



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:25 PM UTC

PDB ID : 6MSD / pdb_00006msd
EMDB ID : EMD-9217
Title : Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome
Authors : Mao, Y.D.
Deposited on : 2018-10-16
Resolution : 3.20 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:

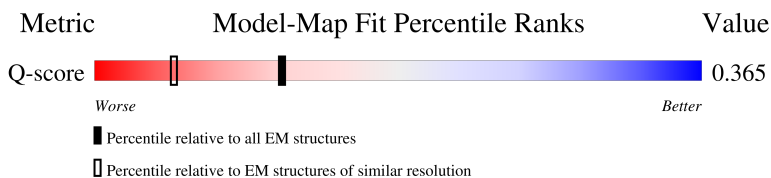
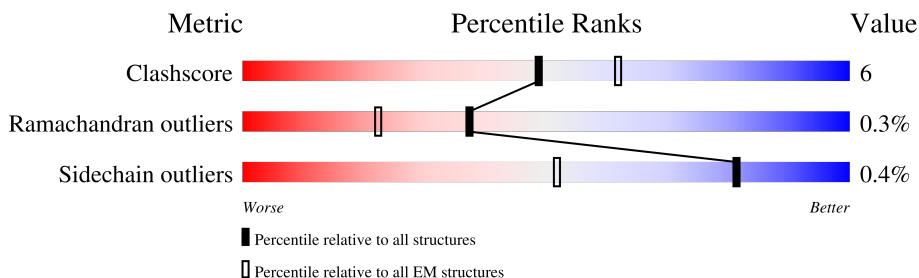
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






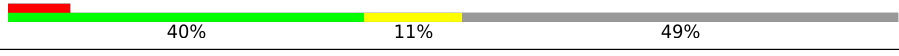
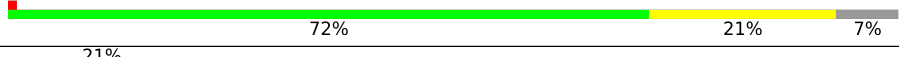

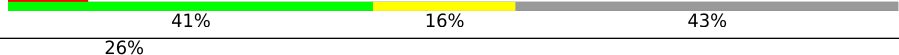

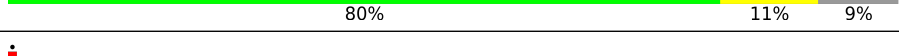
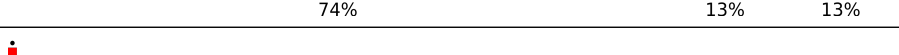
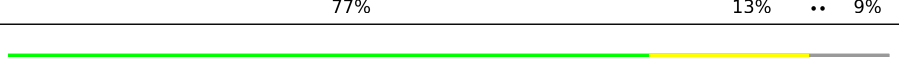
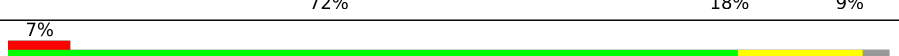

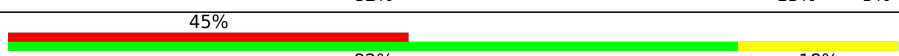
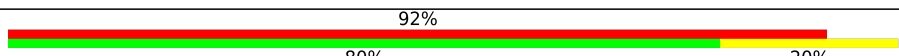
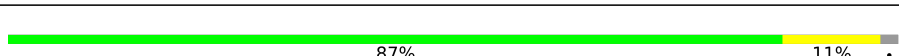

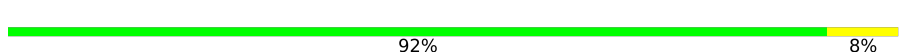
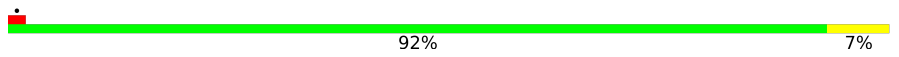


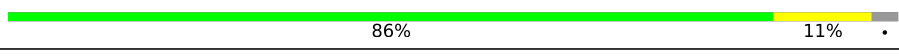

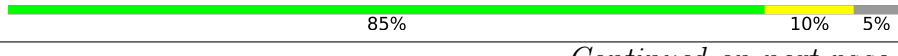

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	U	953	
2	V	534	
3	W	456	
4	X	422	




















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Mol	Chain	Length	Quality of chain
5	Y	389	 80% 17%
6	Z	324	 67% 21% 12%
7	a	376	 77% 22%
8	b	377	 7% 40% 11% 49%
9	c	309	 72% 21% 7%
10	d	349	 21% 58% 15% 26%
11	e	70	 9% 41% 16% 43%
12	f	908	 26% 71% 26%
13	A	433	 80% 11% 9%
14	B	440	 74% 13% 13%
15	C	398	 77% 13% 9%
16	D	418	 72% 18% 9%
17	E	403	 7% 82% 14%
18	F	439	 9% 82% 13% 5%
19	u	76	 45% 82% 18%
19	w	76	 92% 80% 20%
20	G	245	 87% 11%
20	g	245	 87% 11%
21	H	233	 92% 8%
21	h	233	 92% 7%
22	I	260	 83% 13%
22	i	260	 83% 13%
23	J	247	 86% 11%
23	j	247	 85% 12%
24	K	240	 85% 10% 5%

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Mol	Chain	Length	Quality of chain
24	k	240	 84% 11% 5%
25	L	268	 79% 10% 11%
25	l	268	 76% 12% 11%
26	M	254	 83% 11% 6%
26	m	254	 81% 14% 6%
27	N	238	 73% 7% 20%
27	n	238	 74% 7% 20%
28	O	276	 72% 7% 20%
28	o	276	 70% 10% 20%
29	P	204	 89% 11%
29	p	204	 89% 11%
30	Q	201	 88% 11%
30	q	201	 88% 11%
31	R	262	 72% 5% 23%
31	r	262	 72% 5% 23%
32	S	240	 82% 6% 11%
32	s	240	 82% 6% 11%
33	T	263	 72% 10% 18%
33	t	263	 71% 11% 18%

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 105426 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	U	812	6334	4023	1078	1189	44	0	0

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V	480	3852	2444	684	710	14	0	0

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	W	456	3703	2339	635	704	25	0	0

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

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

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	e	40	334	200	55	77	2	0	0

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

- Molecule 13 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	A	394	3096	1951	543	584	18	0	0

- Molecule 14 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	B	384	3018	1901	515	587	15	0	0

- Molecule 15 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	C	363	2864	1808	515	525	16	0	0

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B.

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

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

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

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6A.

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

- Molecule 19 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	u	76	603	378	107	117	1	0	0
19	w	76	603	378	107	117	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	63	ARG	LYS	conflict	UNP P0CG47
w	63	ARG	LYS	conflict	UNP P0CG47

- Molecule 20 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		
20	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 21 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		
21	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 22 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
22	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 23 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	239	Total	C	N	O	S	0	0
			1713	1062	311	335	5		
23	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 24 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		
24	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 25 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	l	238	1850	1159	334	346	11	0	0

- Molecule 26 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	M	240	1856	1178	314	353	11	0	0
26	m	240	1856	1178	314	353	11	0	0

- Molecule 27 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	N	191	1430	893	245	280	12	0	0
27	n	191	1430	893	245	280	12	0	0

- Molecule 28 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	O	220	1643	1033	280	318	12	0	0
28	o	220	1643	1033	280	318	12	0	0

- Molecule 29 is a protein called Proteasome subunit beta type-3.

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

- Molecule 30 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Q	199	1570	1006	265	290	9	0	0
30	q	199	1570	1006	265	290	9	0	0

- Molecule 31 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
31	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 32 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
32	s	213	Total	C	N	O	S	0	0
			1644	1039	282	313	10		

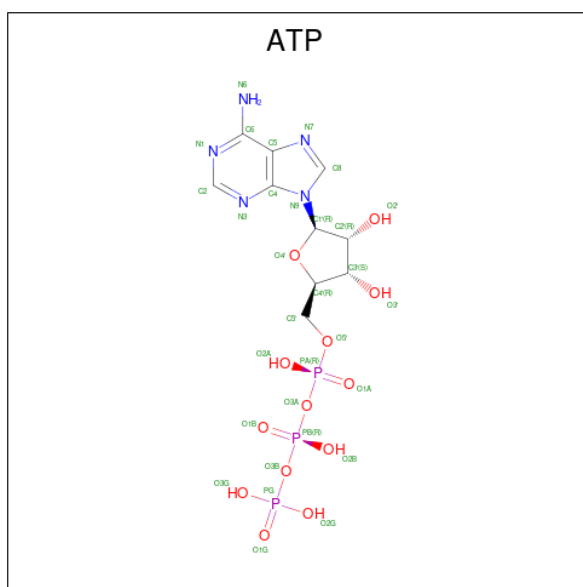
- Molecule 33 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
33	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

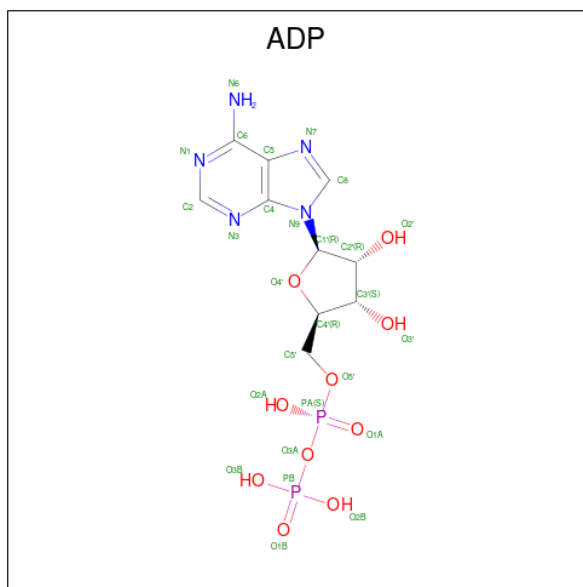


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
35	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

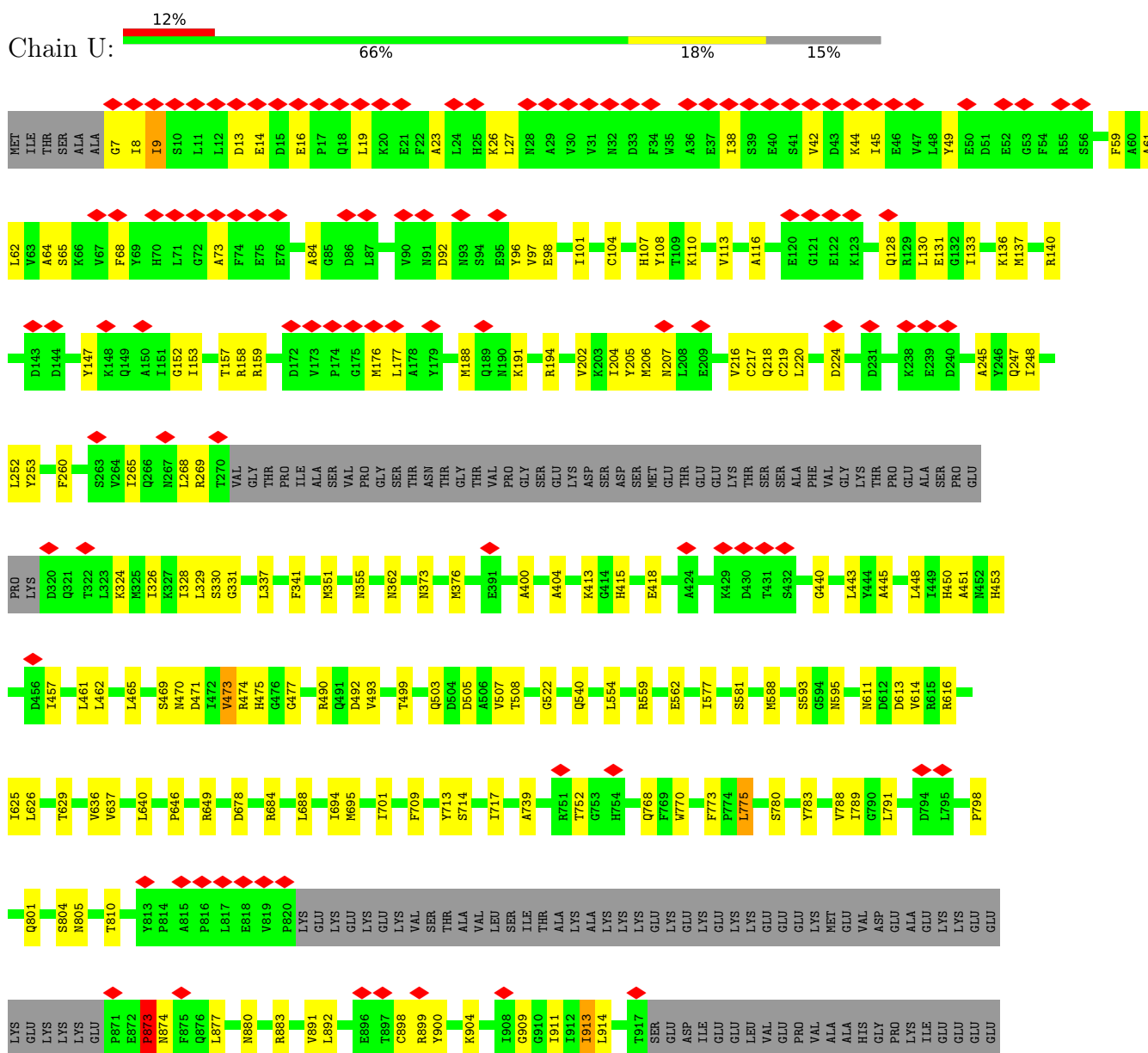


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
37	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
37	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots [i](#)

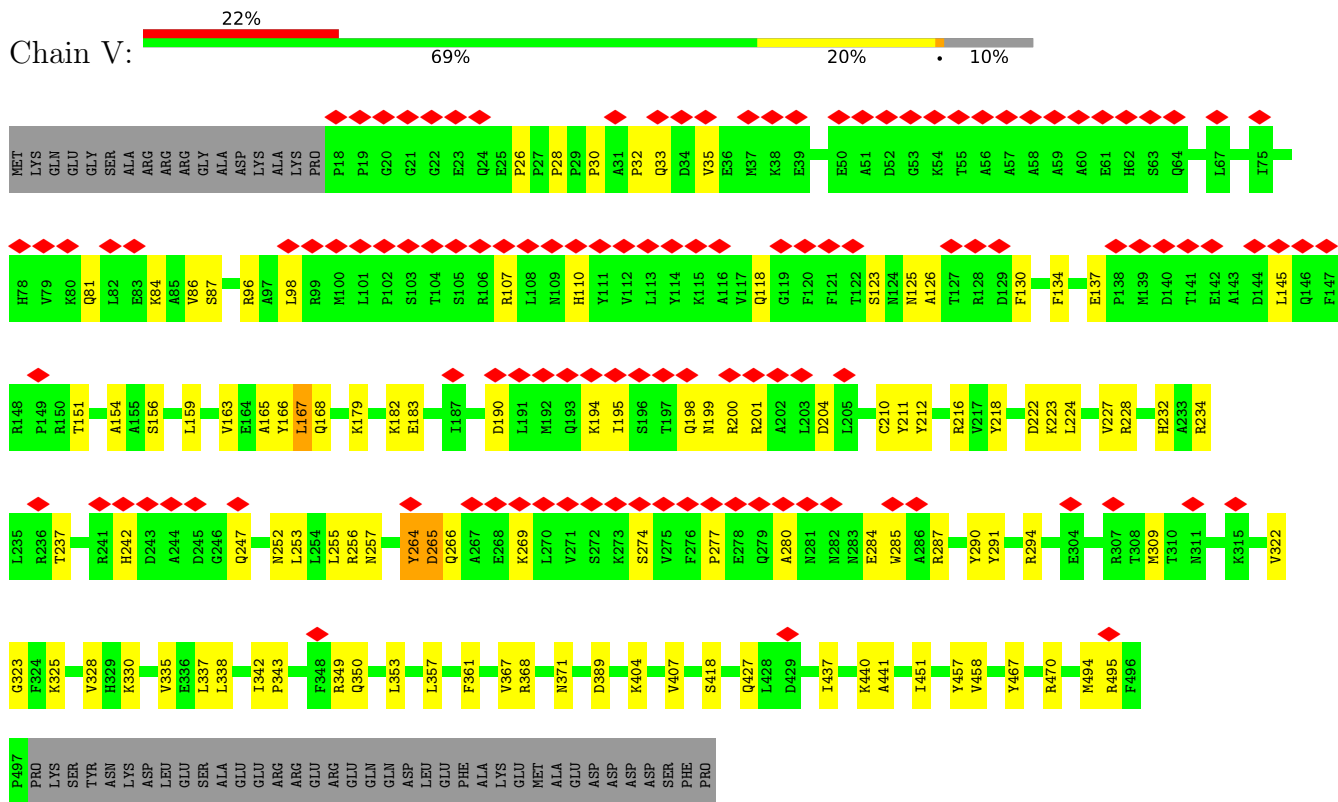
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

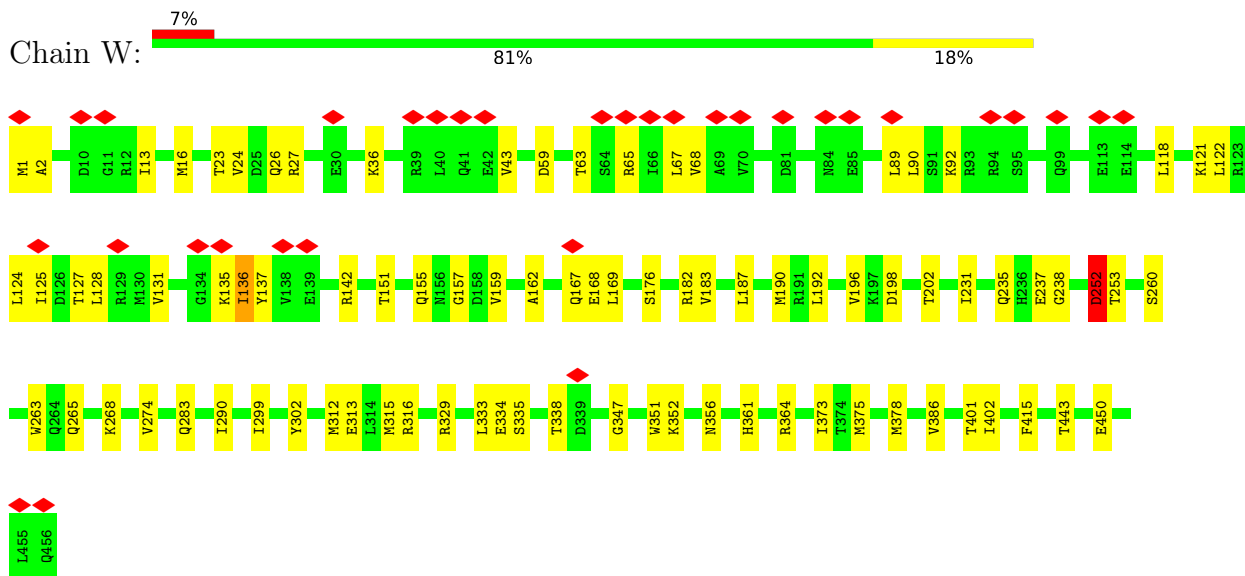


GLN
GLU
PRO
GLU
GLY
PRO
PRO
GLU
GLU
PHE
ARG
GLY
TYR
ILE
ASP
ASP

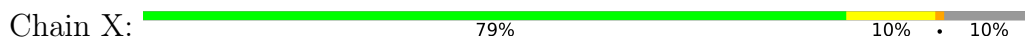
• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

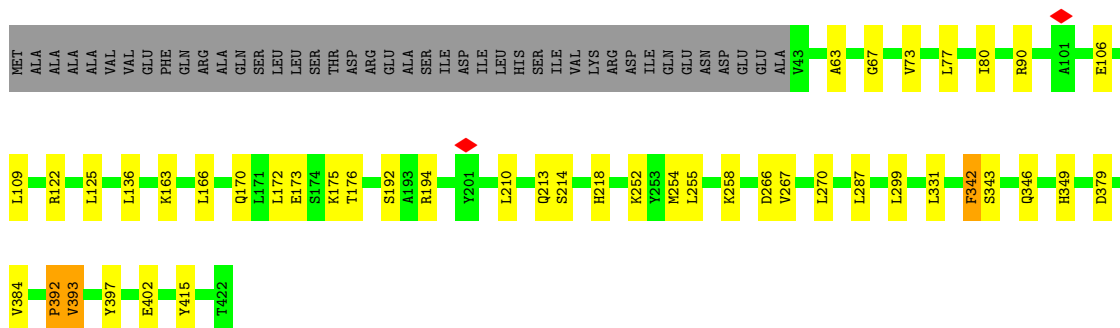


• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

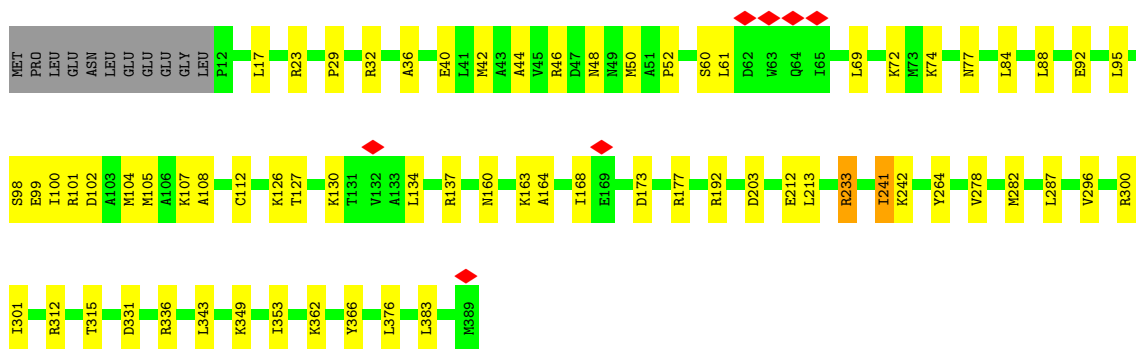
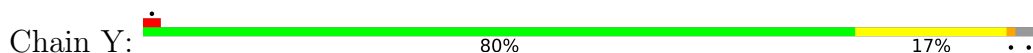


• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

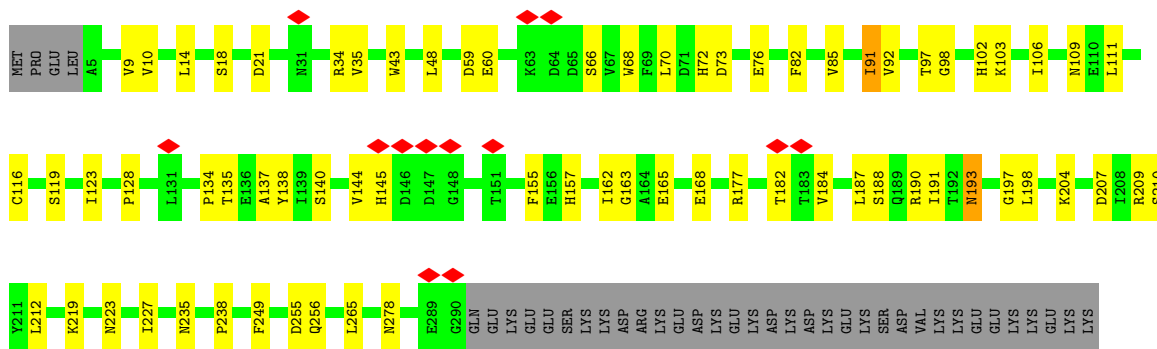




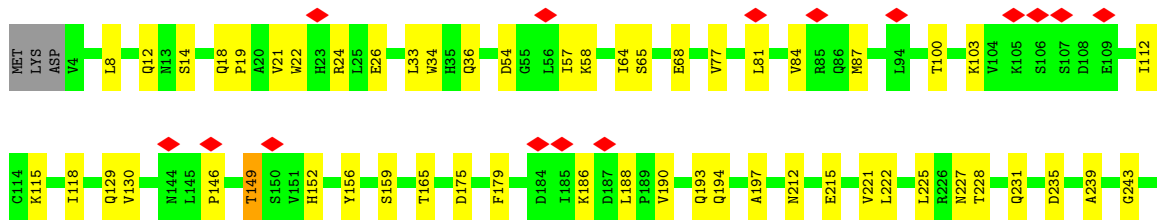
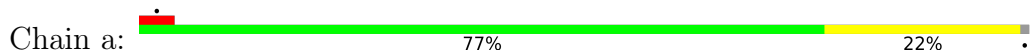
• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6



• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

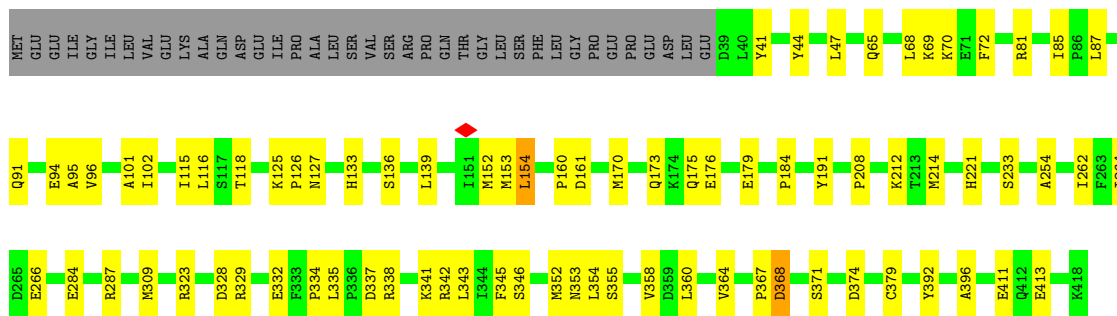


• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13




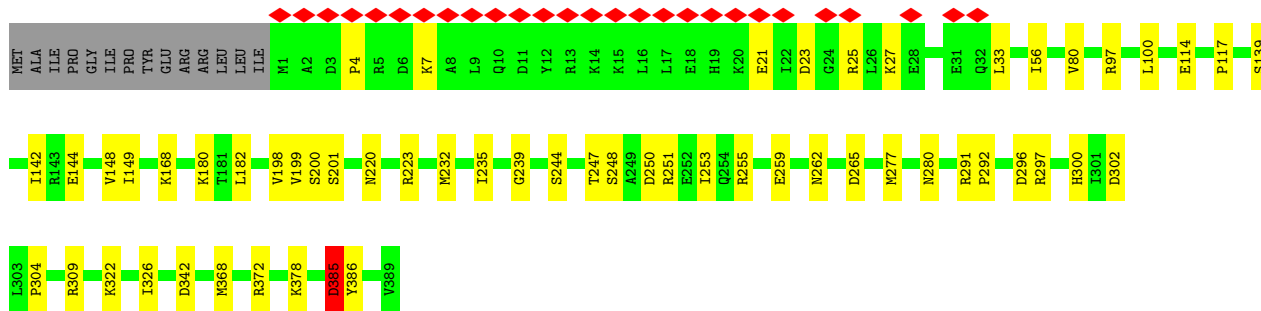
• Molecule 16: 26S proteasome regulatory subunit 6B

