



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:42 PM UTC

PDB ID : 7W3F / pdb_00007w3f
EMDB ID : EMD-32278
Title : Structure of USP14-bound human 26S proteasome in substrate-engaged state
ED1_USP14
Authors : Zhang, S.; Zou, S.; Yin, D.; Wu, Z.; Mao, Y.
Deposited on : 2021-11-25
Resolution : 3.30 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:

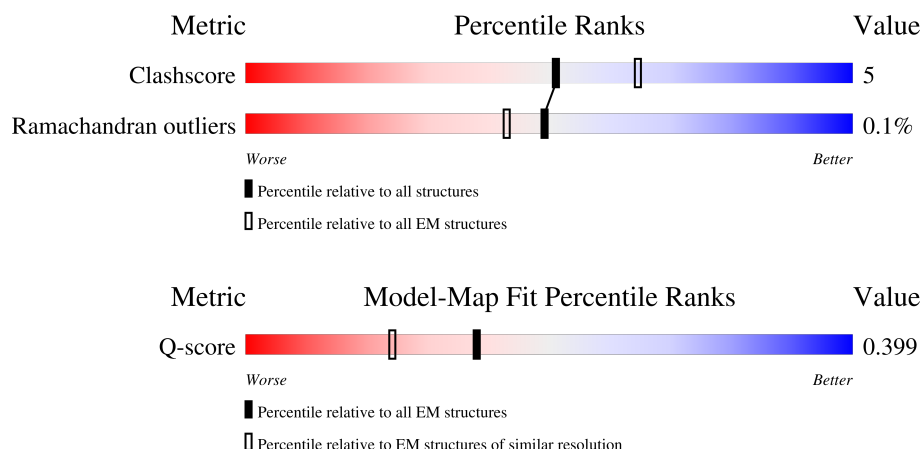
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.30 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.



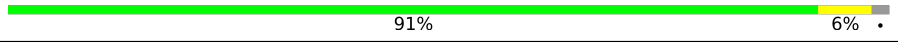
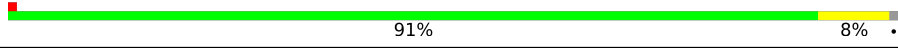
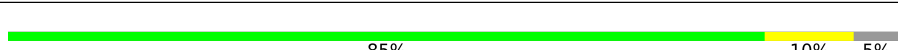
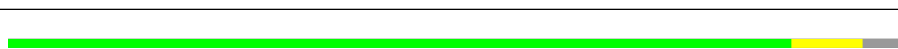
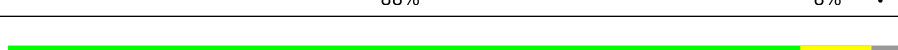
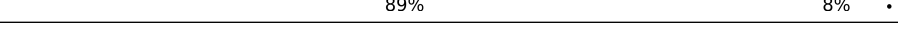
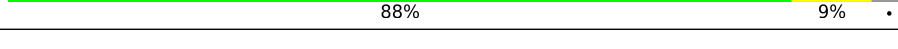
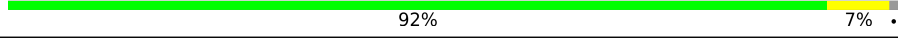
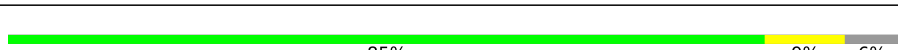
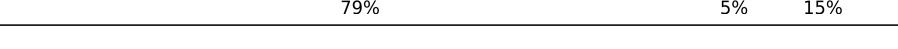
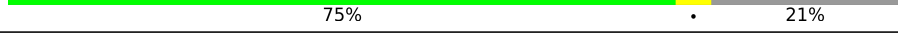
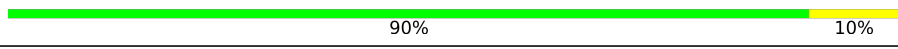
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	 76% 20% 5%
2	B	440	 78% 15% 7%
3	C	398	 82% 17% .
4	D	418	 76% 15% 9%
5	E	403	 76% 21% .

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Mol	Chain	Length	Quality of chain
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	269	
12	l	269	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	
18	r	263	

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Mol	Chain	Length	Quality of chain
19	S	241	
19	s	241	
20	T	264	
20	t	264	
21	U	953	
22	X	422	
23	Y	389	
24	Z	324	
25	a	376	
26	b	377	
27	c	310	
28	d	350	
29	f	908	
30	v	36	
31	x	494	
32	y	76	
33	W	456	
34	V	534	
35	e	70	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 110751 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 26S protease regulatory subunit 7.

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

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

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

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

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

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

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

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1801	1149	304	342	6		
8	h	232	Total	C	N	O	S	0	0
			1805	1154	307	338	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	248	Total	C	N	O	S	0	0
			1933	1222	330	371	10		
9	i	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1861	1166	327	363	5		
10	j	239	Total	C	N	O	S	0	0
			1861	1168	332	356	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	238	Total	C	N	O	S	0	0
			1813	1139	302	361	11		
11	k	234	Total	C	N	O	S	0	0
			1782	1119	295	357	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	240	Total	C	N	O	S	0	0
			1876	1175	338	352	11		
12	l	238	Total	C	N	O	S	0	0
			1861	1165	335	350	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	242	Total	C	N	O	S	0	0
			1890	1200	323	356	11		
13	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	203	Total	C	N	O	S	0	0
			1521	954	259	296	12		
14	n	202	Total	C	N	O	S	0	0
			1510	947	258	293	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1645	1035	278	320	12		
15	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1578	1012	267	290	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
18	r	201	Total	C	N	O	S	0	0
			1549	977	270	293	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		
19	s	213	Total	C	N	O	S	0	0
			1650	1044	283	313	10		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 30 is a protein called Substrate.

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

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

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

- Molecule 32 is a protein called Ubiquitin.

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

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

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

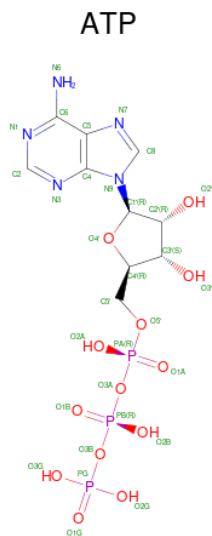
- Molecule 34 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

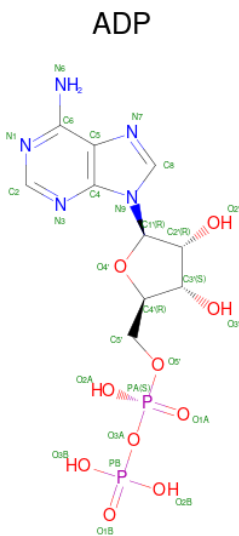
- Molecule 35 is a protein called 26S proteasome complex subunit DSS1.

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

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



- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

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

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

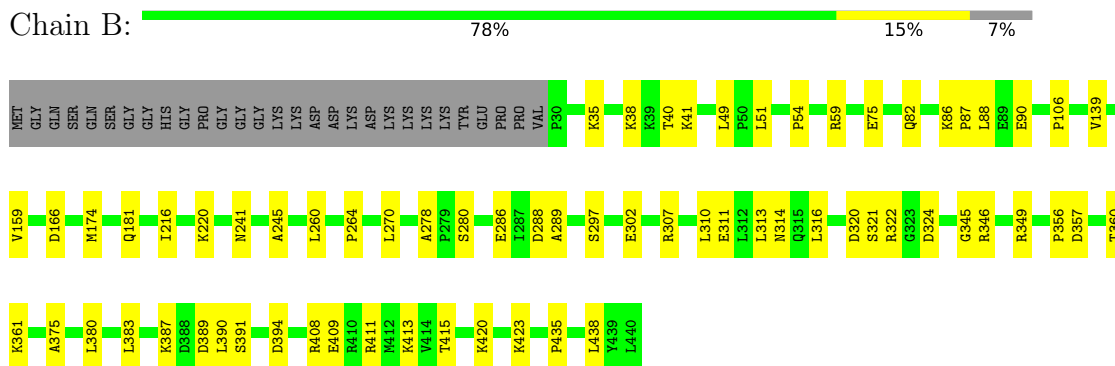
3 Residue-property plots

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

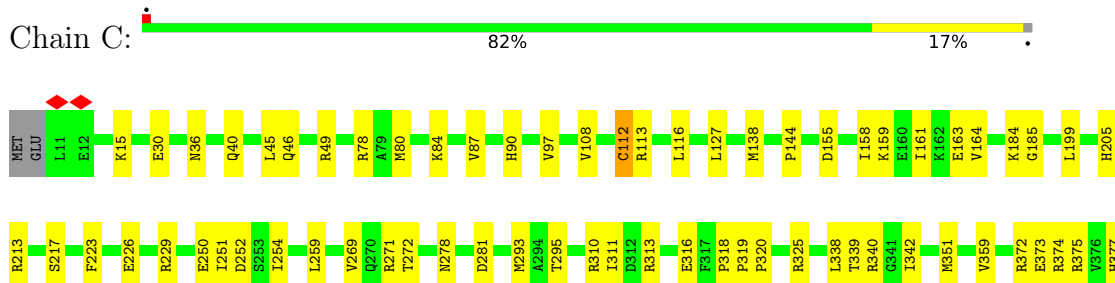
- Molecule 1: 26S protease regulatory subunit 7



- Molecule 2: 26S protease regulatory subunit 4



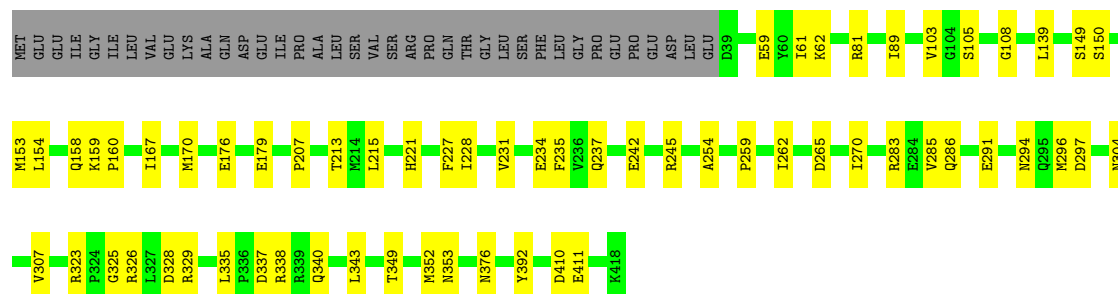
- Molecule 3: Isoform 2 of 26S proteasome regulatory subunit 8





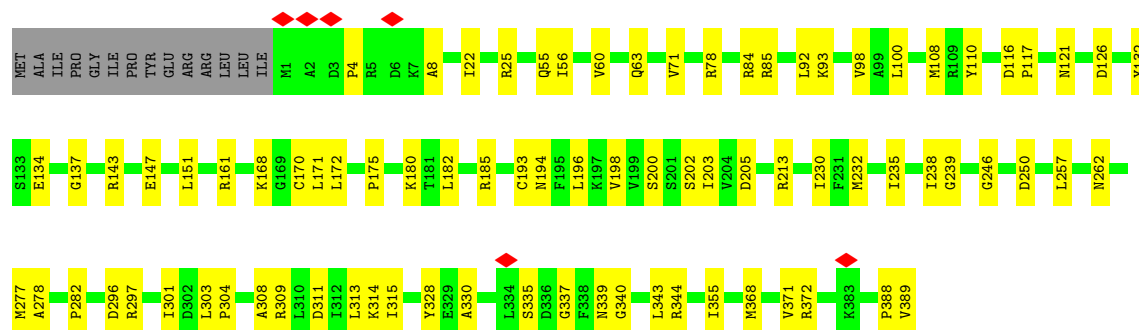
- Molecule 4: 26S protease regulatory subunit 6B

Chain D: 76% 15% 9%



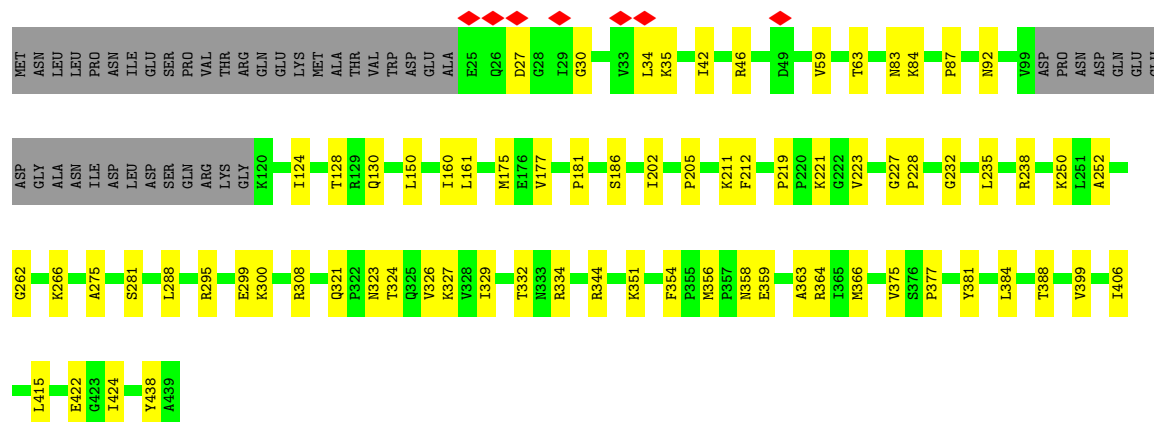
- Molecule 5: 26S proteasome regulatory subunit 10B

Chain E: 76% 21% .



- Molecule 6: 26S protease regulatory subunit 6A

Chain F: 73% 17% 10%



- Molecule 7: Proteasome subunit alpha type-6

Chain G:  91% 6%



- Molecule 7: Proteasome subunit alpha type-6

Chain g:  91% 8%



- Molecule 8: Proteasome subunit alpha type-2

Chain H:  88% 12%



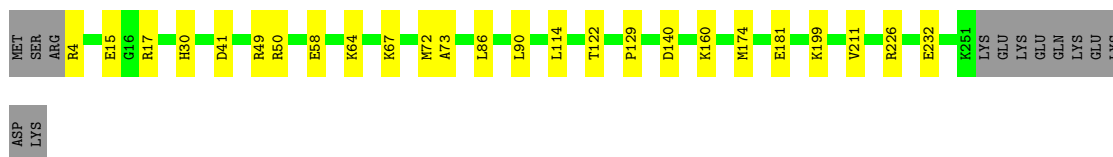
- Molecule 8: Proteasome subunit alpha type-2

Chain h:  91% 8%



- Molecule 9: Proteasome subunit alpha type-4

Chain I:  85% 10% 5%



- Molecule 9: Proteasome subunit alpha type-4

Chain i:  88% 8%



- Molecule 10: Proteasome subunit alpha type-7

Chain J:  89% 8%



- Molecule 10: Proteasome subunit alpha type-7

Chain j:  88% 9%



- Molecule 11: Proteasome subunit alpha type-5

Chain K:  92% 7%



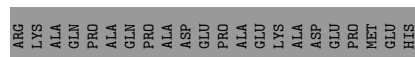
- Molecule 11: Proteasome subunit alpha type-5

Chain k:  89% 8%



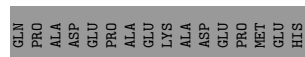
- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

Chain L:  79% 10% 11%



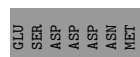
- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

Chain l:  80% 8% 12%

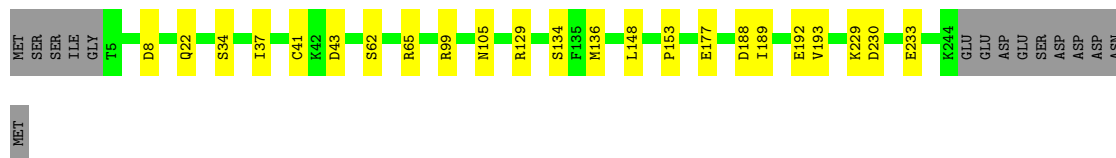


- Molecule 13: Proteasome subunit alpha type-3

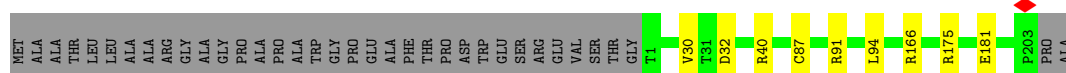
Chain M:  84% 11% 5%



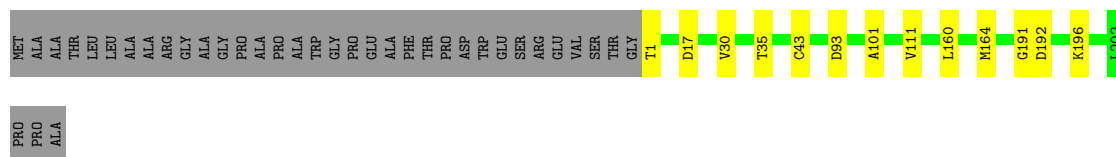
● Molecule 13: Proteasome subunit alpha type-3

Chain m:  85% 9% 6%

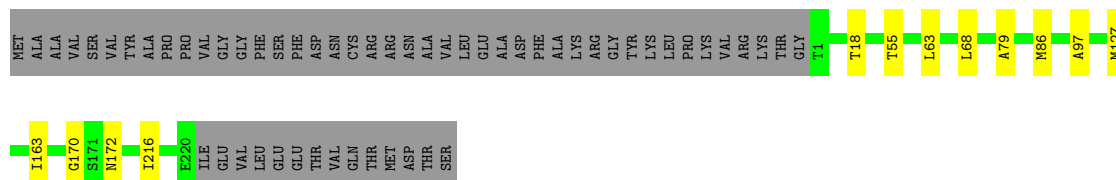
● Molecule 14: Proteasome subunit beta type-6

Chain N:  81% 15%

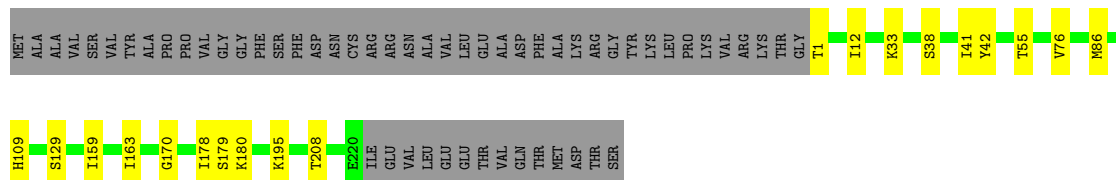
● Molecule 14: Proteasome subunit beta type-6

Chain n:  79% 5% 15%

● Molecule 15: Proteasome subunit beta type-7

Chain O:  75% 21%

● Molecule 15: Proteasome subunit beta type-7

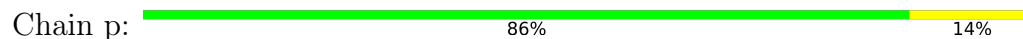
Chain o:  73% 7% 21%

● Molecule 16: Proteasome subunit beta type-3

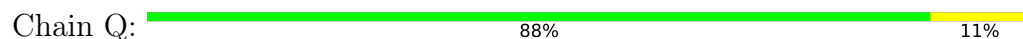
Chain P:  90% 10%



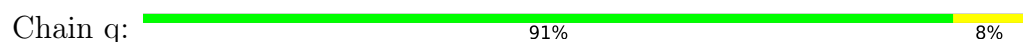
- Molecule 16: Proteasome subunit beta type-3



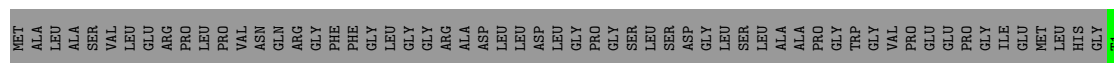
- Molecule 17: Proteasome subunit beta type-2



- Molecule 17: Proteasome subunit beta type-2



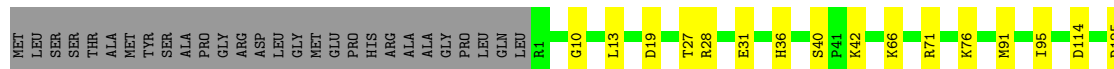
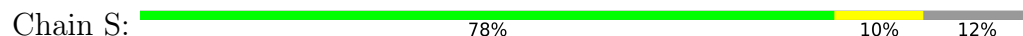
- Molecule 18: Proteasome subunit beta type-5



- Molecule 18: Proteasome subunit beta type-5



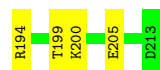
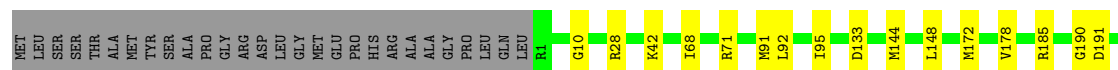
- Molecule 19: Proteasome subunit beta type-1





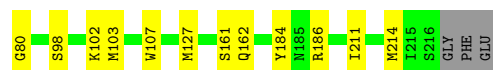
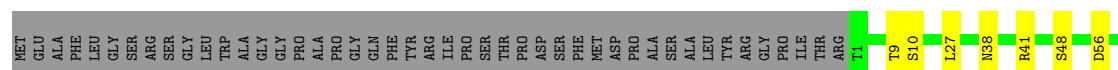
• Molecule 19: Proteasome subunit beta type-1

Chain s: 80% 8% 12%



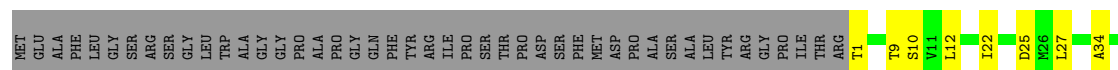
• Molecule 20: Proteasome subunit beta type-4

Chain T: 75% 7% 18%



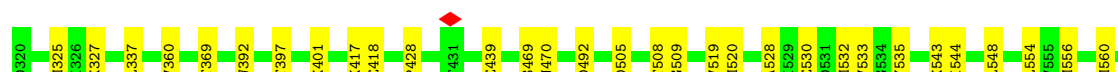
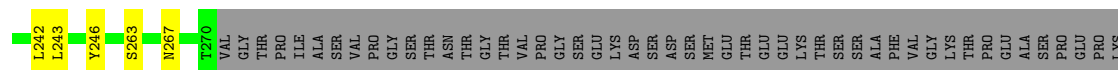
• Molecule 20: Proteasome subunit beta type-4

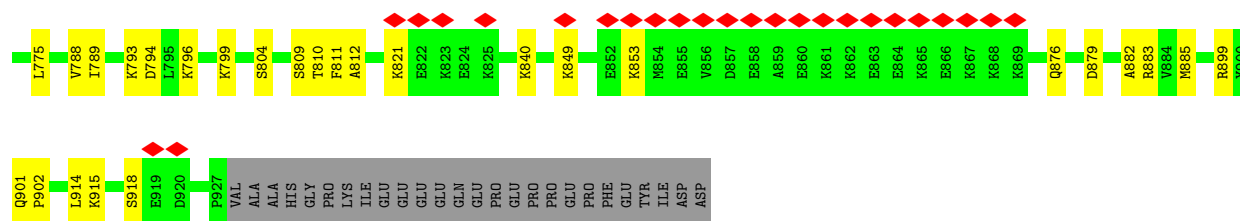
Chain t: 72% 10% 18%



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

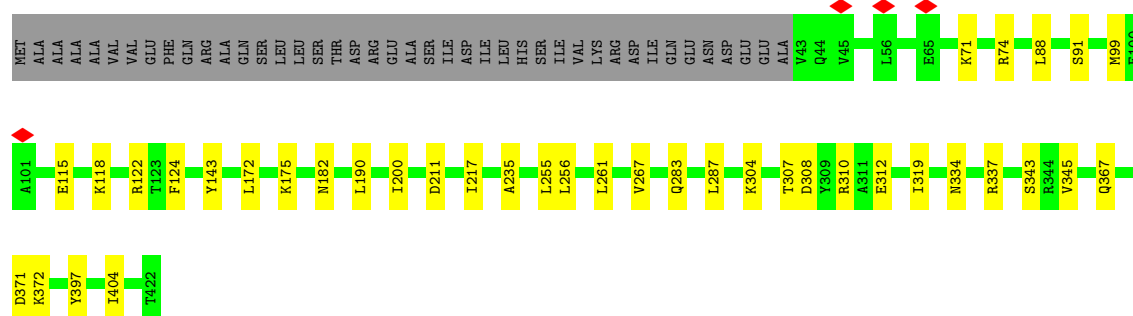
Chain U: 78% 13% 8%





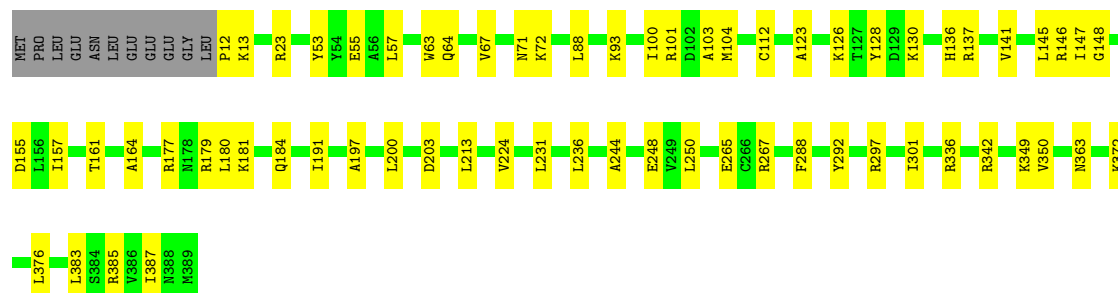
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 81% 9% 10%



