0.46
31:f:180:GLN:HA	31:f:216:MET:HE1	1.97	0.46
1:A:213:LEU:HB3	1:A:337:LEU:HD13	1.98	0.46
1:A:262:GLU:OE2	1:A:265:ARG:NH1	2.49	0.46
25:Y:207:THR:O	25:Y:207:THR:OG1	2.33	0.46
31:f:608:LYS:HB3	31:f:639:LYS:HZ2	1.80	0.46
2:B:168:ASP:OD1	2:B:168:ASP:N	2.43	0.46
4:D:152:MET:HB3	4:D:154:LEU:HD23	1.98	0.46
4:D:274:ARG:NE	5:E:245:GLU:O	2.49	0.46
16:P:14:MET:HE2	16:P:167:ILE:HB	1.98	0.46
27:a:81:LEU:HA	27:a:84:VAL:HG12	1.96	0.46
27:a:322:GLY:HA3	27:a:333:MET:HE2	1.98	0.46
31:f:281:ILE:HB	31:f:284:SER:HB2	1.98	0.46
31:f:680:ARG:HA	31:f:715:HIS:HA	1.97	0.46
5:E:331:ILE:HG23	5:E:371:VAL:HG21	1.97	0.46
17:Q:185:LYS:NZ	17:Q:186:ASN:OD1	2.49	0.46
18:R:192:VAL:HG11	16:p:205:ASP:HB3	1.97	0.46
21:U:376:MET:HE1	21:U:738:ASP:HB2	1.98	0.46
26:Z:9:VAL:HG12	26:Z:48:LEU:HB3	1.98	0.46
8:h:106:PRO:HB2	8:h:109:GLN:HG2	1.98	0.46
31:f:54:ASP:H	31:f:96:LEU:HD21	1.80	0.46
21:U:742:HIS:O	21:U:883:ARG:NE	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:445:LEU:HD13	26:Z:229:GLN:HE22	1.80	0.45
26:Z:176:LEU:HD22	29:c:218:LEU:HD12	1.98	0.45
26:Z:262:LEU:O	26:Z:266:ILE:HG12	2.16	0.45
31:f:560:LEU:HD11	31:f:782:HIS:CE1	2.50	0.45
31:f:603:SER:H	31:f:639:LYS:HA	1.81	0.45
4:D:171:ASP:OD1	4:D:171:ASP:N	2.46	0.45
10:J:39:ASP:OD1	10:J:39:ASP:N	2.48	0.45
23:W:300:PRO:HA	23:W:303:LYS:HE2	1.98	0.45
23:W:325:GLY:O	23:W:329:ARG:NH1	2.49	0.45
24:X:255:LEU:HD12	24:X:287:LEU:HD13	1.97	0.45
26:Z:77:ASN:HB2	29:c:98:MET:HE1	1.99	0.45
15:o:163:ILE:HG12	15:o:170:GLY:HA2	1.98	0.45
16:p:159:ASP:OD1	16:p:159:ASP:N	2.45	0.45
31:f:267:ARG:HB3	31:f:272:LEU:HD12	1.98	0.45
3:C:72:TYR:N	3:C:116:LEU:O	2.47	0.45
21:U:510:GLU:HA	21:U:547:GLY:HA3	1.98	0.45
23:W:112:VAL:HG12	23:W:123:ARG:NH2	2.31	0.45
2:B:125:THR:OG1	2:B:126:SER:N	2.50	0.45
3:C:258:ARG:HB2	3:C:264:GLY:HA3	1.96	0.45
9:I:140:ASP:OD1	9:I:146:GLN:NE2	2.49	0.45
10:J:119:THR:HG22	10:J:126:PRO:HB3	1.98	0.45
17:Q:30:ASP:N	17:Q:30:ASP:OD1	2.50	0.45
21:U:266:GLN:HA	21:U:269:ARG:HG2	1.98	0.45
21:U:536:ALA:HB2	21:U:548:LEU:HD22	1.99	0.45
21:U:744:VAL:HA	21:U:785:PRO:HA	1.99	0.45
23:W:314:LEU:HD22	23:W:365:ILE:HD12	1.98	0.45
27:a:197:ALA:HB1	27:a:226:ARG:HE	1.81	0.45
27:a:352:ARG:HA	27:a:355:PHE:CE2	2.52	0.45
12:l:227:ASP:OD1	12:l:227:ASP:N	2.47	0.45
31:f:616:CYS:HB3	31:f:632:LYS:HE2	1.98	0.45
10:J:90:GLU:HG3	10:J:110:TYR:CZ	2.51	0.45
21:U:367:THR:HA	21:U:370:VAL:HG22	1.98	0.45
21:U:466:LYS:HD3	21:U:466:LYS:HA	1.78	0.45
23:W:153:LYS:NZ	23:W:188:GLU:OE2	2.39	0.45
24:X:82:LYS:HB3	24:X:122:ARG:HH22	1.81	0.45
25:Y:259:TYR:HH	25:Y:295:TYR:HH	1.63	0.45
26:Z:251:LEU:HG	26:Z:252:LYS:HE2	1.98	0.45
27:a:70:ARG:HD2	27:a:70:ARG:HA	1.75	0.45
27:a:106:SER:OG	27:a:107:SER:N	2.50	0.45
31:f:474:SER:HB3	31:f:477:MET:HE3	1.98	0.45
31:f:605:ASN:HD21	31:f:608:LYS:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:49:ARG:NH2	9:I:63:GLU:OE2	2.50	0.45
12:L:47:VAL:HG12	12:L:195:LEU:HD22	1.98	0.45
23:W:417:ARG:HE	23:W:418:PRO:HD2	1.81	0.45
28:b:181:ASP:OD1	28:b:182:ALA:N	2.49	0.45
29:c:41:MET:HE2	29:c:72:VAL:HG21	1.98	0.45
30:d:11:ARG:HE	30:d:12:LYS:H	1.65	0.45
31:f:110:TYR:OH	31:f:118:ASN:ND2	2.40	0.45
33:e:40:GLU:OE1	33:e:40:GLU:N	2.50	0.45
1:A:185:GLU:OE1	1:A:188:ARG:NH2	2.50	0.45
3:C:230:MET:HE2	3:C:230:MET:HB3	1.88	0.45
4:D:56:VAL:HA	21:U:600:ARG:HE	1.82	0.45
6:F:314:LEU:HD21	6:F:342:LEU:HB3	1.99	0.45
23:W:116:THR:OG1	23:W:117:ASP:N	2.50	0.45
28:b:3:LEU:O	28:b:106:LYS:N	2.47	0.45
28:b:124:LEU:HD13	28:b:156:PHE:HB2	1.99	0.45
30:d:58:GLY:O	30:d:62:SER:OG	2.28	0.45
31:f:387:GLN:NE2	31:f:388:ASP:OD1	2.49	0.45
1:A:347:ASP:OD1	1:A:347:ASP:N	2.47	0.45
13:M:8:ASP:OD1	13:M:8:ASP:N	2.49	0.45
25:Y:145:LEU:HD21	25:Y:161:THR:HG23	1.98	0.45
14:n:84:LYS:NZ	14:n:85:GLU:OE2	2.47	0.45
19:s:166:LEU:HD21	19:s:171:ALA:HB2	1.98	0.45
31:f:559:PRO:HB2	31:f:594:LEU:HD22	1.97	0.45
20:T:110:MET:HE2	20:T:110:MET:HB2	1.89	0.45
15:o:40:ASN:OD1	15:o:40:ASN:N	2.50	0.45
17:q:68:LYS:HG3	17:q:74:GLU:HG2	1.97	0.45
21:U:261:LEU:HA	21:U:264:VAL:HG12	1.99	0.45
27:a:227:ASN:O	27:a:231:GLN:NE2	2.42	0.45
30:d:39:THR:O	30:d:86:LYS:NZ	2.46	0.45
21:U:169:GLU:HG3	21:U:171:ASN:H	1.81	0.44
22:V:325:LYS:HA	22:V:328:VAL:HG12	1.98	0.44
8:h:119:GLN:HA	8:h:122:THR:HG22	1.99	0.44
31:f:833:PHE:HE1	31:f:842:VAL:HB	1.81	0.44
21:U:46:GLU:HA	21:U:49:TYR:HB3	1.99	0.44
21:U:408:LEU:HD23	21:U:423:MET:HE1	1.99	0.44
23:W:170:GLN:HG3	23:W:171:VAL:HG23	1.99	0.44
23:W:177:MET:SD	23:W:178:GLU:N	2.84	0.44
23:W:273:TYR:HB2	23:W:276:LEU:HB2	1.99	0.44
25:Y:275:LEU:HD21	25:Y:296:VAL:HG13	1.99	0.44
26:Z:134:PRO:HD2	29:c:220:LEU:HD21	2.00	0.44
4:D:407:ILE:HG13	4:D:408:LYS:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:182:LEU:HD22	34:E:501:ATP:H2'	1.98	0.44
6:F:78:GLU:HA	6:F:81:LYS:HE2	1.98	0.44
9:I:68:LEU:HD11	9:I:74:CYS:HB3	2.00	0.44
20:T:126:ASP:OD1	20:T:130:VAL:N	2.50	0.44
26:Z:243:GLN:HG3	26:Z:244:GLU:H	1.83	0.44
27:a:28:LEU:HG	27:a:33:LEU:HD11	1.99	0.44
28:b:6:THR:HB	28:b:49:VAL:HG22	1.99	0.44
28:b:8:VAL:HA	28:b:110:ILE:HG13	1.98	0.44
31:f:38:ASP:O	31:f:42:GLU:HB2	2.17	0.44
31:f:209:MET:HE2	31:f:211:ILE:HG12	1.99	0.44
31:f:380:PHE:HB3	31:f:752:HIS:CE1	2.52	0.44
31:f:761:MET:HE3	31:f:761:MET:HB2	1.89	0.44
21:U:324:LYS:HA	21:U:327:LYS:HB2	1.99	0.44
21:U:620:GLU:HG2	21:U:654:MET:HB3	1.99	0.44
22:V:131:LEU:HD22	22:V:171:VAL:HG11	1.98	0.44
27:a:342:ASP:OD1	27:a:343:LEU:N	2.46	0.44
14:n:192:ASP:OD1	14:n:192:ASP:N	2.50	0.44
15:o:97:ALA:HB1	15:o:127:MET:HE2	1.99	0.44
31:f:80:ARG:O	31:f:80:ARG:NH1	2.38	0.44
32:x:33:LEU:O	32:x:37:THR:OG1	2.32	0.44
3:C:89:VAL:HG12	3:C:91:PRO:HD2	1.98	0.44
8:H:4:ARG:HD2	8:H:4:ARG:HA	1.86	0.44
22:V:147:PHE:O	22:V:148:ARG:NH1	2.49	0.44
24:X:377:ILE:HD13	25:Y:358:ARG:HH22	1.81	0.44
31:f:75:LEU:HD12	31:f:77:GLU:H	1.82	0.44
31:f:160:ARG:HG3	31:f:189:LYS:HZ1	1.83	0.44
31:f:860:LYS:HD3	31:f:860:LYS:HA	1.77	0.44
7:G:78:CYS:HB3	7:G:140:LEU:HD23	1.99	0.44
16:P:159:ASP:OD1	16:P:159:ASP:N	2.50	0.44
20:T:166:ARG:NH2	20:T:200:GLU:OE2	2.48	0.44
21:U:570:LEU:HD22	21:U:578:LEU:HG	1.99	0.44
21:U:697:GLN:NE2	21:U:744:VAL:O	2.50	0.44
27:a:270:ARG:HD2	27:a:270:ARG:HA	1.81	0.44
7:g:58:ASP:OD1	7:g:58:ASP:N	2.50	0.44
31:f:250:ARG:HH11	31:f:252:ALA:HB3	1.81	0.44
31:f:404:ASP:OD1	31:f:404:ASP:N	2.48	0.44
1:A:41:TYR:HE2	31:f:184:LEU:HD23	1.82	0.44
8:H:55:ILE:HD12	8:H:55:ILE:H	1.82	0.44
22:V:121:PHE:HB3	22:V:128:ARG:HD2	1.99	0.44
31:f:45:LEU:HD23	31:f:56:LEU:HB2	2.00	0.44
31:f:224:ASN:HA	31:f:227:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:346:ASP:HA	31:f:349:TYR:CZ	2.53	0.44
31:f:445:LEU:HD23	31:f:481:SER:HB2	1.98	0.44
1:A:362:MET:HG3	1:A:364:VAL:HG13	1.99	0.44
5:E:322:LYS:HD3	5:E:326:ILE:HG13	1.98	0.44
29:c:25:VAL:HG23	29:c:175:ARG:HA	2.00	0.44
29:c:37:ALA:O	29:c:41:MET:HG2	2.18	0.44
30:d:175:ARG:HH22	30:d:199:PHE:HB2	1.83	0.44
1:A:140:VAL:HG12	1:A:152:PRO:HA	2.00	0.44
1:A:206:ILE:HG22	6:F:373:MET:HE2	1.99	0.44
6:F:231:THR:HG1	6:F:233:LYS:NZ	2.15	0.44
21:U:474:ARG:NH2	21:U:500:ASN:OD1	2.45	0.44
21:U:560:MET:HE2	21:U:560:MET:HB3	1.79	0.44
24:X:143:TYR:HD1	24:X:180:LEU:HD22	1.83	0.44
24:X:317:PRO:O	24:X:321:THR:OG1	2.36	0.44
25:Y:105:MET:HE1	25:Y:140:ILE:HD11	1.99	0.44
27:a:293:PHE:HE1	27:a:331:VAL:HG13	1.82	0.44
10:j:2:SER:OG	10:j:3:TYR:N	2.51	0.44
14:n:166:ARG:HA	14:n:166:ARG:HD3	1.83	0.44
16:p:14:MET:HE3	16:p:154:TRP:HD1	1.82	0.44
18:r:38:ASN:OD1	18:r:41:LEU:N	2.51	0.44
1:A:44:GLN:OE1	1:A:47:GLN:NE2	2.43	0.43
3:C:19:GLY:HA2	3:C:22:GLN:HE21	1.83	0.43
4:D:266:GLU:HG3	5:E:258:MET:HB3	2.00	0.43
6:F:338:LEU:HD13	6:F:342:LEU:HD11	2.00	0.43
10:J:148:ASP:OD1	10:J:152:THR:N	2.44	0.43
21:U:839:ALA:HA	21:U:842:LYS:HE3	1.99	0.43
23:W:137:TYR:O	23:W:141:GLU:HG2	2.18	0.43
26:Z:190:ARG:HH12	29:c:297:VAL:HA	1.83	0.43
27:a:135:ILE:HD13	27:a:158:LEU:HD22	1.99	0.43
28:b:89:GLY:HA2	28:b:92:VAL:HG12	2.00	0.43
32:x:53:LEU:HD12	32:x:57:ASP:HB3	1.99	0.43
4:D:228:ILE:HB	4:D:262:ILE:HD13	1.99	0.43
22:V:122:THR:HG21	22:V:155:ALA:HB1	2.00	0.43
23:W:307:LYS:NZ	23:W:315:MET:SD	2.91	0.43
24:X:409:LYS:HE3	29:c:256:ASN:HD21	1.82	0.43
31:f:496:ASP:OD1	31:f:496:ASP:N	2.51	0.43
31:f:620:PHE:HD2	31:f:629:LYS:HB3	1.83	0.43
31:f:680:ARG:HH22	31:f:762:VAL:HG22	1.83	0.43
31:f:766:GLN:HG2	31:f:768:LEU:H	1.83	0.43
1:A:143:ASP:OD1	1:A:143:ASP:N	2.51	0.43
2:B:59:ARG:H	31:f:184:LEU:HD21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:167:ILE:HG21	4:D:170:MET:HE2	2.00	0.43
