



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:48 AM UTC

PDB ID : 5VGZ / pdb_00005vgz
EMDB ID : EMD-8672
Title : Conformational Landscape of the p28-Bound Human Proteasome Regulatory Particle
Authors : Lu, Y.; Wu, J.; Dong, Y.; Chen, S.; Sun, S.; Ma, Y.B.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.
Deposited on : 2017-04-12
Resolution : 4.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
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

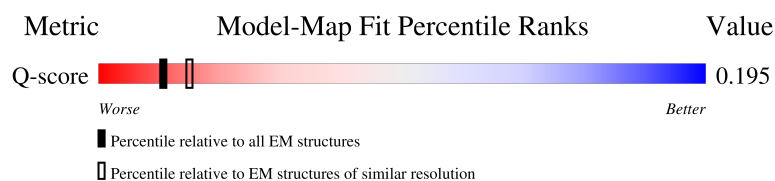
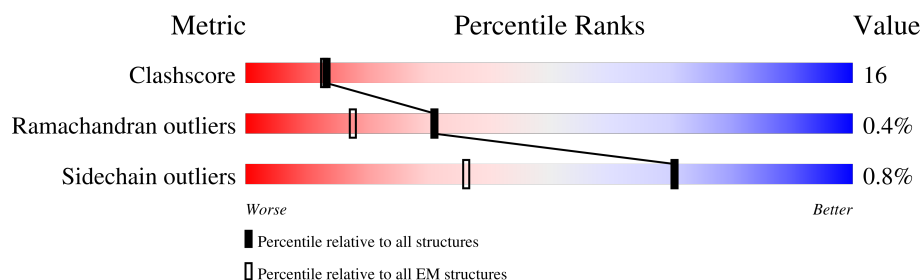
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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

Mol	Chain	Length	Quality of chain
1	A	83	14% 77% 23%
2	B	73	14% 66% 34%
3	C	118	9% 58% 41% .
4	D	107	9% 70% 30%

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Mol	Chain	Length	Quality of chain
5	E	104	
6	F	115	
7	U	935	
8	V	488	
9	W	456	
10	X	385	
11	Y	378	
12	Z	286	
13	a	374	
14	b	191	
15	c	287	
16	d	257	
17	e	70	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 36741 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	83	Total	C	N	O	S	0	0
			654	416	111	125	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	73	Total	C	N	O	S	0	0
			556	346	92	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	118	Total	C	N	O	S	0	0
			954	597	176	179	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	107	Total	C	N	O	0	0
			870	555	147	168		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	104	Total	C	N	O	S	0	0
			853	537	155	158	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	101	Total	C	N	O	S	0	0
			799	512	133	151	3		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	845	Total	C	N	O	S	0	0
			6568	4169	1118	1236	45		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	488	Total	C	N	O	S	0	0
			3919	2487	695	723	14		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	385	Total	C	N	O	S	0	0
			3048	1939	515	582	12		

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	374	Total	C	N	O	S	0	0
			3003	1915	511	562	15		

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

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

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 17 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	e	70	Total	C	N	O	S	0	0
			583	357	89	135	2		

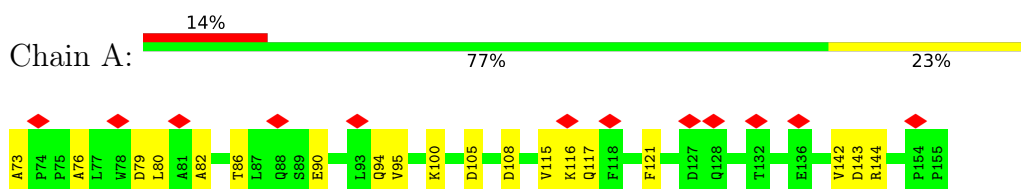
- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

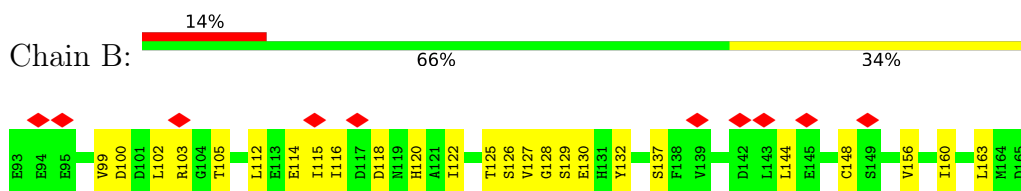
3 Residue-property plots

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.

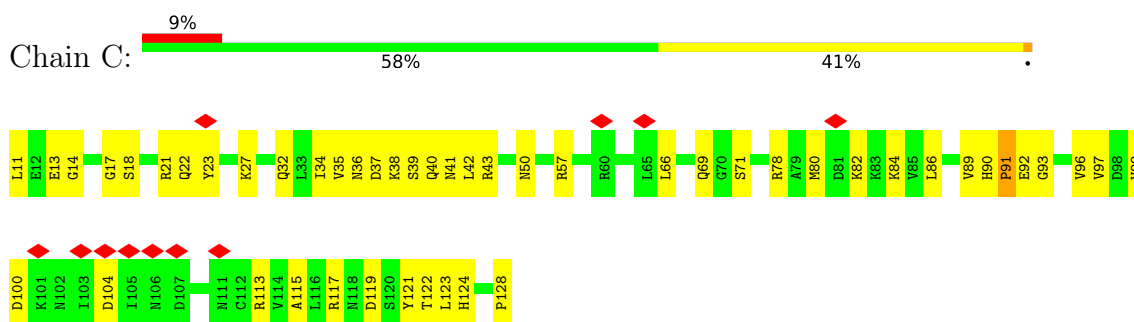
- Molecule 1: 26S proteasome regulatory subunit 7



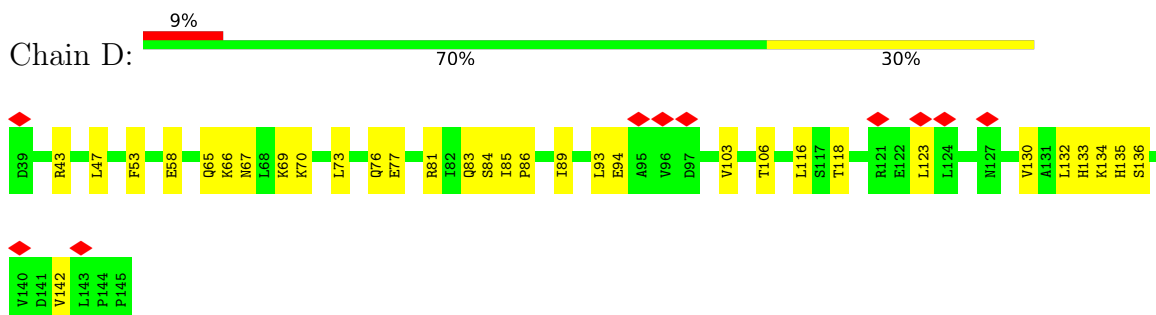
- Molecule 2: 26S proteasome regulatory subunit 4



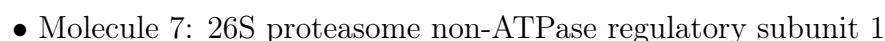
- Molecule 3: 26S proteasome regulatory subunit 8



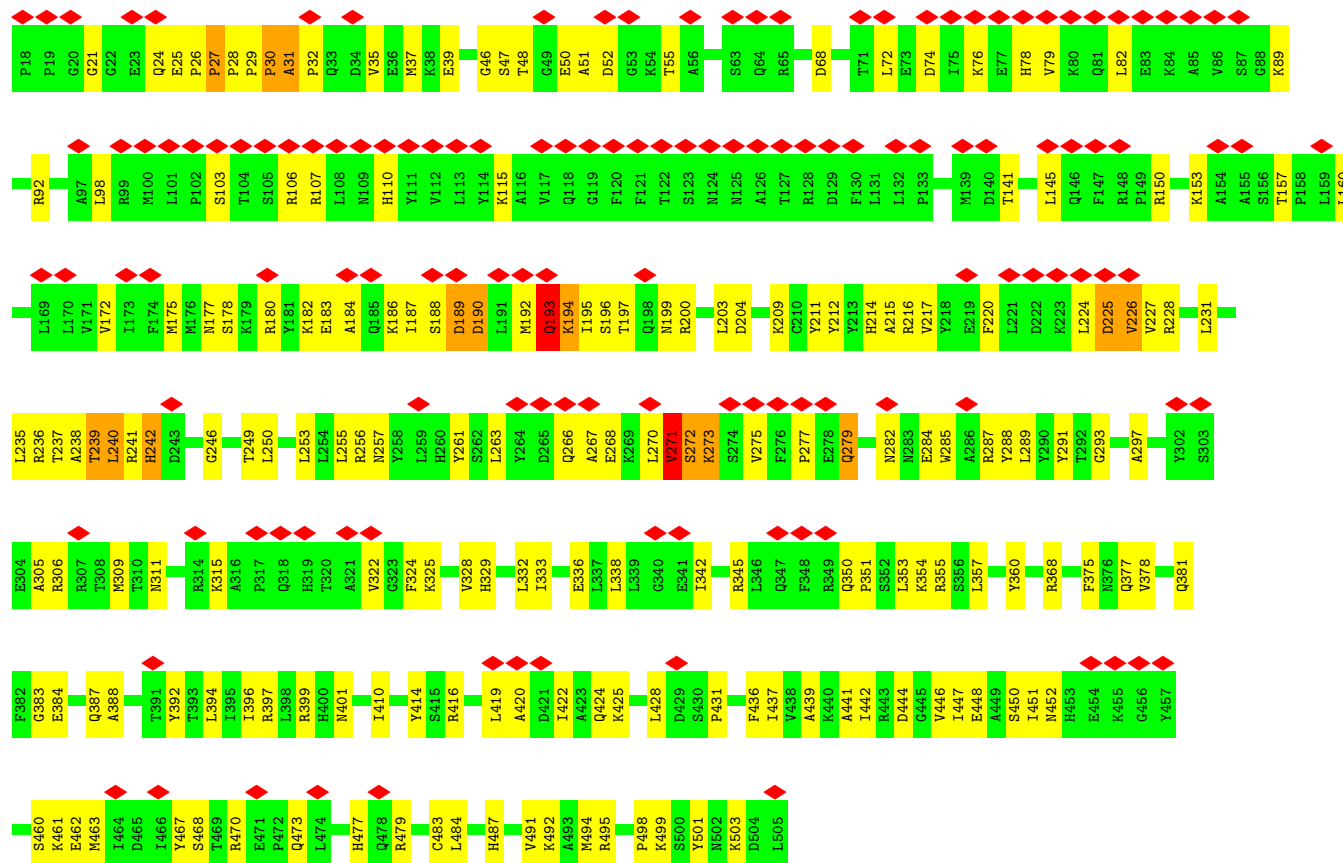
- Molecule 4: 26S proteasome regulatory subunit 6B



Chain E: 26% 66% 33%

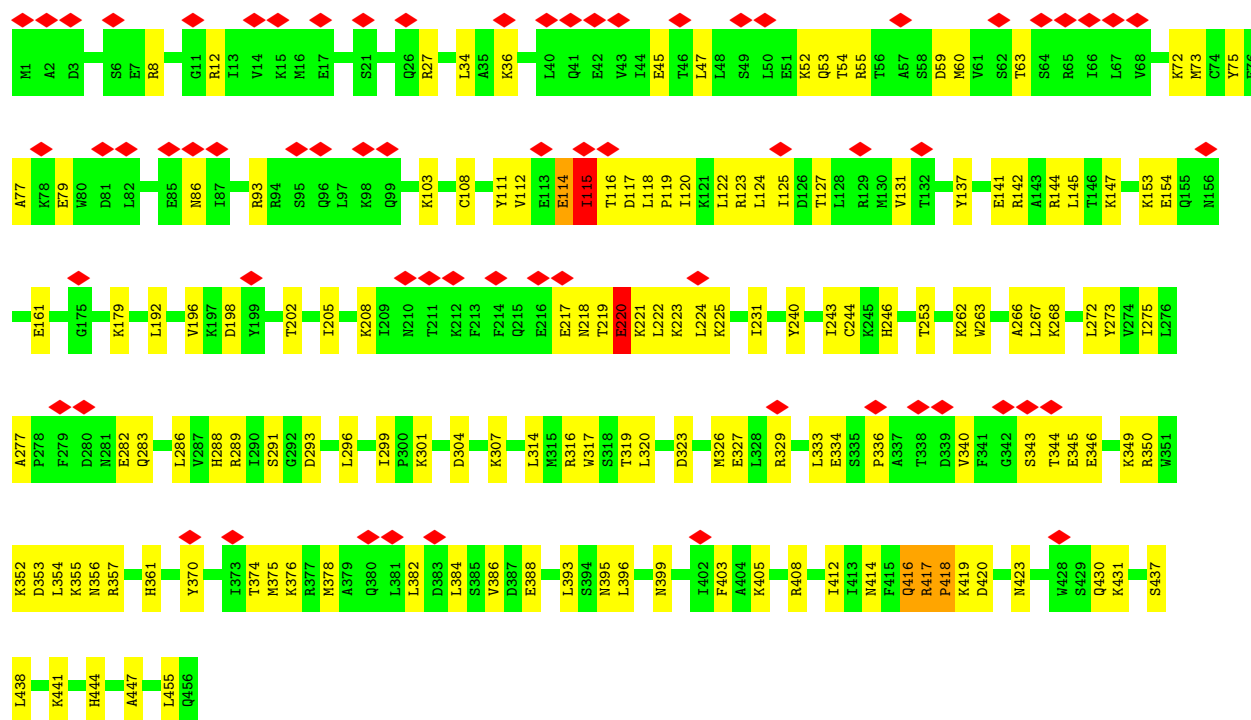


- Molecule 8: 26S proteasome non-ATPase regulatory subunit 3

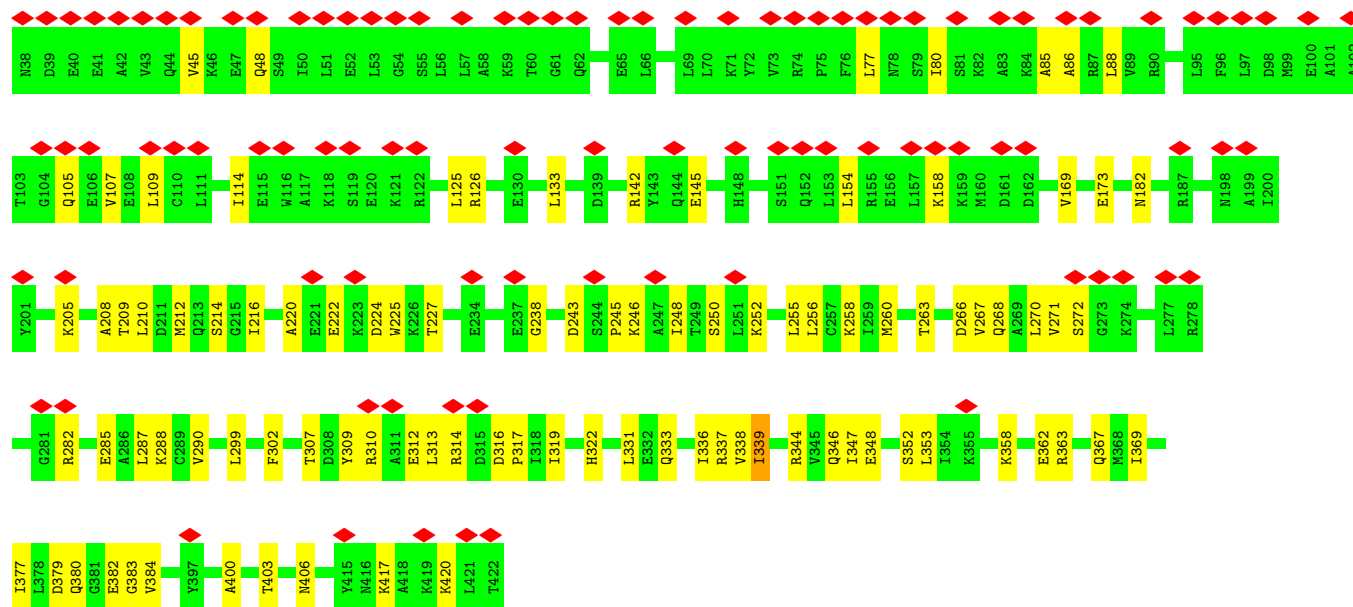
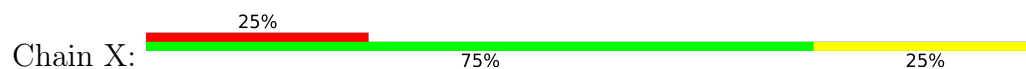


- Molecule 9: 26S proteasome non-ATPase regulatory subunit 12



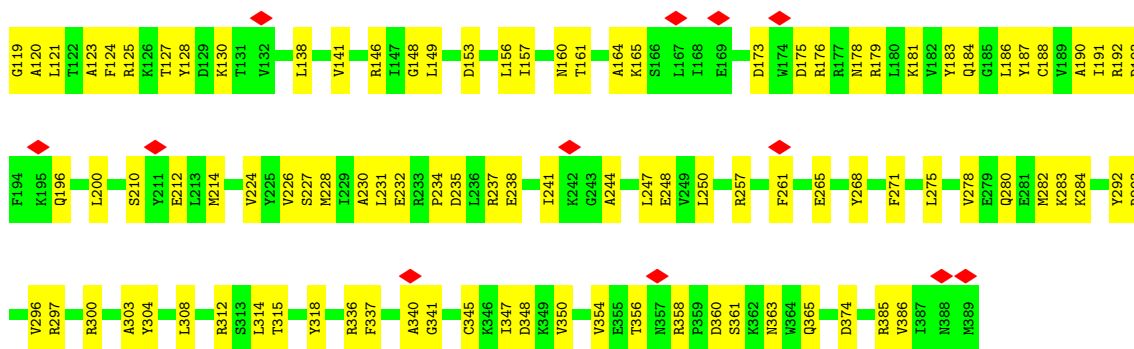


- Molecule 10: 26S proteasome non-ATPase regulatory subunit 11



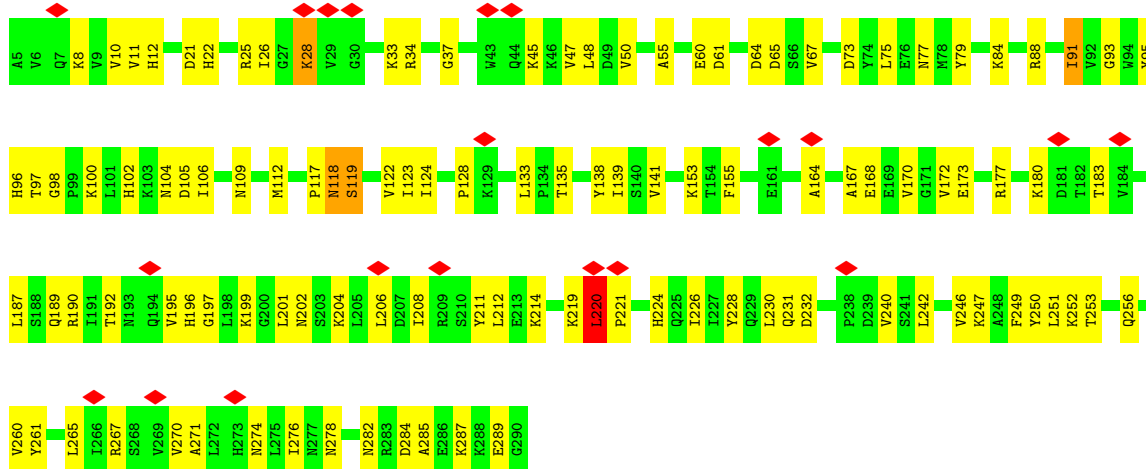
- Molecule 11: 26S proteasome non-ATPase regulatory subunit 6





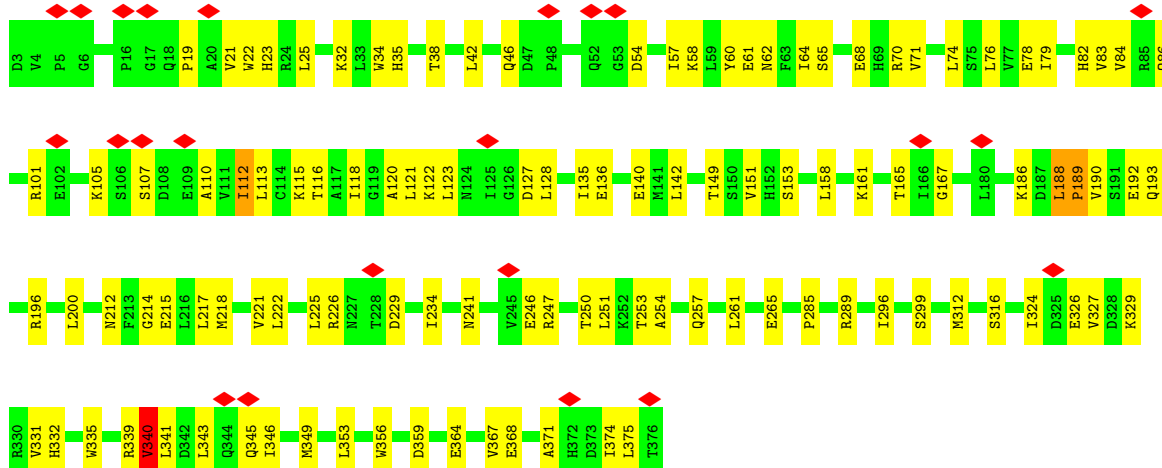
• Molecule 12: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 7% 60% 38% .