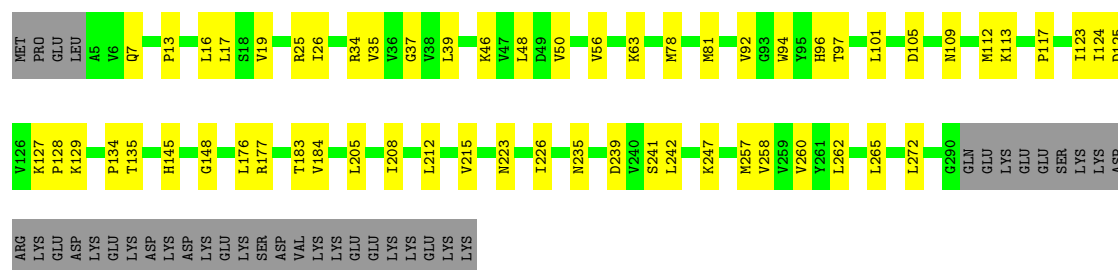
- Molecule 23: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 80% 17%



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

Chain Z: 70% 18% 12%

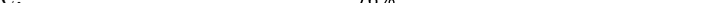


- Molecule 25: 26S proteasome non-ATPase regulatory subunit 13

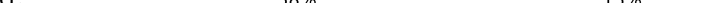
E246	Q249	T253	Q257	L261	K271	Q273	L274	L275	R284	H288	R289	Q290	L291	L310	V320	K321	G322	S323	I324	D325	E326	V327	V331	T334	W335	D342	L343	G344	G345	I346	D370	T376				
Met	Lys	Asp	V4	L8	E26	D54	I57	K58	E66	F67	E68	H69	R70	T88	D89	P90	A93	E102	K105	L123	V130	D137	E140	M141	K161	L180	G181	A197	F211	N212	F213	L216	V221	R226	V232	T236

- Chain b:

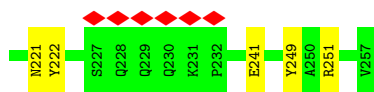
[illegible]

- Chain c:  76% 16% 7%

K152	R161	L162	I163	M164	A195	M166	M167	M168	R175	T178	S179	M190	H183	L194	I189	L192	Y201	S202	K215	M216	L220	K223	Q232	D233	C238	K239	I272	K277	Q278	D279	R282	Q298	K310								
ASP	LEU	LEU	ARG	LEU	GLY	GLY	GLY	PRO	GLY	LEU	GLY	GLN	GLY	PRO	PRO	THR	ASP	ALA	PRO	T27	A28	L36	M54	G55	L56	M57	V72	M75	P76	Q77	V82	M98	R104	P105	E106	W111	H115	F118	I127	Q130	A140

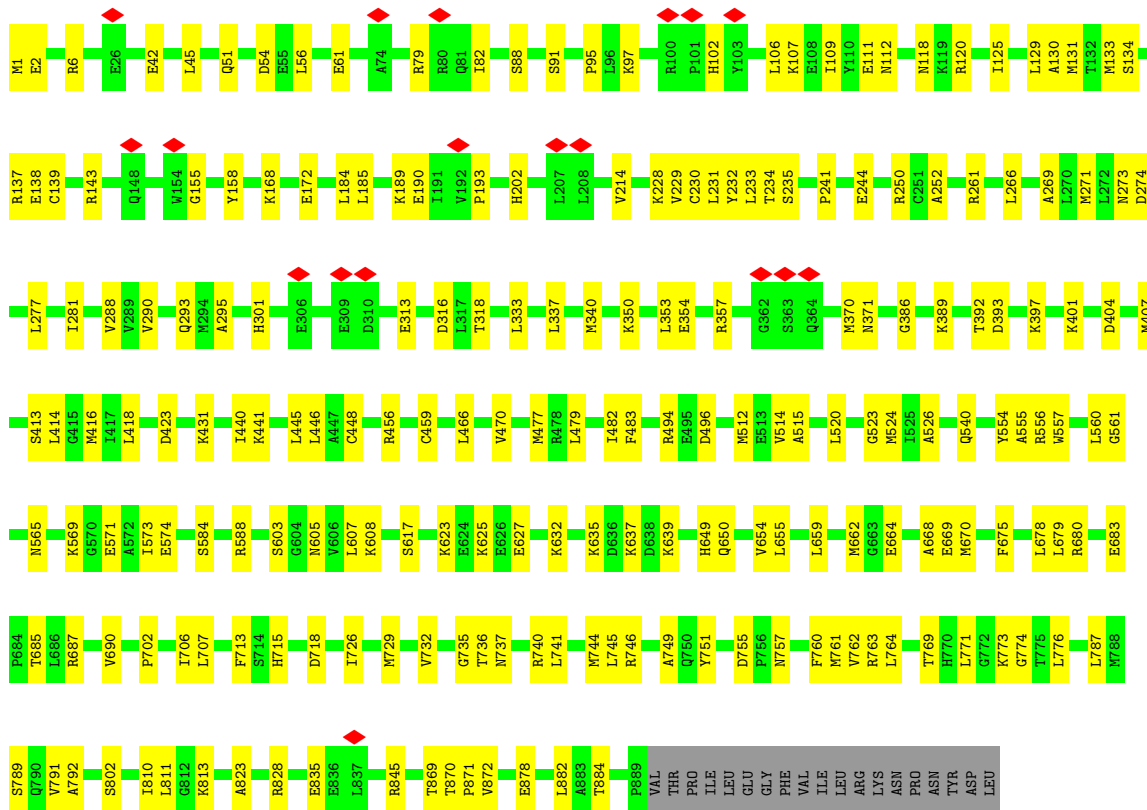
- Chain d:  58% 15% 27%

I49	I54	P69	R73	K79	Y82	F83	Q83	L89	P90	L98	L101	R121	D126	V131	K134	S147	K150	T164	I167	D176	G181	I182	E183	K188	I189	L190	F191	T192	E193	A194	F200	M201	T202	P203	K204	M206	R213									
SER	ARG	LYS	ALA	ALA	VAL	ASN	ALA	GLY	PHE	SER	SER	THR	ARG	ALA	ALA	THR	GLN	VAL	LEU	GLY	K6	M10	R11	K12	S13	P14	M15	K27	L28	V29	E32	L33	L36	T39	G40	T44	K45									
MET	PHE	ILE	LYS	GLY	ARG	ALA	PRO	ARG	ALA	ALA	PRO	GLY	THR	ARG	GLY	GLY	LEU	VAL	ALA	PRO	PRO	ARG	ALA	LEU	GLY	SER	THR	ARG	ARG	PRO	HIS	PHE	ARG	ARG	CYS	VAL	ARG	ARG	LYS	SER	GLY	GLY	LEU	LEU	ALA	ALA



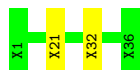
- Molecule 29: 26S proteasome non-ATPase regulatory subunit 2

Chain f: 75% 23%



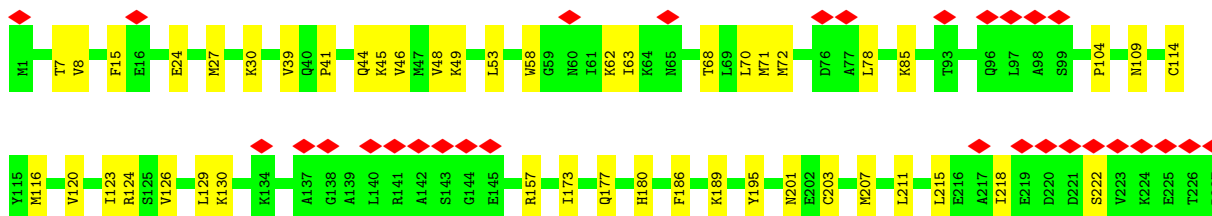
- Molecule 30: Substrate

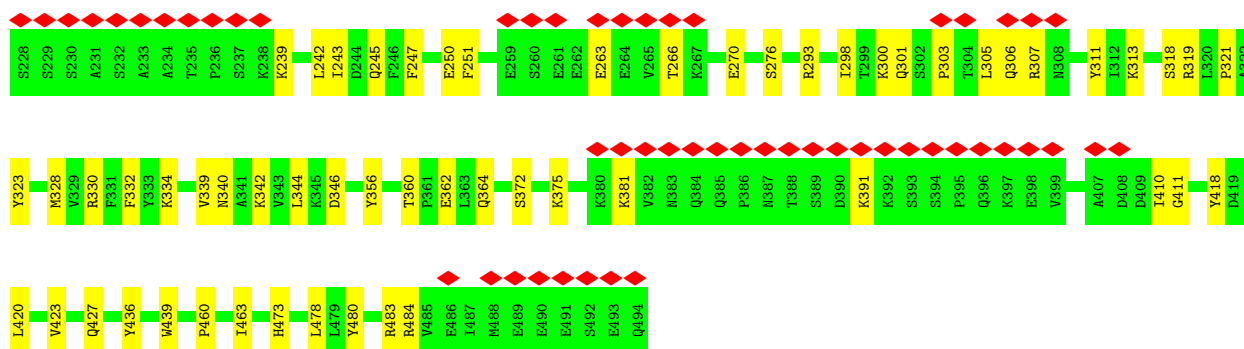
Chain v: 94% 6%



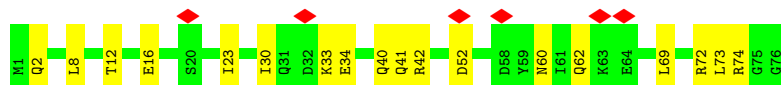
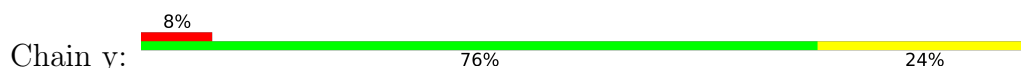
- Molecule 31: Ubiquitin carboxyl-terminal hydrolase 14

Chain x: 17% 79% 21%

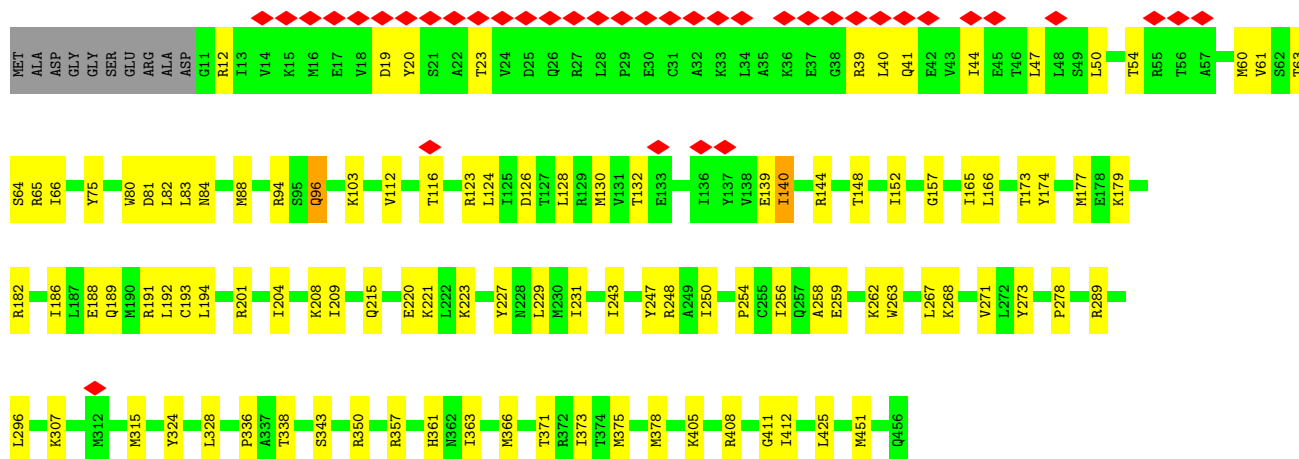
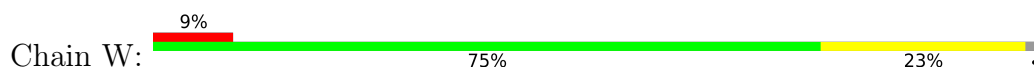




