



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 08:52 AM UTC

PDB ID : 5VHS / pdb_00005vhs
EMDB ID : EMD-8684
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 : 2017-04-13
Resolution : 8.80 Å(reported)

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

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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

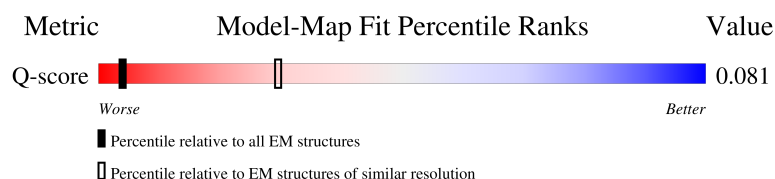
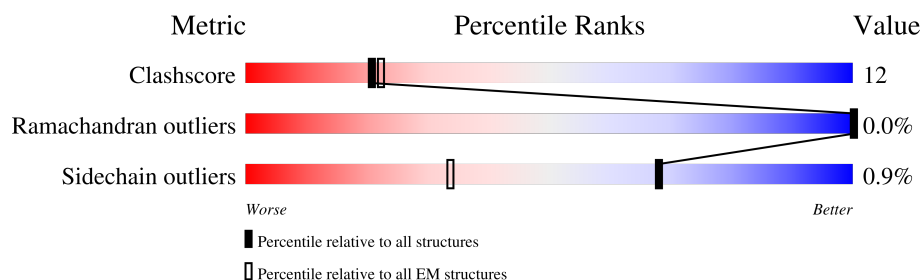
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.80 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.



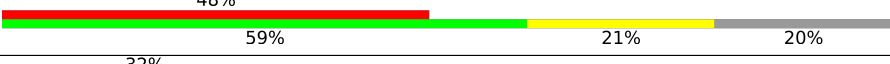
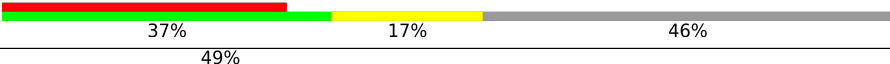
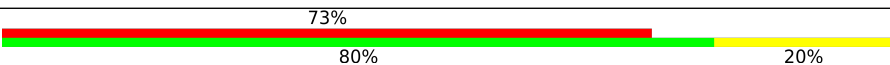
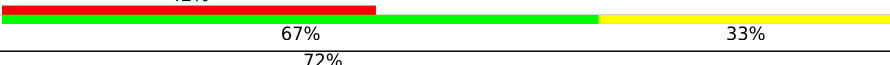
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	265 (8.30 - 9.30)

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	352	73% 66% 28% . .
2	B	341	74% 65% 28% 7%
3	C	385	76% 65% 26% 9%
4	D	368	73% 70% 20% 10%

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Mol	Chain	Length	Quality of chain
5	E	379	
6	F	380	
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	33	
18	f	784	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 47840 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	338	Total	C	N	O	S	0	0
			2665	1682	470	496	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	317	Total	C	N	O	S	0	0
			2476	1557	421	487	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	349	Total	C	N	O	S	0	0
			2752	1724	502	512	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	332	Total	C	N	O	S	0	0
			2649	1677	466	497	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	313	Total	C	N	O	S	0	0
			2493	1566	448	464	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	339	Total	C	N	O	S	0	0
			2647	1673	460	498	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	751	Total	C	N	O	S	0	0
			5829	3696	1001	1088	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	262	Total	C	N	O	S	0	0
			2129	1360	377	385	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	391	Total	C	N	O	S	0	0
			3206	2040	545	600	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	280	Total	C	N	O	S	0	0
			2221	1414	373	425	9		

- 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	176	Total	C	N	O	S	0	0
			1452	943	232	272	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	e	33	Total	C	N	O	S	0	0
			283	172	46	64	1		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	f	636	Total	C	N	O	S	0	0
			4920	3110	830	945	35		

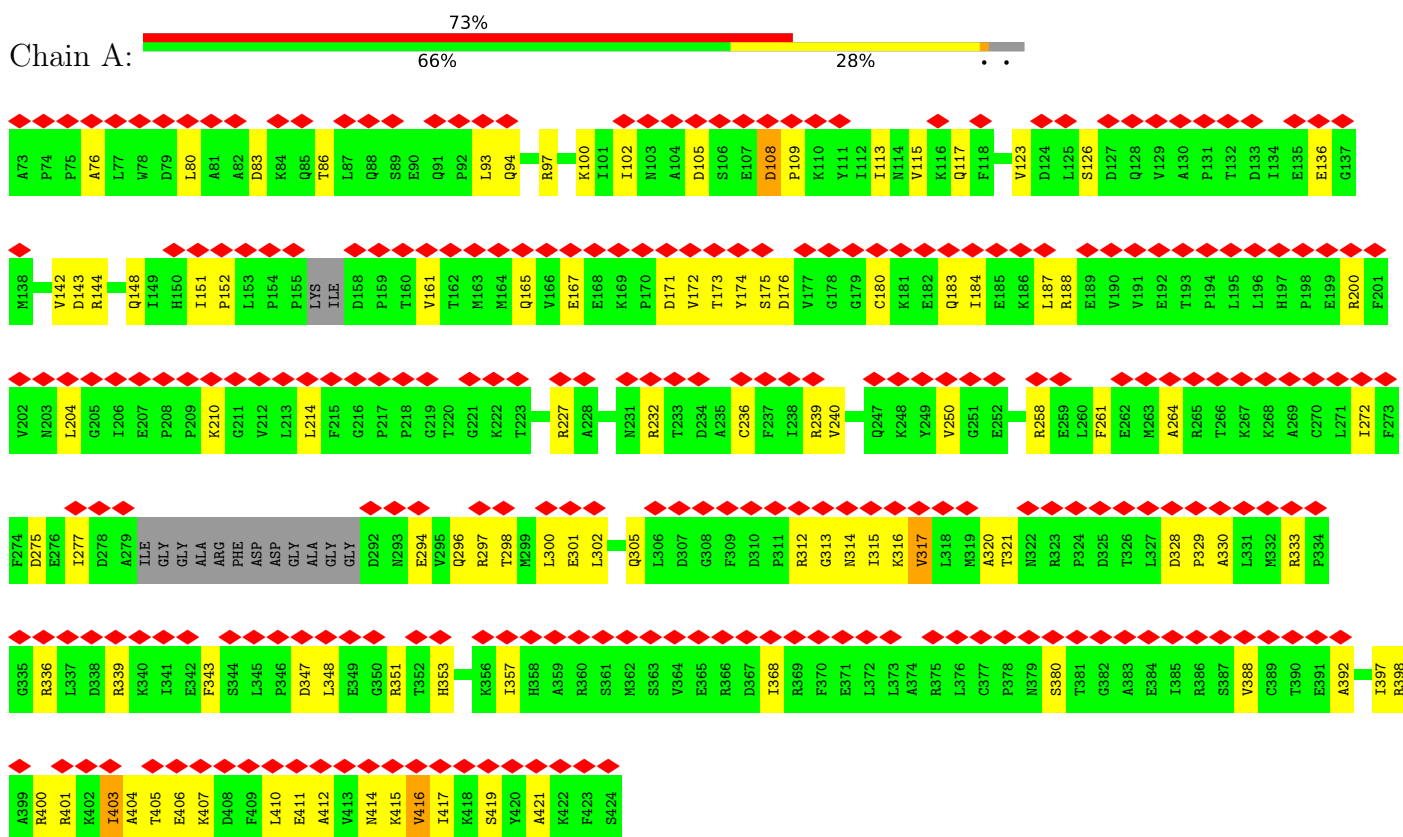
- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

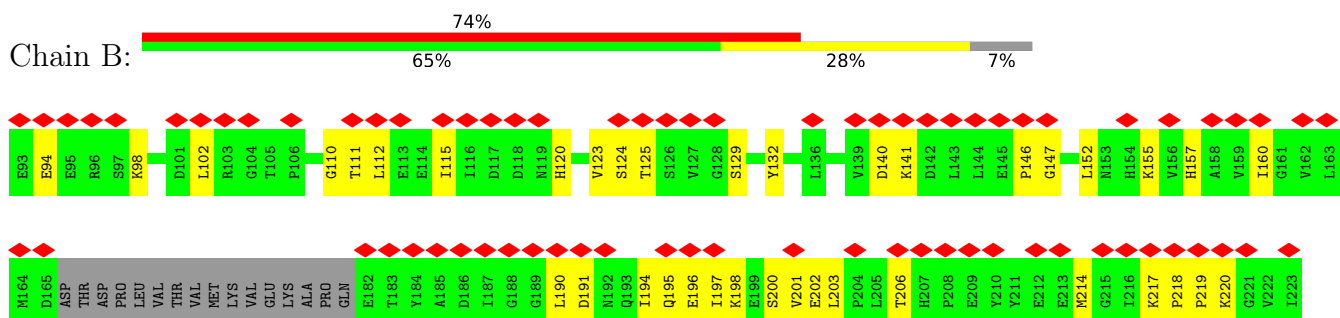
3 Residue-property plots

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

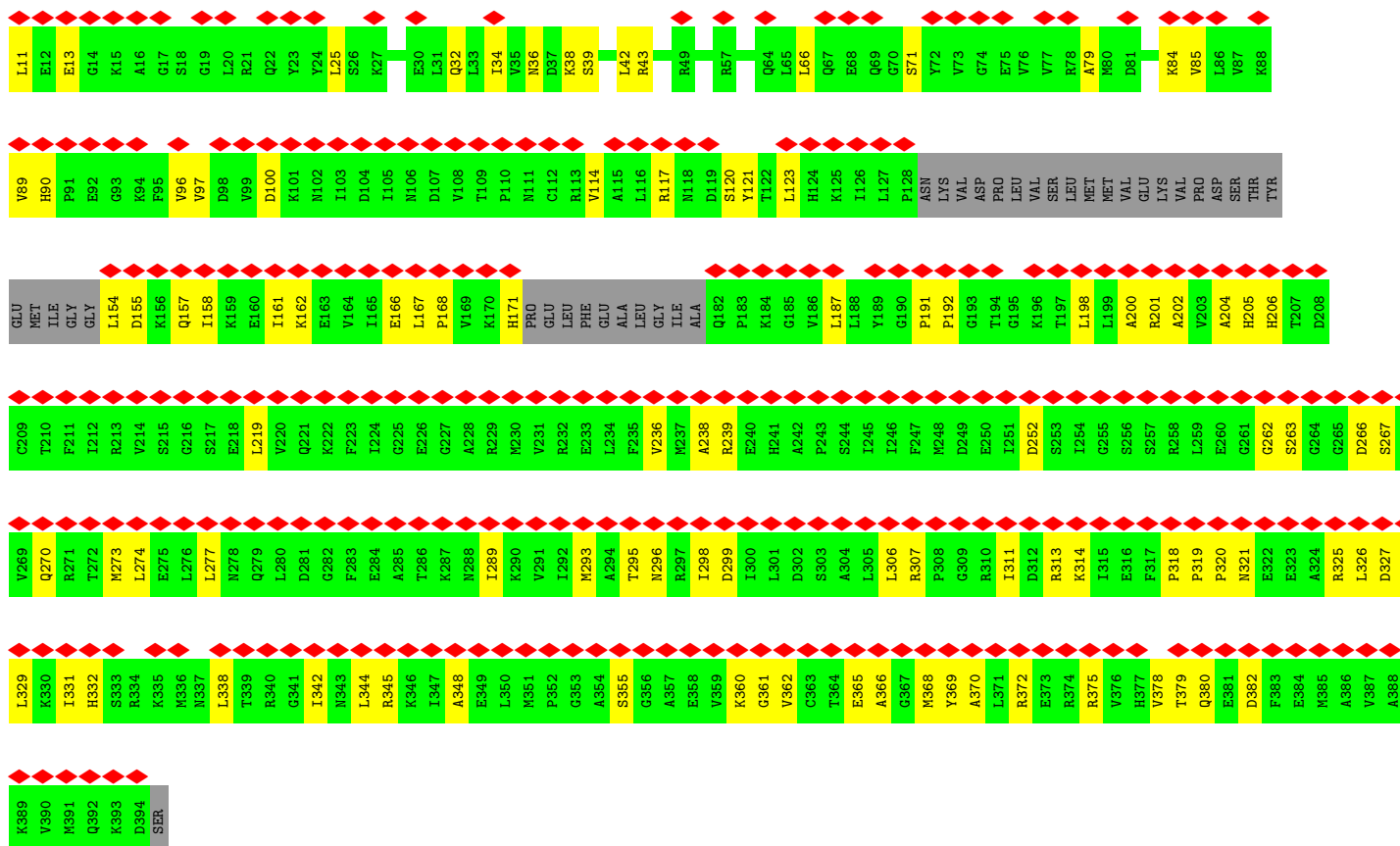
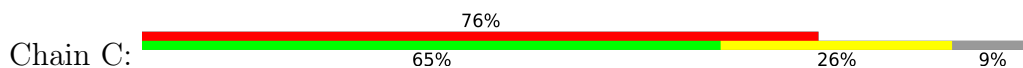


• Molecule 2: 26S proteasome regulatory subunit 4

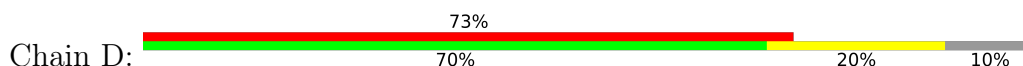


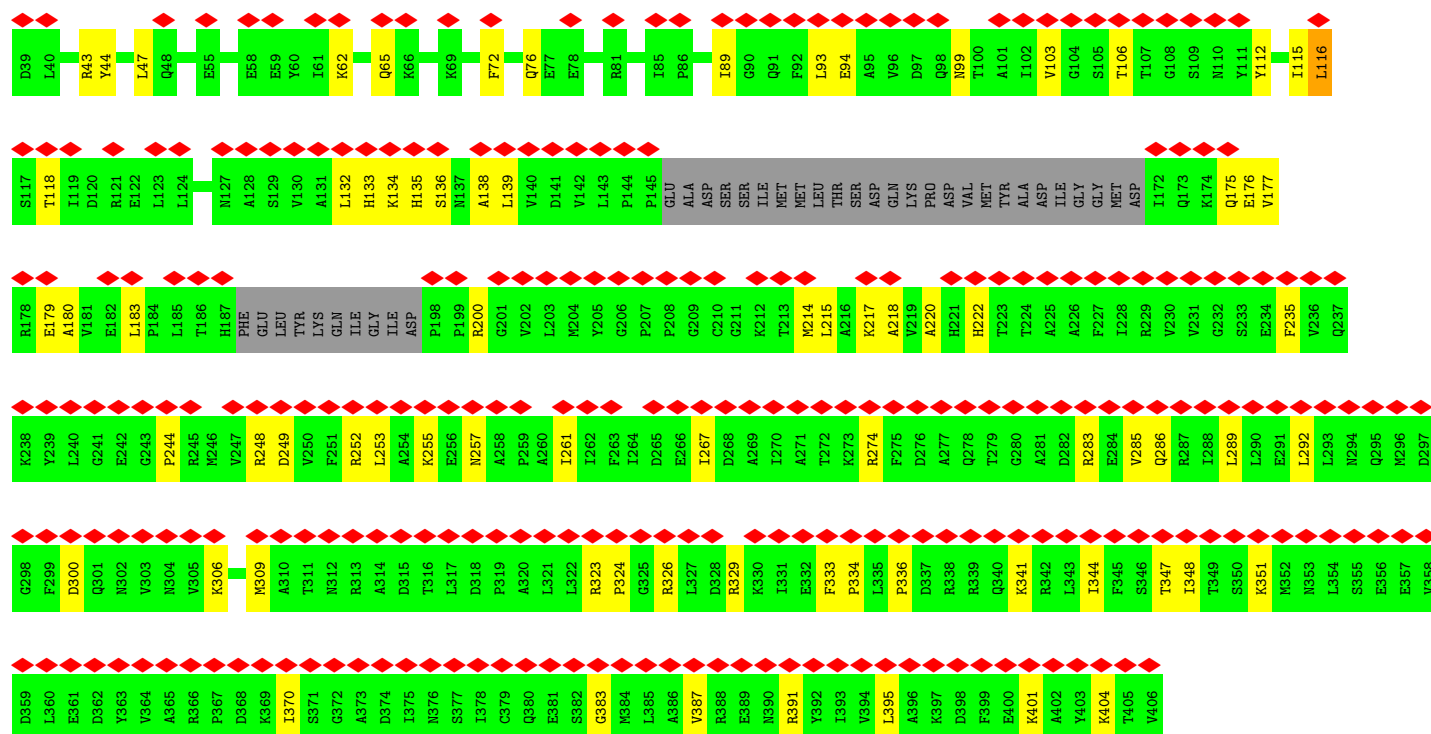


• Molecule 3: 26S proteasome regulatory subunit 8

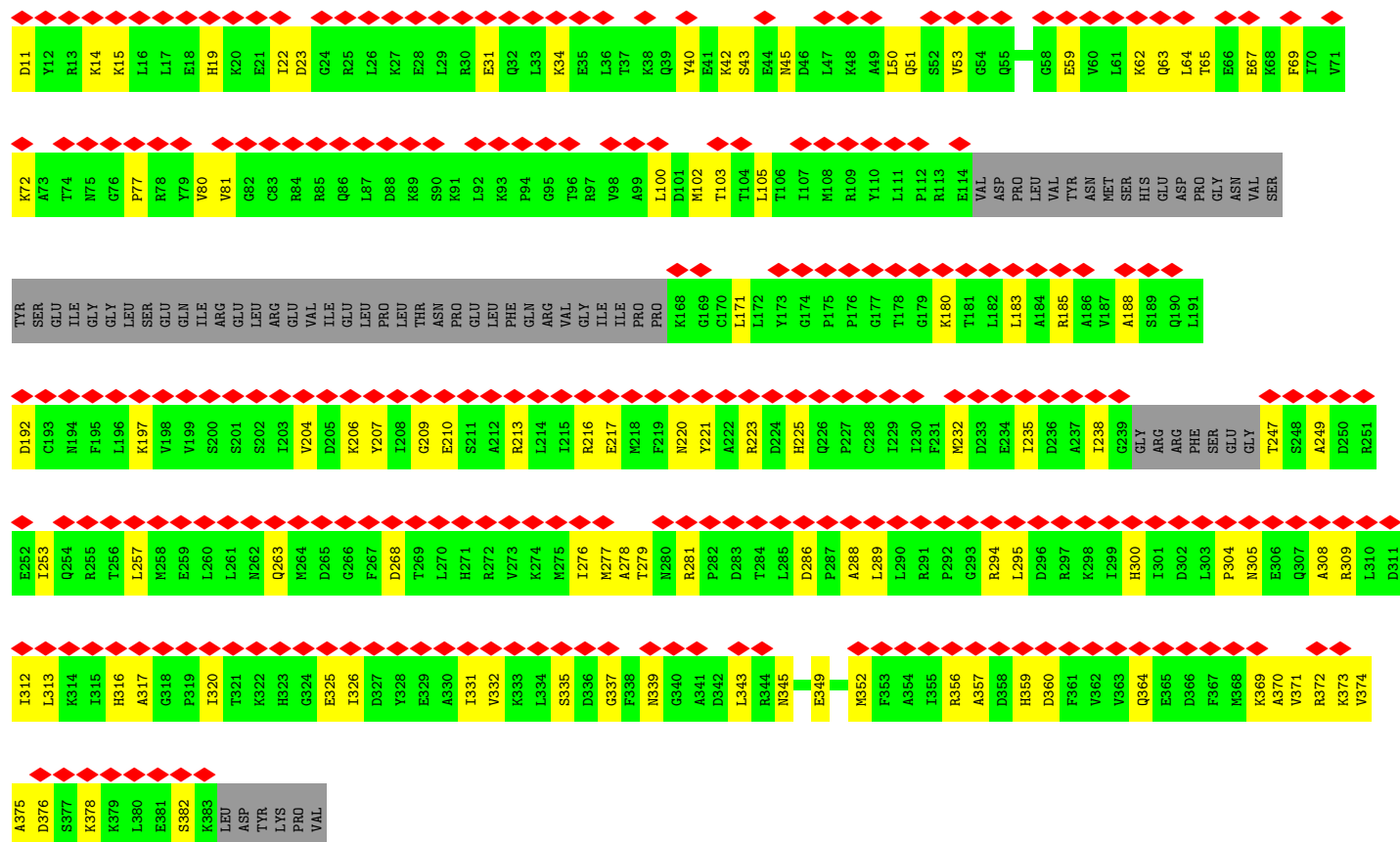


• Molecule 4: 26S proteasome regulatory subunit 6B





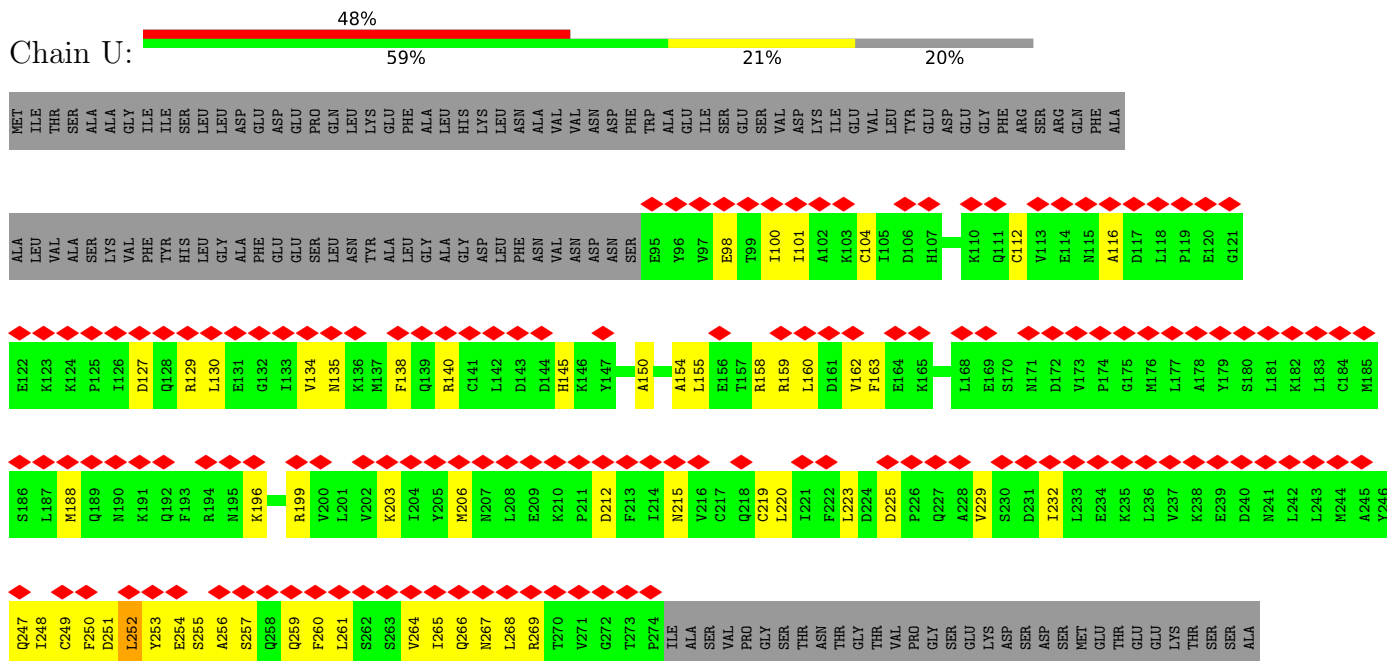
• Molecule 5: 26S proteasome regulatory subunit 10B

