Full wwPDB EM Validation Report ⓘ

Sep 17, 2024 – 03:14 pm BST

PDB ID	:	9GBK
EMDB ID	:	EMD-51221
Title	:	Blm10-20S proteasome complex from pre1-1
Authors	:	Mark, E.; Ramos, P.C.; Kayser, F.; Hoeckendorff, J.; Dohmen, R.J.; Wendler, P.
Deposited on	:	2024-07-31
Resolution	:	2.39 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:

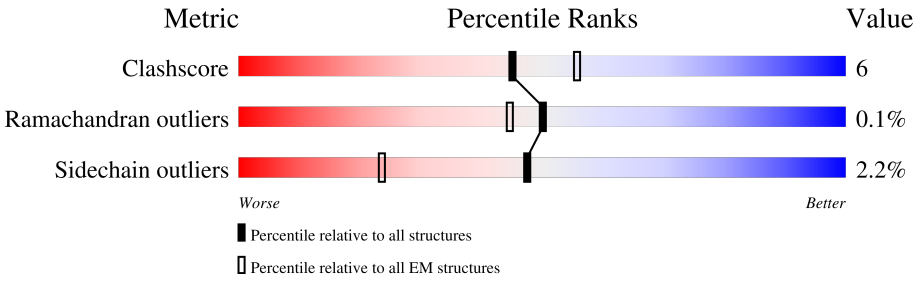
EMDB validation analysis	:	0.0.1.dev112
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 2.39 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	1	222	82% 17%
1	M	222	82% 16%
2	2	233	83% 15%
2	N	233	80% 18%
3	3	2143	5% 74% 13% 13%
4	A	252	85% 10% 5%
4	O	252	8% 73% 20% 6%
5	B	250	80% 13% 7%

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Mol	Chain	Length	Quality of chain
5	P	250	16% 84% 12%
6	C	258	15% 74% 14% 12%
6	Q	258	5% 45% 7% 48%
7	D	254	25% 65% 19% 15%
7	R	254	23% 70% 19% 11%
8	E	260	10% 70% 14% 15%
8	S	260	12% 77% 16% 7%
9	F	234	77% 20%
9	T	234	83% 15%
10	G	288	64% 11% 25%
10	U	288	67% 16% 17%
11	H	196	84% 16%
11	V	196	78% 19%
12	I	232	78% 16% 5%
12	W	232	71% 21% 7%
13	J	205	82% 15%
13	X	205	79% 19%
14	K	212	68% 19% 11%
14	Y	212	8% 75% 16% 9%
15	L	212	86% 13%
15	Z	212	84% 15%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 64984 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 Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	221	Total	C	N	O	S	0	0
			1747	1110	301	332	4		
1	M	220	Total	C	N	O	S	0	0
			1739	1106	300	329	4		

- Molecule 2 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		
2	N	228	Total	C	N	O	S	0	0
			1786	1131	305	343	7		

- Molecule 3 is a protein called Proteasome activator BLM10.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	1875	Total	C	N	O	S	0	0
			15248	9825	2526	2827	70		

- Molecule 4 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	240	Total	C	N	O	S	0	0
			1903	1212	319	364	8		
4	O	236	Total	C	N	O	S	0	0
			1869	1191	313	357	8		

- Molecule 5 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	233	Total	C	N	O	S	0	0
			1780	1134	294	349	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	242	Total 1852	C 1179	N 306	O 363	S 4	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	228	Total 1773	C 1122	N 296	O 352	S 3	0	0
6	Q	133	Total 1059	C 674	N 183	O 201	S 1	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	217	Total 1716	C 1070	N 302	O 341	S 3	0	0
7	R	225	Total 1766	C 1104	N 306	O 352	S 4	0	0

- Molecule 8 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	220	Total 1703	C 1070	N 286	O 340	S 7	0	0
8	S	242	Total 1861	C 1162	N 314	O 378	S 7	0	0

- Molecule 9 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	230	Total 1777	C 1117	N 308	O 347	S 5	1	0
9	T	231	Total 1772	C 1114	N 307	O 347	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	217	Total 1692	C 1076	N 296	O 317	S 3	0	0
10	U	238	Total 1861	C 1185	N 323	O 349	S 4	0	0

- Molecule 11 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	196	Total	C	N	O	S	0	0
			1511	955	250	299	7		
11	V	195	Total	C	N	O	S	0	0
			1503	949	249	298	7		

- Molecule 12 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	221	Total	C	N	O	S	0	0
			1676	1057	292	320	7		
12	W	215	Total	C	N	O	S	0	0
			1633	1030	285	312	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	201	Total	C	N	O	S	0	0
			1559	998	255	298	8		
13	X	203	Total	C	N	O	S	0	0
			1574	1007	257	302	8		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	188	Total	C	N	O	S	0	0
			1511	961	254	290	6		
14	Y	193	Total	C	N	O	S	0	0
			1554	990	262	296	6		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	142	PHE	SER	engineered mutation	UNP P22141
K	199	ASP	-	expression tag	UNP P22141
K	200	TYR	-	expression tag	UNP P22141
K	201	LYS	-	expression tag	UNP P22141
K	202	ASP	-	expression tag	UNP P22141
K	203	ASP	-	expression tag	UNP P22141
K	204	ASP	-	expression tag	UNP P22141
K	205	ASP	-	expression tag	UNP P22141
K	206	LYS	-	expression tag	UNP P22141

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Chain	Residue	Modelled	Actual	Comment	Reference
K	207	HIS	-	expression tag	UNP P22141
K	208	HIS	-	expression tag	UNP P22141
K	209	HIS	-	expression tag	UNP P22141
K	210	HIS	-	expression tag	UNP P22141
K	211	HIS	-	expression tag	UNP P22141
K	212	HIS	-	expression tag	UNP P22141
Y	142	PHE	SER	engineered mutation	UNP P22141
Y	199	ASP	-	expression tag	UNP P22141
Y	200	TYR	-	expression tag	UNP P22141
Y	201	LYS	-	expression tag	UNP P22141
Y	202	ASP	-	expression tag	UNP P22141
Y	203	ASP	-	expression tag	UNP P22141
Y	204	ASP	-	expression tag	UNP P22141
Y	205	ASP	-	expression tag	UNP P22141
Y	206	LYS	-	expression tag	UNP P22141
Y	207	HIS	-	expression tag	UNP P22141
Y	208	HIS	-	expression tag	UNP P22141
Y	209	HIS	-	expression tag	UNP P22141
Y	210	HIS	-	expression tag	UNP P22141
Y	211	HIS	-	expression tag	UNP P22141
Y	212	HIS	-	expression tag	UNP P22141

- Molecule 15 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	212	Total	C	N	O	S	0	0
			1643	1045	280	311	7		
15	Z	212	Total	C	N	O	S	0	0
			1643	1045	280	311	7		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		AltConf
16	1	75	Total	O	0
			75	75	
16	2	85	Total	O	0
			85	85	
16	3	685	Total	O	0
			685	685	
16	A	98	Total	O	0
			98	98	
16	B	57	Total	O	0
			57	57	

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Mol	Chain	Residues	Atoms	AltConf
16	C	58	Total O 58 58	0
16	D	78	Total O 78 78	0
16	E	80	Total O 80 80	0
16	F	55	Total O 55 55	0
16	G	56	Total O 56 56	0
16	H	49	Total O 49 49	0
16	I	70	Total O 70 70	0
16	J	56	Total O 56 56	0
16	K	46	Total O 46 46	0
16	L	55	Total O 55 55	0
16	M	63	Total O 63 63	0
16	N	74	Total O 74 74	0
16	O	70	Total O 70 70	0
16	P	56	Total O 56 56	0
16	Q	37	Total O 37 37	0
16	R	79	Total O 79 79	0
16	S	76	Total O 76 76	0
16	T	61	Total O 61 61	0
16	U	82	Total O 82 82	0
16	V	43	Total O 43 43	0
16	W	64	Total O 64 64	0

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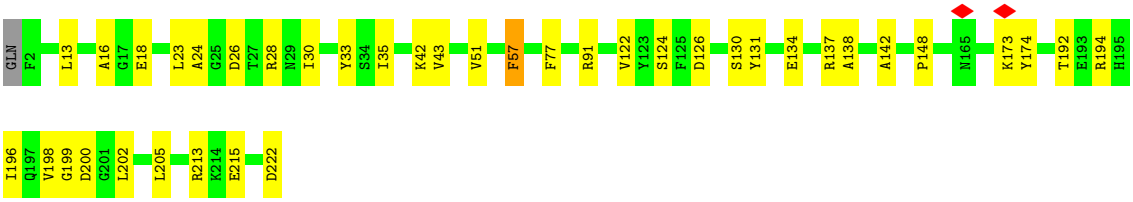
Mol	Chain	Residues	Atoms	AltConf
16	X	43	Total O 43 43	0
16	Y	75	Total O 75 75	0
16	Z	57	Total O 57 57	0

3 Residue-property plots (i)

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

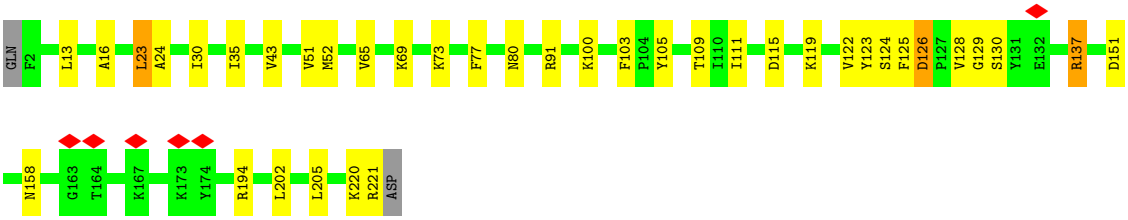
• Molecule 1: Proteasome subunit beta type-6

Chain 1:



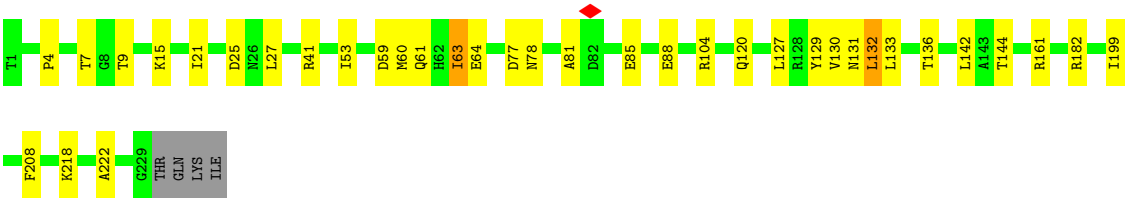
• Molecule 1: Proteasome subunit beta type-6

Chain M:



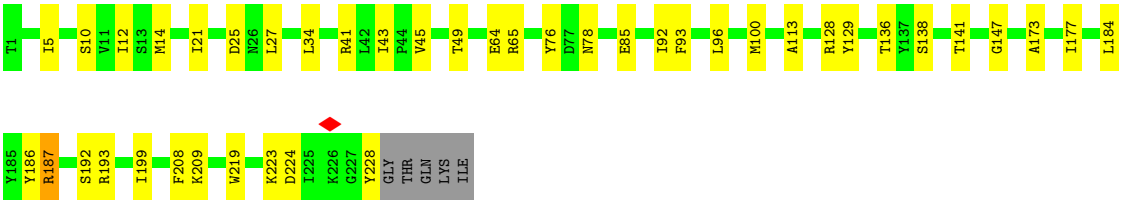
• Molecule 2: Proteasome subunit beta type-7

Chain 2:

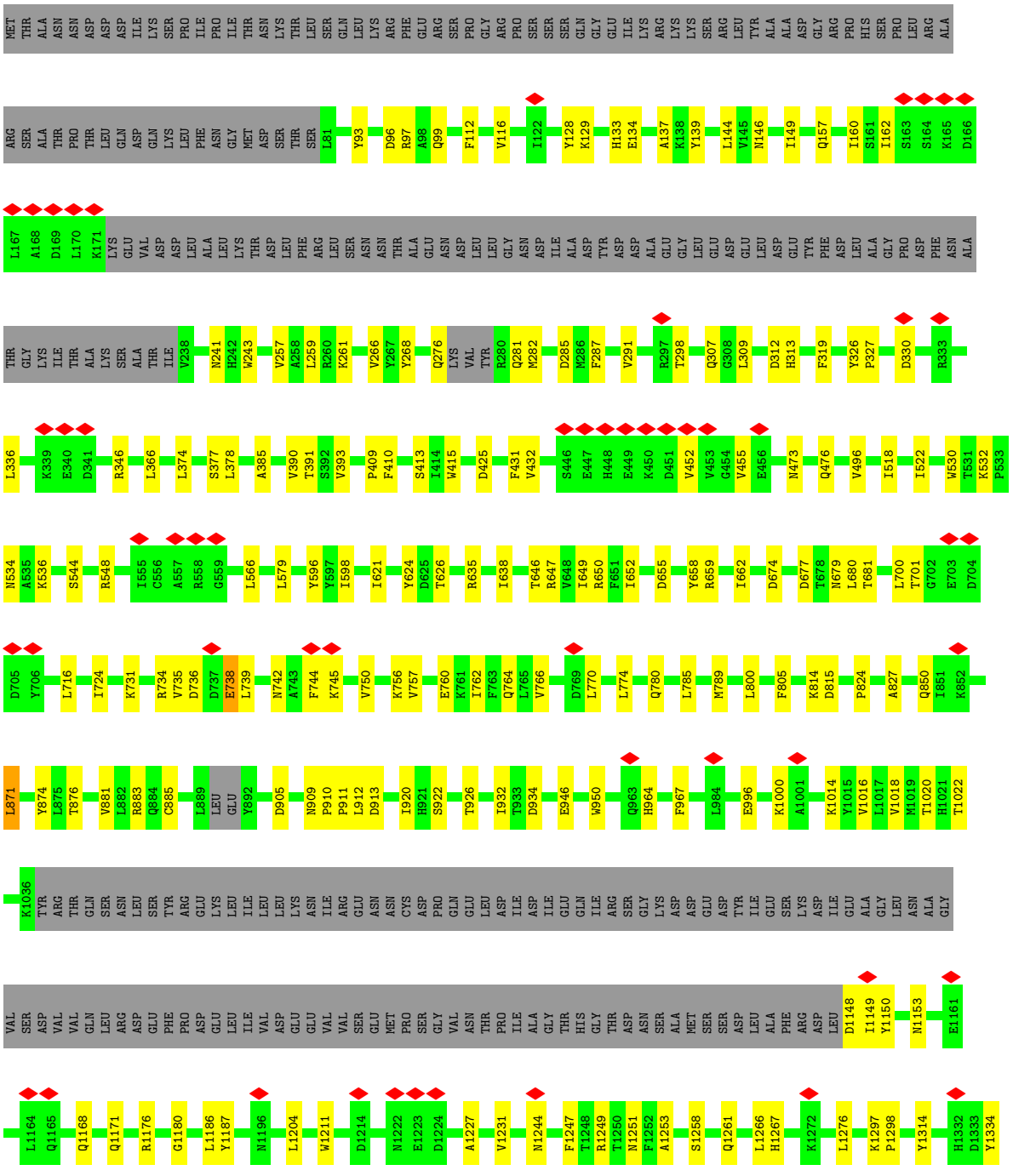


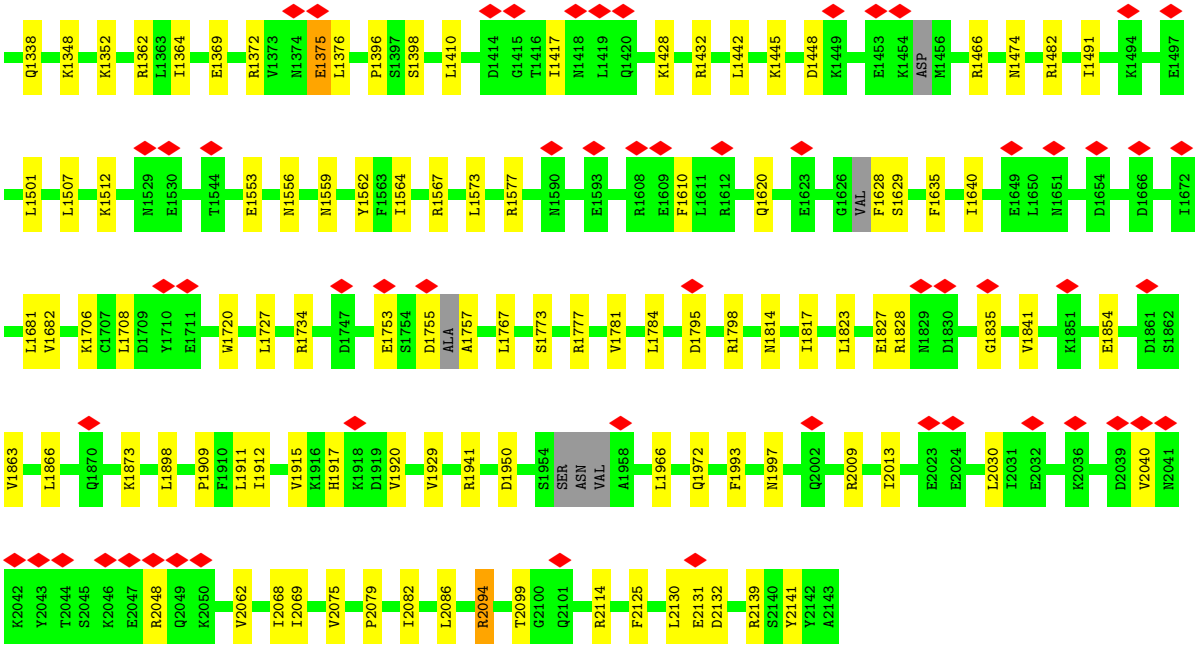
• Molecule 2: Proteasome subunit beta type-7

Chain N:



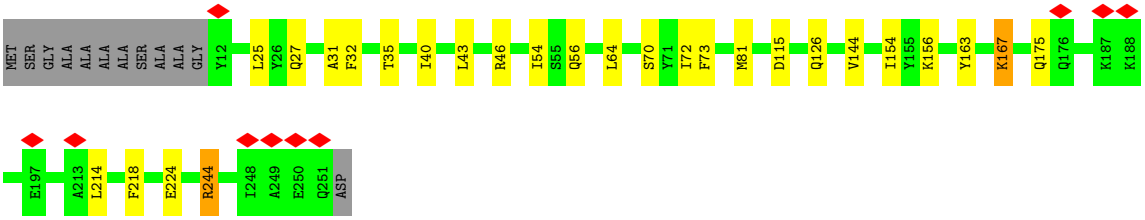
• Molecule 3: Proteasome activator BLM10





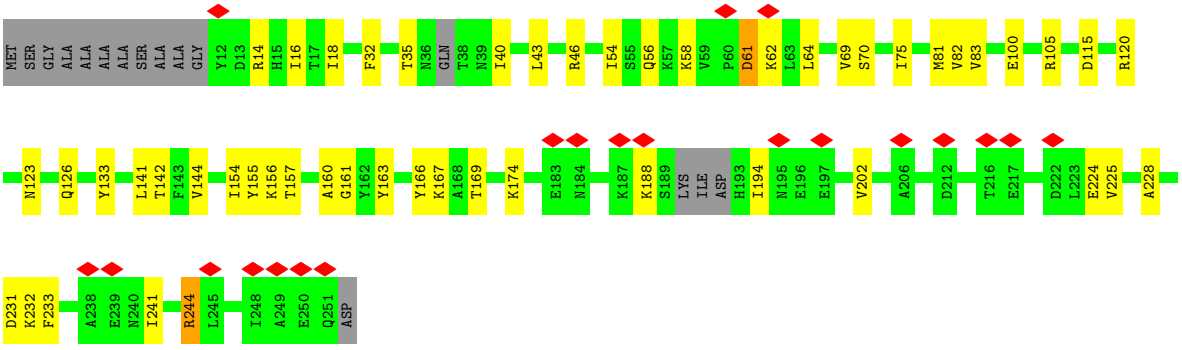
• Molecule 4: Proteasome subunit alpha type-1

Chain A:



