



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:32 PM UTC

PDB ID : 7W39 / pdb_00007w39
EMDB ID : EMD-32274
Title : Structure of USP14-bound human 26S proteasome in state EA2.1_UBL
Authors : Zhang, S.; Zou, S.; Yin, D.; Wu, Z.; Mao, Y.
Deposited on : 2021-11-25
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:

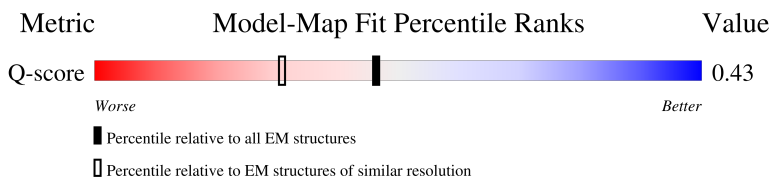
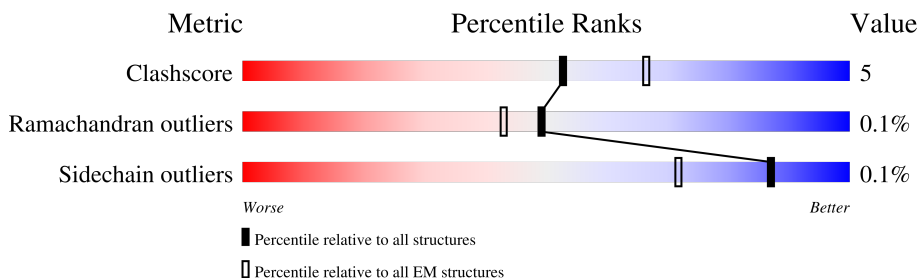
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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	A	433	
2	B	440	
3	C	398	
4	D	418	

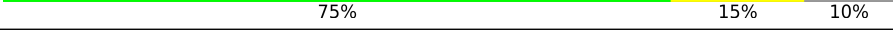
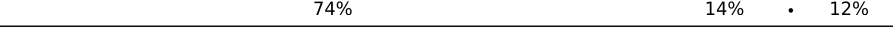
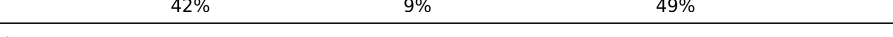
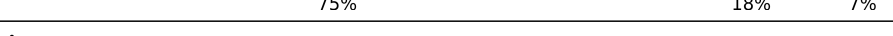
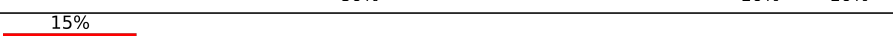
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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	269	
12	l	269	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	

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Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	
21	U	953	
22	V	534	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	310	
30	d	350	
31	e	70	
32	f	908	
33	u	76	
34	v	10	
35	x	494	

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 106442 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	234	Total	C	N	O	S	0	0
			1777	1117	295	354	11		
11	k	234	Total	C	N	O	S	0	0
			1782	1119	295	357	11		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

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

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

- Molecule 33 is a protein called Ubiquitin.

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

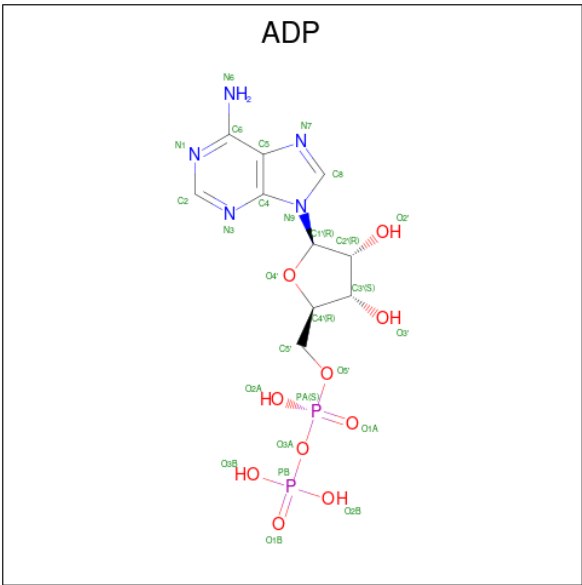
- Molecule 34 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	v	10	Total	C	N	O	0	0
			53	32	11	10		

- Molecule 35 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	x	76	Total	C	N	O	S	0	0
			588	378	96	108	6		

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



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

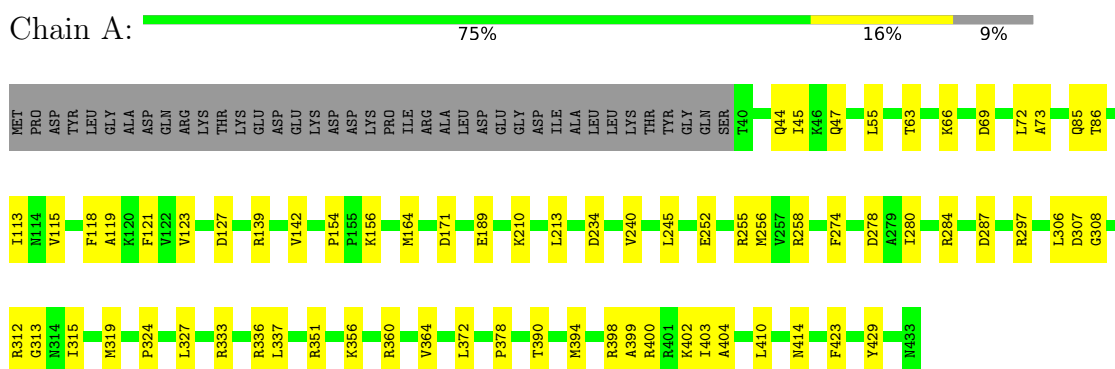
- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

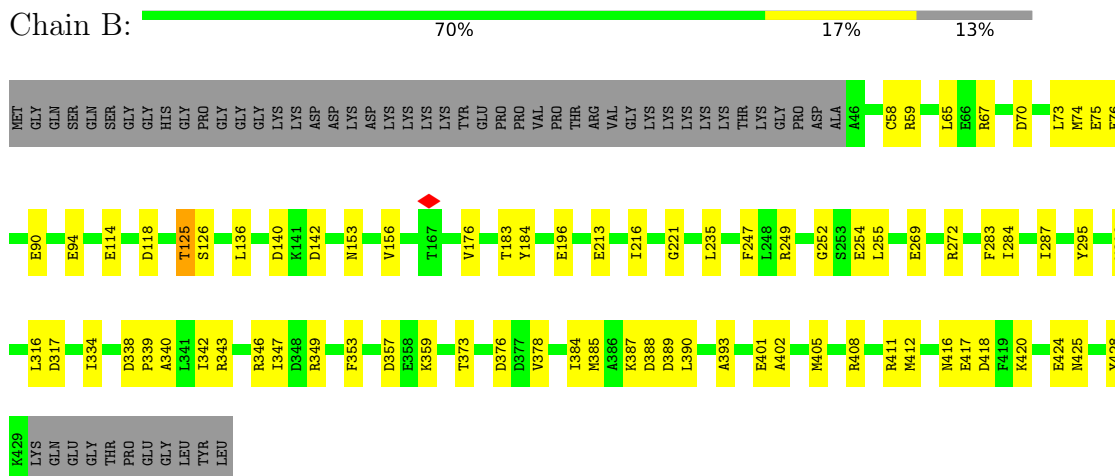
3 Residue-property plots

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

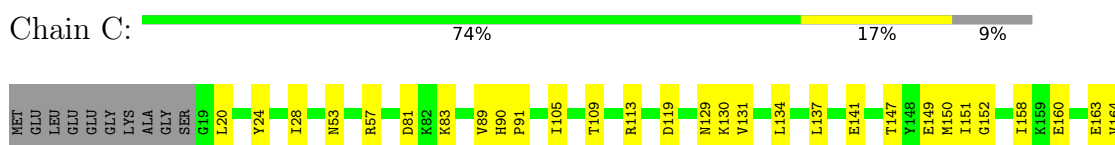
• Molecule 1: 26S protease regulatory subunit 7

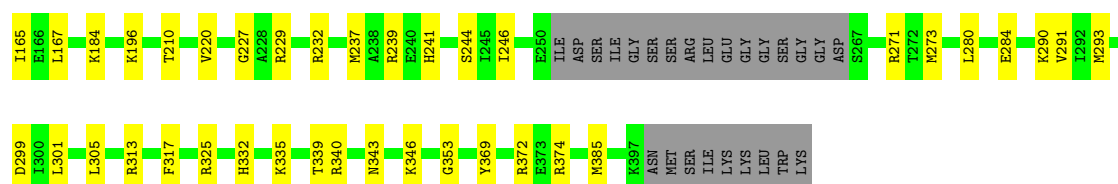


• Molecule 2: 26S protease regulatory subunit 4



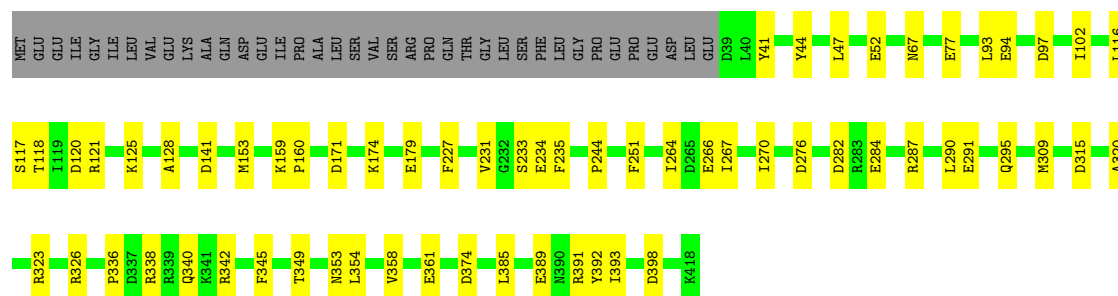
• Molecule 3: Isoform 2 of 26S proteasome regulatory subunit 8





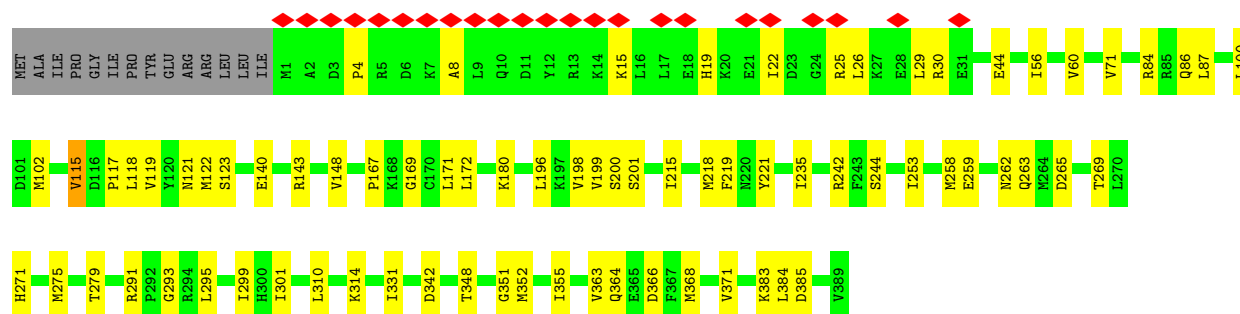
- Molecule 4: 26S protease regulatory subunit 6B

Chain D: 76% 15% 9%



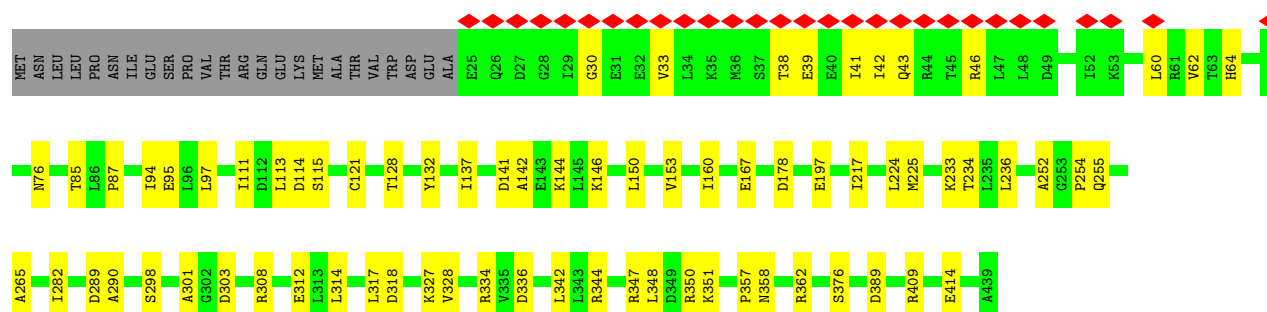
- Molecule 5: 26S proteasome regulatory subunit 10B

Chain E: 6% 78% 19% .



- Molecule 6: 26S protease regulatory subunit 6A

Chain F: 7% 78% 17% 5%



- Molecule 7: Proteasome subunit alpha type-6

Chain G: 92% 7%



- Molecule 7: Proteasome subunit alpha type-6

Chain g: 89% 10% .



- Molecule 8: Proteasome subunit alpha type-2

Chain H: 91% 8% .



- Molecule 8: Proteasome subunit alpha type-2

Chain h: 90% 9% .



- Molecule 9: Proteasome subunit alpha type-4

Chain I: 87% 9% .



- Molecule 9: Proteasome subunit alpha type-4

Chain i: 91% 5% .



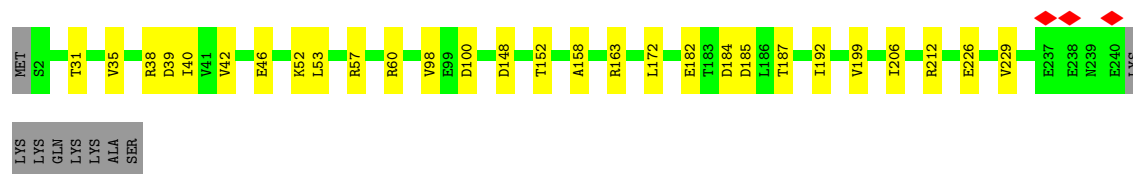
- Molecule 10: Proteasome subunit alpha type-7

Chain J: 91% 5% .



- Molecule 10: Proteasome subunit alpha type-7

Chain j: 85% 11% .



- Molecule 11: Proteasome subunit alpha type-5

Chain K: 87% 10% .



- Molecule 11: Proteasome subunit alpha type-5

Chain k: 91% 6% .



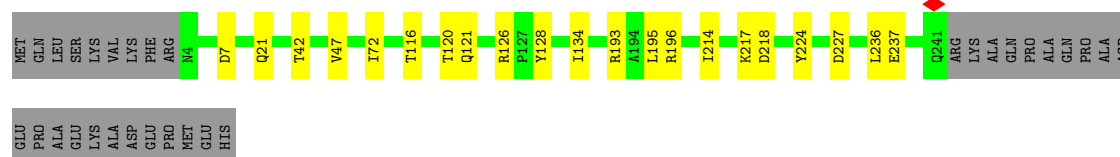
- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

Chain L: 80% 8% 12%



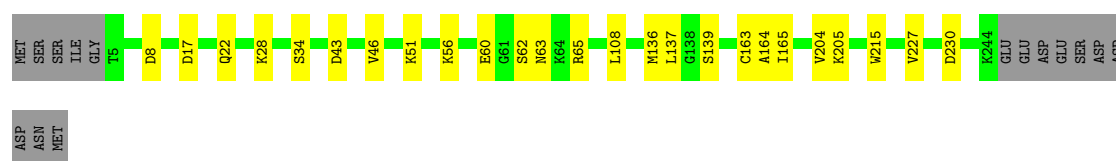
- Molecule 12: Isoform Long of Proteasome subunit alpha type-1

Chain l: 81% 8% 12%



- Molecule 13: Proteasome subunit alpha type-3

Chain M: 84% 10% 6%



- Molecule 13: Proteasome subunit alpha type-3

MET
SER
SER
ILE
GLY
T5
D8
Q22
V23
M27
S34
I39
R65
M75
E93
N97
R129
L137
R169
K173
I176
W215
V227
D230
K240
K244
GLU
GLU
ASP
GLU
SER
SER
ASP
ASP
ASP
ASN
MET

- | | | | | | | | | |
|-----|----|-----|-----|------|------|------|-----|-----|-----|
| MET | ALA | ALA | ALA | THR | LEU | LEU | ALA | ALA | ALA | ARG | GLY | ALA | ALA | GLY | PRO | ALA | PRO | ALA | ALA | TRP | GLY | PRO | GLU | ALA | PHE | THR | PRO | ASP | TRP | GLU | SER | ARG | GLU | VAL | SER | THR | GLY | T1 | I26 | K34 | M120 | R166 | L202 | PRO | PRO | ALA |
|-----|----|-----|-----|------|------|------|-----|-----|-----|

- | | | | | | | | | |
|------|------|------|------|------|------|-----|-----|-----|
| MET | ALA | ALA | THR | LEU | LEU | ALA | ALA | GLY | GLY | PRO | PRO | PRO | TRP | GLY | PRO | GLU | PHE | THR | THR | ASP | TRP | GLU | SER | SER | ARG | GLU | VAL | SER | SER | THR | THR | GLY | TYR | D104 | I127 | Y136 | E165 | R166 | L202 | PRO | PRO | ALA |
|------|------|------|------|------|------|-----|-----|-----|

- [illegible]

- [illegible]

- | | | | | | | | | | | | | | | | |
|-----|----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|
| MET | S2 | K15 | I30 | Q31 | D38 | Q65 | I121 | C122 | S123 | V137 | A143 | M146 | D159 | D193 | D205 |
|-----|----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|

- 



- Molecule 17: Proteasome subunit beta type-2

Chain Q: 87% 12%



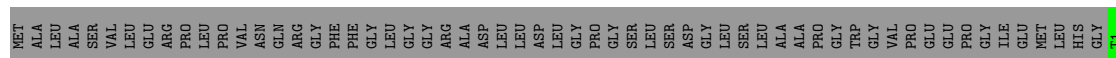
- Molecule 17: Proteasome subunit beta type-2

Chain q: 89% 10%



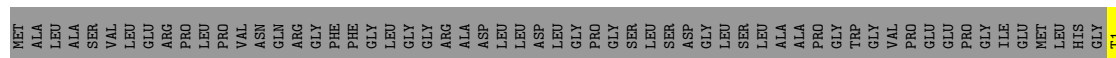
- Molecule 18: Proteasome subunit beta type-5

Chain R: 71% 6% 24%



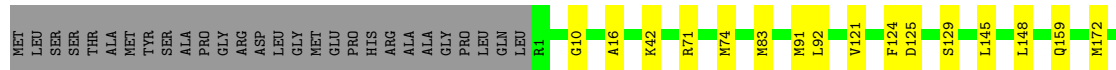
- Molecule 18: Proteasome subunit beta type-5

Chain r: 71% 5% 24%



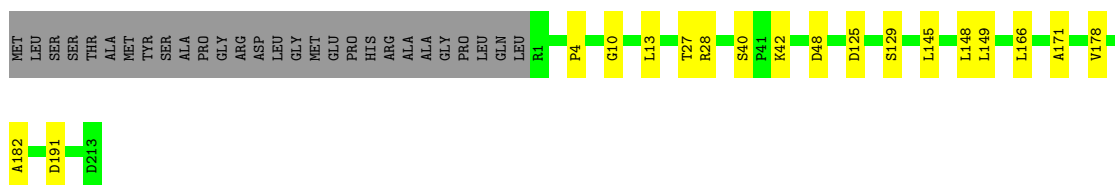
- Molecule 19: Proteasome subunit beta type-1

Chain S: 78% 10% 12%



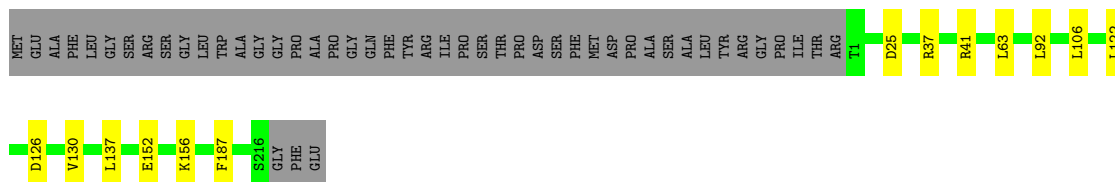
- Molecule 19: Proteasome subunit beta type-1

Chain s: 81% 7% 12%



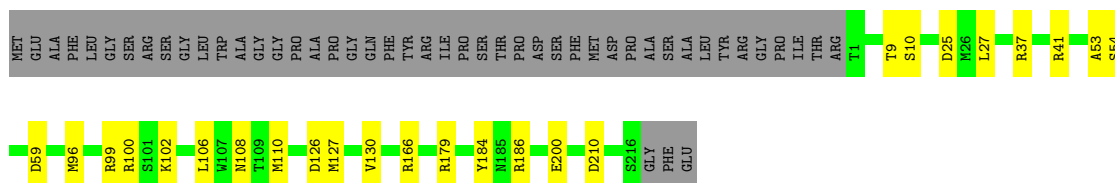
- Molecule 20: Proteasome subunit beta type-4

Chain T: 77% 5% 18%



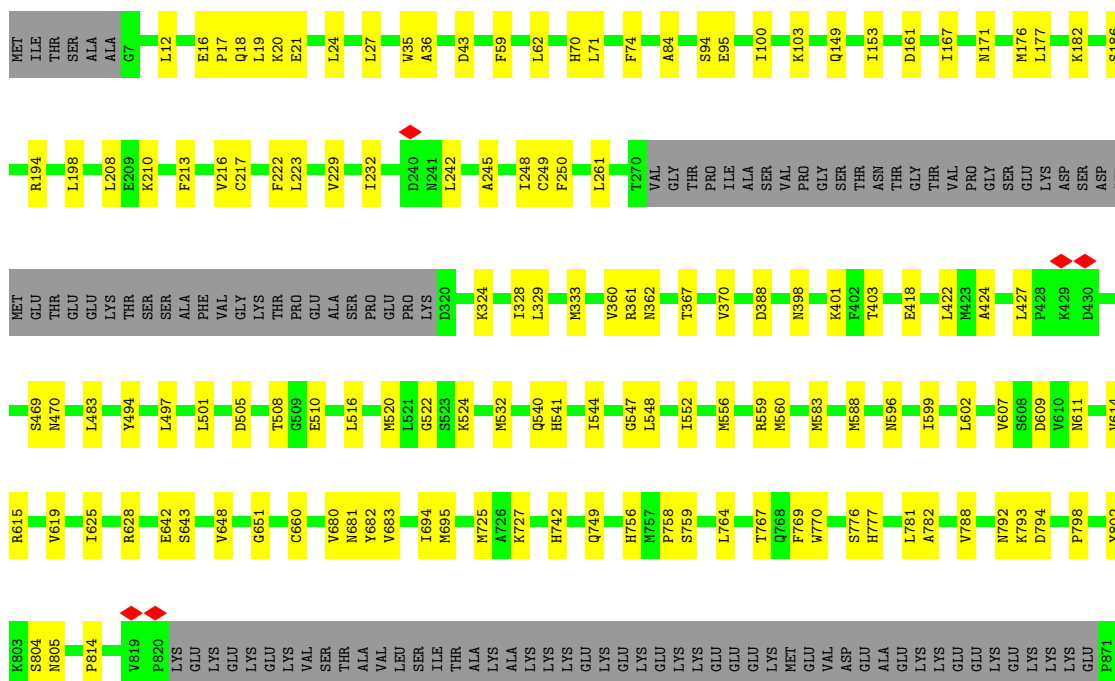
- Molecule 20: Proteasome subunit beta type-4