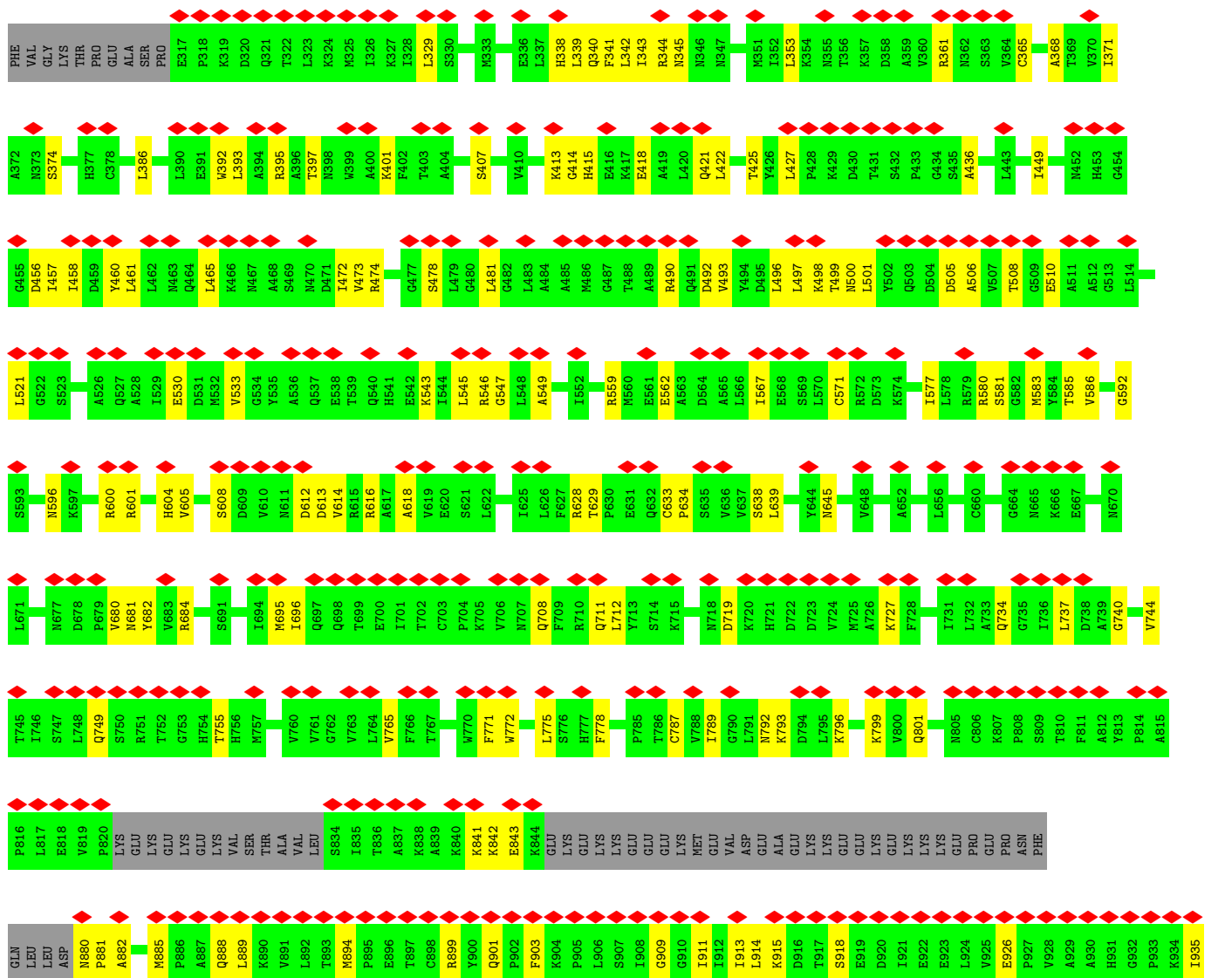


Chain F:

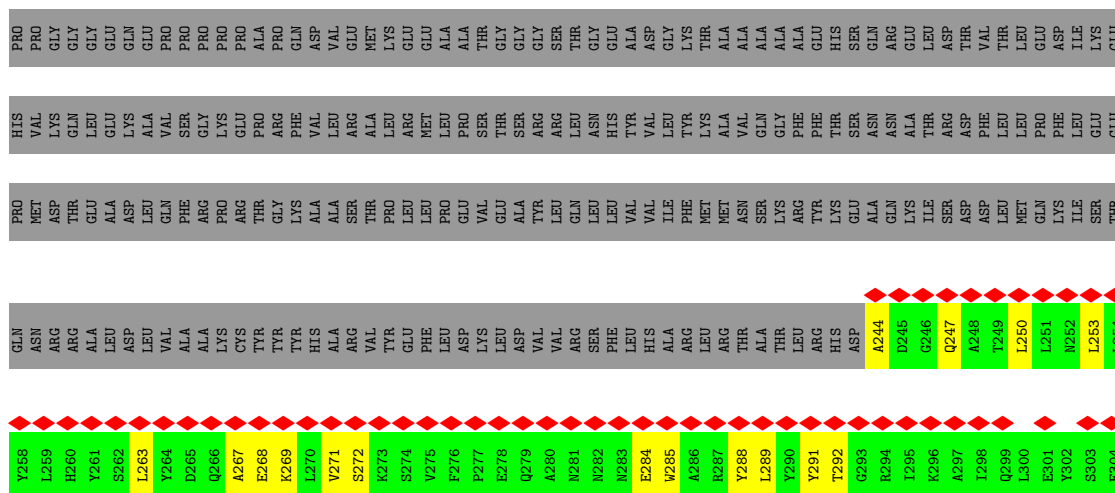
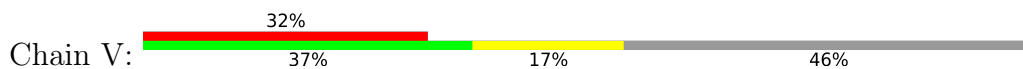


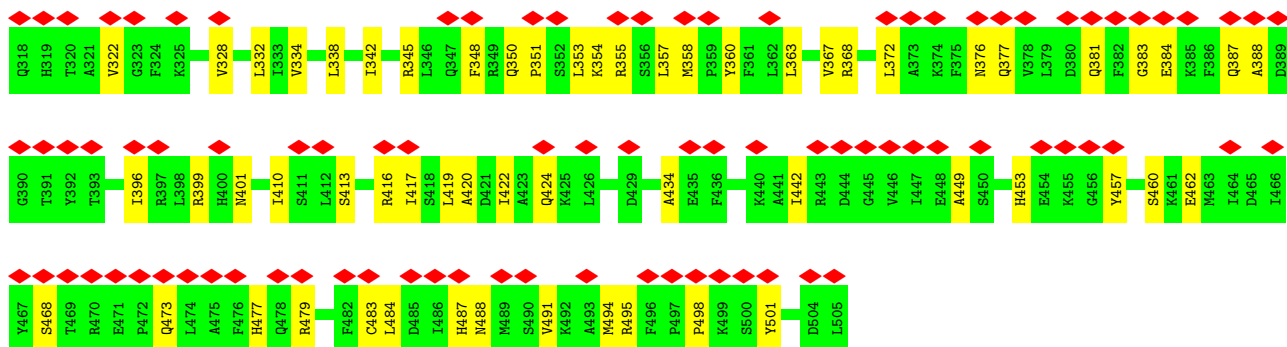
Chain U:



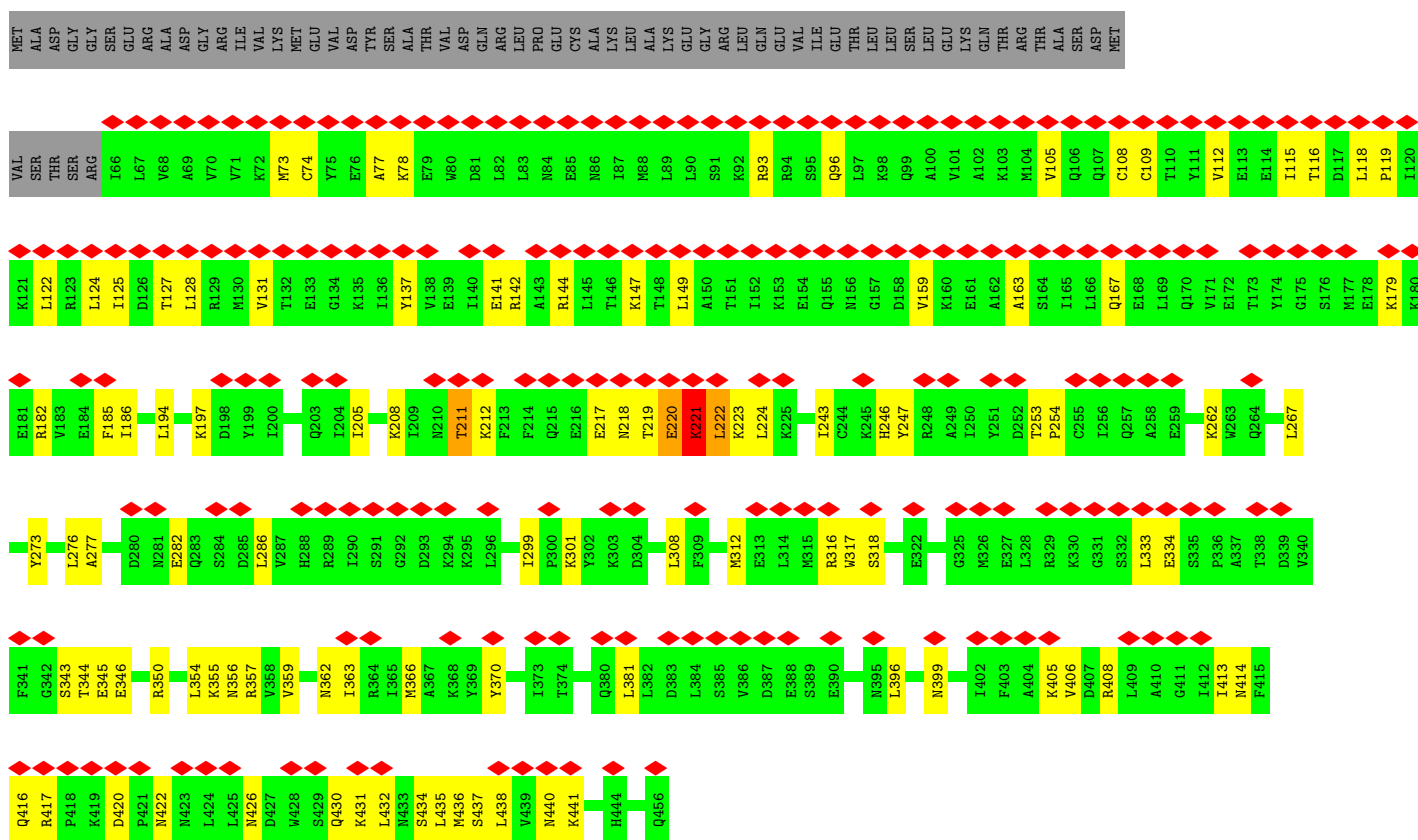


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 3

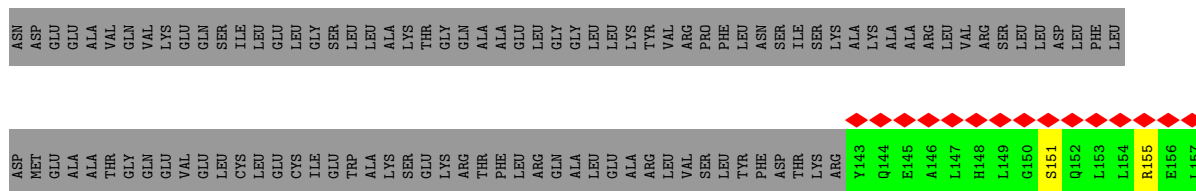


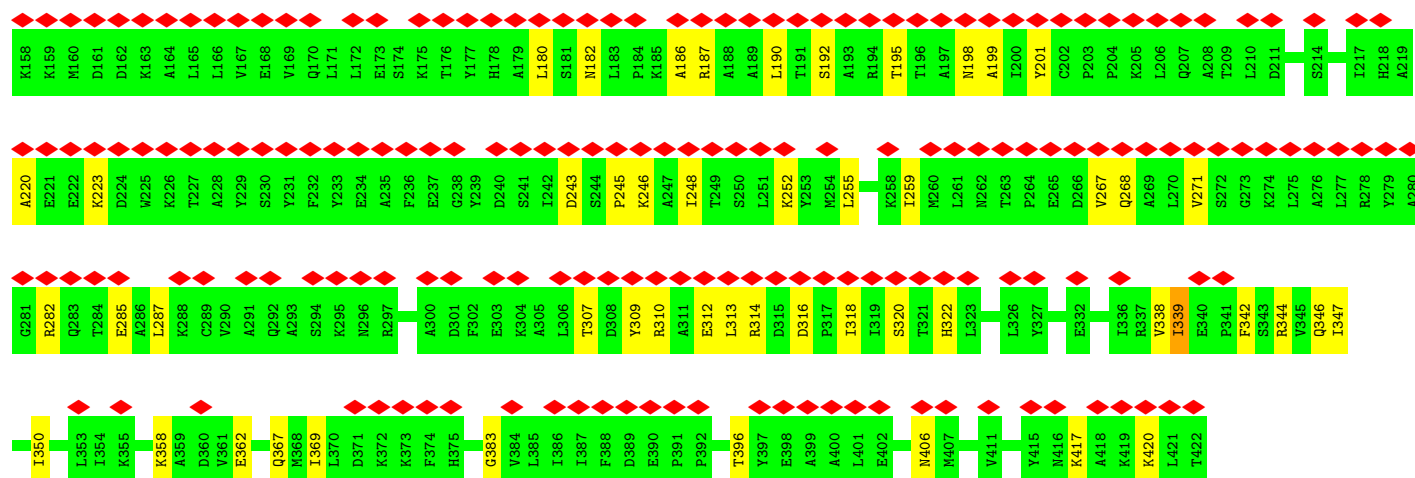


• Molecule 9: 26S proteasome non-ATPase regulatory subunit 12

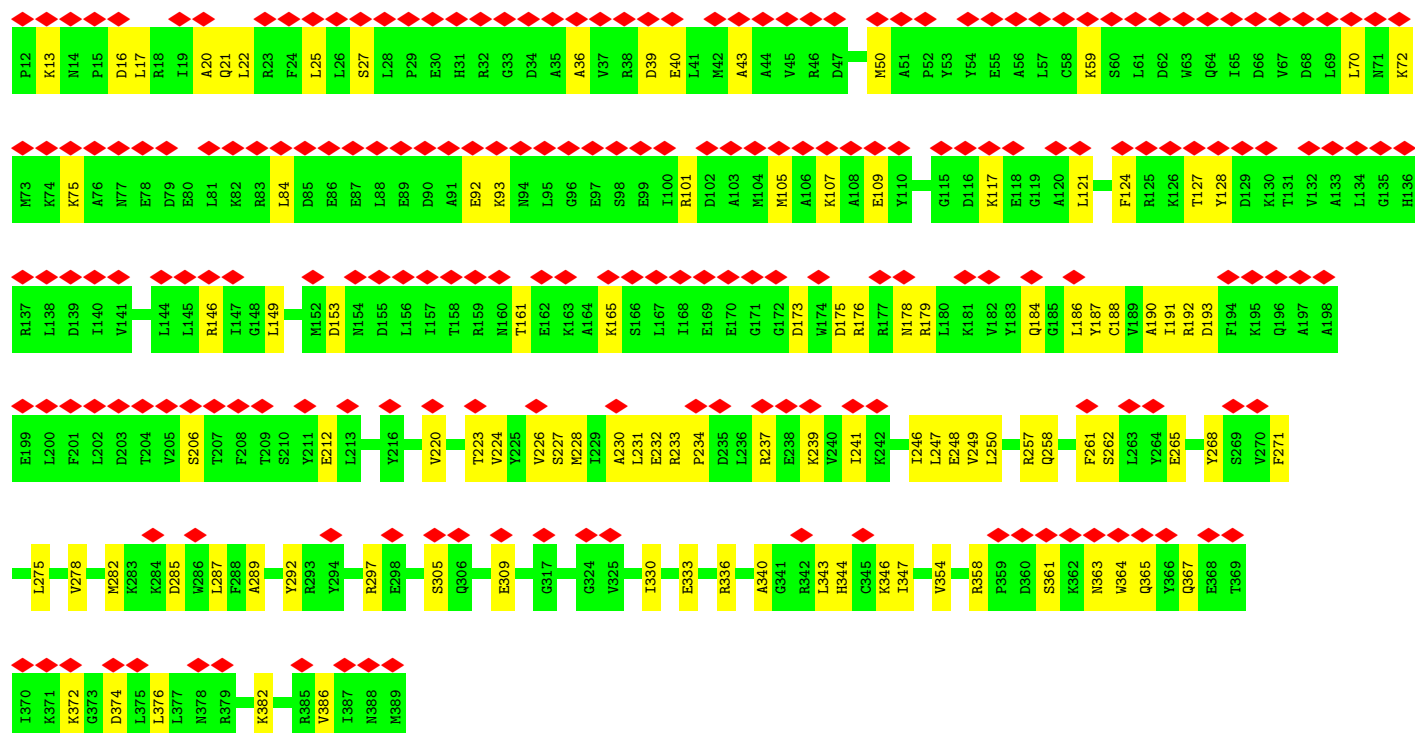
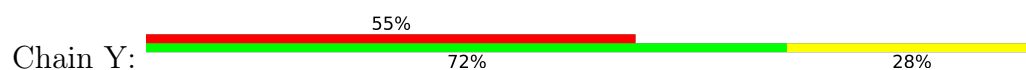


• Molecule 10: 26S proteasome non-ATPase regulatory subunit 11

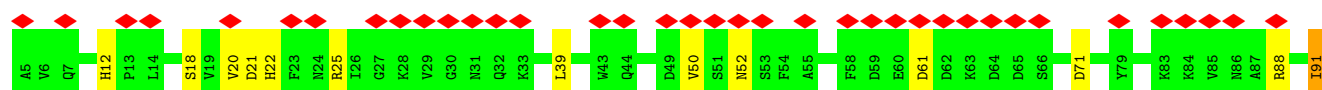
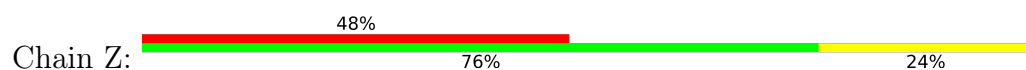


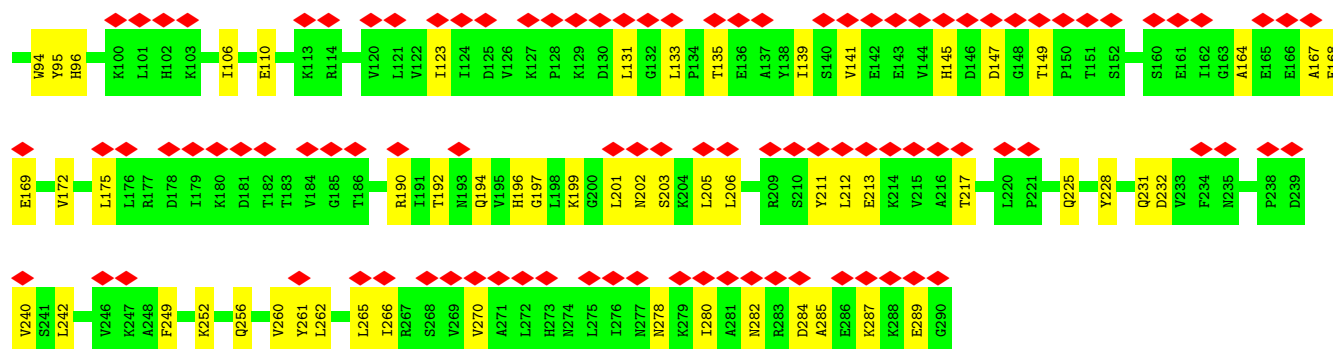


- Molecule 11: 26S proteasome non-ATPase regulatory subunit 6

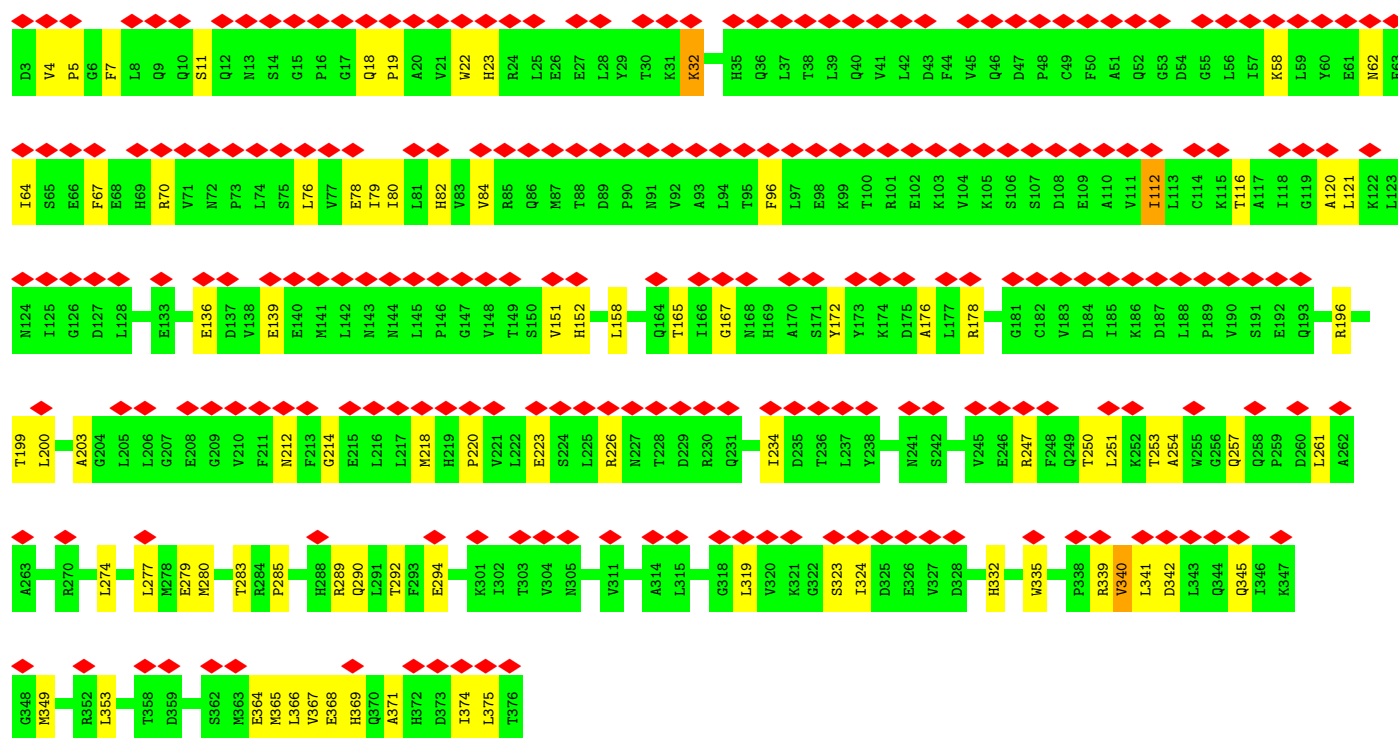
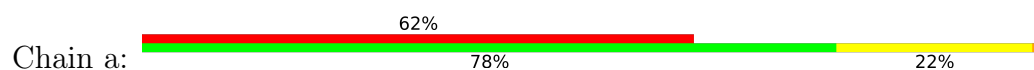


