Full wwPDB EM Validation Report (i)

May 12, 2024 – 05:19 am BST

PDB ID	:	6REY
EMDB ID	:	EMD-4860
Title	:	Human 20S-PA200 Proteasome Complex
Authors	:	Toste Rego, A.; da Fonseca, P.C.A.
Deposited on	:	2019-04-12
Resolution	:	3.00 Å(reported)
Based on initial models	:	?, 5LE5

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 (i) 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 (1)) were used in the production of this report:

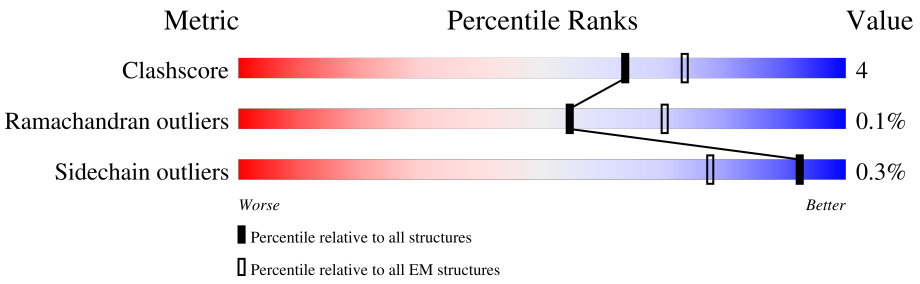
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	246	• 83% 12% 5%
1	O	246	• 83% 12% 5%
2	B	234	88% • 9%
2	P	234	88% • 9%
3	C	261	5% 73% 6% 21%
3	Q	261	• 73% 6% 21%
4	D	248	5% 73% 12% 15%
4	R	248	5% 74% 11% 15%

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Mol	Chain	Length	Quality of chain
5	E	241	85% 10% 6%
5	S	241	84% 10% 6%
6	F	263	78% 11% 10%
6	T	263	79% 11% 10%
7	G	255	87% 7% 5%
7	U	255	87% 8% 5%
8	H	205	87% 10%
8	V	205	87% 9%
9	I	234	87% 8% 6%
9	W	234	84% 10% 6%
10	J	205	90% 9%
10	X	205	91% 9%
11	K	201	81% 16%
11	Y	201	81% 16%
12	L	204	89% 9%
12	Z	204	88% 10%
13	M	213	88% 12%
13	a	213	100%
14	N	219	85% 9% 6%
14	b	219	94% 6%
15	c	1843	10% 95%
15	d	1843	10% 95%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 70722 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 alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	234	1670	1059	293	305	13	0	0
1	O	234	1670	1059	293	305	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	214	1580	1023	278	273	6	0	0
2	P	214	1580	1023	278	273	6	0	0

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	207	1424	911	254	250	9	0	0
3	Q	207	1424	911	254	250	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	210	1508	961	284	258	5	0	0
4	R	210	1508	961	284	258	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	227	1629	1035	276	307	11	0	0
5	S	227	1629	1035	276	307	11	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	236	1745	1115	322	296	12	0	0
6	T	236	1745	1115	322	296	12	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	242	1767	1133	309	314	11	0	0
7	U	242	1767	1133	309	314	11	0	0

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	198	1441	909	251	269	12	0	0
8	V	198	1441	909	251	269	12	0	0

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	221	1591	1008	272	299	12	0	0
9	W	221	1591	1008	272	299	12	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	204	1531	986	263	263	19	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	X	204	1531	986	263	263	19	0	0

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	196	1507	975	258	266	8	0	0
11	Y	196	1507	975	258	266	8	0	0

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	200	1503	956	270	269	8	0	0
12	Z	200	1503	956	270	269	8	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	213	1573	1007	275	281	10	0	0
13	a	213	1573	1007	275	281	10	0	0