10:J:61:LYS:HB3	10:J:61:LYS:HE2	1.85	0.43
23:W:340:VAL:HG13	23:W:350:ARG:HD2	2.00	0.43
27:a:302:ILE:HD12	27:a:302:ILE:HA	1.91	0.43
30:d:67:ASP:OD1	30:d:67:ASP:N	2.51	0.43
15:o:104:ASP:OD1	15:o:104:ASP:N	2.50	0.43
1:A:74:PRO:HG2	1:A:77:LEU:HD13	2.00	0.43
2:B:417:GLU:HA	2:B:420:LYS:HB2	2.00	0.43
23:W:144:ARG:HA	23:W:147:LYS:HG2	2.00	0.43
23:W:243:ILE:HG13	23:W:273:TYR:HE2	1.82	0.43
24:X:120:GLU:OE2	24:X:122:ARG:NH2	2.51	0.43
25:Y:53:TYR:OH	25:Y:66:ASP:OD2	2.37	0.43
26:Z:193:ASN:OD1	26:Z:194:GLN:NE2	2.36	0.43
28:b:157:VAL:HG21	28:b:170:LEU:HD13	2.00	0.43
30:d:131:VAL:HA	30:d:134:LYS:HB3	2.01	0.43
7:g:165:ALA:HB3	8:h:56:LEU:HD22	1.99	0.43
14:n:14:LEU:HD21	14:n:101:ALA:HB3	2.00	0.43
19:s:10:GLY:HA3	19:s:42:LYS:HE2	2.01	0.43
31:f:378:ASN:OD1	31:f:382:ASN:ND2	2.52	0.43
7:G:46:ASP:OD1	7:G:46:ASP:N	2.51	0.43
31:f:209:MET:HE3	31:f:210:GLU:N	2.32	0.43
31:f:834:ASP:OD1	31:f:834:ASP:N	2.51	0.43
4:D:274:ARG:H	5:E:245:GLU:CD	2.26	0.43
4:D:410:ASP:HB2	7:G:173:THR:HG21	2.00	0.43
5:E:333:LYS:HE3	7:G:57:PRO:HA	2.01	0.43
9:I:197:LEU:HA	9:I:200:THR:HG22	1.99	0.43
21:U:177:LEU:HD11	21:U:204:ILE:HG21	2.00	0.43
23:W:409:LEU:HD21	24:X:344:ARG:HE	1.84	0.43
25:Y:141:VAL:HG11	25:Y:164:ALA:HB2	2.00	0.43
26:Z:94:TRP:HB3	26:Z:112:MET:HE3	2.00	0.43
30:d:5:LEU:HD13	30:d:54:ILE:HG12	2.00	0.43
30:d:155:LYS:HE3	30:d:155:LYS:HB2	1.83	0.43
7:g:188:ASP:OD1	7:g:188:ASP:N	2.48	0.43
17:q:53:THR:HG22	17:q:100:VAL:HG12	2.01	0.43
3:C:44:ARG:HE	22:V:495:ARG:HB2	1.83	0.43
8:H:213:CYS:HB2	8:H:218:PHE:HD1	1.83	0.43
12:L:35:THR:HG23	12:L:133:LEU:HD12	2.00	0.43
13:M:230:ASP:N	13:M:230:ASP:OD1	2.51	0.43
21:U:615:ARG:O	21:U:619:VAL:HG22	2.18	0.43
26:Z:187:LEU:HB2	27:a:374:ILE:HG21	2.00	0.43
27:a:163:TYR:HB3	27:a:172:TYR:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:16:ALA:HB2	19:s:121:VAL:HG23	2.01	0.43
31:f:430:ASP:HA	31:f:433:LEU:HB3	2.00	0.43
31:f:523:GLY:HA3	31:f:561:GLY:HA2	2.01	0.43
31:f:725:SER:HB3	31:f:754:LYS:HE3	2.00	0.43
5:E:116:ASP:O	5:E:118:LEU:N	2.52	0.43
8:H:177:ARG:NH1	24:X:161:ASP:O	2.52	0.43
15:O:164:PHE:O	19:s:38:ARG:NH2	2.51	0.43
21:U:764:LEU:O	21:U:767:THR:OG1	2.35	0.43
25:Y:41:LEU:HD13	25:Y:63:TRP:HZ3	1.84	0.43
29:c:154:LYS:HA	29:c:154:LYS:HD3	1.79	0.43
10:j:31:THR:OG1	10:j:163:ARG:O	2.34	0.43
32:x:41:PRO:HA	32:x:44:GLN:HB2	2.01	0.43
9:I:9:THR:HB	9:I:20:GLN:HG3	1.99	0.43
20:T:211:ILE:HG13	14:n:30:VAL:HG11	2.01	0.43
27:a:82:HIS:CD2	27:a:85:ARG:HH12	2.37	0.43
9:i:118:LYS:NZ	9:i:150:SER:OG	2.52	0.43
10:j:39:ASP:OD1	10:j:39:ASP:N	2.52	0.43
31:f:347:ASP:HA	31:f:350:LYS:HB2	2.00	0.43
5:E:264:MET:HE2	5:E:294:ARG:HB3	2.01	0.43
25:Y:144:LEU:HB3	25:Y:160:ASN:HD22	1.84	0.43
9:i:6:ASP:HB3	9:i:8:ARG:HD2	2.00	0.43
11:k:236:GLU:HA	11:k:239:LYS:HE3	2.01	0.43
31:f:347:ASP:N	31:f:347:ASP:OD1	2.52	0.43
31:f:479:LEU:HD13	31:f:514:VAL:HG13	2.00	0.43
31:f:814:SER:HA	31:f:820:GLY:HA2	2.01	0.43
2:B:59:ARG:HA	2:B:62:LEU:HB3	2.01	0.42
2:B:388:ASP:OD1	2:B:388:ASP:N	2.50	0.42
4:D:296:MET:HE3	4:D:326:ARG:HB3	2.01	0.42
13:M:215:TRP:CE3	13:M:227:VAL:HG22	2.54	0.42
22:V:232:HIS:CE1	22:V:254:LEU:HD11	2.54	0.42
23:W:109:CYS:HA	23:W:112:VAL:HG22	2.01	0.42
26:Z:70:LEU:HD12	26:Z:111:LEU:HB3	2.01	0.42
27:a:70:ARG:HE	28:b:17:ARG:HD2	1.84	0.42
30:d:248:GLU:OE1	30:d:251:ARG:NH1	2.52	0.42
17:q:30:ASP:OD1	17:q:30:ASP:N	2.49	0.42
6:F:97:LEU:HB2	6:F:121:CYS:HB2	2.00	0.42
12:L:122:ARG:HB2	12:L:125:ARG:HG3	2.01	0.42
13:M:15:SER:OG	13:M:17:ASP:OD1	2.26	0.42
24:X:394:ASP:OD1	24:X:394:ASP:N	2.50	0.42
26:Z:187:LEU:HD23	30:d:254:GLU:HB3	2.00	0.42
30:d:42:LYS:HE2	30:d:87:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:132:THR:OG1	23:W:133:GLU:N	2.51	0.42
25:Y:124:PHE:HA	25:Y:127:THR:HG22	2.01	0.42
25:Y:262:SER:OG	25:Y:267:ARG:O	2.37	0.42
27:a:277:LEU:HD23	27:a:280:MET:HE3	2.01	0.42
28:b:119:ASP:OD1	28:b:120:ASN:N	2.52	0.42
29:c:255:TYR:O	29:c:259:VAL:HG23	2.19	0.42
23:W:152:ILE:HG13	23:W:165:ILE:HD12	2.01	0.42
23:W:215:GLN:HE21	23:W:223:LYS:HG3	1.85	0.42
27:a:255:TRP:O	27:a:258:GLN:NE2	2.53	0.42
29:c:209:LYS:HE2	29:c:209:LYS:HB2	1.95	0.42
16:p:149:MET:HE2	16:p:173:ASN:HB2	2.01	0.42
15:O:163:ILE:HG12	15:O:170:GLY:HA2	2.02	0.42
16:P:58:THR:O	17:Q:85:ARG:NH2	2.53	0.42
19:S:172:MET:HE3	19:S:172:MET:HB3	1.91	0.42
20:T:96:MET:HE3	20:T:127:MET:HA	2.02	0.42
21:U:898:CYS:SG	21:U:899:ARG:N	2.92	0.42
23:W:108:CYS:O	23:W:112:VAL:HG13	2.19	0.42
23:W:206:SER:OG	23:W:230:MET:SD	2.77	0.42
23:W:359:VAL:HG23	23:W:382:LEU:HD22	2.01	0.42
24:X:415:TYR:HE1	25:Y:383:LEU:HB2	1.84	0.42
31:f:294:MET:SD	31:f:807:ARG:NH1	2.93	0.42
3:C:92:GLU:HG2	3:C:93:GLY:H	1.84	0.42
4:D:133:HIS:HB3	4:D:137:ASN:H	1.85	0.42
5:E:55:GLN:N	6:F:133:PHE:O	2.53	0.42
6:F:223:VAL:HG12	6:F:350:ARG:HB2	2.01	0.42
11:K:78:MET:HE2	11:K:78:MET:HB3	1.82	0.42
23:W:206:SER:HA	23:W:209:ILE:HG12	2.00	0.42
25:Y:228:MET:HE1	25:Y:259:TYR:CZ	2.55	0.42
8:h:65:VAL:O	8:h:220:ARG:NH1	2.45	0.42
17:q:38:MET:HG2	17:q:44:LEU:HB2	2.02	0.42
31:f:322:SER:OG	31:f:455:VAL:O	2.36	0.42
4:D:284:GLU:O	4:D:288:ILE:HG12	2.20	0.42
6:F:342:LEU:HA	6:F:347:ARG:HD2	2.00	0.42
12:L:44:ALA:HB2	12:L:142:PRO:HB3	2.02	0.42
21:U:33:ASP:OD1	21:U:33:ASP:N	2.50	0.42
21:U:616:ARG:HG3	21:U:647:HIS:HB3	2.01	0.42
16:p:7:ASN:ND2	16:p:29:GLY:O	2.52	0.42
20:t:25:ASP:OD1	20:t:41:ARG:NH2	2.38	0.42
31:f:250:ARG:HH21	31:f:874:LEU:HD12	1.84	0.42
31:f:718:ASP:OD1	31:f:755:ASP:HB3	2.20	0.42
6:F:228:PRO:O	6:F:233:LYS:NZ	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:157:ILE:HG23	29:c:158:ASP:H	1.84	0.42
30:d:175:ARG:HD3	30:d:198:LEU:HD13	2.02	0.42
8:h:52:GLN:HB3	8:h:57:TYR:HD2	1.84	0.42
10:j:98:VAL:HG12	10:j:100:ASP:HB2	2.01	0.42
13:m:43:ASP:OD1	13:m:43:ASP:N	2.51	0.42
15:o:63:LEU:HD11	15:o:79:ALA:HB2	2.01	0.42
31:f:19:ALA:O	31:f:23:GLY:N	2.53	0.42
31:f:25:ASP:OD1	31:f:25:ASP:N	2.51	0.42
31:f:305:LEU:O	31:f:308:SER:OG	2.37	0.42
31:f:540:GLN:HA	31:f:543:MET:HG3	2.02	0.42
31:f:779:CYS:HA	31:f:782:HIS:CE1	2.54	0.42
3:C:344:LEU:HA	3:C:347:ILE:HD12	2.02	0.42
4:D:358:VAL:HG11	4:D:399:PHE:HE2	1.85	0.42
5:E:56:ILE:HB	5:E:100:LEU:HB2	2.02	0.42
15:O:48:THR:HB	15:O:51:ASP:HB2	2.02	0.42
20:T:122:LEU:HG	20:T:137:LEU:HD12	2.02	0.42
21:U:710:ARG:NH2	21:U:738:ASP:OD1	2.51	0.42
25:Y:224:VAL:HG21	25:Y:260:LEU:HD12	2.01	0.42
28:b:109:ILE:HD12	28:b:138:VAL:HG22	2.01	0.42
10:j:116:GLN:NE2	11:k:84:ASP:OD1	2.53	0.42
31:f:584:SER:HB2	31:f:588:ARG:HB3	2.01	0.42
1:A:73:ALA:HA	2:B:140:ASP:HB3	2.01	0.42
1:A:312:ARG:HB3	1:A:315:ILE:HB	2.02	0.42
1:A:351:ARG:NH1	1:A:378:PRO:O	2.53	0.42
2:B:235:LEU:HD13	2:B:353:PHE:HZ	1.85	0.42
3:C:147:THR:HG23	3:C:149:GLU:H	1.83	0.42
7:G:38:THR:HG21	7:G:206:LEU:HD21	2.02	0.42
10:J:208:LEU:HD23	10:J:220:LEU:HD12	2.01	0.42
19:S:211:ARG:NH2	19:S:213:ASP:OD2	2.53	0.42
23:W:171:VAL:HG22	23:W:182:ARG:HD3	2.02	0.42
23:W:314:LEU:HD21	27:a:312:MET:HE2	2.01	0.42
19:s:172:MET:HE3	19:s:172:MET:HB3	1.82	0.42
31:f:229:VAL:HG22	31:f:605:ASN:HB2	2.01	0.42
31:f:271:MET:O	31:f:275:MET:N	2.49	0.42
31:f:290:VAL:HG21	31:f:317:LEU:HD21	2.02	0.42
2:B:387:LYS:HA	2:B:387:LYS:HD3	1.87	0.41
4:D:155:THR:HA	4:D:159:LYS:HD3	2.01	0.41
6:F:137:ILE:HD13	6:F:142:ALA:HB2	2.01	0.41
24:X:45:VAL:HA	24:X:48:GLN:HG2	2.01	0.41
27:a:363:MET:HE3	27:a:363:MET:HB2	1.83	0.41
29:c:303:MET:HB3	29:c:303:MET:HE2	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ARG:HG3	2:B:283:PHE:HD2	1.85	0.41
3:C:90:HIS:CG	3:C:91:PRO:HD3	2.55	0.41
5:E:253:ILE:HG21	6:F:308:ARG:NH2	2.36	0.41
12:L:7:ASP:OD1	12:L:7:ASP:N	2.53	0.41
16:P:88:MET:HE2	16:P:88:MET:HB3	1.89	0.41
24:X:347:ILE:HD12	24:X:358:LYS:HD2	2.02	0.41
26:Z:181:ASP:N	26:Z:181:ASP:OD1	2.53	0.41
31:f:637:LYS:HE3	31:f:655:LEU:HD11	2.02	0.41
1:A:86:THR:HG22	2:B:136:LEU:HD12	2.02	0.41
15:O:187:ARG:HA	15:O:188:PRO:HA	1.90	0.41
23:W:247:TYR:CE2	23:W:269:SER:HB2	2.55	0.41
13:m:50:GLU:OE2	13:m:201:HIS:ND1	2.42	0.41
13:m:230:ASP:OD1	13:m:231:ILE:N	2.53	0.41
18:r:58:LEU:HD12	18:r:58:LEU:HA	1.93	0.41
31:f:60:VAL:O	31:f:64:GLY:N	2.41	0.41
31:f:297:MET:O	31:f:301:HIS:ND1	2.53	0.41
32:x:64:LYS:HE3	32:x:67:MET:HB3	2.01	0.41
4:D:374:ASP:O	4:D:378:ILE:HG12	2.20	0.41
19:S:22:ILE:HG12	19:S:197:ILE:HG13	2.01	0.41
23:W:67:LEU:HD12	23:W:100:ALA:HB1	2.02	0.41
29:c:210:ASN:OD1	29:c:210:ASN:N	2.53	0.41
8:h:86:LEU:HD23	8:h:86:LEU:HA	1.92	0.41
8:h:95:GLN:HG3	15:o:65:LEU:HD22	2.03	0.41
5:E:66:GLU:O	5:E:89:LYS:NZ	2.45	0.41
7:G:10:ASP:OD1	7:G:10:ASP:N	2.51	0.41