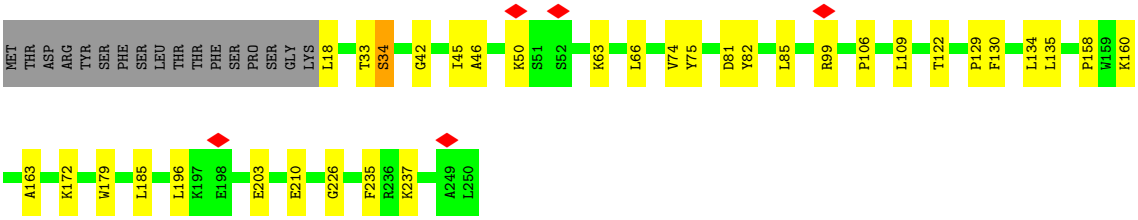
• Molecule 4: Proteasome subunit alpha type-1

Chain O:



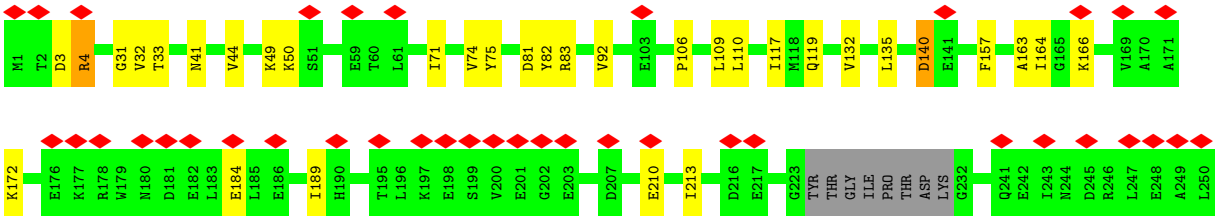
• Molecule 5: Proteasome subunit alpha type-2

Chain B:



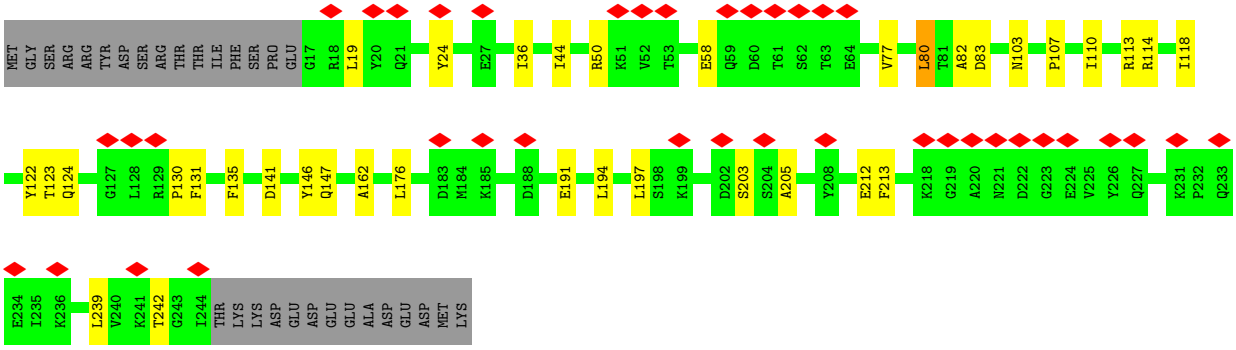
• Molecule 5: Proteasome subunit alpha type-2

Chain P:



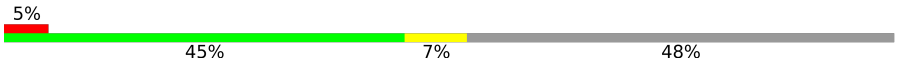
• Molecule 6: Proteasome subunit alpha type-3

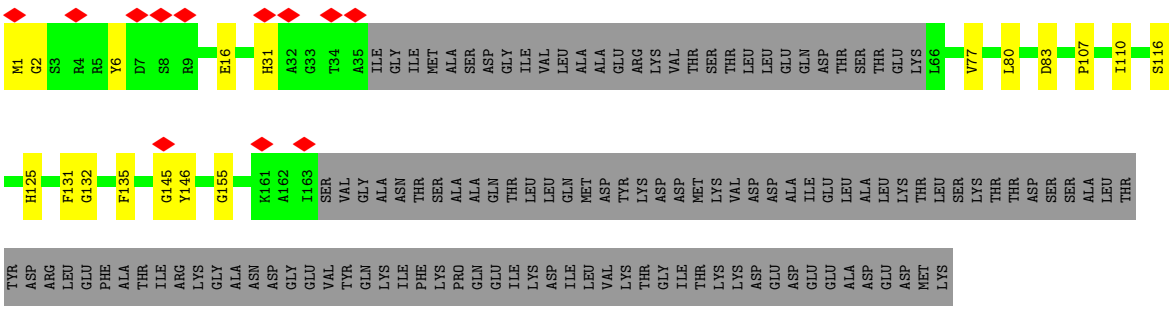
Chain C:



• Molecule 6: Proteasome subunit alpha type-3

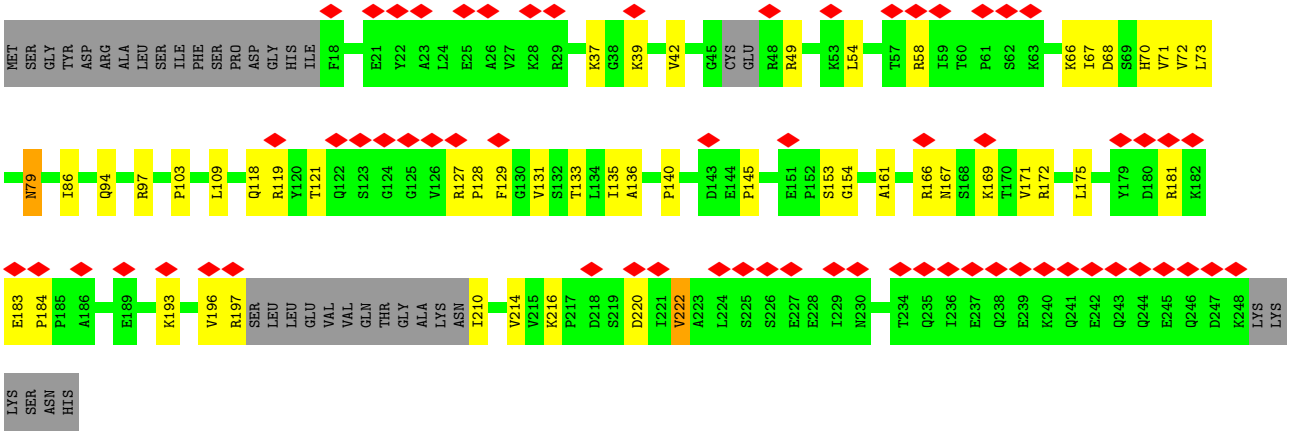
Chain Q:





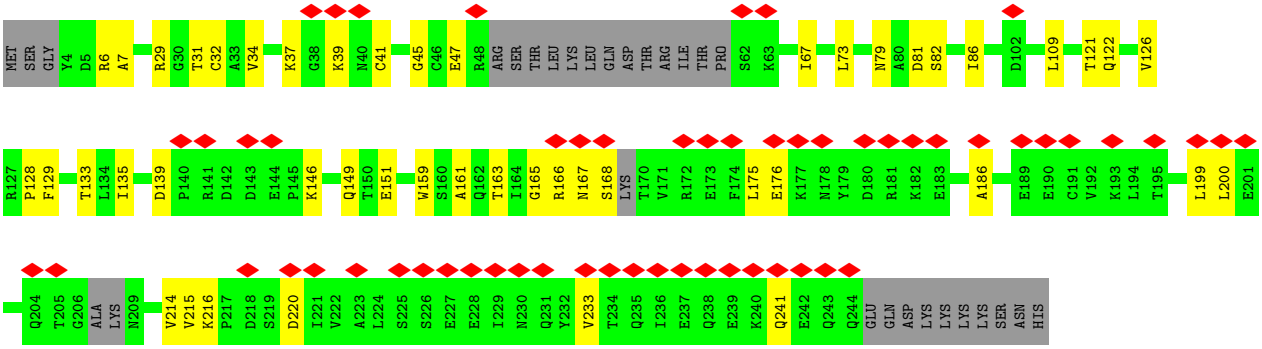
• Molecule 7: Proteasome subunit alpha type-4

Chain D:



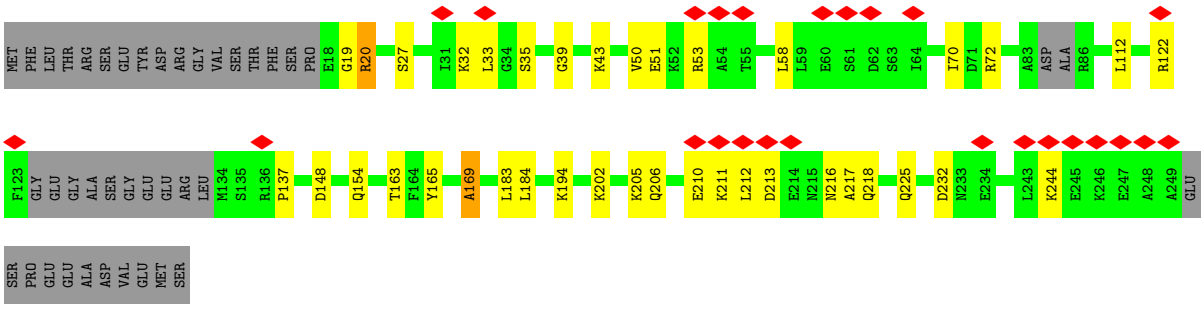
• Molecule 7: Proteasome subunit alpha type-4

Chain R:



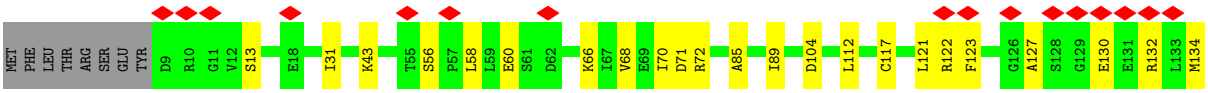
• Molecule 8: Proteasome subunit alpha type-5

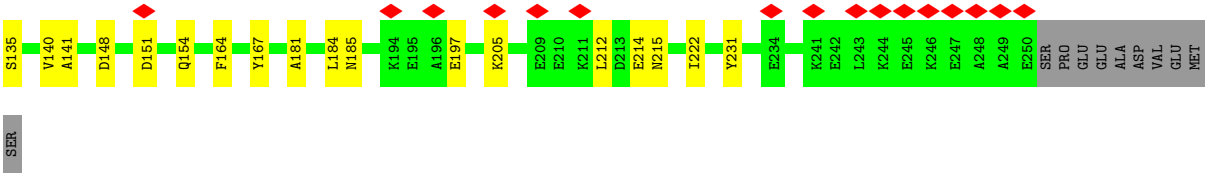
Chain E:



• Molecule 8: Proteasome subunit alpha type-5

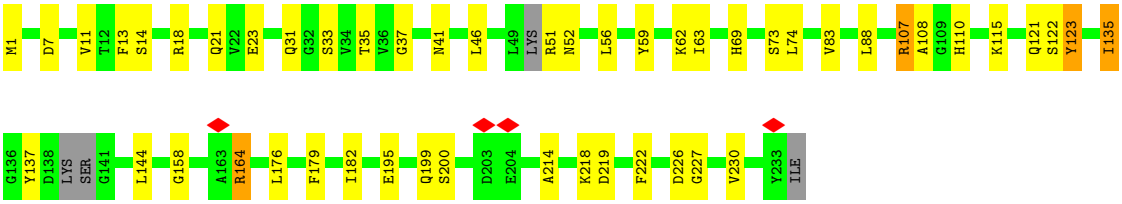
Chain S:





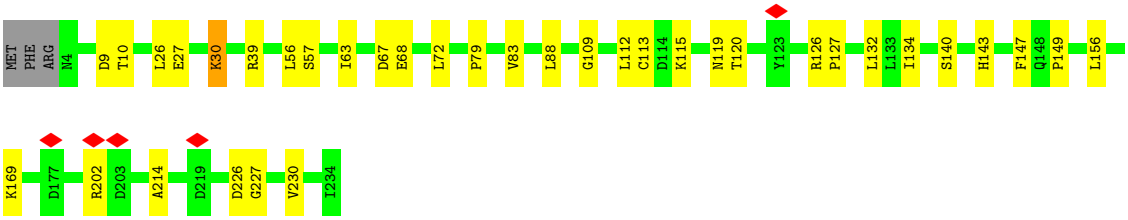
• Molecule 9: Proteasome subunit alpha type-6

Chain F:



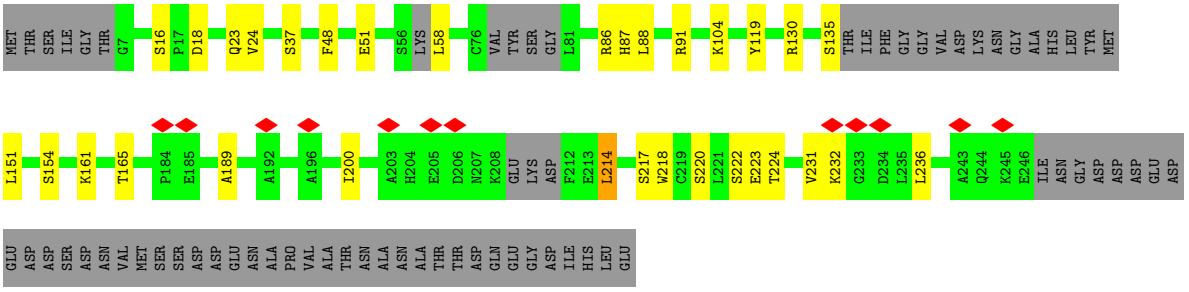
• Molecule 9: Proteasome subunit alpha type-6

Chain T:



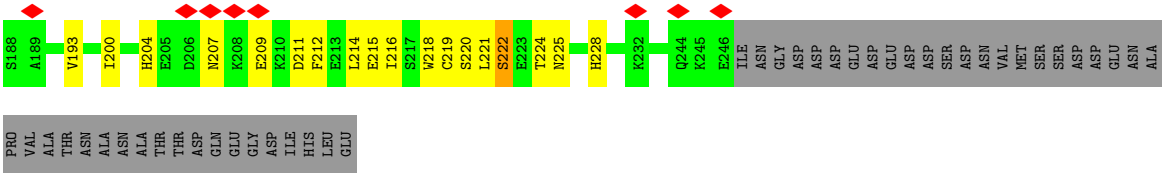
• Molecule 10: Probable proteasome subunit alpha type-7

Chain G:

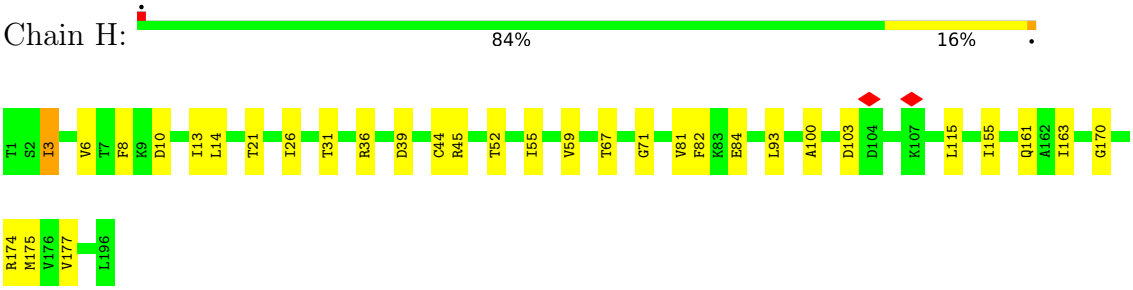


• Molecule 10: Probable proteasome subunit alpha type-7

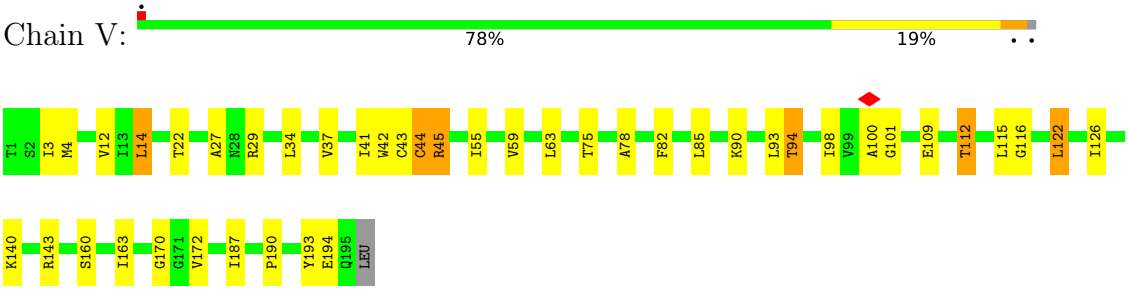
Chain U:



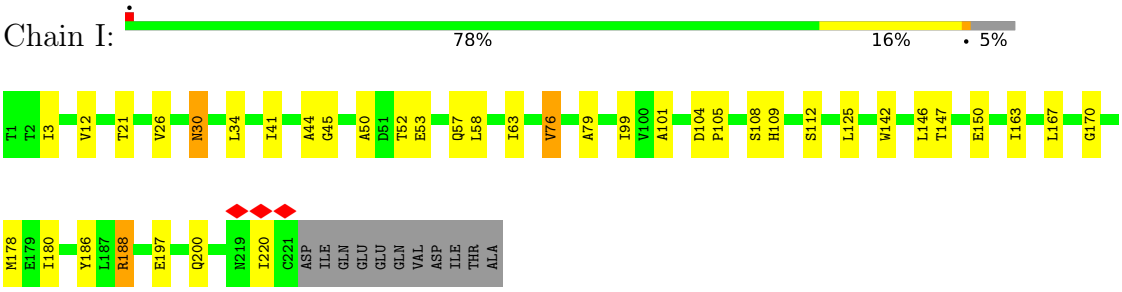
• Molecule 11: Proteasome subunit beta type-1



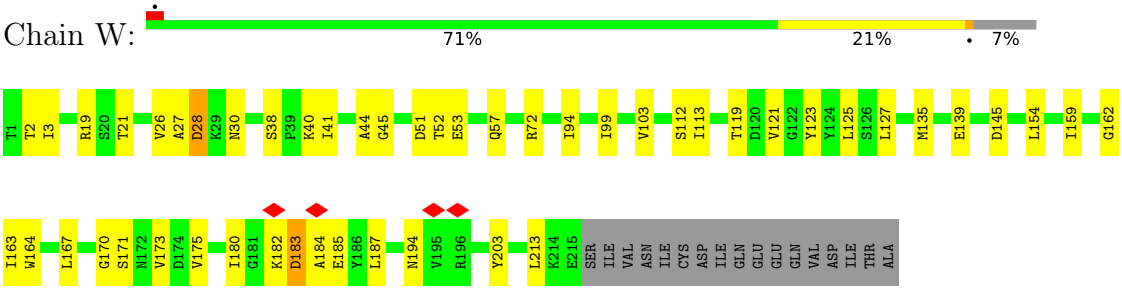
• Molecule 11: Proteasome subunit beta type-1



• Molecule 12: Proteasome subunit beta type-2

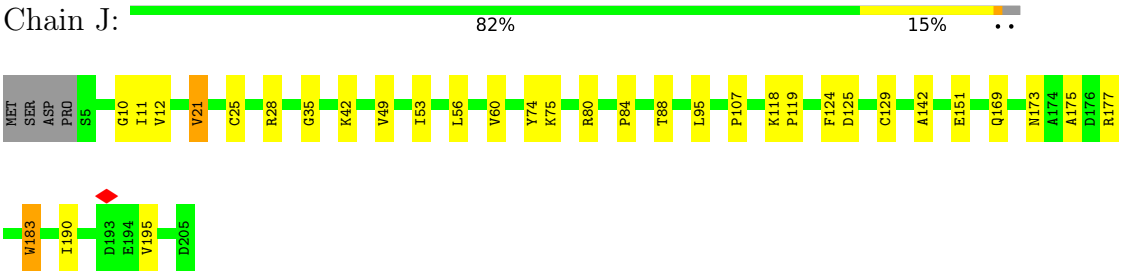


• Molecule 12: Proteasome subunit beta type-2



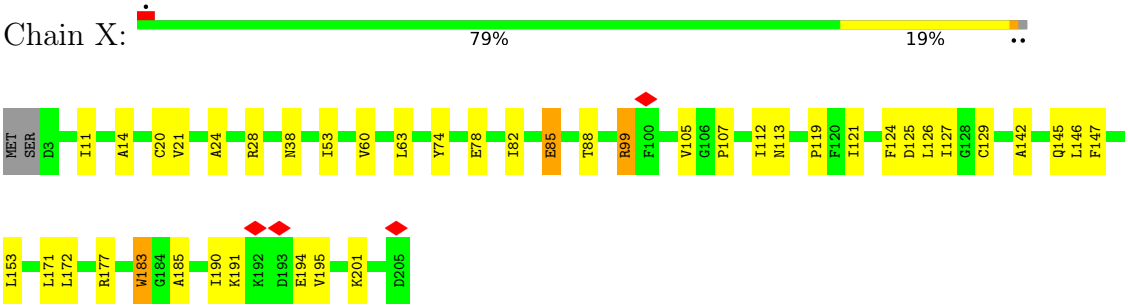
• Molecule 13: Proteasome subunit beta type-3