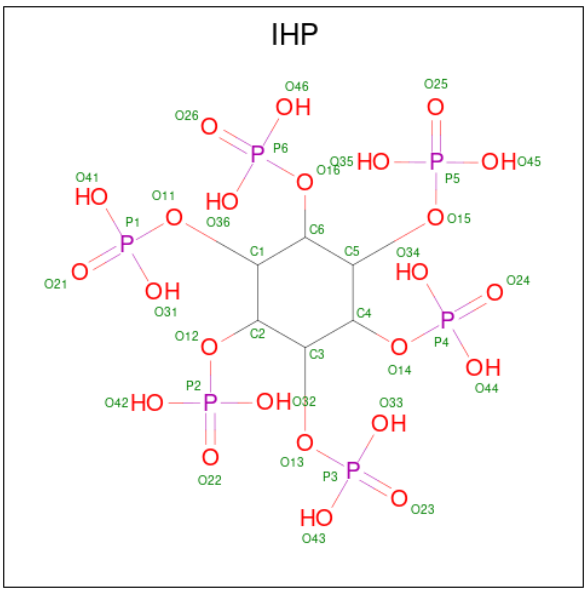
- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	206	1549	984	274	280	11	0	0
14	b	206	1549	984	274	280	11	0	0

- Molecule 15 is a protein called Proteasome activator complex subunit 4.

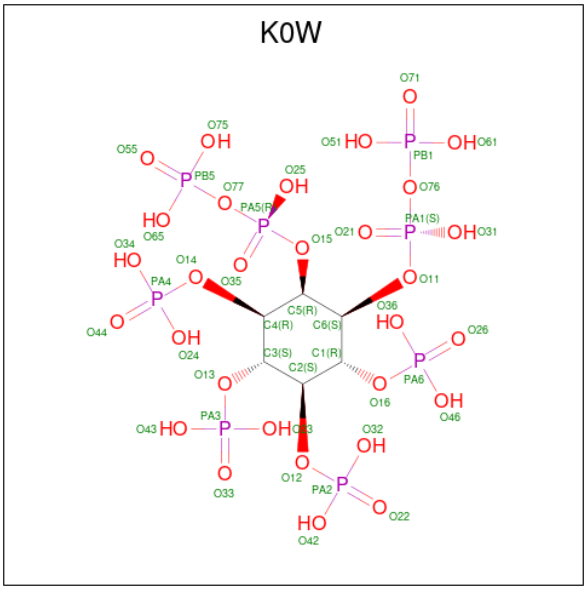
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	c	1773	13263	8666	2329	2194	74	0	0
15	d	1773	13263	8666	2329	2194	74	0	0

- Molecule 16 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
16	c	1	Total	C	O	P	0
			36	6	24	6	
16	d	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 17 is [(1 {S},2 {R},3 {R},4 {S},5 {S},6 {R})-2-[oxidanyl(phosphonooxy)phosphoryl]oxy-3,4,5,6-tetraphosphonooxy-cyclohexyl] phosphono hydrogen phosphate (three-letter code: K0W) (formula: $C_6H_{20}O_{30}P_8$).



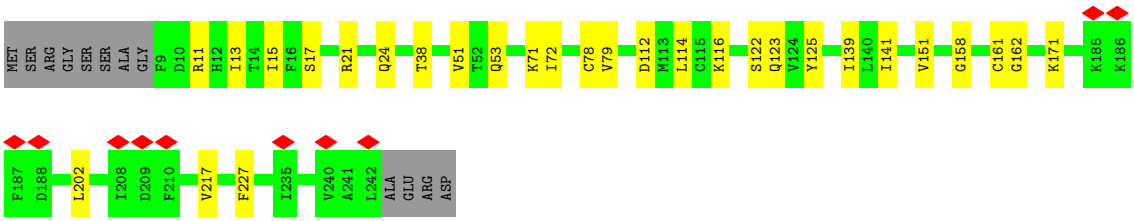
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	c	1	44	6	30	8	0
			Total	C	O	P	
17	d	1	44	6	30	8	0

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.

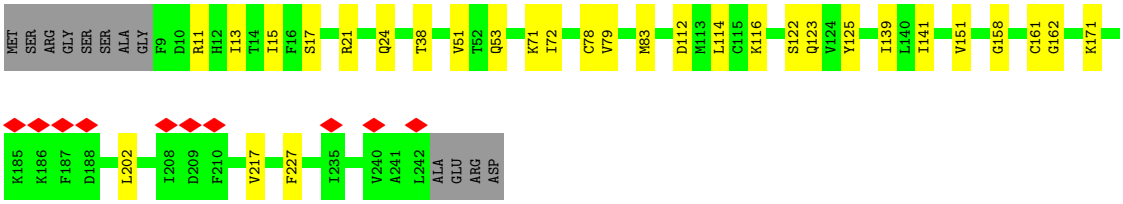
• Molecule 1: Proteasome subunit alpha type-6