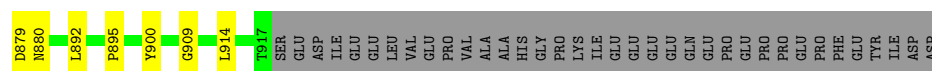
Chain t: 72% 9% 18%



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

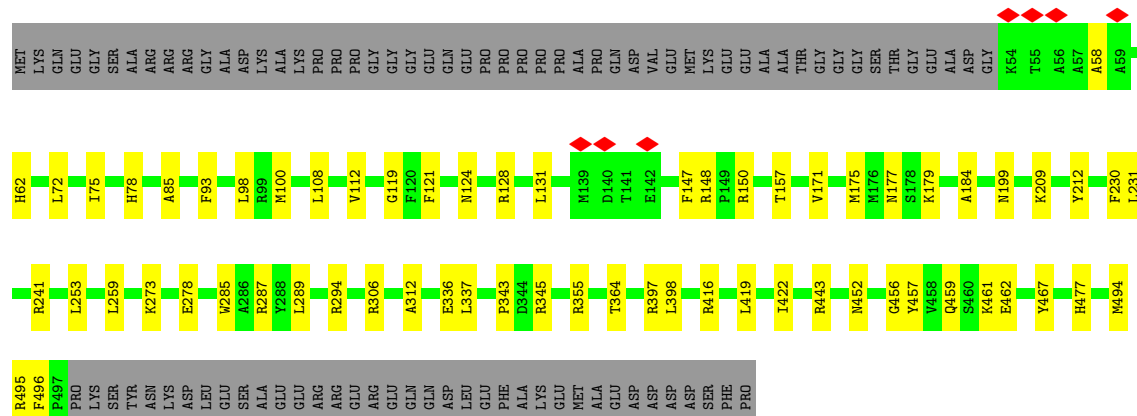
Chain U: 70% 15% 15%





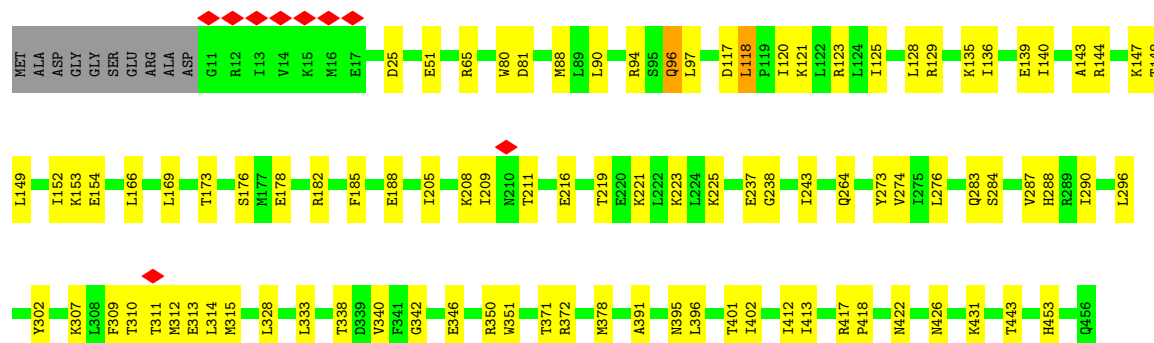
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

Chain V: 71% 12% 17%



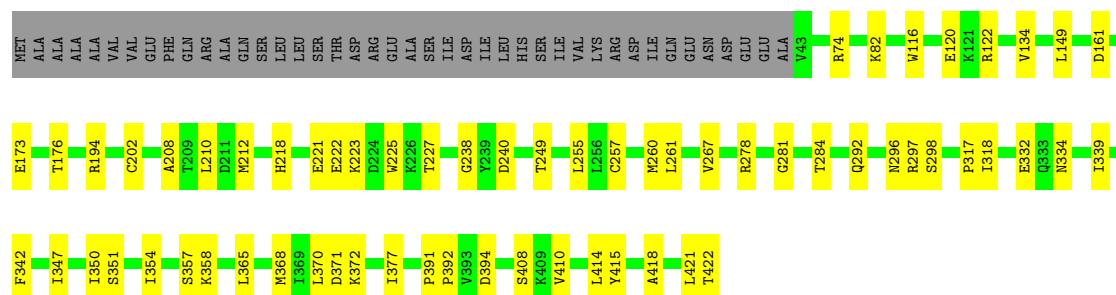
- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

Chain W: 77% 20% 3%

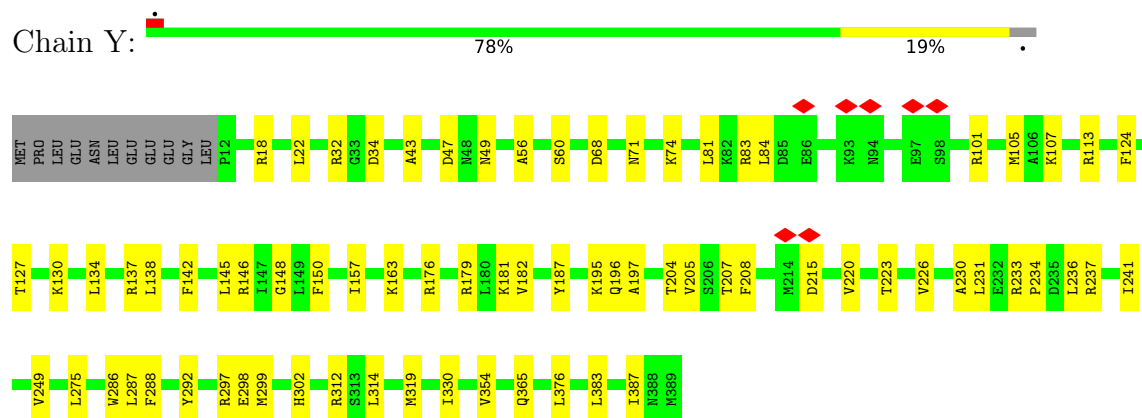


- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

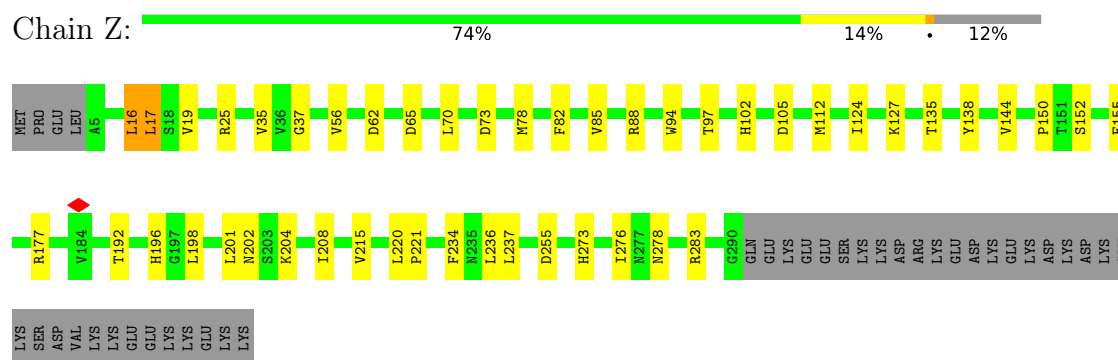
Chain X: 75% 15% 10%



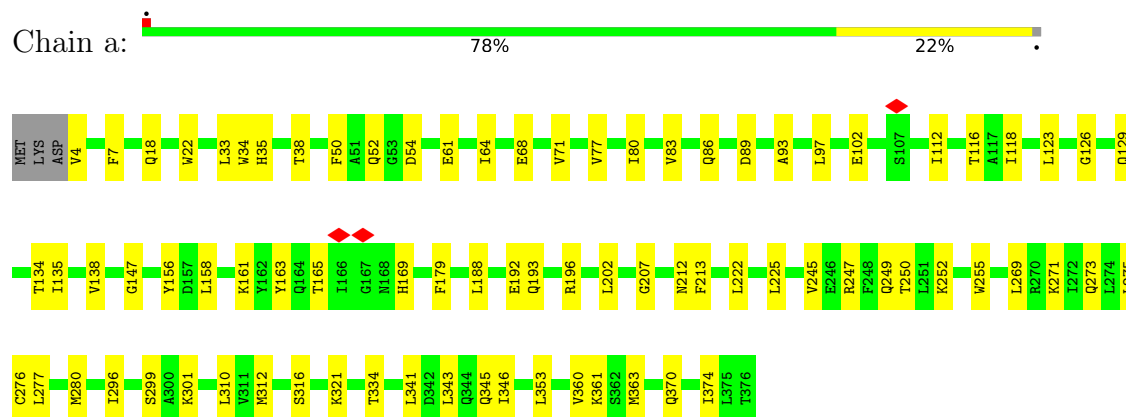
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6



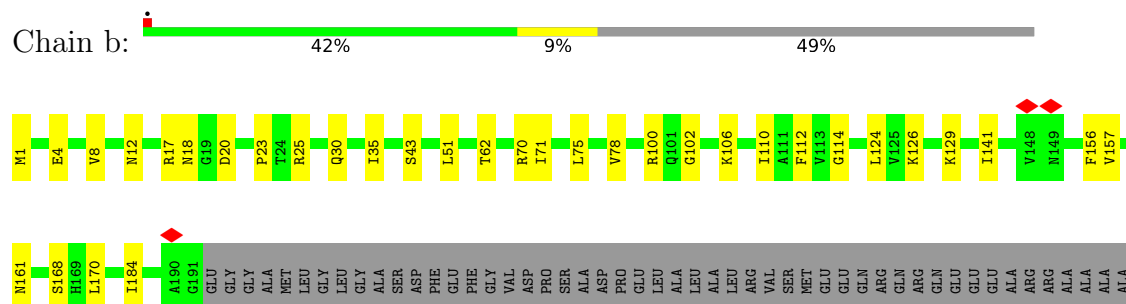
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

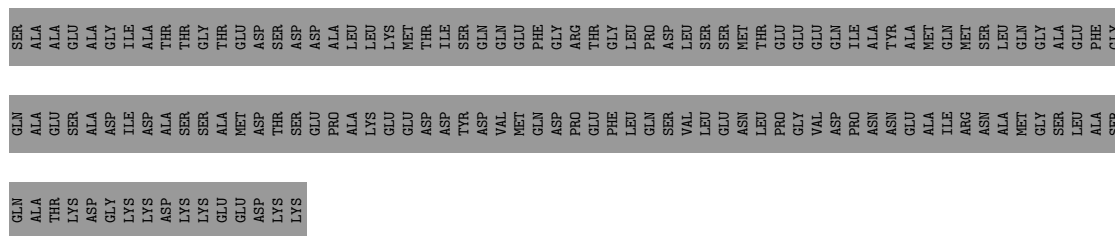


- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

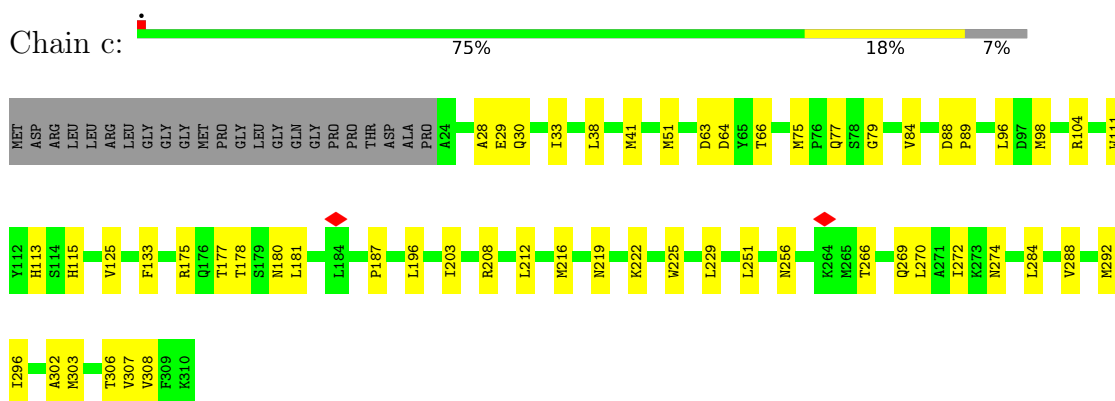


- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

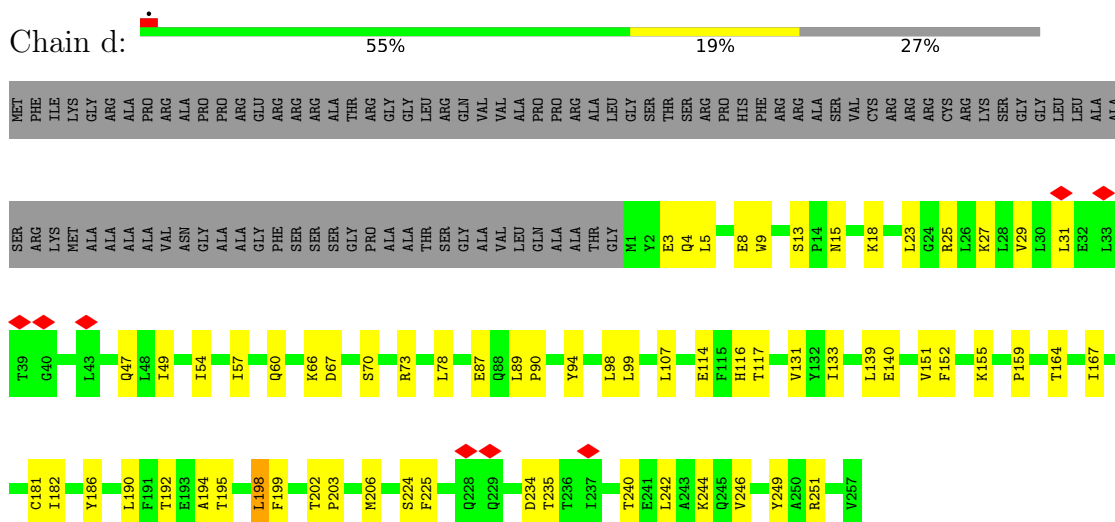




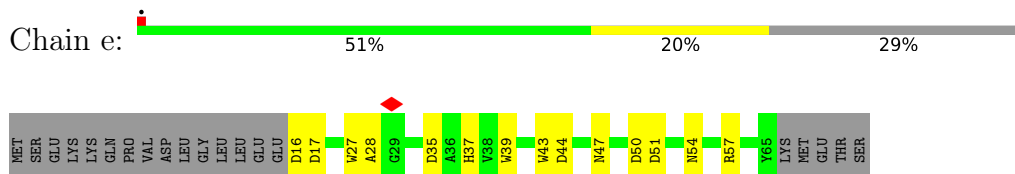
• Molecule 29: 26S proteasome non-ATPase regulatory subunit 14



• Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



• Molecule 31: 26S proteasome complex subunit DSS1



• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	294653	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.003	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/3148	0.51	0/4250
2	B	0.18	0/3061	0.45	0/4129
3	C	0.20	0/2902	0.49	0/3904
4	D	0.20	0/3089	0.48	0/4168
5	E	0.20	0/3145	0.49	1/4233 (0.0%)
6	F	0.19	0/3292	0.43	0/4435
7	G	0.18	0/1923	0.38	0/2601
7	g	0.18	0/1914	0.45	2/2590 (0.1%)
8	H	0.19	0/1844	0.40	0/2499
8	h	0.17	0/1844	0.37	0/2497
9	I	0.19	0/1991	0.44	0/2685
9	i	0.17	0/1985	0.39	0/2677
10	J	0.19	0/1906	0.41	0/2573
10	j	0.17	0/1887	0.39	0/2549
11	K	0.19	0/1804	0.37	0/2436
11	k	0.16	0/1809	0.36	0/2444
12	L	0.18	0/1901	0.36	0/2570
12	l	0.17	0/1896	0.37	0/2565
13	M	0.17	0/1911	0.35	0/2573
13	m	0.17	0/1916	0.33	0/2580
14	N	0.17	0/1540	0.32	0/2085
14	n	0.17	0/1536	0.32	0/2080
15	O	0.18	0/1676	0.39	0/2271
15	o	0.17	0/1686	0.34	0/2282
16	P	0.18	0/1616	0.41	0/2180
16	p	0.18	0/1620	0.38	0/2184
17	Q	0.17	0/1621	0.35	0/2194
17	q	0.17	0/1621	0.36	0/2194
18	R	0.17	0/1590	0.34	0/2147
18	r	0.18	0/1590	0.33	0/2147
19	S	0.19	0/1671	0.42	2/2252 (0.1%)
19	s	0.19	0/1684	0.40	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.18	0/1716	0.35	0/2323
20	t	0.18	0/1720	0.36	0/2328
21	U	0.21	0/6449	0.50	0/8729
22	V	0.17	0/3681	0.39	0/4969
23	W	0.23	0/3683	0.56	1/4952 (0.0%)
24	X	0.18	0/3053	0.46	0/4115
25	Y	0.22	0/3173	0.55	0/4273
26	Z	0.23	0/2324	0.53	0/3150
27	a	0.21	0/3053	0.55	1/4133 (0.0%)
28	b	0.20	0/1478	0.50	0/2001
29	c	0.24	0/2302	0.54	0/3110
30	d	0.21	0/2162	0.56	2/2919 (0.1%)
31	e	0.19	0/437	0.58	1/595 (0.2%)
32	f	0.20	0/6980	0.57	0/9433
33	u	0.21	0/607	0.44	0/816
34	v	0.03	0/8	0.06	0/8
35	x	0.13	0/599	0.31	0/805
All	All	0.19	0/108044	0.45	10/145901 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	g	223	GLU	CA-C-N	6.91	129.86	122.26
7	g	223	GLU	C-N-CA	6.91	129.86	122.26
30	d	198	LEU	CA-C-N	6.55	134.04	121.54
30	d	198	LEU	C-N-CA	6.55	134.04	121.54
5	E	244	SER	N-CA-C	-6.29	102.23	110.53
31	e	28	ALA	CB-CA-C	-6.01	109.63	116.54
23	W	96	GLN	CB-CA-C	-5.58	110.12	116.54
27	a	102	GLU	N-CA-CB	5.43	118.67	110.30
19	S	190	GLY	CA-C-N	5.35	131.77	121.54
19	S	190	GLY	C-N-CA	5.35	131.77	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3096	0	3138	55	0
2	B	3018	0	3081	55	0
3	C	2864	0	2971	50	0
4	D	3039	0	3075	51	0
5	E	3097	0	3173	45	0
6	F	3251	0	3319	53	0
7	G	1889	0	1885	12	0
7	g	1880	0	1875	16	0
8	H	1805	0	1784	13	0
8	h	1805	0	1798	14	0
9	I	1958	0	1960	14	0
9	i	1955	0	1955	9	0
10	J	1880	0	1892	11	0
10	j	1861	0	1865	16	0
11	K	1777	0	1762	14	0
11	k	1782	0	1766	9	0
12	L	1866	0	1852	14	0
12	l	1861	0	1839	14	0
13	M	1876	0	1861	19	0
13	m	1881	0	1868	13	0
14	N	1514	0	1487	3	0
14	n	1510	0	1483	4	0
15	O	1649	0	1659	5	0
15	o	1659	0	1681	12	0
16	P	1587	0	1598	10	0
16	p	1591	0	1609	16	0
17	Q	1588	0	1584	19	0
17	q	1588	0	1584	15	0
18	R	1559	0	1523	11	0
18	r	1559	0	1523	9	0
19	S	1641	0	1639	14	0
19	s	1654	0	1656	11	0
20	T	1683	0	1662	8	0
20	t	1687	0	1666	16	0
21	U	6334	0	6366	97	0
22	V	3612	0	3682	40	0
23	W	3635	0	3762	61	0
24	X	3009	0	3113	42	0
25	Y	3115	0	3120	47	0
26	Z	2281	0	2312	38	0
27	a	2995	0	3012	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	b	1458	0	1505	21	0
29	c	2260	0	2276	43	0
30	d	2116	0	2146	40	0
31	e	425	0	328	12	0
32	f	6866	0	6866	130	0
33	u	601	0	629	6	0
34	v	53	0	21	4	0
35	x	588	0	607	8	0
36	A	31	0	12	1	0
36	B	31	0	12	1	0
36	D	31	0	12	0	0
36	E	31	0	12	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0
37	D	1	0	0	0	0
37	E	1	0	0	0	0
37	F	1	0	0	0	0
38	C	27	0	12	1	0
38	F	27	0	12	0	0
39	c	1	0	0	0	0
All	All	106442	0	106890	1127	0