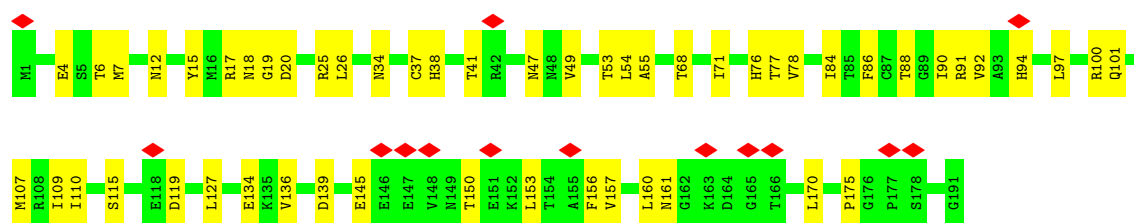
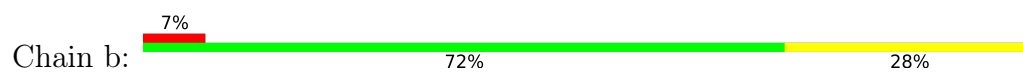


• Molecule 13: 26S proteasome non-ATPase regulatory subunit 13

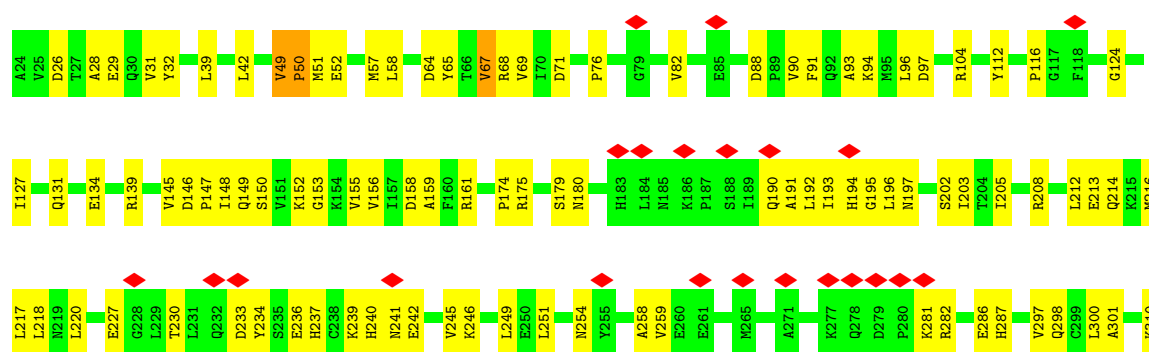
Chain a: 6% 70% 29% .



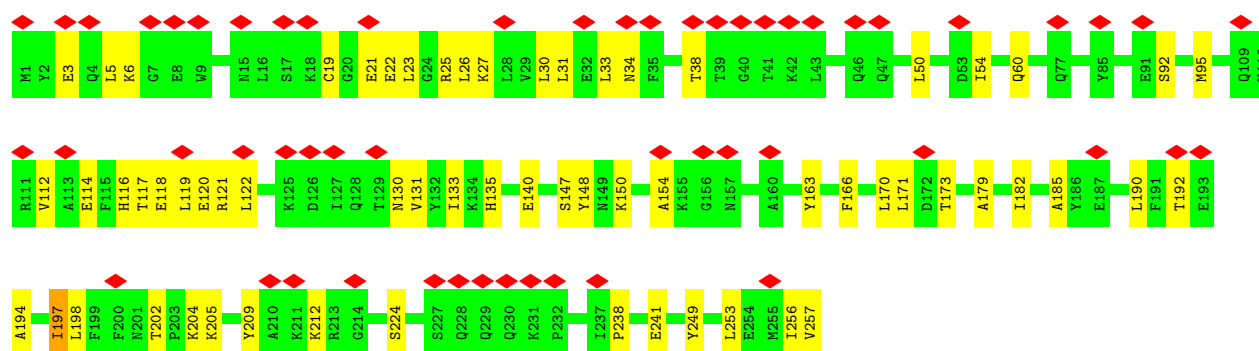
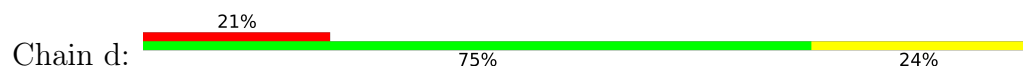
• Molecule 14: 26S proteasome non-ATPase regulatory subunit 4



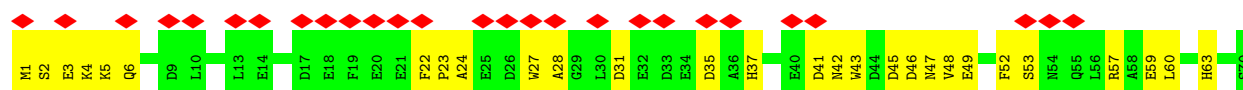
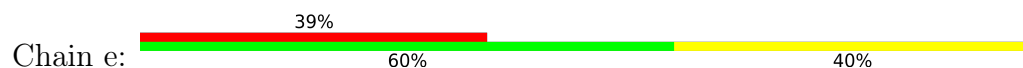
- Molecule 15: 26S proteasome non-ATPase regulatory subunit 14



- Molecule 16: 26S proteasome non-ATPase regulatory subunit 8



- Molecule 17: 26S proteasome complex subunit SEM1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117471	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.015	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	250.88, 250.88, 250.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	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: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/668	0.69	0/911
2	B	0.30	0/563	0.79	0/763
3	C	0.25	0/963	0.67	0/1294
4	D	0.24	0/884	0.60	0/1195
5	E	0.22	0/861	0.56	0/1149
6	F	0.24	0/807	0.63	0/1086
7	U	0.25	0/6684	0.64	3/9043 (0.0%)
8	V	0.30	0/3998	0.83	6/5402 (0.1%)
9	W	0.28	0/3750	0.69	6/5039 (0.1%)
10	X	0.22	0/3091	0.54	0/4165
11	Y	0.25	0/3173	0.62	0/4273
12	Z	0.26	0/2324	0.71	2/3150 (0.1%)
13	a	0.26	0/3061	0.74	7/4144 (0.2%)
14	b	0.25	0/1478	0.61	0/2001
15	c	0.26	0/2302	0.64	2/3110 (0.1%)
16	d	0.24	0/2162	0.65	0/2919
17	e	0.26	0/596	0.62	0/805
All	All	0.26	0/37365	0.67	26/50449 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	188	LEU	CA-C-N	11.48	134.19	119.84
13	a	188	LEU	C-N-CA	11.48	134.19	119.84
13	a	190	VAL	N-CA-C	-9.84	101.28	110.53
12	Z	220	LEU	CA-C-N	9.02	131.12	119.84
12	Z	220	LEU	C-N-CA	9.02	131.12	119.84
8	V	279	GLN	CA-C-N	-7.57	113.43	122.44
8	V	279	GLN	C-N-CA	-7.57	113.43	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	188	SER	N-CA-C	-7.56	102.99	112.90
9	W	220	GLU	N-CA-C	-7.34	101.45	112.54
9	W	219	THR	O-C-N	7.26	132.18	123.24
7	U	457	ILE	N-CA-C	-7.05	105.63	111.91
15	c	49	VAL	CA-C-N	6.92	128.50	119.84
15	c	49	VAL	C-N-CA	6.92	128.50	119.84
13	a	107	SER	N-CA-C	-6.26	104.70	112.72
9	W	219	THR	CA-C-N	6.15	132.52	121.15
9	W	219	THR	C-N-CA	6.15	132.52	121.15
7	U	144	ASP	CA-C-N	5.63	132.30	121.54
7	U	144	ASP	C-N-CA	5.63	132.30	121.54
13	a	327	VAL	N-CA-C	-5.45	106.36	111.48
9	W	231	ILE	N-CA-CB	-5.43	104.17	112.15
8	V	194	LYS	CA-C-N	5.15	127.79	120.53
8	V	194	LYS	C-N-CA	5.15	127.79	120.53
13	a	340	VAL	CA-C-N	5.09	131.27	121.54
13	a	340	VAL	C-N-CA	5.09	131.27	121.54
9	W	231	ILE	CB-CA-C	5.08	118.83	111.88
8	V	271	VAL	N-CA-C	-5.01	106.79	111.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	654	0	657	17	0
2	B	556	0	548	25	0
3	C	954	0	994	57	0
4	D	870	0	883	32	0
5	E	853	0	909	35	0
6	F	799	0	860	34	0
7	U	6568	0	6626	188	0
8	V	3919	0	3960	258	0
9	W	3703	0	3818	130	0
10	X	3048	0	3139	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Y	3115	0	3120	101	0
12	Z	2281	0	2312	117	0
13	a	3003	0	3016	97	0
14	b	1458	0	1505	34	0
15	c	2260	0	2276	85	0
16	d	2116	0	2146	47	0
17	e	583	0	493	29	0
18	c	1	0	0	0	0
All	All	36741	0	37262	1198	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 16.