Chain A:



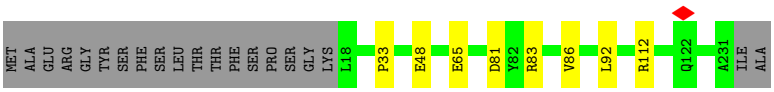
• Molecule 1: Proteasome subunit alpha type-6

Chain O:



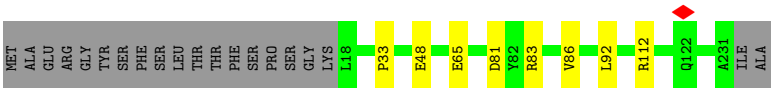
• Molecule 2: Proteasome subunit alpha type-2

Chain B:



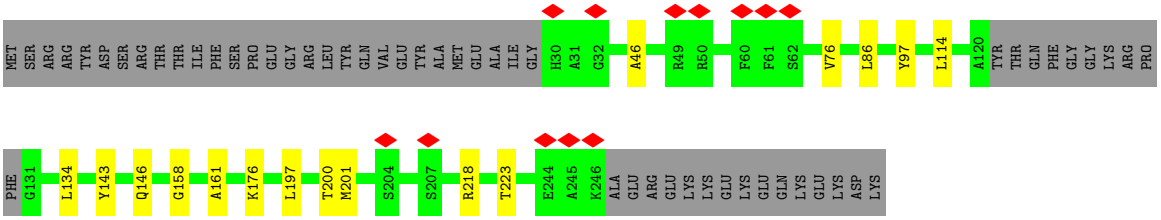
• Molecule 2: Proteasome subunit alpha type-2

Chain P:



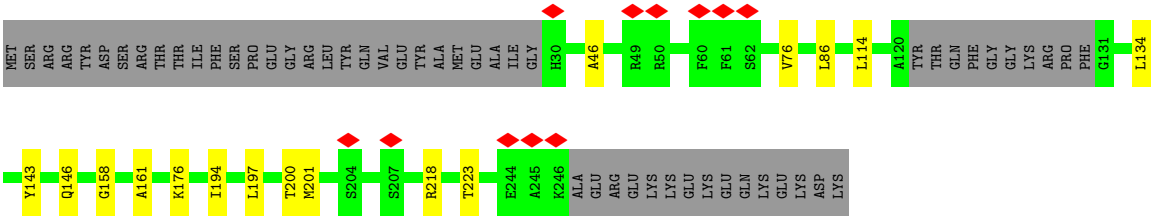
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



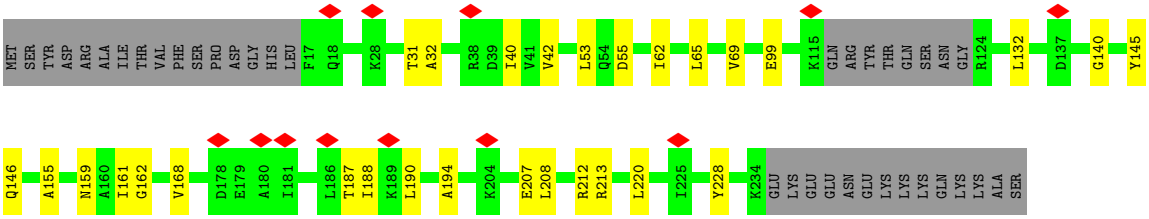
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



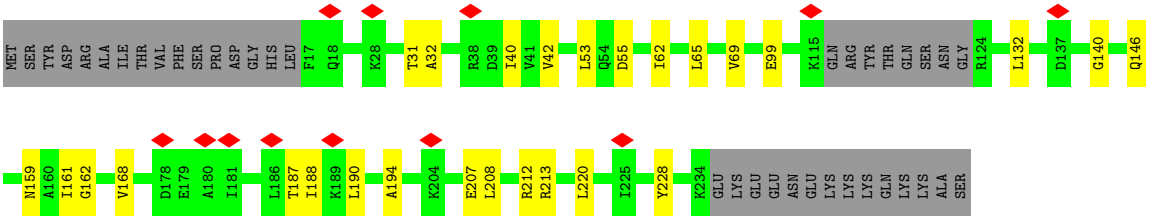
• Molecule 4: Proteasome subunit alpha type-7