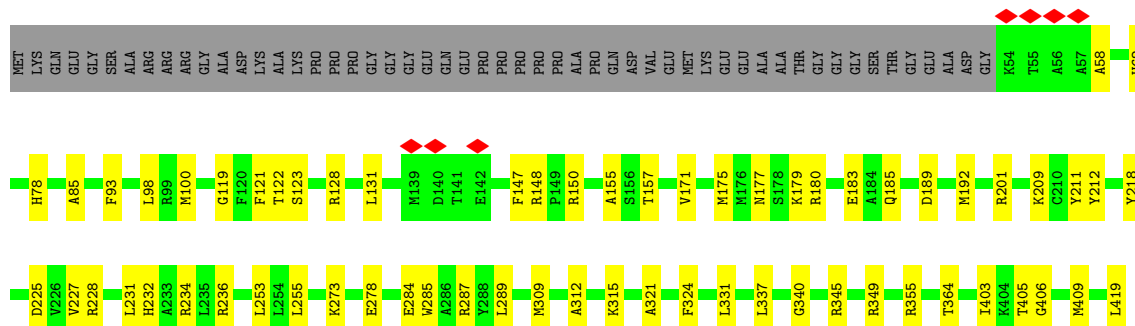
• Molecule 32: Ubiquitin

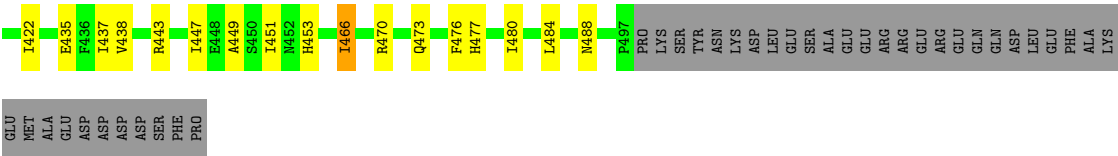


• Molecule 33: 26S proteasome non-ATPase regulatory subunit 12

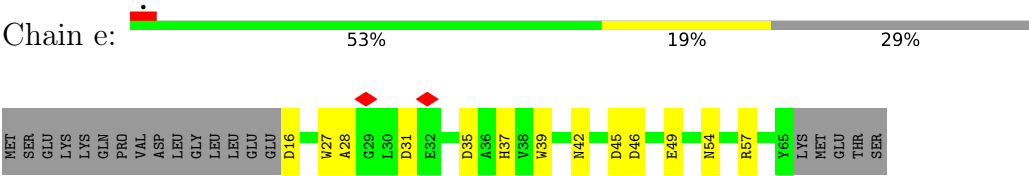


• Molecule 34: 26S proteasome non-ATPase regulatory subunit 3





- Molecule 35: 26S proteasome complex subunit DSS1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124597	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	0.022	Depositor
Minimum map value	-0.004	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/3283	0.50	2/4433 (0.0%)
2	B	0.16	0/3254	0.44	0/4388
3	C	0.19	0/3146	0.51	0/4226
4	D	0.16	0/3090	0.45	0/4168
5	E	0.15	0/3145	0.42	0/4233
6	F	0.16	0/3137	0.43	1/4223 (0.0%)
7	G	0.16	0/1901	0.38	0/2572
7	g	0.16	0/1913	0.39	0/2589
8	H	0.15	0/1840	0.37	0/2495
8	h	0.13	0/1844	0.35	0/2497
9	I	0.14	0/1963	0.36	0/2650
9	i	0.14	0/1985	0.34	0/2677
10	J	0.14	0/1887	0.38	0/2553
10	j	0.15	0/1887	0.38	0/2549
11	K	0.17	0/1841	0.35	0/2486
11	k	0.14	0/1809	0.34	0/2444
12	L	0.14	0/1911	0.32	0/2584
12	l	0.15	0/1896	0.36	0/2565
13	M	0.15	0/1925	0.37	0/2592
13	m	0.13	0/1916	0.31	0/2580
14	N	0.14	0/1548	0.33	0/2097
14	n	0.13	0/1536	0.30	0/2080
15	O	0.14	0/1672	0.37	0/2267
15	o	0.14	0/1686	0.36	0/2282
16	P	0.16	0/1616	0.39	0/2180
16	p	0.15	0/1620	0.38	0/2184
17	Q	0.14	0/1621	0.35	0/2194
17	q	0.14	0/1611	0.36	0/2182
18	R	0.13	0/1590	0.31	0/2147
18	r	0.14	0/1580	0.37	0/2135
19	S	0.14	0/1671	0.36	0/2252
19	s	0.15	0/1680	0.36	2/2264 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.15	0/1716	0.37	0/2323
20	t	0.14	0/1720	0.33	0/2328
21	U	0.15	0/6945	0.41	0/9382
22	X	0.16	0/3053	0.40	0/4115
23	Y	0.17	0/3173	0.47	0/4273
24	Z	0.17	0/2324	0.44	0/3150
25	a	0.16	0/3053	0.48	1/4133 (0.0%)
26	b	0.14	0/1478	0.39	0/2001
27	c	0.18	0/2302	0.47	0/3110
28	d	0.22	0/2162	0.47	0/2919
29	f	0.20	0/6980	0.53	0/9433
31	x	0.16	0/4002	0.39	0/5390
32	y	0.16	0/607	0.41	0/816
33	W	0.18	0/3683	0.48	4/4952 (0.1%)
34	V	0.16	0/3681	0.41	0/4969
35	e	0.20	0/437	0.64	1/595 (0.2%)
All	All	0.16	0/112320	0.42	11/151657 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	326	VAL	N-CA-C	-6.83	106.14	112.43
35	e	28	ALA	CB-CA-C	-6.22	109.39	116.54
1	A	157	ILE	CA-C-N	5.99	136.40	121.80
1	A	157	ILE	C-N-CA	5.99	136.40	121.80
25	a	130	VAL	N-CA-C	-5.80	107.61	113.47
33	W	116	THR	N-CA-C	5.35	117.14	108.26
33	W	96	GLN	CB-CA-C	-5.25	110.08	117.23
33	W	139	GLU	CA-C-N	5.23	131.39	121.97
33	W	139	GLU	C-N-CA	5.23	131.39	121.97
19	s	190	GLY	CA-C-N	5.11	131.29	121.54
19	s	190	GLY	C-N-CA	5.11	131.29	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3229	0	3261	56	0
2	B	3207	0	3278	47	0
3	C	3105	0	3219	50	0
4	D	3040	0	3076	43	0
5	E	3097	0	3174	55	0
6	F	3098	0	3187	48	0
7	G	1867	0	1867	11	0
7	g	1879	0	1872	11	0
8	H	1801	0	1773	16	0
8	h	1805	0	1798	12	0
9	I	1933	0	1923	16	0
9	i	1955	0	1955	17	0
10	J	1861	0	1846	11	0
10	j	1861	0	1865	15	0
11	K	1813	0	1796	12	0
11	k	1782	0	1766	13	0
12	L	1876	0	1856	18	0
12	l	1861	0	1839	15	0
13	M	1890	0	1880	17	0
13	m	1881	0	1868	15	0
14	N	1521	0	1494	7	0
14	n	1510	0	1483	8	0
15	O	1645	0	1648	8	0
15	o	1659	0	1681	13	0
16	P	1587	0	1598	15	0
16	p	1591	0	1609	17	0
17	Q	1588	0	1584	17	0
17	q	1578	0	1569	11	0
18	R	1559	0	1523	6	0
18	r	1549	0	1506	10	0
19	S	1641	0	1639	16	0
19	s	1650	0	1645	12	0
20	T	1683	0	1662	13	0
20	t	1687	0	1666	16	0
21	U	6828	0	6884	76	0
22	X	3009	0	3113	25	0
23	Y	3115	0	3120	44	0
24	Z	2281	0	2312	44	0
25	a	2995	0	3012	40	0
26	b	1458	0	1505	27	0
27	c	2260	0	2276	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	d	2116	0	2146	38	0
29	f	6866	0	6866	139	0
30	v	180	0	45	2	0
31	x	3929	0	3915	67	0
32	y	601	0	629	16	0
33	W	3635	0	3762	72	0
34	V	3612	0	3682	60	0
35	e	425	0	328	14	0
36	A	31	0	12	2	0
36	B	31	0	12	0	0
36	C	31	0	12	0	0
36	D	31	0	12	2	0
37	E	27	0	12	2	0
38	c	1	0	0	0	0
All	All	110751	0	111061	1209	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1209) 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)
6:F:175:MET:HE1	6:F:252:ALA:H	1.53	0.72
29:f:680:ARG:HH22	29:f:762:VAL:HG13	1.56	0.70
31:x:30:LYS:HB3	31:x:41:PRO:HB3	1.73	0.70
17:q:25:ILE:HG23	17:q:26:VAL:HG23	1.75	0.68
6:F:84:LYS:HG3	6:F:161:LEU:HD23	1.77	0.67
11:K:121:LEU:HD23	11:K:160:GLY:HA3	1.76	0.67
29:f:370:MET:SD	29:f:740:ARG:NH2	2.68	0.67
2:B:35:LYS:HZ1	29:f:735:GLY:HA2	1.58	0.67
22:X:122:ARG:HE	22:X:124:PHE:H	1.44	0.66
35:e:35:ASP:HB3	35:e:37:HIS:HD2	1.59	0.66
25:a:273:GLN:HB3	25:a:310:LEU:HD11	1.77	0.66
5:E:355:ILE:HD12	6:F:211:LYS:HG3	1.78	0.65
29:f:736:THR:O	29:f:746:ARG:NH1	2.30	0.65
19:S:147:PRO:HB2	16:p:149:MET:HE3	1.78	0.65
23:Y:177:ARG:NH2	23:Y:203:ASP:O	2.31	0.64
4:D:237:GLN:HG2	5:E:213:ARG:HH22	1.62	0.64
34:V:185:GLN:HG3	34:V:218:TYR:HE1	1.63	0.64
13:M:77:VAL:HG23	13:M:135:PHE:HB3	1.77	0.64
17:Q:25:ILE:HG23	17:Q:26:VAL:HG13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:W:373:ILE:HG12	33:W:378:MET:HE3	1.79	0.64
24:Z:205:LEU:HD13	24:Z:208:ILE:HD11	1.80	0.63
16:p:12:MET:HG3	16:p:138:VAL:HG12	1.78	0.63
4:D:270:ILE:HG12	4:D:285:VAL:HG13	1.79	0.63
22:X:255:LEU:HD22	22:X:267:VAL:HG13	1.81	0.63
6:F:227:GLY:HA3	6:F:354:PHE:HB2	1.80	0.63
21:U:509:GLY:HA3	21:U:544:ILE:HG12	1.81	0.63
21:U:804:SER:HB3	21:U:876:GLN:HB2	1.81	0.63
26:b:40:LYS:HE3	26:b:47:ASN:HD21	1.64	0.63
25:a:68:GLU:HG2	25:a:70:ARG:H	1.64	0.62
29:f:741:LEU:HD22	29:f:792:ALA:HB1	1.80	0.62
3:C:49:ARG:HD2	21:U:639:LEU:HD23	1.80	0.62
24:Z:235:ASN:ND2	25:a:335:TRP:O	2.32	0.62
22:X:71:LYS:HA	22:X:74:ARG:HD3	1.82	0.62
21:U:620:GLU:HA	21:U:655:ALA:HB2	1.80	0.62
6:F:177:VAL:HG21	6:F:250:LYS:HB3	1.82	0.62
5:E:175:PRO:HG3	5:E:303:LEU:HD22	1.82	0.61
22:X:397:TYR:HE1	24:Z:257:MET:HG3	1.65	0.61
2:B:322:ARG:HG2	2:B:324:ASP:H	1.65	0.61
6:F:30:GLY:O	6:F:34:LEU:HB2	2.00	0.61
34:V:309:MET:HE1	34:V:331:LEU:HB3	1.81	0.61
24:Z:37:GLY:HA2	24:Z:56:VAL:HG12	1.82	0.61
1:A:274:PHE:HB3	1:A:277:ILE:HD11	1.81	0.61
8:H:122:THR:HG22	8:H:129:PRO:HB3	1.83	0.61
31:x:126:VAL:HG12	31:x:129:LEU:H	1.64	0.61
1:A:364:VAL:HG12	1:A:404:ALA:HB3	1.81	0.61
23:Y:383:LEU:HD22	24:Z:272:LEU:HD13	1.81	0.61
5:E:134:GLU:HA	5:E:315:ILE:HG21	1.82	0.60
3:C:15:LYS:HB2	21:U:140:ARG:HE	1.66	0.60
29:f:556:ARG:HH12	29:f:627:GLU:HB2	1.66	0.60
5:E:198:VAL:HB	5:E:232:MET:HG3	1.83	0.60
13:M:175:GLU:HB3	13:M:196:ILE:HD12	1.82	0.60
28:d:147:SER:HB3	28:d:150:LYS:HB2	1.82	0.60
3:C:281:ASP:HB2	3:C:310:ARG:HE	1.67	0.60
9:i:53:HIS:HB3	9:i:56:LEU:HD23	1.83	0.60
21:U:417:LYS:HG3	21:U:418:GLU:HG3	1.83	0.60
23:Y:385:ARG:HH12	34:V:315:LYS:HZ3	1.50	0.60
10:j:96:LEU:HB2	17:q:62:LYS:HG3	1.84	0.60
33:W:50:LEU:HG	33:W:66:ILE:HG21	1.84	0.60
21:U:82:LEU:HB3	21:U:129:ARG:HH21	1.67	0.60
31:x:70:LEU:HG	31:x:72:MET:HE3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:277:LYS:HG3	27:c:282:ARG:HH21	1.67	0.59
1:A:163:MET:HG3	1:A:238:ILE:HG23	1.85	0.59
31:x:328:MET:HE3	31:x:330:ARG:HD2	1.84	0.59
2:B:181:GLN:O	2:B:241:ASN:ND2	2.36	0.59
10:J:4:ASP:O	10:J:18:GLN:NE2	2.35	0.59
24:Z:7:GLN:HG2	24:Z:46:LYS:HB3	1.85	0.59
24:Z:26:ILE:HG21	24:Z:35:VAL:HG21	1.84	0.59
29:f:88:SER:OG	29:f:120:ARG:NH2	2.34	0.59
29:f:608:LYS:HB3	29:f:639:LYS:HE3	1.83	0.59
14:N:87:CYS:HA	14:N:94:LEU:HD21	1.84	0.59
16:p:45:MET:HE3	16:p:71:LEU:HD22	1.85	0.59
29:f:185:LEU:HB3	29:f:189:LYS:HE2	1.84	0.59
33:W:363:ILE:HA	33:W:366:MET:HE2	1.85	0.59
11:K:35:SER:HB2	11:K:66:LYS:HE3	1.85	0.58
21:U:519:VAL:HG23	21:U:520:MET:HG2	1.83	0.58
10:j:119:THR:HG22	10:j:126:PRO:HB3	1.85	0.58
33:W:220:GLU:HG3	33:W:221:LYS:HG3	1.85	0.58
25:a:343:LEU:HG	25:a:346:ILE:HD12	1.84	0.58
4:D:265:ASP:OD2	5:E:262:ASN:ND2	2.35	0.58
21:U:127:ASP:HB2	21:U:130:LEU:HD23	1.86	0.58
19:S:71:ARG:HD3	19:S:95:ILE:HD11	1.86	0.58
33:W:128:LEU:O	33:W:132:THR:OG1	2.21	0.58
33:W:273:TYR:OH	33:W:350:ARG:NH1	2.37	0.58
4:D:89:ILE:HB	5:E:78:ARG:HG3	1.85	0.58
33:W:81:ASP:OD1	33:W:123:ARG:NH2	2.36	0.58
27:c:232:GLN:O	27:c:298:GLN:NE2	2.37	0.58
17:Q:35:MET:SD	17:Q:181:ARG:NH1	2.74	0.58
5:E:239:GLY:HA2	5:E:257:LEU:HD13	1.86	0.58
15:o:163:ILE:HD12	15:o:170:GLY:HA2	1.84	0.58
3:C:138:MET:SD	3:C:213:ARG:NH1	2.75	0.57
11:K:85:ALA:HB2	11:K:139:VAL:HG21	1.86	0.57
23:Y:180:LEU:HG	23:Y:200:LEU:HD23	1.86	0.57
24:Z:113:LYS:NZ	24:Z:117:PRO:O	2.35	0.57
29:f:869:THR:HA	29:f:884:THR:HA	1.86	0.57
3:C:217:SER:OG	4:D:291:GLU:OE1	2.21	0.57
1:A:306:LEU:HD13	1:A:336:ARG:HB3	1.87	0.57
22:X:211:ASP:HB2	22:X:235:ALA:HB2	1.85	0.57
23:Y:100:ILE:HG22	23:Y:104:MET:HE2	1.84	0.57
33:W:254:PRO:HG3	33:W:262:LYS:HG2	1.86	0.57
3:C:325:ARG:NH1	3:C:351:MET:O	2.36	0.57
17:Q:59:TYR:O	17:Q:63:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:242:LEU:O	21:U:246:TYR:HB2	2.05	0.57
23:Y:177:ARG:HH22	23:Y:181:LYS:HZ1	1.52	0.57
25:a:212:ASN:HB3	25:a:275:LEU:HD11	1.87	0.57
29:f:91:SER:HA	29:f:109:ILE:HB	1.85	0.57
31:x:189:LYS:HG2	31:x:195:TYR:HB3	1.86	0.57
6:F:321:GLN:HE22	6:F:323:ASN:HB2	1.70	0.57
22:X:343:SER:HB2	33:W:405:LYS:HE3	1.86	0.57
27:c:56:LEU:HA	27:c:111:TRP:HA	1.85	0.57
28:d:6:LYS:O	28:d:10:ASN:ND2	2.37	0.57
29:f:637:LYS:HG3	29:f:678:LEU:HB2	1.86	0.57
29:f:811:LEU:HG	29:f:878:GLU:HA	1.86	0.57
16:p:169:GLN:O	16:p:173:ASN:ND2	2.37	0.57
3:C:30:GLU:OE2	34:V:201:ARG:NH2	2.38	0.57
26:b:24:THR:HG23	26:b:27:GLN:H	1.68	0.57
33:W:41:GLN:HA	33:W:44:ILE:HG12	1.87	0.57
20:T:38:ASN:OD1	20:T:186:ARG:NH2	2.37	0.57
29:f:637:LYS:HE3	29:f:678:LEU:HD22	1.87	0.57
2:B:166:ASP:OD1	3:C:78:ARG:NH1	2.38	0.56
3:C:45:LEU:HD21	4:D:62:LYS:HE3	1.86	0.56
5:E:368:MET:HB3	5:E:372:ARG:HH21	1.70	0.56
2:B:260:LEU:O	2:B:307:ARG:NH1	2.37	0.56
3:C:226:GLU:HA	3:C:229:ARG:HB2	1.86	0.56
9:I:122:THR:HG22	9:I:129:PRO:HB3	1.87	0.56
23:Y:265:GLU:OE1	23:Y:267:ARG:NH1	2.38	0.56
2:B:289:ALA:O	3:C:271:ARG:NH1	2.39	0.56
3:C:113:ARG:HG3	3:C:127:LEU:HB2	1.87	0.56
4:D:376:ASN:ND2	36:D:501:ATP:O2'	2.38	0.56
18:R:9:ARG:HH21	18:R:146:ASP:HB3	1.70	0.56
27:c:167:MET:HG2	27:c:168:MET:HG2	1.86	0.56
27:c:57:MET:HG3	27:c:72:VAL:HG22	1.87	0.56
34:V:192:MET:HE1	34:V:234:ARG:HD3	1.87	0.56
26:b:7:MET:HB3	26:b:109:ILE:HG22	1.86	0.56
28:d:241:GLU:OE2	34:V:470:ARG:NH1	2.39	0.56
18:r:83:LEU:HD13	18:r:101:ILE:HD11	1.87	0.56
33:W:165:ILE:O	33:W:189:GLN:NE2	2.39	0.56
13:M:8:ASP:O	13:M:22:GLN:NE2	2.39	0.56
21:U:576:PRO:HA	21:U:579:ARG:HD3	1.86	0.56
29:f:869:THR:HG22	29:f:882:LEU:HB3	1.88	0.56
29:f:584:SER:HB2	29:f:588:ARG:HB3	1.88	0.56
9:i:153:SER:OG	9:i:155:ASN:ND2	2.39	0.56
3:C:339:THR:OG1	3:C:340:ARG:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:23:ARG:NH2	23:Y:55:GLU:OE1	2.32	0.56
24:Z:13:PRO:HA	24:Z:16:LEU:HD12	1.87	0.56
25:a:70:ARG:HB3	26:b:17:ARG:HG2	1.87	0.56
28:d:192:THR:HG23	28:d:201:ASN:ND2	2.21	0.56
7:G:13:ILE:HG13	7:G:24:GLN:HG2	1.87	0.56
12:L:140:MET:HE3	20:T:80:GLY:HA3	1.88	0.56
15:O:55:THR:HG23	15:O:86:MET:HE1	1.87	0.56
28:d:82:TYR:HB3	28:d:121:ARG:HH22	1.71	0.56
35:e:54:ASN:OD1	35:e:57:ARG:NH2	2.35	0.56
1:A:143:ASP:HB2	1:A:150:HIS:HE1	1.70	0.55
2:B:408:ARG:NH2	3:C:163:GLU:OE2	2.40	0.55
23:Y:67:VAL:O	23:Y:71:ASN:HB2	2.06	0.55
27:c:130:GLN:HG2	27:c:162:LEU:HD23	1.87	0.55
31:x:8:VAL:HB	31:x:15:PHE:HB2	1.87	0.55
34:V:345:ARG:NH2	35:e:46:ASP:OD1	2.39	0.55
29:f:340:MET:HE3	29:f:757:ASN:HD22	1.72	0.55
29:f:670:MET:HE3	29:f:707:LEU:HD22	1.88	0.55
34:V:121:PHE:O	34:V:128:ARG:NH1	2.39	0.55
34:V:289:LEU:HB3	34:V:312:ALA:HB2	1.87	0.55
1:A:329:PRO:HA	1:A:332:MET:HB2	1.87	0.55
21:U:69:TYR:HE2	34:V:236:ARG:HH21	1.51	0.55
23:Y:13:LYS:HE3	23:Y:146:ARG:HH12	1.71	0.55
2:B:245:ALA:HB1	2:B:280:SER:HA	1.89	0.55
5:E:55:GLN:HE22	5:E:108:MET:HG3	1.71	0.55
6:F:375:VAL:HG23	6:F:377:PRO:HD3	1.87	0.55
21:U:899:ARG:NH2	21:U:918:SER:OG	2.39	0.55
28:d:32:GLU:HG2	28:d:33:LEU:HG	1.89	0.55
33:W:152:ILE:HG13	33:W:165:ILE:HD12	1.88	0.55
4:D:337:ASP:HB3	4:D:340:GLN:HB3	1.89	0.55
25:a:232:TRP:HB2	25:a:253:THR:HG22	1.89	0.55
12:l:120:THR:O	13:m:129:ARG:NH1	2.40	0.55
31:x:340:ASN:ND2	32:y:40:GLN:OE1	2.38	0.55
33:W:88:MET:HE1	33:W:130:MET:HB2	1.89	0.55
13:M:50:GLU:OE2	13:M:201:HIS:ND1	2.39	0.55
17:Q:169:LYS:HG3	17:Q:170:ARG:HG2	1.89	0.55
3:C:36:ASN:O	3:C:40:GLN:NE2	2.39	0.55
21:U:616:ARG:HB3	21:U:647:HIS:HB3	1.89	0.55
31:x:423:VAL:HB	31:x:439:TRP:HB2	1.88	0.55
2:B:411:ARG:HH22	2:B:415:THR:HG23	1.70	0.55
16:P:149:MET:HE2	16:P:173:ASN:HB2	1.89	0.55
5:E:282:PRO:HB2	5:E:389:VAL:HG13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:141:CYS:HB3	21:U:150:ALA:HB2	1.89	0.55
25:a:236:THR:HB	25:a:253:THR:HG21	1.88	0.55
29:f:131:MET:SD	29:f:131:MET:N	2.77	0.55
29:f:445:LEU:HD11	29:f:477:MET:HE3	1.87	0.55
10:j:184:ASP:O	10:j:187:THR:OG1	2.24	0.55
7:G:17:SER:HB3	7:G:21:ARG:H	1.71	0.54
8:H:143:ARG:NH1	8:H:144:PRO:O	2.41	0.54
23:Y:13:LYS:HB3	23:Y:146:ARG:HH12	1.70	0.54
29:f:214:VAL:HB	29:f:250:ARG:HH22	1.71	0.54
29:f:252:ALA:HB2	29:f:281:ILE:HG21	1.88	0.54
17:q:168:GLN:NE2	17:q:175:LEU:O	2.39	0.54
2:B:387:LYS:HG3	2:B:389:ASP:H	1.73	0.54
3:C:342:ILE:HG22	3:C:380:GLN:HB2	1.87	0.54
10:J:2:SER:OG	10:J:3:TYR:N	2.40	0.54
21:U:505:ASP:HB2	21:U:508:THR:HG22	1.87	0.54
25:a:327:VAL:HG11	33:W:412:ILE:HD12	1.90	0.54
26:b:97:LEU:HD11	26:b:109:ILE:HG23	1.89	0.54
31:x:24:GLU:O	31:x:58:TRP:NE1	2.38	0.54
5:E:22:ILE:HG22	5:E:25:ARG:HH21	1.71	0.54
20:T:9:THR:HG22	20:T:10:SER:H	1.72	0.54
25:a:123:LEU:HD22	25:a:161:LYS:HB3	1.89	0.54
31:x:251:PHE:HB2	31:x:270:GLU:HB2	1.87	0.54
29:f:828:ARG:HG2	29:f:845:ARG:H	1.72	0.54
15:o:38:SER:HB3	15:o:41:ILE:HB	1.89	0.54
31:x:7:THR:HB	31:x:68:THR:HA	1.88	0.54
34:V:345:ARG:NH1	35:e:42:ASN:O	2.40	0.54
28:d:190:LEU:HA	28:d:221:ASN:HA	1.88	0.54
29:f:95:PRO:HB2	29:f:137:ARG:HH21	1.73	0.54
29:f:354:GLU:HB3	29:f:357:ARG:HD2	1.90	0.54
11:k:44:GLU:HG3	11:k:191:LEU:HG	1.90	0.54
6:F:295:ARG:HA	6:F:300:LYS:HA	1.90	0.54
25:a:342:ASP:O	25:a:345:GLN:N	2.36	0.54
33:W:179:LYS:HZ2	33:W:215:GLN:HG3	1.71	0.54
17:Q:26:VAL:HG21	18:R:136:TYR:HE2	1.72	0.54
21:U:469:SER:OG	21:U:470:ASN:N	2.40	0.54
26:b:97:LEU:HD13	26:b:107:MET:HB3	1.89	0.54
27:c:175:ARG:NH2	27:c:202:SER:O	2.41	0.54
2:B:82:GLN:NE2	29:f:662:MET:O	2.40	0.54
25:a:370:GLN:O	28:d:251:ARG:NH2	2.41	0.54
29:f:2:GLU:O	29:f:6:ARG:NH2	2.41	0.54
7:g:51:VAL:HG22	7:g:217:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:117:PRO:O	5:E:121:ASN:ND2	2.41	0.54
10:J:57:ARG:O	10:J:60:ARG:NH1	2.41	0.54
12:L:132:LEU:HB2	12:L:147:THR:HB	1.89	0.54
29:f:190:GLU:HB3	29:f:193:PRO:HG2	1.90	0.54
29:f:397:LYS:HB3	31:x:85:LYS:HD3	1.89	0.54
29:f:446:LEU:HD11	29:f:483:PHE:HD2	1.72	0.54
2:B:316:LEU:HD23	2:B:346:ARG:HB2	1.88	0.54
4:D:392:TYR:HB3	33:W:204:ILE:HD11	1.89	0.54
28:d:33:LEU:HD13	28:d:44:THR:HG22	1.90	0.54
31:x:222:SER:HB2	31:x:410:ILE:H	1.72	0.54
34:V:85:ALA:HB2	34:V:93:PHE:HB2	1.89	0.54
2:B:380:LEU:HD13	2:B:383:LEU:HD12	1.90	0.53
6:F:288:LEU:HB2	6:F:332:THR:HB	1.90	0.53
23:Y:104:MET:HE1	23:Y:130:LYS:HD2	1.90	0.53
27:c:115:HIS:HB3	27:c:118:PHE:HB2	1.90	0.53
29:f:241:PRO:HA	29:f:244:GLU:HG3	1.90	0.53
31:x:239:LYS:HD2	31:x:245:GLN:HA	1.90	0.53
33:W:247:TYR:HA	33:W:250:ILE:HG12	1.90	0.53
34:V:131:LEU:HD13	34:V:171:VAL:HG21	1.89	0.53
19:S:184:GLU:OE1	19:S:211:ARG:NH1	2.40	0.53
19:s:68:ILE:HD11	19:s:92:LEU:HD13	1.90	0.53
31:x:300:LYS:HE3	32:y:2:GLN:HG2	1.89	0.53
31:x:321:PRO:O	31:x:418:TYR:OH	2.26	0.53
32:y:40:GLN:HG3	32:y:74:ARG:HH21	1.73	0.53
1:A:195:LEU:HD21	1:A:316:LYS:HZ3	1.72	0.53
19:S:13:LEU:HD11	19:S:149:LEU:HD11	1.89	0.53
26:b:61:LEU:HD12	26:b:74:LYS:HD2	1.90	0.53
31:x:46:VAL:HA	31:x:71:MET:HA	1.88	0.53
23:Y:145:LEU:HG	23:Y:179:ARG:HH22	1.74	0.53
29:f:679:LEU:H	29:f:687:ARG:HH22	1.56	0.53
9:i:118:LYS:NZ	9:i:150:SER:OG	2.40	0.53
11:k:129:ASP:N	11:k:129:ASP:OD1	2.42	0.53
32:y:30:ILE:HA	32:y:33:LYS:HG2	1.91	0.53
33:W:267:LEU:HD21	33:W:296:LEU:HD23	1.89	0.53
3:C:372:ARG:NH2	4:D:179:GLU:OE2	2.42	0.53
4:D:353:ASN:ND2	5:E:161:ARG:O	2.41	0.53
33:W:112:VAL:HG11	33:W:124:LEU:HB2	1.90	0.53
6:F:358:ASN:OD1	6:F:359:GLU:N	2.38	0.53
15:O:163:ILE:HG12	15:O:170:GLY:HA2	1.90	0.53
28:d:183:GLU:OE2	28:d:213:ARG:NH1	2.41	0.53
29:f:107:LYS:O	29:f:112:ASN:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:163:ILE:HG23	15:o:170:GLY:HA2	1.91	0.53
4:D:81:ARG:HE	27:c:152:LYS:HD2	1.74	0.53
19:S:184:GLU:HG3	15:o:195:LYS:HE3	1.91	0.53
25:a:211:PHE:HA	25:a:271:LYS:HE3	1.91	0.53
29:f:371:ASN:ND2	29:f:401:LYS:O	2.40	0.53
15:o:42:TYR:HB2	15:o:178:ILE:HD11	1.90	0.53
8:H:185:GLU:OE2	8:H:189:HIS:NE2	2.42	0.53
29:f:138:GLU:HB2	29:f:189:LYS:HD2	1.90	0.53
34:V:58:ALA:O	34:V:62:HIS:ND1	2.42	0.53
9:I:30:HIS:O	9:I:50:ARG:NH1	2.40	0.53
25:a:197:ALA:HB2	25:a:221:VAL:HG12	1.90	0.53
12:l:52:ALA:HB1	12:l:57:ALA:HB3	1.91	0.53
13:m:99:ARG:NH1	13:m:105:ASN:OD1	2.42	0.53
31:x:319:ARG:NH2	31:x:411:GLY:O	2.41	0.53
34:V:349:ARG:HH12	35:e:37:HIS:HE1	1.57	0.53
21:U:337:LEU:HD21	21:U:789:ILE:HG21	1.90	0.53
31:x:332:PHE:HA	32:y:8:LEU:HD13	1.91	0.53
31:x:436:TYR:OH	32:y:73:LEU:O	2.26	0.53
2:B:54:PRO:HA	29:f:835:GLU:HB2	1.91	0.52
3:C:158:ILE:HG22	3:C:199:LEU:HD11	1.90	0.52
9:I:49:ARG:NH1	9:I:58:GLU:OE2	2.42	0.52
29:f:623:LYS:HG3	29:f:625:LYS:H	1.74	0.52
16:p:122:CYS:SG	16:p:123:SER:N	2.82	0.52
1:A:430:MET:HE2	11:K:59:MET:HE1	1.91	0.52
28:d:131:VAL:HA	28:d:134:LYS:HB2	1.90	0.52
33:W:132:THR:OG1	33:W:144:ARG:NH1	2.41	0.52
5:E:132:TYR:HB2	33:W:177:MET:HE1	1.91	0.52
16:P:122:CYS:SG	16:P:123:SER:N	2.82	0.52
18:r:6:PHE:HB3	18:r:139:MET:HE2	1.92	0.52
1:A:127:ASP:HB2	31:x:339:VAL:HG21	1.91	0.52
2:B:86:LYS:HD3	2:B:87:PRO:HD2	1.91	0.52
3:C:251:ILE:HD11	3:C:293:MET:HG3	1.92	0.52
16:P:143:ALA:HA	16:P:146:MET:HE3	1.91	0.52
16:P:193:ASP:OD1	16:P:193:ASP:N	2.42	0.52
34:V:447:ILE:HG13	34:V:449:ALA:H	1.74	0.52
5:E:235:ILE:HB	5:E:277:MET:HE2	1.91	0.52
6:F:202:ILE:O	6:F:327:LYS:NZ	2.42	0.52
23:Y:231:LEU:HB2	23:Y:236:LEU:HD13	1.92	0.52
29:f:79:ARG:H	29:f:82:ILE:HB	1.75	0.52
10:j:152:THR:HG23	11:k:82:ILE:HD11	1.91	0.52
2:B:361:LYS:HE2	2:B:390:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:60:VAL:HG12	5:E:71:VAL:HG22	1.89	0.52
5:E:344:ARG:NH1	37:E:501:ADP:O2'	2.42	0.52
21:U:799:LYS:HZ2	21:U:879:ASP:HB2	1.75	0.52
24:Z:109:ASN:HA	24:Z:112:MET:HE2	1.92	0.52
11:k:41:GLN:NE2	11:k:151:PRO:O	2.42	0.52
31:x:276:SER:OG	31:x:293:ARG:NH1	2.42	0.52
31:x:298:ILE:HD11	31:x:313:LYS:HE3	1.89	0.52
8:H:181:ASP:OD1	8:H:181:ASP:N	2.43	0.52
21:U:666:LYS:O	21:U:670:ASN:ND2	2.42	0.52
24:Z:258:VAL:HA	24:Z:262:LEU:HD13	1.92	0.52
34:V:119:GLY:HA2	34:V:148:ARG:HD3	1.91	0.52
34:V:177:ASN:O	34:V:179:LYS:NZ	2.42	0.52
10:J:119:THR:HG22	10:J:126:PRO:HB3	1.91	0.52
21:U:36:ALA:O	34:V:273:LYS:NZ	2.42	0.52
21:U:530:GLU:HA	21:U:533:VAL:HG12	1.92	0.52
31:x:39:VAL:O	31:x:44:GLN:NE2	2.43	0.52
1:A:368:ILE:HG12	1:A:406:GLU:HB3	1.91	0.52
6:F:399:VAL:HG21	6:F:424:ILE:HD13	1.91	0.52
15:O:216:ILE:HG12	16:P:196:THR:HG22	1.91	0.52
21:U:428:PRO:HG2	21:U:439:GLU:HB3	1.92	0.52
23:Y:53:TYR:OH	23:Y:64:GLN:NE2	2.40	0.52
15:o:55:THR:HG23	15:o:86:MET:HE1	1.91	0.52
32:y:42:ARG:HH12	32:y:72:ARG:HB3	1.73	0.52
33:W:166:LEU:HD13	33:W:201:ARG:HH22	1.75	0.52
10:J:210:VAL:HG13	10:J:220:LEU:HD21	1.92	0.52
24:Z:241:SER:OG	24:Z:242:LEU:N	2.42	0.52
11:k:146:VAL:HG11	11:k:222:PRO:HA	1.92	0.52
16:p:48:ARG:NH1	16:p:192:LYS:O	2.42	0.52
31:x:180:HIS:NE2	31:x:186:PHE:O	2.43	0.52
34:V:321:ALA:HB1	34:V:324:PHE:HB3	1.92	0.52
5:E:313:LEU:HD13	5:E:343:LEU:HD12	1.92	0.51
24:Z:34:ARG:NH1	24:Z:105:ASP:OD1	2.43	0.51
7:g:59:LYS:HE3	13:m:177:GLU:HB2	1.93	0.51
6:F:83:ASN:OD1	27:c:77:GLN:NE2	2.42	0.51
26:b:112:PHE:HE1	26:b:141:ILE:HD12	1.75	0.51
28:d:88:GLN:HG2	28:d:90:PRO:HD3	1.92	0.51
33:W:64:SER:HB3	33:W:103:LYS:HD2	1.92	0.51
5:E:84:ARG:HG3	5:E:85:ARG:H	1.73	0.51
21:U:263:SER:O	21:U:267:ASN:ND2	2.42	0.51
33:W:223:LYS:O	33:W:227:TYR:HB2	2.10	0.51
2:B:139:VAL:HG11	2:B:159:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:137:ASP:HB3	25:a:141:MET:HE1	1.91	0.51
29:f:228:LYS:O	29:f:234:THR:OG1	2.29	0.51
7:g:174:GLU:HG2	7:g:205:VAL:HG22	1.93	0.51
17:q:44:LEU:HD11	17:q:102:LEU:HD22	1.91	0.51
1:A:272:ILE:HB	1:A:317:VAL:HG12	1.93	0.51
2:B:41:LYS:HG3	2:B:278:ALA:HB3	1.92	0.51
29:f:168:LYS:O	29:f:172:GLU:HB3	2.10	0.51
20:t:9:THR:HG22	20:t:10:SER:H	1.74	0.51
1:A:222:LYS:NZ	36:A:501:ATP:O1B	2.44	0.51
3:C:185:GLY:HA3	3:C:311:ILE:HA	1.92	0.51
23:Y:191:ILE:HD13	35:e:39:TRP:HB3	1.93	0.51
27:c:233:ASP:OD1	27:c:233:ASP:N	2.43	0.51
1:A:351:ARG:NH2	1:A:378:PRO:O	2.44	0.51