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

All (1127) 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)
29:c:125:VAL:HG23	34:v:25:LYS:HD3	1.57	0.86
29:c:125:VAL:CG2	34:v:25:LYS:HD3	2.11	0.79
29:c:303:MET:HE1	30:d:242:LEU:HB2	1.65	0.76
32:f:673:ARG:HB3	32:f:707:LEU:HD11	1.67	0.75
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.53	0.73
21:U:694:ILE:HG23	21:U:695:MET:HG3	1.68	0.73
24:X:82:LYS:HB3	24:X:122:ARG:HH22	1.52	0.73
23:W:312:MET:HG2	27:a:312:MET:HB3	1.73	0.71
32:f:223:GLU:O	32:f:227:ALA:HB2	1.91	0.70
30:d:4:GLN:HE22	30:d:18:LYS:HA	1.57	0.70
6:F:111:ILE:HB	29:c:51:MET:HE1	1.74	0.70
21:U:532:MET:HE3	21:U:552:ILE:HG22	1.74	0.70
32:f:253:LEU:HD23	32:f:256:PHE:HB2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:4:PRO:HB2	20:t:100:ARG:HH21	1.58	0.69
3:C:89:VAL:HG12	3:C:91:PRO:HD2	1.75	0.68
32:f:696:LEU:HG	32:f:697:ILE:HG12	1.74	0.68
2:B:402:ALA:HA	2:B:405:MET:HE3	1.75	0.67
22:V:85:ALA:HB2	22:V:93:PHE:HB2	1.76	0.67
1:A:274:PHE:HB2	1:A:319:MET:HG2	1.76	0.67
6:F:60:LEU:O	6:F:64:HIS:ND1	2.25	0.67
25:Y:220:VAL:HG11	25:Y:249:VAL:HG21	1.75	0.67
5:E:198:VAL:HG12	5:E:200:SER:H	1.59	0.67
24:X:212:MET:HE1	24:X:249:THR:HG23	1.77	0.66
21:U:328:ILE:HG13	21:U:329:LEU:HG	1.78	0.66
26:Z:17:LEU:HG	29:c:216:MET:HE1	1.77	0.66
1:A:394:MET:HG2	2:B:349:ARG:HH22	1.61	0.66
6:F:358:ASN:HD21	13:M:205:LYS:HD2	1.60	0.66
27:a:64:ILE:O	27:a:68:GLU:HB2	1.95	0.65
32:f:152:ALA:HB3	32:f:156:HIS:HB2	1.78	0.65
26:Z:144:VAL:HA	26:Z:152:SER:HB3	1.78	0.65
3:C:339:THR:HG22	25:Y:207:THR:HA	1.78	0.65
21:U:70:HIS:HD2	21:U:71:LEU:HD12	1.62	0.64
23:W:417:ARG:HE	23:W:418:PRO:HD2	1.61	0.64
25:Y:181:LYS:HG3	25:Y:204:THR:HG21	1.79	0.64
30:d:87:GLU:HA	30:d:89:LEU:HD23	1.79	0.64
32:f:761:MET:HE3	32:f:763:ARG:HB2	1.79	0.64
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.79	0.64
8:H:111:VAL:HG22	8:H:136:ILE:HD12	1.79	0.64
32:f:271:MET:SD	32:f:300:ARG:NH1	2.71	0.64
8:h:119:GLN:HG3	9:i:81:SER:HB2	1.80	0.64
2:B:58:CYS:SG	2:B:59:ARG:N	2.70	0.64
32:f:491:GLY:HA2	32:f:773:LYS:HE2	1.80	0.63
23:W:307:LYS:NZ	23:W:315:MET:SD	2.72	0.63
11:k:13:ASN:HB2	12:l:126:ARG:HD3	1.80	0.63
1:A:44:GLN:OE1	1:A:47:GLN:NE2	2.31	0.63
16:P:205:ASP:HB3	18:r:192:VAL:HG11	1.81	0.63
29:c:288:VAL:HG12	29:c:292:MET:HE2	1.80	0.63
10:J:96:LEU:HD11	17:Q:58:GLU:HB3	1.79	0.63
32:f:107:LYS:HA	32:f:111:GLU:HB2	1.80	0.63
4:D:67:ASN:ND2	21:U:607:VAL:O	2.31	0.63
24:X:255:LEU:HD22	24:X:267:VAL:HG13	1.81	0.62
19:S:159:GLN:NE2	15:o:207:GLY:O	2.33	0.62
28:b:51:LEU:HD23	28:b:71:ILE:HG23	1.80	0.62
32:f:415:GLY:HA3	32:f:447:ALA:HB1	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:605:ASN:HD21	32:f:639:LYS:HD2	1.63	0.62
3:C:273:MET:HE2	3:C:293:MET:HG3	1.81	0.62
6:F:85:THR:HG22	6:F:87:PRO:HD2	1.81	0.62
24:X:74:ARG:HH22	24:X:116:TRP:HB2	1.63	0.62
12:L:157:ARG:NH2	13:M:60:GLU:OE1	2.32	0.62
19:S:148:LEU:HD23	19:S:178:VAL:HG12	1.81	0.62
23:W:90:LEU:O	23:W:96:GLN:NE2	2.33	0.62
7:G:158:GLY:O	8:H:84:ARG:NH2	2.33	0.62
27:a:341:LEU:HD13	27:a:345:GLN:HB2	1.80	0.61
24:X:365:LEU:HA	24:X:368:MET:HG2	1.82	0.61
31:e:54:ASN:OD1	31:e:57:ARG:NH2	2.33	0.61
26:Z:208:ILE:HG23	27:a:353:LEU:HD21	1.81	0.61
4:D:391:ARG:HG3	23:W:136:ILE:HD11	1.83	0.61
22:V:124:ASN:HA	22:V:128:ARG:HD3	1.83	0.61
32:f:275:MET:SD	32:f:286:LYS:NZ	2.73	0.61
4:D:353:ASN:ND2	4:D:392:TYR:O	2.34	0.61
30:d:78:LEU:HD13	30:d:98:LEU:HD21	1.83	0.61
23:W:80:TRP:HB3	23:W:123:ARG:HE	1.65	0.61
27:a:77:VAL:HA	27:a:80:ILE:HG22	1.83	0.61
5:E:265:ASP:OD2	5:E:291:ARG:NH2	2.33	0.60
18:R:147:LEU:HD12	18:R:151:GLN:HB3	1.83	0.60
22:V:78:HIS:NE2	22:V:100:MET:SD	2.73	0.60
25:Y:43:ALA:O	25:Y:49:ASN:ND2	2.34	0.60
32:f:371:ASN:ND2	32:f:401:LYS:O	2.34	0.60
21:U:609:ASP:O	21:U:615:ARG:NH1	2.33	0.60
4:D:349:THR:HB	4:D:354:LEU:HD11	1.84	0.60
4:D:244:PRO:HB3	4:D:291:GLU:HG3	1.83	0.60
21:U:12:LEU:HD11	21:U:27:LEU:HD11	1.83	0.60
21:U:100:ILE:HA	21:U:103:LYS:HE2	1.84	0.60
27:a:135:ILE:HG12	27:a:158:LEU:HD13	1.84	0.60
32:f:111:GLU:OE2	32:f:137:ARG:NH1	2.31	0.60
4:D:153:MET:HG2	4:D:227:PHE:HB3	1.84	0.60
25:Y:292:TYR:OH	31:e:51:ASP:OD1	2.20	0.60
27:a:54:ASP:HB3	27:a:86:GLN:HG3	1.84	0.59
15:o:55:THR:HG23	15:o:86:MET:HE1	1.84	0.59
23:W:401:THR:HG23	23:W:402:ILE:HD12	1.84	0.59
21:U:599:ILE:HD13	21:U:625:ILE:HD11	1.84	0.59
12:l:120:THR:O	13:m:129:ARG:NH1	2.36	0.59
6:F:197:GLU:OE1	6:F:350:ARG:NH2	2.34	0.59
1:A:390:THR:HA	2:B:216:ILE:HD11	1.85	0.59
30:d:182:ILE:HD12	30:d:186:TYR:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:52:GLU:OE2	21:U:596:ASN:ND2	2.33	0.59
6:F:224:LEU:HB2	6:F:348:LEU:HD23	1.84	0.59
27:a:192:GLU:OE2	27:a:196:ARG:NH1	2.36	0.59
1:A:252:GLU:OE1	1:A:255:ARG:NH1	2.36	0.59
2:B:401:GLU:OE2	2:B:425:ASN:ND2	2.35	0.59
6:F:318:ASP:OD2	6:F:344:ARG:NH2	2.36	0.59
3:C:325:ARG:HD3	3:C:353:GLY:HA2	1.84	0.58
21:U:171:ASN:HD21	21:U:176:MET:HE3	1.66	0.58
25:Y:187:TYR:HE2	25:Y:196:GLN:HB3	1.68	0.58
25:Y:298:GLU:O	25:Y:302:HIS:ND1	2.36	0.58
30:d:60:GLN:NE2	30:d:94:TYR:OH	2.37	0.58
1:A:213:LEU:HD22	1:A:337:LEU:HD23	1.84	0.58
23:W:169:LEU:O	23:W:182:ARG:NH2	2.34	0.58
4:D:267:ILE:HD11	4:D:309:MET:HB3	1.85	0.58
11:K:20:ARG:NH1	11:K:25:GLU:OE1	2.36	0.58
27:a:188:LEU:O	27:a:193:GLN:NE2	2.35	0.58
24:X:120:GLU:OE2	24:X:122:ARG:NH2	2.37	0.58
27:a:89:ASP:O	27:a:93:ALA:HB2	2.03	0.58
32:f:254:GLY:N	32:f:285:CYS:SG	2.77	0.58
7:g:158:GLY:O	8:h:84:ARG:NH2	2.37	0.58
19:s:10:GLY:HA3	19:s:42:LYS:HE2	1.86	0.58
21:U:213:PHE:HA	21:U:216:VAL:HG12	1.85	0.58
25:Y:101:ARG:HB3	25:Y:105:MET:HE1	1.85	0.58
4:D:342:ARG:NH1	24:X:202:CYS:SG	2.77	0.57
21:U:19:LEU:HD13	30:d:23:LEU:HD11	1.85	0.57
21:U:611:ASN:HB3	21:U:614:VAL:HG12	1.86	0.57
32:f:759:LEU:HD23	32:f:761:MET:HB2	1.86	0.57
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.86	0.57
20:t:25:ASP:OD1	20:t:41:ARG:NH2	2.37	0.57
34:v:24:UNK:O	34:v:25:LYS:HB2	2.04	0.57
10:J:50:VAL:HB	10:J:54:GLN:HB2	1.85	0.57
30:d:99:LEU:HB3	30:d:133:ILE:HD11	1.85	0.57
21:U:361:ARG:HH21	21:U:727:LYS:HZ3	1.52	0.57
6:F:153:VAL:HG22	6:F:160:ILE:HG22	1.85	0.57
32:f:748:LEU:O	32:f:752:HIS:ND1	2.38	0.57
13:m:34:SER:OG	13:m:65:ARG:NH1	2.33	0.57
4:D:116:LEU:HD23	4:D:118:THR:H	1.68	0.57
23:W:274:VAL:O	23:W:283:GLN:NE2	2.38	0.57
21:U:660:CYS:HB2	21:U:694:ILE:HD11	1.86	0.57
32:f:486:GLY:HA2	32:f:525:ILE:HD11	1.86	0.57
1:A:156:LYS:HE3	2:B:114:GLU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:GLU:OE2	3:C:232:ARG:NH2	2.38	0.57
1:A:284:ARG:O	6:F:334:ARG:NH1	2.38	0.56
2:B:75:GLU:HB2	32:f:654:VAL:HG22	1.86	0.56
27:a:252:LYS:HA	27:a:255:TRP:HE3	1.69	0.56
3:C:332:HIS:O	3:C:335:LYS:NZ	2.39	0.56
21:U:213:PHE:HB3	21:U:248:ILE:HD13	1.86	0.56
21:U:619:VAL:HG23	21:U:651:GLY:HA3	1.85	0.56
23:W:51:GLU:OE2	23:W:94:ARG:NH2	2.37	0.56
18:r:1:THR:HA	18:r:33:LYS:HZ3	1.70	0.56
20:t:37:ARG:O	20:t:186:ARG:NH1	2.37	0.56
21:U:469:SER:OG	21:U:470:ASN:N	2.38	0.56
25:Y:204:THR:HG23	25:Y:208:PHE:HB3	1.87	0.56
1:A:356:LYS:O	1:A:360:ARG:HB3	2.06	0.56
3:C:343:ASN:HB3	3:C:346:LYS:HB3	1.86	0.56
11:K:91:LYS:HG2	11:K:119:LEU:HD11	1.87	0.56
21:U:770:TRP:O	29:c:177:THR:OG1	2.22	0.56
23:W:312:MET:HB2	27:a:316:SER:HB3	1.88	0.56
7:g:231:THR:OG1	7:g:234:GLU:OE1	2.21	0.56
20:t:54:SER:O	20:t:108:ASN:ND2	2.32	0.56
4:D:77:GLU:OE2	26:Z:177:ARG:NH2	2.38	0.56
5:E:180:LYS:HG2	5:E:301:ILE:HD12	1.86	0.56
19:S:209:SER:OG	19:S:212:LYS:NZ	2.36	0.56
24:X:332:GLU:HB2	24:X:368:MET:HE1	1.87	0.56
29:c:79:GLY:HA3	29:c:84:VAL:HA	1.87	0.56
30:d:29:VAL:HG13	30:d:47:GLN:HB3	1.87	0.56
22:V:177:ASN:O	22:V:179:LYS:NZ	2.39	0.56
25:Y:127:THR:HA	25:Y:130:LYS:HB3	1.88	0.56
32:f:688:ARG:O	32:f:692:LEU:HB2	2.06	0.56
32:f:713:PHE:HB2	32:f:752:HIS:HE1	1.70	0.56
21:U:588:MET:HE1	21:U:764:LEU:HD22	1.88	0.56
2:B:387:LYS:HB3	2:B:390:LEU:HD23	1.87	0.56
13:M:34:SER:OG	13:M:65:ARG:NH1	2.37	0.56
25:Y:176:ARG:HA	25:Y:179:ARG:HB3	1.88	0.56
36:A:501:ATP:O3G	2:B:346:ARG:NH2	2.39	0.55
11:K:52:LYS:NZ	11:K:64:ILE:O	2.39	0.55
1:A:139:ARG:NH1	1:A:154:PRO:O	2.39	0.55
23:W:81:ASP:OD1	23:W:123:ARG:NH2	2.39	0.55
29:c:187:PRO:HB3	29:c:196:LEU:HD12	1.88	0.55
30:d:164:THR:HA	30:d:167:ILE:HG12	1.87	0.55
6:F:282:ILE:HG22	6:F:327:LYS:HB2	1.87	0.55
27:a:247:ARG:HH12	27:a:269:LEU:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:58:ALA:O	22:V:62:HIS:ND1	2.40	0.55
32:f:19:ALA:O	32:f:34:ARG:NH1	2.40	0.55
4:D:284:GLU:OE1	4:D:287:ARG:NH2	2.39	0.55
4:D:320:ALA:O	4:D:326:ARG:NH1	2.39	0.55
23:W:328:LEU:HD11	23:W:351:TRP:HZ2	1.71	0.55
15:o:143:ARG:NH2	15:o:150:GLU:OE1	2.39	0.55
3:C:113:ARG:NH2	3:C:129:ASN:O	2.38	0.55
18:R:64:ARG:NH1	18:R:67:GLU:OE2	2.40	0.54
21:U:770:TRP:CD1	29:c:178:THR:HG1	2.25	0.54
24:X:257:CYS:HA	24:X:260:MET:HE2	1.90	0.54
32:f:625:LYS:NZ	32:f:626:GLU:O	2.40	0.54
9:i:234:GLU:HA	9:i:237:ILE:HG12	1.89	0.54
19:s:145:LEU:HD22	19:s:178:VAL:HB	1.89	0.54
27:a:363:MET:HE3	29:c:307:VAL:HG11	1.89	0.54
32:f:434:TYR:OH	35:x:43:ARG:NH1	2.40	0.54
32:f:625:LYS:O	32:f:629:LYS:NZ	2.40	0.54
32:f:733:GLY:H	32:f:737:ASN:HB3	1.72	0.54
13:m:8:ASP:O	13:m:22:GLN:NE2	2.39	0.54
1:A:306:LEU:O	1:A:312:ARG:NH1	2.40	0.54
6:F:252:ALA:HB3	6:F:255:GLN:HB2	1.89	0.54
10:J:90:GLU:HG3	10:J:110:TYR:CZ	2.42	0.54
18:R:166:ARG:NH1	16:p:34:MET:O	2.40	0.54
25:Y:32:ARG:NH1	25:Y:34:ASP:OD1	2.40	0.54
32:f:202:HIS:O	32:f:206:ASP:HB2	2.07	0.54
8:H:143:ARG:NH1	8:H:144:PRO:O	2.39	0.54
23:W:121:LYS:HE3	23:W:154:GLU:HG2	1.89	0.54
32:f:367:SER:OG	32:f:740:ARG:NH2	2.39	0.54
32:f:512:MET:HE1	32:f:554:TYR:HD2	1.72	0.54
5:E:253:ILE:HG13	6:F:308:ARG:HH22	1.71	0.54
20:T:25:ASP:OD1	20:T:41:ARG:NH2	2.34	0.54
22:V:461:LYS:NZ	22:V:462:GLU:O	2.41	0.54
22:V:150:ARG:NH1	22:V:157:THR:O	2.41	0.54
24:X:297:ARG:O	24:X:334:ASN:ND2	2.41	0.54
32:f:244:GLU:HA	32:f:248:LEU:HD13	1.90	0.54
23:W:221:LYS:HD3	23:W:225:LYS:HD3	1.88	0.54
11:k:52:LYS:NZ	11:k:64:ILE:O	2.40	0.54
12:L:49:LEU:HB2	12:L:195:LEU:HD21	1.90	0.54
32:f:635:LYS:HZ2	32:f:778:LEU:HB3	1.72	0.54
17:q:168:GLN:NE2	17:q:175:LEU:O	2.40	0.54
4:D:354:LEU:HD22	4:D:358:VAL:HG11	1.90	0.53
11:K:41:GLN:NE2	11:K:151:PRO:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:215:ILE:HA	5:E:218:MET:HG2	1.90	0.53
21:U:522:GLY:O	21:U:559:ARG:NH2	2.40	0.53
26:Z:124:ILE:HG22	26:Z:135:THR:HA	1.90	0.53
17:Q:144:ASP:OD2	18:r:166:ARG:NH2	2.41	0.53
26:Z:127:LYS:HG2	29:c:212:LEU:HD11	1.90	0.53
32:f:343:LYS:NZ	32:f:387:GLN:O	2.40	0.53
32:f:828:ARG:NE	32:f:863:THR:OG1	2.35	0.53
16:p:159:ASP:OD1	16:p:159:ASP:N	2.40	0.53
1:A:324:PRO:HA	1:A:327:LEU:HD13	1.91	0.53
4:D:266:GLU:HG3	5:E:258:MET:HB3	1.89	0.53
5:E:86:GLN:OE1	26:Z:88:ARG:NH2	2.41	0.53
24:X:357:SER:OG	24:X:358:LYS:N	2.41	0.53
24:X:394:ASP:N	24:X:394:ASP:OD1	2.42	0.53
32:f:186:THR:HA	32:f:189:LYS:HB3	1.89	0.53
18:r:64:ARG:NH1	18:r:67:GLU:OE1	2.41	0.53
1:A:364:VAL:HG12	1:A:404:ALA:HB3	1.90	0.53
2:B:424:GLU:HA	2:B:428:TYR:HD2	1.73	0.53
19:S:92:LEU:HD23	19:S:124:PHE:HE2	1.73	0.53
25:Y:223:THR:HA	25:Y:226:VAL:HG12	1.91	0.53
7:g:21:ARG:NH2	7:g:23:TYR:OH	2.42	0.53
1:A:351:ARG:NH1	1:A:378:PRO:O	2.42	0.53
14:N:84:LYS:HD3	14:N:120:MET:HB2	1.91	0.53
21:U:242:LEU:HA	21:U:245:ALA:HB3	1.89	0.53
23:W:346:GLU:OE2	23:W:350:ARG:NE	2.40	0.53
25:Y:205:VAL:HG21	25:Y:223:THR:HG21	1.90	0.53
25:Y:237:ARG:O	25:Y:241:ILE:HB	2.07	0.53
28:b:1:MET:N	28:b:43:SER:O	2.38	0.53
32:f:428:GLN:HA	32:f:431:LYS:HE3	1.90	0.53
3:C:20:LEU:HD11	21:U:153:ILE:HG13	1.91	0.53
21:U:900:TYR:HB3	21:U:914:LEU:HG	1.90	0.53
25:Y:124:PHE:HA	25:Y:127:THR:HG22	1.90	0.53
29:c:270:LEU:O	29:c:274:ASN:ND2	2.42	0.53
32:f:180:GLN:NE2	32:f:834:ASP:O	2.41	0.53
17:q:39:SER:OG	17:q:40:GLU:N	2.40	0.53
20:t:96:MET:HE3	20:t:127:MET:HA	1.89	0.53
2:B:252:GLY:HA2	2:B:255:LEU:HD23	1.91	0.53
3:C:164:VAL:HG12	3:C:165:ILE:HG13	1.90	0.53
21:U:596:ASN:HA	21:U:599:ILE:HG22	1.91	0.53
22:V:121:PHE:O	22:V:128:ARG:NH1	2.41	0.53
23:W:340:VAL:HG13	23:W:350:ARG:HD2	1.90	0.53
32:f:482:ILE:HD12	32:f:518:THR:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:MET:HE1	32:f:610:GLN:HB2	1.91	0.53
32:f:695:ALA:HA	32:f:698:SER:HB2	1.90	0.53
35:x:48:VAL:HG11	35:x:61:ILE:HG21	1.90	0.53
26:Z:62:ASP:N	26:Z:62:ASP:OD1	2.40	0.53
6:F:137:ILE:HD13	6:F:142:ALA:HB2	1.91	0.52
13:M:108:LEU:HD11	13:M:137:LEU:HB3	1.91	0.52
27:a:54:ASP:N	27:a:54:ASP:OD1	2.42	0.52
16:p:65:GLN:OE1	17:q:86:ARG:NH2	2.42	0.52
30:d:152:PHE:HA	30:d:155:LYS:HB2	1.91	0.52
5:E:102:MET:HE2	6:F:132:TYR:HE2	1.75	0.52
32:f:57:GLU:HG3	32:f:96:LEU:HD21	1.92	0.52
1:A:55:LEU:HD11	2:B:76:GLU:HG2	1.90	0.52
24:X:221:GLU:O	24:X:223:LYS:NZ	2.41	0.52
9:i:53:HIS:HB3	9:i:56:LEU:HD23	1.91	0.52
16:p:58:THR:O	17:q:85:ARG:NH2	2.42	0.52
1:A:69:ASP:HB2	1:A:72:LEU:H	1.74	0.52
22:V:119:GLY:HA2	22:V:148:ARG:HD3	1.92	0.52
26:Z:78:MET:HG2	29:c:98:MET:HE3	1.92	0.52
28:b:25:ARG:NH1	28:b:114:GLY:O	2.42	0.52
32:f:416:MET:HB3	32:f:450:ILE:HG21	1.91	0.52
24:X:377:ILE:HG12	25:Y:312:ARG:HB3	1.92	0.52
25:Y:56:ALA:HB1	25:Y:60:SER:HB3	1.92	0.52
25:Y:68:ASP:OD1	25:Y:68:ASP:N	2.42	0.52
32:f:45:LEU:HD23	32:f:56:LEU:HB3	1.91	0.52
32:f:790:GLN:HG3	32:f:791:VAL:HG23	1.91	0.52
10:J:116:GLN:NE2	11:K:84:ASP:OD1	2.42	0.52
32:f:94:LYS:HG3	32:f:95:PRO:HD3	1.92	0.52
10:j:31:THR:OG1	10:j:163:ARG:O	2.27	0.52
13:m:230:ASP:OD1	13:m:230:ASP:N	2.42	0.52
2:B:339:PRO:HA	2:B:342:ILE:HG12	1.92	0.52
7:G:120:ASP:OD1	8:H:84:ARG:NH1	2.43	0.52
13:M:230:ASP:N	13:M:230:ASP:OD1	2.42	0.52
4:D:389:GLU:OE1	4:D:391:ARG:NH2	2.43	0.52
5:E:269:THR:O	5:E:271:HIS:ND1	2.43	0.52
6:F:111:ILE:HG12	6:F:113:LEU:H	1.75	0.52
21:U:333:MET:SD	21:U:333:MET:N	2.73	0.52
11:k:41:GLN:NE2	11:k:151:PRO:O	2.43	0.52
15:o:1:THR:N	15:o:168:GLY:O	2.43	0.52
19:s:166:LEU:HD21	19:s:171:ALA:HB2	1.92	0.52
21:U:360:VAL:O	21:U:362:ASN:ND2	2.43	0.52
23:W:25:ASP:OD1	23:W:65:ARG:NH2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:273:TYR:HB2	23:W:276:LEU:HB2	1.92	0.52
25:Y:148:GLY:HA3	25:Y:157:ILE:HG21	1.91	0.52
27:a:126:GLY:HA3	27:a:129:GLN:HE22	1.75	0.52
27:a:249:GLN:HA	27:a:252:LYS:HB2	1.92	0.52
27:a:280:MET:HE3	27:a:299:SER:HB3	1.93	0.52
29:c:89:PRO:HG2	33:u:44:ILE:HD11	1.92	0.52
19:s:27:THR:HB	19:s:40:SER:H	1.73	0.52
4:D:338:ARG:NH2	4:D:361:GLU:OE2	2.43	0.51
4:D:392:TYR:OH	23:W:144:ARG:NH1	2.43	0.51
21:U:24:LEU:HD13	21:U:59:PHE:HB3	1.91	0.51
23:W:431:LYS:NZ	26:Z:236:LEU:O	2.43	0.51
32:f:333:LEU:HD13	32:f:810:ILE:HD12	1.92	0.51
1:A:189:GLU:OE2	6:F:409:ARG:NH2	2.42	0.51
4:D:374:ASP:N	4:D:374:ASP:OD1	2.43	0.51
19:S:125:ASP:OD1	19:S:129:SER:N	2.43	0.51
22:V:131:LEU:HD22	22:V:171:VAL:HG11	1.92	0.51
25:Y:275:LEU:HD11	25:Y:299:MET:HB3	1.91	0.51
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	1.90	0.51
18:r:125:THR:HB	18:r:139:MET:HE3	1.91	0.51
5:E:140:GLU:OE1	5:E:143:ARG:NH2	2.44	0.51
17:Q:83:PHE:O	17:Q:87:ASN:ND2	2.41	0.51
8:h:143:ARG:NH1	8:h:144:PRO:O	2.44	0.51
2:B:373:THR:OG1	2:B:412:MET:O	2.27	0.51
32:f:173:LEU:HD23	32:f:174:ASP:HB2	1.92	0.51
7:g:165:ALA:HB1	7:g:179:LEU:HD13	1.93	0.51
1:A:399:ALA:O	1:A:400:ARG:NE	2.34	0.51
3:C:130:LYS:HG3	3:C:131:VAL:H	1.76	0.51
4:D:233:SER:OG	5:E:259:GLU:OE1	2.28	0.51
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.92	0.51
22:V:419:LEU:HD12	22:V:456:GLY:HA2	1.92	0.51
24:X:298:SER:HA	24:X:334:ASN:HD21	1.75	0.51
32:f:821:LEU:HD11	32:f:869:THR:HG21	1.92	0.51
1:A:119:ALA:HB2	6:F:128:THR:HG23	1.92	0.51
3:C:83:LYS:HD2	3:C:105:ILE:HD11	1.93	0.51
3:C:113:ARG:NH1	4:D:94:GLU:OE2	2.44	0.51
5:E:115:VAL:HG23	6:F:95:GLU:HG3	1.91	0.51
25:Y:71:ASN:HA	25:Y:74:LYS:HG2	1.93	0.51
32:f:637:LYS:HB3	32:f:678:LEU:HD13	1.92	0.51
32:f:828:ARG:HH22	32:f:842:VAL:H	1.59	0.51
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.91	0.51
10:j:148:ASP:OD1	10:j:152:THR:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:THR:OG1	2:B:126:SER:N	2.44	0.51
3:C:239:ARG:NH2	3:C:284:GLU:OE2	2.44	0.51
3:C:372:ARG:NH1	4:D:179:GLU:OE2	2.43	0.51
6:F:336:ASP:OD1	6:F:336:ASP:N	2.43	0.51
16:P:193:ASP:OD1	16:P:193:ASP:N	2.42	0.51
17:Q:137:PHE:HB3	18:r:133:VAL:HG21	1.93	0.51
21:U:804:SER:OG	21:U:805:ASN:N	2.43	0.51
32:f:103:TYR:O	32:f:141:LYS:NZ	2.43	0.51
3:C:163:GLU:HA	3:C:167:LEU:HD13	1.93	0.51
21:U:94:SER:OG	21:U:95:GLU:N	2.44	0.51
22:V:495:ARG:O	26:Z:278:ASN:ND2	2.39	0.51
7:g:147:GLN:OE1	7:g:150:GLN:NE2	2.44	0.51
24:X:281:GLY:H	24:X:284:THR:HG22	1.76	0.51
32:f:320:ILE:O	32:f:325:GLN:NE2	2.44	0.51
32:f:634:LYS:HA	32:f:674:THR:HB	1.92	0.51
7:g:103:TYR:O	15:o:81:ARG:NH2	2.44	0.51
18:r:38:ASN:HD21	18:r:41:LEU:HD12	1.76	0.51
8:H:222:THR:OG1	8:H:225:GLU:OE1	2.21	0.50
22:V:343:PRO:O	31:e:43:TRP:NE1	2.44	0.50
22:V:345:ARG:HH21	31:e:43:TRP:HA	1.75	0.50
13:m:93:GLU:OE2	13:m:97:ASN:ND2	2.44	0.50
5:E:44:GLU:OE2	6:F:76:ASN:ND2	2.43	0.50
10:J:38:ARG:NH2	10:J:178:ASP:O	2.43	0.50
32:f:419:LEU:HD11	32:f:804:LEU:HD21	1.93	0.50
32:f:808:ASN:HB2	32:f:810:ILE:HG12	1.93	0.50
4:D:120:ASP:N	4:D:120:ASP:OD1	2.43	0.50
13:M:51:LYS:NZ	13:M:62:SER:O	2.43	0.50
26:Z:19:VAL:HG11	26:Z:124:ILE:HD11	1.93	0.50
32:f:121:PHE:HD1	32:f:129:LEU:HD13	1.77	0.50
3:C:147:THR:HG23	3:C:149:GLU:H	1.76	0.50
6:F:317:LEU:HD13	6:F:328:VAL:HG21	1.92	0.50
23:W:166:LEU:HA	23:W:169:LEU:HG	1.93	0.50
27:a:61:GLU:HG3	27:a:83:VAL:HG21	1.94	0.50
6:F:318:ASP:HB3	6:F:347:ARG:HG2	1.92	0.50
7:G:112:ASP:N	7:G:112:ASP:OD1	2.44	0.50
23:W:371:THR:HG22	23:W:372:ARG:HG3	1.93	0.50
32:f:400:TYR:HA	32:f:407:MET:HE1	1.92	0.50
7:g:180:GLU:HG2	8:h:55:ILE:HG22	1.93	0.50
25:Y:47:ASP:OD2	25:Y:113:ARG:NH2	2.44	0.50
1:A:73:ALA:HB2	2:B:140:ASP:H	1.77	0.50
26:Z:25:ARG:HB2	29:c:104:ARG:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:194:ALA:HA	30:d:198:LEU:HG	1.92	0.50
9:i:3:ARG:NH2	11:k:125:GLU:OE2	2.43	0.50
6:F:38:THR:HG22	6:F:39:GLU:HG2	1.94	0.50
32:f:80:ARG:HH12	32:f:113:MET:HE1	1.76	0.50
33:u:1:MET:HE1	33:u:63:LYS:HA	1.94	0.50
3:C:246:ILE:HB	3:C:291:VAL:HG12	1.93	0.50
7:G:181:LYS:HA	7:G:184:LYS:HE3	1.94	0.50
8:h:79:MET:H	8:h:132:VAL:HG12	1.77	0.50
15:o:216:ILE:HD11	16:p:194:LYS:HD2	1.93	0.50
35:x:49:LYS:HD2	35:x:67:MET:HG3	1.92	0.50
2:B:196:GLU:OE2	2:B:349:ARG:NH1	2.43	0.49
18:R:80:SER:OG	18:R:120:ARG:NH1	2.42	0.49
24:X:222:GLU:HA	24:X:225:TRP:HE1	1.76	0.49
24:X:408:SER:HB3	25:Y:376:LEU:HD11	1.92	0.49
30:d:27:LYS:O	30:d:31:LEU:HB2	2.12	0.49
3:C:241:HIS:O	3:C:244:SER:OG	2.29	0.49
7:G:46:ASP:OD1	7:G:46:ASP:N	2.45	0.49
13:M:17:ASP:OD1	13:M:17:ASP:N	2.45	0.49
16:P:159:ASP:OD1	16:P:159:ASP:N	2.44	0.49
21:U:388:ASP:OD1	21:U:388:ASP:N	2.44	0.49
22:V:477:HIS:ND1	30:d:249:TYR:OH	2.43	0.49
31:e:37:HIS:HD2	31:e:39:TRP:HB2	1.77	0.49
20:t:59:ASP:HB3	20:t:106:LEU:HD22	1.94	0.49
3:C:151:ILE:HG21	3:C:158:ILE:HD11	1.93	0.49
3:C:184:LYS:HA	3:C:290:LYS:HG3	1.94	0.49
6:F:289:ASP:OD1	6:F:289:ASP:N	2.45	0.49
19:S:172:MET:HE3	19:S:176:LYS:HE3	1.93	0.49
