



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 08:13 PM UTC

PDB ID : 7W3I / pdb_00007w3i
EMDB ID : EMD-32281
Title : Structure of USP14-bound human 26S proteasome in substrate-inhibited state
SB_USP14
Authors : Zhang, S.; Zou, S.; Yin, D.; Wu, Z.; Mao, Y.
Deposited on : 2021-11-25
Resolution : 3.50 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

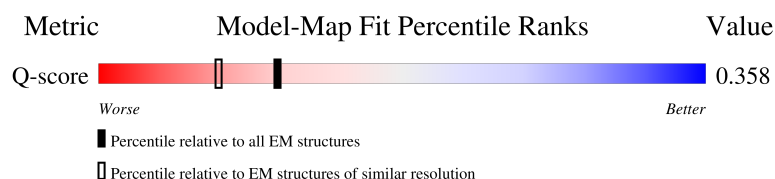
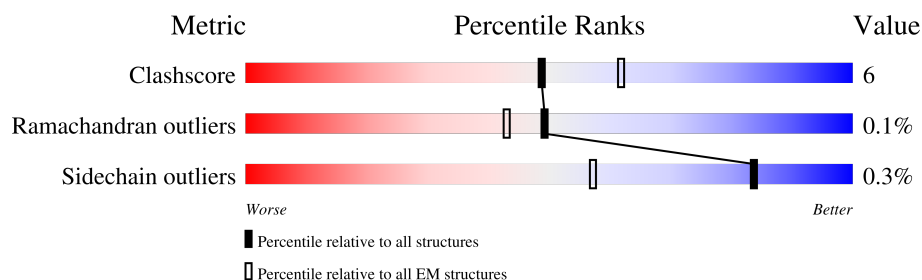
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



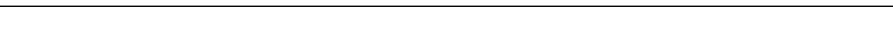
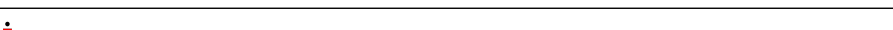
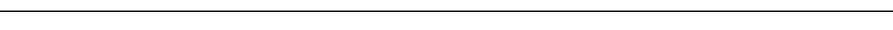
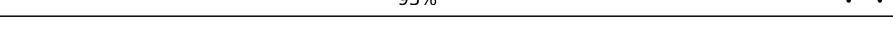
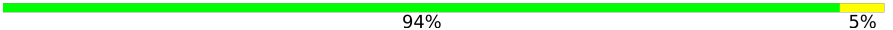
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	x	494	
2	A	433	
3	B	440	
4	C	398	

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Mol	Chain	Length	Quality of chain
5	D	418	
6	E	403	
7	F	439	
8	G	246	
8	g	246	
9	H	234	
9	h	234	
10	I	261	
10	i	261	
11	J	248	
11	j	248	
12	K	241	
12	k	241	
13	L	269	
13	l	269	
14	M	255	
14	m	255	
15	N	239	
15	n	239	
16	O	277	
16	o	277	
17	P	205	
17	p	205	
18	Q	201	
18	q	201	

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

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 110481 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 Ubiquitin carboxyl-terminal hydrolase 14.

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

- Molecule 2 is a protein called 26S protease regulatory subunit 7.

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

- Molecule 3 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	399	Total	C	N	O	S	0	0
			3112	1961	533	603	15		

- Molecule 4 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	386	Total	C	N	O	S	0	0
			3017	1895	543	563	16		

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

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

- Molecule 6 is a protein called 26S proteasome regulatory subunit 10B.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	400	Total	C	N	O	S	0	0
			3133	1972	540	603	18		

- Molecule 8 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	244	Total	C	N	O	S	0	0
			1889	1198	316	362	13		
8	g	244	Total	C	N	O	S	0	0
			1880	1193	318	356	13		

- Molecule 9 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	232	Total	C	N	O	S	0	0
			1805	1152	305	342	6		
9	h	232	Total	C	N	O	S	0	0
			1805	1154	307	338	6		

- Molecule 10 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	250	Total	C	N	O	S	1	0
			1958	1236	336	376	10		
10	i	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		

- Molecule 11 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	239	Total	C	N	O	S	0	0
			1880	1179	333	363	5		
11	j	239	Total	C	N	O	S	0	0
			1861	1168	332	356	5		

- Molecule 12 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	234	Total	C	N	O	S	0	0
			1777	1117	295	354	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	k	234	Total	C	N	O	S	0	0
			1782	1119	295	357	11		

- Molecule 13 is a protein called Isoform Long of Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	238	Total	C	N	O	S	0	0
			1866	1169	336	350	11		
13	l	238	Total	C	N	O	S	0	0
			1861	1165	335	350	11		

- Molecule 14 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	240	Total	C	N	O	S	0	0
			1876	1191	321	353	11		
14	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 15 is a protein called Proteasome subunit beta type-6.

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

- Molecule 16 is a protein called Proteasome subunit beta type-7.

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

- Molecule 17 is a protein called Proteasome subunit beta type-3.

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

- Molecule 18 is a protein called Proteasome subunit beta type-2.

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

- Molecule 19 is a protein called Proteasome subunit beta type-5.

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

- Molecule 20 is a protein called Proteasome subunit beta type-1.

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

- Molecule 21 is a protein called Proteasome subunit beta type-4.

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

- Molecule 22 is a protein called Ubiquitin.

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

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	872	Total	C	N	O	S	0	0
			6828	4328	1157	1298	45		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

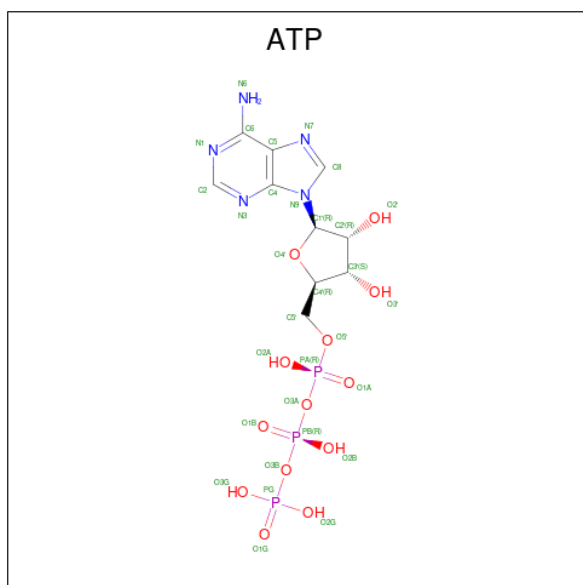
- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

- Molecule 34 is a protein called 26S proteasome complex subunit DSS1.

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

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



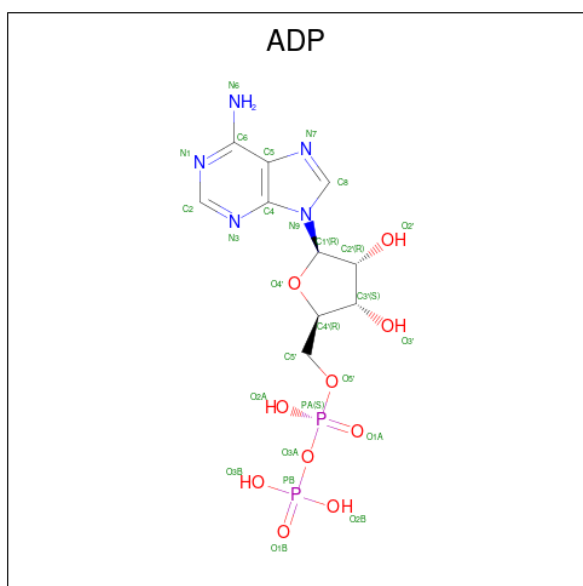
Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

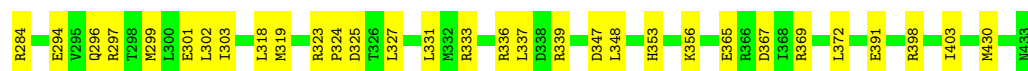
- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



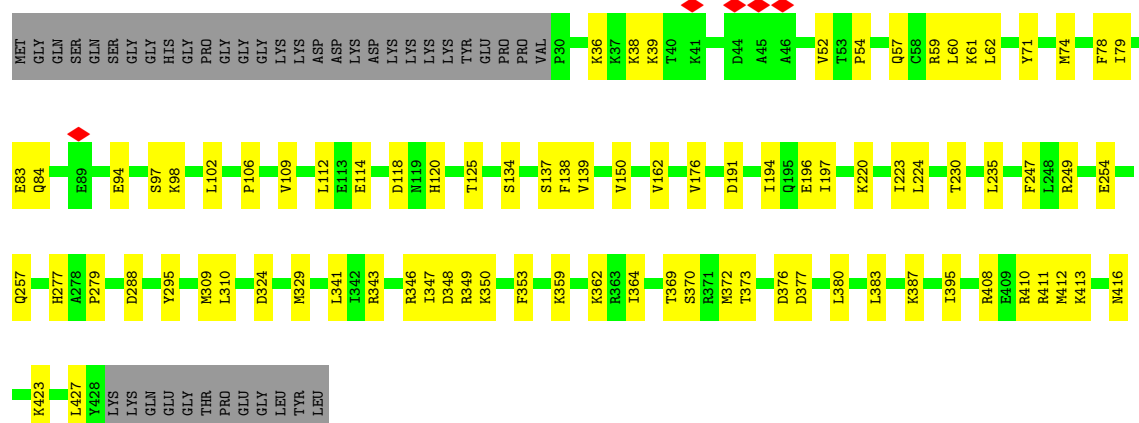
Mol	Chain	Residues	Atoms					AltConf
36	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
36	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

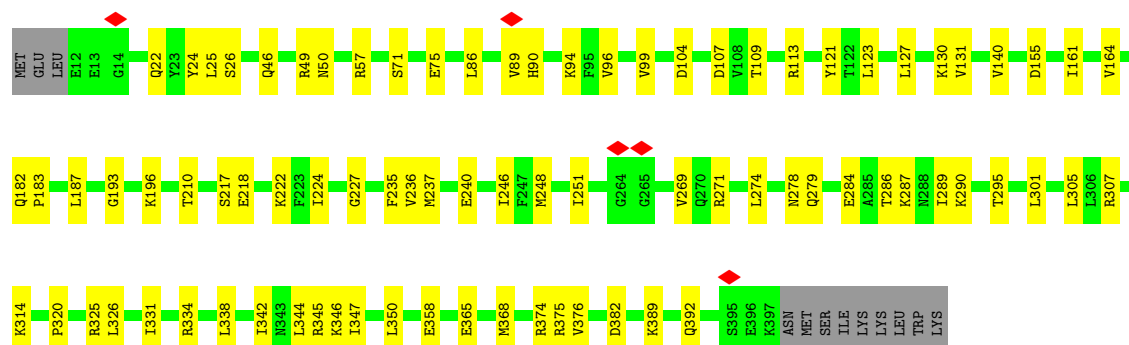
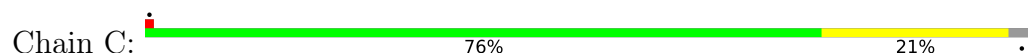
Mol	Chain	Residues	Atoms		AltConf
37	c	1	Total	Zn	0
			1	1	



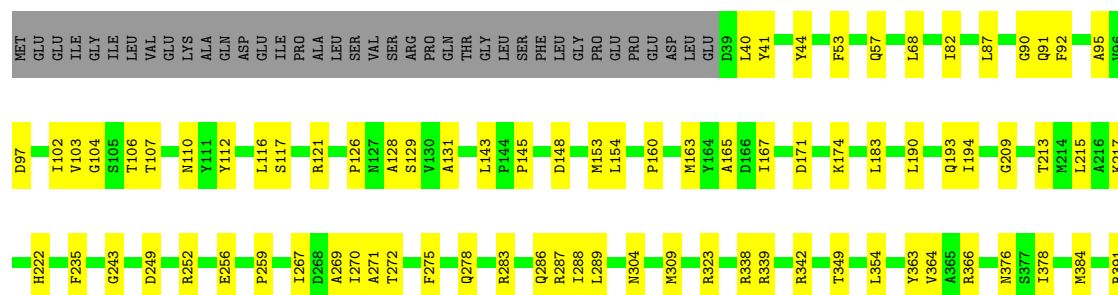
• Molecule 3: 26S protease regulatory subunit 4

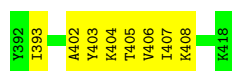


• Molecule 4: Isoform 2 of 26S proteasome regulatory subunit 8



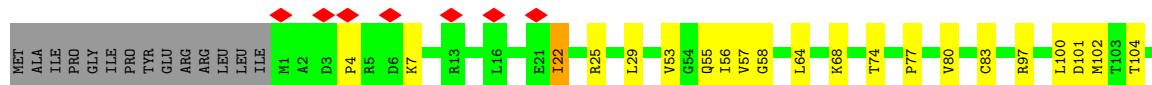
• Molecule 5: 26S protease regulatory subunit 6B





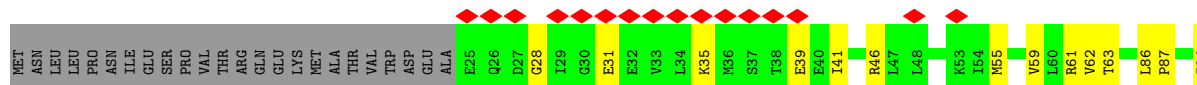
- Molecule 6: 26S proteasome regulatory subunit 10B

Chain E: 79% 17%



- Molecule 7: 26S protease regulatory subunit 6A

Chain F: 76% 15% 9%



- Molecule 8: Proteasome subunit alpha type-6

Chain G: 91% 9%



- Molecule 8: Proteasome subunit alpha type-6

Chain g: 91% 8%



- Molecule 9: Proteasome subunit alpha type-2

Chain H: 91% 9%



• Molecule 9: Proteasome subunit alpha type-2

Chain h: 94% 6%



• Molecule 10: Proteasome subunit alpha type-4

Chain I: 90% 6%



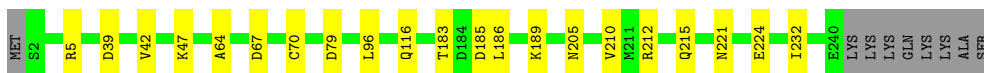
• Molecule 10: Proteasome subunit alpha type-4

Chain i: 90% 6%



• Molecule 11: Proteasome subunit alpha type-7

Chain J: 88% 8%



• Molecule 11: Proteasome subunit alpha type-7

Chain j: 87% 9%



• Molecule 12: Proteasome subunit alpha type-5

Chain K: 87% 10%



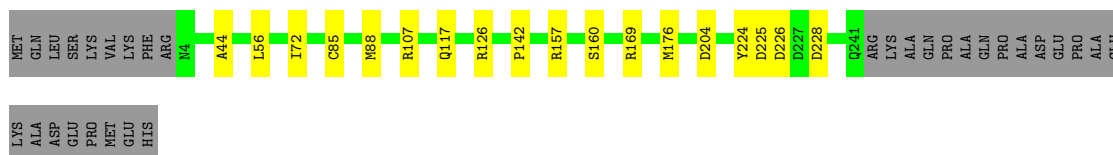
• Molecule 12: Proteasome subunit alpha type-5

Chain k: 93% 6%



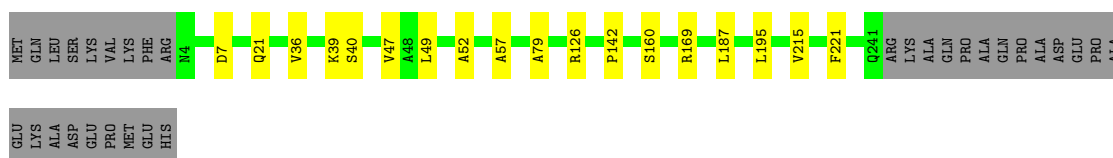
- Molecule 13: Isoform Long of Proteasome subunit alpha type-1

Chain L: 82% 7% 12%



- Molecule 13: Isoform Long of Proteasome subunit alpha type-1

Chain I: 82% 7% 12%



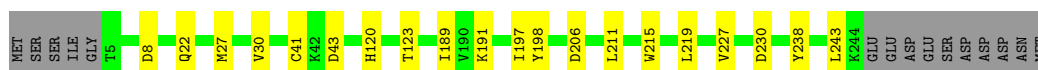
- Molecule 14: Proteasome subunit alpha type-3

Chain M: 87% 7% 6%



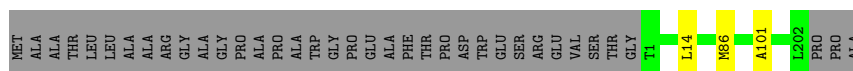
- Molecule 14: Proteasome subunit alpha type-3

Chain m: 86% 8% 6%



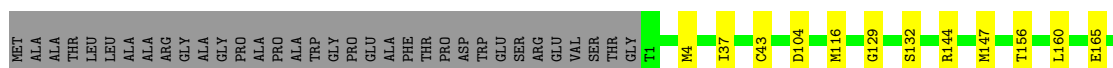
- Molecule 15: Proteasome subunit beta type-6

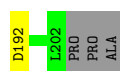
Chain N: 83% 15%



- Molecule 15: Proteasome subunit beta type-6

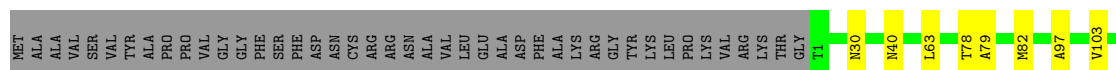
Chain n: 79% 5% 15%





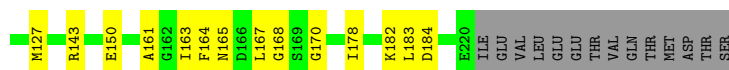
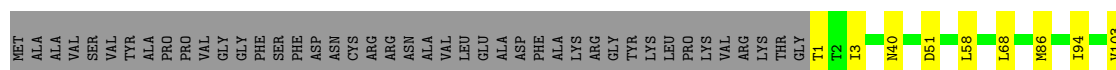
- Molecule 16: Proteasome subunit beta type-7

Chain O: 73% 7% 21%



- Molecule 16: Proteasome subunit beta type-7

Chain o: 71% 8% 21%



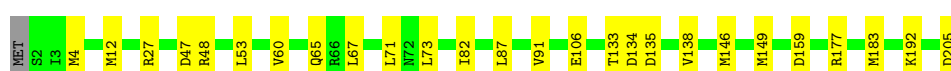
- Molecule 17: Proteasome subunit beta type-3

Chain P: 94% 5%



- Molecule 17: Proteasome subunit beta type-3

Chain p: 87% 13%



- Molecule 18: Proteasome subunit beta type-2

Chain Q: 87% 12%



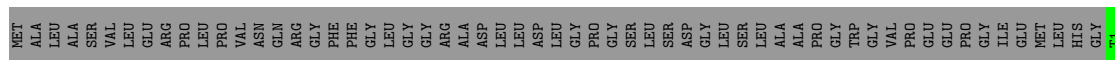
- Molecule 18: Proteasome subunit beta type-2

Chain q: 89% 10%



- Molecule 19: Proteasome subunit beta type-5

Chain R: 72% 5% 24%



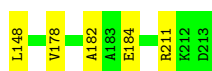
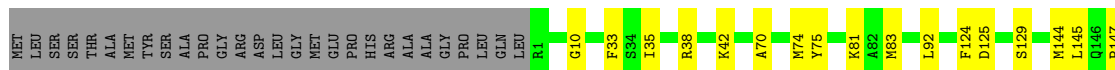
- Molecule 19: Proteasome subunit beta type-5

Chain r: 72% 5% 24%



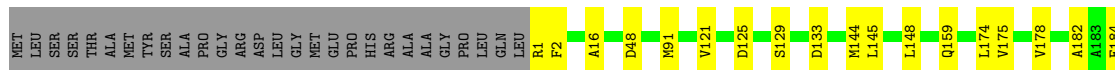
- Molecule 20: Proteasome subunit beta type-1

Chain S: 79% 9% 12%



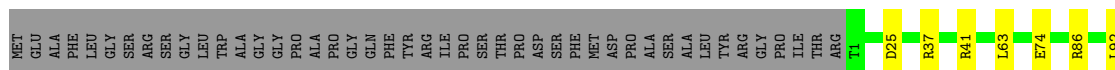
- Molecule 20: Proteasome subunit beta type-1

Chain s: 80% 9% 12%



- Molecule 21: Proteasome subunit beta type-4

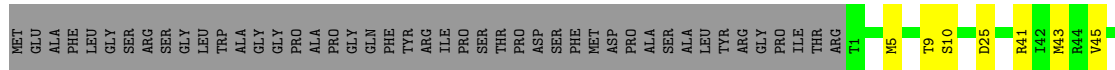
Chain T: 75% 6% 18%





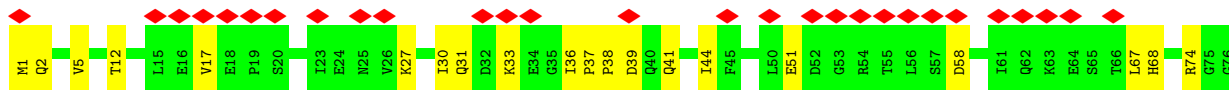
• Molecule 21: Proteasome subunit beta type-4

Chain t: 76% 6% 18%



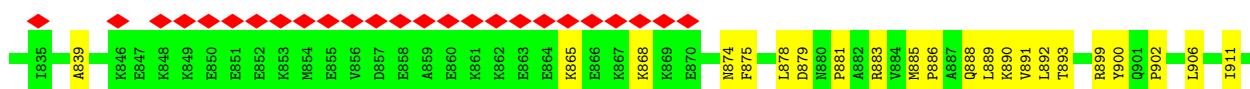
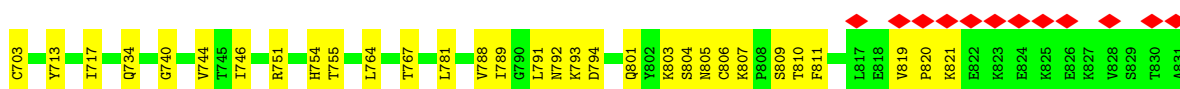
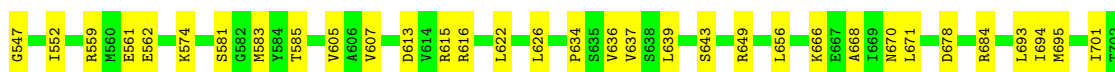
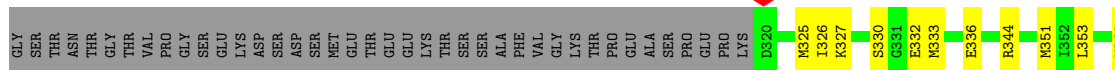
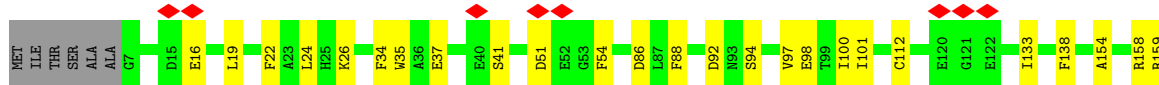
• Molecule 22: Ubiquitin

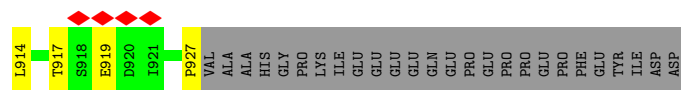
Chain y: 37% 74% 26%



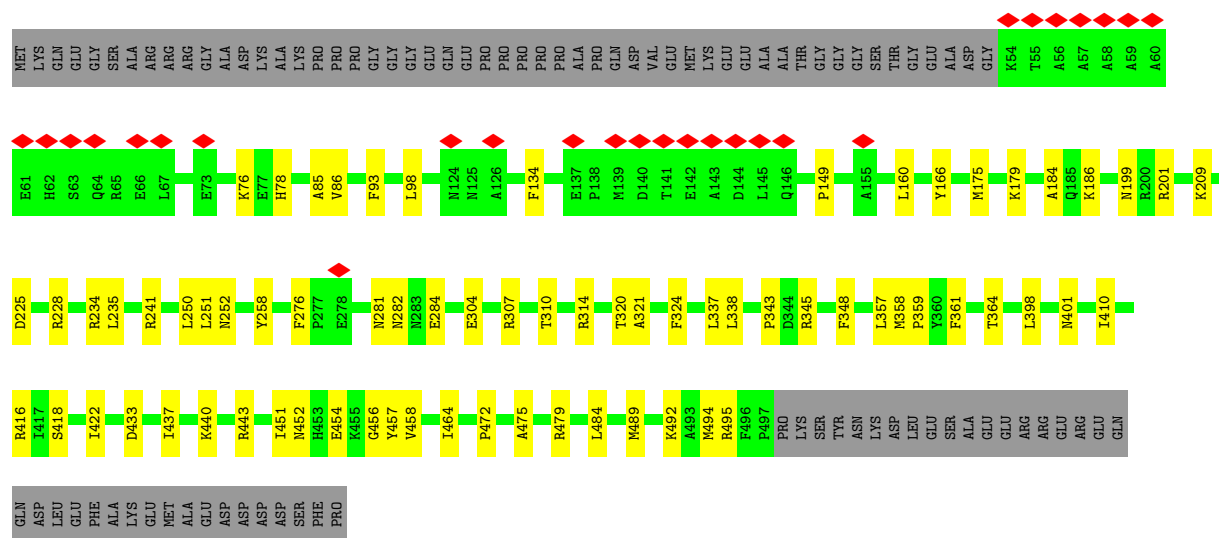
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 5% 72% 20% 8%

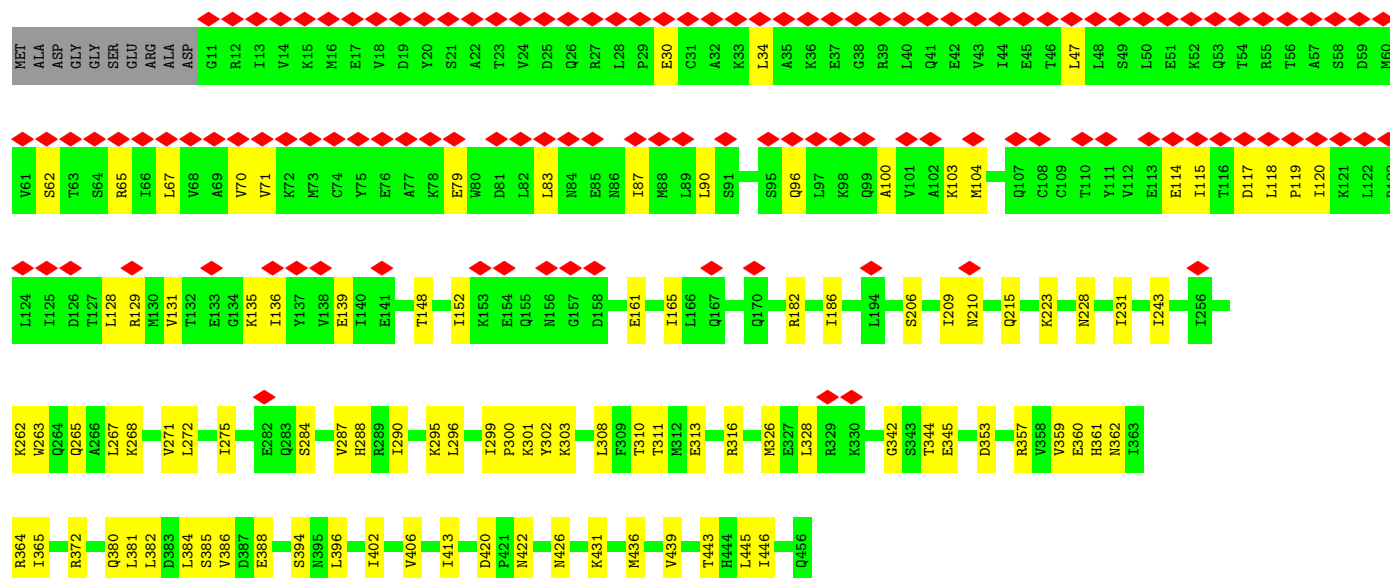
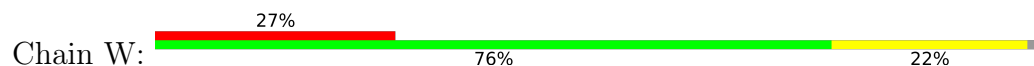