All (1198) 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)
8:V:193:GLN:CD	8:V:194:LYS:H	1.23	1.43
3:C:23:TYR:CE2	8:V:193:GLN:NE2	1.91	1.37
8:V:226:VAL:CG1	8:V:227:VAL:H	1.35	1.35
7:U:145:HIS:O	7:U:146:LYS:HG2	1.11	1.25
8:V:27:PRO:CG	8:V:28:PRO:HD3	1.70	1.20
8:V:268:GLU:O	8:V:272:SER:OG	1.58	1.20
3:C:23:TYR:HE2	8:V:193:GLN:NE2	1.32	1.19
8:V:27:PRO:HD2	8:V:28:PRO:HD2	1.23	1.16
7:U:36:ALA:HB1	8:V:271:VAL:CG1	1.74	1.16
8:V:224:LEU:O	8:V:225:ASP:OD1	1.64	1.16
8:V:29:PRO:HB2	8:V:30:PRO:HD3	1.17	1.15
7:U:146:LYS:HG3	7:U:149:GLN:OE1	1.33	1.14
9:W:220:GLU:O	9:W:222:LEU:N	1.78	1.13
2:B:126:SER:HB3	3:C:92:GLU:OE2	1.46	1.12
8:V:226:VAL:HG13	8:V:227:VAL:N	1.40	1.11
8:V:27:PRO:HG2	8:V:28:PRO:HD3	1.18	1.11
7:U:145:HIS:O	7:U:146:LYS:CG	1.97	1.11
7:U:146:LYS:CG	7:U:149:GLN:OE1	1.89	1.11
8:V:193:GLN:CD	8:V:194:LYS:N	2.07	1.10
7:U:36:ALA:HB1	8:V:271:VAL:HG11	1.31	1.09
8:V:26:PRO:N	8:V:27:PRO:HD3	1.65	1.09
9:W:416:GLN:NE2	9:W:418:PRO:HD3	1.66	1.09
7:U:127:ASP:OD2	7:U:129:ARG:NH1	1.87	1.06
8:V:267:ALA:O	8:V:271:VAL:HB	1.57	1.05
9:W:116:THR:HG23	9:W:119:PRO:HD3	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:27:PRO:CG	8:V:28:PRO:CD	2.38	1.02
8:V:25:GLU:C	8:V:27:PRO:CD	2.34	1.01
8:V:27:PRO:CD	8:V:28:PRO:HD2	1.91	1.00
15:c:191:ALA:O	15:c:195:GLY:HA3	1.61	1.00
1:A:116:LYS:NZ	2:B:130:GLU:OE2	1.95	0.99
8:V:25:GLU:C	8:V:27:PRO:HD3	1.88	0.98
8:V:29:PRO:HB2	8:V:30:PRO:CD	1.94	0.96
8:V:27:PRO:HG2	8:V:28:PRO:CD	1.94	0.96
8:V:239:THR:O	8:V:240:LEU:HB2	1.66	0.96
12:Z:192:THR:O	12:Z:196:HIS:HB3	1.66	0.94
7:U:799:LYS:NZ	7:U:926:GLU:OE2	1.98	0.94
8:V:267:ALA:O	8:V:271:VAL:CB	2.15	0.94
8:V:284:GLU:O	8:V:288:TYR:HB3	1.67	0.93
8:V:27:PRO:CB	8:V:28:PRO:HD3	2.01	0.91
13:a:58:LYS:O	13:a:62:ASN:HB2	1.71	0.91
8:V:186:LYS:O	8:V:190:ASP:HA	1.71	0.91
8:V:268:GLU:O	8:V:273:LYS:CE	2.19	0.90
11:Y:292:TYR:OH	17:e:57:ARG:NH1	2.03	0.90
13:a:189:PRO:HB2	13:a:192:GLU:HB2	1.53	0.90
8:V:473:GLN:O	8:V:477:HIS:HB2	1.71	0.89
7:U:338:HIS:O	7:U:342:LEU:HB2	1.72	0.89
9:W:416:GLN:NE2	9:W:418:PRO:CD	2.36	0.89
11:Y:361:SER:O	11:Y:365:GLN:HB2	1.73	0.89
2:B:126:SER:CB	3:C:92:GLU:OE2	2.21	0.87
8:V:193:GLN:NE2	8:V:194:LYS:H	1.73	0.86
16:d:22:GLU:HG3	16:d:25:ARG:HH11	1.39	0.86
12:Z:26:ILE:CG2	12:Z:28:LYS:NZ	2.39	0.86
7:U:145:HIS:C	7:U:146:LYS:HG2	2.01	0.86
7:U:498:LYS:NZ	7:U:531:ASP:OD2	2.09	0.86
11:Y:278:VAL:O	11:Y:282:MET:HB2	1.76	0.86
11:Y:336:ARG:O	11:Y:340:ALA:HB3	1.76	0.86
6:F:74:LYS:O	6:F:78:GLU:HB2	1.76	0.85
8:V:267:ALA:O	8:V:271:VAL:CG2	2.24	0.85
8:V:27:PRO:CD	8:V:28:PRO:CD	2.53	0.85
8:V:48:THR:O	8:V:52:ASP:HB3	1.76	0.85
17:e:42:ASN:O	17:e:46:ASP:HB2	1.76	0.85
13:a:261:LEU:O	13:a:265:GLU:HB2	1.75	0.85
8:V:26:PRO:N	8:V:27:PRO:CD	2.34	0.85
12:Z:33:LYS:HZ2	12:Z:60:GLU:H	1.22	0.85
5:E:74:THR:OG1	5:E:97:ARG:NH1	2.10	0.85
8:V:311:ASN:OD1	8:V:315:LYS:NZ	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:628:ARG:NH1	7:U:749:GLN:OE1	2.09	0.84
15:c:193:ILE:O	15:c:197:ASN:HB2	1.76	0.84
8:V:193:GLN:OE1	8:V:194:LYS:N	2.09	0.84
7:U:155:LEU:O	7:U:158:ARG:NH1	2.11	0.84
7:U:339:LEU:O	7:U:343:ILE:HB	1.77	0.84
8:V:24:GLN:HA	8:V:27:PRO:HG3	1.60	0.83
1:A:94:GLN:O	1:A:144:ARG:NH1	2.09	0.83
7:U:684:ARG:NH1	7:U:723:ASP:OD2	2.11	0.83
7:U:392:TRP:O	7:U:395:ARG:NH1	2.11	0.82
9:W:282:GLU:O	9:W:286:LEU:HB2	1.79	0.82
9:W:416:GLN:HE22	9:W:418:PRO:CG	1.91	0.82
8:V:194:LYS:HE3	8:V:238:ALA:HA	1.61	0.82
11:Y:161:THR:O	11:Y:165:LYS:HB2	1.79	0.82
10:X:362:GLU:OE2	10:X:380:GLN:NE2	2.12	0.82
11:Y:179:ARG:NH1	11:Y:212:GLU:OE1	2.12	0.82
8:V:377:GLN:O	8:V:381:GLN:HB2	1.80	0.82
8:V:192:MET:C	8:V:193:GLN:OE1	2.23	0.81
12:Z:173:GLU:O	12:Z:177:ARG:NH1	2.13	0.81
11:Y:42:MET:O	11:Y:46:ARG:NH1	2.13	0.81
3:C:32:GLN:O	3:C:36:ASN:HB2	1.80	0.81
9:W:75:TYR:O	9:W:79:GLU:HB3	1.81	0.81
7:U:26:LYS:NZ	16:d:34:ASN:OD1	2.13	0.81
8:V:24:GLN:C	8:V:27:PRO:CG	2.54	0.81
8:V:231:LEU:O	8:V:235:LEU:HB2	1.81	0.80
3:C:90:HIS:O	3:C:91:PRO:O	1.99	0.80
13:a:58:LYS:NZ	13:a:86:GLN:OE1	2.15	0.80
10:X:142:ARG:NE	10:X:145:GLU:OE2	2.13	0.80
1:A:76:ALA:O	1:A:80:LEU:HB2	1.82	0.80
8:V:25:GLU:C	8:V:27:PRO:HD2	2.06	0.80
8:V:29:PRO:CB	8:V:30:PRO:HD3	2.08	0.79
8:V:226:VAL:HG13	8:V:227:VAL:HG23	1.64	0.79
8:V:28:PRO:HB2	8:V:29:PRO:HD3	1.64	0.79
9:W:350:ARG:O	9:W:354:LEU:HB2	1.82	0.79
8:V:224:LEU:O	8:V:225:ASP:CG	2.25	0.79
9:W:417:ARG:HH22	9:W:419:LYS:C	1.90	0.79
10:X:182:ASN:ND2	11:Y:248:GLU:OE2	2.16	0.79
8:V:29:PRO:O	8:V:31:ALA:N	2.16	0.78
8:V:26:PRO:CD	8:V:27:PRO:HD3	2.13	0.78
13:a:35:HIS:HB2	13:a:70:ARG:HH12	1.48	0.78
13:a:70:ARG:HA	14:b:17:ARG:HH12	1.49	0.78
8:V:268:GLU:O	8:V:273:LYS:NZ	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:285:TRP:O	8:V:289:LEU:HB2	1.83	0.78
9:W:417:ARG:HH22	9:W:420:ASP:N	1.82	0.77
8:V:216:ARG:O	8:V:220:PHE:HB2	1.84	0.77
9:W:116:THR:HG23	9:W:119:PRO:CD	2.13	0.77
9:W:108:CYS:O	9:W:112:VAL:HB	1.85	0.77
4:D:86:PRO:O	4:D:134:LYS:NZ	2.17	0.77
8:V:479:ARG:NH1	11:Y:374:ASP:OD1	2.17	0.77
15:c:71:ASP:OD1	15:c:104:ARG:NH1	2.18	0.77
15:c:214:GLN:O	15:c:218:LEU:HB2	1.85	0.76
8:V:153:LYS:NZ	8:V:199:ASN:O	2.19	0.76
5:E:85:ARG:HH12	12:Z:45:LYS:NZ	1.83	0.76
15:c:139:ARG:O	15:c:161:ARG:NH1	2.19	0.76
9:W:417:ARG:NH2	9:W:419:LYS:C	2.44	0.76
12:Z:252:LYS:HZ1	15:c:301:ALA:HB2	1.51	0.76
11:Y:271:PHE:O	11:Y:275:LEU:HB2	1.86	0.76
12:Z:93:GLY:HA2	12:Z:119:SER:HB3	1.67	0.76
8:V:267:ALA:CA	8:V:271:VAL:HG21	2.15	0.75
12:Z:28:LYS:NZ	12:Z:28:LYS:H	1.84	0.75
8:V:226:VAL:HG13	8:V:227:VAL:H	0.63	0.75
13:a:189:PRO:HB2	13:a:192:GLU:CB	2.17	0.75
8:V:46:GLY:O	8:V:50:GLU:HB2	1.87	0.75
12:Z:252:LYS:NZ	15:c:297:VAL:O	2.20	0.75
9:W:220:GLU:C	9:W:222:LEU:H	1.92	0.75
9:W:403:PHE:CZ	9:W:416:GLN:OE1	2.39	0.74
7:U:74:PHE:HZ	8:V:240:LEU:HD22	1.53	0.74
11:Y:124:PHE:O	11:Y:128:TYR:HB2	1.88	0.74
8:V:267:ALA:O	8:V:271:VAL:HG23	1.87	0.73
8:V:268:GLU:C	8:V:272:SER:OG	2.31	0.73
10:X:216:ILE:O	10:X:220:ALA:HB2	1.88	0.73
13:a:196:ARG:O	13:a:200:LEU:HB2	1.89	0.73
11:Y:280:GLN:O	11:Y:284:LYS:NZ	2.19	0.73
15:c:216:MET:O	15:c:220:LEU:HB2	1.89	0.73
15:c:227:GLU:HB2	15:c:230:THR:HA	1.70	0.73
8:V:287:ARG:HH12	17:e:2:SER:H	1.37	0.73
7:U:628:ARG:NH1	7:U:753:GLY:O	2.19	0.72
17:e:45:ASP:O	17:e:49:GLU:HB2	1.89	0.72
8:V:21:GLY:O	8:V:25:GLU:HB2	1.89	0.72
9:W:408:ARG:HH12	10:X:347:ILE:HG23	1.52	0.72
14:b:101:GLN:NE2	15:c:97:ASP:OD2	2.22	0.72
17:e:23:PRO:O	17:e:27:TRP:HB2	1.88	0.72
9:W:218:ASN:O	9:W:223:LYS:NZ	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:VAL:N	3:C:92:GLU:OE2	2.22	0.72
10:X:258:LYS:HZ1	10:X:267:VAL:N	1.87	0.72
13:a:214:GLY:O	13:a:218:MET:HB2	1.89	0.72
8:V:266:GLN:C	8:V:271:VAL:HG21	2.14	0.72
9:W:416:GLN:OE1	9:W:416:GLN:HA	1.90	0.71
16:d:194:ALA:O	16:d:198:LEU:HB2	1.89	0.71
9:W:8:ARG:O	9:W:12:ARG:HB2	1.89	0.71
12:Z:202:ASN:O	12:Z:206:LEU:HB2	1.91	0.71
13:a:247:ARG:O	13:a:251:LEU:HB2	1.89	0.71
5:E:85:ARG:HH12	12:Z:45:LYS:HZ2	1.38	0.70
7:U:212:ASP:OD2	7:U:215:ASN:ND2	2.24	0.70
3:C:21:ARG:NH1	7:U:106:ASP:OD1	2.23	0.70
11:Y:224:VAL:O	11:Y:228:MET:HB2	1.91	0.70
8:V:24:GLN:O	8:V:27:PRO:HG2	1.90	0.70
11:Y:175:ASP:O	11:Y:179:ARG:HB2	1.91	0.70
9:W:395:ASN:O	9:W:399:ASN:HB2	1.92	0.70
10:X:310:ARG:O	10:X:314:ARG:HB2	1.91	0.70
11:Y:226:VAL:O	11:Y:230:ALA:HB3	1.92	0.70
7:U:351:MET:O	7:U:355:ASN:HB2	1.92	0.69
14:b:12:ASN:HD21	14:b:55:ALA:HB2	1.55	0.69
2:B:126:SER:HB3	3:C:92:GLU:CD	2.16	0.69
7:U:337:LEU:HD22	7:U:844:LYS:HZ1	1.56	0.69
8:V:27:PRO:CB	8:V:28:PRO:CD	2.68	0.69
13:a:374:ILE:HG13	13:a:375:LEU:HG	1.74	0.69
8:V:160:LEU:HD13	8:V:182:LYS:HZ1	1.57	0.69
8:V:267:ALA:HA	8:V:271:VAL:HG21	1.73	0.69
9:W:116:THR:O	9:W:118:LEU:N	2.26	0.69
9:W:340:VAL:HG13	9:W:350:ARG:HH11	1.57	0.69
9:W:408:ARG:NH1	10:X:383:GLY:O	2.26	0.69
16:d:198:LEU:HA	16:d:205:LYS:HZ2	1.58	0.69
12:Z:26:ILE:HB	12:Z:28:LYS:HZ1	1.56	0.69
8:V:270:LEU:O	8:V:273:LYS:HG3	1.92	0.69
8:V:189:ASP:O	8:V:190:ASP:HB2	1.92	0.68
3:C:23:TYR:HE2	8:V:193:GLN:CD	2.01	0.68
12:Z:219:LYS:O	12:Z:220:LEU:O	2.10	0.68
12:Z:228:TYR:O	12:Z:232:ASP:HB2	1.93	0.68
9:W:403:PHE:CE2	9:W:416:GLN:OE1	2.46	0.68
11:Y:192:ARG:NE	17:e:41:ASP:OD2	2.27	0.68
8:V:24:GLN:C	8:V:27:PRO:CD	2.67	0.68
8:V:189:ASP:OD1	8:V:190:ASP:N	2.27	0.67
5:E:72:LYS:HZ3	5:E:78:ARG:HE	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:267:ALA:C	8:V:271:VAL:CG2	2.68	0.67
7:U:545:LEU:HB3	7:U:577:ILE:HG21	1.75	0.67
8:V:255:LEU:HD22	8:V:291:TYR:HB3	1.76	0.67
4:D:81:ARG:NH1	15:c:153:GLY:HA2	2.09	0.67
8:V:189:ASP:OD1	8:V:190:ASP:O	2.13	0.67
8:V:270:LEU:O	8:V:273:LYS:CG	2.32	0.67
9:W:63:THR:HG23	9:W:72:LYS:HZ3	1.61	0.66
8:V:305:ALA:O	8:V:309:MET:HB3	1.94	0.66
13:a:186:LYS:HZ3	13:a:221:VAL:HB	1.59	0.66
8:V:271:VAL:N	8:V:273:LYS:HE2	2.09	0.66
5:E:37:THR:HG21	6:F:66:LEU:HD22	1.77	0.66
7:U:772:TRP:HD1	7:U:775:LEU:HG	1.61	0.66
7:U:36:ALA:CB	8:V:271:VAL:CG1	2.65	0.66
7:U:247:GLN:HE21	7:U:913:ILE:H	1.44	0.66
12:Z:33:LYS:NZ	12:Z:60:GLU:H	1.93	0.65
9:W:416:GLN:HE22	9:W:418:PRO:CD	2.06	0.65
3:C:90:HIS:CG	3:C:91:PRO:HD2	2.32	0.65
13:a:222:LEU:HB3	13:a:226:ARG:NH1	2.11	0.65
15:c:212:LEU:O	15:c:216:MET:HB3	1.97	0.65
17:e:24:ALA:O	17:e:28:ALA:HB2	1.95	0.65
3:C:14:GLY:HA2	3:C:18:SER:HB3	1.77	0.65
7:U:36:ALA:HB1	8:V:271:VAL:HG12	1.74	0.65
9:W:317:TRP:HB3	9:W:355:LYS:NZ	2.11	0.65
12:Z:26:ILE:CG2	12:Z:28:LYS:HZ1	2.08	0.65
12:Z:26:ILE:HB	12:Z:28:LYS:NZ	2.12	0.65
11:Y:109:GLU:HG2	11:Y:146:ARG:HH22	1.62	0.64
8:V:392:TYR:O	8:V:396:ILE:HB	1.97	0.64
12:Z:232:ASP:OD2	13:a:335:TRP:NE1	2.30	0.64
13:a:19:PRO:O	13:a:23:HIS:ND1	2.30	0.64
2:B:99:VAL:HB	2:B:160:ILE:HD11	1.80	0.64
7:U:894:MET:SD	7:U:901:GLN:NE2	2.71	0.64
9:W:244:CYS:HA	9:W:273:TYR:HB2	1.78	0.64
7:U:74:PHE:CZ	8:V:240:LEU:HD22	2.32	0.64
11:Y:53:TYR:O	11:Y:57:LEU:HB2	1.97	0.64
15:c:64:ASP:HA	15:c:139:ARG:HH21	1.63	0.64
11:Y:188:CYS:HA	11:Y:191:ILE:HG22	1.78	0.64
7:U:714:SER:O	7:U:718:ASN:HB2	1.97	0.63
8:V:27:PRO:HB2	8:V:28:PRO:HD3	1.80	0.63
9:W:116:THR:C	9:W:118:LEU:H	2.07	0.63
16:d:182:ILE:HG12	16:d:197:ILE:HG21	1.79	0.63
9:W:417:ARG:NH2	9:W:419:LYS:CA	2.56	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:135:ILE:HG12	13:a:158:LEU:HD23	1.81	0.63
15:c:281:LYS:NZ	15:c:286:GLU:OE2	2.29	0.63
9:W:405:LYS:HB3	9:W:414:ASN:HB2	1.79	0.63
4:D:81:ARG:HB2	15:c:152:LYS:HZ2	1.62	0.63
4:D:81:ARG:HB2	15:c:152:LYS:NZ	2.14	0.63
5:E:50:LEU:HD11	6:F:138:GLY:H	1.64	0.63
8:V:226:VAL:CG1	8:V:227:VAL:N	2.12	0.63
10:X:377:ILE:HG23	11:Y:312:ARG:NH1	2.14	0.63
9:W:374:THR:HB	9:W:412:ILE:HD12	1.81	0.62
7:U:115:ASN:HB3	7:U:123:LYS:NZ	2.14	0.62
16:d:27:LYS:O	16:d:31:LEU:HB2	1.99	0.62
7:U:789:ILE:HD12	7:U:911:ILE:HG12	1.82	0.62
9:W:220:GLU:C	9:W:222:LEU:N	2.49	0.62
10:X:282:ARG:NH1	10:X:285:GLU:OE1	2.33	0.62
15:c:146:ASP:OD2	15:c:149:GLN:NE2	2.33	0.62
15:c:236:GLU:O	15:c:240:HIS:ND1	2.32	0.62
12:Z:84:LYS:HE3	15:c:76:PRO:HG3	1.80	0.62
13:a:217:LEU:HD23	13:a:241:ASN:HD22	1.65	0.62
7:U:701:ILE:HD13	7:U:810:THR:HG22	1.82	0.62
15:c:241:ASN:HA	15:c:245:VAL:HB	1.82	0.62
16:d:112:VAL:O	16:d:116:HIS:ND1	2.32	0.62
3:C:90:HIS:ND1	3:C:91:PRO:HD2	2.15	0.61
9:W:205:ILE:O	9:W:208:LYS:N	2.32	0.61
12:Z:112:MET:O	12:Z:119:SER:OG	2.18	0.61
3:C:23:TYR:HE2	8:V:193:GLN:HE21	1.27	0.61
8:V:342:ILE:O	8:V:368:ARG:NH2	2.32	0.61
11:Y:227:SER:HA	11:Y:231:LEU:HD13	1.82	0.61
13:a:222:LEU:HB3	13:a:226:ARG:HH12	1.65	0.61
15:c:90:VAL:O	15:c:94:LYS:HB2	2.00	0.61
9:W:299:ILE:HG22	9:W:301:LYS:H	1.64	0.61
14:b:88:THR:O	14:b:92:VAL:HB	2.00	0.61
13:a:349:MET:O	13:a:353:LEU:HB2	2.01	0.61
4:D:116:LEU:HD23	4:D:118:THR:H	1.66	0.61
7:U:580:ARG:HD3	7:U:613:ASP:HB3	1.83	0.61
7:U:842:LYS:O	7:U:880:ASN:N	2.33	0.61
11:Y:117:LYS:HA	11:Y:120:ALA:HB3	1.81	0.61
7:U:698:GLN:HG2	7:U:705:LYS:NZ	2.16	0.61
8:V:239:THR:O	8:V:240:LEU:CB	2.47	0.61
12:Z:26:ILE:CB	12:Z:28:LYS:HZ1	2.12	0.61
9:W:120:ILE:HG22	9:W:123:ARG:HH21	1.65	0.61
11:Y:138:LEU:HD23	11:Y:176:ARG:HH11	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:141:VAL:HG22	11:Y:160:ASN:HB2	1.83	0.61
16:d:116:HIS:NE2	16:d:140:GLU:OE2	2.33	0.61
9:W:430:GLN:C	15:c:239:LYS:HZ2	2.09	0.61
13:a:189:PRO:HB2	13:a:192:GLU:CG	2.29	0.61
2:B:103:ARG:HB2	3:C:84:LYS:HZ1	1.66	0.61
4:D:86:PRO:HG2	4:D:134:LYS:HZ1	1.66	0.61
2:B:125:THR:HG22	2:B:129:SER:H	1.66	0.60
9:W:63:THR:HG23	9:W:72:LYS:NZ	2.16	0.60
13:a:246:GLU:O	13:a:247:ARG:NH1	2.32	0.60
7:U:708:GLN:HA	7:U:711:GLN:HG2	1.83	0.60
8:V:24:GLN:CA	8:V:27:PRO:HG3	2.31	0.60
11:Y:237:ARG:HA	11:Y:241:ILE:HB	1.83	0.60
9:W:323:ASP:O	9:W:327:GLU:HB2	2.01	0.60
9:W:408:ARG:O	10:X:346:GLN:NE2	2.34	0.60
8:V:442:ILE:HA	8:V:447:ILE:HD11	1.82	0.60
5:E:47:LEU:HD13	6:F:79:LYS:NZ	2.17	0.60
7:U:506:ALA:HB1	7:U:543:LYS:HB2	1.82	0.60
9:W:53:GLN:HG3	9:W:103:LYS:HE2	1.83	0.60
11:Y:261:PHE:O	11:Y:265:GLU:HB2	2.01	0.60
12:Z:26:ILE:HG21	12:Z:28:LYS:NZ	2.14	0.60
8:V:195:ILE:HB	8:V:200:ARG:HB2	1.82	0.60
3:C:89:VAL:HB	3:C:93:GLY:HA3	1.84	0.60
8:V:178:SER:HB3	8:V:182:LYS:NZ	2.17	0.60
8:V:483:CYS:O	8:V:487:HIS:ND1	2.35	0.60
13:a:19:PRO:HA	13:a:22:TRP:HB2	1.83	0.60
10:X:348:GLU:O	10:X:352:SER:HB3	2.02	0.59
15:c:159:ALA:H	15:c:205:ILE:HD11	1.67	0.59
11:Y:173:ASP:OD2	11:Y:176:ARG:NE	2.30	0.59
7:U:58:GLN:O	7:U:62:LEU:HB2	2.01	0.59
8:V:51:ALA:HB3	8:V:150:ARG:HH22	1.66	0.59
8:V:263:LEU:HD22	16:d:121:ARG:HE	1.68	0.59
17:e:43:TRP:O	17:e:47:ASN:HB2	2.01	0.59
7:U:527:GLN:O	7:U:531:ASP:HB2	2.01	0.59
7:U:680:VAL:HG12	7:U:682:TYR:H	1.67	0.59
16:d:6:LYS:NZ	16:d:50:LEU:HD21	2.17	0.59
1:A:95:VAL:HB	1:A:143:ASP:HA	1.85	0.59
7:U:506:ALA:O	7:U:510:GLU:HB2	2.03	0.59
15:c:52:GLU:HB3	15:c:82:VAL:HG23	1.84	0.59
16:d:131:VAL:O	16:d:135:HIS:HB2	2.01	0.59
17:e:45:ASP:O	17:e:49:GLU:CB	2.50	0.59
17:e:52:PHE:HB3	17:e:57:ARG:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:SER:CA	3:C:92:GLU:OE2	2.51	0.59
7:U:74:PHE:O	7:U:78:LEU:HB2	2.02	0.59
10:X:107:VAL:HG23	10:X:133:LEU:HD11	1.85	0.59
11:Y:77:ASN:O	11:Y:81:LEU:HB2	2.03	0.59
15:c:155:VAL:HG22	15:c:155:VAL:O	2.02	0.59
17:e:28:ALA:HA	17:e:31:ASP:HB2	1.85	0.59
8:V:267:ALA:C	8:V:271:VAL:HG23	2.27	0.59
9:W:370:TYR:CZ	9:W:416:GLN:HG2	2.38	0.59
7:U:21:GLU:OE1	7:U:55:ARG:NH1	2.35	0.59
8:V:226:VAL:CG1	8:V:227:VAL:HG23	2.29	0.59
7:U:340:GLN:HE21	7:U:344:ARG:HH12	1.50	0.58
9:W:73:MET:O	9:W:77:ALA:HB3	2.03	0.58
9:W:243:ILE:HA	9:W:246:HIS:HB3	1.84	0.58
6:F:78:GLU:HA	6:F:81:LYS:NZ	2.17	0.58
8:V:24:GLN:O	8:V:27:PRO:CG	2.50	0.58
8:V:468:SER:HA	11:Y:363:ASN:HD22	1.68	0.58
5:E:22:ILE:HG13	5:E:25:ARG:HH11	1.68	0.58
7:U:112:CYS:O	7:U:116:ALA:HB2	2.03	0.58
10:X:154:LEU:HB3	10:X:158:LYS:NZ	2.18	0.58
8:V:24:GLN:C	8:V:27:PRO:HG2	2.27	0.58
11:Y:117:LYS:O	11:Y:121:LEU:HB2	2.03	0.58
12:Z:219:LYS:HG3	12:Z:220:LEU:HD12	1.85	0.58
16:d:92:SER:HB3	16:d:95:MET:HB2	1.85	0.58
7:U:36:ALA:CB	8:V:271:VAL:HG11	2.21	0.58
8:V:473:GLN:NE2	12:Z:246:VAL:O	2.36	0.58
6:F:144:LYS:NZ	6:F:163:THR:HB	2.18	0.58
7:U:127:ASP:HB3	7:U:130:LEU:HD13	1.85	0.58
7:U:683:VAL:O	7:U:687:ALA:HB2	2.04	0.58
8:V:55:THR:OG1	8:V:150:ARG:NH1	2.36	0.58
10:X:252:LYS:O	10:X:256:LEU:HB2	2.03	0.58
12:Z:106:ILE:HG13	12:Z:153:LYS:HD2	1.86	0.58
4:D:65:GLN:NE2	16:d:256:ILE:O	2.36	0.58
12:Z:26:ILE:HG22	12:Z:28:LYS:NZ	2.17	0.58
13:a:64:ILE:O	13:a:68:GLU:HB3	2.03	0.58
7:U:792:ASN:HB3	7:U:914:LEU:HB3	1.86	0.58
12:Z:278:ASN:O	12:Z:282:ASN:ND2	2.37	0.58
7:U:606:ALA:O	7:U:615:ARG:NE	2.36	0.58
17:e:31:ASP:O	17:e:35:ASP:N	2.36	0.58
7:U:415:HIS:HD2	7:U:935:ILE:HG23	1.69	0.58
16:d:5:LEU:HD13	16:d:25:ARG:HH12	1.69	0.58
9:W:286:LEU:HA	9:W:289:ARG:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:333:LEU:HD12	9:W:334:GLU:HG2	1.86	0.57
16:d:26:LEU:HD13	16:d:54:ILE:HD12	1.86	0.57
3:C:50:ASN:ND2	7:U:642:GLU:O	2.36	0.57
8:V:24:GLN:HA	8:V:27:PRO:CG	2.32	0.57
8:V:268:GLU:O	8:V:273:LYS:HE2	2.04	0.57
9:W:268:LYS:NZ	9:W:327:GLU:OE2	2.37	0.57
11:Y:283:LYS:HG3	11:Y:284:LYS:HG3	1.84	0.57
12:Z:202:ASN:O	12:Z:206:LEU:CB	2.52	0.57
5:E:31:GLU:HG3	5:E:34:LYS:HE3	1.86	0.57
6:F:141:ASP:HB3	6:F:144:LYS:HB2	1.84	0.57
7:U:790:GLY:H	7:U:844:LYS:HG3	1.69	0.57
10:X:309:TYR:O	10:X:312:GLU:N	2.37	0.57
13:a:38:THR:HG21	13:a:71:VAL:HG11	1.87	0.57
12:Z:64:ASP:OD2	12:Z:67:VAL:N	2.37	0.57
6:F:121:CYS:HA	6:F:135:PRO:HA	1.85	0.57
7:U:749:GLN:HA	7:U:755:THR:HA	1.85	0.57
1:A:73:ALA:HA	1:A:76:ALA:HB3	1.87	0.57
9:W:115:ILE:HG12	9:W:116:THR:HG22	1.87	0.57
11:Y:347:ILE:HD11	11:Y:354:VAL:HG22	1.85	0.57
2:B:103:ARG:HD3	3:C:84:LYS:HZ1	1.68	0.57
11:Y:104:MET:HG2	11:Y:130:LYS:HZ1	1.70	0.57
11:Y:336:ARG:NH1	17:e:52:PHE:HZ	2.03	0.57
7:U:799:LYS:HB3	7:U:801:GLN:HE22	1.69	0.57
13:a:212:ASN:HD22	13:a:339:ARG:HG3	1.68	0.57
13:a:214:GLY:O	13:a:218:MET:CB	2.53	0.57
2:B:116:ILE:HG22	2:B:118:ASP:H	1.70	0.57
8:V:268:GLU:HA	8:V:272:SER:OG	2.03	0.57
10:X:406:ASN:HD22	12:Z:265:LEU:HD23	1.68	0.57
8:V:216:ARG:NH2	17:e:3:GLU:O	2.38	0.57
8:V:450:SER:H	8:V:460:SER:HA	1.70	0.57
7:U:110:LYS:HE2	7:U:114:GLU:OE2	2.05	0.56
15:c:145:VAL:HG22	15:c:147:PRO:HD3	1.86	0.56
8:V:267:ALA:CA	8:V:271:VAL:CG2	2.84	0.56
15:c:29:GLU:HG3	15:c:65:TYR:HA	1.86	0.56
1:A:121:PHE:HA	6:F:89:LEU:HA	1.87	0.56
7:U:712:LEU:O	7:U:734:GLN:NE2	2.38	0.56
12:Z:65:ASP:O	12:Z:104:ASN:ND2	2.38	0.56
12:Z:195:VAL:HB	12:Z:199:LYS:NZ	2.20	0.56
13:a:186:LYS:NZ	13:a:221:VAL:HB	2.19	0.56
15:c:147:PRO:HA	15:c:150:SER:HB2	1.86	0.56
4:D:103:VAL:HG11	4:D:132:LEU:HD11	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:26:PRO:HD2	8:V:27:PRO:HD3	1.86	0.56
8:V:450:SER:OG	8:V:452:ASN:ND2	2.39	0.56
7:U:801:GLN:HG3	7:U:842:LYS:HG2	1.88	0.56
8:V:193:GLN:OE1	8:V:193:GLN:N	2.38	0.56
10:X:384:VAL:O	11:Y:312:ARG:NH2	2.37	0.56
9:W:384:LEU:HB2	9:W:388:GLU:OE2	2.05	0.56
11:Y:124:PHE:O	11:Y:128:TYR:CB	2.54	0.56
12:Z:28:LYS:H	12:Z:28:LYS:HZ1	1.51	0.56
12:Z:190:ARG:HD2	13:a:375:LEU:HD13	1.86	0.56
15:c:191:ALA:O	15:c:195:GLY:CA	2.46	0.56
3:C:78:ARG:HB3	3:C:86:LEU:HD11	1.87	0.56
5:E:22:ILE:HG13	5:E:25:ARG:NH1	2.21	0.56
5:E:51:GLN:O	12:Z:88:ARG:NH2	2.39	0.56
8:V:263:LEU:HD21	16:d:120:GLU:HB3	1.87	0.56
8:V:345:ARG:NH1	8:V:354:LYS:NZ	2.52	0.56
