



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:02 AM UTC

PDB ID : 7W3C / pdb_00007w3c
EMDB ID : EMD-32277
Title : Structure of USP14-bound human 26S proteasome in substrate-engaged state
ED0_USP14
Authors : Zhang, S.; Zou, S.; Yin, D.; Wu, Z.; Mao, Y.
Deposited on : 2021-11-25
Resolution : 3.40 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:

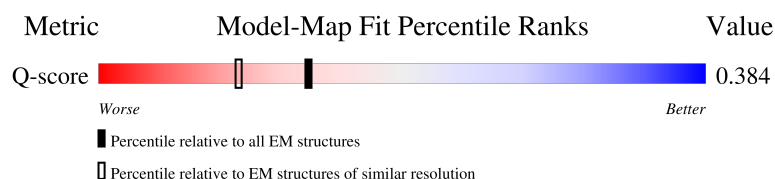
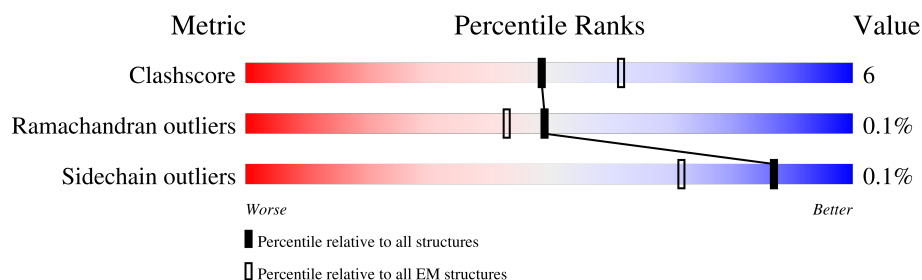
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.40 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.



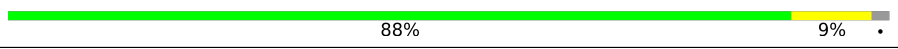
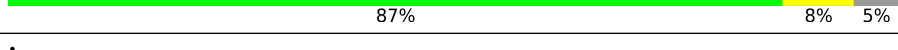
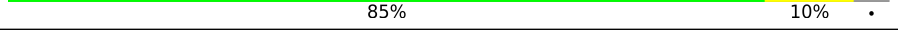
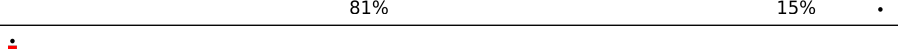
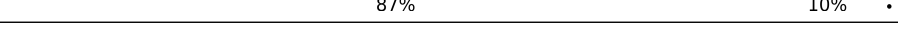
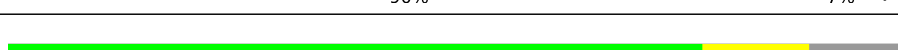
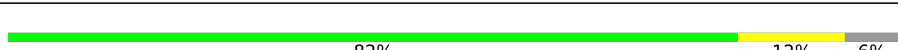
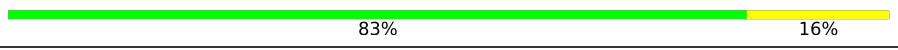
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	B	440	
2	C	398	
3	D	418	
4	E	403	

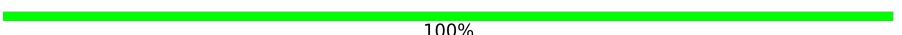
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Mol	Chain	Length	Quality of chain
5	F	439	
6	A	433	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	269	
12	l	269	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	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	X	422	
23	Y	389	
24	Z	324	
25	a	376	
26	b	377	
27	c	310	
28	d	350	
29	f	908	
30	v	36	
31	x	494	
32	y	76	
33	W	456	
34	V	534	
35	e	70	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 110747 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 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	411	Total	C	N	O	S	0	0
			3207	2022	548	622	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	396	Total	C	N	O	S	0	0
			3105	1954	558	576	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

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

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

- Molecule 5 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	395	Total	C	N	O	S	0	0
			3098	1951	533	596	18		

- Molecule 6 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	413	Total	C	N	O	S	0	0
			3229	2034	566	611	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1867	1187	312	355	13		
7	g	244	Total	C	N	O	S	0	0
			1879	1193	318	355	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1801	1149	304	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	248	Total	C	N	O	S	0	0
			1933	1222	330	371	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
			1861	1166	327	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	238	Total	C	N	O	S	0	0
			1813	1139	302	361	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	240	Total	C	N	O	S	0	0
			1876	1175	338	352	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	242	Total	C	N	O	S	0	0
			1890	1200	323	356	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	203	Total	C	N	O	S	0	0
			1521	954	259	296	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
			1645	1035	278	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
			1578	1012	267	290	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
			1549	977	270	293	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
			1650	1044	283	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	872	Total	C	N	O	S	0	0
			6828	4328	1157	1298	45		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

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

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

- Molecule 30 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	v	36	Total	C	N	O	0	0
			180	108	36	36		

- Molecule 31 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	x	494	Total	C	N	O	S	0	0
			3929	2485	647	769	28		

- Molecule 32 is a protein called Ubiquitin.

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

- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

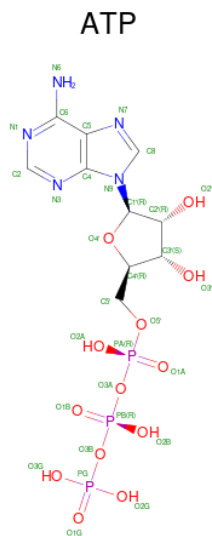
- Molecule 34 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

- Molecule 35 is a protein called 26S proteasome complex subunit DSS1.

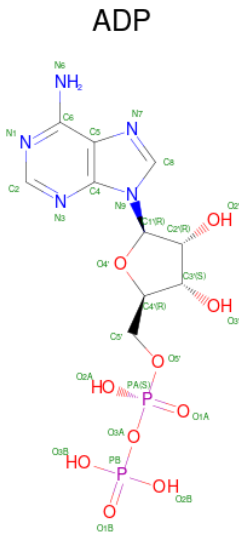
Mol	Chain	Residues	Atoms				AltConf	Trace
35	e	50	Total	C	N	O	0	0
			425	260	65	100		

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 37 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
37	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
37	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

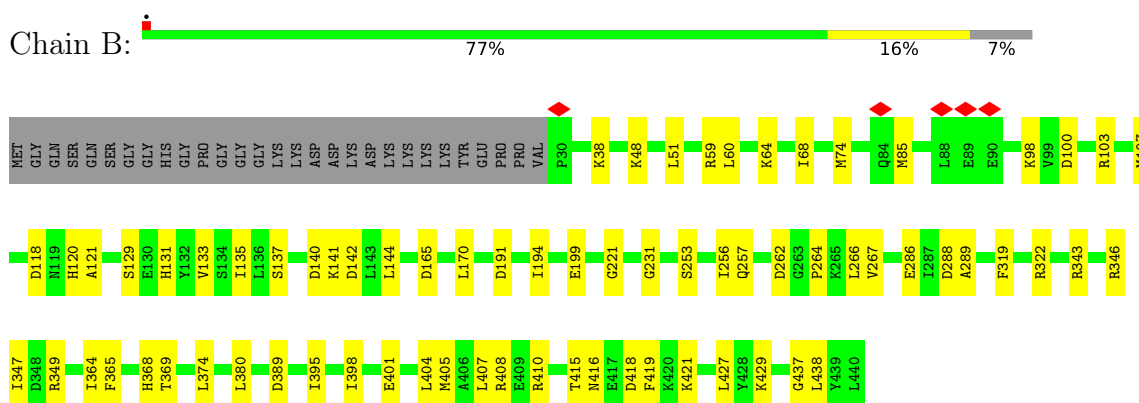
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

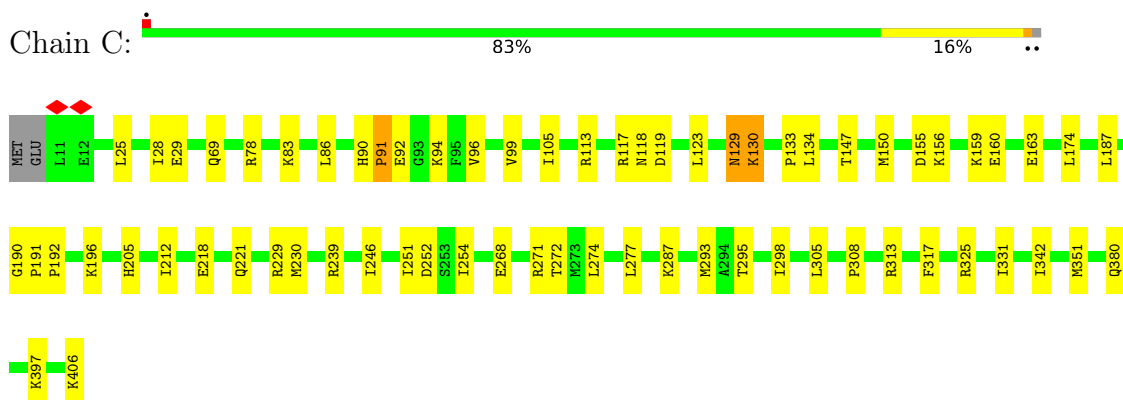
3 Residue-property plots

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

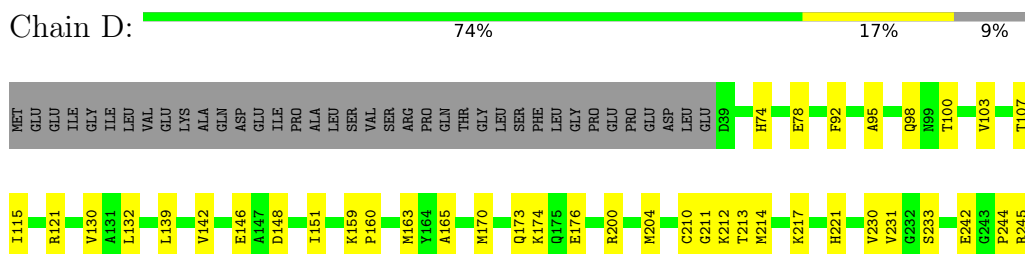
- Molecule 1: 26S protease regulatory subunit 4



- Molecule 2: Isoform 2 of 26S proteasome regulatory subunit 8



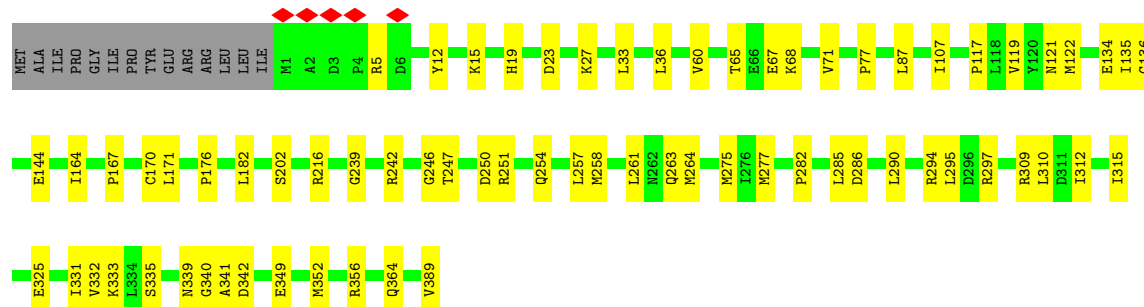
- Molecule 3: 26S protease regulatory subunit 6B





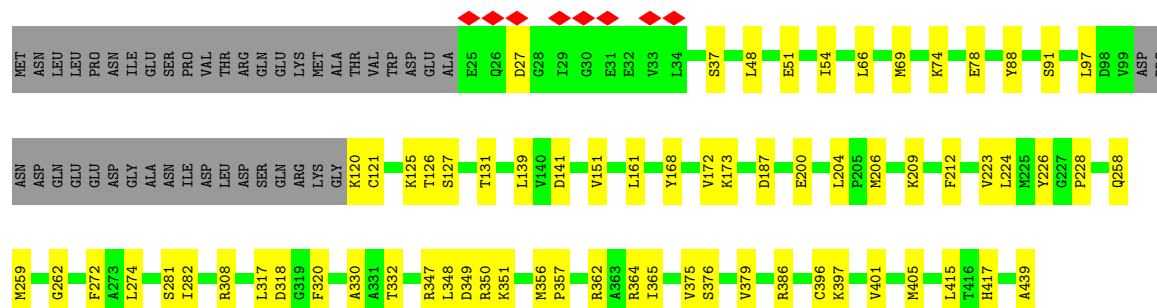
• Molecule 4: 26S proteasome regulatory subunit 10B

Chain E: 79% 18%



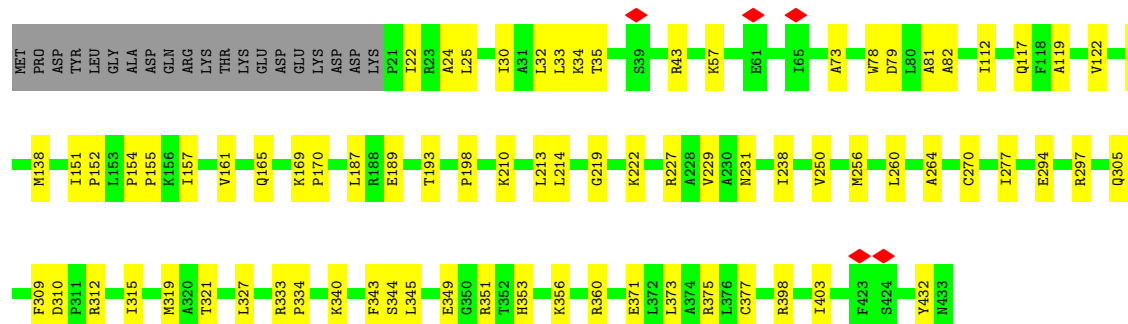
• Molecule 5: 26S protease regulatory subunit 6A

Chain F: 74% 16% 10%



• Molecule 6: 26S protease regulatory subunit 7

Chain A: 78% 18% 5%



• Molecule 7: Proteasome subunit alpha type-6

Chain G: 88% 9%



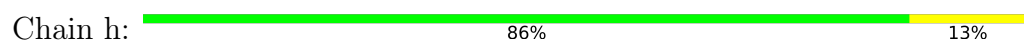
• Molecule 7: Proteasome subunit alpha type-6



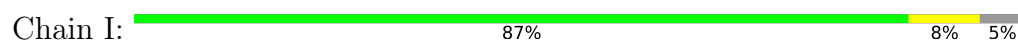
• Molecule 8: Proteasome subunit alpha type-2



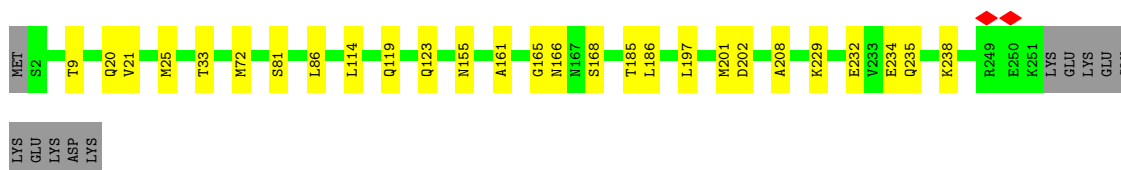
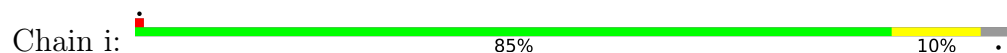
• Molecule 8: Proteasome subunit alpha type-2



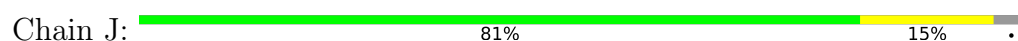
• Molecule 9: Proteasome subunit alpha type-4

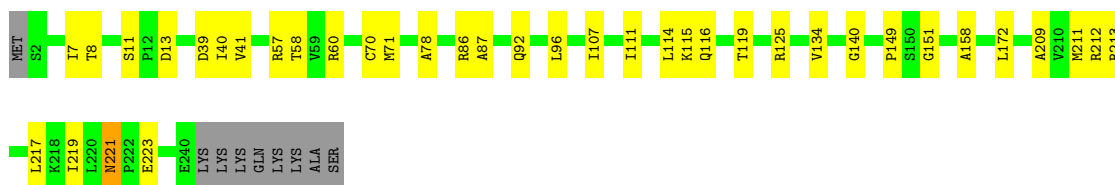


• Molecule 9: Proteasome subunit alpha type-4

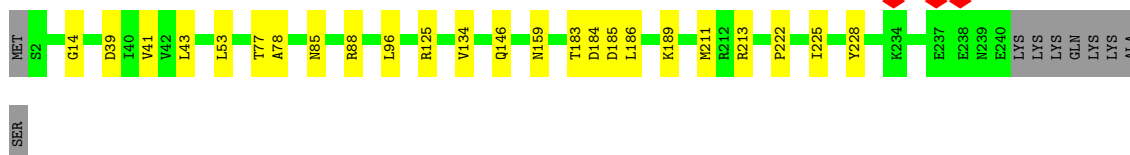
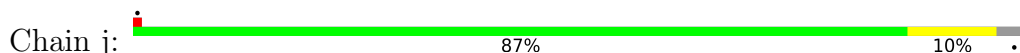


• Molecule 10: Proteasome subunit alpha type-7

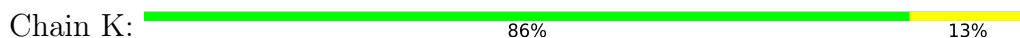




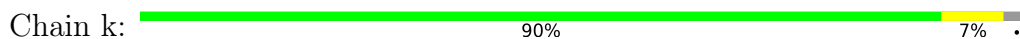
- Molecule 10: Proteasome subunit alpha type-7



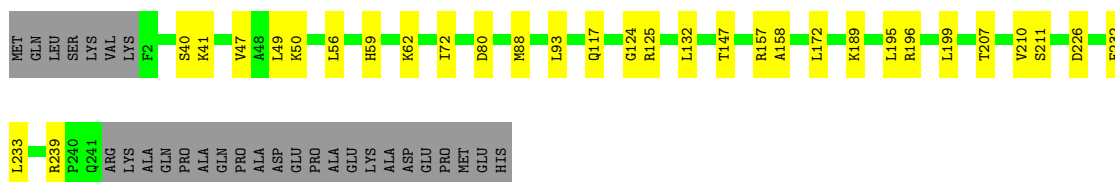
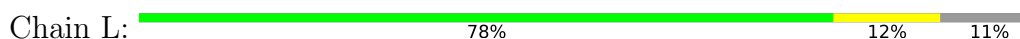
- Molecule 11: Proteasome subunit alpha type-5



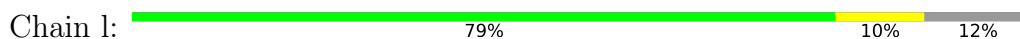
- Molecule 11: Proteasome subunit alpha type-5

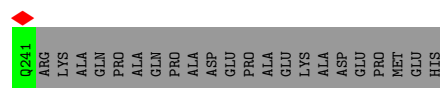


- Molecule 12: Isoform Long of Proteasome subunit alpha type-1



- Molecule 12: Isoform Long of Proteasome subunit alpha type-1





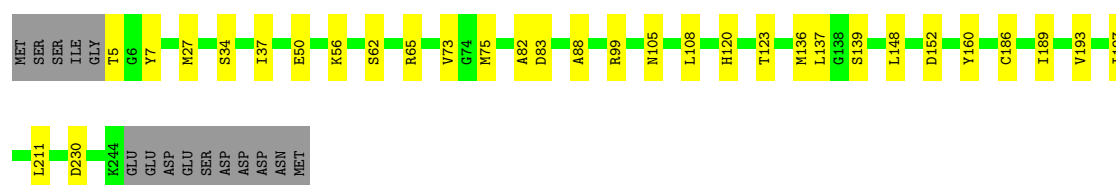
• Molecule 13: Proteasome subunit alpha type-3

Chain M: 85% 10% 5%



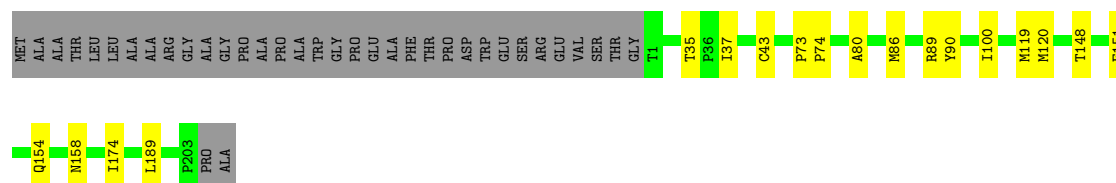
• Molecule 13: Proteasome subunit alpha type-3

Chain m: 82% 12% 6%



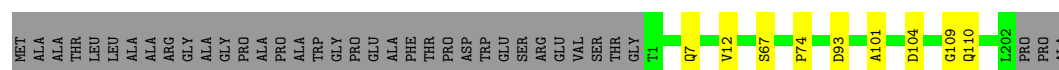
• Molecule 14: Proteasome subunit beta type-6

Chain N: 77% 8% 15%



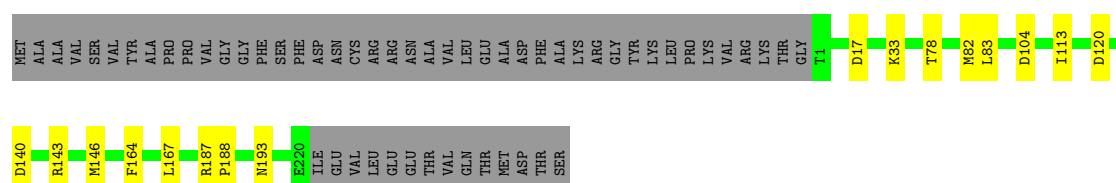
• Molecule 14: Proteasome subunit beta type-6

Chain n: 81% 15% 4%



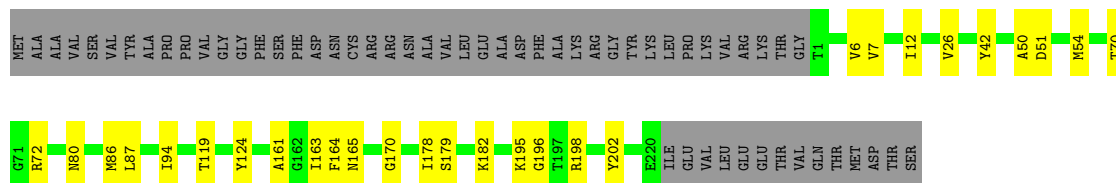
• Molecule 15: Proteasome subunit beta type-7

Chain O: 74% 6% 21%



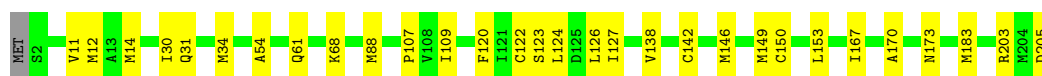
- Molecule 15: Proteasome subunit beta type-7

Chain o:  69% 10% 21%



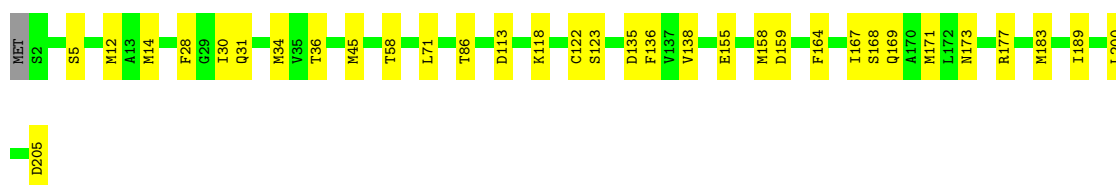
- Molecule 16: Proteasome subunit beta type-3

Chain P:  85% 15%



- Molecule 16: Proteasome subunit beta type-3

Chain p:  83% 16%



- Molecule 17: Proteasome subunit beta type-2

Chain Q:  85% 14%



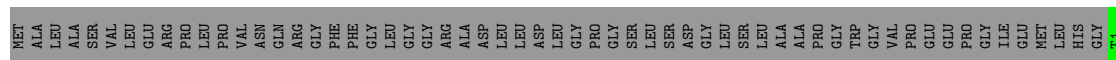
- Molecule 17: Proteasome subunit beta type-2

Chain q:  85% 14%



- Molecule 18: Proteasome subunit beta type-5

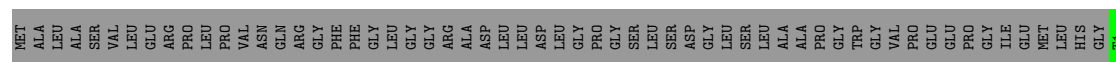
Chain R:  73% 24%





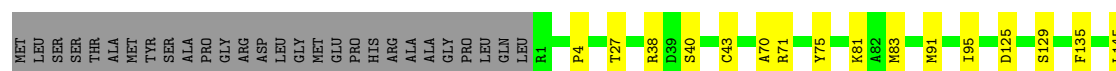
• Molecule 18: Proteasome subunit beta type-5

Chain r: 70% 7% 24%



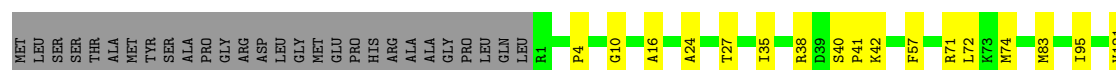
• Molecule 19: Proteasome subunit beta type-1

Chain S: 78% 10% 12%



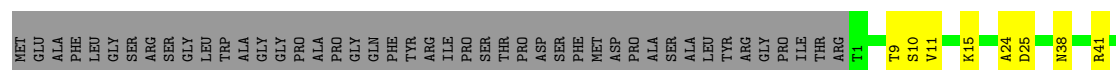
• Molecule 19: Proteasome subunit beta type-1

Chain s: 78% 10% 12%



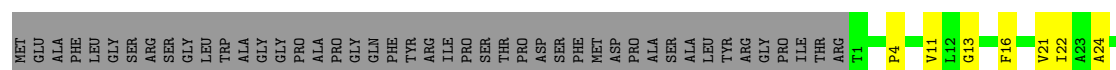
• Molecule 20: Proteasome subunit beta type-4