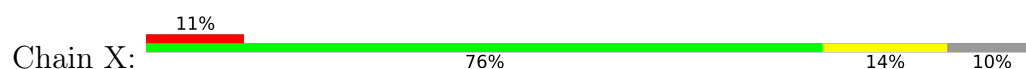
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 3

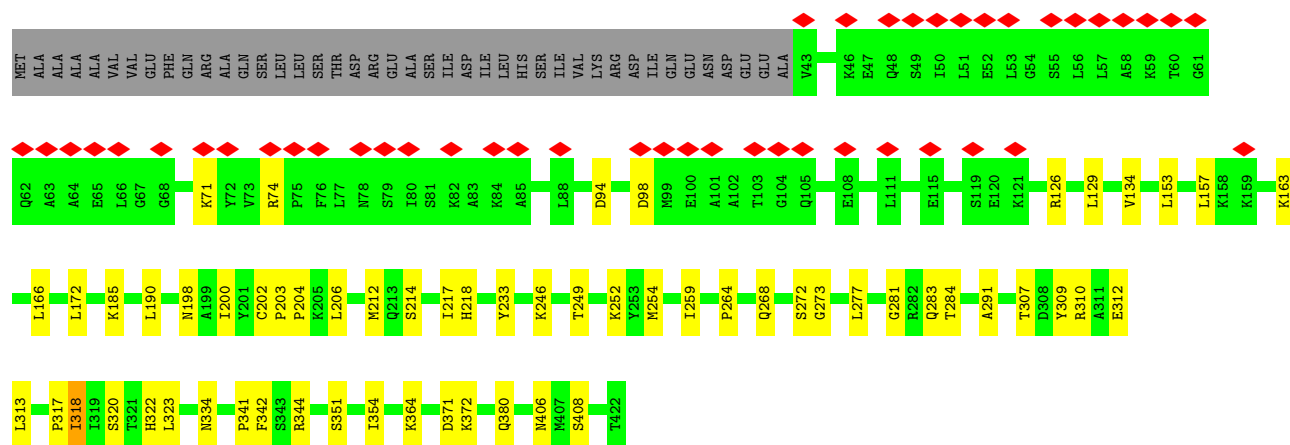


- Molecule 25: 26S proteasome non-ATPase regulatory subunit 12

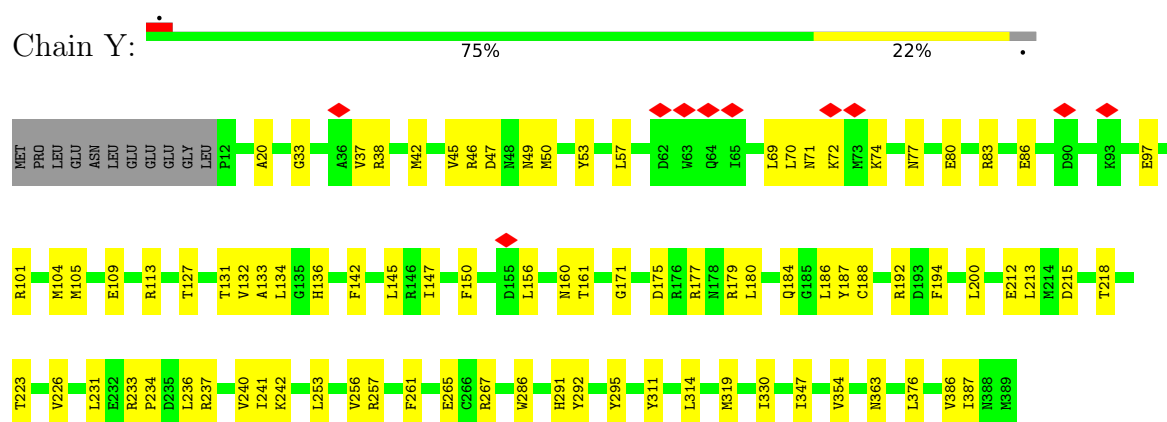


- Molecule 26: 26S proteasome non-ATPase regulatory subunit 11

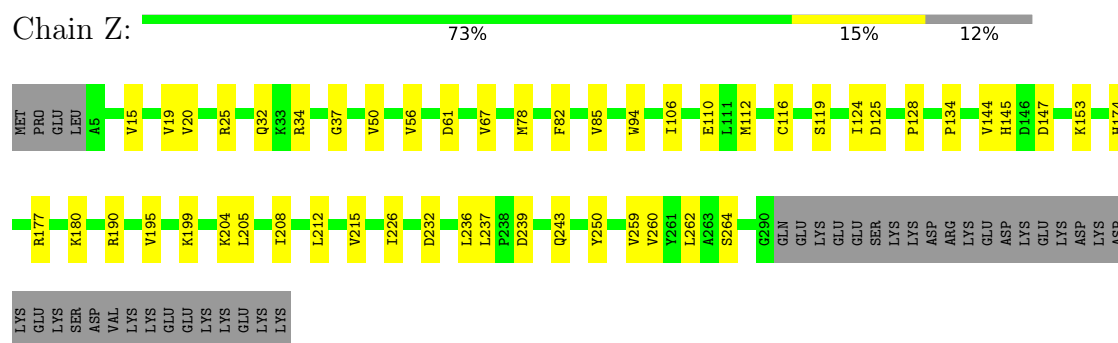




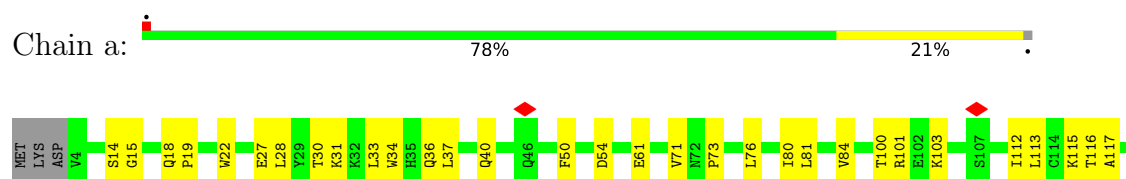
- Molecule 27: 26S proteasome non-ATPase regulatory subunit 6

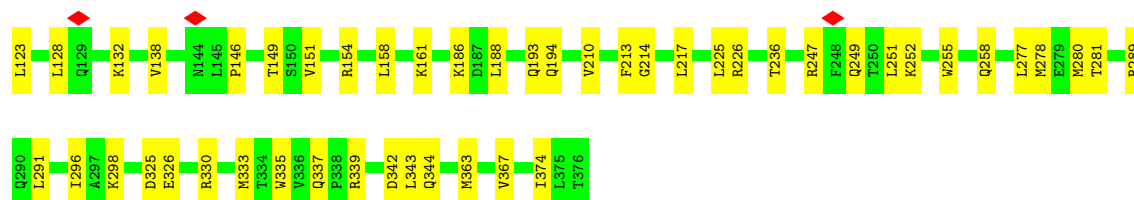


- Molecule 28: 26S proteasome non-ATPase regulatory subunit 7



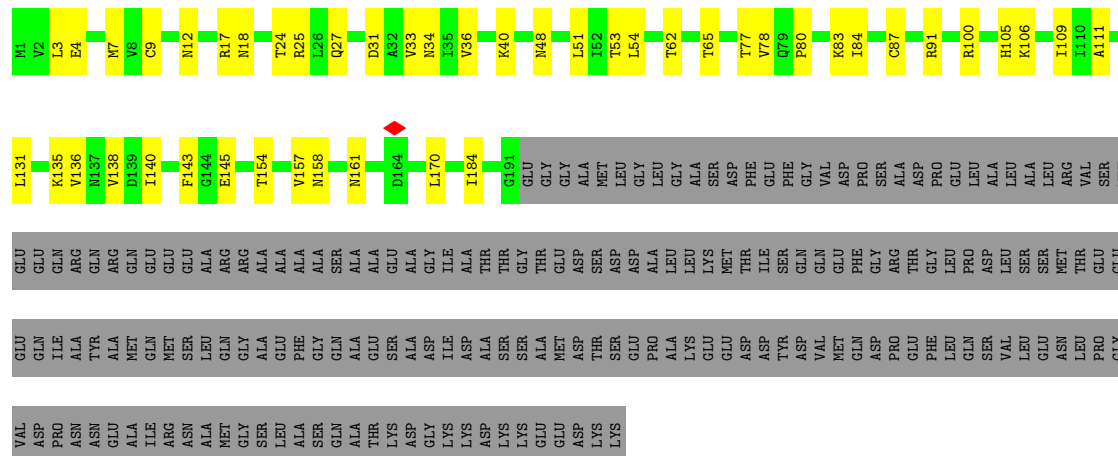
- Molecule 29: 26S proteasome non-ATPase regulatory subunit 13





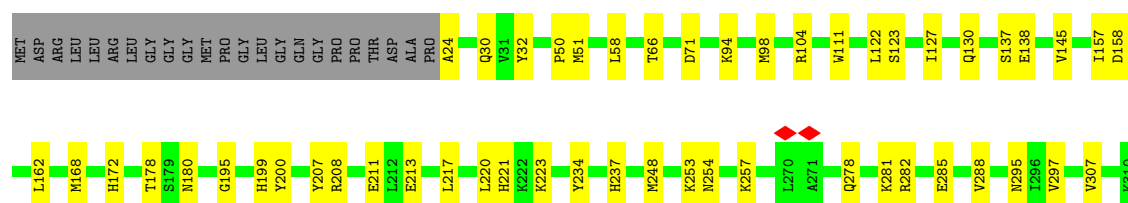
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 4

Chain b: 38% 12% 49%



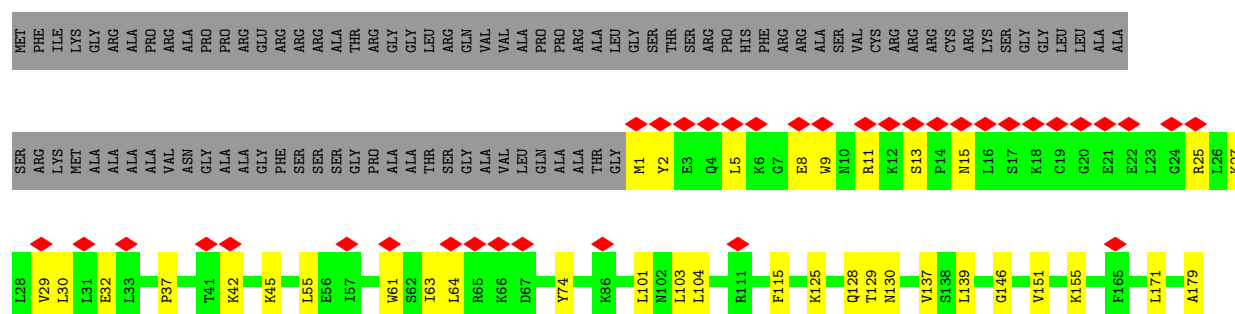
• Molecule 31: 26S proteasome non-ATPase regulatory subunit 14

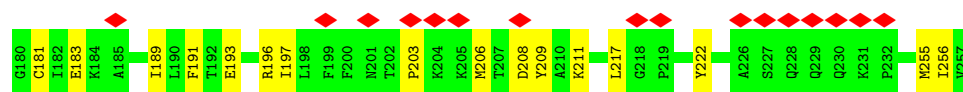
Chain c: 76% 16% 7%



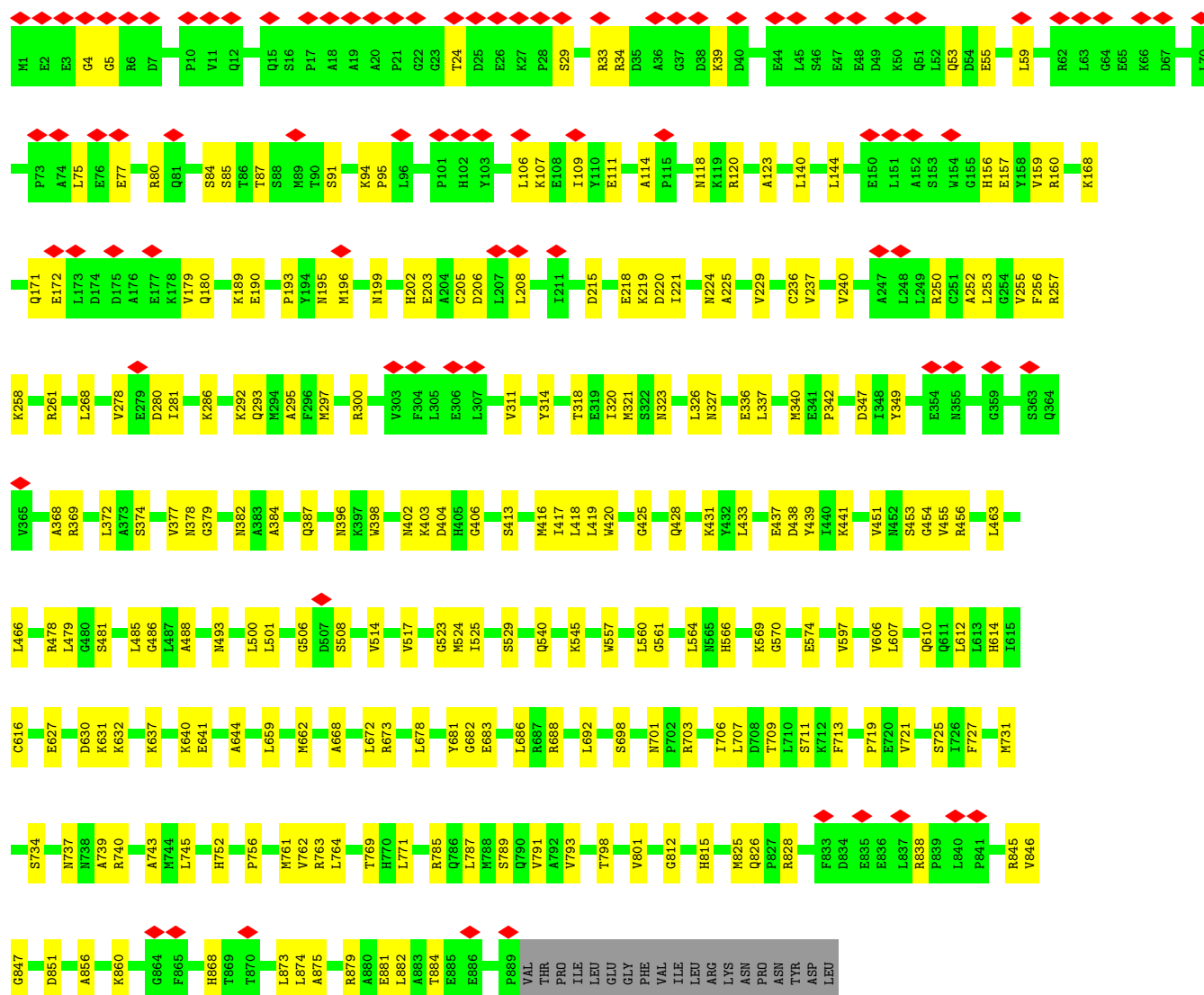
• Molecule 32: 26S proteasome non-ATPase regulatory subunit 8

Chain d: 15% 59% 15% 27%

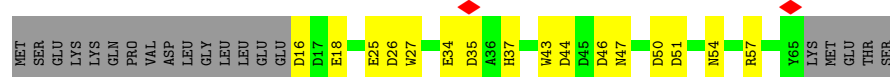




- Molecule 33: 26S proteasome non-ATPase regulatory subunit 2



- Molecule 34: 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	53225	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	-0.005	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, ATP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	x	0.16	0/4002	0.42	0/5390
2	A	0.21	0/3283	0.50	2/4433 (0.0%)
3	B	0.21	0/3157	0.52	0/4258
4	C	0.18	0/3056	0.46	0/4108
5	D	0.18	0/3089	0.47	0/4168
6	E	0.17	0/3145	0.42	0/4233
7	F	0.19	0/3173	0.47	0/4273
8	G	0.25	0/1923	0.38	0/2601
8	g	0.24	0/1914	0.39	0/2590
9	H	0.26	0/1844	0.40	0/2499
9	h	0.25	0/1844	0.38	0/2497
10	I	0.24	0/1991	0.42	0/2685
10	i	0.23	0/1985	0.41	0/2677
11	J	0.20	0/1906	0.41	0/2573
11	j	0.21	0/1887	0.39	0/2549
12	K	0.24	0/1804	0.41	0/2436
12	k	0.22	0/1809	0.35	0/2444
13	L	0.25	0/1901	0.36	0/2570
13	l	0.25	0/1896	0.37	0/2565
14	M	0.25	0/1911	0.39	0/2573
14	m	0.24	0/1916	0.41	0/2580
15	N	0.24	0/1540	0.31	0/2085
15	n	0.24	0/1536	0.35	0/2080
16	O	0.25	0/1676	0.42	0/2271
16	o	0.25	0/1686	0.40	0/2282
17	P	0.26	0/1616	0.42	0/2180
17	p	0.27	0/1620	0.39	0/2184
18	Q	0.25	0/1621	0.37	0/2194
18	q	0.26	0/1621	0.39	0/2194
19	R	0.24	0/1590	0.35	0/2147
19	r	0.24	0/1590	0.36	0/2147
20	S	0.26	0/1671	0.39	0/2252