- Molecule 12: 26S proteasome non-ATPase regulatory subunit 7

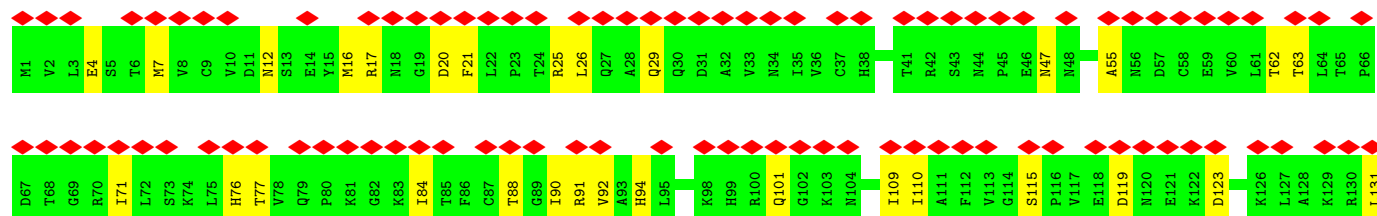
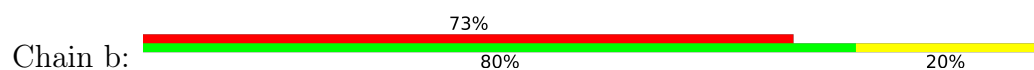


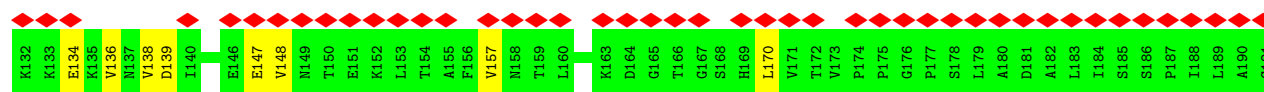


• Molecule 13: 26S proteasome non-ATPase regulatory subunit 13

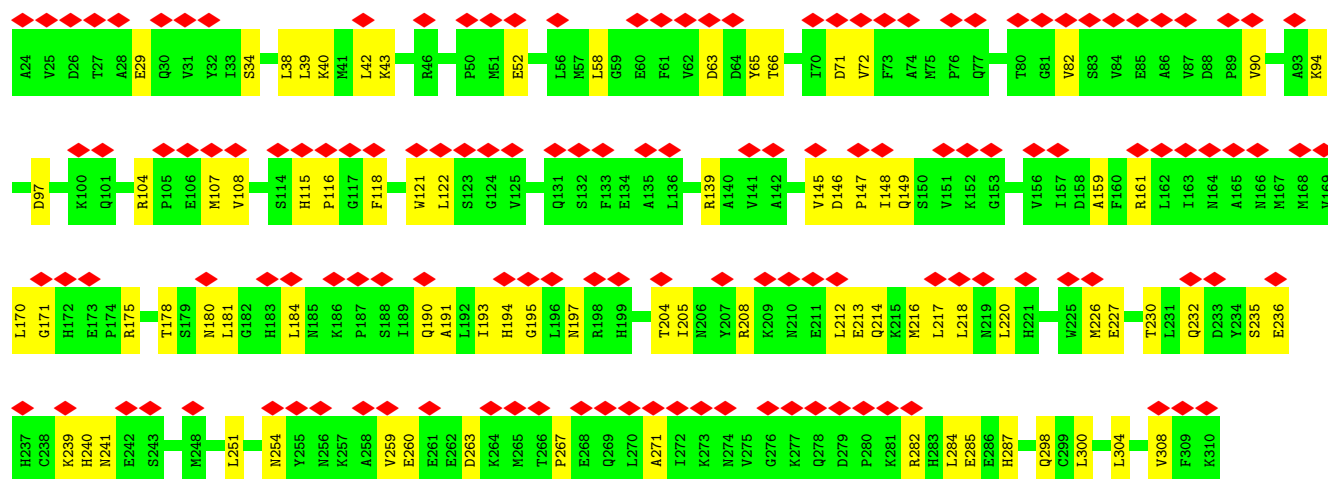


• Molecule 14: 26S proteasome non-ATPase regulatory subunit 4





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



Chain f:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21885	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	0.009	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	258.0, 258.0, 258.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

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	0.12	0/2710	0.35	0/3659
2	B	0.11	0/2509	0.32	0/3383
3	C	0.10	0/2784	0.30	0/3737
4	D	0.11	0/2690	0.31	0/3630
5	E	0.09	0/2525	0.28	0/3387
6	F	0.09	0/2681	0.26	0/3611
7	U	0.08	0/5930	0.27	0/8021
8	V	0.10	0/2170	0.30	0/2929
9	W	0.18	2/3251 (0.1%)	0.38	5/4370 (0.1%)
10	X	0.09	0/2255	0.26	0/3041
11	Y	0.08	0/3173	0.26	0/4273
12	Z	0.08	0/2324	0.23	0/3150
13	a	0.08	0/3061	0.26	0/4144
14	b	0.11	0/1478	0.27	0/2001
15	c	0.08	0/2302	0.22	0/3110
16	d	0.09	0/1486	0.26	0/2010
17	e	0.09	0/289	0.31	0/389
18	f	0.12	0/4989	0.36	0/6729
All	All	0.10	2/48607 (0.0%)	0.30	5/65574 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	220	GLU	CA-C	5.35	1.59	1.52
9	W	221	LYS	N-CA	5.11	1.52	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	221	LYS	CA-C-N	7.84	136.51	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	221	LYS	C-N-CA	7.84	136.51	121.54
9	W	219	THR	CA-C-N	5.37	131.79	121.54
9	W	219	THR	C-N-CA	5.37	131.79	121.54
9	W	219	THR	O-C-N	5.17	129.36	123.31

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	2665	0	2715	73	0
2	B	2476	0	2514	62	0
3	C	2752	0	2855	72	0
4	D	2649	0	2706	52	0
5	E	2493	0	2572	69	0
6	F	2647	0	2749	75	0
7	U	5829	0	5920	130	0
8	V	2129	0	2171	59	0
9	W	3206	0	3314	80	0
10	X	2221	0	2280	40	0
11	Y	3115	0	3120	74	0
12	Z	2281	0	2312	56	0
13	a	3003	0	3016	66	0
14	b	1458	0	1505	24	0
15	c	2260	0	2276	62	0
16	d	1452	0	1445	22	0
17	e	283	0	237	8	0
18	f	4920	0	4956	219	0
19	c	1	0	0	0	0
All	All	47840	0	48663	1160	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 12.