Chain D:  72% 18% 9%




• Molecule 17: 26S proteasome regulatory subunit 10B

Chain E:  7% 82% 14%




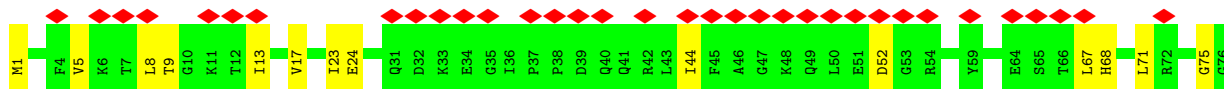
• Molecule 18: 26S proteasome regulatory subunit 6A

Chain F:  9% 82% 13% 5%

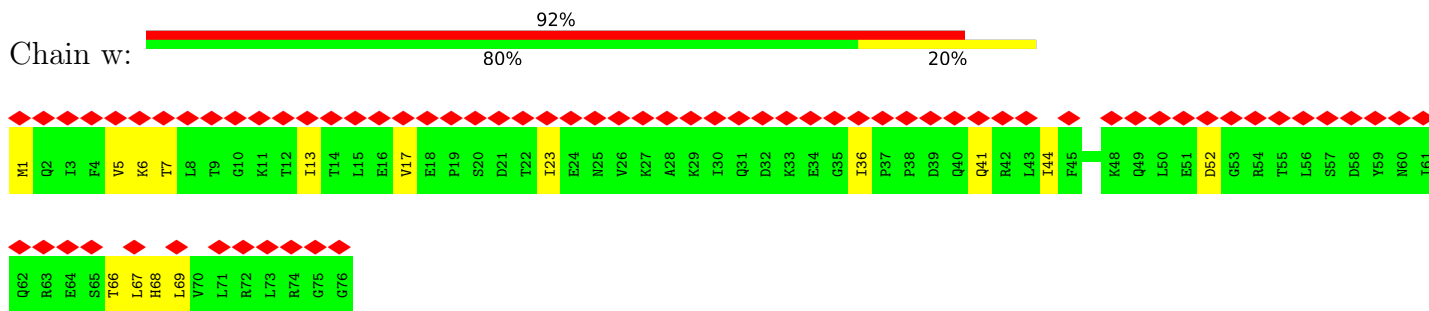


• Molecule 19: Ubiquitin

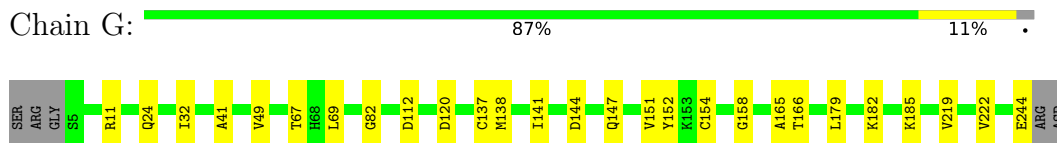
Chain u:  45% 82% 18%



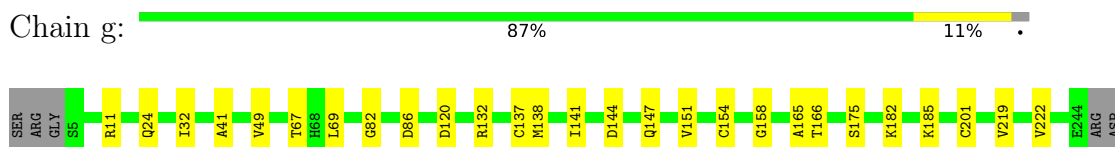
• Molecule 19: Ubiquitin



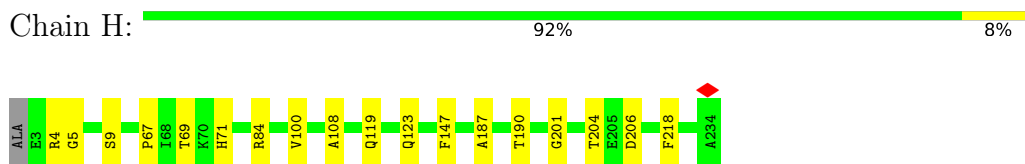
• Molecule 20: Proteasome subunit alpha type-6



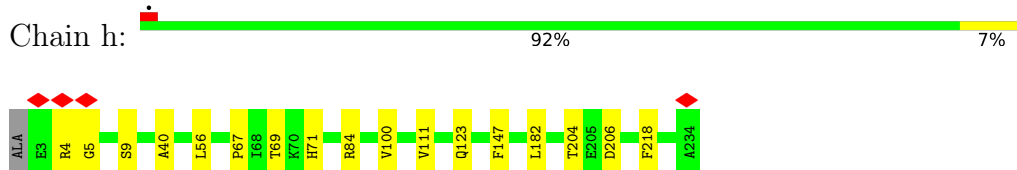
• Molecule 20: Proteasome subunit alpha type-6



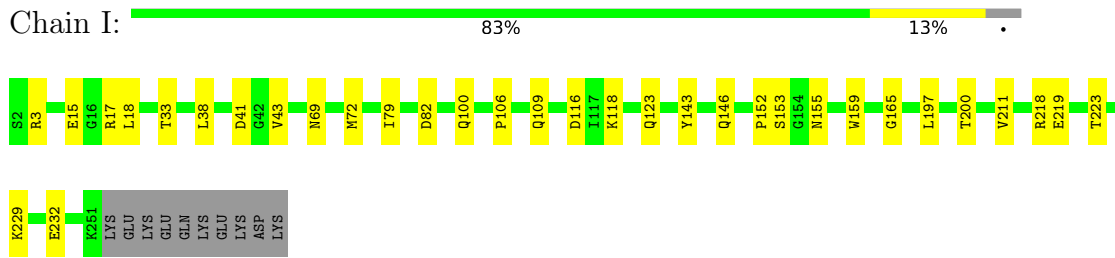
• Molecule 21: Proteasome subunit alpha type-2




• Molecule 21: Proteasome subunit alpha type-2

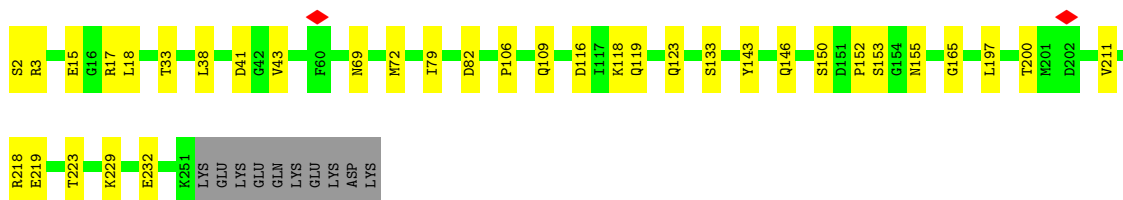


• Molecule 22: Proteasome subunit alpha type-4




• Molecule 22: Proteasome subunit alpha type-4

Chain i:  83% 13%




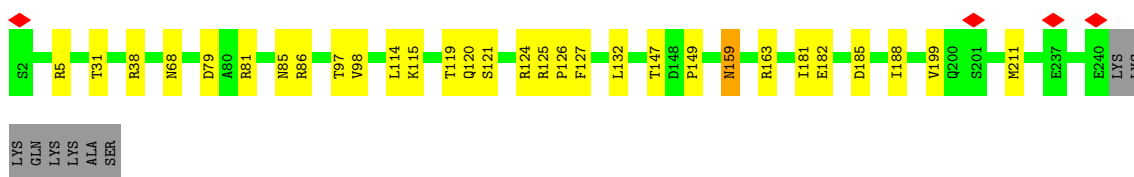
- Molecule 23: Proteasome subunit alpha type-7

Chain J:  86% 11%



- Molecule 23: Proteasome subunit alpha type-7

Chain j:  85% 12%




- Molecule 24: Proteasome subunit alpha type-5

Chain K:  85% 10% 5%




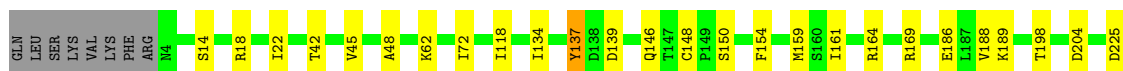
- Molecule 24: Proteasome subunit alpha type-5

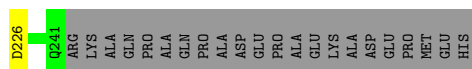
Chain k:  84% 11% 5%



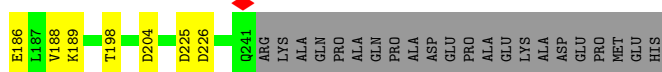
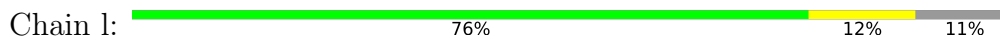
- Molecule 25: Proteasome subunit alpha type-1

Chain L:  79% 10% 11%

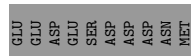
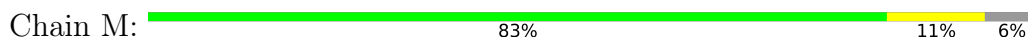




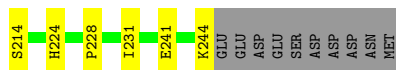
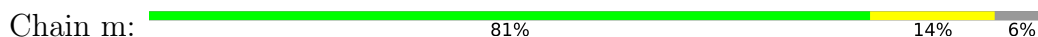
• Molecule 25: Proteasome subunit alpha type-1



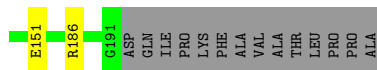
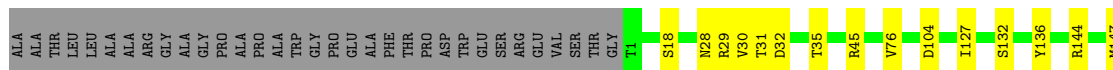
• Molecule 26: Proteasome subunit alpha type-3



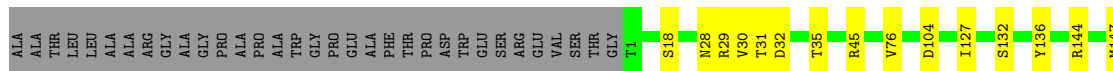
• Molecule 26: Proteasome subunit alpha type-3

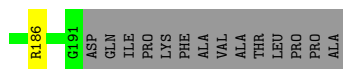


• Molecule 27: Proteasome subunit beta type-6

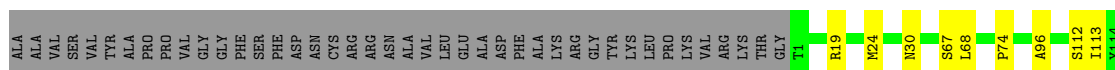


• Molecule 27: Proteasome subunit beta type-6

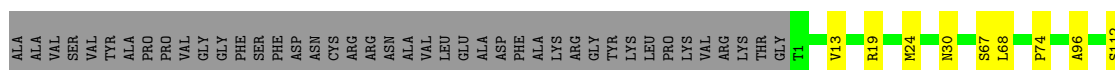




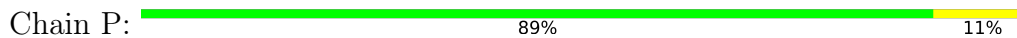
• Molecule 28: Proteasome subunit beta type-7



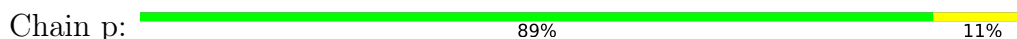
• Molecule 28: Proteasome subunit beta type-7



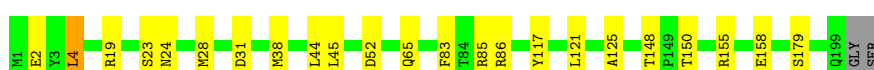
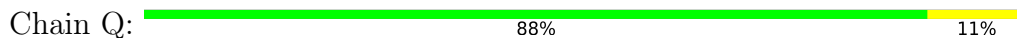
• Molecule 29: Proteasome subunit beta type-3



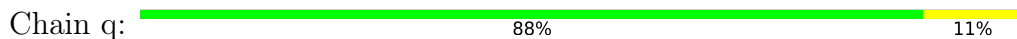
• Molecule 29: Proteasome subunit beta type-3



• Molecule 30: Proteasome subunit beta type-2

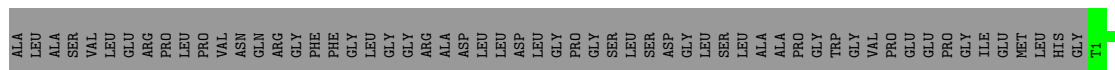


• Molecule 30: Proteasome subunit beta type-2

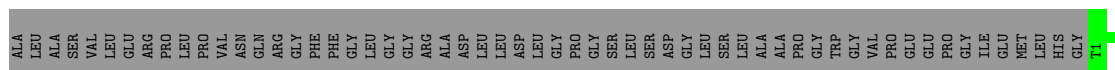




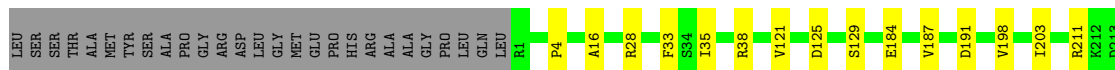
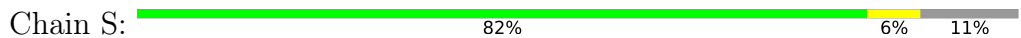
• Molecule 31: Proteasome subunit beta type-5



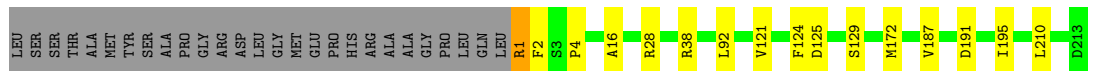
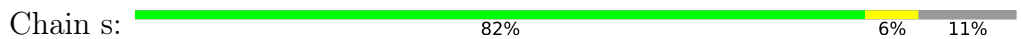
• Molecule 31: Proteasome subunit beta type-5



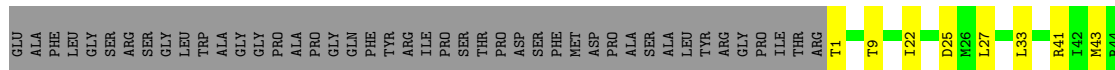
• Molecule 32: Proteasome subunit beta type-1



• Molecule 32: Proteasome subunit beta type-1



• Molecule 33: Proteasome subunit beta type-4



• Molecule 33: Proteasome subunit beta type-4

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	79691	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.023	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0035	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, ADP, 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	U	0.23	0/6449	0.60	4/8729 (0.0%)
2	V	0.28	0/3929	0.72	7/5309 (0.1%)
3	W	0.26	0/3751	0.66	4/5042 (0.1%)
4	X	0.25	0/3053	0.57	4/4115 (0.1%)
5	Y	0.27	0/3173	0.63	1/4273 (0.0%)
6	Z	0.26	0/2324	0.65	1/3150 (0.0%)
7	a	0.23	0/3053	0.61	2/4133 (0.0%)
8	b	0.22	0/1478	0.59	0/2001
9	c	0.30	0/2302	0.72	0/3110
10	d	0.26	0/2162	0.67	0/2919
11	e	0.24	0/338	0.66	0/450
12	f	0.28	0/6980	0.73	2/9433 (0.0%)
13	A	0.39	0/3148	0.68	0/4250
14	B	0.36	0/3061	0.63	2/4129 (0.0%)
15	C	0.33	0/2902	0.65	1/3904 (0.0%)
16	D	0.36	0/3089	0.69	4/4168 (0.1%)
17	E	0.33	0/3145	0.64	2/4233 (0.0%)
18	F	0.34	0/3292	0.60	0/4435
19	u	0.17	0/609	0.49	0/819
19	w	0.21	0/609	0.49	0/819
20	G	0.29	0/1859	0.51	0/2523
20	g	0.29	0/1859	0.51	0/2523
21	H	0.31	0/1743	0.49	0/2372
21	h	0.31	0/1743	0.48	0/2372
22	I	0.29	0/1942	0.57	2/2628 (0.1%)
22	i	0.29	0/1942	0.57	2/2628 (0.1%)
23	J	0.33	0/1737	0.59	0/2369
23	j	0.26	0/1728	0.55	2/2358 (0.1%)
24	K	0.29	0/1747	0.51	0/2364
24	k	0.29	0/1747	0.51	0/2364
25	L	0.36	1/1885 (0.1%)	0.60	2/2552 (0.1%)
25	l	0.36	1/1885 (0.1%)	0.60	2/2552 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	M	0.31	0/1891	0.53	0/2552
26	m	0.31	0/1891	0.53	0/2552
27	N	0.29	0/1454	0.42	0/1967
27	n	0.29	0/1454	0.42	0/1967
28	O	0.28	0/1670	0.46	0/2265
28	o	0.28	0/1670	0.46	0/2265
29	P	0.29	0/1620	0.45	0/2184
29	p	0.29	0/1620	0.46	0/2184
30	Q	0.31	0/1603	0.50	0/2174
30	q	0.31	0/1603	0.49	0/2174
31	R	0.29	0/1579	0.41	0/2134
31	r	0.29	0/1579	0.40	0/2134
32	S	0.29	0/1671	0.45	0/2253
32	s	0.29	0/1674	0.46	0/2257
33	T	0.30	0/1700	0.48	0/2305
33	t	0.30	0/1700	0.49	0/2305
All	All	0.30	2/107043 (0.0%)	0.59	44/144698 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	U	0	1
2	V	0	1
3	W	0	3
5	Y	0	1
6	Z	0	2
8	b	0	1
9	c	0	2
10	d	0	1
12	f	0	11
13	A	0	1
14	B	0	1
15	C	0	4
16	D	0	3
17	E	0	1
18	F	0	2
20	G	0	1
20	g	0	1
23	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	j	0	1
30	Q	0	1
30	q	0	1
33	T	0	1
33	t	0	1
All	All	0	43

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	L	118	ILE	CA-CB	5.71	1.57	1.54
25	l	118	ILE	CA-CB	5.55	1.57	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	106	ILE	N-CA-C	-8.29	105.84	113.71
1	U	473	VAL	N-CA-C	-8.05	104.91	112.96
1	U	873	PRO	CA-C-N	6.99	134.89	121.54
1	U	873	PRO	C-N-CA	6.99	134.89	121.54
16	D	160	PRO	CA-C-N	6.15	131.12	122.46
16	D	160	PRO	C-N-CA	6.15	131.12	122.46
17	E	385	ASP	CA-C-N	5.99	132.98	121.54
17	E	385	ASP	C-N-CA	5.99	132.98	121.54
1	U	8	ILE	N-CA-C	-5.91	106.99	113.43
25	l	225	ASP	CA-C-N	5.84	132.70	121.54
25	l	225	ASP	C-N-CA	5.84	132.70	121.54
25	L	225	ASP	CA-C-N	5.84	132.70	121.54
25	L	225	ASP	C-N-CA	5.84	132.70	121.54
2	V	137	GLU	N-CA-C	5.69	122.38	109.81
2	V	167	LEU	CA-C-N	5.50	132.04	121.54
2	V	167	LEU	C-N-CA	5.50	132.04	121.54
16	D	85	ILE	CA-C-N	-5.47	113.00	119.84
16	D	85	ILE	C-N-CA	-5.47	113.00	119.84
22	i	219	GLU	CA-C-N	5.46	129.00	120.82
22	i	219	GLU	C-N-CA	5.46	129.00	120.82
14	B	53	THR	N-CA-C	5.45	121.86	109.81
22	I	219	GLU	CA-C-N	5.43	128.97	120.82
22	I	219	GLU	C-N-CA	5.43	128.97	120.82
2	V	28	PRO	N-CA-C	5.41	117.31	110.70
23	j	147	THR	CA-C-N	5.38	128.86	120.68
23	j	147	THR	C-N-CA	5.38	128.86	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	252	ASP	CA-C-N	5.35	134.85	121.80
3	W	252	ASP	C-N-CA	5.35	134.85	121.80
2	V	165	ALA	CA-C-N	5.27	131.60	121.54
2	V	165	ALA	C-N-CA	5.27	131.60	121.54
3	W	92	LYS	CA-C-N	5.26	131.59	121.54
3	W	92	LYS	C-N-CA	5.26	131.59	121.54
5	Y	241	ILE	N-CA-C	-5.25	107.28	113.42
4	X	392	PRO	CA-C-N	5.24	131.39	121.97
4	X	392	PRO	C-N-CA	5.24	131.39	121.97
15	C	128	PRO	N-CA-C	5.23	123.24	112.47
14	B	342	ILE	N-CA-C	-5.23	106.33	111.77
12	f	868	HIS	CA-C-N	5.19	131.46	121.54
12	f	868	HIS	C-N-CA	5.19	131.46	121.54
2	V	26	PRO	N-CA-C	5.08	116.89	110.70
7	a	186	LYS	CA-C-N	5.06	131.20	121.54
7	a	186	LYS	C-N-CA	5.06	131.20	121.54
4	X	342	PHE	CA-C-N	5.05	131.19	121.54
4	X	342	PHE	C-N-CA	5.05	131.19	121.54

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	A	400	ARG	Peptide
14	B	278	ALA	Peptide
15	C	127	LEU	Peptide
15	C	129	ASN	Peptide
15	C	89	VAL	Peptide
15	C	90	HIS	Peptide
16	D	125	LYS	Peptide
16	D	354	LEU	Peptide
16	D	368	ASP	Peptide
17	E	385	ASP	Peptide
18	F	344	ARG	Peptide
18	F	86	LEU	Peptide
20	G	222	VAL	Peptide
23	J	199	VAL	Peptide
30	Q	2	GLU	Peptide
33	T	45	VAL	Peptide
1	U	873	PRO	Peptide
2	V	264	TYR	Peptide
3	W	137	TYR	Peptide

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Mol	Chain	Res	Type	Group
3	W	252	ASP	Peptide
3	W	315	MET	Peptide
5	Y	233	ARG	Peptide
6	Z	145	HIS	Peptide
6	Z	223	ASN	Peptide
8	b	149	ASN	Peptide
9	c	155	VAL	Peptide
9	c	34	SER	Peptide
10	d	199	PHE	Peptide
12	f	257	ARG	Peptide
12	f	340	MET	Peptide
12	f	475	ASN	Peptide
12	f	620	PHE	Peptide
12	f	642	ALA	Peptide
12	f	679	LEU	Peptide
12	f	737	ASN	Peptide
12	f	755	ASP	Peptide
12	f	807	ARG	Peptide
12	f	809	ILE	Peptide
12	f	843	SER	Peptide
20	g	222	VAL	Peptide
23	j	199	VAL	Peptide
30	q	2	GLU	Peptide
33	t	45	VAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6334	0	6366	107	0
2	V	3852	0	3893	70	0
3	W	3703	0	3822	48	0
4	X	3009	0	3113	30	0
5	Y	3115	0	3120	42	0
6	Z	2281	0	2312	50	0
7	a	2995	0	3012	53	0
8	b	1458	0	1505	27	0
9	c	2260	0	2276	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	d	2116	0	2146	32	0
11	e	334	0	294	9	0
12	f	6866	0	6866	168	0
13	A	3096	0	3138	30	0
14	B	3018	0	3081	41	0
15	C	2864	0	2971	40	0
16	D	3039	0	3075	47	0
17	E	3097	0	3173	37	0
18	F	3251	0	3319	35	0
19	u	603	0	629	11	0
19	w	603	0	629	22	0
20	G	1826	0	1796	15	0
20	g	1826	0	1796	16	0
21	H	1708	0	1594	13	0
21	h	1708	0	1594	12	0
22	I	1912	0	1851	22	0
22	i	1912	0	1851	22	0
23	J	1713	0	1537	17	0
23	j	1704	0	1517	19	0
24	K	1722	0	1673	16	0
24	k	1722	0	1673	16	0
25	L	1850	0	1822	14	0
25	l	1850	0	1822	19	0
26	M	1856	0	1814	18	0
26	m	1856	0	1814	25	0
27	N	1430	0	1398	10	0
27	n	1430	0	1398	10	0
28	O	1643	0	1644	13	0
28	o	1643	0	1644	17	0
29	P	1591	0	1609	15	0
29	p	1591	0	1609	14	0
30	Q	1570	0	1547	16	0
30	q	1570	0	1547	16	0
31	R	1548	0	1499	10	0
31	r	1548	0	1499	9	0
32	S	1641	0	1616	11	0
32	s	1644	0	1625	12	0
33	T	1667	0	1628	18	0
33	t	1667	0	1628	19	0
34	c	1	0	0	0	0
35	A	31	0	12	1	0
35	B	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	D	31	0	12	2	0
35	E	31	0	12	2	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0
36	F	1	0	0	0	0
37	C	27	0	12	1	0
37	F	27	0	12	1	0
All	All	105426	0	104857	1212	0