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	s	0.25	0/1684	0.36	0/2268
21	T	0.26	0/1716	0.40	0/2323
21	t	0.25	0/1720	0.38	0/2328
22	y	0.20	0/607	0.49	0/816
23	U	0.19	0/6945	0.50	0/9382
24	V	0.17	0/3681	0.44	0/4969
25	W	0.25	0/3683	0.51	0/4952
26	X	0.17	0/3053	0.46	2/4115 (0.0%)
27	Y	0.19	0/3173	0.52	0/4273
28	Z	0.21	0/2324	0.53	0/3150
29	a	0.18	0/3053	0.52	0/4133
30	b	0.20	0/1478	0.51	0/2001
31	c	0.22	0/2302	0.54	0/3110
32	d	0.21	0/2162	0.52	0/2919
33	f	0.20	0/6980	0.52	0/9433
34	e	0.22	0/437	0.53	0/595
All	All	0.22	0/112201	0.45	4/151485 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	48	VAL	N-CA-C	-5.54	107.42	112.96
2	A	37	GLY	N-CA-C	-5.26	104.95	114.46
26	X	317	PRO	CA-C-N	5.19	131.31	121.97
26	X	317	PRO	C-N-CA	5.19	131.31	121.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	x	3929	0	3915	72	0
2	A	3229	0	3261	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3112	0	3181	63	0
4	C	3017	0	3117	56	0
5	D	3039	0	3076	63	0
6	E	3097	0	3174	50	0
7	F	3133	0	3220	46	0
8	G	1889	0	1885	13	0
8	g	1880	0	1875	12	0
9	H	1805	0	1784	13	0
9	h	1805	0	1798	10	0
10	I	1958	0	1960	10	0
10	i	1955	0	1955	10	0
11	J	1880	0	1892	14	0
11	j	1861	0	1865	15	0
12	K	1777	0	1762	16	0
12	k	1782	0	1766	7	0
13	L	1866	0	1852	14	0
13	l	1861	0	1839	11	0
14	M	1876	0	1861	12	0
14	m	1881	0	1868	12	0
15	N	1514	0	1487	2	0
15	n	1510	0	1483	10	0
16	O	1649	0	1659	13	0
16	o	1659	0	1681	13	0
17	P	1587	0	1598	8	0
17	p	1591	0	1609	18	0
18	Q	1588	0	1584	17	0
18	q	1588	0	1584	16	0
19	R	1559	0	1523	10	0
19	r	1559	0	1523	7	0
20	S	1641	0	1639	17	0
20	s	1654	0	1656	14	0
21	T	1683	0	1662	13	0
21	t	1687	0	1666	10	0
22	y	601	0	629	14	0
23	U	6828	0	6884	115	0
24	V	3612	0	3682	47	0
25	W	3635	0	3762	61	0
26	X	3009	0	3113	38	0
27	Y	3115	0	3120	53	0
28	Z	2281	0	2312	34	0
29	a	2995	0	3012	52	0
30	b	1458	0	1505	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	c	2260	0	2276	31	0
32	d	2116	0	2146	35	0
33	f	6866	0	6866	160	0
34	e	425	0	328	9	0
35	A	31	0	12	2	0
35	D	31	0	12	3	0
35	E	31	0	12	1	0
35	F	31	0	12	1	0
36	B	27	0	12	1	0
36	C	27	0	12	2	0
37	c	1	0	0	0	0
All	All	110481	0	110967	1277	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 (1277) 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)
12:K:195:ILE:HD11	12:K:217:LEU:HD11	1.62	0.81
33:f:286:LYS:HG3	33:f:873:LEU:HD12	1.64	0.79
5:D:267:ILE:HG12	5:D:309:MET:HE2	1.69	0.74
23:U:479:LEU:HG	23:U:514:LEU:HD11	1.72	0.72
31:c:50:PRO:HG2	31:c:51:MET:HE2	1.71	0.72
20:S:147:PRO:HB2	17:p:149:MET:HE3	1.72	0.70
23:U:883:ARG:NH1	23:U:885:MET:SD	2.64	0.70
5:D:259:PRO:HB3	5:D:304:ASN:HB2	1.73	0.69
31:c:94:LYS:O	31:c:98:MET:HB2	1.93	0.69
1:x:296:GLU:HB2	1:x:313:LYS:HB3	1.74	0.68
33:f:75:LEU:HD23	33:f:77:GLU:H	1.58	0.68
33:f:189:LYS:HG3	33:f:190:GLU:HG2	1.75	0.68
10:I:8:ARG:HE	11:J:5:ARG:HH21	1.42	0.68
3:B:279:PRO:HB3	3:B:324:ASP:HB3	1.76	0.67
4:C:248:MET:HE1	4:C:269:VAL:HG13	1.76	0.67
23:U:900:TYR:HA	23:U:917:THR:HG21	1.78	0.66
12:K:207:GLU:HG2	12:K:208:GLU:HG3	1.76	0.66
16:o:58:LEU:HD22	16:o:86:MET:HE1	1.78	0.65
26:X:212:MET:HE1	26:X:246:LYS:HB3	1.77	0.65
30:b:100:ARG:HD2	30:b:105:HIS:HB2	1.78	0.65
7:F:61:ARG:HH22	30:b:77:THR:HB	1.62	0.65
18:Q:25:ILE:HG23	18:Q:26:VAL:HG13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:39:LYS:HE3	3:B:277:HIS:HA	1.79	0.65
33:f:828:ARG:HD3	33:f:845:ARG:HB3	1.79	0.64
23:U:373:ASN:HD22	23:U:385:PHE:HD2	1.46	0.64
29:a:247:ARG:HG3	29:a:251:LEU:HD23	1.79	0.64
6:E:282:PRO:HA	6:E:285:LEU:HD23	1.79	0.64
1:x:197:GLN:O	22:y:74:ARG:NH2	2.31	0.64
24:V:494:MET:HG2	24:V:495:ARG:HG2	1.78	0.64
2:A:212:VAL:HG22	2:A:339:ARG:HB3	1.80	0.64
33:f:731:MET:O	33:f:737:ASN:ND2	2.30	0.64
17:p:65:GLN:OE1	18:q:86:ARG:NH2	2.31	0.63
24:V:416:ARG:HA	24:V:458:VAL:HB	1.80	0.63
24:V:321:ALA:HB1	24:V:324:PHE:HB3	1.81	0.63
24:V:440:LYS:HD2	32:d:146:GLY:HA2	1.81	0.63
30:b:87:CYS:SG	30:b:91:ARG:NH1	2.69	0.63
1:x:248:GLY:HA2	1:x:273:LEU:HA	1.80	0.63
25:W:30:GLU:O	25:W:34:LEU:HB2	2.00	0.62
3:B:347:ILE:HG21	3:B:350:LYS:HZ1	1.64	0.62
33:f:261:ARG:HD2	33:f:293:GLN:HE21	1.64	0.62
33:f:323:ASN:HD22	33:f:455:VAL:HA	1.65	0.62
6:E:116:ASP:HB3	6:E:119:VAL:HB	1.82	0.62
19:R:38:ASN:HD21	19:R:41:LEU:HD12	1.63	0.62
16:O:143:ARG:NH2	16:O:150:GLU:OE1	2.32	0.62
24:V:489:MET:HA	24:V:492:LYS:HE2	1.82	0.62
23:U:678:ASP:O	23:U:684:ARG:NH1	2.32	0.62
11:j:211:MET:HG2	11:j:217:LEU:HD13	1.82	0.62
27:Y:231:LEU:HD12	27:Y:234:PRO:HD2	1.82	0.61
28:Z:232:ASP:O	28:Z:236:LEU:HB2	2.00	0.61
33:f:236:CYS:SG	33:f:237:VAL:N	2.72	0.61
33:f:384:ALA:H	33:f:419:LEU:HB3	1.64	0.61
33:f:413:SER:HA	33:f:416:MET:HE2	1.81	0.61
1:x:24:GLU:O	1:x:58:TRP:NE1	2.32	0.61
7:F:294:LYS:HA	7:F:339:ASP:HB3	1.82	0.61
27:Y:101:ARG:HD3	27:Y:131:THR:HG21	1.82	0.61
33:f:24:THR:OG1	33:f:34:ARG:NH2	2.34	0.61
8:g:141:ILE:HG22	8:g:151:VAL:HG22	1.82	0.61
33:f:378:ASN:OD1	33:f:382:ASN:ND2	2.33	0.61
2:A:224:LEU:HD11	35:A:501:ATP:H2'	1.83	0.61
6:E:83:CYS:HB2	6:E:107:ILE:HG13	1.82	0.61
3:B:36:LYS:NZ	3:B:277:HIS:O	2.34	0.61
28:Z:25:ARG:HG2	31:c:104:ARG:HE	1.65	0.61
33:f:369:ARG:HG2	33:f:740:ARG:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:97:ARG:HG2	6:E:111:LEU:HD12	1.83	0.60
5:D:163:MET:SD	5:D:222:HIS:NE2	2.72	0.60
11:J:221:ASN:HB2	11:J:224:GLU:HG3	1.82	0.60
8:g:186:LYS:NZ	8:g:188:ASP:O	2.34	0.60
17:p:48:ARG:NH2	17:p:192:LYS:O	2.34	0.60
33:f:734:SER:H	33:f:737:ASN:HD21	1.48	0.60
10:i:17:ARG:HH21	10:i:19:TYR:HE1	1.47	0.60
15:n:37:ILE:HD11	15:n:43:CYS:HB3	1.84	0.60
23:U:527:GLN:NE2	23:U:531:ASP:OD2	2.34	0.60
29:a:188:LEU:O	29:a:193:GLN:NE2	2.34	0.60
3:B:408:ARG:O	3:B:410:ARG:NH1	2.34	0.60
3:B:411:ARG:NH1	3:B:413:LYS:O	2.31	0.60
23:U:483:LEU:HD11	23:U:781:LEU:HD11	1.83	0.60
33:f:221:ILE:HA	33:f:224:ASN:HB2	1.83	0.60
25:W:47:LEU:HD11	25:W:70:VAL:HG11	1.84	0.60
25:W:215:GLN:HG2	25:W:223:LYS:HE2	1.83	0.60
5:D:269:ALA:HB2	6:E:258:MET:HG3	1.84	0.59
6:E:333:LYS:NZ	8:G:57:PRO:O	2.35	0.59
27:Y:265:GLU:O	27:Y:267:ARG:NH1	2.34	0.59
33:f:428:GLN:HG3	33:f:431:LYS:HE2	1.84	0.59
33:f:721:VAL:HG22	33:f:725:SER:HB2	1.84	0.59
25:W:316:ARG:NH1	25:W:380:GLN:O	2.35	0.59
4:C:331:ILE:HA	4:C:334:ARG:HE	1.67	0.59
6:E:22:ILE:HG22	6:E:25:ARG:HH21	1.67	0.59
11:J:47:LYS:HE2	11:J:205:ASN:HA	1.85	0.59
26:X:203:PRO:HB2	26:X:206:LEU:HB2	1.83	0.59
24:V:343:PRO:O	34:e:43:TRP:NE1	2.35	0.59
5:D:91:GLN:HA	5:D:129:SER:HA	1.84	0.59
23:U:398:ASN:H	23:U:401:LYS:HE2	1.67	0.59
32:d:103:LEU:HD11	32:d:115:PHE:HD1	1.68	0.59
4:C:376:VAL:HG12	5:D:193:GLN:HE22	1.66	0.59
28:Z:243:GLN:OE1	29:a:289:ARG:NH2	2.35	0.59
4:C:237:MET:HE2	4:C:246:ILE:HD11	1.85	0.59
5:D:193:GLN:HG3	5:D:194:ILE:HG13	1.85	0.59
23:U:792:ASN:HB3	23:U:914:LEU:HB3	1.84	0.59
3:B:295:TYR:HE1	4:C:271:ARG:HG3	1.68	0.59
24:V:418:SER:HA	24:V:456:GLY:HA3	1.85	0.59
27:Y:105:MET:HE3	27:Y:109:GLU:HG2	1.85	0.59
30:b:87:CYS:O	30:b:91:ARG:NH1	2.35	0.59
25:W:272:LEU:HA	25:W:301:LYS:HE2	1.86	0.58
28:Z:94:TRP:HD1	28:Z:112:MET:HE2	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:244:SER:HB3	7:F:300:LYS:HD2	1.85	0.58
9:h:143:ARG:NH1	9:h:144:PRO:O	2.36	0.58
4:C:86:LEU:HD11	4:C:94:LYS:HB3	1.85	0.58
8:g:120:ASP:OD1	9:h:84:ARG:NH1	2.35	0.58
10:i:180:LYS:H	10:i:184:MET:HE3	1.68	0.58
4:C:284:GLU:OE2	4:C:287:LYS:NZ	2.36	0.58
16:O:40:ASN:ND2	16:O:103:VAL:O	2.35	0.58
33:f:384:ALA:HA	33:f:420:TRP:HB2	1.86	0.58
33:f:478:ARG:HG2	33:f:514:VAL:HG21	1.84	0.58
1:x:319:ARG:NH2	1:x:410:ILE:O	2.37	0.58
20:s:1:ARG:NH1	20:s:2:PHE:O	2.36	0.58
24:V:437:ILE:HA	32:d:146:GLY:HA3	1.85	0.58
26:X:334:ASN:HB3	26:X:354:ILE:HD11	1.85	0.58
29:a:112:ILE:HB	29:a:138:VAL:HG13	1.84	0.58
5:D:82:ILE:HD11	5:D:116:LEU:HD11	1.86	0.58
8:g:165:ALA:HB1	8:g:179:LEU:HD13	1.86	0.58
28:Z:20:VAL:HG11	31:c:213:GLU:HB3	1.84	0.58
5:D:163:MET:HG3	5:D:165:ALA:H	1.69	0.58
8:g:158:GLY:O	9:h:84:ARG:NH2	2.37	0.58
23:U:164:GLU:HA	23:U:167:ILE:HG12	1.86	0.58
32:d:208:ASP:HA	32:d:211:LYS:HB2	1.86	0.58
33:f:627:GLU:O	33:f:631:LYS:NZ	2.36	0.58
33:f:868:HIS:ND1	33:f:884:THR:OG1	2.32	0.58
1:x:280:ASN:ND2	1:x:282:GLU:OE1	2.37	0.57
3:B:410:ARG:O	33:f:53:GLN:NE2	2.37	0.57
5:D:117:SER:HA	5:D:121:ARG:HH22	1.70	0.57
6:E:210:GLU:HG2	6:E:213:ARG:HH21	1.69	0.57
7:F:362:ARG:NH1	7:F:388:THR:O	2.37	0.57
19:r:64:ARG:NH1	19:r:67:GLU:OE2	2.37	0.57
14:m:198:TYR:HB3	14:m:243:LEU:HD22	1.86	0.57
21:t:43:MET:HE3	21:t:45:VAL:HG22	1.86	0.57
23:U:510:GLU:HA	23:U:547:GLY:HA3	1.86	0.57
24:V:337:LEU:HD21	24:V:364:THR:HG23	1.87	0.57
25:W:406:VAL:HA	25:W:413:ILE:HG22	1.85	0.57
3:B:377:ASP:O	3:B:416:ASN:ND2	2.37	0.57
4:C:57:ARG:NH2	23:U:643:SER:O	2.36	0.57
7:F:304:ARG:HB3	7:F:308:ARG:HH22	1.69	0.57
24:V:252:ASN:ND2	24:V:284:GLU:OE1	2.36	0.57
1:x:152:ILE:HG12	1:x:178:PHE:HB3	1.86	0.57
1:x:361:PRO:HA	1:x:364:GLN:HB2	1.86	0.57
31:c:168:MET:O	31:c:172:HIS:NE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:114:ALA:HA	33:f:118:ASN:HB2	1.87	0.57
21:T:37:ARG:NH1	15:n:165:GLU:OE2	2.36	0.57
28:Z:82:PHE:HA	28:Z:85:VAL:HG12	1.86	0.57
33:f:144:LEU:HD11	33:f:159:VAL:HG21	1.85	0.57
33:f:529:SER:O	33:f:569:LYS:NZ	2.34	0.57
3:B:254:GLU:O	3:B:257:GLN:NE2	2.38	0.57
6:E:198:VAL:HG12	6:E:200:SER:H	1.68	0.57
28:Z:177:ARG:HA	28:Z:180:LYS:HD3	1.85	0.57
14:M:39:ILE:HG23	14:M:181:MET:HE3	1.85	0.57
23:U:24:LEU:HD21	23:U:54:PHE:HZ	1.70	0.57
31:c:195:GLY:O	31:c:199:HIS:ND1	2.38	0.57
33:f:673:ARG:HB3	33:f:707:LEU:HG	1.87	0.57
2:A:66:LYS:NZ	2:A:69:ASP:OD1	2.37	0.57
5:D:278:GLN:NE2	5:D:286:GLN:OE1	2.37	0.57
8:G:141:ILE:HG22	8:G:151:VAL:HG22	1.87	0.56
25:W:300:PRO:HD2	25:W:326:MET:HE1	1.86	0.56
27:Y:33:GLY:HA2	27:Y:37:VAL:HG21	1.87	0.56
1:x:386:PRO:HB2	2:A:232:ARG:HH12	1.69	0.56
1:x:422:ALA:HB3	1:x:479:LEU:HB3	1.87	0.56
29:a:278:MET:SD	29:a:278:MET:N	2.78	0.56
20:s:184:GLU:OE1	20:s:211:ARG:NH1	2.38	0.56
23:U:344:ARG:HE	23:U:927:PRO:HB2	1.70	0.56
32:d:139:LEU:HD11	32:d:151:VAL:HG13	1.87	0.56
6:E:4:PRO:HB2	6:E:7:LYS:HB2	1.87	0.56
31:c:58:LEU:HB3	31:c:71:ASP:HB3	1.86	0.56
2:A:72:LEU:HD11	3:B:162:VAL:HG12	1.86	0.56
2:A:398:ARG:NH2	3:B:196:GLU:OE2	2.38	0.56
12:k:41:GLN:NE2	12:k:151:PRO:O	2.38	0.56
4:C:301:LEU:HD11	4:C:305:LEU:HD23	1.88	0.56
6:E:234:GLU:HG2	7:F:311:LEU:HB3	1.87	0.56
29:a:280:MET:HB3	29:a:333:MET:HE1	1.88	0.56
33:f:29:SER:HB2	33:f:33:ARG:HE	1.69	0.56
1:x:43:ARG:HH22	33:f:433:LEU:HD13	1.69	0.56
4:C:140:VAL:HG13	5:D:323:ARG:HD2	1.87	0.56
10:I:149:GLN:HG3	10:I:164:ILE:HD11	1.88	0.56
25:W:396:LEU:HD13	25:W:402:ILE:HD13	1.86	0.56
33:f:195:ASN:O	33:f:199:ASN:ND2	2.38	0.56
33:f:425:GLY:HA3	33:f:451:VAL:HG21	1.87	0.56
2:A:236:CYS:SG	2:A:267:LYS:NZ	2.74	0.56
33:f:171:GLN:HB3	33:f:208:LEU:HD21	1.86	0.56
2:A:294:GLU:HA	2:A:297:ARG:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:141:ARG:NH1	18:q:165:GLU:OE2	2.39	0.56
24:V:452:ASN:HB3	24:V:457:TYR:HB2	1.87	0.56
14:m:8:ASP:O	14:m:22:GLN:NE2	2.38	0.56
23:U:811:PHE:HA	23:U:885:MET:HE1	1.88	0.56
24:V:398:LEU:HA	24:V:401:ASN:HB2	1.88	0.56
27:Y:142:PHE:HA	27:Y:145:LEU:HD12	1.88	0.56
33:f:681:TYR:HB3	33:f:761:MET:HE3	1.88	0.56
6:E:383:LYS:HD3	6:E:385:ASP:H	1.69	0.55
21:T:122:LEU:HG	21:T:137:LEU:HD12	1.88	0.55
11:j:146:GLN:OE1	11:j:159:ASN:ND2	2.33	0.55
16:o:40:ASN:ND2	16:o:103:VAL:O	2.38	0.55
31:c:111:TRP:NE1	31:c:130:GLN:OE1	2.38	0.55
32:d:8:GLU:HA	32:d:11:ARG:HB2	1.87	0.55
4:C:130:LYS:NZ	4:C:131:VAL:O	2.38	0.55
1:x:119:THR:HG23	1:x:204:TRP:HE3	1.71	0.55
16:O:30:ASN:OD1	16:O:187:ARG:NH2	2.39	0.55
19:R:141:ARG:HH21	18:q:162:LYS:HE3	1.72	0.55
16:o:143:ARG:NH2	16:o:150:GLU:OE1	2.39	0.55
29:a:19:PRO:HA	29:a:22:TRP:HB2	1.87	0.55
23:U:86:ASP:OD1	23:U:86:ASP:N	2.38	0.55
24:V:85:ALA:HB2	24:V:93:PHE:HB2	1.87	0.55
24:V:201:ARG:NH1	24:V:241:ARG:O	2.39	0.55
4:C:222:LYS:HD3	4:C:227:GLY:H	1.72	0.55
5:D:406:VAL:HG12	5:D:407:ILE:HG23	1.89	0.55
7:F:120:LYS:HB2	7:F:137:ILE:HD11	1.89	0.55
23:U:643:SER:O	23:U:649:ARG:NH1	2.40	0.55
2:A:124:ASP:HB3	7:F:86:LEU:HD22	1.89	0.55
9:H:93:LEU:HD13	9:H:113:ARG:HB3	1.88	0.55
3:B:109:VAL:HB	4:C:94:LYS:HB2	1.88	0.55
6:E:245:GLU:OE1	6:E:251:ARG:NH2	2.39	0.55
9:H:139:TRP:NE1	9:H:215:GLU:OE1	2.39	0.55
19:r:9:ARG:NH1	19:r:146:ASP:OD1	2.39	0.55
32:d:42:LYS:O	32:d:45:LYS:NZ	2.32	0.55
23:U:666:LYS:O	23:U:670:ASN:ND2	2.39	0.55
23:U:717:ILE:HD12	23:U:734:GLN:HG3	1.88	0.55
23:U:819:VAL:HG12	23:U:821:LYS:H	1.72	0.55
12:k:13:ASN:HB2	13:l:126:ARG:HD3	1.88	0.54
24:V:454:GLU:HB2	24:V:457:TYR:HE1	1.71	0.54
26:X:318:ILE:HG12	26:X:322:HIS:HE1	1.70	0.54
1:x:109:ASN:H	1:x:452:ASP:HB3	1.72	0.54
2:A:219:GLY:HA2	3:B:343:ARG:HH21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:65:VAL:O	9:H:220:ARG:NH1	2.37	0.54
24:V:304:GLU:OE2	24:V:307:ARG:NH1	2.40	0.54
25:W:296:LEU:HB3	25:W:302:TYR:HB2	1.89	0.54
25:W:380:GLN:HG3	25:W:381:LEU:HD12	1.90	0.54
32:d:29:VAL:HA	32:d:32:GLU:HB2	1.89	0.54
5:D:107:THR:HG22	6:E:77:PRO:HG3	1.89	0.54
9:H:65:VAL:HG22	9:H:75:VAL:HG22	1.88	0.54
13:L:160:SER:O	13:L:169:ARG:NH1	2.40	0.54
22:y:5:VAL:HG22	22:y:67:LEU:HD23	1.90	0.54
3:B:60:LEU:HD11	33:f:219:LYS:HE2	1.90	0.54
11:j:184:ASP:N	11:j:184:ASP:OD1	2.40	0.54
33:f:672:LEU:HB3	33:f:707:LEU:HD23	1.89	0.54
2:A:303:ILE:HD11	2:A:331:LEU:HG	1.88	0.54
7:F:183:GLU:OE1	7:F:238:ARG:NH1	2.41	0.54
11:j:67:ASP:N	11:j:67:ASP:OD1	2.41	0.54
23:U:839:ALA:HB1	33:f:229:VAL:HB	1.89	0.54
24:V:76:LYS:HE3	24:V:149:PRO:HB3	1.88	0.54
33:f:80:ARG:HH12	33:f:84:SER:HB3	1.71	0.54
29:a:34:TRP:O	30:b:17:ARG:NH2	2.41	0.54
16:o:163:ILE:HG12	16:o:170:GLY:HA2	1.90	0.54
3:B:52:VAL:HA	3:B:61:LYS:HD2	1.90	0.54
4:C:22:GLN:HA	4:C:25:LEU:HB2	1.89	0.54
27:Y:347:ILE:HG13	27:Y:354:VAL:HG22	1.89	0.54
2:A:324:PRO:HA	2:A:327:LEU:HD23	1.89	0.54
18:q:168:GLN:HE22	18:q:176:PRO:HA	1.71	0.54
23:U:788:VAL:HG11	23:U:889:LEU:HD21	1.90	0.54
27:Y:134:LEU:HD13	27:Y:171:GLY:HA2	1.89	0.54
2:A:365:GLU:HG2	2:A:367:ASP:H	1.73	0.54
17:P:125:ASP:OD1	17:P:129:CYS:N	2.38	0.54
20:s:145:LEU:HD22	20:s:178:VAL:HB	1.90	0.54
23:U:583:MET:HE3	23:U:605:VAL:HG11	1.89	0.54
34:e:51:ASP:OD2	34:e:54:ASN:ND2	2.41	0.54
5:D:104:GLY:HA2	5:D:110:ASN:HA	1.90	0.53
7:F:243:GLN:O	7:F:245:LYS:NZ	2.39	0.53
28:Z:110:GLU:OE2	28:Z:153:LYS:NZ	2.41	0.53
33:f:218:GLU:HA	33:f:221:ILE:HG12	1.90	0.53
33:f:281:ILE:HA	33:f:286:LYS:HD2	1.90	0.53
19:R:44:THR:HG21	19:R:100:MET:HE3	1.91	0.53
23:U:26:LYS:HD2	32:d:37:PRO:HG3	1.89	0.53
23:U:522:GLY:O	23:U:559:ARG:NH2	2.41	0.53
23:U:764:LEU:O	23:U:767:THR:OG1	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:231:LEU:HG	27:Y:236:LEU:HD12	1.90	0.53
29:a:15:GLY:O	29:a:18:GLN:NE2	2.41	0.53
33:f:682:GLY:HA3	33:f:719:PRO:HA	1.90	0.53
23:U:233:LEU:HD21	23:U:325:MET:HG3	1.90	0.53
29:a:255:TRP:O	29:a:258:GLN:NE2	2.42	0.53
33:f:349:TYR:OH	33:f:374:SER:OG	2.20	0.53
33:f:683:GLU:OE1	33:f:688:ARG:NH2	2.41	0.53
3:B:220:LYS:HB2	3:B:346:ARG:HB2	1.89	0.53
5:D:90:GLY:HA2	5:D:106:THR:HG23	1.90	0.53
5:D:363:TYR:HD1	5:D:366:ARG:HH12	1.57	0.53
6:E:364:GLN:HA	6:E:367:PHE:HD2	1.74	0.53
11:j:96:LEU:HB2	18:q:62:LYS:HG3	1.90	0.53
23:U:265:ILE:HD11	23:U:326:ILE:HG23	1.89	0.53
31:c:254:ASN:HA	31:c:257:LYS:HE2	1.89	0.53
3:B:137:SER:OG	3:B:138:PHE:N	2.41	0.53
4:C:155:ASP:N	4:C:155:ASP:OD1	2.41	0.53
23:U:398:ASN:ND2	31:c:24:ALA:O	2.42	0.53
29:a:116:THR:HA	29:a:158:LEU:HD22	1.91	0.53
32:d:55:LEU:HD22	32:d:74:TYR:HE1	1.73	0.53
18:q:11:ASP:N	18:q:11:ASP:OD1	2.42	0.53
21:t:25:ASP:OD1	21:t:41:ARG:NH2	2.41	0.53
26:X:126:ARG:HH22	26:X:153:LEU:HD11	1.74	0.53
27:Y:104:MET:HE2	27:Y:127:THR:HB	1.91	0.53
29:a:40:GLN:NE2	29:a:61:GLU:OE2	2.42	0.53
32:d:191:PHE:O	32:d:196:ARG:NH1	2.42	0.53
9:H:111:VAL:HG22	9:H:136:ILE:HD12	1.90	0.53
23:U:327:LYS:O	23:U:330:SER:OG	2.24	0.53
30:b:131:LEU:HB3	30:b:136:VAL:HB	1.91	0.53
33:f:257:ARG:O	33:f:261:ARG:NH1	2.41	0.53
33:f:342:PRO:O	33:f:387:GLN:NE2	2.41	0.53
19:R:80:SER:OG	19:R:120:ARG:NH1	2.41	0.52
9:h:119:GLN:HG3	10:i:81:SER:HB2	1.91	0.52
23:U:532:MET:HE1	23:U:552:ILE:HG13	1.91	0.52
26:X:351:SER:HA	26:X:354:ILE:HG22	1.92	0.52
27:Y:237:ARG:HB3	27:Y:242:LYS:HE2	1.91	0.52
33:f:292:LYS:HB3	33:f:771:LEU:HD12	1.91	0.52
33:f:713:PHE:HB2	33:f:752:HIS:CE1	2.45	0.52
5:D:209:GLY:N	35:D:501:ATP:O2G	2.39	0.52
13:l:39:LYS:HE3	13:l:142:PRO:HB2	1.90	0.52
3:B:230:THR:HG21	3:B:353:PHE:HB3	1.91	0.52
8:G:112:ASP:N	8:G:112:ASP:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g:191:PHE:HE1	8:g:219:VAL:HG21	1.74	0.52
23:U:713:TYR:O	23:U:717:ILE:HB	2.09	0.52
2:A:109:PRO:HG3	2:A:125:LEU:HG	1.90	0.52
4:C:182:GLN:HE21	4:C:286:THR:HG23	1.73	0.52
4:C:344:LEU:HA	4:C:347:ILE:HD12	1.91	0.52
14:M:108:LEU:HD22	14:M:139:SER:HB3	1.90	0.52
33:f:221:ILE:HG21	33:f:255:VAL:HG11	1.92	0.52
33:f:508:SER:OG	33:f:545:LYS:NZ	2.39	0.52
11:j:224:GLU:HA	11:j:227:LYS:HE2	1.92	0.52
23:U:803:LYS:HB2	23:U:875:PHE:HA	1.91	0.52
24:V:464:ILE:O	28:Z:250:TYR:OH	2.24	0.52
25:W:313:GLU:HG3	25:W:361:HIS:HD2	1.74	0.52
30:b:109:ILE:HB	30:b:138:VAL:HG22	1.90	0.52
1:x:321:PRO:O	1:x:418:TYR:OH	2.26	0.52
5:D:53:PHE:O	5:D:57:GLN:NE2	2.42	0.52
5:D:275:PHE:O	6:E:251:ARG:NH2	2.42	0.52
32:d:211:LYS:HE2	32:d:217:LEU:HB3	1.91	0.52
2:A:252:GLU:OE1	2:A:255:ARG:NH1	2.43	0.52
7:F:200:GLU:HG2	7:F:204:LEU:HD12	1.92	0.52
20:s:145:LEU:HD21	20:s:182:ALA:HB2	1.92	0.52
33:f:659:LEU:HD12	33:f:668:ALA:HB1	1.92	0.52
4:C:24:TYR:HB3	5:D:40:LEU:HD22	1.92	0.52
6:E:242:ARG:HH21	6:E:258:MET:HE1	1.73	0.52
11:j:230:ALA:HA	11:j:233:GLU:HG2	1.92	0.52
23:U:94:SER:HB3	23:U:97:VAL:HG12	1.91	0.52
23:U:505:ASP:HB3	23:U:508:THR:HG22	1.91	0.52
23:U:740:GLY:HA3	23:U:744:VAL:HG22	1.90	0.52
24:V:484:LEU:HB3	32:d:256:ILE:HD11	1.92	0.52
33:f:347:ASP:N	33:f:347:ASP:OD1	2.43	0.52
33:f:698:SER:OG	33:f:701:ASN:O	2.28	0.52
4:C:86:LEU:HD21	4:C:94:LYS:HD2	1.92	0.51
14:M:230:ASP:N	14:M:230:ASP:OD1	2.42	0.51
22:y:38:PRO:HA	22:y:41:GLN:HE21	1.75	0.51
23:U:138:PHE:HZ	23:U:154:ALA:HB2	1.75	0.51
23:U:251:ASP:OD1	23:U:751:ARG:NH1	2.40	0.51
2:A:296:GLN:HA	2:A:299:MET:HG3	1.93	0.51
5:D:213:THR:OG1	35:D:501:ATP:O3G	2.28	0.51
6:E:360:ASP:N	6:E:360:ASP:OD1	2.43	0.51
28:Z:174:HIS:NE2	31:c:207:TYR:OH	2.39	0.51
2:A:75:PRO:HA	2:A:79:ASP:HB2	1.92	0.51
3:B:79:ILE:HA	3:B:83:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:y:30:ILE:HG22	22:y:33:LYS:HE3	1.91	0.51
23:U:383:ASP:OD2	23:U:387:ARG:NH1	2.43	0.51
24:V:451:ILE:HG13	24:V:458:VAL:HG13	1.92	0.51
29:a:117:ALA:HB2	29:a:154:ARG:HH22	1.76	0.51
33:f:87:THR:O	33:f:91:SER:HB2	2.11	0.51
2:A:217:PRO:O	2:A:222:LYS:NZ	2.44	0.51
4:C:326:LEU:HD21	4:C:345:ARG:HH21	1.75	0.51
4:C:389:LYS:O	4:C:392:GLN:NE2	2.43	0.51
1:x:463:ILE:HA	1:x:466:LEU:HD12	1.93	0.51
4:C:49:ARG:NH1	23:U:639:LEU:O	2.44	0.51
5:D:404:LYS:HA	5:D:408:LYS:HB2	1.91	0.51
23:U:459:ASP:HA	23:U:462:LEU:HB3	1.93	0.51
23:U:803:LYS:HD2	23:U:875:PHE:HB2	1.93	0.51
29:a:27:GLU:OE1	29:a:31:LYS:NZ	2.44	0.51
33:f:323:ASN:ND2	33:f:454:GLY:O	2.43	0.51
1:x:301:GLN:HA	1:x:308:ASN:HA	1.92	0.51
1:x:400:LYS:HB2	1:x:487:ILE:HB	1.92	0.51
1:x:418:TYR:HB3	1:x:480:TYR:HB3	1.93	0.51
14:m:230:ASP:OD1	14:m:230:ASP:N	2.43	0.51
33:f:286:LYS:HB2	33:f:881:GLU:HB3	1.93	0.51
2:A:72:LEU:HD12	3:B:139:VAL:HG22	1.93	0.51
26:X:233:TYR:HA	26:X:254:MET:HE1	1.93	0.51
1:x:305:LEU:O	1:x:307:ARG:NH1	2.44	0.51
2:A:301:GLU:HB2	7:F:254:PRO:HG2	1.91	0.51
3:B:376:ASP:N	3:B:376:ASP:OD1	2.43	0.51
6:E:366:ASP:OD1	6:E:369:LYS:NZ	2.43	0.51
14:M:34:SER:OG	14:M:65:ARG:NH1	2.40	0.51
20:S:145:LEU:HD21	20:S:182:ALA:HB2	1.91	0.51
23:U:330:SER:OG	23:U:332:GLU:OE1	2.29	0.51
23:U:890:LYS:HG3	23:U:891:VAL:HG13	1.91	0.51
3:B:197:ILE:HG21	3:B:235:LEU:HD11	1.92	0.51
5:D:148:ASP:HB3	5:D:252:ARG:HH22	1.75	0.51
6:E:180:LYS:N	35:E:501:ATP:O2B	2.43	0.51
22:y:58:ASP:OD1	22:y:58:ASP:N	2.43	0.51
27:Y:161:THR:HG21	27:Y:186:LEU:HD22	1.92	0.51
31:c:285:GLU:HB2	31:c:288:VAL:HB	1.93	0.51
33:f:323:ASN:HA	33:f:327:ASN:HB2	1.92	0.51
20:S:145:LEU:HD22	20:S:178:VAL:HB	1.92	0.51
25:W:445:LEU:HD11	28:Z:226:ILE:HD12	1.91	0.51
28:Z:212:LEU:HA	28:Z:215:VAL:HG12	1.92	0.51
29:a:277:LEU:HA	29:a:280:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:380:LEU:HD13	3:B:383:LEU:HD12	1.93	0.50
21:T:25:ASP:HA	21:T:187:PHE:HA	1.93	0.50
20:s:48:ASP:OD1	20:s:48:ASP:N	2.44	0.50
30:b:9:CYS:HB3	30:b:111:ALA:HA	1.92	0.50
33:f:311:VAL:HB	33:f:314:TYR:HD1	1.74	0.50
5:D:87:LEU:HB3	6:E:80:VAL:HB	1.93	0.50
13:l:7:ASP:O	13:l:21:GLN:NE2	2.44	0.50
24:V:479:ARG:HH22	28:Z:260:VAL:HB	1.77	0.50
33:f:140:LEU:HD23	33:f:144:LEU:HD23	1.93	0.50
1:x:192:GLN:HG2	1:x:194:GLN:H	1.77	0.50
4:C:375:ARG:NH2	4:C:382:ASP:OD2	2.44	0.50
5:D:160:PRO:HB3	5:D:217:LYS:HE3	1.93	0.50
5:D:338:ARG:NH1	5:D:364:VAL:O	2.44	0.50
12:K:105:GLU:OE2	20:S:75:TYR:OH	2.29	0.50
13:L:157:ARG:HD2	13:L:176:MET:HE3	1.92	0.50
26:X:214:SER:O	26:X:218:HIS:ND1	2.44	0.50
29:a:278:MET:HA	29:a:281:THR:HG22	1.93	0.50
2:A:139:ARG:NH2	3:B:114:GLU:OE1	2.41	0.50
6:E:58:GLY:HA2	6:E:74:THR:HG23	1.92	0.50
7:F:46:ARG:NH2	29:a:103:LYS:O	2.44	0.50
14:M:43:ASP:OD1	14:M:43:ASP:N	2.42	0.50
18:q:39:SER:OG	18:q:40:GLU:N	2.45	0.50
23:U:561:GLU:HG2	23:U:562:GLU:HG3	1.92	0.50
25:W:182:ARG:O	25:W:186:ILE:N	2.38	0.50
25:W:443:THR:HG21	28:Z:204:LYS:HD2	1.94	0.50
33:f:250:ARG:NH1	33:f:253:LEU:H	2.08	0.50
3:B:249:ARG:NH2	4:C:279:GLN:OE1	2.45	0.50
6:E:288:ALA:O	6:E:294:ARG:NH1	2.44	0.50
13:L:117:GLN:NE2	14:M:83:ASP:OD1	2.44	0.50
16:O:171:SER:HA	16:O:193:ASN:HD21	1.77	0.50
12:k:121:LEU:HD12	13:l:79:ALA:HB3	1.94	0.50
28:Z:260:VAL:O	28:Z:264:SER:OG	2.29	0.50
29:a:37:LEU:HD23	29:a:71:VAL:HG11	1.94	0.50
29:a:291:LEU:H	29:a:330:ARG:HH22	1.58	0.50
30:b:12:ASN:ND2	30:b:53:THR:OG1	2.43	0.50
30:b:51:LEU:O	30:b:62:THR:OG1	2.28	0.50
33:f:706:ILE:HG12	33:f:791:VAL:HG11	1.93	0.50
1:x:27:MET:HA	1:x:30:LYS:HD2	1.93	0.50
2:A:189:GLU:O	2:A:193:THR:OG1	2.30	0.50
3:B:373:THR:OG1	3:B:412:MET:O	2.27	0.50
5:D:376:ASN:ND2	35:D:501:ATP:O3'	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:157:ARG:NH2	14:M:60:GLU:OE1	2.43	0.50
14:M:17:ASP:OD1	14:M:17:ASP:N	2.43	0.50
23:U:456:ASP:N	23:U:456:ASP:OD1	2.43	0.50
24:V:234:ARG:HG3	24:V:250:LEU:HD11	1.93	0.50
24:V:345:ARG:NH2	34:e:46:ASP:OD2	2.45	0.50
2:A:79:ASP:O	3:B:98:LYS:NZ	2.45	0.50
2:A:236:CYS:HB3	2:A:270:CYS:HA	1.92	0.50
23:U:794:ASP:OD1	23:U:794:ASP:N	2.44	0.50
24:V:345:ARG:HA	24:V:348:PHE:HD2	1.77	0.50
30:b:78:VAL:HG13	30:b:80:PRO:HD3	1.94	0.50
34:e:44:ASP:OD1	34:e:47:ASN:ND2	2.45	0.50
3:B:118:ASP:O	3:B:120:HIS:ND1	2.41	0.50
4:C:99:VAL:HG12	4:C:123:LEU:HD12	1.93	0.50
18:q:168:GLN:NE2	18:q:175:LEU:O	2.44	0.50
23:U:159:ARG:HE	23:U:162:VAL:HG11	1.76	0.50
33:f:398:TRP:O	33:f:402:ASN:ND2	2.44	0.50
6:E:200:SER:OG	6:E:234:GLU:O	2.30	0.50
12:K:91:LYS:HG2	12:K:119:LEU:HD11	1.94	0.50
28:Z:61:ASP:HB2	28:Z:67:VAL:HB	1.93	0.50
29:a:123:LEU:HD11	29:a:161:LYS:HB3	1.93	0.50
33:f:815:HIS:ND1	33:f:882:LEU:O	2.43	0.50
5:D:249:ASP:OD1	5:D:252:ARG:NH2	2.38	0.49
12:K:118:ASN:O	12:K:122:GLN:NE2	2.45	0.49
29:a:28:LEU:HD22	29:a:36:GLN:HB3	1.93	0.49
32:d:115:PHE:HE1	32:d:137:VAL:HG12	1.77	0.49
32:d:125:LYS:HD2	32:d:130:ASN:HD22	1.76	0.49
1:x:94:GLU:HA	1:x:97:LEU:HD13	1.93	0.49
1:x:185:GLN:NE2	22:y:51:GLU:OE2	2.45	0.49
27:Y:50:MET:HE1	27:Y:70:LEU:HD13	1.94	0.49
33:f:258:LYS:HB2	33:f:769:THR:HG23	1.93	0.49
33:f:570:GLY:O	33:f:574:GLU:N	2.40	0.49
33:f:692:LEU:HD12	33:f:727:PHE:HD2	1.77	0.49
1:x:39:VAL:O	1:x:44:GLN:NE2	2.45	0.49
1:x:324:LEU:HB3	1:x:480:TYR:HB2	1.93	0.49
20:S:125:ASP:OD1	20:S:129:SER:N	2.45	0.49
23:U:367:THR:HA	23:U:370:VAL:HG12	1.93	0.49
23:U:656:LEU:HD21	23:U:671:LEU:HD11	1.94	0.49
25:W:118:LEU:N	25:W:119:PRO:HD2	2.27	0.49
25:W:152:ILE:HG13	25:W:165:ILE:HD12	1.92	0.49
27:Y:71:ASN:HA	27:Y:74:LYS:HG2	1.94	0.49
30:b:33:VAL:HA	30:b:36:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:224:LEU:HD11	3:B:349:ARG:HB2	1.93	0.49
11:j:185:ASP:O	11:j:189:LYS:HG2	2.13	0.49
23:U:791:LEU:HB3	23:U:911:ILE:HD11	1.93	0.49
32:d:9:TRP:HE1	32:d:25:ARG:HD3	1.76	0.49
34:e:50:ASP:N	34:e:50:ASP:OD1	2.46	0.49
1:x:245:GLN:NE2	1:x:410:ILE:O	2.41	0.49
14:M:181:MET:HA	14:M:184:MET:HE2	1.94	0.49
25:W:267:LEU:HD12	25:W:296:LEU:HD23	1.94	0.49
26:X:380:GLN:HB3	27:Y:314:LEU:HA	1.94	0.49
27:Y:192:ARG:HG3	27:Y:194:PHE:HE1	1.77	0.49
30:b:157:VAL:HG21	30:b:170:LEU:HB2	1.95	0.49
33:f:417:ILE:HG22	33:f:418:LEU:HD12	1.93	0.49
2:A:244:GLU:O	2:A:247:GLN:NE2	2.46	0.49
20:s:125:ASP:OD1	20:s:129:SER:N	2.46	0.49
23:U:574:LYS:HD3	31:c:211:GLU:HG3	1.95	0.49
26:X:273:GLY:O	26:X:277:LEU:N	2.43	0.49
33:f:739:ALA:O	33:f:743:ALA:N	2.45	0.49
1:x:113:THR:O	1:x:117:ASN:ND2	2.46	0.49
25:W:186:ILE:HG23	25:W:209:ILE:HD11	1.95	0.49
31:c:137:SER:OG	31:c:138:GLU:N	2.45	0.49
32:d:155:LYS:HD2	32:d:171:LEU:HD11	1.95	0.49
33:f:637:LYS:HB3	33:f:678:LEU:HD13	1.95	0.49
24:V:433:ASP:OD1	24:V:433:ASP:N	2.45	0.49
28:Z:239:ASP:OD1	28:Z:239:ASP:N	2.45	0.49
32:d:2:TYR:HB3	32:d:5:LEU:HD22	1.95	0.49
7:F:289:ASP:OD1	7:F:289:ASP:N	2.44	0.49
23:U:191:LYS:HD3	23:U:194:ARG:HD3	1.95	0.49
24:V:86:VAL:HG21	24:V:160:LEU:HD13	1.95	0.49
31:c:217:LEU:O	31:c:221:HIS:HB2	2.12	0.49
33:f:320:ILE:HB	33:f:326:LEU:HB2	1.94	0.49
6:E:320:ILE:HB	6:E:322:LYS:HE2	1.94	0.49
10:I:119:GLN:NE2	11:J:79:ASP:OD1	2.45	0.49
13:L:107:ARG:HH12	21:T:74:GLU:HG3	1.77	0.49
23:U:219:CYS:SG	23:U:220:LEU:N	2.85	0.49
25:W:420:ASP:N	25:W:420:ASP:OD1	2.45	0.49
31:c:32:TYR:HB3	31:c:208:ARG:HB2	1.95	0.49
33:f:673:ARG:HH12	33:f:785:ARG:HH11	1.59	0.49
1:x:149:ALA:HB3	1:x:214:LYS:HG3	1.95	0.48
4:C:193:GLY:HA2	36:C:501:ADP:H5'1	1.94	0.48
6:E:101:ASP:OD1	6:E:104:THR:N	2.43	0.48
13:l:49:LEU:HG	13:l:195:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:n:116:MET:HE2	15:n:116:MET:HB3	1.76	0.48
25:W:275:ILE:HG21	25:W:308:LEU:HD13	1.95	0.48
28:Z:15:VAL:HG21	28:Z:50:VAL:HG12	1.95	0.48
29:a:374:ILE:HG22	32:d:255:MET:HE1	1.94	0.48
30:b:18:ASN:ND2	30:b:145:GLU:OE2	2.41	0.48
7:F:318:ASP:HB3	7:F:347:ARG:HE	1.78	0.48
12:K:35:SER:HB2	12:K:51:GLU:HG2	1.95	0.48
13:l:215:VAL:HB	13:l:221:PHE:HD1	1.78	0.48
20:s:148:LEU:HD23	20:s:178:VAL:HG12	1.93	0.48
4:C:161:ILE:HA	4:C:164:VAL:HG12	1.94	0.48
16:O:214:GLU:OE2	17:P:198:ARG:NE	2.46	0.48
21:T:174:ARG:NH1	21:T:206:GLU:O	2.47	0.48
33:f:637:LYS:HD2	33:f:678:LEU:HD22	1.96	0.48
1:x:19:GLU:O	1:x:32:GLN:NE2	2.40	0.48
1:x:252:GLU:O	1:x:316:LYS:N	2.46	0.48
13:l:52:ALA:HB1	13:l:57:ALA:HB3	1.95	0.48
23:U:607:VAL:O	23:U:615:ARG:NH1	2.47	0.48
25:W:135:LYS:HB2	25:W:139:GLU:HB2	1.95	0.48
25:W:372:ARG:NH1	29:a:325:ASP:OD2	2.47	0.48
27:Y:175:ASP:OD1	27:Y:175:ASP:N	2.46	0.48
32:d:206:MET:HA	32:d:209:TYR:HB3	1.95	0.48
2:A:369:ARG:HH11	2:A:372:LEU:HD12	1.78	0.48
7:F:141:ASP:OD1	7:F:144:LYS:N	2.43	0.48
12:K:167:ALA:HB3	13:L:56:LEU:HD13	1.95	0.48
23:U:447:GLY:HA3	23:U:480:GLY:HA2	1.95	0.48
27:Y:49:ASN:ND2	27:Y:113:ARG:O	2.36	0.48
28:Z:116:CYS:O	28:Z:119:SER:OG	2.25	0.48
1:x:300:LYS:O	1:x:309:ALA:N	2.38	0.48
1:x:427:GLN:OE1	1:x:473:HIS:NE2	2.46	0.48
14:m:120:HIS:O	14:m:123:THR:OG1	2.30	0.48
23:U:437:TYR:HA	23:U:472:ILE:HG21	1.95	0.48
29:a:128:LEU:O	29:a:132:LYS:NZ	2.41	0.48
33:f:300:ARG:HH22	33:f:318:THR:HG22	1.79	0.48
33:f:404:ASP:OD1	33:f:404:ASP:N	2.46	0.48
1:x:424:LEU:HD11	1:x:436:TYR:HD2	1.79	0.48
4:C:46:GLN:O	4:C:50:ASN:ND2	2.47	0.48
17:p:27:ARG:HB2	17:p:183:MET:HB2	1.95	0.48
25:W:328:LEU:HG	25:W:342:GLY:HA2	1.94	0.48
34:e:35:ASP:HB3	34:e:37:HIS:HD2	1.78	0.48
1:x:251:PHE:HD2	1:x:315:SER:HB3	1.78	0.48
5:D:171:ASP:HA	5:D:174:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:14:LEU:HD21	18:Q:160:LEU:HD22	1.95	0.48
20:s:133:ASP:OD1	20:s:133:ASP:N	2.45	0.48
22:y:31:GLN:NE2	22:y:36:ILE:O	2.31	0.48
28:Z:32:GLN:HG2	28:Z:34:ARG:H	1.78	0.48
29:a:113:LEU:HB2	29:a:154:ARG:HE	1.79	0.48
33:f:486:GLY:HA2	33:f:525:ILE:HD11	1.95	0.48
2:A:280:ILE:HG21	2:A:302:LEU:HD21	1.96	0.48
9:H:148:GLN:OE1	9:H:158:TRP:NE1	2.38	0.48
18:Q:11:ASP:N	18:Q:11:ASP:OD1	2.46	0.48
9:h:206:ASP:OD1	9:h:206:ASP:N	2.47	0.48
12:k:228:MET:HE2	12:k:228:MET:HB2	1.77	0.48
33:f:168:LYS:O	33:f:172:GLU:HB2	2.13	0.48
2:A:151:ILE:HD12	2:A:152:PRO:HD2	1.95	0.48
6:E:29:LEU:HB3	7:F:62:VAL:HG11	1.96	0.48
7:F:314:LEU:HD11	7:F:342:LEU:HA	1.96	0.48
8:G:46:ASP:OD1	8:G:46:ASP:N	2.45	0.48
14:M:43:ASP:HB2	14:M:218:GLU:HG2	1.96	0.48
14:m:215:TRP:CH2	14:m:219:LEU:HD11	2.49	0.48
17:p:138:VAL:HB	17:p:146:MET:HE3	1.96	0.48
25:W:268:LYS:HA	25:W:271:VAL:HG12	1.96	0.48
31:c:281:LYS:HG3	31:c:282:ARG:HG2	1.96	0.48
33:f:438:ASP:OD1	33:f:438:ASP:N	2.47	0.48
33:f:703:ARG:HB2	33:f:787:LEU:HD11	1.94	0.48
3:B:176:VAL:HG21	3:B:247:PHE:HD2	1.78	0.47
22:y:1:MET:N	22:y:17:VAL:O	2.46	0.47
33:f:873:LEU:HD23	33:f:875:ALA:HB3	1.95	0.47
1:x:277:CYS:SG	1:x:278:PHE:N	2.87	0.47
4:C:183:PRO:O	4:C:290:LYS:NZ	2.40	0.47
7:F:288:LEU:HB3	7:F:332:THR:HG22	1.95	0.47
12:K:51:GLU:HA	12:K:215:ILE:HG22	1.95	0.47
12:K:117:SER:HA	12:K:156:MET:HE1	1.95	0.47
33:f:39:LYS:HG3	33:f:85:SER:HA	1.95	0.47
33:f:762:VAL:O	33:f:771:LEU:N	2.34	0.47
7:F:373:MET:HE2	7:F:415:LEU:HD11	1.95	0.47
9:h:86:LEU:HD13	9:h:134:LEU:HD11	1.95	0.47
19:r:179:VAL:HG22	19:r:184:TRP:HB3	1.96	0.47
2:A:45:ILE:HD13	3:B:57:GLN:HB3	1.96	0.47
2:A:213:LEU:HA	2:A:319:MET:HB2	1.96	0.47
3:B:348:ASP:OD1	3:B:349:ARG:HG2	2.15	0.47
12:K:13:ASN:HB3	13:L:126:ARG:HB3	1.96	0.47
18:Q:141:SER:HB3	19:r:138:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:148:LEU:HD23	20:S:178:VAL:HG12	1.97	0.47
33:f:673:ARG:HD2	33:f:707:LEU:HD11	1.96	0.47
5:D:92:PHE:HZ	5:D:95:ALA:HB2	1.79	0.47
8:G:33:ASN:HB2	8:G:170:VAL:HG22	1.94	0.47
25:W:231:ILE:HD12	25:W:243:ILE:HA	1.96	0.47
27:Y:53:TYR:O	27:Y:57:LEU:N	2.47	0.47
29:a:100:THR:HA	29:a:103:LYS:HG2	1.96	0.47
5:D:167:ILE:O	5:D:174:LYS:NZ	2.48	0.47
16:O:110:LEU:HD21	16:O:125:VAL:HG22	1.97	0.47
10:i:71:ASP:OD1	10:i:71:ASP:N	2.48	0.47
10:i:178:ASP:OD2	10:i:195:LYS:NZ	2.47	0.47
23:U:176:MET:HA	23:U:179:TYR:HB3	1.97	0.47
33:f:637:LYS:HD2	33:f:678:LEU:HB2	1.97	0.47
2:A:23:ARG:NH2	33:f:4:GLY:O	2.47	0.47
6:E:175:PRO:HG3	6:E:386:TYR:CZ	2.49	0.47
7:F:383:GLU:OE1	7:F:417:HIS:NE2	2.48	0.47
12:K:52:LYS:NZ	12:K:64:ILE:O	2.48	0.47
15:N:14:LEU:HD21	15:N:101:ALA:HB3	1.96	0.47
18:Q:95:ARG:HG3	18:Q:96:THR:HG23	1.95	0.47
20:S:10:GLY:HA3	20:S:42:LYS:HE2	1.97	0.47
20:s:144:MET:HE1	20:s:185:ARG:HB2	1.95	0.47
23:U:666:LYS:HE2	23:U:703:CYS:HB3	1.95	0.47
23:U:865:LYS:HA	23:U:868:LYS:HG2	1.97	0.47
24:V:472:PRO:HA	24:V:475:ALA:HB3	1.96	0.47
25:W:152:ILE:HD13	25:W:161:GLU:HB3	1.97	0.47
25:W:422:ASN:O	25:W:426:ASN:ND2	2.41	0.47
27:Y:212:GLU:HG2	27:Y:213:LEU:HG	1.96	0.47
31:c:145:VAL:HG22	31:c:157:ILE:HG22	1.95	0.47
32:d:193:GLU:HA	32:d:197:ILE:HG23	1.95	0.47
33:f:171:GLN:HG3	33:f:179:VAL:HG13	1.96	0.47
33:f:463:LEU:HD11	33:f:500:LEU:HD13	1.97	0.47
33:f:764:LEU:HD21	33:f:771:LEU:HB2	1.96	0.47
4:C:237:MET:HE1	4:C:289:ILE:HG12	1.96	0.47
6:E:22:ILE:HD12	7:F:55:MET:HB3	1.96	0.47
6:E:169:GLY:HA3	6:E:295:LEU:HA	1.97	0.47
26:X:190:LEU:HD22	26:X:217:ILE:HG21	1.97	0.47
32:d:128:GLN:HG3	32:d:129:THR:HG22	1.97	0.47
2:A:323:ARG:NH2	2:A:430:MET:SD	2.86	0.47
4:C:346:LYS:O	4:C:350:LEU:HB2	2.15	0.47
11:J:39:ASP:OD1	11:J:39:ASP:N	2.46	0.47
13:L:226:ASP:OD1	13:L:226:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:18:ASN:OD1	30:b:25:ARG:NH1	2.47	0.47
33:f:378:ASN:O	33:f:382:ASN:ND2	2.48	0.47
2:A:21:PRO:HA	33:f:5:GLY:HA2	1.97	0.47
5:D:126:PRO:HG2	5:D:128:ALA:HB3	1.96	0.47
11:J:67:ASP:OD1	11:J:67:ASP:N	2.46	0.47
11:J:116:GLN:HG3	12:K:83:ALA:HB1	1.97	0.47
14:m:206:ASP:OD1	14:m:206:ASP:N	2.47	0.47
23:U:41:SER:O	23:U:41:SER:OG	2.29	0.47
5:D:167:ILE:HG21	5:D:215:LEU:HD21	1.97	0.46
15:n:104:ASP:OD1	15:n:104:ASP:N	2.47	0.46
23:U:35:TRP:HZ3	24:V:235:LEU:HD23	1.79	0.46
24:V:78:HIS:ND1	24:V:166:TYR:OH	2.40	0.46
24:V:225:ASP:OD1	24:V:228:ARG:NH2	2.48	0.46
32:d:203:PRO:HD2	32:d:206:MET:HG2	1.97	0.46
1:x:253:THR:OG1	1:x:268:GLY:O	2.33	0.46
1:x:424:LEU:HB3	1:x:477:VAL:HB	1.97	0.46
2:A:99:THR:HG22	2:A:115:VAL:HG22	1.97	0.46
13:L:225:ASP:H	13:L:228:ASP:HB2	1.80	0.46
18:Q:53:THR:HG22	18:Q:100:VAL:HG12	1.98	0.46
20:S:184:GLU:OE1	20:S:211:ARG:NH2	2.46	0.46
13:l:160:SER:O	13:l:169:ARG:NH1	2.48	0.46
24:V:338:LEU:HG	24:V:398:LEU:HD12	1.97	0.46
32:d:63:ILE:HG12	32:d:101:LEU:HD21	1.98	0.46
33:f:156:HIS:ND1	33:f:157:GLU:OE2	2.35	0.46
33:f:606:VAL:O	33:f:610:GLN:HB2	2.15	0.46
6:E:168:LYS:HA	6:E:274:LYS:HD2	1.97	0.46
18:Q:161:ARG:HD3	18:Q:194:ILE:HD12	1.97	0.46
20:S:147:PRO:HG3	17:p:177:ARG:HG3	1.98	0.46
11:j:195:LEU:HD23	11:j:206:ILE:HG23	1.97	0.46
16:o:161:ALA:O	16:o:165:ASN:ND2	2.43	0.46
22:y:1:MET:SD	22:y:2:GLN:N	2.86	0.46