22:V:212:TYR:HA	22:V:253:LEU:HD11	1.94	0.49
23:W:140:ILE:HG23	23:W:143:ALA:HB3	1.94	0.49
26:Z:192:THR:O	26:Z:196:HIS:ND1	2.38	0.49
28:b:4:GLU:HA	28:b:106:LYS:H	1.77	0.49
32:f:318:THR:HA	32:f:321:MET:HE2	1.92	0.49
32:f:633:GLU:OE2	32:f:673:ARG:NH1	2.45	0.49
16:p:34:MET:HG3	16:p:183:MET:HE2	1.94	0.49
1:A:113:ILE:HG22	1:A:121:PHE:H	1.77	0.49
6:F:97:LEU:N	6:F:121:CYS:O	2.41	0.49
26:Z:35:VAL:H	26:Z:97:THR:HG22	1.77	0.49
28:b:20:ASP:OD1	28:b:20:ASP:N	2.43	0.49
32:f:872:VAL:HG23	32:f:873:LEU:HD23	1.93	0.49
10:j:185:ASP:OD1	10:j:185:ASP:N	2.45	0.49
21:U:742:HIS:CE1	21:U:814:PRO:HG3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:804:SER:HA	21:U:892:LEU:HA	1.93	0.49
23:W:296:LEU:HB3	23:W:302:TYR:HB2	1.95	0.49
27:a:34:TRP:HB3	27:a:71:VAL:HG22	1.94	0.49
27:a:222:LEU:HA	27:a:225:LEU:HD12	1.93	0.49
4:D:267:ILE:HD12	4:D:267:ILE:H	1.78	0.49
15:O:148:GLU:OE2	15:O:182:LYS:NZ	2.46	0.49
20:T:63:LEU:HD21	20:T:106:LEU:HD13	1.93	0.49
21:U:16:GLU:OE1	21:U:18:GLN:NE2	2.39	0.49
33:u:23:ILE:HB	33:u:52:ASP:HA	1.94	0.49
24:X:370:LEU:O	24:X:372:LYS:NZ	2.45	0.49
1:A:113:ILE:HD11	1:A:142:VAL:HG21	1.95	0.49
5:E:29:LEU:HD13	6:F:62:VAL:HG11	1.95	0.49
7:G:67:THR:HG22	7:G:69:LEU:H	1.77	0.49
21:U:792:ASN:OD1	21:U:793:LYS:N	2.46	0.49
27:a:4:VAL:HG23	27:a:7:PHE:H	1.76	0.49
28:b:161:ASN:ND2	28:b:168:SER:O	2.45	0.49
6:F:41:ILE:HB	6:F:42:ILE:HD12	1.94	0.49
27:a:64:ILE:O	27:a:68:GLU:CB	2.61	0.49
27:a:245:VAL:HG11	27:a:301:LYS:HD3	1.95	0.49
29:c:96:LEU:HD12	33:u:8:LEU:HD22	1.93	0.49
29:c:111:TRP:HB3	29:c:133:PHE:HE2	1.77	0.49
32:f:686:LEU:HD12	32:f:687:ARG:HG3	1.94	0.49
9:I:119:GLN:NE2	10:J:79:ASP:OD1	2.44	0.49
12:L:47:VAL:HG12	12:L:195:LEU:HD22	1.94	0.49
19:S:145:LEU:HD21	19:S:182:ALA:HB2	1.95	0.49
21:U:725:MET:HE2	29:c:181:LEU:HD22	1.95	0.49
23:W:88:MET:SD	23:W:129:ARG:NH2	2.84	0.49
15:o:63:LEU:HD11	15:o:79:ALA:HB2	1.93	0.49
19:s:48:ASP:OD1	19:s:48:ASP:N	2.46	0.49
1:A:278:ASP:N	1:A:278:ASP:OD1	2.43	0.48
3:C:53:ASN:ND2	21:U:642:GLU:O	2.45	0.48
4:D:125:LYS:HB2	4:D:128:ALA:HB2	1.95	0.48
4:D:276:ASP:N	4:D:282:ASP:OD2	2.46	0.48
22:V:259:LEU:HD11	22:V:294:ARG:HD3	1.95	0.48
22:V:306:ARG:NH2	22:V:336:GLU:OE2	2.45	0.48
24:X:394:ASP:HB2	25:Y:365:GLN:HE22	1.78	0.48
26:Z:94:TRP:HB3	26:Z:112:MET:HE3	1.95	0.48
27:a:363:MET:HE1	30:d:240:THR:HG22	1.95	0.48
32:f:773:LYS:HA	32:f:776:LEU:HD12	1.94	0.48
32:f:830:LEU:HA	32:f:842:VAL:HG12	1.93	0.48
12:l:42:THR:HA	12:l:217:LYS:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:456:ASP:N	21:U:456:ASP:OD1	2.44	0.48
28:b:112:PHE:HE1	28:b:141:ILE:HD12	1.77	0.48
32:f:372:LEU:HD11	32:f:409:SER:HB2	1.94	0.48
32:f:404:ASP:OD1	32:f:404:ASP:N	2.43	0.48
19:s:125:ASP:OD1	19:s:129:SER:N	2.46	0.48
3:C:28:ILE:HB	4:D:44:TYR:HE1	1.78	0.48
11:K:146:VAL:HG11	11:K:222:PRO:HA	1.93	0.48
23:W:309:PHE:N	23:W:313:GLU:OE2	2.47	0.48
29:c:63:ASP:OD1	29:c:66:THR:OG1	2.27	0.48
32:f:813:LYS:NZ	32:f:852:VAL:O	2.39	0.48
10:j:226:GLU:HA	10:j:229:VAL:HG12	1.96	0.48
16:p:125:ASP:OD1	16:p:129:CYS:N	2.37	0.48
20:t:166:ARG:NH2	20:t:200:GLU:OE1	2.39	0.48
11:K:240:ASP:N	11:K:240:ASP:OD1	2.44	0.48
12:L:122:ARG:HB2	12:L:125:ARG:HG3	1.95	0.48
20:T:126:ASP:OD1	20:T:130:VAL:N	2.44	0.48
23:W:287:VAL:HA	23:W:290:ILE:HG12	1.95	0.48
27:a:321:LYS:O	27:a:334:THR:OG1	2.29	0.48
32:f:403:LYS:HG3	32:f:406:GLY:H	1.78	0.48
1:A:402:LYS:NZ	2:B:213:GLU:OE2	2.43	0.48
5:E:84:ARG:HB2	5:E:87:LEU:HD23	1.94	0.48
5:E:235:ILE:HG22	5:E:279:THR:HB	1.95	0.48
21:U:628:ARG:NE	21:U:749:GLN:OE1	2.46	0.48
22:V:230:PHE:HD2	22:V:231:LEU:HD12	1.77	0.48
24:X:414:LEU:HD22	26:Z:276:ILE:HD11	1.95	0.48
26:Z:215:VAL:HA	26:Z:220:LEU:HB2	1.93	0.48
13:m:215:TRP:CD1	13:m:227:VAL:HG22	2.48	0.48
1:A:429:TYR:HE2	2:B:340:ALA:HB2	1.78	0.48
2:B:67:ARG:HB3	32:f:646:MET:HE1	1.95	0.48
3:C:57:ARG:NH2	21:U:643:SER:O	2.42	0.48
30:d:139:LEU:HD11	30:d:151:VAL:HG13	1.95	0.48
20:T:37:ARG:NH1	14:n:165:GLU:OE2	2.46	0.48
23:W:178:GLU:HB2	23:W:182:ARG:H	1.77	0.48
32:f:157:GLU:O	32:f:161:HIS:ND1	2.47	0.48
32:f:438:ASP:OD1	32:f:438:ASP:N	2.46	0.48
32:f:458:GLU:HB2	35:x:49:LYS:HE2	1.95	0.48
20:t:27:LEU:HD22	20:t:184:TYR:HB2	1.95	0.48
2:B:357:ASP:OD2	2:B:359:LYS:NZ	2.46	0.48
13:M:136:MET:HE3	13:M:165:ILE:HG12	1.94	0.48
18:R:192:VAL:HG11	16:p:205:ASP:HB3	1.96	0.48
21:U:194:ARG:HH12	21:U:222:PHE:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:284:SER:O	23:W:288:HIS:ND1	2.47	0.48
23:W:396:LEU:HD13	23:W:402:ILE:HD13	1.94	0.48
27:a:35:HIS:CE1	28:b:17:ARG:HB2	2.49	0.48
29:c:30:GLN:HB3	29:c:66:THR:HG22	1.95	0.48
2:B:417:GLU:HA	2:B:420:LYS:HB2	1.95	0.48
9:I:180:LYS:H	9:I:184:MET:HE3	1.79	0.48
23:W:149:LEU:HB2	23:W:185:PHE:HE2	1.79	0.48
23:W:219:THR:HG23	23:W:223:LYS:H	1.77	0.48
24:X:347:ILE:HA	24:X:350:ILE:HG22	1.96	0.48
26:Z:102:HIS:N	26:Z:105:ASP:OD2	2.45	0.48
27:a:163:TYR:OH	27:a:169:HIS:ND1	2.46	0.48
21:U:794:ASP:OD1	21:U:794:ASP:N	2.47	0.48
30:d:5:LEU:O	30:d:9:TRP:NE1	2.47	0.48
32:f:112:ASN:OD1	32:f:113:MET:N	2.45	0.48
32:f:701:ASN:HD21	32:f:704:LEU:HD13	1.78	0.48
3:C:141:GLU:O	4:D:323:ARG:NH1	2.46	0.47
4:D:117:SER:O	4:D:121:ARG:NH1	2.46	0.47
21:U:802:TYR:HB3	21:U:895:PRO:HD3	1.96	0.47
27:a:212:ASN:HB3	27:a:275:LEU:HD21	1.96	0.47
32:f:389:LYS:HD2	32:f:393:ASP:HB3	1.95	0.47
1:A:372:LEU:HD11	11:K:207:GLU:HA	1.96	0.47
5:E:15:LYS:O	5:E:19:HIS:ND1	2.41	0.47
21:U:541:HIS:HB2	21:U:544:ILE:HG22	1.97	0.47
23:W:237:GLU:HG2	23:W:238:GLY:H	1.79	0.47
23:W:443:THR:HG21	26:Z:204:LYS:HD2	1.96	0.47
24:X:351:SER:HA	24:X:354:ILE:HG22	1.95	0.47
25:Y:81:LEU:HG	25:Y:107:LYS:HD2	1.95	0.47
8:h:59:GLU:HG2	8:h:60:ARG:HD3	1.96	0.47
3:C:301:LEU:HD13	3:C:305:LEU:HD23	1.97	0.47
6:F:30:GLY:HA2	6:F:33:VAL:HB	1.96	0.47
6:F:357:PRO:O	6:F:362:ARG:NH1	2.47	0.47
23:W:372:ARG:HB3	23:W:412:ILE:HD11	1.96	0.47
25:Y:286:TRP:C	25:Y:288:PHE:H	2.23	0.47
32:f:550:LEU:HD11	32:f:586:PRO:HB2	1.95	0.47
25:Y:195:LYS:NZ	25:Y:230:ALA:O	2.43	0.47
26:Z:37:GLY:HA2	26:Z:56:VAL:HG12	1.96	0.47
6:F:376:SER:HB3	6:F:414:GLU:HG3	1.96	0.47
28:b:124:LEU:HD13	28:b:156:PHE:HB2	1.96	0.47
32:f:393:ASP:OD1	32:f:393:ASP:N	2.44	0.47
32:f:655:LEU:HD23	32:f:659:LEU:HG	1.96	0.47
1:A:245:LEU:HD23	1:A:256:MET:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:41:TYR:HE2	21:U:149:GLN:HA	1.79	0.47
5:E:169:GLY:HA3	5:E:275:MET:HB2	1.97	0.47
6:F:150:LEU:HD21	6:F:167:GLU:HB3	1.96	0.47
21:U:727:LYS:HE2	21:U:727:LYS:HB3	1.77	0.47
22:V:467:TYR:OH	26:Z:255:ASP:OD1	2.31	0.47
24:X:134:VAL:HB	24:X:149:LEU:HD23	1.96	0.47
25:Y:215:ASP:OD1	25:Y:215:ASP:N	2.47	0.47
29:c:125:VAL:HG21	34:v:25:LYS:HD3	1.93	0.47
30:d:114:GLU:HA	30:d:117:THR:HG22	1.97	0.47
31:e:44:ASP:OD1	31:e:47:ASN:ND2	2.40	0.47
32:f:20:ALA:O	32:f:24:THR:OG1	2.29	0.47
32:f:531:ASN:HA	32:f:534:VAL:HB	1.97	0.47
11:k:25:GLU:HA	11:k:28:ILE:HD12	1.97	0.47
12:l:214:ILE:HD12	12:l:224:TYR:HE2	1.80	0.47
2:B:378:VAL:HG12	2:B:416:ASN:HA	1.95	0.47
7:G:10:ASP:OD1	7:G:10:ASP:N	2.48	0.47
21:U:62:LEU:HD12	21:U:84:ALA:HB1	1.95	0.47
26:Z:150:PRO:HB3	27:a:147:GLY:HA2	1.96	0.47
17:q:4:LEU:HD22	17:q:45:LEU:HD23	1.95	0.47
1:A:240:VAL:HB	1:A:274:PHE:HD1	1.79	0.47
2:B:118:ASP:N	2:B:118:ASP:OD1	2.47	0.47
6:F:303:ASP:N	6:F:303:ASP:OD1	2.46	0.47
23:W:310:THR:HG22	23:W:311:THR:H	1.80	0.47
21:U:424:ALA:HA	21:U:427:LEU:HD13	1.97	0.47
21:U:501:LEU:HD11	21:U:548:LEU:HD11	1.97	0.47
7:g:153:LYS:HE2	7:g:163:PHE:HE2	1.80	0.47
9:I:155:ASN:OD1	10:J:77:THR:OG1	2.33	0.46
20:T:25:ASP:HA	20:T:187:PHE:HA	1.97	0.46
22:V:98:LEU:HD22	22:V:209:LYS:HD2	1.96	0.46
29:c:113:HIS:NE2	29:c:115:HIS:CD2	2.83	0.46
29:c:302:ALA:O	29:c:306:THR:HG23	2.15	0.46
32:f:79:ARG:HG2	32:f:82:ILE:HG12	1.97	0.46
32:f:466:LEU:HB3	32:f:485:LEU:HD12	1.97	0.46
17:q:185:LYS:NZ	17:q:186:ASN:OD1	2.45	0.46
1:A:86:THR:HG22	2:B:136:LEU:HD12	1.96	0.46
4:D:171:ASP:OD1	4:D:171:ASP:N	2.47	0.46
7:G:93:ARG:HH21	7:G:121:ILE:HD12	1.80	0.46
9:I:197:LEU:HA	9:I:200:THR:HG22	1.97	0.46
25:Y:138:LEU:HD22	25:Y:176:ARG:HE	1.79	0.46
30:d:8:GLU:HB3	30:d:13:SER:HA	1.96	0.46
32:f:718:ASP:N	32:f:718:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:72:ILE:HG22	12:l:134:ILE:HG12	1.96	0.46
3:C:339:THR:O	3:C:340:ARG:NE	2.41	0.46
4:D:336:PRO:HB3	4:D:340:GLN:HB2	1.98	0.46
5:E:56:ILE:HB	5:E:100:LEU:HB2	1.98	0.46
6:F:114:ASP:OD1	6:F:115:SER:N	2.49	0.46
9:I:33:THR:OG1	9:I:166:ASN:O	2.33	0.46
21:U:161:ASP:OD1	21:U:161:ASP:N	2.47	0.46
32:f:437:GLU:HB3	32:f:440:ILE:HB	1.96	0.46
1:A:306:LEU:HD23	1:A:336:ARG:HB3	1.97	0.46
30:d:195:THR:HB	30:d:202:THR:HG22	1.97	0.46
32:f:520:LEU:O	32:f:524:MET:HG3	2.15	0.46
2:B:389:ASP:OD1	2:B:389:ASP:N	2.48	0.46
6:F:389:ASP:OD1	6:F:389:ASP:N	2.46	0.46
15:O:163:ILE:HG12	15:O:170:GLY:HA2	1.97	0.46
17:Q:169:LYS:O	17:q:27:GLN:NE2	2.48	0.46
21:U:367:THR:HA	21:U:370:VAL:HG22	1.98	0.46
32:f:559:PRO:HG3	32:f:587:PHE:HE2	1.79	0.46
32:f:815:HIS:HB2	32:f:820:GLY:N	2.30	0.46
12:l:121:GLN:HG3	13:m:129:ARG:HG2	1.97	0.46
18:r:182:ASP:OD1	18:r:182:ASP:N	2.43	0.46
3:C:227:GLY:HA3	3:C:229:ARG:HH11	1.80	0.46
5:E:121:ASN:OD1	6:F:146:LYS:NZ	2.48	0.46
21:U:261:LEU:HD22	21:U:329:LEU:HD22	1.96	0.46
27:a:89:ASP:O	27:a:93:ALA:CB	2.64	0.46
32:f:664:GLU:H	32:f:668:ALA:HB3	1.80	0.46
4:D:315:ASP:N	4:D:315:ASP:OD1	2.48	0.46
6:F:348:LEU:O	6:F:351:LYS:NZ	2.48	0.46
22:V:337:LEU:HB3	22:V:398:LEU:HD11	1.98	0.46
26:Z:202:ASN:HD21	27:a:361:LYS:HD2	1.80	0.46
32:f:142:TYR:OH	32:f:190:GLU:N	2.36	0.46
11:k:202:LEU:O	11:k:206:MET:HB2	2.16	0.46
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.97	0.46
8:H:4:ARG:NH2	10:J:4:ASP:OD2	2.49	0.46
11:K:167:ALA:HB3	12:L:56:LEU:HD13	1.98	0.46
13:M:62:SER:OG	13:M:63:ASN:N	2.49	0.46
21:U:217:CYS:HB2	21:U:248:ILE:HD12	1.98	0.46
22:V:337:LEU:HD21	22:V:364:THR:HG23	1.97	0.46
32:f:65:GLU:HB2	32:f:97:LYS:HD3	1.98	0.46
8:h:204:THR:OG1	8:h:206:ASP:OD1	2.29	0.46
2:B:73:LEU:HA	2:B:76:GLU:HG3	1.98	0.46
5:E:291:ARG:HG2	5:E:293:GLY:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:176:MET:HE1	13:M:56:LYS:HB3	1.98	0.46
13:m:8:ASP:OD1	13:m:8:ASP:N	2.48	0.46
5:E:352:MET:HA	5:E:355:ILE:HG22	1.98	0.45
10:J:67:ASP:OD1	10:J:67:ASP:N	2.45	0.45
13:M:204:VAL:HG13	13:M:205:LYS:HG3	1.96	0.45
23:W:216:GLU:OE1	23:W:223:LYS:NZ	2.44	0.45
24:X:208:ALA:HB2	24:X:238:GLY:HA3	1.98	0.45
2:B:90:GLU:HB3	2:B:94:GLU:HB2	1.97	0.45
2:B:221:GLY:HA3	2:B:347:ILE:HG22	1.99	0.45
5:E:348:THR:HA	6:F:217:ILE:HD11	1.98	0.45
9:I:176:LYS:O	10:J:52:LYS:NZ	2.37	0.45
27:a:163:TYR:O	27:a:165:THR:N	2.44	0.45
1:A:312:ARG:HB2	1:A:315:ILE:HB	1.99	0.45
2:B:408:ARG:NH2	3:C:160:GLU:OE2	2.49	0.45
4:D:391:ARG:HG2	4:D:393:ILE:H	1.81	0.45
5:E:219:PHE:HD2	5:E:263:GLN:HB3	1.82	0.45
17:Q:143:LEU:O	17:Q:147:TYR:HB2	2.17	0.45
21:U:418:GLU:HG2	21:U:422:LEU:HB2	1.98	0.45
25:Y:145:LEU:HD13	25:Y:182:VAL:HG11	1.98	0.45
28:b:12:ASN:HB3	28:b:78:VAL:HG22	1.98	0.45
32:f:261:ARG:HH22	32:f:271:MET:HE2	1.81	0.45
20:t:126:ASP:OD1	20:t:130:VAL:N	2.48	0.45
21:U:879:ASP:OD1	21:U:879:ASP:N	2.49	0.45
22:V:416:ARG:HH11	22:V:459:GLN:HE21	1.65	0.45
29:c:296:ILE:HD12	30:d:246:VAL:HG13	1.97	0.45
12:L:88:MET:HG2	12:L:112:ILE:HD11	1.97	0.45
13:M:43:ASP:OD1	13:M:43:ASP:N	2.49	0.45
19:S:145:LEU:HD22	19:S:178:VAL:HB	1.98	0.45
21:U:74:PHE:HB3	21:U:103:LYS:HD2	1.98	0.45
21:U:798:PRO:O	21:U:880:ASN:ND2	2.50	0.45
24:X:240:ASP:OD1	24:X:278:ARG:NH2	2.50	0.45
25:Y:83:ARG:NH1	25:Y:84:LEU:HB2	2.32	0.45
28:b:100:ARG:NH1	28:b:102:GLY:O	2.50	0.45
29:c:251:LEU:HB3	29:c:284:LEU:HD12	1.98	0.45
13:m:169:ARG:HH21	13:m:173:LYS:HE3	1.81	0.45
15:o:86:MET:HB3	15:o:86:MET:HE3	1.81	0.45
1:A:45:ILE:HD12	2:B:65:LEU:HD12	1.99	0.45
1:A:308:GLY:HA2	6:F:234:THR:HG21	1.97	0.45
5:E:351:GLY:HA3	6:F:217:ILE:HD12	1.98	0.45
5:E:364:GLN:NE2	5:E:368:MET:SD	2.89	0.45
8:H:175:GLU:OE2	9:I:53:HIS:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:319:MET:HE2	25:Y:330:ILE:HD12	1.97	0.45
29:c:28:ALA:HB1	29:c:180:ASN:HB2	1.98	0.45
32:f:564:LEU:HD22	32:f:776:LEU:HD23	1.98	0.45
7:g:165:ALA:HB3	8:h:56:LEU:HD22	1.99	0.45
7:g:188:ASP:OD1	7:g:188:ASP:N	2.43	0.45
10:j:57:ARG:O	10:j:60:ARG:NH2	2.49	0.45
5:E:172:LEU:HD23	5:E:299:ILE:HB	1.98	0.45
17:Q:5:ILE:HD11	17:Q:143:LEU:HD11	1.99	0.45
22:V:278:GLU:HA	22:V:285:TRP:HZ2	1.81	0.45
1:A:210:LYS:NZ	1:A:313:GLY:O	2.39	0.45
2:B:317:ASP:HB2	2:B:346:ARG:HG2	1.99	0.45
3:C:28:ILE:HB	4:D:44:TYR:CE1	2.52	0.45
5:E:119:VAL:O	5:E:123:SER:OG	2.28	0.45
5:E:148:VAL:HG23	5:E:167:PRO:HD2	1.99	0.45
6:F:265:ALA:HB1	6:F:312:GLU:OE1	2.17	0.45
12:L:204:ASP:N	12:L:204:ASP:OD1	2.48	0.45
19:S:10:GLY:HA3	19:S:42:LYS:HE2	1.99	0.45
21:U:483:LEU:HD11	21:U:781:LEU:HD11	1.99	0.45
23:W:96:GLN:HB3	23:W:97:LEU:H	1.55	0.45
27:a:33:LEU:HA	28:b:18:ASN:HB2	1.98	0.45
32:f:504:VAL:HG13	32:f:518:THR:HG21	1.99	0.45
16:p:30:ILE:HG22	16:p:31:GLN:H	1.81	0.45
20:t:53:ALA:HB2	20:t:110:MET:HG3	1.98	0.45
13:M:28:LYS:HB3	13:M:28:LYS:HE3	1.83	0.45
21:U:208:LEU:HD23	21:U:210:LYS:H	1.82	0.45
22:V:289:LEU:HB3	22:V:312:ALA:HB2	1.98	0.45
26:Z:138:TYR:HB3	26:Z:155:PHE:HB3	1.99	0.45
29:c:88:ASP:N	29:c:88:ASP:OD1	2.50	0.45
8:H:93:LEU:HD13	8:H:113:ARG:HB3	1.99	0.45
10:J:38:ARG:HH22	10:J:178:ASP:HB3	1.82	0.45
13:M:108:LEU:HD22	13:M:139:SER:HB3	1.98	0.45
22:V:287:ARG:NH2	31:e:17:ASP:OD2	2.50	0.45
24:X:292:GLN:NE2	24:X:296:ASN:OD1	2.44	0.45
27:a:156:TYR:CG	27:a:179:PHE:HB2	2.51	0.45
32:f:75:LEU:HG	32:f:77:GLU:HG3	1.99	0.45
12:l:227:ASP:OD1	12:l:227:ASP:N	2.50	0.45
5:E:310:LEU:HD11	5:E:314:LYS:HE3	1.97	0.44
22:V:452:ASN:HB3	22:V:457:TYR:HB2	1.98	0.44
24:X:218:HIS:NE2	24:X:227:THR:OG1	2.51	0.44
28:b:8:VAL:HA	28:b:110:ILE:HG13	1.99	0.44
31:e:35:ASP:HB3	31:e:37:HIS:ND1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:110:TYR:HD2	32:f:137:ARG:HH12	1.65	0.44
32:f:463:LEU:HD23	35:x:47:MET:HE1	1.99	0.44
32:f:534:VAL:HG13	32:f:562:LEU:HD11	1.98	0.44
32:f:569:LYS:HD2	32:f:573:ILE:HG21	1.99	0.44
20:t:210:ASP:OD1	20:t:210:ASP:N	2.49	0.44
13:M:163:CYS:SG	13:M:164:ALA:N	2.90	0.44
21:U:788:VAL:HG12	21:U:909:GLY:HA2	1.97	0.44
33:u:39:ASP:N	33:u:39:ASP:OD1	2.50	0.44
35:x:30:LYS:NZ	35:x:44:GLN:O	2.47	0.44
12:L:117:GLN:O	12:L:120:THR:OG1	2.29	0.44
19:S:176:LYS:HE2	19:S:208:VAL:HG21	1.99	0.44
21:U:229:VAL:HA	21:U:232:ILE:HG12	1.98	0.44
21:U:249:CYS:HB3	21:U:328:ILE:HB	1.99	0.44
21:U:560:MET:HE2	21:U:560:MET:HB2	1.78	0.44
21:U:681:ASN:OD1	21:U:682:TYR:N	2.51	0.44
22:V:443:ARG:HH21	30:d:181:CYS:HB2	1.82	0.44
23:W:173:THR:N	23:W:182:ARG:HH21	2.15	0.44
29:c:269:GLN:HA	29:c:272:ILE:HG22	1.98	0.44
32:f:466:LEU:HD12	32:f:485:LEU:HB2	1.99	0.44
2:B:284:ILE:HG21	2:B:287:ILE:HD12	2.00	0.44
4:D:264:ILE:HB	4:D:309:MET:HG2	1.98	0.44
6:F:298:SER:OG	6:F:301:ALA:O	2.28	0.44
12:L:158:ALA:HB1	12:L:172:LEU:HD13	2.00	0.44
20:T:152:GLU:OE1	20:T:156:LYS:NZ	2.49	0.44
27:a:18:GLN:HA	27:a:22:TRP:HD1	1.83	0.44
27:a:134:THR:O	27:a:138:VAL:HG23	2.17	0.44
29:c:219:ASN:HB2	29:c:222:LYS:HD3	1.99	0.44
32:f:78:LEU:HB3	32:f:82:ILE:HG13	1.98	0.44
10:j:46:GLU:HG3	10:j:199:VAL:HG22	1.99	0.44
1:A:171:ASP:OD1	1:A:171:ASP:N	2.50	0.44
12:L:226:ASP:OD1	12:L:226:ASP:N	2.51	0.44
17:Q:118:MET:HE2	17:Q:124:LEU:HD13	1.98	0.44
21:U:182:LYS:O	21:U:186:SER:HB3	2.18	0.44
28:b:30:GLN:HG3	28:b:75:LEU:HD13	1.99	0.44
31:e:50:ASP:N	31:e:50:ASP:OD1	2.45	0.44
32:f:90:THR:HG23	32:f:109:ILE:HG23	1.98	0.44
35:x:46:VAL:HG13	35:x:69:LEU:HD22	1.99	0.44
7:G:196:GLU:HG3	7:G:242:LEU:HD12	2.00	0.44
16:P:38:ASP:OD1	16:P:38:ASP:N	2.50	0.44
22:V:199:ASN:OD1	22:V:241:ARG:NH2	2.51	0.44
24:X:415:TYR:HB2	25:Y:383:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:73:ASP:OD2	28:b:70:ARG:NH2	2.50	0.44
29:c:75:MET:SD	29:c:77:GLN:NE2	2.91	0.44
32:f:51:GLN:NE2	32:f:54:ASP:OD1	2.50	0.44
13:m:75:MET:HB2	13:m:137:LEU:HD23	1.99	0.44
1:A:287:ASP:OD1	1:A:287:ASP:N	2.48	0.44
2:B:269:GLU:HA	2:B:272:ARG:HG2	1.99	0.44
7:G:188:ASP:OD1	7:G:188:ASP:N	2.47	0.44
11:K:234:LEU:O	11:K:238:ILE:HG12	2.18	0.44
21:U:21:GLU:HA	21:U:24:LEU:HG	2.00	0.44
24:X:414:LEU:HD21	26:Z:273:HIS:CD2	2.53	0.44
25:Y:187:TYR:CE2	25:Y:196:GLN:HB3	2.51	0.44
11:k:35:SER:HB2	11:k:51:GLU:HG3	1.99	0.44
17:q:38:MET:HE1	17:q:60:ILE:HG22	2.00	0.44
4:D:231:VAL:HG13	5:E:262:ASN:HD22	1.83	0.44
8:H:213:CYS:HB2	8:H:218:PHE:HD1	1.82	0.44
17:Q:1:MET:HE1	17:Q:133:GLY:HA2	1.99	0.44
23:W:148:THR:O	23:W:152:ILE:HG12	2.18	0.44
25:Y:231:LEU:HB2	25:Y:234:PRO:HD2	1.99	0.44
30:d:107:LEU:HD11	30:d:140:GLU:HB2	2.00	0.44
13:m:39:ILE:HD11	13:m:176:ILE:HG12	1.98	0.44
3:C:53:ASN:HD21	21:U:643:SER:HA	1.83	0.44
32:f:631:LYS:HE3	32:f:635:LYS:HG3	2.00	0.44
17:q:22:ALA:HA	17:q:27:GLN:HA	2.00	0.44
2:B:249:ARG:HG3	2:B:283:PHE:HD2	1.83	0.43
2:B:393:ALA:HB2	36:B:501:ATP:H5'1	1.99	0.43
9:I:68:LEU:HD11	9:I:74:CYS:HB3	1.99	0.43
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.51	0.43
26:Z:65:ASP:OD1	26:Z:65:ASP:N	2.44	0.43
31:e:16:ASP:OD1	31:e:16:ASP:N	2.51	0.43
8:h:42:ASN:ND2	8:h:183:GLU:OE2	2.51	0.43
2:B:343:ARG:HE	2:B:346:ARG:NH1	2.16	0.43
5:E:119:VAL:HA	5:E:122:MET:HG2	2.00	0.43
5:E:331:ILE:HG23	5:E:371:VAL:HG21	1.99	0.43
11:K:196:LYS:HE3	11:K:241:ILE:HG21	1.99	0.43
16:P:15:LYS:HE3	16:P:121:ILE:HG12	2.00	0.43
19:S:211:ARG:HH21	15:o:193:ASN:HB3	1.82	0.43
24:X:194:ARG:HG2	24:X:210:LEU:HD21	2.00	0.43
32:f:79:ARG:O	32:f:83:ARG:HG2	2.18	0.43
32:f:334:ALA:HA	32:f:338:ASP:HB2	1.99	0.43
9:i:25:MET:HE1	9:i:151:ASP:HB2	2.01	0.43
9:i:106:PRO:HB2	9:i:109:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:o:163:ILE:HG12	15:o:170:GLY:HA2	2.00	0.43
1:A:63:THR:O	1:A:66:LYS:NZ	2.50	0.43
1:A:69:ASP:OD1	1:A:69:ASP:N	2.51	0.43
1:A:307:ASP:HB2	1:A:336:ARG:NH1	2.33	0.43
5:E:196:LEU:HD11	5:E:221:TYR:HD2	1.84	0.43
5:E:199:VAL:HG23	5:E:201:SER:H	1.83	0.43
30:d:131:VAL:HG22	30:d:159:PRO:HG3	1.99	0.43
1:A:85:GLN:NE2	32:f:700:SER:OG	2.51	0.43
1:A:234:ASP:OD1	1:A:234:ASP:N	2.51	0.43
3:C:150:MET:SD	3:C:150:MET:N	2.91	0.43
4:D:97:ASP:OD1	4:D:97:ASP:N	2.50	0.43
4:D:231:VAL:HB	4:D:234:GLU:HG2	2.00	0.43
21:U:756:HIS:CE1	21:U:758:PRO:HG2	2.53	0.43
23:W:128:LEU:HD22	23:W:147:LYS:HD3	1.99	0.43
23:W:135:LYS:HE3	23:W:139:GLU:HG2	1.99	0.43
32:f:389:LYS:HE3	32:f:417:ILE:HG21	2.00	0.43
32:f:765:ALA:HB2	32:f:877:GLY:HA2	1.99	0.43
12:l:47:VAL:HG12	12:l:195:LEU:HD22	2.00	0.43
1:A:164:MET:HE1	1:A:240:VAL:HG13	2.01	0.43
2:B:153:ASN:HD22	2:B:156:VAL:HG22	1.83	0.43
2:B:376:ASP:N	2:B:376:ASP:OD1	2.50	0.43
22:V:419:LEU:HA	22:V:422:ILE:HG22	2.00	0.43
23:W:153:LYS:NZ	23:W:188:GLU:OE2	2.41	0.43
27:a:34:TRP:O	27:a:38:THR:OG1	2.34	0.43
2:B:176:VAL:HG21	2:B:247:PHE:HD2	1.84	0.43
3:C:152:GLY:H	38:C:501:ADP:HN62	1.65	0.43
4:D:171:ASP:HA	4:D:174:LYS:HD3	1.99	0.43
11:K:209:LYS:O	11:K:214:ASN:ND2	2.48	0.43
21:U:36:ALA:O	22:V:273:LYS:NZ	2.51	0.43
24:X:421:LEU:HB2	26:Z:283:ARG:HH22	1.83	0.43