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

All (1212) 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)
1:U:7:GLY:N	10:d:80:CYS:HG	1.61	0.96
12:f:462:ALA:N	19:w:6:LYS:NZ	2.30	0.80
12:f:462:ALA:HB3	19:w:6:LYS:HZ2	1.46	0.80
12:f:462:ALA:HB3	19:w:6:LYS:NZ	2.00	0.75
26:M:47:PHE:HB2	26:M:214:SER:HB3	1.73	0.70
12:f:691:PRO:HA	12:f:694:LEU:HB2	1.73	0.70
4:X:175:LYS:HG2	4:X:213:GLN:HE22	1.57	0.70
26:m:47:PHE:HB2	26:m:214:SER:HB3	1.73	0.70
12:f:462:ALA:H	19:w:6:LYS:NZ	1.89	0.68
5:Y:29:PRO:HB2	5:Y:32:ARG:HB3	1.76	0.68
2:V:247:GLN:HE21	2:V:274:SER:HA	1.58	0.68
12:f:571:GLU:HG3	12:f:573:ILE:H	1.60	0.66
2:V:223:LYS:HZ2	2:V:227:VAL:HG23	1.61	0.66
11:e:56:LEU:HB2	11:e:59:GLU:HB2	1.77	0.66
2:V:84:LYS:HG2	2:V:123:SER:HB2	1.78	0.65
12:f:463:LEU:CD2	19:w:66:THR:HB	2.26	0.65
12:f:680:ARG:HB2	12:f:763:ARG:HE	1.60	0.65
18:F:224:LEU:HB2	18:F:348:LEU:HD23	1.78	0.65
12:f:462:ALA:H	19:w:6:LYS:HZ3	1.43	0.65
16:D:345:PHE:HB3	16:D:360:LEU:HD23	1.78	0.65
21:H:119:GLN:NE2	22:I:82:ASP:OD1	2.30	0.64
1:U:337:LEU:HD21	1:U:789:ILE:HG21	1.79	0.64
16:D:133:HIS:HD2	16:D:136:SER:H	1.44	0.64
24:K:36:THR:HA	24:K:171:GLY:HA3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:559:ARG:HB3	1:U:562:GLU:HB2	1.79	0.63
12:f:276:GLU:O	12:f:286:LYS:NZ	2.32	0.63
12:f:673:ARG:HH22	12:f:709:THR:HA	1.63	0.63
7:a:14:SER:HB2	7:a:18:GLN:HG2	1.80	0.63
23:j:86:ARG:HE	23:j:114:LEU:HD11	1.61	0.63
12:f:609:VAL:HG12	14:B:74:MET:HE1	1.81	0.63
16:D:411:GLU:HG2	16:D:413:GLU:H	1.64	0.63
24:k:36:THR:HA	24:k:171:GLY:HA3	1.81	0.63
1:U:804:SER:HA	1:U:892:LEU:HA	1.81	0.63
28:O:163:ILE:HG12	28:O:170:GLY:HA2	1.81	0.63
28:o:163:ILE:HG12	28:o:170:GLY:HA2	1.81	0.63
22:i:143:TYR:HB2	22:i:146:GLN:HE21	1.64	0.62
2:V:216:ARG:NH2	11:e:6:GLN:O	2.31	0.62
7:a:227:ASN:O	7:a:231:GLN:NE2	2.31	0.62
8:b:16:MET:HA	8:b:25:ARG:HH11	1.65	0.62
2:V:280:ALA:HB3	2:V:285:TRP:HB2	1.80	0.62
7:a:188:LEU:HD11	7:a:193:GLN:HE21	1.65	0.62
12:f:586:PRO:HA	12:f:589:SER:HB2	1.81	0.62
18:F:439:ALA:HB1	25:L:62:LYS:HD3	1.79	0.62
1:U:131:GLU:OE1	1:U:159:ARG:NH1	2.33	0.62
19:w:23:ILE:HB	19:w:52:ASP:HA	1.81	0.62
7:a:33:LEU:HD13	7:a:36:GLN:HB2	1.82	0.62
29:p:48:ARG:HH12	29:p:114:PRO:HA	1.64	0.62
1:U:694:ILE:HG23	1:U:695:MET:HG3	1.79	0.62
3:W:63:THR:HA	3:W:68:VAL:HG22	1.81	0.62
12:f:425:GLY:HA3	12:f:451:VAL:HG11	1.81	0.62
7:a:255:TRP:O	7:a:258:GLN:NE2	2.33	0.62
2:V:255:LEU:HD22	2:V:291:TYR:HB3	1.81	0.61
16:D:115:ILE:HA	16:D:139:LEU:HB3	1.82	0.61
16:D:91:GLN:HE21	16:D:127:ASN:HB3	1.65	0.61
18:F:120:LYS:HB3	18:F:137:ILE:HD11	1.81	0.61
22:I:123:GLN:HG3	23:J:125:ARG:HE	1.65	0.61
3:W:169:LEU:O	3:W:182:ARG:NH1	2.34	0.61
22:I:143:TYR:HB2	22:I:146:GLN:HE21	1.64	0.61
29:P:48:ARG:HH12	29:P:114:PRO:HA	1.64	0.61
20:g:120:ASP:OD1	21:h:84:ARG:NH1	2.34	0.61
10:d:155:LYS:HE2	10:d:167:ILE:HB	1.83	0.61
25:l:139:ASP:H	33:t:81:HIS:HE1	1.47	0.61
12:f:99:LEU:HG	12:f:101:PRO:HD2	1.81	0.61
33:T:9:THR:O	33:T:41:ARG:NH2	2.34	0.61
3:W:401:THR:HG23	3:W:402:ILE:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:29:ARG:NH1	28:O:139:GLU:OE2	2.33	0.61
7:a:264:ASN:HB3	7:a:267:GLN:HE21	1.66	0.60
12:f:591:ALA:HA	12:f:594:LEU:HD23	1.83	0.60
4:X:379:ASP:HB3	4:X:384:VAL:H	1.66	0.60
7:a:129:GLN:HG3	7:a:130:VAL:HG23	1.83	0.60
22:i:119:GLN:NE2	23:j:79:ASP:OD1	2.34	0.60
1:U:770:TRP:HA	9:c:180:ASN:HB3	1.83	0.60
9:c:197:ASN:ND2	9:c:200:TYR:O	2.35	0.60
33:t:9:THR:O	33:t:41:ARG:NH2	2.34	0.60
12:f:125:ILE:HD11	12:f:128:VAL:HB	1.83	0.60
13:A:398:ARG:HH11	14:B:195:GLN:HE21	1.48	0.60
28:O:164:PHE:O	32:s:38:ARG:NH2	2.35	0.60
27:n:29:ARG:NH1	28:o:139:GLU:OE2	2.34	0.60
12:f:125:ILE:HD13	12:f:129:LEU:HB2	1.83	0.60
13:A:41:TYR:HB2	13:A:44:GLN:HB3	1.84	0.60
22:i:2:SER:N	25:l:123:TYR:HH	1.99	0.60
20:G:158:GLY:O	21:H:84:ARG:NH2	2.34	0.60
20:g:141:ILE:HG22	20:g:151:VAL:HG22	1.84	0.60
25:l:120:THR:O	26:m:129:ARG:NH1	2.34	0.60
19:u:44:ILE:HB	19:u:68:HIS:HB2	1.82	0.60
9:c:25:VAL:O	9:c:176:GLN:NE2	2.34	0.59
18:F:107:ASP:HA	18:F:110:ASN:HB2	1.84	0.59
22:I:218:ARG:NH1	22:I:223:THR:OG1	2.34	0.59
4:X:252:LYS:HA	4:X:287:LEU:HD11	1.84	0.59
13:A:284:ARG:O	18:F:334:ARG:NH2	2.32	0.59
13:A:85:GLN:HA	13:A:88:GLN:HB3	1.83	0.59
13:A:252:GLU:OE2	13:A:255:ARG:NH1	2.35	0.59
22:I:3:ARG:HB2	23:J:5:ARG:HH12	1.66	0.59
7:a:190:VAL:HB	7:a:225:LEU:HD11	1.84	0.59
3:W:162:ALA:HB1	3:W:192:LEU:HB3	1.84	0.59
16:D:332:GLU:HG3	16:D:334:PRO:HD3	1.82	0.59
17:E:56:ILE:HB	17:E:100:LEU:HB2	1.83	0.59
32:s:1:ARG:NH1	32:s:2:PHE:O	2.35	0.59
1:U:625:ILE:HG13	1:U:626:LEU:HG	1.85	0.59
12:f:830:LEU:HB2	12:f:859:PRO:HB2	1.84	0.59
14:B:196:GLU:OE2	14:B:349:ARG:NH1	2.30	0.59
17:E:253:ILE:HG13	18:F:308:ARG:HH22	1.67	0.59
20:G:141:ILE:HG22	20:G:151:VAL:HG22	1.84	0.59
12:f:168:LYS:HD3	12:f:204:ALA:HB1	1.85	0.58
12:f:462:ALA:CB	19:w:6:LYS:NZ	2.64	0.58
12:f:704:LEU:HA	12:f:707:LEU:HB2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:49:LEU:HD13	14:B:51:LEU:H	1.68	0.58
17:E:21:GLU:OE2	17:E:25:ARG:NH2	2.36	0.58
1:U:768:GLN:HB2	1:U:775:LEU:HD12	1.84	0.58
22:I:116:ASP:OD1	23:J:81:ARG:NH1	2.36	0.58
5:Y:160:ASN:HA	5:Y:163:LYS:HB2	1.85	0.58
6:Z:212:LEU:HD11	7:a:350:LYS:HA	1.86	0.58
8:b:15:TYR:O	8:b:25:ARG:NH1	2.36	0.58
12:f:634:LYS:HD2	12:f:637:LYS:HD2	1.85	0.58
18:F:305:GLU:OE1	18:F:308:ARG:NH1	2.36	0.58
1:U:540:GLN:HB2	9:c:68:ARG:HH12	1.69	0.58
5:Y:301:ILE:HG13	5:Y:343:LEU:HD12	1.83	0.58
12:f:593:THR:O	12:f:635:LYS:NZ	2.36	0.58
2:V:224:LEU:HG	2:V:257:ASN:HD22	1.69	0.58
9:c:89:PRO:HG2	19:u:44:ILE:HD11	1.85	0.58
12:f:221:ILE:HA	12:f:224:ASN:HB2	1.85	0.58
12:f:300:ARG:HE	12:f:493:ASN:HB2	1.68	0.58
12:f:679:LEU:HD13	12:f:682:GLY:H	1.68	0.58
3:W:312:MET:HE2	7:a:312:MET:HB3	1.84	0.58
4:X:106:GLU:HB3	4:X:136:LEU:HD21	1.86	0.58
6:Z:73:ASP:H	8:b:63:THR:HG21	1.68	0.58
12:f:39:LYS:HD3	12:f:85:SER:HA	1.86	0.58
12:f:106:LEU:HB2	12:f:141:LYS:HD2	1.85	0.58
20:G:137:CYS:SG	20:G:138:MET:N	2.76	0.58
20:g:137:CYS:SG	20:g:138:MET:N	2.76	0.58
24:k:48:LEU:HD21	24:k:77:ALA:HB2	1.85	0.58
2:V:494:MET:O	6:Z:278:ASN:ND2	2.36	0.58
15:C:24:TYR:O	16:D:44:TYR:OH	2.22	0.58
19:w:44:ILE:HB	19:w:68:HIS:HB2	1.84	0.58
33:T:45:VAL:HB	33:T:49:THR:HG23	1.86	0.58
1:U:13:ASP:OD1	1:U:44:LYS:NZ	2.35	0.58
2:V:325:LYS:HA	2:V:328:VAL:HG12	1.86	0.58
3:W:274:VAL:O	3:W:283:GLN:NE2	2.37	0.58
6:Z:109:ASN:ND2	6:Z:140:SER:OG	2.36	0.58
7:a:342:ASP:OD1	7:a:345:GLN:NE2	2.36	0.58
25:L:186:GLU:HA	25:L:189:LYS:HG2	1.84	0.58
6:Z:249:PHE:HZ	9:c:303:MET:HG2	1.69	0.57
24:K:48:LEU:HD21	24:K:77:ALA:HB2	1.85	0.57
25:l:186:GLU:HA	25:l:189:LYS:HG2	1.84	0.57
1:U:798:PRO:O	1:U:880:ASN:ND2	2.36	0.57
12:f:505:MET:HE3	12:f:537:THR:HG22	1.86	0.57
8:b:24:THR:HG22	8:b:26:LEU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:S:4:PRO:O	33:T:100:ARG:NH2	2.36	0.57
2:V:212:TYR:OH	2:V:287:ARG:NH2	2.38	0.57
12:f:184:LEU:HD21	14:B:58:CYS:HA	1.87	0.57
18:F:282:ILE:HG22	18:F:327:LYS:HB2	1.85	0.57
29:P:62:THR:OG1	30:Q:85:ARG:NH2	2.35	0.57
8:b:142:ASN:HD22	8:b:172:THR:HA	1.70	0.57
12:f:438:ASP:HA	12:f:477:MET:HE2	1.87	0.57
12:f:471:LEU:HD22	12:f:477:MET:HG3	1.86	0.57
12:f:556:ARG:HD3	12:f:786:GLN:HB2	1.86	0.57
16:D:353:ASN:ND2	16:D:392:TYR:O	2.38	0.57
16:D:96:VAL:HG23	16:D:102:ILE:HD11	1.85	0.57
12:f:469:TYR:OH	12:f:478:ARG:NH1	2.38	0.57
22:I:106:PRO:HD2	22:I:109:GLN:HE21	1.70	0.57
6:Z:212:LEU:HD21	7:a:350:LYS:HG3	1.86	0.56
8:b:34:ASN:O	8:b:38:HIS:ND1	2.29	0.56
22:i:218:ARG:NH1	22:i:223:THR:OG1	2.34	0.56
8:b:2:VAL:O	8:b:44:ASN:ND2	2.37	0.56
12:f:482:ILE:HD11	12:f:517:VAL:HG23	1.87	0.56
1:U:471:ASP:HA	1:U:474:ARG:HB2	1.86	0.56
3:W:274:VAL:HG21	3:W:290:ILE:HD13	1.87	0.56
8:b:58:CYS:HB3	8:b:92:VAL:HG21	1.87	0.56
9:c:31:VAL:HB	9:c:205:ILE:HG22	1.86	0.56
16:D:87:LEU:HB3	17:E:80:VAL:HB	1.87	0.56
31:r:26:ILE:HG21	31:r:29:GLN:HE21	1.70	0.56
2:V:349:ARG:HA	2:V:353:LEU:HD23	1.86	0.56
12:f:139:CYS:O	12:f:143:ARG:NH1	2.38	0.56
29:p:65:GLN:OE1	30:q:86:ARG:NH2	2.38	0.56
9:c:54:MET:O	9:c:77:GLN:NE2	2.39	0.56
16:D:212:LYS:NZ	35:D:501:ATP:O1G	2.38	0.56
29:P:126:LEU:HD12	29:P:127:ILE:HG23	1.88	0.56
22:i:106:PRO:HD2	22:i:109:GLN:HE21	1.70	0.56
29:p:126:LEU:HD12	29:p:127:ILE:HG23	1.88	0.56
1:U:362:ASN:HD22	9:c:173:GLU:H	1.54	0.56
2:V:440:LYS:NZ	10:d:143:LEU:O	2.38	0.56
12:f:497:VAL:HA	12:f:500:LEU:HB2	1.88	0.56
16:D:342:ARG:HB3	16:D:364:VAL:HG11	1.88	0.56
17:E:251:ARG:HB3	17:E:255:ARG:HH12	1.70	0.56
30:Q:38:MET:O	30:Q:65:GLN:NE2	2.39	0.56
12:f:469:TYR:O	12:f:472:HIS:ND1	2.32	0.56
31:R:19:ARG:NH2	29:p:205:ASP:OD2	2.39	0.56
27:n:127:ILE:HG12	27:n:132:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:202:VAL:HB	1:U:216:VAL:HG23	1.88	0.56
7:a:252:LYS:HG2	7:a:255:TRP:HE1	1.71	0.56
20:G:11:ARG:O	20:G:24:GLN:NE2	2.39	0.56
26:M:163:CYS:SG	26:M:164:ALA:N	2.79	0.56
28:o:96:ALA:H	28:o:115:PRO:HB3	1.70	0.56
3:W:63:THR:HG22	3:W:68:VAL:HG13	1.87	0.56
4:X:415:TYR:HE1	5:Y:383:LEU:HD13	1.71	0.56
12:f:796:LEU:HA	12:f:799:VAL:HG12	1.88	0.56
13:A:390:THR:HA	14:B:216:ILE:HD11	1.88	0.56
19:u:23:ILE:HB	19:u:52:ASP:HA	1.87	0.56
2:V:212:TYR:HB3	2:V:216:ARG:HH12	1.71	0.55
27:N:127:ILE:HG12	27:N:132:SER:HB2	1.87	0.55
28:O:96:ALA:H	28:O:115:PRO:HB3	1.70	0.55
30:Q:117:TYR:HB3	30:Q:125:ALA:HB3	1.88	0.55
33:t:45:VAL:HB	33:t:49:THR:HG23	1.86	0.55
2:V:200:ARG:HD2	2:V:242:HIS:HB2	1.87	0.55
25:l:48:ALA:HB1	25:l:62:LYS:HE3	1.88	0.55
7:a:8:LEU:HD11	7:a:26:GLU:HB3	1.87	0.55
10:d:212:LYS:HD2	10:d:213:ARG:HG2	1.87	0.55
22:I:15:GLU:OE2	22:I:17:ARG:NE	2.39	0.55
30:q:117:TYR:HB3	30:q:125:ALA:HB3	1.88	0.55
9:c:96:LEU:HD12	19:u:8:LEU:HD22	1.87	0.55
12:f:127:SER:HA	12:f:131:MET:HB2	1.89	0.55
26:m:163:CYS:SG	26:m:164:ALA:N	2.79	0.55
1:U:376:MET:HA	1:U:739:ALA:HA	1.89	0.55
8:b:26:LEU:HD11	8:b:80:PRO:HG3	1.89	0.55
23:J:38:ARG:HH12	23:J:182:GLU:HA	1.72	0.55
29:P:65:GLN:OE1	30:Q:86:ARG:NH2	2.40	0.55
2:V:190:ASP:OD1	2:V:234:ARG:NH1	2.40	0.55
3:W:231:ILE:O	3:W:235:GLN:N	2.40	0.55
18:F:232:GLY:HA2	37:F:501:ADP:H5'2	1.88	0.55
31:R:26:ILE:HG21	31:R:29:GLN:HE21	1.71	0.55
2:V:330:LYS:NZ	2:V:389:ASP:OD2	2.38	0.55
16:D:152:MET:HE3	16:D:154:LEU:HD13	1.88	0.55
25:L:48:ALA:HB1	25:L:62:LYS:HE3	1.88	0.55
5:Y:108:ALA:O	5:Y:112:CYS:N	2.39	0.55
6:Z:82:PHE:HA	6:Z:85:VAL:HG12	1.89	0.55
8:b:21:PHE:HD2	8:b:25:ARG:HG2	1.71	0.55
16:D:374:ASP:HB3	17:E:292:PRO:HG2	1.89	0.55
17:E:97:ARG:HH12	17:E:114:GLU:HB3	1.72	0.55
23:J:68:ASN:HA	23:J:211:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:465:LEU:HD11	1:U:477:GLY:HA3	1.88	0.55
4:X:172:LEU:HD12	4:X:175:LYS:HD3	1.89	0.55
10:d:2:TYR:O	10:d:25:ARG:NH2	2.40	0.55
12:f:370:MET:HE3	12:f:747:GLN:HE22	1.72	0.55
23:J:86:ARG:HE	23:J:114:LEU:HD11	1.72	0.55
33:t:192:VAL:HG12	33:t:197:VAL:HG22	1.89	0.55
16:D:170:MET:HG2	16:D:173:GLN:HB2	1.88	0.55
23:J:115:LYS:HD3	23:J:149:PRO:HA	1.89	0.55
2:V:371:ASN:OD1	2:V:427:GLN:NE2	2.41	0.54
30:q:38:MET:O	30:q:65:GLN:NE2	2.39	0.54
7:a:321:LYS:HB2	7:a:335:TRP:HB3	1.90	0.54
12:f:253:LEU:HD11	12:f:272:LEU:HB3	1.88	0.54
12:f:814:SER:HA	12:f:882:LEU:HD12	1.88	0.54
16:D:264:ILE:HB	16:D:309:MET:HG2	1.89	0.54
24:K:20:ARG:HG2	24:K:21:LEU:H	1.73	0.54
12:f:697:ILE:HG12	12:f:737:ASN:HD21	1.70	0.54
17:E:198:VAL:HG12	17:E:200:SER:H	1.73	0.54
24:k:50:VAL:HG11	24:k:66:LYS:HB2	1.90	0.54
2:V:228:ARG:NH1	2:V:253:LEU:O	2.39	0.54
3:W:375:MET:HE2	3:W:386:VAL:HB	1.88	0.54
4:X:214:SER:O	4:X:218:HIS:ND1	2.39	0.54
5:Y:192:ARG:NH1	11:e:40:GLU:OE1	2.41	0.54
12:f:171:GLN:HG3	12:f:179:VAL:HG22	1.88	0.54
12:f:828:ARG:NH1	12:f:863:THR:OG1	2.40	0.54
22:i:15:GLU:OE2	22:i:17:ARG:NE	2.39	0.54
2:V:368:ARG:NH1	11:e:50:ASP:OD2	2.40	0.54
12:f:679:LEU:HB2	12:f:681:TYR:H	1.73	0.54
17:E:265:ASP:OD2	17:E:291:ARG:NH1	2.38	0.54
30:Q:4:LEU:HD22	30:Q:45:LEU:HB3	1.90	0.54
22:i:197:LEU:HA	22:i:200:THR:HG22	1.89	0.54
30:Q:19:ARG:HH21	30:Q:31:ASP:HB2	1.73	0.54
1:U:107:HIS:HA	1:U:110:LYS:HE3	1.89	0.54
12:f:202:HIS:ND1	12:f:242:GLU:OE2	2.40	0.54
17:E:4:PRO:HG2	17:E:7:LYS:HB3	1.88	0.54
22:I:159:TRP:HA	23:J:54:GLN:HA	1.89	0.54
27:n:18:SER:HB2	27:n:31:THR:H	1.72	0.54
18:F:94:ILE:HD11	18:F:125:LYS:HB2	1.89	0.54
26:m:40:ARG:NH2	26:m:146:ALA:O	2.41	0.54
26:m:241:GLU:O	26:m:244:LYS:NZ	2.41	0.54
2:V:201:ARG:NH2	15:C:29:GLU:OE2	2.41	0.54
3:W:65:ARG:HG3	3:W:67:LEU:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:50:MET:HE2	5:Y:74:LYS:HB3	1.90	0.54
5:Y:104:MET:HA	5:Y:107:LYS:HB2	1.90	0.54
12:f:23:GLY:HA3	12:f:34:ARG:HH22	1.72	0.54
26:M:40:ARG:NH2	26:M:146:ALA:O	2.41	0.54
27:N:18:SER:HB2	27:N:31:THR:H	1.72	0.54
29:P:205:ASP:OD2	31:r:19:ARG:NH2	2.41	0.54
30:q:19:ARG:HH21	30:q:31:ASP:HB2	1.73	0.54
32:s:4:PRO:O	33:t:100:ARG:NH2	2.37	0.54
1:U:245:ALA:O	1:U:324:LYS:NZ	2.41	0.53
13:A:287:ASP:OD1	13:A:287:ASP:N	2.41	0.53
15:C:141:GLU:O	16:D:323:ARG:NH1	2.40	0.53
2:V:252:ASN:ND2	2:V:284:GLU:OE2	2.36	0.53
5:Y:160:ASN:O	5:Y:164:ALA:N	2.39	0.53
12:f:478:ARG:HG3	12:f:514:VAL:HG11	1.88	0.53
12:f:712:LYS:HD2	12:f:781:TYR:HE2	1.73	0.53
19:w:5:VAL:HB	19:w:13:ILE:HB	1.90	0.53
26:m:228:PRO:HD2	26:m:231:ILE:HD12	1.91	0.53
5:Y:99:GLU:HA	5:Y:102:ASP:HB3	1.90	0.53
6:Z:238:PRO:HG2	9:c:309:PHE:HB3	1.90	0.53
1:U:191:LYS:HD2	1:U:194:ARG:HH11	1.74	0.53
13:A:307:ASP:OD2	13:A:333:ARG:NH2	2.41	0.53
3:W:443:THR:HG21	6:Z:204:LYS:HG3	1.89	0.53
12:f:335:ARG:HB3	12:f:853:VAL:HG21	1.89	0.53
29:p:62:THR:OG1	30:q:85:ARG:NH2	2.42	0.53
1:U:780:SER:HA	1:U:783:TYR:HD2	1.74	0.53
5:Y:336:ARG:NH1	11:e:55:GLN:OE1	2.42	0.53
12:f:209:MET:HG3	12:f:211:ILE:H	1.73	0.53
22:I:197:LEU:HA	22:I:200:THR:HG22	1.89	0.53
33:T:192:VAL:HG12	33:T:197:VAL:HG22	1.89	0.53
18:F:228:PRO:O	18:F:233:LYS:NZ	2.41	0.53
3:W:361:HIS:HA	3:W:364:ARG:HE	1.74	0.53
6:Z:235:ASN:OD1	7:a:289:ARG:NH2	2.41	0.53
12:f:198:HIS:O	12:f:202:HIS:N	2.42	0.53
12:f:340:MET:SD	12:f:757:ASN:ND2	2.81	0.53
6:Z:34:ARG:HH12	6:Z:60:GLU:HG3	1.73	0.53
12:f:705:ASN:HB3	12:f:787:LEU:HD21	1.91	0.53
10:d:47:GLN:HG2	10:d:48:LEU:HG	1.91	0.53
12:f:487:LEU:HD11	12:f:804:LEU:HD12	1.90	0.53
16:D:173:GLN:HE22	16:D:334:PRO:HD2	1.74	0.53
26:M:228:PRO:HD2	26:M:231:ILE:HD12	1.91	0.53
26:m:51:LYS:HB3	26:m:210:GLU:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:q:4:LEU:HD22	30:q:45:LEU:HB3	1.90	0.53
4:X:393:VAL:HB	5:Y:362:LYS:HE2	1.91	0.52
8:b:109:ILE:HB	8:b:138:VAL:HG22	1.91	0.52
19:u:5:VAL:HG22	19:u:67:LEU:HD12	1.91	0.52
26:M:168:ALA:HB1	26:M:171:ALA:HB3	1.91	0.52
1:U:65:SER:O	1:U:96:TYR:OH	2.27	0.52
6:Z:98:GLY:HA3	6:Z:123:ILE:HG23	1.91	0.52
12:f:150:GLU:O	12:f:156:HIS:ND1	2.42	0.52
12:f:585:GLU:HG3	12:f:588:ARG:HE	1.74	0.52
24:K:183:GLU:HG3	24:K:184:VAL:HG13	1.91	0.52
28:O:19:ARG:NH1	28:O:169:SER:O	2.42	0.52
23:j:31:THR:OG1	23:j:163:ARG:O	2.27	0.52
1:U:701:ILE:HG21	1:U:810:THR:HA	1.91	0.52
12:f:378:ASN:O	12:f:382:ASN:ND2	2.43	0.52
15:C:28:ILE:HD11	16:D:47:LEU:HD12	1.90	0.52
20:g:11:ARG:O	20:g:24:GLN:NE2	2.39	0.52
21:h:100:VAL:HG13	29:p:93:ASN:HD22	1.74	0.52
24:k:20:ARG:HG2	24:k:21:LEU:H	1.73	0.52
3:W:124:LEU:HD13	3:W:151:THR:HG22	1.92	0.52
4:X:379:ASP:OD2	5:Y:312:ARG:NH1	2.42	0.52
14:B:387:LYS:HB3	14:B:390:LEU:HB3	1.92	0.52
16:D:352:MET:HE1	16:D:379:CYS:HB3	1.92	0.52
24:K:50:VAL:HG11	24:K:66:LYS:HB2	1.90	0.52
2:V:145:LEU:HA	2:V:151:THR:HG21	1.92	0.52
3:W:167:GLN:HG3	3:W:168:GLU:HG3	1.91	0.52
8:b:100:ARG:NH1	8:b:102:GLY:O	2.42	0.52
12:f:726:ILE:O	12:f:730:GLY:N	2.37	0.52
26:m:37:ILE:HD11	26:m:193:VAL:HG13	1.91	0.52
8:b:25:ARG:NH2	8:b:145:GLU:OE1	2.43	0.52
17:E:199:VAL:HG23	17:E:201:SER:H	1.74	0.52
26:M:241:GLU:O	26:M:244:LYS:NZ	2.41	0.52
24:k:183:GLU:HG3	24:k:184:VAL:HG13	1.91	0.52
7:a:221:VAL:HG23	7:a:222:LEU:HG	1.92	0.52
12:f:233:LEU:HD12	12:f:264:GLU:HG3	1.92	0.52
12:f:463:LEU:HD23	19:w:66:THR:HB	1.91	0.52
24:K:76:CYS:SG	24:K:77:ALA:N	2.83	0.52
31:R:141:ARG:NH2	30:q:162:LYS:O	2.43	0.52
23:j:115:LYS:HD3	23:j:149:PRO:HA	1.90	0.52
3:W:24:VAL:HG22	3:W:27:ARG:HH12	1.75	0.52
3:W:159:VAL:HG13	3:W:196:VAL:HG22	1.92	0.52
12:f:288:VAL:HA	12:f:291:GLN:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:737:ASN:O	12:f:746:ARG:NH1	2.42	0.52
12:f:829:MET:H	12:f:845:ARG:HB3	1.74	0.52
1:U:177:LEU:O	1:U:205:TYR:OH	2.27	0.52
2:V:166:TYR:HB3	2:V:168:GLN:HE21	1.74	0.52
2:V:322:VAL:O	2:V:325:LYS:N	2.41	0.52
6:Z:187:LEU:HD23	10:d:254:GLU:HG2	1.92	0.52
12:f:291:GLN:HE22	12:f:324:VAL:HG11	1.75	0.52
26:M:66:LEU:HD21	26:M:214:SER:HB2	1.92	0.52
26:m:66:LEU:HD21	26:m:214:SER:HB2	1.92	0.52
28:o:19:ARG:NH1	28:o:169:SER:O	2.42	0.52
2:V:228:ARG:O	2:V:232:HIS:ND1	2.43	0.52
8:b:100:ARG:HH12	8:b:105:HIS:HB2	1.75	0.52
9:c:84:VAL:O	19:u:75:GLY:N	2.41	0.52
17:E:247:THR:O	17:E:251:ARG:NH2	2.42	0.52
32:S:28:ARG:NH2	32:S:191:ASP:OD1	2.40	0.52
24:k:76:CYS:SG	24:k:77:ALA:N	2.83	0.52
1:U:613:ASP:OD1	1:U:616:ARG:NH2	2.42	0.51
1:U:646:PRO:HA	1:U:649:ARG:HB2	1.93	0.51
7:a:19:PRO:HA	7:a:22:TRP:HD1	1.74	0.51
27:N:32:ASP:OD1	27:N:186:ARG:NH2	2.43	0.51
3:W:378:MET:HE1	3:W:415:PHE:HZ	1.74	0.51
9:c:124:GLY:O	9:c:128:ASN:ND2	2.44	0.51
11:e:53:SER:O	11:e:57:ARG:NH2	2.38	0.51
12:f:790:GLN:HG2	12:f:794:ALA:HB3	1.91	0.51
12:f:813:LYS:HD3	12:f:815:HIS:HE1	1.75	0.51
14:B:58:CYS:SG	14:B:59:ARG:N	2.83	0.51
15:C:89:VAL:HB	15:C:92:GLU:HB3	1.92	0.51
17:E:182:LEU:HD22	35:E:401:ATP:H2'	1.91	0.51
24:K:41:GLN:NE2	24:K:151:PRO:O	2.43	0.51
32:S:187:VAL:HG21	28:o:24:MET:HE3	1.92	0.51
26:m:168:ALA:HB1	26:m:171:ALA:HB3	1.91	0.51
32:s:125:ASP:OD1	32:s:129:SER:N	2.40	0.51
1:U:593:SER:OG	1:U:595:ASN:ND2	2.43	0.51
3:W:118:LEU:HA	3:W:121:LYS:HZ3	1.75	0.51
15:C:69:GLN:HG3	15:C:118:ASN:HD21	1.75	0.51
19:w:5:VAL:HG22	19:w:67:LEU:HD12	1.91	0.51
27:n:32:ASP:OD1	27:n:186:ARG:NH2	2.43	0.51
5:Y:101:ARG:HE	5:Y:127:THR:HA	1.76	0.51
17:E:148:VAL:HG13	17:E:149:ILE:HG23	1.91	0.51
18:F:39:GLU:HA	18:F:42:ILE:HB	1.93	0.51
27:n:144:ARG:H	27:n:147:MET:HE3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:p:2:SER:OG	29:p:3:ILE:N	2.43	0.51
3:W:334:GLU:O	3:W:338:THR:N	2.40	0.51
7:a:197:ALA:HB2	7:a:222:LEU:HD22	1.92	0.51
12:f:414:LEU:HD23	12:f:417:ILE:HD12	1.91	0.51
16:D:233:SER:OG	17:E:259:GLU:OE1	2.28	0.51
19:u:5:VAL:HB	19:u:13:ILE:HB	1.92	0.51
26:M:37:ILE:HD11	26:M:193:VAL:HG13	1.91	0.51
26:M:51:LYS:HB3	26:M:210:GLU:HB3	1.91	0.51
27:N:144:ARG:H	27:N:147:MET:HE3	1.76	0.51
5:Y:69:LEU:HA	5:Y:72:LYS:HE3	1.93	0.51
10:d:175:ARG:HD3	10:d:198:LEU:HD22	1.93	0.51
24:k:41:GLN:NE2	24:k:151:PRO:O	2.43	0.51
3:W:183:VAL:HG12	3:W:187:LEU:HD23	1.91	0.51
5:Y:168:ILE:HG23	5:Y:173:ASP:HB2	1.92	0.51
18:F:336:ASP:OD1	18:F:336:ASP:N	2.42	0.51
33:T:43:MET:HE3	33:T:45:VAL:HG22	1.93	0.51
25:l:148:CYS:SG	25:l:150:SER:OG	2.69	0.51
1:U:204:ILE:HA	1:U:207:ASN:HB2	1.92	0.51
3:W:237:GLU:HG2	3:W:238:GLY:H	1.76	0.51
5:Y:241:ILE:HG23	5:Y:242:LYS:HG2	1.92	0.51
7:a:54:ASP:HA	7:a:57:ILE:HG22	1.93	0.51
11:e:49:GLU:O	11:e:53:SER:OG	2.23	0.51
21:H:4:ARG:NH1	21:H:5:GLY:O	2.43	0.51
1:U:443:LEU:HD22	1:U:461:LEU:HG	1.92	0.51
3:W:347:GLY:O	3:W:351:TRP:N	2.37	0.51
12:f:228:LYS:HB3	12:f:231:LEU:HD13	1.93	0.51
12:f:679:LEU:HD11	12:f:686:LEU:HD21	1.92	0.51
17:E:220:ASN:OD1	17:E:223:ARG:NH2	2.43	0.51