All (1160) 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)
18:f:493:ASN:HA	18:f:525:ILE:CG2	1.62	1.28
18:f:493:ASN:CA	18:f:525:ILE:HG23	1.71	1.19
8:V:267:ALA:O	8:V:271:VAL:HB	1.48	1.09
18:f:301:HIS:O	18:f:305:LEU:HB2	1.50	1.09
18:f:377:VAL:O	18:f:381:VAL:HB	1.54	1.07
15:c:191:ALA:O	15:c:195:GLY:HA3	1.56	1.06
18:f:485:LEU:O	18:f:489:TYR:HD2	1.37	1.05
18:f:95:PRO:O	18:f:99:LEU:HB2	1.55	1.05
9:W:220:GLU:OE1	9:W:222:LEU:N	1.94	1.01
18:f:224:ASN:O	18:f:228:LYS:HB3	1.61	1.00
18:f:318:THR:O	18:f:322:SER:HB3	1.61	0.99
18:f:129:LEU:O	18:f:133:MET:HB2	1.60	0.99
7:U:339:LEU:O	7:U:343:ILE:HB	1.62	0.99
18:f:494:ARG:HG3	18:f:496:ASP:OD1	1.64	0.98
18:f:126:ILE:O	18:f:130:ALA:HB3	1.63	0.96
18:f:228:LYS:O	18:f:232:TYR:HB3	1.68	0.94
18:f:625:LYS:O	18:f:629:LYS:HB2	1.69	0.93
8:V:473:GLN:O	8:V:477:HIS:HB2	1.68	0.92
11:Y:117:LYS:O	11:Y:121:LEU:HB2	1.69	0.92
6:F:272:PHE:O	6:F:276:LYS:HB3	1.69	0.92
1:A:161:VAL:O	1:A:165:GLN:HB2	1.70	0.91
9:W:108:CYS:O	9:W:112:VAL:HB	1.70	0.91
8:V:284:GLU:O	8:V:288:TYR:HB3	1.69	0.91
6:F:74:LYS:O	6:F:78:GLU:HB2	1.71	0.90
18:f:122:ALA:O	18:f:126:ILE:HB	1.71	0.90
5:E:370:ALA:O	5:E:374:VAL:HB	1.72	0.89
9:W:350:ARG:O	9:W:354:LEU:HB2	1.73	0.88
6:F:273:ALA:O	6:F:277:GLU:HB3	1.73	0.88
11:Y:124:PHE:O	11:Y:128:TYR:HB2	1.74	0.87
18:f:493:ASN:ND2	18:f:525:ILE:HG22	1.88	0.87
18:f:624:GLU:O	18:f:628:ASP:HB2	1.75	0.87
18:f:357:ARG:O	18:f:361:SER:HB2	1.75	0.87
18:f:485:LEU:O	18:f:489:TYR:CD2	2.26	0.86
11:Y:17:LEU:O	11:Y:21:GLN:HB2	1.76	0.85
6:F:274:LEU:O	6:F:278:LYS:HB2	1.76	0.85
7:U:338:HIS:O	7:U:342:LEU:HB2	1.76	0.85
18:f:359:GLY:O	18:f:363:SER:HB3	1.77	0.85
15:c:193:ILE:O	15:c:197:ASN:HB2	1.76	0.84
18:f:494:ARG:CG	18:f:496:ASP:OD1	2.25	0.84
7:U:614:VAL:O	7:U:618:ALA:HB2	1.78	0.84
18:f:225:ALA:O	18:f:229:VAL:HB	1.76	0.84
18:f:232:TYR:O	18:f:236:CYS:HB2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:226:VAL:O	11:Y:230:ALA:HB3	1.78	0.83
18:f:494:ARG:HE	18:f:495:GLU:H	1.24	0.83
9:W:182:ARG:O	9:W:186:ILE:HB	1.79	0.83
13:a:365:MET:O	13:a:369:HIS:HB2	1.79	0.81
5:E:312:ILE:O	5:E:316:HIS:HB2	1.80	0.80
13:a:214:GLY:O	13:a:218:MET:HB2	1.81	0.80
17:e:47:ASN:O	17:e:51:ASP:HB2	1.81	0.80
1:A:200:ARG:O	1:A:204:LEU:HB2	1.82	0.80
5:E:378:LYS:O	5:E:382:SER:HB3	1.82	0.80
1:A:298:THR:O	1:A:302:LEU:HB2	1.82	0.80
7:U:250:PHE:O	7:U:254:GLU:HB2	1.82	0.80
3:C:162:LYS:O	3:C:166:GLU:HB2	1.81	0.79
6:F:307:GLN:O	6:F:311:LEU:HB2	1.82	0.79
9:W:220:GLU:OE1	9:W:221:LYS:N	2.15	0.79
5:E:371:VAL:O	5:E:375:ALA:HB3	1.83	0.78
12:Z:164:ALA:HB3	12:Z:169:GLU:HG3	1.65	0.78
3:C:263:SER:O	3:C:267:SER:HB2	1.84	0.78
11:Y:161:THR:O	11:Y:165:LYS:HB2	1.83	0.78
9:W:220:GLU:OE2	9:W:222:LEU:HB2	1.84	0.77
18:f:494:ARG:O	18:f:497:VAL:HG12	1.86	0.75
18:f:127:SER:O	18:f:131:MET:HB2	1.87	0.75
18:f:211:ILE:O	18:f:215:ASP:HB2	1.87	0.75
18:f:493:ASN:ND2	18:f:525:ILE:CG2	2.50	0.75
18:f:252:ALA:O	18:f:256:PHE:HB2	1.88	0.74
18:f:460:ASP:OD1	18:f:460:ASP:N	2.20	0.74
18:f:306:GLU:HB3	18:f:339:ILE:HD12	1.69	0.74
5:E:180:LYS:HD2	5:E:279:THR:H	1.53	0.74
4:D:351:LYS:HB2	10:X:201:TYR:HB3	1.70	0.73
2:B:398:ILE:O	2:B:402:ALA:HB2	1.86	0.73
18:f:494:ARG:HE	18:f:495:GLU:N	1.87	0.73
9:W:220:GLU:CD	9:W:222:LEU:HB2	2.14	0.73
2:B:198:LYS:O	2:B:202:GLU:HB2	1.89	0.73
3:C:120:SER:HB3	15:c:190:GLN:HG3	1.69	0.73
3:C:154:LEU:HA	3:C:327:ASP:HB2	1.70	0.73
9:W:370:TYR:HB2	13:a:323:SER:HB2	1.70	0.73
18:f:618:GLU:HG2	18:f:623:LYS:HD2	1.71	0.72
8:V:484:LEU:O	8:V:488:ASN:HB2	1.90	0.72
3:C:97:VAL:HG11	3:C:121:TYR:HB3	1.72	0.72
6:F:381:TYR:O	6:F:385:ALA:HB3	1.88	0.72
18:f:341:GLU:HG3	18:f:342:PRO:HD3	1.72	0.72
16:d:114:GLU:O	16:d:118:GLU:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:f:675:PHE:O	18:f:679:LEU:HB2	1.91	0.71
7:U:340:GLN:HE21	7:U:344:ARG:HH12	1.37	0.71
18:f:325:GLN:HE21	18:f:328:SER:HA	1.56	0.71
11:Y:336:ARG:O	11:Y:340:ALA:HB3	1.90	0.71
6:F:233:LYS:O	6:F:237:ALA:HB3	1.90	0.71
18:f:313:GLU:O	18:f:317:LEU:HB2	1.89	0.71
18:f:474:SER:O	18:f:478:ARG:HB2	1.91	0.71
7:U:799:LYS:HB3	7:U:801:GLN:HE22	1.55	0.71
8:V:285:TRP:O	8:V:289:LEU:HB2	1.89	0.71
9:W:282:GLU:O	9:W:286:LEU:HB2	1.91	0.70
3:C:362:VAL:O	3:C:366:ALA:HB2	1.92	0.70
3:C:158:ILE:HA	3:C:161:ILE:HG22	1.74	0.70
7:U:493:VAL:O	7:U:497:LEU:HB2	1.92	0.70
7:U:418:GLU:O	7:U:422:LEU:HB2	1.92	0.70
11:Y:361:SER:O	11:Y:365:GLN:HB2	1.90	0.70
13:a:32:LYS:HB3	14:b:20:ASP:HB3	1.71	0.70
4:D:179:GLU:HA	4:D:183:LEU:HD13	1.74	0.70
1:A:102:ILE:HG22	1:A:113:ILE:HG12	1.74	0.69
2:B:387:LYS:HG2	2:B:388:ASP:H	1.58	0.69
11:Y:271:PHE:O	11:Y:275:LEU:HB2	1.91	0.69
7:U:223:LEU:HD12	7:U:225:ASP:H	1.57	0.69
9:W:316:ARG:HG3	9:W:318:SER:H	1.57	0.69
18:f:586:PRO:HA	18:f:589:SER:HB2	1.74	0.69
3:C:368:MET:SD	4:D:329:ARG:NH2	2.66	0.69
18:f:226:TYR:O	18:f:230:CYS:HB2	1.93	0.69
18:f:493:ASN:HA	18:f:525:ILE:HG23	0.79	0.69
3:C:38:LYS:O	3:C:42:LEU:HB2	1.92	0.68
5:E:223:ARG:HH22	5:E:263:GLN:HE21	1.41	0.68
1:A:417:ILE:O	1:A:421:ALA:HB2	1.94	0.68
5:E:369:LYS:O	5:E:373:LYS:HB2	1.94	0.68
7:U:586:VAL:HG21	7:U:601:ARG:HH12	1.59	0.68
9:W:124:LEU:HD13	9:W:149:LEU:HD13	1.74	0.67
13:a:212:ASN:HD22	13:a:339:ARG:HB3	1.58	0.67
18:f:269:ALA:HB2	18:f:277:LEU:HD22	1.76	0.67
1:A:76:ALA:O	1:A:80:LEU:HB2	1.95	0.67
3:C:328:ILE:O	3:C:332:HIS:ND1	2.26	0.67
8:V:416:ARG:HH11	8:V:460:SER:HB2	1.60	0.67
16:d:249:TYR:O	16:d:253:LEU:HB2	1.95	0.67
18:f:129:LEU:O	18:f:133:MET:CB	2.42	0.67
6:F:87:PRO:HB3	6:F:153:VAL:H	1.60	0.66
16:d:119:LEU:HD23	16:d:122:LEU:HD21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:f:494:ARG:HE	18:f:494:ARG:HA	1.60	0.66
7:U:249:CYS:O	7:U:253:TYR:HB2	1.94	0.66
7:U:506:ALA:HB1	7:U:543:LYS:HB2	1.78	0.66
7:U:634:PRO:O	7:U:638:SER:HB3	1.96	0.66
3:C:191:PRO:HB3	3:C:355:SER:HB2	1.76	0.66
11:Y:237:ARG:HA	11:Y:241:ILE:HB	1.78	0.66
13:a:19:PRO:HA	13:a:22:TRP:HB2	1.77	0.66
1:A:172:VAL:HG13	1:A:357:ILE:HD13	1.78	0.66
18:f:229:VAL:O	18:f:233:LEU:CB	2.44	0.66
13:a:58:LYS:O	13:a:62:ASN:HB2	1.96	0.66
7:U:600:ARG:O	7:U:604:HIS:HB2	1.96	0.65
18:f:123:ALA:O	18:f:127:SER:HB2	1.96	0.65
18:f:541:THR:O	18:f:545:LYS:HB2	1.96	0.65
18:f:253:LEU:O	18:f:257:ARG:HB2	1.96	0.65
3:C:34:ILE:HG22	3:C:38:LYS:HE2	1.76	0.65
11:Y:261:PHE:O	11:Y:265:GLU:HB2	1.96	0.65
18:f:534:VAL:HA	18:f:538:ILE:HD11	1.78	0.65
8:V:383:GLY:O	8:V:387:GLN:NE2	2.30	0.65
18:f:608:LYS:HZ3	18:f:634:LYS:HD2	1.61	0.65
4:D:344:ILE:O	4:D:348:ILE:HB	1.97	0.65
11:Y:361:SER:O	11:Y:365:GLN:CB	2.45	0.65
18:f:183:PRO:O	18:f:187:LEU:HB2	1.96	0.65
14:b:88:THR:O	14:b:92:VAL:HB	1.95	0.65
2:B:312:LEU:O	2:B:316:LEU:HB2	1.97	0.65
5:E:50:LEU:HG	6:F:137:ILE:HD12	1.78	0.64
12:Z:106:ILE:O	12:Z:110:GLU:HB2	1.96	0.64
14:b:62:THR:HG21	14:b:71:ILE:HG12	1.78	0.64
9:W:125:ILE:HD12	9:W:128:LEU:HD21	1.78	0.64
18:f:301:HIS:O	18:f:305:LEU:CB	2.37	0.64
5:E:325:GLU:O	5:E:364:GLN:NE2	2.30	0.64
18:f:493:ASN:CA	18:f:525:ILE:CG2	2.51	0.64
4:D:43:ARG:O	4:D:47:LEU:HB2	1.97	0.64
7:U:155:LEU:O	7:U:158:ARG:NH1	2.30	0.64
9:W:431:LYS:O	9:W:435:LEU:HB2	1.97	0.64
1:A:200:ARG:O	1:A:204:LEU:CB	2.46	0.64
5:E:372:ARG:O	5:E:376:ASP:HB2	1.96	0.64
9:W:417:ARG:NH2	9:W:420:ASP:OD2	2.30	0.64
6:F:381:TYR:O	6:F:385:ALA:CB	2.45	0.64
1:A:204:LEU:HD11	6:F:407:ALA:HB3	1.80	0.64
2:B:361:LYS:HG2	2:B:391:SER:HA	1.80	0.64
13:a:19:PRO:O	13:a:23:HIS:ND1	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:236:GLU:O	15:c:240:HIS:ND1	2.30	0.63
18:f:625:LYS:O	18:f:629:LYS:CB	2.46	0.63
9:W:299:ILE:HG22	9:W:301:LYS:H	1.62	0.63
11:Y:124:PHE:O	11:Y:128:TYR:CB	2.46	0.63
8:V:384:GLU:O	8:V:388:ALA:CB	2.47	0.63
2:B:395:ILE:HA	2:B:398:ILE:HG12	1.81	0.63
8:V:384:GLU:O	8:V:388:ALA:HB3	1.98	0.63
9:W:405:LYS:HB3	9:W:414:ASN:HB2	1.80	0.63
18:f:494:ARG:NE	18:f:495:GLU:H	1.97	0.62
12:Z:231:GLN:NE2	13:a:345:GLN:O	2.30	0.62
3:C:32:GLN:O	3:C:36:ASN:HB2	2.00	0.62
4:D:383:GLY:O	4:D:387:VAL:HB	1.99	0.62
13:a:345:GLN:O	13:a:349:MET:HB2	1.99	0.62
7:U:212:ASP:OD2	7:U:215:ASN:ND2	2.31	0.62
3:C:71:SER:HB2	3:C:117:ARG:HA	1.81	0.62
3:C:263:SER:O	3:C:267:SER:CB	2.48	0.62
14:b:12:ASN:HD21	14:b:55:ALA:HB2	1.65	0.62
18:f:366:ASP:H	18:f:370:MET:HB2	1.63	0.62
12:Z:202:ASN:O	12:Z:206:LEU:HB2	2.00	0.62
18:f:654:VAL:HA	18:f:657:ILE:HD12	1.81	0.62
13:a:374:ILE:HD12	16:d:251:ARG:HB2	1.82	0.62
2:B:398:ILE:O	2:B:402:ALA:CB	2.48	0.62
9:W:179:LYS:O	9:W:218:ASN:ND2	2.33	0.62
9:W:333:LEU:HD12	9:W:334:GLU:HG2	1.80	0.62
13:a:172:TYR:O	13:a:176:ALA:HB2	1.99	0.62
18:f:232:TYR:O	18:f:236:CYS:CB	2.47	0.62
3:C:368:MET:O	3:C:372:ARG:HB2	2.00	0.61
12:Z:149:THR:O	13:a:178:ARG:NH1	2.33	0.61
18:f:226:TYR:O	18:f:230:CYS:CB	2.48	0.61
6:F:342:LEU:HD13	6:F:348:LEU:HD12	1.82	0.61
10:X:406:ASN:HD22	12:Z:265:LEU:HD23	1.65	0.61
18:f:125:ILE:HA	18:f:129:LEU:HD12	1.82	0.61
7:U:792:ASN:HB3	7:U:914:LEU:HB3	1.81	0.61
9:W:408:ARG:HB2	10:X:344:ARG:HG2	1.82	0.61
15:c:52:GLU:HB3	15:c:82:VAL:HG23	1.81	0.61
18:f:347:ASP:O	18:f:351:THR:OG1	2.17	0.61
4:D:214:MET:O	4:D:218:ALA:HB2	1.99	0.61
5:E:206:LYS:HG2	6:F:300:LYS:HA	1.82	0.61
7:U:342:LEU:HD23	7:U:345:ASN:HD21	1.65	0.61
9:W:408:ARG:O	10:X:346:GLN:NE2	2.34	0.61
18:f:229:VAL:O	18:f:233:LEU:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG13	1:A:117:GLN:H	1.66	0.61
7:U:789:ILE:HD12	7:U:911:ILE:HG12	1.81	0.61
18:f:493:ASN:HD22	18:f:525:ILE:CG2	2.12	0.61
7:U:127:ASP:OD2	7:U:129:ARG:NH1	2.33	0.61
7:U:392:TRP:O	7:U:395:ARG:NH1	2.34	0.61
15:c:71:ASP:OD1	15:c:104:ARG:NH1	2.33	0.61
15:c:145:VAL:HG22	15:c:147:PRO:HD3	1.83	0.61
1:A:406:GLU:O	1:A:410:LEU:HB3	2.01	0.61
1:A:108:ASP:OD1	1:A:108:ASP:N	2.29	0.60
1:A:261:PHE:HE2	1:A:305:GLN:HB3	1.65	0.60
3:C:154:LEU:HB3	3:C:157:GLN:HB2	1.83	0.60
14:b:16:MET:HE3	14:b:25:ARG:HD3	1.82	0.60
16:d:125:LYS:HG3	16:d:128:GLN:HG3	1.83	0.60
18:f:494:ARG:HA	18:f:494:ARG:NE	2.16	0.60
7:U:708:GLN:HA	7:U:711:GLN:HG2	1.82	0.60
18:f:223:GLU:O	18:f:227:ALA:HB3	2.00	0.60
9:W:115:ILE:HG12	9:W:116:THR:HG22	1.83	0.60
6:F:233:LYS:O	6:F:237:ALA:CB	2.50	0.60
4:D:344:ILE:HA	4:D:347:THR:HG22	1.83	0.60
12:Z:285:ALA:O	12:Z:289:GLU:HB2	2.01	0.60
18:f:493:ASN:CG	18:f:525:ILE:HG22	2.27	0.60
4:D:103:VAL:HG11	4:D:132:LEU:HD11	1.83	0.60
1:A:296:GLN:O	1:A:300:LEU:HB2	2.02	0.60
8:V:372:LEU:O	8:V:376:ASN:HB2	2.01	0.60
10:X:338:VAL:HG23	10:X:339:ILE:HD12	1.84	0.60
7:U:604:HIS:O	7:U:608:SER:HB2	2.01	0.60
8:V:285:TRP:O	8:V:289:LEU:CB	2.49	0.60
11:Y:175:ASP:O	11:Y:179:ARG:HB2	2.01	0.60
18:f:553:THR:HA	18:f:556:ARG:HE	1.67	0.60
13:a:250:THR:O	13:a:254:ALA:HB2	2.02	0.59
5:E:204:VAL:HA	6:F:304:ARG:HH12	1.68	0.59
9:W:438:LEU:HD13	15:c:232:GLN:HA	1.83	0.59
11:Y:372:LYS:O	11:Y:376:LEU:HB2	2.02	0.59
2:B:234:LEU:HD13	2:B:330:ALA:HB1	1.84	0.59
8:V:350:GLN:HE21	8:V:353:LEU:HD13	1.66	0.59
18:f:313:GLU:O	18:f:317:LEU:CB	2.50	0.59
5:E:305:ASN:HB3	5:E:308:ALA:HB3	1.85	0.59
2:B:125:THR:HG22	2:B:129:SER:H	1.67	0.59
6:F:141:ASP:HB3	6:F:144:LYS:HB2	1.84	0.59
13:a:324:ILE:HG12	13:a:332:HIS:H	1.67	0.59
7:U:261:LEU:HA	7:U:264:VAL:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:12:HIS:ND1	12:Z:50:VAL:O	2.33	0.59
18:f:538:ILE:HA	18:f:541:THR:HG22	1.84	0.59
1:A:417:ILE:O	1:A:421:ALA:CB	2.51	0.59
18:f:322:SER:HA	18:f:331:LEU:HD11	1.85	0.59
18:f:493:ASN:ND2	18:f:493:ASN:O	2.36	0.59
4:D:177:VAL:HG21	4:D:215:LEU:HD13	1.85	0.59
9:W:73:MET:O	9:W:77:ALA:CB	2.51	0.59
11:Y:191:ILE:HG23	11:Y:193:ASP:H	1.67	0.59
15:c:191:ALA:O	15:c:195:GLY:CA	2.42	0.59
1:A:312:ARG:HG2	1:A:315:ILE:HG23	1.84	0.58
3:C:277:LEU:HD12	3:C:307:ARG:HH11	1.66	0.58
7:U:259:GLN:NE2	7:U:521:LEU:O	2.36	0.58
15:c:118:PHE:O	15:c:121:TRP:NE1	2.36	0.58
1:A:388:VAL:O	1:A:392:ALA:HB3	2.04	0.58
2:B:112:LEU:HA	2:B:123:VAL:HA	1.85	0.58
6:F:341:ALA:O	6:F:347:ARG:NH2	2.37	0.58
13:a:165:THR:HG22	13:a:167:GLY:H	1.68	0.58
7:U:112:CYS:O	7:U:116:ALA:HB2	2.03	0.58
15:c:63:ASP:OD1	15:c:66:THR:OG1	2.13	0.58
7:U:415:HIS:HD2	7:U:935:ILE:HG23	1.68	0.58
12:Z:18:SER:O	12:Z:22:HIS:ND1	2.33	0.58
15:c:241:ASN:HD21	15:c:300:LEU:HD12	1.68	0.58
18:f:536:SER:O	18:f:540:GLN:HB2	2.04	0.58
5:E:320:ILE:HD13	6:F:217:ILE:HD11	1.85	0.58
12:Z:201:LEU:O	12:Z:205:LEU:HB3	2.03	0.58
1:A:348:LEU:HD12	1:A:351:ARG:HH12	1.68	0.58
12:Z:192:THR:O	12:Z:196:HIS:HB3	2.04	0.58
2:B:382:ASP:O	2:B:386:ALA:HA	2.04	0.58
7:U:842:LYS:O	7:U:880:ASN:N	2.37	0.58
13:a:80:ILE:HD11	13:a:96:PHE:HB3	1.86	0.58
13:a:257:GLN:HB3	13:a:261:LEU:HD22	1.84	0.58
5:E:183:LEU:HD12	5:E:339:ASN:HD21	1.68	0.58
6:F:276:LYS:O	6:F:325:GLN:NE2	2.36	0.58
9:W:205:ILE:O	9:W:208:LYS:N	2.37	0.58
16:d:238:PRO:HA	16:d:241:GLU:HG2	1.86	0.58
6:F:84:LYS:HG3	6:F:161:LEU:HD22	1.84	0.58
12:Z:278:ASN:O	12:Z:282:ASN:ND2	2.37	0.58
18:f:612:LEU:O	18:f:616:CYS:HB2	2.04	0.58
2:B:398:ILE:HA	2:B:401:GLU:HG2	1.86	0.57
7:U:257:SER:HB3	7:U:260:PHE:HB3	1.85	0.57
14:b:110:ILE:HG22	14:b:139:ASP:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:f:502:LEU:HG	18:f:540:GLN:HE22	1.68	0.57
8:V:244:ALA:HB1	8:V:247:GLN:HB3	1.85	0.57
3:C:362:VAL:O	3:C:366:ALA:CB	2.52	0.57
11:Y:178:ASN:ND2	11:Y:206:SER:OG	2.37	0.57
14:b:7:MET:HB2	14:b:109:ILE:HG12	1.87	0.57
9:W:432:LEU:O	9:W:436:MET:HB2	2.05	0.57
10:X:396:THR:HG21	11:Y:365:GLN:HG2	1.86	0.57
11:Y:192:ARG:NH2	17:e:38:VAL:O	2.37	0.57
2:B:231:GLY:O	2:B:235:LEU:HB2	2.04	0.57
11:Y:278:VAL:O	11:Y:282:MET:HB2	2.05	0.57
5:E:371:VAL:O	5:E:375:ALA:CB	2.53	0.57
9:W:147:LYS:HB3	9:W:185:PHE:HE1	1.70	0.57
15:c:282:ARG:NH1	15:c:285:GLU:OE1	2.37	0.57
18:f:321:MET:O	18:f:325:GLN:HB3	2.04	0.57
5:E:331:ILE:HG22	5:E:343:LEU:HD11	1.87	0.57
12:Z:197:GLY:O	12:Z:201:LEU:HB2	2.05	0.57
13:a:367:VAL:O	13:a:371:ALA:CB	2.53	0.57
7:U:889:LEU:HD13	7:U:909:GLY:H	1.69	0.56
18:f:307:LEU:HG	18:f:339:ILE:HD11	1.87	0.56
18:f:566:HIS:ND1	18:f:574:GLU:OE1	2.32	0.56
7:U:583:MET:HE3	7:U:605:VAL:HG11	1.87	0.56
13:a:367:VAL:O	13:a:371:ALA:HB3	2.04	0.56
18:f:236:CYS:HA	18:f:240:VAL:HB	1.87	0.56
1:A:126:SER:HB3	1:A:148:GLN:HB2	1.88	0.56
7:U:265:ILE:HG13	7:U:329:LEU:HD22	1.86	0.56
9:W:416:GLN:HG3	9:W:417:ARG:H	1.70	0.56
12:Z:228:TYR:O	12:Z:232:ASP:HB2	2.05	0.56
2:B:313:LEU:HD22	2:B:341:LEU:HD23	1.88	0.56
8:V:255:LEU:HD22	8:V:291:TYR:HB3	1.86	0.56
9:W:432:LEU:O	9:W:436:MET:CB	2.53	0.56
10:X:310:ARG:HA	10:X:313:LEU:HB2	1.85	0.56
18:f:222:ASP:O	18:f:226:TYR:HB3	2.05	0.56
5:E:213:ARG:NH1	5:E:217:GLU:OE1	2.38	0.56
7:U:799:LYS:HG2	7:U:843:GLU:HA	1.87	0.56
10:X:182:ASN:ND2	11:Y:248:GLU:OE2	2.36	0.56
10:X:309:TYR:O	10:X:312:GLU:N	2.39	0.56
13:a:196:ARG:O	13:a:200:LEU:HB2	2.05	0.56
1:A:339:ARG:NH2	6:F:402:GLU:OE1	2.39	0.56
10:X:252:LYS:HG3	10:X:287:LEU:HD11	1.86	0.56
18:f:494:ARG:HE	18:f:494:ARG:CA	2.18	0.56
8:V:305:ALA:O	8:V:309:MET:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:163:ALA:O	9:W:167:GLN:CB	2.54	0.56
5:E:81:VAL:HG12	5:E:105:LEU:HB3	1.87	0.56
5:E:216:ARG:O	5:E:220:ASN:HB2	2.05	0.56
12:Z:39:LEU:H	12:Z:94:TRP:HA	1.70	0.56
12:Z:133:LEU:HD23	12:Z:135:THR:H	1.70	0.56
15:c:194:HIS:HA	15:c:197:ASN:HB2	1.86	0.56
4:D:65:GLN:NE2	16:d:256:ILE:O	2.39	0.56
7:U:498:LYS:HD3	7:U:501:LEU:HD21	1.88	0.56
7:U:474:ARG:NH2	7:U:500:ASN:O	2.38	0.56
8:V:284:GLU:O	8:V:288:TYR:CB	2.50	0.56
11:Y:232:GLU:HG3	11:Y:234:PRO:HD2	1.88	0.56
2:B:316:LEU:HD11	2:B:327:VAL:HG11	1.87	0.55
18:f:127:SER:O	18:f:131:MET:CB	2.54	0.55
4:D:244:PRO:O	4:D:248:ARG:HB2	2.07	0.55
6:F:363:ALA:O	6:F:367:GLN:HB2	2.06	0.55
11:Y:227:SER:HA	11:Y:231:LEU:HD13	1.87	0.55
12:Z:194:GLN:HE22	13:a:375:LEU:HB2	1.72	0.55
18:f:479:LEU:HA	18:f:517:VAL:HG21	1.88	0.55
11:Y:173:ASP:HB2	11:Y:176:ARG:HB3	1.88	0.55
16:d:182:ILE:HG12	16:d:197:ILE:HG21	1.88	0.55
6:F:60:LEU:O	6:F:64:HIS:ND1	2.31	0.55
15:c:63:ASP:O	15:c:139:ARG:NH2	2.39	0.55
1:A:174:TYR:HD1	1:A:227:ARG:HD2	1.72	0.55
8:V:491:VAL:HA	8:V:494:MET:HG2	1.88	0.55
3:C:89:VAL:HG12	3:C:90:HIS:H	1.71	0.55
8:V:345:ARG:NH2	8:V:348:PHE:O	2.37	0.55
11:Y:101:ARG:O	11:Y:105:MET:HB2	2.07	0.55
11:Y:246:ILE:HA	11:Y:249:VAL:HG22	1.88	0.55
15:c:40:LYS:NZ	15:c:72:VAL:O	2.33	0.55
15:c:193:ILE:O	15:c:197:ASN:CB	2.52	0.55
18:f:517:VAL:O	18:f:521:ALA:HB2	2.06	0.55
3:C:43:ARG:HB2	7:U:639:LEU:HD11	1.88	0.55
8:V:479:ARG:NH1	11:Y:374:ASP:OD1	2.38	0.55
18:f:493:ASN:HD22	18:f:493:ASN:C	2.13	0.55
7:U:894:MET:SD	7:U:901:GLN:NE2	2.80	0.55
9:W:220:GLU:CD	9:W:222:LEU:H	2.14	0.55
10:X:282:ARG:NH1	10:X:285:GLU:OE1	2.40	0.55
18:f:494:ARG:HG2	18:f:496:ASP:OD1	2.07	0.55
3:C:66:LEU:HD23	4:D:136:SER:HB3	1.87	0.55
6:F:308:ARG:O	6:F:312:GLU:HB2	2.07	0.55
8:V:268:GLU:O	8:V:272:SER:OG	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:31:GLU:HG3	5:E:34:LYS:HE3	1.89	0.54
7:U:681:ASN:HA	7:U:684:ARG:HE	1.72	0.54
15:c:175:ARG:HH12	15:c:180:ASN:HD21	1.55	0.54
15:c:214:GLN:O	15:c:218:LEU:HB2	2.07	0.54
18:f:273:ASN:ND2	18:f:310:ASP:OD2	2.40	0.54
3:C:273:MET:HG3	3:C:307:ARG:HH12	1.71	0.54
3:C:295:THR:HG21	3:C:299:ASP:HB2	1.89	0.54
5:E:11:ASP:HA	5:E:14:LYS:HE3	1.89	0.54
6:F:221:LYS:HZ2	6:F:324:THR:HA	1.73	0.54
7:U:248:ILE:HG13	7:U:252:LEU:HD23	1.90	0.54
12:Z:167:ALA:HB1	15:c:42:LEU:HD22	1.88	0.54
15:c:58:LEU:HB2	15:c:71:ASP:HB3	1.89	0.54
18:f:81:GLN:O	18:f:85:SER:HB2	2.08	0.54
18:f:684:PRO:O	18:f:688:ARG:CB	2.55	0.54
5:E:232:MET:HB2	5:E:277:MET:HA	1.88	0.54
10:X:186:ALA:O	10:X:190:LEU:HB2	2.08	0.54
15:c:159:ALA:H	15:c:205:ILE:HD11	1.71	0.54
1:A:100:LYS:HB3	1:A:115:VAL:HG23	1.88	0.54
11:Y:364:TRP:HA	11:Y:367:GLN:HB2	1.89	0.54
12:Z:190:ARG:HD2	13:a:375:LEU:HD13	1.90	0.54
2:B:224:LEU:HD23	2:B:351:ILE:HG12	1.89	0.54
6:F:121:CYS:SG	6:F:122:ALA:N	2.81	0.54
1:A:94:GLN:O	1:A:144:ARG:NH1	2.39	0.54
1:A:97:ARG:HB3	1:A:142:VAL:HG13	1.89	0.54
5:E:180:LYS:HG3	5:E:278:ALA:HB1	1.89	0.54
5:E:232:MET:N	5:E:276:ILE:O	2.41	0.54
9:W:163:ALA:O	9:W:167:GLN:HB2	2.08	0.54
14:b:147:GLU:HG3	14:b:148:VAL:H	1.72	0.54
18:f:138:GLU:O	18:f:142:TYR:HB2	2.08	0.54
1:A:401:ARG:NH1	1:A:403:ILE:O	2.41	0.54
2:B:202:GLU:O	2:B:206:THR:OG1	2.25	0.54
7:U:374:SER:HB3	7:U:407:SER:HB3	1.89	0.54
10:X:255:LEU:O	10:X:259:ILE:HB	2.08	0.54
18:f:664:GLU:HG3	18:f:696:LEU:HB3	1.90	0.54
5:E:59:GLU:O	5:E:72:LYS:N	2.41	0.54
11:Y:109:GLU:HG2	11:Y:146:ARG:HH22	1.72	0.54
11:Y:261:PHE:O	11:Y:265:GLU:CB	2.55	0.54
11:Y:190:ALA:HB2	11:Y:287:LEU:HD21	1.90	0.54
11:Y:305:SER:O	11:Y:309:GLU:HB2	2.08	0.54
18:f:684:PRO:O	18:f:688:ARG:HB2	2.08	0.54
1:A:414:ASN:HA	1:A:417:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:GLU:HB2	7:U:140:ARG:HH12	1.73	0.53
15:c:116:PRO:HB3	15:c:148:ILE:HD13	1.91	0.53
3:C:326:LEU:HD21	3:C:345:ARG:HD3	1.90	0.53
4:D:89:ILE:HD11	5:E:80:VAL:HG13	1.91	0.53
11:Y:124:PHE:HA	11:Y:127:THR:HG22	1.90	0.53
12:Z:21:ASP:OD2	12:Z:25:ARG:NH2	2.41	0.53
15:c:227:GLU:HB2	15:c:230:THR:HA	1.90	0.53
18:f:573:ILE:HG22	18:f:576:ILE:HB	1.90	0.53
3:C:155:ASP:HA	3:C:158:ILE:HG12	1.90	0.53
4:D:261:ILE:HG12	4:D:306:LYS:HB2	1.90	0.53
6:F:121:CYS:HA	6:F:135:PRO:HA	1.90	0.53
9:W:105:VAL:O	9:W:109:CYS:HB2	2.09	0.53
10:X:367:GLN:HG3	11:Y:233:ARG:HH22	1.73	0.53
6:F:69:MET:HA	6:F:72:LYS:HG2	1.90	0.53
7:U:474:ARG:O	7:U:478:SER:CB	2.55	0.53
13:a:342:ASP:HB3	13:a:345:GLN:HB2	1.91	0.53
15:c:29:GLU:HG3	15:c:65:TYR:HA	1.89	0.53
7:U:418:GLU:O	7:U:422:LEU:CB	2.56	0.53
5:E:288:ALA:O	5:E:294:ARG:NH1	2.41	0.53
7:U:457:ILE:HG22	7:U:460:TYR:HB3	1.90	0.53
4:D:252:ARG:HA	4:D:255:LYS:HG2	1.90	0.53
11:Y:101:ARG:O	11:Y:105:MET:CB	2.57	0.53
18:f:221:ILE:O	18:f:225:ALA:HB3	2.08	0.53
2:B:387:LYS:H	2:B:387:LYS:HD2	1.74	0.53
8:V:410:ILE:HD12	8:V:422:ILE:HD11	1.91	0.53
18:f:493:ASN:HB2	18:f:525:ILE:O	2.09	0.53
3:C:71:SER:OG	4:D:112:TYR:O	2.23	0.53
3:C:154:LEU:HG	3:C:331:ILE:HG13	1.90	0.53
15:c:214:GLN:O	15:c:218:LEU:CB	2.56	0.53
18:f:325:GLN:HB2	18:f:330:PHE:HB2	1.90	0.53
1:A:76:ALA:O	1:A:80:LEU:CB	2.57	0.53
7:U:799:LYS:NZ	7:U:926:GLU:OE2	2.42	0.53
10:X:307:THR:HA	10:X:310:ARG:HE	1.73	0.53
6:F:205:PRO:HA	6:F:212:PHE:HE2	1.75	0.52
7:U:793:LYS:HB3	7:U:796:LYS:HB2	1.91	0.52
15:c:226:MET:HG3	15:c:227:GLU:H	1.75	0.52
1:A:214:LEU:HB3	1:A:343:PHE:HD1	1.73	0.52
3:C:361:GLY:O	3:C:365:GLU:HB2	2.09	0.52
8:V:267:ALA:O	8:V:271:VAL:CB	2.40	0.52
1:A:412:ALA:O	1:A:416:VAL:HB	2.09	0.52
7:U:580:ARG:HD3	7:U:613:ASP:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:289:LEU:HD21	8:V:308:THR:HG23	1.92	0.52
9:W:356:ASN:HA	9:W:359:VAL:HG12	1.91	0.52
9:W:430:GLN:NE2	9:W:434:SER:OG	2.42	0.52
13:a:112:ILE:HD13	13:a:151:VAL:HG21	1.91	0.52
18:f:466:LEU:HA	18:f:474:SER:HB3	1.91	0.52
6:F:167:GLU:HG3	6:F:274:LEU:HD11	1.91	0.52
7:U:749:GLN:HA	7:U:755:THR:HA	1.90	0.52
9:W:144:ARG:HD3	9:W:147:LYS:HZ3	1.74	0.52
11:Y:39:ASP:O	11:Y:43:ALA:HB3	2.09	0.52
13:a:285:PRO:O	13:a:289:ARG:NH2	2.43	0.52
1:A:388:VAL:O	1:A:392:ALA:CB	2.58	0.52
1:A:411:GLU:O	1:A:415:LYS:CB	2.58	0.52
2:B:217:LYS:O	2:B:219:PRO:HD3	2.09	0.52
3:C:167:LEU:HB3	3:C:168:PRO:HD3	1.90	0.52
7:U:497:LEU:HD23	7:U:501:LEU:HD23	1.91	0.52
11:Y:184:GLN:O	11:Y:188:CYS:HB2	2.09	0.52
18:f:780:PRO:O	18:f:784:ASP:HB2	2.10	0.52
3:C:325:ARG:O	3:C:329:LEU:HB2	2.10	0.52
9:W:436:MET:O	9:W:440:ASN:CB	2.57	0.52
12:Z:20:VAL:HG13	15:c:212:LEU:HD22	1.90	0.52
3:C:369:TYR:HA	3:C:372:ARG:HB3	1.90	0.52
18:f:477:MET:O	18:f:481:SER:HB2	2.10	0.52
5:E:15:LYS:O	5:E:19:HIS:ND1	2.36	0.52
5:E:223:ARG:NH1	5:E:268:ASP:OD1	2.43	0.52
6:F:224:LEU:HD13	6:F:348:LEU:HD13	1.92	0.52
7:U:414:GLY:H	7:U:449:ILE:HG23	1.75	0.52
9:W:247:TYR:HB2	9:W:273:TYR:HB3	1.90	0.52
18:f:229:VAL:O	18:f:233:LEU:HB3	2.08	0.52
18:f:629:LYS:HE3	18:f:785:ARG:HD2	1.92	0.52
4:D:274:ARG:O	4:D:283:ARG:NH2	2.41	0.52
18:f:278:VAL:HA	18:f:281:ILE:HG22	1.92	0.52
7:U:695:MET:HE1	7:U:712:LEU:HD13	1.92	0.51
10:X:198:ASN:OD1	10:X:199:ALA:N	2.43	0.51
12:Z:240:VAL:HG12	12:Z:242:LEU:H	1.76	0.51
15:c:39:LEU:HD23	15:c:42:LEU:HD12	1.90	0.51
18:f:80:ARG:O	18:f:84:SER:HB3	2.10	0.51
5:E:207:TYR:HD1	5:E:209:GLY:H	1.57	0.51
7:U:885:MET:HB3	7:U:888:GLN:HG3	1.92	0.51
11:Y:268:TYR:HA	11:Y:271:PHE:HB3	1.91	0.51
14:b:4:GLU:O	14:b:47:ASN:ND2	2.41	0.51
4:D:218:ALA:O	4:D:222:HIS:ND1	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:510:GLU:HA	7:U:547:GLY:HA3	1.92	0.51
11:Y:372:LYS:O	11:Y:376:LEU:CB	2.59	0.51
8:V:305:ALA:O	8:V:309:MET:CB	2.58	0.51
11:Y:27:SER:OG	11:Y:59:LYS:NZ	2.39	0.51
5:E:349:GLU:HA	5:E:352:MET:HE3	1.92	0.51
7:U:188:MET:HE1	7:U:596:ASN:HB2	1.93	0.51
8:V:351:PRO:HB2	8:V:355:ARG:HH22	1.76	0.51
18:f:76:GLU:OE1	18:f:79:ARG:NH2	2.44	0.51
18:f:723:TYR:HB3	18:f:746:ARG:HE	1.75	0.51
7:U:614:VAL:O	7:U:618:ALA:CB	2.57	0.51
13:a:374:ILE:HG13	13:a:375:LEU:HG	1.92	0.51
18:f:170:TRP:HE1	18:f:190:GLU:HB2	1.76	0.51
2:B:358:GLU:O	2:B:362:LYS:HB2	2.11	0.51
3:C:79:ALA:HA	3:C:85:VAL:HG13	1.93	0.51
11:Y:84:LEU:HD13	11:Y:107:LYS:HA	1.92	0.51
18:f:303:VAL:HA	18:f:339:ILE:HG13	1.92	0.51
1:A:330:ALA:O	1:A:333:ARG:NH1	2.44	0.51
7:U:361:ARG:N	7:U:365:CYS:SG	2.82	0.51
8:V:377:GLN:O	8:V:381:GLN:HB2	2.10	0.51
9:W:224:LEU:HD22	9:W:253:THR:HG23	1.93	0.51
9:W:408:ARG:NH1	10:X:383:GLY:O	2.43	0.51
13:a:250:THR:HA	13:a:253:THR:HG22	1.92	0.51
15:c:190:GLN:HA	15:c:194:HIS:CE1	2.46	0.51
18:f:187:LEU:HD13	18:f:228:LYS:HD3	1.93	0.51
1:A:232:ARG:HG2	1:A:236:CYS:HA	1.93	0.51
11:Y:330:ILE:HA	11:Y:333:GLU:HB2	1.91	0.51
18:f:331:LEU:HD22	18:f:335:ARG:HH21	1.74	0.51
5:E:51:GLN:O	12:Z:88:ARG:NH2	2.43	0.51
7:U:581:SER:O	7:U:585:THR:OG1	2.19	0.51
18:f:584:SER:O	18:f:589:SER:OG	2.28	0.51
5:E:309:ARG:NH1	5:E:339:ASN:O	2.44	0.50
7:U:772:TRP:HD1	7:U:775:LEU:HG	1.75	0.50
12:Z:131:LEU:HD21	12:Z:199:LYS:HG2	1.92	0.50
13:a:152:HIS:CD2	13:a:178:ARG:HG2	2.46	0.50
18:f:228:LYS:O	18:f:232:TYR:CB	2.50	0.50
3:C:360:LYS:HE2	4:D:324:PRO:HB2	1.93	0.50
15:c:213:GLU:O	15:c:217:LEU:HB3	2.11	0.50
1:A:397:ILE:HG13	2:B:214:MET:HG3	1.93	0.50
3:C:327:ASP:OD1	3:C:328:ILE:N	2.45	0.50
5:E:309:ARG:HD2	5:E:332:VAL:HG13	1.92	0.50
10:X:187:ARG:HH22	10:X:223:LYS:HE3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:316:ASP:OD2	10:X:320:SER:OG	2.26	0.50
18:f:536:SER:O	18:f:540:GLN:CB	2.59	0.50
3:C:318:PRO:HG2	3:C:321:ASN:HB2	1.93	0.50
4:D:289:LEU:HD12	4:D:292:LEU:HD11	1.92	0.50
9:W:267:LEU:HD23	9:W:299:ILE:HD11	1.92	0.50
11:Y:72:LYS:HA	11:Y:75:LYS:HE3	1.92	0.50
13:a:120:ALA:HB2	13:a:158:LEU:HD11	1.94	0.50
18:f:724:ASN:O	18:f:728:ALA:C	2.54	0.50
6:F:362:ARG:HD3	6:F:365:ILE:HD11	1.92	0.50
8:V:342:ILE:O	8:V:368:ARG:NH2	2.40	0.50
12:Z:145:HIS:HD1	12:Z:147:ASP:H	1.59	0.50
18:f:315:GLU:HA	18:f:318:THR:HG22	1.92	0.50
18:f:509:LYS:O	18:f:554:TYR:OH	2.28	0.50
2:B:333:ARG:HB3	2:B:336:THR:HG23	1.93	0.50
6:F:273:ALA:O	6:F:277:GLU:CB	2.54	0.50
6:F:301:ALA:HB3	6:F:304:ARG:HE	1.76	0.50
7:U:250:PHE:O	7:U:254:GLU:CB	2.58	0.50
8:V:410:ILE:HA	8:V:413:SER:HB3	1.93	0.50
11:Y:292:TYR:OH	17:e:57:ARG:NH1	2.45	0.50
2:B:333:ARG:HG2	2:B:335:GLU:H	1.75	0.50
7:U:719:ASP:HB2	7:U:727:LYS:HE2	1.94	0.50
9:W:118:LEU:HB3	9:W:119:PRO:HD3	1.93	0.50
7:U:247:GLN:HE21	7:U:913:ILE:H	1.59	0.50
12:Z:232:ASP:OD2	13:a:335:TRP:NE1	2.45	0.50
14:b:90:ILE:HG23	14:b:94:HIS:CD2	2.47	0.50
18:f:317:LEU:O	18:f:321:MET:HB2	2.11	0.50
2:B:224:LEU:N	2:B:329:MET:O	2.45	0.50
3:C:262:GLY:O	3:C:266:ASP:CB	2.60	0.50
7:U:505:ASP:HB2	7:U:508:THR:HG22	1.94	0.50
8:V:419:LEU:HD13	8:V:457:TYR:HA	1.94	0.50
4:D:200:ARG:NH1	4:D:300:ASP:OD1	2.45	0.49
8:V:263:LEU:HB3	16:d:124:ALA:HA	1.93	0.49
13:a:199:THR:O	13:a:203:ALA:CB	2.59	0.49
13:a:247:ARG:O	13:a:251:LEU:HB2	2.12	0.49
18:f:80:ARG:HD2	18:f:133:MET:HE1	1.94	0.49
18:f:403:LYS:HG2	18:f:404:ASP:H	1.76	0.49
2:B:398:ILE:HD13	2:B:423:LYS:HD3	1.94	0.49
5:E:65:THR:HG22	5:E:67:GLU:H	1.77	0.49
6:F:374:ASN:HB3	6:F:414:GLU:HG3	1.94	0.49
7:U:680:VAL:HG12	7:U:682:TYR:H	1.77	0.49
17:e:42:ASN:O	17:e:46:ASP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:f:652:VAL:HA	18:f:655:LEU:HD13	1.94	0.49
2:B:198:LYS:HD3	2:B:202:GLU:HG3	1.93	0.49
3:C:167:LEU:HA	3:C:171:HIS:HB2	1.92	0.49
4:D:323:ARG:HE	4:D:326:ARG:HE	1.59	0.49
12:Z:172:VAL:HG13	15:c:217:LEU:HD21	1.93	0.49
13:a:274:LEU:HD13	13:a:319:LEU:HD21	1.93	0.49
14:b:101:GLN:NE2	15:c:97:ASP:OD2	2.45	0.49
2:B:231:GLY:O	2:B:235:LEU:CB	2.60	0.49
2:B:390:LEU:HD21	2:B:394:ASP:H	1.77	0.49
9:W:73:MET:O	9:W:77:ALA:HB3	2.13	0.49
18:f:298:LEU:HA	18:f:301:HIS:HD2	1.77	0.49
18:f:671:ALA:O	18:f:674:THR:OG1	2.26	0.49
1:A:415:LYS:O	1:A:419:SER:OG	2.23	0.49
3:C:344:LEU:O	3:C:348:ALA:CB	2.61	0.49
5:E:63:GLN:HG3	5:E:69:PHE:HB3	1.94	0.49
9:W:437:SER:O	9:W:441:LYS:CB	2.61	0.49
13:a:70:ARG:HA	14:b:17:ARG:HH12	1.77	0.49