29:c:104:ARG:H	29:c:104:ARG:HD3	1.84	0.43
30:d:70:SER:OG	30:d:73:ARG:NH2	2.50	0.43
9:i:161:ALA:HB3	10:j:53:LEU:HD23	2.01	0.43
17:q:167:LEU:HD23	17:q:167:LEU:HA	1.89	0.43
1:A:115:VAL:HG21	1:A:118:PHE:HB2	2.00	0.43
3:C:369:TYR:CE2	3:C:385:MET:HB3	2.53	0.43
9:I:194:ILE:HD12	9:I:194:ILE:HA	1.93	0.43
19:S:16:ALA:HB2	19:S:121:VAL:HG23	2.01	0.43
21:U:759:SER:HA	21:U:782:ALA:HA	1.99	0.43
32:f:448:CYS:HA	32:f:451:VAL:HG12	2.01	0.43
10:j:40:ILE:HG22	10:j:212:ARG:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:p:70:ARG:HB3	16:p:90:MET:HE2	2.01	0.43
19:s:145:LEU:HD21	19:s:182:ALA:HB2	2.01	0.43
33:u:5:VAL:HB	33:u:13:ILE:HG23	2.00	0.43
1:A:410:LEU:O	1:A:414:ASN:ND2	2.52	0.43
18:R:38:ASN:HD21	18:R:41:LEU:HD12	1.82	0.43
27:a:50:PHE:HD2	27:a:52:GLN:HB3	1.83	0.43
27:a:161:LYS:HD2	27:a:161:LYS:HA	1.78	0.43
29:c:64:ASP:OD1	29:c:64:ASP:N	2.50	0.43
30:d:175:ARG:HE	30:d:199:PHE:HD2	1.65	0.43
1:A:127:ASP:OD1	1:A:127:ASP:N	2.42	0.43
5:E:60:VAL:HA	5:E:71:VAL:HG12	2.01	0.43
6:F:225:MET:HE2	6:F:233:LYS:HB3	2.00	0.43
17:Q:31:ASP:OD1	17:Q:31:ASP:N	2.51	0.43
20:T:122:LEU:HG	20:T:137:LEU:HD12	2.01	0.43
21:U:524:LYS:HB2	21:U:556:MET:HE2	2.01	0.43
7:g:127:GLN:NE2	8:h:128:ARG:O	2.49	0.43
10:j:184:ASP:O	10:j:187:THR:OG1	2.29	0.43
13:m:23:VAL:O	13:m:27:MET:HG2	2.17	0.43
35:x:10:TRP:CD1	35:x:72:MET:HA	2.54	0.43
1:A:73:ALA:HA	2:B:140:ASP:HB3	2.00	0.43
2:B:140:ASP:O	2:B:142:ASP:N	2.47	0.43
3:C:134:LEU:HD22	3:C:237:MET:HE2	2.00	0.43
23:W:422:ASN:O	23:W:426:ASN:ND2	2.51	0.43
25:Y:142:PHE:HB3	25:Y:146:ARG:HH22	1.84	0.43
30:d:224:SER:OG	30:d:225:PHE:N	2.51	0.43
32:f:87:THR:HA	32:f:90:THR:HG22	2.01	0.43
32:f:655:LEU:HA	32:f:659:LEU:HD23	2.00	0.43
8:h:86:LEU:HD23	8:h:86:LEU:HA	1.89	0.43
4:D:93:LEU:HD12	4:D:102:ILE:HG22	2.01	0.42
4:D:141:ASP:N	4:D:141:ASP:OD1	2.52	0.42
5:E:364:GLN:O	5:E:368:MET:HG2	2.19	0.42
17:Q:25:ILE:HG22	17:Q:26:VAL:HG13	2.01	0.42
17:Q:26:VAL:HG21	18:R:136:TYR:HE2	1.83	0.42
17:Q:167:LEU:HD23	17:Q:167:LEU:HA	1.91	0.42
21:U:403:THR:HG23	21:U:777:HIS:HE1	1.84	0.42
21:U:764:LEU:O	21:U:767:THR:OG1	2.33	0.42
22:V:355:ARG:NH1	31:e:27:TRP:O	2.41	0.42
24:X:414:LEU:HD11	26:Z:273:HIS:CE1	2.54	0.42
27:a:97:LEU:HD22	27:a:118:ILE:HG13	2.00	0.42
32:f:285:CYS:HB3	32:f:872:VAL:HB	2.00	0.42
7:g:58:ASP:OD1	7:g:58:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:218:ASP:OD1	12:l:218:ASP:N	2.45	0.42
3:C:81:ASP:OD1	3:C:81:ASP:N	2.49	0.42
16:P:205:ASP:OD1	16:P:205:ASP:N	2.50	0.42
27:a:370:GLN:OE1	30:d:244:LYS:NZ	2.45	0.42
32:f:408:LEU:HD21	32:f:446:LEU:HD13	2.01	0.42
32:f:485:LEU:HD21	32:f:497:VAL:HG13	2.02	0.42
32:f:828:ARG:HB3	32:f:843:SER:HB2	2.02	0.42
3:C:184:LYS:HD2	3:C:280:LEU:HD13	2.00	0.42
11:K:78:MET:HE2	11:K:78:MET:HB3	1.97	0.42
12:L:215:VAL:HB	12:L:221:PHE:HD1	1.83	0.42
23:W:243:ILE:HG13	23:W:273:TYR:HE2	1.85	0.42
26:Z:201:LEU:HD22	29:c:225:TRP:HD1	1.83	0.42
27:a:112:ILE:O	27:a:116:THR:HG23	2.19	0.42
27:a:277:LEU:HD21	27:a:296:ILE:HG23	2.01	0.42
12:l:116:THR:HG22	12:l:128:TYR:HD2	1.85	0.42
12:l:236:LEU:HG	12:l:237:GLU:HG3	2.01	0.42
5:E:4:PRO:HG2	5:E:8:ALA:H	1.84	0.42
6:F:224:LEU:HD23	6:F:351:LYS:HG2	2.01	0.42
6:F:236:LEU:HD23	6:F:236:LEU:HA	1.89	0.42
13:M:8:ASP:O	13:M:22:GLN:NE2	2.46	0.42
14:N:166:ARG:HA	14:N:166:ARG:HD3	1.81	0.42
21:U:680:VAL:HB	21:U:683:VAL:HG12	2.00	0.42
21:U:798:PRO:HG2	21:U:880:ASN:HD21	1.84	0.42
22:V:461:LYS:HD2	22:V:461:LYS:HA	1.89	0.42
25:Y:146:ARG:HG2	25:Y:150:PHE:CZ	2.55	0.42
27:a:207:GLY:O	27:a:271:LYS:NZ	2.44	0.42
32:f:786:GLN:HG2	32:f:788:MET:H	1.83	0.42
14:n:127:ILE:HD11	14:n:136:TYR:CE1	2.54	0.42
1:A:333:ARG:HH21	1:A:336:ARG:CZ	2.32	0.42
2:B:411:ARG:NH2	2:B:418:ASP:OD2	2.52	0.42
3:C:374:ARG:HA	3:C:374:ARG:HD3	1.85	0.42
6:F:314:LEU:HD21	6:F:342:LEU:HB3	2.02	0.42
19:s:13:LEU:HD11	19:s:149:LEU:HD11	2.02	0.42
20:t:96:MET:HE2	20:t:110:MET:HE1	2.01	0.42
2:B:235:LEU:HD13	2:B:353:PHE:HZ	1.83	0.42
18:R:71:LYS:HE2	18:R:71:LYS:HB2	1.92	0.42
23:W:176:SER:HB3	23:W:178:GLU:HG2	2.01	0.42
7:g:43:ARG:HH21	7:g:164:LYS:HG2	1.85	0.42
10:j:38:ARG:NH1	10:j:182:GLU:O	2.52	0.42
14:n:166:ARG:HA	14:n:166:ARG:HD3	1.80	0.42
18:r:105:ASP:OD1	18:r:105:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ARG:NH2	6:F:254:PRO:O	2.52	0.42
1:A:319:MET:HE1	1:A:337:LEU:HD11	2.01	0.42
3:C:119:ASP:OD1	3:C:119:ASP:N	2.53	0.42
21:U:324:LYS:O	21:U:328:ILE:HG12	2.18	0.42
24:X:225:TRP:HB2	24:X:261:LEU:HD13	2.02	0.42
7:g:54:LYS:HE3	7:g:66:VAL:HG23	2.00	0.42
10:j:35:VAL:HG12	10:j:42:VAL:HB	2.02	0.42
12:l:7:ASP:O	12:l:21:GLN:NE2	2.50	0.42
4:D:345:PHE:O	4:D:349:THR:OG1	2.29	0.42
6:F:314:LEU:HD22	6:F:347:ARG:HD3	2.02	0.42
13:M:46:VAL:HG22	13:M:215:TRP:HB3	2.01	0.42
18:R:133:VAL:HG21	17:q:137:PHE:HB3	2.00	0.42
27:a:247:ARG:HA	27:a:250:THR:HG22	2.02	0.42
27:a:276:CYS:SG	27:a:277:LEU:N	2.93	0.42
30:d:195:THR:HG22	30:d:206:MET:HB3	2.02	0.42
32:f:763:ARG:O	32:f:807:ARG:NH2	2.52	0.42
10:j:158:ALA:HB3	10:j:172:LEU:HD21	2.02	0.42
3:C:369:TYR:HA	3:C:372:ARG:HG2	2.02	0.42
5:E:123:SER:HA	5:E:196:LEU:HD23	2.02	0.42
19:S:83:MET:HE1	19:S:91:MET:SD	2.60	0.42
21:U:35:TRP:HB3	21:U:70:HIS:CD2	2.55	0.42
21:U:398:ASN:H	21:U:401:LYS:HE2	1.85	0.42
21:U:588:MET:HE2	21:U:588:MET:HB2	1.82	0.42
22:V:175:MET:HB3	22:V:184:ALA:HB2	2.02	0.42
30:d:8:GLU:O	30:d:13:SER:OG	2.38	0.42
7:g:41:ALA:HB3	7:g:166:THR:HB	2.01	0.42
14:n:104:ASP:OD1	14:n:104:ASP:N	2.51	0.42
16:p:135:ASP:OD1	16:p:135:ASP:N	2.50	0.42
5:E:22:ILE:HD12	5:E:25:ARG:HD2	2.02	0.42
5:E:171:LEU:HB3	5:E:295:LEU:HD13	2.01	0.42
6:F:60:LEU:HB3	6:F:64:HIS:CE1	2.55	0.42
13:M:8:ASP:OD1	13:M:8:ASP:N	2.53	0.42
17:Q:44:LEU:HD11	17:Q:102:LEU:HD22	2.02	0.42
21:U:583:MET:HE1	21:U:602:LEU:HA	2.02	0.42
22:V:72:LEU:HG	22:V:112:VAL:HG13	2.02	0.42
26:Z:70:LEU:HD23	26:Z:70:LEU:HA	1.84	0.42
26:Z:234:PHE:HA	26:Z:237:LEU:HD23	2.01	0.42
32:f:535:THR:HA	32:f:538:ILE:HG22	2.02	0.42
17:q:31:ASP:OD1	17:q:31:ASP:N	2.51	0.42
17:q:102:LEU:HB2	17:q:118:MET:HB3	2.01	0.42
2:B:295:TYR:CZ	3:C:271:ARG:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:250:PHE:HE1	21:U:328:ILE:HA	1.84	0.41
24:X:371:ASP:OD1	25:Y:233:ARG:NH1	2.53	0.41
28:b:157:VAL:HG21	28:b:170:LEU:HB2	2.02	0.41
30:d:3:GLU:O	30:d:25:ARG:NH2	2.53	0.41
20:t:102:LYS:HB2	20:t:102:LYS:HE2	1.81	0.41
1:A:394:MET:O	1:A:398:ARG:HG3	2.20	0.41
4:D:235:PHE:HB2	4:D:270:ILE:HD11	2.02	0.41
4:D:290:LEU:HD23	4:D:290:LEU:HA	1.91	0.41
8:H:177:ARG:HE	24:X:161:ASP:HB3	1.84	0.41
21:U:198:LEU:HD23	21:U:223:LEU:HD13	2.02	0.41
29:c:41:MET:HE3	29:c:41:MET:HB3	1.93	0.41
10:j:98:VAL:HG12	10:j:100:ASP:HB2	2.02	0.41
16:p:15:LYS:HE3	16:p:121:ILE:HG12	2.02	0.41
1:A:245:LEU:HB2	1:A:280:ILE:HD13	2.02	0.41
2:B:316:LEU:HD23	2:B:346:ARG:HB3	2.02	0.41
2:B:388:ASP:N	2:B:388:ASP:OD1	2.48	0.41
3:C:273:MET:HE3	3:C:273:MET:HB2	1.84	0.41
19:S:71:ARG:HA	19:S:74:MET:HE3	2.02	0.41
24:X:418:ALA:O	24:X:422:THR:OG1	2.33	0.41
8:h:50:LYS:HG2	8:h:52:GLN:HE21	1.85	0.41
10:j:39:ASP:OD1	10:j:39:ASP:N	2.52	0.41
10:j:192:ILE:HD12	10:j:206:ILE:HD12	2.02	0.41
3:C:137:LEU:HD11	3:C:220:VAL:HA	2.02	0.41
6:F:178:ASP:N	6:F:178:ASP:OD1	2.52	0.41
8:H:119:GLN:NE2	9:I:82:ASP:OD1	2.53	0.41
17:Q:27:GLN:HE21	17:q:172:ILE:HA	1.85	0.41
18:R:114:VAL:HG22	18:R:120:ARG:HG3	2.01	0.41
21:U:333:MET:HE3	21:U:333:MET:HB3	1.90	0.41
25:Y:387:ILE:HG21	26:Z:276:ILE:HG22	2.03	0.41
27:a:156:TYR:HE2	27:a:196:ARG:HH21	1.68	0.41
30:d:67:ASP:OD1	30:d:70:SER:HB2	2.20	0.41
32:f:42:GLU:HB2	32:f:89:MET:HE1	2.02	0.41
2:B:384:ILE:HG22	2:B:385:MET:HE2	2.03	0.41
3:C:160:GLU:OE1	3:C:313:ARG:NH1	2.54	0.41
3:C:299:ASP:N	3:C:299:ASP:OD1	2.53	0.41
16:P:143:ALA:HA	16:P:146:MET:HE3	2.02	0.41
17:Q:30:ASP:OD1	17:Q:30:ASP:N	2.53	0.41
22:V:494:MET:HE2	22:V:494:MET:HB2	1.91	0.41
23:W:378:MET:HE3	23:W:378:MET:HB2	1.89	0.41
23:W:378:MET:HE1	23:W:413:ILE:HD11	2.03	0.41
25:Y:187:TYR:HD2	25:Y:197:ALA:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:35:ILE:HD11	28:b:184:ILE:HD11	2.02	0.41
28:b:62:THR:HA	28:b:70:ARG:HH12	1.85	0.41
32:f:745:LEU:HD23	32:f:745:LEU:HA	1.90	0.41
1:A:297:ARG:HG3	6:F:290:ALA:HB1	2.01	0.41
11:K:235:GLU:O	11:K:239:LYS:HG3	2.20	0.41
12:L:116:THR:HG22	12:L:128:TYR:HD2	1.85	0.41
21:U:497:LEU:HB3	21:U:516:LEU:HD13	2.03	0.41
25:Y:231:LEU:HG	25:Y:236:LEU:HD12	2.02	0.41
25:Y:297:ARG:NH1	31:e:44:ASP:OD2	2.53	0.41
32:f:94:LYS:HD2	32:f:109:ILE:HD13	2.03	0.41
17:q:44:LEU:HD11	17:q:102:LEU:HD22	2.03	0.41
1:A:423:PHE:HZ	2:B:334:ILE:HG23	1.85	0.41
4:D:251:PHE:HD2	4:D:295:GLN:HB3	1.86	0.41
5:E:342:ASP:OD1	5:E:342:ASP:N	2.54	0.41
9:I:25:MET:HE1	9:I:152:PRO:HD2	2.03	0.41
15:O:143:ARG:NH2	15:O:150:GLU:OE1	2.52	0.41
21:U:494:TYR:CD1	21:U:516:LEU:HD11	2.56	0.41
21:U:524:LYS:HB2	21:U:524:LYS:HE3	1.94	0.41
23:W:205:ILE:O	23:W:209:ILE:HG12	2.20	0.41
24:X:410:VAL:HG12	29:c:256:ASN:HA	2.03	0.41
26:Z:198:LEU:HD22	29:c:229:LEU:HD21	2.02	0.41
28:b:106:LYS:HD2	28:b:106:LYS:HA	1.94	0.41
30:d:54:ILE:HA	30:d:57:ILE:HG22	2.03	0.41
32:f:569:LYS:H	32:f:569:LYS:HG2	1.53	0.41
32:f:829:MET:HE3	32:f:845:ARG:HH12	1.86	0.41
9:i:186:LEU:HD12	9:i:186:LEU:HA	1.92	0.41
12:l:7:ASP:OD1	12:l:7:ASP:N	2.52	0.41
20:t:99:ARG:HD2	20:t:99:ARG:HA	1.93	0.41
13:M:215:TRP:CE3	13:M:227:VAL:HG22	2.56	0.41
15:O:187:ARG:HA	15:O:188:PRO:HA	1.89	0.41
21:U:43:ASP:OD1	21:U:43:ASP:N	2.54	0.41
21:U:167:ILE:HB	21:U:177:LEU:HD11	2.02	0.41
23:W:312:MET:HE2	27:a:312:MET:SD	2.61	0.41
23:W:338:THR:HA	23:W:342:GLY:HA3	2.02	0.41
25:Y:163:LYS:HD3	25:Y:163:LYS:HA	1.89	0.41
25:Y:314:LEU:O	25:Y:354:VAL:N	2.43	0.41
8:h:166:ASN:OD1	8:h:169:ASN:ND2	2.39	0.41
3:C:24:TYR:HB3	4:D:44:TYR:OH	2.20	0.41
3:C:28:ILE:HD13	4:D:44:TYR:HD1	1.86	0.41
9:I:208:ALA:HB3	9:I:230:GLN:HE21	1.85	0.41
15:O:112:SER:HB2	15:O:127:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:123:SER:HB3	16:P:137:VAL:HB	2.03	0.41
21:U:17:PRO:HA	21:U:20:LYS:HB2	2.02	0.41
21:U:494:TYR:CD1	21:U:520:MET:HE3	2.56	0.41
21:U:619:VAL:HG11	21:U:648:VAL:HG13	2.03	0.41
23:W:208:LYS:O	23:W:211:THR:OG1	2.37	0.41
23:W:264:GLN:HB3	23:W:333:LEU:HD21	2.02	0.41
23:W:453:HIS:CE1	26:Z:221:PRO:HG2	2.56	0.41
24:X:173:GLU:HA	24:X:176:THR:HG22	2.03	0.41
25:Y:18:ARG:HG3	25:Y:22:LEU:HD13	2.02	0.41
25:Y:134:LEU:HA	25:Y:137:ARG:HD2	2.02	0.41
26:Z:16:LEU:HD13	26:Z:16:LEU:HA	1.89	0.41
27:a:374:ILE:HD11	30:d:251:ARG:HD2	2.02	0.41
29:c:33:ILE:HD11	29:c:38:LEU:HD12	2.02	0.41
29:c:266:THR:HG22	29:c:269:GLN:H	1.85	0.41
32:f:45:LEU:HD11	32:f:55:GLU:HB2	2.03	0.41
32:f:673:ARG:O	32:f:781:TYR:OH	2.34	0.41
32:f:679:LEU:HD21	32:f:715:HIS:CE1	2.56	0.41
8:h:95:GLN:HG3	15:o:65:LEU:HG	2.02	0.41
9:i:181:GLU:HG2	10:j:52:LYS:HZ3	1.84	0.41
11:k:129:ASP:OD1	11:k:129:ASP:N	2.54	0.41
16:p:35:VAL:HG12	16:p:36:THR:HG23	2.03	0.41
1:A:319:MET:HE3	1:A:319:MET:HB2	1.96	0.41
2:B:70:ASP:O	2:B:74:MET:HG2	2.21	0.41
5:E:363:VAL:HG13	5:E:366:ASP:H	1.87	0.41
8:H:79:MET:H	8:H:132:VAL:HG12	1.85	0.41
22:V:147:PHE:O	22:V:148:ARG:NH1	2.45	0.41
24:X:391:PRO:HA	24:X:392:PRO:HD3	1.83	0.41
27:a:212:ASN:OD1	27:a:213:PHE:N	2.48	0.41
28:b:126:LYS:HA	28:b:129:LYS:HG2	2.03	0.41
30:d:234:ASP:OD1	30:d:235:THR:N	2.53	0.41
20:t:9:THR:OG1	20:t:10:SER:N	2.54	0.41
2:B:183:THR:OG1	2:B:184:TYR:N	2.47	0.40
2:B:334:ILE:HD12	2:B:334:ILE:HA	1.95	0.40
3:C:196:LYS:HA	3:C:317:PHE:HE2	1.87	0.40
6:F:141:ASP:OD1	6:F:144:LYS:NZ	2.37	0.40
12:L:35:THR:HG23	12:L:133:LEU:HD12	2.02	0.40
14:N:26:ILE:O	20:t:179:ARG:NH1	2.48	0.40
16:P:30:ILE:HG22	16:P:31:GLN:H	1.86	0.40
23:W:312:MET:HG3	23:W:314:LEU:HD23	2.02	0.40
28:b:12:ASN:OD1	28:b:12:ASN:N	2.52	0.40
30:d:15:ASN:HB2	30:d:18:LYS:HE2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:66:LYS:HE3	30:d:66:LYS:HB3	1.91	0.40
16:p:45:MET:HE3	16:p:67:LEU:HD22	2.03	0.40
16:p:47:ASP:OD1	16:p:47:ASP:N	2.54	0.40
19:s:28:ARG:NH2	19:s:191:ASP:OD1	2.51	0.40
2:B:309:MET:HE3	2:B:338:ASP:HB2	2.04	0.40
5:E:26:LEU:HD21	5:E:30:ARG:HE	1.85	0.40
17:Q:4:LEU:HD22	17:Q:45:LEU:HD23	2.03	0.40
22:V:75:ILE:HD11	22:V:108:LEU:HD21	2.03	0.40
23:W:125:ILE:HD12	23:W:125:ILE:HA	1.96	0.40
23:W:153:LYS:HA	23:W:153:LYS:HD3	1.77	0.40
23:W:173:THR:HG23	23:W:182:ARG:NH2	2.37	0.40
23:W:391:ALA:O	23:W:395:ASN:ND2	2.54	0.40
27:a:273:GLN:HB3	27:a:310:LEU:HD11	2.03	0.40
27:a:360:VAL:HG22	29:c:308:VAL:HG13	2.04	0.40
29:c:175:ARG:HD3	29:c:181:LEU:HD12	2.03	0.40
30:d:190:LEU:HD22	30:d:192:THR:HG22	2.03	0.40
32:f:24:THR:HG21	32:f:71:TYR:HE1	1.86	0.40
32:f:246:SER:HA	32:f:253:LEU:HD22	2.03	0.40
32:f:530:CYS:SG	32:f:533:ASP:HB2	2.61	0.40
13:m:240:LYS:HE3	13:m:240:LYS:HB2	1.86	0.40
3:C:90:HIS:CG	3:C:91:PRO:HD3	2.55	0.40
4:D:159:LYS:HA	4:D:160:PRO:HD3	1.90	0.40
21:U:510:GLU:HA	21:U:547:GLY:HA3	2.03	0.40
27:a:202:LEU:HD23	27:a:202:LEU:HA	1.94	0.40
27:a:343:LEU:HA	27:a:346:ILE:HD12	2.03	0.40
15:o:81:ARG:HA	15:o:81:ARG:HD2	1.96	0.40
1:A:113:ILE:HD12	1:A:123:VAL:HG21	2.04	0.40
9:I:241:GLU:HA	9:I:244:GLU:HG3	2.04	0.40
17:Q:11:ASP:OD1	17:Q:11:ASP:N	2.54	0.40
21:U:540:GLN:O	29:c:208:ARG:NH1	2.46	0.40
21:U:769:PHE:HB3	21:U:776:SER:OG	2.21	0.40
22:V:397:ARG:HH21	30:d:116:HIS:HB3	1.87	0.40
23:W:118:LEU:HD13	23:W:118:LEU:HA	1.87	0.40
29:c:29:GLU:HB2	29:c:203:ILE:HD11	2.02	0.40
32:f:6:ARG:HD2	32:f:6:ARG:HA	1.98	0.40
32:f:372:LEU:HD12	32:f:372:LEU:HA	1.86	0.40
11:k:189:MET:HE3	11:k:194:ALA:HB2	2.03	0.40
12:l:193:ARG:HG2	12:l:196:ARG:HH12	1.87	0.40
3:C:90:HIS:CD2	3:C:90:HIS:H	2.38	0.40
4:D:47:LEU:HD23	4:D:47:LEU:HA	1.86	0.40
4:D:385:LEU:HD23	4:D:398:ASP:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:117:PRO:HD3	6:F:94:ILE:HG23	2.04	0.40
6:F:43:GLN:HA	6:F:46:ARG:HG2	2.02	0.40
18:R:27:ALA:O	16:p:177:ARG:NH1	2.52	0.40
20:T:92:LEU:HD23	20:T:92:LEU:HA	1.92	0.40
24:X:317:PRO:HG2	24:X:318:ILE:HD12	2.02	0.40
24:X:339:ILE:HA	24:X:342:PHE:CZ	2.57	0.40
30:d:49:ILE:HD11	30:d:90:PRO:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/433 (90%)	344 (88%)	48 (12%)	0	100	100
2	B	382/440 (87%)	359 (94%)	23 (6%)	0	100	100
3	C	359/398 (90%)	330 (92%)	29 (8%)	0	100	100
4	D	378/418 (90%)	343 (91%)	35 (9%)	0	100	100
5	E	387/403 (96%)	362 (94%)	24 (6%)	1 (0%)	36	68
6	F	413/439 (94%)	387 (94%)	26 (6%)	0	100	100
7	G	242/246 (98%)	231 (96%)	11 (4%)	0	100	100
7	g	242/246 (98%)	226 (93%)	16 (7%)	0	100	100
8	H	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
8	h	230/234 (98%)	217 (94%)	13 (6%)	0	100	100
9	I	249/261 (95%)	240 (96%)	9 (4%)	0	100	100
9	i	248/261 (95%)	241 (97%)	7 (3%)	0	100	100
10	J	237/248 (96%)	226 (95%)	11 (5%)	0	100	100
10	j	237/248 (96%)	223 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	232/241 (96%)	220 (95%)	11 (5%)	1 (0%)	30	62
11	k	232/241 (96%)	225 (97%)	7 (3%)	0	100	100
12	L	236/269 (88%)	231 (98%)	5 (2%)	0	100	100
12	l	236/269 (88%)	228 (97%)	8 (3%)	0	100	100
13	M	238/255 (93%)	237 (100%)	1 (0%)	0	100	100
13	m	238/255 (93%)	237 (100%)	1 (0%)	0	100	100
14	N	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
14	n	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
15	O	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
15	o	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
16	P	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
16	p	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
17	Q	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
17	q	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
18	R	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
18	r	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
19	S	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
19	s	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
20	T	214/264 (81%)	207 (97%)	7 (3%)	0	100	100
20	t	214/264 (81%)	205 (96%)	9 (4%)	0	100	100
21	U	806/953 (85%)	765 (95%)	41 (5%)	0	100	100
22	V	442/534 (83%)	434 (98%)	7 (2%)	1 (0%)	43	73
23	W	444/456 (97%)	421 (95%)	23 (5%)	0	100	100
24	X	378/422 (90%)	357 (94%)	21 (6%)	0	100	100
25	Y	376/389 (97%)	335 (89%)	41 (11%)	0	100	100
26	Z	284/324 (88%)	261 (92%)	23 (8%)	0	100	100
27	a	371/376 (99%)	343 (92%)	28 (8%)	0	100	100
28	b	189/377 (50%)	172 (91%)	16 (8%)	1 (0%)	24	59
29	c	285/310 (92%)	259 (91%)	26 (9%)	0	100	100
30	d	255/350 (73%)	225 (88%)	29 (11%)	1 (0%)	30	62
31	e	48/70 (69%)	42 (88%)	6 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	f	887/908 (98%)	760 (86%)	126 (14%)	1 (0%)	48	79
33	u	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
34	v	1/10 (10%)	0	0	1 (100%)	0	0
35	x	74/494 (15%)	71 (96%)	3 (4%)	0	100	100
All	All	13434/15468 (87%)	12634 (94%)	793 (6%)	7 (0%)	49	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	d	203	PRO
5	E	242	ARG
22	V	496	PHE
34	v	25	LYS
32	f	871	PRO
28	b	23	PRO
11	K	130	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	337/372 (91%)	336 (100%)	1 (0%)	86	88
2	B	339/385 (88%)	338 (100%)	1 (0%)	86	88
3	C	314/346 (91%)	312 (99%)	2 (1%)	78	84
4	D	333/366 (91%)	333 (100%)	0	100	100
5	E	341/353 (97%)	336 (98%)	5 (2%)	57	76
6	F	357/379 (94%)	357 (100%)	0	100	100
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	202 (100%)	0	100	100
8	H	188/191 (98%)	188 (100%)	0	100	100
8	h	188/191 (98%)	188 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	207/221 (94%)	205 (99%)	2 (1%)	68	80
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	201/211 (95%)	201 (100%)	0	100	100
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	193/203 (95%)	193 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/230 (88%)	202 (100%)	0	100	100
12	l	201/230 (87%)	201 (100%)	0	100	100
13	M	196/212 (92%)	196 (100%)	0	100	100
13	m	198/212 (93%)	198 (100%)	0	100	100
14	N	157/181 (87%)	157 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	179/228 (78%)	179 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	168/171 (98%)	168 (100%)	0	100	100
17	q	168/171 (98%)	168 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	156/202 (77%)	156 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	178/199 (89%)	178 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	692/816 (85%)	692 (100%)	0	100	100
22	V	390/460 (85%)	390 (100%)	0	100	100
23	W	410/416 (99%)	407 (99%)	3 (1%)	76	83
24	X	327/362 (90%)	327 (100%)	0	100	100
25	Y	334/344 (97%)	333 (100%)	1 (0%)	86	88
26	Z	257/295 (87%)	255 (99%)	2 (1%)	73	82
27	a	333/336 (99%)	332 (100%)	1 (0%)	86	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/268 (94%)	252 (100%)	0	100	100
30	d	231/294 (79%)	231 (100%)	0	100	100
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	745/763 (98%)	745 (100%)	0	100	100
33	u	68/68 (100%)	68 (100%)	0	100	100
34	v	1/1 (100%)	1 (100%)	0	100	100
35	x	64/439 (15%)	64 (100%)	0	100	100
All	All	11490/13134 (88%)	11472 (100%)	18 (0%)	87	89