8:V:467:TYR:HA	8:V:470:ARG:HB3	1.88	0.56
11:Y:337:PHE:HD1	11:Y:341:GLY:HA3	1.71	0.56
13:a:78:GLU:O	13:a:82:HIS:ND1	2.38	0.56
13:a:250:THR:O	13:a:254:ALA:HB2	2.06	0.56
13:a:345:GLN:O	13:a:349:MET:HB2	2.06	0.56
7:U:724:VAL:HA	7:U:727:LYS:HE3	1.88	0.56
8:V:396:ILE:HD12	8:V:399:ARG:HD3	1.89	0.56
8:V:422:ILE:HG13	8:V:425:LYS:HE3	1.88	0.56
12:Z:12:HIS:ND1	12:Z:50:VAL:O	2.34	0.56
12:Z:190:ARG:HE	13:a:375:LEU:HB3	1.70	0.56
14:b:7:MET:HB2	14:b:109:ILE:HG12	1.88	0.56
13:a:247:ARG:NH2	13:a:299:SER:O	2.39	0.55
8:V:29:PRO:CB	8:V:30:PRO:CD	2.69	0.55
9:W:423:ASN:HD22	15:c:246:LYS:NZ	2.04	0.55
10:X:417:LYS:HD2	11:Y:386:VAL:HG11	1.88	0.55
13:a:364:GLU:O	13:a:368:GLU:HB2	2.06	0.55
4:D:66:LYS:O	4:D:70:LYS:NZ	2.32	0.55
8:V:282:ASN:O	11:Y:385:ARG:NH1	2.39	0.55
9:W:293:ASP:HB3	9:W:296:LEU:HB2	1.87	0.55
3:C:23:TYR:CD2	8:V:193:GLN:NE2	2.66	0.55
9:W:34:LEU:HG	9:W:47:LEU:HD21	1.88	0.55
10:X:420:LYS:HZ3	12:Z:276:ILE:HG23	1.70	0.55
11:Y:361:SER:O	11:Y:365:GLN:CB	2.51	0.55
12:Z:164:ALA:HB1	12:Z:168:GLU:HB3	1.87	0.55
2:B:125:THR:H	2:B:128:GLY:HA2	1.72	0.55
3:C:43:ARG:HB2	7:U:639:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:121:CYS:SG	6:F:122:ALA:N	2.80	0.55
8:V:287:ARG:NH1	17:e:2:SER:H	2.03	0.55
7:U:36:ALA:HB1	8:V:271:VAL:CB	2.37	0.55
8:V:68:ASP:O	8:V:72:LEU:HB2	2.07	0.55
8:V:211:TYR:O	8:V:215:ALA:HB2	2.06	0.55
8:V:491:VAL:HG13	12:Z:267:ARG:HH21	1.71	0.55
12:Z:204:LYS:NZ	13:a:356:TRP:HB3	2.21	0.55
12:Z:261:TYR:O	12:Z:265:LEU:HB2	2.07	0.55
13:a:196:ARG:O	13:a:200:LEU:CB	2.53	0.55
3:C:71:SER:HB2	3:C:117:ARG:HA	1.88	0.55
9:W:116:THR:O	9:W:119:PRO:CD	2.55	0.55
8:V:46:GLY:O	8:V:50:GLU:CB	2.55	0.55
9:W:317:TRP:HB3	9:W:355:LYS:HZ1	1.72	0.55
10:X:417:LYS:HA	10:X:420:LYS:HG2	1.89	0.55
13:a:118:ILE:HG23	13:a:122:LYS:HZ3	1.71	0.55
7:U:242:LEU:HA	7:U:324:LYS:HZ3	1.72	0.55
7:U:899:ARG:O	7:U:917:THR:OG1	2.25	0.55
8:V:226:VAL:HG13	8:V:227:VAL:CG2	2.36	0.55
8:V:338:LEU:HD11	8:V:394:LEU:HD21	1.88	0.55
8:V:351:PRO:O	8:V:355:ARG:NH2	2.40	0.55
13:a:123:LEU:HD13	13:a:161:LYS:HB2	1.88	0.55
15:c:216:MET:O	15:c:220:LEU:CB	2.55	0.55
16:d:130:ASN:HB3	16:d:133:ILE:HG12	1.89	0.55
4:D:81:ARG:HH12	15:c:153:GLY:HA2	1.70	0.55
6:F:144:LYS:HZ1	6:F:163:THR:HB	1.72	0.55
7:U:802:TYR:HA	7:U:895:PRO:HD3	1.89	0.55
8:V:420:ALA:O	8:V:424:GLN:HB3	2.07	0.55
9:W:116:THR:O	9:W:119:PRO:HD2	2.07	0.55
8:V:51:ALA:HB1	8:V:55:THR:HA	1.89	0.54
9:W:343:SER:HB2	9:W:346:GLU:HB3	1.89	0.54
12:Z:26:ILE:CB	12:Z:28:LYS:NZ	2.68	0.54
13:a:34:TRP:HB2	13:a:70:ARG:HD3	1.88	0.54
16:d:238:PRO:HA	16:d:241:GLU:HG2	1.88	0.54
9:W:119:PRO:O	9:W:123:ARG:HB3	2.08	0.54
11:Y:84:LEU:HD13	11:Y:107:LYS:HA	1.88	0.54
13:a:349:MET:O	13:a:353:LEU:CB	2.55	0.54
16:d:60:GLN:NE2	16:d:163:TYR:OH	2.41	0.54
7:U:383:ASP:HB3	7:U:387:ARG:NH1	2.23	0.54
7:U:474:ARG:NH2	7:U:503:GLN:OE1	2.41	0.54
7:U:115:ASN:HB3	7:U:123:LYS:HZ2	1.72	0.54
8:V:25:GLU:N	8:V:27:PRO:HD3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:268:GLU:CA	8:V:272:SER:OG	2.56	0.54
14:b:6:THR:HB	14:b:49:VAL:HG22	1.88	0.54
3:C:69:GLN:HE22	4:D:135:HIS:HA	1.72	0.54
6:F:60:LEU:O	6:F:64:HIS:ND1	2.33	0.54
12:Z:118:ASN:OD1	12:Z:118:ASN:N	2.38	0.54
9:W:277:ALA:O	9:W:357:ARG:NH2	2.40	0.54
5:E:87:LEU:HD22	5:E:91:LYS:NZ	2.22	0.54
7:U:242:LEU:HA	7:U:324:LYS:NZ	2.23	0.54
8:V:306:ARG:NH2	8:V:336:GLU:OE2	2.41	0.54
8:V:410:ILE:HD12	8:V:422:ILE:HD11	1.90	0.54
9:W:263:TRP:HA	9:W:267:LEU:HB2	1.90	0.54
16:d:6:LYS:HZ1	16:d:50:LEU:HD21	1.73	0.54
16:d:114:GLU:HA	16:d:117:THR:HG22	1.90	0.54
8:V:106:ARG:O	8:V:110:HIS:ND1	2.37	0.54
8:V:204:ASP:HB3	8:V:246:GLY:HA3	1.88	0.54
8:V:263:LEU:HB2	16:d:121:ARG:HH21	1.73	0.54
9:W:116:THR:C	9:W:118:LEU:N	2.63	0.54
14:b:54:LEU:HD13	14:b:84:ILE:HG13	1.89	0.54
16:d:205:LYS:O	16:d:209:TYR:HB2	2.07	0.54
17:e:24:ALA:O	17:e:28:ALA:CB	2.56	0.54
6:F:151:VAL:HA	6:F:163:THR:HA	1.90	0.53
7:U:506:ALA:HB2	7:U:541:HIS:HB3	1.89	0.53
9:W:73:MET:O	9:W:77:ALA:CB	2.55	0.53
9:W:137:TYR:HE2	9:W:141:GLU:H	1.55	0.53
15:c:227:GLU:OE2	15:c:233:ASP:HB2	2.08	0.53
5:E:63:GLN:HG3	5:E:69:PHE:HB3	1.91	0.53
8:V:194:LYS:CE	8:V:238:ALA:HA	2.36	0.53
9:W:36:LYS:HD3	9:W:86:ASN:HD22	1.73	0.53
2:B:103:ARG:HB2	3:C:84:LYS:NZ	2.24	0.53
5:E:85:ARG:HH22	12:Z:45:LYS:NZ	2.07	0.53
7:U:242:LEU:HG	7:U:324:LYS:HD2	1.89	0.53
7:U:586:VAL:HG21	7:U:601:ARG:NH1	2.24	0.53
7:U:666:LYS:HA	7:U:669:ILE:HD12	1.89	0.53
11:Y:345:CYS:HG	11:Y:356:THR:HG1	1.55	0.53
12:Z:34:ARG:HB2	12:Z:96:HIS:HB2	1.90	0.53
15:c:158:ASP:OD2	15:c:202:SER:OG	2.18	0.53
3:C:84:LYS:HG2	3:C:96:VAL:HG22	1.90	0.53
8:V:180:ARG:O	8:V:184:ALA:HB2	2.08	0.53
15:c:31:VAL:HA	15:c:67:VAL:HG13	1.91	0.53
7:U:681:ASN:HB3	7:U:684:ARG:HH11	1.74	0.53
8:V:383:GLY:O	8:V:387:GLN:NE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:127:THR:HG23	9:W:145:LEU:HD13	1.90	0.53
11:Y:224:VAL:O	11:Y:228:MET:CB	2.56	0.53
8:V:29:PRO:O	8:V:32:PRO:HD2	2.08	0.53
12:Z:61:ASP:OD2	14:b:91:ARG:NH1	2.41	0.53
13:a:226:ARG:HB3	13:a:234:ILE:HD11	1.91	0.53
16:d:148:TYR:HE1	16:d:171:LEU:HD22	1.74	0.53
7:U:356:THR:HB	7:U:369:THR:HG22	1.90	0.53
11:Y:234:PRO:O	11:Y:238:GLU:HB2	2.09	0.53
12:Z:240:VAL:HG12	12:Z:242:LEU:H	1.74	0.53
7:U:533:VAL:HG23	7:U:578:LEU:HD11	1.91	0.52
8:V:231:LEU:HD21	8:V:250:LEU:HB3	1.91	0.52
3:C:22:GLN:CD	4:D:43:ARG:HH11	2.17	0.52
7:U:389:ASN:HB2	7:U:391:GLU:HG2	1.91	0.52
9:W:403:PHE:HZ	9:W:418:PRO:HG3	1.74	0.52
10:X:310:ARG:HA	10:X:313:LEU:HB2	1.90	0.52
12:Z:271:ALA:HA	12:Z:274:ASN:HD22	1.73	0.52
6:F:80:ILE:O	6:F:84:LYS:HB2	2.09	0.52
7:U:573:ASP:O	7:U:579:ARG:NH2	2.41	0.52
7:U:705:LYS:HG3	7:U:708:GLN:HE21	1.74	0.52
8:V:24:GLN:CA	8:V:27:PRO:CG	2.87	0.52
12:Z:73:ASP:OD1	12:Z:77:ASN:ND2	2.43	0.52
8:V:368:ARG:HH22	17:e:43:TRP:HZ2	1.55	0.52
12:Z:249:PHE:O	12:Z:253:THR:OG1	2.25	0.52
16:d:249:TYR:O	16:d:253:LEU:HB2	2.09	0.52
1:A:143:ASP:OD1	1:A:144:ARG:N	2.43	0.52
4:D:130:VAL:HA	4:D:142:VAL:HG12	1.92	0.52
6:F:87:PRO:HB3	6:F:152:GLY:HA2	1.91	0.52
8:V:483:CYS:SG	8:V:484:LEU:N	2.82	0.52
10:X:313:LEU:HA	10:X:316:ASP:HB2	1.92	0.52
11:Y:358:ARG:HG2	11:Y:360:ASP:OD2	2.09	0.52
12:Z:172:VAL:HG13	15:c:217:LEU:HD21	1.90	0.52
2:B:163:LEU:HD11	3:C:80:MET:HE3	1.91	0.52
7:U:142:LEU:HD21	7:U:166:THR:HG22	1.92	0.52
8:V:305:ALA:O	8:V:309:MET:CB	2.57	0.52
11:Y:337:PHE:HA	11:Y:341:GLY:H	1.75	0.52
12:Z:170:VAL:HG12	15:c:155:VAL:HB	1.91	0.52
13:a:123:LEU:HD11	13:a:135:ILE:HD11	1.92	0.52
2:B:100:ASP:HA	2:B:103:ARG:HG2	1.92	0.52
8:V:103:SER:O	8:V:107:ARG:NH1	2.42	0.52
8:V:492:LYS:NZ	8:V:495:ARG:NH1	2.58	0.52
9:W:179:LYS:HD2	9:W:217:GLU:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:379:ASP:OD2	10:X:382:GLU:HB2	2.09	0.52
13:a:42:LEU:O	13:a:46:GLN:HB2	2.10	0.52
13:a:257:GLN:HB3	13:a:261:LEU:HD22	1.90	0.52
5:E:27:LYS:HB2	5:E:30:ARG:HH12	1.74	0.52
8:V:186:LYS:HG3	8:V:187:ILE:HG23	1.92	0.52
1:A:86:THR:O	1:A:90:GLU:HB2	2.10	0.52
9:W:431:LYS:HA	15:c:239:LYS:HZ1	1.74	0.52
11:Y:175:ASP:HA	11:Y:178:ASN:HB3	1.92	0.52
12:Z:138:TYR:HB3	12:Z:155:PHE:HB3	1.91	0.52
16:d:30:LEU:HA	16:d:33:LEU:HB2	1.90	0.52
8:V:266:GLN:O	8:V:271:VAL:HG21	2.08	0.52
11:Y:181:LYS:HE3	11:Y:200:LEU:HA	1.92	0.52
12:Z:128:PRO:HG2	15:c:216:MET:HB2	1.92	0.52
13:a:112:ILE:HD13	13:a:151:VAL:HG21	1.92	0.52
7:U:135:ASN:HA	7:U:138:PHE:HB3	1.91	0.51
7:U:146:LYS:CB	7:U:146:LYS:NZ	2.73	0.51
7:U:543:LYS:HA	7:U:546:ARG:HG2	1.91	0.51
12:Z:28:LYS:CE	12:Z:28:LYS:N	2.73	0.51
12:Z:34:ARG:NH1	12:Z:100:LYS:O	2.43	0.51
14:b:26:LEU:HD21	14:b:78:VAL:HG11	1.92	0.51
17:e:42:ASN:O	17:e:46:ASP:CB	2.52	0.51
4:D:106:THR:HG21	5:E:77:PRO:HA	1.91	0.51
8:V:28:PRO:HB2	8:V:29:PRO:CD	2.36	0.51
8:V:284:GLU:O	8:V:288:TYR:CB	2.51	0.51
11:Y:43:ALA:HA	11:Y:46:ARG:HH11	1.75	0.51
11:Y:193:ASP:OD2	11:Y:196:GLN:HB2	2.10	0.51
14:b:84:ILE:HD12	14:b:115:SER:HB2	1.91	0.51
3:C:37:ASP:HB2	8:V:503:LYS:HB2	1.93	0.51
7:U:637:VAL:HA	7:U:640:LEU:HD13	1.91	0.51
7:U:885:MET:HB3	7:U:888:GLN:HG3	1.93	0.51
8:V:238:ALA:HB1	8:V:242:HIS:HD2	1.75	0.51
12:Z:189:GLN:O	12:Z:192:THR:OG1	2.28	0.51
2:B:120:HIS:HB2	2:B:132:TYR:HB2	1.92	0.51
3:C:66:LEU:HD23	4:D:136:SER:HB3	1.92	0.51
8:V:28:PRO:CB	8:V:29:PRO:HD3	2.38	0.51
12:Z:208:ILE:HA	12:Z:211:TYR:HB3	1.92	0.51
8:V:98:LEU:O	8:V:107:ARG:NE	2.43	0.51
8:V:224:LEU:HA	8:V:228:ARG:HD2	1.92	0.51
12:Z:285:ALA:O	12:Z:289:GLU:HB2	2.10	0.51
11:Y:268:TYR:HE1	11:Y:303:ALA:HB1	1.75	0.51
4:D:123:LEU:HD23	4:D:142:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:116:GLN:HE21	6:F:118:LYS:HB3	1.75	0.51
7:U:340:GLN:NE2	7:U:344:ARG:HH12	2.08	0.51
9:W:52:LYS:HE3	9:W:55:ARG:HH21	1.75	0.51
16:d:19:CYS:O	16:d:23:LEU:HB2	2.11	0.51
16:d:185:ALA:HB1	16:d:224:SER:HB2	1.92	0.51
6:F:69:MET:HA	6:F:72:LYS:HG2	1.92	0.51
7:U:70:HIS:O	8:V:236:ARG:NH1	2.44	0.51
8:V:322:VAL:HG13	8:V:350:GLN:HG3	1.93	0.51
13:a:149:THR:O	13:a:153:SER:N	2.41	0.51
16:d:34:ASN:ND2	16:d:38:THR:OG1	2.44	0.51
7:U:793:LYS:HB3	7:U:796:LYS:HB2	1.92	0.50
8:V:384:GLU:O	8:V:388:ALA:CB	2.59	0.50
8:V:420:ALA:O	8:V:424:GLN:CB	2.59	0.50
9:W:408:ARG:NH1	10:X:346:GLN:HA	2.25	0.50
10:X:420:LYS:NZ	12:Z:276:ILE:HG23	2.26	0.50
4:D:69:LYS:NZ	16:d:257:VAL:HG12	2.26	0.50
8:V:172:VAL:HG13	8:V:217:VAL:HG13	1.92	0.50
9:W:144:ARG:HA	9:W:147:LYS:NZ	2.26	0.50
13:a:165:THR:HG22	13:a:167:GLY:H	1.76	0.50
1:A:76:ALA:HB1	2:B:137:SER:HB3	1.93	0.50
2:B:126:SER:C	3:C:92:GLU:OE2	2.54	0.50
7:U:889:LEU:HD13	7:U:909:GLY:H	1.76	0.50
8:V:193:GLN:NE2	8:V:194:LYS:N	2.48	0.50
9:W:403:PHE:HZ	9:W:416:GLN:OE1	1.92	0.50
3:C:13:GLU:O	3:C:18:SER:N	2.44	0.50
8:V:345:ARG:NH1	8:V:354:LYS:HZ3	2.09	0.50
9:W:196:VAL:HG12	9:W:198:ASP:HB2	1.94	0.50
9:W:340:VAL:HA	9:W:350:ARG:NH1	2.25	0.50
7:U:98:GLU:O	7:U:102:ALA:HB2	2.12	0.50
7:U:139:GLN:HA	7:U:142:LEU:HB2	1.94	0.50
7:U:473:VAL:O	7:U:477:GLY:HA3	2.11	0.50
8:V:328:VAL:O	8:V:332:LEU:HB2	2.12	0.50
12:Z:105:ASP:O	12:Z:109:ASN:HB2	2.11	0.50
8:V:74:ASP:OD1	17:e:6:GLN:NE2	2.44	0.50
12:Z:252:LYS:NZ	15:c:301:ALA:HB2	2.24	0.50
15:c:116:PRO:HB3	15:c:148:ILE:HD13	1.92	0.50
8:V:183:GLU:HA	8:V:187:ILE:HG13	1.93	0.50
9:W:455:LEU:HD22	12:Z:214:LYS:NZ	2.27	0.50
14:b:145:GLU:OE2	14:b:175:PRO:HG3	2.11	0.50
15:c:212:LEU:O	15:c:216:MET:CB	2.60	0.50
7:U:337:LEU:HD22	7:U:844:LYS:NZ	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:698:GLN:HG2	7:U:705:LYS:HZ3	1.77	0.49
8:V:224:LEU:HB2	8:V:257:ASN:HD21	1.76	0.49
8:V:267:ALA:N	8:V:271:VAL:HG21	2.25	0.49
8:V:419:LEU:HD11	8:V:431:PRO:HG3	1.94	0.49
10:X:338:VAL:HG23	10:X:339:ILE:HD12	1.94	0.49
12:Z:28:LYS:H	12:Z:28:LYS:CE	2.24	0.49
15:c:175:ARG:HH22	15:c:180:ASN:HD21	1.60	0.49
3:C:57:ARG:NH1	7:U:644:TYR:OH	2.24	0.49
6:F:90:VAL:O	6:F:127:SER:OG	2.26	0.49
12:Z:34:ARG:NH1	12:Z:98:GLY:HA3	2.27	0.49
15:c:214:GLN:O	15:c:218:LEU:CB	2.56	0.49
7:U:604:HIS:O	7:U:608:SER:HB2	2.12	0.49
8:V:24:GLN:O	8:V:27:PRO:CD	2.60	0.49
8:V:180:ARG:O	8:V:184:ALA:CB	2.61	0.49
8:V:273:LYS:NZ	8:V:273:LYS:H	2.10	0.49
2:B:115:ILE:HD11	2:B:144:LEU:HD23	1.94	0.49
3:C:40:GLN:HA	3:C:43:ARG:NH1	2.28	0.49
7:U:482:GLY:HA3	7:U:515:ALA:HB1	1.94	0.49
7:U:728:PHE:O	7:U:732:LEU:HB2	2.12	0.49
7:U:745:THR:O	7:U:784:THR:N	2.42	0.49
8:V:271:VAL:H	8:V:273:LYS:HE2	1.77	0.49
9:W:370:TYR:CE1	9:W:416:GLN:HG2	2.47	0.49
12:Z:28:LYS:N	12:Z:28:LYS:HE2	2.28	0.49
5:E:85:ARG:NH1	12:Z:45:LYS:HZ2	2.09	0.49
7:U:836:THR:OG1	7:U:838:LYS:O	2.29	0.49
7:U:261:LEU:HA	7:U:264:VAL:HG12	1.93	0.49
7:U:344:ARG:HD2	7:U:880:ASN:HB3	1.95	0.49
9:W:444:HIS:HA	9:W:447:ALA:HB3	1.95	0.49
13:a:367:VAL:O	13:a:371:ALA:HB2	2.13	0.49
5:E:68:LYS:HG2	5:E:82:GLY:HA2	1.95	0.49
7:U:681:ASN:HB3	7:U:723:ASP:OD2	2.12	0.49
10:X:271:VAL:HG21	10:X:288:LYS:NZ	2.28	0.49
13:a:212:ASN:HD21	13:a:340:VAL:HB	1.78	0.49
7:U:493:VAL:O	7:U:497:LEU:HB2	2.12	0.49
9:W:224:LEU:HD13	9:W:253:THR:HG23	1.93	0.49
9:W:423:ASN:HB3	15:c:246:LYS:HZ2	1.78	0.49
15:c:32:TYR:HB2	15:c:68:ARG:HA	1.94	0.49
6:F:73:ILE:O	6:F:77:SER:OG	2.29	0.49
8:V:324:PHE:HB2	17:e:5:LYS:HG2	1.94	0.49
9:W:317:TRP:HA	9:W:320:LEU:HD13	1.95	0.49
12:Z:10:VAL:N	12:Z:48:LEU:O	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:176:MET:O	7:U:180:SER:HB2	2.13	0.49
8:V:197:THR:OG1	8:V:199:ASN:OD1	2.28	0.49
9:W:124:LEU:HA	9:W:127:THR:HG22	1.95	0.49
9:W:417:ARG:C	9:W:417:ARG:CZ	2.86	0.49
11:Y:148:GLY:HA3	11:Y:157:ILE:HG21	1.94	0.49
12:Z:208:ILE:O	12:Z:212:LEU:HB2	2.13	0.49
15:c:58:LEU:HB2	15:c:71:ASP:HB3	1.95	0.49
7:U:142:LEU:HG	7:U:145:HIS:HD1	1.77	0.48
7:U:350:LEU:O	7:U:354:LYS:CB	2.62	0.48
8:V:48:THR:O	8:V:52:ASP:CB	2.56	0.48
8:V:231:LEU:HD13	8:V:253:LEU:HD11	1.95	0.48
11:Y:124:PHE:HA	11:Y:127:THR:HG22	1.95	0.48
12:Z:11:VAL:HA	12:Z:50:VAL:HB	1.94	0.48
13:a:54:ASP:OD1	13:a:86:GLN:NE2	2.45	0.48
13:a:84:VAL:HG11	13:a:121:LEU:HD21	1.94	0.48
7:U:198:LEU:HD23	7:U:219:CYS:HA	1.95	0.48
8:V:79:VAL:HG23	8:V:82:LEU:HB2	1.93	0.48
8:V:273:LYS:NZ	8:V:273:LYS:N	2.60	0.48
10:X:258:LYS:HZ1	10:X:266:ASP:C	2.21	0.48
3:C:27:LYS:NZ	8:V:241:ARG:HB2	2.27	0.48
5:E:101:ASP:OD1	5:E:102:MET:N	2.45	0.48
7:U:226:PRO:HA	7:U:229:VAL:HG12	1.95	0.48
12:Z:251:LEU:HD21	15:c:246:LYS:NZ	2.28	0.48
12:Z:256:GLN:HE22	15:c:298:GLN:HG2	1.77	0.48
7:U:150:ALA:O	7:U:154:ALA:HB2	2.13	0.48
7:U:583:MET:HE3	7:U:605:VAL:HG11	1.95	0.48
7:U:681:ASN:HA	7:U:684:ARG:HE	1.78	0.48
12:Z:21:ASP:OD2	12:Z:25:ARG:NH2	2.46	0.48
15:c:26:ASP:HB3	15:c:174:PRO:HG2	1.96	0.48
4:D:89:ILE:HB	5:E:78:ARG:HG3	1.94	0.48
7:U:213:PHE:HA	7:U:216:VAL:HG12	1.96	0.48
11:Y:283:LYS:HG3	11:Y:284:LYS:HZ2	1.79	0.48
11:Y:297:ARG:HH11	17:e:48:VAL:CG2	2.27	0.48
3:C:35:VAL:HG13	4:D:58:GLU:OE2	2.13	0.48
6:F:88:TYR:HB3	6:F:155:LYS:HZ1	1.78	0.48
7:U:350:LEU:O	7:U:354:LYS:HB3	2.13	0.48
9:W:267:LEU:HD23	9:W:299:ILE:HD11	1.95	0.48
9:W:393:LEU:HA	9:W:396:LEU:HB2	1.95	0.48
10:X:210:LEU:O	10:X:214:SER:OG	2.29	0.48
15:c:282:ARG:HE	15:c:286:GLU:HG3	1.79	0.48
16:d:21:GLU:O	16:d:25:ARG:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:138:PHE:HE2	7:U:165:LYS:NZ	2.10	0.48
7:U:138:PHE:HE2	7:U:165:LYS:HZ1	1.61	0.48
8:V:410:ILE:HD11	8:V:425:LYS:NZ	2.27	0.48
9:W:115:ILE:CG1	9:W:116:THR:HG22	2.43	0.48
12:Z:75:LEU:O	12:Z:79:TYR:HB3	2.13	0.48
12:Z:270:VAL:O	12:Z:274:ASN:ND2	2.47	0.48
16:d:5:LEU:HD11	16:d:26:LEU:HD11	1.96	0.48
2:B:105:THR:HA	3:C:97:VAL:HG23	1.95	0.48
9:W:59:ASP:O	9:W:63:THR:OG1	2.32	0.48
9:W:423:ASN:HD22	15:c:246:LYS:HZ3	1.61	0.48
9:W:438:LEU:HA	9:W:441:LYS:HE3	1.94	0.48
10:X:290:VAL:HG13	10:X:302:PHE:HE1	1.78	0.48
15:c:194:HIS:HA	15:c:197:ASN:HB2	1.95	0.48
5:E:74:THR:HG1	5:E:97:ARG:NH1	2.12	0.48
6:F:151:VAL:HG12	6:F:163:THR:HG23	1.94	0.48
9:W:8:ARG:O	9:W:12:ARG:CB	2.59	0.48
14:b:90:ILE:HD12	14:b:127:LEU:HD13	1.96	0.48
7:U:496:LEU:HA	7:U:499:THR:HG22	1.95	0.48
10:X:271:VAL:HG21	10:X:288:LYS:HZ3	1.79	0.48
11:Y:345:CYS:SG	11:Y:356:THR:OG1	2.63	0.48
13:a:70:ARG:HH21	14:b:15:TYR:HA	1.78	0.48
14:b:110:ILE:HG22	14:b:139:ASP:HB2	1.96	0.48
6:F:152:GLY:HA3	6:F:162:GLU:H	1.79	0.47
8:V:24:GLN:C	8:V:27:PRO:HG3	2.38	0.47
9:W:202:THR:HA	9:W:205:ILE:HG12	1.96	0.47
13:a:74:LEU:HD21	13:a:110:ALA:HB1	1.96	0.47
13:a:359:ASP:HB3	15:c:310:LYS:HG3	1.95	0.47
14:b:107:MET:HB3	14:b:136:VAL:HG13	1.96	0.47
7:U:257:SER:HB2	7:U:261:LEU:HG	1.95	0.47
11:Y:280:GLN:HA	11:Y:283:LYS:HE2	1.96	0.47
2:B:102:LEU:HD22	2:B:160:ILE:HD13	1.96	0.47
7:U:397:THR:HA	7:U:401:LYS:HE2	1.95	0.47
7:U:885:MET:HG2	7:U:887:ALA:H	1.80	0.47
8:V:416:ARG:HE	11:Y:350:VAL:HG12	1.79	0.47
12:Z:33:LYS:HZ2	12:Z:60:GLU:N	2.01	0.47
17:e:59:GLU:HG3	17:e:63:HIS:CE1	2.50	0.47
6:F:55:MET:HB2	13:a:105:LYS:HZ2	1.79	0.47
15:c:28:ALA:HA	15:c:175:ARG:HG3	1.96	0.47
3:C:23:TYR:CE2	8:V:193:GLN:CD	2.78	0.47
9:W:283:GLN:HE22	9:W:361:HIS:CE1	2.31	0.47
7:U:457:ILE:HG22	7:U:460:TYR:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:474:ARG:NH2	7:U:500:ASN:O	2.48	0.47
8:V:492:LYS:HZ2	8:V:495:ARG:HH11	1.62	0.47
9:W:222:LEU:HG	9:W:225:LYS:HD2	1.95	0.47
13:a:186:LYS:HZ2	13:a:225:LEU:CD1	2.27	0.47
4:D:69:LYS:HZ1	16:d:257:VAL:C	2.23	0.47
5:E:81:VAL:HG12	5:E:105:LEU:HB3	1.96	0.47
7:U:740:GLY:HA3	7:U:744:VAL:HG22	1.95	0.47
7:U:799:LYS:HA	7:U:843:GLU:HA	1.97	0.47
8:V:25:GLU:CA	8:V:27:PRO:HD3	2.45	0.47
8:V:350:GLN:HE21	8:V:353:LEU:HD13	1.78	0.47
8:V:357:LEU:HG	8:V:360:TYR:HB3	1.97	0.47
9:W:288:HIS:HA	9:W:291:SER:HB3	1.96	0.47
12:Z:22:HIS:CD2	12:Z:25:ARG:HH12	2.32	0.47
12:Z:197:GLY:O	12:Z:201:LEU:HB2	2.14	0.47
13:a:76:LEU:HA	13:a:79:ILE:HG22	1.95	0.47
13:a:112:ILE:HG12	13:a:142:LEU:HD12	1.97	0.47
15:c:88:ASP:HB3	15:c:91:PHE:HB3	1.96	0.47
15:c:251:LEU:HA	15:c:254:ASN:HD22	1.80	0.47
10:X:377:ILE:HG23	11:Y:312:ARG:HH11	1.79	0.47
13:a:359:ASP:OD2	15:c:310:LYS:HE2	2.14	0.47
14:b:150:THR:HA	14:b:153:LEU:HB2	1.97	0.47
1:A:76:ALA:O	1:A:80:LEU:CB	2.58	0.47
8:V:160:LEU:HD13	8:V:182:LYS:NZ	2.28	0.47
8:V:177:ASN:HA	8:V:180:ARG:HH11	1.79	0.47
12:Z:26:ILE:CG2	12:Z:28:LYS:HZ3	2.24	0.47
15:c:245:VAL:O	15:c:249:LEU:N	2.48	0.47
7:U:205:TYR:HD2	7:U:211:PRO:HA	1.80	0.47
8:V:287:ARG:NH1	17:e:1:MET:HB2	2.30	0.47
10:X:169:VAL:O	10:X:173:GLU:HB2	2.15	0.47
11:Y:283:LYS:HE3	11:Y:284:LYS:HZ2	1.79	0.47
12:Z:123:ILE:HD12	12:Z:138:TYR:HE2	1.79	0.47
14:b:97:LEU:O	14:b:100:ARG:NH1	2.47	0.47
1:A:144:ARG:HH22	2:B:156:VAL:HG13	1.80	0.46
8:V:153:LYS:HZ3	8:V:203:LEU:HB2	1.78	0.46
13:a:35:HIS:CB	13:a:70:ARG:HH12	2.22	0.46
10:X:282:ARG:HB3	10:X:312:GLU:OE2	2.15	0.46
13:a:193:GLN:HA	13:a:196:ARG:HB2	1.97	0.46
3:C:34:ILE:HG22	3:C:38:LYS:HE2	1.97	0.46
4:D:67:ASN:HA	4:D:70:LYS:NZ	2.30	0.46
7:U:520:MET:HE2	7:U:520:MET:HB3	1.80	0.46
7:U:535:TYR:HA	7:U:538:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:765:VAL:HG11	7:U:778:PHE:HD2	1.80	0.46
8:V:256:ARG:HE	17:e:4:LYS:HZ3	1.62	0.46
9:W:154:GLU:HG2	9:W:192:LEU:HD21	1.98	0.46
9:W:417:ARG:C	9:W:417:ARG:NE	2.73	0.46
12:Z:26:ILE:HG22	12:Z:28:LYS:HZ1	1.77	0.46
13:a:21:VAL:O	13:a:25:LEU:HB2	2.15	0.46
4:D:85:ILE:HG21	5:E:68:LYS:HD2	1.98	0.46
10:X:45:VAL:HA	10:X:48:GLN:HG2	1.97	0.46
11:Y:92:GLU:HG2	11:Y:93:LYS:HD2	1.97	0.46
11:Y:234:PRO:O	11:Y:238:GLU:CB	2.63	0.46