10:J:5:ARG:HA	10:J:5:ARG:HD3	1.80	0.41
11:K:52:LYS:NZ	11:K:64:ILE:O	2.53	0.41
12:L:62:LYS:HE2	12:L:62:LYS:HB3	1.95	0.41
16:P:62:THR:HG23	17:Q:86:ARG:HH12	1.86	0.41
21:U:844:LYS:O	21:U:848:LYS:HG2	2.20	0.41
29:c:33:ILE:HD11	29:c:205:ILE:HD12	2.03	0.41
30:d:139:LEU:HD11	30:d:151:VAL:HG13	2.03	0.41
30:d:235:THR:O	30:d:239:SER:N	2.46	0.41
9:i:41:ASP:OD1	9:i:41:ASP:N	2.48	0.41
31:f:148:GLN:HG2	31:f:149:GLU:HG2	2.01	0.41
31:f:442:SER:HB2	31:f:477:MET:HA	2.01	0.41
31:f:448:CYS:HA	31:f:451:VAL:HG12	2.03	0.41
1:A:414:ASN:C	1:A:414:ASN:HD22	2.28	0.41
3:C:147:THR:OG1	3:C:206:HIS:NE2	2.47	0.41
3:C:235:PHE:HA	3:C:238:ALA:HB3	2.03	0.41
4:D:285:VAL:HG21	5:E:255:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:127:SER:HB3	18:R:136:TYR:CE1	2.56	0.41
23:W:152:ILE:HG13	23:W:165:ILE:HB	2.02	0.41
23:W:357:ARG:HD3	23:W:357:ARG:HA	1.90	0.41
26:Z:64:ASP:OD2	28:b:91:ARG:NH2	2.49	0.41
29:c:296:ILE:HD13	29:c:296:ILE:HA	1.92	0.41
13:m:39:ILE:HD11	13:m:176:ILE:HG12	2.01	0.41
2:B:317:ASP:HB2	2:B:346:ARG:HG2	2.03	0.41
7:G:206:LEU:HB3	7:G:208:ILE:HG13	2.03	0.41
21:U:11:LEU:HD13	21:U:19:LEU:HD11	2.02	0.41
23:W:153:LYS:HA	23:W:153:LYS:HD3	1.78	0.41
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	2.02	0.41
29:c:70:ILE:HG12	29:c:104:ARG:HH22	1.85	0.41
7:g:80:MET:HE2	7:g:87:SER:HA	2.03	0.41
8:h:160:ALA:HB1	8:h:174:LEU:HD13	2.03	0.41
31:f:805:ASP:OD1	31:f:805:ASP:N	2.54	0.41
1:A:119:ALA:HB2	6:F:128:THR:HG23	2.02	0.41
4:D:154:LEU:H	4:D:154:LEU:HG	1.56	0.41
17:Q:108:ASP:HB3	17:Q:112:GLY:H	1.85	0.41
22:V:287:ARG:NH1	33:e:21:GLU:OE2	2.48	0.41
23:W:103:LYS:HA	23:W:103:LYS:HD3	1.85	0.41
27:a:70:ARG:O	28:b:17:ARG:NH1	2.54	0.41
27:a:273:GLN:HB3	27:a:310:LEU:HD11	2.03	0.41
30:d:2:TYR:O	30:d:25:ARG:NH2	2.53	0.41
30:d:103:LEU:HD23	30:d:136:PRO:HB2	2.03	0.41
11:k:97:GLN:HG3	18:r:65:ILE:HG13	2.03	0.41
13:m:175:GLU:HB3	13:m:196:ILE:HG12	2.03	0.41
20:t:179:ARG:HA	20:t:179:ARG:HD3	1.85	0.41
31:f:468:ASP:OD1	31:f:468:ASP:N	2.53	0.41
1:A:356:LYS:O	1:A:360:ARG:HB3	2.20	0.41
1:A:372:LEU:HD11	11:K:207:GLU:HG2	2.02	0.41
4:D:161:ASP:HA	4:D:221:HIS:CD2	2.56	0.41
5:E:167:PRO:O	5:E:274:LYS:NZ	2.48	0.41
13:M:43:ASP:OD1	13:M:43:ASP:N	2.53	0.41
21:U:906:LEU:HD12	21:U:906:LEU:HA	1.91	0.41
22:V:128:ARG:HH21	22:V:132:LEU:HD11	1.86	0.41
23:W:406:VAL:HG22	24:X:342:PHE:HB3	2.03	0.41
26:Z:79:TYR:HE1	26:Z:90:ARG:HA	1.86	0.41
29:c:55:GLY:HA2	29:c:75:MET:HG2	2.03	0.41
9:i:175:LEU:O	9:i:179:TYR:HB2	2.21	0.41
15:o:50:ALA:O	15:o:54:MET:HG2	2.20	0.41
17:q:44:LEU:HD11	17:q:102:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:r:127:SER:HB3	18:r:136:TYR:CE1	2.56	0.41
32:x:23:ASP:OD1	32:x:23:ASP:N	2.53	0.41
4:D:97:ASP:OD1	4:D:97:ASP:N	2.53	0.41
21:U:465:LEU:HD11	21:U:477:GLY:HA3	2.03	0.41
21:U:808:PRO:HB3	21:U:876:GLN:HG2	2.01	0.41
25:Y:371:LYS:HD3	25:Y:371:LYS:HA	1.88	0.41
26:Z:13:PRO:HA	26:Z:16:LEU:HB3	2.03	0.41
29:c:303:MET:O	29:c:306:THR:OG1	2.39	0.41
7:g:132:ARG:HA	7:g:133:PRO:HD3	1.90	0.41
31:f:127:SER:O	31:f:127:SER:OG	2.39	0.41
3:C:73:VAL:HG11	4:D:110:ASN:HB2	2.02	0.40
4:D:183:LEU:HD12	4:D:183:LEU:HA	1.92	0.40
18:R:1:THR:HA	18:R:33:LYS:HZ3	1.86	0.40
23:W:276:LEU:HD12	23:W:353:ASP:HB3	2.03	0.40
23:W:422:ASN:OD1	23:W:423:ASN:N	2.54	0.40
24:X:93:LEU:HD23	24:X:129:LEU:HD22	2.03	0.40
11:k:147:ASP:N	11:k:147:ASP:OD1	2.54	0.40
18:r:106:LYS:HE2	18:r:106:LYS:HB2	1.89	0.40
5:E:196:LEU:HD23	5:E:196:LEU:HA	1.92	0.40
6:F:236:LEU:HD23	6:F:236:LEU:HA	1.94	0.40
6:F:317:LEU:HD13	6:F:328:VAL:HG21	2.03	0.40
13:M:87:LEU:HD23	13:M:87:LEU:HA	1.92	0.40
19:S:168:LEU:O	19:S:172:MET:HG2	2.21	0.40
21:U:229:VAL:HA	21:U:232:ILE:HG12	2.02	0.40
24:X:157:LEU:HD21	24:X:165:LEU:HD23	2.02	0.40
25:Y:138:LEU:HD12	25:Y:138:LEU:HA	1.95	0.40
27:a:7:PHE:HE2	27:a:60:TYR:HB2	1.86	0.40
27:a:20:ALA:HB1	27:a:24:ARG:NH1	2.35	0.40
30:d:170:LEU:HA	30:d:173:THR:HG22	2.01	0.40
8:h:124:SER:OG	8:h:125:GLY:N	2.55	0.40
10:j:186:LEU:HD12	10:j:186:LEU:HA	1.93	0.40
31:f:373:ALA:HA	31:f:748:LEU:HD12	2.03	0.40
3:C:267:SER:HB2	3:C:270:GLN:HG3	2.03	0.40
5:E:177:GLY:N	6:F:344:ARG:HD2	2.36	0.40
6:F:206:MET:HE1	6:F:246:ALA:HB2	2.01	0.40
9:I:161:ALA:HB1	9:I:175:LEU:HD13	2.04	0.40
13:M:81:LEU:HD23	13:M:81:LEU:HA	1.90	0.40
21:U:249:CYS:HB3	21:U:328:ILE:HB	2.03	0.40
25:Y:317:GLY:N	25:Y:352:GLU:OE2	2.53	0.40
26:Z:237:LEU:HA	26:Z:238:PRO:HD3	1.95	0.40
30:d:42:LYS:HG3	30:d:86:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:55:LEU:HD23	30:d:55:LEU:HA	1.94	0.40
10:j:212:ARG:O	10:j:214:ASP:N	2.54	0.40
12:l:39:LYS:HE3	12:l:142:PRO:HB2	2.04	0.40
16:p:12:MET:HE2	16:p:146:MET:HE2	2.04	0.40
19:s:68:ILE:HD13	19:s:68:ILE:HA	1.92	0.40
31:f:680:ARG:HH21	31:f:762:VAL:HG13	1.87	0.40
31:f:771:LEU:HD12	31:f:771:LEU:HA	1.88	0.40
1:A:45:ILE:HD13	1:A:45:ILE:HA	1.93	0.40
7:G:45:LYS:HB3	7:G:45:LYS:HE2	1.80	0.40
10:J:189:LYS:HA	10:J:232:ILE:HD11	2.03	0.40
10:J:195:LEU:HD23	10:J:195:LEU:HA	1.98	0.40
21:U:572:ARG:HD3	21:U:572:ARG:HA	1.84	0.40
21:U:587:ALA:HB2	21:U:621:SER:HB3	2.04	0.40
21:U:612:ASP:HB3	21:U:647:HIS:CG	2.57	0.40
21:U:756:HIS:CE1	21:U:758:PRO:HG2	2.56	0.40
26:Z:260:VAL:HG13	29:c:292:MET:HE1	2.03	0.40
29:c:151:VAL:HG23	29:c:152:LYS:H	1.86	0.40
29:c:264:LYS:HA	29:c:264:LYS:HD2	1.93	0.40
10:j:40:ILE:HG22	10:j:212:ARG:HG2	2.02	0.40
11:k:25:GLU:HA	11:k:28:ILE:HD12	2.04	0.40
18:r:139:MET:O	18:r:143:TYR:HB2	2.21	0.40
31:f:343:LYS:HB3	31:f:388:ASP:HA	2.03	0.40
31:f:380:PHE:HB3	31:f:752:HIS:NE2	2.36	0.40
1:A:115:VAL:HG21	1:A:118:PHE:HB2	2.03	0.40
4:D:306:LYS:HA	4:D:306:LYS:HD3	1.86	0.40
9:I:205:LYS:HD3	9:I:205:LYS:HA	1.84	0.40
23:W:148:THR:O	23:W:152:ILE:HG12	2.22	0.40
23:W:205:ILE:O	23:W:209:ILE:HG12	2.21	0.40
24:X:173:GLU:HA	24:X:176:THR:HG22	2.04	0.40
24:X:212:MET:HE2	24:X:212:MET:HB2	1.98	0.40
29:c:34:SER:HB2	29:c:36:LEU:H	1.87	0.40
30:d:82:TYR:CG	30:d:95:MET:HE1	2.56	0.40
20:t:69:GLN:NE2	20:t:73:ASP:OD1	2.55	0.40
31:f:73:PRO:HA	31:f:76:GLU:HG2	2.03	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	411/433 (95%)	367 (89%)	44 (11%)	0	100	100
2	B	386/440 (88%)	357 (92%)	29 (8%)	0	100	100
3	C	377/398 (95%)	344 (91%)	33 (9%)	0	100	100
4	D	378/418 (90%)	347 (92%)	31 (8%)	0	100	100
5	E	373/403 (93%)	347 (93%)	26 (7%)	0	100	100
6	F	372/439 (85%)	346 (93%)	26 (7%)	0	100	100
7	G	242/246 (98%)	233 (96%)	9 (4%)	0	100	100
7	g	242/246 (98%)	232 (96%)	10 (4%)	0	100	100
8	H	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
8	h	230/234 (98%)	218 (95%)	12 (5%)	0	100	100
9	I	249/261 (95%)	242 (97%)	7 (3%)	0	100	100
9	i	248/261 (95%)	243 (98%)	5 (2%)	0	100	100
10	J	237/248 (96%)	227 (96%)	10 (4%)	0	100	100
10	j	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
11	K	232/241 (96%)	222 (96%)	9 (4%)	1 (0%)	30	65
11	k	232/241 (96%)	224 (97%)	8 (3%)	0	100	100
12	L	236/269 (88%)	232 (98%)	4 (2%)	0	100	100
12	l	236/269 (88%)	226 (96%)	10 (4%)	0	100	100
13	M	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
13	m	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
14	N	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
14	n	200/239 (84%)	196 (98%)	4 (2%)	0	100	100
15	O	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
15	o	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
16	P	202/205 (98%)	194 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	p	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
17	Q	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
17	q	197/201 (98%)	193 (98%)	4 (2%)	0	100	100
18	R	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
18	r	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
19	S	211/241 (88%)	204 (97%)	7 (3%)	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%)	206 (96%)	8 (4%)	0	100	100
21	U	858/953 (90%)	808 (94%)	49 (6%)	1 (0%)	48	80
22	V	470/534 (88%)	456 (97%)	13 (3%)	1 (0%)	43	76
23	W	444/456 (97%)	408 (92%)	33 (7%)	3 (1%)	18	53
24	X	378/422 (90%)	360 (95%)	18 (5%)	0	100	100
25	Y	376/389 (97%)	350 (93%)	26 (7%)	0	100	100
26	Z	284/324 (88%)	259 (91%)	24 (8%)	1 (0%)	30	65
27	a	371/376 (99%)	345 (93%)	26 (7%)	0	100	100
28	b	189/377 (50%)	178 (94%)	10 (5%)	1 (0%)	24	60
29	c	285/310 (92%)	254 (89%)	30 (10%)	1 (0%)	30	65
30	d	255/350 (73%)	224 (88%)	31 (12%)	0	100	100
31	f	887/908 (98%)	772 (87%)	115 (13%)	0	100	100
32	x	79/494 (16%)	68 (86%)	11 (14%)	0	100	100
33	e	48/70 (69%)	40 (83%)	8 (17%)	0	100	100
All	All	13430/15382 (87%)	12638 (94%)	783 (6%)	9 (0%)	49	80