Chain J:



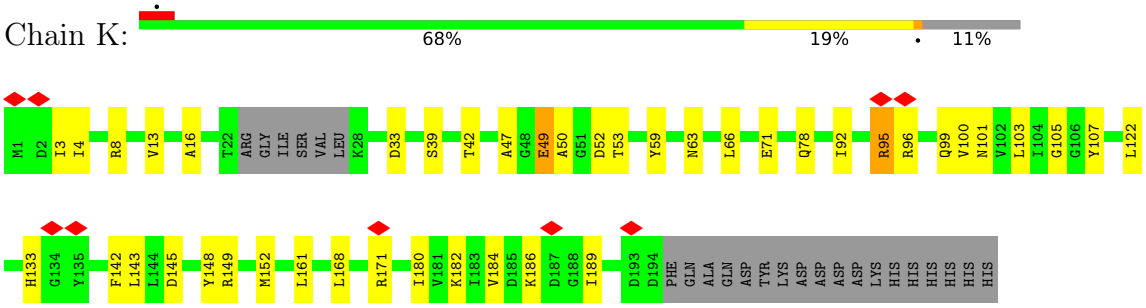
• Molecule 13: Proteasome subunit beta type-3

Chain X:



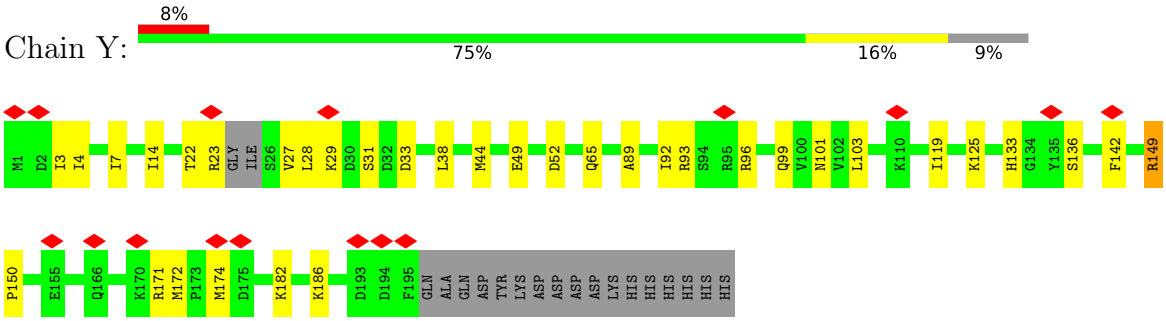
• Molecule 14: Proteasome subunit beta type-4

Chain K:



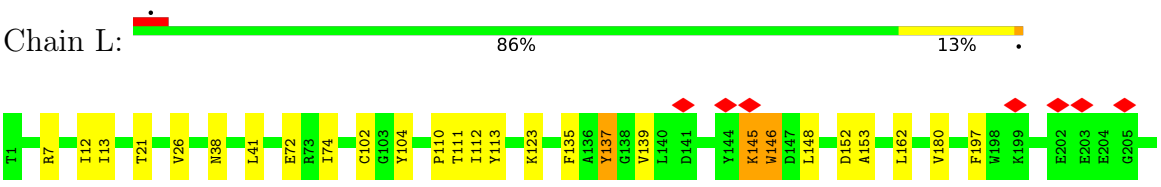
• Molecule 14: Proteasome subunit beta type-4

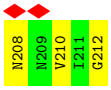
Chain Y:



• Molecule 15: Proteasome subunit beta type-5

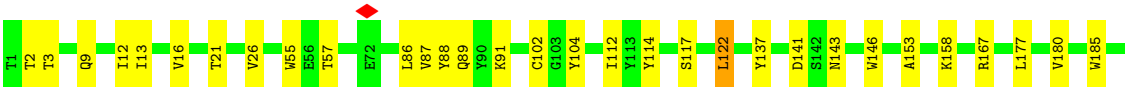
Chain L:





• Molecule 15: Proteasome subunit beta type-5

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	129737	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.104	Depositor
Minimum map value	-1.371	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	500.4, 500.4, 500.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

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	1	0.24	0/1785	0.46	0/2408
1	M	0.24	0/1777	0.47	0/2397
2	2	0.24	0/1821	0.49	0/2470
2	N	0.24	0/1817	0.48	0/2465
3	3	0.24	0/15586	0.42	0/21106
4	A	0.24	0/1941	0.45	0/2629
4	O	0.24	0/1905	0.46	0/2578
5	B	0.24	0/1813	0.45	0/2456
5	P	0.24	0/1886	0.46	0/2551
6	C	0.24	0/1800	0.45	0/2437
6	Q	0.24	0/1082	0.49	0/1466
7	D	0.23	0/1739	0.48	0/2349
7	R	0.24	0/1791	0.47	0/2422
8	E	0.23	0/1724	0.46	0/2320
8	S	0.23	0/1886	0.45	0/2541
9	F	0.24	0/1803	0.49	0/2436
9	T	0.24	0/1799	0.48	0/2433
10	G	0.24	0/1724	0.43	0/2323
10	U	0.24	0/1900	0.45	0/2564
11	H	0.24	0/1540	0.45	0/2087
11	V	0.24	0/1532	0.46	0/2076
12	I	0.23	0/1707	0.46	0/2315
12	W	0.24	0/1664	0.46	0/2256
13	J	0.25	0/1588	0.46	0/2143
13	X	0.24	0/1604	0.46	0/2166
14	K	0.23	0/1538	0.46	0/2072
14	Y	0.24	0/1582	0.46	0/2131
15	L	0.24	0/1680	0.46	0/2274
15	Z	0.24	0/1680	0.46	0/2274
All	All	0.24	0/63694	0.45	0/86145

There are no bond length outliers.

There are no bond angle outliers.

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	1	1747	0	1700	24	0
1	M	1739	0	1696	22	0
2	2	1790	0	1793	23	0
2	N	1786	0	1790	26	0
3	3	15248	0	15246	153	0
4	A	1903	0	1898	17	0
4	O	1869	0	1860	33	0
5	B	1780	0	1798	19	0
5	P	1852	0	1867	22	0
6	C	1773	0	1777	22	0
6	Q	1059	0	1035	10	0
7	D	1716	0	1726	37	0
7	R	1766	0	1754	32	0
8	E	1703	0	1696	22	0
8	S	1861	0	1836	33	0
9	F	1777	0	1771	30	0
9	T	1772	0	1775	24	0
10	G	1692	0	1684	22	0
10	U	1861	0	1852	27	0
11	H	1511	0	1481	21	0
11	V	1503	0	1470	27	0
12	I	1676	0	1684	23	0
12	W	1633	0	1637	33	0
13	J	1559	0	1555	21	0
13	X	1574	0	1566	30	0
14	K	1511	0	1511	28	0
14	Y	1554	0	1558	22	0
15	L	1643	0	1595	19	0
15	Z	1643	0	1595	21	0
16	1	75	0	0	1	0
16	2	85	0	0	1	0
16	3	685	0	0	11	0
16	A	98	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	57	0	0	1	0
16	C	58	0	0	1	0
16	D	78	0	0	6	0
16	E	80	0	0	5	0
16	F	55	0	0	1	0
16	G	56	0	0	2	0
16	H	49	0	0	2	0
16	I	70	0	0	1	0
16	J	56	0	0	0	0
16	K	46	0	0	2	0
16	L	55	0	0	0	0
16	M	63	0	0	2	0
16	N	74	0	0	0	0
16	O	70	0	0	1	0
16	P	56	0	0	0	0
16	Q	37	0	0	0	0
16	R	79	0	0	2	0
16	S	76	0	0	2	0
16	T	61	0	0	2	0
16	U	82	0	0	2	0
16	V	43	0	0	1	0
16	W	64	0	0	1	0
16	X	43	0	0	0	0
16	Y	75	0	0	3	0
16	Z	57	0	0	2	0
All	All	64984	0	62206	760	0