23:U:792:ASN:OD1	23:U:793:LYS:N	2.48	0.46
25:W:287:VAL:HA	25:W:290:ILE:HG12	1.98	0.46
27:Y:127:THR:O	27:Y:131:THR:OG1	2.30	0.46
27:Y:179:ARG:NH1	27:Y:212:GLU:OE1	2.47	0.46
31:c:220:LEU:HA	31:c:223:LYS:HG2	1.97	0.46
33:f:80:ARG:O	33:f:80:ARG:NH1	2.48	0.46
33:f:253:LEU:HB3	33:f:256:PHE:HB2	1.96	0.46
7:F:28:GLY:HA2	7:F:31:GLU:HG2	1.98	0.46
8:g:210:PHE:HB3	8:g:214:GLU:HB2	1.96	0.46
23:U:807:LYS:HE2	23:U:874:ASN:HD21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:309:TYR:HB2	26:X:313:LEU:HD13	1.96	0.46
28:Z:106:ILE:HG23	28:Z:153:LYS:HB2	1.98	0.46
35:A:501:ATP:O5'	3:B:343:ARG:NH2	2.39	0.46
3:B:78:PHE:HB2	33:f:614:HIS:CD2	2.50	0.46
3:B:369:THR:HA	3:B:372:MET:HG2	1.96	0.46
4:C:89:VAL:HG23	4:C:90:HIS:H	1.80	0.46
4:C:320:PRO:O	4:C:325:ARG:NH1	2.48	0.46
4:C:326:LEU:HD11	4:C:345:ARG:HH21	1.80	0.46
5:D:235:PHE:HD2	5:D:288:ILE:HD13	1.81	0.46
6:E:280:ASN:HB2	7:F:295:ARG:HH12	1.80	0.46
14:M:66:LEU:HD12	14:M:212:GLU:HG2	1.97	0.46
29:a:363:MET:HE3	29:a:367:VAL:HG23	1.96	0.46
30:b:54:LEU:HD13	30:b:84:ILE:HA	1.97	0.46
30:b:143:PHE:HZ	30:b:184:ILE:HD13	1.79	0.46
1:x:149:ALA:HA	1:x:152:ILE:HB	1.98	0.46
1:x:220:ASP:HB2	1:x:223:VAL:HG23	1.97	0.46
6:E:216:ARG:HA	6:E:263:GLN:HE22	1.80	0.46
8:G:224:ASN:OD1	8:G:228:ARG:NH1	2.48	0.46
21:T:25:ASP:OD1	21:T:41:ARG:NH2	2.38	0.46
9:h:124:SER:OG	9:h:125:GLY:N	2.48	0.46
23:U:804:SER:OG	23:U:805:ASN:N	2.49	0.46
30:b:48:ASN:OD1	30:b:65:THR:N	2.49	0.46
33:f:225:ALA:HB1	33:f:644:ALA:HA	1.97	0.46
1:x:334:LYS:HD3	1:x:339:VAL:HG23	1.98	0.46
19:R:91:LYS:NZ	19:R:117:GLU:OE1	2.49	0.46
13:l:36:VAL:HG22	13:l:160:SER:HB2	1.96	0.46
23:U:613:ASP:OD1	23:U:616:ARG:NH1	2.48	0.46
29:a:249:GLN:HA	29:a:252:LYS:HG2	1.97	0.46
33:f:789:SER:HA	33:f:793:VAL:HG13	1.98	0.46
4:C:104:ASP:HB3	4:C:107:ASP:HB2	1.96	0.46
10:I:21:VAL:O	10:I:25:MET:HG2	2.15	0.46
17:p:159:ASP:OD1	17:p:159:ASP:N	2.41	0.46
22:y:44:ILE:HB	22:y:68:HIS:HB3	1.97	0.46
23:U:694:ILE:HG23	23:U:695:MET:SD	2.56	0.46
25:W:360:GLU:HG2	25:W:364:ARG:HE	1.80	0.46
27:Y:180:LEU:HD23	27:Y:200:LEU:HD12	1.97	0.46
33:f:160:ARG:HG3	33:f:196:MET:HE3	1.98	0.46
33:f:229:VAL:HG21	33:f:607:LEU:HD13	1.97	0.46
33:f:323:ASN:HD21	33:f:420:TRP:CG	2.34	0.46
11:J:212:ARG:HB2	11:J:215:GLN:HB3	1.97	0.46
13:L:204:ASP:N	13:L:204:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:i:67:LYS:HE3	10:i:225:ILE:HD12	1.97	0.46
23:U:806:CYS:SG	23:U:809:SER:OG	2.70	0.46
25:W:310:THR:HG22	25:W:311:THR:HG23	1.97	0.46
29:a:278:MET:HG3	29:a:339:ARG:HH12	1.79	0.46
32:d:211:LYS:HD3	32:d:211:LYS:HA	1.82	0.46
33:f:202:HIS:NE2	33:f:240:VAL:O	2.46	0.46
33:f:297:MET:HE1	33:f:321:MET:HB3	1.98	0.46
33:f:856:ALA:HA	33:f:860:LYS:HD3	1.97	0.46
3:B:120:HIS:HA	3:B:134:SER:HA	1.97	0.46
17:P:38:ASP:OD1	17:P:38:ASP:N	2.48	0.46
9:h:204:THR:OG1	9:h:206:ASP:OD1	2.27	0.46
1:x:163:MET:HA	1:x:166:THR:HG22	1.97	0.45
2:A:146:LYS:HB3	2:A:148:GLN:HG3	1.99	0.45
4:C:187:LEU:HD23	4:C:314:LYS:HE3	1.98	0.45
5:D:145:PRO:HB2	5:D:256:GLU:HG3	1.98	0.45
5:D:272:THR:HB	6:E:251:ARG:HE	1.81	0.45
18:q:21:ALA:O	18:q:28:MET:N	2.49	0.45
23:U:210:LYS:HD3	23:U:211:PRO:HD2	1.97	0.45
26:X:71:LYS:HA	26:X:74:ARG:HD2	1.98	0.45
26:X:249:THR:HA	26:X:252:LYS:HD3	1.99	0.45
26:X:406:ASN:HD21	31:c:253:LYS:HA	1.81	0.45
23:U:754:HIS:CG	23:U:755:THR:H	2.35	0.45
27:Y:42:MET:SD	27:Y:42:MET:N	2.87	0.45
31:c:158:ASP:OD1	31:c:158:ASP:N	2.48	0.45
33:f:566:HIS:HA	33:f:569:LYS:HG3	1.97	0.45
2:A:347:ASP:OD1	2:A:348:LEU:N	2.45	0.45
20:S:70:ALA:O	20:S:74:MET:HG3	2.16	0.45
14:m:43:ASP:OD1	14:m:43:ASP:N	2.47	0.45
23:U:197:VAL:HA	23:U:200:VAL:HG12	1.98	0.45
25:W:115:ILE:HB	25:W:120:ILE:HD12	1.98	0.45
26:X:320:SER:HA	26:X:323:LEU:HB2	1.98	0.45
26:X:371:ASP:OD1	27:Y:233:ARG:NH2	2.49	0.45
33:f:203:GLU:HA	33:f:206:ASP:HB2	1.98	0.45
1:x:184:PRO:HA	1:x:187:ALA:HB3	1.97	0.45
11:j:146:GLN:HG3	11:j:161:ILE:HD11	1.97	0.45
21:t:96:MET:HE3	21:t:110:MET:HE1	1.98	0.45
28:Z:262:LEU:HD13	31:c:248:MET:HE1	1.98	0.45
30:b:7:MET:HB2	30:b:109:ILE:HG23	1.98	0.45
33:f:698:SER:OG	33:f:698:SER:O	2.34	0.45
6:E:197:LYS:HE2	6:E:231:PHE:HE2	1.81	0.45
10:I:38:LEU:HD23	10:I:160:LYS:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:90:LEU:HB2	25:W:96:GLN:HE22	1.82	0.45
25:W:118:LEU:H	25:W:119:PRO:HD2	1.80	0.45
25:W:384:LEU:HD13	25:W:388:GLU:HB2	1.98	0.45
27:Y:231:LEU:HB2	27:Y:234:PRO:HD2	1.98	0.45
33:f:87:THR:O	33:f:91:SER:CB	2.65	0.45
33:f:368:ALA:O	33:f:372:LEU:HB2	2.17	0.45
1:x:425:THR:OG1	1:x:437:VAL:O	2.33	0.45
17:p:47:ASP:HB3	17:p:48:ARG:HD2	1.98	0.45
21:t:25:ASP:HA	21:t:187:PHE:HA	1.98	0.45
27:Y:97:GLU:OE2	27:Y:132:VAL:N	2.50	0.45
29:a:194:GLN:HB2	29:a:226:ARG:HD2	1.99	0.45
3:B:423:LYS:HG2	3:B:427:LEU:HD23	1.99	0.45
7:F:272:PHE:HD2	7:F:316:GLN:HG3	1.81	0.45
7:F:368:ILE:HG23	7:F:371:ARG:HH12	1.82	0.45
8:G:131:MET:SD	8:G:131:MET:N	2.89	0.45
18:Q:197:PRO:HD2	18:q:199:GLN:HA	1.97	0.45
20:S:38:ARG:NH2	16:o:164:PHE:O	2.49	0.45
20:S:92:LEU:HD23	20:S:124:PHE:HE2	1.82	0.45
21:T:86:ARG:NH1	21:T:133:GLU:OE2	2.50	0.45
23:U:167:ILE:HD12	23:U:204:ILE:HG21	1.97	0.45
29:a:113:LEU:O	29:a:154:ARG:NH2	2.42	0.45
2:A:353:HIS:HA	2:A:356:LYS:HD2	1.98	0.45
3:B:387:LYS:HD3	3:B:387:LYS:HA	1.82	0.45
7:F:134:LEU:HD12	7:F:134:LEU:HA	1.83	0.45
15:N:86:MET:HE3	15:N:86:MET:HB2	1.79	0.45
20:S:144:MET:HE2	20:S:144:MET:HB3	1.79	0.45
10:i:95:GLN:HG3	17:p:73:LEU:HG	1.97	0.45
10:i:140:ASP:OD2	10:i:146:GLN:NE2	2.50	0.45
10:i:161:ALA:HB3	11:j:53:LEU:HD23	1.99	0.45
23:U:97:VAL:HA	23:U:100:ILE:HG12	1.99	0.45
23:U:801:GLN:NE2	23:U:879:ASP:OD1	2.49	0.45
32:d:103:LEU:HD12	32:d:103:LEU:HA	1.81	0.45
33:f:454:GLY:HA2	33:f:456:ARG:HH21	1.80	0.45
4:C:71:SER:HB3	5:D:112:TYR:HB3	1.97	0.45
5:D:190:LEU:HA	5:D:193:GLN:HG2	1.99	0.45
15:n:116:MET:HB2	21:t:5:MET:HE2	1.99	0.45
19:r:12:VAL:HG22	19:r:179:VAL:HB	1.98	0.45
24:V:199:ASN:OD1	24:V:241:ARG:NH2	2.49	0.45
26:X:264:PRO:HB2	26:X:291:ALA:HB1	1.99	0.45
29:a:186:LYS:HE3	29:a:225:LEU:HD11	1.99	0.45
30:b:154:THR:O	30:b:158:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:224:LYS:O	1:x:228:SER:OG	2.35	0.45
3:B:79:ILE:O	3:B:84:GLN:N	2.50	0.45
23:U:208:LEU:HD23	23:U:210:LYS:H	1.82	0.45
23:U:333:MET:HA	23:U:336:GLU:HG3	1.98	0.45
33:f:160:ARG:HH21	33:f:193:PRO:HB2	1.81	0.45
4:C:326:LEU:HD11	4:C:345:ARG:NH2	2.32	0.44
5:D:384:MET:SD	6:E:297:ARG:NH2	2.86	0.44
7:F:178:ASP:N	7:F:178:ASP:OD1	2.50	0.44
23:U:634:PRO:HG3	23:U:668:ALA:HB2	1.99	0.44
31:c:162:LEU:HA	31:c:200:TYR:CZ	2.53	0.44
33:f:845:ARG:NH1	33:f:847:GLY:H	2.15	0.44
1:x:427:GLN:HB2	1:x:473:HIS:CG	2.52	0.44
7:F:35:LYS:HA	7:F:39:GLU:HB2	2.00	0.44
8:G:123:GLN:O	8:G:126:THR:OG1	2.35	0.44
18:q:44:LEU:HD11	18:q:102:LEU:HD22	1.98	0.44
20:s:91:MET:HE2	20:s:91:MET:HB3	1.82	0.44
26:X:342:PHE:HB2	26:X:344:ARG:H	1.82	0.44
28:Z:259:VAL:HG12	28:Z:260:VAL:HG13	1.98	0.44
31:c:278:GLN:H	31:c:281:LYS:NZ	2.15	0.44
32:d:61:TRP:HD1	32:d:64:LEU:HD21	1.82	0.44
4:C:193:GLY:N	36:C:501:ADP:O2B	2.49	0.44
4:C:374:ARG:HH22	5:D:183:LEU:HD11	1.82	0.44
5:D:339:ARG:NH1	26:X:198:ASN:O	2.51	0.44
12:K:148:GLU:OE2	20:S:81:LYS:NZ	2.39	0.44
11:j:79:ASP:HB3	11:j:127:PHE:HD1	1.81	0.44
23:U:811:PHE:HE2	23:U:878:LEU:HD21	1.83	0.44
25:W:436:MET:HA	25:W:439:VAL:HG12	1.98	0.44
25:W:443:THR:HA	25:W:446:ILE:HG12	1.99	0.44
27:Y:311:TYR:CG	27:Y:314:LEU:HD12	2.52	0.44
28:Z:190:ARG:HH11	31:c:297:VAL:HG11	1.81	0.44
5:D:129:SER:HB2	5:D:143:LEU:HD11	1.99	0.44
12:K:195:ILE:HA	12:K:195:ILE:HD12	1.85	0.44
18:Q:169:LYS:O	18:q:27:GLN:NE2	2.50	0.44
8:g:132:ARG:HA	8:g:133:PRO:HD3	1.88	0.44
18:q:31:ASP:OD1	18:q:31:ASP:N	2.47	0.44
23:U:886:PRO:HA	23:U:889:LEU:HD12	1.99	0.44
26:X:153:LEU:O	26:X:157:LEU:HB2	2.18	0.44
29:a:54:ASP:N	29:a:54:ASP:OD1	2.48	0.44
33:f:278:VAL:HG23	33:f:280:ASP:H	1.82	0.44
1:x:249:VAL:HG22	1:x:321:PRO:HD3	1.99	0.44
2:A:190:VAL:HG11	2:A:212:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:288:LEU:O	7:F:292:GLY:N	2.48	0.44
23:U:373:ASN:OD1	23:U:374:SER:N	2.50	0.44
24:V:175:MET:O	24:V:179:LYS:N	2.50	0.44
24:V:310:THR:HG22	24:V:314:ARG:HH21	1.82	0.44
25:W:131:VAL:HG22	25:W:136:ILE:HD13	1.99	0.44
27:Y:69:LEU:HA	27:Y:72:LYS:HE3	2.00	0.44
7:F:169:ASP:HB3	7:F:172:VAL:HG23	1.99	0.44
9:H:175:GLU:HG2	10:I:54:LYS:HE3	1.99	0.44
23:U:98:GLU:HA	23:U:101:ILE:HG12	2.00	0.44
28:Z:236:LEU:HD11	29:a:335:TRP:HE3	1.82	0.44
32:d:27:LYS:HA	32:d:27:LYS:HD3	1.85	0.44
33:f:641:GLU:HB3	33:f:763:ARG:HH12	1.83	0.44
3:B:74:MET:HB3	33:f:614:HIS:CE1	2.53	0.44
7:F:154:ASN:ND2	7:F:157:SER:OG	2.44	0.44
11:J:185:ASP:OD1	11:J:185:ASP:N	2.48	0.44
18:Q:4:LEU:HD22	18:Q:45:LEU:HD23	1.99	0.44
20:s:175:VAL:HG11	20:s:195:ILE:HD12	1.99	0.44
21:t:178:TYR:HE1	21:t:207:THR:HG23	1.83	0.44
24:V:98:LEU:HD22	24:V:209:LYS:HD2	1.98	0.44
26:X:281:GLY:H	26:X:284:THR:HG22	1.83	0.44
33:f:292:LYS:HZ2	33:f:764:LEU:HD22	1.83	0.44
1:x:377:LEU:HA	1:x:380:LYS:HE3	2.00	0.44
4:C:338:LEU:HD22	4:C:342:ILE:HG21	1.99	0.44
13:l:47:VAL:HG12	13:l:195:LEU:HD22	2.00	0.44
16:o:1:THR:N	16:o:168:GLY:O	2.50	0.44
28:Z:37:GLY:HA2	28:Z:56:VAL:HG12	1.98	0.44
7:F:134:LEU:HD21	7:F:159:LEU:HA	2.00	0.44
16:o:51:ASP:HB3	16:o:94:ILE:HG23	2.00	0.44
23:U:229:VAL:HA	23:U:232:ILE:HG12	2.00	0.44
27:Y:184:GLN:HA	27:Y:187:TYR:HD2	1.83	0.44
33:f:709:THR:HG21	33:f:745:LEU:HB3	2.00	0.44
25:W:385:SER:OG	25:W:386:VAL:N	2.51	0.43
28:Z:232:ASP:O	28:Z:236:LEU:CB	2.66	0.43
33:f:433:LEU:HA	33:f:441:LYS:HA	2.01	0.43
3:B:191:ASP:HA	3:B:194:ILE:HB	1.99	0.43
4:C:217:SER:OG	4:C:218:GLU:N	2.51	0.43
5:D:339:ARG:HA	5:D:342:ARG:HH21	1.83	0.43
7:F:154:ASN:HD22	7:F:157:SER:HG	1.63	0.43
8:G:199:ILE:HG23	8:G:210:PHE:HZ	1.82	0.43
9:H:159:LYS:HE3	10:I:57:ASP:HA	2.00	0.43
30:b:4:GLU:OE2	30:b:40:LYS:NZ	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:205:CYS:HA	33:f:208:LEU:HG	1.99	0.43
33:f:524:MET:HB3	33:f:564:LEU:HD13	2.00	0.43
9:H:119:GLN:HG3	10:I:81:SER:HB2	2.00	0.43
16:O:63:LEU:HD11	16:O:79:ALA:HB2	1.99	0.43
23:U:701:ILE:HG21	23:U:810:THR:HG23	2.00	0.43
24:V:357:LEU:O	24:V:361:PHE:N	2.48	0.43
33:f:403:LYS:HB2	33:f:406:GLY:H	1.83	0.43
33:f:798:THR:HA	33:f:801:VAL:HG22	2.00	0.43
2:A:187:LEU:HD11	2:A:318:LEU:HD11	2.00	0.43
5:D:402:ALA:HA	5:D:405:THR:HG22	2.00	0.43
17:P:49:LEU:HD21	17:P:87:LEU:HD22	2.01	0.43
20:s:16:ALA:HB2	20:s:121:VAL:HG23	2.00	0.43
21:t:50:MET:HE3	21:t:50:MET:HB2	1.84	0.43
24:V:281:ASN:OD1	24:V:282:ASN:N	2.51	0.43
29:a:236:THR:HG22	29:a:249:GLN:HG3	2.01	0.43
2:A:279:ALA:HB2	3:B:310:LEU:HD23	2.00	0.43
11:J:189:LYS:HA	11:J:232:ILE:HD11	1.99	0.43
19:R:192:VAL:HG11	17:p:205:ASP:HB3	2.00	0.43
23:U:636:VAL:HG23	23:U:637:VAL:HG23	2.00	0.43
24:V:410:ILE:HG21	24:V:422:ILE:HG13	2.01	0.43
29:a:298:LYS:HA	29:a:298:LYS:HD3	1.84	0.43
1:x:423:VAL:HB	1:x:439:TRP:HB2	2.00	0.43
3:B:106:PRO:HB3	4:C:121:TYR:HB2	2.01	0.43
5:D:153:MET:SD	5:D:154:LEU:N	2.91	0.43
8:G:206:LEU:HB3	8:G:208:ILE:HG13	2.00	0.43
19:R:105:ASP:OD1	19:R:105:ASP:N	2.49	0.43
14:m:197:ILE:HG21	14:m:211:LEU:HD13	2.00	0.43
23:U:383:ASP:HB3	23:U:386:LEU:HB2	2.00	0.43
26:X:134:VAL:HG13	26:X:172:LEU:HD23	1.99	0.43
30:b:135:LYS:HA	30:b:135:LYS:HD2	1.82	0.43
32:d:179:ALA:O	32:d:183:GLU:N	2.50	0.43
4:C:22:GLN:O	4:C:26:SER:N	2.51	0.43
4:C:196:LYS:NZ	4:C:295:THR:O	2.45	0.43
5:D:391:ARG:NH1	5:D:393:ILE:O	2.52	0.43
11:J:64:ALA:HA	11:J:70:CYS:HA	2.01	0.43
26:X:157:LEU:HB3	26:X:166:LEU:HD11	2.01	0.43
32:d:104:LEU:HD12	32:d:104:LEU:HA	1.88	0.43
1:x:364:GLN:O	1:x:368:VAL:HG23	2.18	0.43
1:x:397:LYS:HE2	1:x:491:GLU:HB2	1.99	0.43
4:C:251:ILE:HD13	4:C:251:ILE:HA	1.91	0.43
5:D:97:ASP:OD1	5:D:97:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:267:ILE:HB	5:D:270:ILE:HB	2.00	0.43
6:E:64:LEU:HB3	6:E:68:LYS:HB3	2.00	0.43
17:P:65:GLN:OE1	18:Q:86:ARG:NH2	2.50	0.43
19:R:44:THR:OG1	19:R:100:MET:N	2.49	0.43
23:U:216:VAL:HG23	23:U:220:LEU:HD13	2.00	0.43
28:Z:125:ASP:HB3	28:Z:128:PRO:HD2	2.01	0.43
29:a:81:LEU:HA	29:a:84:VAL:HG12	2.01	0.43
4:C:86:LEU:HD12	4:C:96:VAL:HG23	2.00	0.43
4:C:127:LEU:HD11	5:D:102:ILE:HG12	2.00	0.43
4:C:236:VAL:HA	4:C:240:GLU:HB3	2.00	0.43
6:E:237:ALA:HB2	7:F:311:LEU:HD12	1.99	0.43
7:F:41:ILE:HG22	7:F:46:ARG:HD2	2.00	0.43
10:I:144:GLY:O	10:I:146:GLN:NE2	2.51	0.43
15:n:144:ARG:HD3	15:n:147:MET:HE3	2.00	0.43
25:W:262:LYS:HA	25:W:265:GLN:HG2	2.01	0.43
26:X:307:THR:HA	26:X:310:ARG:HD3	2.01	0.43
27:Y:319:MET:HE3	27:Y:330:ILE:HG21	2.00	0.43
33:f:220:ASP:O	33:f:224:ASN:N	2.50	0.43
1:x:159:LEU:O	1:x:162:SER:OG	2.33	0.43
1:x:242:LEU:O	1:x:246:PHE:HB2	2.18	0.43
1:x:298:ILE:HG12	22:y:12:THR:HG21	2.01	0.43
2:A:54:GLN:HG3	2:A:55:LEU:HD12	2.00	0.43
5:D:160:PRO:HB3	5:D:217:LYS:HB2	2.00	0.43
17:P:30:ILE:HG22	17:P:31:GLN:H	1.84	0.43
18:Q:59:TYR:O	18:Q:63:ASN:ND2	2.51	0.43
23:U:885:MET:HE2	23:U:888:GLN:HG3	2.01	0.43
25:W:67:LEU:HD12	25:W:100:ALA:HB1	2.01	0.43
28:Z:205:LEU:HA	28:Z:208:ILE:HG22	2.01	0.43
33:f:688:ARG:HB3	33:f:692:LEU:HD23	2.01	0.43
13:L:85:CYS:HA	13:L:88:MET:HE2	2.01	0.42
14:M:46:VAL:HG22	14:M:215:TRP:HB3	2.01	0.42
21:T:179:ARG:HA	21:T:179:ARG:HD3	1.79	0.42
16:o:182:LYS:NZ	16:o:184:ASP:OD2	2.40	0.42
24:V:228:ARG:HD3	24:V:258:TYR:HE1	1.83	0.42
26:X:364:LYS:HD2	26:X:364:LYS:HA	1.86	0.42
30:b:83:LYS:HA	30:b:83:LYS:HD2	1.91	0.42
1:x:336:LYS:H	1:x:336:LYS:HG3	1.50	0.42
4:C:365:GLU:HA	4:C:368:MET:HG3	2.01	0.42
9:H:203:MET:HA	9:H:207:ASN:HD21	1.83	0.42
21:T:92:LEU:HD23	21:T:92:LEU:HA	1.90	0.42
17:p:53:LEU:HB3	17:p:60:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:693:LEU:HG	23:U:746:ILE:HD11	2.01	0.42
25:W:362:ASN:HA	25:W:365:ILE:HG12	2.00	0.42
26:X:268:GLN:O	26:X:272:SER:OG	2.30	0.42
2:A:42:SER:OG	2:A:43:ARG:NH1	2.51	0.42
3:B:78:PHE:HE2	33:f:659:LEU:HD11	1.84	0.42
3:B:370:SER:HB2	33:f:838:ARG:HH12	1.84	0.42
5:D:87:LEU:HD11	5:D:131:ALA:HB1	2.01	0.42
6:E:145:LEU:HA	6:E:148:VAL:HG12	2.01	0.42
12:K:212:ALA:HB3	12:K:231:LYS:HE2	2.02	0.42
18:q:1:MET:HE1	18:q:134:TYR:CZ	2.54	0.42
23:U:92:ASP:OD1	23:U:92:ASP:N	2.49	0.42
27:Y:215:ASP:HB3	27:Y:218:THR:HG23	2.00	0.42
30:b:24:THR:HG22	30:b:27:GLN:H	1.85	0.42
33:f:256:PHE:CZ	33:f:268:LEU:HB2	2.54	0.42
3:B:364:ILE:HG22	3:B:395:ILE:HG21	2.01	0.42
4:C:71:SER:HB3	5:D:112:TYR:HD2	1.84	0.42
11:J:183:THR:H	11:J:186:LEU:HD12	1.84	0.42
21:t:157:GLN:NE2	21:t:159:VAL:O	2.52	0.42
25:W:79:GLU:O	25:W:83:LEU:N	2.49	0.42
25:W:129:ARG:HA	25:W:129:ARG:HD2	1.75	0.42
26:X:259:ILE:HD13	26:X:259:ILE:HA	1.89	0.42
33:f:379:GLY:HA3	33:f:416:MET:HE3	2.01	0.42
1:x:124:ARG:NH2	1:x:164:ASP:OD1	2.47	0.42
2:A:67:GLU:CD	2:A:68:SER:H	2.28	0.42
4:C:75:GLU:OE2	4:C:113:ARG:NH1	2.53	0.42
5:D:87:LEU:HD23	6:E:80:VAL:HG21	2.02	0.42
8:G:43:ARG:HH21	8:G:164:LYS:HG2	1.85	0.42
8:G:80:MET:SD	8:G:138:MET:HG3	2.59	0.42
9:H:64:LYS:HG2	9:H:76:TYR:HE1	1.84	0.42
8:g:10:ASP:OD1	8:g:10:ASP:N	2.47	0.42
18:q:103:LEU:HD23	18:q:103:LEU:HA	1.94	0.42
21:t:9:THR:OG1	21:t:10:SER:N	2.52	0.42
24:V:464:ILE:HD13	27:Y:363:ASN:HB3	2.00	0.42
25:W:206:SER:O	25:W:210:ASN:ND2	2.52	0.42
25:W:300:PRO:HA	25:W:303:LYS:HE2	2.01	0.42
29:a:280:MET:HE3	29:a:296:ILE:HG13	2.02	0.42
3:B:94:GLU:O	3:B:97:SER:OG	2.33	0.42
5:D:243:GLY:HA3	5:D:288:ILE:HD11	2.01	0.42
7:F:358:ASN:OD1	7:F:359:GLU:N	2.49	0.42
13:l:40:SER:HB3	13:l:187:LEU:HD22	2.02	0.42
23:U:165:LYS:HA	23:U:168:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:353:LEU:HB3	23:U:385:PHE:HZ	1.83	0.42
23:U:360:VAL:HG13	23:U:365:CYS:HB3	2.01	0.42
27:Y:188:CYS:SG	27:Y:286:TRP:NE1	2.92	0.42
29:a:14:SER:HA	29:a:50:PHE:HE2	1.83	0.42
31:c:248:MET:HE3	31:c:248:MET:HB3	1.89	0.42
33:f:340:MET:HE2	33:f:756:PRO:HG2	2.01	0.42
33:f:673:ARG:HA	33:f:711:SER:HB3	2.01	0.42
34:e:16:ASP:OD1	34:e:16:ASP:N	2.50	0.42
1:x:421:GLN:HA	1:x:441:LYS:HB3	2.02	0.42
6:E:55:GLN:HB2	7:F:133:PHE:HB3	2.02	0.42
6:E:56:ILE:O	6:E:100:LEU:N	2.51	0.42
16:O:63:LEU:HG	16:O:82:MET:HE1	2.02	0.42
16:O:147:GLU:HB2	16:O:150:GLU:HG3	2.02	0.42
17:p:133:THR:OG1	17:p:134:ASP:N	2.52	0.42
23:U:789:ILE:HG12	23:U:881:PRO:HA	2.01	0.42
25:W:128:LEU:HD21	25:W:148:THR:HB	2.02	0.42
25:W:394:SER:HA	26:X:341:PRO:HG3	2.00	0.42
27:Y:291:HIS:HB3	27:Y:295:TYR:HB2	2.01	0.42
29:a:33:LEU:HA	30:b:18:ASN:HD22	1.84	0.42
29:a:101:ARG:HH12	29:a:115:LYS:HG2	1.84	0.42
29:a:214:GLY:HA2	29:a:217:LEU:HD13	2.00	0.42
30:b:31:ASP:HA	30:b:34:ASN:HD22	1.84	0.42
33:f:120:ARG:HA	33:f:123:ALA:HB3	2.00	0.42
33:f:557:TRP:HA	33:f:560:LEU:HD12	2.02	0.42
1:x:153:THR:HA	1:x:156:LEU:HG	2.02	0.42
2:A:22:ILE:HD13	3:B:408:ARG:HH22	1.84	0.42
8:G:202:LEU:O	8:G:206:LEU:HB2	2.20	0.42
11:j:39:ASP:OD1	11:j:39:ASP:N	2.53	0.42
23:U:112:CYS:HB3	23:U:158:ARG:HB2	2.02	0.42
23:U:236:LEU:HD13	23:U:244:MET:HG2	2.02	0.42
24:V:320:THR:HB	34:e:18:GLU:HA	2.01	0.42
25:W:103:LYS:HA	25:W:103:LYS:HD3	1.82	0.42
25:W:353:ASP:OD1	25:W:357:ARG:NH2	2.53	0.42
27:Y:37:VAL:HG23	27:Y:38:ARG:HD3	2.01	0.42
27:Y:187:TYR:HD1	27:Y:192:ARG:HB3	1.85	0.42
29:a:73:PRO:HA	29:a:76:LEU:HB3	2.00	0.42
32:d:1:MET:HE2	32:d:1:MET:HB2	1.95	0.42
33:f:91:SER:HA	33:f:94:LYS:HD3	2.01	0.42
33:f:107:LYS:O	33:f:111:GLU:N	2.45	0.42
1:x:171:PRO:HB2	1:x:173:ILE:HG13	2.02	0.42
1:x:239:LYS:HB3	1:x:244:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:322:ALA:HB2	1:x:411:GLY:HA2	2.01	0.42
2:A:169:LYS:NZ	2:A:231:ASN:O	2.40	0.42
2:A:333:ARG:HH21	2:A:336:ARG:CZ	2.32	0.42
3:B:54:PRO:HG3	3:B:60:LEU:HB2	2.00	0.42
6:E:237:ALA:HB1	7:F:308:ARG:HG3	2.02	0.42
11:J:42:VAL:HG22	11:J:210:VAL:HG12	2.02	0.42
19:R:95:LEU:HD23	19:R:95:LEU:HA	1.93	0.42
11:j:41:VAL:HG13	11:j:136:PHE:HE1	1.84	0.42
17:p:135:ASP:OD1	17:p:135:ASP:N	2.51	0.42
21:t:10:SER:OG	21:t:139:THR:O	2.34	0.42
23:U:265:ILE:HG13	23:U:326:ILE:HD12	2.02	0.42
24:V:451:ILE:HG23	24:V:458:VAL:HG22	2.01	0.42
25:W:446:ILE:HD13	28:Z:208:ILE:HG13	2.02	0.42
26:X:283:GLN:HG2	26:X:312:GLU:HG2	2.01	0.42
6:E:53:VAL:HG22	6:E:102:MET:HE3	2.01	0.42
11:J:96:LEU:HD22	18:Q:62:LYS:HD3	2.01	0.42
17:P:135:ASP:OD1	17:P:135:ASP:N	2.48	0.42
9:h:182:LEU:HD23	9:h:182:LEU:HA	1.94	0.42
10:i:158:GLY:O	11:j:54:GLN:NE2	2.46	0.42
14:m:27:MET:HA	14:m:30:VAL:HG12	2.00	0.42
15:n:192:ASP:N	15:n:192:ASP:OD1	2.51	0.42
17:p:4:MET:HE1	17:p:106:GLU:HG3	2.01	0.42
27:Y:223:THR:HA	27:Y:226:VAL:HG12	2.02	0.42
33:f:523:GLY:HA3	33:f:561:GLY:HA2	2.02	0.42
33:f:812:GLY:HA3	33:f:879:ARG:HD3	2.02	0.42
1:x:208:MET:HE2	1:x:208:MET:HB3	1.95	0.41
4:C:274:LEU:O	4:C:278:ASN:ND2	2.53	0.41
16:O:78:THR:HG22	16:O:82:MET:HE2	2.01	0.41
24:V:443:ARG:HE	32:d:181:CYS:HA	1.84	0.41
27:Y:47:ASP:OD2	27:Y:49:ASN:ND2	2.44	0.41
27:Y:147:ILE:HD12	27:Y:147:ILE:HA	1.94	0.41
29:a:363:MET:HG2	31:c:307:VAL:HG11	2.01	0.41
32:d:13:SER:OG	32:d:15:ASN:OD1	2.31	0.41
33:f:215:ASP:N	33:f:215:ASP:OD1	2.53	0.41
2:A:34:LYS:HA	2:A:34:LYS:HD3	1.70	0.41
2:A:50:ASP:OD1	2:A:50:ASP:N	2.53	0.41
6:E:199:VAL:HG23	6:E:201:SER:H	1.84	0.41
12:k:32:LYS:NZ	12:k:175:GLU:OE1	2.53	0.41
14:m:215:TRP:CD1	14:m:227:VAL:HG22	2.56	0.41
23:U:34:PHE:HD2	23:U:37:GLU:HG3	1.85	0.41
23:U:429:LYS:HB3	23:U:439:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:431:LYS:HE2	28:Z:237:LEU:HB3	2.02	0.41
26:X:318:ILE:HG12	26:X:322:HIS:CE1	2.53	0.41
27:Y:177:ARG:HA	27:Y:180:LEU:HD13	2.02	0.41
27:Y:386:VAL:HG12	27:Y:387:ILE:HG12	2.02	0.41
29:a:325:ASP:OD1	29:a:326:GLU:N	2.53	0.41
32:d:189:ILE:HG13	32:d:222:TYR:HB2	2.02	0.41
33:f:94:LYS:HG3	33:f:95:PRO:HD3	2.01	0.41
33:f:336:GLU:HG3	33:f:337:LEU:HD12	2.01	0.41
3:B:71:TYR:CZ	33:f:640:LYS:HE2	2.55	0.41
5:D:349:THR:HB	5:D:354:LEU:HD12	2.01	0.41
9:H:50:LYS:HB3	9:H:64:LYS:HD3	2.02	0.41
18:Q:31:ASP:OD1	18:Q:31:ASP:N	2.53	0.41
14:m:41:CYS:HB3	14:m:189:ILE:HG13	2.02	0.41
22:y:37:PRO:HA	22:y:38:PRO:HD3	1.87	0.41
23:U:494:TYR:CZ	23:U:498:LYS:HD2	2.55	0.41
23:U:803:LYS:HG3	23:U:893:THR:HB	2.02	0.41
23:U:804:SER:HA	23:U:892:LEU:HA	2.01	0.41
23:U:892:LEU:HD21	23:U:906:LEU:HG	2.02	0.41
25:W:71:VAL:HG21	25:W:104:MET:SD	2.60	0.41
26:X:163:LYS:HB3	26:X:200:ILE:HD11	2.02	0.41
30:b:3:LEU:O	30:b:106:LYS:N	2.43	0.41
33:f:55:GLU:O	33:f:59:LEU:HB2	2.20	0.41
33:f:692:LEU:HD12	33:f:727:PHE:CD2	2.55	0.41
33:f:826:GLN:NE2	33:f:846:VAL:HG13	2.35	0.41
1:x:333:TYR:HA	1:x:340:ASN:HA	2.01	0.41
3:B:59:ARG:HA	3:B:62:LEU:HB3	2.03	0.41
3:B:359:LYS:HA	3:B:362:LYS:HD2	2.02	0.41
18:Q:161:ARG:HD2	18:Q:161:ARG:HA	1.89	0.41
21:T:92:LEU:HD12	21:T:112:ILE:HD11	2.03	0.41
23:U:581:SER:O	23:U:585:THR:OG1	2.31	0.41
25:W:284:SER:O	25:W:288:HIS:ND1	2.33	0.41
27:Y:45:VAL:HG23	27:Y:46:ARG:HD3	2.01	0.41
28:Z:78:MET:HB2	28:Z:78:MET:HE2	1.88	0.41
29:a:113:LEU:HB3	29:a:151:VAL:HG23	2.02	0.41
29:a:146:PRO:O	29:a:149:THR:OG1	2.38	0.41
29:a:342:ASP:O	29:a:344:GLN:N	2.54	0.41
31:c:237:HIS:NE2	31:c:295:ASN:OD1	2.54	0.41
33:f:180:GLN:HE22	33:f:219:LYS:HE3	1.85	0.41
33:f:466:LEU:HD12	33:f:481:SER:HA	2.03	0.41
1:x:334:LYS:H	1:x:334:LYS:HG3	1.61	0.41
3:B:112:LEU:HG	3:B:150:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:288:ASP:OD1	3:B:288:ASP:N	2.53	0.41
7:F:168:TYR:HB2	7:F:173:LYS:HE2	2.01	0.41
15:n:129:GLY:O	15:n:132:SER:OG	2.38	0.41
16:o:178:ILE:HG23	16:o:183:LEU:HD12	2.03	0.41
17:p:67:LEU:HD11	17:p:91:VAL:HG22	2.01	0.41
18:q:170:ARG:HA	18:q:170:ARG:HD3	1.91	0.41
19:r:2:THR:HG21	19:r:163:ALA:HB1	2.01	0.41
27:Y:133:ALA:HB3	27:Y:136:HIS:HB2	2.02	0.41
27:Y:253:LEU:HD13	27:Y:256:VAL:HG21	2.03	0.41
33:f:437:GLU:HG2	33:f:439:TYR:H	1.86	0.41
33:f:485:LEU:HD22	33:f:501:LEU:HD11	2.02	0.41
2:A:391:GLU:OE2	3:B:349:ARG:NH1	2.53	0.41
5:D:267:ILE:HD12	5:D:271:ALA:HB2	2.02	0.41
7:F:59:VAL:O	7:F:63:THR:OG1	2.27	0.41
13:L:44:ALA:HB2	13:L:142:PRO:HB3	2.01	0.41
21:T:99:ARG:HD2	21:T:99:ARG:HA	1.86	0.41
8:g:141:ILE:HD12	8:g:220:VAL:HG12	2.02	0.41
23:U:88:PHE:CD2	23:U:133:ILE:HD12	2.55	0.41
27:Y:156:LEU:O	27:Y:160:ASN:ND2	2.53	0.41
29:a:80:ILE:HD12	29:a:100:THR:HG21	2.03	0.41
29:a:210:VAL:HG11	29:a:213:PHE:HB2	2.03	0.41
33:f:295:ALA:O	33:f:493:ASN:ND2	2.37	0.41
33:f:825:MET:HB3	33:f:851:ASP:HB2	2.01	0.41
1:x:468:GLY:HA2	1:x:474:ILE:HG12	2.02	0.41
6:E:280:ASN:HB3	7:F:295:ARG:HH22	1.86	0.41
13:L:72:ILE:HG21	13:L:88:MET:HE1	2.03	0.41
16:O:97:ALA:HB1	16:O:127:MET:SD	2.61	0.41
8:g:202:LEU:HA	8:g:205:VAL:HG12	2.02	0.41
17:p:67:LEU:HD21	17:p:87:LEU:HD11	2.03	0.41
23:U:16:GLU:HB3	23:U:19:LEU:HB3	2.01	0.41
23:U:622:LEU:HD21	23:U:626:LEU:HD12	2.01	0.41
24:V:134:PHE:HZ	24:V:186:LYS:HD3	1.85	0.41
25:W:228:ASN:HA	25:W:231:ILE:HG12	2.03	0.41
25:W:422:ASN:HA	31:c:234:TYR:HD2	1.86	0.41
29:a:335:TRP:CE2	29:a:337:GLN:HB3	2.56	0.41
33:f:453:SER:HA	33:f:488:ALA:HA	2.02	0.41
33:f:683:GLU:HB3	33:f:686:LEU:HD21	2.03	0.41
1:x:76:ASP:OD1	1:x:76:ASP:N	2.47	0.41
1:x:439:TRP:HZ3	1:x:458:VAL:HG11	1.86	0.41
5:D:283:ARG:HB3	5:D:287:ARG:HH21	1.85	0.41
25:W:263:TRP:HZ2	25:W:295:LYS:HG2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:77:ASN:HA	27:Y:80:GLU:HG2	2.01	0.41
33:f:106:LEU:HB2	33:f:109:ILE:HD12	2.03	0.41
3:B:38:LYS:HA	3:B:38:LYS:HD2	1.75	0.41
4:C:235:PHE:O	4:C:240:GLU:N	2.53	0.41
12:K:66:LYS:HA	12:K:78:MET:HE2	2.02	0.41
13:L:224:TYR:HD2	13:L:228:ASP:HB3	1.86	0.41
17:P:193:ASP:OD1	17:P:193:ASP:N	2.53	0.41
12:k:52:LYS:NZ	12:k:61:PRO:O	2.46	0.41
14:m:191:LYS:HB3	14:m:238:TYR:CD2	2.56	0.41
22:y:27:LYS:O	22:y:31:GLN:HG2	2.21	0.41
23:U:51:ASP:HB2	23:U:54:PHE:HB2	2.03	0.41
23:U:231:ASP:HB3	23:U:235:LYS:NZ	2.35	0.41
23:U:234:GLU:O	23:U:238:LYS:HG2	2.21	0.41
24:V:251:LEU:HD23	24:V:276:PHE:HD1	1.86	0.41
25:W:62:SER:HA	25:W:65:ARG:HE	1.86	0.41
25:W:344:THR:OG1	25:W:345:GLU:OE2	2.35	0.41
25:W:359:VAL:HG23	25:W:382:LEU:HD12	2.03	0.41
26:X:372:LYS:HD3	26:X:372:LYS:HA	1.84	0.41
27:Y:45:VAL:HG12	27:Y:70:LEU:HD21	2.03	0.41
29:a:27:GLU:O	29:a:30:THR:OG1	2.29	0.41
33:f:433:LEU:HG	33:f:441:LYS:HG3	2.02	0.41
33:f:479:LEU:HG	33:f:517:VAL:HG21	2.03	0.41
33:f:506:GLY:HA2	33:f:540:GLN:HE21	1.86	0.41
33:f:597:VAL:HG21	33:f:612:LEU:HD13	2.02	0.41
33:f:627:GLU:N	33:f:630:ASP:OD1	2.49	0.41
33:f:826:GLN:HE21	33:f:846:VAL:HG13	1.84	0.41
1:x:40:GLN:HA	1:x:41:PRO:HD3	1.91	0.41
2:A:160:THR:HG21	2:A:256:MET:HE2	2.02	0.41
2:A:211:GLY:HA3	2:A:337:LEU:HA	2.02	0.41
2:A:325:ASP:OD1	2:A:325:ASP:N	2.51	0.41
3:B:309:MET:SD	3:B:341:LEU:HD11	2.61	0.41
3:B:343:ARG:O	3:B:346:ARG:NH1	2.53	0.41
36:B:501:ADP:O1B	4:C:307:ARG:NE	2.54	0.41
5:D:41:TYR:HA	5:D:44:TYR:CE1	2.55	0.41
6:E:57:VAL:HG21	7:F:123:VAL:HG13	2.02	0.41
20:S:33:PHE:HA	16:o:167:LEU:HD12	2.03	0.41
12:k:147:ASP:OD1	12:k:147:ASP:N	2.54	0.41
17:p:71:LEU:HD11	17:p:82:ILE:HG21	2.02	0.41
26:X:202:CYS:O	26:X:204:PRO:HD3	2.21	0.41
26:X:408:SER:HB2	27:Y:376:LEU:HD12	2.02	0.41
27:Y:257:ARG:HH21	27:Y:261:PHE:HE2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:171:GLN:HG2	33:f:208:LEU:HD11	2.02	0.41
34:e:54:ASN:OD1	34:e:57:ARG:NH2	2.42	0.41
1:x:371:ARG:NH1	2:A:199:GLU:OE2	2.54	0.40
3:B:359:LYS:HB2	3:B:359:LYS:HE2	1.90	0.40
6:E:175:PRO:HD2	6:E:178:THR:HG21	2.02	0.40
7:F:94:ILE:HD11	7:F:125:LYS:HB2	2.02	0.40
9:H:230:LEU:HD23	9:H:230:LEU:HA	1.89	0.40
16:O:210:ALA:HB2	20:s:159:GLN:HG3	2.02	0.40
17:p:12:MET:HE2	17:p:12:MET:HB2	1.91	0.40
27:Y:20:ALA:HB2	27:Y:150:PHE:CD1	2.56	0.40
27:Y:83:ARG:NH2	27:Y:86:GLU:OE1	2.54	0.40
28:Z:19:VAL:HG21	28:Z:124:ILE:HG13	2.03	0.40
31:c:178:THR:OG1	31:c:180:ASN:OD1	2.28	0.40
33:f:250:ARG:HH12	33:f:252:ALA:HB3	1.85	0.40
1:x:280:ASN:HD21	1:x:282:GLU:HB2	1.87	0.40
2:A:122:VAL:O	7:F:87:PRO:HA	2.22	0.40
5:D:378:ILE:HD13	5:D:403:TYR:CE1	2.57	0.40
10:I:140:ASP:OD1	10:I:146:GLN:NE2	2.35	0.40
18:Q:144:ASP:OD2	19:r:166:ARG:NH2	2.54	0.40
20:S:35:ILE:O	21:T:151:ARG:NH2	2.41	0.40
9:h:65:VAL:O	9:h:220:ARG:NH1	2.47	0.40
16:o:3:ILE:HD11	16:o:127:MET:HB2	2.03	0.40
16:o:68:LEU:HD23	16:o:68:LEU:HA	1.90	0.40
23:U:351:MET:HE3	23:U:820:PRO:HD2	2.03	0.40
23:U:803:LYS:O	23:U:893:THR:N	2.42	0.40
24:V:358:MET:HE3	24:V:359:PRO:HD3	2.04	0.40
28:Z:195:VAL:HG12	28:Z:199:LYS:HE2	2.03	0.40
30:b:111:ALA:HB3	30:b:140:ILE:HA	2.03	0.40
2:A:284:ARG:HH21	7:F:334:ARG:HG3	1.87	0.40
3:B:223:ILE:HA	3:B:329:MET:HB3	2.04	0.40
4:C:358:GLU:H	4:C:358:GLU:HG2	1.71	0.40
6:E:123:SER:OG	6:E:124:HIS:N	2.54	0.40
16:O:193:ASN:OD1	16:O:193:ASN:N	2.54	0.40
20:s:174:LEU:HD23	20:s:174:LEU:HA	1.92	0.40
23:U:216:VAL:HG21	23:U:232:ILE:HD11	2.03	0.40
23:U:899:ARG:NH2	23:U:919:GLU:O	2.54	0.40
25:W:87:ILE:HG12	25:W:104:MET:HE2	2.03	0.40
25:W:271:VAL:HG11	25:W:299:ILE:HG21	2.04	0.40
26:X:185:LYS:HD3	26:X:185:LYS:HA	1.87	0.40
27:Y:240:VAL:HG13	27:Y:241:ILE:HG13	2.02	0.40
31:c:30:GLN:H	31:c:66:THR:HG22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:336:ARG:HH22	35:F:501:ATP:PG	2.44	0.40
3:B:84:GLN:HA	33:f:662:MET:HE1	2.04	0.40
3:B:223:ILE:HG23	3:B:329:MET:HB3	2.04	0.40
5:D:68:LEU:HA	5:D:68:LEU:HD23	1.85	0.40
5:D:92:PHE:HA	5:D:103:VAL:HG12	2.03	0.40
18:Q:68:LYS:HG3	18:Q:74:GLU:HG2	2.03	0.40
20:S:75:TYR:CD1	20:S:83:MET:HG2	2.56	0.40
21:T:63:LEU:HD23	21:T:63:LEU:HA	1.93	0.40
15:n:4:MET:HG2	15:n:156:THR:HG23	2.02	0.40
15:n:160:LEU:HA	15:n:160:LEU:HD23	1.90	0.40
23:U:902:PRO:HA	23:U:914:LEU:HD12	2.04	0.40
26:X:94:ASP:O	26:X:98:ASP:HB2	2.22	0.40
26:X:126:ARG:HA	26:X:129:LEU:HD12	2.02	0.40
33:f:377:VAL:HG22	33:f:752:HIS:HB3	2.03	0.40
33:f:616:CYS:HB2	33:f:632:LYS:HG3	2.03	0.40
1:x:27:MET:HA	1:x:30:LYS:HB2	2.04	0.40
1:x:78:LEU:HD11	33:f:396:ASN:HD22	1.86	0.40
1:x:351:LEU:HD11	1:x:464:LEU:HD21	2.03	0.40
2:A:337:LEU:HA	2:A:337:LEU:HD23	1.83	0.40
5:D:270:ILE:HG22	5:D:289:LEU:HD21	2.03	0.40
8:g:49:VAL:HG22	8:g:219:VAL:HG23	2.04	0.40
22:y:39:ASP:N	22:y:39:ASP:OD1	2.54	0.40
23:U:22:PHE:HB3	32:d:30:LEU:HD11	2.03	0.40
24:V:175:MET:SD	24:V:184:ALA:HB2	2.62	0.40
33:f:606:VAL:O	33:f:610:GLN:CB	2.69	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	x	492/494 (100%)	463 (94%)	29 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	411/433 (95%)	365 (89%)	46 (11%)	0	100	100
3	B	397/440 (90%)	352 (89%)	45 (11%)	0	100	100
4	C	384/398 (96%)	341 (89%)	42 (11%)	1 (0%)	36	67
5	D	378/418 (90%)	344 (91%)	34 (9%)	0	100	100
6	E	387/403 (96%)	353 (91%)	33 (8%)	1 (0%)	36	67
7	F	396/439 (90%)	356 (90%)	40 (10%)	0	100	100
8	G	242/246 (98%)	231 (96%)	11 (4%)	0	100	100
8	g	242/246 (98%)	226 (93%)	16 (7%)	0	100	100
9	H	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
9	h	230/234 (98%)	217 (94%)	13 (6%)	0	100	100
10	I	249/261 (95%)	240 (96%)	9 (4%)	0	100	100
10	i	248/261 (95%)	240 (97%)	8 (3%)	0	100	100
11	J	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
11	j	237/248 (96%)	221 (93%)	16 (7%)	0	100	100
12	K	232/241 (96%)	215 (93%)	16 (7%)	1 (0%)	30	62
12	k	232/241 (96%)	221 (95%)	11 (5%)	0	100	100
13	L	236/269 (88%)	231 (98%)	5 (2%)	0	100	100
13	l	236/269 (88%)	227 (96%)	9 (4%)	0	100	100
14	M	238/255 (93%)	231 (97%)	7 (3%)	0	100	100
14	m	238/255 (93%)	232 (98%)	6 (2%)	0	100	100
15	N	200/239 (84%)	197 (98%)	3 (2%)	0	100	100
15	n	200/239 (84%)	190 (95%)	10 (5%)	0	100	100
16	O	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
16	o	218/277 (79%)	210 (96%)	8 (4%)	0	100	100
17	P	202/205 (98%)	189 (94%)	13 (6%)	0	100	100
17	p	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
18	Q	197/201 (98%)	190 (96%)	7 (4%)	0	100	100
18	q	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
19	R	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
19	r	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
20	S	211/241 (88%)	203 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	s	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
21	T	214/264 (81%)	209 (98%)	5 (2%)	0	100	100
21	t	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
22	y	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
23	U	868/953 (91%)	806 (93%)	62 (7%)	0	100	100
24	V	442/534 (83%)	428 (97%)	14 (3%)	0	100	100
25	W	444/456 (97%)	417 (94%)	27 (6%)	0	100	100
26	X	378/422 (90%)	366 (97%)	11 (3%)	1 (0%)	36	67
27	Y	376/389 (97%)	338 (90%)	37 (10%)	1 (0%)	36	67
28	Z	284/324 (88%)	248 (87%)	34 (12%)	2 (1%)	18	51
29	a	371/376 (99%)	339 (91%)	31 (8%)	1 (0%)	36	67
30	b	189/377 (50%)	172 (91%)	17 (9%)	0	100	100
31	c	285/310 (92%)	248 (87%)	37 (13%)	0	100	100
32	d	255/350 (73%)	218 (86%)	37 (14%)	0	100	100
33	f	887/908 (98%)	792 (89%)	95 (11%)	0	100	100
34	e	48/70 (69%)	43 (90%)	5 (10%)	0	100	100
All	All	13955/15458 (90%)	13009 (93%)	938 (7%)	8 (0%)	49	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	X	318	ILE
28	Z	134	PRO
29	a	343	LEU
27	Y	292	TYR
28	Z	145	HIS
6	E	22	ILE
4	C	224	ILE
12	K	130	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	x	439/439 (100%)	431 (98%)	8 (2%)	51	69
2	A	348/372 (94%)	344 (99%)	4 (1%)	65	74
3	B	347/385 (90%)	345 (99%)	2 (1%)	78	79
4	C	330/346 (95%)	328 (99%)	2 (1%)	78	79
5	D	333/366 (91%)	333 (100%)	0	100	100
6	E	341/353 (97%)	341 (100%)	0	100	100
7	F	344/379 (91%)	343 (100%)	1 (0%)	86	83
8	G	205/210 (98%)	205 (100%)	0	100	100
8	g	202/210 (96%)	202 (100%)	0	100	100
9	H	188/191 (98%)	188 (100%)	0	100	100
9	h	188/191 (98%)	188 (100%)	0	100	100
10	I	207/221 (94%)	205 (99%)	2 (1%)	68	75
10	i	206/221 (93%)	206 (100%)	0	100	100
11	J	201/211 (95%)	201 (100%)	0	100	100
11	j	196/211 (93%)	196 (100%)	0	100	100
12	K	193/203 (95%)	193 (100%)	0	100	100
12	k	195/203 (96%)	195 (100%)	0	100	100
13	L	202/230 (88%)	202 (100%)	0	100	100
13	l	201/230 (87%)	201 (100%)	0	100	100
14	M	196/212 (92%)	196 (100%)	0	100	100
14	m	198/212 (93%)	198 (100%)	0	100	100
15	N	157/181 (87%)	157 (100%)	0	100	100
15	n	156/181 (86%)	156 (100%)	0	100	100
16	O	179/228 (78%)	179 (100%)	0	100	100
16	o	181/228 (79%)	181 (100%)	0	100	100
17	P	172/174 (99%)	172 (100%)	0	100	100
17	p	173/174 (99%)	173 (100%)	0	100	100
18	Q	168/171 (98%)	168 (100%)	0	100	100
18	q	168/171 (98%)	168 (100%)	0	100	100
19	R	156/202 (77%)	156 (100%)	0	100	100
19	r	156/202 (77%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	S	175/199 (88%)	175 (100%)	0	100	100
20	s	178/199 (89%)	178 (100%)	0	100	100
21	T	178/215 (83%)	178 (100%)	0	100	100
21	t	179/215 (83%)	179 (100%)	0	100	100
22	y	68/68 (100%)	68 (100%)	0	100	100
23	U	748/816 (92%)	748 (100%)	0	100	100
24	V	390/460 (85%)	390 (100%)	0	100	100
25	W	410/416 (99%)	408 (100%)	2 (0%)	81	80
26	X	327/362 (90%)	327 (100%)	0	100	100
27	Y	334/344 (97%)	334 (100%)	0	100	100
28	Z	257/295 (87%)	255 (99%)	2 (1%)	73	77
29	a	333/336 (99%)	333 (100%)	0	100	100
30	b	167/312 (54%)	166 (99%)	1 (1%)	78	79
31	c	252/268 (94%)	249 (99%)	3 (1%)	63	73
32	d	231/294 (79%)	231 (100%)	0	100	100
33	f	745/763 (98%)	744 (100%)	1 (0%)	88	87
34	e	44/63 (70%)	40 (91%)	4 (9%)	9	32
All	All	11942/13133 (91%)	11910 (100%)	32 (0%)	84	83