Chain T: 73% 9% 18%



• Molecule 20: Proteasome subunit beta type-4

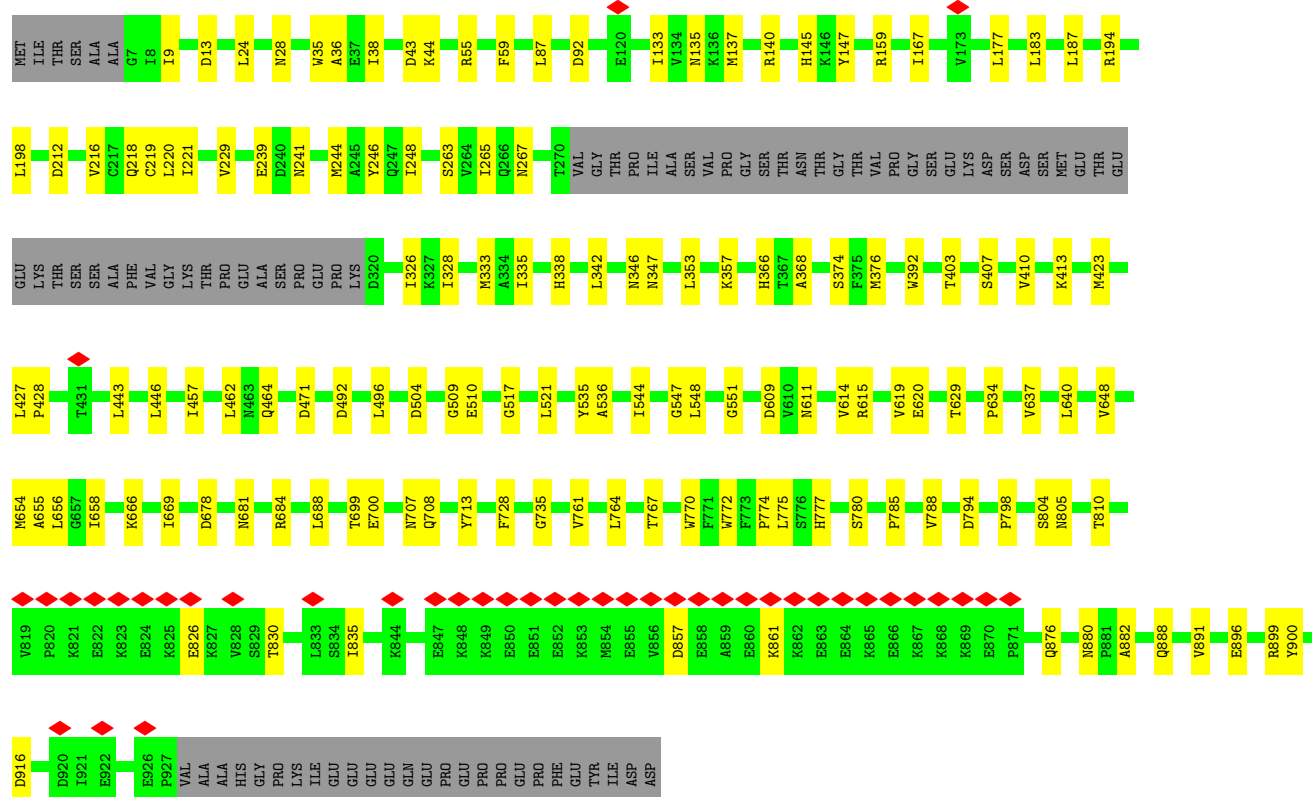
Chain t: 72% 10% 18%





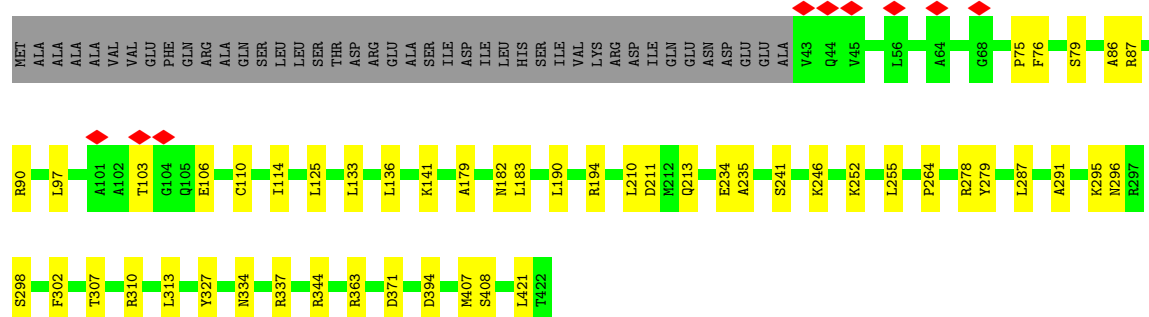
- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 77% 15% 8%



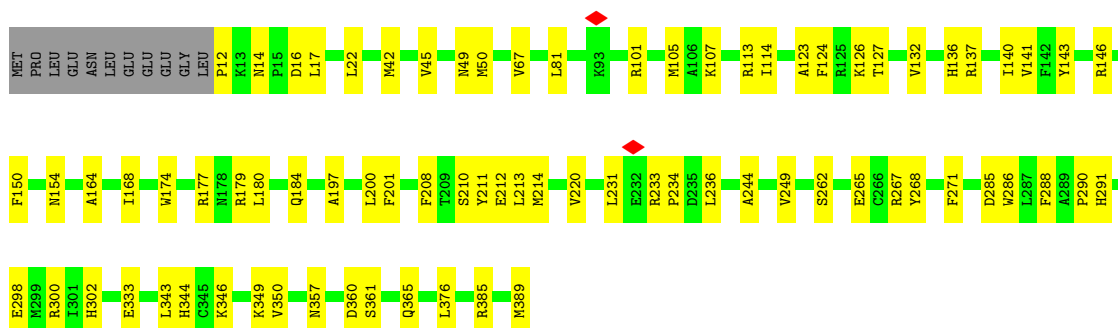
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 78% 12% 10%



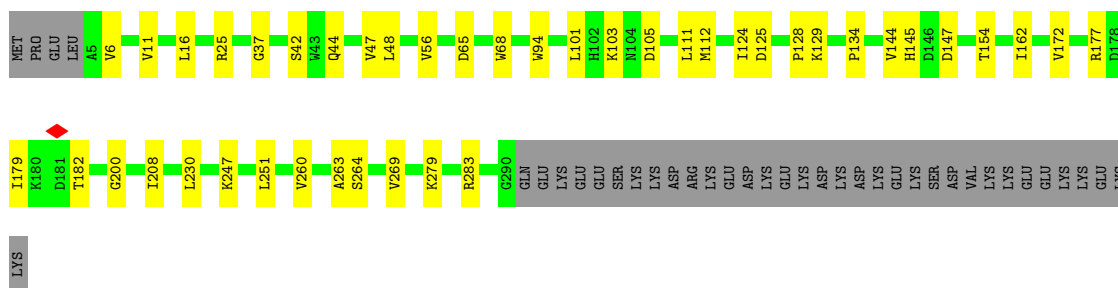
- Molecule 23: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 77% 20% 3%



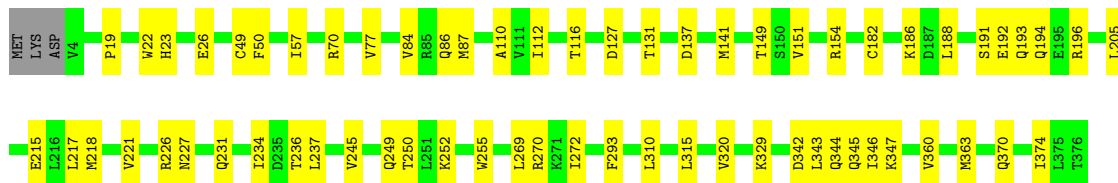
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 75% 13% 12%



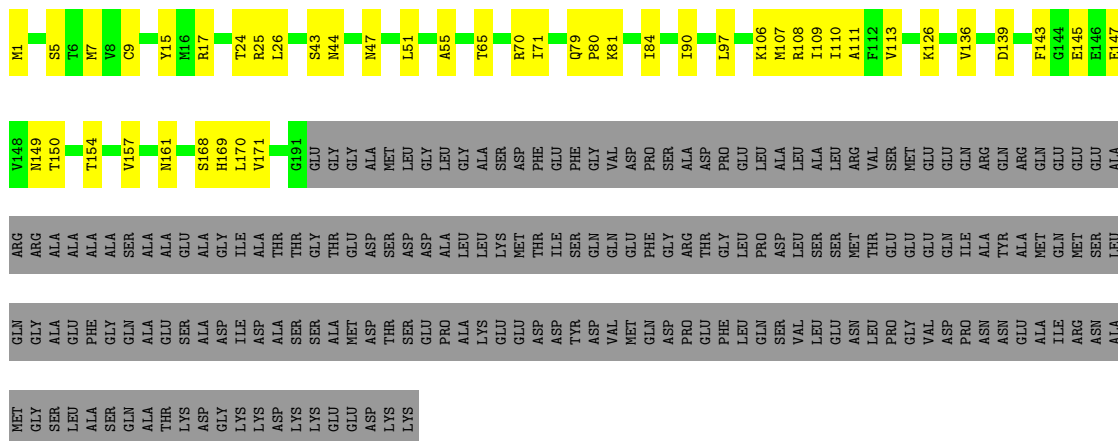
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 82% 17% .

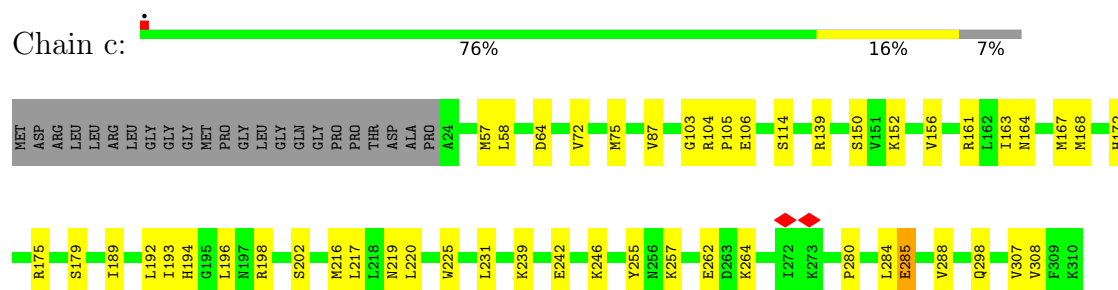


- Molecule 26: 26S proteasome non-ATPase regulatory subunit 4

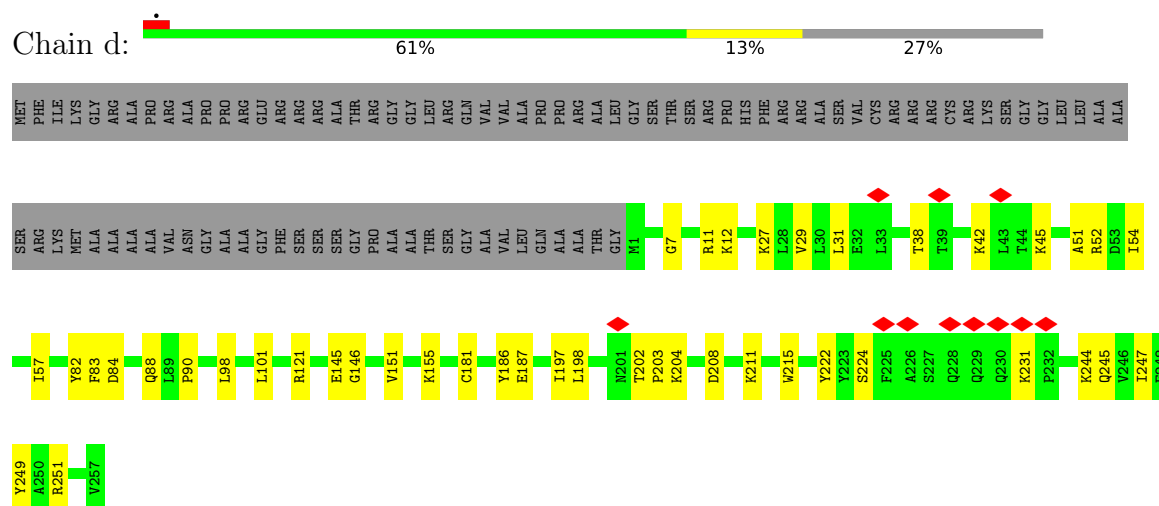
Chain b: 39% 12% 49%



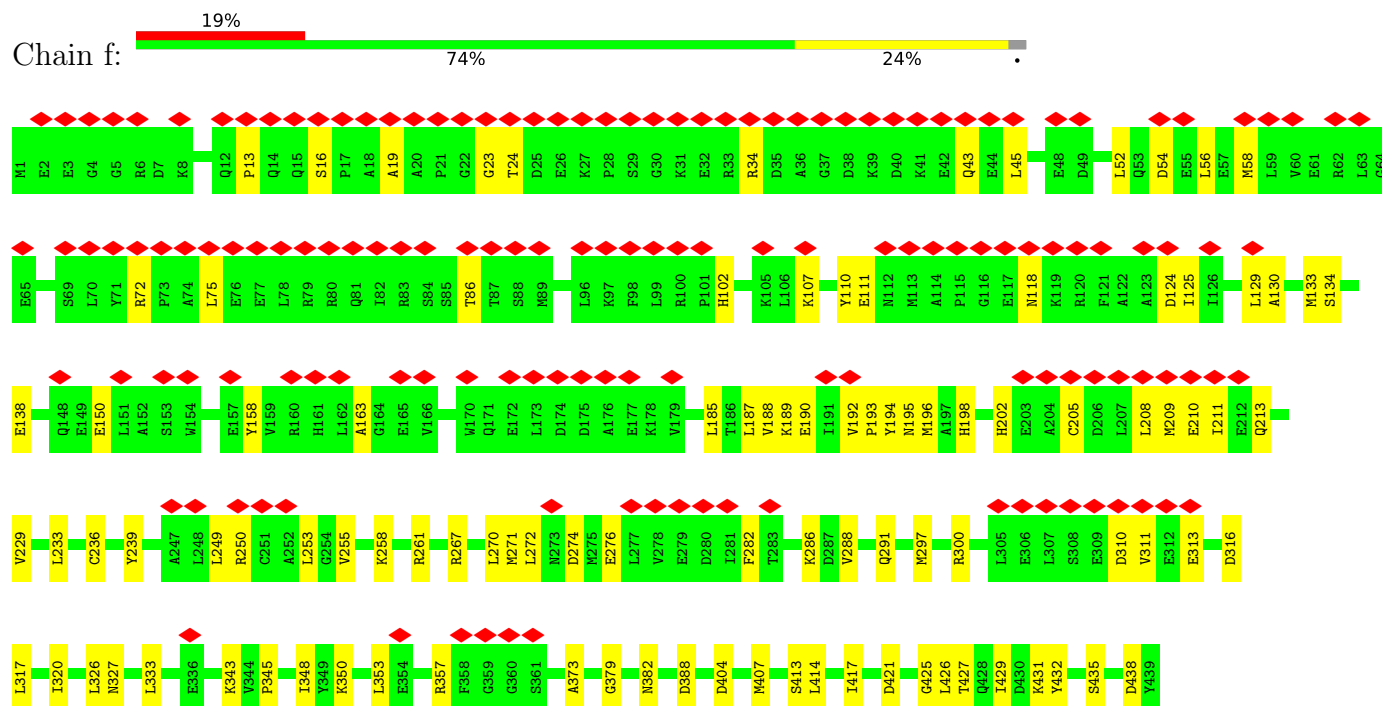
- Molecule 27: 26S proteasome non-ATPase regulatory subunit 14

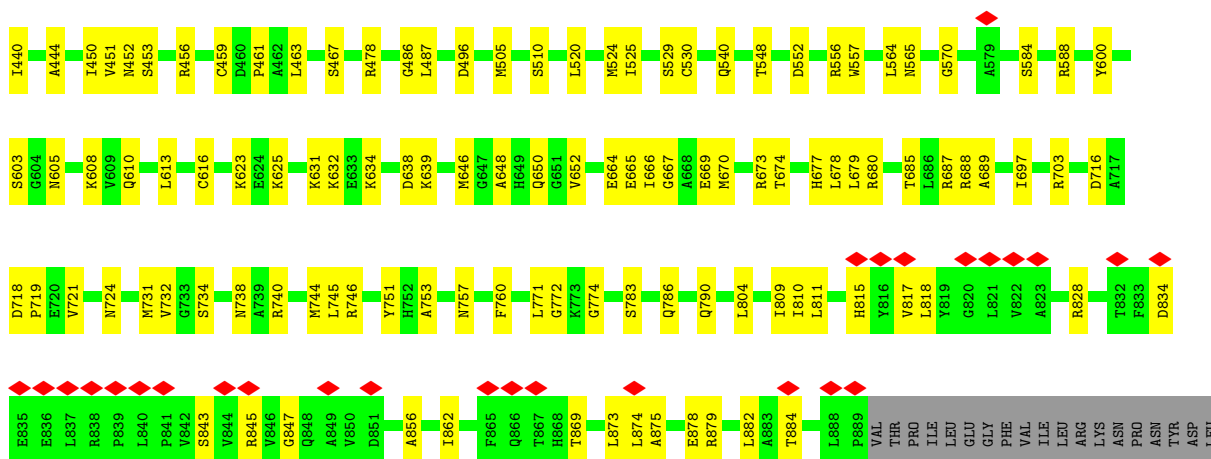


- Molecule 28: 26S proteasome non-ATPase regulatory subunit 8



- Molecule 29: 26S proteasome non-ATPase regulatory subunit 2





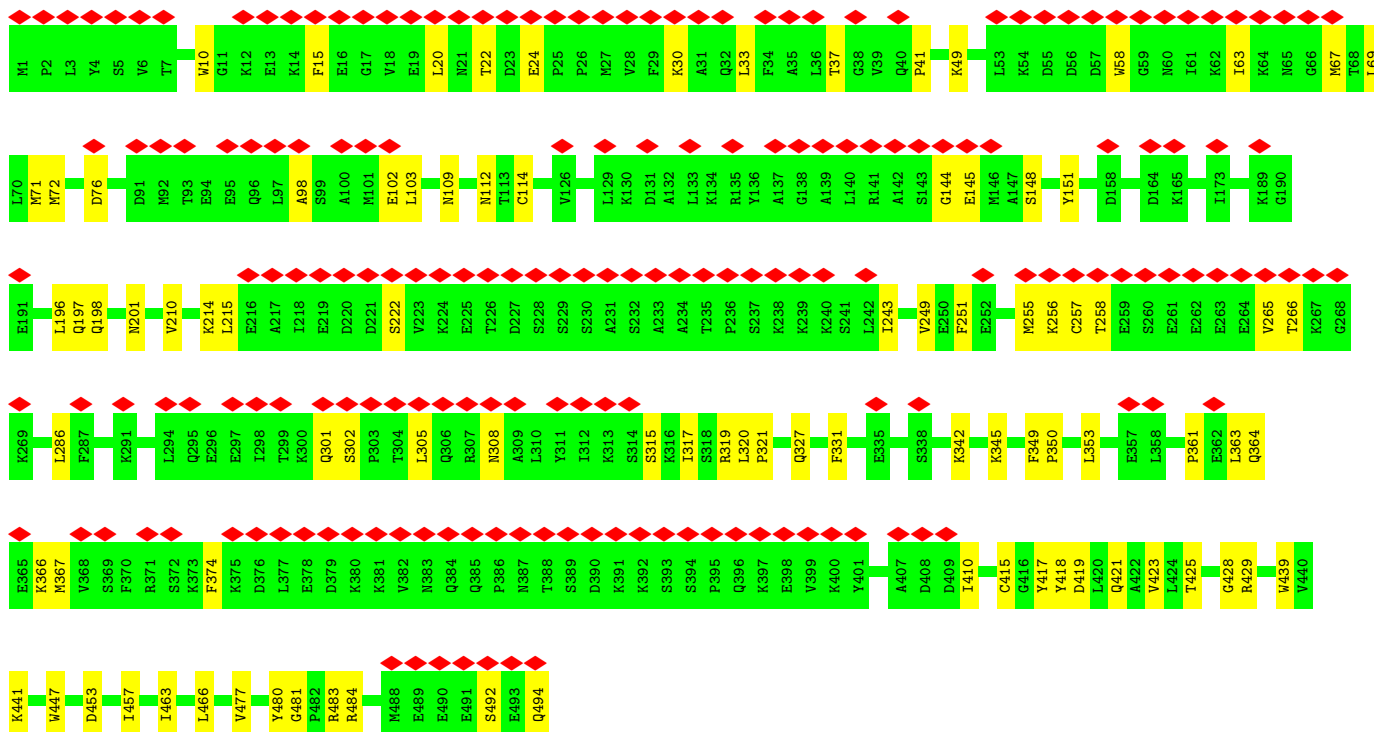
- Molecule 30: Substrate

Chain v: 100%

There are no outlier residues recorded for this chain.

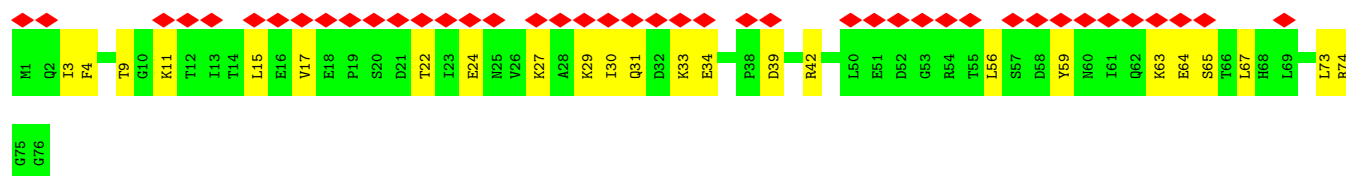
- Molecule 31: Ubiquitin carboxyl-terminal hydrolase 14

Chain x: 38% 82% 18%

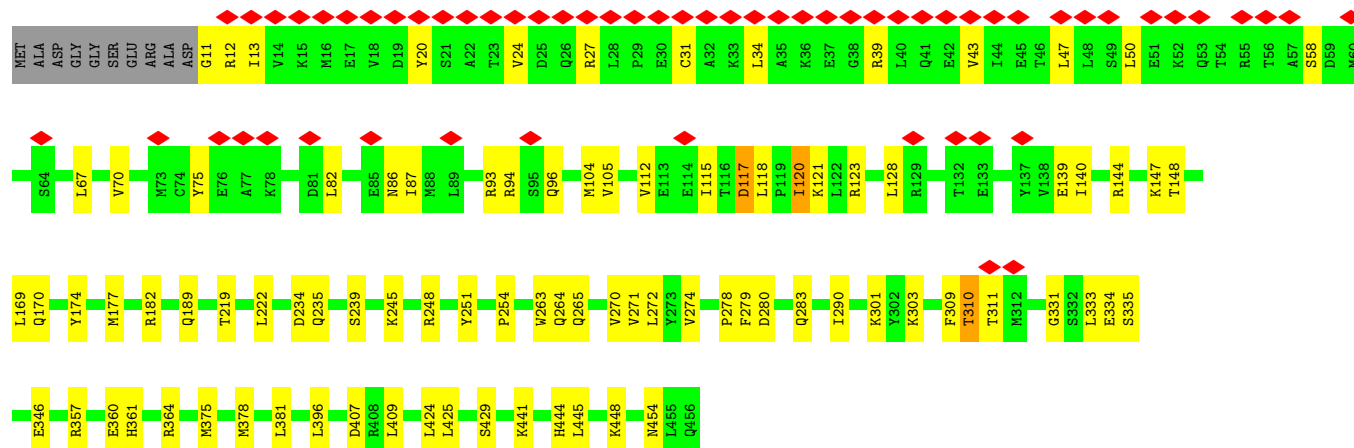
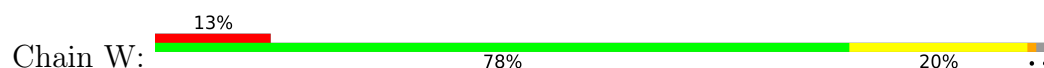


- Molecule 32: Ubiquitin

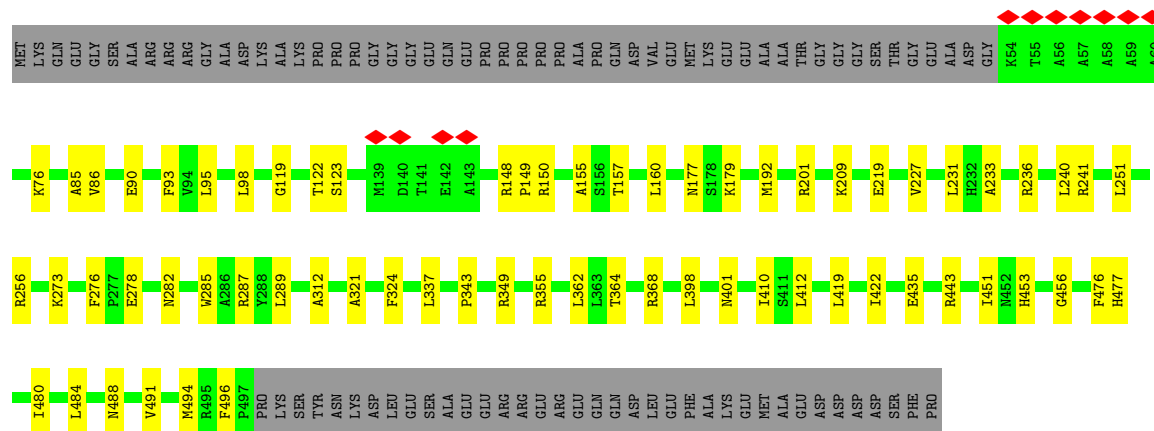
Chain y: 55% 68% 32%



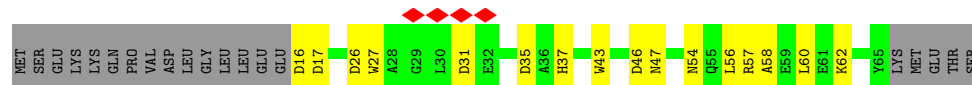
- Molecule 33: 26S proteasome non-ATPase regulatory subunit 12



- Molecule 34: 26S proteasome non-ATPase regulatory subunit 3



- Molecule 35: 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	142577	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	0.020	Depositor
Minimum map value	-0.004	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.16	0/3254	0.44	0/4388
2	C	0.19	0/3146	0.50	2/4226 (0.0%)
3	D	0.17	0/3090	0.44	0/4168
4	E	0.16	0/3145	0.43	0/4233
5	F	0.16	0/3137	0.43	0/4223
6	A	0.16	0/3283	0.43	0/4433
7	G	0.18	0/1901	0.39	0/2572
7	g	0.17	0/1913	0.37	0/2589
8	H	0.17	0/1840	0.39	0/2495
8	h	0.17	0/1844	0.38	0/2497
9	I	0.17	0/1963	0.35	0/2650
9	i	0.16	0/1985	0.33	0/2677
10	J	0.17	0/1887	0.41	0/2553
10	j	0.16	0/1887	0.41	0/2549
11	K	0.18	0/1841	0.37	0/2486
11	k	0.16	0/1809	0.36	0/2444
12	L	0.18	0/1911	0.35	0/2584
12	l	0.17	0/1896	0.35	0/2565
13	M	0.17	0/1925	0.34	0/2592
13	m	0.16	0/1916	0.35	0/2580
14	N	0.18	0/1548	0.33	0/2097
14	n	0.18	0/1536	0.33	0/2080
15	O	0.17	0/1672	0.40	0/2267
15	o	0.17	0/1686	0.38	0/2282
16	P	0.20	0/1616	0.39	0/2180
16	p	0.18	0/1620	0.40	0/2184
17	Q	0.17	0/1621	0.37	0/2194
17	q	0.19	0/1611	0.41	0/2182
18	R	0.17	0/1590	0.35	0/2147
18	r	0.18	0/1580	0.36	0/2135
19	S	0.18	0/1671	0.38	0/2252
19	s	0.19	0/1680	0.39	0/2264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.18	0/1716	0.38	0/2323
20	t	0.19	0/1720	0.40	0/2328
21	U	0.16	0/6945	0.44	0/9382
22	X	0.16	0/3053	0.40	0/4115
23	Y	0.18	0/3173	0.47	0/4273
24	Z	0.17	0/2324	0.43	0/3150
25	a	0.18	0/3053	0.48	0/4133
26	b	0.16	0/1478	0.41	0/2001
27	c	0.20	0/2302	0.54	1/3110 (0.0%)
28	d	0.22	0/2162	0.51	0/2919
29	f	0.20	0/6980	0.51	1/9433 (0.0%)
31	x	0.13	0/4002	0.37	0/5390
32	y	0.22	0/607	0.63	2/816 (0.2%)
33	W	0.20	0/3683	0.50	0/4952
34	V	0.16	0/3681	0.38	0/4969
35	e	0.16	0/437	0.41	0/595
All	All	0.17	0/112320	0.42	6/151657 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f	875	ALA	N-CA-C	-5.32	108.56	114.62
32	y	31	GLN	CA-CB-CG	5.14	124.39	114.10
32	y	31	GLN	N-CA-CB	5.09	118.16	110.28
2	C	397	LYS	CA-C-N	5.07	131.22	121.54
2	C	397	LYS	C-N-CA	5.07	131.22	121.54
27	c	114	SER	N-CA-C	5.03	116.51	108.41