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	V	224	LEU
23	W	132	THR
23	W	117	ASP
23	W	137	TYR
26	Z	222	ILE
29	c	156	VAL
28	b	23	PRO

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Mol	Chain	Res	Type
11	K	130	PRO
21	U	174	PRO

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	352/372 (95%)	350 (99%)	2 (1%)	78	88
2	B	341/385 (89%)	340 (100%)	1 (0%)	86	91
3	C	325/346 (94%)	323 (99%)	2 (1%)	78	88
4	D	333/366 (91%)	331 (99%)	2 (1%)	78	88
5	E	298/353 (84%)	295 (99%)	3 (1%)	68	84
6	F	296/379 (78%)	295 (100%)	1 (0%)	86	91
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	202 (100%)	0	100	100
8	H	188/191 (98%)	188 (100%)	0	100	100
8	h	188/191 (98%)	188 (100%)	0	100	100
9	I	207/221 (94%)	205 (99%)	2 (1%)	68	84
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	201/211 (95%)	201 (100%)	0	100	100
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	193/203 (95%)	193 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/230 (88%)	202 (100%)	0	100	100
12	l	201/230 (87%)	201 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	168 (100%)	0	100	100
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	738/816 (90%)	736 (100%)	2 (0%)	86	91
22	V	391/460 (85%)	390 (100%)	1 (0%)	86	91
23	W	410/416 (99%)	409 (100%)	1 (0%)	87	92
24	X	327/362 (90%)	327 (100%)	0	100	100
25	Y	334/344 (97%)	334 (100%)	0	100	100
26	Z	257/295 (87%)	257 (100%)	0	100	100
27	a	333/336 (99%)	333 (100%)	0	100	100
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/268 (94%)	252 (100%)	0	100	100
30	d	231/294 (79%)	231 (100%)	0	100	100
31	f	745/763 (98%)	745 (100%)	0	100	100
32	x	68/439 (16%)	68 (100%)	0	100	100
33	e	44/63 (70%)	44 (100%)	0	100	100
All	All	11396/13065 (87%)	11379 (100%)	17 (0%)	87	93

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	403	ILE
1	A	414	ASN
2	B	125	THR

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Mol	Chain	Res	Type
3	C	109	THR
3	C	210	THR
4	D	153	MET
4	D	154	LEU
5	E	283	ASP
5	E	384	LEU
5	E	387	LYS
6	F	416	THR
9	I	7[A]	SER
9	I	7[B]	SER
21	U	496	LEU
21	U	497	LEU
22	V	106	ARG
23	W	26	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	94	GLN
1	A	148	GLN
1	A	247	GLN
1	A	296	GLN
2	B	57	GLN
2	B	314	ASN
3	C	22	GLN
3	C	64	GLN
3	C	102	ASN
4	D	65	GLN
4	D	83	GLN
4	D	98	GLN
4	D	237	GLN
4	D	295	GLN
6	F	208	HIS
6	F	243	GLN
7	G	75	ASN
7	G	128	ASN
9	I	102	GLN
9	I	123	GLN
10	J	92	GLN
10	J	154	HIS
11	K	73	HIS

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Mol	Chain	Res	Type
12	L	16	GLN
15	O	91	GLN
15	O	193	ASN
16	P	7	ASN
17	Q	82	ASN
17	Q	101	ASN
18	R	70	ASN
19	S	79	ASN
19	S	151	ASN
21	U	79	ASN
21	U	89	ASN
21	U	111	GLN
21	U	135	ASN
21	U	207	ASN
21	U	340	GLN
21	U	346	ASN
21	U	355	ASN
21	U	452	ASN
21	U	604	HIS
21	U	888	GLN
22	V	62	HIS
22	V	260	HIS
22	V	365	GLN
22	V	427	GLN
22	V	473	GLN
23	W	86	ASN
23	W	210	ASN
23	W	215	GLN
23	W	395	ASN
24	X	207	GLN
24	X	322	HIS
24	X	329	ASN
24	X	334	ASN
25	Y	273	GLN
25	Y	291	HIS
25	Y	302	HIS
26	Z	86	ASN
26	Z	243	GLN
26	Z	254	ASN
26	Z	282	ASN
27	a	9	GLN
27	a	164	GLN

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Mol	Chain	Res	Type
27	a	169	HIS
27	a	264	ASN
27	a	288	HIS
28	b	34	ASN
28	b	142	ASN
29	c	92	GLN
29	c	240	HIS
29	c	269	GLN
30	d	88	GLN
8	h	102	GLN
9	i	40	ASN
9	i	142	HIS
9	i	167	ASN
9	i	177	GLN
10	j	92	GLN
10	j	122	ASN
10	j	175	ASN
12	l	59	HIS
12	l	90	GLN
14	n	110	GLN
14	n	158	ASN
16	p	7	ASN
17	q	71	ASN
17	q	99	HIS
17	q	189	HIS
18	r	196	HIS
19	s	79	ASN
19	s	108	ASN
19	s	152	GLN
20	t	3	ASN
31	f	224	ASN
31	f	238	ASN
31	f	323	ASN
31	f	382	ASN
31	f	452	ASN
31	f	457	ASN
31	f	677	HIS
31	f	705	ASN
31	f	715	HIS
32	x	21	ASN
32	x	65	ASN

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 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
36	ADP	C	501	35	28,29,29	1.40	4 (14%)	43,45,45	1.87	8 (18%)
34	ATP	E	501	35	32,33,33	1.38	4 (12%)	48,52,52	1.81	7 (14%)
34	ATP	A	501	35	32,33,33	0.36	0	48,52,52	0.30	0
34	ATP	B	501	35	32,33,33	0.37	0	48,52,52	0.30	0
36	ADP	F	501	35	28,29,29	1.43	3 (10%)	43,45,45	1.99	8 (18%)
34	ATP	D	501	35	32,33,33	0.39	0	48,52,52	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ADP	C	501	35	-	5/16/32/32	0/3/3/3
34	ATP	E	501	35	-	3/22/38/38	0/3/3/3
34	ATP	A	501	35	-	0/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ATP	B	501	35	-	5/22/38/38	0/3/3/3
36	ADP	F	501	35	-	3/16/32/32	0/3/3/3
34	ATP	D	501	35	-	2/22/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	F	501	ADP	C5-C4	4.77	1.47	1.39
36	C	501	ADP	C5-C4	4.64	1.47	1.39
34	E	501	ATP	C5-C4	4.64	1.47	1.39
36	F	501	ADP	C5-C6	2.77	1.48	1.41
36	F	501	ADP	C5-N7	-2.61	1.34	1.39
34	E	501	ATP	C5-C6	2.61	1.48	1.41
36	C	501	ADP	C5-C6	2.60	1.48	1.41
34	E	501	ATP	C5-N7	-2.57	1.34	1.39
36	C	501	ADP	C5-N7	-2.43	1.34	1.39
36	C	501	ADP	C8-N7	2.23	1.36	1.31
34	E	501	ATP	C8-N7	2.09	1.35	1.31

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	F	501	ADP	C5-C4-N3	-6.69	117.51	126.72
36	C	501	ADP	C5-C4-N3	-6.15	118.24	126.72
34	E	501	ATP	C5-C4-N3	-6.09	118.33	126.72
36	F	501	ADP	N3-C4-N9	5.28	136.15	127.17
36	C	501	ADP	N3-C4-N9	4.92	135.53	127.17
34	E	501	ATP	N3-C4-N9	4.89	135.49	127.17
36	F	501	ADP	C2-N3-C4	4.01	121.62	111.83
36	C	501	ADP	C2-N3-C4	3.79	121.08	111.83
34	E	501	ATP	C2-N3-C4	3.78	121.06	111.83
36	F	501	ADP	C4-C5-N7	-3.65	106.41	110.58
36	C	501	ADP	C4-C5-N7	-3.42	106.67	110.58
34	E	501	ATP	C4-C5-N7	-3.41	106.69	110.58
34	E	501	ATP	N3-C2-N1	-3.26	123.65	128.58
36	F	501	ADP	N3-C2-N1	-3.24	123.67	128.58
36	C	501	ADP	N3-C2-N1	-3.20	123.74	128.58
36	F	501	ADP	C5-N7-C8	2.81	107.86	103.45
34	E	501	ATP	C5-N7-C8	2.67	107.65	103.45
36	C	501	ADP	C3'-C2'-C1'	2.56	106.31	101.46
36	C	501	ADP	C4-N9-C8	2.55	108.42	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	501	ADP	C5'-N7-C8	2.52	107.42	103.45
34	E	501	ATP	C4'-N9-C8	2.43	108.29	105.74
36	F	501	ADP	C5'-C4'-C3'	-2.25	107.10	115.21
36	F	501	ADP	C3'-C2'-C1'	2.19	105.61	101.46