6:Z:137:ALA:O	6:Z:157:HIS:ND1	2.44	0.51
7:a:273:GLN:HB3	7:a:310:LEU:HD11	1.93	0.50
16:D:266:GLU:OE2	17:E:262:ASN:ND2	2.45	0.50
25:l:146:GLN:HE21	25:l:154:PHE:HD2	1.59	0.50
3:W:268:LYS:HD3	3:W:333:LEU:HD13	1.92	0.50
5:Y:84:LEU:HD22	5:Y:104:MET:HE2	1.94	0.50
17:E:148:VAL:HB	17:E:297:ARG:HH21	1.76	0.50
1:U:19:LEU:O	1:U:23:ALA:N	2.44	0.50
6:Z:135:THR:HG21	6:Z:162:ILE:HD11	1.93	0.50
10:d:162:SER:OG	10:d:164:THR:OG1	2.27	0.50
12:f:305:LEU:HB2	12:f:317:LEU:HD22	1.92	0.50
12:f:447:ALA:HA	12:f:450:ILE:HD12	1.93	0.50
13:A:324:PRO:HA	13:A:327:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:h:4:ARG:NH1	21:h:5:GLY:O	2.43	0.50
7:a:58:LYS:NZ	7:a:87:MET:SD	2.84	0.50
15:C:246:ILE:HB	15:C:291:VAL:HG12	1.94	0.50
16:D:335:LEU:HD11	16:D:371:SER:HA	1.93	0.50
18:F:435:LEU:HD11	24:K:20:ARG:HB3	1.92	0.50
31:R:77:ALA:O	31:R:120:ARG:NH2	2.44	0.50
21:h:69:THR:HG23	21:h:71:HIS:H	1.77	0.50
9:c:79:GLY:HA2	9:c:84:VAL:HA	1.94	0.50
12:f:704:LEU:O	12:f:708:ASP:N	2.43	0.50
15:C:88:LYS:HB3	15:C:94:LYS:HG2	1.93	0.50
32:s:92:LEU:HD23	32:s:124:PHE:HE2	1.77	0.50
12:f:628:ASP:O	12:f:632:LYS:N	2.40	0.50
14:B:117:ASP:OD1	14:B:117:ASP:N	2.43	0.50
1:U:45:ILE:O	1:U:49:TYR:N	2.45	0.50
1:U:104:CYS:O	1:U:108:TYR:N	2.45	0.50
21:H:69:THR:HG23	21:H:71:HIS:H	1.77	0.50
23:J:119:THR:HG22	23:J:126:PRO:HB3	1.94	0.50
25:l:204:ASP:OD1	25:l:204:ASP:N	2.45	0.50
4:X:254:MET:HG3	4:X:255:LEU:HG	1.94	0.50
25:L:204:ASP:OD1	25:L:204:ASP:N	2.45	0.50
21:h:204:THR:OG1	21:h:206:ASP:OD1	2.30	0.50
23:j:68:ASN:HA	23:j:211:MET:HE1	1.93	0.50
33:t:43:MET:HE3	33:t:45:VAL:HG22	1.93	0.50
1:U:554:LEU:HG	1:U:588:MET:HE1	1.94	0.50
5:Y:233:ARG:NH1	5:Y:264:TYR:O	2.45	0.50
7:a:115:LYS:HD3	7:a:118:ILE:HD12	1.93	0.50
12:f:240:VAL:HA	12:f:257:ARG:HH21	1.76	0.50
17:E:244:SER:H	18:F:300:LYS:HA	1.77	0.50
18:F:153:VAL:HG22	18:F:160:ILE:HG22	1.94	0.50
1:U:791:LEU:HD22	1:U:911:ILE:HD11	1.93	0.49
6:Z:9:VAL:HA	6:Z:48:LEU:HB3	1.94	0.49
25:L:146:GLN:HE21	25:L:154:PHE:HD2	1.59	0.49
27:n:136:TYR:HE2	33:t:33:LEU:HD21	1.76	0.49
16:D:214:MET:N	35:D:501:ATP:O2A	2.45	0.49
19:u:1:MET:N	19:u:17:VAL:O	2.36	0.49
22:I:69:ASN:HD22	22:I:72:MET:HE3	1.77	0.49
32:S:38:ARG:HH12	33:T:151:ARG:HD3	1.77	0.49
20:g:32:ILE:HA	20:g:82:GLY:HA2	1.94	0.49
4:X:299:LEU:HD21	4:X:331:LEU:HA	1.92	0.49
27:N:76:VAL:HG23	27:N:104:ASP:HB2	1.94	0.49
1:U:469:SER:OG	1:U:470:ASN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:714:SER:HA	1:U:717:ILE:HG22	1.94	0.49
6:Z:68:TRP:HE1	6:Z:111:LEU:HD22	1.76	0.49
12:f:752:HIS:HE1	12:f:803:PHE:HZ	1.61	0.49
12:f:872:VAL:HG21	12:f:882:LEU:H	1.76	0.49
5:Y:203:ASP:OD1	5:Y:203:ASP:N	2.46	0.49
5:Y:315:THR:HA	5:Y:353:ILE:HA	1.93	0.49
12:f:191:ILE:HG22	12:f:231:LEU:HD11	1.94	0.49
12:f:711:SER:HA	12:f:749:ALA:HB2	1.94	0.49
21:H:204:THR:OG1	21:H:206:ASP:OD1	2.30	0.49
1:U:108:TYR:HD1	1:U:130:LEU:HG	1.77	0.49
1:U:128:GLN:HA	1:U:131:GLU:HG2	1.93	0.49
2:V:418:SER:HA	2:V:457:TYR:HA	1.95	0.49
15:C:147:THR:HG22	15:C:150:MET:HE3	1.94	0.49
15:C:232:ARG:HD3	15:C:279:GLN:HE21	1.77	0.49
1:U:62:LEU:HD12	1:U:84:ALA:HB1	1.95	0.49
1:U:451:ALA:O	1:U:453:HIS:ND1	2.45	0.49
20:G:32:ILE:HA	20:G:82:GLY:HA2	1.94	0.49
31:r:77:ALA:O	31:r:120:ARG:NH2	2.44	0.49
2:V:467:TYR:OH	4:X:397:TYR:OH	2.28	0.49
12:f:564:LEU:HD22	12:f:776:LEU:HG	1.94	0.49
18:F:272:PHE:HD2	18:F:316:GLN:HG3	1.77	0.49
12:f:353:LEU:HD11	13:A:268:LYS:HD3	1.95	0.49
12:f:743:ALA:HA	12:f:746:ARG:HH21	1.78	0.49
1:U:9:ILE:HD11	1:U:38:ILE:HG13	1.95	0.49
1:U:14:GLU:HG2	1:U:16:GLU:H	1.77	0.49
7:a:341:LEU:HB2	7:a:345:GLN:HE21	1.78	0.49
8:b:124:LEU:HD21	8:b:152:LYS:HB3	1.95	0.49
12:f:119:LYS:HA	12:f:122:ALA:HB3	1.95	0.49
17:E:23:ASP:OD2	17:E:27:LYS:NZ	2.46	0.49
27:n:76:VAL:HG23	27:n:104:ASP:HB2	1.94	0.49
2:V:200:ARG:NH2	2:V:237:THR:OG1	2.46	0.48
10:d:91:GLU:OE1	10:d:96:HIS:NE2	2.46	0.48
13:A:213:LEU:HD22	13:A:337:LEU:HD23	1.95	0.48
33:T:92:LEU:HD23	33:T:112:ILE:HD11	1.95	0.48
33:t:92:LEU:HD23	33:t:112:ILE:HD11	1.95	0.48
1:U:217:CYS:HB2	1:U:248:ILE:HD12	1.95	0.48
1:U:695:MET:HE1	1:U:709:PHE:HD2	1.78	0.48
7:a:292:THR:HG23	7:a:295:GLU:H	1.77	0.48
12:f:552:ASP:HB3	12:f:556:ARG:HG3	1.95	0.48
13:A:140:VAL:HG12	13:A:152:PRO:HA	1.95	0.48
22:I:38:LEU:HB3	22:I:43:VAL:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:g:86:ASP:OD1	26:m:120:HIS:NE2	2.31	0.48
22:i:33:THR:HA	22:i:165:GLY:HA2	1.95	0.48
10:d:49:ILE:HG23	10:d:50:LEU:HD12	1.95	0.48
14:B:262:ASP:OD1	14:B:265:LYS:NZ	2.47	0.48
15:C:373:GLU:HG3	15:C:375:ARG:HG3	1.94	0.48
30:Q:38:MET:HE1	30:Q:44:LEU:HB2	1.95	0.48
22:i:69:ASN:HD22	22:i:72:MET:HE3	1.77	0.48
9:c:115:HIS:HB3	9:c:118:PHE:HB2	1.95	0.48
25:l:164:ARG:O	25:l:198:THR:OG1	2.27	0.48
5:Y:362:LYS:O	5:Y:366:TYR:N	2.44	0.48
6:Z:134:PRO:HG2	9:c:220:LEU:HG	1.95	0.48
23:j:121:SER:HB3	23:j:124:ARG:HD2	1.96	0.48
30:q:38:MET:HE1	30:q:44:LEU:HB2	1.95	0.48
12:f:462:ALA:N	19:w:6:LYS:HZ1	2.08	0.48
12:f:811:LEU:HD21	12:f:862:ILE:HD13	1.96	0.48
14:B:107:MET:HB2	15:C:96:VAL:HB	1.94	0.48
17:E:304:PRO:O	17:E:309:ARG:NH1	2.46	0.48
25:l:14:SER:HB3	25:l:18:ARG:H	1.78	0.48
3:W:312:MET:HG3	3:W:313:GLU:H	1.79	0.48
10:d:116:HIS:HA	10:d:119:LEU:HD23	1.94	0.48
17:E:368:MET:HB3	17:E:372:ARG:HH12	1.79	0.48
22:I:33:THR:HA	22:I:165:GLY:HA2	1.95	0.48
22:i:123:GLN:HG3	23:j:125:ARG:HE	1.77	0.48
1:U:400:ALA:O	1:U:404:ALA:N	2.45	0.48
4:X:67:GLY:HA2	4:X:109:LEU:HD21	1.95	0.48
7:a:290:GLN:O	7:a:330:ARG:NH2	2.47	0.48
15:C:273:MET:HE2	15:C:277:LEU:HD11	1.94	0.48
28:O:143:ARG:NH2	28:O:150:GLU:OE1	2.47	0.48
5:Y:40:GLU:O	5:Y:44:ALA:N	2.47	0.48
5:Y:60:SER:OG	5:Y:61:LEU:N	2.47	0.48
6:Z:128:PRO:O	9:c:215:LYS:NZ	2.42	0.48
12:f:94:LYS:HA	12:f:97:LYS:HB2	1.95	0.48
13:A:261:PHE:O	13:A:265:ARG:NH2	2.46	0.48
14:B:342:ILE:HG22	14:B:350:LYS:HE3	1.95	0.48
15:C:307:ARG:HH21	15:C:310:ARG:CZ	2.27	0.48
17:E:248:SER:HA	17:E:251:ARG:HD3	1.95	0.48
31:R:19:ARG:HE	31:R:29:GLN:HE22	1.60	0.48
1:U:490:ARG:HB2	1:U:493:VAL:HG12	1.96	0.48
7:a:12:GLN:HE21	7:a:19:PRO:HB3	1.79	0.48
10:d:178:ILE:O	10:d:182:ILE:N	2.47	0.48
18:F:117:ARG:NH2	18:F:135:PRO:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:H:100:VAL:HG13	29:P:93:ASN:HD22	1.78	0.48
29:P:2:SER:OG	29:P:3:ILE:N	2.43	0.48
25:l:117:GLN:NE2	26:m:83:ASP:OD1	2.47	0.48
1:U:499:THR:O	1:U:503:GLN:NE2	2.39	0.47
2:V:494:MET:SD	2:V:495:ARG:NH1	2.87	0.47
7:a:255:TRP:HB3	7:a:261:LEU:HD11	1.96	0.47
7:a:278:MET:HE2	7:a:319:LEU:HB2	1.96	0.47
12:f:619:HIS:H	14:B:85:MET:HE1	1.79	0.47
13:A:368:ILE:HG22	13:A:406:GLU:HB2	1.96	0.47
17:E:180:LYS:NZ	35:E:401:ATP:O2G	2.47	0.47
18:F:433:ALA:HB3	24:K:20:ARG:HH22	1.79	0.47
25:L:14:SER:HB3	25:L:18:ARG:H	1.78	0.47
22:i:38:LEU:HB3	22:i:43:VAL:HG23	1.94	0.47
31:r:19:ARG:HE	31:r:29:GLN:HE22	1.60	0.47
32:S:125:ASP:OD1	32:S:129:SER:N	2.41	0.47
23:j:120:GLN:O	24:k:134:SER:OG	2.29	0.47
2:V:195:ILE:HG13	15:C:25:LEU:HD22	1.95	0.47
5:Y:48:ASN:HD21	5:Y:77:ASN:HA	1.78	0.47
8:b:50:GLY:HA3	8:b:64:LEU:HA	1.96	0.47
8:b:180:ALA:HA	8:b:183:LEU:HD13	1.96	0.47
3:W:187:LEU:HA	3:W:190:MET:HE3	1.96	0.47
14:B:145:GLU:HG2	14:B:148:CYS:HB2	1.97	0.47
14:B:173:VAL:HG21	15:C:233:GLU:HG3	1.97	0.47
25:l:72:ILE:HG22	25:l:134:ILE:HG12	1.97	0.47
1:U:59:PHE:HA	1:U:62:LEU:HD13	1.96	0.47
4:X:73:VAL:O	4:X:77:LEU:N	2.47	0.47
10:d:234:ASP:OD1	10:d:234:ASP:N	2.45	0.47
12:f:462:ALA:CB	19:w:6:LYS:HZ2	2.20	0.47
13:A:73:ALA:HA	14:B:140:ASP:HB3	1.96	0.47
17:E:117:PRO:HD3	18:F:94:ILE:HG23	1.97	0.47
25:L:139:ASP:H	33:T:81:HIS:HE1	1.60	0.47
28:o:143:ARG:NH2	28:o:150:GLU:OE1	2.47	0.47
20:g:49:VAL:HG22	20:g:219:VAL:HG23	1.97	0.47
1:U:788:VAL:HG12	1:U:909:GLY:HA2	1.96	0.47
2:V:467:TYR:OH	6:Z:255:ASP:OD1	2.31	0.47
4:X:170:GLN:NE2	4:X:192:SER:OG	2.39	0.47
10:d:191:PHE:N	10:d:220:ASN:OD1	2.37	0.47
14:B:170:LEU:HD13	15:C:229:ARG:HH11	1.79	0.47
30:Q:52:ASP:OD1	31:R:88:TYR:OH	2.28	0.47
23:j:132:LEU:HD21	23:j:159:ASN:HB3	1.97	0.47
3:W:124:LEU:HA	3:W:127:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:101:ARG:NH2	5:Y:126:LYS:O	2.38	0.47
16:D:338:ARG:HH12	21:H:201:GLY:HA3	1.79	0.47
22:I:229:LYS:N	22:I:232:GLU:OE2	2.47	0.47
25:L:72:ILE:HG22	25:L:134:ILE:HG12	1.97	0.47
32:S:38:ARG:NH2	28:o:164:PHE:O	2.48	0.47
33:t:79:ASP:HB3	33:t:81:HIS:HD2	1.79	0.47
2:V:200:ARG:O	2:V:204:ASP:N	2.48	0.47
3:W:142:ARG:HH12	3:W:176:SER:HB3	1.80	0.47
5:Y:88:LEU:HA	5:Y:100:ILE:HG12	1.96	0.47
6:Z:116:CYS:O	6:Z:119:SER:OG	2.32	0.47
7:a:194:GLN:HB3	7:a:225:LEU:HG	1.96	0.47
9:c:291:LEU:O	9:c:295:ASN:ND2	2.48	0.47
28:o:120:ASP:OD1	28:o:120:ASP:N	2.48	0.47
33:t:49:THR:HB	33:t:85:PRO:HG3	1.97	0.47
1:U:415:HIS:CD2	1:U:418:GLU:H	2.32	0.47
1:U:462:LEU:HD11	1:U:492:ASP:HB3	1.97	0.47
12:f:281:ILE:HA	12:f:282:PHE:HA	1.63	0.47
12:f:524:MET:HA	12:f:776:LEU:HD23	1.96	0.47
18:F:103:ASP:HA	18:F:104:GLN:HA	1.71	0.47
24:k:199:LEU:HD11	24:k:217:LEU:HD11	1.97	0.47
1:U:218:GLN:HG3	1:U:752:THR:HB	1.97	0.46
1:U:247:GLN:HG3	1:U:904:LYS:HD2	1.97	0.46
1:U:900:TYR:HB3	1:U:914:LEU:HG	1.98	0.46
10:d:122:LEU:HB2	10:d:125:LYS:HB2	1.96	0.46
14:B:337:LEU:HD11	14:B:342:ILE:HD11	1.96	0.46
15:C:344:LEU:HD23	15:C:347:ILE:HD12	1.97	0.46
33:T:49:THR:HB	33:T:85:PRO:HG3	1.97	0.46
33:T:79:ASP:HB3	33:T:81:HIS:HD2	1.79	0.46
1:U:157:THR:HG23	1:U:159:ARG:H	1.79	0.46
9:c:33:ILE:HG23	9:c:69:VAL:HG13	1.95	0.46
12:f:302:GLY:HA2	12:f:317:LEU:HD11	1.96	0.46
12:f:373:ALA:HB2	12:f:744:MET:HA	1.97	0.46
12:f:608:LYS:HA	12:f:611:GLN:HG2	1.98	0.46
26:M:65:ARG:HH21	26:M:78:ALA:HA	1.81	0.46
1:U:801:GLN:HB3	1:U:877:LEU:HD22	1.97	0.46
2:V:194:LYS:HA	2:V:199:ASN:HB2	1.97	0.46
2:V:470:ARG:HD2	10:d:238:PRO:HG3	1.97	0.46
2:V:470:ARG:HE	10:d:242:LEU:HD21	1.81	0.46
6:Z:256:GLN:NE2	9:c:295:ASN:O	2.48	0.46
7:a:228:THR:HA	7:a:231:GLN:HE21	1.80	0.46
8:b:157:VAL:HG21	8:b:170:LEU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:378:ASN:OD1	12:f:382:ASN:ND2	2.47	0.46
14:B:56:THR:OG1	14:B:57:GLN:N	2.48	0.46
14:B:183:THR:OG1	14:B:184:TYR:N	2.48	0.46
15:C:151:ILE:HG21	15:C:158:ILE:HD11	1.96	0.46
17:E:144:GLU:OE2	17:E:297:ARG:NH1	2.48	0.46
18:F:35:LYS:HB2	18:F:38:THR:HB	1.97	0.46
24:K:199:LEU:HD11	24:K:217:LEU:HD11	1.97	0.46
25:L:148:CYS:SG	25:L:150:SER:OG	2.69	0.46
29:p:135:ASP:OD1	29:p:135:ASP:N	2.46	0.46
1:U:220:LEU:O	1:U:224:ASP:N	2.47	0.46
15:C:113:ARG:HB3	15:C:127:LEU:HB3	1.97	0.46
25:l:121:GLN:HG3	26:m:129:ARG:HG2	1.97	0.46
26:m:214:SER:HG	26:m:224:HIS:HE2	1.59	0.46
28:o:112:SER:OG	28:o:120:ASP:OD1	2.34	0.46
1:U:475:HIS:NE2	1:U:507:VAL:O	2.33	0.46
4:X:163:LYS:HA	4:X:166:LEU:HD13	1.98	0.46
14:B:140:ASP:O	14:B:142:ASP:N	2.45	0.46
21:h:67:PRO:HG2	28:o:68:LEU:HD11	1.98	0.46
22:i:229:LYS:N	22:i:232:GLU:OE2	2.47	0.46
1:U:113:VAL:HA	1:U:158:ARG:HG3	1.98	0.46
3:W:265:GLN:OE1	3:W:335:SER:OG	2.33	0.46
4:X:255:LEU:HD13	4:X:267:VAL:HG13	1.97	0.46
10:d:18:LYS:O	10:d:22:GLU:N	2.48	0.46
20:g:41:ALA:HB3	20:g:166:THR:HB	1.98	0.46
7:a:159:SER:OG	7:a:175:ASP:OD2	2.34	0.46
7:a:280:MET:HB3	7:a:280:MET:HE2	1.77	0.46
10:d:101:LEU:HG	10:d:166:PHE:HE2	1.81	0.46
12:f:149:GLU:HG3	12:f:152:ALA:HB2	1.98	0.46
12:f:831:VAL:HG12	12:f:843:SER:HB3	1.98	0.46
13:A:368:ILE:HD13	13:A:409:PHE:HE2	1.81	0.46
1:U:326:ILE:O	1:U:330:SER:OG	2.29	0.46
6:Z:198:LEU:HD22	9:c:229:LEU:HD21	1.98	0.46
7:a:65:SER:HA	7:a:68:GLU:HB2	1.97	0.46
9:c:75:MET:SD	9:c:75:MET:N	2.89	0.46
17:E:232:MET:HB3	17:E:277:MET:HG2	1.96	0.46
18:F:289:ASP:OD1	18:F:289:ASP:N	2.49	0.46
32:S:198:VAL:HG22	32:S:203:ILE:HG12	1.98	0.46
32:s:28:ARG:NH2	32:s:191:ASP:OD1	2.48	0.46
1:U:97:VAL:HG22	1:U:101:ILE:HG23	1.97	0.46
1:U:577:ILE:O	1:U:581:SER:N	2.47	0.46
2:V:156:SER:HA	2:V:159:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:81:LEU:HA	7:a:84:VAL:HG12	1.98	0.46
7:a:269:LEU:HD12	7:a:272:ILE:HD11	1.98	0.46
12:f:382:ASN:ND2	12:f:388:ASP:OD2	2.49	0.46
35:A:501:ATP:O1G	14:B:343:ARG:NH2	2.47	0.46
15:C:198:LEU:HD23	37:C:501:ADP:H5'2	1.98	0.46
16:D:328:ASP:OD1	16:D:328:ASP:N	2.44	0.46
19:w:7:THR:HG22	19:w:69:LEU:HD23	1.98	0.46
25:L:164:ARG:O	25:L:198:THR:OG1	2.27	0.46
1:U:206:MET:HE3	1:U:216:VAL:HG21	1.98	0.46
1:U:341:PHE:HZ	1:U:883:ARG:HB3	1.80	0.46
12:f:594:LEU:O	12:f:635:LYS:NZ	2.43	0.46
22:I:123:GLN:NE2	23:J:118:TYR:OH	2.49	0.46
32:S:33:PHE:HA	28:o:167:LEU:HD12	1.98	0.46
26:m:214:SER:OG	26:m:224:HIS:NE2	2.31	0.46
2:V:30:PRO:HA	2:V:33:GLN:HB2	1.97	0.45
2:V:218:TYR:HA	2:V:222:ASP:HB2	1.98	0.45
4:X:63:ALA:O	4:X:67:GLY:N	2.43	0.45
4:X:173:GLU:HA	4:X:176:THR:HG22	1.97	0.45
6:Z:72:HIS:O	6:Z:76:GLU:N	2.46	0.45
16:D:65:GLN:OE1	16:D:69:LYS:NZ	2.50	0.45
20:G:120:ASP:OD1	21:H:84:ARG:NH1	2.49	0.45
29:P:7:ASN:ND2	29:P:29:GLY:O	2.39	0.45
24:k:37:ALA:HB2	24:k:50:VAL:HG23	1.98	0.45
26:m:65:ARG:HH21	26:m:78:ALA:HA	1.81	0.45
32:s:38:ARG:HH12	33:t:151:ARG:HD3	1.81	0.45
1:U:611:ASN:HB3	1:U:614:VAL:HG12	1.98	0.45
3:W:128:LEU:HD13	3:W:131:VAL:HG21	1.98	0.45
6:Z:193:ASN:ND2	6:Z:197:GLY:HA3	2.32	0.45
8:b:93:ALA:HB1	8:b:109:ILE:HD13	1.98	0.45
12:f:253:LEU:HD21	12:f:272:LEU:HD22	1.97	0.45
12:f:384:ALA:HB2	12:f:759:LEU:HD13	1.97	0.45
22:i:153:SER:OG	22:i:155:ASN:OD1	2.35	0.45
23:j:115:LYS:HG3	23:j:127:PHE:HD2	1.82	0.45
29:p:125:ASP:OD1	29:p:129:CYS:N	2.39	0.45
7:a:100:THR:HA	7:a:103:LYS:HE2	1.98	0.45
8:b:95:LEU:O	8:b:99:HIS:ND1	2.38	0.45
12:f:242:GLU:O	12:f:246:SER:OG	2.30	0.45
13:A:429:TYR:HE2	14:B:340:ALA:HB2	1.81	0.45
16:D:175:GLN:NE2	16:D:179:GLU:OE2	2.46	0.45
20:G:41:ALA:HB3	20:G:166:THR:HB	1.98	0.45
22:I:153:SER:OG	22:I:155:ASN:OD1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:114:GLU:HA	10:d:117:THR:HG22	1.99	0.45
12:f:463:LEU:HD23	19:w:66:THR:CG2	2.47	0.45
12:f:548:THR:HG21	12:f:554:TYR:HE2	1.81	0.45
17:E:342:ASP:OD2	17:E:378:LYS:NZ	2.38	0.45
28:O:112:SER:OG	28:O:120:ASP:OD1	2.34	0.45
28:O:113:ILE:HG12	28:O:119:THR:HG22	1.99	0.45
32:S:35:ILE:HB	33:T:151:ARG:HH12	1.81	0.45
23:j:185:ASP:HA	23:j:188:ILE:HD12	1.97	0.45
32:s:16:ALA:HB2	32:s:121:VAL:HG23	1.98	0.45
1:U:445:ALA:HA	1:U:448:LEU:HD12	1.99	0.45
2:V:151:THR:HA	2:V:154:ALA:HB3	1.99	0.45
2:V:290:TYR:OH	2:V:294:ARG:NH2	2.49	0.45
5:Y:376:LEU:HD22	6:Z:265:LEU:HD11	1.98	0.45
8:b:3:LEU:HB3	8:b:105:HIS:HA	1.98	0.45
12:f:460:ASP:N	12:f:460:ASP:OD1	2.49	0.45
26:M:175:GLU:HA	26:M:178:LYS:HD3	1.99	0.45
23:j:119:THR:HG22	23:j:126:PRO:HB3	1.98	0.45
1:U:471:ASP:HB2	1:U:507:VAL:HG13	1.99	0.45
2:V:84:LYS:HE3	2:V:125:ASN:HB2	1.99	0.45
3:W:36:LYS:NZ	20:G:244:GLU:O	2.49	0.45
12:f:57:GLU:HG2	12:f:93:PRO:HB3	1.98	0.45
12:f:429:ILE:HG23	12:f:444:ALA:HB1	1.99	0.45
14:B:297:SER:OG	15:C:268:GLU:OE2	2.35	0.45
16:D:358:VAL:HG22	16:D:396:ALA:HB2	1.98	0.45
20:G:49:VAL:HG22	20:G:219:VAL:HG23	1.97	0.45
24:K:37:ALA:HB2	24:K:50:VAL:HG23	1.99	0.45
29:P:58:THR:O	30:Q:85:ARG:NH2	2.50	0.45
1:U:373:ASN:HA	1:U:376:MET:HG2	1.99	0.45
4:X:402:GLU:HB2	9:c:249:LEU:HD11	1.99	0.45
17:E:280:ASN:HB2	18:F:295:ARG:HH12	1.81	0.45
24:K:60:GLU:OE1	24:K:63:SER:N	2.50	0.45
21:h:71:HIS:HA	21:h:218:PHE:H	1.81	0.45
5:Y:101:ARG:O	5:Y:105:MET:N	2.49	0.45
8:b:151:GLU:OE1	8:b:152:LYS:NZ	2.39	0.45
13:A:425:ALA:HA	14:B:339:PRO:HB2	1.99	0.45
30:Q:23:SER:HB2	30:Q:28:MET:HG2	1.99	0.45
22:i:133:SER:OG	22:i:150:SER:O	2.33	0.45
1:U:61:ALA:HA	1:U:64:ALA:HB3	1.99	0.45
1:U:153:ILE:O	1:U:157:THR:N	2.42	0.45
1:U:218:GLN:NE2	1:U:752:THR:O	2.48	0.45
9:c:59:GLY:HA2	9:c:70:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:107:MET:HE2	19:u:9:THR:HB	1.97	0.45
13:A:74:PRO:HA	13:A:75:PRO:HD3	1.81	0.45
15:C:25:LEU:HA	15:C:28:ILE:HG22	1.98	0.45
30:q:148:THR:HG22	30:q:150:THR:H	1.82	0.45
3:W:1:MET:HG3	3:W:43:VAL:HG21	1.98	0.45
3:W:23:THR:HA	3:W:26:GLN:HB2	1.97	0.45
22:I:100:GLN:HE21	30:Q:83:PHE:HE1	1.65	0.45
29:P:125:ASP:OD1	29:P:129:CYS:N	2.39	0.45
26:m:175:GLU:HA	26:m:178:LYS:HD3	1.99	0.45
1:U:898:CYS:SG	1:U:899:ARG:N	2.90	0.44
21:H:71:HIS:HA	21:H:218:PHE:H	1.81	0.44
24:K:210:LEU:HD11	24:K:215:ILE:HG12	1.99	0.44
27:N:28:ASN:ND2	27:N:30:VAL:O	2.50	0.44
24:k:60:GLU:OE1	24:k:63:SER:N	2.50	0.44
28:o:113:ILE:HG12	28:o:119:THR:HG22	1.99	0.44
30:q:81:ALA:O	30:q:84:THR:OG1	2.35	0.44
1:U:42:VAL:HG22	1:U:68:PHE:HZ	1.82	0.44
1:U:253:TYR:CZ	1:U:331:GLY:HA3	2.52	0.44
1:U:328:ILE:HG13	1:U:329:LEU:HG	1.98	0.44
6:Z:43:TRP:HB3	6:Z:48:LEU:HD22	1.99	0.44
12:f:388:ASP:HB3	12:f:391:LEU:HB2	1.99	0.44
12:f:531:ASN:HD22	12:f:534:VAL:HB	1.81	0.44
12:f:755:ASP:OD1	12:f:755:ASP:N	2.49	0.44
22:I:197:LEU:HD13	22:I:211:VAL:HG11	1.99	0.44
3:W:260:SER:HA	3:W:263:TRP:HB3	1.99	0.44
9:c:196:LEU:HA	9:c:197:ASN:HA	1.63	0.44
10:d:194:ALA:HB3	10:d:222:TYR:HE2	1.82	0.44
12:f:729:MET:HA	12:f:732:VAL:HG12	2.00	0.44
13:A:99:THR:HG22	13:A:115:VAL:HG12	1.99	0.44
17:E:168:LYS:N	17:E:296:ASP:OD2	2.51	0.44
20:g:165:ALA:HB3	21:h:56:LEU:HD22	1.99	0.44
20:g:182:LYS:HD3	20:g:185:LYS:HE2	1.99	0.44
33:t:46:ASN:OD1	33:t:46:ASN:N	2.50	0.44
1:U:177:LEU:HD23	1:U:205:TYR:HE1	1.83	0.44
2:V:247:GLN:HB3	2:V:277:PRO:HB3	1.98	0.44
2:V:404:LYS:HA	2:V:407:VAL:HG12	1.99	0.44
3:W:373:ILE:HA	7:a:326:GLU:HB3	1.99	0.44
4:X:346:GLN:HE21	4:X:349:HIS:CE1	2.34	0.44
6:Z:34:ARG:HE	6:Z:102:HIS:CD2	2.36	0.44
6:Z:43:TRP:HE3	6:Z:92:VAL:HG23	1.82	0.44
9:c:136:LEU:HD23	19:u:71:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:w:36:ILE:HB	19:w:41:GLN:HE21	1.82	0.44
23:J:154:HIS:NE2	24:K:59:MET:SD	2.89	0.44
1:U:351:MET:O	1:U:355:ASN:N	2.43	0.44
1:U:678:ASP:O	1:U:684:ARG:NH1	2.49	0.44
10:d:176:ASP:O	10:d:180:GLY:N	2.51	0.44
12:f:437:GLU:HG3	12:f:440:ILE:HD12	1.99	0.44
20:G:182:LYS:HD3	20:G:185:LYS:HE2	1.99	0.44
30:Q:148:THR:HG22	30:Q:150:THR:H	1.82	0.44
29:p:107:PRO:HG2	29:p:124:LEU:HB2	2.00	0.44
1:U:68:PHE:O	1:U:73:ALA:N	2.51	0.44
1:U:252:LEU:HD11	1:U:260:PHE:HE2	1.83	0.44
2:V:211:TYR:HD2	2:V:253:LEU:HD13	1.83	0.44
3:W:329:ARG:NH1	3:W:334:GLU:OE1	2.51	0.44
3:W:450:GLU:OE2	6:Z:219:LYS:NZ	2.47	0.44
4:X:90:ARG:HH21	4:X:125:LEU:HD12	1.82	0.44
14:B:221:GLY:HA3	14:B:347:ILE:HA	2.00	0.44
31:r:83:LEU:HD11	31:r:97:MET:HE1	1.99	0.44
4:X:194:ARG:HD2	4:X:210:LEU:HD21	2.00	0.44
5:Y:32:ARG:HH12	5:Y:36:ALA:N	2.15	0.44
7:a:18:GLN:HG3	7:a:22:TRP:HE1	1.82	0.44
9:c:161:ARG:HB3	9:c:201:TYR:CZ	2.52	0.44
12:f:859:PRO:HD2	12:f:860:LYS:HD2	1.99	0.44
15:C:83:LYS:HD2	15:C:105:ILE:HD11	1.99	0.44
24:k:99:HIS:HB2	24:k:107:MET:HE3	2.00	0.44
27:n:28:ASN:HD21	28:o:122:LEU:HD21	1.83	0.44
1:U:26:LYS:HE2	10:d:30:LEU:HD13	2.00	0.44
2:V:33:GLN:NE2	2:V:118:GLN:OE1	2.51	0.44
2:V:335:VAL:HA	2:V:338:LEU:HD12	1.99	0.44
12:f:269:ALA:O	12:f:273:ASN:N	2.45	0.44
14:B:249:ARG:HG3	14:B:283:PHE:HD2	1.81	0.44
29:P:36:THR:OG1	29:P:38:ASP:OD1	2.33	0.44
5:Y:23:ARG:NH1	5:Y:52:PRO:O	2.40	0.44
5:Y:278:VAL:O	5:Y:282:MET:N	2.48	0.44
6:Z:66:SER:OG	6:Z:103:LYS:NZ	2.51	0.44
16:D:184:PRO:HG3	16:D:191:TYR:CZ	2.53	0.44
25:L:42:THR:O	25:L:137:TYR:OH	2.36	0.44
28:O:67:SER:HB3	28:O:74:PRO:HG3	2.00	0.44
33:T:1:THR:N	33:T:105:PRO:O	2.50	0.44
22:i:218:ARG:HH11	22:i:223:THR:HG1	1.65	0.44
2:V:437:ILE:HG13	10:d:146:GLY:H	1.83	0.43
9:c:51:MET:HE3	9:c:51:MET:HB2	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:e:45:ASP:O	11:e:49:GLU:N	2.43	0.43
12:f:202:HIS:CE1	12:f:241:PRO:HB2	2.53	0.43