15:c:235:SER:HB2	15:c:239:LYS:HE2	1.95	0.49
18:f:89:MET:HG2	18:f:90:THR:HG23	1.93	0.49
1:A:298:THR:O	1:A:302:LEU:CB	2.59	0.49
3:C:238:ALA:HB1	3:C:289:ILE:HD12	1.94	0.49
16:d:131:VAL:O	16:d:135:HIS:HB2	2.13	0.49
18:f:248:LEU:O	18:f:252:ALA:CB	2.60	0.49
3:C:198:LEU:O	3:C:202:ALA:HB2	2.12	0.49
9:W:243:ILE:HD11	9:W:276:LEU:HD12	1.95	0.49
18:f:93:PRO:HB2	18:f:137:ARG:HE	1.76	0.49
6:F:274:LEU:O	6:F:278:LYS:CB	2.53	0.49
12:Z:225:GLN:HE22	13:a:339:ARG:HD2	1.77	0.49
1:A:250:VAL:HG11	1:A:294:GLU:HB2	1.94	0.49
6:F:288:LEU:HD12	6:F:291:ILE:HD11	1.94	0.49
7:U:413:LYS:HG3	7:U:449:ILE:HA	1.94	0.49
9:W:211:THR:HG23	9:W:212:LYS:H	1.77	0.49
16:d:205:LYS:O	16:d:209:TYR:HB2	2.12	0.49
18:f:503:PRO:O	18:f:507:ASP:HB2	2.13	0.49
1:A:167:GLU:OE1	1:A:239:ARG:NE	2.40	0.49
1:A:347:ASP:O	1:A:351:ARG:NH2	2.46	0.49
3:C:187:LEU:HB3	3:C:293:MET:HB2	1.95	0.49
3:C:267:SER:HA	3:C:270:GLN:HB2	1.95	0.49
6:F:373:MET:SD	6:F:373:MET:N	2.86	0.49
7:U:397:THR:HA	7:U:401:LYS:HE2	1.95	0.49
9:W:220:GLU:OE1	9:W:222:LEU:CA	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:36:ALA:O	11:Y:40:GLU:CB	2.61	0.49
18:f:336:GLU:HG3	18:f:337:LEU:HD22	1.95	0.49
18:f:545:LYS:HE2	18:f:555:ALA:HA	1.95	0.49
18:f:632:LYS:HB3	18:f:661:ALA:HA	1.94	0.49
5:E:349:GLU:HG2	5:E:374:VAL:HG21	1.94	0.48
6:F:73:ILE:O	6:F:77:SER:OG	2.20	0.48
7:U:134:VAL:O	7:U:138:PHE:HB2	2.13	0.48
8:V:322:VAL:HG13	8:V:350:GLN:HG3	1.95	0.48
18:f:584:SER:OG	18:f:588:ARG:HB2	2.12	0.48
3:C:11:LEU:O	7:U:140:ARG:NH1	2.45	0.48
6:F:153:VAL:HG23	6:F:158:TYR:HA	1.93	0.48
12:Z:252:LYS:HE3	15:c:304:LEU:HD12	1.94	0.48
4:D:106:THR:HG21	5:E:77:PRO:HA	1.95	0.48
7:U:100:ILE:O	7:U:104:CYS:HB2	2.13	0.48
7:U:496:LEU:HA	7:U:499:THR:HG22	1.95	0.48
9:W:350:ARG:O	9:W:354:LEU:CB	2.55	0.48
11:Y:250:LEU:HD13	11:Y:257:ARG:HD3	1.95	0.48
16:d:122:LEU:HG	16:d:123:PRO:HD3	1.95	0.48
18:f:253:LEU:O	18:f:257:ARG:CB	2.61	0.48
18:f:470:VAL:HG13	18:f:471:LEU:H	1.78	0.48
5:E:40:TYR:O	5:E:43:SER:OG	2.25	0.48
8:V:313:LEU:HD12	8:V:328:VAL:HG13	1.94	0.48
8:V:328:VAL:O	8:V:332:LEU:HB2	2.13	0.48
18:f:88:SER:HB2	18:f:92:VAL:HG23	1.95	0.48
2:B:255:LEU:HA	2:B:258:LYS:HG2	1.95	0.48
4:D:244:PRO:O	4:D:248:ARG:CB	2.62	0.48
5:E:304:PRO:HB2	5:E:309:ARG:HH21	1.79	0.48
6:F:151:VAL:HG12	6:F:163:THR:HG23	1.96	0.48
8:V:420:ALA:O	8:V:424:GLN:HB3	2.14	0.48
10:X:259:ILE:HD13	10:X:267:VAL:HG21	1.96	0.48
10:X:417:LYS:HA	10:X:420:LYS:HG2	1.94	0.48
16:d:202:THR:HG22	16:d:204:LYS:HG2	1.95	0.48
18:f:536:SER:HA	18:f:539:LEU:HB3	1.94	0.48
1:A:312:ARG:HG3	1:A:314:ASN:H	1.78	0.48
5:E:207:TYR:HE1	5:E:210:GLU:H	1.60	0.48
7:U:340:GLN:O	7:U:343:ILE:HG22	2.13	0.48
7:U:545:LEU:O	7:U:549:ALA:HB2	2.13	0.48
9:W:422:ASN:OD1	9:W:426:ASN:ND2	2.45	0.48
12:Z:52:ASN:HD22	15:c:43:LYS:HE2	1.77	0.48
12:Z:270:VAL:HG13	15:c:284:LEU:HD22	1.94	0.48
18:f:94:LYS:HB3	18:f:95:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:368:MET:O	3:C:372:ARG:CB	2.62	0.48
4:D:116:LEU:HD23	4:D:118:THR:H	1.77	0.48
6:F:367:GLN:O	6:F:371:ARG:HB3	2.13	0.48
7:U:145:HIS:HB3	7:U:150:ALA:HB2	1.94	0.48
7:U:841:LYS:NZ	7:U:882:ALA:O	2.47	0.48
9:W:74:CYS:HB3	9:W:78:LYS:HE2	1.94	0.48
13:a:76:LEU:HA	13:a:79:ILE:HG22	1.96	0.48
18:f:337:LEU:O	18:f:341:GLU:HB3	2.13	0.48
5:E:62:LYS:HE3	5:E:64:LEU:HD11	1.96	0.48
5:E:253:ILE:O	5:E:257:LEU:HB2	2.14	0.48
10:X:358:LYS:O	10:X:362:GLU:CB	2.61	0.48
15:c:267:PRO:O	15:c:271:ALA:CB	2.61	0.48
18:f:527:VAL:HG11	18:f:775:THR:HG21	1.95	0.48
2:B:369:THR:HG22	2:B:374:LEU:HD21	1.95	0.48
6:F:271:ALA:O	6:F:275:ALA:HB3	2.13	0.48
8:V:453:HIS:O	16:d:188:LYS:NZ	2.47	0.48
11:Y:247:LEU:HA	11:Y:250:LEU:HD23	1.96	0.48
2:B:417:GLU:O	2:B:421:LYS:HB2	2.13	0.48
4:D:336:PRO:HA	4:D:341:LYS:HE2	1.96	0.48
5:E:188:ALA:HA	5:E:192:ASP:HB2	1.96	0.48
12:Z:213:GLU:O	12:Z:217:THR:OG1	2.27	0.48
15:c:139:ARG:HB3	15:c:161:ARG:HH12	1.79	0.48
15:c:178:THR:HA	15:c:181:LEU:HD13	1.95	0.48
2:B:195:GLN:HA	2:B:198:LYS:HB3	1.96	0.47
7:U:543:LYS:HA	7:U:546:ARG:HG2	1.95	0.47
9:W:436:MET:O	9:W:440:ASN:HB2	2.14	0.47
3:C:36:ASN:O	3:C:39:SER:OG	2.30	0.47
5:E:281:ARG:HH12	6:F:296:PHE:HE1	1.62	0.47
15:c:170:LEU:HG	15:c:171:GLY:H	1.79	0.47
18:f:221:ILE:O	18:f:225:ALA:CB	2.62	0.47
3:C:43:ARG:HB2	7:U:639:LEU:HD21	1.95	0.47
5:E:185:ARG:NH1	5:E:345:ASN:OD1	2.47	0.47
6:F:357:PRO:HA	6:F:361:ALA:HB3	1.96	0.47
9:W:344:THR:HG23	9:W:345:GLU:HG2	1.96	0.47
16:d:194:ALA:O	16:d:198:LEU:HB2	2.13	0.47
2:B:94:GLU:O	2:B:98:LYS:HB3	2.15	0.47
6:F:403:ALA:HB1	6:F:415:LEU:HD11	1.95	0.47
7:U:266:GLN:HA	7:U:269:ARG:HB3	1.95	0.47
9:W:317:TRP:CD1	9:W:355:LYS:HZ2	2.32	0.47
12:Z:96:HIS:CE1	12:Z:123:ILE:HG12	2.50	0.47
12:Z:231:GLN:HE22	13:a:345:GLN:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ILE:HA	1:A:113:ILE:HA	1.96	0.47
3:C:313:ARG:NH1	3:C:314:LYS:O	2.48	0.47
7:U:344:ARG:HD2	7:U:880:ASN:HB3	1.96	0.47
8:V:311:ASN:OD1	8:V:315:LYS:NZ	2.48	0.47
11:Y:153:ASP:OD1	11:Y:153:ASP:N	2.47	0.47
18:f:365:VAL:HG11	18:f:374:SER:HB2	1.96	0.47
18:f:481:SER:O	18:f:485:LEU:HB2	2.14	0.47
1:A:136:GLU:OE1	1:A:258:ARG:NH2	2.48	0.47
1:A:240:VAL:O	1:A:275:ASP:N	2.47	0.47
6:F:204:LEU:HD23	6:F:205:PRO:HD3	1.96	0.47
18:f:86:THR:HG23	18:f:87:THR:H	1.79	0.47
4:D:62:LYS:HD3	4:D:65:GLN:NE2	2.29	0.47
9:W:405:LYS:N	9:W:414:ASN:O	2.47	0.47
16:d:114:GLU:HA	16:d:117:THR:HG22	1.94	0.47
18:f:138:GLU:O	18:f:142:TYR:CB	2.62	0.47
18:f:211:ILE:HA	18:f:214:VAL:HG22	1.97	0.47
2:B:409:GLU:OE1	2:B:411:ARG:NH1	2.48	0.47
5:E:206:LYS:NZ	6:F:301:ALA:O	2.47	0.47
7:U:154:ALA:HB1	7:U:163:PHE:HB3	1.97	0.47
9:W:124:LEU:HA	9:W:127:THR:HG22	1.97	0.47
18:f:478:ARG:O	18:f:482:ILE:HB	2.15	0.47
4:D:99:ASN:HA	4:D:115:ILE:HD11	1.96	0.47
5:E:312:ILE:HG23	5:E:316:HIS:CD2	2.50	0.47
6:F:379:VAL:HG13	6:F:384:LEU:HD21	1.97	0.47
12:Z:201:LEU:O	12:Z:205:LEU:CB	2.63	0.47
13:a:349:MET:O	13:a:353:LEU:HB2	2.14	0.47
2:B:191:ASP:HA	2:B:194:ILE:HG22	1.97	0.47
4:D:176:GLU:O	4:D:180:ALA:CB	2.63	0.47
6:F:272:PHE:O	6:F:276:LYS:CB	2.52	0.47
6:F:391:PHE:HE2	6:F:424:ILE:HG23	1.79	0.47
7:U:545:LEU:HB3	7:U:577:ILE:HG21	1.95	0.47
18:f:502:LEU:HB3	18:f:503:PRO:HD3	1.97	0.47
18:f:743:ALA:HA	18:f:746:ARG:HG2	1.97	0.47
1:A:315:ILE:HG13	1:A:316:LYS:H	1.79	0.46
3:C:198:LEU:O	3:C:202:ALA:CB	2.63	0.46
3:C:375:ARG:HH22	3:C:382:ASP:HB2	1.79	0.46
5:E:335:SER:HB2	5:E:343:LEU:HD13	1.97	0.46
7:U:247:GLN:HE21	7:U:913:ILE:HG13	1.80	0.46
8:V:501:TYR:HA	12:Z:282:ASN:HD21	1.80	0.46
9:W:406:VAL:HG12	9:W:413:ILE:HG22	1.97	0.46
18:f:188:VAL:HA	18:f:191:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:f:620:PHE:CE2	18:f:622:SER:HB3	2.50	0.46
5:E:378:LYS:O	5:E:382:SER:CB	2.57	0.46
7:U:474:ARG:O	7:U:478:SER:HB2	2.14	0.46
7:U:490:ARG:NH2	7:U:492:ASP:OD2	2.47	0.46
9:W:220:GLU:OE2	9:W:222:LEU:HD13	2.15	0.46
10:X:358:LYS:O	10:X:362:GLU:HB2	2.16	0.46
13:a:18:GLN:HB3	13:a:22:TRP:CD1	2.50	0.46
18:f:749:ALA:HA	18:f:752:HIS:HB2	1.97	0.46
3:C:338:LEU:HD11	3:C:342:ILE:HD13	1.97	0.46
7:U:251:ASP:OD1	7:U:252:LEU:N	2.48	0.46
10:X:268:GLN:HA	10:X:271:VAL:HG22	1.96	0.46
15:c:216:MET:O	15:c:220:LEU:HB2	2.16	0.46
18:f:229:VAL:HG21	18:f:256:PHE:CZ	2.51	0.46
18:f:494:ARG:NE	18:f:494:ARG:CA	2.77	0.46
1:A:368:ILE:HD11	1:A:405:THR:HG23	1.97	0.46
5:E:304:PRO:HG2	5:E:337:GLY:H	1.81	0.46
12:Z:139:ILE:HG12	12:Z:141:VAL:HG13	1.97	0.46
12:Z:256:GLN:HE22	15:c:298:GLN:HG2	1.81	0.46
3:C:25:LEU:HD13	4:D:44:TYR:HD1	1.80	0.46
4:D:43:ARG:O	4:D:47:LEU:CB	2.64	0.46
5:E:235:ILE:HG13	5:E:238:ILE:HD11	1.97	0.46
7:U:229:VAL:HG23	7:U:232:ILE:HD11	1.98	0.46
11:Y:50:MET:HE3	11:Y:70:LEU:HD22	1.98	0.46
13:a:196:ARG:O	13:a:200:LEU:CB	2.63	0.46
13:a:292:THR:HG23	13:a:294:GLU:H	1.81	0.46
18:f:281:ILE:O	18:f:285:CYS:CB	2.63	0.46
2:B:219:PRO:HB3	2:B:323:GLY:HA2	1.98	0.46
7:U:135:ASN:HA	7:U:138:PHE:HB3	1.97	0.46
7:U:386:LEU:HD22	7:U:393:LEU:HD11	1.97	0.46
11:Y:22:LEU:HD22	11:Y:25:LEU:HD21	1.97	0.46
15:c:184:LEU:HB2	15:c:204:THR:HG22	1.97	0.46
15:c:260:GLU:HA	15:c:263:ASP:HB2	1.96	0.46
3:C:201:ARG:O	3:C:205:HIS:HB2	2.16	0.46
4:D:175:GLN:HB2	10:X:195:THR:HG21	1.96	0.46
5:E:171:LEU:HD13	5:E:295:LEU:HD13	1.98	0.46
5:E:356:ARG:HD2	6:F:350:ARG:HH12	1.79	0.46
9:W:218:ASN:O	9:W:223:LYS:NZ	2.48	0.46
13:a:84:VAL:HG11	13:a:121:LEU:HD21	1.97	0.46
13:a:199:THR:O	13:a:203:ALA:HB2	2.16	0.46
13:a:250:THR:O	13:a:254:ALA:CB	2.63	0.46
13:a:340:VAL:HG13	13:a:341:LEU:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:e:45:ASP:O	17:e:49:GLU:CB	2.64	0.46
18:f:531:ASN:HA	18:f:569:LYS:HA	1.97	0.46
2:B:194:ILE:HA	2:B:197:ILE:HG22	1.97	0.46
2:B:382:ASP:O	2:B:386:ALA:CA	2.64	0.46
3:C:319:PRO:N	3:C:320:PRO:HD2	2.31	0.46
6:F:249:LEU:HB2	6:F:283:ILE:HG13	1.97	0.46
10:X:180:LEU:HB3	11:Y:248:GLU:HG2	1.98	0.46
10:X:310:ARG:O	10:X:314:ARG:HB2	2.15	0.46
11:Y:220:VAL:HA	11:Y:223:THR:HG22	1.97	0.46
18:f:493:ASN:ND2	18:f:493:ASN:C	2.73	0.46
4:D:333:PHE:CG	4:D:334:PRO:HD2	2.51	0.46
8:V:484:LEU:HD21	12:Z:260:VAL:HG22	1.97	0.46
11:Y:258:GLN:O	11:Y:262:SER:OG	2.34	0.46
1:A:264:ALA:HB2	1:A:272:ILE:HD11	1.97	0.46
2:B:197:ILE:O	2:B:201:VAL:HG22	2.16	0.46
6:F:304:ARG:HA	6:F:307:GLN:HB2	1.97	0.46
7:U:421:GLN:O	7:U:425:THR:OG1	2.20	0.46
9:W:316:ARG:NH2	9:W:381:LEU:O	2.49	0.46
18:f:248:LEU:O	18:f:252:ALA:HB3	2.16	0.46
18:f:523:GLY:O	18:f:527:VAL:HG13	2.16	0.46
2:B:147:GLY:O	2:B:265:LYS:NZ	2.34	0.45
7:U:903:PHE:HB3	7:U:915:LYS:HD2	1.98	0.45
11:Y:92:GLU:HG2	11:Y:93:LYS:HD2	1.98	0.45
12:Z:39:LEU:HB2	12:Z:95:TYR:HD1	1.81	0.45
18:f:95:PRO:O	18:f:99:LEU:CB	2.44	0.45
18:f:350:LYS:HG3	18:f:351:THR:HG23	1.98	0.45
1:A:176:ASP:HA	1:A:353:HIS:HB3	1.99	0.45
1:A:214:LEU:HB2	1:A:320:ALA:HA	1.98	0.45
1:A:351:ARG:HD3	1:A:380:SER:HB2	1.98	0.45
6:F:194:GLN:O	6:F:194:GLN:HG2	2.16	0.45
17:e:43:TRP:O	17:e:47:ASN:HB2	2.17	0.45
2:B:392:GLY:O	2:B:396:LYS:HB2	2.16	0.45
4:D:253:LEU:O	4:D:257:ASN:HB3	2.16	0.45
4:D:401:LYS:HA	4:D:404:LYS:HE2	1.97	0.45
18:f:316:ASP:O	18:f:319:GLU:HG2	2.17	0.45
18:f:585:GLU:HB2	18:f:586:PRO:HD2	1.98	0.45
3:C:202:ALA:O	3:C:206:HIS:ND1	2.41	0.45
5:E:360:ASP:N	5:E:360:ASP:OD1	2.49	0.45
8:V:250:LEU:HD23	8:V:253:LEU:HD21	1.99	0.45
11:Y:179:ARG:NH1	11:Y:212:GLU:OE1	2.45	0.45
12:Z:164:ALA:HB1	12:Z:168:GLU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:f:624:GLU:O	18:f:628:ASP:CB	2.58	0.45
4:D:283:ARG:HG3	4:D:286:GLN:HE21	1.81	0.45
7:U:792:ASN:OD1	7:U:793:LYS:N	2.47	0.45
15:c:282:ARG:H	15:c:282:ARG:HD3	1.82	0.45
18:f:102:HIS:CG	18:f:103:TYR:H	2.33	0.45
18:f:496:ASP:OD1	18:f:497:VAL:N	2.49	0.45
2:B:120:HIS:HB2	2:B:132:TYR:HB2	1.99	0.45
3:C:379:THR:HG23	3:C:382:ASP:H	1.82	0.45
8:V:417:ILE:HD13	8:V:434:ALA:HB1	1.99	0.45
11:Y:226:VAL:O	11:Y:230:ALA:CB	2.59	0.45
18:f:675:PHE:CG	18:f:694:LEU:HD23	2.52	0.45
18:f:744:MET:O	18:f:748:LEU:HB2	2.17	0.45
2:B:270:LEU:HA	2:B:273:VAL:HG12	1.99	0.45
5:E:286:ASP:O	5:E:289:LEU:N	2.50	0.45
6:F:74:LYS:O	6:F:78:GLU:CB	2.54	0.45
7:U:787:CYS:HB2	7:U:881:PRO:HB2	1.97	0.45
3:C:236:VAL:HG22	3:C:239:ARG:HH12	1.82	0.45
10:X:151:SER:O	10:X:155:ARG:HG2	2.17	0.45
11:Y:36:ALA:O	11:Y:40:GLU:HB2	2.16	0.45
18:f:273:ASN:ND2	18:f:312:GLU:OE1	2.50	0.45
7:U:456:ASP:HB3	7:U:458:ILE:HG13	1.98	0.45
10:X:245:PRO:HA	10:X:248:ILE:HG22	1.98	0.45
13:a:349:MET:O	13:a:353:LEU:CB	2.65	0.45
13:a:366:LEU:HD21	16:d:244:LYS:HE2	1.98	0.45
7:U:493:VAL:O	7:U:497:LEU:CB	2.63	0.45
11:Y:13:LYS:HB2	11:Y:212:GLU:HG2	1.98	0.45
18:f:92:VAL:O	18:f:95:PRO:HD2	2.17	0.45
18:f:623:LYS:O	18:f:627:GLU:HB3	2.17	0.45
18:f:778:LEU:HA	18:f:781:TYR:HE1	1.82	0.45
1:A:105:ASP:OD1	1:A:105:ASP:N	2.49	0.44
2:B:140:ASP:O	2:B:141:LYS:HG2	2.17	0.44
2:B:402:ALA:O	2:B:406:ALA:CB	2.65	0.44
7:U:368:ALA:HA	7:U:371:ILE:HG22	1.99	0.44
14:b:76:HIS:CG	14:b:77:THR:H	2.35	0.44
18:f:651:GLY:O	18:f:654:VAL:N	2.45	0.44
1:A:411:GLU:O	1:A:415:LYS:HB3	2.17	0.44
5:E:42:LYS:HA	5:E:45:ASN:HD22	1.83	0.44
8:V:396:ILE:HD12	8:V:399:ARG:HD3	1.99	0.44
8:V:483:CYS:O	8:V:487:HIS:ND1	2.36	0.44
12:Z:249:PHE:HZ	15:c:308:VAL:HG11	1.81	0.44
12:Z:261:TYR:O	12:Z:265:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:f:102:HIS:CD2	18:f:103:TYR:H	2.36	0.44
18:f:140:LEU:O	18:f:144:LEU:CB	2.65	0.44
18:f:517:VAL:O	18:f:521:ALA:CB	2.65	0.44
1:A:143:ASP:OD1	1:A:144:ARG:N	2.50	0.44
3:C:344:LEU:O	3:C:348:ALA:HB3	2.17	0.44
4:D:283:ARG:HA	4:D:286:GLN:HG2	1.98	0.44
6:F:234:THR:OG1	6:F:286:ASP:OD2	2.34	0.44
7:U:127:ASP:HB3	7:U:130:LEU:HD13	1.99	0.44
8:V:468:SER:HA	11:Y:363:ASN:HD22	1.82	0.44
9:W:408:ARG:HH12	10:X:347:ILE:HG23	1.82	0.44
11:Y:347:ILE:HD11	11:Y:354:VAL:HG22	1.98	0.44
13:a:226:ARG:HB3	13:a:234:ILE:HD11	2.00	0.44
18:f:268:LEU:O	18:f:272:LEU:HB2	2.17	0.44
2:B:155:LYS:C	2:B:157:HIS:H	2.25	0.44
2:B:357:ASP:O	2:B:358:GLU:HG2	2.17	0.44
3:C:370:ALA:HB2	3:C:378:VAL:HG22	1.98	0.44
6:F:88:TYR:CE1	6:F:155:LYS:HA	2.53	0.44
7:U:196:LYS:HA	7:U:199:ARG:HG2	2.00	0.44
9:W:73:MET:O	9:W:77:ALA:HB2	2.15	0.44
10:X:342:PHE:HD2	10:X:350:ILE:HD12	1.81	0.44
13:a:64:ILE:HA	13:a:67:PHE:CE1	2.52	0.44
18:f:232:TYR:CE2	18:f:248:LEU:HD12	2.53	0.44
1:A:108:ASP:OD1	1:A:109:PRO:HD3	2.17	0.44
7:U:338:HIS:HA	7:U:341:PHE:CE1	2.52	0.44
10:X:186:ALA:O	10:X:190:LEU:CB	2.65	0.44
10:X:255:LEU:HD22	10:X:267:VAL:HG13	1.99	0.44
7:U:633:CYS:HB2	7:U:634:PRO:HD3	1.99	0.44
10:X:417:LYS:HA	10:X:420:LYS:HE3	1.99	0.44
14:b:26:LEU:HD12	14:b:29:GLN:HE21	1.82	0.44
14:b:76:HIS:CD2	14:b:77:THR:H	2.34	0.44
15:c:213:GLU:O	15:c:217:LEU:CB	2.65	0.44
7:U:98:GLU:HA	7:U:101:ILE:HG12	2.00	0.44
7:U:474:ARG:O	7:U:478:SER:HB3	2.18	0.44
18:f:414:LEU:HA	18:f:417:ILE:HG12	1.99	0.44
2:B:283:PHE:CE2	2:B:285:ASP:HB2	2.53	0.44
4:D:133:HIS:HD2	4:D:138:ALA:HB3	1.83	0.44
5:E:197:LYS:HB3	6:F:315:ASN:HD21	1.83	0.44
7:U:465:LEU:HD13	7:U:481:LEU:HD22	1.99	0.44
8:V:462:GLU:HB2	11:Y:346:LYS:NZ	2.32	0.44
18:f:477:MET:O	18:f:481:SER:CB	2.66	0.44
3:C:262:GLY:O	3:C:266:ASP:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:214:MET:O	4:D:218:ALA:CB	2.65	0.44
5:E:23:ASP:HB3	6:F:56:LYS:HE2	2.00	0.44
9:W:277:ALA:O	9:W:357:ARG:NH2	2.51	0.44
18:f:92:VAL:HG12	18:f:133:MET:HG3	2.00	0.44
18:f:249:LEU:HD23	18:f:272:LEU:HG	1.99	0.44
18:f:261:ARG:O	18:f:264:GLU:HG2	2.18	0.44
18:f:778:LEU:HA	18:f:781:TYR:CE1	2.53	0.44
3:C:298:ILE:HD12	3:C:298:ILE:H	1.82	0.43
5:E:81:VAL:HG11	5:E:100:LEU:HD22	1.99	0.43
6:F:100:ASP:HB3	6:F:101:PRO:HD3	1.99	0.43
7:U:696:ILE:HG22	7:U:737:LEU:HA	1.99	0.43
18:f:546:SER:HB3	18:f:588:ARG:HD3	2.00	0.43
1:A:187:LEU:HD22	1:A:214:LEU:HD11	1.99	0.43
2:B:401:GLU:O	2:B:405:MET:CB	2.66	0.43
12:Z:25:ARG:HD3	15:c:104:ARG:HE	1.83	0.43
15:c:115:HIS:HE1	15:c:122:LEU:HD23	1.83	0.43
18:f:273:ASN:HD21	18:f:312:GLU:HB3	1.84	0.43
1:A:277:ILE:HG22	1:A:321:THR:HG21	1.99	0.43
5:E:102:MET:HG3	5:E:103:THR:HG23	2.00	0.43
7:U:772:TRP:CD1	7:U:775:LEU:HG	2.53	0.43
9:W:220:GLU:CD	9:W:220:GLU:C	2.86	0.43
12:Z:71:ASP:OD1	14:b:63:THR:OG1	2.35	0.43
12:Z:91:ILE:H	12:Z:91:ILE:HG13	1.67	0.43
13:a:247:ARG:HA	13:a:250:THR:HG22	2.00	0.43
18:f:93:PRO:HB2	18:f:137:ARG:NE	2.34	0.43
18:f:357:ARG:O	18:f:361:SER:CB	2.59	0.43
18:f:446:LEU:HD13	18:f:480:GLY:HA2	2.00	0.43
4:D:93:LEU:HD23	4:D:94:GLU:HG3	2.01	0.43
7:U:600:ARG:O	7:U:604:HIS:CB	2.63	0.43
11:Y:149:LEU:HD13	11:Y:186:LEU:HD23	2.00	0.43
15:c:146:ASP:OD2	15:c:149:GLN:NE2	2.42	0.43
5:E:313:LEU:O	5:E:317:ALA:CB	2.65	0.43
8:V:354:LYS:O	8:V:358:MET:HG3	2.19	0.43
9:W:194:LEU:HA	9:W:197:LYS:HE3	1.99	0.43
12:Z:202:ASN:O	12:Z:206:LEU:CB	2.65	0.43
18:f:187:LEU:HA	18:f:190:GLU:HG2	2.01	0.43
18:f:417:ILE:HG13	18:f:418:LEU:HG	2.00	0.43
18:f:620:PHE:HB3	18:f:623:LYS:HG2	2.00	0.43
18:f:623:LYS:O	18:f:627:GLU:CB	2.67	0.43
18:f:658:ALA:HA	18:f:661:ALA:HB3	2.01	0.43
7:U:712:LEU:HD21	7:U:734:GLN:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:184:GLN:HA	11:Y:187:TYR:CD1	2.53	0.43
12:Z:175:LEU:HD21	15:c:38:LEU:HD13	2.01	0.43
18:f:79:ARG:HH21	18:f:95:PRO:HG3	1.84	0.43
18:f:138:GLU:HB3	18:f:193:PRO:HG3	2.00	0.43
3:C:274:LEU:HD11	3:C:306:LEU:HD23	2.00	0.43
5:E:313:LEU:O	5:E:317:ALA:HB2	2.19	0.43
7:U:264:VAL:HA	7:U:267:ASN:HB2	2.01	0.43
9:W:122:LEU:HA	9:W:125:ILE:HG22	2.00	0.43
12:Z:199:LYS:HD3	15:c:230:THR:HG21	2.01	0.43
12:Z:211:TYR:HD2	12:Z:212:LEU:HD12	1.84	0.43
13:a:7:PHE:O	13:a:11:SER:HB3	2.19	0.43
15:c:212:LEU:O	15:c:216:MET:HB3	2.19	0.43
4:D:134:LYS:HG3	4:D:135:HIS:ND1	2.33	0.43
6:F:152:GLY:HA3	6:F:161:LEU:HG	2.01	0.43
9:W:253:THR:HG22	9:W:262:LYS:HE3	2.00	0.43
12:Z:284:ASP:HA	12:Z:287:LYS:HG2	2.01	0.43
15:c:90:VAL:O	15:c:94:LYS:HB2	2.19	0.43
18:f:646:MET:HB3	18:f:654:VAL:HG12	2.01	0.43
2:B:102:LEU:HD22	2:B:160:ILE:HD13	2.01	0.43
6:F:363:ALA:O	6:F:367:GLN:CB	2.67	0.43
7:U:159:ARG:HD2	7:U:160:LEU:H	1.84	0.43
9:W:131:VAL:HG22	9:W:142:ARG:HD2	2.00	0.43
15:c:107:MET:HE3	15:c:108:VAL:HG22	2.01	0.43
6:F:233:LYS:HD3	6:F:331:ALA:HB1	2.00	0.43
9:W:437:SER:O	9:W:441:LYS:HB2	2.19	0.43
13:a:78:GLU:O	13:a:82:HIS:ND1	2.50	0.43
5:E:247:THR:HG23	5:E:249:ALA:H	1.84	0.42
7:U:341:PHE:HB2	7:U:880:ASN:HA	2.01	0.42
13:a:4:VAL:HB	13:a:5:PRO:HD3	2.01	0.42
18:f:301:HIS:HA	18:f:304:PHE:CE2	2.54	0.42
18:f:373:ALA:O	18:f:377:VAL:HG23	2.19	0.42
18:f:446:LEU:HD21	18:f:799:VAL:HG11	2.01	0.42
1:A:151:ILE:HD12	1:A:152:PRO:HD2	2.00	0.42
1:A:317:VAL:HG11	1:A:336:ARG:HH22	1.83	0.42
4:D:115:ILE:HG22	4:D:139:LEU:HD21	2.01	0.42
9:W:93:ARG:HE	9:W:96:GLN:HB2	1.84	0.42
18:f:130:ALA:HA	18:f:133:MET:HB3	2.01	0.42
2:B:356:PRO:HB3	2:B:360:THR:HB	2.00	0.42
3:C:252:ASP:OD1	3:C:296:ASN:ND2	2.52	0.42
7:U:841:LYS:HG2	7:U:881:PRO:HA	2.00	0.42
8:V:289:LEU:HA	8:V:292:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:f:190:GLU:C	18:f:193:PRO:HD2	2.44	0.42
7:U:613:ASP:O	7:U:616:ARG:HD2	2.19	0.42
9:W:363:ILE:HA	9:W:366:MET:HG2	2.01	0.42
16:d:127:ILE:HG22	16:d:129:THR:H	1.85	0.42
18:f:625:LYS:HA	18:f:657:ILE:HD11	2.01	0.42
1:A:184:ILE:O	1:A:188:ARG:HB2	2.19	0.42
1:A:411:GLU:O	1:A:415:LYS:HB2	2.19	0.42
6:F:362:ARG:NH1	6:F:396:CYS:SG	2.93	0.42
7:U:899:ARG:NH2	7:U:918:SER:OG	2.52	0.42
11:Y:297:ARG:HH12	17:e:44:ASP:C	2.27	0.42
13:a:364:GLU:O	13:a:368:GLU:HB3	2.20	0.42
15:c:259:VAL:HG11	15:c:287:HIS:HE1	1.83	0.42
18:f:242:GLU:N	18:f:243:PRO:HD2	2.35	0.42
18:f:262:PHE:HB3	18:f:281:ILE:HD11	2.02	0.42
18:f:481:SER:O	18:f:485:LEU:CB	2.67	0.42
2:B:387:LYS:HG2	2:B:388:ASP:N	2.32	0.42
9:W:408:ARG:H	10:X:344:ARG:HE	1.67	0.42
13:a:112:ILE:H	13:a:112:ILE:HG13	1.46	0.42
13:a:112:ILE:O	13:a:116:THR:OG1	2.21	0.42
15:c:34:SER:HB3	15:c:208:ARG:CZ	2.49	0.42
16:d:150:LYS:O	16:d:154:ALA:CB	2.68	0.42
18:f:92:VAL:HB	18:f:93:PRO:HD3	2.01	0.42
18:f:184:LEU:HD23	18:f:184:LEU:H	1.85	0.42
18:f:605:ASN:N	18:f:605:ASN:OD1	2.52	0.42
18:f:605:ASN:OD1	18:f:608:LYS:HE3	2.20	0.42
8:V:360:TYR:CZ	8:V:363:LEU:HD11	2.55	0.42
11:Y:258:GLN:O	11:Y:262:SER:CB	2.68	0.42
13:a:214:GLY:O	13:a:218:MET:CB	2.61	0.42
13:a:290:GLN:HE22	13:a:332:HIS:HB2	1.83	0.42
18:f:82:ILE:O	18:f:86:THR:HG22	2.20	0.42
18:f:94:LYS:HA	18:f:97:LYS:HG2	2.00	0.42
1:A:397:ILE:O	1:A:400:ARG:NH1	2.53	0.42
8:V:268:GLU:HA	8:V:272:SER:HB3	2.02	0.42
8:V:338:LEU:HD22	8:V:401:ASN:HD22	1.84	0.42
8:V:360:TYR:CE1	8:V:363:LEU:HD11	2.55	0.42
10:X:243:ASP:HB3	10:X:246:LYS:HB2	2.01	0.42
14:b:84:ILE:HD12	14:b:115:SER:HB2	2.02	0.42
1:A:398:ARG:HH12	2:B:196:GLU:HA	1.85	0.42
2:B:251:VAL:HG13	2:B:285:ASP:HB3	2.02	0.42
14:b:20:ASP:OD1	14:b:21:PHE:N	2.53	0.42
14:b:157:VAL:HG21	14:b:170:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:d:175:ARG:O	16:d:179:ALA:HB3	2.20	0.42
1:A:407:LYS:HA	1:A:410:LEU:HD23	2.01	0.42
2:B:196:GLU:O	2:B:200:SER:HB2	2.20	0.42
4:D:249:ASP:HA	4:D:252:ARG:HG2	2.01	0.42
4:D:267:ILE:HD13	4:D:309:MET:SD	2.60	0.42
4:D:333:PHE:CD1	4:D:334:PRO:HD2	2.55	0.42
6:F:325:GLN:HG2	6:F:326:VAL:H	1.85	0.42
7:U:203:LYS:HA	7:U:206:MET:HE3	2.01	0.42
9:W:254:PRO:HA	9:W:262:LYS:HE2	2.01	0.42
17:e:45:ASP:O	17:e:49:GLU:HB2	2.20	0.42
18:f:253:LEU:HD12	18:f:277:LEU:HD12	2.01	0.42
2:B:111:THR:O	2:B:124:SER:N	2.53	0.41
2:B:220:LYS:HB3	2:B:348:ASP:HB2	2.01	0.41
2:B:269:GLU:HA	2:B:272:ARG:HG2	2.02	0.41
3:C:342:ILE:HG13	3:C:380:GLN:HB2	2.02	0.41
7:U:159:ARG:HB3	7:U:162:VAL:HB	2.00	0.41
8:V:363:LEU:O	8:V:367:VAL:HG23	2.20	0.41
13:a:136:GLU:HA	13:a:139:GLU:HG2	2.02	0.41
14:b:131:LEU:HD13	14:b:138:VAL:HG21	2.02	0.41
18:f:329:ASN:HA	18:f:332:ALA:HB3	2.01	0.41
4:D:72:PHE:O	4:D:76:GLN:HB2	2.20	0.41
6:F:90:VAL:HG13	6:F:150:LEU:HA	2.03	0.41
6:F:314:LEU:HD21	6:F:342:LEU:HD23	2.01	0.41
7:U:530:GLU:HA	7:U:533:VAL:HG12	2.01	0.41
7:U:604:HIS:O	7:U:608:SER:CB	2.68	0.41
2:B:115:ILE:HD12	2:B:146:PRO:HG3	2.03	0.41
3:C:191:PRO:HA	3:C:192:PRO:HD3	1.87	0.41
3:C:200:ALA:O	3:C:204:ALA:CB	2.68	0.41
4:D:391:ARG:NH2	4:D:395:LEU:H	2.18	0.41
6:F:88:TYR:CZ	6:F:89:LEU:HD23	2.54	0.41
7:U:458:ILE:HA	7:U:461:LEU:HB2	2.02	0.41
7:U:546:ARG:HE	7:U:771:PHE:HD2	1.67	0.41
9:W:179:LYS:HD2	9:W:217:GLU:HB2	2.03	0.41
9:W:362:ASN:OD1	9:W:363:ILE:N	2.53	0.41
11:Y:231:LEU:HD21	11:Y:239:LYS:HD2	2.03	0.41
1:A:171:ASP:OD1	1:A:171:ASP:N	2.50	0.41
1:A:210:LYS:NZ	1:A:313:GLY:O	2.38	0.41
1:A:401:ARG:HH12	1:A:404:ALA:HA	1.86	0.41
5:E:357:ALA:O	5:E:359:HIS:ND1	2.40	0.41
8:V:305:ALA:HA	8:V:308:THR:HG22	2.03	0.41
8:V:473:GLN:O	8:V:477:HIS:CB	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:224:VAL:O	11:Y:228:MET:CB	2.68	0.41
12:Z:202:ASN:OD1	12:Z:203:SER:N	2.53	0.41
14:b:134:GLU:HG3	14:b:136:VAL:HG23	2.00	0.41
15:c:29:GLU:O	15:c:175:ARG:NH2	2.50	0.41
4:D:217:LYS:HA	4:D:220:ALA:HB3	2.02	0.41
7:U:601:ARG:HA	7:U:604:HIS:HB3	2.02	0.41
10:X:192:SER:HA	10:X:195:THR:HG22	2.03	0.41
10:X:318:ILE:HD12	10:X:318:ILE:H	1.85	0.41
18:f:84:SER:HB2	18:f:92:VAL:HG13	2.03	0.41
1:A:328:ASP:HB3	1:A:329:PRO:HD3	2.02	0.41
3:C:25:LEU:HD11	4:D:47:LEU:HD23	2.01	0.41
3:C:100:ASP:OD1	3:C:100:ASP:N	2.52	0.41
4:D:176:GLU:O	4:D:180:ALA:HB3	2.20	0.41
6:F:134:LEU:HD22	6:F:158:TYR:O	2.21	0.41
6:F:298:SER:OG	6:F:304:ARG:NH1	2.53	0.41
7:U:134:VAL:O	7:U:138:PHE:CB	2.69	0.41
7:U:229:VAL:HA	7:U:232:ILE:HG12	2.02	0.41
7:U:255:SER:OG	7:U:256:ALA:N	2.54	0.41
8:V:495:ARG:C	8:V:498:PRO:HD2	2.45	0.41
10:X:220:ALA:HA	10:X:322:HIS:HE2	1.85	0.41
11:Y:16:ASP:O	11:Y:20:ALA:HB3	2.20	0.41
12:Z:61:ASP:OD2	14:b:91:ARG:NH1	2.52	0.41
15:c:267:PRO:O	15:c:271:ALA:HB2	2.19	0.41
18:f:282:PHE:HD1	18:f:282:PHE:HA	1.74	0.41
18:f:790:GLN:HG3	18:f:791:VAL:H	1.85	0.41
11:Y:285:ASP:H	11:Y:289:ALA:HB2	1.84	0.41
18:f:324:VAL:C	18:f:326:LEU:H	2.27	0.41
1:A:180:CYS:SG	1:A:183:GLN:HB2	2.61	0.41
7:U:472:ILE:HD12	7:U:473:VAL:HG23	2.02	0.41
18:f:403:LYS:O	18:f:407:MET:N	2.53	0.41
1:A:83:ASP:O	1:A:86:THR:OG1	2.31	0.41
1:A:297:ARG:O	1:A:301:GLU:HB3	2.20	0.41
2:B:110:GLY:HA3	2:B:152:LEU:HD13	2.02	0.41
5:E:221:TYR:O	5:E:225:HIS:HB2	2.21	0.41
7:U:559:ARG:HB3	7:U:562:GLU:HB3	2.02	0.41
8:V:313:LEU:HD13	8:V:332:LEU:HD22	2.03	0.41
11:Y:188:CYS:HA	11:Y:191:ILE:HG22	2.03	0.41
11:Y:233:ARG:HB2	11:Y:234:PRO:HD3	2.02	0.41
12:Z:262:LEU:O	12:Z:266:ILE:HB	2.21	0.41
13:a:364:GLU:O	13:a:368:GLU:CB	2.69	0.41
14:b:119:ASP:HB3	14:b:123:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:f:501:LEU:HD22	18:f:518:THR:HG23	2.03	0.41
18:f:607:LEU:HG	18:f:610:GLN:HE21	1.86	0.41
5:E:300:HIS:NE2	9:W:93:ARG:HA	2.36	0.41
6:F:73:ILE:O	6:F:77:SER:CB	2.69	0.41
7:U:219:CYS:SG	7:U:220:LEU:N	2.93	0.41
7:U:567:ILE:O	7:U:571:CYS:HB2	2.21	0.41
7:U:592:GLY:HA2	7:U:628:ARG:HE	1.85	0.41
7:U:740:GLY:HA3	7:U:744:VAL:HG22	2.03	0.41
11:Y:224:VAL:O	11:Y:228:MET:HB2	2.21	0.41
11:Y:382:LYS:O	11:Y:386:VAL:HG23	2.21	0.41
13:a:279:GLU:O	13:a:283:THR:OG1	2.25	0.41
15:c:251:LEU:HA	15:c:254:ASN:HD22	1.86	0.41
16:d:179:ALA:HA	16:d:182:ILE:HG22	2.03	0.41
18:f:80:ARG:HB3	18:f:95:PRO:HB2	2.03	0.41
18:f:557:TRP:HE1	18:f:786:GLN:HB2	1.86	0.41
1:A:108:ASP:CG	1:A:109:PRO:HD3	2.47	0.40
2:B:218:PRO:O	2:B:326:LYS:NZ	2.54	0.40
8:V:353:LEU:O	8:V:357:LEU:HB2	2.21	0.40
9:W:220:GLU:O	9:W:221:LYS:CB	2.70	0.40
9:W:308:LEU:HD23	9:W:312:MET:HE2	2.03	0.40
15:c:58:LEU:HA	15:c:108:VAL:HA	2.01	0.40
18:f:87:THR:O	18:f:88:SER:OG	2.37	0.40
3:C:84:LYS:HG2	3:C:96:VAL:HG22	2.03	0.40
3:C:325:ARG:O	3:C:329:LEU:CB	2.68	0.40
5:E:53:VAL:HG11	6:F:157:SER:HB2	2.04	0.40
7:U:765:VAL:HG11	7:U:778:PHE:HD2	1.86	0.40
9:W:137:TYR:HE2	9:W:141:GLU:H	1.69	0.40
9:W:243:ILE:HA	9:W:246:HIS:HB3	2.02	0.40
9:W:343:SER:HB2	9:W:346:GLU:HB3	2.03	0.40
9:W:396:LEU:HA	9:W:399:ASN:HB3	2.03	0.40
13:a:172:TYR:O	13:a:176:ALA:CB	2.67	0.40
14:b:4:GLU:H	14:b:47:ASN:ND2	2.19	0.40
1:A:173:THR:HG23	1:A:175:SER:H	1.86	0.40
7:U:436:ALA:HB1	7:U:472:ILE:HG12	2.03	0.40
8:V:268:GLU:HG2	8:V:269:LYS:N	2.37	0.40
8:V:334:VAL:HG22	8:V:360:TYR:CZ	2.56	0.40
11:Y:344:HIS:CD2	11:Y:358:ARG:HG3	2.57	0.40
12:Z:231:GLN:NE2	13:a:345:GLN:HB3	2.37	0.40
1:A:123:VAL:HA	6:F:86:LEU:HD13	2.04	0.40
4:D:235:PHE:CE2	4:D:285:VAL:HB	2.56	0.40
6:F:241:ALA:O	6:F:244:THR:OG1	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:442:ILE:HD11	8:V:449:ALA:HB3	2.03	0.40
10:X:420:LYS:HZ3	12:Z:280:ILE:HG23	1.86	0.40
13:a:220:PRO:HA	13:a:223:GLU:HG2	2.03	0.40
13:a:277:LEU:O	13:a:280:MET:HG2	2.22	0.40
16:d:171:LEU:HA	16:d:174:ILE:HG12	2.04	0.40
1:A:400:ARG:CZ	2:B:203:LEU:HD13	2.51	0.40
3:C:114:VAL:HG11	3:C:123:LEU:HD11	2.04	0.40
7:U:264:VAL:HG22	7:U:268:LEU:HD13	2.04	0.40
7:U:612:ASP:OD1	7:U:645:ASN:ND2	2.55	0.40
11:Y:117:LYS:O	11:Y:121:LEU:CB	2.55	0.40
18:f:746:ARG:O	18:f:750:GLN:HG3	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	332/352 (94%)	299 (90%)	33 (10%)	0	100	100
2	B	311/341 (91%)	271 (87%)	40 (13%)	0	100	100
3	C	343/385 (89%)	323 (94%)	20 (6%)	0	100	100
4	D	326/368 (89%)	315 (97%)	11 (3%)	0	100	100
5	E	307/379 (81%)	290 (94%)	17 (6%)	0	100	100
6	F	333/380 (88%)	311 (93%)	22 (7%)	0	100	100
7	U	743/935 (80%)	716 (96%)	27 (4%)	0	100	100
8	V	260/488 (53%)	237 (91%)	23 (9%)	0	100	100
9	W	387/456 (85%)	359 (93%)	26 (7%)	2 (0%)	24	63
10	X	276/385 (72%)	269 (98%)	7 (2%)	0	100	100
11	Y	376/378 (100%)	359 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Z	284/286 (99%)	272 (96%)	12 (4%)	0	100	100
13	a	372/374 (100%)	351 (94%)	21 (6%)	0	100	100
14	b	189/191 (99%)	175 (93%)	14 (7%)	0	100	100
15	c	285/287 (99%)	277 (97%)	8 (3%)	0	100	100
16	d	174/257 (68%)	160 (92%)	14 (8%)	0	100	100
17	e	31/33 (94%)	28 (90%)	3 (10%)	0	100	100
18	f	616/784 (79%)	556 (90%)	60 (10%)	0	100	100
All	All	5945/7059 (84%)	5568 (94%)	375 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	W	221	LYS
9	W	222	LEU