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	B	501	ATP	C5'-O5'-PA-O1A
34	B	501	ATP	C5'-O5'-PA-O3A
34	E	501	ATP	O4'-C4'-C5'-O5'
36	C	501	ADP	C5'-O5'-PA-O1A
36	C	501	ADP	C5'-O5'-PA-O2A
36	C	501	ADP	C5'-O5'-PA-O3A
36	F	501	ADP	C5'-O5'-PA-O3A
34	E	501	ATP	C3'-C4'-C5'-O5'
36	C	501	ADP	O4'-C4'-C5'-O5'
34	B	501	ATP	PB-O3B-PG-O3G
34	D	501	ATP	PA-O3A-PB-O2B
34	B	501	ATP	C5'-O5'-PA-O2A
34	E	501	ATP	C5'-O5'-PA-O1A
36	F	501	ADP	C5'-O5'-PA-O1A
36	C	501	ADP	C3'-C4'-C5'-O5'
36	F	501	ADP	C4'-C5'-O5'-PA
34	B	501	ATP	PG-O3B-PB-O2B
34	D	501	ATP	PA-O3A-PB-O1B

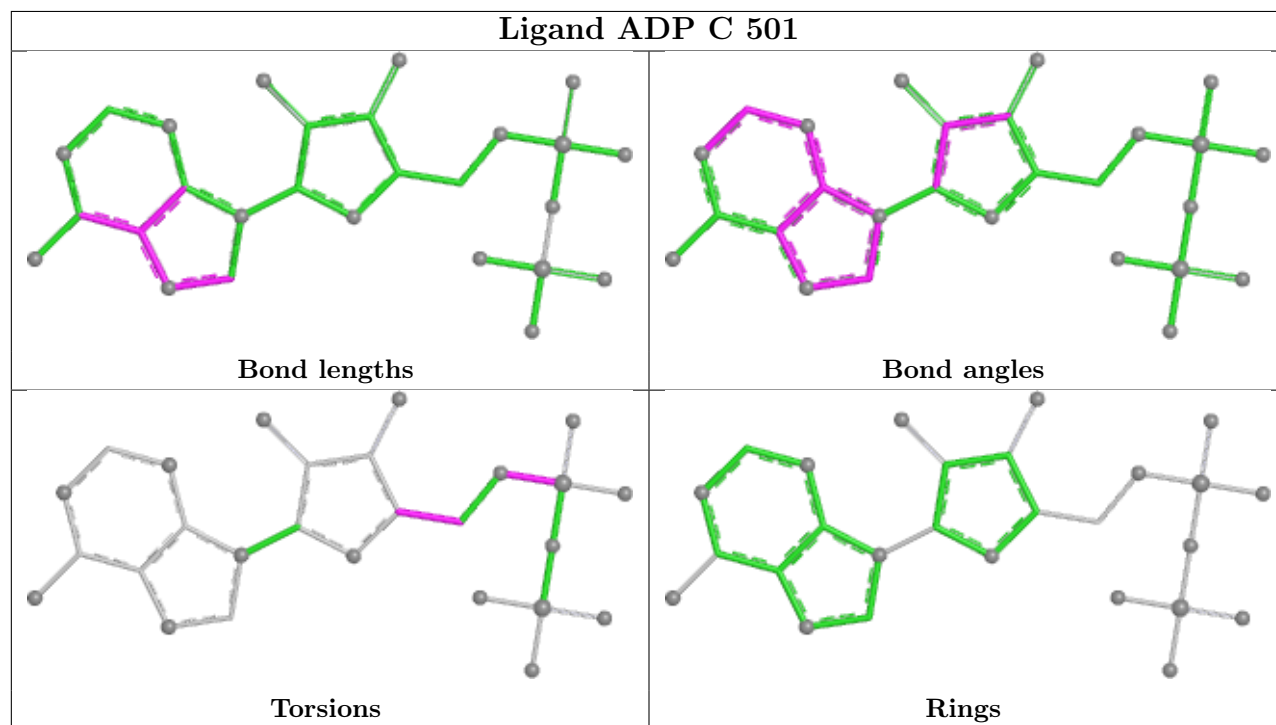
There are no ring outliers.

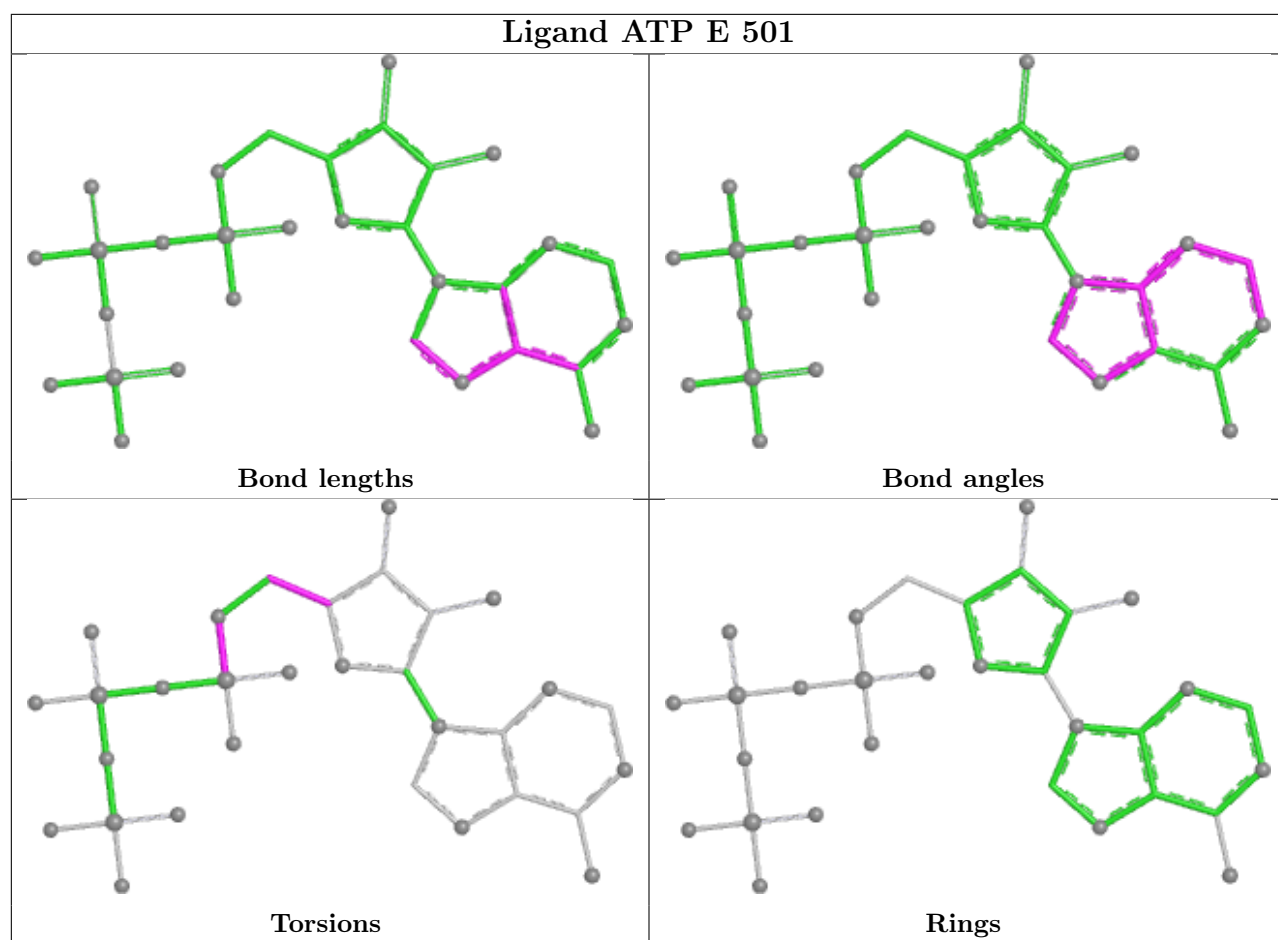
2 monomers are involved in 2 short contacts:

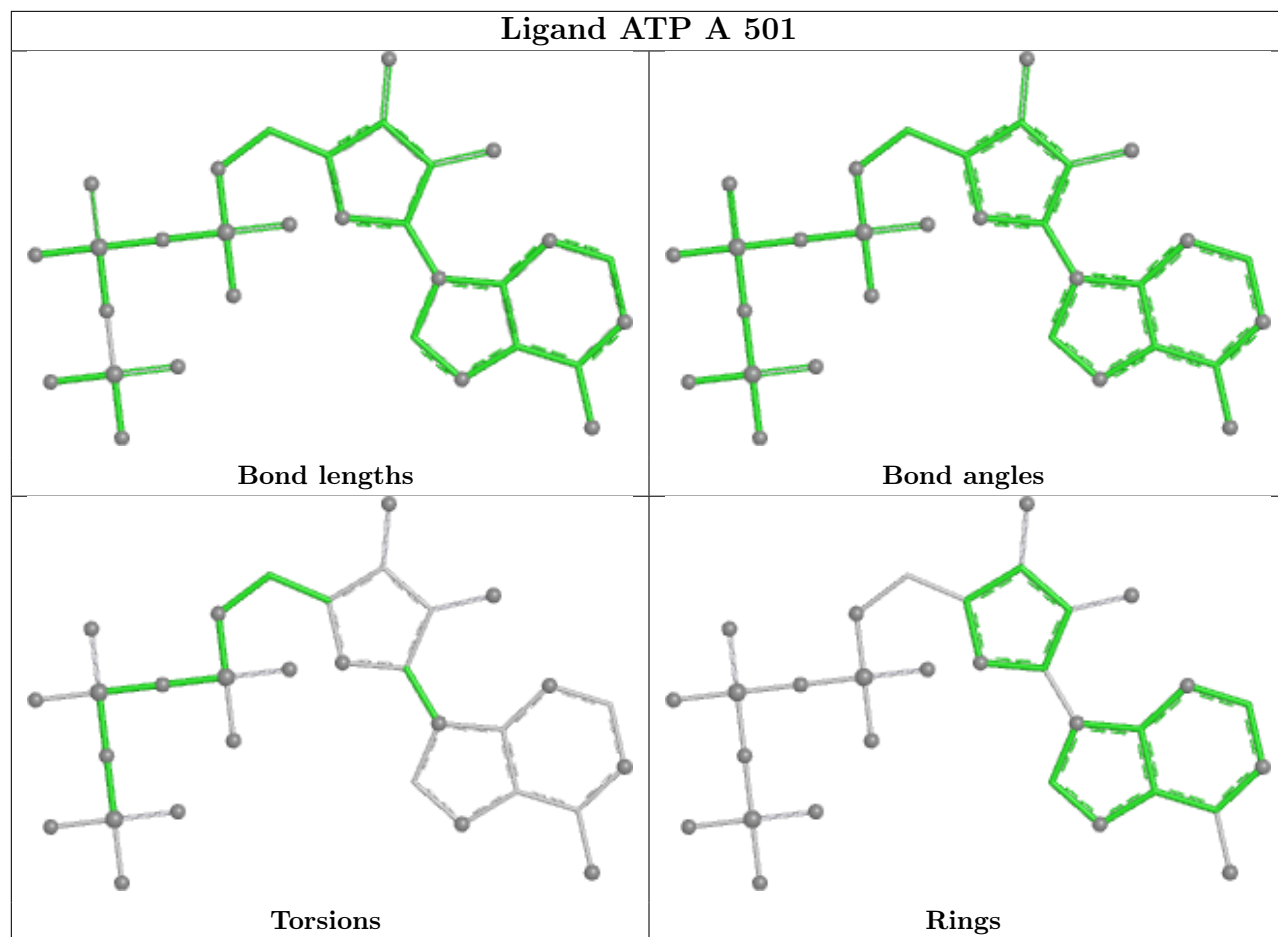
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	C	501	ADP	1	0
34	E	501	ATP	1	0