12:f:465:LEU:O	12:f:481:SER:OG	2.35	0.43
14:B:125:THR:OG1	14:B:126:SER:N	2.50	0.43
14:B:412:MET:HE1	15:C:177:ALA:HB1	2.00	0.43
15:C:90:HIS:CD2	15:C:90:HIS:H	2.36	0.43
18:F:358:ASN:O	18:F:362:ARG:NH1	2.50	0.43
28:O:120:ASP:OD1	28:O:120:ASP:N	2.48	0.43
29:P:189:ILE:HG23	29:P:196:THR:HB	2.00	0.43
27:n:28:ASN:ND2	27:n:30:VAL:O	2.50	0.43
28:o:67:SER:HB3	28:o:74:PRO:HG3	2.00	0.43
29:p:189:ILE:HG23	29:p:196:THR:HB	2.00	0.43
1:U:522:GLY:O	1:U:559:ARG:NH2	2.51	0.43
1:U:695:MET:HE3	1:U:695:MET:HB2	1.88	0.43
3:W:142:ARG:HE	3:W:182:ARG:HB2	1.83	0.43
6:Z:207:ASP:O	6:Z:210:SER:OG	2.29	0.43
8:b:121:GLU:HB3	8:b:152:LYS:HG2	2.00	0.43
9:c:225:TRP:CD1	9:c:226:MET:HG3	2.52	0.43
12:f:827:PRO:HA	12:f:862:ILE:HG13	2.00	0.43
12:f:833:PHE:HB2	12:f:840:LEU:HD23	2.01	0.43
15:C:301:LEU:HD13	15:C:305:LEU:HD23	2.01	0.43
16:D:284:GLU:OE1	16:D:287:ARG:NH1	2.50	0.43
16:D:337:ASP:O	16:D:341:LYS:NZ	2.39	0.43
31:R:83:LEU:HD11	31:R:97:MET:HE1	1.99	0.43
30:q:23:SER:HB2	30:q:28:MET:HG2	1.99	0.43
1:U:413:LYS:HD2	1:U:780:SER:HB2	2.00	0.43
2:V:264:TYR:O	2:V:266:GLN:N	2.50	0.43
3:W:352:LYS:O	3:W:356:ASN:N	2.51	0.43
5:Y:296:VAL:O	5:Y:300:ARG:N	2.40	0.43
6:Z:184:VAL:HG13	6:Z:188:SER:HB3	2.00	0.43
7:a:212:ASN:HD21	7:a:215:GLU:HB3	1.83	0.43
14:B:203:LEU:HA	14:B:206:THR:HG22	2.01	0.43
15:C:86:LEU:HD11	15:C:94:LYS:HD3	2.00	0.43
16:D:95:ALA:HA	16:D:101:ALA:HA	2.00	0.43
16:D:208:PRO:HB2	17:E:291:ARG:HD3	1.99	0.43
22:i:41:ASP:OD1	22:i:41:ASP:N	2.51	0.43
2:V:179:LYS:O	2:V:183:GLU:N	2.42	0.43
2:V:290:TYR:HE1	2:V:309:MET:HE1	1.84	0.43
7:a:156:TYR:HB3	7:a:179:PHE:HB2	1.99	0.43
7:a:273:GLN:HE22	7:a:302:ILE:HD13	1.83	0.43
9:c:100:LYS:HG2	9:c:105:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:417:ILE:HG22	12:f:418:LEU:HD12	2.00	0.43
30:Q:23:SER:OG	30:Q:24:ASN:N	2.52	0.43
1:U:92:ASP:OD2	1:U:140:ARG:NH1	2.51	0.43
1:U:116:ALA:HB2	1:U:158:ARG:HB3	2.01	0.43
1:U:133:ILE:O	1:U:137:MET:N	2.47	0.43
1:U:450:HIS:HB2	1:U:457:ILE:HG21	2.01	0.43
2:V:198:GLN:HB3	2:V:201:ARG:HB2	2.00	0.43
5:Y:101:ARG:HD3	5:Y:130:LYS:HD3	2.00	0.43
5:Y:173:ASP:O	5:Y:177:ARG:N	2.51	0.43
6:Z:138:TYR:HB3	6:Z:155:PHE:HB3	2.01	0.43
6:Z:227:ILE:H	6:Z:227:ILE:HG13	1.74	0.43
12:f:267:ARG:O	12:f:271:MET:N	2.45	0.43
17:E:235:ILE:O	17:E:239:GLY:N	2.45	0.43
21:H:9:SER:OG	21:H:123:GLN:O	2.31	0.43
22:i:197:LEU:HD13	22:i:211:VAL:HG11	1.99	0.43
2:V:253:LEU:HD23	2:V:256:ARG:HD3	2.00	0.43
5:Y:331:ASP:OD2	5:Y:349:LYS:NZ	2.52	0.43
12:f:31:LYS:HE2	12:f:31:LYS:HB3	1.88	0.43
12:f:625:LYS:HG3	12:f:629:LYS:HE3	2.01	0.43
14:B:388:ASP:N	14:B:388:ASP:OD1	2.52	0.43
15:C:113:ARG:HH21	15:C:129:ASN:H	1.66	0.43
15:C:175:PHE:O	15:C:179:GLY:N	2.48	0.43
23:J:121:SER:OG	23:J:122:ASN:N	2.50	0.43
25:L:159:MET:HE1	25:L:169:ARG:HE	1.84	0.43
25:l:146:GLN:HE22	25:l:159:MET:HE2	1.83	0.43
31:r:97:MET:HB3	31:r:116:SER:HB3	2.01	0.43
1:U:505:ASP:HB3	1:U:508:THR:HG22	2.01	0.43
1:U:688:LEU:HB3	1:U:713:TYR:HE1	1.83	0.43
10:d:5:LEU:HD12	10:d:25:ARG:HG2	2.01	0.43
12:f:742:ALA:O	12:f:746:ARG:NE	2.51	0.43
25:l:42:THR:O	25:l:137:TYR:OH	2.36	0.43
3:W:2:ALA:HB2	3:W:43:VAL:HG22	2.00	0.43
6:Z:144:VAL:HG22	7:a:146:PRO:HB3	2.01	0.43
7:a:100:THR:HG22	7:a:103:LYS:HE2	2.01	0.43
12:f:332:ALA:HA	12:f:336:GLU:HB2	2.01	0.43
14:B:183:THR:HG23	14:B:185:ALA:H	1.82	0.43
18:F:210:GLU:O	18:F:214:ASN:N	2.49	0.43
24:k:210:LEU:HD11	24:k:215:ILE:HG12	1.99	0.43
29:p:36:THR:OG1	29:p:38:ASP:OD1	2.33	0.43
33:t:1:THR:N	33:t:105:PRO:O	2.50	0.43
1:U:133:ILE:HA	1:U:136:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:84:LYS:HA	2:V:87:SER:HB2	2.00	0.43
9:c:54:MET:H	9:c:77:GLN:HE22	1.66	0.43
9:c:118:PHE:HB3	9:c:121:TRP:CH2	2.54	0.43
12:f:182:GLU:OE2	12:f:186:THR:OG1	2.36	0.43
15:C:338:LEU:HD13	15:C:338:LEU:HA	1.91	0.43
23:j:98:VAL:HG22	31:r:78:ALA:HB1	2.00	0.43
1:U:188:MET:HG2	1:U:194:ARG:HB2	2.00	0.43
9:c:216:MET:HE3	9:c:216:MET:HB2	1.78	0.43
10:d:125:LYS:HB3	10:d:130:ASN:HD22	1.84	0.43
11:e:59:GLU:HG3	11:e:63:HIS:HE1	1.83	0.43
12:f:218:GLU:HA	12:f:221:ILE:HG22	2.01	0.43
18:F:314:LEU:HD21	18:F:342:LEU:HB3	2.01	0.43
25:L:146:GLN:HE22	25:L:159:MET:HE2	1.83	0.43
31:R:97:MET:HB3	31:R:116:SER:HB3	2.01	0.43
22:i:116:ASP:OD1	23:j:81:ARG:NH1	2.52	0.43
1:U:791:LEU:O	1:U:914:LEU:N	2.42	0.42
2:V:87:SER:HB3	2:V:126:ALA:H	1.82	0.42
6:Z:10:VAL:HG13	6:Z:163:GLY:HA3	2.00	0.42
6:Z:190:ARG:HH11	9:c:296:ILE:HG22	1.84	0.42
7:a:258:GLN:HA	7:a:261:LEU:HD13	2.01	0.42
9:c:54:MET:HE2	9:c:54:MET:HB2	1.72	0.42
9:c:163:ILE:HG12	9:c:174:PRO:HG3	2.01	0.42
12:f:408:LEU:HD21	12:f:797:LEU:HD13	2.01	0.42
12:f:823:ALA:HB1	12:f:825:MET:HG3	2.00	0.42
14:B:135:ILE:HG22	14:B:139:VAL:HG11	2.01	0.42
15:C:132:ASP:HB2	15:C:135:VAL:HG23	2.00	0.42
22:I:41:ASP:N	22:I:41:ASP:OD1	2.51	0.42
25:L:45:VAL:HG11	25:L:188:VAL:HG22	2.01	0.42
26:M:136:MET:HE3	26:M:163:CYS:HB3	2.01	0.42
26:M:214:SER:HG	26:M:224:HIS:HE2	1.59	0.42
30:Q:19:ARG:HH11	30:Q:179:SER:HB3	1.83	0.42
27:n:35:THR:OG1	27:n:45:ARG:NH2	2.53	0.42
1:U:913:ILE:H	1:U:913:ILE:HG13	1.64	0.42
6:Z:182:THR:OG1	16:D:70:LYS:NZ	2.42	0.42
7:a:235:ASP:HB3	7:a:251:LEU:HD11	2.00	0.42
8:b:89:GLY:HA2	8:b:92:VAL:HG12	2.00	0.42
12:f:61:GLU:HB2	12:f:65:GLU:HB2	2.00	0.42
13:A:240:VAL:HG21	13:A:260:LEU:HD11	2.01	0.42
20:g:158:GLY:O	21:h:84:ARG:NH2	2.53	0.42
1:U:640:LEU:HD23	1:U:640:LEU:HA	1.86	0.42
2:V:32:PRO:HA	2:V:35:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:194:LYS:H	2:V:194:LYS:HD2	1.84	0.42
2:V:451:ILE:HG13	2:V:458:VAL:HG13	2.01	0.42
9:c:46:ARG:HA	9:c:49:VAL:HB	2.01	0.42
12:f:462:ALA:CB	19:w:6:LYS:HZ1	2.31	0.42
12:f:733:GLY:O	12:f:746:ARG:NH1	2.50	0.42
16:D:116:LEU:HD13	16:D:118:THR:H	1.84	0.42
23:J:81:ARG:O	23:J:85:ASN:ND2	2.52	0.42
26:M:40:ARG:HA	26:M:45:VAL:HA	2.01	0.42
2:V:81:GLN:HG3	2:V:86:VAL:HB	2.02	0.42
9:c:252:ALA:O	9:c:256:ASN:N	2.51	0.42
12:f:253:LEU:HD22	12:f:257:ARG:HD3	2.00	0.42
13:A:75:PRO:HA	13:A:78:TRP:HE1	1.83	0.42
18:F:212:PHE:HD1	18:F:217:ILE:HD11	1.84	0.42
24:K:99:HIS:HB2	24:K:107:MET:HE3	2.00	0.42
32:S:16:ALA:HB2	32:S:121:VAL:HG23	2.00	0.42
22:i:3:ARG:HB2	23:j:5:ARG:HH12	1.84	0.42
3:W:13:ILE:HA	3:W:16:MET:HG2	2.02	0.42
4:X:255:LEU:HB2	4:X:287:LEU:HD13	2.00	0.42
7:a:346:ILE:O	7:a:350:LYS:N	2.52	0.42
9:c:104:ARG:NH2	9:c:106:GLU:OE2	2.39	0.42
9:c:303:MET:HE2	10:d:239:SER:HA	2.01	0.42
12:f:475:ASN:O	12:f:477:MET:N	2.52	0.42
29:P:107:PRO:HG2	29:P:124:LEU:HB2	2.00	0.42
29:p:58:THR:O	30:q:85:ARG:NH2	2.52	0.42
31:r:6:PHE:HE1	31:r:156:ALA:HB2	1.85	0.42
32:s:1:ARG:HH21	33:t:2:GLN:HE22	1.66	0.42
1:U:147:TYR:HB3	1:U:176:MET:HE1	2.02	0.42
2:V:337:LEU:HD22	2:V:367:VAL:HG11	2.02	0.42
6:Z:70:LEU:HD12	6:Z:111:LEU:HD23	2.02	0.42
7:a:112:ILE:H	7:a:112:ILE:HG13	1.75	0.42
12:f:171:GLN:HE21	12:f:179:VAL:HG13	1.84	0.42
12:f:189:LYS:HG2	12:f:190:GLU:HG2	2.02	0.42
12:f:414:LEU:HA	12:f:417:ILE:HD12	2.01	0.42
12:f:637:LYS:HE2	12:f:673:ARG:HB2	2.00	0.42
13:A:95:VAL:HG23	14:B:133:VAL:HG12	2.00	0.42
15:C:125:LYS:HZ2	16:D:96:VAL:HG11	1.85	0.42
31:R:6:PHE:HE1	31:R:156:ALA:HB2	1.85	0.42
32:S:184:GLU:OE1	32:S:211:ARG:NH1	2.52	0.42
25:l:45:VAL:HG11	25:l:188:VAL:HG22	2.01	0.42
28:o:30:ASN:OD1	28:o:187:ARG:NH2	2.53	0.42
2:V:96:ARG:HB3	2:V:98:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:149:THR:HA	7:a:152:HIS:HB3	2.01	0.42
8:b:124:LEU:O	8:b:128:ALA:N	2.52	0.42
12:f:463:LEU:HD23	19:w:66:THR:CB	2.50	0.42
17:E:33:LEU:HD13	18:F:66:LEU:HA	2.01	0.42
22:I:79:ILE:HG22	22:I:82:ASP:H	1.85	0.42
20:g:132:ARG:HB2	26:m:12:SER:HA	2.02	0.42
25:l:159:MET:HE1	25:l:169:ARG:HE	1.84	0.42
26:m:35:THR:HA	26:m:166:GLY:HA3	2.01	0.42
5:Y:134:LEU:HA	5:Y:137:ARG:HB2	2.01	0.42
6:Z:35:VAL:HB	6:Z:97:THR:HB	2.02	0.42
6:Z:91:ILE:H	6:Z:91:ILE:HG13	1.57	0.42
6:Z:109:ASN:HD22	6:Z:155:PHE:HE1	1.66	0.42
10:d:109:GLN:OE1	10:d:111:ARG:NH1	2.52	0.42
13:A:258:ARG:O	13:A:262:GLU:N	2.51	0.42
16:D:343:LEU:O	16:D:346:SER:OG	2.36	0.42
26:M:51:LYS:O	26:M:210:GLU:N	2.49	0.42
30:Q:155:ARG:HA	30:Q:158:GLU:HG2	2.01	0.42
2:V:107:ARG:HA	2:V:110:HIS:HB2	2.02	0.42
3:W:135:LYS:HB3	3:W:136:ILE:H	1.67	0.42
3:W:198:ASP:O	3:W:202:THR:OG1	2.30	0.42
5:Y:92:GLU:HB3	5:Y:100:ILE:HD11	2.01	0.42
10:d:178:ILE:HA	10:d:181:CYS:SG	2.60	0.42
12:f:327:ASN:HD22	12:f:330:PHE:HB3	1.85	0.42
12:f:369:ARG:HA	12:f:372:LEU:HD13	2.01	0.42
12:f:673:ARG:NH1	12:f:708:ASP:OD2	2.53	0.42
13:A:258:ARG:HH22	18:F:255:GLN:HA	1.84	0.42
15:C:187:LEU:HB3	15:C:314:LYS:HG2	2.02	0.42
18:F:43:GLN:HA	18:F:46:ARG:HG3	2.02	0.42
26:m:136:MET:HE3	26:m:163:CYS:HB3	2.01	0.42
26:m:139:SER:OG	26:m:140:TYR:N	2.53	0.42
30:q:19:ARG:HH11	30:q:179:SER:HB3	1.83	0.42
7:a:21:VAL:HA	7:a:24:ARG:HB3	2.01	0.42
7:a:34:TRP:HZ3	7:a:64:ILE:HG23	1.85	0.42
10:d:61:TRP:HZ3	10:d:65:ARG:HH21	1.67	0.42
12:f:705:ASN:OD1	12:f:706:ILE:N	2.53	0.42
27:N:136:TYR:HE2	33:T:33:LEU:HD21	1.85	0.42
28:O:24:MET:HE3	32:s:187:VAL:HG21	2.02	0.42
22:i:18:LEU:HD22	23:j:125:ARG:HH12	1.85	0.42
29:p:7:ASN:ND2	29:p:29:GLY:O	2.39	0.42
1:U:23:ALA:O	1:U:27:LEU:N	2.53	0.41
1:U:773:PHE:HE1	9:c:180:ASN:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:299:ILE:HG22	3:W:302:TYR:H	1.84	0.41
5:Y:17:LEU:HD22	5:Y:212:GLU:HB2	2.01	0.41
21:H:67:PRO:HG2	28:O:68:LEU:HD11	2.02	0.41
22:I:18:LEU:HD22	23:J:125:ARG:HH12	1.85	0.41
26:M:35:THR:HA	26:M:166:GLY:HA3	2.01	0.41
20:g:144:ASP:HB3	20:g:147:GLN:HB2	2.02	0.41
26:m:40:ARG:HA	26:m:45:VAL:HA	2.01	0.41
33:t:22:ILE:HD12	33:t:50:MET:HE3	2.02	0.41
1:U:805:ASN:N	1:U:891:VAL:O	2.49	0.41
2:V:350:GLN:H	2:V:353:LEU:HB3	1.85	0.41
2:V:437:ILE:O	2:V:441:ALA:N	2.51	0.41
3:W:59:ASP:O	3:W:63:THR:OG1	2.30	0.41
12:f:462:ALA:CA	19:w:6:LYS:NZ	2.83	0.41
12:f:875:ALA:O	12:f:876:HIS:ND1	2.53	0.41
19:u:24:GLU:HB3	19:u:52:ASP:HB3	2.02	0.41
29:P:58:THR:OG1	30:Q:121:LEU:O	2.22	0.41
22:i:79:ILE:HG22	22:i:82:ASP:H	1.85	0.41
4:X:342:PHE:HB2	4:X:343:SER:H	1.60	0.41
12:f:378:ASN:HD21	12:f:392:THR:HG22	1.85	0.41
26:M:139:SER:OG	26:M:140:TYR:N	2.53	0.41
28:O:30:ASN:OD1	28:O:187:ARG:NH2	2.53	0.41
33:T:46:ASN:OD1	33:T:46:ASN:N	2.50	0.41
1:U:219:CYS:SG	1:U:220:LEU:N	2.93	0.41
1:U:268:LEU:HD22	1:U:329:LEU:HD11	2.01	0.41
2:V:265:ASP:O	2:V:269:LYS:NZ	2.45	0.41
2:V:342:ILE:HD12	2:V:343:PRO:HD2	2.01	0.41
9:c:32:TYR:HB3	9:c:208:ARG:HD2	2.02	0.41
13:A:236:CYS:SG	13:A:267:LYS:HG2	2.60	0.41
14:B:387:LYS:HB3	14:B:390:LEU:HD23	2.02	0.41
27:N:35:THR:OG1	27:N:45:ARG:NH2	2.53	0.41
20:g:67:THR:HG22	20:g:69:LEU:H	1.85	0.41
20:g:175:SER:OG	20:g:201:CYS:SG	2.74	0.41
30:q:155:ARG:HA	30:q:158:GLU:HG2	2.01	0.41
33:t:136:SER:HB2	33:t:150:LEU:HD13	2.02	0.41
4:X:397:TYR:OH	6:Z:255:ASP:OD1	2.36	0.41
12:f:296:PHE:O	12:f:807:ARG:NH2	2.54	0.41
14:B:234:LEU:HG	35:B:501:ATP:H2'	2.02	0.41
16:D:176:GLU:OE2	16:D:329:ARG:NH1	2.45	0.41
18:F:119:GLY:HA2	18:F:120:LYS:HA	1.81	0.41
20:G:144:ASP:HB3	20:G:147:GLN:HB2	2.02	0.41
21:h:9:SER:OG	21:h:123:GLN:O	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:k:117:SER:HB2	25:l:82:ARG:HH12	1.85	0.41
1:U:440:GLY:HA2	1:U:473:VAL:HG13	2.02	0.41
2:V:357:LEU:O	2:V:361:PHE:N	2.38	0.41
6:Z:209:ARG:HD2	6:Z:212:LEU:HD22	2.02	0.41
8:b:138:VAL:H	8:b:160:LEU:HD21	1.84	0.41
12:f:814:SER:OG	12:f:822:VAL:O	2.38	0.41
13:A:312:ARG:HB2	13:A:315:ILE:HD12	2.03	0.41
19:w:1:MET:N	19:w:17:VAL:O	2.37	0.41
23:J:31:THR:OG1	23:J:163:ARG:O	2.38	0.41
32:s:191:ASP:O	32:s:210:LEU:N	2.47	0.41
33:t:4:PRO:HG3	33:t:107:TRP:CE2	2.56	0.41
1:U:152:GLY:HA3	16:D:41:TYR:CD2	2.56	0.41
1:U:649:ARG:HD3	15:C:57:ARG:NH1	2.36	0.41
3:W:122:LEU:HA	3:W:125:ILE:HG22	2.03	0.41
12:f:93:PRO:HB2	12:f:97:LYS:HG3	2.03	0.41
12:f:325:GLN:HE21	12:f:420:TRP:HE3	1.69	0.41
13:A:294:GLU:HA	13:A:297:ARG:HH11	1.85	0.41
14:B:93:GLU:HA	14:B:96:ARG:HB2	2.03	0.41
16:D:68:LEU:O	16:D:72:PHE:N	2.46	0.41
16:D:254:ALA:HB2	16:D:262:ILE:HD11	2.03	0.41
33:T:22:ILE:HD12	33:T:50:MET:HE3	2.02	0.41
31:r:9:ARG:NH2	31:r:146:ASP:OD1	2.42	0.41
3:W:155:GLN:HG2	3:W:157:GLY:H	1.85	0.41
4:X:122:ARG:HD2	4:X:125:LEU:HB2	2.02	0.41
12:f:372:LEU:HD11	12:f:403:LYS:HE3	2.02	0.41
13:A:191:VAL:HG13	13:A:271:LEU:HD21	2.03	0.41
14:B:112:LEU:HD23	14:B:123:VAL:HG12	2.03	0.41
16:D:94:GLU:HG2	16:D:102:ILE:HD13	2.01	0.41
17:E:250:ASP:OD1	17:E:250:ASP:N	2.53	0.41
18:F:226:TYR:CZ	18:F:353:GLU:HB3	2.55	0.41
19:w:36:ILE:O	19:w:41:GLN:NE2	2.54	0.41
23:J:98:VAL:HG22	31:R:78:ALA:HB1	2.02	0.41
29:P:135:ASP:OD1	29:P:135:ASP:N	2.46	0.41
33:T:136:SER:HB2	33:T:150:LEU:HD13	2.02	0.41
23:j:38:ARG:NH1	23:j:181:ILE:O	2.54	0.41
23:j:81:ARG:O	23:j:85:ASN:ND2	2.54	0.41
2:V:126:ALA:HA	2:V:130:PHE:HB2	2.02	0.41
2:V:277:PRO:HD2	2:V:285:TRP:HZ3	1.86	0.41
6:Z:165:GLU:HB3	6:Z:168:GLU:HG2	2.03	0.41
10:d:36:LEU:HD23	10:d:38:THR:H	1.86	0.41
12:f:322:SER:HA	12:f:325:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:281:GLY:HA3	13:A:299:MET:HG3	2.03	0.41
15:C:21:ARG:HA	15:C:24:TYR:HD2	1.84	0.41
15:C:327:ASP:OD1	15:C:327:ASP:N	2.53	0.41
17:E:322:LYS:HD3	17:E:326:ILE:HG13	2.02	0.41
21:H:108:ALA:HA	21:H:147:PHE:HE2	1.85	0.41
28:o:13:VAL:HG22	28:o:177:VAL:HG22	2.03	0.41
32:s:172:MET:HE1	32:s:195:ILE:HG21	2.02	0.41
33:t:27:LEU:HD22	33:t:184:TYR:HB2	2.03	0.41
5:Y:95:LEU:HD11	5:Y:98:SER:HA	2.02	0.41
7:a:239:ALA:O	7:a:243:GLY:N	2.53	0.41
12:f:441:LYS:HB2	12:f:477:MET:HE1	2.03	0.41
12:f:669:GLU:CD	12:f:705:ASN:HD22	2.29	0.41
12:f:809:ILE:HG23	12:f:810:ILE:HG23	2.03	0.41
14:B:212:GLU:N	14:B:212:GLU:OE1	2.54	0.41
16:D:153:MET:SD	16:D:153:MET:N	2.93	0.41
17:E:300:HIS:NE2	17:E:302:ASP:OD1	2.53	0.41
18:F:81:LYS:HE2	18:F:81:LYS:HB3	1.96	0.41
24:K:20:ARG:H	24:K:20:ARG:HD2	1.86	0.41
26:M:40:ARG:HD2	26:M:161:TRP:CE3	2.56	0.41
33:T:25:ASP:HA	33:T:187:PHE:HA	2.03	0.41
26:m:40:ARG:HD2	26:m:161:TRP:CE3	2.56	0.41
28:o:204:CYS:HB2	28:o:208:THR:HG21	2.03	0.41
1:U:98:GLU:HB2	15:C:19:GLY:HA2	2.01	0.40
1:U:636:VAL:HG23	1:U:637:VAL:HG23	2.02	0.40
5:Y:42:MET:SD	5:Y:46:ARG:NH2	2.95	0.40
6:Z:21:ASP:OD1	6:Z:21:ASP:N	2.53	0.40
9:c:31:VAL:HG23	9:c:203:ILE:HG21	2.03	0.40
12:f:220:ASP:O	12:f:224:ASN:N	2.54	0.40
14:B:253:SER:O	15:C:271:ARG:NH2	2.54	0.40
14:B:264:PRO:HG3	14:B:308:THR:HA	2.02	0.40
20:G:165:ALA:HB1	20:G:179:LEU:HD13	2.03	0.40
20:g:138:MET:HB3	20:g:154:CYS:HB3	2.03	0.40
23:j:38:ARG:HH12	23:j:182:GLU:HA	1.86	0.40
26:m:51:LYS:O	26:m:210:GLU:N	2.49	0.40
33:t:25:ASP:HA	33:t:187:PHE:HA	2.03	0.40
4:X:258:LYS:HD3	4:X:266:ASP:HB2	2.03	0.40
9:c:244:VAL:HB	9:c:291:LEU:HD21	2.03	0.40
12:f:248:LEU:HD13	12:f:248:LEU:HA	1.98	0.40
12:f:412:ALA:HA	12:f:447:ALA:HB2	2.02	0.40
12:f:712:LYS:HA	12:f:715:HIS:HB2	2.03	0.40
15:C:372:ARG:HH22	16:D:175:GLN:NE2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:161:ASP:HA	16:D:221:HIS:CD2	2.56	0.40
20:G:67:THR:HG22	20:G:69:LEU:H	1.85	0.40
20:G:112:ASP:HB3	20:G:152:TYR:CZ	2.56	0.40
24:k:20:ARG:H	24:k:20:ARG:HD2	1.86	0.40
1:U:265:ILE:HG23	1:U:269:ARG:HH12	1.87	0.40
5:Y:213:LEU:HD23	5:Y:213:LEU:HA	1.94	0.40
6:Z:14:LEU:O	6:Z:18:SER:N	2.52	0.40
12:f:121:PHE:CD2	12:f:129:LEU:HD11	2.57	0.40
12:f:250:ARG:NH1	12:f:285:CYS:SG	2.94	0.40
12:f:269:ALA:HA	12:f:272:LEU:HB2	2.03	0.40
12:f:394:ASP:OD1	12:f:394:ASP:N	2.54	0.40
12:f:478:ARG:NH2	12:f:507:ASP:OD2	2.55	0.40
21:h:111:VAL:HG21	21:h:147:PHE:HD2	1.86	0.40
22:i:118:LYS:HD3	22:i:152:PRO:HA	2.02	0.40
30:q:31:ASP:N	30:q:31:ASP:OD1	2.54	0.40
30:q:81:ALA:HB2	30:q:104:LEU:HD22	2.04	0.40
2:V:126:ALA:HB2	2:V:134:PHE:HE2	1.86	0.40
2:V:182:LYS:NZ	2:V:210:CYS:SG	2.74	0.40
4:X:175:LYS:HG2	4:X:213:GLN:NE2	2.30	0.40
4:X:255:LEU:HD21	4:X:270:LEU:HD12	2.03	0.40
6:Z:59:ASP:HB2	8:b:99:HIS:CE1	2.56	0.40
6:Z:177:ARG:HD2	6:Z:177:ARG:HA	1.90	0.40
7:a:77:VAL:HG21	7:a:113:LEU:HD13	2.03	0.40
12:f:265:ALA:HB3	12:f:268:LEU:HB2	2.03	0.40
17:E:139:SER:HA	17:E:142:ILE:HD12	2.03	0.40
20:G:138:MET:HB3	20:G:154:CYS:HB3	2.03	0.40
27:N:144:ARG:NH2	27:N:151:GLU:OE1	2.55	0.40
24:k:54:ILE:HG23	24:k:59:MET:HE2	2.03	0.40
25:l:105:VAL:N	25:l:138:ASP:OD1	2.43	0.40
26:m:39:ILE:HD11	26:m:189:ILE:HD12	2.04	0.40
3:W:361:HIS:HA	3:W:364:ARG:HH11	1.87	0.40
9:c:44:HIS:CE1	9:c:53:VAL:HB	2.56	0.40
9:c:156:VAL:HG21	16:D:81:ARG:HH12	1.86	0.40
12:f:75:LEU:HD12	12:f:78:LEU:HD13	2.04	0.40
18:F:311:LEU:HD23	18:F:314:LEU:HD12	2.04	0.40
21:H:187:ALA:HA	21:H:190:THR:HG22	2.03	0.40
22:I:118:LYS:HD3	22:I:152:PRO:HA	2.02	0.40
23:J:108:THR:HG22	23:J:133:ILE:HD13	2.04	0.40
33:T:27:LEU:HD22	33:T:184:TYR:HB2	2.03	0.40
21:h:40:ALA:HB1	21:h:182:LEU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	806/953 (85%)	752 (93%)	52 (6%)	2 (0%)	43	73
2	V	478/534 (90%)	420 (88%)	55 (12%)	3 (1%)	21	56
3	W	454/456 (100%)	407 (90%)	43 (10%)	4 (1%)	14	47
4	X	378/422 (90%)	355 (94%)	22 (6%)	1 (0%)	36	68
5	Y	376/389 (97%)	343 (91%)	33 (9%)	0	100	100
6	Z	284/324 (88%)	244 (86%)	40 (14%)	0	100	100
7	a	371/376 (99%)	335 (90%)	35 (9%)	1 (0%)	36	68
8	b	189/377 (50%)	174 (92%)	15 (8%)	0	100	100
9	c	285/309 (92%)	243 (85%)	42 (15%)	0	100	100
10	d	255/349 (73%)	217 (85%)	38 (15%)	0	100	100
11	e	36/70 (51%)	25 (69%)	11 (31%)	0	100	100
12	f	887/908 (98%)	717 (81%)	164 (18%)	6 (1%)	18	52
13	A	392/433 (90%)	343 (88%)	47 (12%)	2 (0%)	24	59
14	B	382/440 (87%)	341 (89%)	40 (10%)	1 (0%)	36	68
15	C	359/398 (90%)	330 (92%)	27 (8%)	2 (1%)	21	56
16	D	378/418 (90%)	335 (89%)	38 (10%)	5 (1%)	9	40
17	E	387/403 (96%)	347 (90%)	38 (10%)	2 (0%)	24	59
18	F	413/439 (94%)	380 (92%)	32 (8%)	1 (0%)	43	73
19	u	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
19	w	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
20	G	238/245 (97%)	223 (94%)	15 (6%)	0	100	100
20	g	238/245 (97%)	223 (94%)	15 (6%)	0	100	100
21	H	230/233 (99%)	223 (97%)	7 (3%)	0	100	100
21	h	230/233 (99%)	223 (97%)	7 (3%)	0	100	100
22	I	248/260 (95%)	227 (92%)	21 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	i	248/260 (95%)	227 (92%)	21 (8%)	0	100	100
23	J	237/247 (96%)	218 (92%)	18 (8%)	1 (0%)	30	62
23	j	237/247 (96%)	222 (94%)	14 (6%)	1 (0%)	30	62
24	K	224/240 (93%)	212 (95%)	12 (5%)	0	100	100
24	k	224/240 (93%)	212 (95%)	12 (5%)	0	100	100
25	L	236/268 (88%)	221 (94%)	14 (6%)	1 (0%)	30	62
25	l	236/268 (88%)	220 (93%)	15 (6%)	1 (0%)	30	62
26	M	238/254 (94%)	223 (94%)	15 (6%)	0	100	100
26	m	238/254 (94%)	223 (94%)	15 (6%)	0	100	100
27	N	189/238 (79%)	182 (96%)	7 (4%)	0	100	100
27	n	189/238 (79%)	182 (96%)	7 (4%)	0	100	100
28	O	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
28	o	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
29	P	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
29	p	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
30	Q	197/201 (98%)	182 (92%)	15 (8%)	0	100	100
30	q	197/201 (98%)	182 (92%)	15 (8%)	0	100	100
31	R	199/262 (76%)	191 (96%)	8 (4%)	0	100	100
31	r	199/262 (76%)	191 (96%)	8 (4%)	0	100	100
32	S	211/240 (88%)	202 (96%)	9 (4%)	0	100	100
32	s	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
33	T	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
33	t	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
All	All	13418/15012 (89%)	12272 (92%)	1112 (8%)	34 (0%)	37	68