15:c:193:ILE:O	15:c:197:ASN:CB	2.58	0.46
16:d:114:GLU:O	16:d:118:GLU:HB2	2.15	0.46
7:U:132:GLY:O	7:U:136:LYS:HB2	2.16	0.46
7:U:219:CYS:SG	7:U:220:LEU:N	2.89	0.46
8:V:473:GLN:HE21	12:Z:250:TYR:N	2.14	0.46
10:X:317:PRO:HD2	10:X:319:ILE:HD11	1.96	0.46
7:U:625:ILE:HG13	7:U:626:LEU:HG	1.98	0.46
11:Y:179:ARG:HH12	11:Y:212:GLU:CD	2.17	0.46
14:b:157:VAL:HG21	14:b:170:LEU:HD13	1.98	0.46
7:U:666:LYS:NZ	7:U:704:PRO:HD2	2.30	0.46
8:V:293:GLY:O	8:V:297:ALA:HB2	2.15	0.46
11:Y:175:ASP:O	11:Y:179:ARG:CB	2.62	0.46
12:Z:97:THR:HA	12:Z:124:ILE:HG13	1.98	0.46
12:Z:284:ASP:HA	12:Z:287:LYS:HG2	1.96	0.46
13:a:367:VAL:O	13:a:371:ALA:CB	2.63	0.46
8:V:212:TYR:OH	8:V:249:THR:O	2.28	0.46
5:E:112:PRO:HG2	6:F:96:LEU:HD21	1.97	0.46
7:U:841:LYS:HG2	7:U:882:ALA:H	1.81	0.46
9:W:114:GLU:OE1	9:W:114:GLU:HA	2.14	0.46
10:X:400:ALA:O	10:X:403:THR:OG1	2.28	0.46
12:Z:228:TYR:OH	13:a:340:VAL:O	2.34	0.46
16:d:209:TYR:HA	16:d:212:LYS:HB3	1.98	0.46
7:U:150:ALA:O	7:U:154:ALA:CB	2.64	0.46
7:U:504:ASP:OD1	7:U:535:TYR:OH	2.34	0.46
8:V:47:SER:O	8:V:150:ARG:NH2	2.49	0.46
9:W:304:ASP:HA	9:W:307:LYS:HE3	1.97	0.46
9:W:416:GLN:HE22	9:W:418:PRO:HG3	1.76	0.46
11:Y:278:VAL:HG12	11:Y:282:MET:HE3	1.98	0.46
12:Z:37:GLY:HA2	12:Z:55:ALA:HA	1.98	0.46
12:Z:196:HIS:HB2	15:c:234:TYR:HE2	1.81	0.46
4:D:70:LYS:HD2	12:Z:180:LYS:HZ1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:47:LEU:HD11	6:F:80:ILE:HD11	1.98	0.45
9:W:45:GLU:OE2	9:W:93:ARG:HG3	2.15	0.45
10:X:216:ILE:O	10:X:220:ALA:CB	2.60	0.45
11:Y:110:TYR:HA	11:Y:113:ARG:HH11	1.80	0.45
12:Z:64:ASP:OD2	12:Z:67:VAL:HG23	2.16	0.45
7:U:799:LYS:HZ3	7:U:924:LEU:HB3	1.80	0.45
8:V:501:TYR:HA	12:Z:282:ASN:HD21	1.81	0.45
9:W:131:VAL:HA	9:W:142:ARG:HD2	1.98	0.45
9:W:349:LYS:O	9:W:353:ASP:CB	2.65	0.45
10:X:255:LEU:HD22	10:X:267:VAL:HG13	1.98	0.45
14:b:68:THR:HA	14:b:71:ILE:HD12	1.98	0.45
7:U:12:LEU:HD22	7:U:41:SER:HB3	1.98	0.45
8:V:309:MET:HE3	8:V:332:LEU:HA	1.99	0.45
10:X:222:GLU:OE2	10:X:322:HIS:HD2	1.98	0.45
11:Y:191:ILE:HG23	11:Y:193:ASP:H	1.81	0.45
15:c:124:GLY:HA2	15:c:127:ILE:HG22	1.97	0.45
7:U:103:LYS:O	7:U:107:HIS:ND1	2.34	0.45
8:V:89:LYS:HG3	8:V:92:ARG:HH21	1.81	0.45
8:V:273:LYS:N	8:V:273:LYS:HZ3	2.14	0.45
9:W:314:LEU:HD11	9:W:382:LEU:HD21	1.98	0.45
10:X:337:ARG:HH22	10:X:353:LEU:HD21	1.80	0.45
11:Y:210:SER:O	11:Y:214:MET:N	2.50	0.45
8:V:397:ARG:O	8:V:401:ASN:HB2	2.16	0.45
8:V:491:VAL:HA	8:V:494:MET:HG2	1.98	0.45
9:W:153:LYS:HE2	9:W:161:GLU:HG3	1.99	0.45
15:c:241:ASN:HD21	15:c:300:LEU:HD12	1.80	0.45
7:U:36:ALA:CB	8:V:271:VAL:HG12	2.41	0.45
7:U:101:ILE:HA	7:U:104:CYS:HB3	1.99	0.45
7:U:490:ARG:HB2	7:U:493:VAL:HG12	1.99	0.45
8:V:76:LYS:HE3	8:V:78:HIS:HB2	1.99	0.45
8:V:436:PHE:HE2	16:d:147:SER:HA	1.81	0.45
10:X:246:LYS:O	10:X:250:SER:OG	2.31	0.45
3:C:115:ALA:HB3	3:C:124:HIS:HB2	1.99	0.45
7:U:21:GLU:OE2	7:U:55:ARG:NE	2.49	0.45
7:U:184:CYS:HA	7:U:187:LEU:HD23	1.99	0.45
7:U:353:LEU:HD12	7:U:357:LYS:HZ1	1.82	0.45
8:V:28:PRO:CB	8:V:29:PRO:CD	2.94	0.45
8:V:228:ARG:HD3	8:V:257:ASN:ND2	2.31	0.45
8:V:439:ALA:HA	8:V:442:ILE:HD12	1.99	0.45
8:V:484:LEU:HD11	12:Z:260:VAL:HG22	1.99	0.45
10:X:417:LYS:HA	10:X:420:LYS:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:121:LEU:O	11:Y:125:ARG:HB2	2.17	0.45
5:E:62:LYS:HE3	5:E:64:LEU:HD11	1.98	0.45
5:E:85:ARG:HH22	12:Z:45:LYS:HZ3	1.65	0.45
7:U:2:ILE:HD13	7:U:5:ALA:HB3	1.98	0.45
10:X:154:LEU:HB3	10:X:158:LYS:HZ2	1.82	0.45
10:X:344:ARG:HG3	10:X:384:VAL:HG13	1.97	0.45
11:Y:119:GLY:O	11:Y:123:ALA:HB2	2.17	0.45
4:D:89:ILE:HD11	5:E:80:VAL:HG13	1.99	0.45
7:U:147:TYR:O	7:U:147:TYR:CD1	2.70	0.45
8:V:25:GLU:O	8:V:27:PRO:HD2	2.16	0.45
8:V:153:LYS:NZ	8:V:203:LEU:HB2	2.32	0.45
8:V:193:GLN:NE2	8:V:194:LYS:HB3	2.32	0.45
8:V:325:LYS:O	8:V:329:HIS:HB2	2.16	0.45
9:W:437:SER:O	9:W:441:LYS:CB	2.64	0.45
12:Z:133:LEU:HD23	12:Z:135:THR:H	1.81	0.45
15:c:39:LEU:HD23	15:c:42:LEU:HD12	1.98	0.45
11:Y:314:LEU:HB2	11:Y:354:VAL:HB	1.99	0.45
11:Y:315:THR:HG23	11:Y:318:TYR:H	1.82	0.45
7:U:64:ALA:HA	7:U:67:VAL:HG12	1.99	0.44
7:U:421:GLN:O	7:U:425:THR:OG1	2.31	0.44
8:V:209:LYS:HA	8:V:212:TYR:HD2	1.82	0.44
8:V:261:TYR:HE1	16:d:121:ARG:HB3	1.82	0.44
10:X:77:LEU:HD22	10:X:85:ALA:HA	1.99	0.44
3:C:99:VAL:HB	3:C:123:LEU:H	1.82	0.44
12:Z:28:LYS:HZ3	12:Z:28:LYS:HA	1.82	0.44
14:b:53:THR:OG1	14:b:54:LEU:N	2.51	0.44
2:B:112:LEU:N	2:B:148:CYS:O	2.50	0.44
3:C:90:HIS:O	3:C:91:PRO:C	2.60	0.44
5:E:15:LYS:O	5:E:19:HIS:ND1	2.37	0.44
5:E:38:LYS:O	5:E:42:LYS:HB2	2.17	0.44
5:E:87:LEU:HD22	5:E:91:LYS:HZ3	1.82	0.44
8:V:282:ASN:C	11:Y:385:ARG:HH12	2.26	0.44
13:a:364:GLU:O	13:a:368:GLU:CB	2.65	0.44
16:d:119:LEU:HD23	16:d:122:LEU:HD21	1.99	0.44
1:A:108:ASP:OD1	1:A:108:ASP:N	2.47	0.44
8:V:89:LYS:HG3	8:V:92:ARG:HE	1.82	0.44
10:X:243:ASP:HB3	10:X:246:LYS:HB2	1.99	0.44
11:Y:153:ASP:OD2	11:Y:156:LEU:HB2	2.17	0.44
12:Z:8:LYS:HG3	12:Z:47:VAL:HG23	2.00	0.44
12:Z:22:HIS:CG	12:Z:25:ARG:HH12	2.35	0.44
6:F:79:LYS:HA	6:F:82:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:24:GLN:O	8:V:28:PRO:CD	2.65	0.44
8:V:28:PRO:N	8:V:29:PRO:HD2	2.32	0.44
10:X:208:ALA:HB2	10:X:238:GLY:HA3	1.99	0.44
10:X:255:LEU:HB2	10:X:287:LEU:HD13	1.99	0.44
13:a:112:ILE:H	13:a:112:ILE:HG13	1.47	0.44
13:a:324:ILE:HG12	13:a:332:HIS:H	1.82	0.44
15:c:131:GLN:HA	15:c:134:GLU:OE2	2.16	0.44
4:D:43:ARG:O	4:D:47:LEU:HB2	2.17	0.44
8:V:441:ALA:HA	8:V:444:ASP:OD2	2.17	0.44
11:Y:232:GLU:HG2	11:Y:235:ASP:OD2	2.18	0.44
11:Y:250:LEU:HD13	11:Y:257:ARG:HD3	1.99	0.44
13:a:70:ARG:HA	14:b:17:ARG:NH1	2.24	0.44
13:a:326:GLU:HG3	13:a:329:LYS:HA	2.00	0.44
15:c:69:VAL:O	15:c:208:ARG:NH2	2.36	0.44
5:E:40:TYR:HE2	6:F:70:LYS:HE3	1.82	0.44
7:U:61:ALA:O	7:U:65:SER:HB3	2.17	0.44
7:U:803:LYS:HA	7:U:839:ALA:H	1.83	0.44
10:X:268:GLN:O	10:X:272:SER:HB2	2.18	0.44
11:Y:244:ALA:HA	11:Y:247:LEU:HD12	1.99	0.44
12:Z:219:LYS:O	12:Z:220:LEU:C	2.61	0.44
13:a:22:TRP:HA	13:a:25:LEU:HB3	1.99	0.44
15:c:190:GLN:HA	15:c:194:HIS:CE1	2.53	0.44
7:U:418:GLU:O	7:U:422:LEU:HB2	2.18	0.44
8:V:428:LEU:HD11	8:V:437:ILE:HD12	1.99	0.44
9:W:108:CYS:HB3	9:W:123:ARG:NH1	2.33	0.44
10:X:258:LYS:HE2	10:X:270:LEU:HD12	1.99	0.44
12:Z:139:ILE:HG12	12:Z:141:VAL:HG13	1.98	0.44
13:a:312:MET:O	13:a:316:SER:OG	2.32	0.44
15:c:57:MET:HE2	15:c:112:TYR:HB3	1.99	0.44
7:U:196:LYS:HA	7:U:199:ARG:HG2	2.00	0.44
8:V:446:VAL:HG23	8:V:447:ILE:HG23	2.00	0.44
8:V:448:GLU:OE2	8:V:463:MET:HB3	2.17	0.44
10:X:209:THR:HG23	10:X:212:MET:HE2	1.99	0.44
11:Y:50:MET:HE3	11:Y:70:LEU:HB3	2.00	0.44
12:Z:247:LYS:NZ	12:Z:250:TYR:HD2	2.15	0.44
15:c:156:VAL:O	15:c:156:VAL:HG12	2.17	0.44
16:d:190:LEU:HD22	16:d:192:THR:HG22	1.99	0.44
7:U:477:GLY:O	7:U:481:LEU:HB3	2.18	0.43
7:U:770:TRP:O	15:c:179:SER:OG	2.27	0.43
8:V:196:SER:H	8:V:200:ARG:HG3	1.82	0.43
8:V:315:LYS:HD2	11:Y:385:ARG:HE	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:442:ILE:HG21	8:V:451:ILE:HD11	2.00	0.43
9:W:262:LYS:O	9:W:266:ALA:HB3	2.18	0.43
7:U:666:LYS:HZ3	7:U:704:PRO:HD2	1.83	0.43
8:V:268:GLU:O	8:V:273:LYS:HE3	2.10	0.43
8:V:277:PRO:HD2	8:V:279:GLN:NE2	2.33	0.43
9:W:352:LYS:O	9:W:356:ASN:HB2	2.18	0.43
11:Y:160:ASN:O	11:Y:164:ALA:HB3	2.18	0.43
11:Y:184:GLN:HA	11:Y:187:TYR:CE2	2.52	0.43
9:W:75:TYR:O	9:W:79:GLU:CB	2.57	0.43
11:Y:149:LEU:HD13	11:Y:186:LEU:HD23	2.00	0.43
12:Z:231:GLN:NE2	13:a:345:GLN:O	2.49	0.43
13:a:112:ILE:O	13:a:116:THR:OG1	2.27	0.43
13:a:343:LEU:HA	13:a:346:ILE:HD12	2.00	0.43
3:C:80:MET:HG3	3:C:82:LYS:HG2	2.00	0.43
6:F:94:ILE:HD12	6:F:125:LYS:HE2	1.99	0.43
7:U:12:LEU:HD21	7:U:45:ILE:HG13	2.01	0.43
9:W:27:ARG:HH12	9:W:54:THR:C	2.26	0.43
9:W:119:PRO:O	9:W:123:ARG:CB	2.66	0.43
9:W:416:GLN:CD	9:W:418:PRO:HD3	2.39	0.43
12:Z:180:LYS:HG2	12:Z:183:THR:HG21	2.00	0.43
3:C:113:ARG:NH2	3:C:128:PRO:O	2.51	0.43
7:U:698:GLN:OE1	7:U:702:THR:OG1	2.36	0.43
15:c:49:VAL:HB	15:c:50:PRO:HD2	1.99	0.43
1:A:115:VAL:HG13	1:A:117:GLN:H	1.83	0.43
6:F:78:GLU:HA	6:F:81:LYS:HZ3	1.83	0.43
7:U:362:ASN:HA	7:U:395:ARG:HH21	1.83	0.43
7:U:698:GLN:HG2	7:U:705:LYS:HZ2	1.82	0.43
10:X:263:THR:HG22	10:X:266:ASP:H	1.84	0.43
11:Y:72:LYS:HA	11:Y:75:LYS:HE3	1.99	0.43
11:Y:98:SER:HA	11:Y:101:ARG:HB3	1.99	0.43
12:Z:102:HIS:N	12:Z:105:ASP:OD2	2.50	0.43
12:Z:204:LYS:HZ2	13:a:356:TRP:CD1	2.37	0.43
13:a:296:ILE:HD12	13:a:331:VAL:HG21	2.00	0.43
14:b:20:ASP:OD1	14:b:20:ASP:N	2.49	0.43
7:U:142:LEU:HA	7:U:145:HIS:HA	2.01	0.43
7:U:146:LYS:NZ	7:U:146:LYS:HB3	2.32	0.43
7:U:841:LYS:NZ	7:U:882:ALA:O	2.50	0.43
9:W:240:TYR:HE1	9:W:350:ARG:HG2	1.83	0.43
9:W:272:LEU:HD23	9:W:275:ILE:HD12	2.00	0.43
9:W:417:ARG:NE	9:W:417:ARG:O	2.51	0.43
9:W:437:SER:O	9:W:441:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:258:LYS:HZ3	10:X:266:ASP:HB2	1.83	0.43
12:Z:21:ASP:OD2	15:c:104:ARG:NH2	2.51	0.43
13:a:101:ARG:HH12	13:a:115:LYS:HG3	1.84	0.43
14:b:18:ASN:OD1	14:b:25:ARG:NH2	2.52	0.43
7:U:683:VAL:O	7:U:687:ALA:CB	2.66	0.43
8:V:141:THR:HG22	8:V:145:LEU:HB2	2.01	0.43
8:V:194:LYS:NZ	8:V:237:THR:HG23	2.34	0.43
9:W:416:GLN:NE2	9:W:418:PRO:CG	2.64	0.43
10:X:114:ILE:HG23	10:X:126:ARG:HB2	2.00	0.43
11:Y:190:ALA:O	17:e:37:HIS:NE2	2.40	0.43
13:a:127:ASP:OD1	13:a:128:LEU:N	2.52	0.43
15:c:49:VAL:O	15:c:51:MET:N	2.52	0.43
7:U:221:ILE:HG22	7:U:256:ALA:HB2	1.99	0.43
9:W:122:LEU:HA	9:W:125:ILE:HG22	2.01	0.43
8:V:98:LEU:HD13	8:V:98:LEU:HA	1.90	0.43
10:X:319:ILE:H	10:X:319:ILE:HG13	1.66	0.43
13:a:57:ILE:HA	13:a:60:TYR:HB2	2.00	0.43
14:b:134:GLU:HG3	14:b:136:VAL:HG23	2.00	0.43
1:A:105:ASP:OD1	1:A:105:ASP:N	2.52	0.42
3:C:38:LYS:O	3:C:42:LEU:HB2	2.19	0.42
3:C:41:ASN:ND2	8:V:499:LYS:O	2.52	0.42
3:C:104:ASP:OD1	3:C:104:ASP:N	2.52	0.42
7:U:80:TYR:O	7:U:84:ALA:HB2	2.19	0.42
8:V:333:ILE:HA	8:V:336:GLU:HB2	2.00	0.42
9:W:116:THR:HG23	9:W:116:THR:O	2.19	0.42
9:W:403:PHE:CZ	9:W:418:PRO:HG3	2.51	0.42
12:Z:28:LYS:CE	12:Z:28:LYS:CA	2.95	0.42
13:a:285:PRO:O	13:a:289:ARG:NH2	2.52	0.42
3:C:11:LEU:O	7:U:140:ARG:NH1	2.51	0.42
3:C:13:GLU:O	3:C:17:GLY:N	2.52	0.42
4:D:73:LEU:HA	4:D:76:GLN:HB3	2.00	0.42
4:D:93:LEU:HD23	4:D:94:GLU:HG3	2.00	0.42
7:U:256:ALA:HA	7:U:754:HIS:CD2	2.55	0.42
8:V:267:ALA:HA	8:V:271:VAL:CG2	2.45	0.42
9:W:272:LEU:HA	9:W:275:ILE:HD12	2.01	0.42
12:Z:204:LYS:NZ	13:a:356:TRP:CD1	2.87	0.42
13:a:136:GLU:O	13:a:140:GLU:HB2	2.19	0.42
1:A:100:LYS:HG2	1:A:142:VAL:HG11	2.02	0.42
3:C:100:ASP:HB3	3:C:122:THR:HB	2.02	0.42
7:U:117:ASP:N	7:U:117:ASP:OD1	2.51	0.42
7:U:559:ARG:HB3	7:U:562:GLU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:225:TRP:HE1	10:X:260:MET:HE2	1.85	0.42
11:Y:44:ALA:HA	11:Y:49:ASN:HD22	1.85	0.42
3:C:119:ASP:OD1	3:C:119:ASP:N	2.51	0.42
4:D:77:GLU:OE2	12:Z:183:THR:HG22	2.19	0.42
8:V:375:PHE:HA	8:V:378:VAL:HB	2.01	0.42
3:C:36:ASN:O	3:C:39:SER:OG	2.36	0.42
7:U:353:LEU:C	7:U:357:LYS:HZ3	2.26	0.42
9:W:344:THR:HG23	9:W:345:GLU:HG2	2.02	0.42
13:a:58:LYS:O	13:a:62:ASN:CB	2.57	0.42
15:c:93:ALA:HA	15:c:96:LEU:HD12	2.02	0.42
7:U:368:ALA:HA	7:U:371:ILE:HG22	2.00	0.42
7:U:458:ILE:HG23	7:U:481:LEU:HD11	2.01	0.42
10:X:309:TYR:O	10:X:313:LEU:N	2.44	0.42
13:a:340:VAL:HG13	13:a:341:LEU:H	1.85	0.42
15:c:155:VAL:O	15:c:155:VAL:HG13	2.20	0.42
15:c:192:LEU:O	15:c:196:LEU:HB2	2.20	0.42
15:c:213:GLU:O	15:c:217:LEU:CB	2.68	0.42
7:U:374:SER:HB3	7:U:407:SER:HB3	2.01	0.42
8:V:186:LYS:O	8:V:190:ASP:CA	2.57	0.42
8:V:492:LYS:NZ	8:V:495:ARG:HH11	2.18	0.42
9:W:60:MET:SD	9:W:111:TYR:OH	2.72	0.42
11:Y:173:ASP:HB2	11:Y:176:ARG:HB3	2.02	0.42
12:Z:167:ALA:HB1	15:c:42:LEU:HD22	2.01	0.42
3:C:27:LYS:HZ2	8:V:241:ARG:HB2	1.84	0.42
4:D:84:SER:H	4:D:133:HIS:HE1	1.68	0.42
5:E:85:ARG:NH1	12:Z:45:LYS:NZ	2.60	0.42
8:V:226:VAL:HG13	8:V:227:VAL:CA	2.37	0.42
10:X:245:PRO:HA	10:X:248:ILE:HG22	2.01	0.42
12:Z:28:LYS:HA	12:Z:28:LYS:HD3	1.66	0.42
16:d:202:THR:HG22	16:d:204:LYS:HG2	2.02	0.42
17:e:49:GLU:O	17:e:53:SER:N	2.52	0.42
6:F:78:GLU:HA	6:F:81:LYS:HZ1	1.84	0.42
8:V:384:GLU:O	8:V:388:ALA:HB2	2.18	0.42
9:W:317:TRP:HB3	9:W:355:LYS:HZ2	1.82	0.42
9:W:376:LYS:NZ	9:W:386:VAL:HG11	2.35	0.42
9:W:417:ARG:HA	9:W:417:ARG:HD2	1.85	0.42
13:a:34:TRP:CD1	14:b:19:GLY:H	2.37	0.42
16:d:163:TYR:HA	16:d:166:PHE:HD2	1.85	0.42
16:d:179:ALA:HA	16:d:182:ILE:HG22	2.01	0.42
9:W:326:MET:HA	9:W:329:ARG:HB2	2.02	0.42
12:Z:224:HIS:NE2	12:Z:228:TYR:OH	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:237:HIS:HA	15:c:240:HIS:HB2	2.01	0.42
7:U:92:ASP:HB3	7:U:97:VAL:HG11	2.01	0.41
7:U:462:LEU:HD12	7:U:481:LEU:HD21	2.01	0.41
8:V:153:LYS:O	8:V:157:THR:OG1	2.23	0.41
10:X:86:ALA:HA	10:X:125:LEU:HD13	2.02	0.41
13:a:215:GLU:HA	13:a:218:MET:HE2	2.01	0.41
1:A:79:ASP:HA	1:A:82:ALA:HB3	2.03	0.41
4:D:66:LYS:C	4:D:70:LYS:HZ3	2.20	0.41
7:U:20:LYS:NZ	7:U:48:LEU:HD22	2.35	0.41
8:V:35:VAL:O	8:V:39:GLU:HB2	2.20	0.41
8:V:462:GLU:OE2	11:Y:348:ASP:HA	2.20	0.41
10:X:205:LYS:O	10:X:209:THR:OG1	2.35	0.41
15:c:259:VAL:HG11	15:c:287:HIS:CE1	2.55	0.41
2:B:114:GLU:OE2	2:B:122:ILE:HD12	2.20	0.41
7:U:141:CYS:HB3	7:U:149:GLN:HE21	1.85	0.41
12:Z:226:ILE:O	12:Z:230:LEU:HB2	2.20	0.41
13:a:250:THR:HA	13:a:253:THR:HG22	2.01	0.41
14:b:37:CYS:O	14:b:41:THR:OG1	2.31	0.41
14:b:157:VAL:O	14:b:161:ASN:N	2.53	0.41
9:W:52:LYS:HA	9:W:55:ARG:HG2	2.02	0.41
10:X:299:LEU:HD21	10:X:331:LEU:HD13	2.02	0.41
11:Y:293:ARG:HH22	17:e:52:PHE:HB2	1.84	0.41
15:c:139:ARG:C	15:c:161:ARG:HH12	2.29	0.41
16:d:170:LEU:HA	16:d:173:THR:HG22	2.01	0.41
3:C:90:HIS:C	3:C:91:PRO:O	2.62	0.41
7:U:36:ALA:O	7:U:39:SER:OG	2.38	0.41
7:U:516:LEU:HA	7:U:519:VAL:HG22	2.02	0.41
8:V:175:MET:HE2	8:V:214:HIS:HB3	2.01	0.41
8:V:447:ILE:H	8:V:447:ILE:HG13	1.80	0.41
10:X:224:ASP:OD2	10:X:227:THR:HG23	2.21	0.41
12:Z:91:ILE:H	12:Z:91:ILE:HG13	1.54	0.41
14:b:34:ASN:O	14:b:38:HIS:ND1	2.37	0.41
14:b:94:HIS:CE1	14:b:109:ILE:HD12	2.56	0.41
15:c:202:SER:OG	15:c:203:ILE:N	2.53	0.41
5:E:47:LEU:HD13	6:F:79:LYS:HZ3	1.84	0.41
6:F:88:TYR:HB3	6:F:155:LYS:NZ	2.35	0.41
8:V:273:LYS:CE	8:V:273:LYS:H	2.34	0.41
9:W:316:ARG:O	9:W:319:THR:OG1	2.27	0.41
10:X:307:THR:HA	10:X:310:ARG:HE	1.84	0.41
10:X:363:ARG:O	10:X:367:GLN:HB2	2.20	0.41
12:Z:95:TYR:HB3	12:Z:122:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:d:150:LYS:O	16:d:154:ALA:HB2	2.21	0.41
4:D:53:PHE:CE2	7:U:632:GLN:HB3	2.56	0.41
8:V:28:PRO:N	8:V:29:PRO:CD	2.83	0.41
10:X:333:GLN:HA	10:X:336:ILE:HG12	2.01	0.41
13:a:226:ARG:HG2	13:a:229:ASP:OD2	2.20	0.41
15:c:254:ASN:O	15:c:258:ALA:CB	2.68	0.41
13:a:54:ASP:O	13:a:58:LYS:HG2	2.21	0.41
8:V:29:PRO:O	8:V:32:PRO:CD	2.68	0.41
8:V:37:MET:HE3	8:V:115:LYS:HZ2	1.86	0.41
8:V:226:VAL:HG13	8:V:227:VAL:CB	2.50	0.41
8:V:448:GLU:OE2	8:V:461:LYS:HE2	2.21	0.41
8:V:498:PRO:HG3	12:Z:274:ASN:HB3	2.02	0.41
11:Y:57:LEU:HD12	11:Y:60:SER:HB2	2.01	0.41
11:Y:111:LEU:HA	11:Y:114:ILE:HG22	2.03	0.41
11:Y:300:ARG:NH1	17:e:60:LEU:HD11	2.36	0.41
11:Y:304:TYR:O	11:Y:308:LEU:HB2	2.20	0.41
12:Z:249:PHE:O	12:Z:253:THR:CB	2.69	0.41
13:a:61:GLU:O	13:a:65:SER:OG	2.35	0.41
13:a:113:LEU:HD23	13:a:113:LEU:HA	1.90	0.41
13:a:296:ILE:HD11	13:a:331:VAL:HG11	2.03	0.41
14:b:76:HIS:CD2	14:b:77:THR:H	2.39	0.41
15:c:90:VAL:O	15:c:94:LYS:CB	2.67	0.41
8:V:177:ASN:HA	8:V:180:ARG:NH1	2.35	0.41
8:V:263:LEU:HD23	16:d:118:GLU:HA	2.03	0.41
9:W:408:ARG:CZ	10:X:346:GLN:HA	2.51	0.41
11:Y:231:LEU:HD23	11:Y:235:ASP:HB3	2.02	0.41
11:Y:261:PHE:O	11:Y:265:GLU:CB	2.68	0.41
11:Y:296:VAL:O	11:Y:300:ARG:HG2	2.20	0.41
13:a:35:HIS:N	13:a:70:ARG:HH12	2.19	0.41
13:a:247:ARG:O	13:a:251:LEU:CB	2.65	0.41
14:b:4:GLU:H	14:b:47:ASN:ND2	2.19	0.41
3:C:97:VAL:HG11	3:C:121:TYR:HB3	2.03	0.40
3:C:97:VAL:HG21	3:C:121:TYR:HB2	2.03	0.40
7:U:762:GLY:O	7:U:766:PHE:CB	2.70	0.40
9:W:268:LYS:HD3	9:W:336:PRO:HG2	2.04	0.40
10:X:347:ILE:HD12	10:X:358:LYS:HG2	2.03	0.40
10:X:379:ASP:OD1	10:X:380:GLN:N	2.54	0.40
15:c:242:GLU:HA	15:c:246:LYS:HE3	2.02	0.40
16:d:150:LYS:O	16:d:154:ALA:CB	2.69	0.40
3:C:92:GLU:OE1	3:C:92:GLU:HA	2.19	0.40
6:F:61:ARG:HB2	14:b:76:HIS:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:567:ILE:HG21	7:U:586:VAL:HB	2.03	0.40
10:X:77:LEU:HD21	10:X:88:LEU:HD23	2.03	0.40
10:X:105:GLN:O	10:X:109:LEU:HB2	2.20	0.40
11:Y:183:TYR:HA	11:Y:186:LEU:HD13	2.03	0.40
4:D:83:GLN:HA	4:D:133:HIS:CE1	2.57	0.40
7:U:442:GLY:O	7:U:446:LEU:HB2	2.21	0.40
7:U:762:GLY:O	7:U:766:PHE:HB2	2.21	0.40
8:V:178:SER:HB3	8:V:182:LYS:HZ3	1.84	0.40
11:Y:292:TYR:CZ	17:e:57:ARG:NH1	2.89	0.40
13:a:58:LYS:HB3	13:a:83:VAL:HG22	2.04	0.40
13:a:120:ALA:HB2	13:a:158:LEU:HD11	2.03	0.40
14:b:86:PHE:HB3	14:b:119:ASP:OD2	2.21	0.40
16:d:3:GLU:OE2	16:d:5:LEU:HB2	2.22	0.40
7:U:567:ILE:CG2	7:U:601:ARG:HH12	2.35	0.40
11:Y:304:TYR:O	11:Y:308:LEU:CB	2.69	0.40
13:a:188:LEU:HA	13:a:189:PRO:HD2	1.75	0.40
1:A:116:LYS:HZ1	2:B:128:GLY:HA3	1.87	0.40
5:E:72:LYS:NZ	5:E:78:ARG:HE	2.16	0.40
6:F:152:GLY:N	6:F:162:GLU:O	2.54	0.40
7:U:109:THR:OG1	7:U:156:GLU:O	2.39	0.40
7:U:264:VAL:HA	7:U:267:ASN:HD22	1.86	0.40
8:V:414:TYR:HE1	11:Y:347:ILE:HG12	1.86	0.40
9:W:375:MET:HA	9:W:378:MET:HB3	2.04	0.40
11:Y:119:GLY:O	11:Y:123:ALA:CB	2.70	0.40
14:b:156:PHE:O	14:b:160:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	81/83 (98%)	73 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	71/73 (97%)	57 (80%)	14 (20%)	0	100	100
3	C	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14	49
4	D	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
5	E	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
6	F	97/115 (84%)	91 (94%)	6 (6%)	0	100	100
7	U	837/935 (90%)	790 (94%)	46 (6%)	1 (0%)	48	83
8	V	486/488 (100%)	410 (84%)	67 (14%)	9 (2%)	6	32
9	W	452/456 (99%)	410 (91%)	38 (8%)	4 (1%)	14	49
10	X	381/385 (99%)	371 (97%)	10 (3%)	0	100	100
11	Y	376/378 (100%)	355 (94%)	21 (6%)	0	100	100
12	Z	284/286 (99%)	260 (92%)	21 (7%)	3 (1%)	11	45
13	a	372/374 (100%)	346 (93%)	25 (7%)	1 (0%)	36	71
14	b	189/191 (99%)	174 (92%)	15 (8%)	0	100	100
15	c	285/287 (99%)	259 (91%)	25 (9%)	1 (0%)	30	67
16	d	255/257 (99%)	230 (90%)	25 (10%)	0	100	100
17	e	68/70 (97%)	61 (90%)	7 (10%)	0	100	100
All	All	4557/4707 (97%)	4196 (92%)	341 (8%)	20 (0%)	31	67