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	B	3207	0	3278	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3105	0	3219	44	0
3	D	3040	0	3076	47	0
4	E	3097	0	3174	52	0
5	F	3098	0	3187	48	0
6	A	3229	0	3261	52	0
7	G	1867	0	1867	14	0
7	g	1879	0	1872	16	0
8	H	1801	0	1773	17	0
8	h	1805	0	1798	20	0
9	I	1933	0	1923	16	0
9	i	1955	0	1955	17	0
10	J	1861	0	1846	27	0
10	j	1861	0	1865	17	0
11	K	1813	0	1796	21	0
11	k	1782	0	1766	10	0
12	L	1876	0	1856	23	0
12	l	1861	0	1839	18	0
13	M	1890	0	1880	18	0
13	m	1881	0	1868	21	0
14	N	1521	0	1494	11	0
14	n	1510	0	1483	5	0
15	O	1645	0	1648	11	0
15	o	1659	0	1681	17	0
16	P	1587	0	1598	20	0
16	p	1591	0	1609	23	0
17	Q	1588	0	1584	20	0
17	q	1578	0	1569	21	0
18	R	1559	0	1523	6	0
18	r	1549	0	1506	13	0
19	S	1641	0	1639	17	0
19	s	1650	0	1645	17	0
20	T	1683	0	1662	14	0
20	t	1687	0	1666	19	0
21	U	6828	0	6884	88	0
22	X	3009	0	3113	33	0
23	Y	3115	0	3120	51	0
24	Z	2281	0	2312	36	0
25	a	2995	0	3012	42	0
26	b	1458	0	1505	33	0
27	c	2260	0	2276	37	0
28	d	2116	0	2146	27	0
29	f	6866	0	6866	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	v	180	0	45	0	0
31	x	3929	0	3915	58	0
32	y	601	0	629	16	0
33	W	3635	0	3762	60	0
34	V	3612	0	3682	44	0
35	e	425	0	328	15	0
36	B	31	0	12	2	0
36	C	31	0	12	0	0
36	D	31	0	12	3	0
37	E	27	0	12	6	0
37	F	27	0	12	1	0
38	c	1	0	0	0	0
All	All	110747	0	111061	1280	0