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	403	ILE
2	B	125	THR
3	C	109	THR
3	C	210	THR
5	E	115	VAL
5	E	118	LEU
5	E	383	LYS
5	E	384	LEU
5	E	385	ASP
9	I	7[A]	SER
9	I	7[B]	SER
23	W	117	ASP
23	W	118	LEU
23	W	120	ILE
25	Y	287	LEU
26	Z	16	LEU
26	Z	17	LEU
27	a	123	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	117	GLN
1	A	203	ASN

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Mol	Chain	Res	Type
1	A	296	GLN
1	A	353	HIS
1	A	414	ASN
1	A	433	ASN
2	B	55	HIS
2	B	181	GLN
2	B	241	ASN
2	B	242	GLN
2	B	257	GLN
2	B	277	HIS
2	B	314	ASN
3	C	53	ASN
3	C	64	GLN
3	C	221	GLN
3	C	337	ASN
4	D	98	GLN
4	D	193	GLN
4	D	237	GLN
4	D	412	GLN
4	D	414	HIS
5	E	55	GLN
5	E	225	HIS
5	E	226	GLN
5	E	359	HIS
6	F	83	ASN
6	F	321	GLN
6	F	380	ASN
7	G	75	ASN
7	G	92	GLN
7	G	128	ASN
9	I	95	GLN
9	I	102	GLN
9	I	230	GLN
10	J	92	GLN
10	J	154	HIS
11	K	73	HIS
11	K	152	GLN
11	K	204	GLN
12	L	90	GLN
13	M	180	GLN
16	P	7	ASN
17	Q	61	GLN

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Mol	Chain	Res	Type
17	Q	82	ASN
18	R	70	ASN
18	R	162	GLN
19	S	79	ASN
19	S	151	ASN
19	S	160	ASN
20	T	69	GLN
20	T	81	HIS
20	T	213	HIS
21	U	70	HIS
21	U	79	ASN
21	U	128	GLN
21	U	192	GLN
21	U	207	ASN
21	U	647	HIS
21	U	734	GLN
21	U	777	HIS
22	V	124	ASN
22	V	168	GLN
22	V	185	GLN
22	V	319	HIS
22	V	453	HIS
22	V	459	GLN
23	W	210	ASN
23	W	218	ASN
23	W	356	ASN
23	W	395	ASN
24	X	198	ASN
24	X	262	ASN
24	X	292	GLN
24	X	296	ASN
24	X	334	ASN
24	X	406	ASN
25	Y	273	GLN
25	Y	365	GLN
26	Z	77	ASN
26	Z	104	ASN
26	Z	109	ASN
26	Z	202	ASN
27	a	9	GLN
27	a	241	ASN
27	a	249	GLN

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Mol	Chain	Res	Type
27	a	258	GLN
27	a	264	ASN
27	a	305	ASN
28	b	30	GLN
28	b	34	ASN
28	b	76	HIS
29	c	92	GLN
29	c	128	ASN
29	c	274	ASN
30	d	4	GLN
30	d	60	GLN
30	d	77	GLN
30	d	88	GLN
32	f	148	GLN
32	f	352	HIS
32	f	382	ASN
32	f	790	GLN
7	g	33	ASN
7	g	150	GLN
9	i	30	HIS
9	i	40	ASN
9	i	95	GLN
9	i	177	GLN
10	j	92	GLN
10	j	154	HIS
10	j	175	ASN
11	k	41	GLN
11	k	186	HIS
13	m	32	ASN
13	m	143	ASN
14	n	66	HIS
14	n	193	GLN
15	o	35	HIS
15	o	165	ASN
17	q	71	ASN
18	r	85	ASN
18	r	196	HIS
20	t	213	HIS
33	u	2	GLN
33	u	41	GLN
33	u	49	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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
38	ADP	F	501	37	28,29,29	1.37	4 (14%)	43,45,45	1.94	8 (18%)
38	ADP	C	501	-	28,29,29	1.39	4 (14%)	43,45,45	1.93	8 (18%)
36	ATP	B	501	37	32,33,33	0.43	0	48,52,52	0.29	0
36	ATP	A	501	37	32,33,33	0.62	2 (6%)	48,52,52	0.37	0
36	ATP	D	501	37	32,33,33	1.38	4 (12%)	48,52,52	1.81	8 (16%)
36	ATP	E	501	37	32,33,33	0.57	1 (3%)	48,52,52	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	ADP	F	501	37	-	5/16/32/32	0/3/3/3
38	ADP	C	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	B	501	37	-	5/22/38/38	0/3/3/3
36	ATP	A	501	37	-	4/22/38/38	0/3/3/3
36	ATP	D	501	37	-	3/22/38/38	0/3/3/3
36	ATP	E	501	37	-	5/22/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	501	ATP	C5-C4	4.68	1.47	1.39
38	F	501	ADP	C5-C4	4.65	1.47	1.39
38	C	501	ADP	C5-C4	4.63	1.47	1.39
38	C	501	ADP	C5-C6	2.64	1.48	1.41
36	D	501	ATP	C5-C6	2.57	1.48	1.41
38	F	501	ADP	C5-N7	-2.56	1.34	1.39
38	C	501	ADP	C5-N7	-2.51	1.34	1.39
38	F	501	ADP	C5-C6	2.49	1.47	1.41
36	D	501	ATP	C5-N7	-2.44	1.34	1.39
36	A	501	ATP	PA-O3A	-2.21	1.57	1.59
36	E	501	ATP	PB-O3B	-2.20	1.57	1.59
38	C	501	ADP	C8-N7	2.18	1.35	1.31
36	D	501	ATP	C8-N7	2.11	1.35	1.31
38	F	501	ADP	C8-N7	2.10	1.35	1.31
36	A	501	ATP	PB-O3B	-2.10	1.57	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	F	501	ADP	C5-C4-N3	-6.53	117.72	126.72
36	D	501	ATP	C5-C4-N3	-6.39	117.91	126.72
38	C	501	ADP	C5-C4-N3	-6.36	117.96	126.72
38	F	501	ADP	N3-C4-N9	5.32	136.22	127.17
36	D	501	ATP	N3-C4-N9	5.22	136.04	127.17
38	C	501	ADP	N3-C4-N9	5.11	135.86	127.17
38	F	501	ADP	C2-N3-C4	3.97	121.53	111.83
36	D	501	ATP	C2-N3-C4	3.96	121.50	111.83
38	C	501	ADP	C2-N3-C4	3.91	121.38	111.83
38	C	501	ADP	C4-C5-N7	-3.34	106.76	110.58
38	F	501	ADP	N3-C2-N1	-3.30	123.59	128.58
38	C	501	ADP	N3-C2-N1	-3.27	123.64	128.58
36	D	501	ATP	N3-C2-N1	-3.22	123.71	128.58
38	F	501	ADP	C4-C5-N7	-3.14	107.00	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	501	ATP	C4-C5-N7	-2.93	107.23	110.58
38	C	501	ADP	C3'-C2'-C1'	2.85	106.85	101.46
38	F	501	ADP	C3'-C2'-C1'	2.73	106.63	101.46
38	C	501	ADP	C5-N7-C8	2.53	107.42	103.45
38	C	501	ADP	C4-N9-C8	2.34	108.20	105.74
38	F	501	ADP	C5-N7-C8	2.33	107.12	103.45
38	F	501	ADP	C4-N9-C8	2.24	108.09	105.74
36	D	501	ATP	C5-N7-C8	2.15	106.83	103.45
36	D	501	ATP	C4-N9-C8	2.09	107.94	105.74
36	D	501	ATP	C3'-C2'-C1'	2.05	105.35	101.46

There are no chirality outliers.