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	x	326	ILE
1	x	327	GLN
1	x	330	ARG
1	x	334	LYS
1	x	336	LYS
1	x	338	SER
1	x	339	VAL
1	x	342	LYS
2	A	34	LYS
2	A	38	GLN
2	A	40	THR
2	A	403	ILE
3	B	102	LEU
3	B	125	THR

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Mol	Chain	Res	Type
4	C	109	THR
4	C	210	THR
7	F	416	THR
10	I	7[A]	SER
10	I	7[B]	SER
25	W	114	GLU
25	W	117	ASP
28	Z	144	VAL
28	Z	147	ASP
30	b	161	ASN
31	c	122	LEU
31	c	123	SER
31	c	127	ILE
33	f	874	LEU
34	e	25	GLU
34	e	26	ASP
34	e	27	TRP
34	e	34	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	x	44	GLN
1	x	117	ASN
1	x	177	GLN
1	x	180	HIS
1	x	201	ASN
1	x	271	ASN
1	x	306	GLN
1	x	308	ASN
1	x	340	ASN
1	x	384	GLN
2	A	94	GLN
3	B	81	ASN
3	B	154	HIS
3	B	241	ASN
3	B	314	ASN
4	C	50	ASN
4	C	53	ASN
4	C	182	GLN
4	C	332	HIS
4	C	377	HIS