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	293/300 (98%)	288 (98%)	5 (2%)	53	69
2	B	276/298 (93%)	272 (99%)	4 (1%)	59	72
3	C	302/333 (91%)	300 (99%)	2 (1%)	76	81
4	D	290/321 (90%)	288 (99%)	2 (1%)	76	81
5	E	273/333 (82%)	271 (99%)	2 (1%)	76	81
6	F	291/326 (89%)	289 (99%)	2 (1%)	76	81
7	U	639/798 (80%)	635 (99%)	4 (1%)	78	83
8	V	231/422 (55%)	231 (100%)	0	100	100
9	W	361/416 (87%)	359 (99%)	2 (1%)	78	83
10	X	243/331 (73%)	241 (99%)	2 (1%)	73	80
11	Y	334/334 (100%)	333 (100%)	1 (0%)	86	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Z	257/257 (100%)	256 (100%)	1 (0%)	84	84
13	a	334/334 (100%)	331 (99%)	3 (1%)	70	79
14	b	167/167 (100%)	167 (100%)	0	100	100
15	c	252/252 (100%)	252 (100%)	0	100	100
16	d	158/231 (68%)	155 (98%)	3 (2%)	50	67
17	e	31/31 (100%)	30 (97%)	1 (3%)	34	56
18	f	538/660 (82%)	527 (98%)	11 (2%)	48	66
All	All	5270/6144 (86%)	5225 (99%)	45 (1%)	68	79