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	91	PRO
8	V	27	PRO
8	V	190	ASP
8	V	193	GLN
8	V	225	ASP
8	V	226	VAL
9	W	115	ILE
9	W	221	LYS
12	Z	221	PRO
15	c	50	PRO
8	V	30	PRO
8	V	31	ALA
9	W	117	ASP
8	V	240	LEU
13	a	189	PRO

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Mol	Chain	Res	Type
12	Z	220	LEU
7	U	148	LYS
9	W	418	PRO
8	V	275	VAL
12	Z	117	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	73/73 (100%)	73 (100%)	0	100	100
2	B	66/66 (100%)	66 (100%)	0	100	100
3	C	107/107 (100%)	107 (100%)	0	100	100
4	D	98/98 (100%)	98 (100%)	0	100	100
5	E	95/95 (100%)	94 (99%)	1 (1%)	65	74
6	F	94/106 (89%)	94 (100%)	0	100	100
7	U	717/798 (90%)	711 (99%)	6 (1%)	73	77
8	V	422/422 (100%)	415 (98%)	7 (2%)	53	67
9	W	416/416 (100%)	411 (99%)	5 (1%)	63	73
10	X	331/331 (100%)	328 (99%)	3 (1%)	70	76
11	Y	334/334 (100%)	334 (100%)	0	100	100
12	Z	257/257 (100%)	252 (98%)	5 (2%)	50	66
13	a	334/334 (100%)	331 (99%)	3 (1%)	70	76
14	b	167/167 (100%)	167 (100%)	0	100	100
15	c	252/252 (100%)	251 (100%)	1 (0%)	84	82
16	d	231/231 (100%)	230 (100%)	1 (0%)	84	82
17	e	63/63 (100%)	62 (98%)	1 (2%)	55	69
All	All	4057/4150 (98%)	4024 (99%)	33 (1%)	70	77