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

All (1280) 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)
10:J:221:ASN:HB2	10:J:223:GLU:OE1	1.78	0.83
23:Y:197:ALA:O	23:Y:201:PHE:HB2	1.77	0.83
4:E:340:GLY:HA3	37:E:501:ADP:N3	2.01	0.76
4:E:341:ALA:HB2	37:E:501:ADP:H4'	1.68	0.74
29:f:267:ARG:O	29:f:271:MET:HB3	1.88	0.73
2:C:239:ARG:HH12	2:C:287:LYS:H	1.36	0.73
4:E:136:GLY:H	37:E:501:ADP:HN62	1.39	0.70
24:Z:260:VAL:HG21	34:V:476:PHE:HB3	1.71	0.70
6:A:161:VAL:O	6:A:165:GLN:HB2	1.92	0.70
28:d:27:LYS:O	28:d:31:LEU:HB2	1.91	0.70
3:D:230:VAL:HB	3:D:264:ILE:HG22	1.75	0.68
14:n:12:VAL:HG11	14:n:101:ALA:HB1	1.76	0.68
19:s:4:PRO:HB2	20:t:100:ARG:HH21	1.59	0.68
9:I:174:MET:HE3	9:I:196:VAL:HG22	1.76	0.67
8:h:119:GLN:HG3	9:i:81:SER:HB2	1.77	0.67
13:M:77:VAL:HG23	13:M:135:PHE:HB3	1.77	0.67
28:d:42:LYS:HG3	28:d:45:LYS:HD2	1.77	0.66
5:F:187:ASP:O	5:F:364:ARG:NH1	2.29	0.65
31:x:286:LEU:HD13	31:x:349:PHE:HB3	1.78	0.65
33:W:170:GLN:HA	33:W:182:ARG:HH22	1.62	0.65
29:f:487:LEU:HD22	29:f:524:MET:HE1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:34:SER:HB3	13:m:65:ARG:HH12	1.62	0.64
5:F:357:PRO:HG2	5:F:362:ARG:HE	1.62	0.64
33:W:219:THR:HG23	33:W:222:LEU:H	1.62	0.64
29:f:150:GLU:HB3	29:f:192:VAL:HG11	1.80	0.63
21:U:346:ASN:HD22	21:U:347:ASN:N	1.95	0.63
22:X:394:ASP:OD2	23:Y:365:GLN:NE2	2.30	0.63
16:P:142:CYS:HB2	16:P:146:MET:HE2	1.81	0.63
29:f:288:VAL:HA	29:f:291:GLN:HB3	1.80	0.63
12:L:50:LYS:HD2	12:L:211:SER:HB2	1.81	0.63
16:p:168:SER:HB2	16:p:200:LEU:HD21	1.81	0.63
33:W:264:GLN:OE1	33:W:265:GLN:NE2	2.32	0.63
23:Y:385:ARG:HB3	34:V:282:ASN:HD21	1.63	0.62
16:p:12:MET:HG3	16:p:138:VAL:HG12	1.81	0.62
31:x:201:ASN:HB3	32:y:42:ARG:HH12	1.63	0.62
11:k:202:LEU:HD13	11:k:215:ILE:HD11	1.81	0.62
18:r:114:VAL:HG12	18:r:120:ARG:HB3	1.82	0.62
31:x:109:ASN:ND2	31:x:114:CYS:SG	2.72	0.62
24:Z:263:ALA:HB1	27:c:288:VAL:HG13	1.80	0.62
28:d:181:CYS:HB2	34:V:443:ARG:HH21	1.64	0.62
25:a:112:ILE:HG21	25:a:151:VAL:HG23	1.80	0.62
26:b:97:LEU:HD22	26:b:109:ILE:HG23	1.81	0.62
21:U:805:ASN:HB2	21:U:891:VAL:HB	1.81	0.62
28:d:181:CYS:HG	28:d:186:TYR:HH	1.45	0.62
20:T:92:LEU:HD12	20:T:112:ILE:HD11	1.82	0.61
2:C:212:ILE:HD12	2:C:246:ILE:HG12	1.82	0.61
10:J:87:ALA:HB2	10:J:111:ILE:HD11	1.83	0.61
29:f:811:LEU:HD21	29:f:862:ILE:HD13	1.81	0.61
21:U:810:THR:O	21:U:888:GLN:NE2	2.34	0.61
29:f:487:LEU:HD12	29:f:804:LEU:HB2	1.83	0.61
34:V:419:LEU:HD12	34:V:456:GLY:HA2	1.81	0.61
10:J:96:LEU:HB2	17:Q:62:LYS:HG3	1.82	0.61
29:f:666:ILE:HG13	29:f:703:ARG:HH22	1.66	0.61
10:j:43:LEU:HD11	10:j:134:VAL:HG21	1.83	0.61
8:H:203:MET:HA	8:H:207:ASN:HD22	1.66	0.61
25:a:70:ARG:HB3	26:b:17:ARG:HB3	1.82	0.61
29:f:233:LEU:HA	29:f:236:CYS:HB2	1.83	0.61
33:W:75:TYR:OH	33:W:123:ARG:NH1	2.33	0.61
3:D:170:MET:HE1	3:D:174:LYS:HB3	1.82	0.60
33:W:144:ARG:HD2	33:W:147:LYS:HD3	1.82	0.60
23:Y:346:LYS:NZ	34:V:412:LEU:O	2.34	0.60
27:c:104:ARG:NH1	27:c:105:PRO:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LYS:HA	1:B:144:LEU:HD13	1.84	0.60
3:D:384:MET:HG3	4:E:297:ARG:HH12	1.66	0.60
25:a:215:GLU:HA	25:a:218:MET:HB2	1.83	0.60
2:C:117:ARG:HE	27:c:189:ILE:HD11	1.65	0.60
21:U:9:ILE:HD11	21:U:38:ILE:HG22	1.83	0.60
12:L:189:LYS:NZ	12:L:232:PHE:O	2.35	0.60
21:U:263:SER:O	21:U:267:ASN:ND2	2.34	0.60
23:Y:361:SER:O	23:Y:365:GLN:NE2	2.34	0.60
29:f:326:LEU:HA	29:f:879:ARG:HH22	1.65	0.60
14:N:37:ILE:HD11	14:N:43:CYS:HB3	1.83	0.60
25:a:194:GLN:O	25:a:226:ARG:NH2	2.35	0.60
22:X:110:CYS:HB3	22:X:133:LEU:HD21	1.83	0.60
1:B:319:PHE:H	1:B:322:ARG:HH22	1.50	0.60
25:a:49:CYS:SG	25:a:50:PHE:N	2.74	0.59
17:q:38:MET:HB2	17:q:42:ILE:HB	1.83	0.59
33:W:34:LEU:HB2	33:W:39:ARG:HH12	1.66	0.59
9:I:218:ARG:NH1	9:I:223:THR:OG1	2.35	0.59
8:H:205:GLU:HB3	8:H:227:LYS:HB3	1.84	0.59
13:M:93:GLU:OE2	13:M:97:ASN:ND2	2.35	0.59
29:f:664:GLU:HG3	29:f:667:GLY:H	1.68	0.59
16:p:12:MET:HE3	16:p:171:MET:HG2	1.85	0.59
19:s:35:ILE:O	20:t:151:ARG:NH2	2.33	0.59
3:D:148:ASP:HA	3:D:151:ILE:HB	1.84	0.59
8:H:10:LEU:HD11	8:H:129:PRO:HD3	1.85	0.59
20:T:9:THR:HG22	20:T:10:SER:H	1.68	0.59
7:g:120:ASP:OD1	8:h:84:ARG:NH1	2.35	0.59
21:U:509:GLY:HA3	21:U:544:ILE:HG12	1.85	0.59
24:Z:162:ILE:HG21	27:c:220:LEU:HB3	1.85	0.59
29:f:459:CYS:HA	31:x:49:LYS:HG2	1.85	0.59
2:C:86:LEU:HD22	2:C:94:LYS:HB3	1.85	0.59
29:f:297:MET:HG2	29:f:456:ARG:HG3	1.84	0.59
24:Z:65:ASP:HB2	24:Z:103:LYS:HD2	1.85	0.59
31:x:441:LYS:HA	31:x:447:TRP:HA	1.83	0.59
3:D:248:ARG:NH1	3:D:295:GLN:OE1	2.35	0.58
5:F:88:TYR:HB2	6:A:122:VAL:HB	1.85	0.58
21:U:24:LEU:O	21:U:28:ASN:ND2	2.34	0.58
29:f:425:GLY:HA3	29:f:451:VAL:HG21	1.83	0.58
29:f:631:LYS:HA	29:f:634:LYS:HB2	1.85	0.58
2:C:99:VAL:HG12	2:C:123:LEU:HD13	1.85	0.58
12:L:157:ARG:NH2	13:M:56:LYS:O	2.35	0.58
13:M:211:LEU:O	13:M:232:ARG:NH2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:251:LEU:HD12	33:W:425:LEU:HD12	1.85	0.58
31:x:30:LYS:HB3	31:x:41:PRO:HB3	1.86	0.58
31:x:317:ILE:HD12	31:x:320:LEU:HB3	1.86	0.58
35:e:58:ALA:O	35:e:62:LYS:HB2	2.03	0.58
16:P:109:ILE:HB	16:P:122:CYS:HB3	1.86	0.58
17:Q:83:PHE:O	17:Q:87:ASN:ND2	2.37	0.58
27:c:164:ASN:HB3	27:c:167:MET:HE1	1.86	0.58
29:f:685:THR:H	29:f:689:ALA:HB3	1.68	0.58
2:C:187:LEU:HD21	2:C:298:ILE:HD11	1.84	0.58
21:U:413:LYS:NZ	21:U:780:SER:O	2.35	0.58
22:X:190:LEU:HD12	22:X:213:GLN:HG3	1.85	0.58
10:j:39:ASP:OD1	10:j:213:ARG:NH1	2.36	0.58
19:S:194:ARG:NH2	19:S:196:CYS:SG	2.76	0.58
21:U:133:ILE:HG22	21:U:137:MET:HE1	1.84	0.58
20:t:107:TRP:HA	20:t:127:MET:HE2	1.86	0.58
32:y:33:LYS:HG3	32:y:34:GLU:HG2	1.86	0.58
3:D:268:ASP:HB2	4:E:258:MET:HE1	1.85	0.58
27:c:139:ARG:HA	27:c:161:ARG:HH21	1.69	0.58
6:A:351:ARG:NH1	6:A:377:CYS:O	2.37	0.57
21:U:446:LEU:HB3	21:U:457:ILE:HD11	1.84	0.57
25:a:50:PHE:O	25:a:86:GLN:NE2	2.36	0.57
5:F:318:ASP:OD1	5:F:347:ARG:NH1	2.38	0.57
8:H:122:THR:HG22	8:H:129:PRO:HB3	1.87	0.57
31:x:321:PRO:O	31:x:418:TYR:OH	2.22	0.57
18:R:192:VAL:HG11	16:p:205:ASP:HB3	1.86	0.57
4:E:325:GLU:O	4:E:364:GLN:NE2	2.36	0.57
23:Y:184:GLN:NE2	23:Y:200:LEU:O	2.37	0.57
29:f:680:ARG:NH2	29:f:760:PHE:O	2.38	0.57
33:W:105:VAL:HB	33:W:140:ILE:HG21	1.87	0.57
27:c:242:GLU:O	27:c:246:LYS:NZ	2.38	0.57
29:f:189:LYS:HG3	29:f:190:GLU:HG3	1.86	0.57
29:f:634:LYS:HA	29:f:674:THR:HG22	1.87	0.57
33:W:360:GLU:HG3	33:W:396:LEU:HD21	1.85	0.57
13:M:8:ASP:O	13:M:22:GLN:NE2	2.38	0.57
26:b:26:LEU:HD11	26:b:80:PRO:HG3	1.86	0.57
26:b:147:GLU:HG3	26:b:150:THR:HG22	1.86	0.57
10:j:41:VAL:HB	10:j:211:MET:HB2	1.85	0.57
20:t:54:SER:O	20:t:108:ASN:ND2	2.37	0.57
2:C:218:GLU:O	2:C:221:GLN:NE2	2.38	0.57
23:Y:101:ARG:NH1	23:Y:127:THR:OG1	2.37	0.57
29:f:209:MET:HG2	29:f:211:ILE:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.87	0.57
31:x:364:GLN:HA	31:x:367:MET:HB2	1.87	0.57
34:V:491:VAL:HA	34:V:494:MET:HE3	1.86	0.57
13:M:108:LEU:HD11	13:M:137:LEU:HB3	1.87	0.57
21:U:764:LEU:O	21:U:767:THR:OG1	2.21	0.57
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.87	0.57
5:F:281:SER:OG	5:F:282:ILE:N	2.38	0.56
6:A:30:ILE:HG13	6:A:34:LYS:HD3	1.87	0.56
23:Y:132:VAL:O	23:Y:137:ARG:NH2	2.37	0.56
28:d:7:GLY:O	28:d:11:ARG:NH1	2.36	0.56
28:d:145:GLU:HG2	28:d:146:GLY:H	1.70	0.56
31:x:69:LEU:HB3	31:x:71:MET:HE3	1.86	0.56
10:J:140:GLY:O	10:J:213:ARG:NH1	2.39	0.56
22:X:194:ARG:HH21	22:X:210:LEU:HG	1.69	0.56
22:X:363:ARG:NH2	23:Y:265:GLU:O	2.37	0.56
23:Y:300:ARG:NH1	23:Y:333:GLU:OE2	2.38	0.56
24:Z:16:LEU:HD22	24:Z:124:ILE:HD12	1.86	0.56
29:f:249:LEU:HD23	29:f:253:LEU:HD11	1.87	0.56
34:V:355:ARG:NH2	35:e:31:ASP:OD1	2.37	0.56
2:C:268:GLU:HA	2:C:271:ARG:HE	1.71	0.56
29:f:311:VAL:HG12	29:f:313:GLU:H	1.69	0.56
10:j:183:THR:HG22	10:j:185:ASP:H	1.71	0.56
12:l:132:LEU:HB2	12:l:147:THR:HB	1.88	0.56
21:U:896:GLU:O	21:U:899:ARG:NH2	2.39	0.56
1:B:51:LEU:HD21	29:f:646:MET:HB2	1.88	0.56
3:D:200:ARG:NH1	3:D:302:ASN:O	2.39	0.56
5:F:272:PHE:HB3	5:F:320:PHE:HZ	1.71	0.56
21:U:216:VAL:HG11	21:U:248:ILE:HG23	1.88	0.56
29:f:190:GLU:HB3	29:f:193:PRO:HG2	1.87	0.56
15:o:163:ILE:HG12	15:o:170:GLY:HA2	1.86	0.56
31:x:24:GLU:O	31:x:58:TRP:NE1	2.38	0.56
23:Y:285:ASP:HB3	23:Y:288:PHE:HB3	1.86	0.56
25:a:186:LYS:HG2	25:a:221:VAL:HG23	1.88	0.56
29:f:107:LYS:O	29:f:111:GLU:HB3	2.06	0.56
29:f:811:LEU:HD12	29:f:878:GLU:HA	1.88	0.56
6:A:344:SER:OG	6:A:345:LEU:N	2.39	0.55
31:x:301:GLN:HA	31:x:308:ASN:HA	1.87	0.55
6:A:375:ARG:HH11	11:K:173:ALA:HB2	1.71	0.55
29:f:731:MET:O	29:f:746:ARG:NH1	2.39	0.55
7:g:158:GLY:O	8:h:84:ARG:NH2	2.40	0.55
15:o:7:VAL:HG12	15:o:12:ILE:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:W:87:ILE:HG21	33:W:123:ARG:HH22	1.71	0.55
34:V:85:ALA:HB2	34:V:93:PHE:HB2	1.87	0.55
34:V:177:ASN:O	34:V:179:LYS:NZ	2.39	0.55
1:B:415:THR:HG23	1:B:418:ASP:H	1.71	0.55
6:A:238:ILE:HG13	6:A:260:LEU:HD21	1.88	0.55
24:Z:37:GLY:HA2	24:Z:56:VAL:HG12	1.88	0.55
25:a:370:GLN:HG3	28:d:244:LYS:HD3	1.88	0.55
27:c:194:HIS:O	27:c:198:ARG:NH2	2.38	0.55
9:i:155:ASN:ND2	10:j:77:THR:OG1	2.39	0.55
15:o:51:ASP:HB3	15:o:94:ILE:HG23	1.88	0.55
16:p:45:MET:HE3	16:p:71:LEU:HD22	1.89	0.55
21:U:772:TRP:HB3	21:U:775:LEU:HD13	1.88	0.55
23:Y:49:ASN:HA	23:Y:114:ILE:HG23	1.88	0.55
26:b:90:ILE:HD11	26:b:109:ILE:HD12	1.89	0.55
19:s:27:THR:HB	19:s:40:SER:H	1.72	0.55
1:B:98:LYS:NZ	6:A:82:ALA:O	2.39	0.55
20:T:11:VAL:HG13	20:T:24:ALA:HB2	1.88	0.55
20:T:41:ARG:NH1	20:T:53:ALA:O	2.39	0.55
24:Z:200:GLY:HA3	27:c:225:TRP:HE1	1.71	0.55
29:f:102:HIS:NE2	29:f:133:MET:SD	2.80	0.55
31:x:421:GLN:HG2	31:x:441:LYS:HE2	1.88	0.55
32:y:9:THR:HG23	32:y:11:LYS:HG2	1.89	0.55
13:m:73:VAL:HG22	13:m:139:SER:HB2	1.89	0.55
33:W:303:LYS:O	33:W:310:THR:OG1	2.25	0.55
26:b:44:ASN:HB3	26:b:47:ASN:HB2	1.88	0.55
29:f:845:ARG:HD3	29:f:847:GLY:H	1.71	0.55
31:x:353:LEU:HB3	31:x:418:TYR:HB2	1.88	0.55
17:Q:166:GLU:HB2	18:r:141:ARG:HH21	1.72	0.55
7:g:132:ARG:NH1	13:m:123:THR:O	2.40	0.55
26:b:24:THR:HG22	26:b:26:LEU:H	1.71	0.55
13:m:5:THR:HG22	13:m:7:TYR:H	1.72	0.55
3:D:342:ARG:NH2	22:X:234:GLU:OE2	2.39	0.55
4:E:171:LEU:HB2	4:E:295:LEU:HD22	1.89	0.55
4:E:171:LEU:HD22	4:E:295:LEU:HD13	1.88	0.55
21:U:770:TRP:O	27:c:179:SER:OG	2.25	0.55
26:b:161:ASN:ND2	26:b:168:SER:OG	2.38	0.55
33:W:82:LEU:O	33:W:86:ASN:ND2	2.39	0.55
16:P:149:MET:HE2	16:P:173:ASN:HB2	1.89	0.54
21:U:265:ILE:HG23	21:U:326:ILE:HD12	1.88	0.54
17:q:26:VAL:HG21	18:r:136:TYR:HE2	1.70	0.54
33:W:251:TYR:HE1	33:W:270:VAL:HG21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:231:VAL:HG12	3:D:233:SER:H	1.71	0.54
6:A:157:ILE:HG21	6:A:256:MET:HE3	1.88	0.54
34:V:287:ARG:NH2	35:e:17:ASP:OD2	2.40	0.54
6:A:305:GLN:O	6:A:309:PHE:HB2	2.08	0.54
24:Z:125:ASP:HB3	24:Z:128:PRO:HD2	1.90	0.54
9:i:208:ALA:HB2	9:i:234:GLU:HB3	1.90	0.54
32:y:39:ASP:OD2	32:y:74:ARG:NH1	2.41	0.54
33:W:34:LEU:O	33:W:39:ARG:NH1	2.40	0.54
6:A:250:VAL:HG21	6:A:297:ARG:HG3	1.88	0.54
15:O:83:LEU:HD22	15:O:113:ILE:HD13	1.90	0.54
21:U:521:LEU:HD21	21:U:761:VAL:HG21	1.89	0.54
1:B:401:GLU:HG3	1:B:405:MET:HE1	1.88	0.54
26:b:107:MET:HE3	26:b:136:VAL:HG22	1.89	0.54
29:f:584:SER:HB2	29:f:588:ARG:HB3	1.88	0.54
8:h:51:LYS:NZ	8:h:200:GLU:O	2.41	0.54
12:l:200:PRO:O	12:l:239:ARG:NH2	2.40	0.54
3:D:332:GLU:HG3	3:D:334:PRO:HD3	1.88	0.54
2:C:221:GLN:HE22	2:C:230:MET:HG3	1.72	0.54
16:P:203:ARG:NH1	16:P:205:ASP:OD2	2.40	0.54
21:U:135:ASN:OD1	21:U:159:ARG:NH2	2.41	0.54
23:Y:123:ALA:HA	23:Y:126:LYS:HE3	1.90	0.54
28:d:208:ASP:HA	28:d:211:LYS:HD2	1.89	0.54
1:B:343:ARG:HH22	1:B:346:ARG:HH21	1.55	0.54
20:T:38:ASN:OD1	20:T:186:ARG:NH2	2.38	0.54
34:V:321:ALA:HB1	34:V:324:PHE:HB3	1.88	0.54
6:A:170:PRO:O	6:A:231:ASN:ND2	2.41	0.54
21:U:620:GLU:HA	21:U:655:ALA:HB2	1.89	0.54
23:Y:344:HIS:ND1	23:Y:357:ASN:O	2.31	0.54
24:Z:247:LYS:HD3	33:W:424:LEU:HB3	1.89	0.54
2:C:254:ILE:HD11	2:C:272:THR:HB	1.90	0.53
4:E:309:ARG:HD2	4:E:332:VAL:HG13	1.90	0.53
5:F:172:VAL:HG11	5:F:274:LEU:HD23	1.90	0.53
9:I:108:GLU:OE1	10:J:57:ARG:NH2	2.40	0.53
34:V:368:ARG:NH1	35:e:43:TRP:O	2.41	0.53
25:a:227:ASN:O	25:a:231:GLN:NE2	2.40	0.53
5:F:330:ALA:HB3	5:F:348:LEU:HD11	1.91	0.53
23:Y:141:VAL:HG11	23:Y:164:ALA:HB2	1.89	0.53
25:a:250:THR:HG21	25:a:272:ILE:HD13	1.90	0.53
29:f:282:PHE:HA	29:f:286:LYS:HB2	1.89	0.53
29:f:486:GLY:HA2	29:f:525:ILE:HD11	1.89	0.53
33:W:333:LEU:HD23	33:W:335:SER:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:150:SER:HB3	27:c:156:VAL:HG23	1.89	0.53
29:f:815:HIS:ND1	29:f:882:LEU:O	2.37	0.53
10:j:14:GLY:HA3	11:k:30:ALA:HB2	1.91	0.53
16:p:34:MET:HG3	16:p:183:MET:HE2	1.90	0.53
31:x:423:VAL:HB	31:x:439:TRP:HB2	1.91	0.53
1:B:231:GLY:N	36:B:501:ATP:O2A	2.42	0.53
4:E:23:ASP:OD2	4:E:27:LYS:NZ	2.41	0.53
6:A:213:LEU:HD23	6:A:340:LYS:HG3	1.91	0.53
17:Q:58:GLU:OE1	17:Q:62:LYS:NZ	2.41	0.53
21:U:43:ASP:N	21:U:43:ASP:OD1	2.40	0.53
26:b:149:ASN:ND2	26:b:171:VAL:O	2.39	0.53
15:o:86:MET:HE2	15:o:87:LEU:HD12	1.91	0.53
1:B:286:GLU:HB3	2:C:274:LEU:HD13	1.91	0.53
29:f:43:GLN:NE2	29:f:124:ASP:OD2	2.42	0.53
29:f:333:LEU:HD13	29:f:810:ILE:HD12	1.90	0.53
29:f:688:ARG:NH1	29:f:724:ASN:OD1	2.42	0.53
2:C:119:ASP:HB3	27:c:193:ILE:HG13	1.91	0.53
16:P:138:VAL:HG11	16:P:146:MET:HB3	1.91	0.53
23:Y:14:ASN:ND2	23:Y:213:LEU:O	2.34	0.53
29:f:638:ASP:OD1	29:f:677:HIS:NE2	2.38	0.53
10:j:146:GLN:OE1	10:j:159:ASN:ND2	2.41	0.53
26:b:5:SER:HB3	26:b:107:MET:HA	1.91	0.53
33:W:93:ARG:NH1	33:W:96:GLN:OE1	2.42	0.53
8:H:39:LYS:NZ	9:I:57:ASP:OD2	2.38	0.53
12:L:72:ILE:HD13	12:L:88:MET:HE1	1.91	0.53
23:Y:231:LEU:HD23	23:Y:234:PRO:HG2	1.91	0.53
24:Z:105:ASP:OD1	24:Z:105:ASP:N	2.40	0.53
23:Y:177:ARG:HA	23:Y:180:LEU:HB2	1.90	0.53
10:j:184:ASP:N	10:j:184:ASP:OD1	2.42	0.53
31:x:144:GLY:O	31:x:148:SER:N	2.40	0.53
32:y:56:LEU:HD23	32:y:59:TYR:HD2	1.73	0.53
2:C:406:LYS:HB2	9:I:80:THR:HG22	1.90	0.52
21:U:678:ASP:O	21:U:684:ARG:NH1	2.42	0.52
29:f:194:TYR:O	29:f:198:HIS:ND1	2.37	0.52
29:f:453:SER:HB3	29:f:804:LEU:HD13	1.90	0.52
7:g:165:ALA:HB1	7:g:179:LEU:HD13	1.90	0.52
32:y:63:LYS:HG3	32:y:64:GLU:HG2	1.91	0.52
4:E:170:CYS:SG	4:E:171:LEU:N	2.82	0.52
21:U:619:VAL:HG13	21:U:640:LEU:HD13	1.92	0.52
15:o:198:ARG:NH1	16:p:155:GLU:OE2	2.42	0.52
17:q:19:ARG:NH2	17:q:31:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:x:256:LYS:HB2	31:x:265:VAL:HG13	1.91	0.52
3:D:204:MET:HG2	3:D:333:PHE:HE2	1.74	0.52
4:E:176:PRO:O	4:E:339:ASN:ND2	2.42	0.52
3:D:98:GLN:OE1	3:D:121:ARG:NH1	2.43	0.52
17:Q:11:ASP:N	17:Q:11:ASP:OD1	2.43	0.52
19:S:194:ARG:NH2	19:S:205:GLU:OE1	2.42	0.52
24:Z:154:THR:HG22	33:W:448:LYS:HZ2	1.74	0.52
4:E:356:ARG:NH1	5:F:200:GLU:OE2	2.43	0.52
10:J:40:ILE:HG13	10:J:212:ARG:HG3	1.91	0.52
2:C:160:GLU:OE1	2:C:313:ARG:NH1	2.41	0.52
4:E:136:GLY:N	37:E:501:ADP:HN62	2.07	0.52
22:X:264:PRO:HG2	22:X:295:LYS:HB2	1.91	0.52
24:Z:172:VAL:HG22	27:c:217:LEU:HD21	1.92	0.52
34:V:76:LYS:HE3	34:V:149:PRO:HB3	1.91	0.52
5:F:262:GLY:O	5:F:308:ARG:NH2	2.43	0.52
23:Y:101:ARG:HH21	23:Y:136:HIS:HB3	1.75	0.52
29:f:110:TYR:OH	29:f:118:ASN:ND2	2.42	0.52
10:j:96:LEU:HB2	17:q:62:LYS:HG3	1.92	0.52
20:t:43:MET:HE3	20:t:45:VAL:HG22	1.90	0.52
5:F:258:GLN:HG3	5:F:259:MET:HG2	1.90	0.52
19:S:150:ASP:OD2	16:p:177:ARG:NH2	2.39	0.52
22:X:182:ASN:HA	23:Y:244:ALA:HB1	1.91	0.52
27:c:285:GLU:HA	27:c:288:VAL:HB	1.90	0.52
33:W:274:VAL:O	33:W:283:GLN:NE2	2.41	0.52
17:Q:59:TYR:O	17:Q:63:ASN:ND2	2.43	0.52
20:T:25:ASP:OD1	20:T:41:ARG:NH2	2.38	0.52
18:r:35:ILE:HD11	18:r:45:MET:HB3	1.92	0.52
33:W:279:PHE:HA	33:W:283:GLN:HG2	1.92	0.52
4:E:333:LYS:HE2	33:W:12:ARG:HB3	1.91	0.52
12:L:72:ILE:HG21	12:L:88:MET:HE1	1.91	0.52
23:Y:389:MET:HG3	34:V:95:LEU:HD11	1.92	0.52
25:a:363:MET:HE2	27:c:307:VAL:HG11	1.91	0.52
29:f:261:ARG:HH21	29:f:772:GLY:H	1.58	0.52
3:D:242:GLU:OE1	3:D:245:ARG:NH1	2.43	0.51
9:i:235:GLN:HA	9:i:238:LYS:HG2	1.92	0.51
13:M:171:ALA:O	13:M:174:THR:OG1	2.28	0.51
29:f:353:LEU:O	29:f:357:ARG:NH1	2.43	0.51
29:f:548:THR:HA	29:f:552:ASP:HB2	1.91	0.51
15:o:6:VAL:HG23	15:o:124:TYR:HB3	1.92	0.51
18:r:164:THR:HG23	18:r:171:GLY:HA2	1.92	0.51
4:E:242:ARG:NH2	4:E:286:ASP:OD2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:43:ARG:HH21	7:G:164:LYS:HG2	1.75	0.51
10:J:86:ARG:HD2	10:J:114:LEU:HD22	1.93	0.51
21:U:335:ILE:HA	21:U:338:HIS:CE1	2.45	0.51
23:Y:174:TRP:O	23:Y:177:ARG:NH1	2.43	0.51
12:l:36:VAL:HG12	12:l:160:SER:HB2	1.93	0.51
31:x:417:TYR:HB2	31:x:483:ARG:HG2	1.92	0.51
1:B:199:GLU:OE2	1:B:349:ARG:NH2	2.44	0.51
11:K:121:LEU:HD23	11:K:160:GLY:HA3	1.91	0.51
21:U:798:PRO:O	21:U:880:ASN:ND2	2.43	0.51
25:a:245:VAL:HG13	25:a:272:ILE:HD12	1.92	0.51
29:f:524:MET:HB3	29:f:564:LEU:HD13	1.93	0.51
11:k:221:GLN:NE2	11:k:224:GLN:OE1	2.44	0.51
32:y:3:ILE:HD13	32:y:17:VAL:HB	1.91	0.51
3:D:380:GLN:HA	4:E:164:ILE:HD12	1.92	0.51
6:A:210:LYS:NZ	6:A:310:ASP:O	2.41	0.51
12:L:50:LYS:HB3	12:L:59:HIS:HB3	1.92	0.51
3:D:210:CYS:HB3	3:D:335:LEU:HD23	1.92	0.51
5:F:97:LEU:HB2	5:F:121:CYS:HB2	1.93	0.51
6:A:349:GLU:O	6:A:353:HIS:ND1	2.41	0.51
15:O:164:PHE:O	19:s:38:ARG:NH2	2.44	0.51
17:Q:39:SER:OG	17:Q:40:GLU:N	2.44	0.51
21:U:609:ASP:O	21:U:615:ARG:NH1	2.44	0.51
27:c:75:MET:HE1	27:c:87:VAL:HG13	1.93	0.51
31:x:98:ALA:O	31:x:102:GLU:HB3	2.11	0.51
33:W:245:LYS:HG2	33:W:248:ARG:HH12	1.75	0.51
8:H:111:VAL:HG22	8:H:136:ILE:HD12	1.92	0.51
25:a:193:GLN:OE1	25:a:196:ARG:NH2	2.44	0.51
27:c:57:MET:HB3	27:c:72:VAL:HG12	1.92	0.51
9:i:123:GLN:OE1	10:j:125:ARG:NH2	2.43	0.51
31:x:222:SER:HB2	31:x:410:ILE:HB	1.93	0.51
3:D:176:GLU:OE1	3:D:329:ARG:NH1	2.39	0.51
3:D:211:GLY:HA3	3:D:214:MET:HE2	1.93	0.51
8:h:68:ILE:HB	8:h:72:ILE:HG23	1.91	0.51
31:x:249:VAL:HB	31:x:321:PRO:HD3	1.93	0.51
7:G:180:GLU:HA	7:G:183:VAL:HG12	1.92	0.51
17:Q:26:VAL:HG21	18:R:136:TYR:HE2	1.76	0.51
29:f:600:TYR:HB3	29:f:603:SER:HB3	1.93	0.51
12:l:165:SER:OG	12:l:169:ARG:NH2	2.43	0.51
35:e:54:ASN:OD1	35:e:57:ARG:NH2	2.43	0.51
8:h:133:SER:OG	8:h:149:SER:O	2.25	0.51
2:C:251:ILE:H	2:C:295:THR:HB	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:247:LYS:HD2	33:W:425:LEU:HG	1.92	0.50
28:d:52:ARG:HH12	28:d:82:TYR:HD1	1.57	0.50
29:f:125:ILE:HG21	29:f:129:LEU:H	1.76	0.50
11:k:101:PHE:O	18:r:57:ARG:NH2	2.43	0.50
2:C:86:LEU:HD13	2:C:94:LYS:HD3	1.93	0.50
29:f:719:PRO:O	29:f:724:ASN:ND2	2.44	0.50
32:y:22:THR:HG23	32:y:24:GLU:H	1.77	0.50
1:B:68:ILE:HD12	29:f:650:GLN:HG3	1.94	0.50
1:B:74:MET:HE2	29:f:613:LEU:HD23	1.93	0.50
4:E:19:HIS:ND1	5:F:51:GLU:OE1	2.39	0.50
17:Q:118:MET:HE2	17:Q:124:LEU:HD13	1.92	0.50
21:U:328:ILE:HG22	21:U:333:MET:HG2	1.93	0.50
29:f:771:LEU:HG	29:f:774:GLY:H	1.77	0.50
17:q:153:ARG:NH1	17:q:184:ASP:OD2	2.43	0.50
31:x:419:ASP:O	31:x:481:GLY:N	2.44	0.50
21:U:376:MET:HE3	21:U:735:GLY:HA2	1.92	0.50
13:m:230:ASP:OD1	13:m:230:ASP:N	2.43	0.50
15:o:80:ASN:HD21	15:o:119:THR:HG21	1.76	0.50
10:J:221:ASN:CB	10:J:223:GLU:OE1	2.53	0.50
21:U:353:LEU:HD21	21:U:376:MET:HG3	1.93	0.50
23:Y:50:MET:HB2	23:Y:67:VAL:HG23	1.92	0.50
26:b:15:TYR:HE2	26:b:145:GLU:HB3	1.76	0.50
13:m:148:LEU:HD22	13:m:160:TYR:HB2	1.94	0.50
33:W:280:ASP:H	33:W:283:GLN:HB3	1.77	0.50
8:H:51:LYS:NZ	8:H:200:GLU:O	2.41	0.50
25:a:249:GLN:HA	25:a:252:LYS:HG2	1.92	0.50
17:q:52:ASP:OD1	18:r:88:TYR:OH	2.30	0.50
31:x:103:LEU:HD21	31:x:457:ILE:HG23	1.94	0.50
31:x:319:ARG:NH1	31:x:410:ILE:O	2.45	0.50
21:U:346:ASN:HD22	21:U:347:ASN:H	1.58	0.50
24:Z:6:VAL:HG23	24:Z:47:VAL:HA	1.93	0.50
24:Z:42:SER:O	24:Z:44:GLN:NE2	2.45	0.50
25:a:374:ILE:HD11	28:d:251:ARG:HA	1.94	0.50
29:f:379:GLY:HA3	29:f:413:SER:HB3	1.93	0.50
17:q:83:PHE:O	17:q:87:ASN:ND2	2.44	0.50
19:s:71:ARG:HD3	19:s:95:ILE:HD11	1.93	0.50
31:x:20:LEU:HD22	31:x:63:ILE:HG21	1.92	0.50
31:x:374:PHE:HD2	31:x:415:CYS:HB3	1.77	0.50
33:W:67:LEU:HB3	33:W:104:MET:SD	2.50	0.50
6:A:250:VAL:HB	6:A:294:GLU:HG2	1.93	0.50
29:f:19:ALA:O	29:f:23:GLY:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:W:235:GLN:NE2	33:W:346:GLU:OE2	2.37	0.50
34:V:289:LEU:HB3	34:V:312:ALA:HB2	1.94	0.50
3:D:160:PRO:HB3	3:D:217:LYS:HD2	1.94	0.50
19:S:125:ASP:OD2	19:S:129:SER:OG	2.30	0.50
25:a:70:ARG:HD3	26:b:24:THR:HG23	1.94	0.50
29:f:250:ARG:HG3	29:f:253:LEU:HG	1.92	0.50
29:f:404:ASP:OD1	29:f:404:ASP:N	2.44	0.50
16:p:122:CYS:SG	16:p:123:SER:N	2.85	0.50
18:r:37:ILE:HD11	18:r:56:GLU:HB3	1.93	0.50
31:x:49:LYS:HD2	31:x:67:MET:HB2	1.93	0.50
12:L:158:ALA:HB1	12:L:172:LEU:HD13	1.94	0.49
22:X:211:ASP:HB2	22:X:235:ALA:HB2	1.94	0.49
29:f:130:ALA:O	29:f:134:SER:N	2.39	0.49
31:x:112:ASN:HB3	31:x:197:GLN:HB2	1.94	0.49
19:S:38:ARG:NH2	15:o:164:PHE:O	2.46	0.49
21:U:471:ASP:OD1	21:U:471:ASP:N	2.42	0.49
32:y:27:LYS:HA	32:y:30:ILE:HG22	1.94	0.49
5:F:187:ASP:OD1	5:F:187:ASP:N	2.46	0.49
6:A:371:GLU:OE2	11:K:204:GLN:NE2	2.45	0.49
12:L:93:LEU:HD21	19:S:70:ALA:HB1	1.94	0.49
23:Y:298:GLU:O	23:Y:302:HIS:ND1	2.43	0.49
8:h:64:LYS:HG2	8:h:76:TYR:HE1	1.77	0.49
10:j:189:LYS:NZ	10:j:228:TYR:O	2.46	0.49
13:m:197:ILE:HG21	13:m:211:LEU:HD13	1.95	0.49
1:B:398:ILE:HD11	1:B:427:LEU:HD22	1.93	0.49
3:D:335:LEU:HD13	3:D:371:SER:HB3	1.95	0.49
12:L:199:LEU:O	12:L:239:ARG:NH2	2.46	0.49