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	LEU
1	A	108	ASP
1	A	317	VAL
1	A	403	ILE
1	A	416	VAL
2	B	190	LEU
2	B	260	LEU
2	B	355	LEU
2	B	387	LYS
3	C	219	LEU
3	C	311	ILE
4	D	116	LEU
4	D	370	ILE
5	E	22	ILE
5	E	326	ILE
6	F	85	THR
6	F	204	LEU
7	U	252	LEU
7	U	353	LEU
7	U	427	LEU
7	U	629	THR
9	W	159	VAL
9	W	211	THR
10	X	339	ILE
10	X	369	ILE
11	Y	343	LEU
12	Z	91	ILE
13	a	32	LYS

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Mol	Chain	Res	Type
13	a	112	ILE
13	a	340	VAL
16	d	189	ILE
16	d	190	LEU
16	d	197	ILE
17	e	56	LEU
18	f	75	LEU
18	f	188	VAL
18	f	282	PHE
18	f	325	GLN
18	f	353	LEU
18	f	391	LEU
18	f	403	LYS
18	f	460	ASP
18	f	470	VAL
18	f	583	VAL
18	f	745	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
1	A	293	ASN
1	A	353	HIS
2	B	131	HIS
2	B	193	GLN
3	C	22	GLN
3	C	50	ASN
3	C	270	GLN
3	C	278	ASN
3	C	296	ASN
4	D	65	GLN
4	D	74	HIS
4	D	133	HIS
4	D	221	HIS
5	E	55	GLN
5	E	262	ASN
5	E	263	GLN
5	E	316	HIS
5	E	364	GLN
6	F	83	ASN
6	F	316	GLN

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Mol	Chain	Res	Type
6	F	323	ASN
6	F	374	ASN
7	U	139	GLN
7	U	247	GLN
7	U	259	GLN
7	U	340	GLN
7	U	373	ASN
7	U	415	HIS
7	U	438	GLN
7	U	450	HIS
7	U	464	GLN
7	U	743	ASN
7	U	754	HIS
7	U	801	GLN
8	V	329	HIS
8	V	477	HIS
8	V	488	ASN
9	W	257	GLN
9	W	288	HIS
9	W	395	ASN
10	X	406	ASN
11	Y	136	HIS
11	Y	178	ASN
11	Y	251	HIS
11	Y	306	GLN
11	Y	365	GLN
12	Z	189	GLN
12	Z	194	GLN
12	Z	229	GLN
12	Z	231	GLN
12	Z	273	HIS
12	Z	282	ASN
13	a	35	HIS
13	a	129	GLN
13	a	152	HIS
13	a	241	ASN
13	a	290	GLN
13	a	332	HIS
14	b	12	ASN
14	b	29	GLN
14	b	34	ASN
14	b	76	HIS

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Mol	Chain	Res	Type
15	c	183	HIS
15	c	194	HIS
15	c	241	ASN
15	c	254	ASN
15	c	256	ASN
15	c	283	HIS
18	f	102	HIS
18	f	180	GLN
18	f	273	ASN
18	f	301	HIS
18	f	325	GLN
18	f	327	ASN
18	f	493	ASN
18	f	540	GLN
18	f	565	ASN
18	f	610	GLN
18	f	752	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	3.20

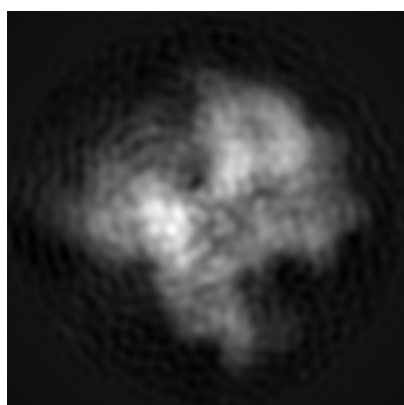
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8684. These allow visual inspection of the internal detail of the map and identification of artifacts.

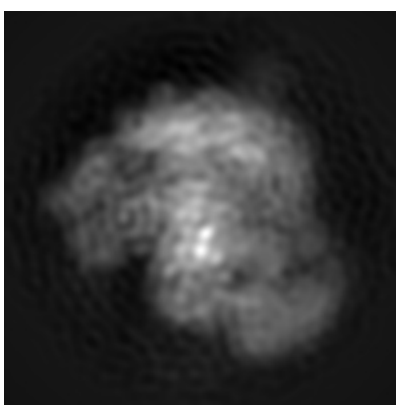
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

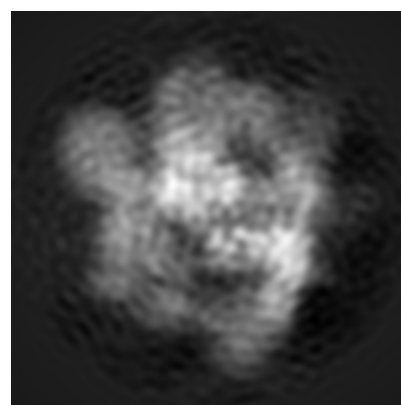
6.1.1 Primary map



X



Y

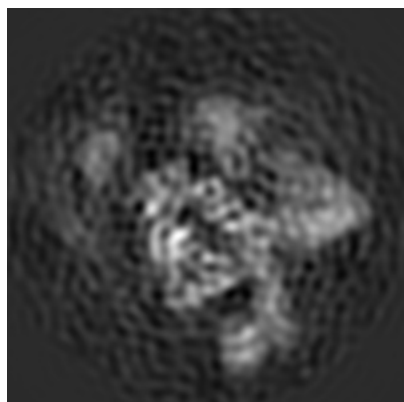


Z

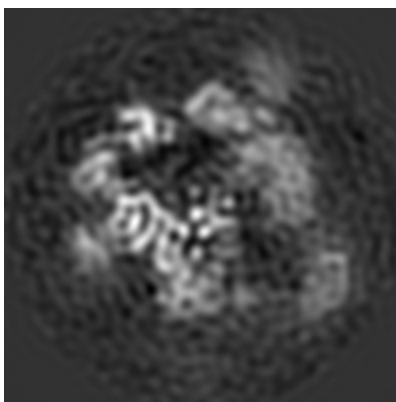
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

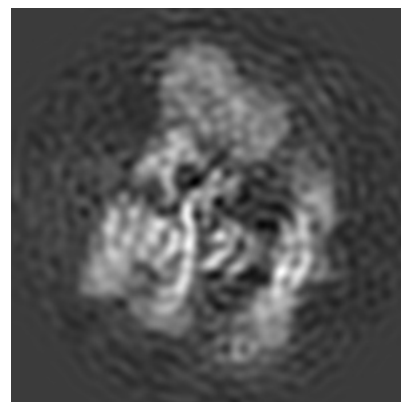
6.2.1 Primary map



X Index: 150



Y Index: 150

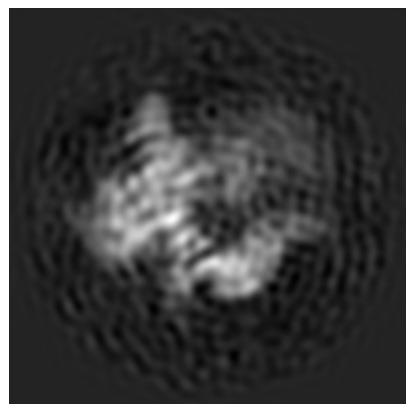


Z Index: 150

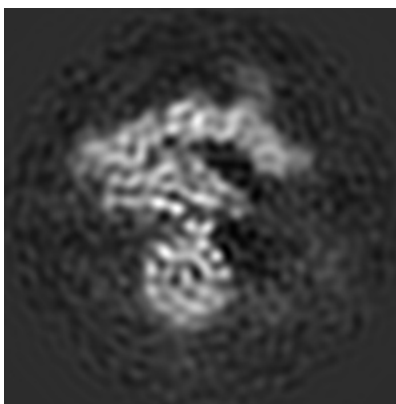
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

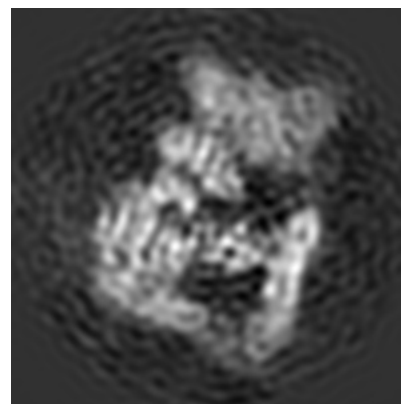
6.3.1 Primary map



X Index: 209



Y Index: 128

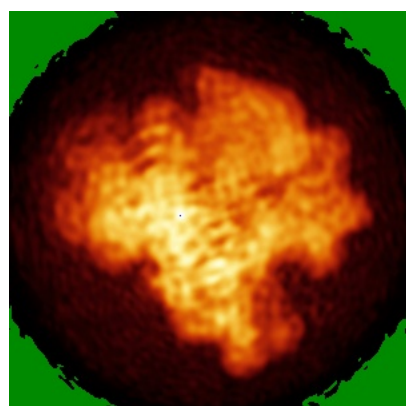


Z Index: 135

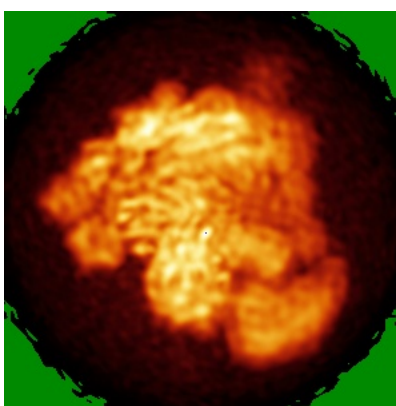
The images above show the largest variance slices of the map in three orthogonal directions.