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	167	LEU
1	U	874	ASN
12	f	476	THR
15	C	90	HIS
16	D	126	PRO
17	E	386	TYR

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Mol	Chain	Res	Type
2	V	265	ASP
3	W	252	ASP
4	X	392	PRO
7	a	149	THR
12	f	808	ASN
13	A	425	ALA
15	C	128	PRO
16	D	154	LEU
17	E	385	ASP
12	f	118	ASN
12	f	859	PRO
16	D	368	ASP
1	U	873	PRO
13	A	109	PRO
14	B	87	PRO
16	D	355	SER
23	j	97	THR
3	W	316	ARG
12	f	853	VAL
16	D	367	PRO
23	J	97	THR
25	L	226	ASP
25	l	226	ASP
2	V	323	GLY
3	W	136	ILE
18	F	165	PRO
12	f	755	ASP
3	W	253	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	U	692/816 (85%)	688 (99%)	4 (1%)	78 84
2	V	414/460 (90%)	413 (100%)	1 (0%)	87 89
3	W	393/416 (94%)	391 (100%)	2 (0%)	81 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	X	327/362 (90%)	325 (99%)	2 (1%)	78	84
5	Y	334/344 (97%)	333 (100%)	1 (0%)	86	88
6	Z	257/295 (87%)	254 (99%)	3 (1%)	63	79
7	a	333/336 (99%)	331 (99%)	2 (1%)	78	84
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	248 (98%)	4 (2%)	55	75
10	d	231/293 (79%)	228 (99%)	3 (1%)	61	78
11	e	38/63 (60%)	38 (100%)	0	100	100
12	f	60/763 (8%)	60 (100%)	0	100	100
15	C	11/346 (3%)	10 (91%)	1 (9%)	9	34
17	E	10/353 (3%)	10 (100%)	0	100	100
20	g	193/209 (92%)	193 (100%)	0	100	100
21	h	164/190 (86%)	164 (100%)	0	100	100
22	i	193/220 (88%)	193 (100%)	0	100	100
23	j	152/210 (72%)	151 (99%)	1 (1%)	76	83
24	K	62/202 (31%)	62 (100%)	0	100	100
24	k	186/202 (92%)	186 (100%)	0	100	100
25	L	198/229 (86%)	195 (98%)	3 (2%)	57	76
25	l	198/229 (86%)	195 (98%)	3 (2%)	57	76
26	M	192/211 (91%)	192 (100%)	0	100	100
26	m	192/211 (91%)	192 (100%)	0	100	100
27	N	148/180 (82%)	148 (100%)	0	100	100
27	n	148/180 (82%)	148 (100%)	0	100	100
28	O	177/227 (78%)	177 (100%)	0	100	100
28	o	177/227 (78%)	176 (99%)	1 (1%)	78	84
29	P	173/173 (100%)	173 (100%)	0	100	100
29	p	173/173 (100%)	173 (100%)	0	100	100
30	Q	164/171 (96%)	163 (99%)	1 (1%)	78	84
30	q	164/171 (96%)	163 (99%)	1 (1%)	78	84
31	R	153/201 (76%)	153 (100%)	0	100	100
31	r	153/201 (76%)	153 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	S	174/198 (88%)	174 (100%)	0	100	100
32	s	175/198 (88%)	174 (99%)	1 (1%)	78	84
33	T	175/214 (82%)	175 (100%)	0	100	100
33	t	175/214 (82%)	175 (100%)	0	100	100
All	All	7578/10267 (74%)	7544 (100%)	34 (0%)	81	86

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	9	ILE
1	U	629	THR
1	U	775	LEU
1	U	913	ILE
2	V	163	VAL
3	W	89	LEU
3	W	90	LEU
4	X	80	ILE
4	X	393	VAL
5	Y	287	LEU
6	Z	91	ILE
6	Z	191	ILE
6	Z	193	ASN
7	a	165	THR
7	a	374	ILE
9	c	69	VAL
9	c	151	VAL
9	c	251	LEU
9	c	284	LEU
10	d	122	LEU
10	d	178	ILE
10	d	202	THR
15	C	89	VAL
25	L	22	ILE
25	L	137	TYR
25	L	161	ILE
30	Q	4	LEU
23	j	159	ASN
25	l	22	ILE
25	l	137	TYR
25	l	161	ILE
28	o	186	LEU

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Mol	Chain	Res	Type
30	q	4	LEU
32	s	1	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	267	ASN
1	U	340	GLN
1	U	345	ASN
1	U	355	ASN
1	U	362	ASN
1	U	377	HIS
1	U	415	HIS
1	U	595	ASN
2	V	125	ASN
2	V	168	GLN
2	V	247	GLN
2	V	400	HIS
2	V	427	GLN
3	W	86	ASN
3	W	106	GLN
3	W	107	GLN
3	W	399	ASN
3	W	430	GLN
3	W	440	ASN
4	X	48	GLN
4	X	213	GLN
4	X	262	ASN
4	X	329	ASN
4	X	333	GLN
4	X	349	HIS
4	X	406	ASN
5	Y	48	ASN
5	Y	136	HIS
5	Y	178	ASN
5	Y	306	GLN
5	Y	363	ASN
6	Z	77	ASN
6	Z	109	ASN
6	Z	193	ASN
6	Z	196	HIS
6	Z	202	ASN

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Mol	Chain	Res	Type
6	Z	274	ASN
6	Z	277	ASN
7	a	9	GLN
7	a	12	GLN
7	a	18	GLN
7	a	144	ASN
7	a	164	GLN
7	a	193	GLN
7	a	212	ASN
7	a	231	GLN
7	a	249	GLN
7	a	273	GLN
7	a	345	GLN
8	b	142	ASN
9	c	44	HIS
9	c	113	HIS
9	c	128	ASN
9	c	130	GLN
9	c	149	GLN
9	c	164	ASN
9	c	166	ASN
9	c	172	HIS
9	c	180	ASN
9	c	197	ASN
9	c	199	HIS
9	c	221	HIS
9	c	232	GLN
9	c	241	ASN
9	c	254	ASN
9	c	274	ASN
10	d	149	ASN
10	d	229	GLN
11	e	63	HIS
12	f	43	GLN
15	C	90	HIS
25	L	4	ASN
25	L	21	GLN
25	L	90	GLN
25	L	146	GLN
26	M	97	ASN
26	M	221	ASN
27	N	28	ASN

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Mol	Chain	Res	Type
27	N	110	GLN
28	O	35	HIS
28	O	66	HIS
29	P	93	ASN
30	Q	8	GLN
31	R	29	GLN
32	S	163	HIS
33	T	69	GLN
33	T	81	HIS
20	g	12	HIS
20	g	33	ASN
20	g	75	ASN
20	g	92	GLN
20	g	123	GLN
20	g	127	GLN
20	g	128	ASN
21	h	63	HIS
21	h	88	HIS
21	h	169	ASN
21	h	214	ASN
22	i	40	ASN
22	i	53	HIS
22	i	84	ASN
22	i	119	GLN
22	i	167	ASN
23	j	15	HIS
23	j	85	ASN
23	j	122	ASN
23	j	159	ASN
24	k	118	ASN
24	k	155	HIS
24	k	227	HIS
25	l	4	ASN
25	l	90	GLN
25	l	146	GLN
25	l	166	GLN
26	m	72	HIS
26	m	97	ASN
26	m	221	ASN
27	n	28	ASN
27	n	110	GLN
28	o	35	HIS

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Mol	Chain	Res	Type
28	o	116	HIS
29	p	93	ASN
30	q	8	GLN
30	q	82	ASN
31	r	29	GLN
33	t	69	GLN
33	t	81	HIS