4:D:105:SER:OG	4:D:108:GLY:O	2.28	0.51
29:f:107:LYS:HA	29:f:111:GLU:HB2	1.92	0.51
13:m:8:ASP:O	13:m:22:GLN:NE2	2.44	0.51
19:s:10:GLY:HA3	19:s:42:LYS:HE3	1.92	0.51
31:x:203:CYS:O	31:x:207:MET:HG2	2.11	0.51
3:C:46:GLN:HG2	21:U:639:LEU:HD11	1.93	0.51
3:C:250:GLU:HA	3:C:295:THR:HB	1.93	0.51
24:Z:127:LYS:O	24:Z:129:LYS:NZ	2.43	0.51
19:s:194:ARG:NH2	19:s:205:GLU:OE2	2.44	0.51
1:A:152:PRO:HD2	31:x:344:LEU:HD11	1.91	0.51
5:E:335:SER:HB2	5:E:371:VAL:HG13	1.92	0.51
9:I:4:ARG:O	10:J:5:ARG:NH1	2.44	0.51
21:U:360:VAL:HG21	21:U:392:TRP:HZ2	1.76	0.51
21:U:811:PHE:HB2	21:U:885:MET:HE1	1.93	0.51
22:X:307:THR:HA	22:X:310:ARG:HH11	1.76	0.51
31:x:263:GLU:OE2	31:x:266:THR:OG1	2.29	0.51
34:V:470:ARG:HE	34:V:473:GLN:HG2	1.76	0.51
19:S:27:THR:HB	19:S:40:SER:H	1.75	0.51
10:j:43:LEU:HD11	10:j:134:VAL:HG21	1.92	0.51
12:l:50:LYS:HE3	12:l:59:HIS:HB3	1.92	0.51
1:A:223:THR:OG1	36:A:501:ATP:O2A	2.29	0.50
2:B:409:GLU:HB2	2:B:411:ARG:HD3	1.93	0.50
10:j:65:LEU:HD11	10:j:71:MET:HE3	1.92	0.50
11:k:31:ILE:HD13	11:k:140:ALA:HB2	1.92	0.50
14:n:35:THR:OG1	14:n:43:CYS:SG	2.69	0.50
5:E:193:CYS:SG	5:E:194:ASN:N	2.81	0.50
18:R:146:ASP:OD1	18:R:146:ASP:N	2.43	0.50
26:b:95:LEU:HA	26:b:98:LYS:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:108:ARG:NH1	26:b:139:ASP:OD1	2.43	0.50
7:g:33:ASN:HB3	7:g:170:VAL:HG12	1.92	0.50
34:V:484:LEU:O	34:V:488:ASN:ND2	2.44	0.50
23:Y:363:ASN:ND2	34:V:466:ILE:O	2.45	0.50
28:d:126:ASP:OD1	28:d:126:ASP:N	2.44	0.50
29:f:231:LEU:HD22	29:f:235:SER:HB3	1.94	0.50
16:p:14:MET:HE3	16:p:154:TRP:HD1	1.76	0.50
2:B:49:LEU:HD11	29:f:650:GLN:HB2	1.92	0.50
4:D:149:SER:OG	4:D:150:SER:N	2.45	0.50
6:F:228:PRO:HG3	6:F:356:MET:HE1	1.93	0.50
24:Z:96:HIS:ND1	24:Z:97:THR:O	2.45	0.50
27:c:104:ARG:NH1	27:c:106:GLU:OE2	2.44	0.50
11:k:99:HIS:HB2	11:k:107:MET:HE3	1.93	0.50
6:F:128:THR:HG23	6:F:130:GLN:HG2	1.92	0.50
21:U:623:GLY:HA3	21:U:658:ILE:HG13	1.94	0.50
23:Y:88:LEU:HD21	23:Y:103:ALA:HB2	1.94	0.50
26:b:19:GLY:HA2	26:b:24:THR:HA	1.93	0.50
31:x:360:THR:HG22	31:x:362:GLU:H	1.76	0.50
12:L:54:SER:OG	12:L:55:GLU:N	2.41	0.50
26:b:20:ASP:OD1	26:b:20:ASP:N	2.44	0.50
29:f:664:GLU:H	29:f:668:ALA:HB3	1.76	0.50
7:g:123:GLN:HG3	8:h:81:PRO:HB2	1.94	0.50
33:W:271:VAL:HG12	33:W:307:LYS:HE3	1.92	0.50
34:V:349:ARG:NH2	35:e:39:TRP:O	2.45	0.50
1:A:194:PRO:HG2	1:A:208:PRO:HB3	1.94	0.50
6:F:366:MET:HE1	6:F:384:LEU:HB2	1.92	0.50
16:P:2:SER:OG	16:P:3:ILE:N	2.45	0.50
25:a:197:ALA:HB3	25:a:226:ARG:HH22	1.75	0.50
28:d:192:THR:HG22	28:d:201:ASN:HD21	1.76	0.50
8:H:65:VAL:O	8:H:220:ARG:NH1	2.45	0.50
10:J:140:GLY:O	10:J:213:ARG:NH1	2.45	0.50
19:S:125:ASP:OD1	19:S:129:SER:N	2.44	0.50
22:X:143:TYR:OH	23:Y:248:GLU:O	2.29	0.50
26:b:15:TYR:HD2	26:b:115:SER:HA	1.76	0.50
29:f:273:ASN:HA	29:f:277:LEU:HD13	1.94	0.50
29:f:353:LEU:HD13	29:f:729:MET:HE3	1.93	0.50
9:i:119:GLN:NE2	10:j:79:ASP:OD1	2.44	0.50
31:x:342:LYS:HD2	32:y:73:LEU:HD11	1.92	0.50
32:y:41:GLN:HB2	32:y:69:LEU:HD11	1.93	0.50
5:E:337:GLY:O	5:E:339:ASN:ND2	2.45	0.50
7:G:112:ASP:N	7:G:112:ASP:OD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:32:ASN:OD1	34:V:236:ARG:NH1	2.45	0.50
25:a:102:GLU:O	25:a:105:LYS:NZ	2.44	0.50
28:d:182:ILE:HG21	28:d:189:ILE:HD13	1.94	0.50
28:d:192:THR:CG2	28:d:201:ASN:HD21	2.25	0.50
29:f:333:LEU:HG	29:f:337:LEU:HB2	1.92	0.50
29:f:393:ASP:OD1	29:f:393:ASP:N	2.45	0.50
6:F:27:ASP:N	6:F:27:ASP:OD1	2.44	0.49
29:f:389:LYS:HE2	29:f:393:ASP:HB3	1.94	0.49
7:g:90:GLN:HE21	7:g:134:LEU:HD23	1.77	0.49
5:E:309:ARG:HB3	33:W:12:ARG:HH22	1.77	0.49
6:F:181:PRO:HG2	6:F:238:ARG:HG2	1.94	0.49
27:c:278:GLN:HG2	27:c:279:ASP:H	1.77	0.49
9:i:150:SER:OG	9:i:151:ASP:N	2.45	0.49
16:p:7:ASN:ND2	16:p:29:GLY:O	2.41	0.49
34:V:278:GLU:HA	34:V:285:TRP:HZ2	1.78	0.49
1:A:43:ARG:HA	1:A:46:LYS:HE3	1.93	0.49
21:U:634:PRO:O	21:U:638:SER:OG	2.23	0.49
8:h:50:LYS:NZ	8:h:206:ASP:O	2.38	0.49
9:i:202:ASP:N	9:i:202:ASP:OD1	2.45	0.49
6:F:30:GLY:O	6:F:34:LEU:CB	2.61	0.49
15:O:18:THR:HB	15:O:172:ASN:HB2	1.93	0.49
24:Z:19:VAL:HG21	24:Z:124:ILE:HG13	1.93	0.49
29:f:675:PHE:HB3	29:f:715:HIS:CE1	2.47	0.49
19:s:28:ARG:NH2	19:s:191:ASP:OD1	2.44	0.49
19:s:144:MET:HE1	19:s:185:ARG:HB3	1.93	0.49
33:W:193:CYS:SG	33:W:201:ARG:NH2	2.83	0.49
3:C:254:ILE:HD11	3:C:272:THR:HB	1.93	0.49
29:f:404:ASP:HA	29:f:407:MET:HE1	1.95	0.49
15:o:1:THR:HG23	15:o:33:LYS:HZ3	1.76	0.49
1:A:359:ALA:HA	1:A:362:MET:HE3	1.95	0.49
2:B:264:PRO:HB3	2:B:311:GLU:HG3	1.93	0.49
3:C:144:PRO:O	3:C:205:HIS:ND1	2.39	0.49
21:U:201:LEU:HA	21:U:204:ILE:HG22	1.94	0.49
25:a:212:ASN:OD1	25:a:213:PHE:N	2.46	0.49
28:d:189:ILE:HG13	28:d:222:TYR:HB2	1.94	0.49
29:f:45:LEU:HB3	29:f:54:ASP:HB3	1.95	0.49
29:f:202:HIS:ND1	29:f:244:GLU:HG2	2.28	0.49
2:B:88:LEU:HB3	2:B:90:GLU:HG2	1.95	0.49
4:D:296:MET:HE2	4:D:326:ARG:HG3	1.94	0.49
6:F:205:PRO:HB3	6:F:324:THR:HG22	1.95	0.49
11:K:203:LYS:HB2	11:K:210:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:54:ASP:O	25:a:58:LYS:N	2.46	0.49
29:f:229:VAL:HG11	29:f:605:ASN:HD22	1.77	0.49
29:f:828:ARG:HH21	29:f:845:ARG:HE	1.61	0.49
12:l:47:VAL:HG12	12:l:195:LEU:HD22	1.95	0.49
15:o:12:ILE:HD11	15:o:178:ILE:HD12	1.95	0.49
34:V:355:ARG:HH22	35:e:31:ASP:H	1.60	0.49
21:U:564:ASP:OD1	21:U:564:ASP:N	2.45	0.49
4:D:325:GLY:H	4:D:328:ASP:HB3	1.76	0.48
21:U:27:LEU:HD11	21:U:38:ILE:HG21	1.95	0.48
21:U:556:MET:HE1	21:U:566:LEU:HD12	1.95	0.48
28:d:12:LYS:HG3	28:d:14:PRO:HD3	1.94	0.48
29:f:42:GLU:HA	29:f:56:LEU:HD21	1.93	0.48
29:f:483:PHE:HE2	29:f:802:SER:HB2	1.77	0.48
29:f:764:LEU:HB2	29:f:769:THR:HB	1.95	0.48
15:o:76:VAL:HG11	15:o:109:HIS:HB2	1.95	0.48
35:e:16:ASP:OD1	35:e:16:ASP:N	2.46	0.48
3:C:49:ARG:NH1	21:U:639:LEU:O	2.46	0.48
4:D:297:ASP:OD2	4:D:323:ARG:NH2	2.38	0.48
21:U:554:LEU:HD21	21:U:764:LEU:HD22	1.95	0.48
24:Z:48:LEU:HD21	24:Z:92:VAL:HG11	1.96	0.48
28:d:28:LEU:O	28:d:32:GLU:HB2	2.12	0.48
24:Z:25:ARG:NH2	27:c:104:ARG:O	2.44	0.48
29:f:459:CYS:HA	31:x:49:LYS:HG2	1.94	0.48
12:l:49:LEU:HB2	12:l:195:LEU:HD21	1.95	0.48
31:x:45:LYS:N	31:x:72:MET:O	2.44	0.48
17:Q:168:GLN:NE2	17:Q:175:LEU:O	2.40	0.48
21:U:560:MET:HG2	21:U:590:TYR:HA	1.95	0.48
21:U:688:LEU:HD22	21:U:713:TYR:HE1	1.78	0.48
23:Y:336:ARG:NH1	35:e:49:GLU:OE2	2.47	0.48
29:f:584:SER:H	29:f:588:ARG:HD3	1.79	0.48
8:h:14:SER:HB3	8:h:18:LYS:H	1.79	0.48
14:n:93:ASP:N	14:n:93:ASP:OD1	2.45	0.48
3:C:45:LEU:HB3	4:D:61:ILE:HG21	1.95	0.48
4:D:170:MET:HE3	4:D:215:LEU:HD12	1.95	0.48
20:T:9:THR:O	20:T:41:ARG:NH2	2.46	0.48
29:f:713:PHE:HD2	29:f:749:ALA:HA	1.78	0.48
33:W:258:ALA:HA	33:W:263:TRP:HE1	1.77	0.48
6:F:275:ALA:O	6:F:281:SER:OG	2.25	0.48
14:N:175:ARG:HH22	20:t:215:ILE:HD11	1.79	0.48
29:f:95:PRO:O	29:f:102:HIS:NE2	2.47	0.48
29:f:202:HIS:CE1	29:f:244:GLU:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:732:VAL:HG22	29:f:746:ARG:HE	1.79	0.48
2:B:106:PRO:HA	3:C:97:VAL:HG12	1.96	0.48
4:D:103:VAL:HG11	4:D:139:LEU:HD21	1.96	0.48
4:D:167:ILE:HG21	4:D:170:MET:HE2	1.96	0.48
5:E:330:ALA:HB1	5:E:371:VAL:HG11	1.95	0.48
8:H:39:LYS:HE2	8:H:144:PRO:HG2	1.94	0.48
21:U:49:TYR:O	21:U:57:ARG:NE	2.37	0.48
21:U:788:VAL:HB	21:U:882:ALA:HB3	1.95	0.48
22:X:304:LYS:O	22:X:308:ASP:HB2	2.13	0.48
23:Y:145:LEU:HD11	23:Y:161:THR:HG23	1.96	0.48
25:a:180:LEU:HD13	25:a:221:VAL:HG21	1.96	0.48
11:k:210:LEU:HG	11:k:238:ILE:HD11	1.95	0.48
31:x:130:LYS:O	31:x:157:ARG:NH2	2.46	0.48
31:x:298:ILE:HB	31:x:311:TYR:HB2	1.95	0.48
34:V:175:MET:HE2	34:V:183:GLU:HB2	1.95	0.48
1:A:213:LEU:HA	1:A:319:MET:HB2	1.96	0.48
3:C:252:ASP:O	4:D:286:GLN:NE2	2.46	0.48
7:G:191:PHE:HE1	7:G:219:VAL:HG11	1.78	0.48
23:Y:184:GLN:NE2	23:Y:197:ALA:O	2.40	0.48
23:Y:297:ARG:NH2	35:e:45:ASP:OD1	2.47	0.48
28:d:164:THR:HA	28:d:167:ILE:HG12	1.96	0.48
11:k:9:ASP:OD1	11:k:9:ASP:N	2.47	0.48
18:r:127:SER:HB2	18:r:136:TYR:CE1	2.48	0.48
32:y:30:ILE:HG22	32:y:33:LYS:HE3	1.95	0.48
6:F:223:VAL:HB	6:F:329:ILE:HG22	1.94	0.48
11:K:41:GLN:NE2	11:K:151:PRO:O	2.47	0.48
17:Q:155:ARG:NH1	17:Q:158:GLU:OE2	2.46	0.48
22:X:99:MET:HE3	22:X:99:MET:HB3	1.64	0.48
22:X:345:VAL:HA	33:W:408:ARG:HB3	1.95	0.48
31:x:303:PRO:O	31:x:306:GLN:NE2	2.47	0.48
33:W:128:LEU:HG	33:W:144:ARG:HH22	1.79	0.48
14:N:30:VAL:HG11	20:t:211:ILE:HG13	1.95	0.48
19:S:31:GLU:OE1	19:S:36:HIS:NE2	2.42	0.48
29:f:494:ARG:NH2	29:f:496:ASP:OD2	2.47	0.48
7:g:88:ARG:HA	7:g:91:VAL:HG12	1.95	0.48
9:i:71:ASP:HB3	9:i:223:THR:HG21	1.96	0.48
13:m:230:ASP:OD1	13:m:230:ASP:N	2.46	0.48
33:W:23:THR:HG21	33:W:50:LEU:HD11	1.96	0.48
4:D:231:VAL:HB	4:D:234:GLU:HB2	1.96	0.47
7:G:22:LEU:HD12	8:H:79:MET:HE1	1.96	0.47
19:S:114:ASP:OD2	19:S:132:ARG:NH2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:125:ASP:HB3	24:Z:128:PRO:HD2	1.96	0.47
25:a:284:ARG:NH1	25:a:288:HIS:O	2.47	0.47
1:A:144:ARG:NE	30:v:32:UNK:O	2.47	0.47
29:f:813:LYS:NZ	29:f:823:ALA:O	2.47	0.47
12:l:7:ASP:OD1	12:l:7:ASP:N	2.45	0.47
31:x:218:ILE:HB	31:x:242:LEU:HB2	1.95	0.47
34:V:119:GLY:O	34:V:122:THR:OG1	2.30	0.47
1:A:213:LEU:HD23	1:A:340:LYS:HE2	1.96	0.47
1:A:362:MET:HG3	1:A:364:VAL:HG13	1.95	0.47
2:B:41:LYS:HG2	2:B:245:ALA:HA	1.96	0.47
5:E:172:LEU:HD23	5:E:301:ILE:HD11	1.95	0.47
12:L:105:VAL:HG11	12:L:136:GLY:HA3	1.95	0.47
24:Z:94:TRP:CD2	24:Z:112:MET:HE1	2.49	0.47
29:f:479:LEU:HD12	29:f:514:VAL:HG22	1.96	0.47
34:V:189:ASP:OD1	34:V:218:TYR:OH	2.32	0.47
4:D:410:ASP:OD1	4:D:411:GLU:N	2.44	0.47
5:E:143:ARG:HB3	33:W:174:TYR:HE2	1.79	0.47
6:F:388:THR:HG22	6:F:424:ILE:HD11	1.96	0.47
12:L:47:VAL:HG12	12:L:195:LEU:HD22	1.96	0.47
21:U:492:ASP:OD1	21:U:492:ASP:N	2.47	0.47
22:X:115:GLU:HA	22:X:118:LYS:HE3	1.97	0.47
24:Z:260:VAL:HG11	34:V:476:PHE:CG	2.48	0.47
28:d:192:THR:CG2	28:d:201:ASN:ND2	2.77	0.47
29:f:569:LYS:HE3	29:f:573:ILE:HG21	1.96	0.47
8:h:74:LEU:HD11	8:h:134:LEU:HB3	1.96	0.47
16:P:38:ASP:OD1	16:P:38:ASP:N	2.47	0.47
16:P:61:GLN:HB2	17:Q:85:ARG:NH2	2.29	0.47
17:Q:43:LEU:HB2	17:Q:183:ILE:HD11	1.95	0.47
21:U:528:ALA:O	21:U:532:MET:HG3	2.14	0.47
25:a:325:ASP:OD1	33:W:371:THR:OG1	2.26	0.47
27:c:127:ILE:HD12	27:c:162:LEU:HD11	1.96	0.47
1:A:357:ILE:HD12	1:A:360:ARG:HH21	1.79	0.47
2:B:286:GLU:OE1	3:C:278:ASN:ND2	2.47	0.47
2:B:409:GLU:O	29:f:51:GLN:NE2	2.47	0.47
13:M:197:ILE:HG21	13:M:211:LEU:HD13	1.96	0.47
17:Q:118:MET:HE2	17:Q:118:MET:HB3	1.78	0.47
19:S:19:ASP:OD1	19:S:19:ASP:N	2.47	0.47
20:T:161:SER:OG	20:T:162:GLN:N	2.48	0.47
7:g:112:ASP:OD1	7:g:112:ASP:N	2.46	0.47
31:x:62:LYS:NZ	31:x:63:ILE:O	2.47	0.47
31:x:201:ASN:OD1	32:y:42:ARG:NH2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:W:20:TYR:HB2	33:W:61:VAL:HB	1.97	0.47
1:A:180:CYS:HB2	1:A:183:GLN:HE22	1.80	0.47
5:E:116:ASP:N	5:E:116:ASP:OD1	2.48	0.47
6:F:366:MET:HE3	6:F:381:TYR:HD1	1.78	0.47
21:U:159:ARG:HH21	21:U:162:VAL:HG13	1.79	0.47
29:f:228:LYS:HD2	29:f:233:LEU:HD22	1.97	0.47
29:f:271:MET:HA	29:f:274:ASP:HB2	1.96	0.47
29:f:520:LEU:HB2	29:f:557:TRP:HB3	1.96	0.47
29:f:737:ASN:OD1	29:f:746:ARG:NH2	2.48	0.47
29:f:773:LYS:HA	29:f:776:LEU:HD13	1.96	0.47
11:k:235:GLU:HA	11:k:238:ILE:HG22	1.97	0.47
31:x:109:ASN:ND2	31:x:114:CYS:SG	2.88	0.47
33:W:19:ASP:N	33:W:19:ASP:OD1	2.47	0.47
33:W:338:THR:O	33:W:343:SER:N	2.47	0.47
2:B:375:ALA:HB2	2:B:413:LYS:HB3	1.96	0.47
29:f:680:ARG:NH2	29:f:760:PHE:O	2.33	0.47
29:f:685:THR:HA	29:f:690:VAL:H	1.80	0.47
15:o:179:SER:OG	15:o:180:LYS:N	2.48	0.47
31:x:173:ILE:O	31:x:177:GLN:HB2	2.15	0.47
34:V:211:TYR:OH	34:V:234:ARG:NE	2.45	0.47
1:A:143:ASP:OD2	1:A:146:LYS:N	2.41	0.47
1:A:236:CYS:HB3	1:A:270:CYS:HB2	1.74	0.47
1:A:295:VAL:HA	1:A:298:THR:HG22	1.97	0.47
2:B:357:ASP:OD1	2:B:360:THR:OG1	2.24	0.47
24:Z:260:VAL:HG23	34:V:480:ILE:HB	1.97	0.47
29:f:231:LEU:HD23	29:f:234:THR:HB	1.96	0.47
29:f:515:ALA:HB1	29:f:540:GLN:HE22	1.79	0.47
29:f:787:LEU:HD12	29:f:791:VAL:HB	1.96	0.47
33:W:80:TRP:HA	33:W:83:LEU:HD12	1.97	0.47
33:W:315:MET:HE1	33:W:361:HIS:ND1	2.30	0.47
34:V:212:TYR:HA	34:V:253:LEU:HD11	1.96	0.47
34:V:227:VAL:HG12	34:V:231:LEU:HD13	1.96	0.47
1:A:242:GLY:H	1:A:276:GLU:HB2	1.79	0.47
1:A:278:ASP:N	1:A:278:ASP:OD1	2.46	0.47
1:A:347:ASP:N	1:A:347:ASP:OD1	2.48	0.47
5:E:205:ASP:HA	6:F:299:GLU:HA	1.97	0.47
24:Z:101:LEU:HD22	33:W:451:MET:HG3	1.96	0.47
20:t:63:LEU:HD21	20:t:106:LEU:HD13	1.97	0.47
2:B:59:ARG:HB2	29:f:184:LEU:HG	1.97	0.46
16:P:58:THR:O	17:Q:85:ARG:NH2	2.47	0.46
20:T:211:ILE:HG13	14:n:30:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:290:VAL:HA	29:f:293:GLN:HB2	1.96	0.46
12:l:41:LYS:NZ	12:l:180:MET:O	2.47	0.46
33:W:40:LEU:HD22	33:W:82:LEU:HD13	1.96	0.46
33:W:60:MET:O	33:W:64:SER:OG	2.23	0.46
5:E:296:ASP:HB2	5:E:297:ARG:HH11	1.80	0.46
6:F:232:GLY:HA2	6:F:235:LEU:HD13	1.96	0.46
6:F:406:ILE:HD13	6:F:422:GLU:HG3	1.97	0.46
13:M:52:LEU:HA	13:M:209:PHE:HA	1.97	0.46
24:Z:212:LEU:HA	24:Z:215:VAL:HG12	1.97	0.46
29:f:125:ILE:HG21	29:f:129:LEU:HB2	1.96	0.46
29:f:726:ILE:HD12	29:f:726:ILE:HA	1.79	0.46
1:A:187:LEU:HG	1:A:341:ILE:HD13	1.97	0.46
3:C:374:ARG:HA	3:C:374:ARG:HD3	1.72	0.46
13:M:108:LEU:HD11	13:M:137:LEU:HB3	1.97	0.46
19:S:10:GLY:HA3	19:S:42:LYS:HE2	1.97	0.46
1:A:394:MET:HG2	2:B:349:ARG:HH21	1.79	0.46
12:L:9:ASP:N	12:L:9:ASP:OD1	2.46	0.46
29:f:1:MET:SD	29:f:1:MET:N	2.83	0.46
9:i:176:LYS:HZ1	10:j:52:LYS:HB2	1.80	0.46
12:l:226:ASP:OD1	12:l:226:ASP:N	2.49	0.46
14:n:1:THR:N	14:n:17:ASP:OD2	2.48	0.46
3:C:87:VAL:HG21	3:C:116:LEU:HD13	1.98	0.46
25:a:66:GLU:O	25:a:69:HIS:NE2	2.49	0.46
29:f:470:VAL:HG13	29:f:482:ILE:HD11	1.97	0.46
20:t:25:ASP:H	20:t:41:ARG:HH21	1.64	0.46
33:W:208:LYS:HB3	33:W:208:LYS:HE2	1.83	0.46
2:B:387:LYS:HB3	2:B:390:LEU:HG	1.98	0.46
5:E:282:PRO:HG2	5:E:388:PRO:HA	1.96	0.46
5:E:328:TYR:OH	33:W:60:MET:SD	2.69	0.46
22:X:182:ASN:HA	23:Y:244:ALA:HB1	1.97	0.46
29:f:386:GLY:HA2	29:f:418:LEU:HG	1.98	0.46
34:V:147:PHE:O	34:V:148:ARG:NH1	2.47	0.46
1:A:433:ASN:HB3	11:K:66:LYS:HE2	1.97	0.46
24:Z:123:ILE:O	24:Z:135:THR:OG1	2.30	0.46
28:d:98:LEU:HA	28:d:101:LEU:HD12	1.97	0.46
28:d:176:ASP:OD1	28:d:213:ARG:NH2	2.49	0.46
29:f:202:HIS:HE1	29:f:244:GLU:HA	1.80	0.46
29:f:423:ASP:OD1	29:f:423:ASP:N	2.48	0.46
33:W:54:THR:HG21	33:W:63:THR:HB	1.98	0.46
3:C:373:GLU:OE1	3:C:375:ARG:NE	2.44	0.46
17:Q:30:ASP:OD1	17:Q:30:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:376:LEU:HD23	24:Z:265:LEU:HD13	1.98	0.46
25:a:90:PRO:HA	25:a:93:ALA:HB3	1.97	0.46
31:x:48:VAL:HG23	31:x:53:LEU:HB2	1.97	0.46
33:W:375:MET:HE1	33:W:411:GLY:HA2	1.98	0.46
1:A:259:GLU:O	1:A:263:MET:HG3	2.16	0.46
2:B:75:GLU:HG3	29:f:654:VAL:HG22	1.97	0.46
9:I:15:GLU:HG3	9:I:17:ARG:HD3	1.98	0.46
19:S:13:LEU:HD13	19:S:145:LEU:HD23	1.97	0.46
25:a:320:VAL:HG12	25:a:322:GLY:H	1.81	0.46
25:a:324:ILE:HG23	25:a:331:VAL:HG12	1.98	0.46
26:b:4:GLU:HA	26:b:106:LYS:H	1.80	0.46
29:f:524:MET:HE2	29:f:776:LEU:HD23	1.97	0.46
29:f:571:GLU:HA	29:f:574:GLU:HB2	1.97	0.46
13:m:41:CYS:HB3	13:m:189:ILE:HG13	1.98	0.46
31:x:420:LEU:HD21	31:x:478:LEU:HD23	1.97	0.46
9:i:70:GLU:O	9:i:223:THR:OG1	2.34	0.46
2:B:288:ASP:OD1	2:B:288:ASP:N	2.47	0.45
5:E:180:LYS:HG2	5:E:301:ILE:HD12	1.98	0.45
13:M:3:ILE:HG23	13:M:5:THR:H	1.80	0.45
21:U:794:ASP:OD1	21:U:794:ASP:N	2.45	0.45
22:X:404:ILE:HG21	23:Y:372:LYS:HB3	1.97	0.45
15:o:159:ILE:O	15:o:163:ILE:HG12	2.16	0.45
2:B:313:LEU:HD11	2:B:346:ARG:HH11	1.81	0.45
12:L:72:ILE:HG21	12:L:88:MET:HE1	1.98	0.45
12:L:196:ARG:HH21	12:L:239:ARG:HB3	1.81	0.45
13:m:136:MET:HE2	13:m:148:LEU:HD11	1.99	0.45
14:n:191:GLY:O	14:n:196:LYS:NZ	2.50	0.45
31:x:116:MET:HE1	31:x:180:HIS:HB2	1.98	0.45
1:A:351:ARG:NH1	1:A:377:CYS:O	2.50	0.45
3:C:338:LEU:HB3	3:C:342:ILE:HD11	1.98	0.45
6:F:344:ARG:HE	6:F:351:LYS:HE2	1.81	0.45
9:I:86:LEU:HD22	9:I:114:LEU:HD11	1.97	0.45
11:K:167:ALA:HB3	12:L:56:LEU:HD13	1.97	0.45
13:M:139:SER:OG	13:M:140:TYR:N	2.48	0.45
7:g:2:SER:OG	7:g:3:ARG:N	2.48	0.45
1:A:73:ALA:HB3	1:A:78:TRP:HD1	1.82	0.45
1:A:248:LYS:HE3	1:A:290:GLY:HA3	1.99	0.45
2:B:174:MET:HE1	2:B:270:LEU:HD13	1.98	0.45
2:B:220:LYS:NZ	2:B:345:GLY:O	2.45	0.45
2:B:310:LEU:O	2:B:314:ASN:ND2	2.48	0.45
3:C:184:LYS:HE3	3:C:184:LYS:HB2	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:259:LEU:HG	4:D:283:ARG:HH21	1.80	0.45
12:L:158:ALA:HB1	12:L:172:LEU:HD13	1.97	0.45
17:Q:78:THR:O	17:Q:82:ASN:ND2	2.42	0.45
16:p:113:ASP:OD2	16:p:116:THR:N	2.42	0.45
34:V:284:GLU:OE2	34:V:287:ARG:NH1	2.48	0.45
3:C:339:THR:HG22	3:C:377:HIS:HB2	1.97	0.45
12:L:215:VAL:HB	12:L:221:PHE:HD1	1.81	0.45
21:U:763:VAL:O	21:U:767:THR:OG1	2.33	0.45
9:i:68:LEU:HD11	9:i:74:CYS:HB3	1.98	0.45
31:x:120:VAL:HA	31:x:123:ILE:HD12	1.98	0.45
32:y:33:LYS:HG3	32:y:34:GLU:HG2	1.99	0.45
33:W:188:GLU:HG2	33:W:191:ARG:HH12	1.81	0.45
34:V:234:ARG:HD2	34:V:234:ARG:HA	1.70	0.45
1:A:143:ASP:HB2	1:A:150:HIS:CE1	2.51	0.45
6:F:35:LYS:HD3	6:F:35:LYS:HA	1.82	0.45
23:Y:112:CYS:HB2	23:Y:147:ILE:HD11	1.99	0.45
24:Z:78:MET:SD	27:c:98:MET:HG2	2.57	0.45
29:f:301:HIS:HB3	29:f:456:ARG:HD2	1.98	0.45
8:h:39:LYS:HG3	8:h:44:VAL:HG22	1.99	0.45
16:p:143:ALA:HA	16:p:146:MET:HE3	1.98	0.45
17:q:172:ILE:HG13	17:q:173:LEU:HD12	1.99	0.45
34:V:98:LEU:HD22	34:V:209:LYS:HD2	1.99	0.45
6:F:221:LYS:HD2	6:F:327:LYS:HB3	1.99	0.45
8:H:139:TRP:NE1	8:H:215:GLU:OE1	2.48	0.45
23:Y:145:LEU:HG	23:Y:179:ARG:HH12	1.80	0.45
23:Y:288:PHE:HD2	23:Y:292:TYR:HE1	1.65	0.45
29:f:106:LEU:HD23	29:f:137:ARG:HD2	1.99	0.45
29:f:523:GLY:HA3	29:f:561:GLY:HA2	1.98	0.45
29:f:557:TRP:HA	29:f:560:LEU:HD12	1.99	0.45
20:t:49:THR:HG21	20:t:88:ILE:HD12	1.99	0.45
10:J:36:ARG:HD2	10:J:144:LEU:HB3	1.99	0.45
14:N:166:ARG:NH1	20:t:34:ALA:O	2.48	0.45
23:Y:12:PRO:HB2	23:Y:13:LYS:H	1.61	0.45
23:Y:224:VAL:HG21	23:Y:250:LEU:HD21	1.98	0.45
25:a:137:ASP:HA	25:a:140:GLU:HG2	1.98	0.45
9:i:69:ASN:HB2	9:i:72:MET:HB2	1.99	0.45
9:i:155:ASN:OD1	10:j:77:THR:OG1	2.35	0.45
17:q:86:ARG:NH2	17:q:90:ASP:OD1	2.49	0.45
31:x:298:ILE:HG13	32:y:12:THR:HG21	1.98	0.45
33:W:39:ARG:HG3	33:W:41:GLN:H	1.82	0.45
4:D:159:LYS:HD2	4:D:221:HIS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:155:ASP:N	23:Y:155:ASP:OD1	2.50	0.45
26:b:138:VAL:H	26:b:160:LEU:HD21	1.82	0.45
13:m:43:ASP:OD1	13:m:43:ASP:N	2.46	0.45
16:p:88:MET:HE2	16:p:88:MET:HB3	1.83	0.45
18:r:37:ILE:HD11	18:r:56:GLU:HB3	1.98	0.45
33:W:231:ILE:HG23	33:W:243:ILE:HG23	1.99	0.45
4:D:254:ALA:HB2	4:D:262:ILE:HD11	1.99	0.45
6:F:124:ILE:HD11	6:F:160:ILE:HD11	1.98	0.45
21:U:327:LYS:HE2	21:U:327:LYS:HB2	1.86	0.45
27:c:189:ILE:HA	27:c:192:LEU:HB2	1.99	0.45
8:h:124:SER:OG	8:h:125:GLY:N	2.50	0.45
16:p:58:THR:OG1	17:q:121:LEU:O	2.31	0.45
18:r:182:ASP:OD1	18:r:182:ASP:N	2.46	0.45
19:s:172:MET:HE3	19:s:172:MET:HB3	1.79	0.45
34:V:438:VAL:HG11	34:V:451:ILE:HD13	1.99	0.45
5:E:56:ILE:N	5:E:100:LEU:O	2.45	0.44
16:P:25:ASP:O	16:P:41:LYS:NZ	2.49	0.44
29:f:318:THR:HB	29:f:456:ARG:HH22	1.81	0.44
29:f:350:LYS:HA	29:f:751:TYR:CZ	2.52	0.44
8:h:163:MET:HE3	8:h:163:MET:HB2	1.88	0.44
13:m:8:ASP:OD1	13:m:8:ASP:N	2.48	0.44
17:Q:22:ALA:HA	17:Q:27:GLN:HA	2.00	0.44
20:T:27:LEU:HD22	20:T:184:TYR:HB2	1.99	0.44
27:c:161:ARG:NH1	27:c:201:TYR:OH	2.45	0.44
27:c:163:ILE:HG22	27:c:201:TYR:HD1	1.82	0.44
9:i:119:GLN:HG3	10:j:78:ALA:HB1	1.99	0.44
33:W:278:PRO:HG3	33:W:357:ARG:HH21	1.81	0.44
34:V:340:GLY:HA2	34:V:405:THR:HB	1.98	0.44
1:A:229:VAL:O	1:A:233:THR:OG1	2.33	0.44
3:C:108:VAL:HB	3:C:112:CYS:HB2	1.98	0.44
21:U:26:LYS:HG2	28:d:36:LEU:HG	1.99	0.44
29:f:718:ASP:HB3	29:f:755:ASP:HB3	1.98	0.44
9:i:3:ARG:NH1	11:k:9:ASP:O	2.49	0.44
8:H:148:GLN:OE1	8:H:158:TRP:NE1	2.50	0.44
9:I:226:ARG:NH2	9:I:232:GLU:OE2	2.50	0.44
12:L:233:LEU:HA	12:L:236:LEU:HD13	1.99	0.44
29:f:512:MET:HE1	29:f:555:ALA:HB2	1.99	0.44
29:f:764:LEU:HD23	29:f:764:LEU:HA	1.85	0.44
9:i:239:LYS:HE3	9:i:239:LYS:HB2	1.83	0.44
33:W:248:ARG:HE	33:W:289:ARG:CZ	2.31	0.44
34:V:225:ASP:OD1	34:V:228:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:303:LEU:HD23	5:E:304:PRO:HD3	1.98	0.44
17:Q:27:GLN:NE2	17:q:169:LYS:O	2.45	0.44
22:X:172:LEU:HD23	22:X:175:LYS:HD3	1.99	0.44
28:d:11:ARG:HG2	28:d:12:LYS:HG2	1.99	0.44
29:f:313:GLU:HB3	29:f:316:ASP:HB3	2.00	0.44
34:V:123:SER:OG	34:V:155:ALA:O	2.35	0.44
34:V:355:ARG:HH11	35:e:27:TRP:HB2	1.83	0.44
1:A:381:THR:HG22	1:A:384:GLU:HG3	2.00	0.44
4:D:242:GLU:OE1	4:D:245:ARG:NH1	2.41	0.44
21:U:660:CYS:HB3	21:U:663:THR:HB	1.99	0.44
21:U:809:SER:OG	21:U:810:THR:N	2.51	0.44
21:U:902:PRO:HA	21:U:914:LEU:HA	1.99	0.44
28:d:29:VAL:HG11	28:d:54:ILE:HD11	1.98	0.44
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.99	0.44
31:x:418:TYR:HB3	31:x:480:TYR:HB3	2.00	0.44