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

All (760) 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)
2:2:15:LYS:HE2	2:2:127:LEU:HB3	1.64	0.79
11:V:14:LEU:HD13	11:V:43:CYS:HA	1.70	0.73
10:G:87:HIS:HE2	10:G:119:TYR:HH	1.37	0.71
1:1:91:ARG:HD2	8:S:104:ASP:HB2	1.71	0.70
8:E:39:GLY:O	8:E:169:ALA:HA	1.91	0.70
11:V:14:LEU:HD12	11:V:34:LEU:HD22	1.74	0.70
3:3:635:ARG:HH22	3:3:679:ASN:HB2	1.57	0.69
7:D:67:ILE:HG21	7:D:109:LEU:HD21	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:261:LYS:HG3	3:3:309:LEU:HD13	1.74	0.69
11:V:4:MET:SD	16:V:239:HOH:O	2.51	0.69
11:H:115:LEU:HB3	2:N:5:ILE:HD13	1.75	0.69
1:M:158:ASN:HD22	13:X:172:LEU:HB3	1.59	0.68
2:N:27:LEU:HD21	2:N:34:LEU:HD22	1.76	0.67
7:D:216:LYS:HB2	7:D:220:ASP:HB3	1.75	0.67
11:H:55:ILE:HD11	11:H:93:LEU:HD13	1.75	0.67
14:K:149:ARG:NH1	15:Z:205:GLY:O	2.28	0.66
1:1:30:ILE:HG22	1:1:35:ILE:HA	1.76	0.66
5:B:122:THR:HG22	5:B:129:PRO:HB3	1.78	0.66
1:1:26:ASP:O	1:1:42:LYS:NZ	2.29	0.65
3:3:496:VAL:O	3:3:548:ARG:NH1	2.29	0.65
7:D:73:LEU:HD11	7:D:133:THR:HB	1.78	0.65
5:P:4:ARG:NH1	10:U:128:SER:OG	2.29	0.65
12:W:38:SER:HB3	12:W:41:ILE:HB	1.78	0.65
2:2:131:ASN:ND2	2:2:132:LEU:O	2.29	0.65
3:3:716:LEU:HD22	3:3:742:ASN:HD22	1.61	0.65
1:M:30:ILE:HG22	1:M:35:ILE:HA	1.78	0.65
12:I:163:ILE:HG23	12:I:170:GLY:HA2	1.77	0.65
7:R:32:CYS:HA	7:R:165:GLY:HA3	1.78	0.64
14:Y:3:ILE:HD12	14:Y:136:SER:HB3	1.78	0.64
3:3:731:LYS:O	3:3:734:ARG:NH1	2.31	0.64
2:2:25:ASP:OD1	2:2:41:ARG:NH2	2.29	0.64
3:3:1150:TYR:O	3:3:1267:HIS:NE2	2.30	0.64
10:U:43:ASN:ND2	10:U:187:LEU:O	2.31	0.64
15:Z:158:LYS:HG3	15:Z:177:LEU:HD11	1.80	0.64
13:J:107:PRO:HD2	13:J:124:PHE:HB2	1.79	0.64
1:M:111:ILE:HG22	1:M:123:TYR:HB2	1.78	0.64
7:R:161:ALA:HB1	7:R:175:LEU:HD13	1.80	0.64
11:V:90:LYS:NZ	11:V:116:GLY:O	2.30	0.63
1:M:126:ASP:OD1	1:M:130:SER:N	2.32	0.63
5:P:163:ALA:O	5:P:172:LYS:NZ	2.30	0.63
3:3:1348:LYS:HE2	3:3:1352:LYS:HZ3	1.61	0.63
13:X:38:ASN:HB3	13:X:183:TRP:HD1	1.63	0.63
9:F:135:ILE:HD11	9:F:222:PHE:HE1	1.63	0.63
12:W:19:ARG:NH2	12:W:167:LEU:O	2.30	0.63
2:N:128:ARG:HG2	2:N:138:SER:HB2	1.80	0.63
13:X:11:ILE:HG23	13:X:146:LEU:HD11	1.81	0.63
12:I:3:ILE:HG22	12:I:99:ILE:HD12	1.81	0.63
14:Y:52:ASP:OD1	15:Z:91:LYS:NZ	2.31	0.63
4:O:225:VAL:HG21	4:O:244:ARG:HH12	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:184:VAL:HG22	14:K:189:ILE:HG13	1.81	0.62
15:L:7:ARG:O	15:L:146:TRP:NE1	2.32	0.62
13:X:24:ALA:HB1	13:X:171:LEU:HD22	1.79	0.62
2:N:187:ARG:NH1	12:W:135:MET:SD	2.72	0.62
2:2:131:ASN:HD22	2:2:132:LEU:HD12	1.62	0.62
1:1:126:ASP:OD1	1:1:130:SER:N	2.24	0.62
15:L:162:LEU:HD21	15:L:197:PHE:HB2	1.82	0.62
1:1:148:PRO:HG3	13:J:177:ARG:HG3	1.81	0.62
8:E:212:LEU:HD11	8:E:217:ALA:HB2	1.80	0.62
7:D:214:VAL:HB	7:D:222:VAL:HG23	1.82	0.62
13:J:21:VAL:HG23	13:J:190:ILE:HB	1.81	0.61
11:H:161:GLN:HE21	11:V:140:LYS:HE2	1.64	0.61
10:G:189:ALA:HB1	10:G:218:TRP:HE1	1.66	0.61
3:3:1993:PHE:O	3:3:1997:ASN:ND2	2.30	0.61
9:F:7:ASP:O	9:F:21:GLN:NE2	2.33	0.61
3:3:1929:VAL:HG13	3:3:1966:LEU:HD13	1.82	0.61
4:O:133:TYR:HB2	5:P:4:ARG:HH21	1.64	0.61
3:3:1972:GLN:HB2	3:3:2013:ILE:HD12	1.83	0.60
6:C:124:GLN:NE2	7:D:128:PRO:O	2.34	0.60
7:R:41:CYS:HA	7:R:215:VAL:O	2.02	0.60
7:R:216:LYS:HB2	7:R:220:ASP:HB3	1.83	0.60
7:R:81:ASP:HB3	7:R:129:PHE:HD1	1.65	0.60
12:I:21:THR:HG22	12:I:26:VAL:HA	1.81	0.60
5:P:74:VAL:HG12	5:P:135:LEU:HB2	1.83	0.60
5:P:119:GLN:NE2	6:Q:83:ASP:OD1	2.34	0.60
3:3:1474:ASN:O	3:3:1512:LYS:NZ	2.33	0.60
13:X:21:VAL:HG13	13:X:119:PRO:HB3	1.84	0.60
12:I:147:THR:OG1	12:I:150:GLU:OE1	2.20	0.60
2:N:224:ASP:OD1	2:N:224:ASP:N	2.35	0.60
4:O:46:ARG:HE	4:O:167:LYS:HA	1.66	0.60
3:3:1795:ASP:HA	3:3:1798:ARG:HE	1.67	0.60
3:3:2040:VAL:HB	3:3:2048:ARG:HH21	1.66	0.60
15:L:111:THR:HG23	15:L:123:LYS:HE2	1.82	0.60
1:1:23:LEU:HD23	1:1:51:VAL:HG12	1.84	0.59
1:M:124:SER:HB2	1:M:137:ARG:HG3	1.84	0.59
12:W:28:ASP:OD1	12:W:28:ASP:N	2.35	0.59
12:W:213:LEU:HD21	13:X:201:LYS:HD3	1.84	0.59
4:A:43:LEU:HD23	4:A:54:ILE:HD11	1.85	0.59
12:W:171:SER:O	12:W:194:ASN:ND2	2.34	0.59
3:3:2094:ARG:NH2	3:3:2132:ASP:O	2.36	0.59
6:C:123:THR:HG22	6:C:130:PRO:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:50:ARG:NH1	6:C:212:GLU:OE2	2.36	0.59
9:T:156:LEU:HG	10:U:59:LEU:HD23	1.85	0.59
3:3:964:HIS:O	3:3:1249:ARG:NH1	2.35	0.59
7:D:73:LEU:HD13	7:D:135:ILE:HG12	1.83	0.59
12:W:203:TYR:HB2	13:X:153:LEU:HA	1.85	0.59
4:A:46:ARG:HE	4:A:167:LYS:HA	1.68	0.59
4:O:123:ASN:OD1	5:P:83:ARG:NH1	2.35	0.59
12:W:183:ASP:OD1	12:W:183:ASP:N	2.36	0.59
3:3:652:ILE:HG23	3:3:658:TYR:HB3	1.85	0.59
5:B:63:LYS:HD3	5:B:75:TYR:HE1	1.67	0.58
8:E:148:ASP:OD2	8:E:154:GLN:NE2	2.34	0.58
13:J:28:ARG:HB2	13:J:183:TRP:HB2	1.86	0.58
4:O:61:ASP:HB2	4:O:64:LEU:HD13	1.85	0.58
7:D:73:LEU:HD23	7:D:86:ILE:HG12	1.84	0.58
15:L:21:THR:HG22	15:L:26:VAL:HA	1.84	0.58
4:O:54:ILE:HG22	4:O:225:VAL:HG22	1.86	0.58
3:3:530:TRP:O	3:3:534:ASN:ND2	2.26	0.58
13:J:74:TYR:OH	13:J:80:ARG:NH2	2.37	0.58
13:X:21:VAL:HG23	13:X:190:ILE:HB	1.84	0.58
6:Q:2:GLY:O	10:U:127:ASN:ND2	2.37	0.58
7:D:118:GLN:HB2	7:D:154:GLY:HA3	1.86	0.58
15:L:208:ASN:HD22	14:Y:150:PRO:HD3	1.69	0.58
1:M:109:THR:HB	1:M:125:PHE:HB2	1.86	0.58
1:1:134:GLU:OE2	1:1:137:ARG:NH2	2.36	0.58
7:R:139:ASP:OD2	7:R:146:LYS:NZ	2.37	0.58
13:X:191:LYS:HB2	13:X:194:GLU:HB2	1.85	0.58
12:W:112:SER:HB3	12:W:125:LEU:HD13	1.86	0.57
9:F:176:LEU:HD13	10:G:58:LEU:HD23	1.87	0.57
14:K:59:TYR:O	14:K:63:ASN:ND2	2.33	0.57
5:P:109:LEU:HD11	13:X:78:GLU:HG2	1.87	0.57
7:R:122:GLN:NE2	8:S:134:MET:SD	2.77	0.57
9:T:109:GLY:HA2	9:T:147:PHE:CE2	2.39	0.57
3:3:1369:GLU:OE1	3:3:1372:ARG:NH2	2.35	0.57
7:D:79:ASN:N	7:D:79:ASN:OD1	2.38	0.57
2:N:25:ASP:OD1	2:N:41:ARG:NH2	2.33	0.57
5:P:31:GLY:O	5:P:166:LYS:NZ	2.33	0.57
5:P:49:LYS:HD2	5:P:210:GLU:HB2	1.85	0.57
8:S:121:LEU:HG	9:T:79:PRO:HB3	1.85	0.57
8:E:35:SER:HB3	8:E:53:ARG:HE	1.69	0.57
13:X:85:GLU:OE2	13:X:113:ASN:ND2	2.37	0.57
9:F:11:VAL:HA	10:G:130:ARG:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:X:107:PRO:HG2	13:X:124:PHE:HB2	1.87	0.57
3:3:1016:VAL:O	3:3:1020:THR:HG23	2.04	0.57
3:3:621:ILE:HD11	3:3:724:ILE:HG22	1.86	0.57
8:E:194:LYS:NZ	16:E:301:HOH:O	2.37	0.57
7:R:166:ARG:HD2	7:R:168:SER:H	1.70	0.57
11:V:34:LEU:HD23	11:V:44:CYS:HB3	1.86	0.57
15:L:38:ASN:HD21	15:L:41:LEU:HD12	1.69	0.56
3:3:1348:LYS:HG2	3:3:1352:LYS:HE2	1.87	0.56
11:H:84:GLU:OE2	2:N:65:ARG:NH1	2.31	0.56
13:J:35:GLY:O	15:Z:167:ARG:NH1	2.38	0.56
9:T:88:LEU:HD11	9:T:112:LEU:HD11	1.87	0.56
3:3:1835:GLY:O	3:3:1941:ARG:NH2	2.39	0.56
9:F:14:SER:HB3	9:F:18:ARG:H	1.70	0.56
13:J:21:VAL:HG13	13:J:119:PRO:HB3	1.87	0.56
14:Y:7:ILE:HG22	14:Y:14:ILE:HB	1.88	0.56
3:3:920:ILE:HD12	3:3:1022:THR:HG23	1.86	0.56
12:W:45:GLY:HA3	12:W:52:THR:HG21	1.87	0.56
2:2:21:ILE:HG12	2:2:199:ILE:HG12	1.88	0.56
5:P:106:PRO:HD2	5:P:109:LEU:HD12	1.88	0.56
7:R:31:THR:HB	7:R:47:GLU:HB2	1.88	0.56
8:S:123:PHE:HA	8:S:132:ARG:HA	1.88	0.56
2:N:14:MET:HG3	2:N:141:THR:HG22	1.88	0.56
12:W:163:ILE:HG23	12:W:170:GLY:HA2	1.87	0.56
2:2:77:ASP:OD2	10:U:86:ARG:NH2	2.39	0.55
7:R:161:ALA:HB3	8:S:58:LEU:HD23	1.88	0.55
3:3:378:LEU:HD23	3:3:1573:LEU:HD22	1.88	0.55
3:3:2131:GLU:HG2	9:F:164:ARG:HG3	1.87	0.55
7:D:42:VAL:HG11	7:D:136:ALA:HB1	1.89	0.55
15:Z:21:THR:HG22	15:Z:26:VAL:HA	1.88	0.55
7:D:97:ARG:NH1	16:D:301:HOH:O	2.34	0.55
7:D:210:ILE:N	16:D:304:HOH:O	2.39	0.55
10:U:67:ILE:HG12	10:U:77:VAL:HG12	1.88	0.55
14:Y:33:ASP:OD1	14:Y:182:LYS:NZ	2.37	0.55
12:I:30:ASN:O	12:I:188:ARG:NH2	2.38	0.55
3:3:336:LEU:HD11	3:3:385:ALA:HB2	1.89	0.55
3:3:1231:VAL:HG21	3:3:1258:SER:HB2	1.89	0.55
4:A:144:VAL:HG12	4:A:154:ILE:HG12	1.88	0.55
3:3:932:ILE:HD11	3:3:967:PHE:HB3	1.88	0.55
8:E:244:LYS:NZ	16:E:310:HOH:O	2.40	0.55
11:V:163:ILE:HG23	11:V:170:GLY:HA3	1.87	0.55
15:L:208:ASN:OD1	15:L:208:ASN:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:132:LEU:HB2	9:T:147:PHE:HB2	1.89	0.54
2:2:218:LYS:NZ	12:I:142:TRP:O	2.40	0.54
4:A:244:ARG:NH1	16:A:312:HOH:O	2.40	0.54
11:H:3:ILE:HG12	11:H:44:CYS:HB3	1.89	0.54
12:W:30:ASN:ND2	16:W:305:HOH:O	2.40	0.54
12:I:112:SER:HB3	12:I:125:LEU:HD13	1.88	0.54
4:O:40:ILE:HG23	4:O:56:GLN:HB2	1.89	0.54
5:P:140:ASP:OD1	5:P:140:ASP:N	2.40	0.54
3:3:2062:VAL:HG21	3:3:2099:THR:HG23	1.89	0.54
10:G:151:LEU:N	16:G:307:HOH:O	2.40	0.54
9:T:27:GLU:HA	9:T:30:LYS:HE3	1.90	0.54
12:I:45:GLY:HA3	12:I:52:THR:HG21	1.90	0.54
14:K:8:ARG:NH1	14:K:148:TYR:OH	2.40	0.54
2:N:43:ILE:HG13	2:N:64:GLU:HG2	1.89	0.54
5:P:3:ASP:O	5:P:4:ARG:NE	2.40	0.54
8:S:148:ASP:OD2	8:S:154:GLN:NE2	2.40	0.54
8:E:122:ARG:NH2	16:E:311:HOH:O	2.40	0.54
10:G:37:SER:OG	10:G:165:THR:OG1	2.26	0.54
14:K:16:ALA:HB2	14:K:161:LEU:HD11	1.90	0.54
14:K:171:ARG:HD2	15:Z:137:TYR:HE2	1.71	0.54
4:O:32:PHE:O	4:O:35:THR:OG1	2.19	0.54
3:3:1314:TYR:HB2	3:3:1352:LYS:HZ1	1.73	0.54
2:N:27:LEU:HB2	2:N:192:SER:HB2	1.89	0.54
10:U:70:VAL:HB	10:U:74:ILE:HB	1.89	0.54
10:U:193:VAL:HG13	10:U:216:ILE:HG21	1.89	0.54
13:X:20:CYS:HA	13:X:112:ILE:HD11	1.89	0.54
13:X:171:LEU:HD21	13:X:185:ALA:HB1	1.90	0.54
11:H:45:ARG:HD2	11:H:52:THR:HB	1.89	0.54
3:3:473:ASN:O	3:3:476:GLN:HG3	2.08	0.54
4:O:157:THR:HG22	4:O:163:TYR:HB2	1.90	0.54
15:Z:12:ILE:HB	15:Z:180:VAL:HB	1.88	0.54
3:3:934:ASP:OD2	3:3:1249:ARG:NH2	2.34	0.54
3:3:1682:VAL:HG11	3:3:1727:LEU:HD21	1.90	0.53
8:E:19:GLY:O	8:E:20:ARG:NH1	2.40	0.53
3:3:266:VAL:HG21	3:3:1410:LEU:HG	1.90	0.53
7:D:94:GLN:HG3	14:K:66:LEU:HB2	1.90	0.53
3:3:646:THR:HA	3:3:649:ILE:HD12	1.91	0.53
8:E:35:SER:HB2	8:E:51:GLU:HB3	1.90	0.53
10:G:200:ILE:HG21	10:G:214:LEU:HG	1.90	0.53
3:3:1396:PRO:HB2	3:3:1432:ARG:HG3	1.89	0.53
8:S:13:SER:HB3	9:T:126:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:226:GLY:HA3	12:I:186:TYR:HB3	1.91	0.53
8:S:127:ALA:HA	9:T:83:VAL:HG22	1.91	0.53
12:I:53:GLU:OE2	12:I:57:GLN:NE2	2.42	0.53
1:M:151:ASP:OD2	13:X:177:ARG:NH1	2.41	0.53
7:R:47:GLU:OE1	7:R:167:ASN:ND2	2.38	0.53
11:V:75:THR:OG1	11:V:109:GLU:OE1	2.20	0.53
3:3:2009:ARG:O	3:3:2013:ILE:HG12	2.09	0.53
9:F:88:LEU:HD11	9:F:108:ALA:HB1	1.90	0.53
8:S:205:LYS:HB2	8:S:212:LEU:HD22	1.90	0.53
3:3:756:LYS:HA	3:3:800:LEU:HD21	1.91	0.53
7:D:161:ALA:HB1	7:D:175:LEU:HD13	1.89	0.53
1:M:115:ASP:OD1	1:M:119:LYS:N	2.42	0.53
13:X:125:ASP:OD1	13:X:129:CYS:N	2.34	0.53
11:V:22:THR:HG22	11:V:27:ALA:HB2	1.91	0.53
2:2:130:VAL:HG23	2:2:136:THR:HG22	1.91	0.52
2:2:222:ALA:O	11:H:174:ARG:NH2	2.37	0.52
6:C:80:LEU:HD13	6:C:82:ALA:H	1.73	0.52
14:K:99:GLN:NE2	16:K:306:HOH:O	2.42	0.52
9:T:115:LYS:O	9:T:119:ASN:ND2	2.42	0.52
11:V:172:VAL:HG12	11:V:190:PRO:HD3	1.91	0.52
3:3:1507:LEU:HD21	3:3:1635:PHE:HA	1.91	0.52
10:G:51:GLU:HG2	10:G:200:ILE:HG23	1.91	0.52
4:O:100:GLU:OE1	4:O:120:ARG:NH1	2.42	0.52
5:P:75:TYR:HB3	5:P:82:TYR:CD1	2.45	0.52
11:V:37:VAL:H	11:V:42:TRP:HB3	1.74	0.52
13:X:14:ALA:HB1	13:X:121:ILE:HD13	1.91	0.52
3:3:1620:GLN:NE2	16:3:2246:HOH:O	2.42	0.52
5:B:106:PRO:HD2	5:B:109:LEU:HD12	1.91	0.52
1:M:43:VAL:HG12	1:M:205:LEU:HD12	1.89	0.52
6:C:113:ARG:NH2	14:K:71:GLU:OE2	2.43	0.52
3:3:144:LEU:HD11	3:3:259:LEU:HD21	1.92	0.52
7:D:118:GLN:NE2	16:D:306:HOH:O	2.41	0.52
12:W:103:VAL:HG11	12:W:180:ILE:HA	1.91	0.52
13:J:10:GLY:HA3	13:J:42:LYS:HE2	1.90	0.52
14:K:3:ILE:HD13	14:K:168:LEU:HD13	1.91	0.52
3:3:1176:ARG:NH2	3:3:1211:TRP:O	2.40	0.52
9:F:164:ARG:O	9:F:200:SER:OG	2.20	0.52
14:K:92:ILE:HG21	14:K:122:LEU:HA	1.91	0.52
3:3:162:ILE:HD11	3:3:1428:LYS:HG3	1.90	0.52
9:F:83:VAL:HG12	9:F:115:LYS:HZ3	1.74	0.52
14:K:145:ASP:O	15:Z:206:SER:OG	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:171:ARG:NH2	15:Z:141:ASP:OD1	2.43	0.52
9:T:67:ASP:OD1	9:T:68:GLU:N	2.42	0.52
9:T:109:GLY:HA2	9:T:147:PHE:HE2	1.75	0.52
15:L:148:LEU:HB3	15:L:152:ASP:HB2	1.92	0.52
14:Y:65:GLN:NE2	16:Y:308:HOH:O	2.42	0.52
3:3:116:VAL:H	3:3:298:THR:HG22	1.75	0.52
3:3:1261:GLN:NE2	16:3:2253:HOH:O	2.43	0.52
1:M:24:ALA:HB1	1:M:202:LEU:HD11	1.90	0.52
7:D:129:PHE:HB3	7:D:131:VAL:HG12	1.92	0.51
10:G:88:LEU:HD21	10:G:151:LEU:HD23	1.92	0.51
4:O:241:ILE:O	4:O:244:ARG:NE	2.42	0.51
9:T:72:LEU:HB3	9:T:134:ILE:HG12	1.91	0.51
3:3:409:PRO:HG2	3:3:1828:ARG:HG2	1.91	0.51
3:3:1168:GLN:HA	3:3:1171:GLN:HG2	1.92	0.51
3:3:2069:ILE:HD13	3:3:2086:LEU:HD22	1.90	0.51
6:C:19:LEU:HD21	7:D:127:ARG:HD3	1.92	0.51
7:D:37:LYS:HE2	7:D:145:PRO:HB2	1.91	0.51
14:K:96:ARG:NH2	16:K:304:HOH:O	2.41	0.51
4:A:32:PHE:O	4:A:35:THR:OG1	2.22	0.51
4:A:73:PHE:HB2	4:A:81:MET:HG2	1.92	0.51
15:L:7:ARG:HG3	15:L:110:PRO:HB2	1.91	0.51
2:N:224:ASP:OD2	12:W:123:TYR:OH	2.23	0.51
4:O:82:VAL:HG13	4:O:142:THR:HB	1.92	0.51
8:S:31:ILE:HD13	8:S:141:ALA:HB2	1.93	0.51
3:3:659:ARG:HA	3:3:662:ILE:HD13	1.93	0.51
3:3:1640:ILE:HD11	3:3:1681:LEU:HD23	1.92	0.51
6:C:141:ASP:OD1	6:C:147:GLN:NE2	2.42	0.51
9:T:169:LYS:NZ	16:T:308:HOH:O	2.44	0.51
1:1:173:LYS:NZ	16:1:306:HOH:O	2.37	0.51
4:A:25:LEU:O	4:A:27:GLN:N	2.36	0.51
4:O:75:ILE:HD11	4:O:81:MET:HE2	1.93	0.51
7:R:149:GLN:HG2	7:R:159:TRP:CD1	2.45	0.51
15:Z:9:GLN:NE2	15:Z:146:TRP:O	2.43	0.51
3:3:1567:ARG:NH1	3:3:1773:SER:O	2.44	0.51
7:D:167:ASN:O	7:D:169:LYS:N	2.42	0.51
15:L:12:ILE:HG21	15:L:102:CYS:HB3	1.93	0.51
8:S:70:ILE:HG21	8:S:112:LEU:HD21	1.92	0.51
3:3:909:ASN:O	3:3:913:ASP:N	2.37	0.51
15:L:210:VAL:HG12	15:L:212:GLY:H	1.76	0.51
11:V:94:THR:HA	11:V:115:LEU:HD11	1.92	0.51
14:Y:49:GLU:HB2	14:Y:99:GLN:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:738:GLU:OE1	3:3:739:LEU:N	2.44	0.51
9:F:62:LYS:NZ	9:F:74:LEU:O	2.44	0.51
7:R:200:LEU:HD11	7:R:233:VAL:HG22	1.93	0.51
8:S:184:LEU:HD23	9:T:56:LEU:HG	1.92	0.51
11:V:160:SER:HB3	11:V:193:TYR:HB2	1.92	0.51
12:W:94:ILE:HG12	13:X:99:ARG:HH12	1.75	0.51
3:3:1817:ILE:HG13	3:3:1823:LEU:HD13	1.92	0.51
9:F:69:HIS:HB2	9:F:137:TYR:HB3	1.92	0.51
12:I:76:VAL:HG21	12:I:109:HIS:HB2	1.93	0.51
3:3:652:ILE:HG22	3:3:662:ILE:HD11	1.93	0.50
4:O:126:GLN:NE2	5:P:81:ASP:OD1	2.39	0.50
11:V:4:MET:HG3	11:V:126:ILE:HG22	1.93	0.50
12:W:21:THR:HG22	12:W:26:VAL:HA	1.93	0.50
1:M:220:LYS:NZ	16:M:307:HOH:O	2.43	0.50
3:3:1187:TYR:HB2	3:3:1204:LEU:HD21	1.93	0.50
1:M:126:ASP:OD1	1:M:129:GLY:N	2.44	0.50
14:Y:89:ALA:O	14:Y:92:ILE:HG22	2.11	0.50
3:3:1553:GLU:OE2	3:3:1734:ARG:NH2	2.44	0.50
11:H:13:ILE:HG12	11:H:177:VAL:HG22	1.93	0.50
7:R:122:GLN:HG2	8:S:134:MET:HB2	1.92	0.50
8:S:122:ARG:HD3	8:S:130:GLU:HG3	1.92	0.50
4:O:14:ARG:NH2	16:O:1707:HOH:O	2.42	0.50
7:R:34:VAL:HG22	7:R:163:THR:HG22	1.92	0.50
4:A:115:ASP:OD1	4:A:115:ASP:N	2.43	0.50
3:3:330:ASP:N	3:3:330:ASP:OD1	2.42	0.50
3:3:883:ARG:NE	3:3:1227:ALA:HB3	2.27	0.50
9:F:31:GLN:O	9:F:51:ARG:NH2	2.45	0.50
5:P:92:VAL:HG21	5:P:117:ILE:HD11	1.94	0.50
3:3:2075:VAL:O	3:3:2114:ARG:NH2	2.42	0.50
4:O:43:LEU:HD23	4:O:54:ILE:HD11	1.93	0.50
2:2:59:ASP:O	2:2:63:ILE:HG23	2.12	0.50
3:3:374:LEU:HD13	3:3:390:VAL:HG22	1.94	0.50
6:C:162:ALA:HB3	7:D:54:LEU:HD13	1.93	0.50
7:D:121:THR:HA	7:D:128:PRO:HB3	1.94	0.50
6:Q:125:HIS:HB3	7:R:126:VAL:HG12	1.94	0.50
10:U:20:ARG:NH2	16:U:314:HOH:O	2.43	0.50
14:Y:186:LYS:NZ	16:Y:311:HOH:O	2.45	0.50
9:F:63:ILE:HG21	9:F:214:ALA:HB2	1.94	0.49
10:U:225:ASN:ND2	16:U:311:HOH:O	2.37	0.49
9:F:37:GLY:O	9:F:158:GLY:HA2	2.12	0.49
13:J:11:ILE:HG21	13:J:142:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:161:GLY:O	5:P:83:ARG:NH2	2.46	0.49
9:F:179:PHE:HA	9:F:182:ILE:HD11	1.94	0.49
1:M:52:MET:HE1	1:M:65:VAL:HA	1.94	0.49
10:U:32:GLU:HG3	10:U:169:ARG:HH12	1.76	0.49
3:3:1180:GLY:HA3	3:3:1276:LEU:HD21	1.94	0.49
5:B:81:ASP:HB3	5:B:130:PHE:HD1	1.77	0.49
14:K:39:SER:HB3	14:K:42:THR:HB	1.95	0.49
5:P:33:THR:HA	5:P:164:ILE:O	2.12	0.49
1:1:28:ARG:NH2	1:1:196:ILE:O	2.45	0.49
2:N:10:SER:HB3	2:N:147:GLY:H	1.78	0.49
15:Z:13:ILE:HG13	15:Z:153:ALA:HB1	1.94	0.49
3:3:701:THR:OG1	3:3:745:LYS:O	2.30	0.49
5:B:18:LEU:N	16:B:301:HOH:O	2.45	0.49
7:D:118:GLN:O	7:D:121:THR:OG1	2.29	0.49
5:P:44:VAL:HG22	5:P:213:ILE:HG22	1.95	0.49
14:Y:119:ILE:HG12	14:Y:125:LYS:HG3	1.94	0.49
1:1:142:ALA:HB2	1:1:198:VAL:HG21	1.95	0.49
15:L:137:TYR:HB3	14:Y:171:ARG:CZ	2.43	0.49
7:D:58:ARG:NH2	16:D:307:HOH:O	2.41	0.49
2:N:78:ASN:HD21	2:N:85:GLU:HB3	1.78	0.49
2:2:182:ARG:NH1	16:2:311:HOH:O	2.45	0.49
3:3:770:LEU:HD22	3:3:774:LEU:HD23	1.94	0.49
2:N:21:ILE:HG12	2:N:199:ILE:HG12	1.95	0.49
10:U:50:VAL:HG23	10:U:215:GLU:HB3	1.95	0.49
3:3:1708:LEU:HD21	3:3:1720:TRP:CD1	2.48	0.48
6:C:107:PRO:HD2	6:C:110:ILE:HD12	1.95	0.48
8:E:202:LYS:NZ	8:E:206:GLN:OE1	2.39	0.48
10:G:16:SER:OG	10:G:18:ASP:OD1	2.22	0.48
11:H:163:ILE:HG23	11:H:170:GLY:HA2	1.95	0.48
11:V:112:THR:HG21	11:V:122:LEU:HD12	1.95	0.48
12:W:145:ASP:OD1	12:W:145:ASP:N	2.43	0.48
1:M:100:LYS:HE2	1:M:105:TYR:CZ	2.48	0.48
2:2:129:TYR:HE2	2:2:144:THR:HG22	1.78	0.48
6:C:83:ASP:HB3	6:C:131:PHE:HD1	1.78	0.48
10:G:232:LYS:HG3	10:G:236:LEU:HD22	1.95	0.48
15:L:135:PHE:O	15:L:139:VAL:HG23	2.13	0.48
1:1:43:VAL:HG12	1:1:205:LEU:HD12	1.95	0.48
3:3:655:ASP:O	3:3:659:ARG:HG3	2.14	0.48
11:H:103:ASP:OD1	11:H:103:ASP:N	2.46	0.48
12:I:104:ASP:HB2	12:I:105:PRO:HD2	1.96	0.48
8:S:181:ALA:O	8:S:185:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:2079:PRO:HD2	3:3:2082:ILE:HD12	1.96	0.48
6:C:114:ARG:HE	6:C:118:ILE:HD11	1.78	0.48
9:F:63:ILE:HD13	9:F:214:ALA:HB2	1.96	0.48
2:N:193:ARG:NH1	11:V:194:GLU:OE1	2.47	0.48
3:3:1567:ARG:NH1	16:3:2271:HOH:O	2.47	0.48
4:O:144:VAL:HG12	4:O:154:ILE:HG12	1.94	0.48
7:R:39:LYS:HB3	7:R:186:ALA:HA	1.94	0.48
7:D:181:ARG:HG3	8:E:58:LEU:HA	1.95	0.48
8:S:151:ASP:HB2	8:S:154:GLN:HE21	1.78	0.48
8:S:197:GLU:OE2	8:S:231:TYR:OH	2.28	0.48
7:D:39:LYS:HE3	7:D:184:PRO:HG2	1.95	0.48
9:F:107:ARG:NH1	16:F:310:HOH:O	2.46	0.48
8:S:151:ASP:HB2	8:S:154:GLN:NE2	2.29	0.48
12:W:2:THR:HG21	12:W:162:GLY:HA3	1.95	0.48
3:3:96:ASP:HB3	3:3:99:GLN:HB3	1.95	0.48
6:C:194:LEU:HD12	6:C:242:THR:HG21	1.95	0.48
8:S:132:ARG:NH1	16:S:310:HOH:O	2.47	0.48
13:X:53:ILE:HB	13:X:60:VAL:HG13	1.95	0.48
3:3:1014:LYS:NZ	16:3:2263:HOH:O	2.44	0.47
10:U:51:GLU:OE2	10:U:204:HIS:ND1	2.40	0.47