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Mol	Chain	Res	Type
5	D	74	HIS
5	D	110	ASN
5	D	175	GLN
5	D	193	GLN
5	D	353	ASN
6	E	45	ASN
6	E	339	ASN
7	F	43	GLN
7	F	83	ASN
7	F	208	HIS
7	F	243	GLN
8	G	68	HIS
10	I	84	ASN
11	J	54	GLN
12	K	41	GLN
12	K	155	HIS
12	K	204	GLN
13	L	4	ASN
13	L	21	GLN
13	L	43	HIS
13	L	59	HIS
15	N	158	ASN
15	N	193	GLN
16	O	91	GLN
16	O	165	ASN
18	Q	63	ASN
18	Q	82	ASN
19	R	62	GLN
19	R	119	ASN
19	R	151	GLN
20	S	151	ASN
20	S	152	GLN
21	T	147	GLN
8	g	75	ASN
8	g	128	ASN
9	h	95	GLN
9	h	102	GLN
9	h	123	GLN
9	h	202	GLN
10	i	95	GLN
11	j	122	ASN
11	j	154	HIS

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Mol	Chain	Res	Type
11	j	215	GLN
12	k	41	GLN
12	k	155	HIS
13	l	20	HIS
13	l	21	GLN
13	l	86	ASN
13	l	90	GLN
14	m	32	ASN
15	n	66	HIS
17	p	31	GLN
17	p	169	GLN
18	q	82	ASN
18	q	99	HIS
18	q	168	GLN
20	s	80	ASN
20	s	146	GLN
20	s	160	ASN
21	t	3	ASN
21	t	81	HIS
22	y	60	ASN
23	U	259	GLN
23	U	267	ASN
23	U	389	ASN
23	U	421	GLN
23	U	467	ASN
23	U	670	ASN
23	U	718	ASN
23	U	743	ASN
23	U	874	ASN
25	W	96	GLN
25	W	235	GLN
25	W	361	HIS
26	X	144	GLN
26	X	207	GLN
26	X	292	GLN
26	X	296	ASN
26	X	334	ASN
26	X	380	GLN
26	X	405	GLN
27	Y	64	GLN
27	Y	196	GLN
27	Y	273	GLN