25:a:370:GLN:HB3	28:d:247:ILE:HG21	1.94	0.49
33:W:13:ILE:HB	33:W:58:SER:HB2	1.95	0.49
34:V:119:GLY:HA2	34:V:148:ARG:HD3	1.95	0.49
1:B:408:ARG:NH2	2:C:163:GLU:OE1	2.45	0.49
5:F:97:LEU:O	5:F:120:LYS:N	2.46	0.49
5:F:376:SER:HB3	5:F:379:VAL:HG23	1.93	0.49
10:J:7:ILE:HG23	10:J:8:THR:HG23	1.95	0.49
16:P:122:CYS:SG	16:P:123:SER:N	2.84	0.49
19:s:145:LEU:HD21	19:s:182:ALA:HB2	1.95	0.49
33:W:144:ARG:O	33:W:148:THR:OG1	2.26	0.49
36:D:501:ATP:O2G	4:E:294:ARG:NH2	2.46	0.49
4:E:282:PRO:HG2	4:E:389:VAL:HG13	1.94	0.49
19:s:41:PRO:HB3	19:s:194:ARG:HD2	1.95	0.49
33:W:11:GLY:N	33:W:94:ARG:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:W:20:TYR:HB3	33:W:24:VAL:HG13	1.95	0.49
34:V:119:GLY:O	34:V:122:THR:OG1	2.29	0.49
2:C:239:ARG:NH2	2:C:287:LYS:O	2.44	0.49
5:F:125:LYS:HA	5:F:131:THR:HA	1.94	0.49
12:L:117:GLN:NE2	13:M:83:ASP:OD1	2.46	0.49
21:U:246:TYR:HE2	21:U:794:ASP:HB2	1.78	0.49
19:s:192:ALA:HA	19:s:209:SER:HA	1.95	0.49
33:W:27:ARG:HD2	33:W:50:LEU:HD13	1.95	0.49
29:f:438:ASP:OD1	29:f:438:ASP:N	2.45	0.49
31:x:257:CYS:SG	31:x:258:THR:N	2.86	0.49
7:g:220:VAL:HG22	7:g:227:PHE:HA	1.95	0.49
22:X:75:PRO:O	22:X:79:SER:CB	2.61	0.49
28:d:187:GLU:OE1	28:d:224:SER:OG	2.26	0.49
34:V:337:LEU:HD21	34:V:364:THR:HG23	1.94	0.49
3:D:92:PHE:HZ	3:D:95:ALA:HB2	1.78	0.48
25:a:84:VAL:HG22	25:a:87:MET:HE2	1.95	0.48
28:d:83:PHE:HZ	28:d:121:ARG:HD2	1.78	0.48
14:n:93:ASP:N	14:n:93:ASP:OD1	2.46	0.48
5:F:74:LYS:NZ	5:F:78:GLU:OE1	2.42	0.48
5:F:228:PRO:HG3	5:F:356:MET:HE1	1.95	0.48
29:f:13:PRO:HG3	29:f:56:LEU:HD22	1.95	0.48
34:V:435:GLU:HG2	34:V:453:HIS:CD2	2.48	0.48
3:D:159:LYS:HE3	3:D:221:HIS:HA	1.95	0.48
3:D:170:MET:SD	3:D:173:GLN:HB2	2.54	0.48
7:G:40:VAL:HG23	7:G:167:ALA:HB2	1.96	0.48
22:X:371:ASP:OD1	23:Y:233:ARG:NH2	2.40	0.48
23:Y:233:ARG:HA	23:Y:236:LEU:HD22	1.94	0.48
29:f:616:CYS:HB3	29:f:632:LYS:HG3	1.94	0.48
31:x:419:ASP:OD1	31:x:419:ASP:N	2.46	0.48
4:E:246:GLY:HA3	4:E:250:ASP:HB2	1.96	0.48
6:A:260:LEU:O	6:A:264:ALA:CB	2.61	0.48
15:O:193:ASN:OD1	19:s:211:ARG:NH2	2.47	0.48
20:T:15:LYS:HE2	20:T:135:PRO:HA	1.95	0.48
21:U:239:GLU:OE2	21:U:241:ASN:ND2	2.47	0.48
21:U:517:GLY:HA3	21:U:551:GLY:HA2	1.96	0.48
28:d:88:GLN:HG3	28:d:90:PRO:HD3	1.95	0.48
29:f:310:ASP:OD1	29:f:310:ASP:N	2.47	0.48
29:f:463:LEU:O	29:f:467:SER:OG	2.28	0.48
8:h:50:LYS:HB3	8:h:64:LYS:HD2	1.96	0.48
13:m:108:LEU:HD22	13:m:139:SER:HB3	1.96	0.48
15:o:161:ALA:O	15:o:165:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:y:29:LYS:HE2	32:y:29:LYS:HB2	1.67	0.48
21:U:634:PRO:HA	21:U:637:VAL:HG12	1.94	0.48
29:f:665:GLU:HA	29:f:669:GLU:HB2	1.96	0.48
12:l:26:MET:HE1	12:l:148:CYS:HB3	1.95	0.48
12:L:80:ASP:OD1	12:L:125:ARG:NH2	2.47	0.48
12:l:117:GLN:NE2	13:m:83:ASP:OD1	2.46	0.48
13:m:27:MET:HE1	13:m:152:ASP:HB3	1.94	0.48
35:e:16:ASP:OD1	35:e:16:ASP:N	2.46	0.48
2:C:69:GLN:OE1	2:C:118:ASN:ND2	2.47	0.48
23:Y:262:SER:OG	23:Y:267:ARG:O	2.31	0.48
11:k:236:GLU:HA	11:k:239:LYS:HG2	1.95	0.48
6:A:112:ILE:HG12	6:A:122:VAL:HG22	1.94	0.48
14:N:35:THR:OG1	14:N:43:CYS:SG	2.72	0.48
9:i:119:GLN:HG3	10:j:78:ALA:HB1	1.95	0.48
9:i:202:ASP:N	9:i:202:ASP:OD1	2.46	0.48
19:s:125:ASP:OD1	19:s:129:SER:N	2.47	0.48
34:V:150:ARG:NH1	34:V:157:THR:O	2.47	0.48
4:E:87:LEU:HG	4:E:107:ILE:HG13	1.94	0.48
15:O:167:LEU:HD21	19:s:35:ILE:HD11	1.96	0.48
22:X:76:PHE:HA	22:X:79:SER:HB3	1.95	0.48
1:B:199:GLU:OE1	6:A:398:ARG:NH1	2.47	0.48
4:E:15:LYS:HG3	5:F:48:LEU:HD13	1.96	0.48
23:Y:42:MET:HA	23:Y:45:VAL:HG22	1.96	0.48
26:b:79:GLN:OE1	26:b:81:LYS:NZ	2.46	0.48
16:p:12:MET:HB2	16:p:171:MET:HE2	1.95	0.48
31:x:425:THR:HG21	31:x:466:LEU:HD22	1.96	0.48
21:U:619:VAL:HG21	21:U:648:VAL:HG13	1.96	0.47
29:f:718:ASP:N	29:f:718:ASP:OD1	2.46	0.47
7:g:67:THR:HG22	7:g:69:LEU:H	1.79	0.47
11:K:52:LYS:NZ	11:K:216:GLU:OE2	2.43	0.47
11:K:215:ILE:HD11	11:K:238:ILE:HD11	1.95	0.47
29:f:600:TYR:HB2	29:f:639:LYS:HG2	1.95	0.47
18:r:144:SER:OG	18:r:146:ASP:OD1	2.31	0.47
33:W:441:LYS:HA	33:W:444:HIS:CD2	2.49	0.47
3:D:115:ILE:HG23	3:D:139:LEU:HD22	1.95	0.47
7:G:71:LYS:HA	7:G:77:GLY:HA2	1.95	0.47
21:U:536:ALA:HB2	21:U:548:LEU:HD22	1.95	0.47
12:l:176:MET:HE1	13:m:56:LYS:HB2	1.96	0.47
4:E:117:PRO:O	4:E:121:ASN:ND2	2.40	0.47
4:E:310:LEU:HB2	4:E:332:VAL:HG21	1.96	0.47
12:L:207:THR:OG1	12:L:226:ASP:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:12:MET:HE2	16:P:167:ILE:HD12	1.95	0.47
25:a:344:GLN:HA	25:a:347:LYS:HD2	1.96	0.47
27:c:64:ASP:HA	27:c:139:ARG:HH12	1.79	0.47
29:f:738:ASN:O	29:f:740:ARG:NH1	2.47	0.47
13:m:37:ILE:HD11	13:m:193:VAL:HG13	1.96	0.47
17:q:152:SER:OG	17:q:154:GLU:OE1	2.30	0.47
4:E:135:ILE:HA	37:E:501:ADP:N6	2.30	0.47
13:M:108:LEU:HD22	13:M:139:SER:HB3	1.97	0.47
16:P:107:PRO:HB2	16:P:124:LEU:HD12	1.96	0.47
19:S:177:ASP:OD2	15:o:202:TYR:OH	2.27	0.47
21:U:368:ALA:HB2	21:U:728:PHE:HD1	1.78	0.47
29:f:198:HIS:O	29:f:202:HIS:ND1	2.47	0.47
12:l:155:ASP:HB3	13:m:62:SER:HB2	1.96	0.47
31:x:215:LEU:HD22	31:x:243:ILE:HG12	1.97	0.47
31:x:463:ILE:HA	31:x:466:LEU:HD12	1.97	0.47
33:W:274:VAL:HG21	33:W:290:ILE:HD13	1.95	0.47
33:W:331:GLY:HA3	33:W:334:GLU:HG3	1.96	0.47
1:B:59:ARG:HE	29:f:187:LEU:HD22	1.79	0.47
4:E:239:GLY:HA2	4:E:257:LEU:HD13	1.96	0.47
21:U:35:TRP:HA	21:U:38:ILE:HG12	1.95	0.47
21:U:366:HIS:NE2	21:U:392:TRP:O	2.47	0.47
23:Y:268:TYR:HA	23:Y:271:PHE:HB3	1.96	0.47
13:m:75:MET:HE1	13:m:88:ALA:HB2	1.96	0.47
16:p:159:ASP:OD1	16:p:159:ASP:N	2.45	0.47
4:E:182:LEU:HD22	37:E:501:ADP:N7	2.28	0.47
18:R:97:MET:N	18:R:116:SER:OG	2.44	0.47
22:X:103:THR:HA	22:X:106:GLU:HB2	1.97	0.47
27:c:58:LEU:HD13	27:c:106:GLU:H	1.78	0.47
29:f:427:THR:O	29:f:431:LYS:NZ	2.48	0.47
12:l:158:ALA:HB1	12:l:172:LEU:HD13	1.96	0.47
12:l:218:ASP:OD1	12:l:218:ASP:N	2.47	0.47
16:p:14:MET:HG2	16:p:167:ILE:HD12	1.97	0.47
19:s:10:GLY:HA3	19:s:42:LYS:HE3	1.95	0.47
34:V:233:ALA:HA	34:V:236:ARG:HD3	1.96	0.47
34:V:355:ARG:NH1	35:e:27:TRP:O	2.47	0.47
1:B:107:MET:HG2	2:C:96:VAL:HB	1.97	0.47
3:D:385:LEU:HD13	3:D:401:LYS:HE2	1.97	0.47
28:d:245:GLN:NE2	28:d:249:TYR:OH	2.47	0.47
29:f:205:CYS:HA	29:f:208:LEU:HD12	1.97	0.47
29:f:426:LEU:HD23	31:x:72:MET:HG2	1.95	0.47
7:g:191:PHE:HE1	7:g:219:VAL:HG21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:V:410:ILE:HG21	34:V:422:ILE:HG13	1.97	0.47
6:A:35:THR:O	6:A:43:ARG:NH2	2.48	0.47
11:K:182:GLN:HA	12:L:56:LEU:HD11	1.95	0.47
16:P:126:LEU:HD12	16:P:127:ILE:HG23	1.97	0.47
17:Q:22:ALA:HA	17:Q:27:GLN:HA	1.97	0.47
25:a:360:VAL:HG22	27:c:308:VAL:HG13	1.97	0.47
7:g:86:ASP:OD1	13:m:120:HIS:NE2	2.44	0.47
8:h:9:SER:OG	8:h:123:GLN:O	2.33	0.47
8:h:204:THR:OG1	8:h:206:ASP:OD1	2.32	0.47
16:p:164:PHE:HB2	16:p:189:ILE:HD11	1.96	0.47
31:x:222:SER:H	31:x:410:ILE:HD13	1.78	0.47
1:B:429:LYS:HE3	2:C:308:PRO:HG3	1.96	0.47
1:B:437:GLY:O	9:I:155:ASN:ND2	2.48	0.47
6:A:79:ASP:OD1	6:A:79:ASP:N	2.47	0.47
6:A:277:ILE:HG12	6:A:319:MET:HE1	1.97	0.47
27:c:280:PRO:HA	27:c:284:LEU:HB2	1.97	0.47
20:t:11:VAL:HG23	20:t:24:ALA:HB2	1.96	0.47
33:W:174:TYR:HA	33:W:177:MET:HE1	1.97	0.47
34:V:86:VAL:HG21	34:V:160:LEU:HD13	1.97	0.47
34:V:227:VAL:HG12	34:V:231:LEU:HD13	1.95	0.47
7:G:102:LYS:NZ	7:G:108:GLU:OE2	2.42	0.46
10:J:211:MET:HG2	10:J:217:LEU:HD13	1.96	0.46
19:S:135:PHE:HB2	19:S:149:LEU:HD23	1.97	0.46
21:U:36:ALA:O	34:V:273:LYS:NZ	2.44	0.46
17:q:11:ASP:N	17:q:11:ASP:OD1	2.49	0.46
19:s:72:LEU:HD13	19:s:83:MET:HE3	1.97	0.46
34:V:278:GLU:HA	34:V:285:TRP:HZ2	1.79	0.46
34:V:484:LEU:O	34:V:488:ASN:ND2	2.47	0.46
1:B:100:ASP:HA	1:B:103:ARG:HE	1.80	0.46
21:U:655:ALA:HA	21:U:658:ILE:HG12	1.97	0.46
28:d:29:VAL:HG11	28:d:51:ALA:HB2	1.97	0.46
29:f:138:GLU:HG2	29:f:163:ALA:HB2	1.96	0.46
19:s:24:ALA:HB1	19:s:193:LEU:HD11	1.97	0.46
2:C:91:PRO:HD2	2:C:92:GLU:HG2	1.97	0.46
6:A:73:ALA:HB3	6:A:78:TRP:HD1	1.80	0.46
8:H:9:SER:HG	8:H:12:THR:HG1	1.60	0.46
11:K:85:ALA:HB2	11:K:139:VAL:HG21	1.96	0.46
13:M:83:ASP:HB3	13:M:131:PHE:HD2	1.80	0.46
20:T:193:THR:OG1	20:T:194:GLU:N	2.49	0.46
29:f:426:LEU:HA	29:f:429:ILE:HG22	1.97	0.46
6:A:138:MET:HE1	6:A:152:PRO:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:119:GLN:HG3	9:I:81:SER:HB2	1.97	0.46
14:N:154:GLN:NE2	14:N:158:ASN:OD1	2.44	0.46
21:U:335:ILE:HD13	21:U:338:HIS:HE1	1.79	0.46
22:X:421:LEU:HB3	24:Z:283:ARG:HH22	1.80	0.46
8:h:93:LEU:HD13	8:h:113:ARG:HB3	1.98	0.46
5:F:127:SER:HB2	6:A:119:ALA:HB1	1.97	0.46
21:U:443:LEU:HD21	21:U:464:GLN:HG2	1.98	0.46
22:X:408:SER:HA	23:Y:376:LEU:HD11	1.97	0.46
23:Y:124:PHE:HA	23:Y:127:THR:HG22	1.98	0.46
25:a:22:TRP:O	25:a:26:GLU:HG2	2.15	0.46
25:a:227:ASN:OD1	25:a:227:ASN:N	2.49	0.46
25:a:315:LEU:HD12	25:a:320:VAL:HG23	1.98	0.46
29:f:271:MET:SD	29:f:300:ARG:NH2	2.88	0.46
29:f:605:ASN:HD21	29:f:608:LYS:HB2	1.80	0.46
13:m:99:ARG:NH2	13:m:105:ASN:OD1	2.41	0.46
34:V:419:LEU:HD11	34:V:451:ILE:HD11	1.97	0.46
3:D:146:GLU:HG3	3:D:253:LEU:HA	1.96	0.46
3:D:244:PRO:HD3	3:D:288:ILE:HG12	1.97	0.46
21:U:220:LEU:HD22	21:U:229:VAL:HG22	1.97	0.46
22:X:344:ARG:NH1	33:W:407:ASP:OD2	2.49	0.46
25:a:191:SER:O	25:a:194:GLN:NE2	2.46	0.46
7:g:186:LYS:HZ3	7:g:189:TRP:HE1	1.63	0.46
33:W:254:PRO:HD3	33:W:263:TRP:HB2	1.97	0.46
5:F:141:ASP:OD1	5:F:141:ASP:N	2.47	0.46
8:H:222:THR:OG1	8:H:225:GLU:OE2	2.31	0.46
13:M:230:ASP:N	13:M:230:ASP:OD1	2.48	0.46
21:U:403:THR:HG23	21:U:777:HIS:HE1	1.81	0.46
26:b:1:MET:N	26:b:43:SER:O	2.45	0.46
15:o:12:ILE:HD11	15:o:178:ILE:HD12	1.97	0.46
34:V:419:LEU:HA	34:V:422:ILE:HG22	1.98	0.46
1:B:118:ASP:O	1:B:120:HIS:ND1	2.46	0.46
2:C:187:LEU:HA	2:C:293:MET:HB2	1.98	0.46
4:E:12:TYR:OH	5:F:27:ASP:OD2	2.34	0.46
12:L:132:LEU:HB3	12:L:147:THR:HB	1.97	0.46
21:U:216:VAL:HG11	21:U:248:ILE:HD12	1.97	0.46
22:X:264:PRO:HB3	22:X:291:ALA:HB1	1.97	0.46
25:a:226:ARG:HG3	25:a:234:ILE:HG12	1.97	0.46
28:d:42:LYS:HA	28:d:45:LYS:HB3	1.97	0.46
29:f:16:SER:HB3	29:f:34:ARG:HD3	1.97	0.46
29:f:429:ILE:HD11	29:f:444:ALA:HA	1.98	0.46
1:B:253:SER:HB3	1:B:289:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ILE:O	2:C:229:ARG:NH2	2.49	0.46
1:B:257:GLN:HB2	1:B:262:ASP:HB2	1.98	0.46
3:D:309:MET:HG3	3:D:327:LEU:HD21	1.96	0.46
24:Z:129:LYS:HD3	27:c:216:MET:HB3	1.98	0.46
12:l:49:LEU:HB2	12:l:195:LEU:HD21	1.97	0.46
18:r:176:LEU:HB3	18:r:187:VAL:HB	1.97	0.46
31:x:302:SER:HB3	31:x:305:LEU:HB2	1.97	0.46
15:O:140:ASP:OD2	20:t:171:ARG:NH2	2.49	0.46
25:a:205:LEU:HD21	25:a:236:THR:HG21	1.98	0.46
1:B:60:LEU:HG	1:B:64:LYS:HE3	1.98	0.45
8:H:213:CYS:HB2	8:H:218:PHE:HD1	1.80	0.45
22:X:87:ARG:HG2	22:X:90:ARG:HH21	1.81	0.45
23:Y:12:PRO:HD2	23:Y:211:TYR:HB3	1.98	0.45
28:d:151:VAL:O	28:d:155:LYS:HB2	2.16	0.45
9:i:9:THR:HG23	9:i:20:GLN:HG3	1.98	0.45
11:k:117:SER:OG	11:k:160:GLY:O	2.32	0.45
1:B:140:ASP:O	1:B:142:ASP:N	2.47	0.45
3:D:204:MET:HG2	3:D:333:PHE:CE2	2.51	0.45
3:D:274:ARG:NH2	3:D:276:ASP:O	2.42	0.45
16:P:11:VAL:HG23	16:P:54:ALA:HB2	1.98	0.45
21:U:666:LYS:HA	21:U:669:ILE:HD12	1.97	0.45
25:a:137:ASP:O	25:a:141:MET:HG3	2.17	0.45
29:f:783:SER:HB2	29:f:790:GLN:HB3	1.98	0.45
12:l:7:ASP:OD1	12:l:7:ASP:N	2.49	0.45
32:y:15:LEU:HD13	32:y:29:LYS:HD2	1.98	0.45
1:B:264:PRO:HA	1:B:267:VAL:HG12	1.98	0.45
1:B:389:ASP:OD1	1:B:389:ASP:N	2.48	0.45
2:C:29:GLU:OE1	34:V:201:ARG:NE	2.47	0.45
11:K:103:TYR:HE1	19:S:91:MET:HE2	1.81	0.45
21:U:699:THR:OG1	21:U:700:GLU:N	2.48	0.45
22:X:97:LEU:HD13	22:X:136:LEU:HD11	1.98	0.45
15:O:78:THR:O	15:O:82:MET:HG2	2.16	0.45
21:U:629:THR:O	21:U:629:THR:OG1	2.34	0.45
24:Z:144:VAL:HG23	24:Z:145:HIS:H	1.81	0.45
29:f:414:LEU:HA	29:f:417:ILE:HD12	1.98	0.45
29:f:570:GLY:HA2	29:f:600:TYR:HE1	1.81	0.45
9:i:33:THR:OG1	9:i:166:ASN:OD1	2.34	0.45
10:j:222:PRO:HA	10:j:225:ILE:HD12	1.98	0.45
13:m:34:SER:OG	13:m:50:GLU:O	2.32	0.45
16:p:58:THR:OG1	17:q:121:LEU:O	2.25	0.45
1:B:410:ARG:HH22	6:A:25:LEU:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:333:ARG:NH1	6:A:334:PRO:O	2.49	0.45
17:Q:78:THR:O	17:Q:82:ASN:ND2	2.46	0.45
21:U:183:LEU:HD12	21:U:187:LEU:HB2	1.98	0.45
21:U:688:LEU:HD22	21:U:713:TYR:HE1	1.81	0.45
26:b:9:CYS:HB2	26:b:111:ALA:HA	1.99	0.45
29:f:111:GLU:O	29:f:158:TYR:OH	2.33	0.45
29:f:373:ALA:HB2	29:f:744:MET:HG3	1.99	0.45
29:f:452:ASN:HD21	29:f:461:PRO:HD2	1.81	0.45
12:l:39:LYS:HG3	12:l:142:PRO:HB2	1.99	0.45
34:V:398:LEU:HA	34:V:401:ASN:HB2	1.99	0.45
1:B:165:ASP:O	2:C:78:ARG:NH2	2.50	0.45
2:C:25:LEU:HA	2:C:28:ILE:HG12	1.98	0.45
2:C:252:ASP:OD2	2:C:295:THR:OG1	2.34	0.45
3:D:212:LYS:NZ	3:D:311:THR:O	2.42	0.45
11:K:186:HIS:HB2	11:K:189:MET:HE3	1.98	0.45
11:K:203:LYS:HB2	11:K:210:LEU:HD22	1.98	0.45
25:a:217:LEU:HD11	25:a:237:LEU:HB3	1.98	0.45
2:C:159:LYS:HG3	6:A:22:ILE:HD12	1.99	0.45
3:D:369:LYS:H	3:D:369:LYS:HG2	1.58	0.45
7:G:196:GLU:HG3	7:G:242:LEU:HD13	1.97	0.45
29:f:195:ASN:OD1	29:f:196:MET:N	2.50	0.45
14:n:67:SER:HB2	14:n:74:PRO:HG3	1.99	0.45
33:W:310:THR:HG22	33:W:311:THR:HG23	1.98	0.45
33:W:441:LYS:O	33:W:445:LEU:HB2	2.17	0.45
1:B:416:ASN:N	1:B:416:ASN:OD1	2.50	0.45
5:F:317:LEU:HB3	5:F:347:ARG:HA	1.98	0.45
6:A:133:ASP:HB3	31:x:345:LYS:HB2	1.99	0.45
6:A:219:GLY:H	6:A:222:LYS:HZ2	1.63	0.45
16:P:153:LEU:HD12	16:P:170:ALA:HB2	1.99	0.45
19:S:71:ARG:HD3	19:S:95:ILE:HD11	1.97	0.45
29:f:350:LYS:HA	29:f:751:TYR:HE2	1.82	0.45
3:D:103:VAL:HG21	3:D:132:LEU:HD11	1.98	0.45
4:E:5:ARG:HH12	5:F:37:SER:HB2	1.82	0.45
5:F:224:LEU:HD11	5:F:332:THR:HG22	1.99	0.45
9:I:175:LEU:HD13	9:I:196:VAL:HG21	1.99	0.45
19:S:185:ARG:HA	15:o:26:VAL:HG22	1.98	0.45
21:U:504:ASP:OD1	21:U:535:TYR:OH	2.31	0.45
21:U:611:ASN:HB3	21:U:614:VAL:HG22	1.98	0.45
25:a:293:PHE:HB2	25:a:329:LYS:HB3	1.98	0.45
28:d:249:TYR:HH	34:V:477:HIS:HD1	1.63	0.45
10:j:88:ARG:HH11	17:q:70:ARG:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:x:255:MET:HB2	31:x:266:THR:HB	1.99	0.45
33:W:309:PHE:HB3	33:W:361:HIS:CE1	2.52	0.45
3:D:100:THR:HB	3:D:112:TYR:HE1	1.81	0.45
5:F:375:VAL:HA	5:F:415:LEU:H	1.82	0.45
19:S:4:PRO:O	20:T:100:ARG:NH1	2.50	0.45
23:Y:17:LEU:HD23	23:Y:214:MET:HG2	1.98	0.45
24:Z:25:ARG:HD3	27:c:103:GLY:HA3	1.99	0.45
32:y:3:ILE:HG23	32:y:65:SER:HB3	1.99	0.45
34:V:98:LEU:HD22	34:V:209:LYS:HD2	1.99	0.45
4:E:246:GLY:O	4:E:251:ARG:N	2.49	0.44
4:E:261:LEU:HA	4:E:264:MET:HG2	1.98	0.44
10:J:116:GLN:O	10:J:119:THR:OG1	2.31	0.44
12:L:196:ARG:O	12:L:239:ARG:NH2	2.50	0.44
21:U:13:ASP:OD1	21:U:44:LYS:NZ	2.40	0.44
29:f:45:LEU:HD21	29:f:54:ASP:HB3	1.98	0.44
34:V:343:PRO:O	35:e:43:TRP:NE1	2.48	0.44
2:C:277:LEU:HD11	2:C:305:LEU:HB3	2.00	0.44
7:G:80:MET:HE2	7:G:87:SER:HA	1.98	0.44
14:N:86:MET:HE2	14:N:86:MET:HB2	1.92	0.44
16:P:12:MET:HE3	16:P:150:CYS:SG	2.57	0.44
21:U:212:ASP:HB2	21:U:244:MET:HE3	1.98	0.44
22:X:86:ALA:HA	22:X:125:LEU:HD21	1.99	0.44
24:Z:162:ILE:HG13	27:c:220:LEU:HD22	2.00	0.44
25:a:19:PRO:O	25:a:23:HIS:ND1	2.38	0.44
26:b:169:HIS:HB3	26:b:171:VAL:HG13	2.00	0.44
27:c:175:ARG:NH2	27:c:202:SER:O	2.51	0.44
29:f:210:GLU:HA	29:f:213:GLN:HE21	1.82	0.44
29:f:450:ILE:HG12	29:f:804:LEU:HD11	2.00	0.44
15:o:42:TYR:HB2	15:o:178:ILE:HD11	1.98	0.44
20:t:4:PRO:HG3	20:t:107:TRP:CE2	2.52	0.44
31:x:196:LEU:O	31:x:198:GLN:NE2	2.50	0.44
3:D:107:THR:HG23	4:E:77:PRO:HB3	1.99	0.44
5:F:396:CYS:SG	5:F:397:LYS:N	2.90	0.44
10:J:158:ALA:HB3	11:K:58:LEU:HD23	1.99	0.44
11:K:167:ALA:HB3	12:L:56:LEU:HD13	1.99	0.44
23:Y:143:TYR:HD1	23:Y:146:ARG:HH21	1.65	0.44
24:Z:134:PRO:HG3	27:c:219:ASN:HD21	1.82	0.44
25:a:77:VAL:HG21	25:a:110:ALA:HB1	1.98	0.44
29:f:286:LYS:HA	29:f:286:LYS:HD2	1.81	0.44
8:h:111:VAL:HG22	8:h:136:ILE:HD12	1.98	0.44
9:i:229:LYS:NZ	9:i:232:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:x:483:ARG:NH1	31:x:484:ARG:O	2.51	0.44
14:N:119:MET:HE3	14:N:119:MET:HB2	1.86	0.44
21:U:244:MET:O	21:U:248:ILE:HG12	2.17	0.44
24:Z:177:ARG:HA	24:Z:177:ARG:HD3	1.77	0.44
25:a:127:ASP:O	25:a:131:THR:OG1	2.33	0.44
16:p:113:ASP:HB2	16:p:118:LYS:H	1.81	0.44
31:x:251:PHE:HB3	31:x:315:SER:HB3	1.99	0.44
1:B:48:LYS:HA	1:B:48:LYS:HD3	1.78	0.44
4:E:216:ARG:HA	4:E:263:GLN:HE22	1.82	0.44
6:A:57:LYS:HB3	6:A:57:LYS:HE2	1.77	0.44
12:L:210:VAL:HG21	12:L:233:LEU:HD21	1.99	0.44
15:O:143:ARG:HG2	15:O:146:MET:HE2	1.99	0.44
19:S:27:THR:HB	19:S:40:SER:H	1.83	0.44
21:U:357:LYS:HE3	21:U:392:TRP:CG	2.53	0.44
21:U:857:ASP:OD1	21:U:857:ASP:N	2.51	0.44
25:a:188:LEU:HD13	25:a:192:GLU:HG2	1.99	0.44
29:f:732:VAL:HG22	29:f:746:ARG:HB3	1.99	0.44
12:l:27:GLU:HG2	12:l:30:LYS:HZ3	1.83	0.44
17:q:161:ARG:HE	17:q:161:ARG:HB3	1.67	0.44
33:W:278:PRO:HD3	33:W:357:ARG:HH21	1.82	0.44
9:I:119:GLN:HG3	10:J:78:ALA:HB1	2.00	0.44
12:L:72:ILE:HD12	12:L:132:LEU:HD11	1.99	0.44
17:Q:170:ARG:NH1	17:q:27:GLN:O	2.47	0.44
21:U:342:LEU:HD11	21:U:785:PRO:HB3	2.00	0.44
29:f:255:VAL:HG12	29:f:258:LYS:HD3	1.99	0.44
11:k:36:THR:HA	11:k:171:GLY:HA3	1.99	0.44
12:l:101:ARG:HH21	20:t:83:TYR:HE1	1.65	0.44
33:W:31:CYS:HB2	33:W:43:VAL:HG23	1.98	0.44
25:a:149:THR:HB	25:a:182:CYS:HB3	1.98	0.44
29:f:623:LYS:HG2	29:f:625:LYS:H	1.83	0.44
17:q:88:LEU:HD22	17:q:122:ALA:HB2	2.00	0.44
31:x:453:ASP:OD1	31:x:453:ASP:N	2.49	0.44
1:B:137:SER:HB2	6:A:81:ALA:HB2	2.00	0.44
2:C:134:LEU:HB2	2:C:230:MET:HE1	2.00	0.44
21:U:59:PHE:HD1	21:U:87:LEU:HD21	1.83	0.44
24:Z:44:GLN:HE21	24:Z:48:LEU:HA	1.82	0.44
24:Z:260:VAL:HA	34:V:480:ILE:HD13	2.00	0.44
17:q:35:MET:HG2	17:q:45:LEU:HG	2.00	0.44
31:x:145:GLU:HA	31:x:148:SER:HB2	1.98	0.44
35:e:35:ASP:HB3	35:e:37:HIS:CD2	2.52	0.44
21:U:194:ARG:HH21	21:U:198:LEU:HD13	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:407:MET:HE1	24:Z:269:VAL:HB	1.99	0.44
26:b:5:SER:O	26:b:108:ARG:N	2.51	0.44
29:f:272:LEU:O	29:f:276:GLU:HB3	2.17	0.44
1:B:51:LEU:HD22	1:B:64:LYS:HD3	2.00	0.43
1:B:129:SER:HB2	6:A:117:GLN:HG2	2.00	0.43
1:B:131:HIS:HB3	1:B:133:VAL:HG13	1.99	0.43
4:E:254:GLN:O	4:E:258:MET:HG3	2.17	0.43
5:F:139:LEU:HG	5:F:161:LEU:HD12	2.00	0.43
5:F:365:ILE:HG21	37:F:501:ADP:C2	2.53	0.43
6:A:161:VAL:O	6:A:165:GLN:CB	2.65	0.43
15:O:120:ASP:OD1	15:O:120:ASP:N	2.50	0.43
12:l:196:ARG:HE	12:l:239:ARG:HD3	1.83	0.43
34:V:123:SER:OG	34:V:155:ALA:O	2.36	0.43
3:D:274:ARG:HD2	3:D:274:ARG:HA	1.88	0.43
5:F:168:TYR:HB3	5:F:173:LYS:HZ1	1.83	0.43
9:I:7:SER:HB2	9:I:11:ILE:HD12	2.00	0.43
18:R:127:SER:HB3	18:R:136:TYR:CE1	2.52	0.43
19:S:43:CYS:HB2	19:S:194:ARG:HH12	1.82	0.43
21:U:92:ASP:OD2	21:U:140:ARG:NH2	2.51	0.43
23:Y:113:ARG:O	23:Y:113:ARG:NH1	2.43	0.43
26:b:51:LEU:HD21	26:b:71:ILE:HG23	2.00	0.43
8:h:49:GLU:HA	8:h:208:ILE:HA	2.00	0.43
31:x:342:LYS:NZ	31:x:428:GLY:O	2.47	0.43
33:W:378:MET:HA	33:W:381:LEU:HB2	2.00	0.43
4:E:349:GLU:HA	4:E:352:MET:HG3	2.00	0.43
6:A:321:THR:HG21	6:A:327:LEU:HD21	2.00	0.43
9:I:197:LEU:HA	9:I:200:THR:HG22	2.00	0.43
12:L:40:SER:OG	12:L:41:LYS:N	2.51	0.43
14:N:89:ARG:NH2	14:N:90:TYR:OH	2.50	0.43
28:d:231:LYS:HE2	28:d:231:LYS:HB2	1.89	0.43
14:n:104:ASP:OD2	14:n:110:GLN:NE2	2.51	0.43
19:s:57:PHE:HZ	20:t:128:LEU:HB3	1.84	0.43
31:x:327:GLN:HG3	31:x:477:VAL:HG23	2.00	0.43
1:B:85:MET:HB2	21:U:826:GLU:HB3	2.00	0.43
12:L:47:VAL:HG12	12:L:195:LEU:HD22	2.00	0.43
21:U:427:LEU:HD12	21:U:428:PRO:HD2	2.01	0.43
29:f:239:TYR:HE1	29:f:270:LEU:HD11	1.80	0.43
29:f:382:ASN:ND2	29:f:388:ASP:OD1	2.39	0.43
29:f:716:ASP:HB3	29:f:753:ALA:HA	2.00	0.43
7:g:90:GLN:HE22	7:g:118:ILE:HG23	1.84	0.43
16:p:28:PHE:HD2	16:p:36:THR:HG22	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:PHE:HD2	1:B:380:LEU:HD13	1.84	0.43
4:E:331:ILE:O	4:E:335:SER:OG	2.35	0.43
6:A:151:ILE:HD11	31:x:429:ARG:HH11	1.84	0.43
6:A:432:TYR:O	11:K:53:ARG:NH2	2.52	0.43
10:J:92:GLN:HG3	17:Q:66:LEU:HB2	1.99	0.43
15:O:17:ASP:OD1	15:O:33:LYS:NZ	2.52	0.43
18:R:196:HIS:O	18:R:200:SER:OG	2.30	0.43
25:a:116:THR:HG21	25:a:154:ARG:HB3	2.01	0.43
29:f:745:LEU:HD23	29:f:745:LEU:HA	1.83	0.43
33:W:169:LEU:O	33:W:182:ARG:NH1	2.48	0.43
4:E:60:VAL:HG12	4:E:71:VAL:HG22	2.00	0.43
5:F:379:VAL:HA	5:F:417:HIS:HE1	1.83	0.43
22:X:296:ASN:OD1	22:X:298:SER:OG	2.27	0.43
24:Z:208:ILE:HD11	24:Z:230:LEU:HD21	2.01	0.43
29:f:317:LEU:HA	29:f:320:ILE:HG12	2.00	0.43
9:i:161:ALA:HB3	10:j:53:LEU:HD23	2.01	0.43
20:t:100:ARG:HD2	20:t:128:LEU:HA	2.00	0.43
33:W:112:VAL:HA	33:W:115:ILE:HG12	2.01	0.43
34:V:90:GLU:HG3	34:V:496:PHE:HE2	1.82	0.43
3:D:214:MET:HE1	36:D:501:ATP:C5	2.53	0.43
3:D:264:ILE:HD12	3:D:267:ILE:HD13	2.01	0.43
8:H:46:LEU:HD12	8:H:75:VAL:HG12	2.01	0.43
10:J:116:GLN:HB2	10:J:151:GLY:HA3	1.99	0.43
13:M:136:MET:HE3	13:M:165:ILE:HG12	2.01	0.43
23:Y:220:VAL:HG11	23:Y:249:VAL:HB	2.00	0.43
7:g:123:GLN:NE2	8:h:82:ASP:OD1	2.42	0.43
20:t:22:ILE:HG12	20:t:50:MET:HE3	2.00	0.43
17:Q:180:VAL:HG13	17:Q:191:LEU:HB2	2.01	0.43
21:U:167:ILE:HD12	21:U:177:LEU:HG	2.01	0.43
21:U:366:HIS:HE1	21:U:392:TRP:HB3	1.83	0.43
26:b:5:SER:N	26:b:106:LYS:O	2.46	0.43
27:c:255:TYR:HD1	27:c:280:PRO:HG3	1.84	0.43
31:x:33:LEU:O	31:x:37:THR:OG1	2.29	0.43
4:E:36:LEU:C	5:F:69:MET:HE1	2.44	0.43
4:E:339:ASN:HB2	4:E:342:ASP:HB2	2.00	0.43
5:F:91:SER:HB3	5:F:126:THR:HG22	2.01	0.43
5:F:365:ILE:HD12	5:F:396:CYS:SG	2.59	0.43
29:f:345:PRO:HG2	29:f:348:ILE:HB	1.99	0.43