11:V:12:VAL:HG21	11:V:100:ALA:HB1	1.94	0.47
12:W:53:GLU:OE2	12:W:57:GLN:NE2	2.47	0.47
14:Y:29:LYS:HG2	14:Y:31:SER:H	1.78	0.47
2:2:61:GLN:O	2:2:64:GLU:HG2	2.15	0.47
5:B:99:ARG:HH21	12:I:58:LEU:HB2	1.79	0.47
10:G:135:SER:HB2	10:G:165:THR:HG21	1.95	0.47
4:O:228:ALA:HB2	4:O:233:PHE:HD1	1.79	0.47
1:1:57:PHE:HZ	2:2:133:LEU:HB3	1.79	0.47
5:B:85:LEU:HD23	5:B:134:LEU:HD11	1.96	0.47
14:Y:96:ARG:NH2	15:Z:88:TYR:O	2.38	0.47
9:T:63:ILE:HG21	9:T:214:ALA:HB2	1.96	0.47
7:R:176:GLU:HG2	8:S:58:LEU:HD13	1.96	0.47
11:V:55:ILE:HD12	11:V:85:LEU:HB3	1.96	0.47
7:D:71:VAL:HG11	7:D:109:LEU:HD23	1.96	0.47
11:H:31:THR:O	11:H:174:ARG:NH1	2.48	0.47
9:T:10:THR:HG21	9:T:127:PRO:HD3	1.97	0.47
4:A:126:GLN:NE2	5:B:81:ASP:OD1	2.43	0.47
14:K:4:ILE:HG22	14:K:103:LEU:HD12	1.97	0.47
12:W:3:ILE:HG22	12:W:99:ILE:HD12	1.96	0.47
14:Y:101:ASN:HB3	14:Y:133:HIS:CE1	2.49	0.47
5:B:163:ALA:O	5:B:172:LYS:NZ	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:121:THR:HG21	7:D:153:SER:HA	1.97	0.47
9:F:227:GLY:O	9:F:230:VAL:HG22	2.15	0.47
15:L:139:VAL:HG22	14:Y:142:PHE:CD1	2.49	0.47
7:R:37:LYS:NZ	8:S:60:GLU:OE2	2.42	0.47
10:G:24:VAL:HG11	10:G:154:SER:HB3	1.97	0.47
6:Q:80:LEU:HD12	6:Q:132:GLY:HA3	1.96	0.47
7:R:73:LEU:HD23	7:R:86:ILE:HG12	1.97	0.47
15:Z:3:THR:HA	15:Z:16:VAL:HG12	1.97	0.47
14:K:107:TYR:CZ	14:K:186:LYS:HG2	2.50	0.47
3:3:241:ASN:HA	3:3:282:MET:HE3	1.95	0.46
3:3:241:ASN:ND2	16:3:2245:HOH:O	2.41	0.46
3:3:1334:TYR:CD2	3:3:1375:GLU:HG3	2.50	0.46
3:3:1375:GLU:HG2	3:3:1376:LEU:HG	1.97	0.46
12:I:12:VAL:HG21	12:I:101:ALA:HB1	1.96	0.46
12:I:108:SER:HB3	12:I:180:ILE:HD11	1.98	0.46
13:X:28:ARG:HB2	13:X:183:TRP:HB2	1.98	0.46
3:3:1362:ARG:NH1	16:3:2270:HOH:O	2.46	0.46
8:S:85:ALA:HB2	8:S:140:VAL:HG11	1.97	0.46
9:T:88:LEU:HD21	9:T:112:LEU:HG	1.97	0.46
3:3:1564:ILE:O	3:3:1777:ARG:NH1	2.33	0.46
5:B:42:GLY:HA3	5:B:185:LEU:HD13	1.97	0.46
13:J:95:LEU:HD11	13:J:107:PRO:HG2	1.96	0.46
11:V:59:VAL:HG11	11:V:82:PHE:CE2	2.51	0.46
14:Y:92:ILE:HG23	14:Y:93:ARG:HG3	1.96	0.46
1:1:124:SER:O	1:1:131:TYR:HA	2.15	0.46
3:3:261:LYS:NZ	3:3:307:GLN:O	2.44	0.46
3:3:281:GLN:NE2	3:3:285:ASP:OD1	2.48	0.46
11:H:8:PHE:CE2	11:H:10:ASP:HB2	2.51	0.46
13:J:12:VAL:HG22	13:J:25:CYS:HB2	1.96	0.46
14:K:149:ARG:HB2	14:K:152:MET:HG3	1.96	0.46
2:N:223:LYS:HG3	11:V:187:ILE:HG21	1.97	0.46
10:U:142:ASP:OD1	10:U:147:HIS:NE2	2.48	0.46
13:X:11:ILE:HD11	13:X:142:ALA:HB3	1.97	0.46
3:3:1917:HIS:HB3	3:3:1920:VAL:HB	1.96	0.46
11:H:59:VAL:HG22	11:H:81:VAL:HG12	1.98	0.46
7:R:45:GLY:HA3	7:R:199:LEU:HD11	1.97	0.46
12:W:184:ALA:O	12:W:185:GLU:HG2	2.15	0.46
3:3:757:VAL:O	3:3:760:GLU:HG3	2.15	0.46
8:S:123:PHE:HB3	8:S:134:MET:H	1.81	0.46
4:O:115:ASP:OD2	12:W:72:ARG:NH2	2.49	0.46
10:U:207:ASN:O	10:U:209:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:43:CYS:O	11:V:45:ARG:NH2	2.47	0.46
13:X:126:LEU:HG	13:X:127:ILE:HG23	1.98	0.46
13:J:53:ILE:HB	13:J:60:VAL:HG13	1.98	0.46
1:M:80:ASN:ND2	16:M:312:HOH:O	2.49	0.46
7:R:6:ARG:NH1	16:R:312:HOH:O	2.48	0.46
3:3:1297:LYS:HB2	3:3:1298:PRO:HD3	1.97	0.46
3:3:2139:ARG:NH2	16:E:308:HOH:O	2.48	0.46
4:A:214:LEU:HD12	4:A:218:PHE:HZ	1.80	0.46
12:I:146:LEU:HD22	12:I:150:GLU:HB3	1.97	0.46
6:Q:107:PRO:HD2	6:Q:110:ILE:HD12	1.98	0.46
3:3:146:ASN:HB3	3:3:243:TRP:CE2	2.51	0.45
9:F:121:GLN:HG3	10:G:130:ARG:HB3	1.97	0.45
7:R:241:GLN:NE2	16:R:313:HOH:O	2.49	0.45
3:3:377:SER:OG	3:3:1577:ARG:NH1	2.48	0.45
3:3:1755:ASP:OD1	3:3:1757:ALA:N	2.50	0.45
3:3:1911:LEU:O	3:3:1915:VAL:HG23	2.16	0.45
11:H:6:VAL:HG12	11:H:155:ILE:HD11	1.98	0.45
13:J:125:ASP:OD1	13:J:129:CYS:N	2.28	0.45
3:3:413:SER:OG	3:3:1827:GLU:OE1	2.32	0.45
6:C:103:ASN:HB3	14:K:78:GLN:HE22	1.81	0.45
8:E:184:LEU:HD23	9:F:56:LEU:HG	1.98	0.45
13:J:11:ILE:HD11	13:J:175:ALA:HB2	1.99	0.45
15:Z:12:ILE:HG23	15:Z:112:ILE:HD11	1.98	0.45
8:E:50:VAL:HG12	8:E:218:GLN:HB3	1.98	0.45
12:I:41:ILE:HG12	12:I:76:VAL:HG12	1.99	0.45
13:J:169:GLN:O	13:J:173:ASN:ND2	2.40	0.45
2:2:78:ASN:HD21	2:2:85:GLU:HB3	1.81	0.45
3:3:1338:GLN:NE2	16:3:2280:HOH:O	2.49	0.45
3:3:1448:ASP:OD1	3:3:1482:ARG:NH2	2.45	0.45
15:L:12:ILE:HB	15:L:180:VAL:HB	1.98	0.45
4:O:115:ASP:OD1	4:O:115:ASP:N	2.46	0.45
10:U:214:LEU:HD21	10:U:216:ILE:HD11	1.99	0.45
12:I:34:LEU:HD12	12:I:186:TYR:HE1	1.81	0.45
9:F:52:ASN:HB2	9:F:59:TYR:CE2	2.51	0.45
1:M:221:ARG:HG2	12:W:164:TRP:HZ3	1.82	0.45
5:P:189:ILE:HD11	5:P:213:ILE:HG21	1.99	0.45
1:1:213:ARG:NH1	1:1:215:GLU:OE2	2.45	0.45
6:C:77:VAL:HG22	6:C:135:PHE:HE1	1.82	0.45
14:K:53:THR:HG22	14:K:100:VAL:HG22	1.98	0.45
6:Q:116:SER:HB2	6:Q:155:GLY:O	2.17	0.45
11:V:29:ARG:NH2	12:W:139:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:1706:LYS:NZ	16:3:2262:HOH:O	2.44	0.45
14:K:95:ARG:HD3	14:K:96:ARG:HG3	1.99	0.45
7:R:79:ASN:O	7:R:82:SER:OG	2.25	0.45
3:3:157:GLN:HG3	3:3:276:GLN:HG3	2.00	0.44
4:A:72:ILE:HD12	4:A:224:GLU:HG2	1.99	0.44
5:B:158:PRO:HB2	6:C:58:GLU:HB2	1.98	0.44
6:C:194:LEU:HD13	6:C:239:LEU:HD23	1.99	0.44
2:N:45:VAL:HG11	2:N:92:ILE:HG12	2.00	0.44
2:N:113:ALA:HB1	2:N:129:TYR:CE2	2.52	0.44
4:O:231:ASP:OD2	4:O:232:LYS:NZ	2.48	0.44
9:T:39:ARG:NE	16:T:306:HOH:O	2.40	0.44
15:Z:89:GLN:NE2	16:Z:311:HOH:O	2.49	0.44
1:1:16:ALA:HB2	1:1:122:VAL:HG23	1.98	0.44
9:F:122:SER:O	9:F:123:TYR:HB3	2.17	0.44
1:1:194:ARG:HG2	13:J:151:GLU:HG3	1.99	0.44
2:2:4:PRO:HB2	2:2:7:THR:HG22	1.99	0.44
2:2:127:LEU:HG	2:2:142:LEU:HD12	2.00	0.44
3:3:920:ILE:HD13	3:3:1018:VAL:HG13	1.99	0.44
3:3:1247:PHE:HB3	3:3:1251:ASN:HB3	1.98	0.44
5:B:33:THR:O	5:B:34:SER:OG	2.31	0.44
7:D:68:ASP:OD1	7:D:71:VAL:HB	2.17	0.44
10:G:220:SER:O	10:G:224:THR:OG1	2.29	0.44
6:Q:16:GLU:O	7:R:29:ARG:NH2	2.31	0.44
11:V:43:CYS:HB2	11:V:100:ALA:H	1.81	0.44
14:Y:22:THR:HB	14:Y:27:VAL:HG22	2.00	0.44
3:3:518:ILE:O	3:3:522:ILE:HG13	2.18	0.44
4:A:31:ALA:O	4:A:35:THR:HG23	2.18	0.44
6:C:203:SER:O	6:C:205:ALA:N	2.51	0.44
9:F:176:LEU:HA	9:F:179:PHE:CE2	2.53	0.44
9:T:120:THR:HG22	9:T:127:PRO:HB3	1.98	0.44
13:X:38:ASN:HB3	13:X:183:TRP:CD1	2.47	0.44
13:X:88:THR:HG23	13:X:124:PHE:CZ	2.52	0.44
3:3:659:ARG:HD2	3:3:744:PHE:HZ	1.81	0.44
4:A:64:LEU:O	10:G:161:LYS:NZ	2.50	0.44
7:D:171:VAL:HG13	7:D:197:ARG:HH22	1.83	0.44
14:K:49:GLU:HB2	14:K:99:GLN:HB2	1.98	0.44
3:3:496:VAL:HG21	3:3:544:SER:HB2	2.00	0.44
8:E:169:ALA:HB1	8:E:183:LEU:HD22	1.99	0.44
12:I:50:ALA:HB2	13:J:129:CYS:HB2	2.00	0.44
7:R:151:GLU:N	7:R:151:GLU:OE1	2.51	0.44
3:3:881:VAL:O	3:3:926:THR:OG1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:36:ARG:NH2	11:H:39:ASP:OD1	2.38	0.44
1:M:16:ALA:HB2	1:M:122:VAL:HG23	2.00	0.44
1:1:33:TYR:HA	12:I:167:LEU:HD12	2.00	0.44
6:C:191:GLU:HG2	6:C:242:THR:HG22	1.98	0.44
4:O:194:ILE:HD12	4:O:202:VAL:HG13	2.00	0.44
10:U:42:CYS:HB2	10:U:187:LEU:O	2.17	0.44
3:3:762:ILE:O	3:3:766:VAL:HG23	2.18	0.44
3:3:1244:ASN:ND2	16:3:2288:HOH:O	2.51	0.44
4:O:115:ASP:HB3	4:O:155:TYR:CZ	2.52	0.44
3:3:313:HIS:CD2	3:3:366:LEU:HD11	2.53	0.43
3:3:1767:LEU:HD21	3:3:1784:LEU:HD11	2.00	0.43
5:B:74:VAL:HG12	5:B:135:LEU:HB2	1.99	0.43
1:M:23:LEU:HD12	1:M:51:VAL:HG23	2.00	0.43
4:O:156:LYS:HB3	4:O:166:TYR:HE1	1.83	0.43
7:R:121:THR:HG22	7:R:128:PRO:HB3	2.00	0.43
8:S:68:VAL:HG11	8:S:89:ILE:HG21	1.99	0.43
12:W:175:VAL:O	12:W:187:LEU:HB2	2.18	0.43
4:A:175:GLN:NE2	16:A:311:HOH:O	2.40	0.43
15:Z:143:ASN:ND2	16:Z:310:HOH:O	2.46	0.43
3:3:674:ASP:H	3:3:681:THR:HG22	1.84	0.43
3:3:780:GLN:NE2	16:3:2289:HOH:O	2.51	0.43
3:3:1148:ASP:O	3:3:1150:TYR:N	2.47	0.43
9:F:33:SER:HB3	9:F:62:LYS:HE3	1.99	0.43
11:V:3:ILE:HG22	11:V:98:ILE:HD12	2.00	0.43
3:3:1553:GLU:HG2	3:3:1562:TYR:CZ	2.53	0.43
13:X:145:GLN:OE1	13:X:145:GLN:N	2.43	0.43
13:X:177:ARG:HD2	13:X:177:ARG:HA	1.82	0.43
3:3:326:TYR:CG	3:3:327:PRO:HD2	2.53	0.43
3:3:579:LEU:HD23	3:3:579:LEU:HA	1.87	0.43
5:B:46:ALA:HB1	5:B:196:LEU:HD11	2.00	0.43
6:C:44:ILE:HD11	6:C:146:TYR:HB3	2.00	0.43
2:N:129:TYR:O	2:N:136:THR:HA	2.18	0.43
8:S:43:LYS:NZ	16:S:312:HOH:O	2.50	0.43
15:Z:55:TRP:CE3	15:Z:86:LEU:HD21	2.54	0.43
3:3:93:TYR:CD2	3:3:137:ALA:HB2	2.54	0.43
12:I:63:ILE:HD12	12:I:79:ALA:HB2	1.99	0.43
9:T:227:GLY:O	9:T:230:VAL:HG22	2.19	0.43
14:Y:172:MET:HG3	14:Y:174:MET:H	1.84	0.43
3:3:785:LEU:O	3:3:789:MET:HG3	2.19	0.43
3:3:910:PRO:HB2	3:3:911:PRO:HD3	2.00	0.43
3:3:932:ILE:HD13	3:3:1253:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:216:ASN:ND2	16:E:305:HOH:O	2.37	0.43
2:2:53:ILE:HD11	2:2:63:ILE:HD11	2.01	0.43
3:3:112:PHE:O	3:3:257:VAL:HG23	2.19	0.43
3:3:967:PHE:HE1	3:3:1249:ARG:HG3	1.84	0.43
3:3:1466:ARG:HG3	3:3:1501:LEU:HD21	2.00	0.43
3:3:1909:PRO:HA	3:3:1912:ILE:HG22	2.01	0.43
12:I:200:GLN:NE2	16:I:314:HOH:O	2.50	0.43
7:R:159:TRP:CZ3	8:S:56:SER:HB3	2.53	0.43
1:1:24:ALA:HB1	1:1:202:LEU:HD11	1.99	0.43
1:1:192:THR:HG23	1:1:199:GLY:HA3	2.01	0.43
1:M:194:ARG:HG2	13:X:147:PHE:HB3	2.01	0.43
6:Q:83:ASP:HB3	6:Q:131:PHE:HD1	1.83	0.43
11:V:41:ILE:HG22	11:V:101:GLY:HA3	2.00	0.43
15:Z:114:TYR:HB3	15:Z:122:LEU:HD12	2.01	0.43
3:3:391:THR:HG22	3:3:431:PHE:HB2	2.01	0.43
6:C:36:ILE:HD12	6:C:197:LEU:HG	2.00	0.43
11:H:14:LEU:HD21	11:H:100:ALA:HB3	2.01	0.43
12:W:3:ILE:HD13	12:W:44:ALA:HB1	2.01	0.43
14:Y:4:ILE:HG22	14:Y:103:LEU:HD12	2.01	0.43
15:Z:12:ILE:HG21	15:Z:102:CYS:HB3	2.01	0.43
3:3:133:HIS:NE2	3:3:134:GLU:OE2	2.52	0.42
5:B:66:LEU:HD12	5:B:235:PHE:CD1	2.54	0.42
10:U:211:ASP:OD1	10:U:212:PHE:N	2.52	0.42
3:3:1556:ASN:ND2	3:3:1559:ASN:O	2.49	0.42
7:D:172:ARG:NH2	16:D:309:HOH:O	2.45	0.42
15:L:145:LYS:HD3	15:L:148:LEU:HD21	2.01	0.42
6:Q:77:VAL:HG12	6:Q:135:PHE:HE1	1.85	0.42
3:3:452:VAL:HG12	3:3:455:VAL:HB	2.00	0.42
3:3:2125:PHE:HB2	3:3:2130:LEU:HG	2.01	0.42
4:A:40:ILE:HG23	4:A:56:GLN:HB2	2.01	0.42
13:J:88:THR:HG23	13:J:124:PHE:CZ	2.55	0.42
1:M:13:LEU:HD12	1:M:137:ARG:O	2.18	0.42
5:P:32:VAL:HG22	5:P:50:LYS:HE2	2.01	0.42
3:3:139:TYR:HB2	3:3:1149:ILE:HD11	2.00	0.42
3:3:2030:LEU:HG	3:3:2068:ILE:HD11	2.02	0.42
5:B:75:TYR:HB3	5:B:82:TYR:CD1	2.55	0.42
7:D:66:LYS:HA	7:D:72:VAL:HG13	2.02	0.42
10:G:151:LEU:N	16:G:312:HOH:O	2.52	0.42
13:J:190:ILE:HG23	13:J:195:VAL:HG22	2.01	0.42
1:M:65:VAL:HG12	1:M:69:LYS:HE2	2.01	0.42
2:N:45:VAL:HB	2:N:49:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:598:ILE:HG22	3:3:647:ARG:HG3	2.01	0.42
3:3:1841:VAL:HG23	3:3:1898:LEU:HD22	2.02	0.42
3:3:2141:TYR:HA	8:E:163:THR:HG21	2.02	0.42
8:E:205:LYS:HG3	8:E:210:GLU:HA	2.01	0.42
10:U:141:VAL:HG21	10:U:220:SER:HA	2.02	0.42
15:Z:87:VAL:HG11	15:Z:117:SER:HA	2.01	0.42
2:2:78:ASN:HB3	2:2:81:ALA:HB2	2.02	0.42
3:3:1186:LEU:HD23	3:3:1204:LEU:HD13	2.01	0.42
11:H:67:THR:HA	11:H:71:GLY:O	2.19	0.42
15:L:12:ILE:HG23	15:L:112:ILE:HD11	2.02	0.42
4:O:16:ILE:HG13	4:O:18:ILE:HG12	2.02	0.42
12:W:51:ASP:HB3	12:W:94:ILE:HG23	2.01	0.42
3:3:871:LEU:HD11	3:3:912:LEU:HD22	2.01	0.42
3:3:871:LEU:HD12	3:3:874:TYR:HD2	1.84	0.42
3:3:1781:VAL:HG22	3:3:1784:LEU:HG	2.02	0.42
7:D:67:ILE:HD11	7:D:73:LEU:HB2	2.01	0.42
14:K:101:ASN:HB3	14:K:133:HIS:CE1	2.54	0.42
2:N:228:TYR:HA	12:W:121:VAL:HG23	2.01	0.42
13:X:105:VAL:HG23	13:X:107:PRO:HD3	2.02	0.42
3:3:532:LYS:HE3	3:3:536:LYS:HE3	2.01	0.42
3:3:824:PRO:O	3:3:827:ALA:HB3	2.20	0.42
3:3:1364:ILE:HD12	3:3:1442:LEU:HD21	2.01	0.42
9:T:26:LEU:HD23	9:T:149:PRO:HD2	2.01	0.42
12:W:113:ILE:HG12	12:W:119:THR:HG22	2.02	0.42
2:2:104:ARG:HG3	2:2:133:LEU:HA	2.02	0.42
3:3:128:TYR:CD1	3:3:1153:ASN:HB2	2.55	0.42
3:3:160:ILE:HG21	3:3:1428:LYS:HA	2.02	0.42
4:A:156:LYS:O	4:A:163:TYR:HA	2.19	0.42
7:D:49:ARG:HH22	7:D:166:ARG:CZ	2.33	0.42
7:D:216:LYS:HE2	7:D:216:LYS:HB3	1.95	0.42
8:E:232:ASP:OD1	8:E:232:ASP:N	2.50	0.42
14:K:4:ILE:HG13	14:K:47:ALA:HB2	2.01	0.42
4:O:83:VAL:HG13	4:O:141:LEU:HD23	2.01	0.42
7:R:73:LEU:HD13	7:R:135:ILE:HG12	2.00	0.42
3:3:885:CYS:H	3:3:926:THR:CG2	2.32	0.42
10:G:232:LYS:HA	10:G:236:LEU:HB2	2.00	0.42
4:O:69:VAL:HA	10:U:158:TRP:CZ3	2.55	0.42
10:U:221:LEU:O	10:U:222:SER:OG	2.31	0.42
12:W:175:VAL:HB	12:W:187:LEU:HG	2.02	0.42
11:H:21:THR:HG22	11:H:26:ILE:HG12	2.02	0.41
4:O:40:ILE:HG12	4:O:58:LYS:HZ1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:63:LEU:HD11	11:V:78:ALA:HB2	2.02	0.41
1:1:13:LEU:HD13	1:1:138:ALA:HB2	2.01	0.41
3:3:805:PHE:CZ	3:3:876:THR:HG21	2.55	0.41
13:J:56:LEU:O	13:J:60:VAL:HG23	2.20	0.41
8:S:117:CYS:SG	8:S:164:PHE:HB3	2.60	0.41
12:W:21:THR:HA	12:W:27:ALA:H	1.85	0.41
1:1:18:GLU:HB3	1:1:174:TYR:HE1	1.85	0.41
1:1:91:ARG:HH21	15:Z:57:THR:HG21	1.84	0.41
3:3:922:SER:O	3:3:926:THR:OG1	2.31	0.41
3:3:1863:VAL:HG12	3:3:1866:LEU:HD12	2.01	0.41
3:3:2086:LEU:HD13	3:3:2086:LEU:HA	1.94	0.41
9:F:18:ARG:NH2	9:F:23:GLU:OE1	2.53	0.41
4:O:32:PHE:HE2	4:O:160:ALA:HB2	1.86	0.41
10:U:32:GLU:HG3	10:U:169:ARG:NH1	2.35	0.41
14:Y:23:ARG:HH22	14:Y:28:LEU:HD12	1.86	0.41
10:G:48:PHE:HB2	10:G:217:SER:OG	2.20	0.41
14:K:50:ALA:O	14:K:52:ASP:N	2.53	0.41
2:N:173:ALA:O	2:N:177:ILE:HG12	2.20	0.41
3:3:268:TYR:OH	3:3:312:ASP:O	2.33	0.41
5:B:210:GLU:OE2	5:B:237:LYS:NZ	2.43	0.41
9:F:13:PHE:N	10:G:23:GLN:OE1	2.35	0.41
10:G:222:SER:OG	10:G:223:GLU:OE1	2.33	0.41
11:H:59:VAL:HG11	11:H:82:PHE:CE2	2.56	0.41
14:K:13:VAL:HG11	14:K:105:GLY:HA3	2.02	0.41
14:K:142:PHE:CE2	14:K:143:LEU:HG	2.56	0.41
2:N:12:ILE:HD11	2:N:184:LEU:HD12	2.02	0.41
7:R:7:ALA:HB2	8:S:135:SER:HB2	2.02	0.41
3:3:700:LEU:HD22	3:3:946:GLU:HB3	2.02	0.41
3:3:850:GLN:NE2	16:3:2272:HOH:O	2.47	0.41
6:C:114:ARG:NH2	16:C:306:HOH:O	2.47	0.41
14:K:180:ILE:HD11	14:K:182:LYS:HE3	2.02	0.41
8:S:167:TYR:CE2	9:T:57:SER:HB3	2.55	0.41
12:W:99:ILE:HG13	12:W:127:LEU:HD12	2.02	0.41
14:Y:149:ARG:NH1	16:Y:317:HOH:O	2.53	0.41
2:N:96:LEU:O	2:N:100:MET:HG2	2.20	0.41
8:S:123:PHE:CB	8:S:134:MET:HG2	2.50	0.41
8:E:27:SER:HB3	8:E:137:PRO:HG3	2.02	0.41
7:R:67:ILE:HG21	7:R:109:LEU:HD21	2.01	0.41
8:S:214:GLU:OE2	8:S:215:ASN:ND2	2.53	0.41
10:U:200:ILE:HG21	10:U:214:LEU:HD13	2.02	0.41
11:V:190:PRO:HA	11:V:193:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:659:ARG:HD2	3:3:744:PHE:CZ	2.56	0.41
3:3:736:ASP:HB3	3:3:738:GLU:HG3	2.02	0.41
3:3:1398:SER:HA	3:3:1432:ARG:NH1	2.36	0.41
3:3:1491:ILE:HD13	3:3:1610:PHE:CD1	2.55	0.41
3:3:1628:PHE:HB2	3:3:1629:SER:H	1.66	0.41
9:F:195:GLU:O	9:F:199:GLN:HG2	2.21	0.41
11:H:175:MET:HB3	16:H:218:HOH:O	2.21	0.41
13:J:49:VAL:HG12	13:J:84:PRO:HG3	2.01	0.41
4:O:70:SER:OG	4:O:224:GLU:OE2	2.26	0.41
8:S:71:ASP:OD1	8:S:72:ARG:N	2.48	0.41
10:U:219:CYS:HB2	10:U:228:HIS:HA	2.02	0.41
13:X:63:LEU:HD11	13:X:105:VAL:HG21	2.03	0.41
14:Y:38:LEU:HD21	14:Y:44:MET:HE2	2.02	0.41
2:2:88:GLU:OE1	2:2:120:GLN:NE2	2.50	0.41
15:L:13:ILE:HG13	15:L:153:ALA:HB1	2.03	0.41
1:M:52:MET:HE3	1:M:65:VAL:HG22	2.03	0.41
5:P:71:ILE:HG21	5:P:110:LEU:HD23	2.03	0.41
3:3:760:GLU:OE1	3:3:764:GLN:NE2	2.54	0.40
5:B:160:LYS:HD3	5:B:179:TRP:CH2	2.55	0.40
6:C:162:ALA:HB1	6:C:176:LEU:HD13	2.02	0.40
8:E:211:LYS:HA	8:E:211:LYS:HD2	1.87	0.40
9:F:46:LEU:HD13	9:F:73:SER:HB3	2.03	0.40
5:P:41:ASN:ND2	5:P:184:GLU:OE1	2.52	0.40
9:T:226:ASP:OD1	9:T:227:GLY:N	2.54	0.40
10:U:27:ALA:O	10:U:31:VAL:HG23	2.22	0.40
1:1:222:ASP:HB3	2:2:161:ARG:HH22	1.86	0.40
2:2:53:ILE:HD12	2:2:60:MET:HG3	2.02	0.40
3:3:1445:LYS:HE3	3:3:1445:LYS:HB2	1.88	0.40
7:D:70:HIS:CD2	7:D:71:VAL:HG23	2.56	0.40
7:D:103:PRO:HG2	7:D:140:PRO:HG3	2.04	0.40
8:E:72:ARG:NH2	8:E:225:GLN:O	2.55	0.40
9:F:110:HIS:HA	10:G:86:ARG:NH2	2.35	0.40
9:F:135:ILE:HG22	9:F:144:LEU:HD13	2.03	0.40
2:N:93:PHE:HZ	2:N:136:THR:HB	1.87	0.40
2:N:113:ALA:HB1	2:N:129:TYR:HE2	1.86	0.40
7:R:159:TRP:HZ3	8:S:56:SER:HB3	1.87	0.40
9:T:140:SER:OG	9:T:143:HIS:NE2	2.48	0.40
8:E:70:ILE:HG21	8:E:112:LEU:HD21	2.03	0.40
11:H:13:ILE:HG23	16:H:218:HOH:O	2.20	0.40
4:O:43:LEU:HD12	4:O:169:THR:O	2.21	0.40
4:O:156:LYS:O	4:O:163:TYR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:145:GLY:O	6:Q:146:TYR:HB2	2.22	0.40
13:X:74:TYR:CD1	13:X:82:ILE:HG12	2.56	0.40
3:3:149:ILE:HG12	3:3:1417:ILE:HD11	2.04	0.40
3:3:626:THR:HG23	3:3:638:ILE:HG12	2.04	0.40
7:D:119:ARG:NH2	16:D:315:HOH:O	2.54	0.40
10:U:158:TRP:HB2	10:U:160:TYR:CE1	2.56	0.40
12:W:159:ILE:HG21	12:W:173:VAL:HG13	2.03	0.40
1:1:28:ARG:HD3	1:1:200:ASP:OD2	2.22	0.40
3:3:287:PHE:O	3:3:291:VAL:HG22	2.22	0.40
3:3:996:GLU:O	3:3:1000:LYS:HG3	2.22	0.40
4:A:70:SER:OG	4:A:224:GLU:OE2	2.23	0.40
12:I:3:ILE:HG12	12:I:44:ALA:HB1	2.04	0.40
15:L:113:TYR:CE1	15:L:123:LYS:HB2	2.57	0.40
10:U:127:ASN:OD1	10:U:127:ASN:N	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	219/222 (99%)	216 (99%)	3 (1%)	0	100	100
1	M	218/222 (98%)	209 (96%)	9 (4%)	0	100	100
2	2	227/233 (97%)	222 (98%)	5 (2%)	0	100	100
2	N	226/233 (97%)	218 (96%)	8 (4%)	0	100	100
3	3	1857/2143 (87%)	1795 (97%)	62 (3%)	0	100	100
4	A	238/252 (94%)	230 (97%)	8 (3%)	0	100	100
4	O	230/252 (91%)	219 (95%)	11 (5%)	0	100	100
5	B	231/250 (92%)	224 (97%)	5 (2%)	2 (1%)	14	22
5	P	238/250 (95%)	235 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	226/258 (88%)	218 (96%)	8 (4%)	0	100	100
6	Q	129/258 (50%)	120 (93%)	9 (7%)	0	100	100
7	D	211/254 (83%)	197 (93%)	14 (7%)	0	100	100
7	R	217/254 (85%)	209 (96%)	8 (4%)	0	100	100
8	E	214/260 (82%)	206 (96%)	7 (3%)	1 (0%)	25	38
8	S	240/260 (92%)	236 (98%)	4 (2%)	0	100	100
9	F	225/234 (96%)	213 (95%)	11 (5%)	1 (0%)	30	44
9	T	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
10	G	207/288 (72%)	199 (96%)	8 (4%)	0	100	100
10	U	234/288 (81%)	224 (96%)	9 (4%)	1 (0%)	30	44
11	H	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
11	V	193/196 (98%)	179 (93%)	13 (7%)	1 (0%)	25	38
12	I	219/232 (94%)	214 (98%)	5 (2%)	0	100	100
12	W	213/232 (92%)	207 (97%)	6 (3%)	0	100	100
13	J	199/205 (97%)	190 (96%)	9 (4%)	0	100	100
13	X	201/205 (98%)	189 (94%)	11 (6%)	1 (0%)	25	38
14	K	184/212 (87%)	172 (94%)	12 (6%)	0	100	100
14	Y	189/212 (89%)	186 (98%)	3 (2%)	0	100	100
15	L	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
15	Z	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
All	All	7828/8759 (89%)	7548 (96%)	273 (4%)	7 (0%)	50	65