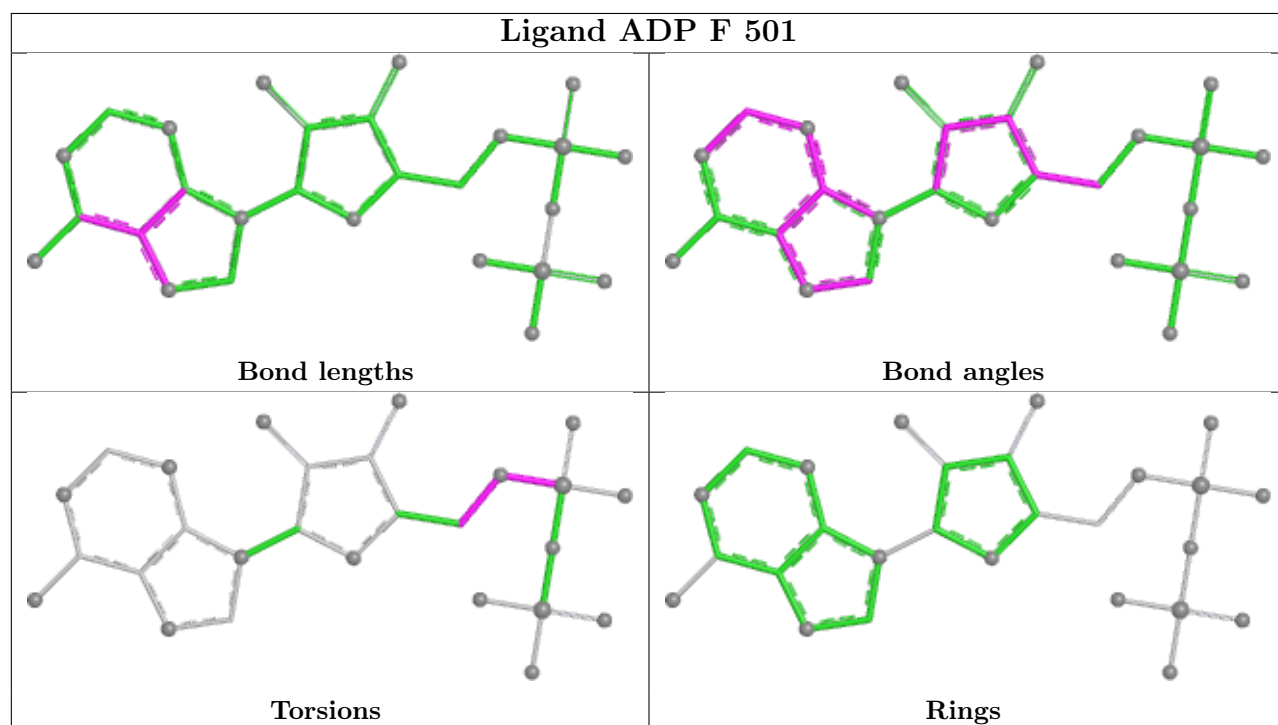
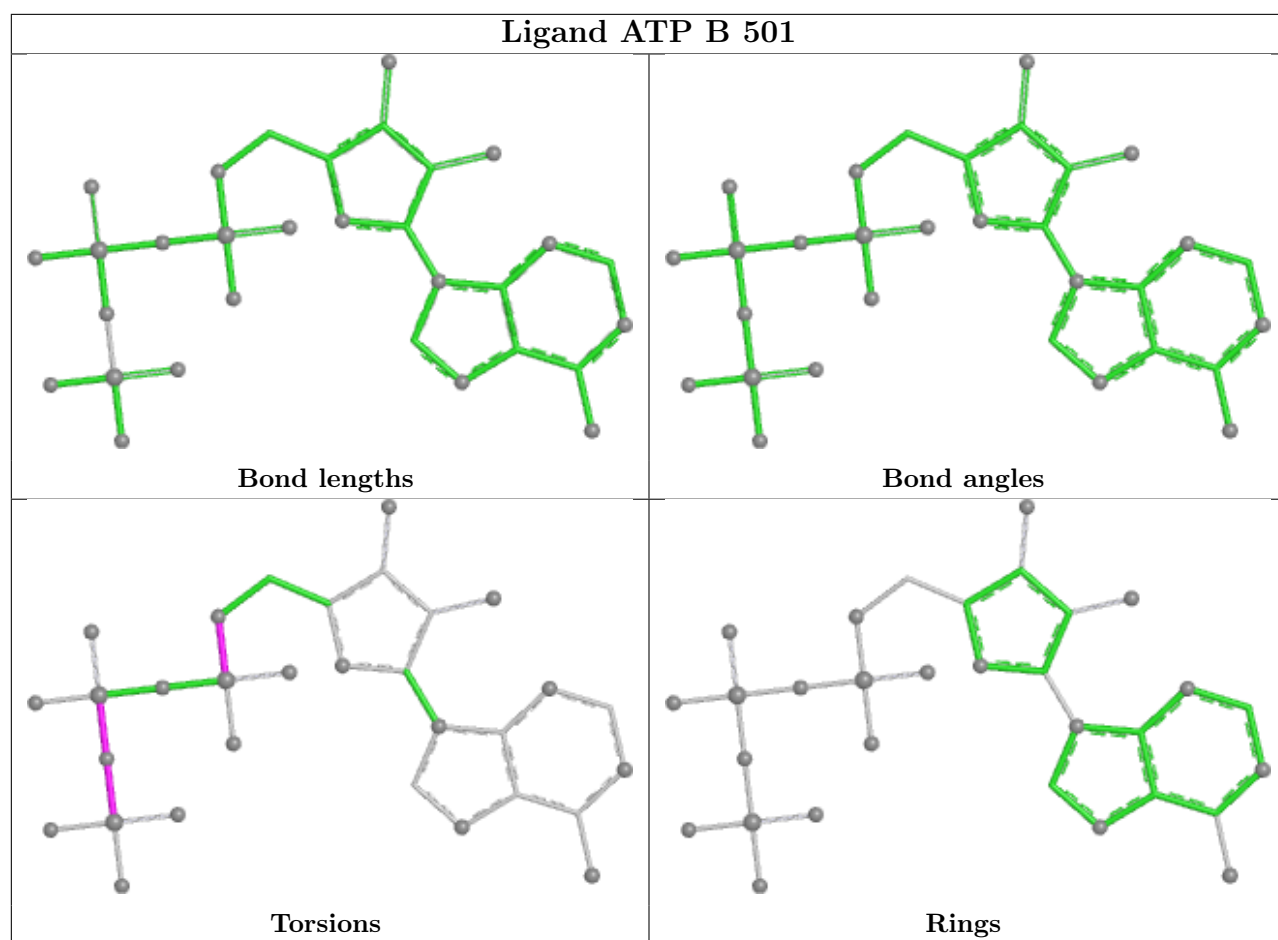
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

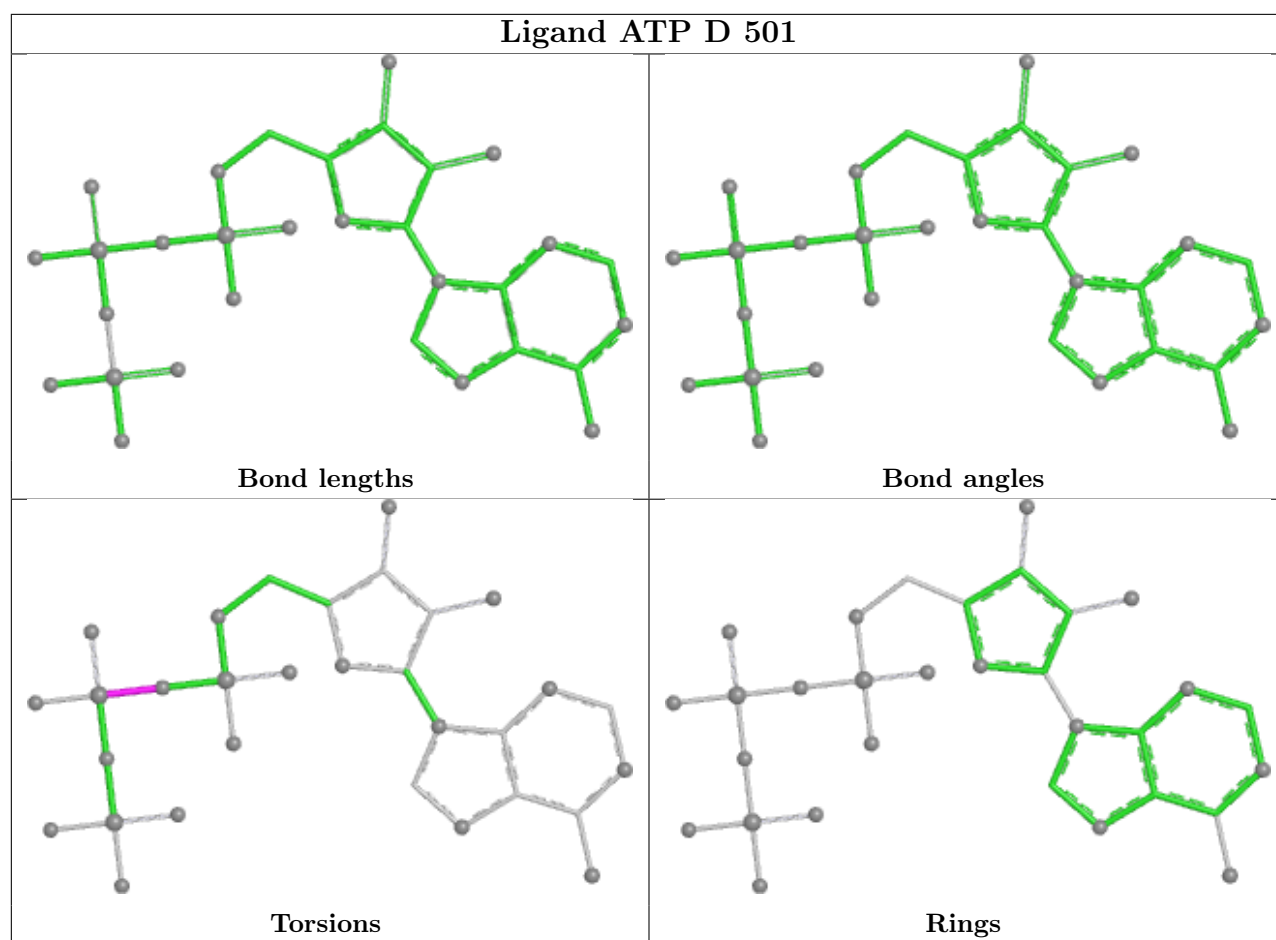
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

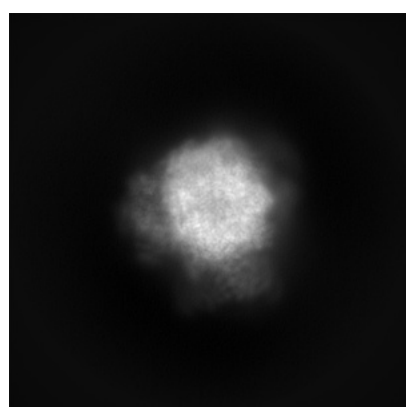
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32272. These allow visual inspection of the internal detail of the map and identification of artifacts.

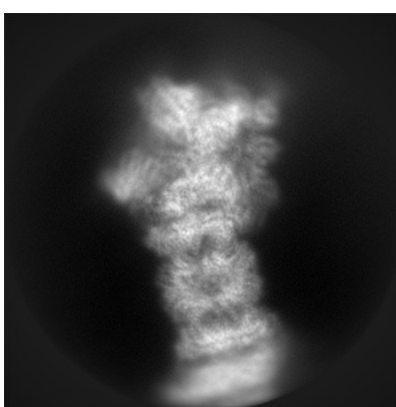
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

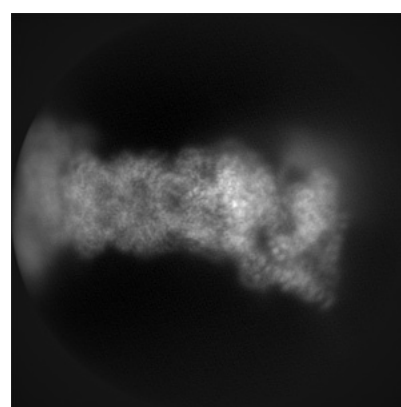
6.1.1 Primary map



X



Y

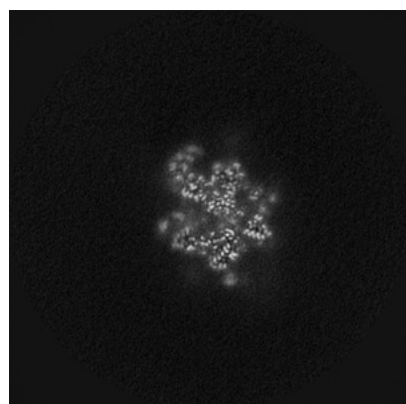


Z

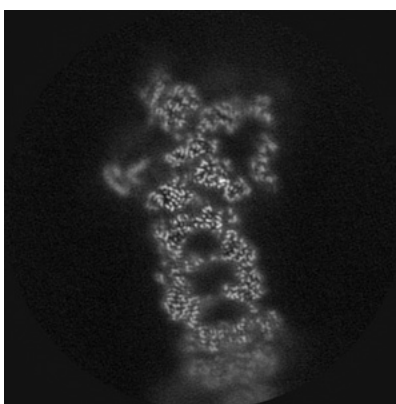
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

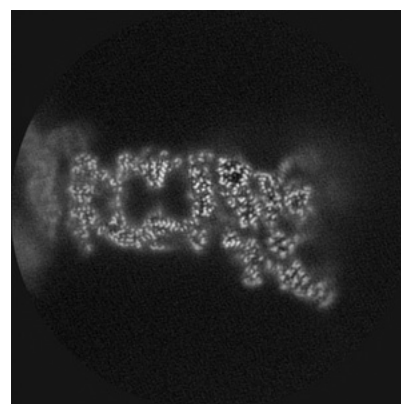
6.2.1 Primary map



X Index: 320



Y Index: 320

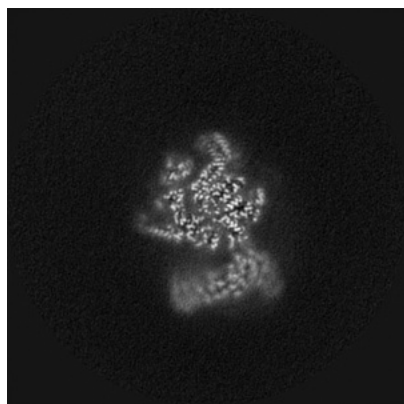


Z Index: 320

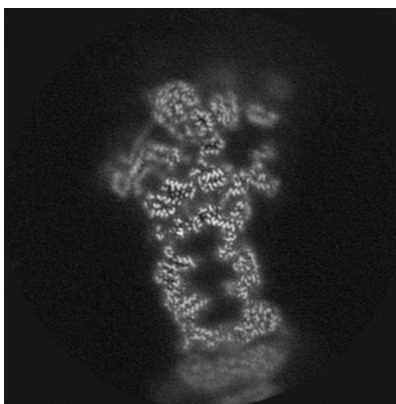
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