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	22	ILE
7	U	146	LYS
7	U	427	LEU
7	U	507	VAL
7	U	529	ILE
7	U	554	LEU
7	U	935	ILE
8	V	189	ASP
8	V	193	GLN
8	V	239	THR
8	V	242	HIS
8	V	271	VAL
8	V	272	SER
8	V	273	LYS
9	W	114	GLU
9	W	115	ILE
9	W	220	GLU
9	W	416	GLN
9	W	417	ARG
10	X	80	ILE
10	X	339	ILE
10	X	369	ILE
12	Z	28	LYS
12	Z	91	ILE
12	Z	118	ASN
12	Z	119	SER
12	Z	187	LEU
13	a	32	LYS
13	a	112	ILE
13	a	340	VAL
15	c	67	VAL
16	d	197	ILE
17	e	22	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	131	HIS
3	C	22	GLN
3	C	69	GLN
4	D	83	GLN
4	D	133	HIS
5	E	45	ASN

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Mol	Chain	Res	Type
6	F	116	GLN
6	F	154	ASN
7	U	79	ASN
7	U	139	GLN
7	U	247	GLN
7	U	267	ASN
7	U	340	GLN
7	U	373	ASN
7	U	415	HIS
7	U	438	GLN
7	U	450	HIS
7	U	604	HIS
7	U	708	GLN
7	U	743	ASN
7	U	805	ASN
7	U	901	GLN
8	V	78	HIS
8	V	109	ASN
8	V	125	ASN
8	V	242	HIS
8	V	257	ASN
8	V	260	HIS
8	V	279	GLN
8	V	377	GLN
8	V	452	ASN
8	V	473	GLN
9	W	86	ASN
9	W	96	GLN
9	W	99	GLN
9	W	257	GLN
9	W	288	HIS
9	W	361	HIS
9	W	395	ASN
9	W	416	GLN
9	W	423	ASN
10	X	148	HIS
10	X	170	GLN
10	X	182	ASN
10	X	333	GLN
10	X	406	ASN
10	X	416	ASN
11	Y	48	ASN

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Mol	Chain	Res	Type
11	Y	71	ASN
11	Y	273	GLN
11	Y	291	HIS
11	Y	363	ASN
11	Y	367	GLN
12	Z	196	HIS
12	Z	229	GLN
12	Z	231	GLN
12	Z	274	ASN
12	Z	282	ASN
13	a	35	HIS
13	a	40	GLN
13	a	258	GLN
13	a	288	HIS
13	a	290	GLN
13	a	372	HIS
14	b	12	ASN
14	b	29	GLN
14	b	34	ASN
14	b	76	HIS
14	b	99	HIS
14	b	149	ASN
14	b	158	ASN
15	c	44	HIS
15	c	130	GLN
15	c	183	HIS
15	c	214	GLN
15	c	241	ASN
15	c	254	ASN
16	d	60	GLN
16	d	96	HIS
16	d	97	GLN
17	e	6	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	W	1
10	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	205:ILE	C	206:SER	N	3.21
1	X	311:ALA	C	312:GLU	N	3.21

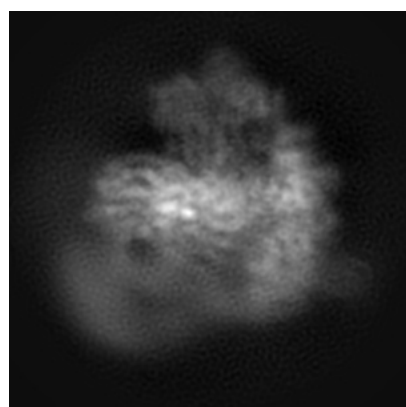
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8672. These allow visual inspection of the internal detail of the map and identification of artifacts.

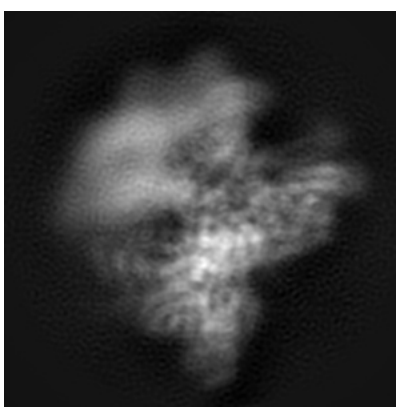
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

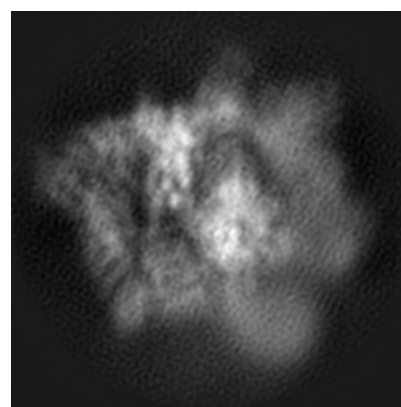
6.1.1 Primary map



X



Y

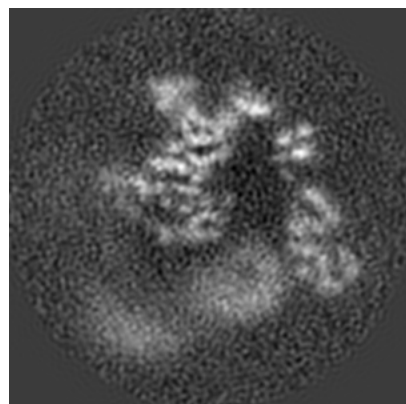


Z

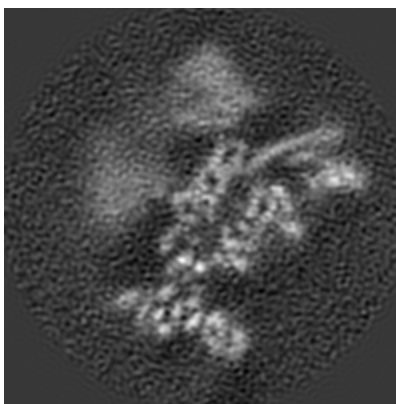
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

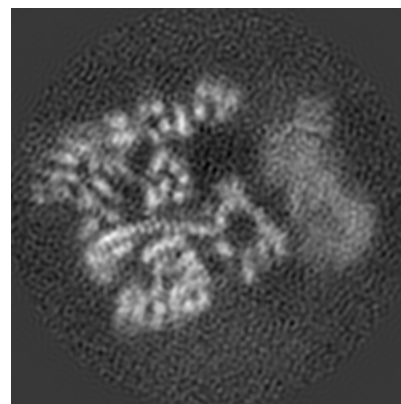
6.2.1 Primary map



X Index: 128



Y Index: 128

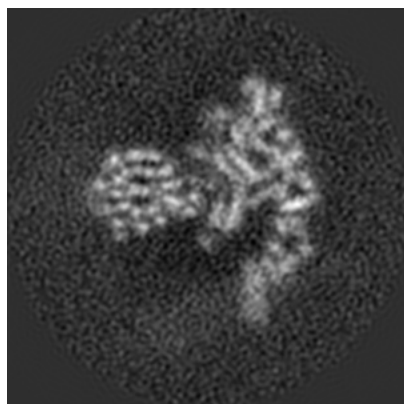


Z Index: 128

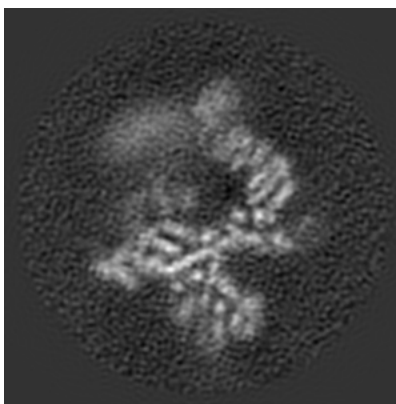
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

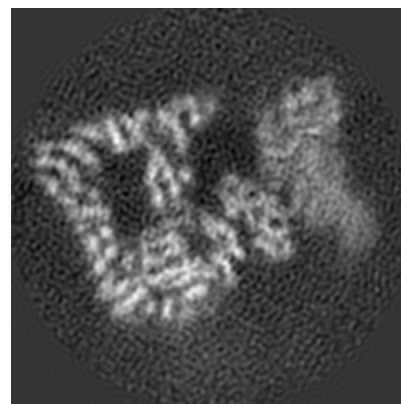
6.3.1 Primary map



X Index: 109



Y Index: 179

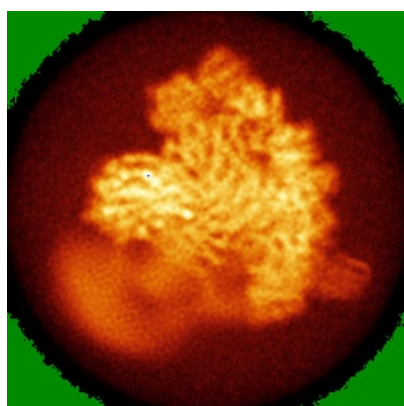


Z Index: 139

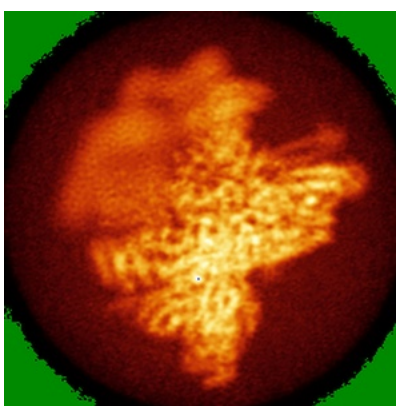
The images above show the largest variance slices of the map in three orthogonal directions.