7:G:180:GLU:HA	7:G:183:VAL:HG12	2.00	0.44
22:X:283:GLN:HG3	22:X:312:GLU:HG3	1.98	0.44
22:X:372:LYS:HD3	22:X:372:LYS:HA	1.72	0.44
26:b:129:LYS:HD3	26:b:129:LYS:HA	1.79	0.44
27:c:223:LYS:HD2	27:c:223:LYS:HA	1.79	0.44
29:f:431:LYS:HG3	31:x:78:LEU:HB3	2.00	0.44
10:j:94:HIS:ND1	10:j:102:VAL:HG22	2.33	0.44
31:x:71:MET:O	31:x:72:MET:HE2	2.17	0.44
1:A:198:PRO:HA	1:A:201:PHE:HD2	1.83	0.44
5:E:98:VAL:HA	5:E:110:TYR:HA	1.99	0.44
29:f:130:ALA:O	29:f:134:SER:N	2.41	0.44
8:H:74:LEU:HD11	8:H:134:LEU:HD22	2.00	0.44
10:J:195:LEU:HD23	10:J:195:LEU:HA	1.90	0.44
23:Y:141:VAL:HG11	23:Y:164:ALA:HB2	2.00	0.44
23:Y:301:ILE:HD13	23:Y:342:ARG:HD2	2.00	0.44
24:Z:247:LYS:HD3	33:W:425:LEU:HB2	1.99	0.44
28:d:249:TYR:OH	34:V:477:HIS:ND1	2.47	0.44
29:f:761:MET:HG2	29:f:763:ARG:H	1.82	0.44
29:f:771:LEU:HG	29:f:774:GLY:H	1.83	0.44
18:r:59:LEU:HD22	18:r:83:LEU:HD12	2.00	0.44
20:t:103:MET:HE3	20:t:103:MET:HB3	1.84	0.44
1:A:346:PRO:O	1:A:351:ARG:NE	2.51	0.43
5:E:168:LYS:HA	5:E:168:LYS:HD3	1.76	0.43
12:L:100:ASP:OD1	19:S:66:LYS:NZ	2.51	0.43
21:U:840:LYS:HB2	29:f:607:LEU:HD11	2.00	0.43
21:U:849:LYS:HA	21:U:853:LYS:HZ3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:134:PRO:HB3	27:c:220:LEU:HG	2.00	0.43
25:a:54:ASP:HA	25:a:57:ILE:HG22	2.00	0.43
25:a:284:ARG:HH21	25:a:291:LEU:HB2	1.83	0.43
29:f:133:MET:O	29:f:137:ARG:HG2	2.18	0.43
29:f:526:ALA:O	29:f:565:ASN:ND2	2.51	0.43
15:o:1:THR:O	15:o:129:SER:N	2.51	0.43
17:q:62:LYS:HA	17:q:62:LYS:HD3	1.78	0.43
31:x:372:SER:HA	31:x:375:LYS:HE3	2.00	0.43
31:x:381:LYS:HA	31:x:381:LYS:HD3	1.80	0.43
33:W:144:ARG:HH21	33:W:148:THR:HG23	1.81	0.43
1:A:125:LEU:HA	1:A:149:ILE:HB	2.00	0.43
2:B:420:LYS:HA	2:B:423:LYS:HE2	1.99	0.43
8:H:77:SER:HB2	8:H:163:MET:HE3	1.99	0.43
9:I:41:ASP:OD1	9:I:41:ASP:N	2.51	0.43
14:N:91:ARG:NH2	20:T:56:ASP:OD2	2.50	0.43
22:X:256:LEU:HD12	22:X:319:ILE:HG13	1.99	0.43
23:Y:349:LYS:HG3	23:Y:350:VAL:HG22	2.00	0.43
24:Z:129:LYS:HG3	27:c:215:LYS:HE3	1.98	0.43
12:l:207:THR:OG1	12:l:226:ASP:O	2.36	0.43
31:x:427:GLN:HB2	31:x:473:HIS:CD2	2.53	0.43
33:W:140:ILE:HD13	33:W:140:ILE:HA	1.88	0.43
34:V:355:ARG:NH1	35:e:27:TRP:O	2.51	0.43
34:V:406:GLY:HA2	34:V:409:MET:HE3	2.00	0.43
3:C:155:ASP:OD1	3:C:155:ASP:N	2.51	0.43
5:E:137:GLY:HA3	5:E:308:ALA:HB2	1.99	0.43
5:E:311:ASP:HA	5:E:314:LYS:HG2	2.01	0.43
9:I:140:ASP:OD1	9:I:140:ASP:N	2.52	0.43
29:f:441:LYS:HB3	29:f:477:MET:HE1	2.00	0.43
17:q:5:ILE:HD11	17:q:143:LEU:HD11	2.01	0.43
32:y:23:ILE:HD11	32:y:52:ASP:HA	2.00	0.43
33:W:75:TYR:HA	33:W:83:LEU:HD11	1.99	0.43
2:B:320:ASP:OD1	2:B:321:SER:N	2.51	0.43
5:E:196:LEU:HD12	5:E:230:ILE:HG12	2.00	0.43
6:F:334:ARG:HA	6:F:334:ARG:HD3	1.84	0.43
9:I:67:LYS:HA	9:I:73:ALA:HA	2.01	0.43
25:a:89:ASP:OD1	25:a:89:ASP:N	2.51	0.43
12:l:81:ALA:HB2	12:l:130:VAL:HG21	2.01	0.43
20:t:27:LEU:HD11	20:t:34:ALA:HB1	2.00	0.43
31:x:126:VAL:HG13	31:x:323:TYR:HE2	1.83	0.43
31:x:483:ARG:NH1	31:x:484:ARG:O	2.51	0.43
23:Y:128:TYR:CZ	23:Y:137:ARG:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:d:45:LYS:O	28:d:49:ILE:HG12	2.18	0.43
29:f:407:MET:HB3	29:f:440:ILE:HG12	2.00	0.43
8:h:196:LYS:HA	8:h:203:MET:HE1	2.00	0.43
11:k:78:MET:HE2	11:k:78:MET:HB3	1.93	0.43
31:x:346:ASP:OD1	31:x:346:ASP:N	2.51	0.43
14:N:32:ASP:OD1	14:N:32:ASP:N	2.51	0.43
17:Q:180:VAL:HG13	17:Q:191:LEU:HB2	2.00	0.43
21:U:233:LEU:HD21	21:U:325:MET:HG3	2.01	0.43
23:Y:123:ALA:HA	23:Y:126:LYS:HE3	1.99	0.43
3:C:164:VAL:HG11	3:C:313:ARG:HE	1.83	0.43
10:J:221:ASN:HB3	10:J:224:GLU:HG3	2.01	0.43
13:M:37:ILE:HD11	13:M:193:VAL:HG13	1.99	0.43
21:U:619:VAL:HG23	21:U:651:GLY:HA3	1.99	0.43
24:Z:177:ARG:HA	24:Z:177:ARG:HD3	1.81	0.43
24:Z:239:ASP:HB2	25:a:289:ARG:HH21	1.83	0.43
10:j:4:ASP:OD1	10:j:4:ASP:N	2.52	0.43
16:p:53:LEU:HB3	16:p:60:VAL:HG22	2.01	0.43
34:V:150:ARG:NH1	34:V:157:THR:O	2.52	0.43
18:R:127:SER:HB3	18:R:136:TYR:CE1	2.54	0.43
20:T:103:MET:HE2	20:T:103:MET:H	1.83	0.43
21:U:91:ASN:HD21	21:U:97:VAL:HG21	1.83	0.43
22:X:190:LEU:HD22	22:X:217:ILE:HD12	2.00	0.43
24:Z:94:TRP:CG	24:Z:112:MET:HE1	2.54	0.43
26:b:33:VAL:HG11	26:b:75:LEU:HD21	2.00	0.43
29:f:229:VAL:HB	29:f:605:ASN:HB3	2.01	0.43
33:W:194:LEU:HD23	33:W:194:LEU:HA	1.87	0.43
4:D:235:PHE:HE1	4:D:270:ILE:HD12	1.84	0.43
6:F:92:ASN:HA	6:F:150:LEU:HA	2.00	0.43
6:F:262:GLY:H	6:F:308:ARG:HD3	1.83	0.43
8:H:130:PHE:HB3	8:H:132:VAL:HG12	2.01	0.43
15:O:63:LEU:HD11	15:O:79:ALA:HB2	2.01	0.43
21:U:18:GLN:HE22	28:d:27:LYS:HD2	1.83	0.43
21:U:617:ALA:HA	21:U:620:GLU:HG3	2.01	0.43
24:Z:148:GLY:HA2	25:a:181:GLY:CA	2.49	0.43
26:b:117:VAL:O	26:b:152:LYS:NZ	2.51	0.43
33:W:61:VAL:HG12	33:W:65:ARG:HE	1.83	0.43
34:V:435:GLU:HG2	34:V:453:HIS:HD2	1.83	0.43
1:A:386:ARG:HH22	2:B:216:ILE:HG22	1.83	0.43
3:C:223:PHE:HA	30:v:21:UNK:HA	2.01	0.43
4:D:207:PRO:HG2	4:D:335:LEU:HB2	2.01	0.43
5:E:355:ILE:HG13	6:F:212:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:45:VAL:HG21	12:L:188:VAL:HG22	2.01	0.43
29:f:675:PHE:O	29:f:715:HIS:NE2	2.51	0.43
13:m:34:SER:HB3	13:m:65:ARG:HH12	1.84	0.43
16:p:30:ILE:HG22	16:p:31:GLN:H	1.83	0.43
18:r:1:THR:N	18:r:169:TYR:O	2.52	0.43
33:W:268:LYS:HB3	33:W:336:PRO:HG2	2.01	0.43
1:A:286:ASP:OD1	1:A:287:ASP:N	2.50	0.42
2:B:435:PRO:HD2	2:B:438:LEU:HD12	2.01	0.42
3:C:80:MET:HB2	3:C:84:LYS:HB2	2.00	0.42
5:E:202:SER:HB2	6:F:300:LYS:HD2	2.01	0.42
8:H:120:GLU:OE2	8:H:123:GLN:NE2	2.51	0.42
14:N:40:ARG:NH2	14:N:181:GLU:O	2.45	0.42
27:c:54:MET:HB2	27:c:82:VAL:HG12	2.01	0.42
27:c:75:MET:HB2	27:c:75:MET:HE2	1.78	0.42
27:c:238:CYS:SG	27:c:239:LYS:N	2.92	0.42
29:f:61:GLU:HG3	29:f:97:LYS:HB2	2.01	0.42
29:f:350:LYS:HB2	29:f:350:LYS:HE3	1.74	0.42
20:t:122:LEU:HG	20:t:137:LEU:HD12	2.01	0.42
3:C:254:ILE:HG13	3:C:269:VAL:HB	2.01	0.42
5:E:246:GLY:HA3	5:E:250:ASP:HB2	2.01	0.42
7:G:14:THR:HB	8:H:128:ARG:HB3	2.01	0.42
7:G:112:ASP:HB3	7:G:152:TYR:CZ	2.54	0.42
21:U:397:THR:OG1	21:U:401:LYS:NZ	2.52	0.42
23:Y:57:LEU:HD23	23:Y:63:TRP:HA	2.00	0.42
26:b:107:MET:HB2	26:b:136:VAL:HG12	2.00	0.42
10:j:8:THR:HG22	10:j:18:GLN:HB2	2.01	0.42
19:s:199:THR:OG1	19:s:200:LYS:N	2.52	0.42
20:t:22:ILE:HG12	20:t:50:MET:HE3	2.01	0.42
31:x:211:LEU:HG	31:x:215:LEU:HD13	2.01	0.42
33:W:324:TYR:HB3	33:W:328:LEU:HD13	2.01	0.42
4:D:349:THR:HA	4:D:352:MET:HG2	2.01	0.42
5:E:340:GLY:HA3	37:E:501:ADP:C5	2.53	0.42
7:G:132:ARG:HG3	13:M:12:SER:HA	2.01	0.42
12:L:176:MET:HE1	13:M:56:LYS:HB3	2.01	0.42
29:f:230:CYS:HB3	29:f:232:TYR:CE1	2.54	0.42
29:f:655:LEU:HG	29:f:659:LEU:HD12	2.00	0.42
7:g:143:ILE:HG12	7:g:220:VAL:HG13	2.00	0.42
7:g:155:ASP:OD1	7:g:159:TYR:N	2.43	0.42
20:t:45:VAL:HB	20:t:49:THR:HG23	2.01	0.42
4:D:176:GLU:OE1	4:D:329:ARG:NH1	2.53	0.42
7:G:46:ASP:OD1	7:G:46:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:119:GLN:HB3	8:H:153:GLY:HA3	2.02	0.42
20:T:211:ILE:HA	20:T:214:MET:HE2	2.00	0.42
21:U:720:LYS:HB3	21:U:720:LYS:HE3	1.81	0.42
22:X:255:LEU:HB2	22:X:287:LEU:HD13	2.02	0.42
23:Y:148:GLY:HA3	23:Y:157:ILE:HD11	2.01	0.42
28:d:69:PRO:O	28:d:73:ARG:HG2	2.19	0.42
29:f:448:CYS:HB2	29:f:466:LEU:HD21	2.01	0.42
11:k:196:LYS:O	11:k:200:ILE:HG12	2.19	0.42
31:x:305:LEU:HG	31:x:307:ARG:HG2	2.01	0.42
34:V:337:LEU:HD21	34:V:364:THR:HG23	2.00	0.42
34:V:419:LEU:HD13	34:V:435:GLU:HG3	1.99	0.42
6:F:186:SER:O	6:F:364:ARG:NH1	2.52	0.42
6:F:438:TYR:OH	11:K:19:GLY:O	2.38	0.42
24:Z:183:THR:OG1	24:Z:184:VAL:N	2.51	0.42
27:c:178:THR:OG1	27:c:179:SER:N	2.52	0.42
27:c:183:HIS:HD2	27:c:184:LEU:HD23	1.83	0.42
4:D:159:LYS:HD3	4:D:160:PRO:HD2	2.02	0.42
6:F:42:ILE:HD12	25:a:66:GLU:HG2	2.00	0.42
16:P:30:ILE:HG22	16:P:31:GLN:H	1.85	0.42
21:U:812:ALA:HB3	21:U:883:ARG:HH22	1.84	0.42
23:Y:72:LYS:HD2	23:Y:72:LYS:HA	1.79	0.42
24:Z:7:GLN:N	24:Z:46:LYS:O	2.51	0.42
24:Z:223:ASN:HB3	24:Z:226:ILE:HB	2.02	0.42
29:f:744:MET:HE3	29:f:744:MET:HB3	1.96	0.42
13:m:134:SER:HB2	13:m:153:PRO:HD3	2.02	0.42
20:t:126:ASP:OD1	20:t:130:VAL:N	2.52	0.42
33:W:173:THR:HG23	33:W:182:ARG:HG2	2.00	0.42
1:A:141:GLY:N	1:A:151:ILE:O	2.48	0.42
2:B:297:SER:HB3	2:B:302:GLU:HG3	2.00	0.42
3:C:46:GLN:HG2	21:U:639:LEU:HD21	2.01	0.42
3:C:159:LYS:HD3	3:C:159:LYS:HA	1.93	0.42
3:C:351:MET:HE1	3:C:359:VAL:HG22	2.02	0.42
4:D:153:MET:HE1	4:D:227:PHE:H	1.85	0.42
12:L:7:ASP:OD1	12:L:7:ASP:N	2.51	0.42
21:U:793:LYS:H	21:U:796:LYS:HB3	1.85	0.42
22:X:367:GLN:NE2	22:X:371:ASP:OD2	2.51	0.42
24:Z:39:LEU:HD11	24:Z:50:VAL:HB	2.01	0.42
24:Z:63:LYS:HD3	26:b:91:ARG:HH22	1.85	0.42
26:b:130:ARG:HA	26:b:130:ARG:HD3	1.76	0.42
29:f:392:THR:HG22	29:f:414:LEU:HD12	2.00	0.42
19:s:91:MET:HE2	19:s:91:MET:HB3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LEU:HD21	11:K:207:GLU:HA	2.00	0.42
4:D:259:PRO:HB3	4:D:304:ASN:HB3	2.01	0.42
11:K:28:ILE:O	11:K:31:ILE:HG12	2.19	0.42
22:X:88:LEU:O	22:X:91:SER:OG	2.29	0.42
25:a:213:PHE:HD2	25:a:216:LEU:HB2	1.85	0.42
26:b:171:VAL:HG11	26:b:187:PRO:HG3	2.01	0.42
29:f:702:PRO:O	29:f:706:ILE:HG12	2.20	0.42
4:D:228:ILE:HB	4:D:262:ILE:HD13	2.01	0.42
4:D:262:ILE:HB	4:D:307:VAL:HG12	2.02	0.42
6:F:266:LYS:HE2	6:F:266:LYS:HB3	1.95	0.42
27:c:130:GLN:NE2	27:c:140:ALA:O	2.35	0.42
29:f:431:LYS:HD3	31:x:78:LEU:HD13	2.01	0.42
29:f:637:LYS:HD2	29:f:678:LEU:HD13	2.01	0.42
29:f:745:LEU:HD23	29:f:745:LEU:HA	1.75	0.42
8:h:9:SER:HA	8:h:125:GLY:HA2	2.01	0.42
14:n:101:ALA:HB2	14:n:111:VAL:HG23	2.02	0.42
14:n:192:ASP:OD1	14:n:192:ASP:N	2.52	0.42
31:x:460:PRO:HA	31:x:463:ILE:HG12	2.02	0.42
33:W:44:ILE:HA	33:W:47:LEU:HB2	2.01	0.42
3:C:391:MET:SD	3:C:391:MET:N	2.93	0.42
9:I:64:LYS:HB3	9:I:64:LYS:HE2	1.83	0.42
13:M:163:CYS:SG	13:M:164:ALA:N	2.93	0.42
16:P:151:GLU:OE1	19:s:185:ARG:NH2	2.46	0.42
20:T:98:SER:O	20:T:102:LYS:NZ	2.53	0.42
28:d:189:ILE:HB	28:d:194:ALA:HB2	2.02	0.42
29:f:139:CYS:SG	29:f:143:ARG:NH2	2.92	0.42
20:t:1:THR:N	20:t:105:PRO:O	2.52	0.42
31:x:27:MET:HE3	31:x:27:MET:O	2.20	0.42
31:x:483:ARG:HD2	31:x:483:ARG:HA	1.93	0.42
33:W:259:GLU:HG3	33:W:262:LYS:H	1.84	0.42
34:V:355:ARG:NH2	35:e:31:ASP:OD1	2.53	0.42
1:A:123:VAL:HG12	6:F:87:PRO:HB3	2.02	0.41
5:E:147:GLU:HA	5:E:151:LEU:HD23	2.01	0.41
7:G:132:ARG:HA	7:G:133:PRO:HD3	1.92	0.41
16:P:25:ASP:OD1	16:P:41:LYS:NZ	2.54	0.41
19:S:76:LYS:HE3	19:S:76:LYS:HB2	1.76	0.41
28:d:79:LYS:O	28:d:83:PHE:N	2.53	0.41
29:f:683:GLU:HB3	29:f:687:ARG:HG3	2.02	0.41
15:o:208:THR:OG1	16:p:165:GLU:OE1	2.36	0.41
34:V:403:ILE:HG21	34:V:437:ILE:HD13	2.01	0.41
5:E:182:LEU:HD23	5:E:185:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:190:ASP:OD1	18:R:190:ASP:N	2.52	0.41
20:T:107:TRP:HA	20:T:127:MET:HE2	2.01	0.41
23:Y:387:ILE:HD12	23:Y:387:ILE:HA	1.91	0.41
24:Z:16:LEU:HB3	27:c:216:MET:HE1	2.01	0.41
26:b:40:LYS:O	26:b:43:SER:OG	2.29	0.41
27:c:27:THR:OG1	27:c:28:ALA:N	2.53	0.41
14:n:160:LEU:O	14:n:164:MET:HG3	2.20	0.41
18:r:7:LYS:NZ	18:r:123:GLY:O	2.53	0.41
19:s:133:ASP:OD1	19:s:133:ASP:N	2.51	0.41
33:W:84:ASN:ND2	33:W:126:ASP:OD2	2.36	0.41
1:A:127:ASP:OD1	1:A:127:ASP:N	2.52	0.41
6:F:377:PRO:HB3	6:F:415:LEU:HD12	2.02	0.41
9:I:160:LYS:NZ	9:I:181:GLU:OE2	2.46	0.41
12:L:172:LEU:O	12:L:176:MET:HB3	2.20	0.41
21:U:772:TRP:HD1	21:U:775:LEU:HG	1.84	0.41
26:b:25:ARG:NH1	26:b:114:GLY:O	2.53	0.41
13:m:37:ILE:HD11	13:m:193:VAL:HG13	2.02	0.41
19:s:71:ARG:HH11	19:s:95:ILE:HD11	1.86	0.41
33:W:174:TYR:HA	33:W:177:MET:HE3	2.02	0.41
33:W:194:LEU:HD12	33:W:229:LEU:HD12	2.02	0.41
3:C:259:LEU:HD23	3:C:259:LEU:HA	1.90	0.41
4:D:338:ARG:HA	4:D:338:ARG:HD2	1.93	0.41
5:E:93:LYS:HA	5:E:93:LYS:HD2	1.85	0.41
6:F:363:ALA:HA	6:F:366:MET:HE2	2.02	0.41
12:L:6:TYR:OH	13:M:8:ASP:OD2	2.27	0.41
27:c:180:ASN:OD1	27:c:183:HIS:NE2	2.53	0.41
28:d:181:CYS:HB2	34:V:443:ARG:HH21	1.85	0.41
29:f:266:LEU:HB3	29:f:269:ALA:HB3	2.02	0.41
12:l:155:ASP:HB3	13:m:62:SER:HB2	2.03	0.41
31:x:250:GLU:O	31:x:318:SER:N	2.53	0.41
33:W:157:GLY:HA3	33:W:192:LEU:HD22	2.02	0.41
33:W:256:ILE:HD13	33:W:256:ILE:HA	1.95	0.41
33:W:268:LYS:HD2	33:W:336:PRO:HD2	2.02	0.41
34:V:255:LEU:HD23	34:V:255:LEU:HA	1.93	0.41
2:B:40:THR:HA	2:B:278:ALA:HB2	2.03	0.41
5:E:161:ARG:HD3	5:E:161:ARG:HA	1.83	0.41
9:I:49:ARG:NH2	9:I:211:VAL:O	2.47	0.41
22:X:261:LEU:HD23	22:X:261:LEU:HA	1.88	0.41
24:Z:17:LEU:HB3	27:c:36:LEU:HB3	2.02	0.41
26:b:44:ASN:ND2	26:b:46:GLU:OE1	2.51	0.41
28:d:15:ASN:OD1	28:d:15:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:d:203:PRO:HG2	28:d:206:MET:HG3	2.02	0.41
29:f:288:VAL:HG11	29:f:872:VAL:HG23	2.01	0.41
8:h:119:GLN:HG3	9:i:81:SER:HB3	2.03	0.41
12:l:158:ALA:HB1	12:l:172:LEU:HD13	2.02	0.41
12:l:172:LEU:O	12:l:176:MET:HB3	2.20	0.41
31:x:243:ILE:O	31:x:247:PHE:HB2	2.20	0.41
33:W:315:MET:HE2	33:W:315:MET:HB2	1.89	0.41
3:C:319:PRO:HA	3:C:320:PRO:HD3	1.89	0.41
5:E:63:GLN:NE2	5:E:92:LEU:O	2.51	0.41
9:I:72:MET:HE3	9:I:72:MET:HB3	1.85	0.41
21:U:243:LEU:HD13	21:U:915:LYS:HE2	2.01	0.41
22:X:334:ASN:OD1	22:X:337:ARG:NH2	2.53	0.41
23:Y:93:LYS:HD3	23:Y:93:LYS:HA	1.89	0.41
26:b:18:ASN:O	26:b:24:THR:OG1	2.34	0.41
8:h:86:LEU:HD13	8:h:134:LEU:HD11	2.02	0.41
34:V:175:MET:HE3	34:V:180:ARG:HB2	2.01	0.41
2:B:49:LEU:HD21	29:f:649:HIS:HB2	2.02	0.41
4:D:154:LEU:HA	4:D:158:GLN:HE21	1.85	0.41
20:T:48:SER:O	20:T:48:SER:OG	2.39	0.41
21:U:369:THR:HG23	21:U:731:ILE:HD13	2.02	0.41
24:Z:81:MET:HE2	24:Z:81:MET:HB2	1.85	0.41
29:f:333:LEU:HD13	29:f:810:ILE:HD12	2.03	0.41
10:j:41:VAL:HG11	10:j:134:VAL:HB	2.02	0.41
34:V:185:GLN:HG3	34:V:218:TYR:CE1	2.49	0.41
34:V:419:LEU:HA	34:V:422:ILE:HG22	2.02	0.41
4:D:213:THR:OG1	36:D:501:ATP:O1A	2.37	0.41
5:E:4:PRO:HG2	5:E:8:ALA:HB2	2.01	0.41
5:E:198:VAL:HG12	5:E:200:SER:H	1.86	0.41
10:J:13:ASP:OD1	10:J:13:ASP:N	2.52	0.41
13:M:23:VAL:O	13:M:27:MET:HG2	2.21	0.41
25:a:257:GLN:HB3	25:a:261:LEU:HD12	2.03	0.41
28:d:204:LYS:HA	28:d:204:LYS:HD2	1.87	0.41
29:f:664:GLU:O	29:f:669:GLU:N	2.52	0.41
12:l:40:SER:HB3	12:l:187:LEU:HD11	2.02	0.41
1:A:129:VAL:O	31:x:334:LYS:NZ	2.47	0.41
1:A:172:VAL:O	1:A:231:ASN:ND2	2.51	0.41
1:A:236:CYS:HB2	1:A:267:LYS:HD2	2.02	0.41
4:D:59:GLU:OE1	21:U:600:ARG:NH1	2.54	0.41
6:F:46:ARG:HB2	25:a:66:GLU:HA	2.03	0.41
11:K:50:VAL:HB	11:K:66:LYS:HD3	2.03	0.41
15:O:68:LEU:HD23	15:O:68:LEU:HA	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:210:LYS:HE3	21:U:210:LYS:HB2	1.85	0.41
21:U:901:GLN:N	21:U:915:LYS:O	2.53	0.41
23:Y:101:ARG:NH2	23:Y:136:HIS:HB3	2.35	0.41
25:a:326:GLU:HG2	33:W:373:ILE:HD12	2.01	0.41
27:c:164:ASN:ND2	27:c:166:ASN:OD1	2.53	0.41
29:f:155:GLY:HA2	29:f:158:TYR:HB2	2.02	0.41
29:f:870:THR:HA	29:f:871:PRO:HD3	1.91	0.41
9:i:187:LYS:H	9:i:187:LYS:HG2	1.68	0.41
31:x:356:TYR:HD2	31:x:364:GLN:HG3	1.86	0.41
31:x:391:LYS:HA	31:x:391:LYS:HD2	1.94	0.41
33:W:94:ARG:HD3	33:W:96:GLN:H	1.84	0.41
1:A:139:ARG:NH2	1:A:154:PRO:O	2.54	0.41
1:A:403:ILE:HD13	1:A:403:ILE:HA	1.88	0.41
3:C:158:ILE:HA	3:C:161:ILE:HG22	2.03	0.41
15:O:86:MET:HB3	15:O:86:MET:HE3	1.79	0.41
15:O:97:ALA:HB1	15:O:127:MET:HE2	2.02	0.41
21:U:92:ASP:OD1	21:U:92:ASP:N	2.54	0.41
21:U:115:ASN:HD21	21:U:124:LYS:H	1.68	0.41
29:f:413:SER:HA	29:f:416:MET:HG3	2.03	0.41
8:h:223:PRO:HA	8:h:226:VAL:HG12	2.03	0.41
13:m:188:ASP:O	13:m:192:GLU:HG2	2.21	0.41
2:B:35:LYS:HB2	2:B:38:LYS:HD3	2.03	0.40
5:E:203:ILE:HD11	5:E:238:ILE:HD13	2.04	0.40
9:I:174:MET:HE1	9:I:199:LYS:HB3	2.03	0.40
18:R:18:SER:HB3	18:R:173:ALA:H	1.86	0.40
19:S:91:MET:HE2	19:S:91:MET:HB3	1.96	0.40
21:U:821:LYS:HE3	21:U:821:LYS:HB3	1.90	0.40
25:a:246:GLU:HB3	25:a:249:GLN:HB2	2.02	0.40
29:f:603:SER:H	29:f:639:LYS:HA	1.86	0.40
12:l:117:GLN:O	12:l:120:THR:OG1	2.32	0.40
16:p:14:MET:HG2	16:p:136:PHE:HB3	2.04	0.40
20:t:185:ASN:OD1	20:t:204:SER:OG	2.35	0.40
33:W:186:ILE:HB	33:W:209:ILE:HD11	2.04	0.40
1:A:219:GLY:O	1:A:381:THR:OG1	2.32	0.40
2:B:51:LEU:HD12	2:B:51:LEU:HA	1.88	0.40
2:B:391:SER:OG	2:B:394:ASP:OD2	2.32	0.40
3:C:316:GLU:HG2	3:C:318:PRO:HD3	2.03	0.40
4:D:294:ASN:O	4:D:294:ASN:ND2	2.54	0.40
5:E:170:CYS:SG	5:E:171:LEU:N	2.94	0.40
6:F:295:ARG:HE	6:F:300:LYS:HZ1	1.67	0.40
8:H:82:ASP:HB3	8:H:130:PHE:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:192:GLU:O	13:M:196:ILE:HG12	2.21	0.40
16:P:14:MET:HB3	16:P:163:LEU:HD11	2.03	0.40
22:X:200:ILE:HD12	22:X:200:ILE:HA	1.98	0.40
23:Y:181:LYS:NZ	23:Y:213:LEU:HD11	2.36	0.40
24:Z:272:LEU:HD23	24:Z:272:LEU:HA	1.95	0.40
25:a:8:LEU:HD22	25:a:26:GLU:HB2	2.02	0.40
26:b:7:MET:HE1	26:b:93:ALA:HA	2.03	0.40
28:d:188:LYS:HB2	28:d:188:LYS:HE3	1.86	0.40
29:f:118:ASN:OD1	29:f:118:ASN:N	2.54	0.40
13:m:229:LYS:O	13:m:233:GLU:HG2	2.22	0.40
20:t:12:LEU:HD13	20:t:173:MET:HE2	2.03	0.40
31:x:301:GLN:NE2	32:y:16:GLU:OE1	2.50	0.40
33:W:254:PRO:HB3	33:W:263:TRP:CG	2.56	0.40
34:V:78:HIS:NE2	34:V:100:MET:HE3	2.36	0.40
1:A:213:LEU:HD11	1:A:321:THR:HG22	2.04	0.40
6:F:219:PRO:HG2	6:F:221:LYS:HE2	2.03	0.40
16:P:58:THR:HA	17:Q:85:ARG:HH21	1.86	0.40
21:U:543:LYS:NZ	21:U:771:PHE:O	2.54	0.40
24:Z:176:LEU:HD23	24:Z:176:LEU:HA	1.92	0.40
25:a:321:LYS:HB2	25:a:334:THR:HB	2.04	0.40
28:d:203:PRO:HB2	28:d:204:LYS:H	1.71	0.40
16:p:68:LYS:HD2	16:p:68:LYS:HA	1.91	0.40
17:q:52:ASP:OD1	18:r:88:TYR:OH	2.32	0.40
18:r:127:SER:HB2	18:r:136:TYR:HE1	1.87	0.40
4:D:340:GLN:HA	4:D:343:LEU:HD12	2.03	0.40
6:F:59:VAL:O	6:F:63:THR:OG1	2.30	0.40
9:I:90:LEU:HG	9:I:114:LEU:HD13	2.02	0.40
19:S:28:ARG:NH2	19:S:191:ASP:OD1	2.45	0.40
21:U:535:TYR:HD2	21:U:548:LEU:HD11	1.86	0.40
21:U:579:ARG:NH2	21:U:609:ASP:OD1	2.43	0.40
21:U:727:LYS:HB3	21:U:727:LYS:HE2	1.87	0.40
29:f:261:ARG:HH12	29:f:295:ALA:C	2.30	0.40
29:f:554:TYR:OH	29:f:789:SER:O	2.36	0.40
29:f:617:SER:HB2	29:f:632:LYS:HE2	2.04	0.40
10:j:201:SER:OG	10:j:205:ASN:OD1	2.32	0.40
31:x:104:PRO:HB3	31:x:124:ARG:HH22	1.86	0.40
5:E:126:ASP:OD1	5:E:126:ASP:N	2.55	0.40
5:E:180:LYS:HB3	5:E:278:ALA:HB1	2.04	0.40
13:M:70:ASP:HB3	13:M:73:VAL:HG12	2.04	0.40
21:U:35:TRP:HH2	34:V:232:HIS:HB3	1.87	0.40
29:f:632:LYS:HA	29:f:635:LYS:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:y:60:ASN:O	32:y:62:GLN:NE2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/433 (95%)	371 (90%)	39 (10%)	1 (0%)	43	71
2	B	409/440 (93%)	367 (90%)	41 (10%)	1 (0%)	43	71
3	C	394/398 (99%)	351 (89%)	41 (10%)	2 (0%)	24	55
4	D	378/418 (90%)	336 (89%)	42 (11%)	0	100	100
5	E	387/403 (96%)	348 (90%)	39 (10%)	0	100	100
6	F	391/439 (89%)	364 (93%)	27 (7%)	0	100	100
7	G	238/246 (97%)	224 (94%)	14 (6%)	0	100	100
7	g	242/246 (98%)	235 (97%)	7 (3%)	0	100	100
8	H	230/234 (98%)	215 (94%)	15 (6%)	0	100	100
8	h	230/234 (98%)	218 (95%)	12 (5%)	0	100	100
9	I	246/261 (94%)	236 (96%)	10 (4%)	0	100	100
9	i	248/261 (95%)	241 (97%)	7 (3%)	0	100	100
10	J	237/248 (96%)	230 (97%)	7 (3%)	0	100	100
10	j	237/248 (96%)	227 (96%)	10 (4%)	0	100	100
11	K	236/241 (98%)	231 (98%)	5 (2%)	0	100	100
11	k	232/241 (96%)	223 (96%)	9 (4%)	0	100	100
12	L	75/269 (28%)	73 (97%)	2 (3%)	0	100	100
12	l	236/269 (88%)	228 (97%)	8 (3%)	0	100	100
13	M	171/255 (67%)	166 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	238/255 (93%)	236 (99%)	2 (1%)	0	100	100
14	N	201/239 (84%)	195 (97%)	6 (3%)	0	100	100
14	n	200/239 (84%)	192 (96%)	8 (4%)	0	100	100
15	O	218/277 (79%)	215 (99%)	3 (1%)	0	100	100
15	o	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
16	P	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
16	p	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
17	Q	197/201 (98%)	189 (96%)	8 (4%)	0	100	100
17	q	197/201 (98%)	189 (96%)	8 (4%)	0	100	100
18	R	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
18	r	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
19	S	211/241 (88%)	206 (98%)	5 (2%)	0	100	100
19	s	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
20	T	214/264 (81%)	210 (98%)	4 (2%)	0	100	100
20	t	214/264 (81%)	210 (98%)	4 (2%)	0	100	100
21	U	868/953 (91%)	816 (94%)	52 (6%)	0	100	100
22	X	378/422 (90%)	363 (96%)	15 (4%)	0	100	100
23	Y	376/389 (97%)	339 (90%)	37 (10%)	0	100	100
24	Z	284/324 (88%)	256 (90%)	27 (10%)	1 (0%)	30	60
25	a	371/376 (99%)	348 (94%)	22 (6%)	1 (0%)	36	65
26	b	189/377 (50%)	173 (92%)	16 (8%)	0	100	100
27	c	285/310 (92%)	255 (90%)	30 (10%)	0	100	100
28	d	255/350 (73%)	221 (87%)	32 (12%)	2 (1%)	16	45
29	f	887/908 (98%)	771 (87%)	116 (13%)	0	100	100
31	x	492/494 (100%)	455 (92%)	37 (8%)	0	100	100
32	y	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
33	W	444/456 (97%)	420 (95%)	23 (5%)	1 (0%)	43	71
34	V	442/534 (83%)	432 (98%)	9 (2%)	1 (0%)	43	71
35	e	48/70 (69%)	42 (88%)	6 (12%)	0	100	100
All	All	13742/15458 (89%)	12874 (94%)	858 (6%)	10 (0%)	49	75