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Mol	Chain	Res	Type
28	Z	193	ASN
28	Z	194	GLN
28	Z	202	ASN
28	Z	231	GLN
29	a	40	GLN
29	a	143	ASN
30	b	12	ASN
30	b	34	ASN
30	b	101	GLN
30	b	161	ASN
31	c	30	GLN
31	c	166	ASN
32	d	228	GLN
33	f	195	ASN
33	f	213	GLN
33	f	323	ASN
33	f	352	HIS
33	f	382	ASN
33	f	540	GLN
33	f	610	GLN
33	f	649	HIS
33	f	650	GLN
33	f	724	ASN
33	f	737	ASN
33	f	758	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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	ATP	D	501	-	32,33,33	0.32	0	48,52,52	0.30	0
36	ADP	C	501	-	28,29,29	1.37	3 (10%)	43,45,45	1.96	9 (20%)
35	ATP	F	501	-	32,33,33	0.63	1 (3%)	48,52,52	0.36	0
35	ATP	E	501	-	32,33,33	0.46	0	48,52,52	0.32	0
35	ATP	A	501	-	32,33,33	0.60	1 (3%)	48,52,52	0.34	0
36	ADP	B	501	-	28,29,29	1.37	4 (14%)	43,45,45	1.94	9 (20%)

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
35	ATP	D	501	-	-	5/22/38/38	0/3/3/3
36	ADP	C	501	-	-	3/16/32/32	0/3/3/3
35	ATP	F	501	-	-	6/22/38/38	0/3/3/3
35	ATP	E	501	-	-	2/22/38/38	0/3/3/3
35	ATP	A	501	-	-	6/22/38/38	0/3/3/3
36	ADP	B	501	-	-	3/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	501	ADP	C5-C4	4.67	1.47	1.39
36	C	501	ADP	C5-C4	4.51	1.47	1.39
36	C	501	ADP	C5-N7	-2.62	1.34	1.39
35	F	501	ATP	PA-O3A	-2.59	1.56	1.59
36	C	501	ADP	C5-C6	2.52	1.48	1.41
36	B	501	ADP	C5-N7	-2.51	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	501	ADP	C5-C6	2.50	1.47	1.41
35	A	501	ATP	PB-O3B	-2.45	1.56	1.59
36	B	501	ADP	C8-N7	2.05	1.35	1.31

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	501	ADP	C5-C4-N3	-6.61	117.61	126.72
36	C	501	ADP	C5-C4-N3	-6.27	118.08	126.72
36	B	501	ADP	N3-C4-N9	5.55	136.60	127.17
36	C	501	ADP	N3-C4-N9	5.27	136.14	127.17
36	B	501	ADP	C2-N3-C4	3.92	121.42	111.83
36	C	501	ADP	C2-N3-C4	3.70	120.87	111.83
36	C	501	ADP	C4-C5-N7	-3.39	106.71	110.58
36	B	501	ADP	N3-C2-N1	-3.10	123.89	128.58
36	C	501	ADP	N3-C2-N1	-3.03	123.99	128.58
36	C	501	ADP	C4-N9-C8	2.99	108.88	105.74
36	B	501	ADP	C4-C5-N7	-2.98	107.18	110.58
36	C	501	ADP	C3'-C2'-C1'	2.76	106.68	101.46
36	C	501	ADP	C5-N7-C8	2.75	107.77	103.45
36	B	501	ADP	C3'-C2'-C1'	2.72	106.62	101.46
36	B	501	ADP	C4-N9-C8	2.41	108.27	105.74
36	B	501	ADP	C5-N7-C8	2.32	107.10	103.45
36	C	501	ADP	N9-C8-N7	-2.16	110.87	113.94
36	B	501	ADP	C1'-N9-C8	-2.04	122.58	127.09

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	501	ATP	C5'-O5'-PA-O1A
35	A	501	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	C5'-O5'-PA-O3A
35	E	501	ATP	PB-O3B-PG-O2G
35	F	501	ATP	C5'-O5'-PA-O1A
35	F	501	ATP	C5'-O5'-PA-O2A
35	F	501	ATP	C5'-O5'-PA-O3A
36	B	501	ADP	C5'-O5'-PA-O1A
36	C	501	ADP	C5'-O5'-PA-O1A
36	C	501	ADP	C5'-O5'-PA-O2A
36	C	501	ADP	C5'-O5'-PA-O3A
35	F	501	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
35	F	501	ATP	C3'-C4'-C5'-O5'
35	A	501	ATP	PA-O3A-PB-O1B
36	B	501	ADP	PB-O3A-PA-O5'
35	D	501	ATP	C4'-C5'-O5'-PA
35	A	501	ATP	C5'-O5'-PA-O2A
35	D	501	ATP	C5'-O5'-PA-O1A
36	B	501	ADP	C5'-O5'-PA-O3A
35	F	501	ATP	C4'-C5'-O5'-PA
35	A	501	ATP	PA-O3A-PB-O2B
35	D	501	ATP	PB-O3A-PA-O2A
35	E	501	ATP	PB-O3B-PG-O1G
35	D	501	ATP	PB-O3A-PA-O1A
35	A	501	ATP	C3'-C4'-C5'-O5'

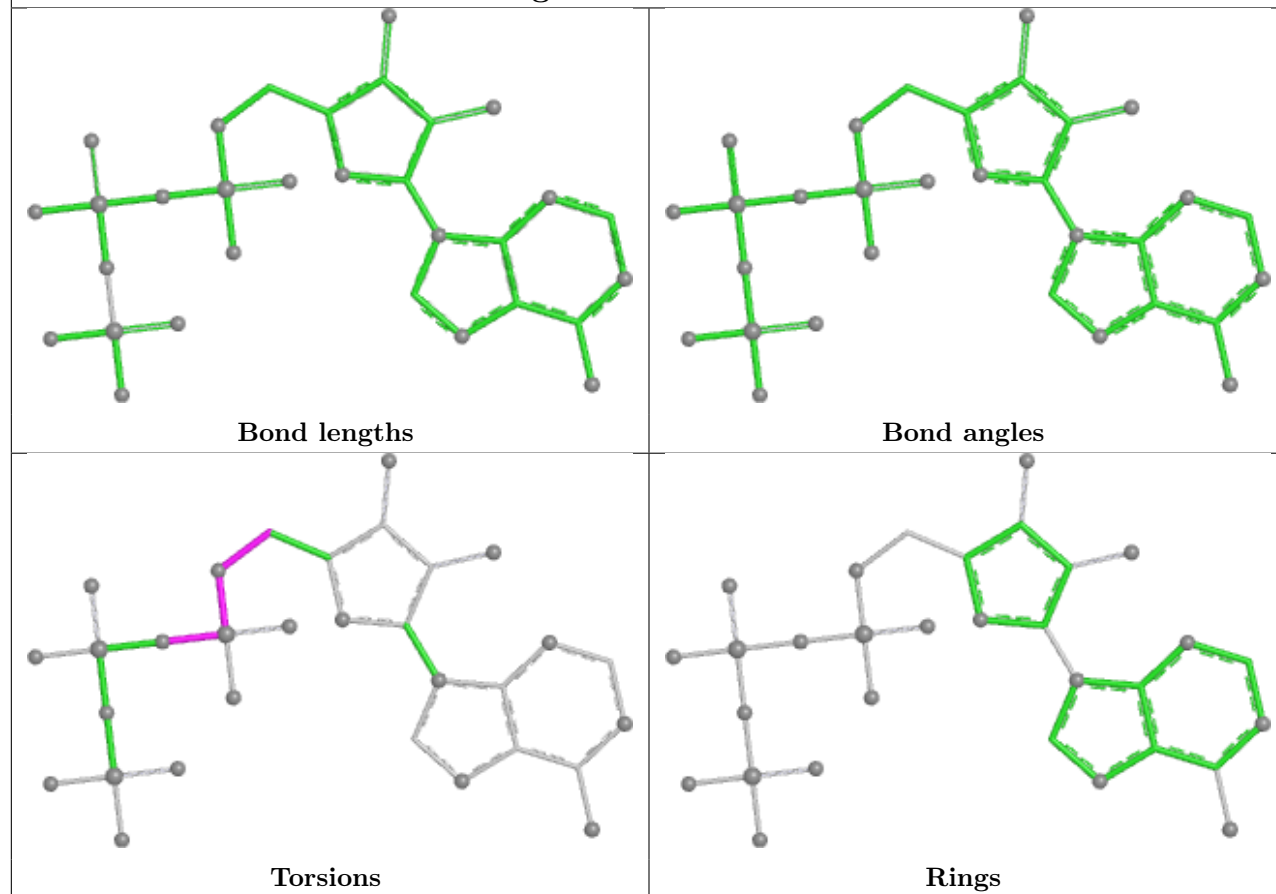
There are no ring outliers.

6 monomers are involved in 10 short contacts:

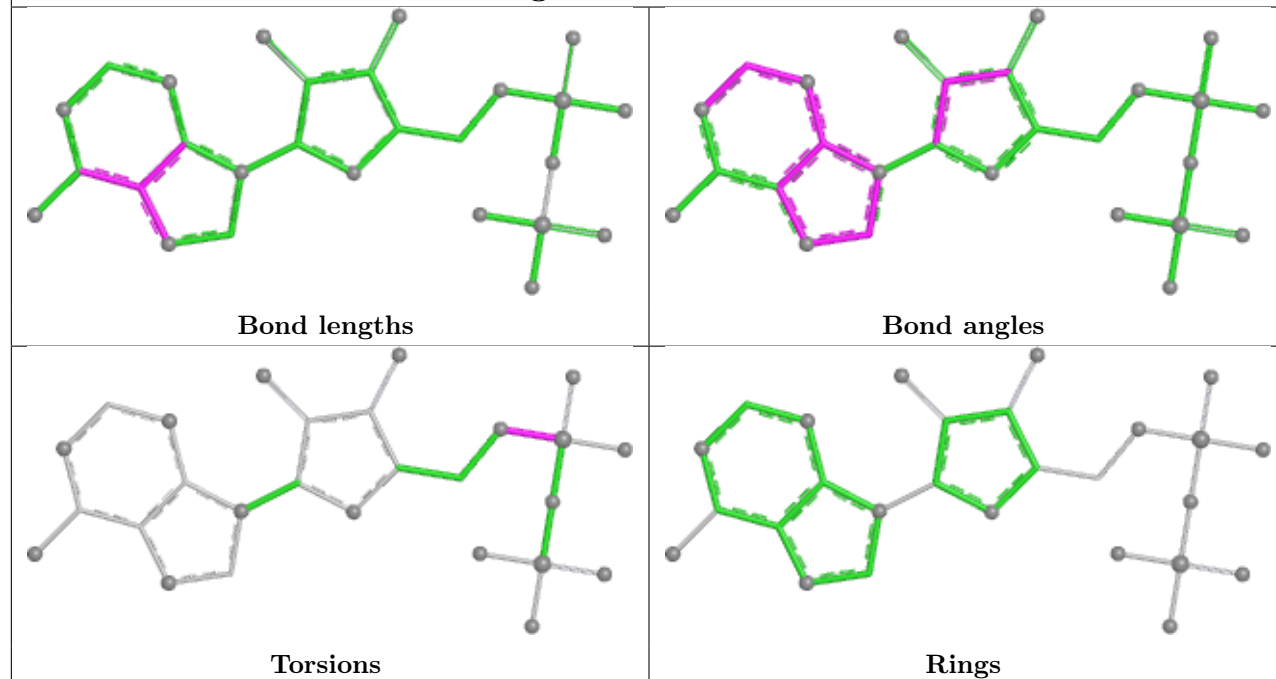
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	D	501	ATP	3	0
36	C	501	ADP	2	0
35	F	501	ATP	1	0
35	E	501	ATP	1	0
35	A	501	ATP	2	0
36	B	501	ADP	1	0

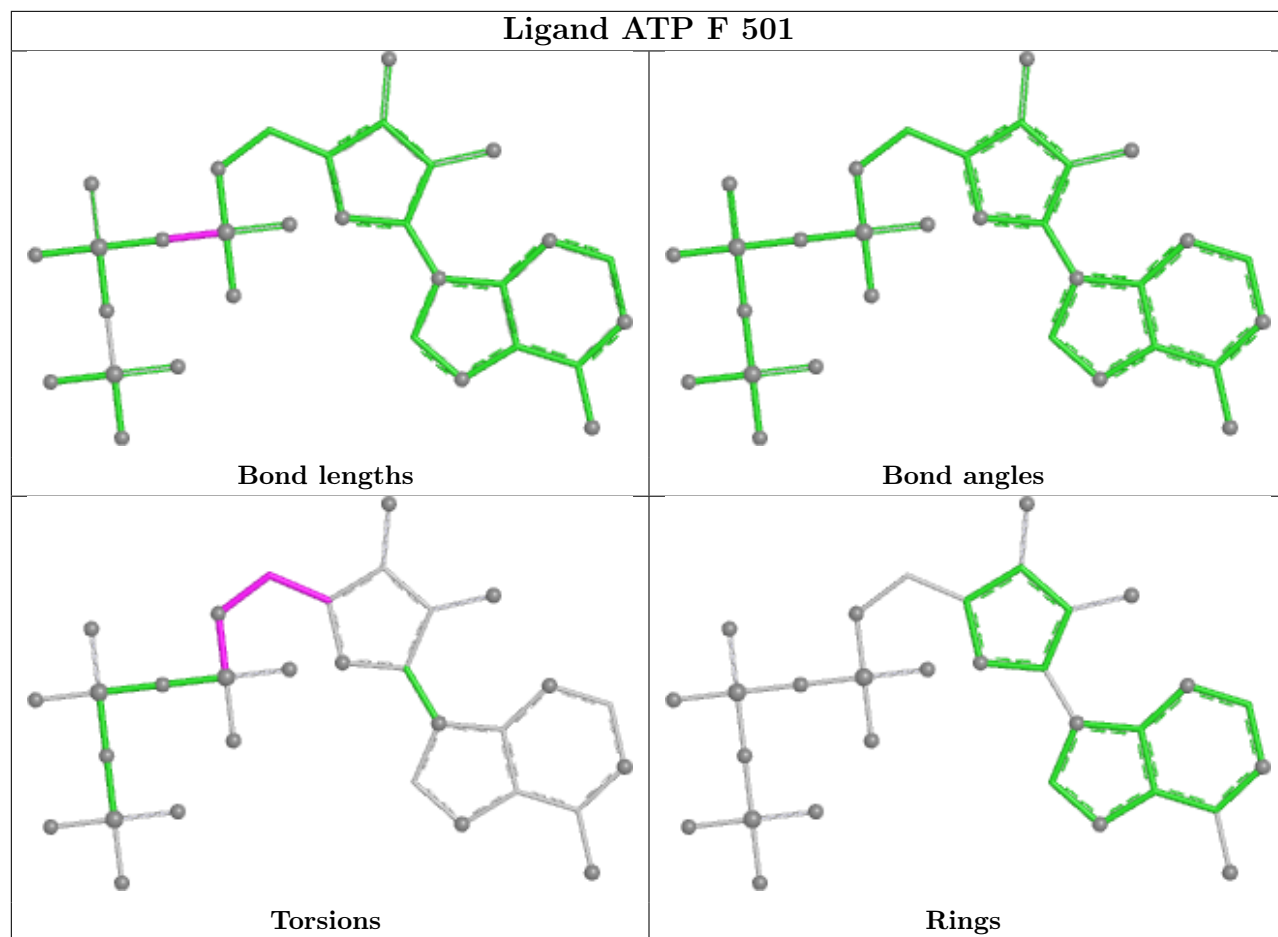
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

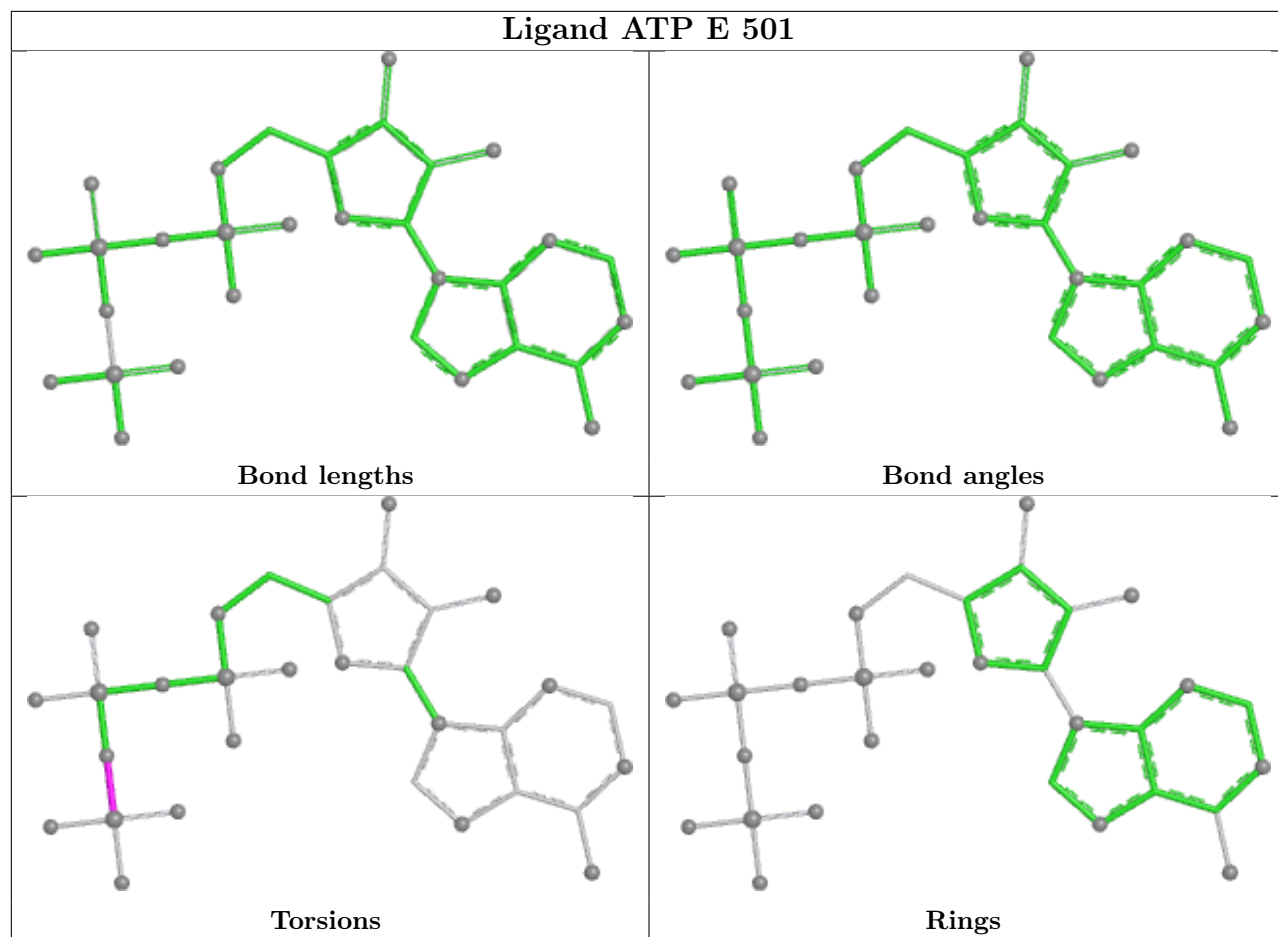
Ligand ATP D 501



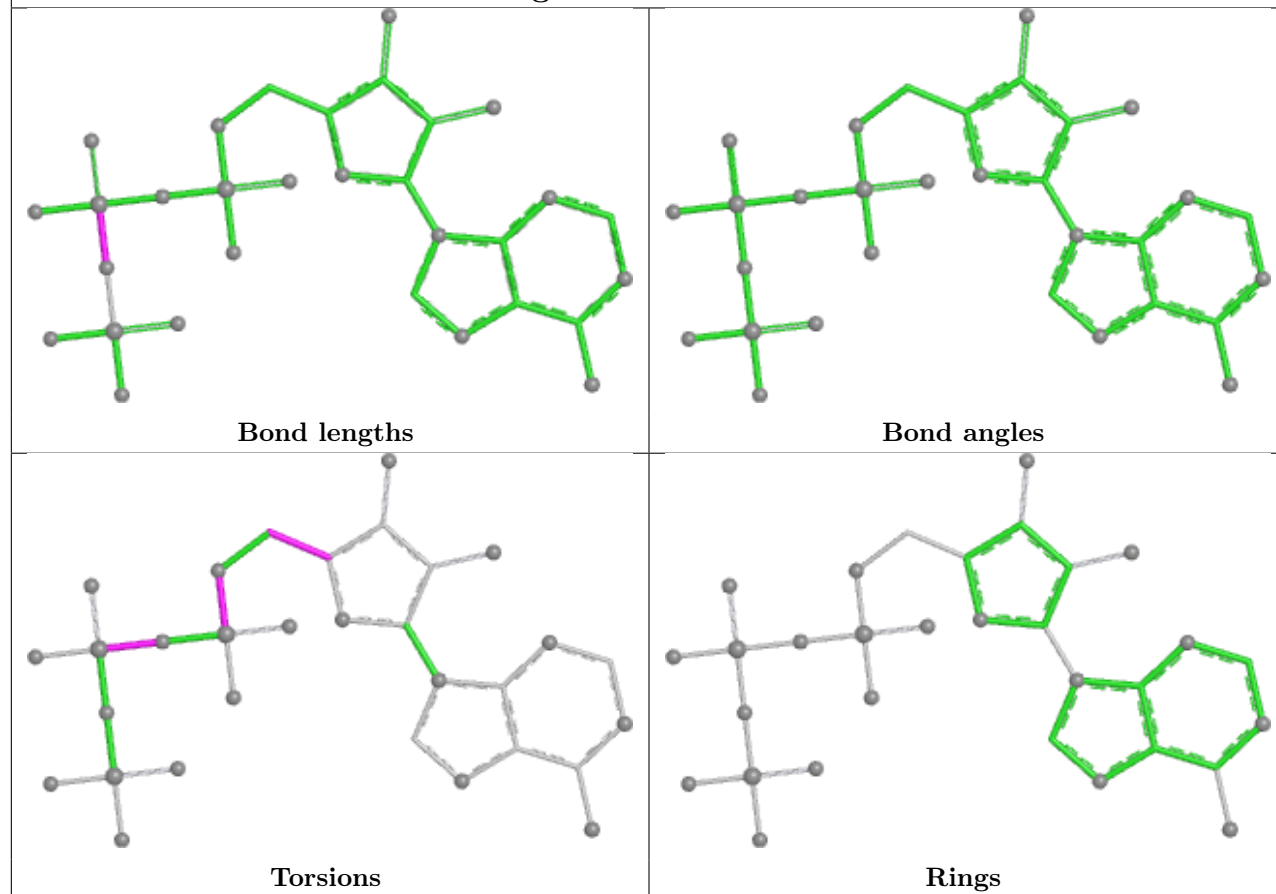
Ligand ADP C 501



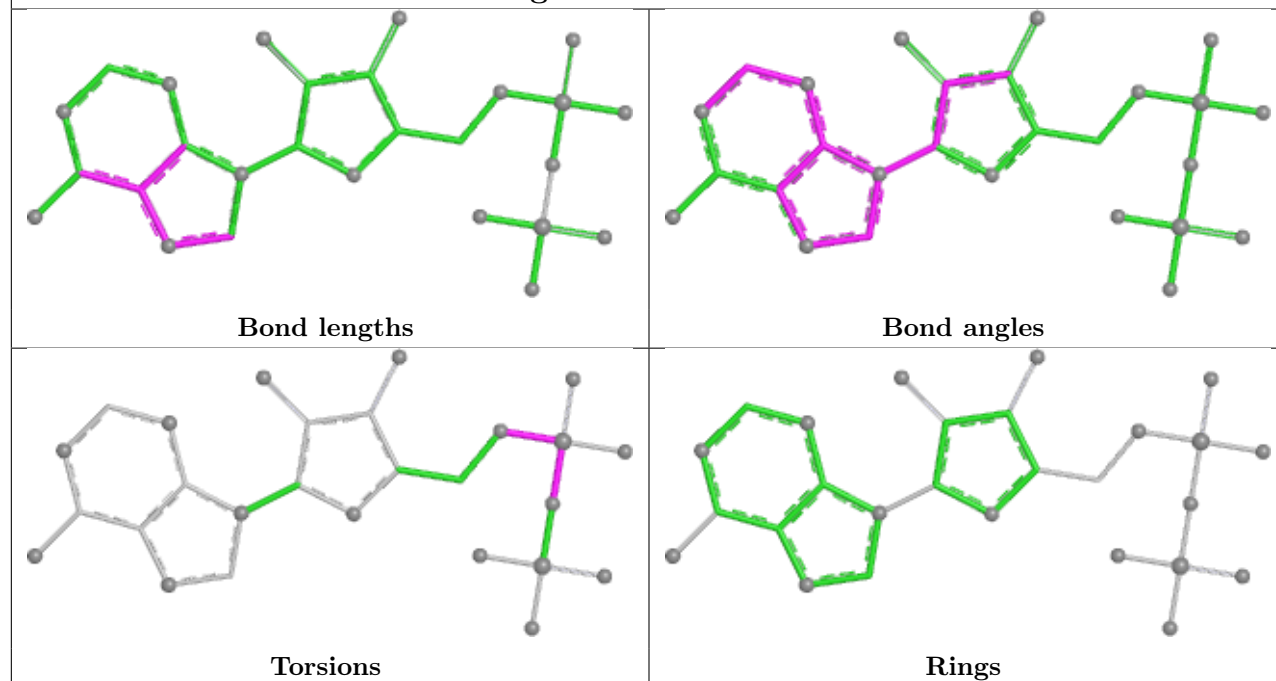




Ligand ATP A 501



Ligand ADP B 501



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

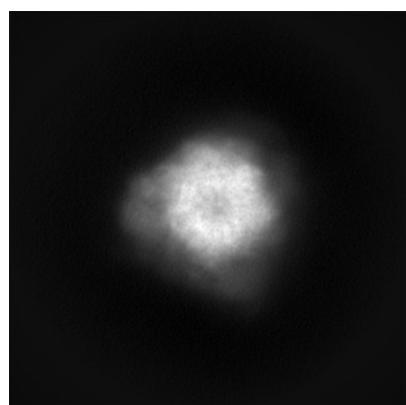
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32281. 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](#)

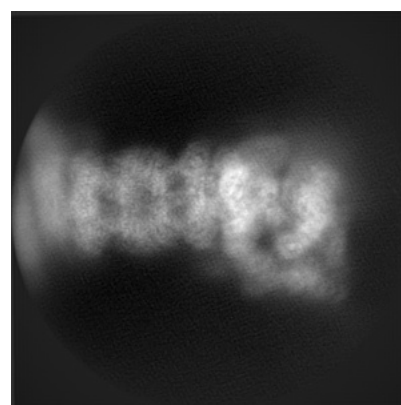
6.1.1 Primary map



X



Y

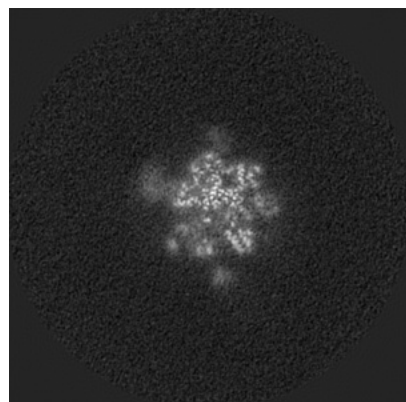


Z

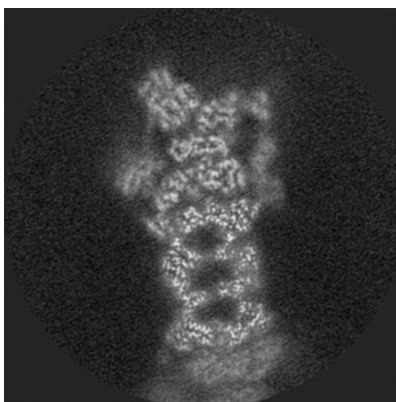
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

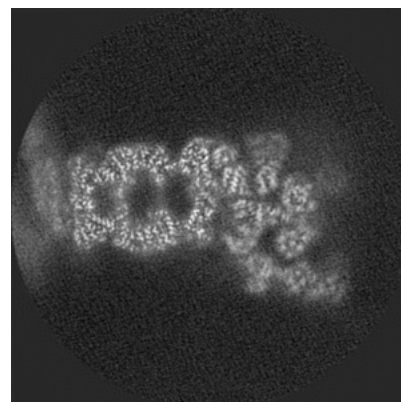
6.2.1 Primary map



X Index: 320



Y Index: 320

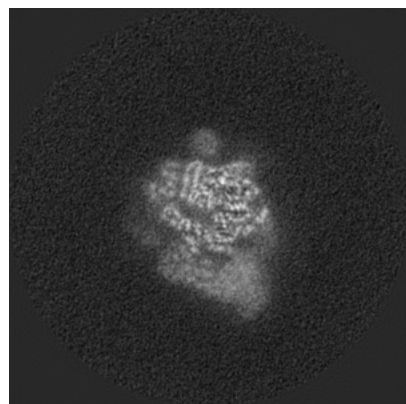


Z Index: 320

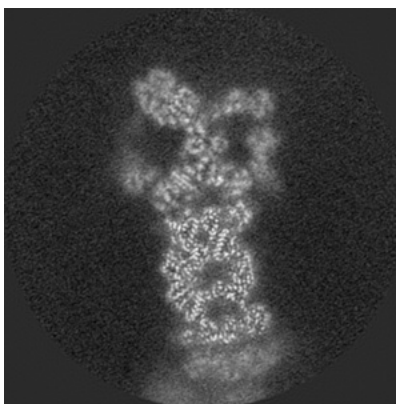
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

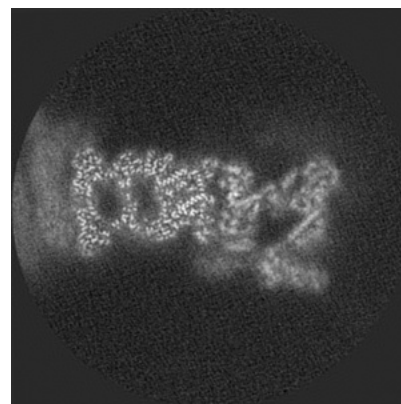
6.3.1 Primary map



X Index: 359



Y Index: 302

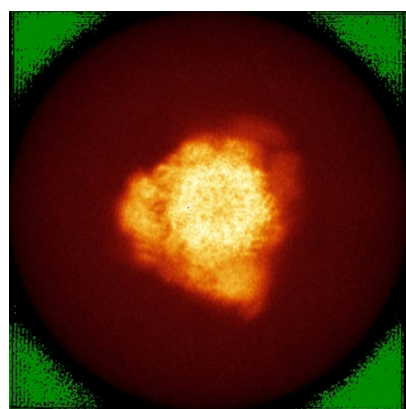


Z Index: 360

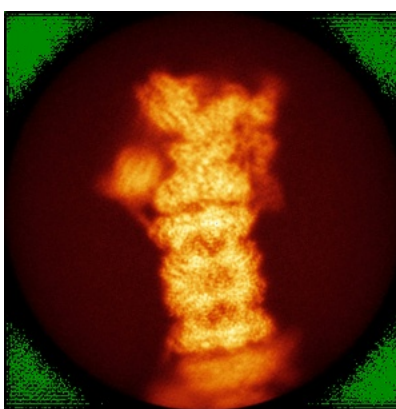
The images above show the largest variance slices of the map in three orthogonal directions.