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	203	GLU
13	X	195	VAL
5	B	34	SER
8	E	169	ALA
9	F	123	TYR
10	U	222	SER
11	V	122	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	184/185 (100%)	182 (99%)	2 (1%)	70 84
1	M	183/185 (99%)	175 (96%)	8 (4%)	24 41
2	2	195/199 (98%)	190 (97%)	5 (3%)	41 62
2	N	195/199 (98%)	189 (97%)	6 (3%)	35 56
3	3	1728/1963 (88%)	1697 (98%)	31 (2%)	54 73
4	A	206/210 (98%)	204 (99%)	2 (1%)	73 86
4	O	202/210 (96%)	196 (97%)	6 (3%)	36 57
5	B	193/209 (92%)	191 (99%)	2 (1%)	73 86
5	P	202/209 (97%)	198 (98%)	4 (2%)	50 70
6	C	188/216 (87%)	184 (98%)	4 (2%)	48 69
6	Q	109/216 (50%)	106 (97%)	3 (3%)	38 59
7	D	194/226 (86%)	189 (97%)	5 (3%)	41 62
7	R	199/226 (88%)	197 (99%)	2 (1%)	73 86
8	E	182/215 (85%)	176 (97%)	6 (3%)	33 53
8	S	198/215 (92%)	196 (99%)	2 (1%)	73 86
9	F	190/193 (98%)	181 (95%)	9 (5%)	22 38
9	T	190/193 (98%)	186 (98%)	4 (2%)	48 69
10	G	180/239 (75%)	176 (98%)	4 (2%)	47 67
10	U	198/239 (83%)	191 (96%)	7 (4%)	31 51
11	H	162/162 (100%)	161 (99%)	1 (1%)	84 92
11	V	161/162 (99%)	154 (96%)	7 (4%)	25 42
12	I	180/190 (95%)	174 (97%)	6 (3%)	33 53
12	W	174/190 (92%)	169 (97%)	5 (3%)	37 58
13	J	169/173 (98%)	165 (98%)	4 (2%)	44 64
13	X	171/173 (99%)	168 (98%)	3 (2%)	54 73
14	K	167/189 (88%)	164 (98%)	3 (2%)	54 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	Y	172/189 (91%)	171 (99%)	1 (1%)	84 92
15	L	169/169 (100%)	163 (96%)	6 (4%)	30 49
15	Z	169/169 (100%)	165 (98%)	4 (2%)	44 64
All	All	6810/7513 (91%)	6658 (98%)	152 (2%)	47 67

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	57	PHE
1	1	77	PHE
2	2	9	THR
2	2	27	LEU
2	2	63	ILE
2	2	132	LEU
2	2	208	PHE
3	3	97	ARG
3	3	129	LYS
3	3	319	PHE
3	3	346	ARG
3	3	393	VAL
3	3	410	PHE
3	3	415	TRP
3	3	425	ASP
3	3	432	VAL
3	3	566	LEU
3	3	596	TYR
3	3	624	TYR
3	3	650	ARG
3	3	677	ASP
3	3	680	LEU
3	3	735	VAL
3	3	738	GLU
3	3	750	VAL
3	3	814	LYS
3	3	815	ASP
3	3	871	LEU
3	3	905	ASP
3	3	950	TRP
3	3	1266	LEU
3	3	1375	GLU
3	3	1753	GLU

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Mol	Chain	Res	Type
3	3	1814	ASN
3	3	1854	GLU
3	3	1873	LYS
3	3	1950	ASP
3	3	2094	ARG
4	A	167	LYS
4	A	244	ARG
5	B	45	ILE
5	B	50	LYS
6	C	24	TYR
6	C	80	LEU
6	C	122	TYR
6	C	213	PHE
7	D	79	ASN
7	D	183	GLU
7	D	193	LYS
7	D	196	VAL
7	D	222	VAL
8	E	20	ARG
8	E	32	LYS
8	E	33	LEU
8	E	43	LYS
8	E	165	TYR
8	E	213	ASP
9	F	1	MET
9	F	35	THR
9	F	41	ASN
9	F	107	ARG
9	F	135	ILE
9	F	164	ARG
9	F	218	LYS
9	F	219	ASP
9	F	226	ASP
10	G	91	ARG
10	G	104	LYS
10	G	214	LEU
10	G	231	VAL
11	H	3	ILE
12	I	30	ASN
12	I	76	VAL
12	I	178	MET
12	I	188	ARG

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Mol	Chain	Res	Type
12	I	197	GLU
12	I	220	ILE
13	J	21	VAL
13	J	75	LYS
13	J	118	LYS
13	J	183	TRP
14	K	33	ASP
14	K	49	GLU
14	K	95	ARG
15	L	72	GLU
15	L	74	ILE
15	L	104	TYR
15	L	137	TYR
15	L	145	LYS
15	L	146	TRP
1	M	23	LEU
1	M	73	LYS
1	M	77	PHE
1	M	91	ARG
1	M	103	PHE
1	M	126	ASP
1	M	128	VAL
1	M	137	ARG
2	N	76	TYR
2	N	186	TYR
2	N	187	ARG
2	N	208	PHE
2	N	209	LYS
2	N	219	TRP
4	O	61	ASP
4	O	62	LYS
4	O	105	ARG
4	O	174	LYS
4	O	188	LYS
4	O	244	ARG
5	P	4	ARG
5	P	132	VAL
5	P	140	ASP
5	P	157	PHE
6	Q	1	MET
6	Q	6	TYR
6	Q	31	HIS

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Mol	Chain	Res	Type
7	R	133	THR
7	R	214	VAL
8	S	66	LYS
8	S	222	ILE
9	T	9	ASP
9	T	30	LYS
9	T	113	CYS
9	T	202	ARG
10	U	18	ASP
10	U	44	ASP
10	U	104	LYS
10	U	134	VAL
10	U	185	GLU
10	U	218	TRP
10	U	224	THR
11	V	14	LEU
11	V	44	CYS
11	V	45	ARG
11	V	93	LEU
11	V	94	THR
11	V	112	THR
11	V	143	ARG
12	W	28	ASP
12	W	40	LYS
12	W	154	LEU
12	W	182	LYS
12	W	183	ASP
13	X	85	GLU
13	X	99	ARG
13	X	183	TRP
14	Y	149	ARG
15	Z	2	THR
15	Z	104	TYR
15	Z	122	LEU
15	Z	185	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	131	ASN
12	I	194	ASN
4	O	56	GLN

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Mol	Chain	Res	Type
7	R	122	GLN
8	S	154	GLN
10	U	43	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

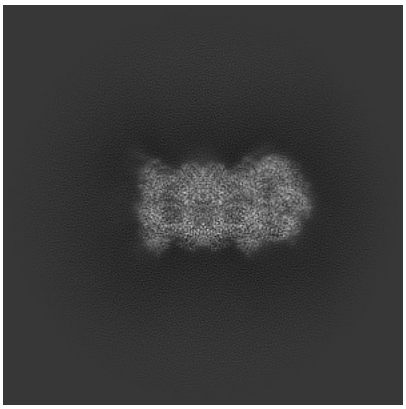
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51221. These allow visual inspection of the internal detail of the map and identification of artifacts.