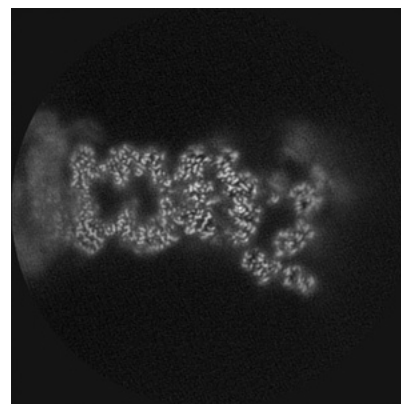
6.3.1 Primary map



X Index: 362



Y Index: 334

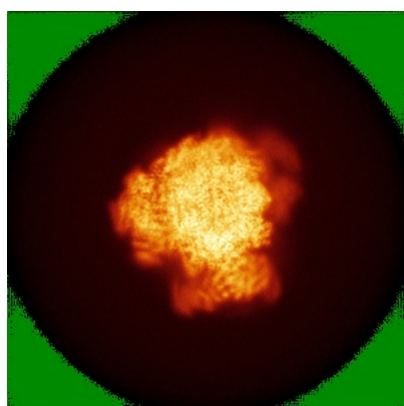


Z Index: 349

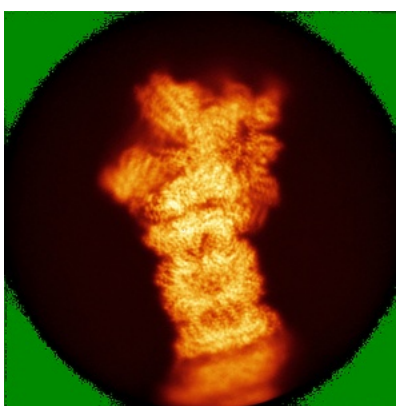
The images above show the largest variance slices of the map in three orthogonal directions.

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

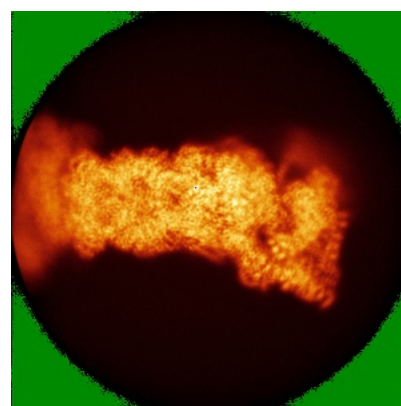
6.4.1 Primary map



X



Y

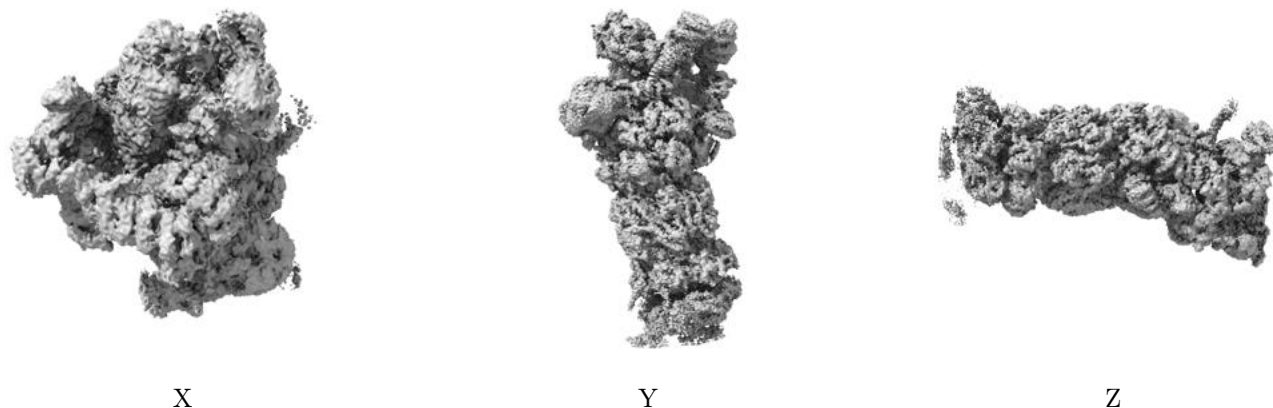


Z

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 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

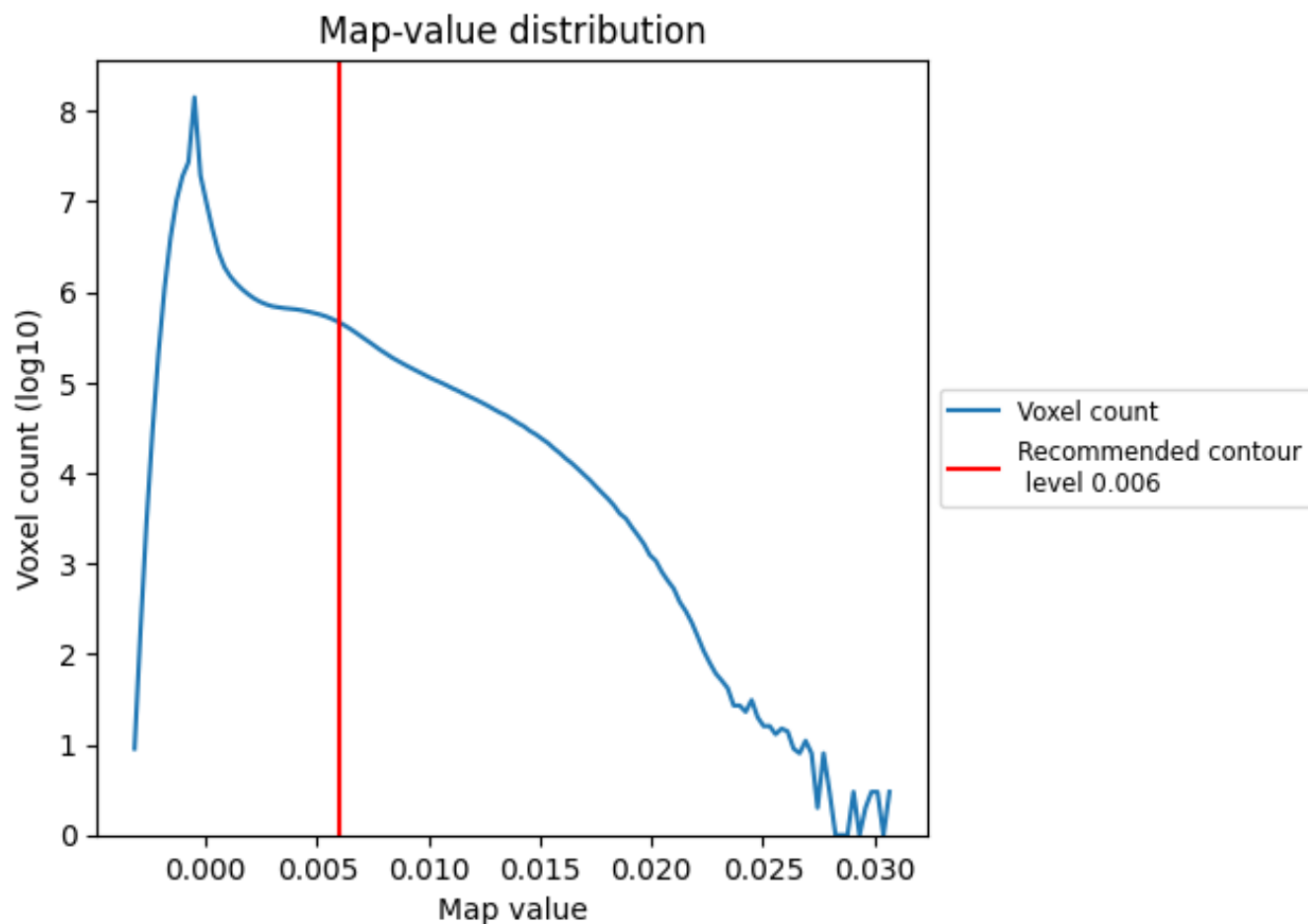
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

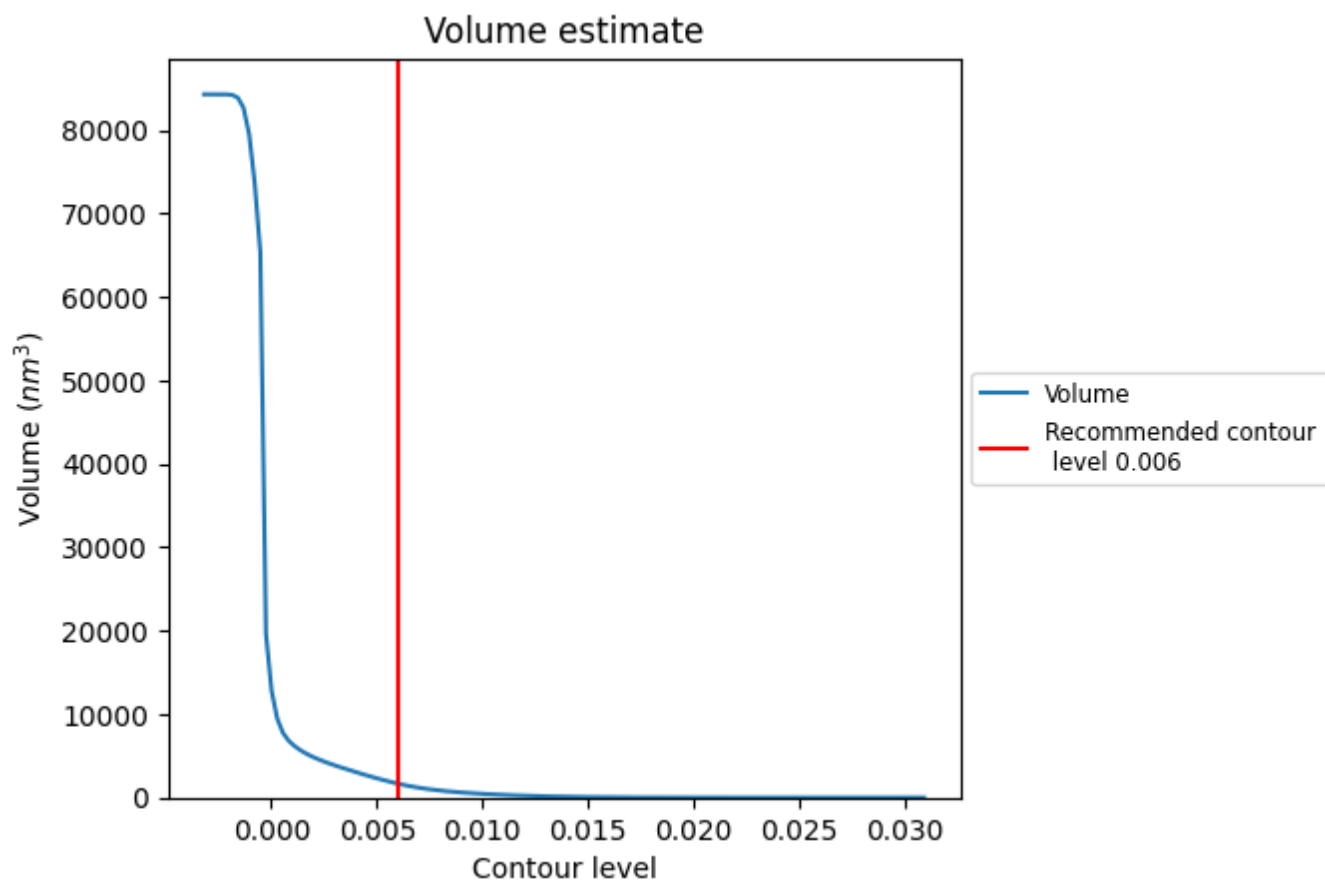
This section contains the results of statistical analysis of the map.

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.