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

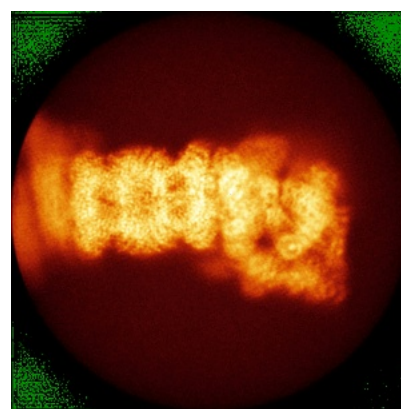
6.4.1 Primary map



X



Y

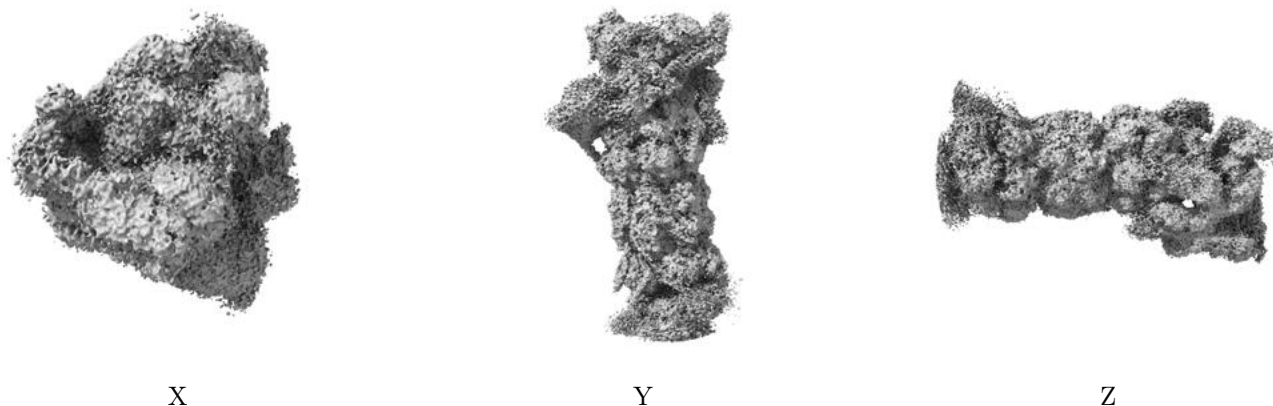


Z

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.

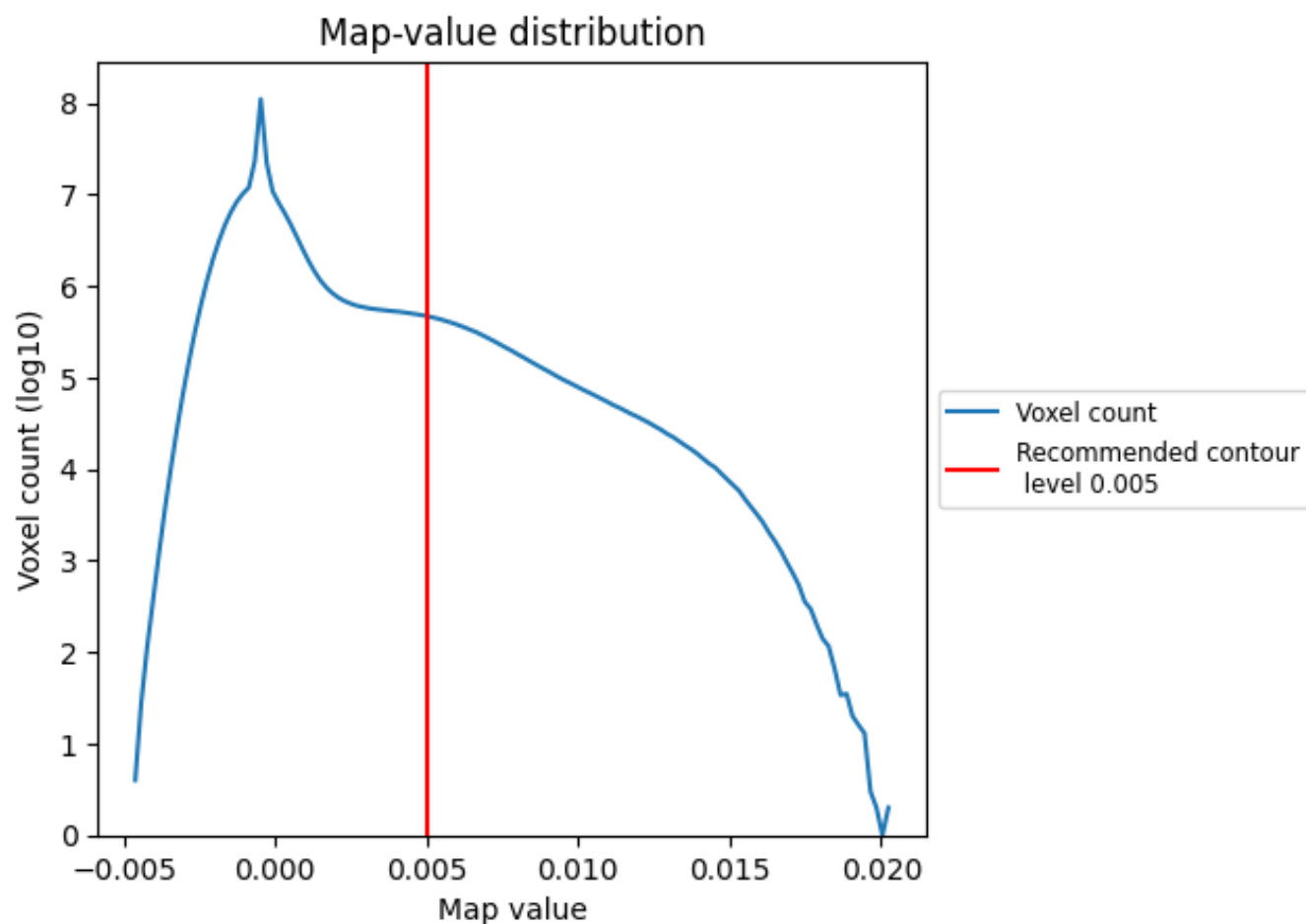
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

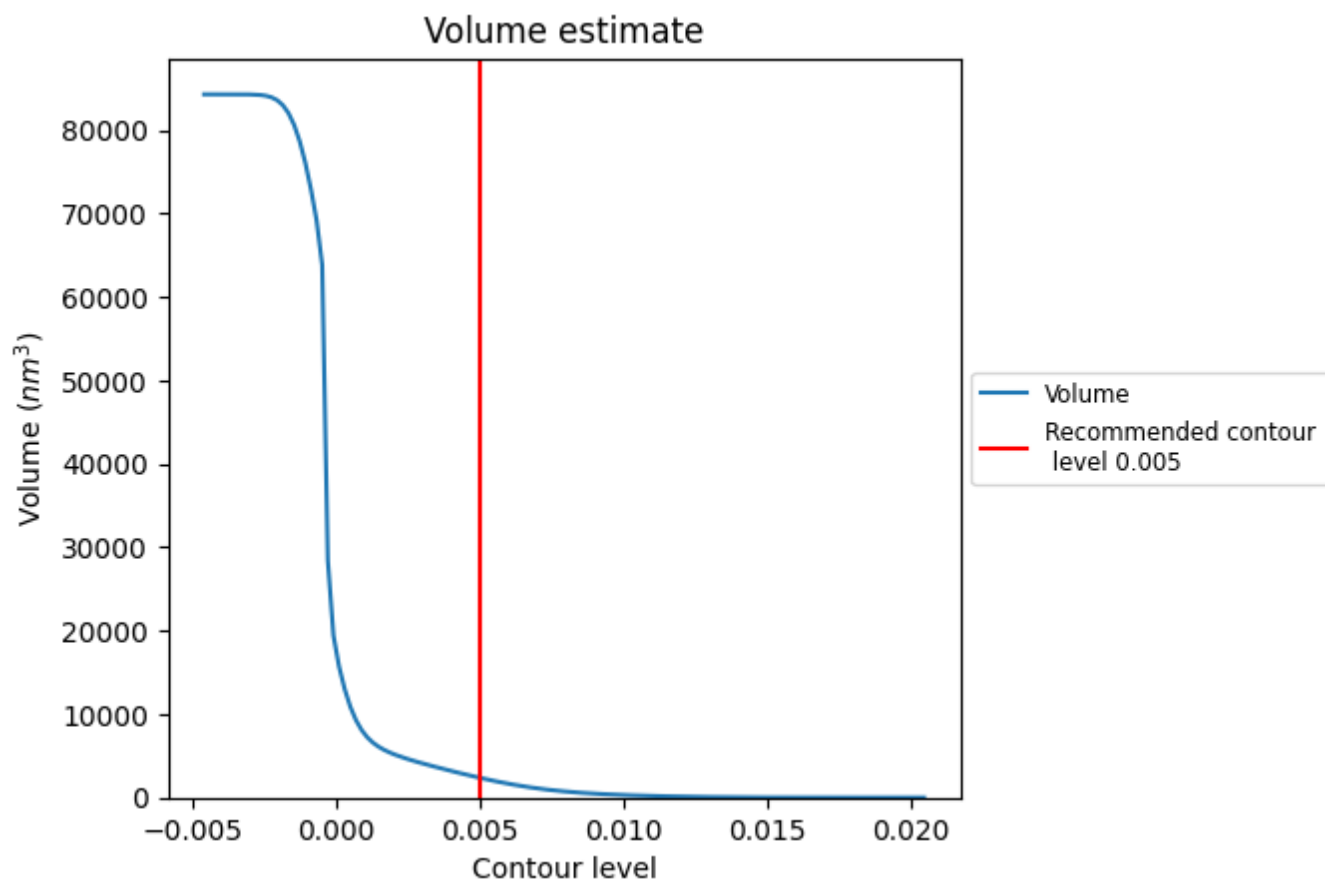
This section contains the results of statistical analysis of the map.

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.

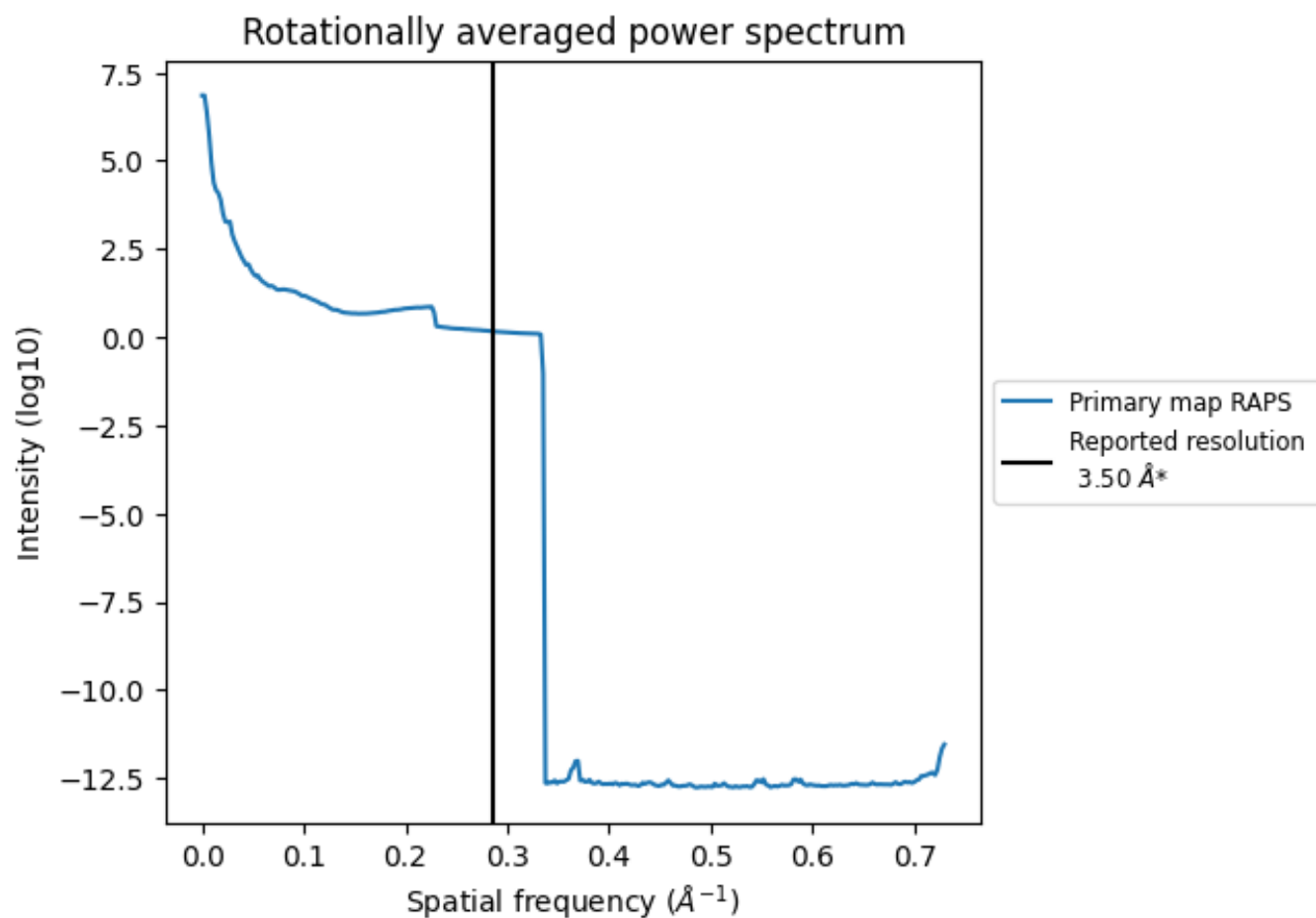
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2347 nm³; this corresponds to an approximate mass of 2121 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 0.286 Å⁻¹

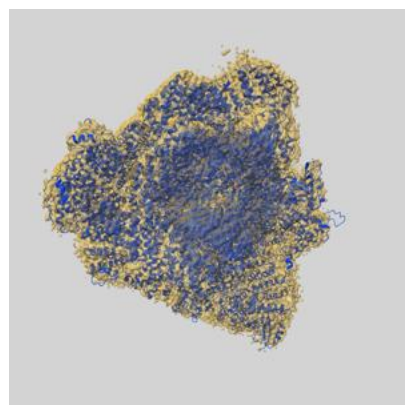
8 Fourier-Shell correlation

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

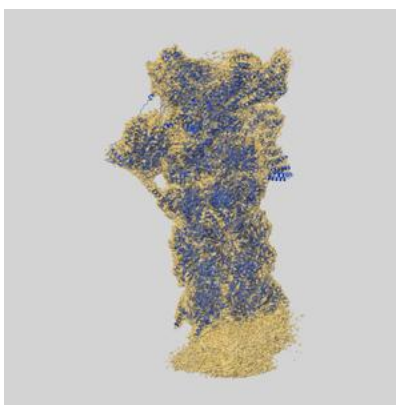
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32281 and PDB model 7W3I. Per-residue inclusion information can be found in section [3](#) on page [12](#).

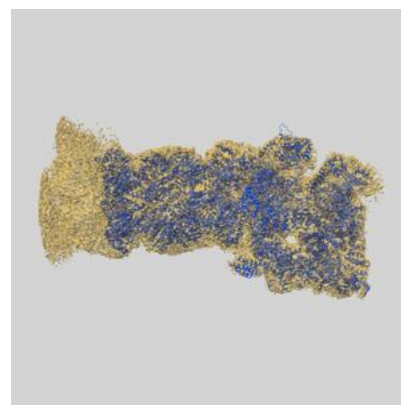
9.1 Map-model overlay [i](#)



X



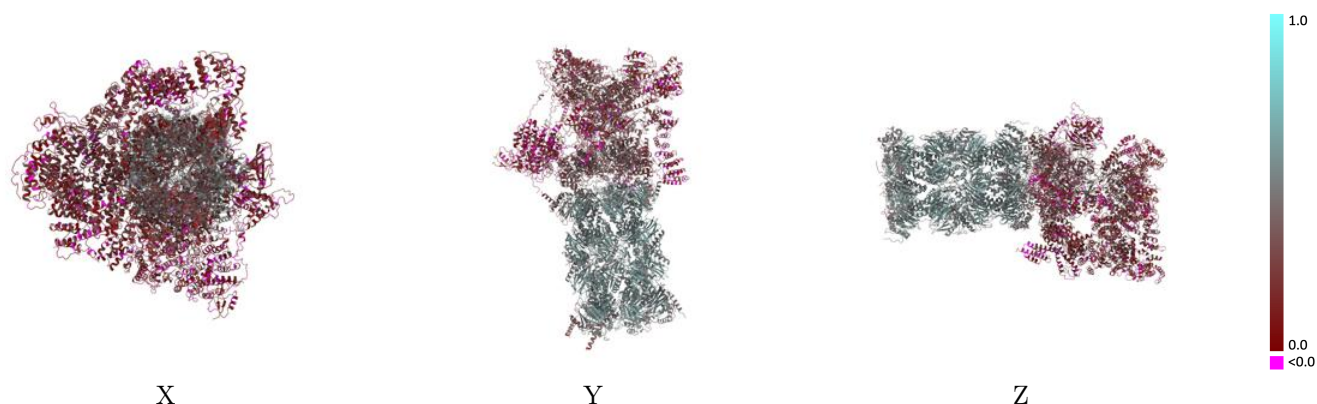
Y



Z

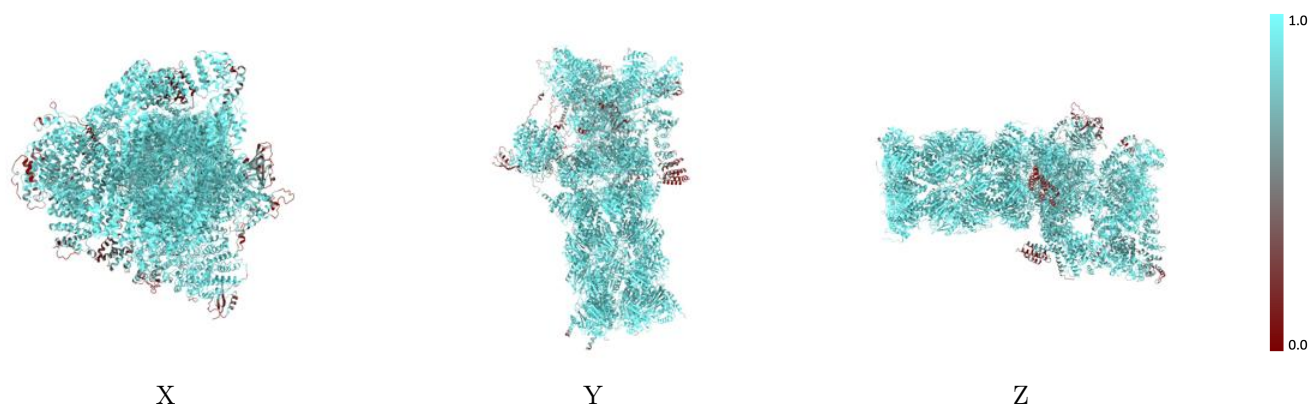
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



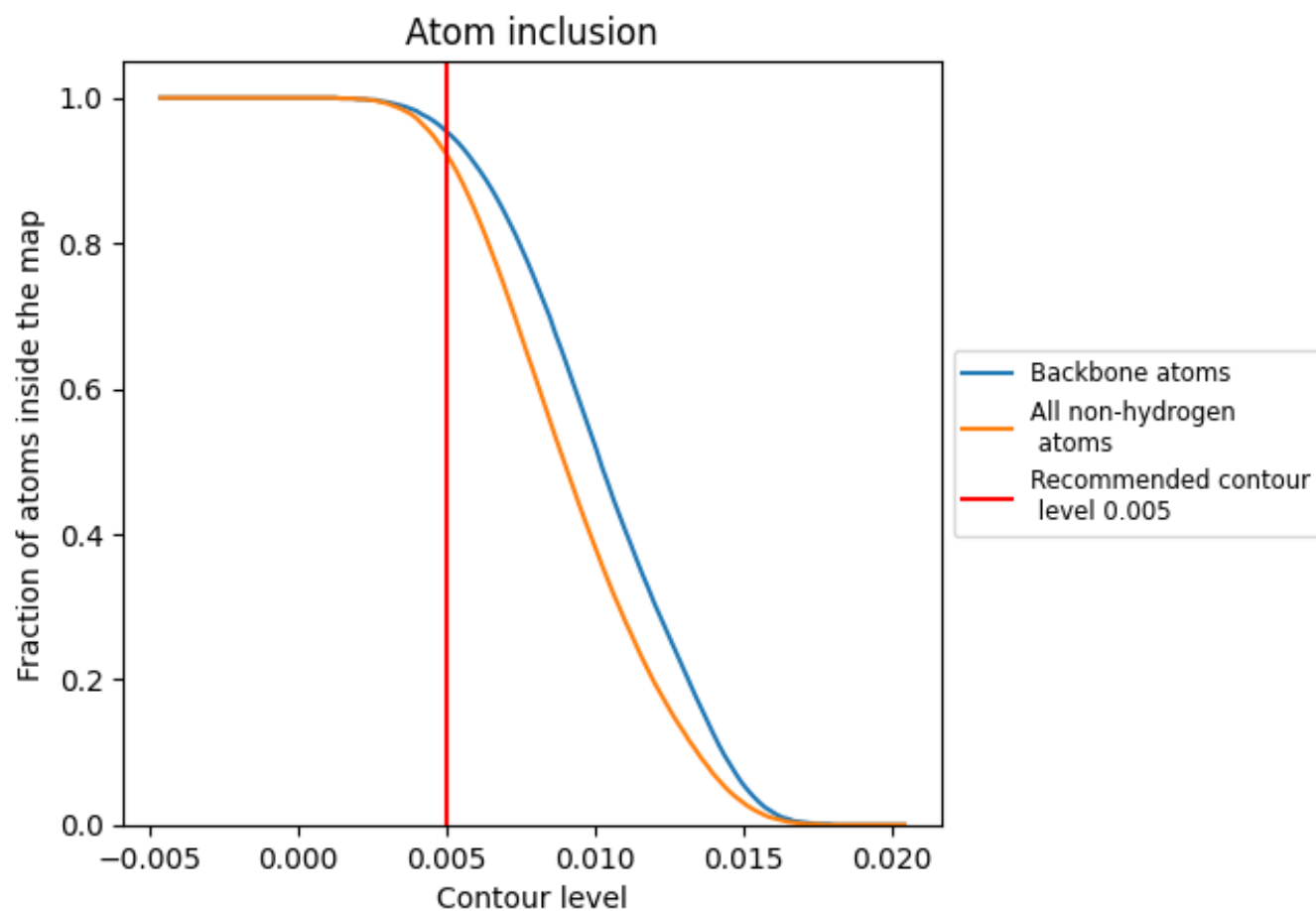
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% 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	 0.9230	 0.3580
A	 0.9590	 0.3330
B	 0.9540	 0.2960
C	 0.9510	 0.2920
D	 0.9810	 0.3000
E	 0.9450	 0.3040
F	 0.9370	 0.3270
G	 0.9890	 0.5060
H	 0.9930	 0.5170
I	 0.9810	 0.4850
J	 0.9730	 0.4510
K	 0.9780	 0.4970
L	 0.9910	 0.5310
M	 0.9830	 0.5140
N	 0.9910	 0.5430
O	 0.9960	 0.5360
P	 0.9970	 0.5420
Q	 0.9920	 0.5350
R	 0.9900	 0.5390
S	 0.9840	 0.5330
T	 0.9840	 0.5470
U	 0.8980	 0.2470
V	 0.8670	 0.2150
W	 0.6990	 0.1590
X	 0.8180	 0.2020
Y	 0.9320	 0.1970
Z	 0.9730	 0.2790
a	 0.9130	 0.1860
b	 0.9240	 0.2210
c	 0.9630	 0.2800
d	 0.7080	 0.1640
e	 0.8970	 0.2030
f	 0.8490	 0.1320
g	 0.9710	 0.5090
h	 0.9850	 0.5240



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Chain	Atom inclusion	Q-score
i	 0.9540	 0.4950
j	 0.9500	 0.4460
k	 0.9790	 0.5130
l	 0.9910	 0.5330
m	 0.9820	 0.5140
n	 0.9930	 0.5450
o	 0.9820	 0.5410
p	 0.9870	 0.5420
q	 0.9880	 0.5400
r	 0.9920	 0.5370
s	 0.9930	 0.5380
t	 0.9920	 0.5490
x	 0.6640	 0.1620
y	 0.4920	 0.1750