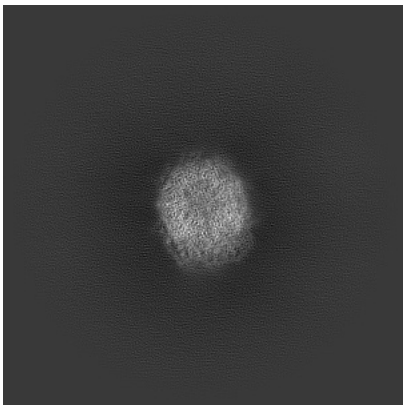
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

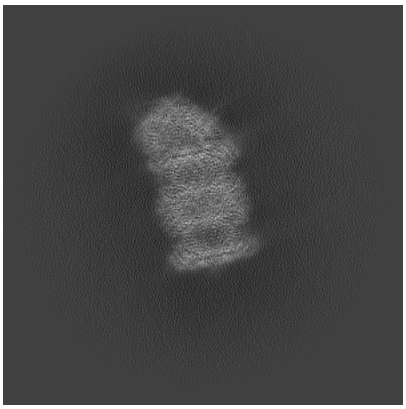
6.1.1 Primary map



X

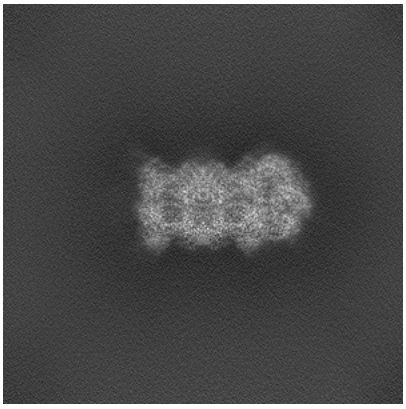


Y

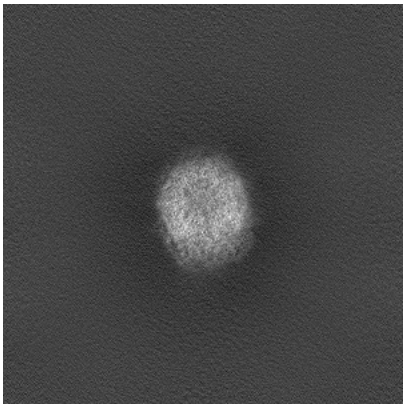


Z

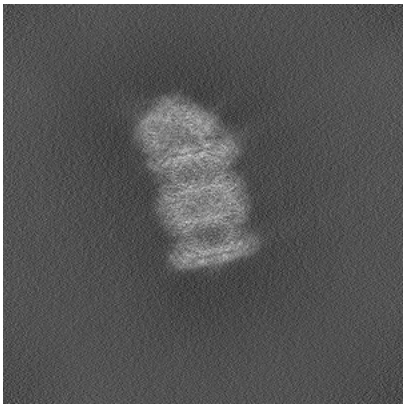
6.1.2 Raw map



X



Y

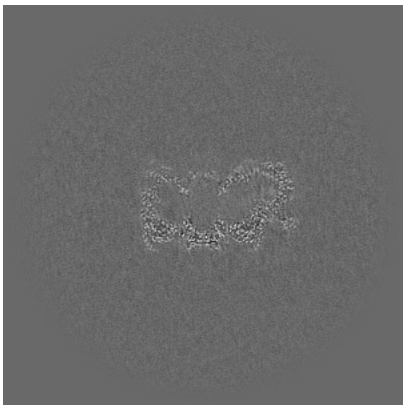


Z

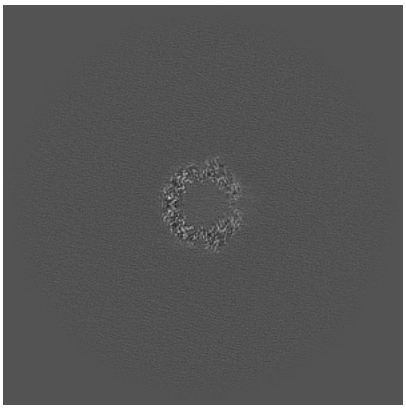
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

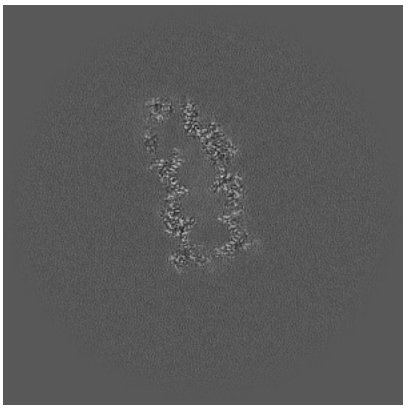
6.2.1 Primary map



X Index: 300

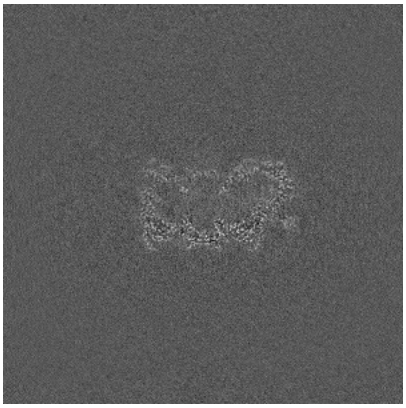


Y Index: 300

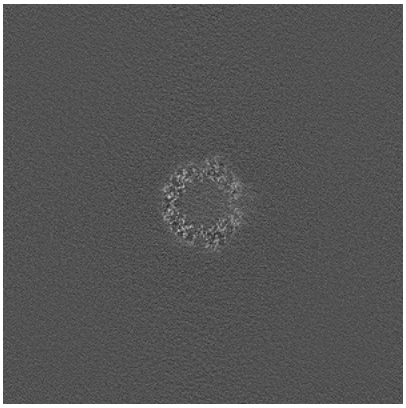


Z Index: 300

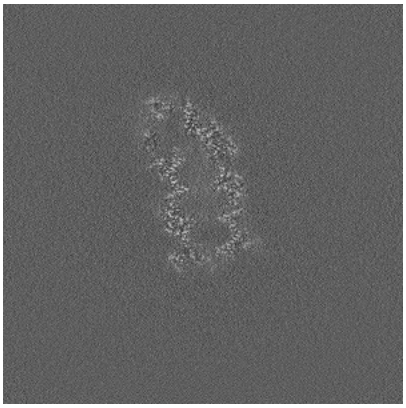
6.2.2 Raw map



X Index: 300



Y Index: 300

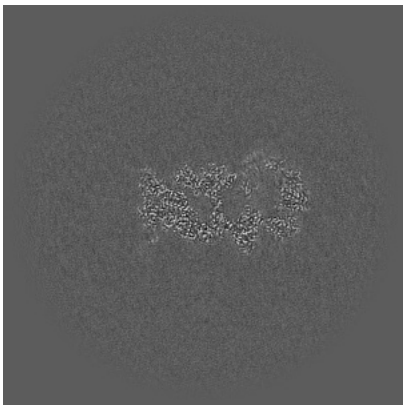


Z Index: 300

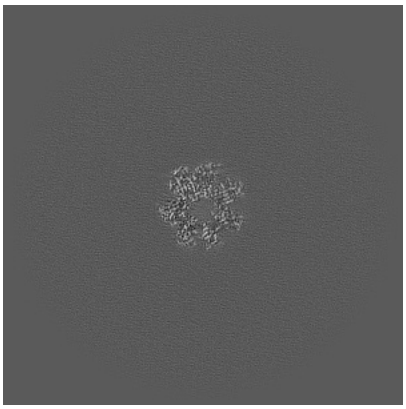
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

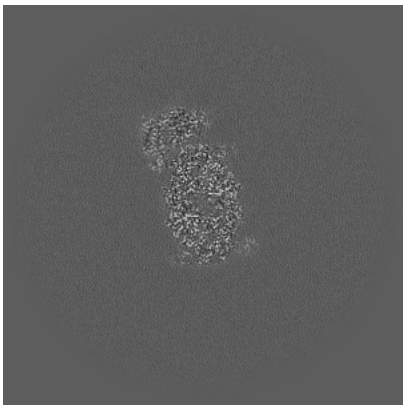
6.3.1 Primary map



X Index: 272

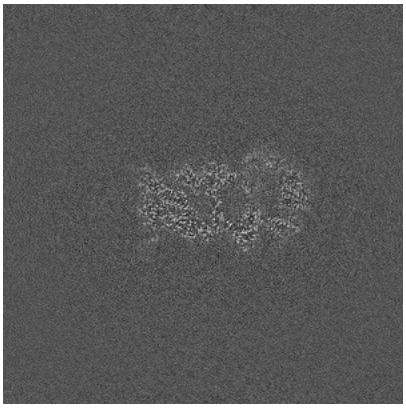


Y Index: 327

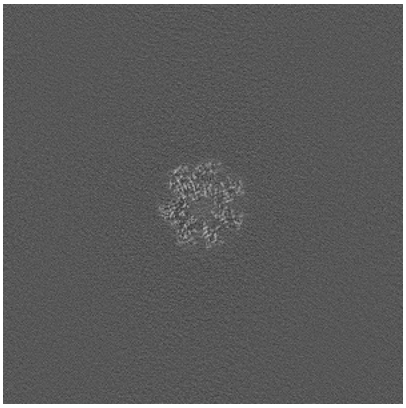


Z Index: 268

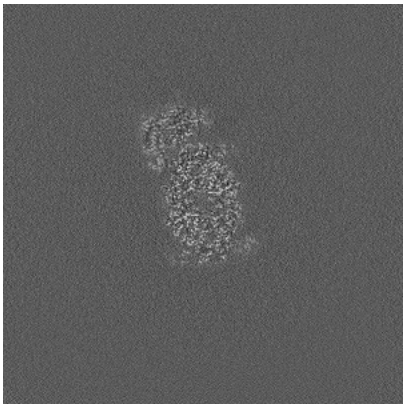
6.3.2 Raw map



X Index: 272



Y Index: 327

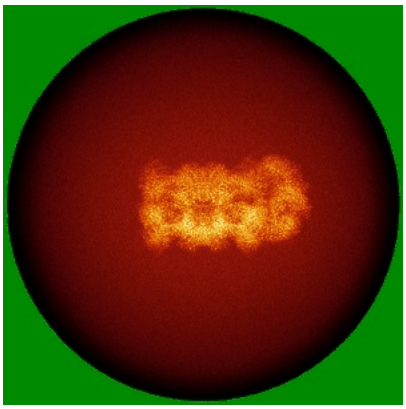


Z Index: 268

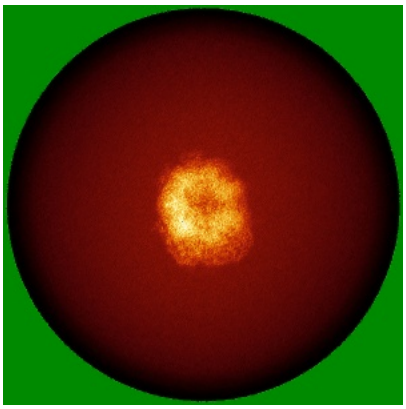
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

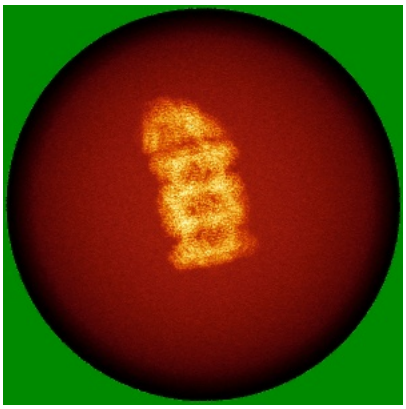
6.4.1 Primary map



X

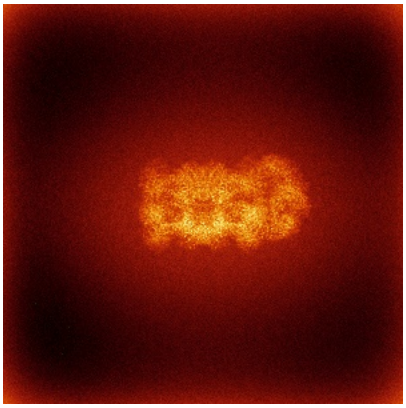


Y

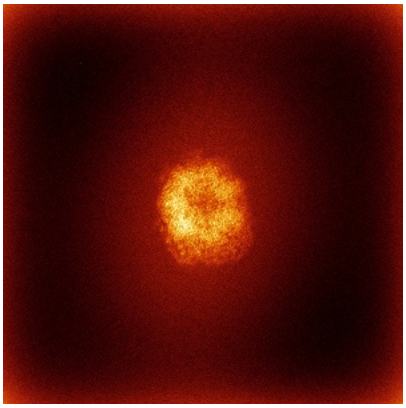


Z

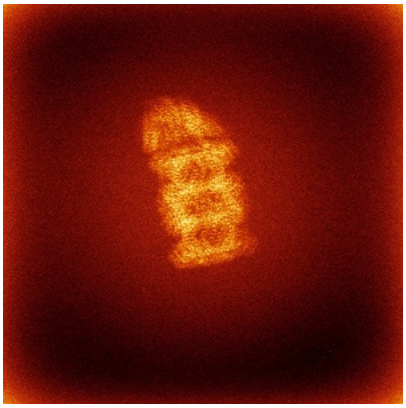
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

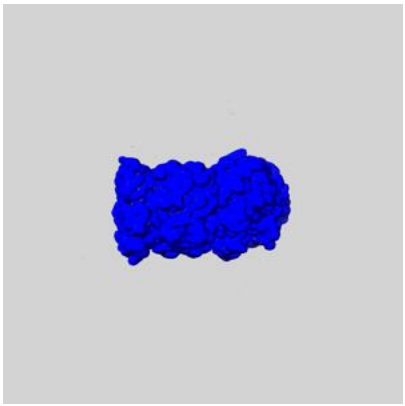
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

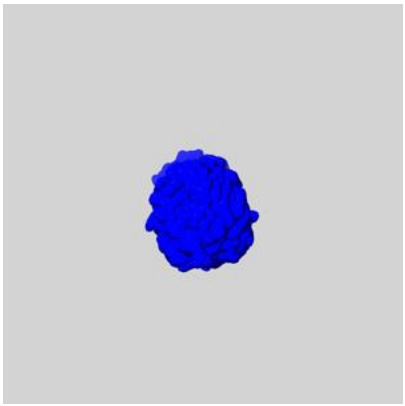
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

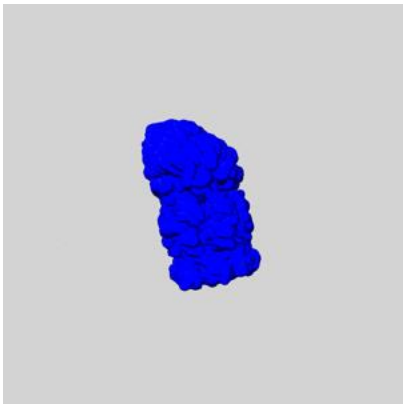
6.6.1 emd_51221_msk_1.map (i)



X



Y

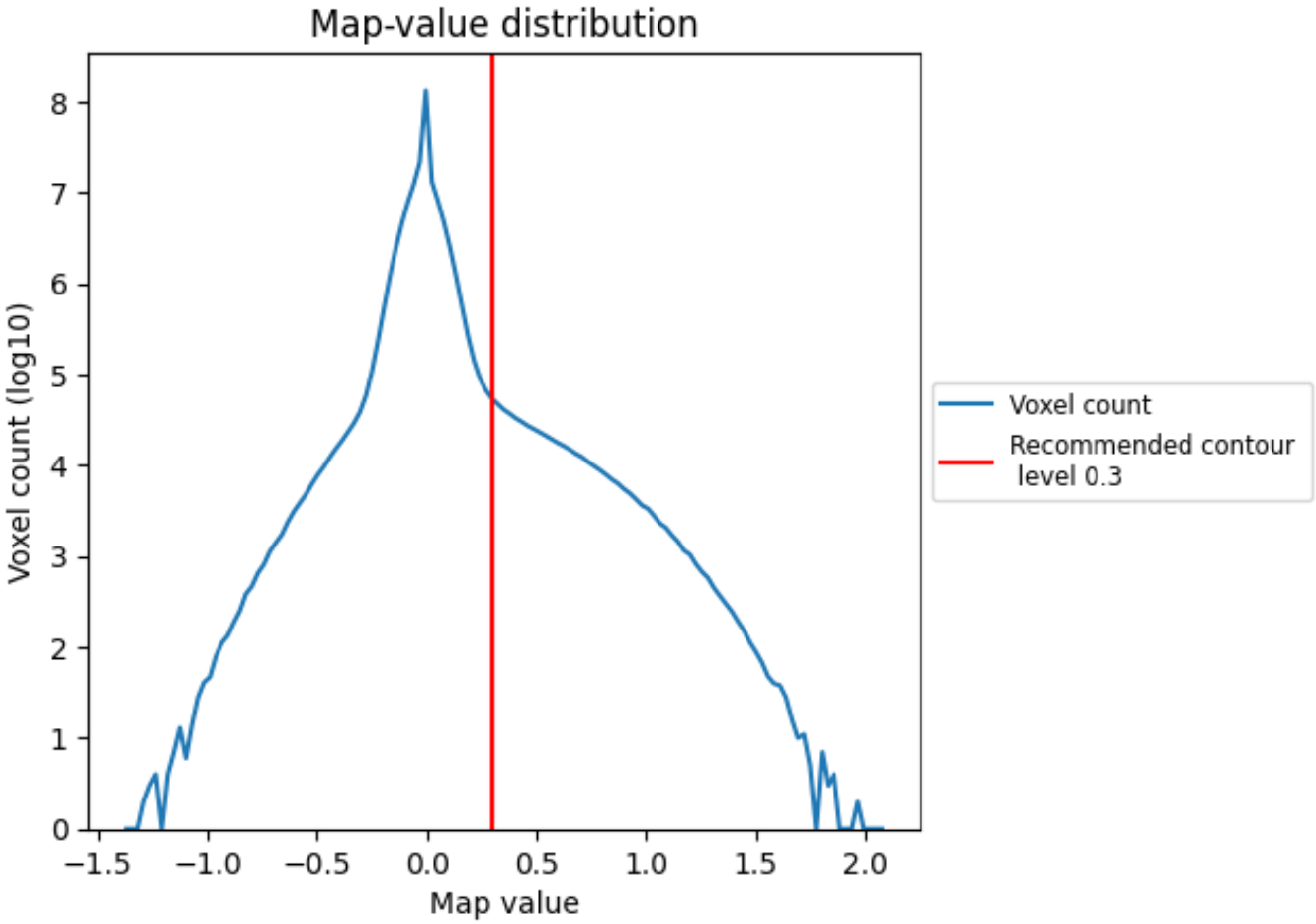


Z

7 Map analysis

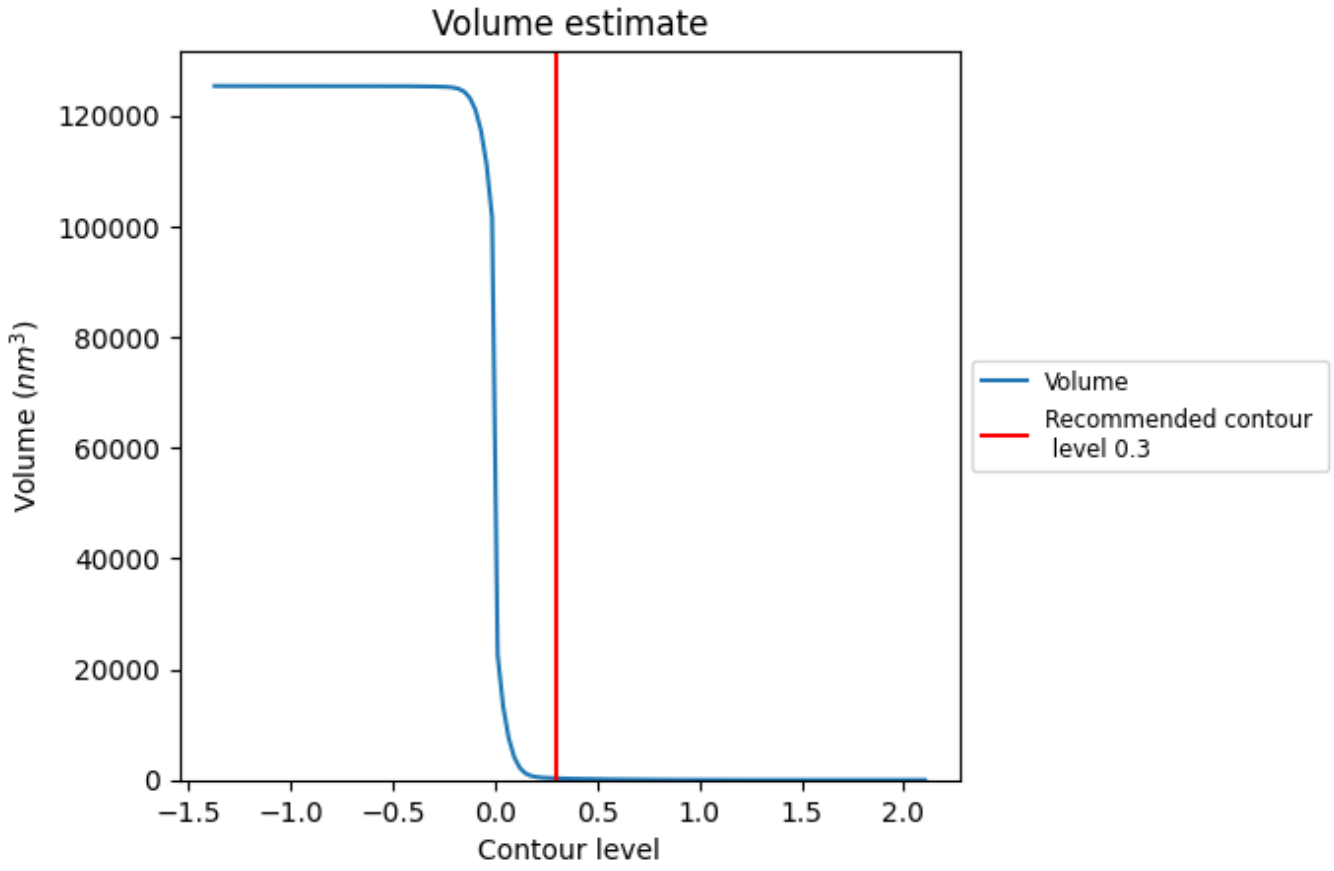
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