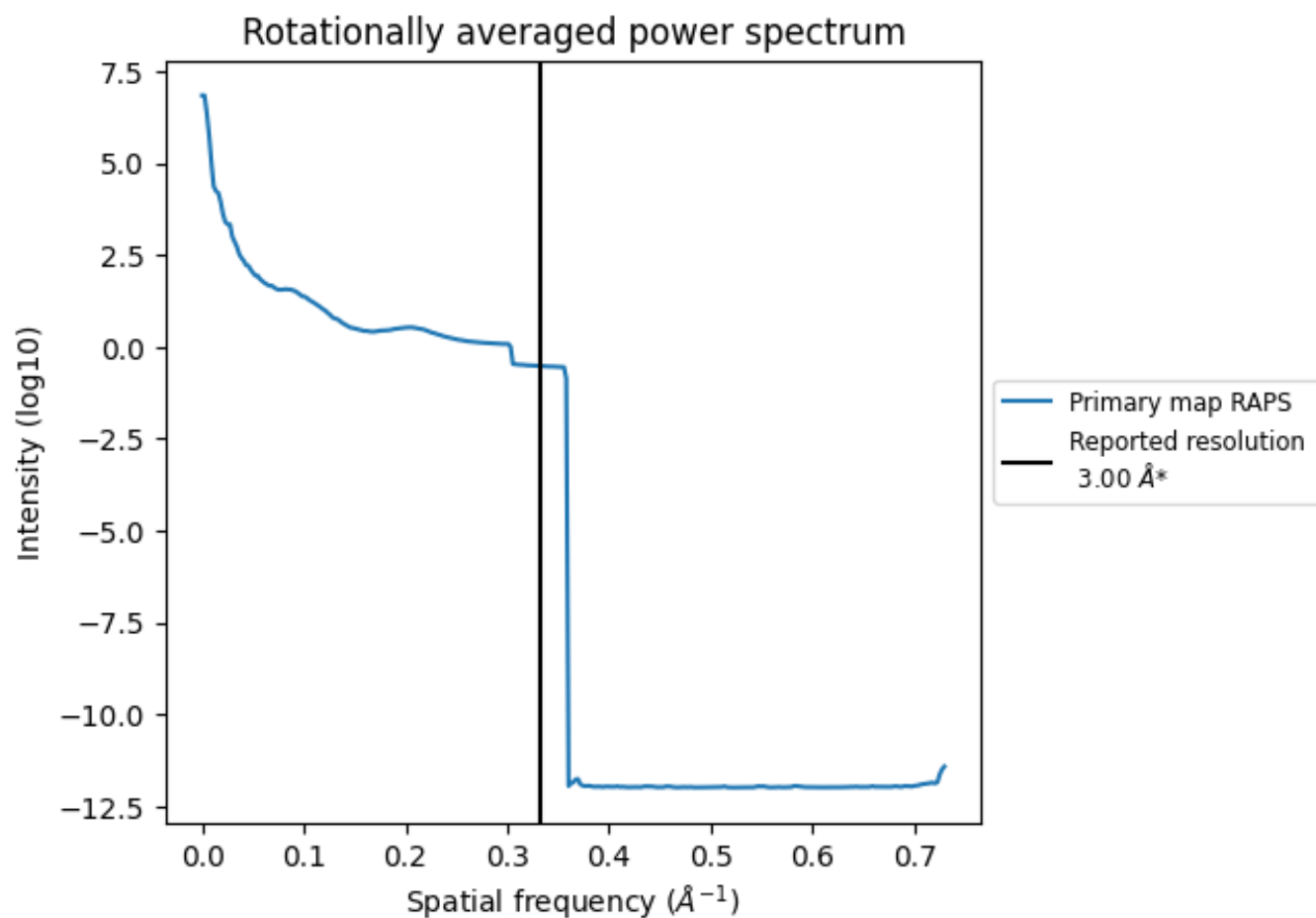
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1666 nm³; this corresponds to an approximate mass of 1505 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

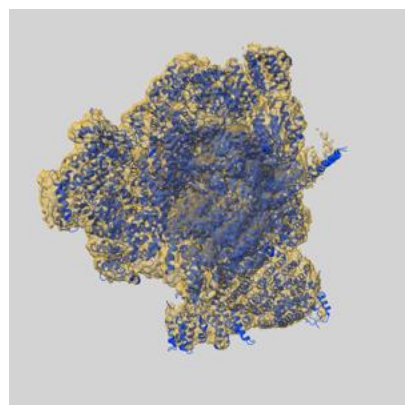
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

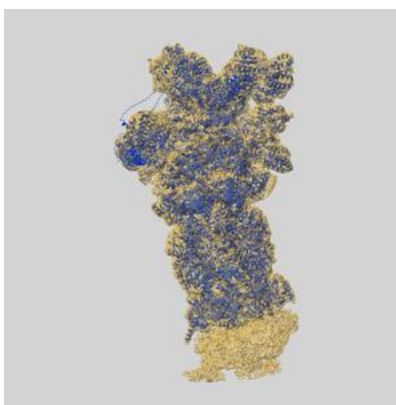
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32272 and PDB model 7W37. Per-residue inclusion information can be found in section [3](#) on page [13](#).

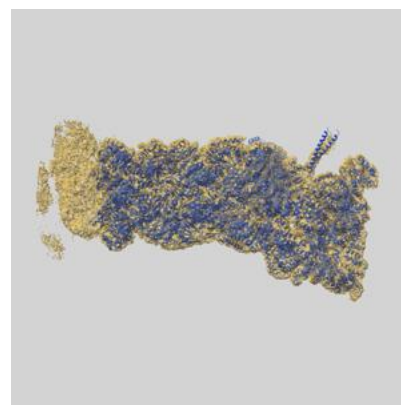
9.1 Map-model overlay [i](#)



X



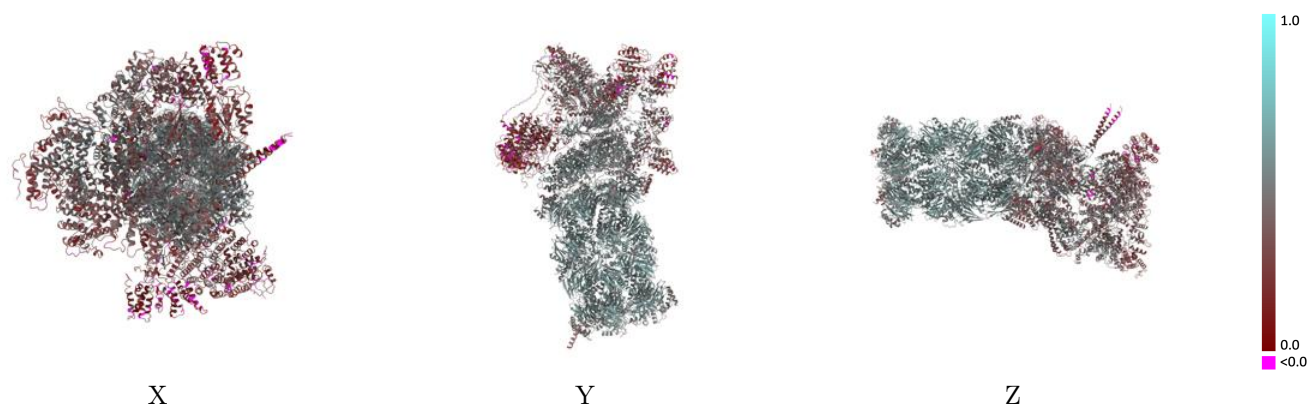
Y



Z

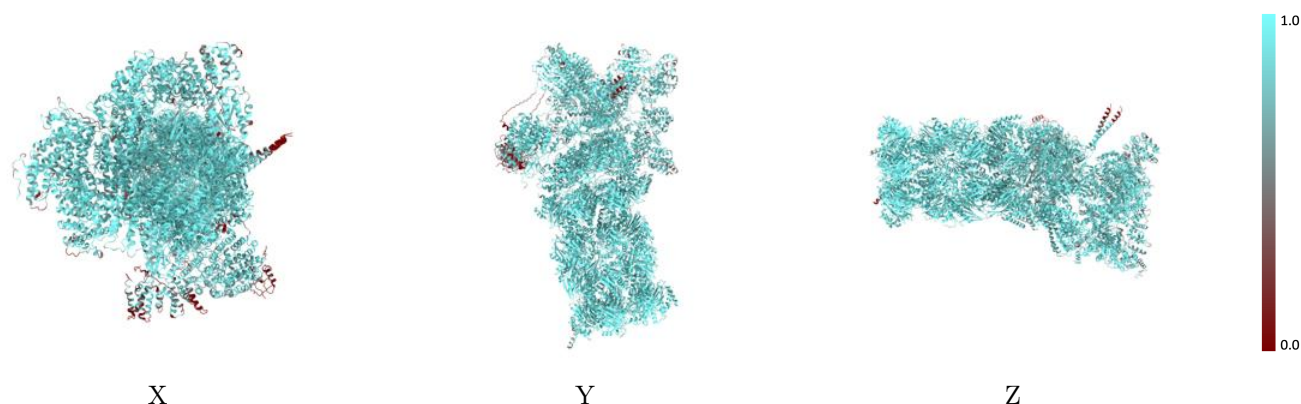
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



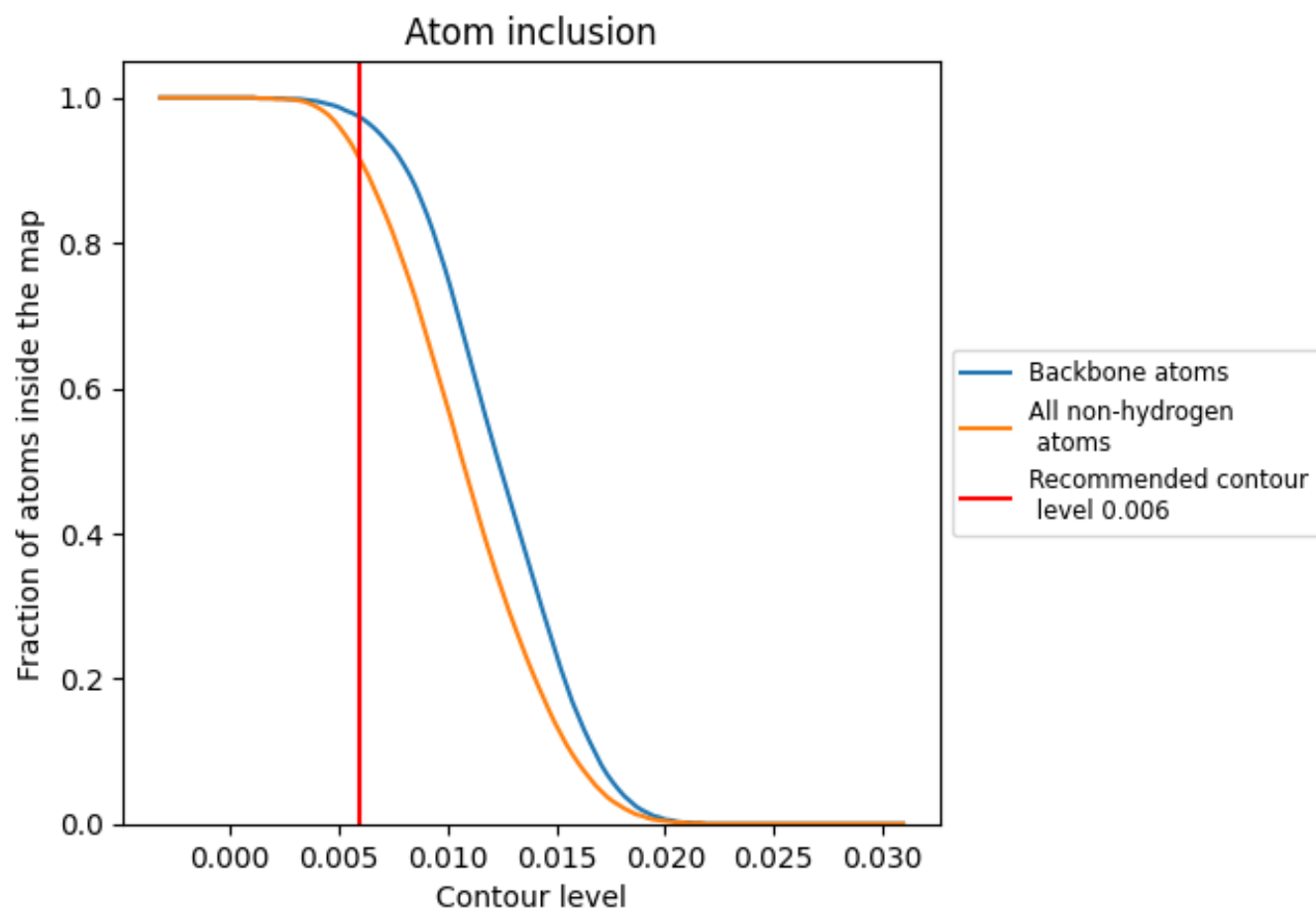
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 91% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9140	 0.4440
A	 0.9210	 0.4430
B	 0.9390	 0.4520
C	 0.9460	 0.4590
D	 0.9530	 0.4620
E	 0.9360	 0.4590
F	 0.9280	 0.4660
G	 0.9670	 0.5270
H	 0.9750	 0.5280
I	 0.9620	 0.5130
J	 0.9550	 0.4910
K	 0.9590	 0.5270
L	 0.9740	 0.5440
M	 0.9700	 0.5280
N	 0.9790	 0.5560
O	 0.9780	 0.5460
P	 0.9840	 0.5470
Q	 0.9780	 0.5460
R	 0.9850	 0.5390
S	 0.9790	 0.5430
T	 0.9760	 0.5580
U	 0.8460	 0.3550
V	 0.8880	 0.3710
W	 0.8230	 0.3310
X	 0.8900	 0.3890
Y	 0.9230	 0.4240
Z	 0.8910	 0.3420
a	 0.8210	 0.3010
b	 0.8000	 0.2600
c	 0.9190	 0.4140
d	 0.7870	 0.2950
e	 0.7920	 0.3520
f	 0.8120	 0.2170
g	 0.9610	 0.5250
h	 0.9660	 0.5320



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Chain	Atom inclusion	Q-score
i	 0.9330	 0.4990
j	 0.9130	 0.4630
k	 0.9410	 0.5130
l	 0.9670	 0.5350
m	 0.9500	 0.5270
n	 0.9820	 0.5670
o	 0.9760	 0.5520
p	 0.9870	 0.5540
q	 0.9810	 0.5500
r	 0.9840	 0.5520
s	 0.9720	 0.5520
t	 0.9720	 0.5600
x	 0.1340	 0.1550