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
3	C	112	CYS
28	d	203	PRO
33	W	140	ILE
24	Z	145	HIS
28	d	200	PHE
3	C	90	HIS
25	a	343	LEU
2	B	356	PRO
34	V	466	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	ADP	E	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.85	10 (23%)
36	ATP	A	501	-	32,33,33	0.31	0	48,52,52	0.32	0
36	ATP	D	501	-	32,33,33	0.33	0	48,52,52	0.32	0
36	ATP	B	501	-	32,33,33	0.34	0	48,52,52	0.29	0
36	ATP	C	501	-	32,33,33	0.39	0	48,52,52	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ADP	E	501	-	-	4/16/32/32	0/3/3/3
36	ATP	A	501	-	-	4/22/38/38	0/3/3/3
36	ATP	D	501	-	-	0/22/38/38	0/3/3/3
36	ATP	B	501	-	-	6/22/38/38	0/3/3/3
36	ATP	C	501	-	-	4/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	E	501	ADP	C5-C4	4.67	1.47	1.39
37	E	501	ADP	C5-C6	2.66	1.48	1.41
37	E	501	ADP	C5-N7	-2.37	1.34	1.39
37	E	501	ADP	C8-N7	2.27	1.36	1.31

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	E	501	ADP	C5-C4-N3	-5.98	118.48	126.72
37	E	501	ADP	N3-C4-N9	4.73	135.21	127.17
37	E	501	ADP	C2-N3-C4	3.66	120.78	111.83
37	E	501	ADP	C4-C5-N7	-3.61	106.46	110.58
37	E	501	ADP	N3-C2-N1	-3.11	123.87	128.58
37	E	501	ADP	C5-N7-C8	2.71	107.72	103.45
37	E	501	ADP	C4-N9-C8	2.66	108.54	105.74
37	E	501	ADP	C3'-C2'-C1'	2.51	106.20	101.46
37	E	501	ADP	N9-C8-N7	-2.08	110.98	113.94
37	E	501	ADP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (18) torsion outliers are listed below:

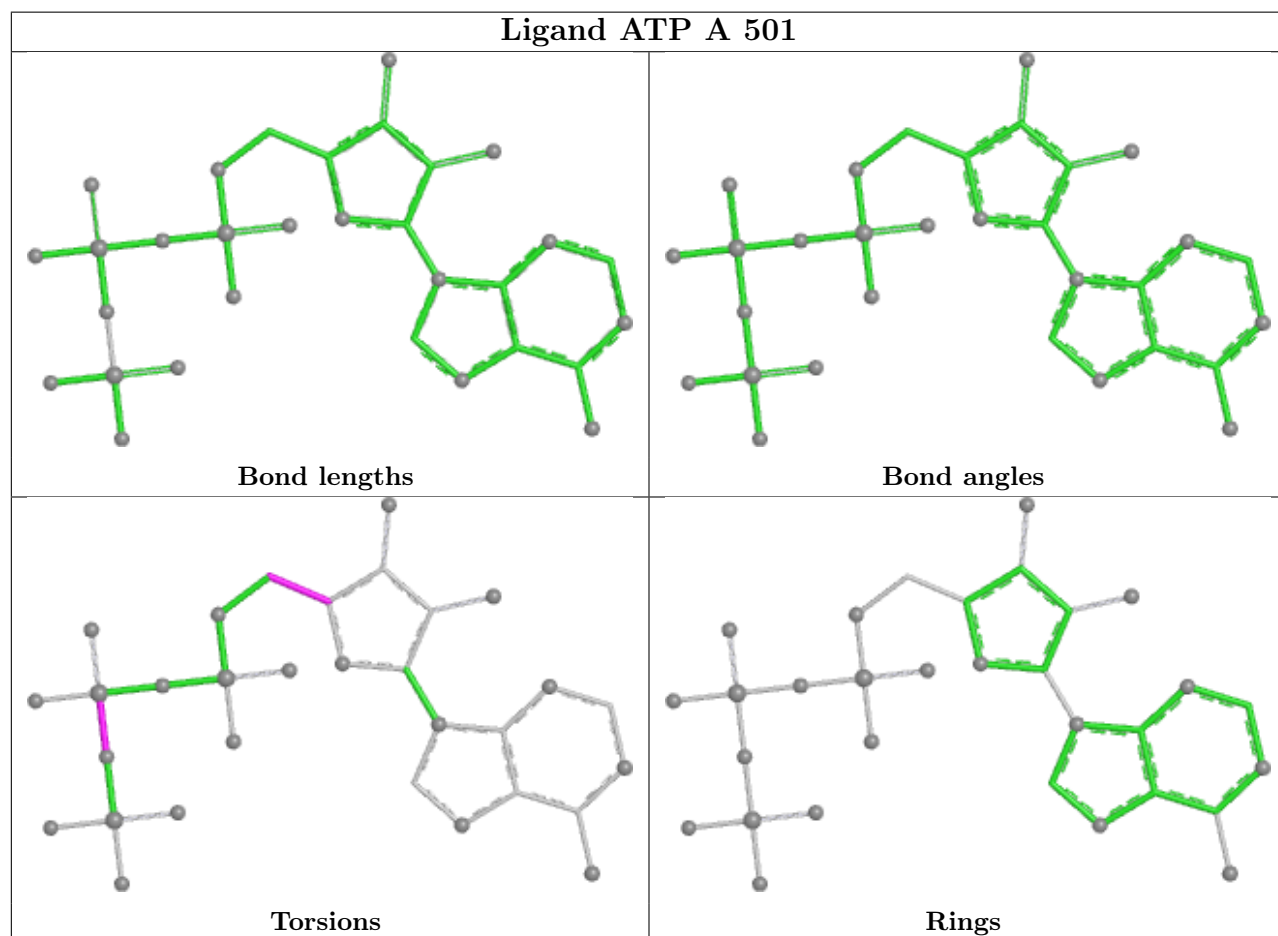
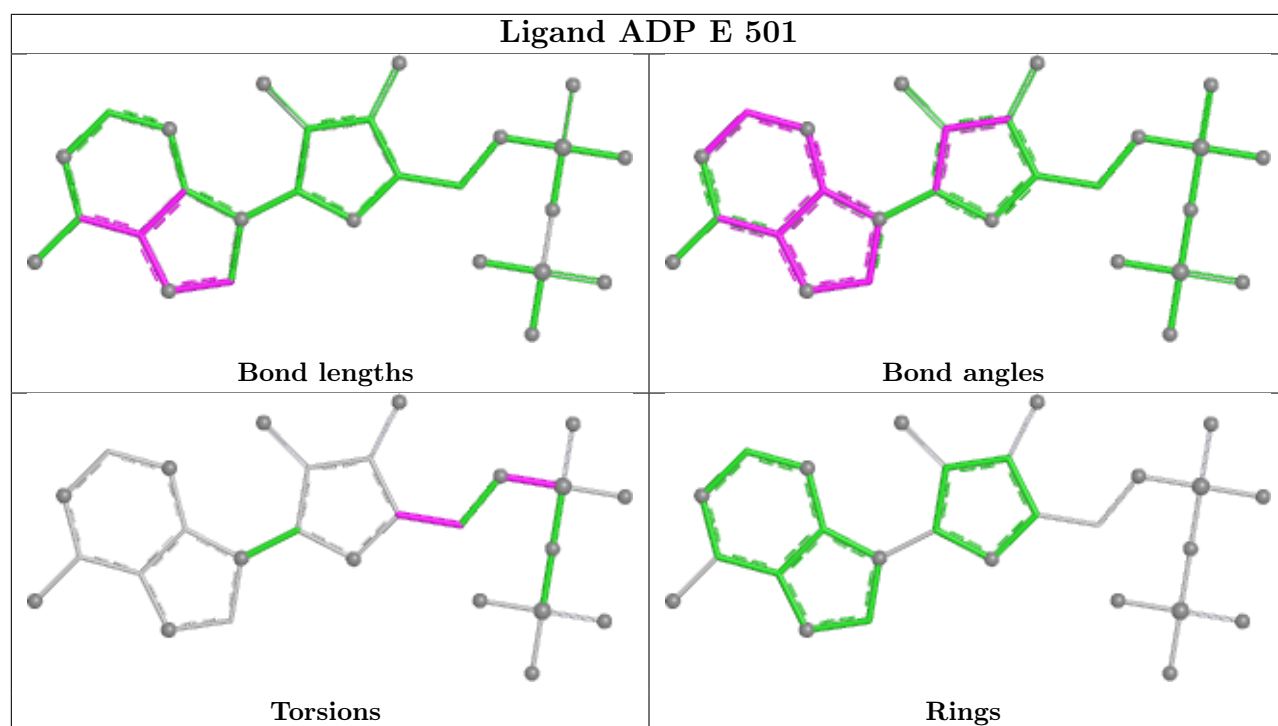
Mol	Chain	Res	Type	Atoms
36	B	501	ATP	C5'-O5'-PA-O1A
36	B	501	ATP	C5'-O5'-PA-O2A
36	B	501	ATP	C5'-O5'-PA-O3A
37	E	501	ADP	C5'-O5'-PA-O1A
36	A	501	ATP	C3'-C4'-C5'-O5'
36	B	501	ATP	O4'-C4'-C5'-O5'
36	B	501	ATP	C3'-C4'-C5'-O5'
36	A	501	ATP	O4'-C4'-C5'-O5'
37	E	501	ADP	O4'-C4'-C5'-O5'
37	E	501	ADP	C3'-C4'-C5'-O5'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

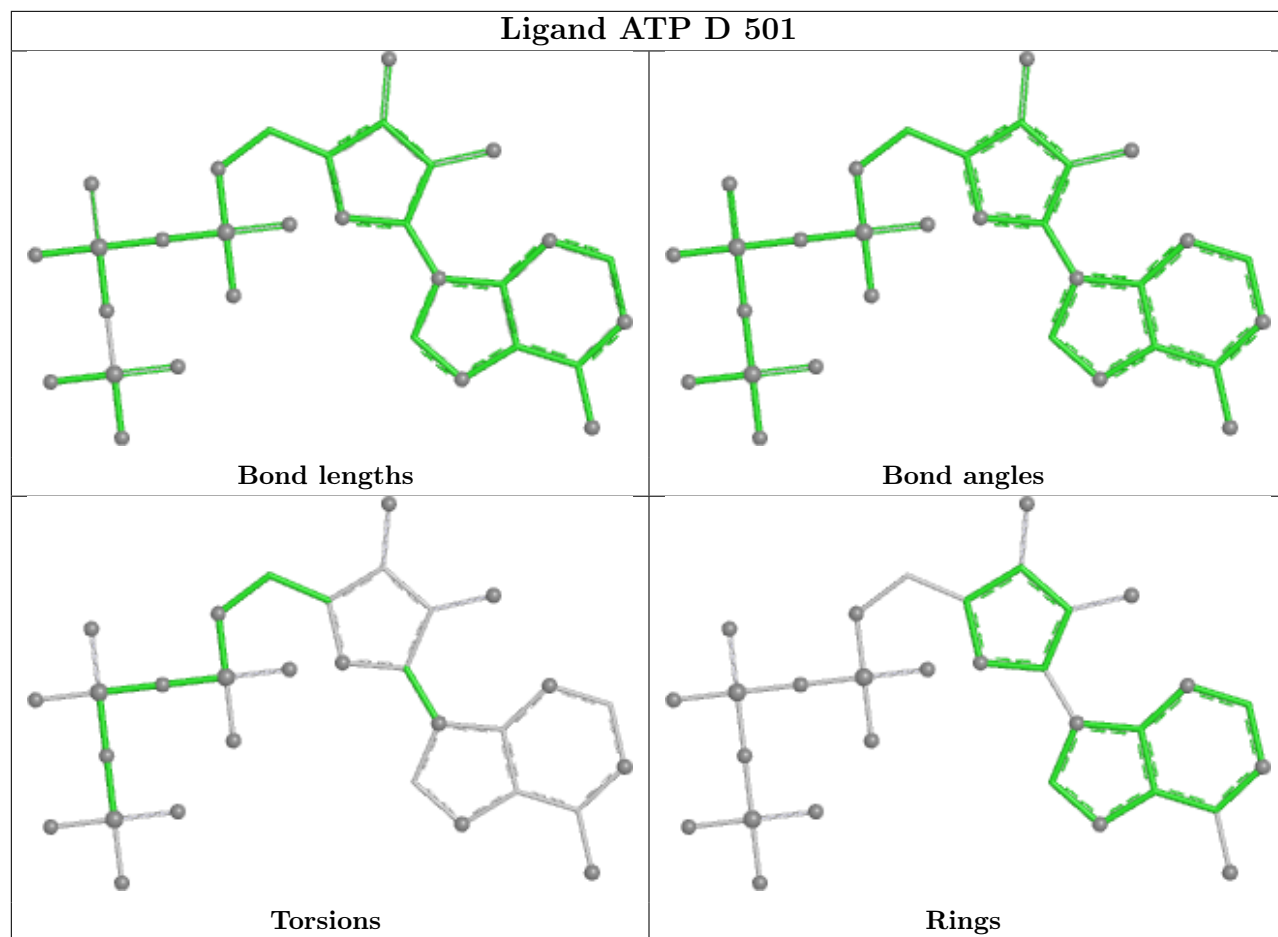
There are no ring outliers.

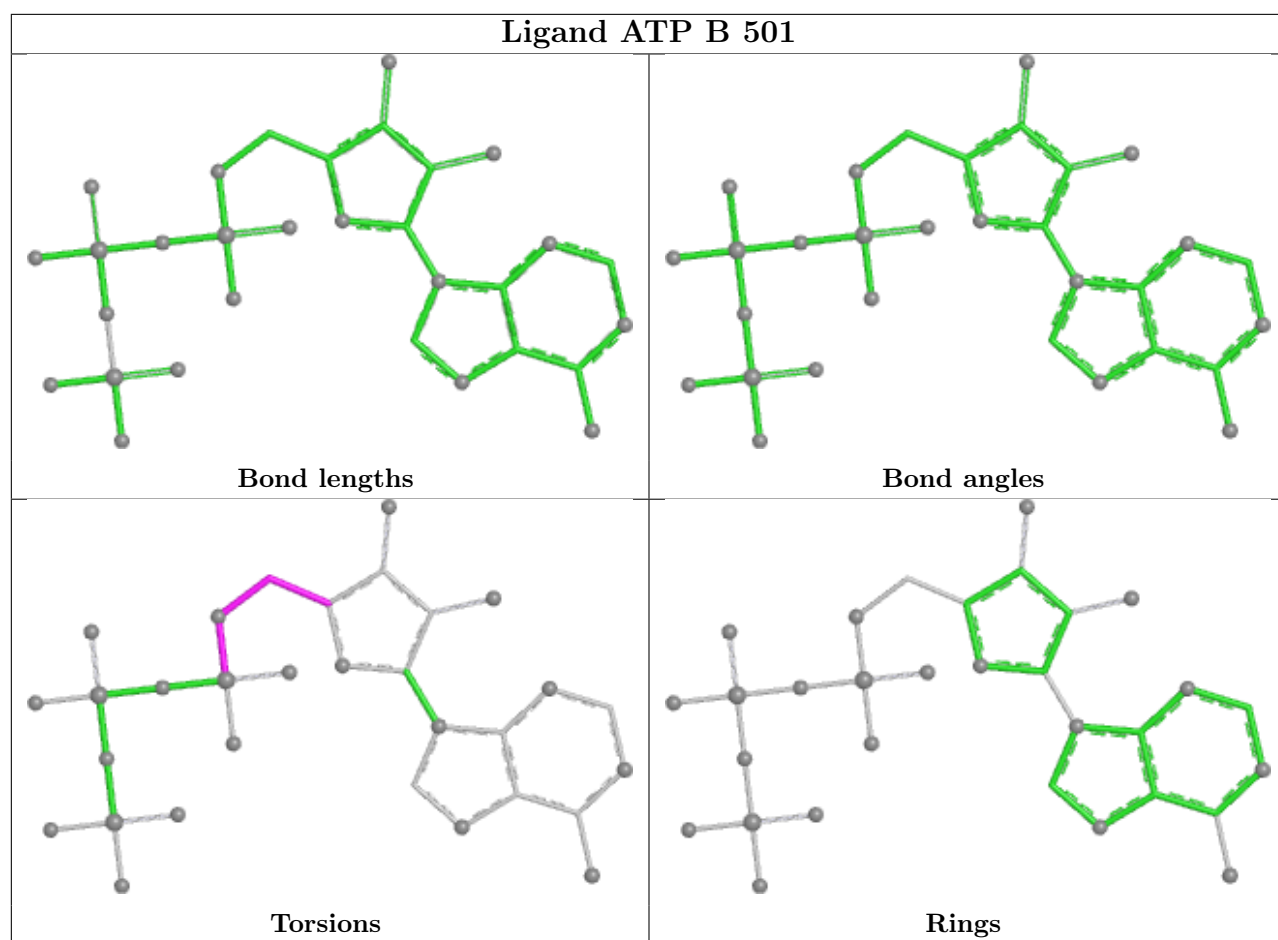
3 monomers are involved in 6 short contacts:

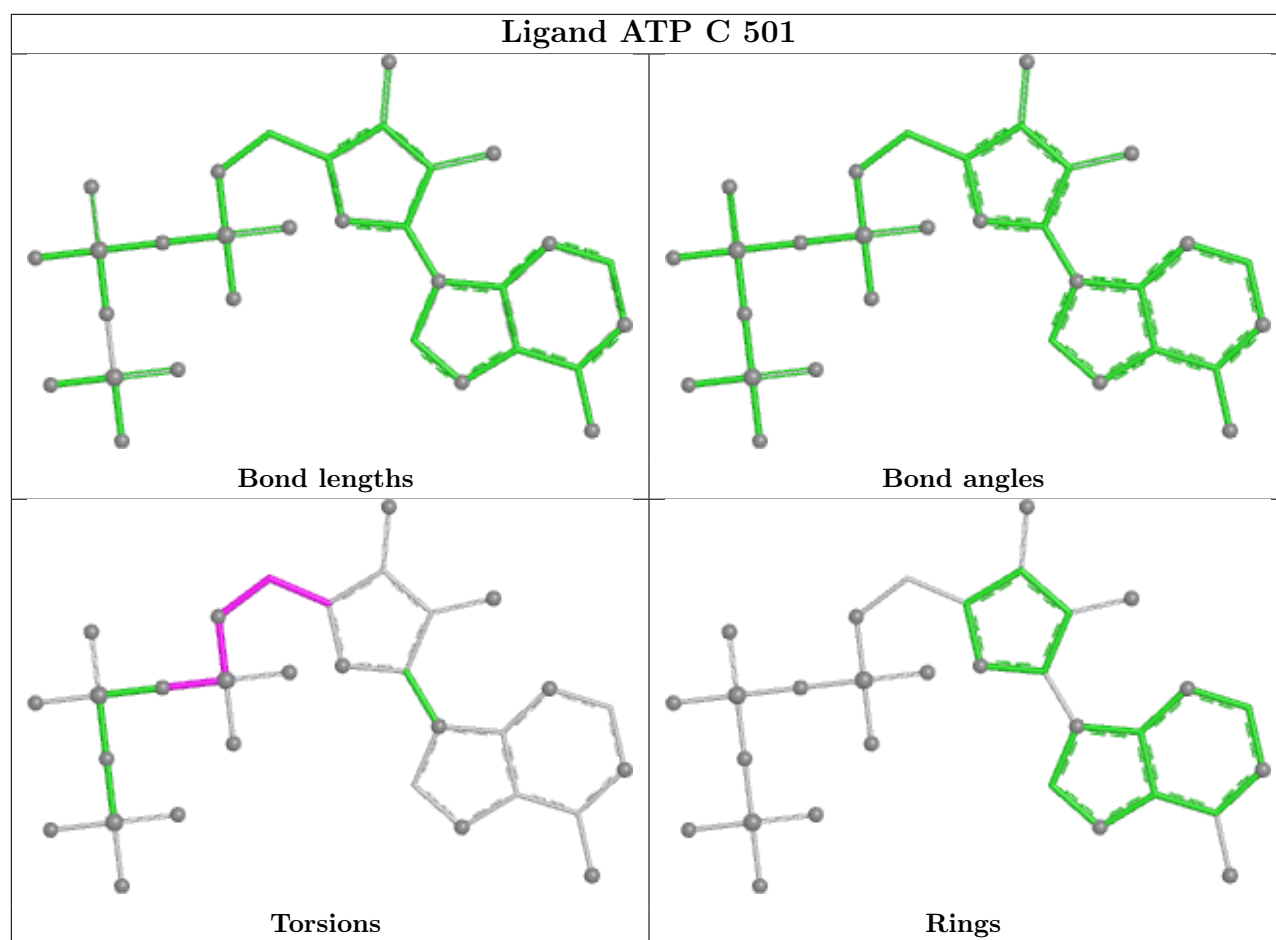
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	E	501	ADP	2	0
36	A	501	ATP	2	0
36	D	501	ATP	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

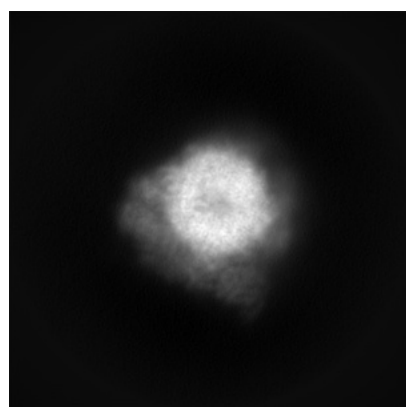
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32278. 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](#)

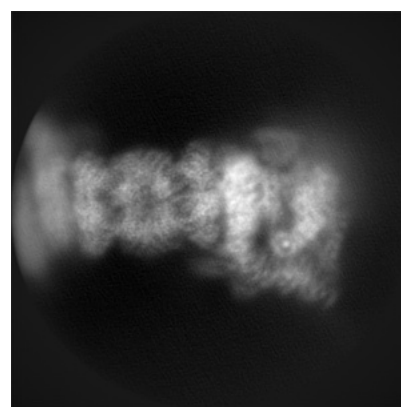
6.1.1 Primary map



X



Y

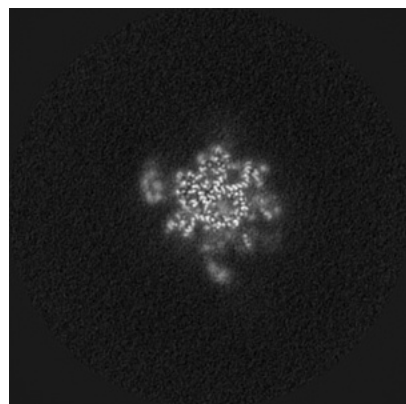


Z

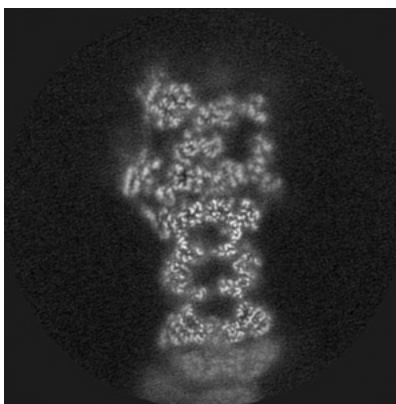
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