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	ATP	A	501	36	32,33,33	1.31	4 (12%)	48,52,52	1.88	9 (18%)
35	ATP	B	501	36	32,33,33	1.29	5 (15%)	48,52,52	1.78	11 (22%)
37	ADP	C	501	-	28,29,29	1.35	3 (10%)	43,45,45	2.05	9 (20%)
35	ATP	E	401	36	32,33,33	1.28	4 (12%)	48,52,52	1.77	9 (18%)
35	ATP	D	501	36	32,33,33	1.30	5 (15%)	48,52,52	1.75	7 (14%)
37	ADP	F	501	36	28,29,29	1.36	6 (21%)	43,45,45	1.83	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	A	501	36	-	1/22/38/38	0/3/3/3
35	ATP	B	501	36	-	3/22/38/38	0/3/3/3
37	ADP	C	501	-	-	4/16/32/32	0/3/3/3
35	ATP	E	401	36	-	2/22/38/38	0/3/3/3
35	ATP	D	501	36	-	8/22/38/38	0/3/3/3
37	ADP	F	501	36	-	8/16/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C	501	ADP	C5-C4	4.41	1.47	1.39
35	D	501	ATP	C5-C4	4.34	1.46	1.39
35	E	401	ATP	C5-C4	4.25	1.46	1.39
35	A	501	ATP	C5-C4	4.19	1.46	1.39
35	B	501	ATP	C5-C4	4.17	1.46	1.39
37	F	501	ADP	C5-C4	4.15	1.46	1.39
35	A	501	ATP	C5-N7	-3.03	1.33	1.39
37	F	501	ADP	C5-N7	-2.83	1.33	1.39
37	C	501	ADP	C5-N7	-2.76	1.34	1.39
35	B	501	ATP	C5-N7	-2.75	1.34	1.39
35	E	401	ATP	C5-N7	-2.71	1.34	1.39
35	D	501	ATP	C5-N7	-2.67	1.34	1.39
37	C	501	ADP	C5-C6	2.47	1.47	1.41
37	F	501	ADP	C4-N9	-2.38	1.32	1.37
35	A	501	ATP	C5-C6	2.36	1.47	1.41
35	D	501	ATP	C5-C6	2.33	1.47	1.41
35	B	501	ATP	C4-N9	-2.31	1.32	1.37
35	A	501	ATP	C8-N9	-2.28	1.33	1.37
35	E	401	ATP	C5-C6	2.27	1.47	1.41
35	E	401	ATP	C4-N9	-2.25	1.33	1.37
35	B	501	ATP	C5-C6	2.17	1.47	1.41
35	B	501	ATP	C8-N9	-2.15	1.33	1.37
37	F	501	ADP	C8-N9	-2.14	1.33	1.37
35	D	501	ATP	C8-N7	2.11	1.35	1.31
37	F	501	ADP	C8-N7	2.11	1.35	1.31
37	F	501	ADP	C5-C6	2.11	1.46	1.41
35	D	501	ATP	C4-N9	-2.06	1.33	1.37

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	501	ADP	C5-C4-N3	-7.04	117.02	126.72
35	A	501	ATP	C5-C4-N3	-6.65	117.56	126.72
35	D	501	ATP	C5-C4-N3	-5.98	118.48	126.72
37	F	501	ADP	C5-C4-N3	-5.96	118.51	126.72
37	C	501	ADP	N3-C4-N9	5.75	136.94	127.17
35	E	401	ATP	C5-C4-N3	-5.73	118.83	126.72
35	B	501	ATP	C5-C4-N3	-5.69	118.88	126.72
35	A	501	ATP	N3-C4-N9	5.56	136.63	127.17
35	B	501	ATP	N3-C4-N9	4.85	135.41	127.17
35	E	401	ATP	N3-C4-N9	4.78	135.30	127.17
35	D	501	ATP	N3-C4-N9	4.75	135.24	127.17
37	F	501	ADP	N3-C4-N9	4.69	135.14	127.17
37	C	501	ADP	C2-N3-C4	4.13	121.91	111.83
35	A	501	ATP	C2-N3-C4	3.81	121.14	111.83
35	D	501	ATP	C2-N3-C4	3.71	120.90	111.83
35	B	501	ATP	C2-N3-C4	3.56	120.53	111.83
37	F	501	ADP	C2-N3-C4	3.54	120.49	111.83
35	E	401	ATP	C2-N3-C4	3.50	120.37	111.83
35	B	501	ATP	N3-C2-N1	-3.32	123.55	128.58
35	D	501	ATP	C4-C5-N7	-3.29	106.83	110.58
37	F	501	ADP	C4-C5-N7	-3.28	106.84	110.58
35	A	501	ATP	C4-C5-N7	-3.26	106.86	110.58
37	C	501	ADP	C4-C5-N7	-3.25	106.87	110.58
35	D	501	ATP	N3-C2-N1	-3.18	123.76	128.58
37	C	501	ADP	N3-C2-N1	-3.18	123.77	128.58
35	B	501	ATP	C4-N9-C8	3.14	109.03	105.74
35	E	401	ATP	C4-C5-N7	-3.03	107.11	110.58
35	E	401	ATP	N3-C2-N1	-3.00	124.04	128.58
35	B	501	ATP	C4-C5-N7	-2.99	107.16	110.58
35	E	401	ATP	C4-N9-C8	2.90	108.78	105.74
35	A	501	ATP	N3-C2-N1	-2.83	124.30	128.58
37	F	501	ADP	N3-C2-N1	-2.80	124.35	128.58
37	C	501	ADP	C3'-C2'-C1'	2.72	106.62	101.46
35	B	501	ATP	C3'-C2'-C1'	2.63	106.45	101.46
35	A	501	ATP	C4-N9-C8	2.62	108.49	105.74
37	F	501	ADP	C4-N9-C8	2.61	108.47	105.74
35	E	401	ATP	C3'-C2'-C1'	2.59	106.36	101.46
35	A	501	ATP	C5-N7-C8	2.58	107.50	103.45
37	C	501	ADP	C5-N7-C8	2.52	107.41	103.45
35	D	501	ATP	C4-N9-C8	2.50	108.37	105.74
35	D	501	ATP	C5-N7-C8	2.40	107.22	103.45
35	B	501	ATP	C2'-C1'-N9	-2.40	107.34	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	501	ADP	C1'-N9-C8	-2.36	121.85	127.09
35	E	401	ATP	C5-N7-C8	2.29	107.05	103.45
37	F	501	ADP	C5-N7-C8	2.28	107.03	103.45
35	B	501	ATP	C5-N7-C8	2.27	107.02	103.45
37	C	501	ADP	C4-N9-C8	2.23	108.08	105.74
35	A	501	ATP	C1'-N9-C8	-2.13	122.36	127.09
35	A	501	ATP	C3'-C2'-C1'	2.13	105.49	101.46
37	F	501	ADP	C2'-C1'-N9	-2.10	108.09	113.30
35	E	401	ATP	O3G-PG-O2G	2.03	115.41	107.80
35	B	501	ATP	C2-N1-C6	2.03	122.06	118.73
35	B	501	ATP	N9-C8-N7	-2.01	111.08	113.94

There are no chirality outliers.

All (26) torsion outliers are listed below:

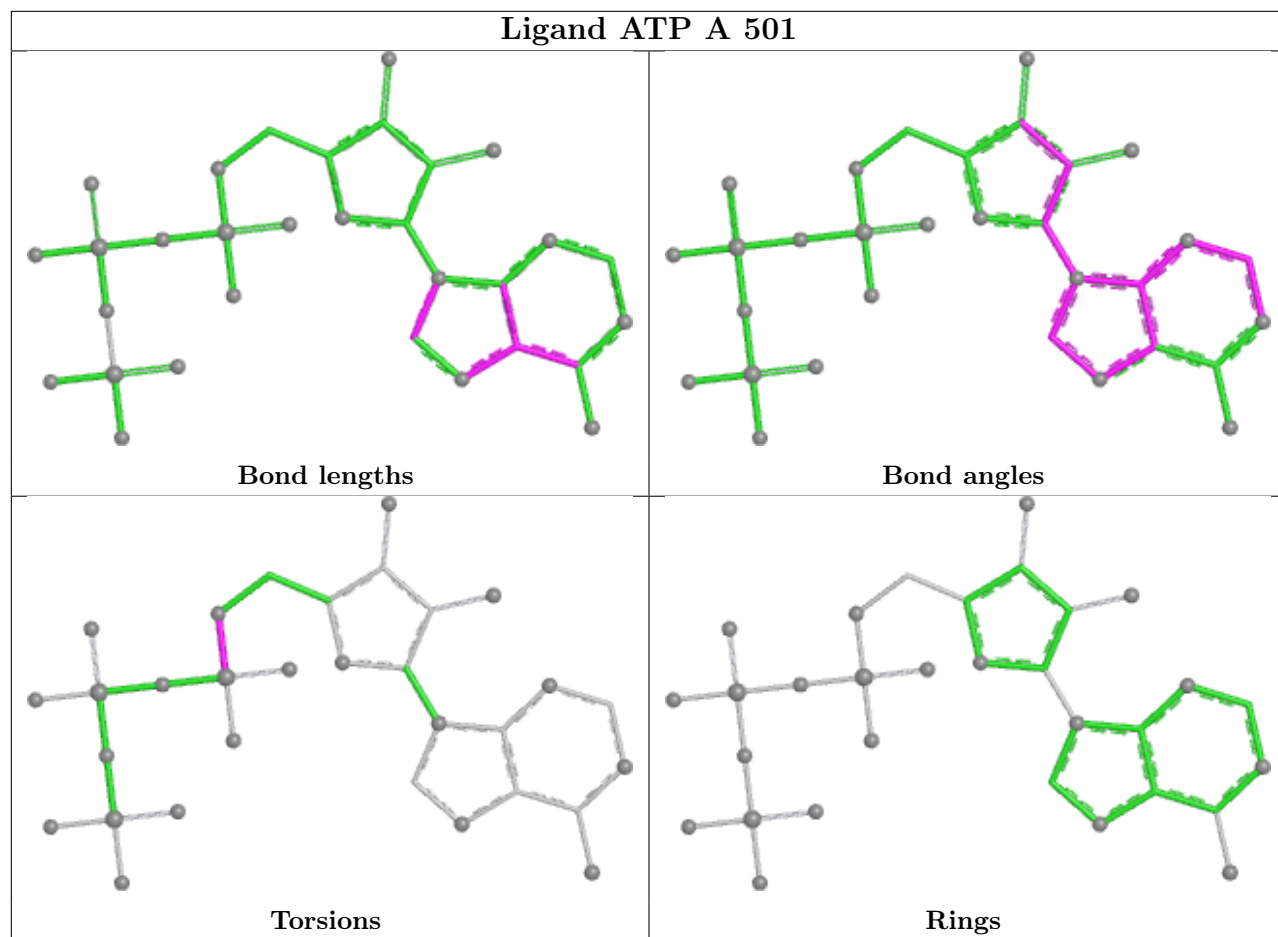
Mol	Chain	Res	Type	Atoms
35	B	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	C5'-O5'-PA-O2A
35	B	501	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	C5'-O5'-PA-O1A
35	D	501	ATP	C5'-O5'-PA-O3A
37	C	501	ADP	PA-O3A-PB-O3B
37	C	501	ADP	C5'-O5'-PA-O2A
37	C	501	ADP	C5'-O5'-PA-O3A
37	F	501	ADP	PA-O3A-PB-O2B
37	F	501	ADP	C5'-O5'-PA-O1A
37	F	501	ADP	O4'-C4'-C5'-O5'
37	F	501	ADP	C3'-C4'-C5'-O5'
35	D	501	ATP	O4'-C1'-N9-C4
35	D	501	ATP	O4'-C1'-N9-C8
37	F	501	ADP	PA-O3A-PB-O1B
35	D	501	ATP	O4'-C4'-C5'-O5'
37	F	501	ADP	C2'-C1'-N9-C8
35	D	501	ATP	C3'-C4'-C5'-O5'
35	A	501	ATP	C5'-O5'-PA-O1A
37	F	501	ADP	O4'-C1'-N9-C8
37	F	501	ADP	O4'-C1'-N9-C4
37	C	501	ADP	PA-O3A-PB-O2B
35	D	501	ATP	C2'-C1'-N9-C8
35	D	501	ATP	PA-O3A-PB-O2B
35	E	401	ATP	PG-O3B-PB-O2B
35	E	401	ATP	PA-O3A-PB-O2B

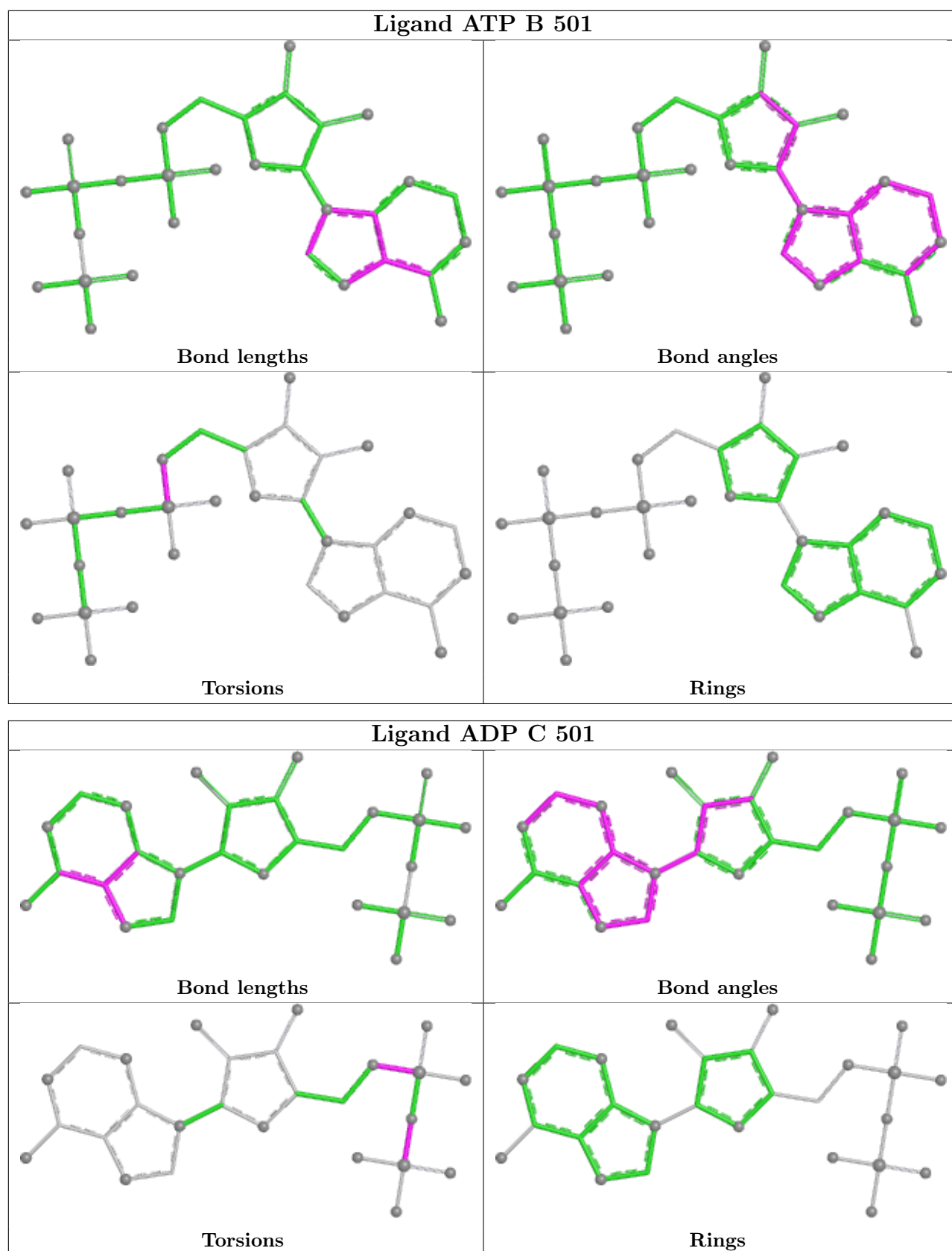
There are no ring outliers.

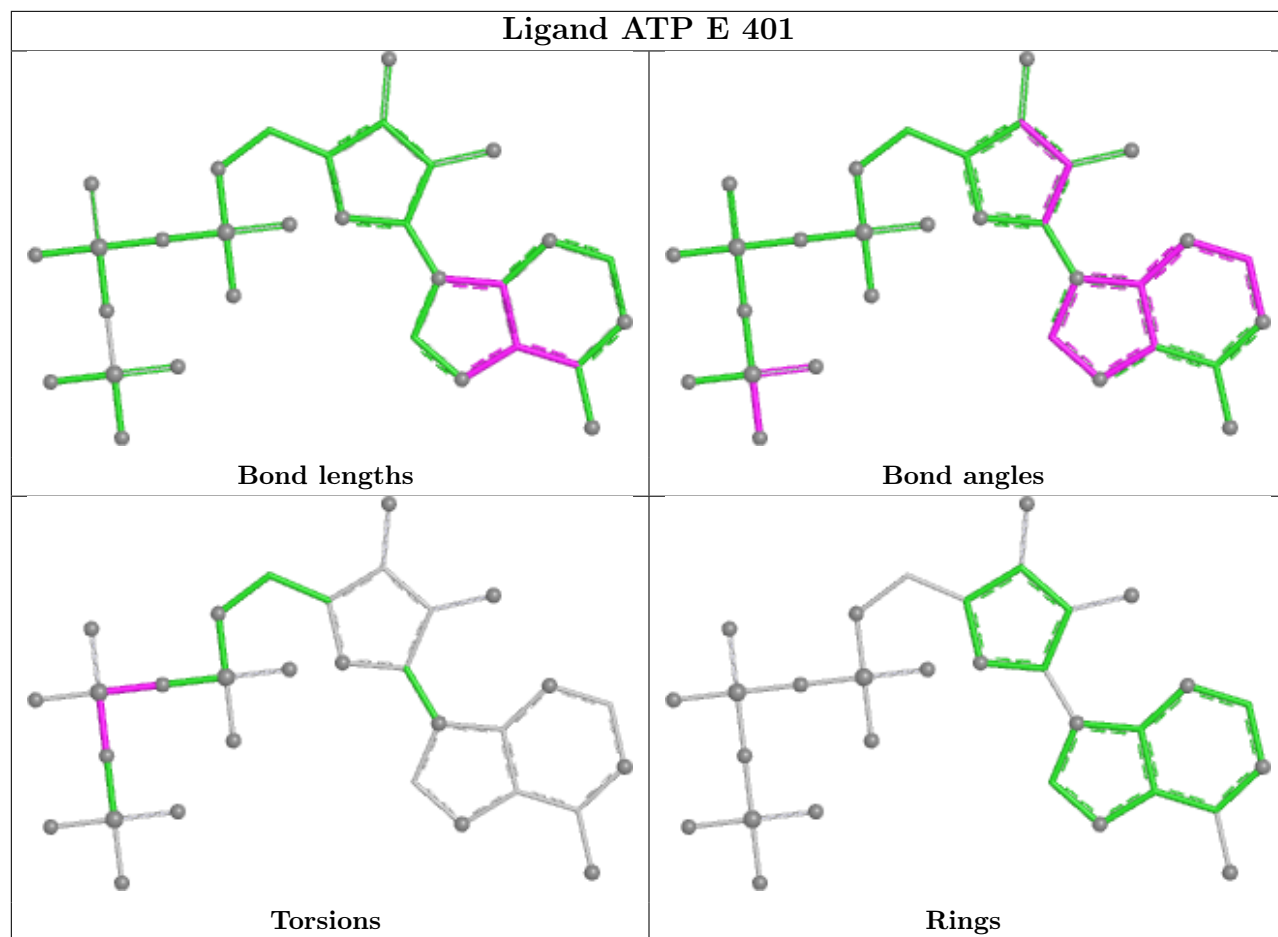
6 monomers are involved in 8 short contacts:

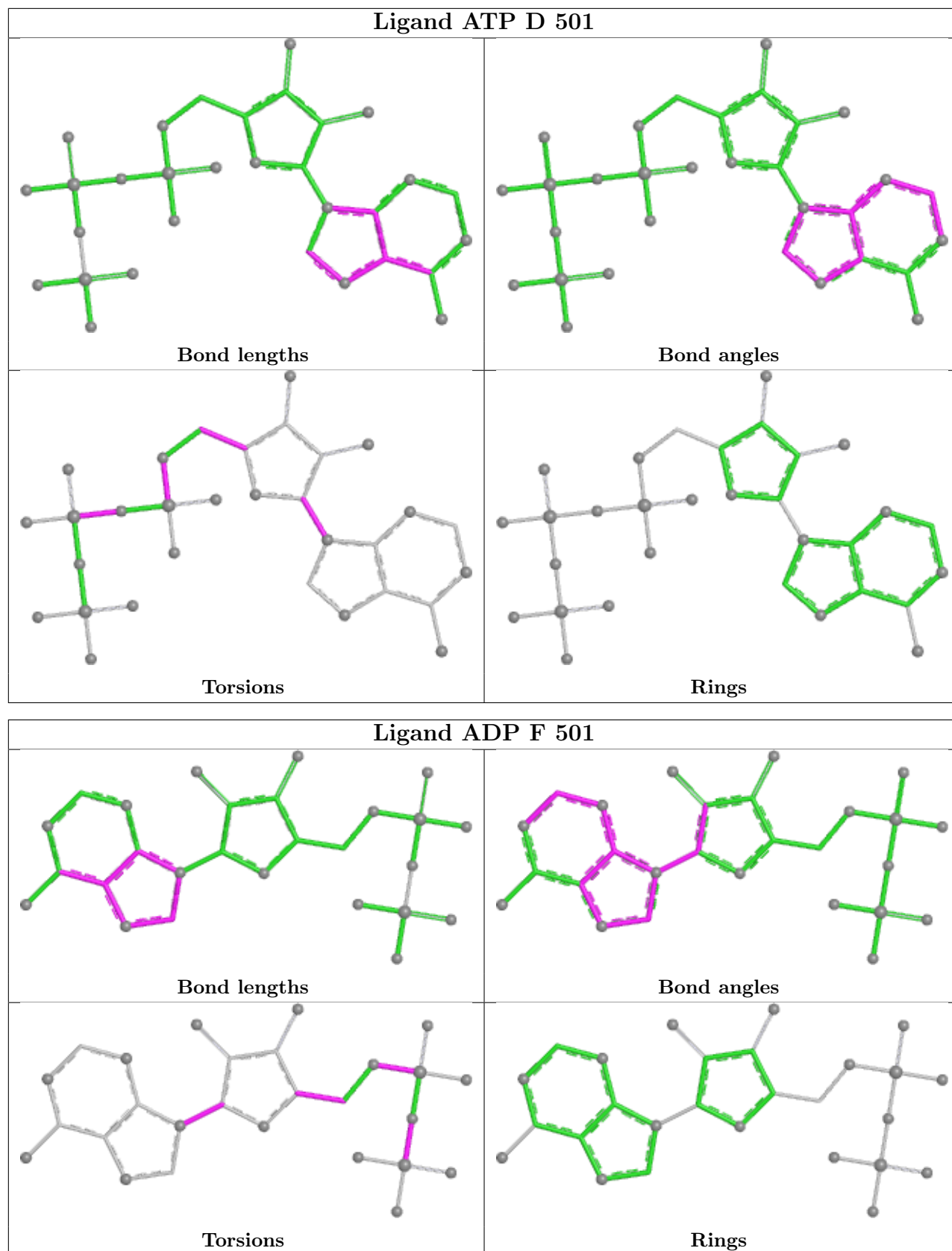
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	501	ATP	1	0
35	B	501	ATP	1	0
37	C	501	ADP	1	0
35	E	401	ATP	2	0
35	D	501	ATP	2	0
37	F	501	ADP	1	0

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









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.

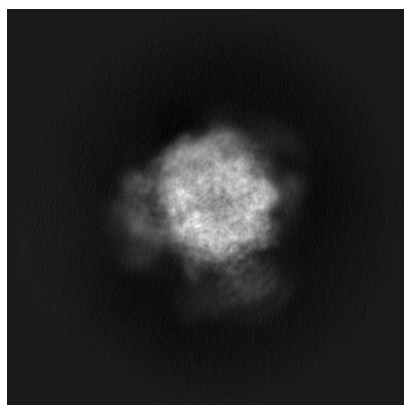
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9217. These allow visual inspection of the internal detail of the map and identification of artifacts.

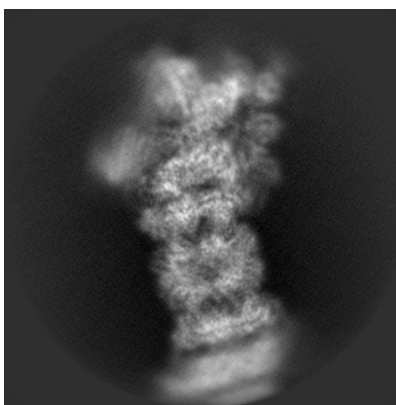
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

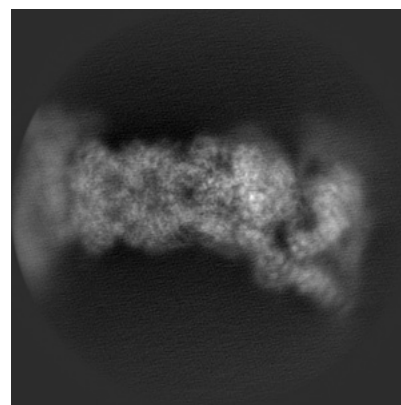
6.1.1 Primary map



X



Y

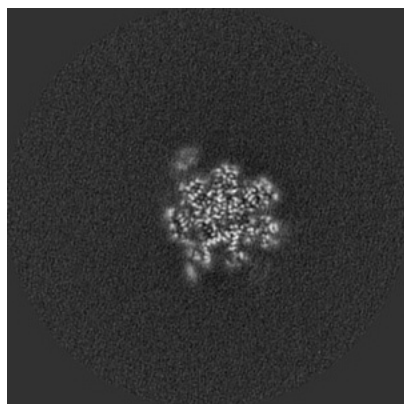


Z

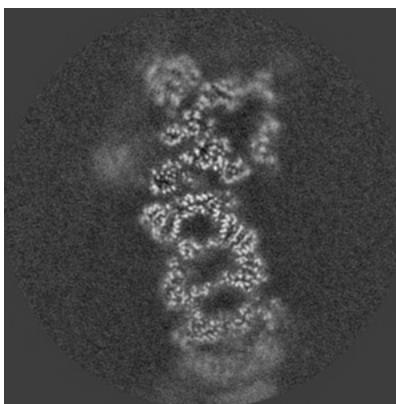
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

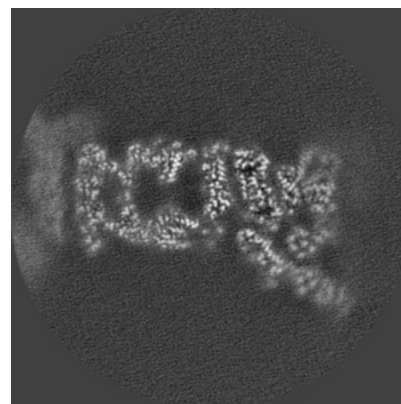
6.2.1 Primary map



X Index: 300



Y Index: 300

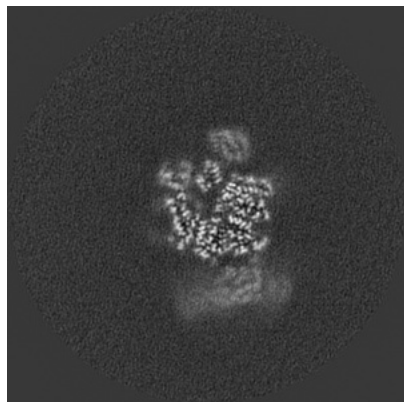


Z Index: 300

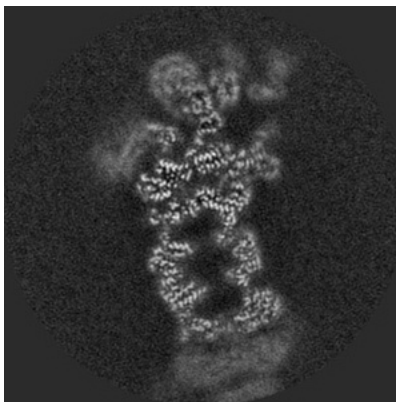
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

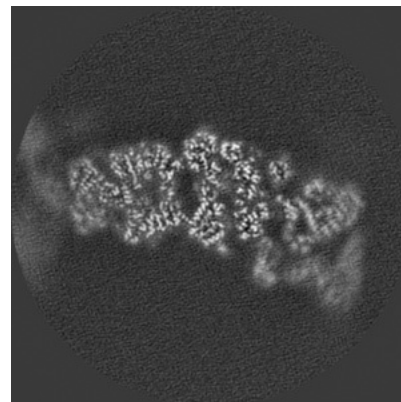
6.3.1 Primary map



X Index: 352



Y Index: 319

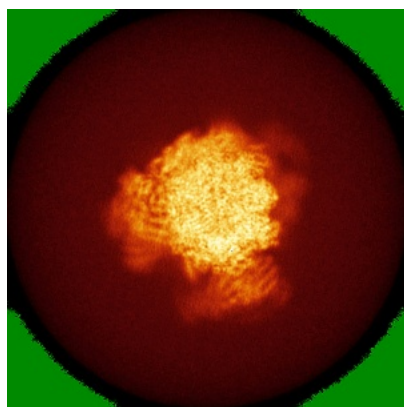


Z Index: 273

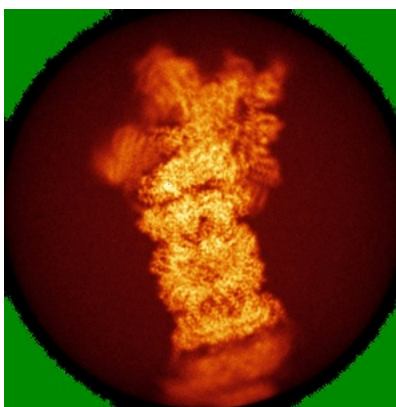
The images above show the largest variance slices of the map in three orthogonal directions.