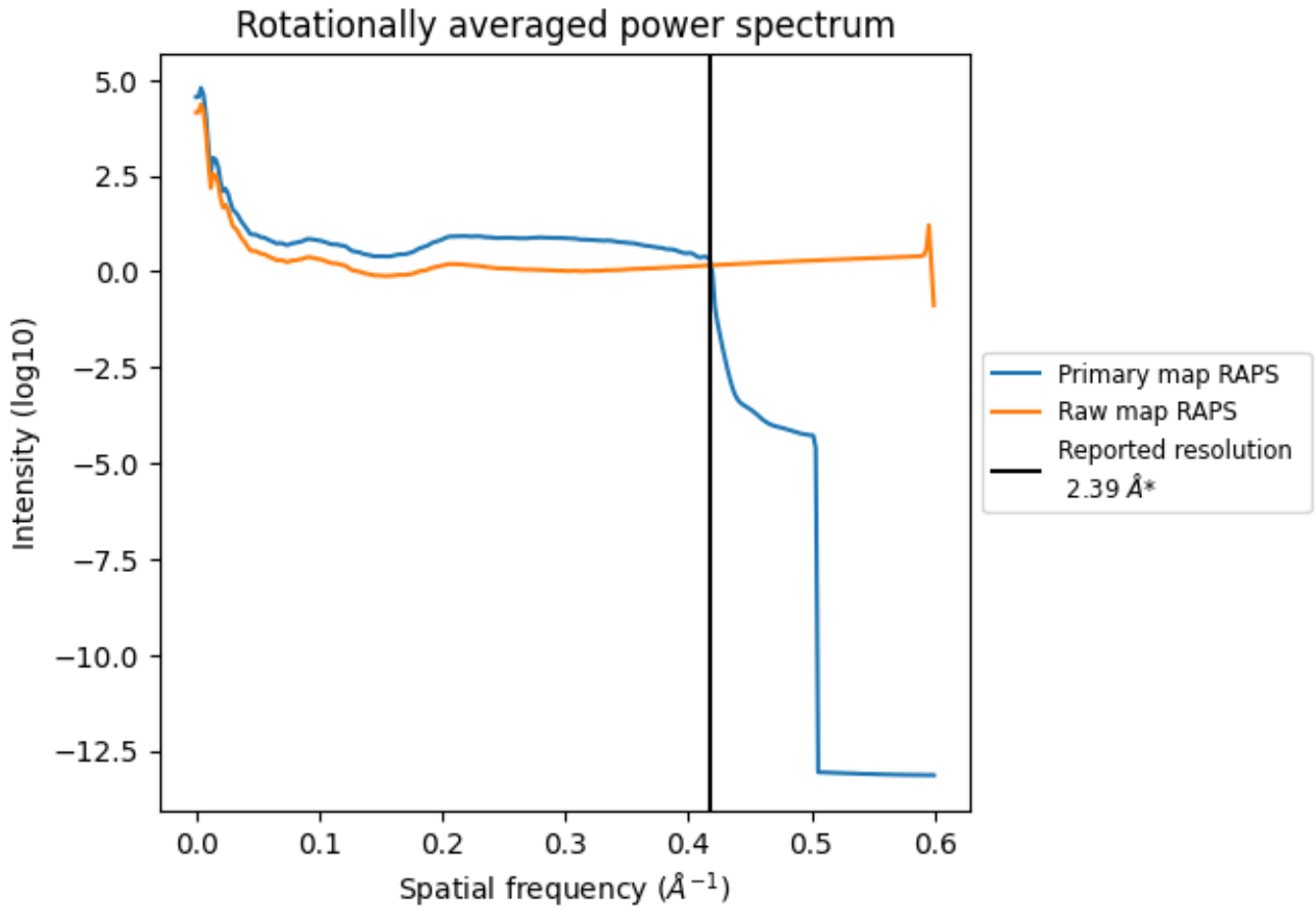
7.2 Volume estimate



The volume at the recommended contour level is 302 nm^3; this corresponds to an approximate mass of 273 kDa.

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

7.3 Rotationally averaged power spectrum (i)

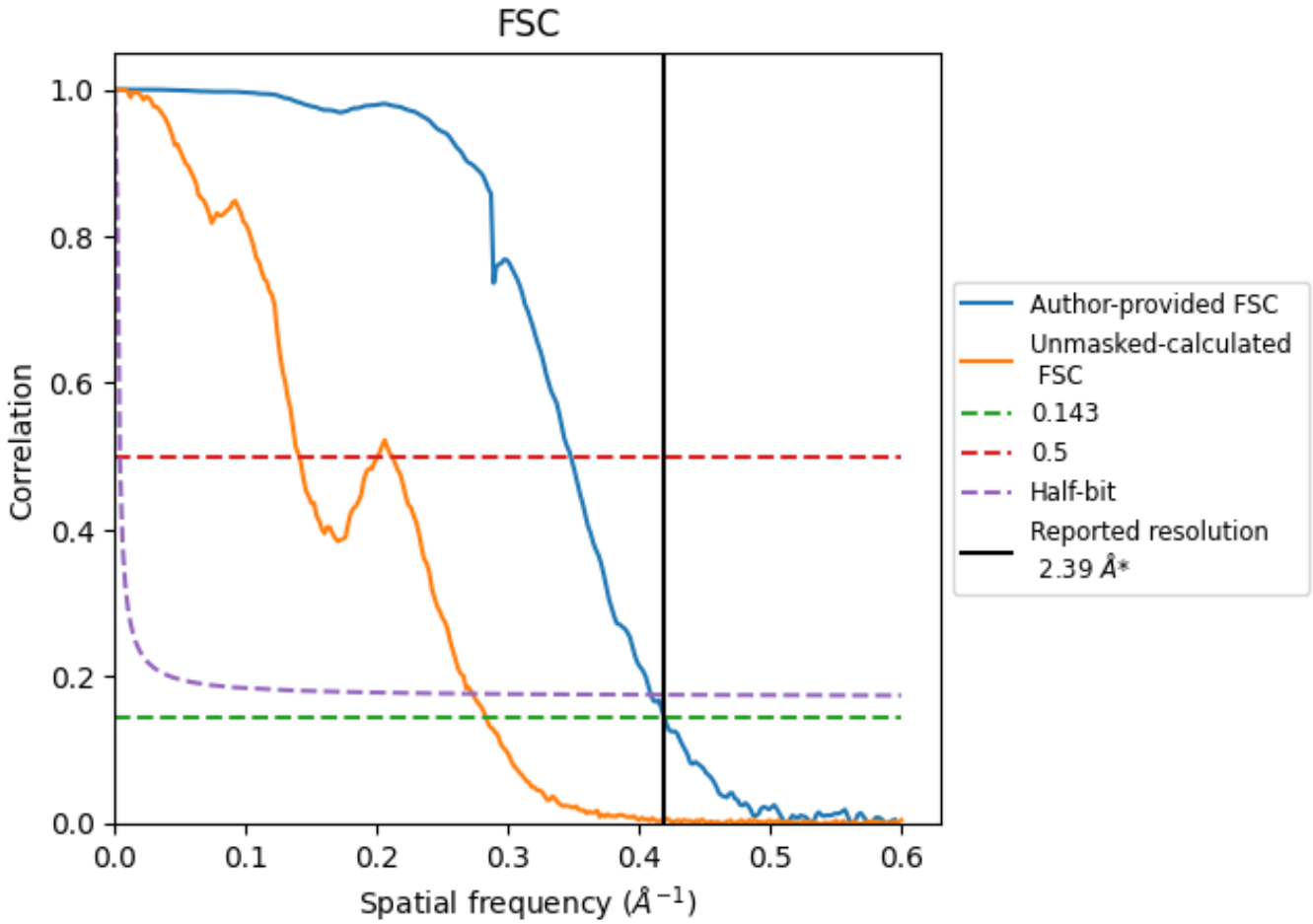


*Reported resolution corresponds to spatial frequency of 0.418 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.418 Å^{-1}

8.2 Resolution estimates (i)

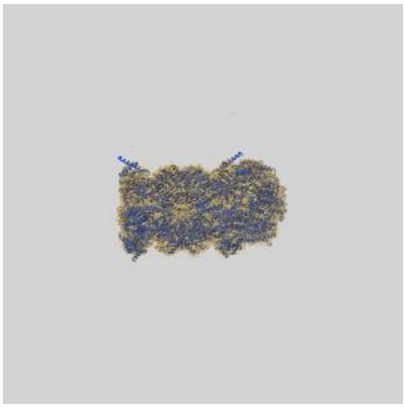
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	2.39	2.88	2.45
Unmasked-calculated*	3.53	7.12	3.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 2.39 by more than 10 %

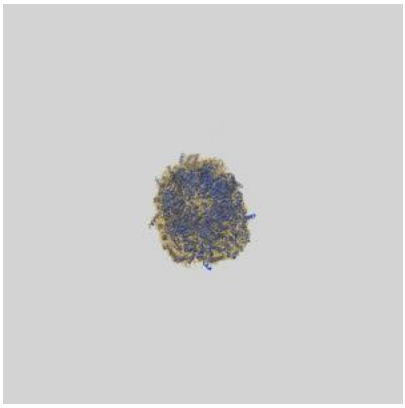
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51221 and PDB model 9GBK. Per-residue inclusion information can be found in section 3 on page 10.

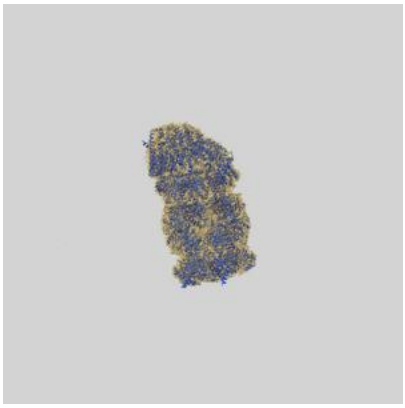
9.1 Map-model overlay



X



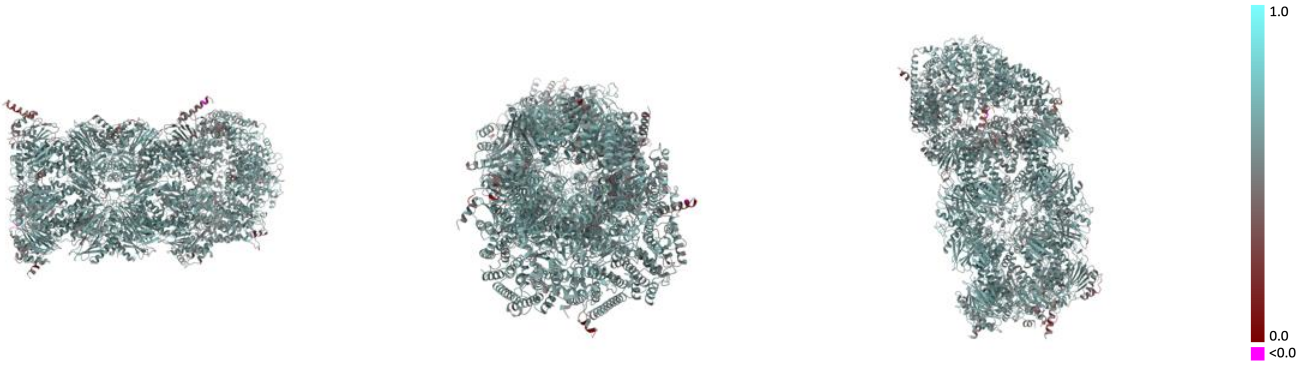
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

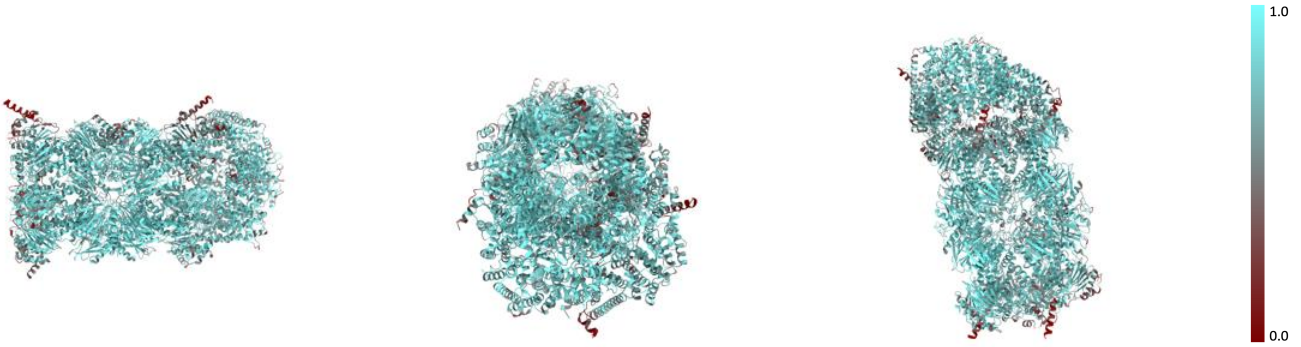
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

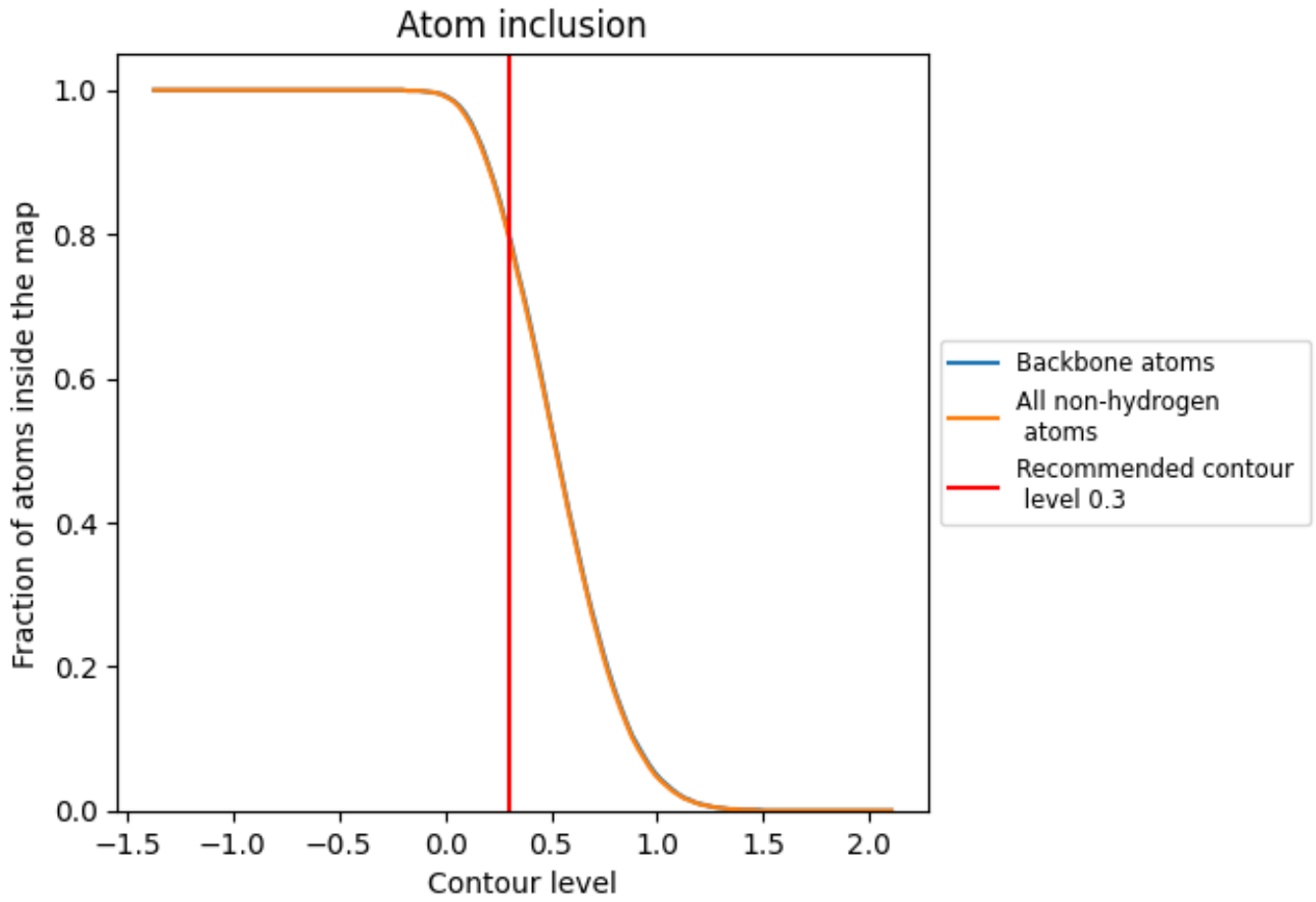
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7970	0.5850
1	0.9010	0.6330
2	0.9250	0.6370
3	0.7760	0.5720
A	0.8440	0.6020
B	0.8510	0.6110
C	0.7090	0.5570
D	0.5600	0.4820
E	0.7420	0.5620
F	0.8470	0.5850
G	0.8140	0.5760
H	0.8930	0.6120
I	0.8920	0.6170
J	0.9100	0.6400
K	0.8020	0.5870
L	0.8250	0.5930
M	0.8520	0.6020
N	0.8990	0.6180
O	0.7770	0.5760
P	0.6970	0.5590
Q	0.7380	0.5660
R	0.6110	0.5340
S	0.7360	0.5840
T	0.8410	0.6080
U	0.8310	0.6030
V	0.8680	0.5840
W	0.8450	0.5850
X	0.8280	0.5930
Y	0.7630	0.5790
Z	0.8610	0.6090