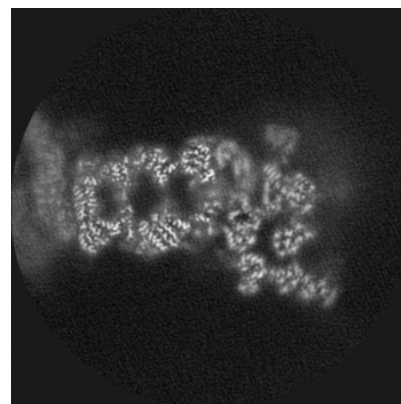
6.2.1 Primary map



X Index: 320



Y Index: 320

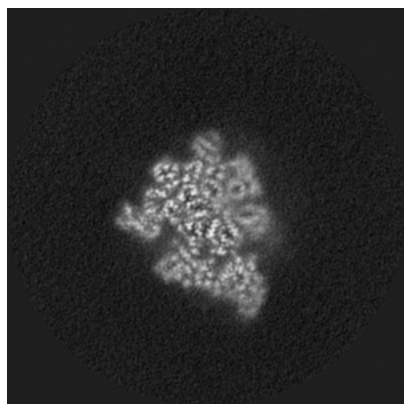


Z Index: 320

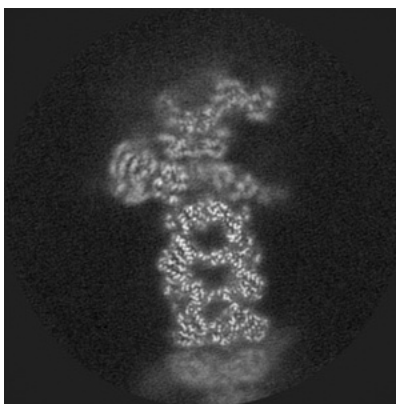
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

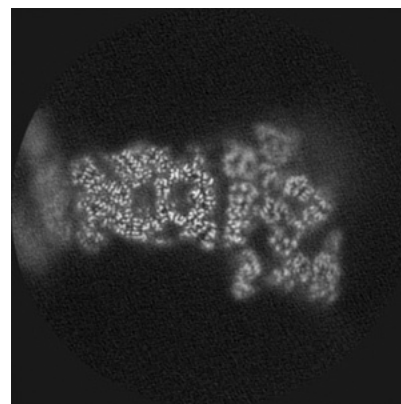
6.3.1 Primary map



X Index: 368



Y Index: 361

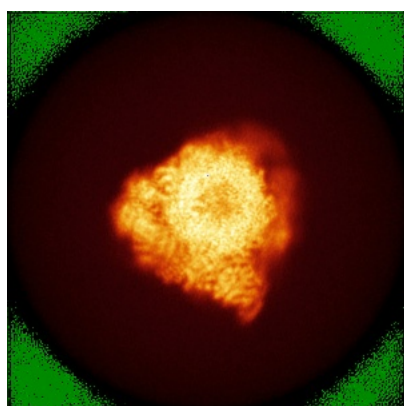


Z Index: 297

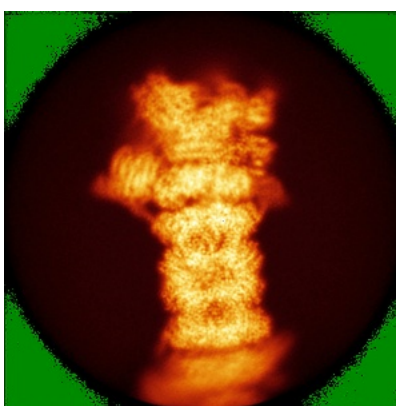
The images above show the largest variance slices of the map in three orthogonal directions.

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

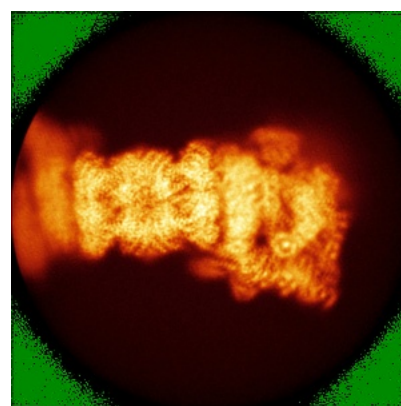
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

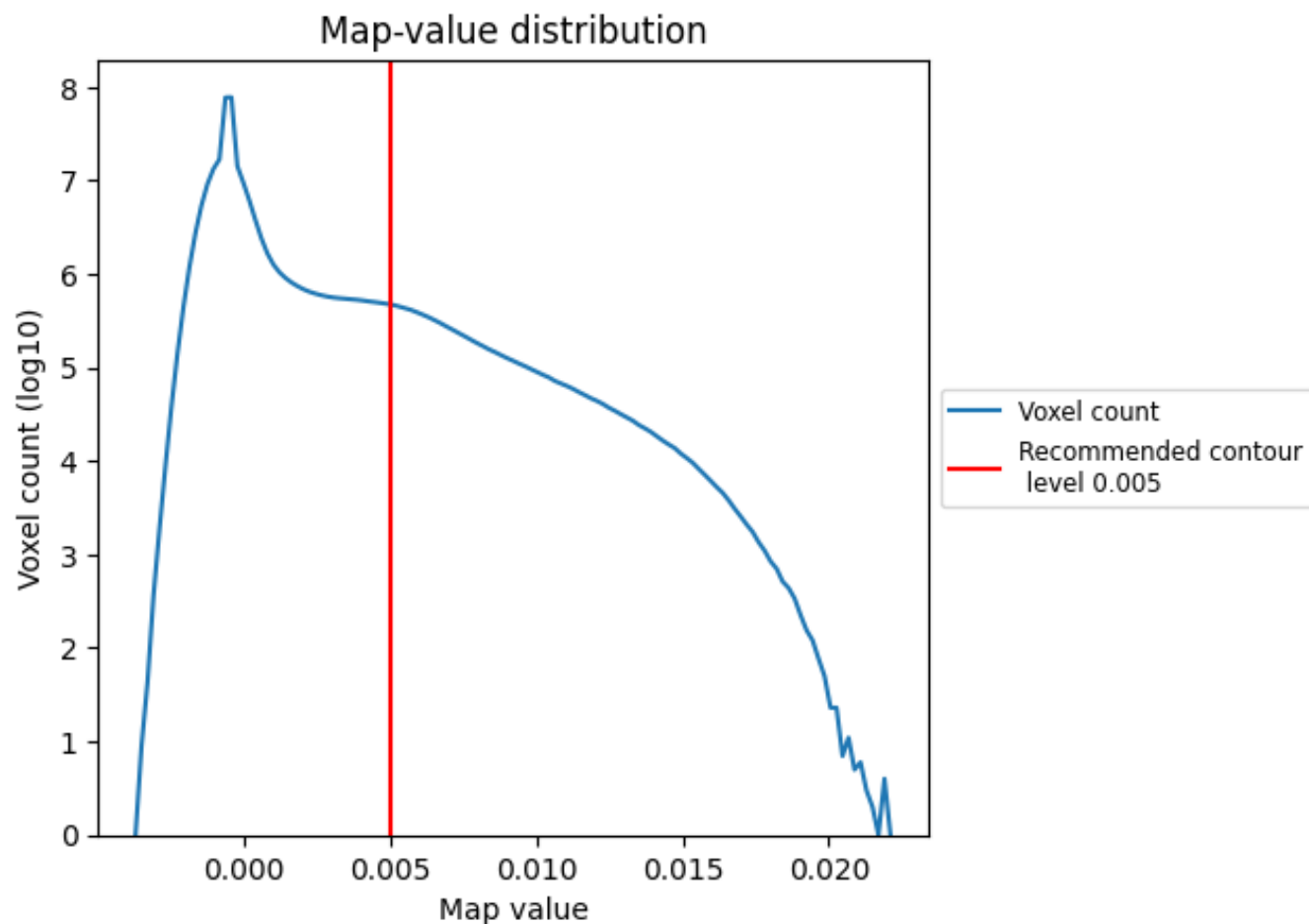
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

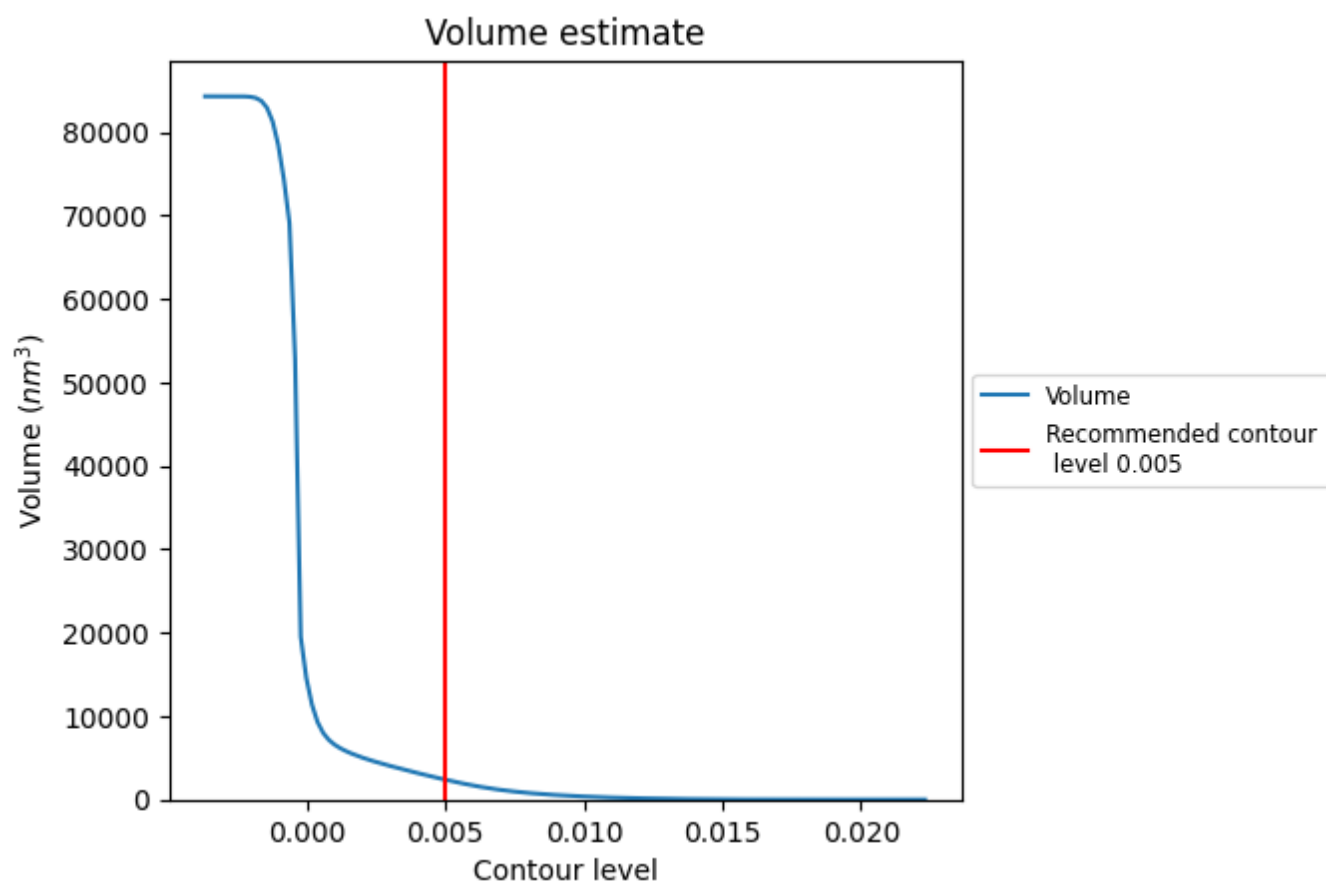
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

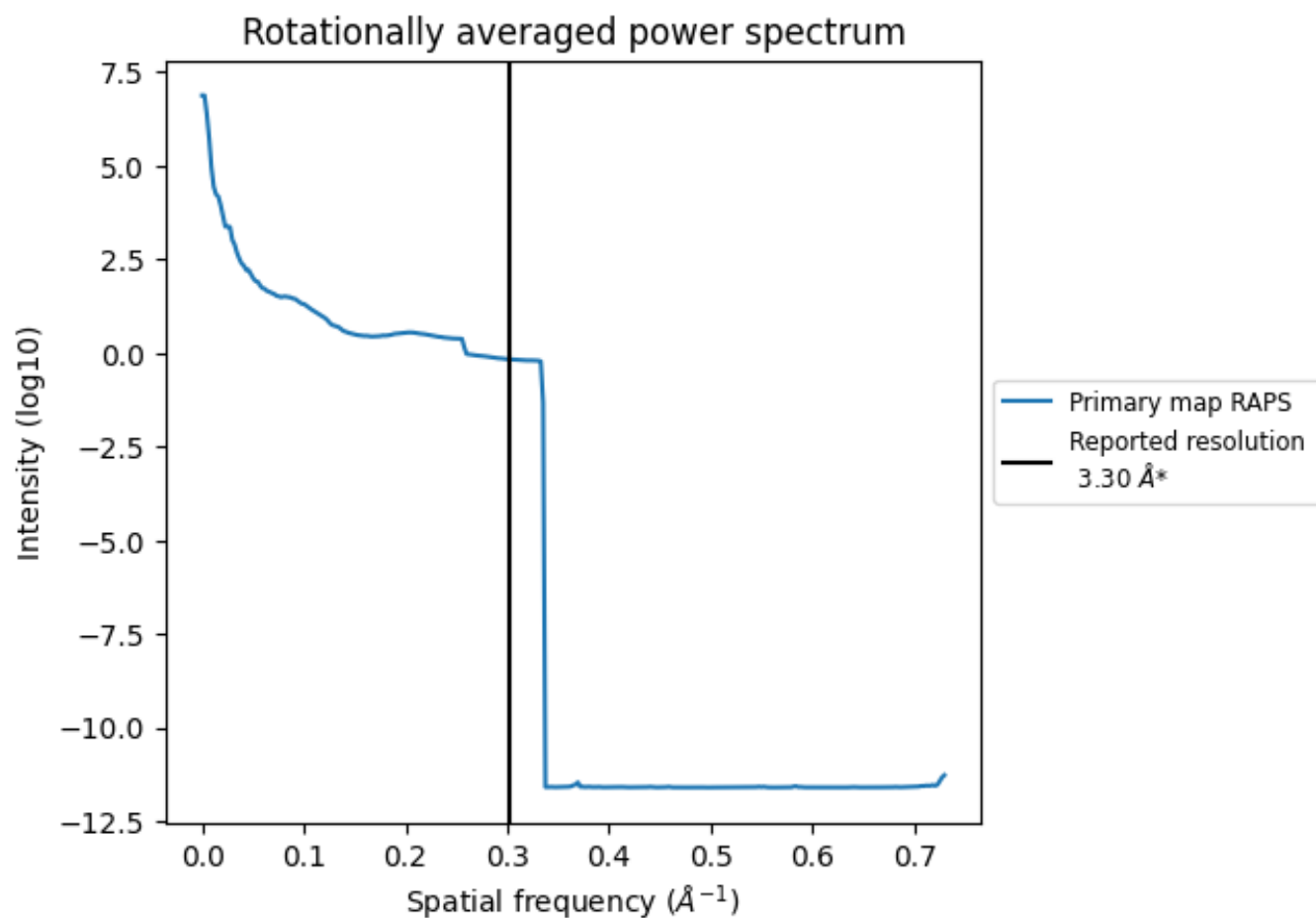
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2376 nm^3 ; this corresponds to an approximate mass of 2146 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 0.303 Å⁻¹

8 Fourier-Shell correlation

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

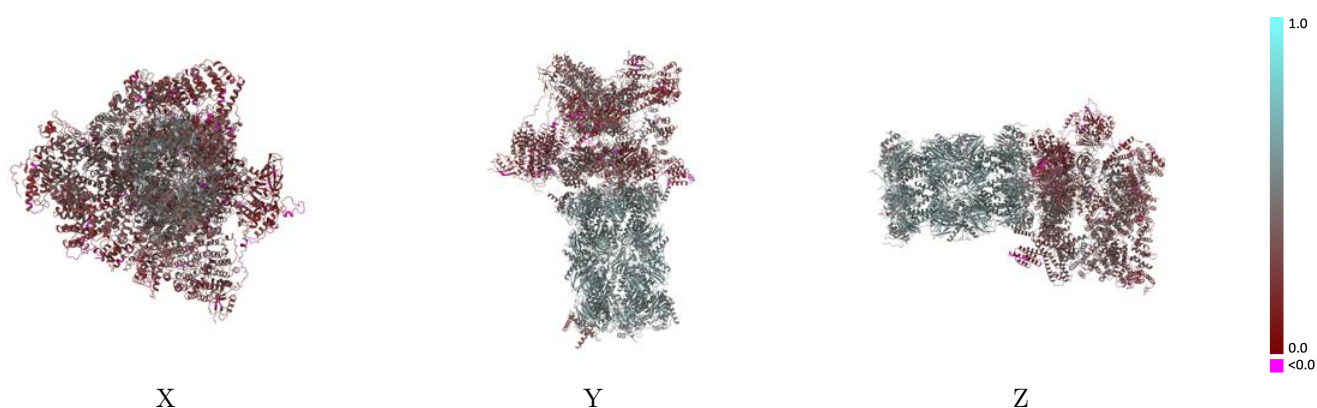
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-32278 and PDB model 7W3F. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

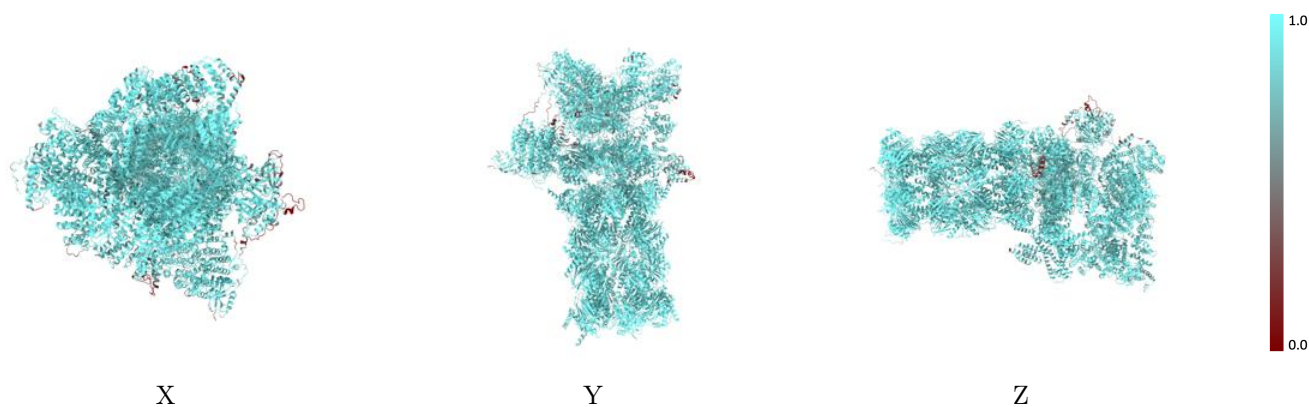
This section was not generated.

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



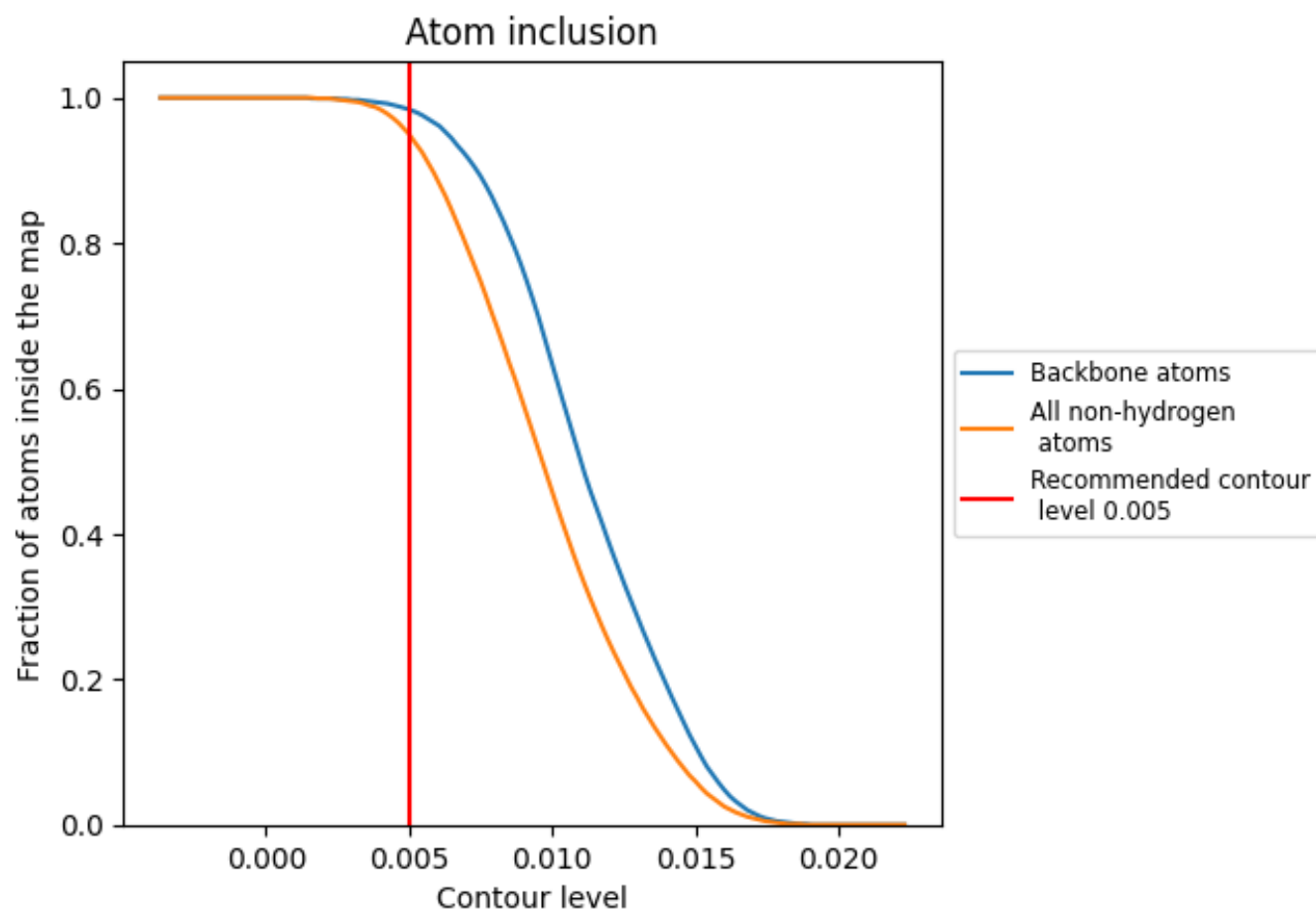
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 98% of all backbone atoms, 95% 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	 0.9500	 0.3990
A	 0.9700	 0.2880
B	 0.9640	 0.3620
C	 0.9680	 0.3860
D	 0.9770	 0.3870
E	 0.9400	 0.3080
F	 0.9460	 0.2300
G	 0.9860	 0.5120
H	 0.9930	 0.5130
I	 0.9770	 0.5000
J	 0.9760	 0.4850
K	 0.9820	 0.5030
L	 0.9860	 0.5230
M	 0.9810	 0.5110
N	 0.9910	 0.5420
O	 0.9940	 0.5330
P	 0.9940	 0.5420
Q	 0.9920	 0.5370
R	 0.9950	 0.5390
S	 0.9910	 0.5340
T	 0.9860	 0.5430
U	 0.9220	 0.3380
V	 0.9320	 0.3150
W	 0.8470	 0.2750
X	 0.9440	 0.3210
Y	 0.9530	 0.3440
Z	 0.9720	 0.3510
a	 0.9240	 0.2800
b	 0.9400	 0.2870
c	 0.9620	 0.3580
d	 0.8560	 0.2470
e	 0.9280	 0.3210
f	 0.9240	 0.2440
g	 0.9740	 0.5140
h	 0.9820	 0.5230



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Chain	Atom inclusion	Q-score
i	 0.9610	 0.4970
j	 0.9650	 0.4680
k	 0.9770	 0.5110
l	 0.9860	 0.5280
m	 0.9830	 0.5190
n	 0.9950	 0.5500
o	 0.9910	 0.5360
p	 0.9960	 0.5480
q	 0.9940	 0.5480
r	 0.9960	 0.5490
s	 0.9910	 0.5380
t	 0.9850	 0.5470
v	 0.9780	 0.3210
x	 0.7510	 0.2040
y	 0.7870	 0.1750