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

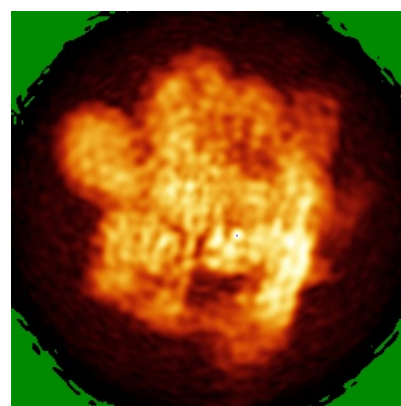
6.4.1 Primary map



X



Y

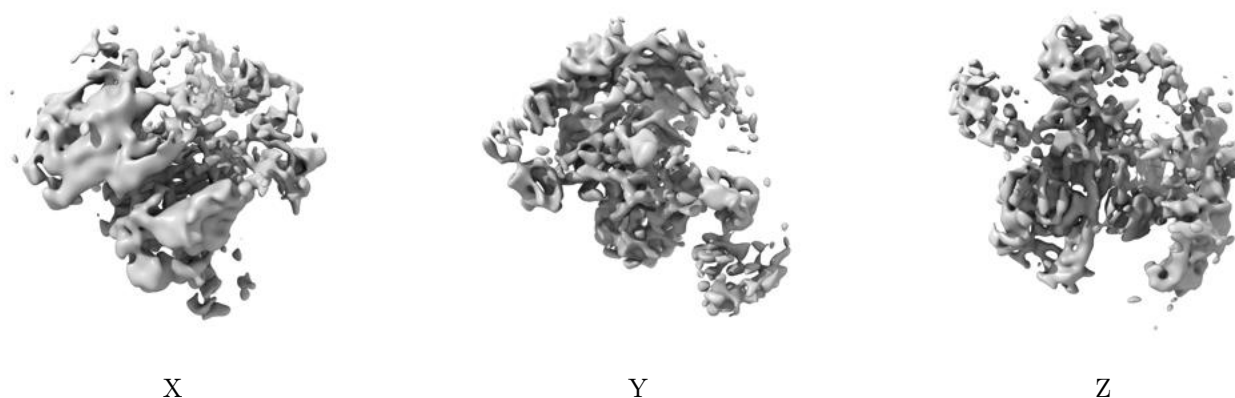


Z

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.

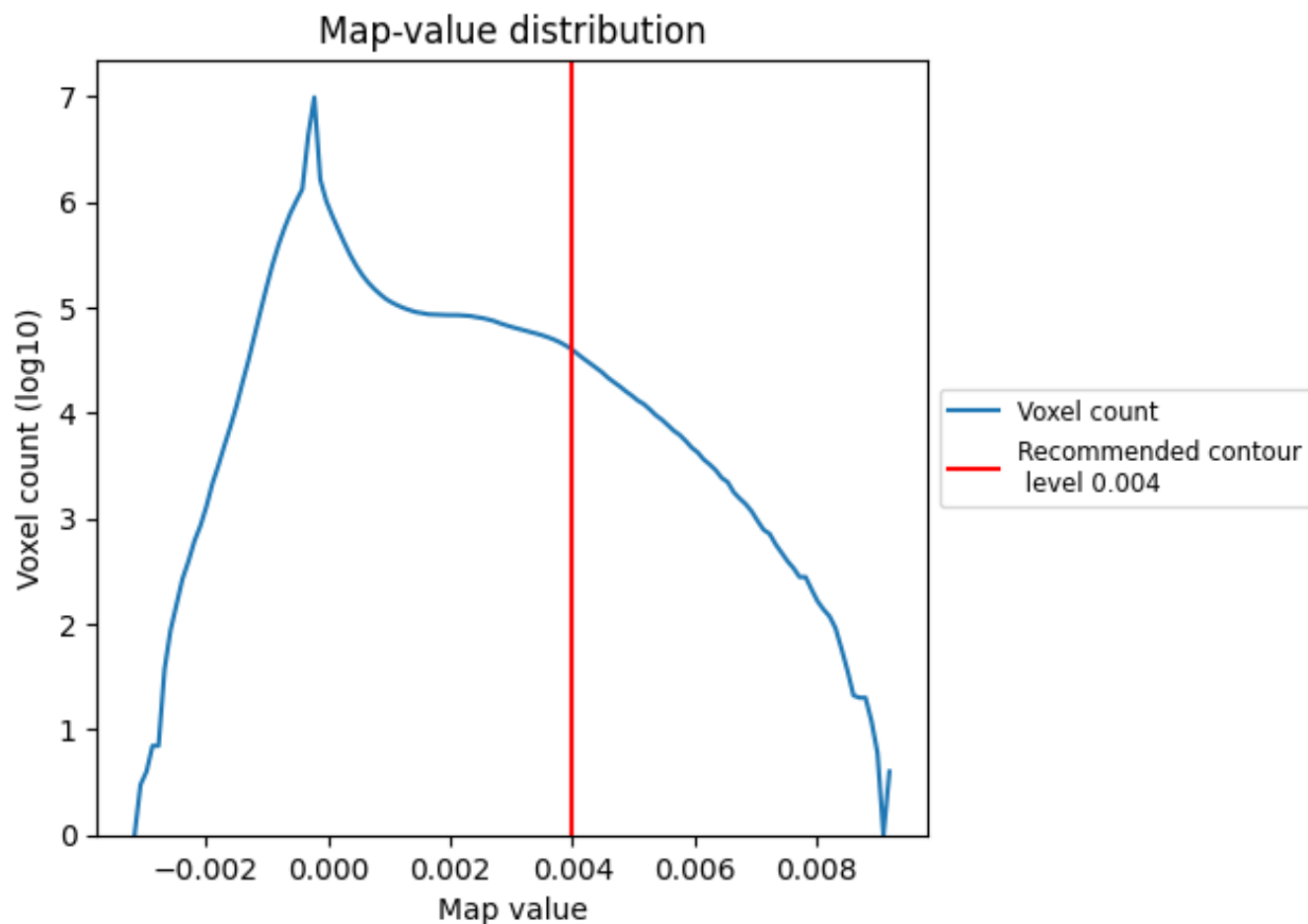
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

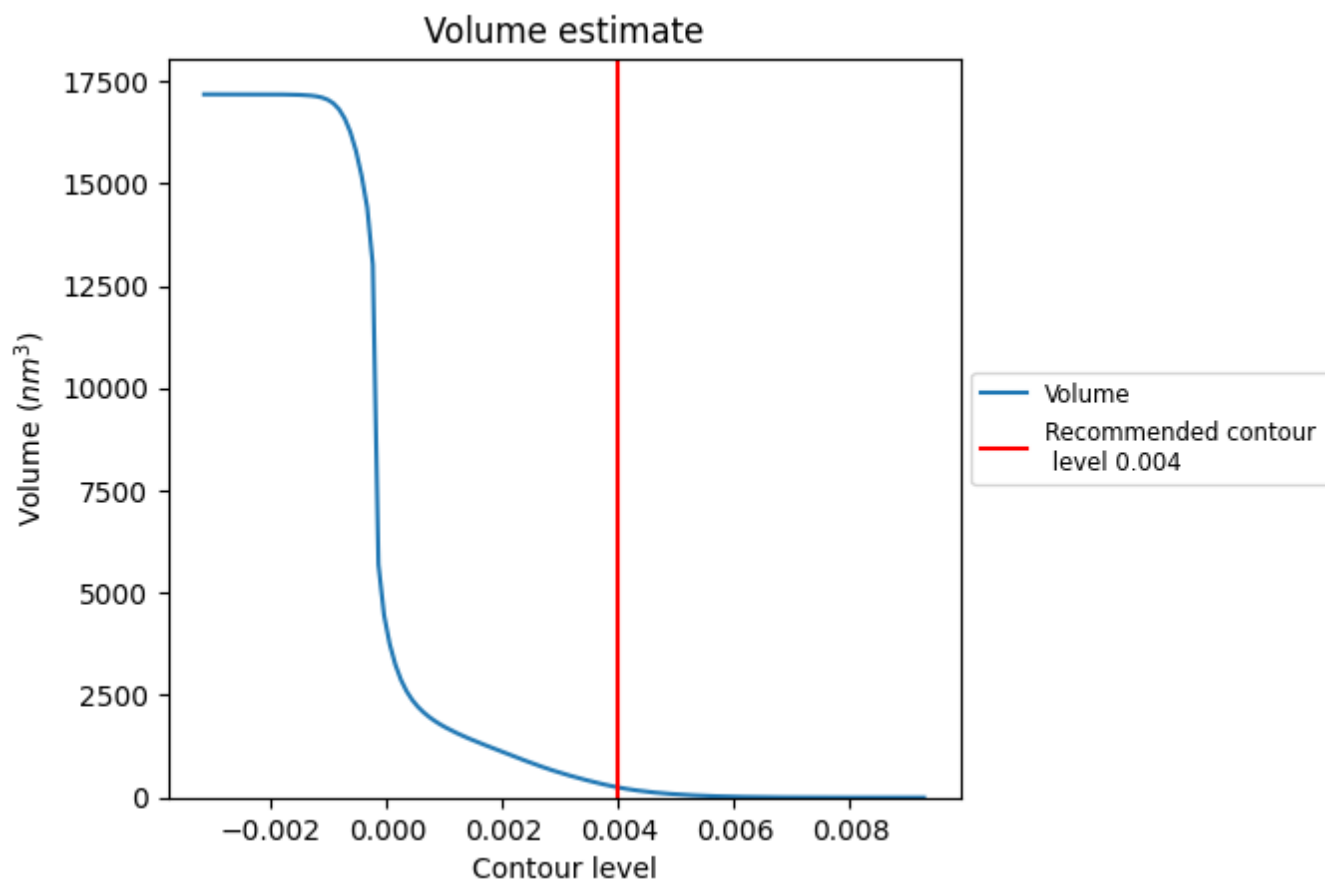
This section contains the results of statistical analysis of the map.

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.

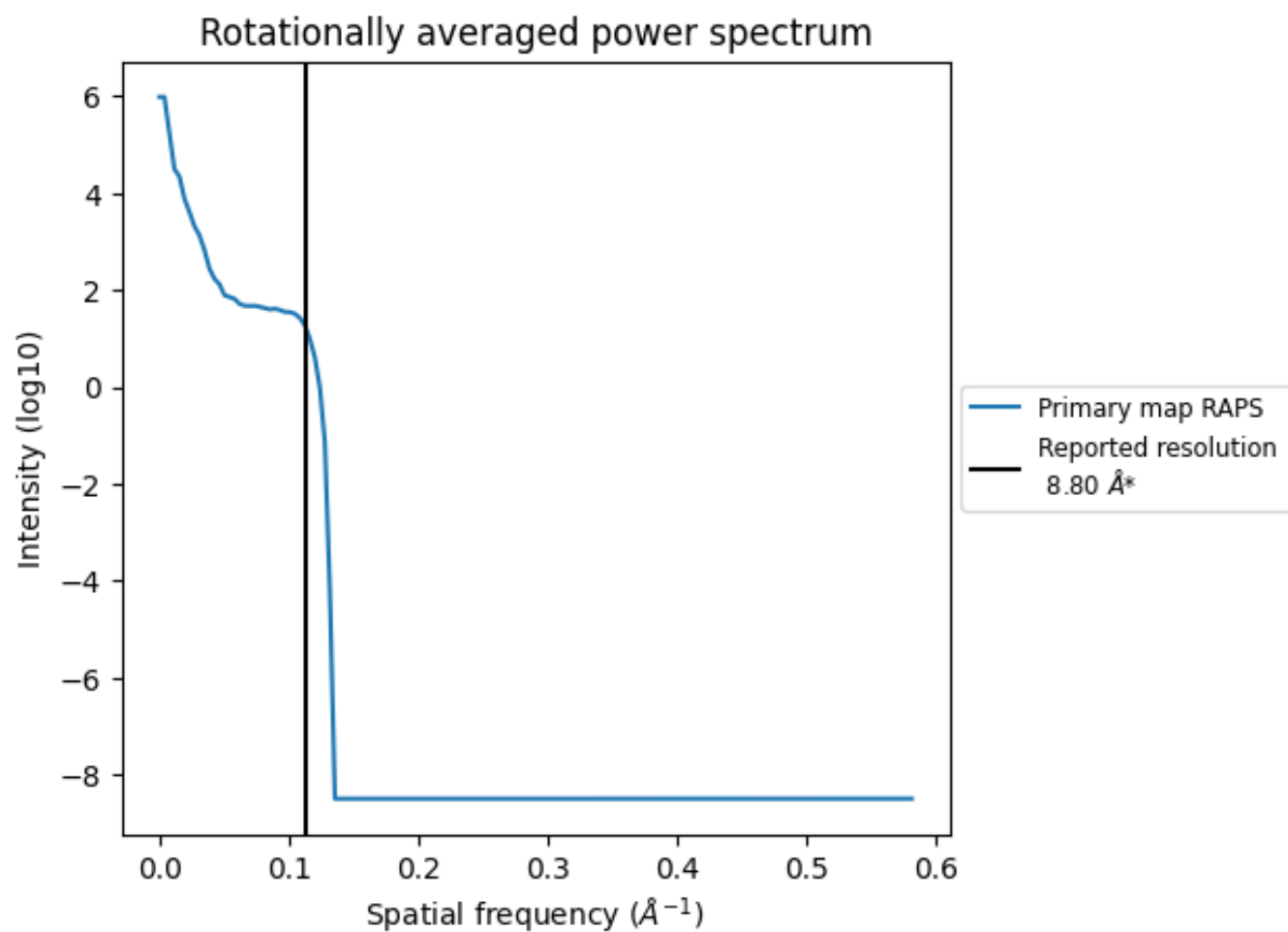
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 248 nm³; this corresponds to an approximate mass of 224 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 0.114 Å⁻¹

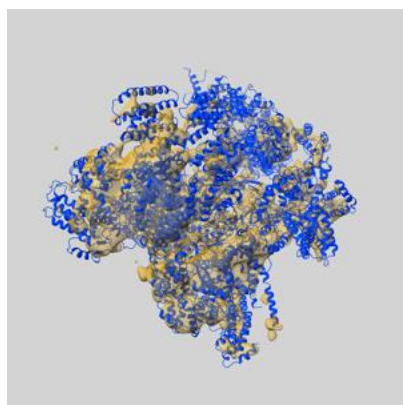
8 Fourier-Shell correlation

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

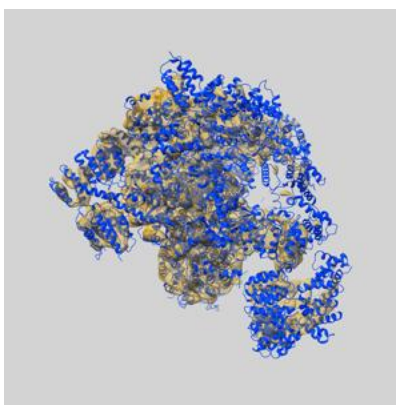
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8684 and PDB model 5VHS. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

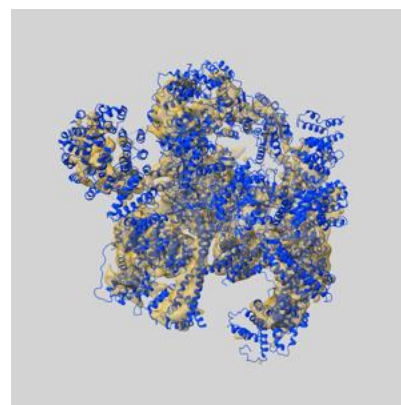
9.1 Map-model overlay [i](#)



X



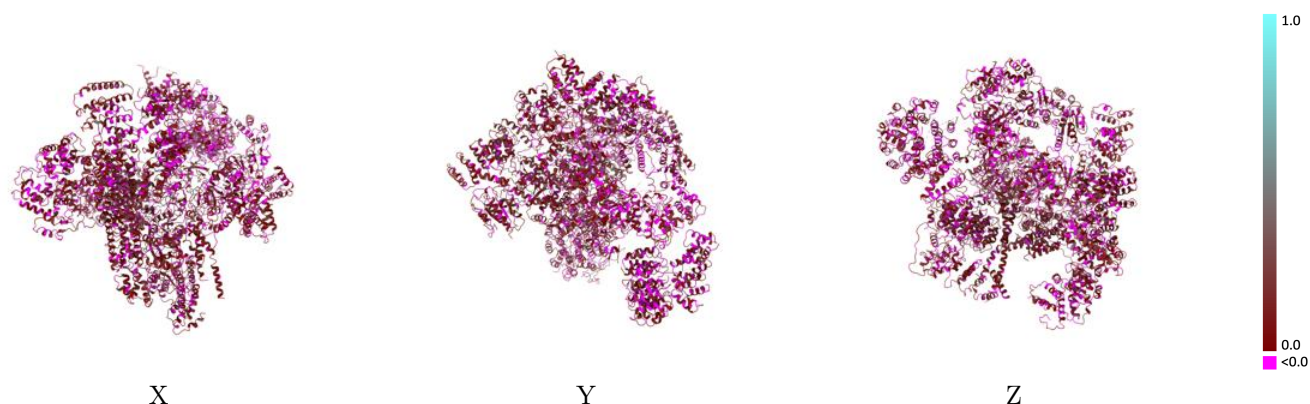
Y



Z

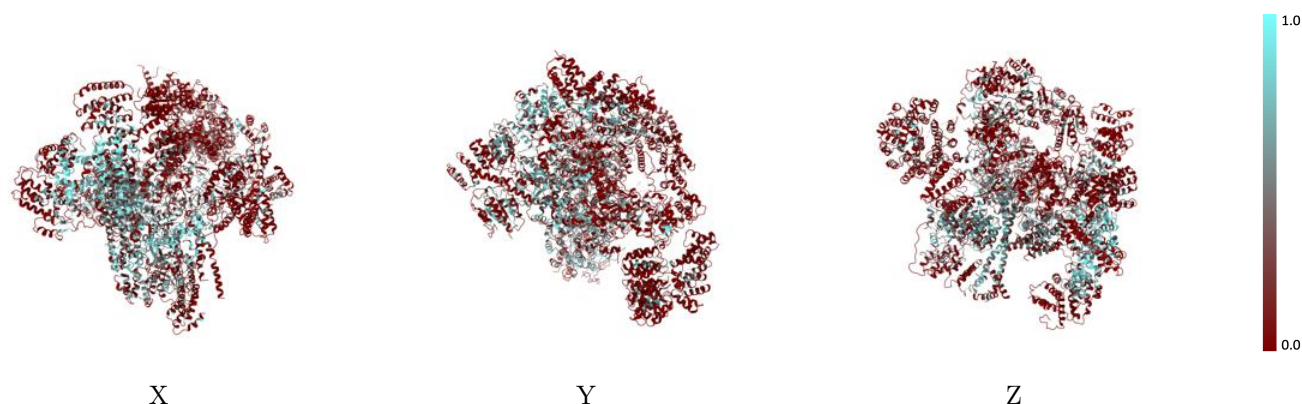
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



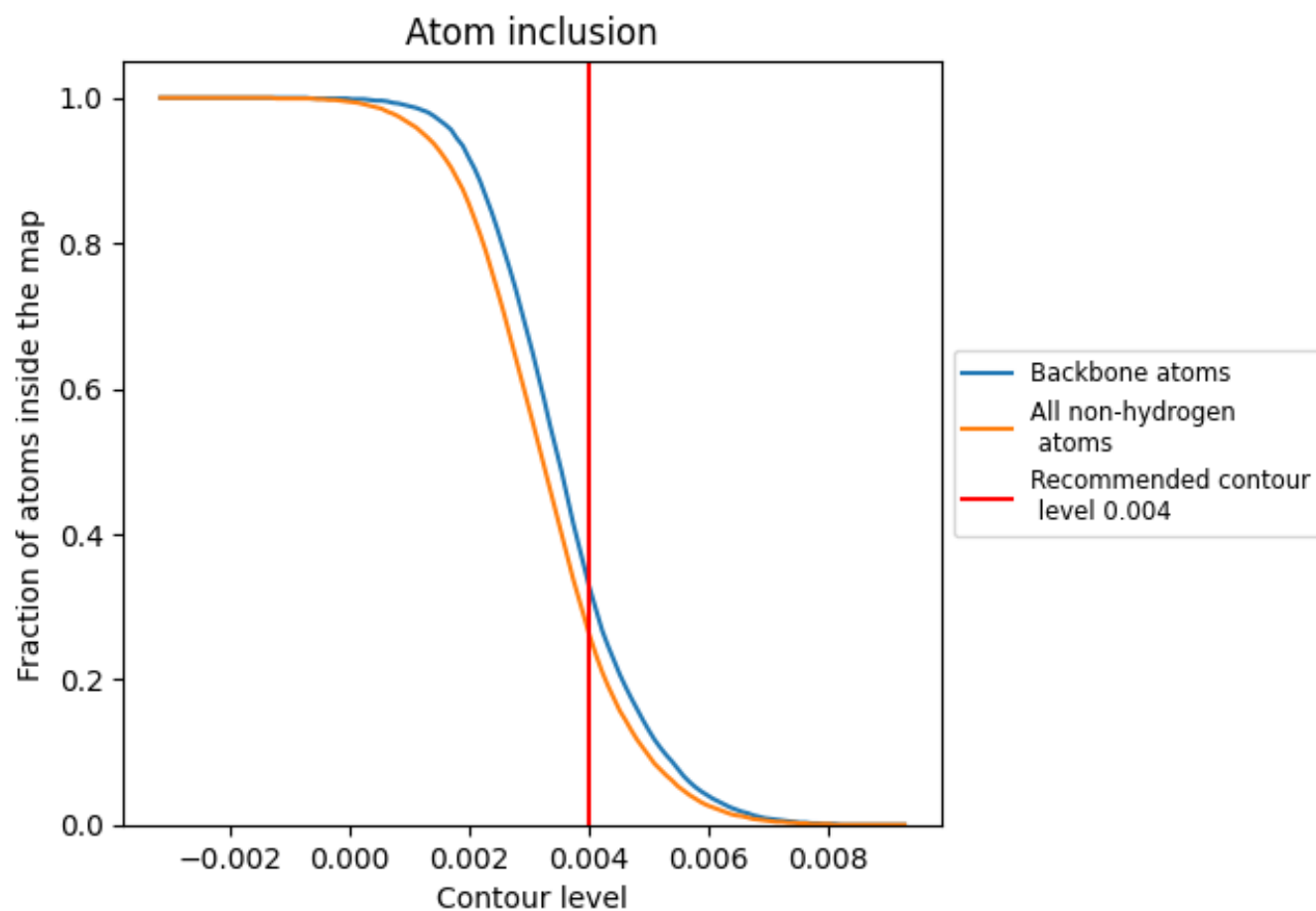
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 33% of all backbone atoms, 26% 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	 0.2640	 0.0810
A	 0.2060	 0.0660
B	 0.1870	 0.0520
C	 0.1350	 0.0890
D	 0.1710	 0.0710
E	 0.1210	 0.0800
F	 0.1970	 0.0870
U	 0.3520	 0.0840
V	 0.3630	 0.0530
W	 0.3720	 0.1050
X	 0.2600	 0.0780
Y	 0.4020	 0.0940
Z	 0.4240	 0.1220
a	 0.3310	 0.1080
b	 0.2460	 0.0840
c	 0.4200	 0.1130
d	 0.1420	 0.0550
e	 0.5290	 0.1110
f	 0.1040	 0.0460