All (24) torsion outliers are listed below:

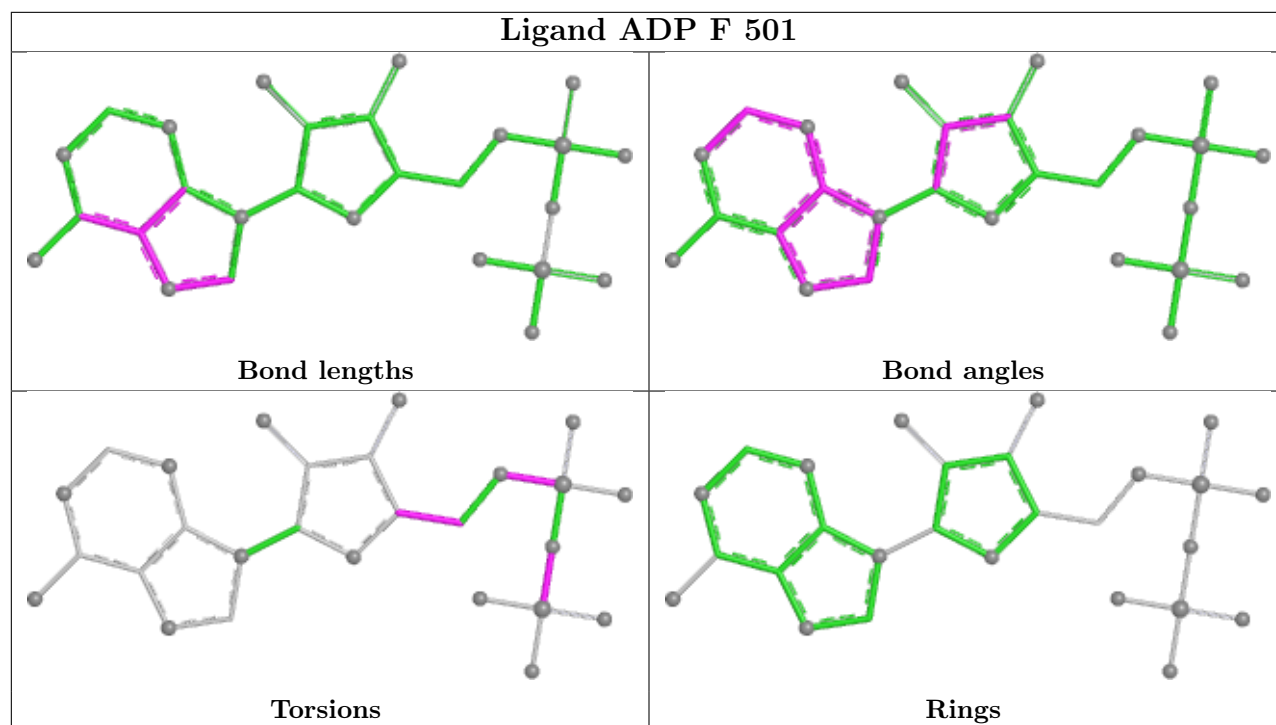
Mol	Chain	Res	Type	Atoms
36	A	501	ATP	C5'-O5'-PA-O2A
36	A	501	ATP	C5'-O5'-PA-O3A
36	B	501	ATP	C5'-O5'-PA-O1A
36	B	501	ATP	C5'-O5'-PA-O3A
36	D	501	ATP	C5'-O5'-PA-O1A
36	E	501	ATP	C5'-O5'-PA-O3A
38	C	501	ADP	C5'-O5'-PA-O2A
38	C	501	ADP	C5'-O5'-PA-O3A
38	F	501	ADP	PA-O3A-PB-O3B
38	F	501	ADP	C5'-O5'-PA-O2A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

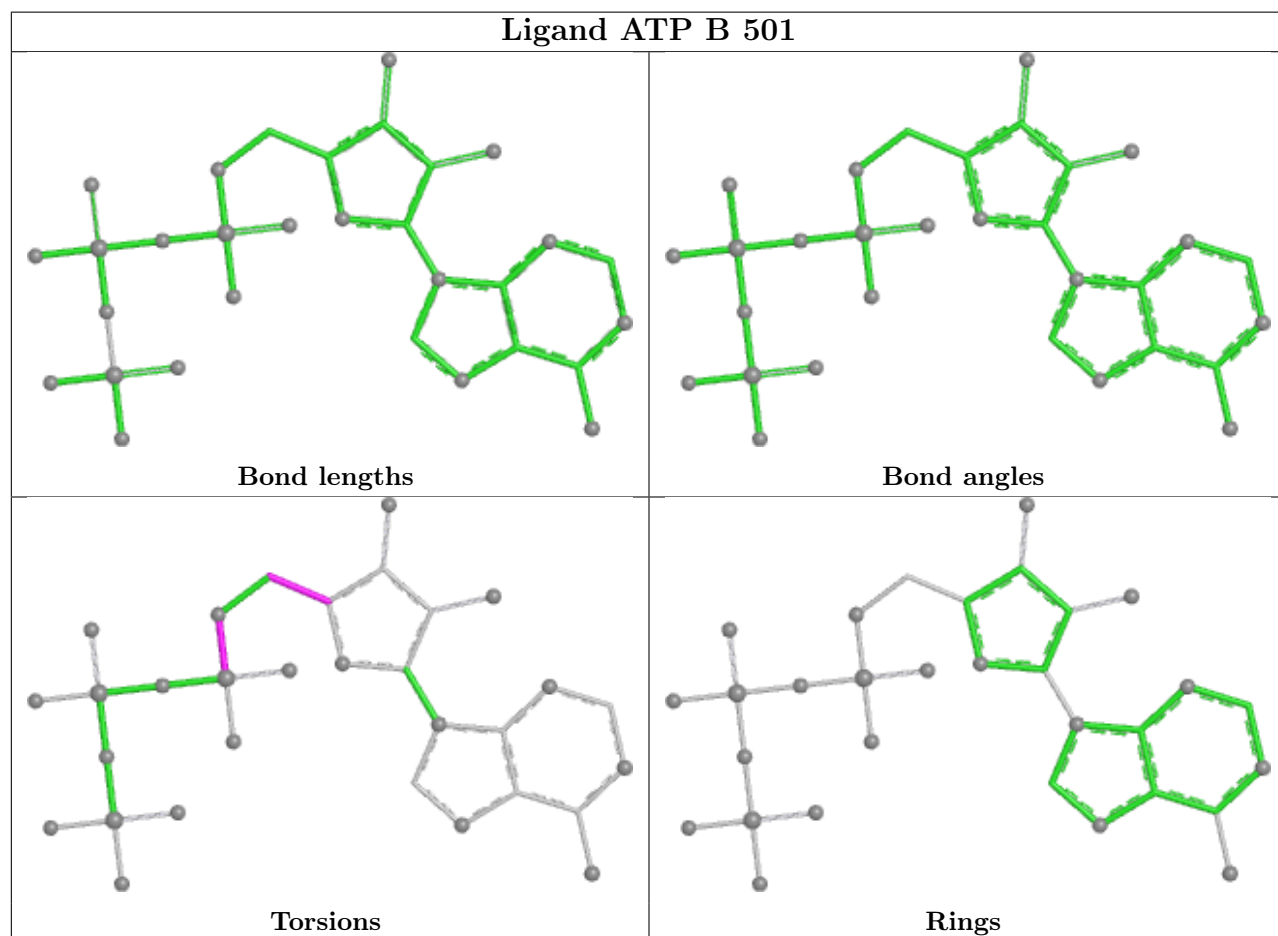
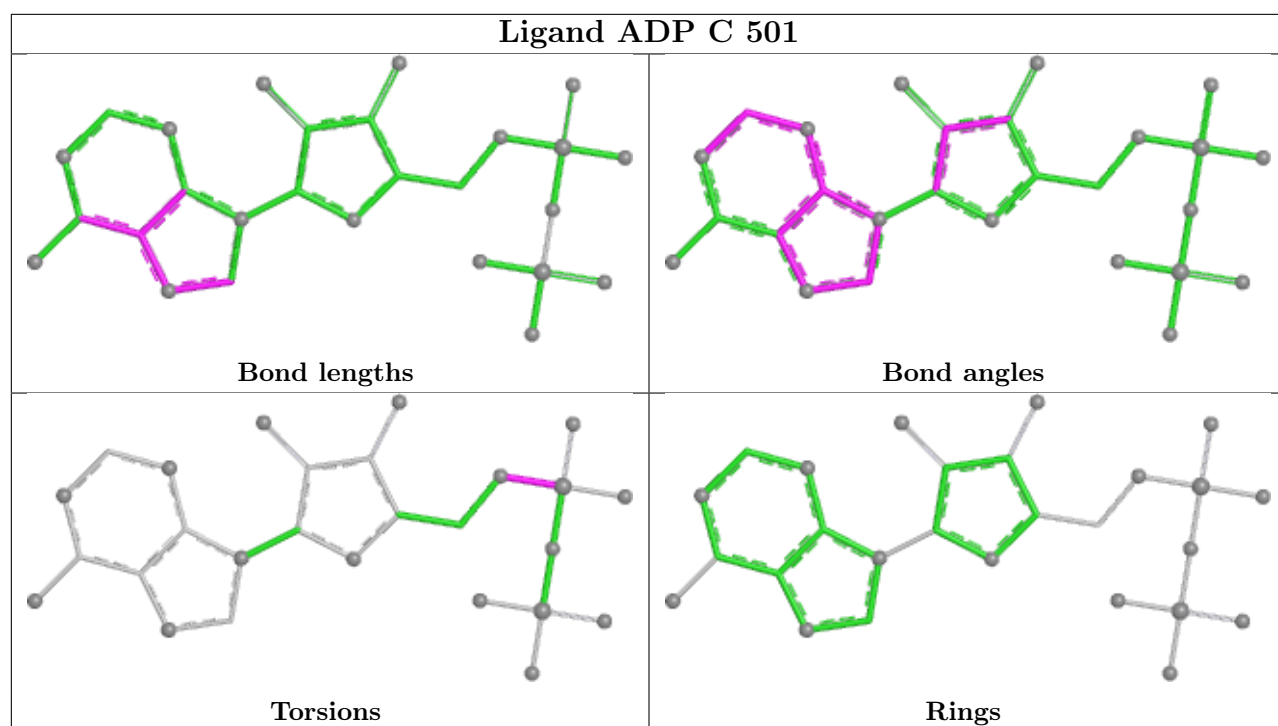
There are no ring outliers.

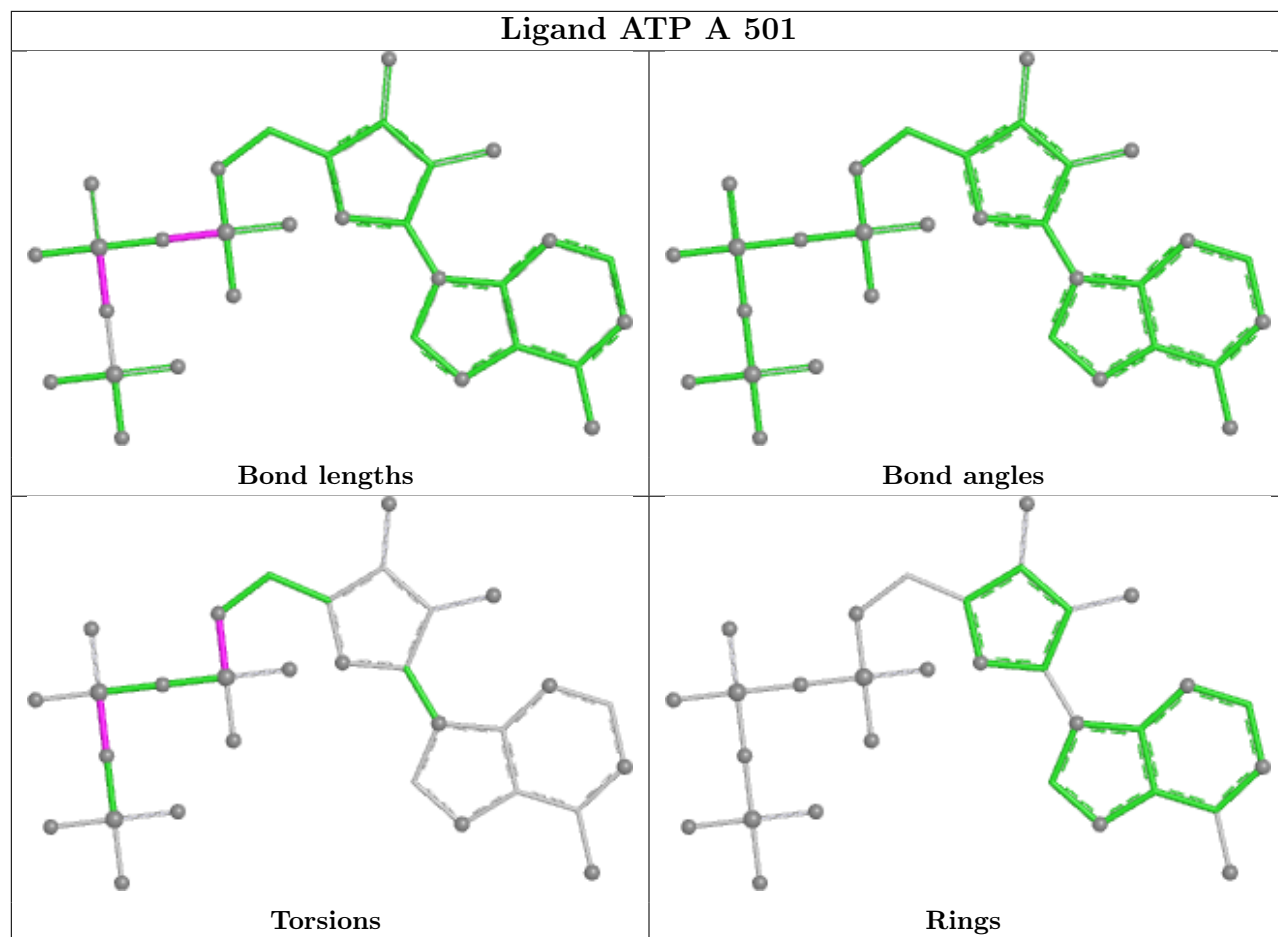
3 monomers are involved in 3 short contacts:

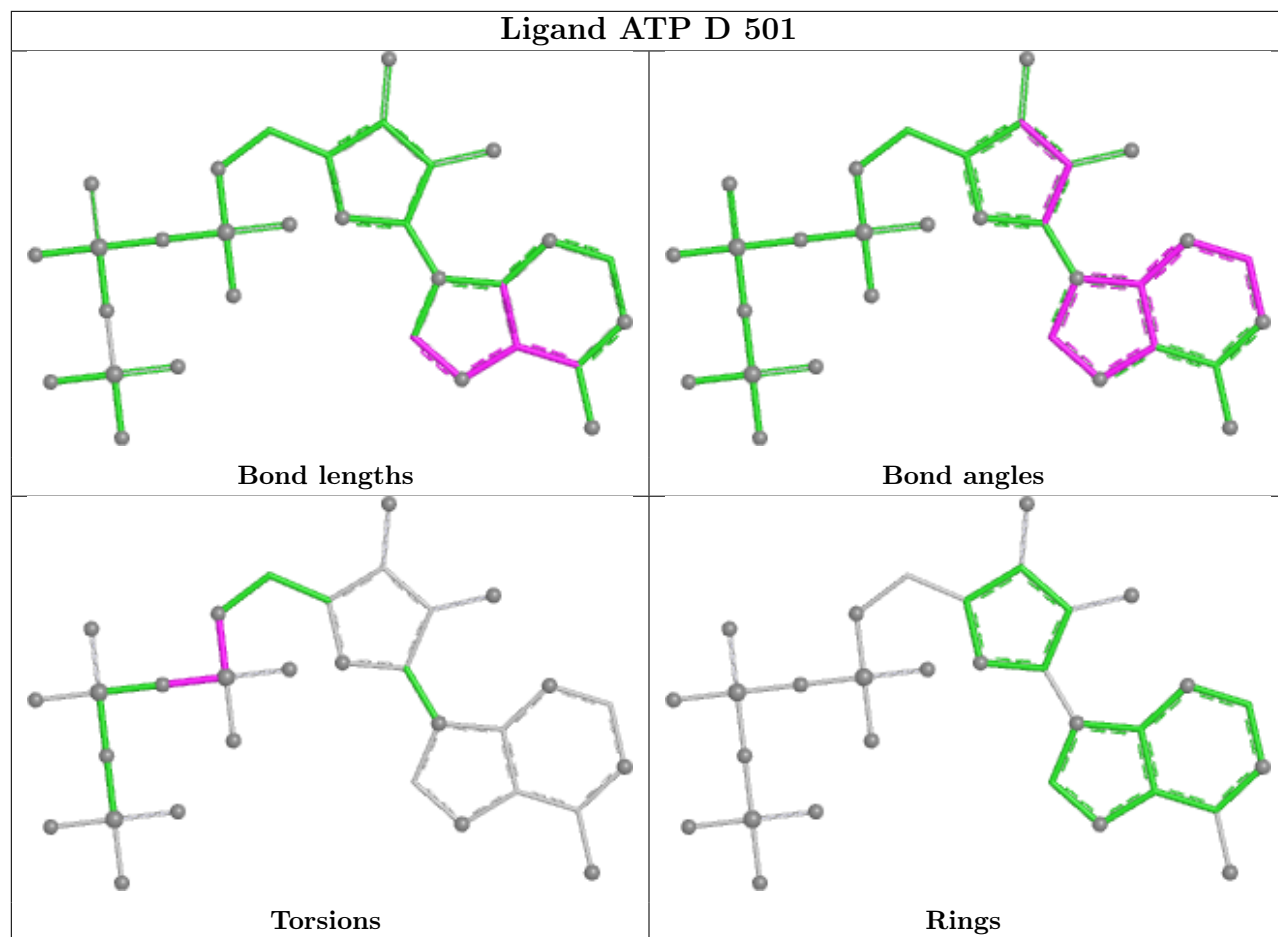
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	C	501	ADP	1	0
36	B	501	ATP	1	0
36	A	501	ATP	1	0

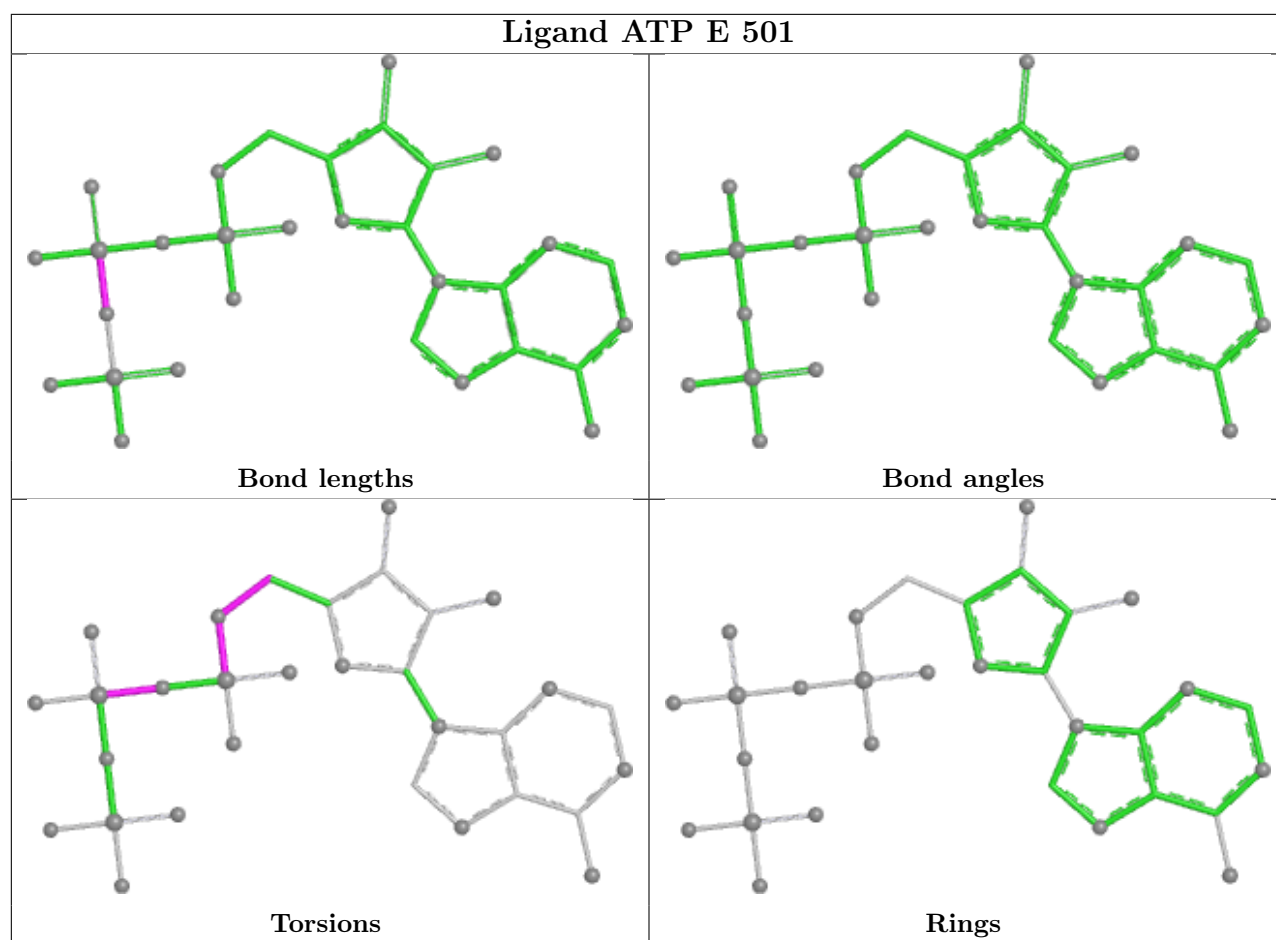
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

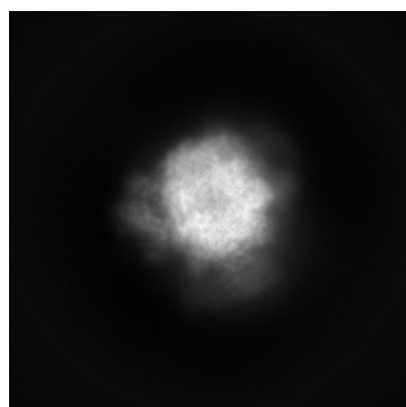
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32274. These allow visual inspection of the internal detail of the map and identification of artifacts.