1:B:410:ARG:NH2	6:A:24:ALA:O	2.52	0.43
2:C:325:ARG:HD3	2:C:351:MET:HB2	2.01	0.43
4:E:119:VAL:HA	4:E:122:MET:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:362:ARG:HA	5:F:365:ILE:HG12	2.01	0.43
5:F:439:ALA:OXT	12:L:62:LYS:NZ	2.51	0.43
6:A:214:LEU:HB3	6:A:343:PHE:HE1	1.83	0.43
6:A:356:LYS:O	6:A:360:ARG:HB2	2.18	0.43
10:J:70:CYS:SG	10:J:71:MET:N	2.92	0.43
20:T:135:PRO:HB2	20:T:154:LEU:HD21	2.01	0.43
23:Y:360:ASP:OD1	23:Y:360:ASP:N	2.50	0.43
25:a:269:LEU:HD23	25:a:272:ILE:HD11	2.00	0.43
26:b:157:VAL:HG21	26:b:170:LEU:HG	2.01	0.43
28:d:12:LYS:HD2	28:d:12:LYS:HA	1.77	0.43
29:f:407:MET:HG3	29:f:440:ILE:HG12	1.99	0.43
29:f:505:MET:HE3	29:f:540:GLN:HG3	2.00	0.43
20:t:16:PHE:HE1	20:t:21:VAL:HG23	1.84	0.43
20:t:43:MET:HE2	20:t:51:LEU:HD22	2.01	0.43
33:W:128:LEU:HG	33:W:147:LYS:HE2	2.01	0.43
1:B:170:LEU:HD12	1:B:266:LEU:HD21	2.01	0.42
3:D:74:HIS:NE2	24:Z:179:ILE:O	2.52	0.42
7:G:164:LYS:NZ	8:H:55:ILE:O	2.47	0.42
10:J:41:VAL:HG11	10:J:134:VAL:HB	2.00	0.42
10:J:221:ASN:HB2	10:J:223:GLU:CD	2.43	0.42
21:U:835:ILE:HD11	29:f:229:VAL:HG13	2.00	0.42
23:Y:105:MET:HE1	23:Y:140:ILE:HD11	2.00	0.42
27:c:163:ILE:HD12	27:c:163:ILE:HA	1.91	0.42
28:d:98:LEU:HA	28:d:101:LEU:HD12	2.00	0.42
29:f:817:VAL:HG23	29:f:818:LEU:HD23	2.00	0.42
8:h:103:GLU:OE2	16:p:86:THR:OG1	2.37	0.42
9:i:165:GLY:O	9:i:168:SER:OG	2.34	0.42
31:x:76:ASP:OD1	31:x:76:ASP:N	2.51	0.42
1:B:369:THR:HB	1:B:374:LEU:HD11	2.02	0.42
2:C:342:ILE:HG13	2:C:380:GLN:HB3	2.00	0.42
4:E:144:GLU:OE2	4:E:297:ARG:NH2	2.46	0.42
7:G:80:MET:HE3	7:G:80:MET:HB3	1.87	0.42
17:Q:31:ASP:OD1	17:Q:31:ASP:N	2.49	0.42
17:Q:66:LEU:HD21	17:Q:70:ARG:HH21	1.84	0.42
24:Z:179:ILE:HB	24:Z:182:THR:HG22	2.01	0.42
31:x:210:VAL:O	31:x:214:LYS:HB2	2.19	0.42
1:B:288:ASP:OD1	1:B:288:ASP:N	2.52	0.42
11:K:240:ASP:OD1	11:K:241:ILE:N	2.52	0.42
17:Q:193:ASN:OD1	17:Q:193:ASN:N	2.47	0.42
21:U:788:VAL:HB	21:U:882:ALA:HB3	2.01	0.42
29:f:869:THR:HA	29:f:884:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:195:LYS:NZ	15:o:196:GLY:O	2.50	0.42
17:q:59:TYR:O	17:q:63:ASN:ND2	2.48	0.42
17:q:62:LYS:HA	17:q:62:LYS:HD3	1.75	0.42
1:B:364:ILE:HG22	1:B:395:ILE:HG21	2.02	0.42
4:E:65:THR:HG23	4:E:67:GLU:H	1.84	0.42
4:E:202:SER:O	5:F:308:ARG:NH1	2.52	0.42
21:U:510:GLU:HA	21:U:547:GLY:HA3	2.02	0.42
21:U:900:TYR:HD1	21:U:916:ASP:HA	1.85	0.42
27:c:231:LEU:O	27:c:298:GLN:NE2	2.47	0.42
28:d:197:ILE:HG22	28:d:198:LEU:HD23	2.02	0.42
29:f:432:TYR:O	29:f:435:SER:OG	2.28	0.42
29:f:679:LEU:HD23	29:f:687:ARG:HH22	1.84	0.42
19:s:16:ALA:HB2	19:s:121:VAL:HG23	2.01	0.42
20:t:122:LEU:HG	20:t:137:LEU:HD12	2.02	0.42
33:W:272:LEU:HD21	33:W:301:LYS:HE3	2.01	0.42
2:C:155:ASP:OD1	2:C:156:LYS:N	2.51	0.42
2:C:268:GLU:HB3	2:C:271:ARG:HH21	1.84	0.42
6:A:33:LEU:HD23	29:f:52:LEU:HD23	2.00	0.42
10:J:11:SER:OG	10:J:13:ASP:OD1	2.36	0.42
21:U:423:MET:HG3	21:U:446:LEU:HD11	2.00	0.42
26:b:7:MET:HB3	26:b:109:ILE:HG22	2.01	0.42
26:b:79:GLN:HB3	26:b:81:LYS:HZ3	1.84	0.42
28:d:181:CYS:SG	28:d:186:TYR:OH	2.65	0.42
9:i:197:LEU:HD22	9:i:201:MET:HE3	2.02	0.42
4:E:247:THR:HG22	4:E:251:ARG:HH12	1.85	0.42
10:J:58:THR:HA	10:J:60:ARG:NH1	2.33	0.42
16:P:34:MET:HE2	16:P:183:MET:HE1	2.02	0.42
21:U:830:THR:HB	29:f:610:GLN:HE21	1.85	0.42
22:X:307:THR:HA	22:X:310:ARG:HG2	2.01	0.42
23:Y:81:LEU:HD13	23:Y:107:LYS:HA	2.01	0.42
26:b:97:LEU:HG	26:b:107:MET:HB2	2.01	0.42
29:f:124:ASP:OD1	29:f:124:ASP:N	2.53	0.42
29:f:271:MET:HA	29:f:274:ASP:HB2	2.00	0.42
29:f:343:LYS:HB3	29:f:388:ASP:HA	2.01	0.42
8:h:43:GLY:HA3	8:h:184:LEU:HD21	2.00	0.42
33:W:375:MET:SD	33:W:375:MET:N	2.93	0.42
34:V:251:LEU:HD23	34:V:276:PHE:HD1	1.84	0.42
2:C:150:MET:HA	2:C:331:ILE:HD12	2.02	0.42
3:D:121:ARG:HA	3:D:121:ARG:HD3	1.85	0.42
3:D:327:LEU:HD23	3:D:327:LEU:HA	1.88	0.42
3:D:408:LYS:HD3	3:D:408:LYS:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:8:ASP:N	13:M:8:ASP:OD1	2.52	0.42
20:T:108:ASN:HB3	20:T:110:MET:HE3	2.01	0.42
22:X:252:LYS:HD3	22:X:313:LEU:HD13	2.01	0.42
26:b:113:VAL:O	26:b:143:PHE:N	2.45	0.42
26:b:154:THR:HA	26:b:170:LEU:HD11	2.02	0.42
29:f:24:THR:HG21	29:f:75:LEU:HD13	2.01	0.42
29:f:229:VAL:HG12	29:f:605:ASN:HB2	2.02	0.42
29:f:520:LEU:HD22	29:f:557:TRP:CD1	2.55	0.42
14:n:7:GLN:NE2	14:n:109:GLY:O	2.53	0.42
33:W:357:ARG:HD3	33:W:357:ARG:HA	1.82	0.42
6:A:189:GLU:O	6:A:193:THR:OG1	2.35	0.42
21:U:145:HIS:ND1	21:U:147:TYR:OH	2.43	0.42
22:X:334:ASN:OD1	22:X:337:ARG:NH1	2.51	0.42
23:Y:113:ARG:HD2	23:Y:113:ARG:HA	1.81	0.42
26:b:126:LYS:HA	26:b:126:LYS:HD2	1.95	0.42
28:d:215:TRP:HD1	28:d:222:TYR:HB3	1.85	0.42
29:f:556:ARG:CZ	29:f:786:GLN:HG3	2.50	0.42
11:k:234:LEU:HD23	11:k:234:LEU:HA	1.90	0.42
34:V:349:ARG:HH12	35:e:37:HIS:HE1	1.67	0.42
1:B:407:LEU:HD11	2:C:174:LEU:HD13	2.01	0.42
9:I:197:LEU:HA	9:I:197:LEU:HD12	1.90	0.42
13:M:191:LYS:H	13:M:191:LYS:HG2	1.66	0.42
19:S:75:TYR:CE1	19:S:83:MET:HB3	2.54	0.42
22:X:114:ILE:HD11	22:X:133:LEU:HG	2.02	0.42
22:X:255:LEU:HB2	22:X:287:LEU:HD13	2.02	0.42
8:h:206:ASP:OD1	8:h:206:ASP:N	2.49	0.42
31:x:15:PHE:HE2	31:x:37:THR:HG22	1.84	0.42
33:W:47:LEU:HD13	33:W:70:VAL:HG13	2.02	0.42
34:V:192:MET:HE3	34:V:192:MET:HB2	1.85	0.42
1:B:38:LYS:HG2	29:f:697:ILE:HG21	2.01	0.42
2:C:130:LYS:HD3	2:C:130:LYS:HA	1.51	0.42
4:E:65:THR:HG22	4:E:68:LYS:HB2	2.02	0.42
10:J:209:ALA:HB2	10:J:219:ILE:HD13	2.02	0.42
11:K:66:LYS:HE3	11:K:66:LYS:HB3	1.85	0.42
14:N:148:THR:OG1	14:N:151:GLU:OE1	2.27	0.42
21:U:218:GLN:HA	21:U:221:ILE:HD11	2.02	0.42
21:U:410:VAL:HG21	21:U:777:HIS:HD2	1.84	0.42
21:U:804:SER:HB3	21:U:876:GLN:HB2	2.02	0.42
22:X:302:PHE:CE2	22:X:327:TYR:HB2	2.55	0.42
24:Z:11:VAL:HB	24:Z:162:ILE:HD13	2.02	0.42
29:f:327:ASN:ND2	29:f:421:ASP:OD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:734:SER:O	29:f:734:SER:OG	2.31	0.42
9:i:72:MET:HE2	9:i:72:MET:HB3	1.90	0.42
10:j:85:ASN:OD1	17:q:70:ARG:NH1	2.44	0.42
11:k:13:ASN:HB3	12:l:126:ARG:HB3	2.02	0.42
20:t:92:LEU:HD23	20:t:112:ILE:HD11	2.02	0.42
32:y:24:GLU:HA	32:y:27:LYS:HG2	2.01	0.42
33:W:279:PHE:CZ	33:W:364:ARG:HG3	2.55	0.42
34:V:219:GLU:OE2	34:V:256:ARG:NH1	2.53	0.42
5:F:224:LEU:HG	5:F:226:TYR:HD2	1.85	0.41
6:A:227:ARG:HA	6:A:227:ARG:HD3	1.92	0.41
10:J:107:ILE:HD12	10:J:107:ILE:HA	1.93	0.41
11:K:81:LEU:HD12	11:K:138:GLY:HA3	2.00	0.41
21:U:492:ASP:OD1	21:U:492:ASP:N	2.53	0.41
22:X:241:SER:O	22:X:241:SER:OG	2.33	0.41
27:c:152:LYS:HE3	27:c:152:LYS:HB3	1.86	0.41
16:p:135:ASP:OD1	16:p:136:PHE:N	2.51	0.41
31:x:22:THR:HG22	31:x:63:ILE:HD12	2.02	0.41
31:x:350:PRO:O	31:x:480:TYR:OH	2.32	0.41
2:C:190:GLY:O	2:C:196:LYS:NZ	2.41	0.41
2:C:190:GLY:HA2	2:C:191:PRO:HD3	1.87	0.41
4:E:242:ARG:HH11	4:E:258:MET:HE3	1.85	0.41
6:A:187:LEU:HD23	6:A:229:VAL:HG21	2.02	0.41
7:G:13:ILE:HG13	7:G:14:THR:HG23	2.02	0.41
7:G:112:ASP:OD1	7:G:113:MET:N	2.53	0.41
16:P:88:MET:HE3	16:P:120:PHE:HZ	1.85	0.41
21:U:55:ARG:H	21:U:55:ARG:HG2	1.66	0.41
29:f:757:ASN:HA	29:f:809:ILE:HG22	2.02	0.41
8:h:39:LYS:HG3	8:h:44:VAL:HG22	2.00	0.41
17:q:101:ASN:HB3	17:q:132:HIS:CE1	2.56	0.41
31:x:148:SER:HA	31:x:151:TYR:CE2	2.54	0.41
32:y:4:PHE:O	32:y:67:LEU:N	2.48	0.41
33:W:121:LYS:HE2	33:W:121:LYS:HB3	1.85	0.41
6:A:169:LYS:HB2	6:A:169:LYS:HE3	1.74	0.41
10:J:158:ALA:HB1	10:J:172:LEU:HD13	2.01	0.41
11:K:42:THR:OG1	11:K:189:MET:O	2.38	0.41
13:M:120:HIS:O	13:M:123:THR:OG1	2.35	0.41
16:P:14:MET:HG2	16:P:167:ILE:HD13	2.01	0.41
21:U:535:TYR:HE2	21:U:544:ILE:HG21	1.85	0.41
26:b:65:THR:OG1	26:b:70:ARG:NH1	2.42	0.41
7:g:58:ASP:OD1	7:g:58:ASP:N	2.53	0.41
13:m:75:MET:HB2	13:m:137:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:x:331:PHE:HE1	32:y:73:LEU:HB2	1.85	0.41
31:x:361:PRO:HA	31:x:364:GLN:HB2	2.02	0.41
33:W:409:LEU:HD23	33:W:409:LEU:HA	1.87	0.41
35:e:26:ASP:OD1	35:e:26:ASP:N	2.52	0.41
8:H:82:ASP:HB3	8:H:130:PHE:HD2	1.85	0.41
8:H:196:LYS:HA	8:H:203:MET:HE1	2.01	0.41
14:N:80:ALA:HA	14:N:100:ILE:HD13	2.02	0.41
16:P:12:MET:HE1	16:P:170:ALA:HB3	2.02	0.41
26:b:1:MET:SD	26:b:43:SER:OG	2.76	0.41
29:f:353:LEU:HD23	29:f:353:LEU:HA	1.93	0.41
29:f:721:VAL:HA	29:f:724:ASN:HD22	1.83	0.41
29:f:828:ARG:HB3	29:f:843:SER:HA	2.02	0.41
9:i:185:THR:OG1	9:i:186:LEU:N	2.52	0.41
13:m:186:CYS:HA	13:m:189:ILE:HG22	2.02	0.41
16:p:155:GLU:HB2	16:p:158:MET:HE3	2.01	0.41
2:C:83:LYS:HA	2:C:105:ILE:HD12	2.03	0.41
3:D:296:MET:SD	3:D:326:ARG:HB2	2.61	0.41
6:A:170:PRO:HD2	6:A:231:ASN:HA	2.02	0.41
20:T:126:ASP:OD1	20:T:130:VAL:N	2.48	0.41
21:U:707:ASN:OD1	21:U:708:GLN:N	2.53	0.41
21:U:772:TRP:CD1	21:U:774:PRO:HD2	2.54	0.41
23:Y:290:PRO:HG2	23:Y:291:HIS:NE2	2.35	0.41
23:Y:349:LYS:HD3	23:Y:349:LYS:HA	1.95	0.41
24:Z:260:VAL:O	24:Z:264:SER:OG	2.30	0.41
27:c:262:GLU:O	27:c:264:LYS:NZ	2.38	0.41
29:f:478:ARG:HH11	29:f:510:SER:HB3	1.85	0.41
29:f:529:SER:O	29:f:565:ASN:ND2	2.54	0.41
9:i:21:VAL:O	9:i:25:MET:HG2	2.21	0.41
9:i:86:LEU:HG	9:i:114:LEU:HD11	2.02	0.41
20:t:127:MET:HB2	20:t:127:MET:HE3	1.84	0.41
2:C:147:THR:HA	2:C:205:HIS:HD2	1.85	0.41
5:F:223:VAL:HG22	5:F:350:ARG:HD3	2.03	0.41
9:I:41:ASP:OD1	9:I:41:ASP:N	2.52	0.41
21:U:198:LEU:HD21	21:U:219:CYS:HA	2.02	0.41
22:X:246:LYS:HA	22:X:246:LYS:HD3	1.93	0.41
27:c:239:LYS:HD2	27:c:239:LYS:HA	1.84	0.41
28:d:54:ILE:HA	28:d:57:ILE:HG12	2.01	0.41
29:f:72:ARG:HH21	29:f:86:THR:HB	1.85	0.41
29:f:496:ASP:OD1	29:f:496:ASP:N	2.53	0.41
29:f:834:ASP:OD1	29:f:834:ASP:N	2.52	0.41
33:W:271:VAL:HG12	33:W:290:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:275:MET:HG3	4:E:277:MET:HE2	2.02	0.41
5:F:204:LEU:HB3	5:F:212:PHE:HZ	1.85	0.41
16:P:88:MET:HE2	16:P:122:CYS:SG	2.61	0.41
21:U:462:LEU:HD12	21:U:496:LEU:HD13	2.03	0.41
21:U:861:LYS:HD3	21:U:861:LYS:HA	1.92	0.41
25:a:252:LYS:HA	25:a:255:TRP:NE1	2.35	0.41
25:a:342:ASP:O	25:a:345:GLN:N	2.38	0.41
29:f:316:ASP:OD1	29:f:316:ASP:N	2.52	0.41
29:f:530:CYS:HB2	29:f:565:ASN:HD21	1.86	0.41
7:g:7:ALA:N	7:g:10:ASP:OD1	2.50	0.41
13:m:136:MET:HE3	13:m:136:MET:HB2	1.88	0.41
15:o:70:THR:HG23	15:o:72:ARG:H	1.85	0.41
16:p:169:GLN:O	16:p:173:ASN:ND2	2.49	0.41
1:B:191:ASP:HA	1:B:194:ILE:HD12	2.02	0.41
9:I:123:GLN:OE1	10:J:125:ARG:NH2	2.54	0.41
11:K:13:ASN:ND2	12:L:124:GLY:O	2.54	0.41
11:K:228:MET:HE3	11:K:228:MET:HB2	1.93	0.41
21:U:374:SER:HB3	21:U:407:SER:HB3	2.03	0.41
23:Y:208:PHE:N	23:Y:212:GLU:OE2	2.48	0.41
25:a:343:LEU:HA	25:a:346:ILE:HD12	2.02	0.41
26:b:25:ARG:HD2	26:b:143:PHE:HB3	2.02	0.41
8:h:189:HIS:HA	8:h:233:ILE:HD11	2.03	0.41
16:p:5:SER:O	16:p:5:SER:OG	2.37	0.41
16:p:58:THR:O	17:q:85:ARG:NH2	2.54	0.41
18:r:42:LEU:HD23	18:r:42:LEU:HA	1.95	0.41
33:W:24:VAL:HA	33:W:50:LEU:HD11	2.03	0.41
33:W:117:ASP:HA	33:W:120:ILE:HB	2.03	0.41
34:V:362:LEU:HD12	34:V:362:LEU:HA	1.93	0.41
1:B:404:LEU:HD23	1:B:404:LEU:HA	1.93	0.41
3:D:78:GLU:OE2	27:c:152:LYS:NZ	2.48	0.41
3:D:163:MET:HG3	3:D:165:ALA:H	1.86	0.41
4:E:33:LEU:HA	5:F:66:LEU:HD21	2.03	0.41
5:F:54:ILE:HD13	5:F:54:ILE:HA	1.96	0.41
5:F:206:MET:O	5:F:209:LYS:NZ	2.51	0.41
5:F:349:ASP:O	5:F:351:LYS:NZ	2.52	0.41
6:A:154:PRO:HA	6:A:155:PRO:HD3	1.96	0.41
8:H:230:LEU:HD23	8:H:230:LEU:HA	1.97	0.41
13:M:114:ARG:HD2	13:M:114:ARG:HA	1.85	0.41
14:N:174:ILE:HB	14:N:189:LEU:HB2	2.03	0.41
17:Q:140:LEU:HD23	17:Q:140:LEU:HA	1.91	0.41
22:X:141:LYS:HE2	22:X:179:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:278:ARG:NH2	22:X:279:TYR:OH	2.38	0.41
24:Z:101:LEU:O	33:W:454:ASN:ND2	2.54	0.41
24:Z:279:LYS:HB3	24:Z:279:LYS:HE2	1.89	0.41
26:b:55:ALA:HA	26:b:84:ILE:HA	2.03	0.41
29:f:828:ARG:NH1	29:f:845:ARG:HB3	2.36	0.41
29:f:879:ARG:HA	29:f:879:ARG:HD3	1.84	0.41
15:o:179:SER:HB3	15:o:182:LYS:HB2	2.02	0.41
17:q:7:ILE:HD11	17:q:156:ALA:HB1	2.03	0.41
18:r:141:ARG:HD3	18:r:141:ARG:HA	1.87	0.41
31:x:10:TRP:HD1	31:x:72:MET:HA	1.85	0.41
31:x:363:LEU:HD12	31:x:366:LYS:HD3	2.01	0.41
35:e:56:LEU:O	35:e:60:LEU:HB2	2.21	0.41
1:B:221:GLY:HA3	1:B:347:ILE:HD13	2.03	0.41
2:C:190:GLY:HA3	2:C:317:PHE:HB2	2.02	0.41
6:A:270:CYS:H	6:A:315:ILE:HG22	1.86	0.41
8:H:114:VAL:HA	8:H:117:VAL:HG22	2.02	0.41
10:J:111:ILE:HD13	10:J:111:ILE:HA	1.91	0.41
11:K:105:GLU:OE2	19:S:81:LYS:NZ	2.44	0.41
11:K:209:LYS:O	11:K:214:ASN:ND2	2.53	0.41
13:M:45:VAL:HG21	13:M:148:LEU:HD13	2.01	0.41
15:O:187:ARG:HA	15:O:188:PRO:HA	1.91	0.41
17:Q:43:LEU:HD13	17:Q:188:ILE:HD13	2.03	0.41
20:T:110:MET:HB2	20:T:125:VAL:HB	2.02	0.41
23:Y:137:ARG:HD2	23:Y:168:ILE:HD11	2.03	0.41
24:Z:94:TRP:HB3	24:Z:112:MET:HE3	2.03	0.41
29:f:670:MET:HG2	29:f:673:ARG:NH1	2.36	0.41
3:D:110:ASN:OD1	3:D:110:ASN:N	2.55	0.40
3:D:130:VAL:HG12	3:D:142:VAL:HG12	2.03	0.40
4:E:134:GLU:HA	4:E:315:ILE:HD13	2.03	0.40
6:A:78:TRP:O	6:A:82:ALA:N	2.50	0.40
7:G:51:VAL:HG22	7:G:217:VAL:HG22	2.03	0.40
10:J:115:LYS:HE2	10:J:149:PRO:HA	2.03	0.40
18:R:100:MET:HE2	18:R:126:PHE:HB3	2.03	0.40
21:U:637:VAL:HG11	21:U:656:LEU:HD13	2.03	0.40
21:U:681:ASN:OD1	21:U:681:ASN:N	2.53	0.40
23:Y:285:ASP:OD1	23:Y:286:TRP:N	2.52	0.40
23:Y:343:LEU:HD12	23:Y:343:LEU:HA	1.95	0.40
24:Z:68:TRP:HH2	24:Z:111:LEU:HG	1.86	0.40
29:f:648:ALA:HB1	29:f:678:LEU:HD21	2.03	0.40
16:p:30:ILE:HG22	16:p:31:GLN:H	1.87	0.40
18:r:82:LEU:HD23	18:r:82:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:t:189:ILE:HG23	20:t:200:GLU:HB2	2.03	0.40
1:B:416:ASN:HA	1:B:419:PHE:HD2	1.84	0.40
1:B:421:LYS:HA	1:B:421:LYS:HD2	1.85	0.40
2:C:113:ARG:HH21	2:C:129:ASN:C	2.29	0.40
6:A:198:PRO:HB3	6:A:312:ARG:HH21	1.85	0.40
7:G:10:ASP:OD1	7:G:10:ASP:N	2.48	0.40
9:I:214:ALA:HB2	9:I:227:VAL:HG12	2.02	0.40
10:J:39:ASP:OD1	10:J:39:ASP:N	2.53	0.40
12:L:49:LEU:HB2	12:L:195:LEU:HD21	2.03	0.40
14:N:73:PRO:HA	14:N:74:PRO:HD3	1.86	0.40
15:O:104:ASP:OD1	15:O:104:ASP:N	2.54	0.40
16:P:68:LYS:HD2	16:P:68:LYS:HA	1.92	0.40
23:Y:22:LEU:HD12	23:Y:22:LEU:HA	1.90	0.40
25:a:57:ILE:HD12	25:a:57:ILE:HA	2.00	0.40
25:a:270:ARG:HH21	25:a:310:LEU:HD13	1.85	0.40
26:b:110:ILE:HG12	26:b:139:ASP:HB3	2.02	0.40
26:b:157:VAL:HG13	26:b:168:SER:HG	1.85	0.40
27:c:192:LEU:HD22	27:c:196:LEU:HD23	2.03	0.40
27:c:231:LEU:HD12	33:W:429:SER:HB3	2.03	0.40
29:f:639:LYS:HB2	29:f:639:LYS:HE3	1.78	0.40
29:f:811:LEU:HD22	29:f:856:ALA:HB2	2.03	0.40
8:h:46:LEU:HD11	8:h:137:CYS:HB3	2.02	0.40
31:x:492:SER:OG	31:x:494:GLN:OE1	2.39	0.40
34:V:240:LEU:HD12	34:V:241:ARG:HG3	2.02	0.40
35:e:47:ASN:OD1	35:e:47:ASN:N	2.54	0.40
1:B:365:PHE:HB3	1:B:380:LEU:HD22	2.03	0.40
1:B:368:HIS:HE1	36:B:501:ATP:H2	1.69	0.40
4:E:285:LEU:HD13	4:E:290:LEU:HD21	2.01	0.40
4:E:309:ARG:HA	4:E:312:ILE:HG22	2.03	0.40
5:F:386:ARG:HH22	13:M:54:LEU:HG	1.85	0.40
16:P:61:GLN:HB2	17:Q:85:ARG:NH2	2.36	0.40
21:U:654:MET:HE1	21:U:767:THR:HA	2.03	0.40
23:Y:168:ILE:HG21	23:Y:179:ARG:HH22	1.86	0.40
28:d:38:THR:HG21	28:d:84:ASP:HB2	2.04	0.40
29:f:652:VAL:HG21	29:f:687:ARG:HD2	2.03	0.40
7:g:202:LEU:HD12	7:g:202:LEU:HA	1.91	0.40
10:j:183:THR:H	10:j:186:LEU:HD12	1.86	0.40
12:l:117:GLN:HG3	13:m:82:ALA:HB1	2.04	0.40
19:s:71:ARG:HA	19:s:74:MET:HE3	2.04	0.40
20:t:13:GLY:HA3	20:t:22:ILE:HG22	2.03	0.40
32:y:4:PHE:N	32:y:65:SER:O	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:W:31:CYS:HA	33:W:34:LEU:HG	2.03	0.40
33:W:234:ASP:HB3	33:W:239:SER:HB2	2.03	0.40
35:e:46:ASP:N	35:e:46:ASP:OD1	2.47	0.40
35:e:58:ALA:O	35:e:62:LYS:CB	2.68	0.40
1:B:438:LEU:HD12	1:B:438:LEU:HA	1.92	0.40
3:D:213:THR:OG1	36:D:501:ATP:O1G	2.40	0.40
6:A:32:LEU:HD22	29:f:58:MET:HE3	2.04	0.40
14:N:120:MET:HE3	14:N:120:MET:HB2	1.91	0.40
22:X:183:LEU:HD12	22:X:183:LEU:HA	1.95	0.40
25:a:252:LYS:HA	25:a:255:TRP:CE2	2.56	0.40
27:c:168:MET:O	27:c:172:HIS:NE2	2.54	0.40
27:c:257:LYS:HD2	27:c:257:LYS:HA	1.83	0.40
29:f:185:LEU:HA	29:f:188:VAL:HG12	2.03	0.40
11:k:50:VAL:HG11	11:k:66:LYS:HB2	2.03	0.40
15:o:50:ALA:O	15:o:54:MET:HG2	2.21	0.40
1:B:121:ALA:HB2	1:B:135:ILE:HD11	2.03	0.40
1:B:322:ARG:HA	1:B:322:ARG:HD3	1.72	0.40
5:F:91:SER:O	5:F:151:VAL:N	2.52	0.40
5:F:401:VAL:O	5:F:405:MET:HG3	2.21	0.40
9:I:76:VAL:HG12	9:I:134:LEU:HG	2.02	0.40
16:P:30:ILE:HG22	16:P:31:GLN:H	1.86	0.40
19:S:145:LEU:HD22	19:S:178:VAL:HB	2.04	0.40
20:T:174:ARG:NH1	20:T:206:GLU:O	2.55	0.40
23:Y:16:ASP:HB2	23:Y:150:PHE:CZ	2.57	0.40
23:Y:154:ASN:OD1	23:Y:154:ASN:N	2.51	0.40
23:Y:210:SER:OG	23:Y:211:TYR:N	2.52	0.40
24:Z:147:ASP:OD1	24:Z:147:ASP:N	2.51	0.40
29:f:253:LEU:HD23	29:f:253:LEU:HA	1.85	0.40
7:g:189:TRP:HB3	7:g:194:THR:HG23	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	B	409/440 (93%)	377 (92%)	32 (8%)	0	100	100
2	C	394/398 (99%)	357 (91%)	33 (8%)	4 (1%)	12	40
3	D	378/418 (90%)	331 (88%)	47 (12%)	0	100	100
4	E	387/403 (96%)	348 (90%)	38 (10%)	1 (0%)	36	65
5	F	391/439 (89%)	353 (90%)	38 (10%)	0	100	100
6	A	411/433 (95%)	371 (90%)	40 (10%)	0	100	100
7	G	238/246 (97%)	225 (94%)	13 (6%)	0	100	100
7	g	242/246 (98%)	231 (96%)	11 (4%)	0	100	100
8	H	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
8	h	230/234 (98%)	221 (96%)	9 (4%)	0	100	100
9	I	246/261 (94%)	238 (97%)	8 (3%)	0	100	100
9	i	248/261 (95%)	242 (98%)	6 (2%)	0	100	100
10	J	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
10	j	237/248 (96%)	225 (95%)	12 (5%)	0	100	100
11	K	236/241 (98%)	228 (97%)	8 (3%)	0	100	100
11	k	232/241 (96%)	225 (97%)	7 (3%)	0	100	100
12	L	238/269 (88%)	228 (96%)	10 (4%)	0	100	100
12	l	236/269 (88%)	228 (97%)	8 (3%)	0	100	100
13	M	240/255 (94%)	235 (98%)	5 (2%)	0	100	100
13	m	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
14	N	201/239 (84%)	196 (98%)	5 (2%)	0	100	100
14	n	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
15	O	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
15	o	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
16	P	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
16	p	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
17	Q	197/201 (98%)	190 (96%)	7 (4%)	0	100	100
17	q	197/201 (98%)	189 (96%)	8 (4%)	0	100	100
18	R	199/263 (76%)	196 (98%)	3 (2%)	0	100	100
18	r	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
19	S	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
19	s	211/241 (88%)	204 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	214/264 (81%)	210 (98%)	4 (2%)	0	100	100
20	t	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
21	U	868/953 (91%)	802 (92%)	66 (8%)	0	100	100
22	X	378/422 (90%)	362 (96%)	16 (4%)	0	100	100
23	Y	376/389 (97%)	343 (91%)	32 (8%)	1 (0%)	36	65
24	Z	284/324 (88%)	257 (90%)	27 (10%)	0	100	100
25	a	371/376 (99%)	349 (94%)	22 (6%)	0	100	100
26	b	189/377 (50%)	168 (89%)	21 (11%)	0	100	100
27	c	285/310 (92%)	253 (89%)	31 (11%)	1 (0%)	30	59
28	d	255/350 (73%)	221 (87%)	33 (13%)	1 (0%)	30	59
29	f	887/908 (98%)	770 (87%)	117 (13%)	0	100	100
31	x	492/494 (100%)	466 (95%)	26 (5%)	0	100	100
32	y	74/76 (97%)	65 (88%)	9 (12%)	0	100	100
33	W	444/456 (97%)	407 (92%)	35 (8%)	2 (0%)	24	54
34	V	442/534 (83%)	432 (98%)	10 (2%)	0	100	100
35	e	48/70 (69%)	41 (85%)	7 (15%)	0	100	100
All	All	13974/15458 (90%)	13071 (94%)	893 (6%)	10 (0%)	49	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	167	PRO
27	c	285	GLU
2	C	133	PRO
2	C	192	PRO
2	C	90	HIS
33	W	310	THR
33	W	139	GLU
28	d	203	PRO
23	Y	350	VAL
2	C	91	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	B	357/385 (93%)	357 (100%)	0	100	100
2	C	340/346 (98%)	338 (99%)	2 (1%)	78	80
3	D	333/366 (91%)	333 (100%)	0	100	100
4	E	341/353 (97%)	341 (100%)	0	100	100
5	F	340/379 (90%)	340 (100%)	0	100	100
6	A	349/372 (94%)	347 (99%)	2 (1%)	78	80
7	G	202/210 (96%)	202 (100%)	0	100	100
7	g	201/210 (96%)	201 (100%)	0	100	100
8	H	187/191 (98%)	187 (100%)	0	100	100
8	h	188/191 (98%)	188 (100%)	0	100	100
9	I	202/221 (91%)	202 (100%)	0	100	100
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	197/211 (93%)	196 (100%)	1 (0%)	81	81
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	197/203 (97%)	196 (100%)	1 (0%)	81	81
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	198/212 (93%)	198 (100%)	0	100	100
13	m	198/212 (93%)	198 (100%)	0	100	100
14	N	158/181 (87%)	158 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	178/228 (78%)	178 (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	166/171 (97%)	166 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	r	154/202 (76%)	154 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	177/199 (89%)	176 (99%)	1 (1%)	78	80
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	748/816 (92%)	748 (100%)	0	100	100
22	X	327/362 (90%)	327 (100%)	0	100	100
23	Y	334/344 (97%)	334 (100%)	0	100	100
24	Z	257/295 (87%)	257 (100%)	0	100	100
25	a	333/336 (99%)	333 (100%)	0	100	100
26	b	167/312 (54%)	167 (100%)	0	100	100
27	c	252/268 (94%)	252 (100%)	0	100	100
28	d	231/294 (79%)	229 (99%)	2 (1%)	70	76
29	f	745/763 (98%)	743 (100%)	2 (0%)	86	84
31	x	439/439 (100%)	439 (100%)	0	100	100
32	y	68/68 (100%)	68 (100%)	0	100	100
33	W	410/416 (99%)	406 (99%)	4 (1%)	68	75
34	V	390/460 (85%)	390 (100%)	0	100	100
35	e	44/63 (70%)	44 (100%)	0	100	100
All	All	11946/13133 (91%)	11931 (100%)	15 (0%)	87	89