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

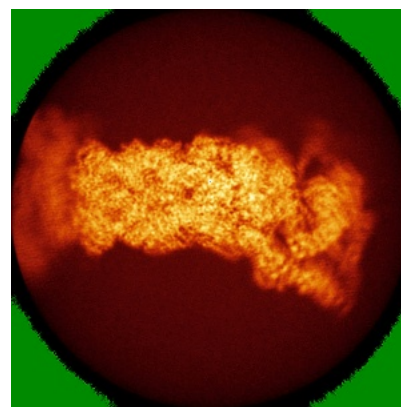
6.4.1 Primary map



X



Y

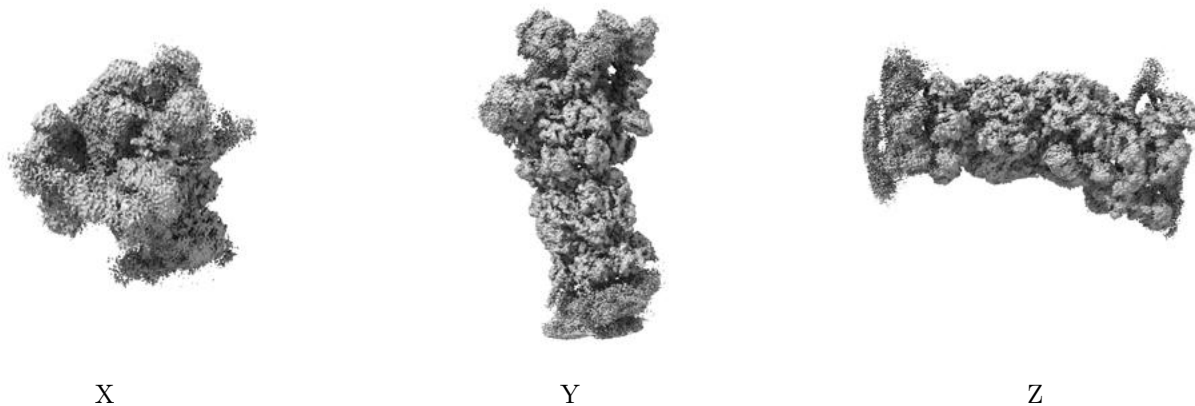


Z

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 0.0035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

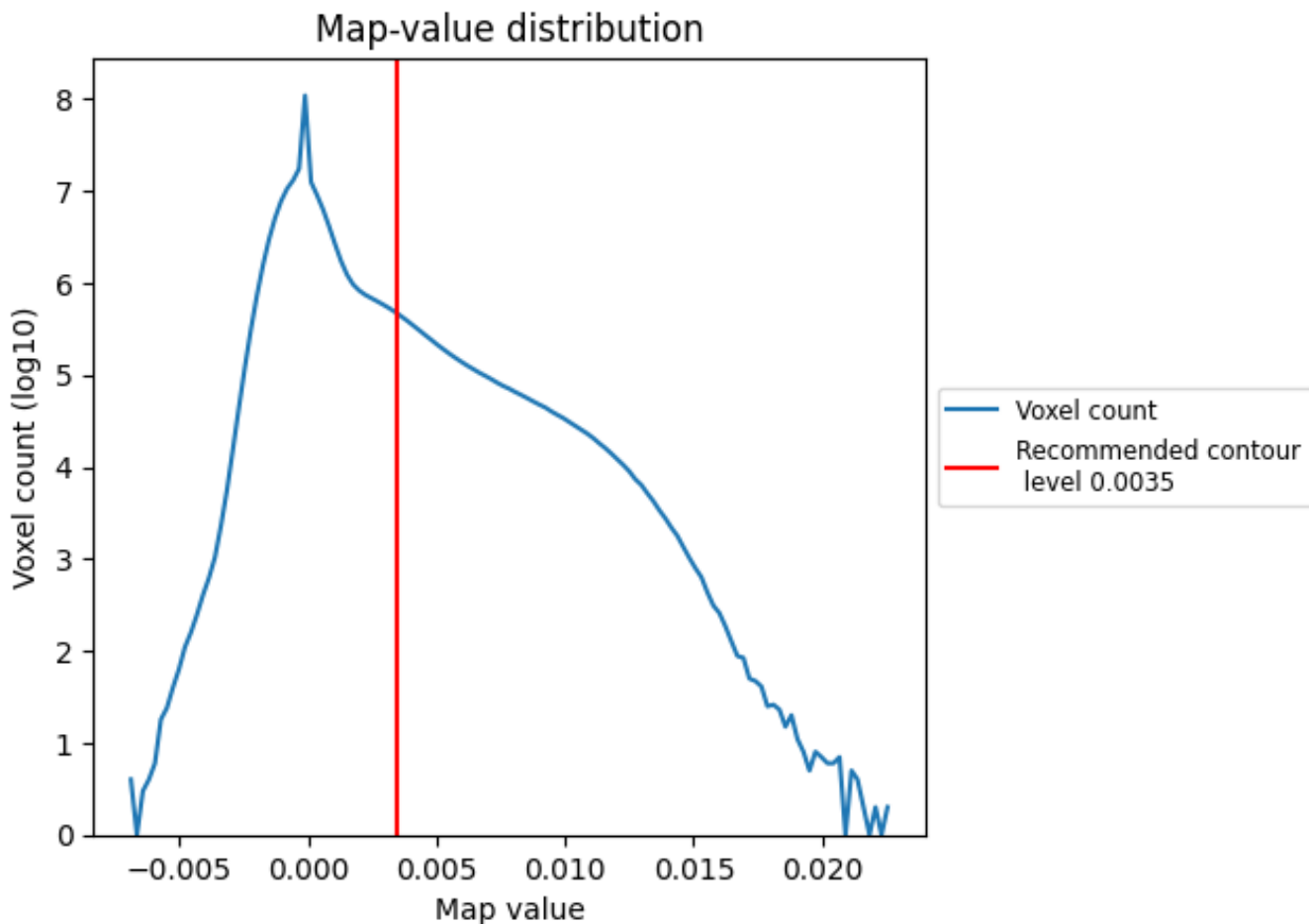
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

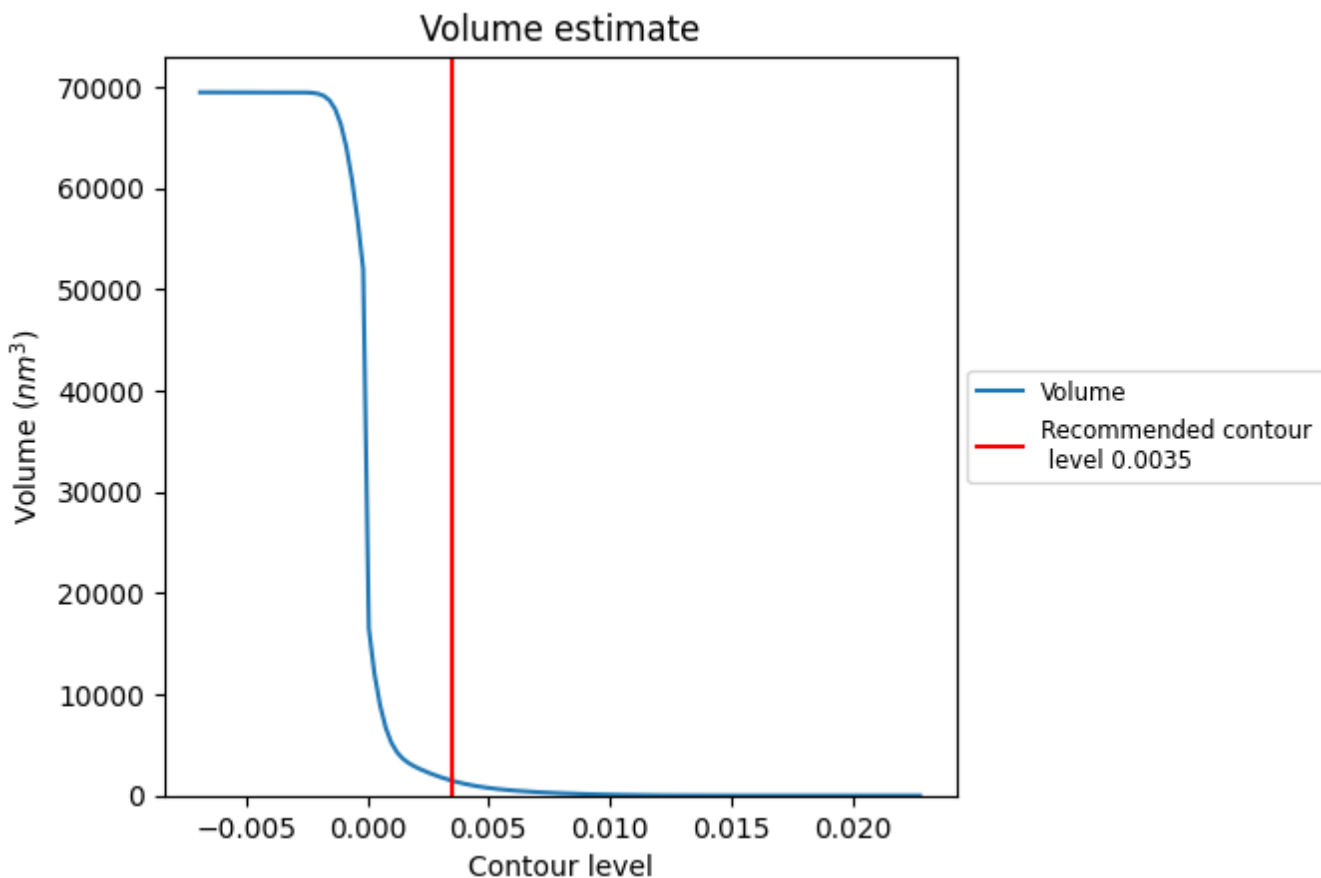
This section contains the results of statistical analysis of the map.

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.

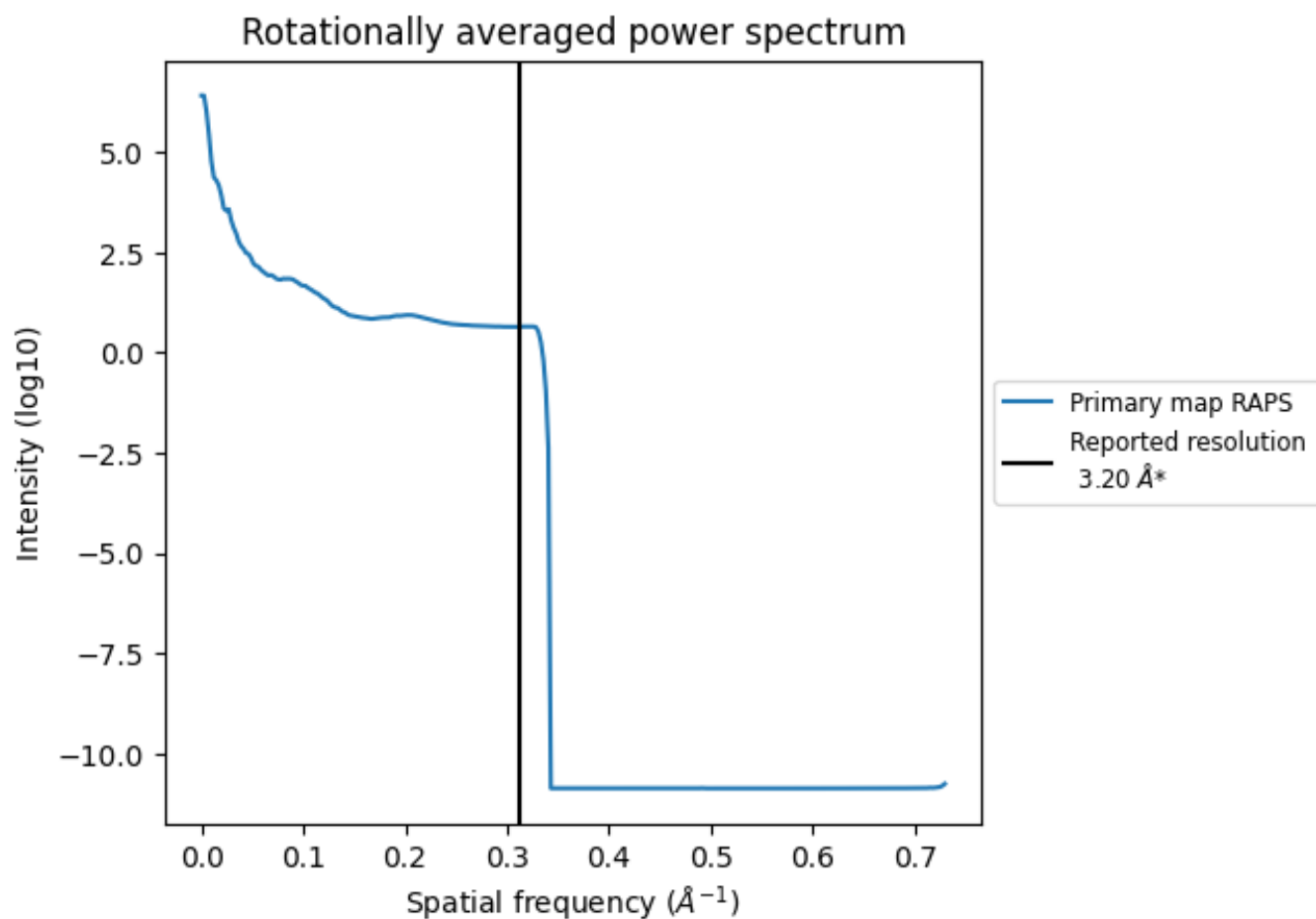
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1467 nm^3 ; this corresponds to an approximate mass of 1325 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

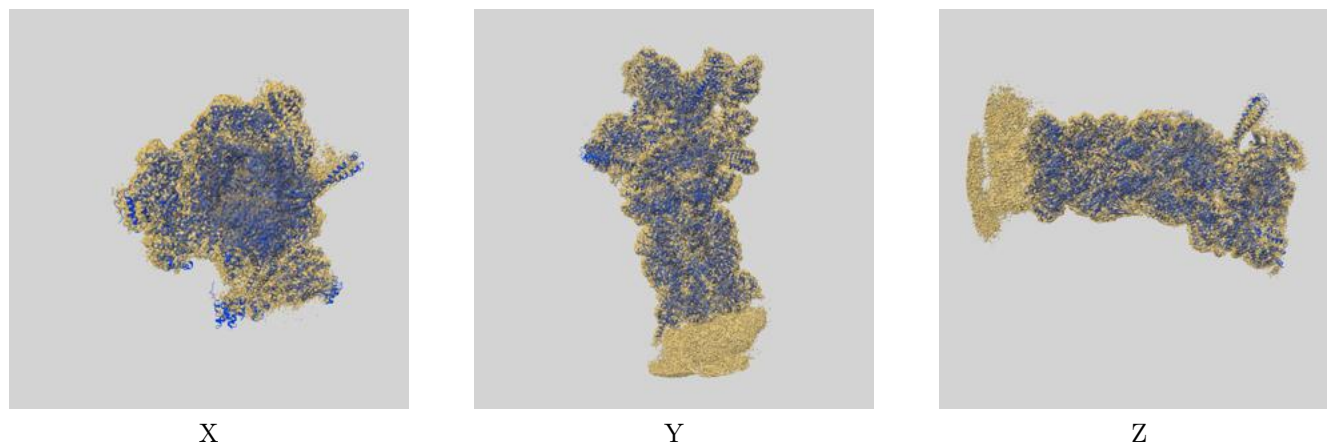
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

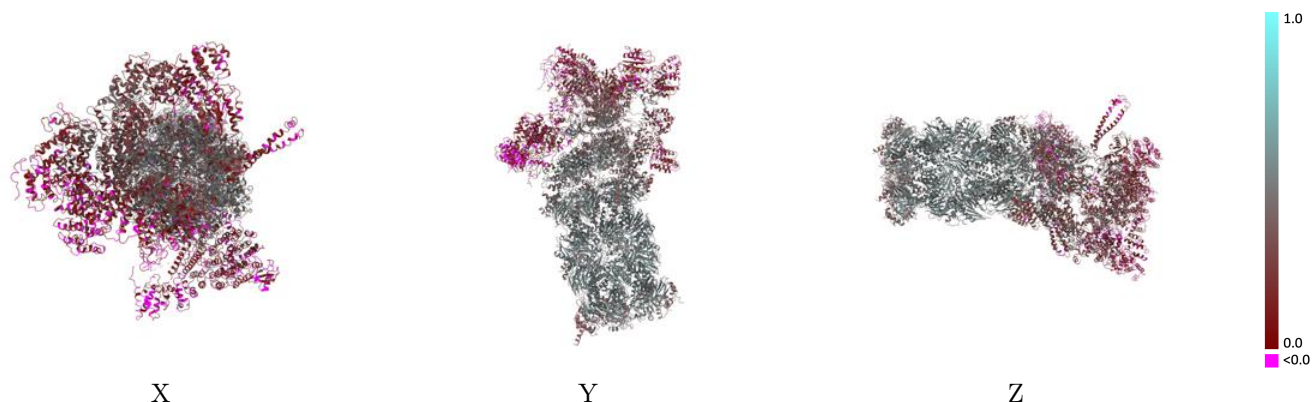
This section contains information regarding the fit between EMDB map EMD-9217 and PDB model 6MSD. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



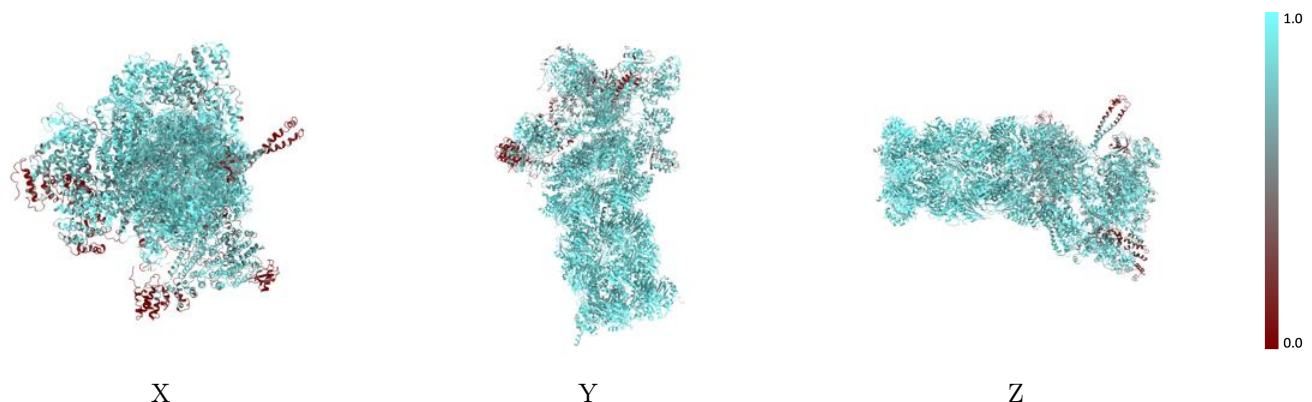
The images above show the 3D surface view of the map at the recommended contour level 0.0035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



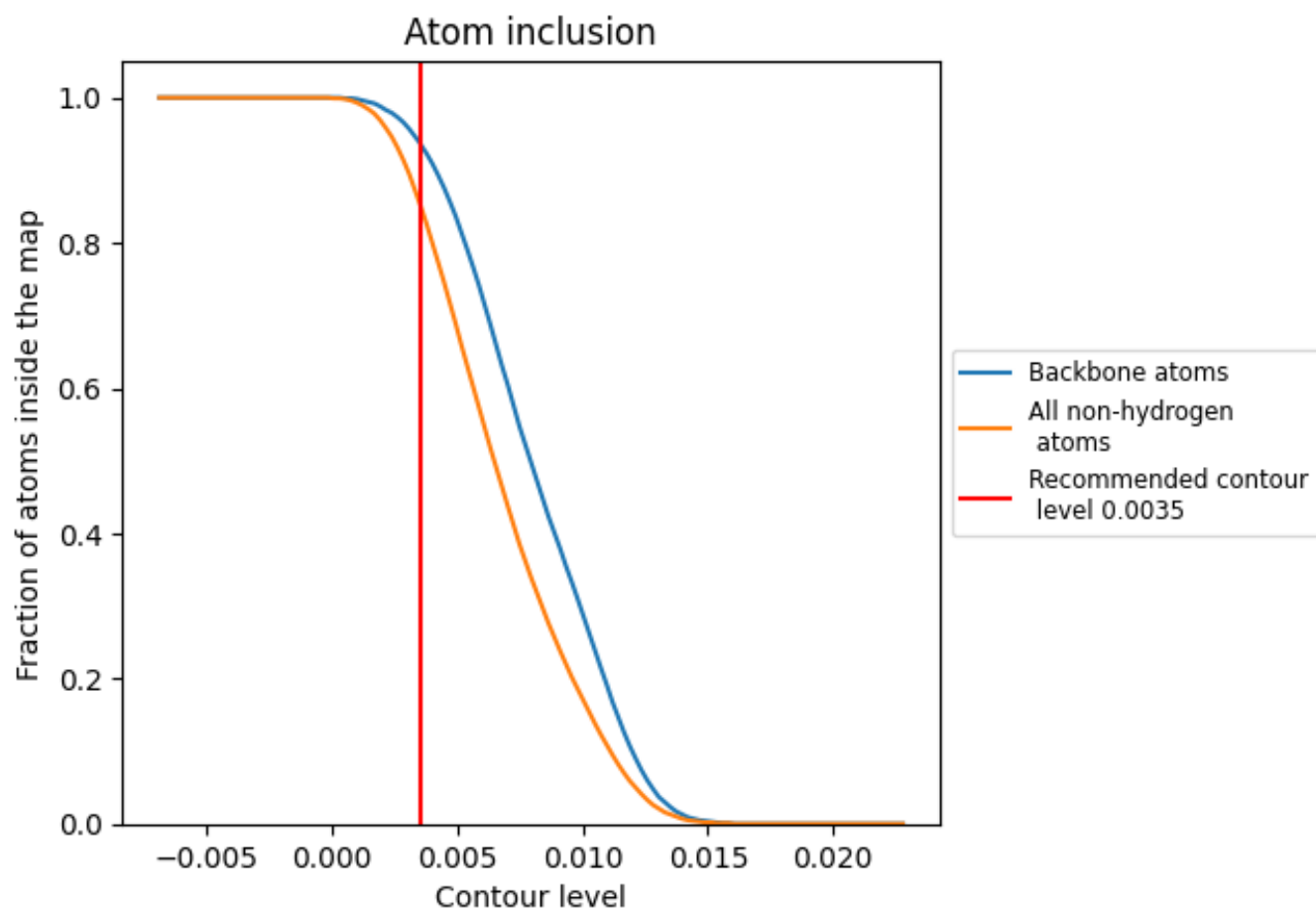
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0035).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 86% 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 (0.0035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.3650
A	 0.8890	 0.4230
B	 0.8930	 0.4050
C	 0.8960	 0.4030
D	 0.8940	 0.4090
E	 0.8450	 0.3910
F	 0.8230	 0.3970
G	 0.9480	 0.4870
H	 0.9580	 0.4950
I	 0.9390	 0.4530
J	 0.9580	 0.4570
K	 0.9420	 0.4760
L	 0.9580	 0.4870
M	 0.9430	 0.4670
N	 0.9640	 0.5050
O	 0.9720	 0.5050
P	 0.9710	 0.5130
Q	 0.9670	 0.4980
R	 0.9700	 0.5060
S	 0.9630	 0.5000
T	 0.9620	 0.5090
U	 0.7490	 0.1650
V	 0.6530	 0.1560
W	 0.7770	 0.2270
X	 0.8380	 0.2990
Y	 0.8810	 0.2920
Z	 0.8260	 0.2860
a	 0.8260	 0.2290
b	 0.7160	 0.1570
c	 0.8400	 0.3090
d	 0.6060	 0.1350
e	 0.7390	 0.1420
f	 0.6090	 0.1320
g	 0.9450	 0.4710
h	 0.9460	 0.4780



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Chain	Atom inclusion	Q-score
i	 0.9080	 0.4320
j	 0.9290	 0.4040
k	 0.9290	 0.4510
l	 0.9530	 0.4660
m	 0.9430	 0.4640
n	 0.9720	 0.5160
o	 0.9770	 0.5170
p	 0.9720	 0.5150
q	 0.9690	 0.5100
r	 0.9780	 0.5140
s	 0.9690	 0.5100
t	 0.9690	 0.5160
u	 0.4150	 0.2430
w	 0.1120	 0.0080