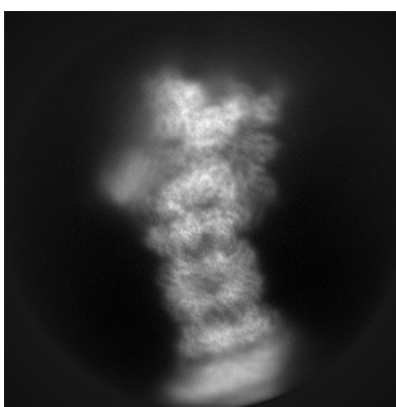
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

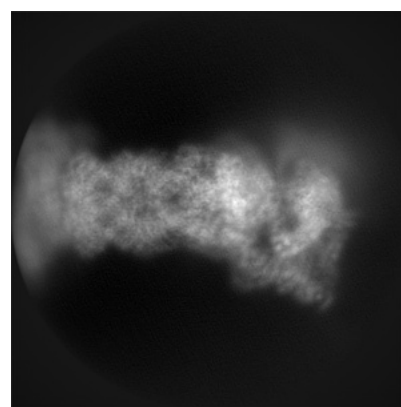
6.1.1 Primary map



X



Y

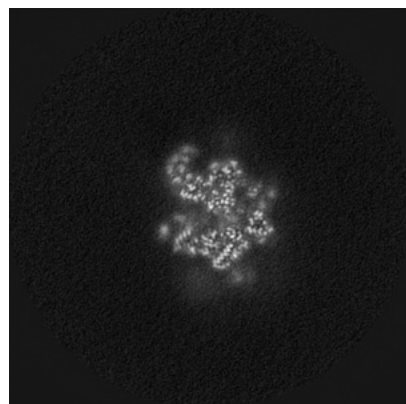


Z

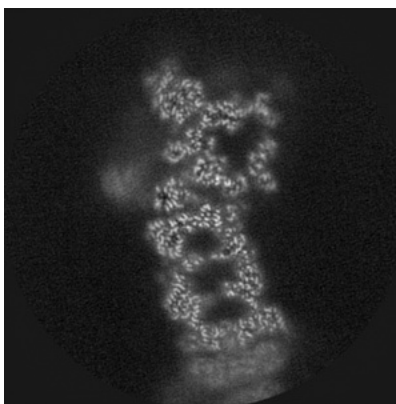
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

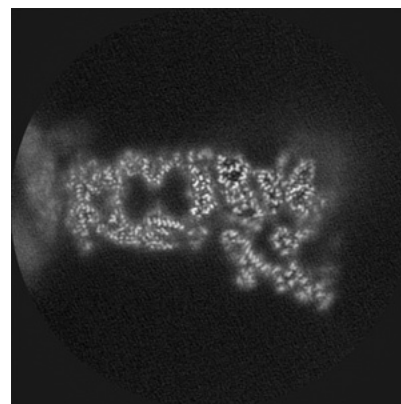
6.2.1 Primary map



X Index: 320



Y Index: 320

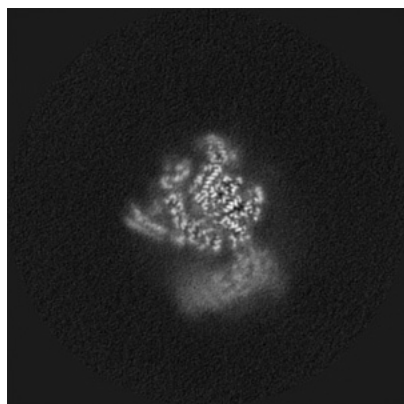


Z Index: 320

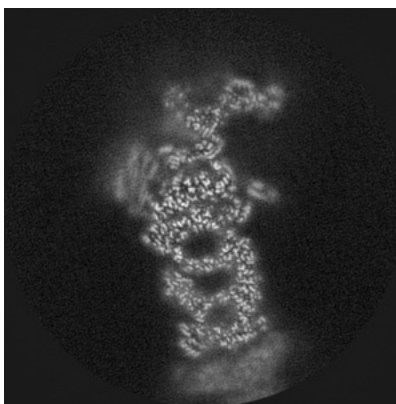
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

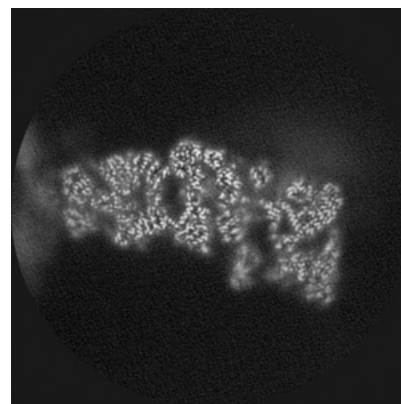
6.3.1 Primary map



X Index: 360



Y Index: 360

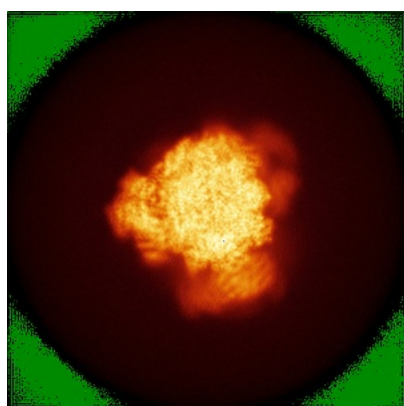


Z Index: 296

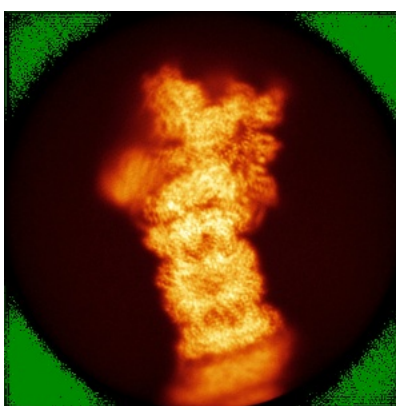
The images above show the largest variance slices of the map in three orthogonal directions.

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

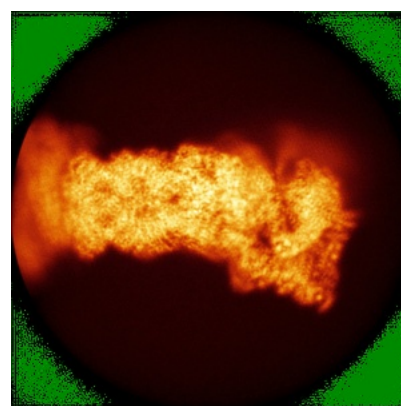
6.4.1 Primary map



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

This section was not generated.

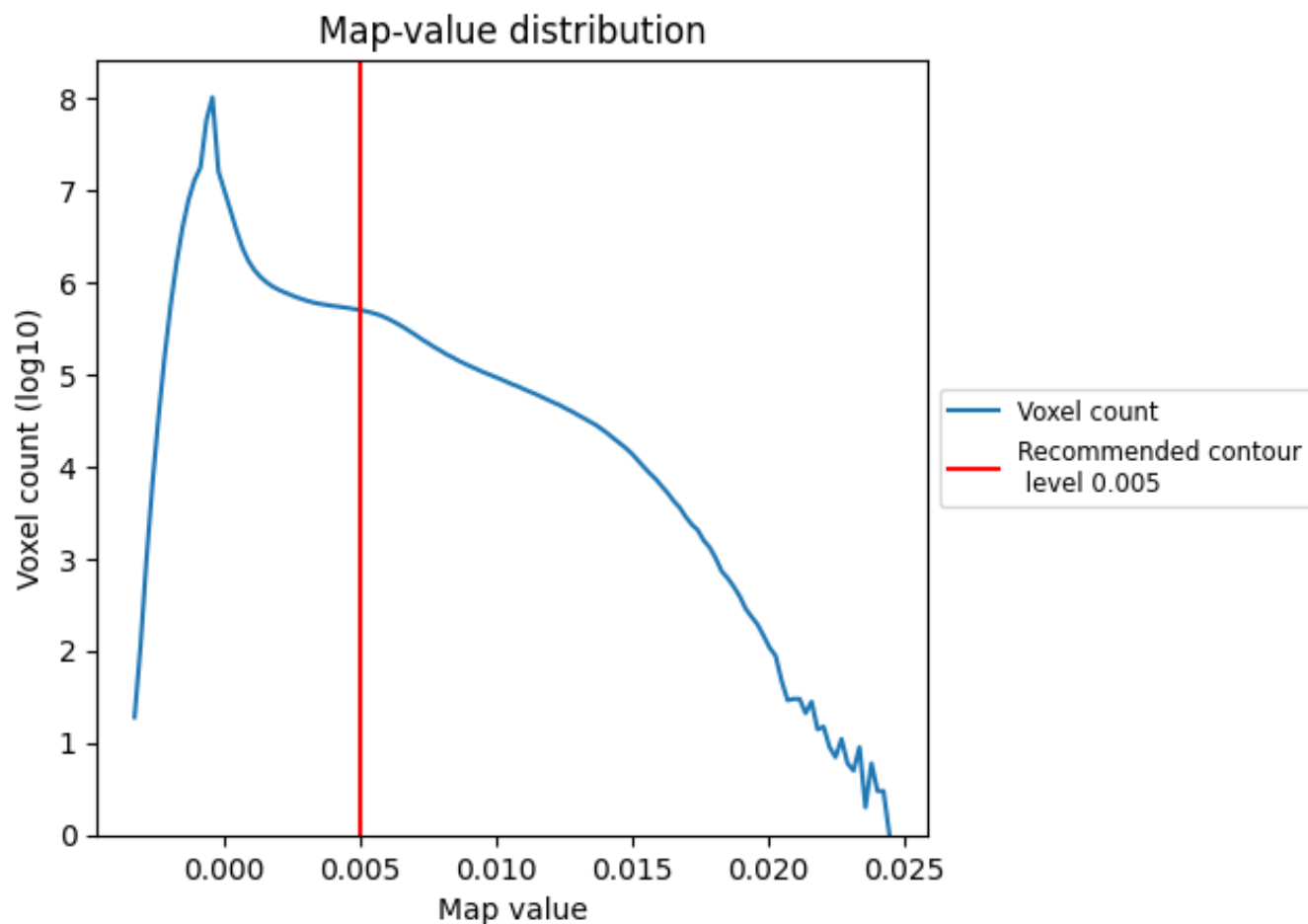
6.6 Mask visualisation

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

7 Map analysis [i](#)

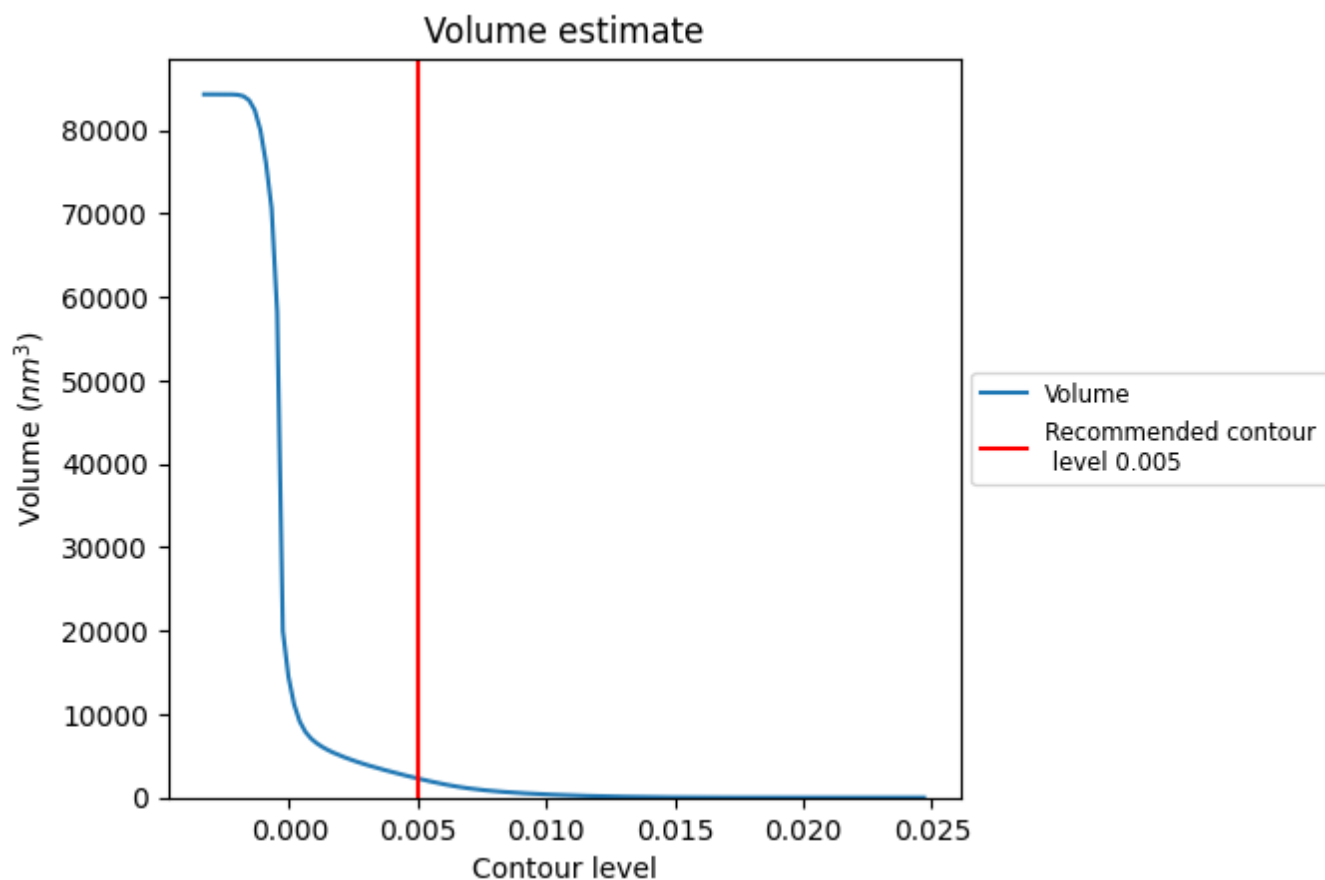
This section contains the results of statistical analysis of the map.

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.

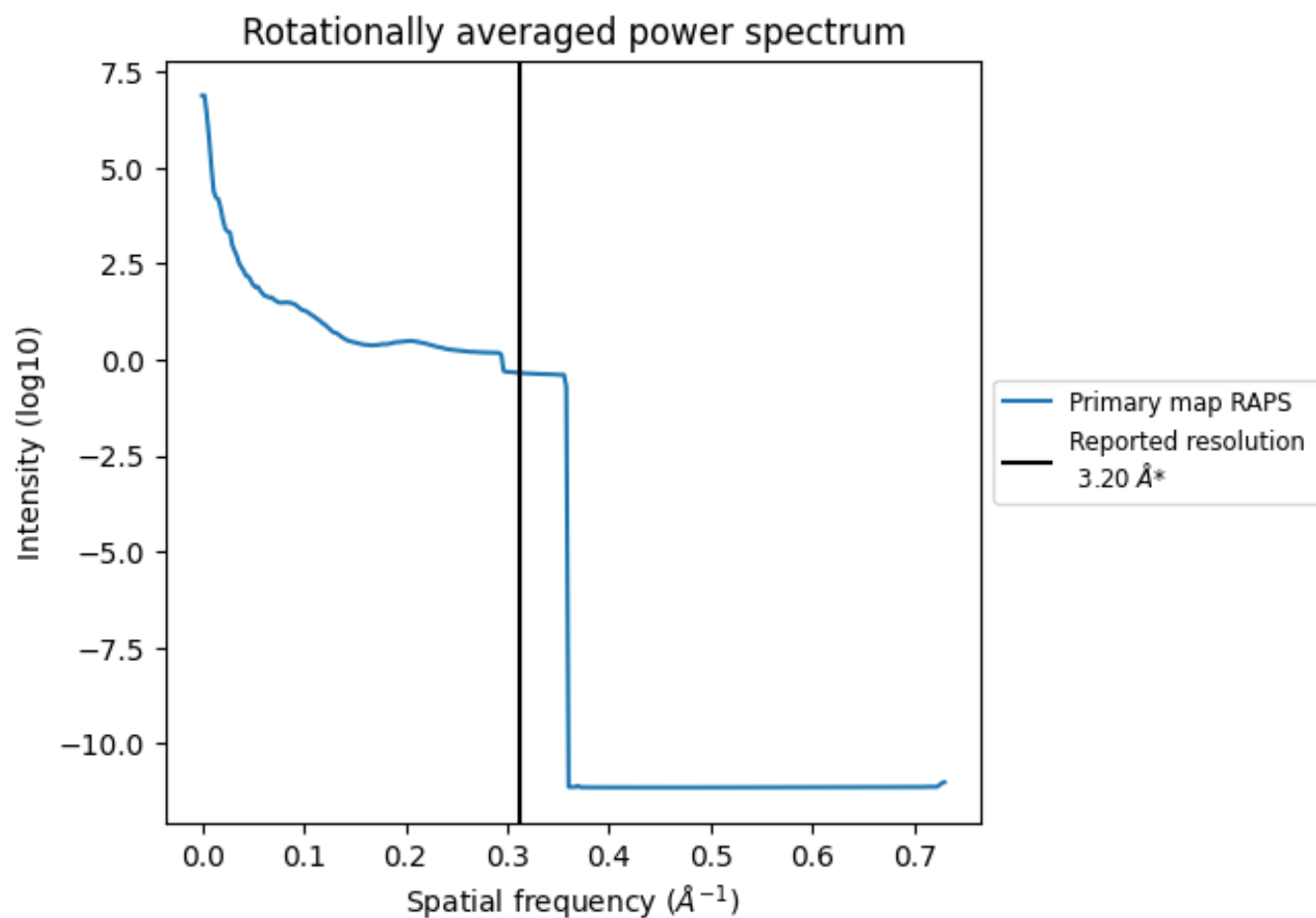
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2293 nm^3 ; this corresponds to an approximate mass of 2072 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

8 Fourier-Shell correlation ⓘ

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

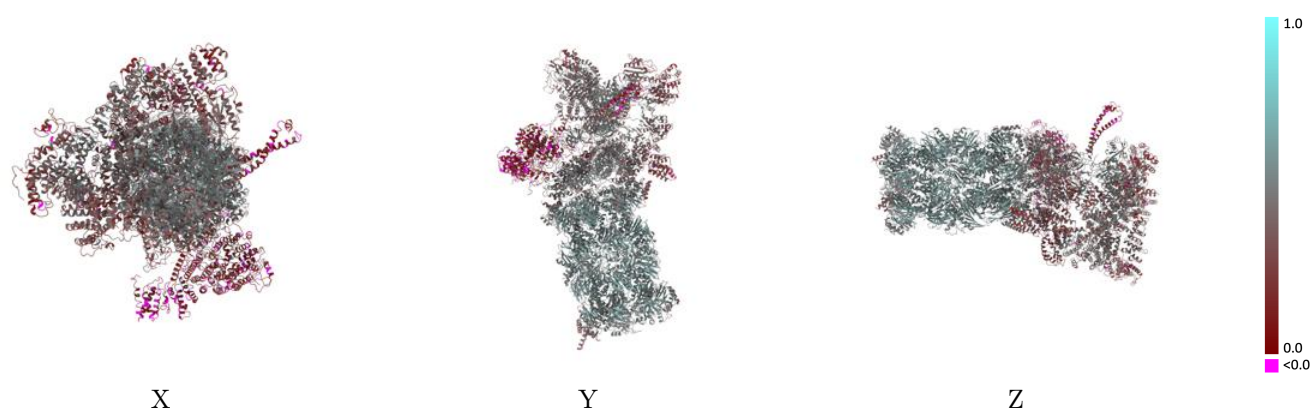
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-32274 and PDB model 7W39. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

This section was not generated.

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

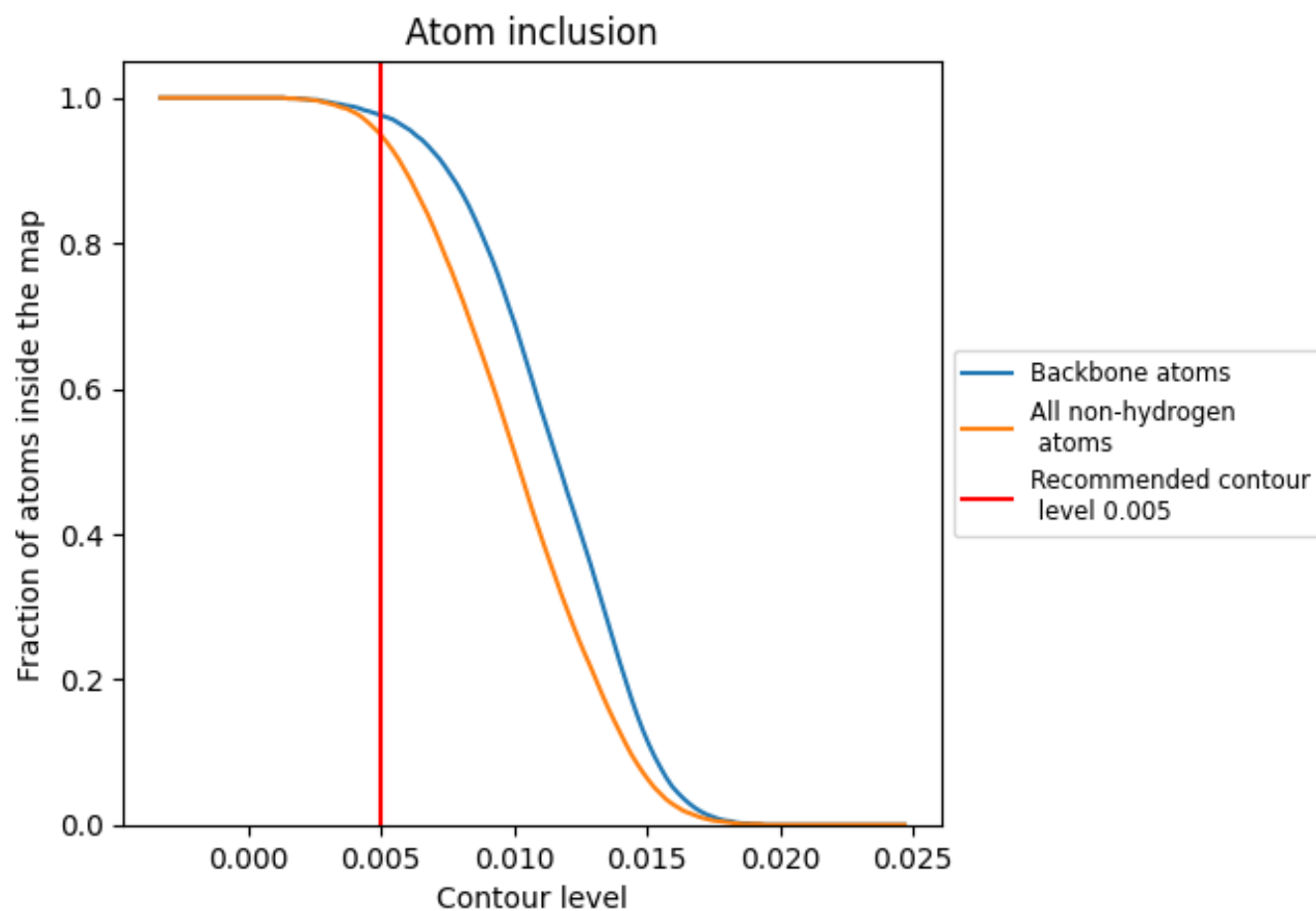


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.4300
A	 0.9720	 0.4240
B	 0.9710	 0.3860
C	 0.9810	 0.3870
D	 0.9810	 0.4160
E	 0.9210	 0.4150
F	 0.8970	 0.4180
G	 0.9840	 0.5180
H	 0.9860	 0.5230
I	 0.9840	 0.5070
J	 0.9760	 0.4870
K	 0.9810	 0.5210
L	 0.9890	 0.5360
M	 0.9900	 0.5200
N	 0.9910	 0.5510
O	 0.9920	 0.5430
P	 0.9950	 0.5460
Q	 0.9900	 0.5400
R	 0.9930	 0.5370
S	 0.9910	 0.5410
T	 0.9900	 0.5540
U	 0.9590	 0.3940
V	 0.9500	 0.3900
W	 0.9120	 0.3110
X	 0.9470	 0.3350
Y	 0.9410	 0.3110
Z	 0.9650	 0.4110
a	 0.9280	 0.3210
b	 0.9360	 0.3480
c	 0.9680	 0.4440
d	 0.8940	 0.2820
e	 0.9430	 0.3440
f	 0.7910	 0.1480
g	 0.9770	 0.5220
h	 0.9850	 0.5180



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Chain	Atom inclusion	Q-score
i	 0.9620	 0.4920
j	 0.9570	 0.4590
k	 0.9760	 0.5060
l	 0.9860	 0.5290
m	 0.9800	 0.5160
n	 0.9950	 0.5610
o	 0.9910	 0.5490
p	 0.9970	 0.5530
q	 0.9950	 0.5480
r	 0.9940	 0.5510
s	 0.9860	 0.5440
t	 0.9870	 0.5570
u	 0.9780	 0.4550
v	 1.0000	 0.2250
x	 0.0240	 0.1320