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	129	ASN
2	C	130	LYS
6	A	373	LEU
6	A	403	ILE
10	J	221	ASN
11	K	156	MET
28	d	202	THR
28	d	204	LYS
29	f	873	LEU
29	f	874	LEU
19	s	193	LEU

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Mol	Chain	Res	Type
33	W	117	ASP
33	W	118	LEU
33	W	120	ILE
33	W	189	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	ASN
2	C	171	HIS
2	C	278	ASN
3	D	48	GLN
3	D	135	HIS
4	E	129	ASN
4	E	194	ASN
5	F	395	GLN
5	F	428	GLN
6	A	94	GLN
6	A	117	GLN
6	A	414	ASN
7	G	68	HIS
8	H	207	ASN
9	I	51	ASN
9	I	95	GLN
10	J	92	GLN
10	J	122	ASN
11	K	97	GLN
11	K	155	HIS
11	K	186	HIS
11	K	204	GLN
11	K	224	GLN
12	L	68	ASN
12	L	146	GLN
12	L	175	HIS
12	L	203	GLN
12	L	209	ASN
16	P	18	ASN
16	P	169	GLN
17	Q	71	ASN
18	R	62	GLN
18	R	175	ASN
19	S	80	ASN

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Mol	Chain	Res	Type
19	S	152	GLN
20	T	147	GLN
21	U	32	ASN
21	U	111	GLN
21	U	128	GLN
21	U	207	ASN
21	U	345	ASN
21	U	346	ASN
21	U	347	ASN
21	U	421	GLN
21	U	611	ASN
21	U	708	GLN
21	U	743	ASN
21	U	801	GLN
21	U	805	ASN
21	U	888	GLN
23	Y	49	ASN
23	Y	71	ASN
23	Y	178	ASN
23	Y	351	ASN
23	Y	357	ASN
23	Y	365	GLN
24	Z	44	GLN
24	Z	196	HIS
24	Z	273	HIS
24	Z	277	ASN
24	Z	278	ASN
25	a	18	GLN
25	a	124	ASN
25	a	264	ASN
25	a	337	GLN
26	b	48	ASN
26	b	137	ASN
27	c	128	ASN
27	c	274	ASN
28	d	228	GLN
28	d	252	GLN
29	f	118	ASN
29	f	224	ASN
29	f	238	ASN
29	f	371	ASN
29	f	387	GLN

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Mol	Chain	Res	Type
29	f	402	ASN
29	f	565	ASN
29	f	650	GLN
7	g	68	HIS
7	g	75	ASN
7	g	128	ASN
8	h	21	GLN
8	h	109	GLN
9	i	40	ASN
9	i	102	GLN
10	j	154	HIS
10	j	175	ASN
10	j	215	GLN
11	k	98	ASN
11	k	99	HIS
11	k	211	ASN
12	l	5	GLN
12	l	59	HIS
12	l	175	HIS
13	m	147	GLN
13	m	180	GLN
14	n	7	GLN
14	n	66	HIS
14	n	123	GLN
14	n	154	GLN
14	n	158	ASN
15	o	62	ASN
16	p	72	ASN
17	q	82	ASN
17	q	101	ASN
17	q	132	HIS
17	q	174	ASN
18	r	162	GLN
19	s	108	ASN
20	t	61	GLN
20	t	147	GLN
31	x	272	GLN
31	x	308	ASN
31	x	327	GLN
32	y	25	ASN
33	W	107	GLN
33	W	189	GLN

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Mol	Chain	Res	Type
33	W	356	ASN
34	V	124	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 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	ADP	E	501	-	28,29,29	1.33	5 (17%)	43,45,45	2.41	12 (27%)
37	ADP	F	501	-	28,29,29	1.44	3 (10%)	43,45,45	1.82	7 (16%)
36	ATP	D	501	-	32,33,33	0.43	0	48,52,52	0.31	0
36	ATP	C	501	-	32,33,33	0.38	0	48,52,52	0.33	0
36	ATP	B	501	-	32,33,33	0.41	0	48,52,52	0.36	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
37	ADP	E	501	-	-	8/16/32/32	0/3/3/3
37	ADP	F	501	-	-	6/16/32/32	0/3/3/3
36	ATP	D	501	-	-	4/22/38/38	0/3/3/3
36	ATP	C	501	-	-	11/22/38/38	0/3/3/3
36	ATP	B	501	-	-	3/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	F	501	ADP	C5-C4	4.84	1.47	1.39
37	E	501	ADP	C5-N7	-3.04	1.33	1.39
37	E	501	ADP	C5-C4	2.90	1.44	1.39
37	F	501	ADP	C5-C6	2.76	1.48	1.41
37	F	501	ADP	C5-N7	-2.72	1.34	1.39
37	E	501	ADP	C5-C6	2.36	1.47	1.41
37	E	501	ADP	C8-N9	-2.11	1.34	1.37
37	E	501	ADP	PA-O3A	2.00	1.61	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	E	501	ADP	C5-C4-N3	-8.70	114.74	126.72
37	E	501	ADP	N3-C4-N9	6.61	138.40	127.17
37	F	501	ADP	C5-C4-N3	-6.28	118.07	126.72
37	E	501	ADP	C2-N3-C4	5.26	124.67	111.83
37	F	501	ADP	N3-C4-N9	4.83	135.37	127.17
37	E	501	ADP	C4-C5-N7	-3.90	106.13	110.58
37	F	501	ADP	C4-C5-N7	-3.90	106.13	110.58
37	F	501	ADP	C2-N3-C4	3.44	120.24	111.83
37	E	501	ADP	C5-N7-C8	3.32	108.67	103.45
37	E	501	ADP	N3-C2-N1	-2.93	124.15	128.58
37	E	501	ADP	N9-C8-N7	-2.90	109.82	113.94
37	F	501	ADP	C5-N7-C8	2.69	107.68	103.45
37	E	501	ADP	C6-C5-N7	2.63	137.15	132.09
37	E	501	ADP	C4-N9-C8	2.59	108.46	105.74
37	F	501	ADP	C3'-C2'-C1'	2.52	106.23	101.46
37	E	501	ADP	C3'-C2'-C1'	2.32	105.86	101.46
37	F	501	ADP	N3-C2-N1	-2.23	125.21	128.58
37	E	501	ADP	O3B-PB-O2B	2.20	116.05	107.80
37	E	501	ADP	C5-C6-N1	2.19	123.06	117.51

There are no chirality outliers.

All (32) torsion outliers are listed below:

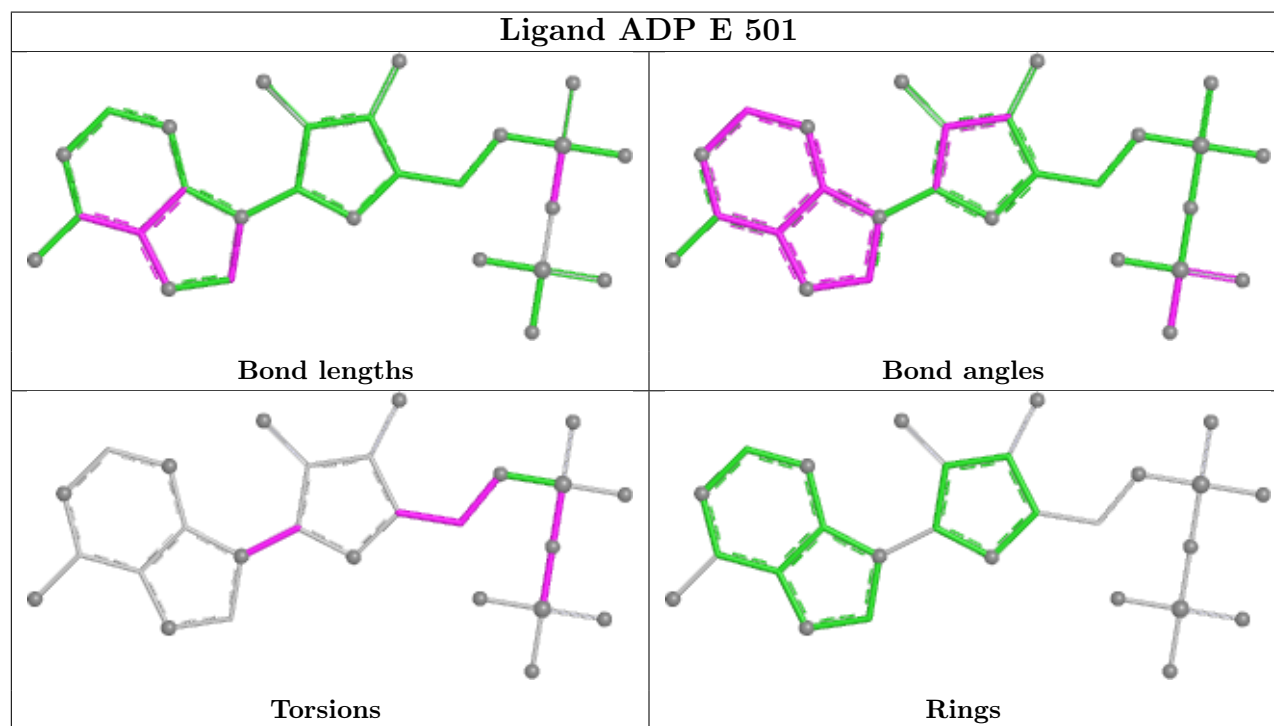
Mol	Chain	Res	Type	Atoms
36	B	501	ATP	PB-O3A-PA-O5'
36	B	501	ATP	C5'-O5'-PA-O2A
36	C	501	ATP	C5'-O5'-PA-O1A
36	C	501	ATP	C5'-O5'-PA-O3A
37	E	501	ADP	PA-O3A-PB-O3B
37	E	501	ADP	O4'-C4'-C5'-O5'
37	F	501	ADP	C5'-O5'-PA-O1A
37	F	501	ADP	C5'-O5'-PA-O2A
37	F	501	ADP	C5'-O5'-PA-O3A
36	D	501	ATP	O4'-C4'-C5'-O5'
36	D	501	ATP	C3'-C4'-C5'-O5'
37	F	501	ADP	O4'-C4'-C5'-O5'
37	F	501	ADP	C3'-C4'-C5'-O5'
37	E	501	ADP	C3'-C4'-C5'-O5'
37	E	501	ADP	C2'-C1'-N9-C8
37	E	501	ADP	C2'-C1'-N9-C4
36	C	501	ATP	C4'-C5'-O5'-PA
37	E	501	ADP	PB-O3A-PA-O5'
36	C	501	ATP	PB-O3B-PG-O2G
36	C	501	ATP	PB-O3A-PA-O2A
36	C	501	ATP	C5'-O5'-PA-O2A
37	F	501	ADP	C4'-C5'-O5'-PA
37	E	501	ADP	C4'-C5'-O5'-PA
36	B	501	ATP	C4'-C5'-O5'-PA
36	C	501	ATP	PB-O3B-PG-O3G
36	C	501	ATP	PA-O3A-PB-O1B
36	C	501	ATP	PA-O3A-PB-O2B
36	C	501	ATP	PB-O3A-PA-O1A
36	D	501	ATP	PB-O3A-PA-O1A
36	D	501	ATP	PB-O3A-PA-O2A
36	C	501	ATP	PB-O3B-PG-O1G
37	E	501	ADP	PA-O3A-PB-O1B

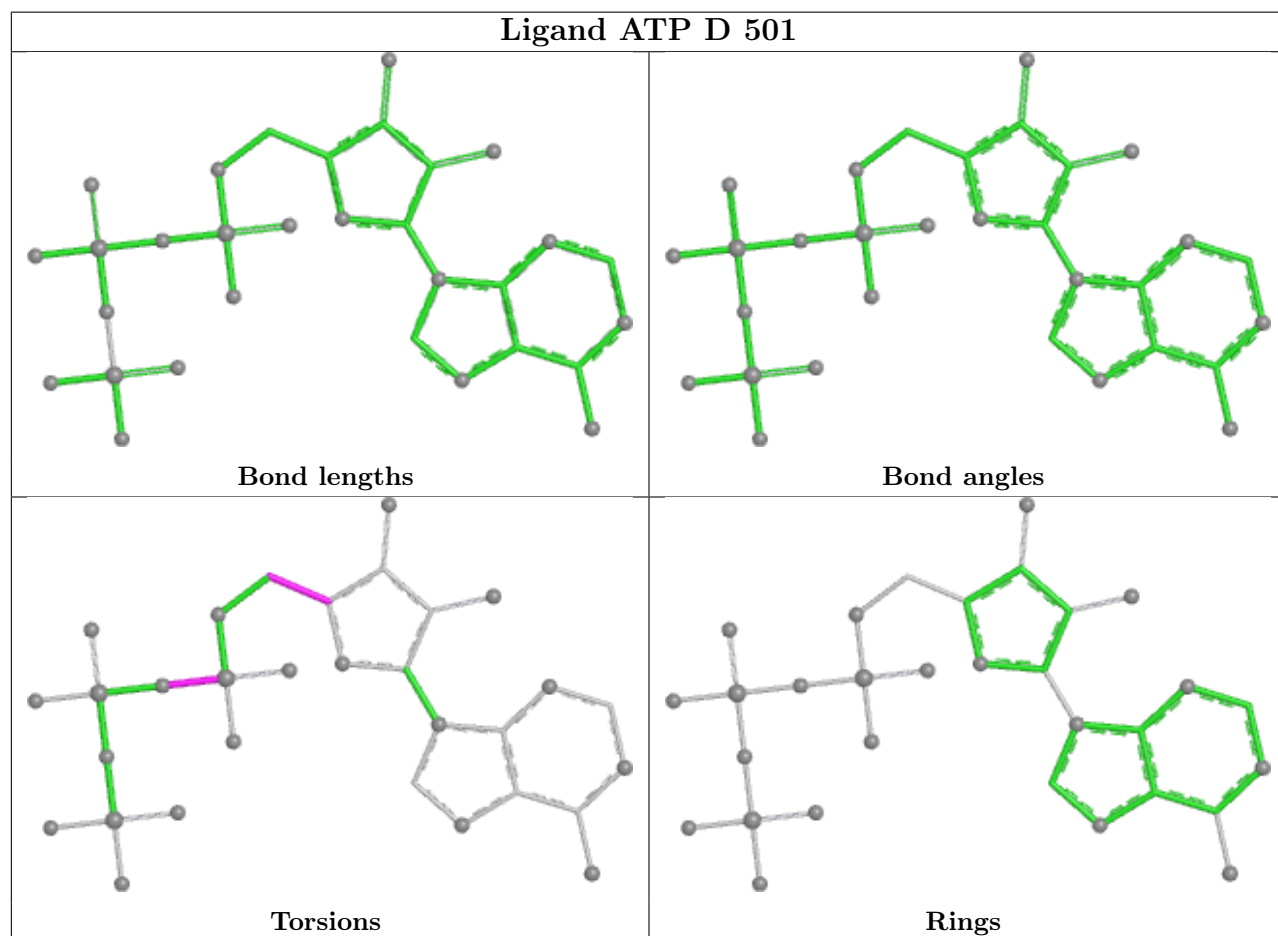
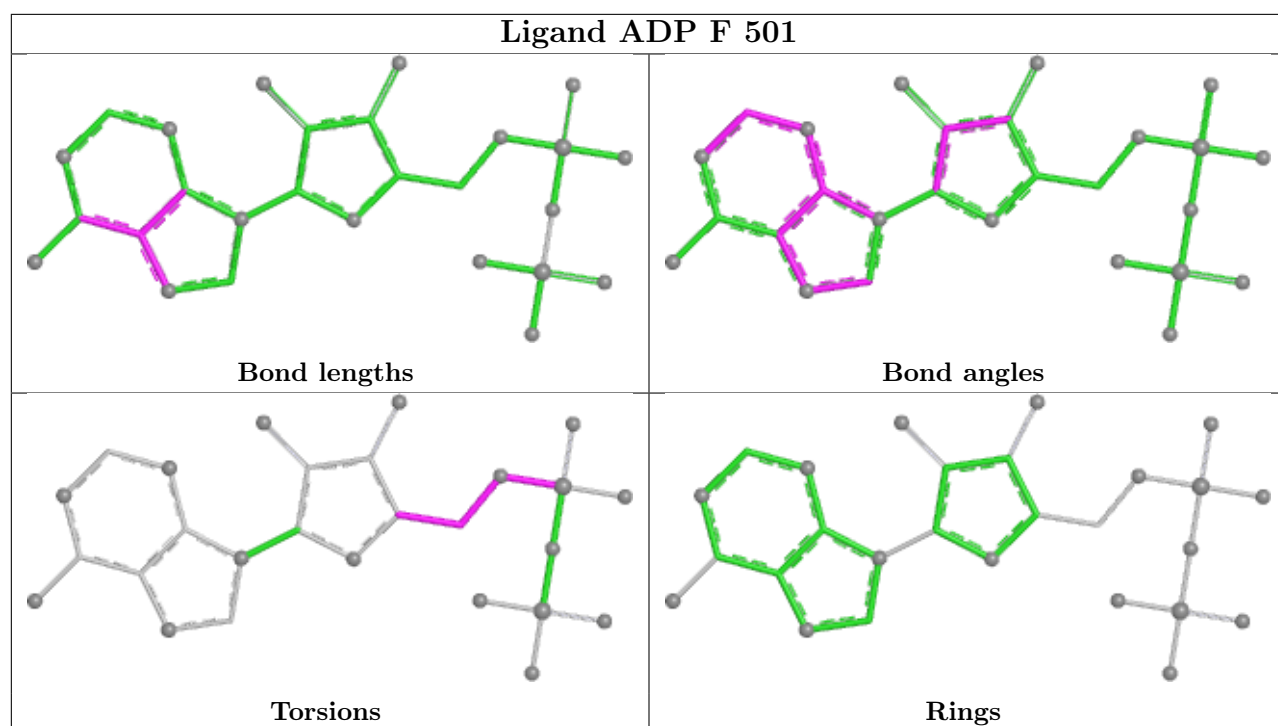
There are no ring outliers.

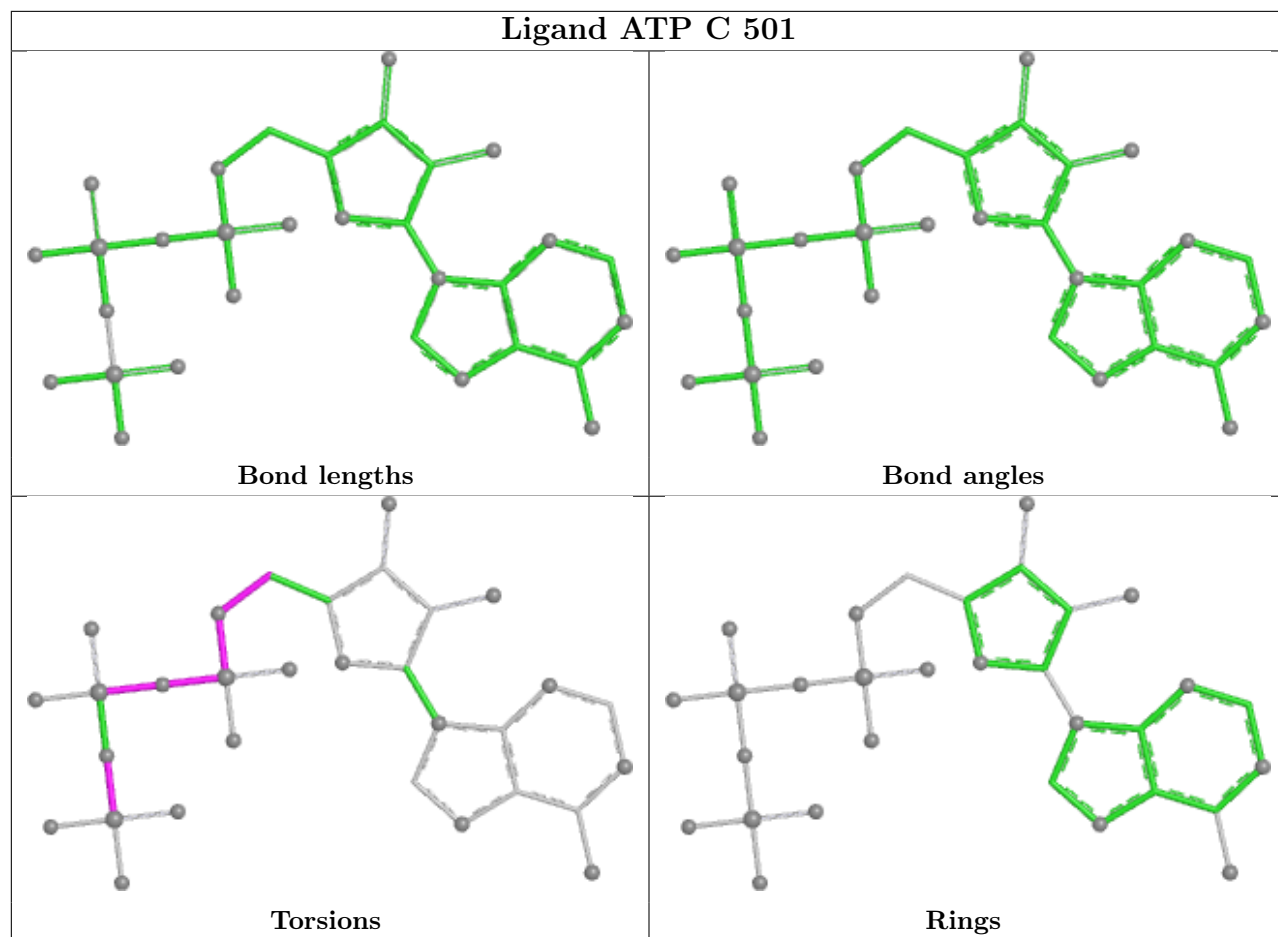
4 monomers are involved in 12 short contacts:

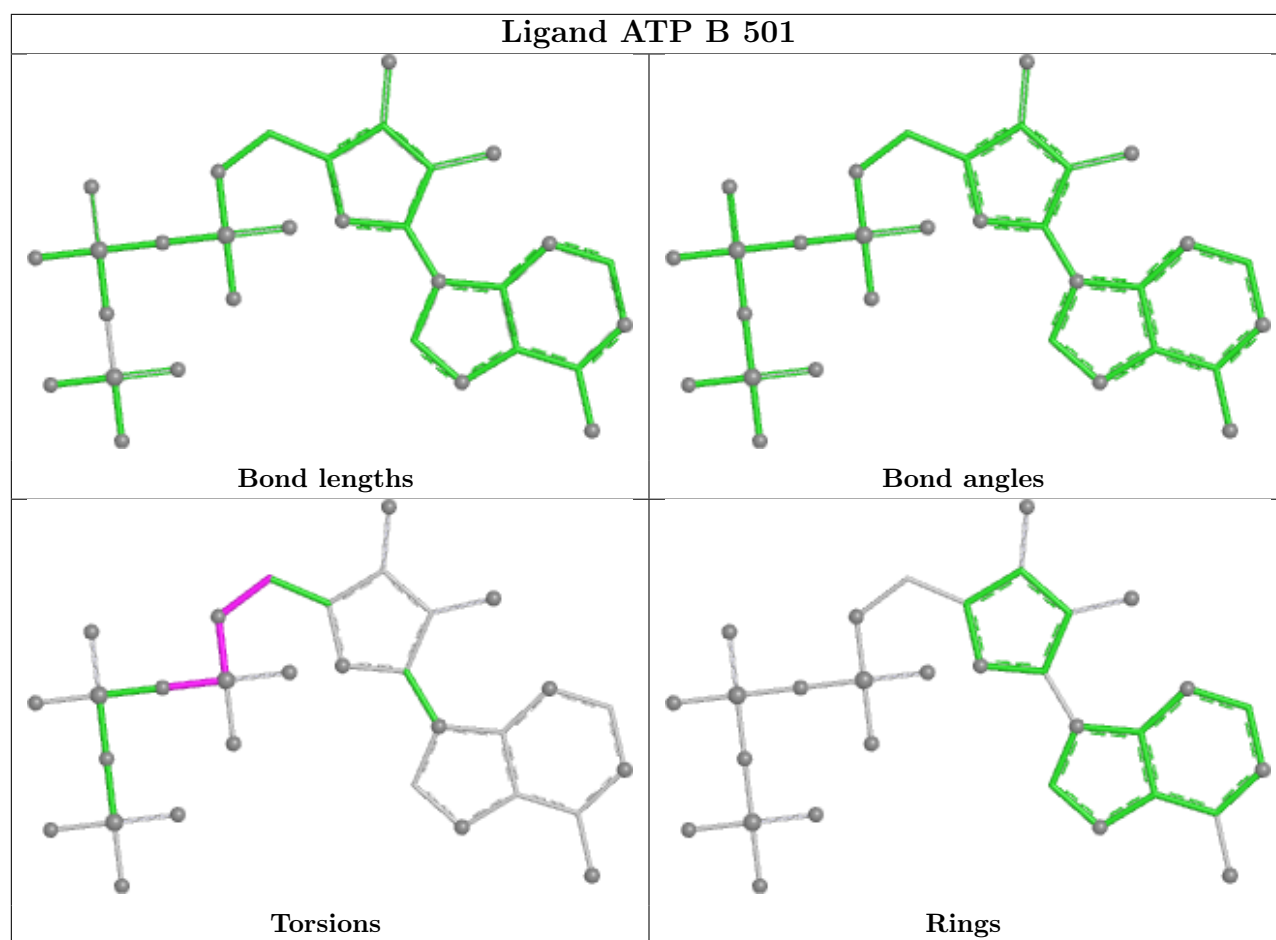
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	E	501	ADP	6	0
37	F	501	ADP	1	0
36	D	501	ATP	3	0
36	B	501	ATP	2	0

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.