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

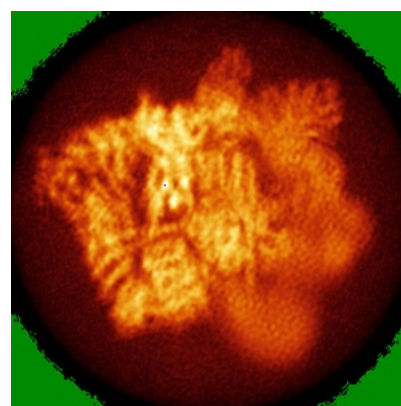
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

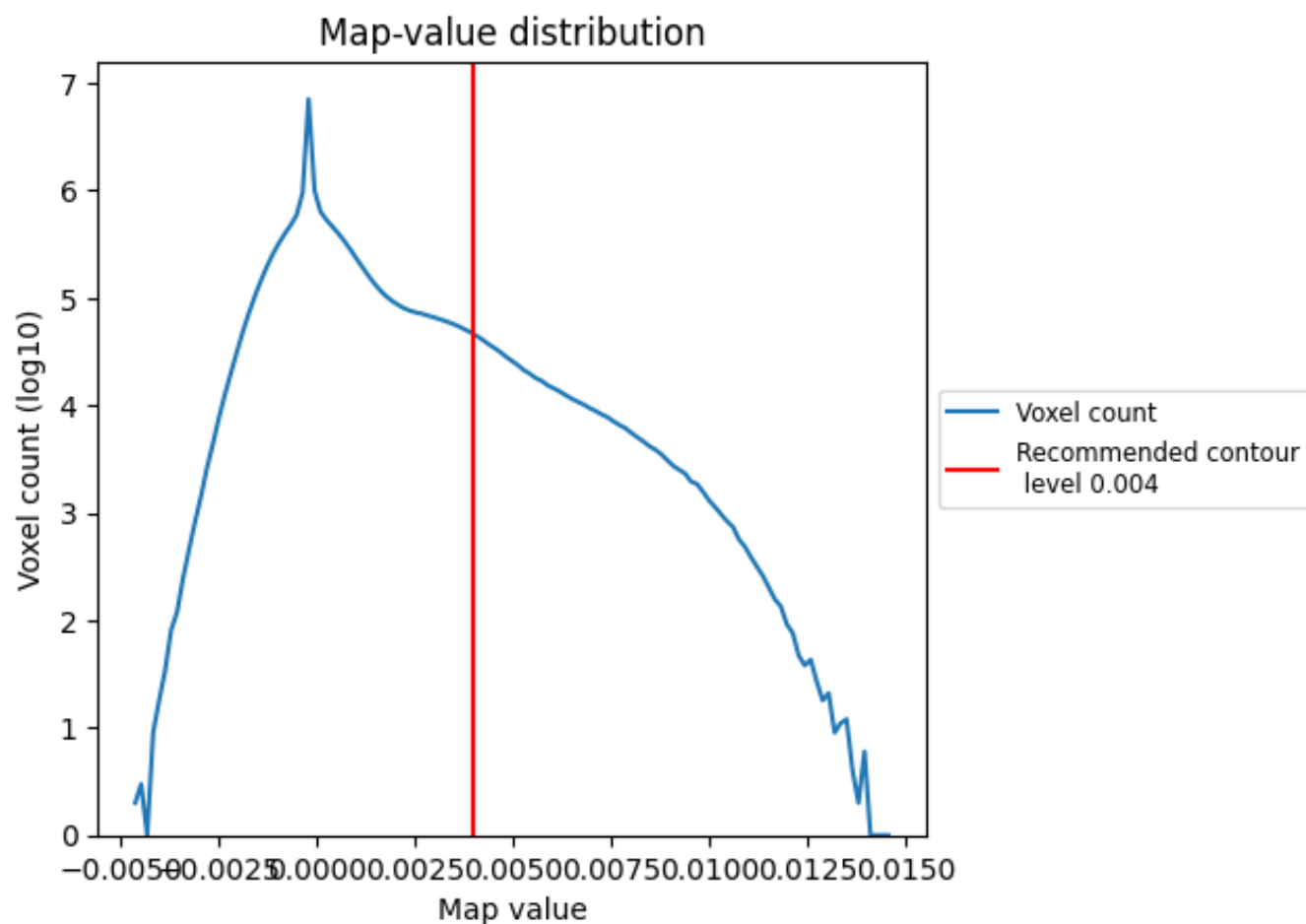
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

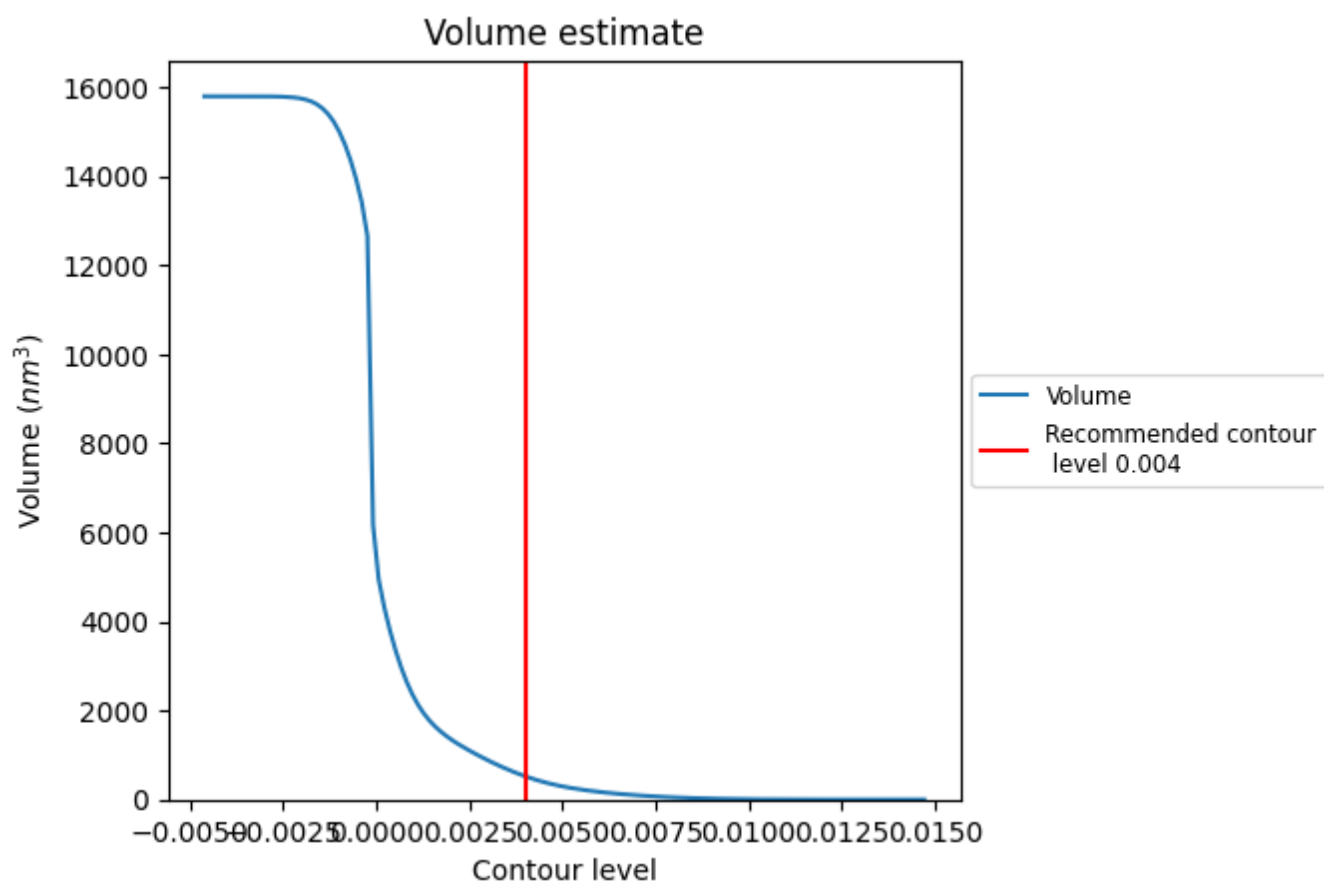
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

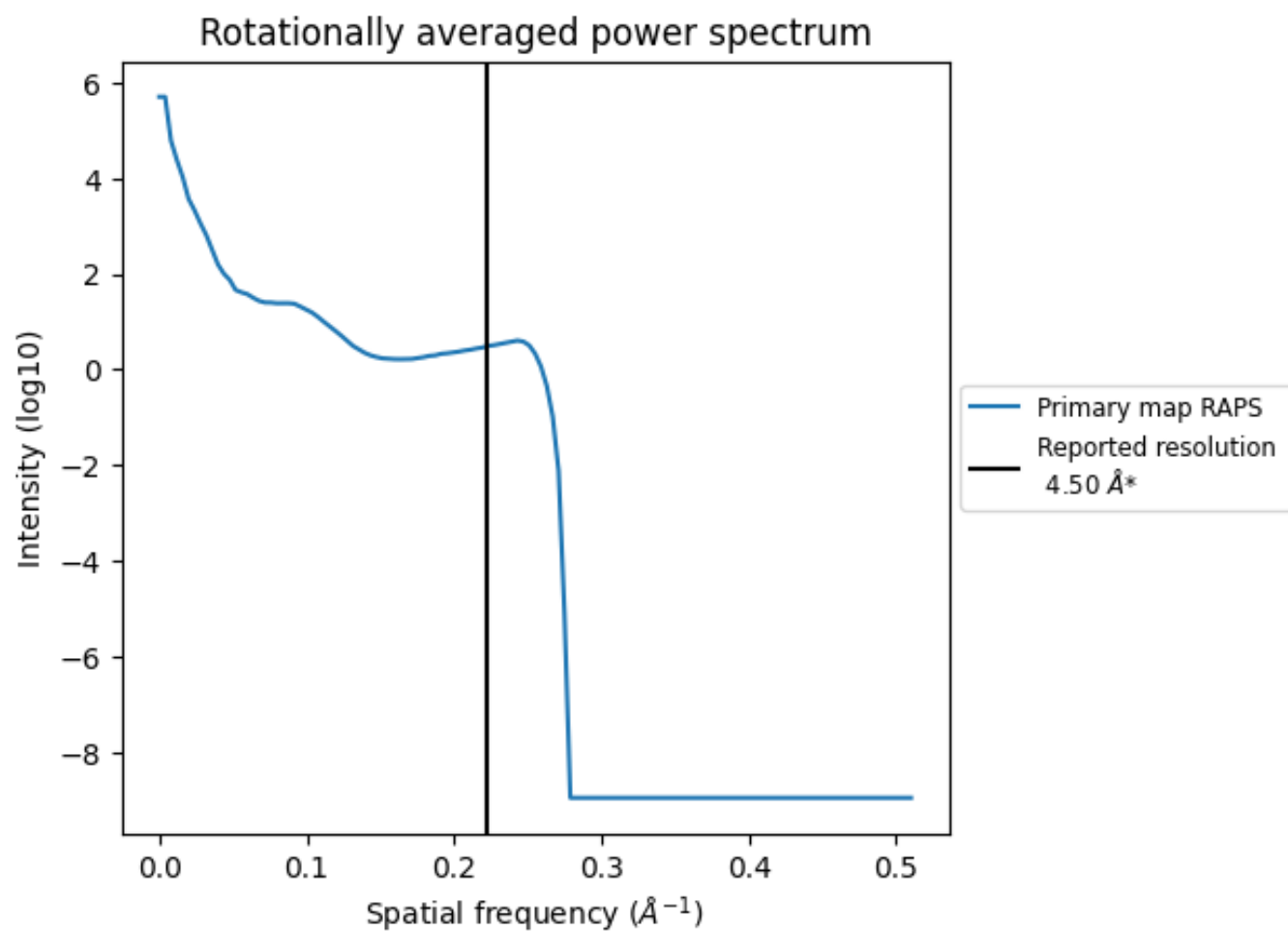
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 523 nm³; this corresponds to an approximate mass of 472 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 0.222 Å⁻¹

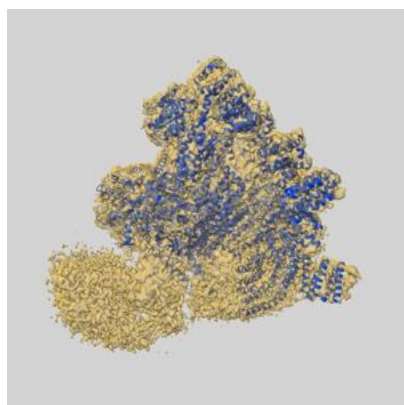
8 Fourier-Shell correlation

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

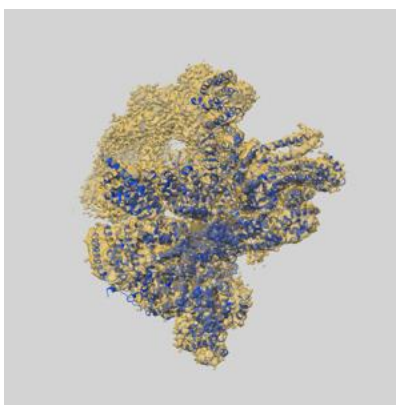
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8672 and PDB model 5VGZ. Per-residue inclusion information can be found in section 3 on page 7.

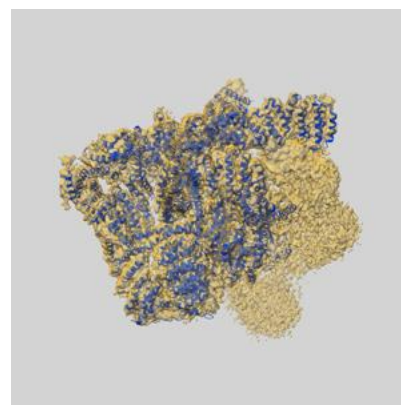
9.1 Map-model overlay [i](#)



X



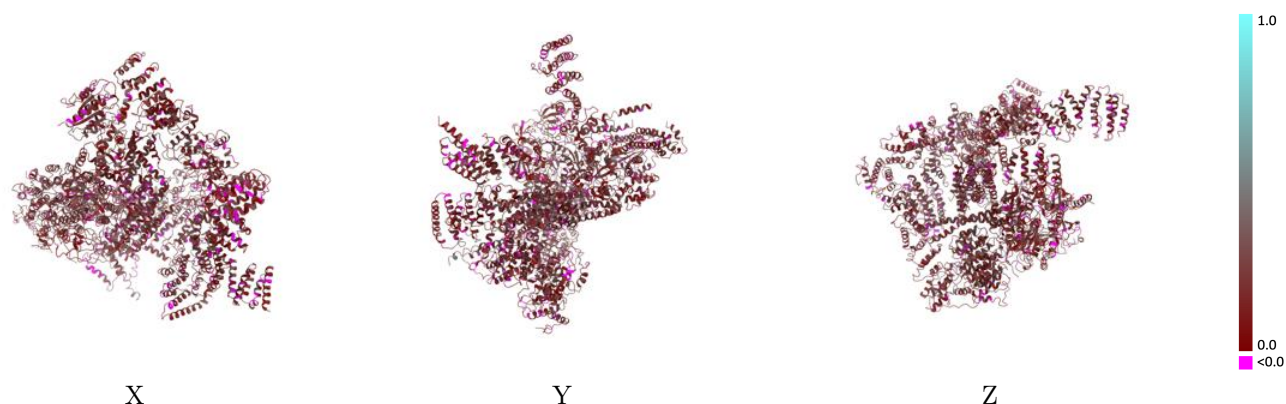
Y



Z

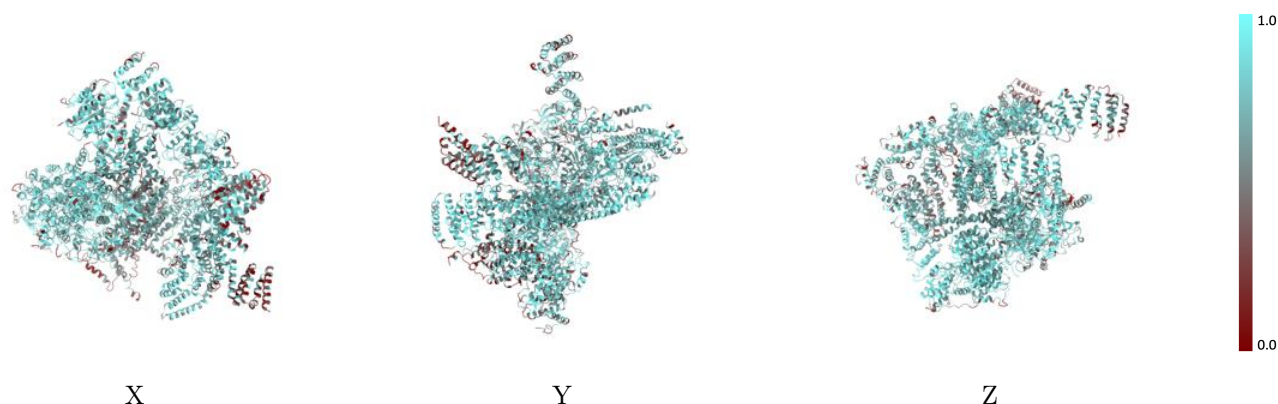
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



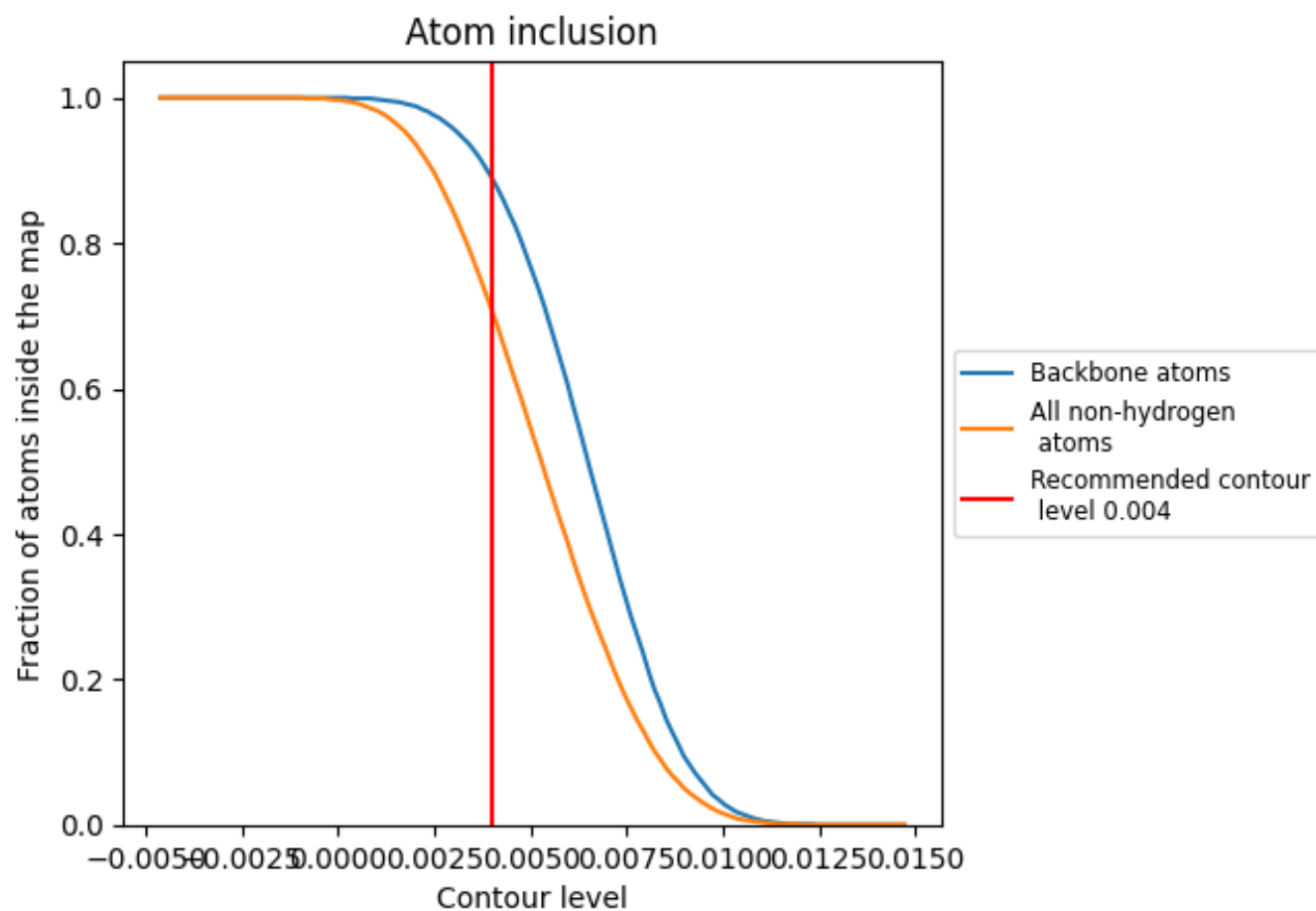
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 71% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7070	 0.1950
A	 0.6990	 0.1900
B	 0.6620	 0.1800
C	 0.7190	 0.2040
D	 0.6900	 0.2120
E	 0.5930	 0.2090
F	 0.6080	 0.2080
U	 0.8110	 0.2220
V	 0.5810	 0.1630
W	 0.6780	 0.1800
X	 0.6060	 0.1790
Y	 0.7920	 0.1890
Z	 0.7400	 0.2040
a	 0.7750	 0.1950
b	 0.7640	 0.1930
c	 0.7240	 0.2160
d	 0.6430	 0.1900
e	 0.5290	 0.1680