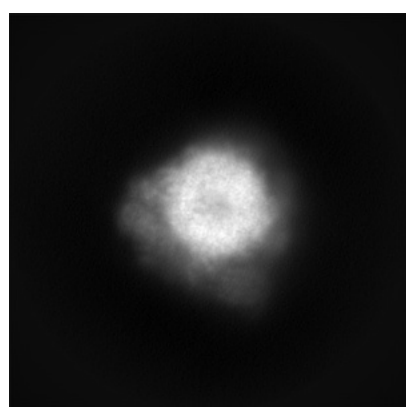
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32277. 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](#)

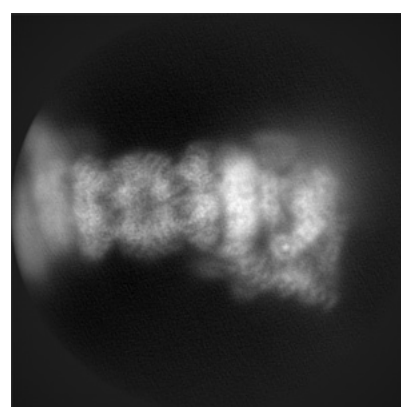
6.1.1 Primary map



X



Y

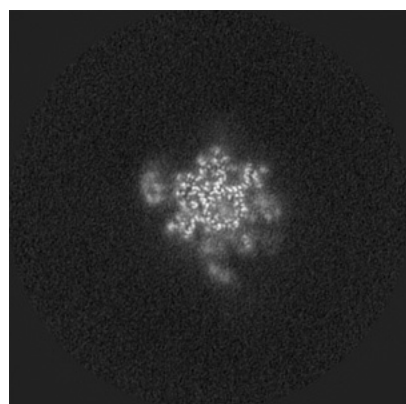


Z

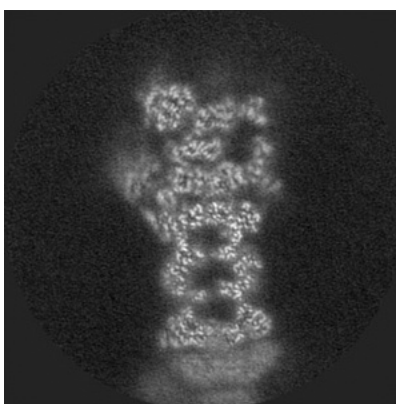
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

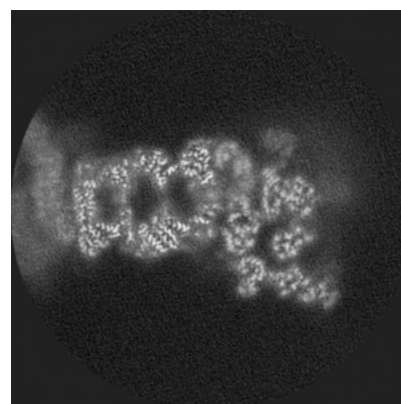
6.2.1 Primary map



X Index: 320



Y Index: 320

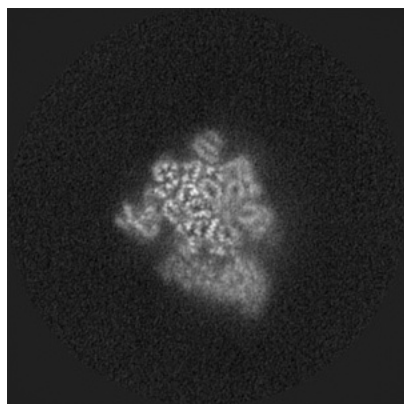


Z Index: 320

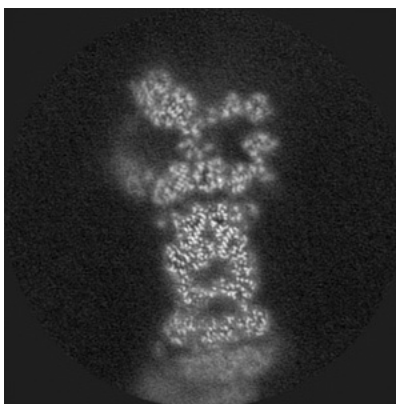
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

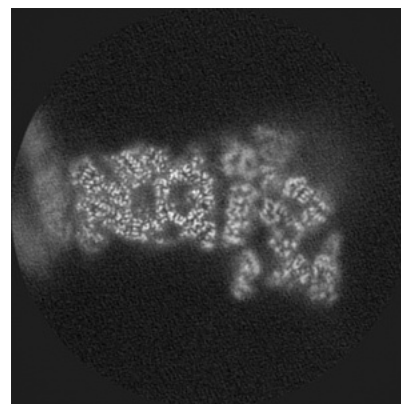
6.3.1 Primary map



X Index: 366



Y Index: 303

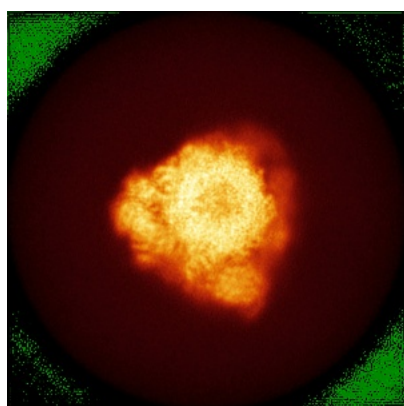


Z Index: 297

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

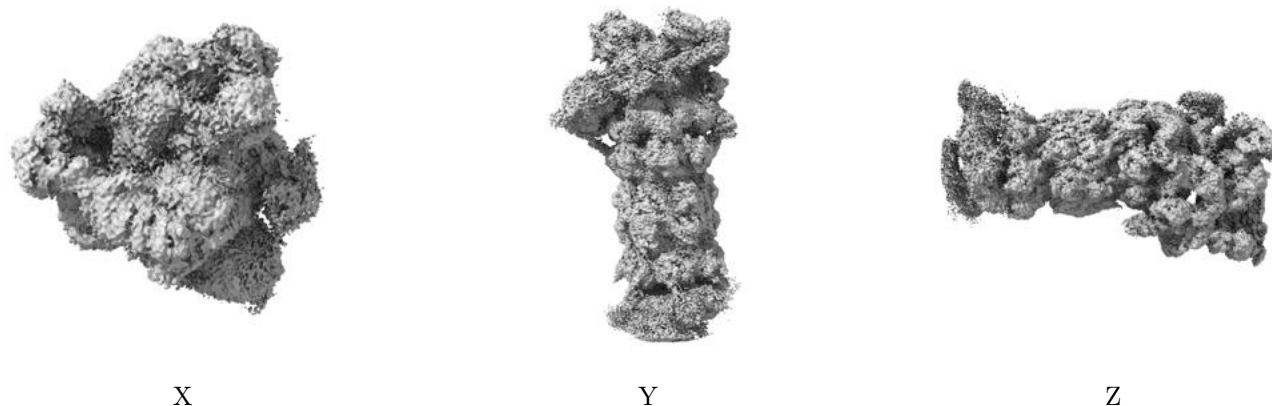


Z

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

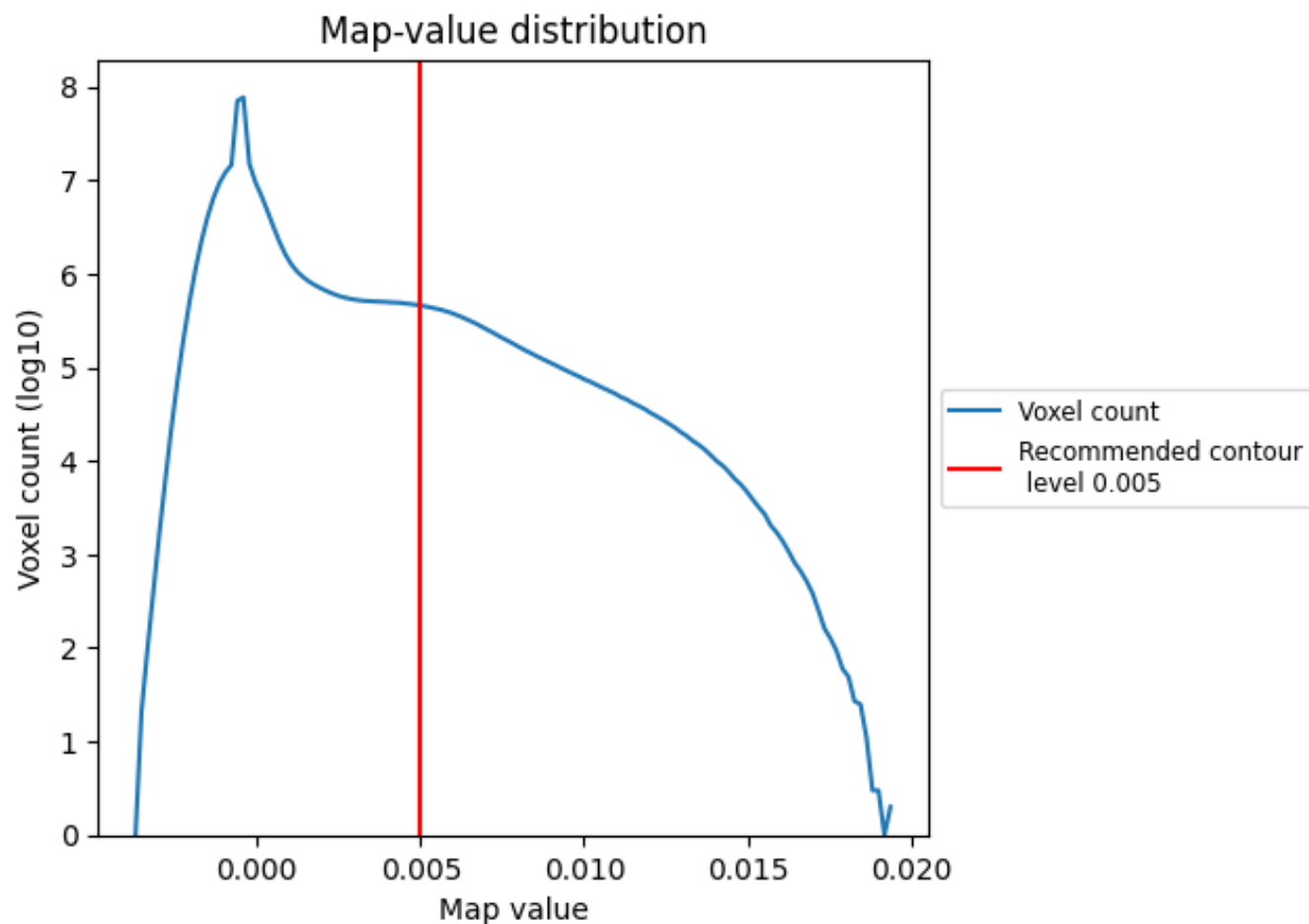
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

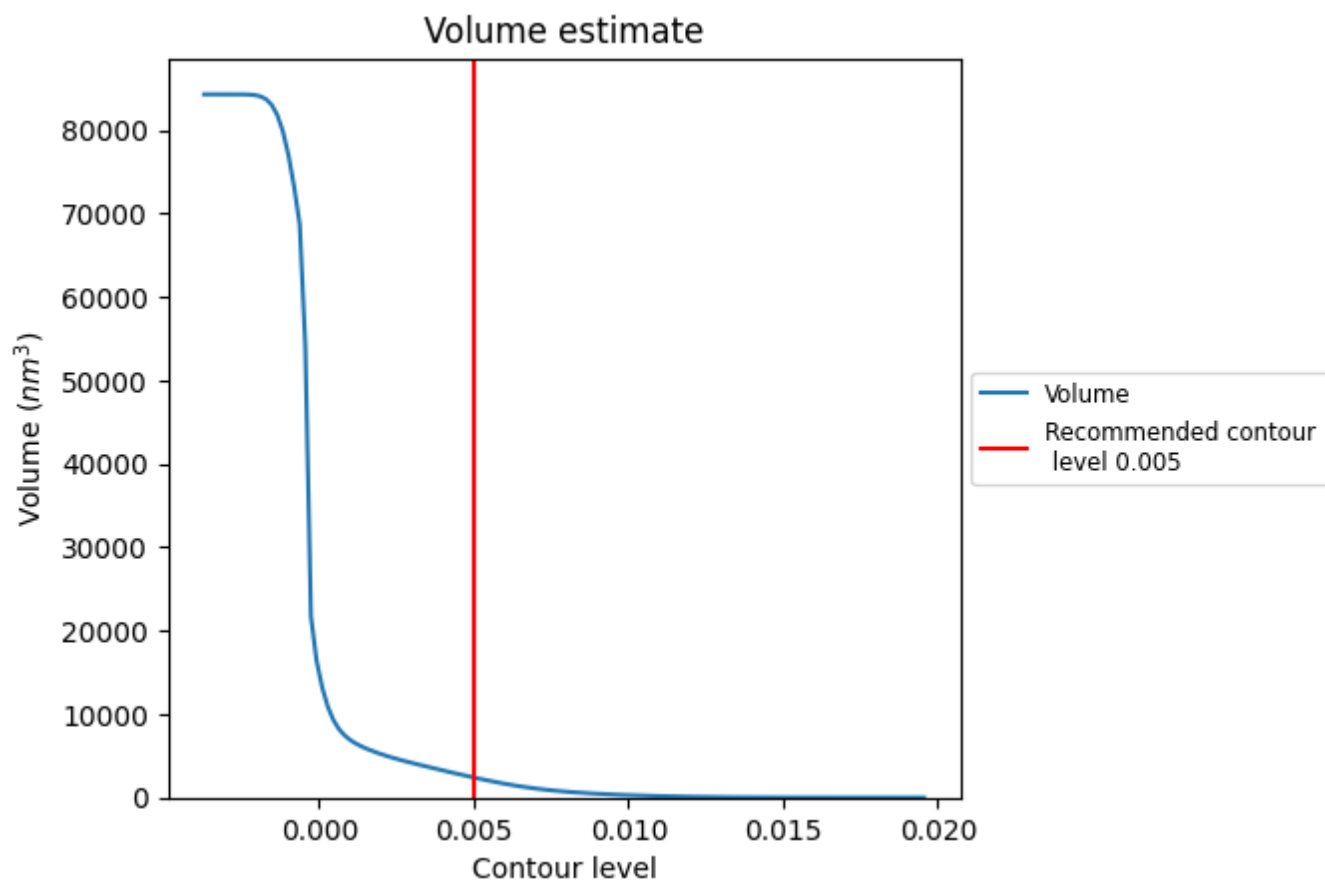
This section contains the results of statistical analysis of the map.

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.

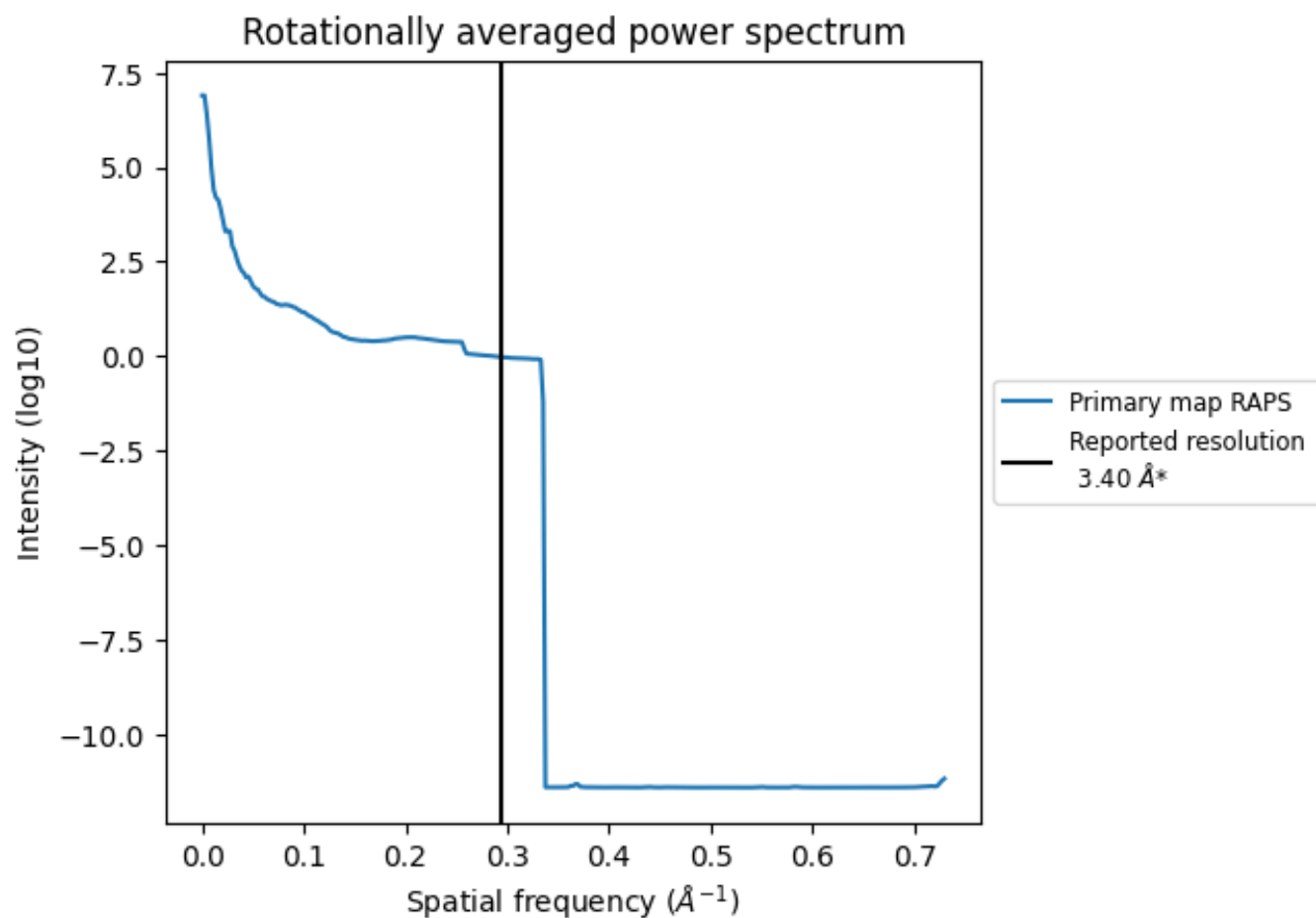
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2400 nm^3 ; this corresponds to an approximate mass of 2168 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 0.294 Å⁻¹

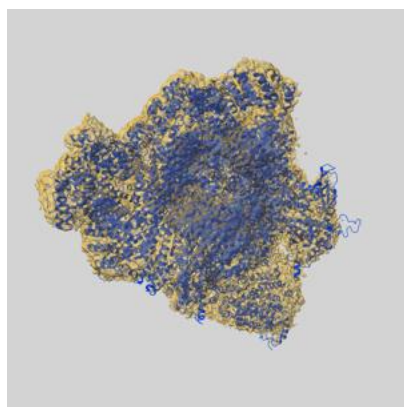
8 Fourier-Shell correlation ⓘ

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

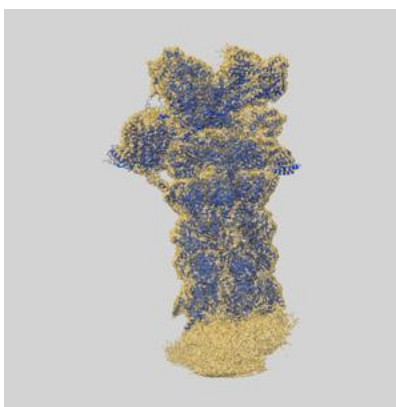
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32277 and PDB model 7W3C. Per-residue inclusion information can be found in section [3](#) on page [13](#).

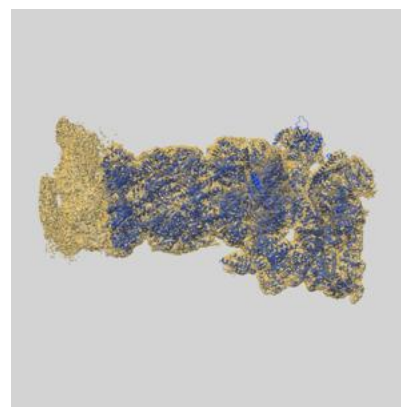
9.1 Map-model overlay [i](#)



X



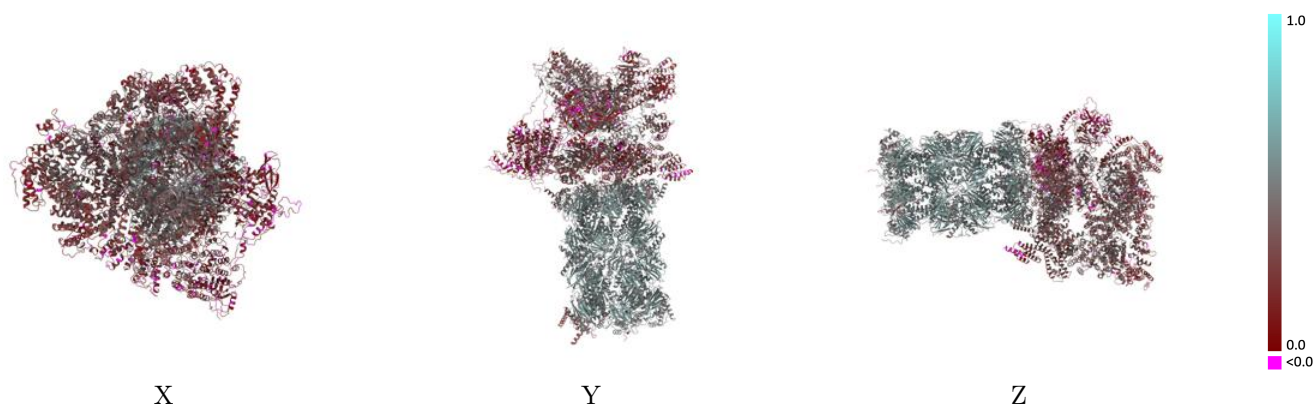
Y



Z

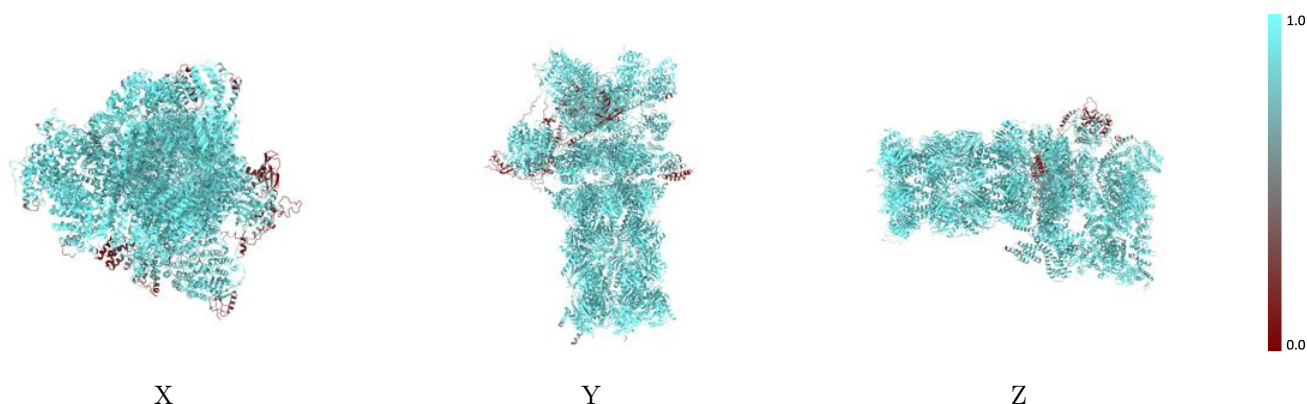
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



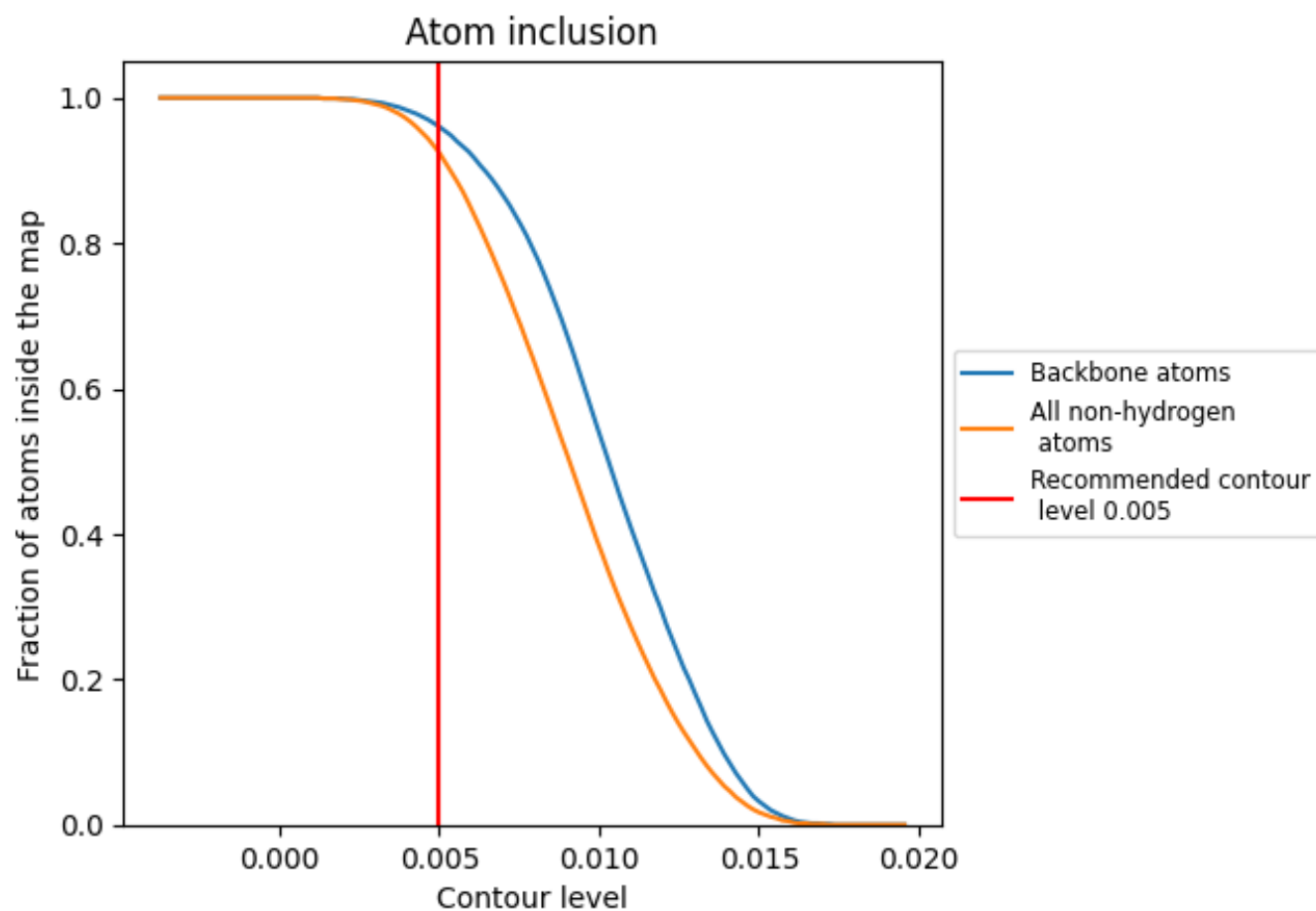
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9240	 0.3840
A	 0.9550	 0.2570
B	 0.9540	 0.3150
C	 0.9720	 0.3580
D	 0.9760	 0.3740
E	 0.9490	 0.3210
F	 0.9430	 0.2170
G	 0.9810	 0.5090
H	 0.9890	 0.5110
I	 0.9770	 0.4780
J	 0.9790	 0.4720
K	 0.9790	 0.4860
L	 0.9880	 0.5220
M	 0.9780	 0.5080
N	 0.9850	 0.5340
O	 0.9910	 0.5310
P	 0.9950	 0.5380
Q	 0.9940	 0.5270
R	 0.9960	 0.5280
S	 0.9840	 0.5270
T	 0.9860	 0.5400
U	 0.9110	 0.3260
V	 0.9380	 0.3260
W	 0.7880	 0.2650
X	 0.9250	 0.3160
Y	 0.9350	 0.3210
Z	 0.9650	 0.3280
a	 0.9330	 0.2760
b	 0.9510	 0.2720
c	 0.9570	 0.3500
d	 0.8610	 0.2380
e	 0.9040	 0.3230
f	 0.7510	 0.1900
g	 0.9700	 0.5100
h	 0.9830	 0.5150



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Chain	Atom inclusion	Q-score
i	 0.9520	 0.4860
j	 0.9530	 0.4480
k	 0.9680	 0.4940
l	 0.9860	 0.5200
m	 0.9780	 0.5060
n	 0.9900	 0.5400
o	 0.9850	 0.5300
p	 0.9940	 0.5380
q	 0.9910	 0.5310
r	 0.9950	 0.5420
s	 0.9900	 0.5260
t	 0.9820	 0.5320
v	 0.9830	 0.3400
x	 0.5410	 0.1600
y	 0.3830	 0.1560