Chain D:



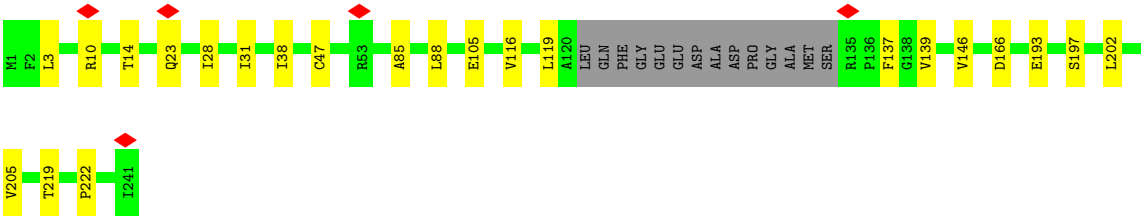
• Molecule 4: Proteasome subunit alpha type-7

Chain R:



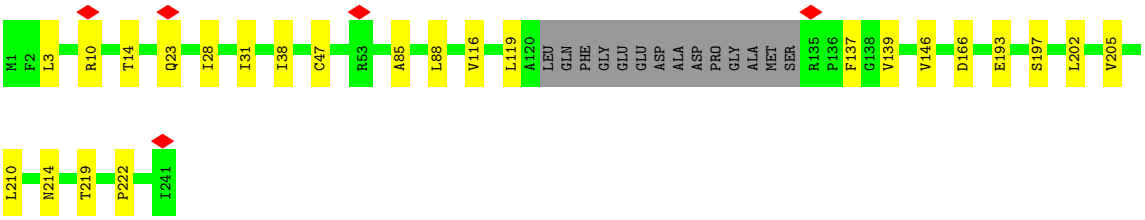
• Molecule 5: Proteasome subunit alpha type-5

Chain E:



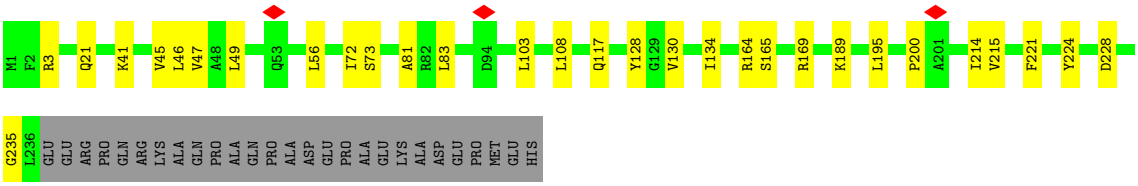
• Molecule 5: Proteasome subunit alpha type-5

Chain S:



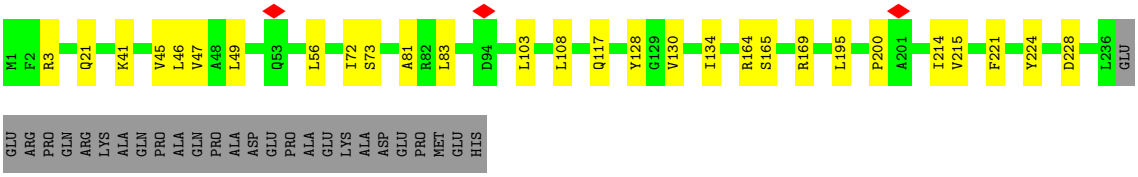
• Molecule 6: Proteasome subunit alpha type-1

Chain F:



• Molecule 6: Proteasome subunit alpha type-1

Chain T:

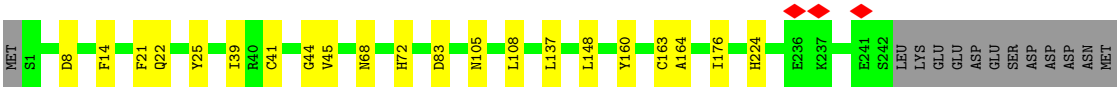


• Molecule 7: Proteasome subunit alpha type-3

Chain G:

• Molecule 7: Proteasome subunit alpha type-3

Chain U:

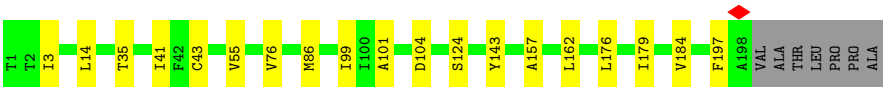


• Molecule 8: Proteasome subunit beta type-6

Chain H:

• Molecule 8: Proteasome subunit beta type-6

Chain V:



• Molecule 9: Proteasome subunit beta type-7

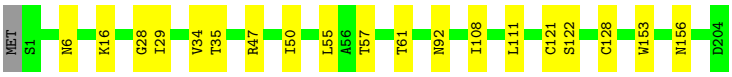
Chain I:

• Molecule 9: Proteasome subunit beta type-7

Chain W:

• Molecule 10: Proteasome subunit beta type-3

Chain J:

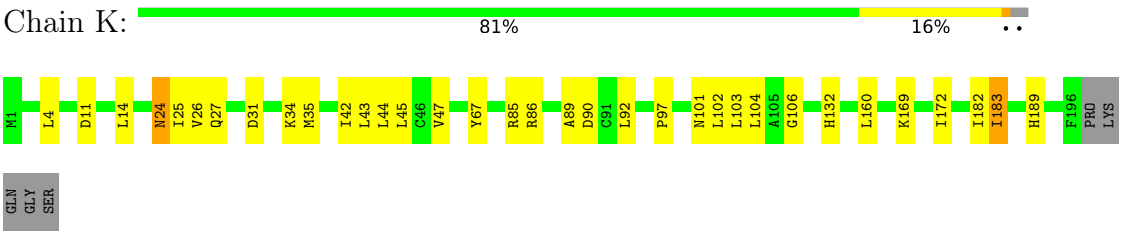


• Molecule 10: Proteasome subunit beta type-3

Chain X:

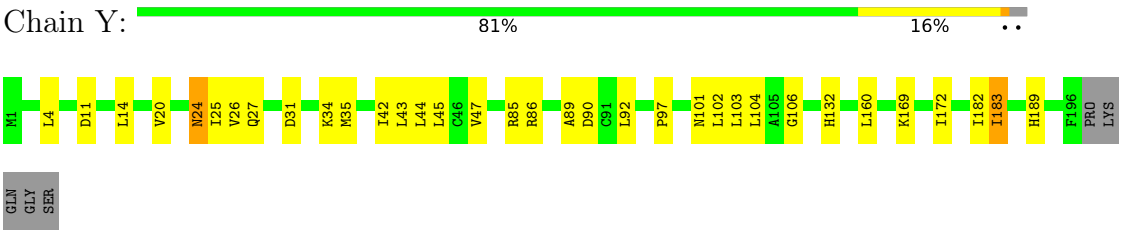
• Molecule 11: Proteasome subunit beta type-2

Chain K:



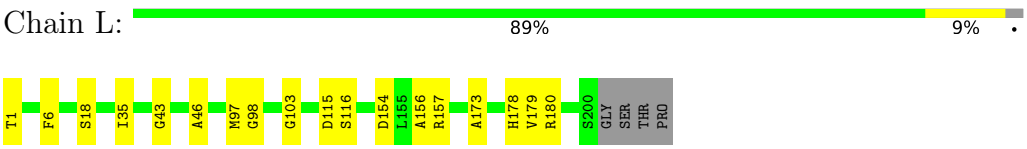
• Molecule 11: Proteasome subunit beta type-2

Chain Y:



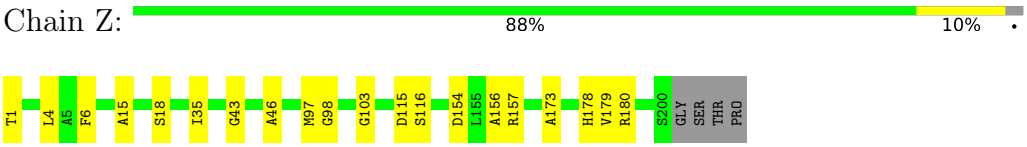
• Molecule 12: Proteasome subunit beta type-5

Chain L:



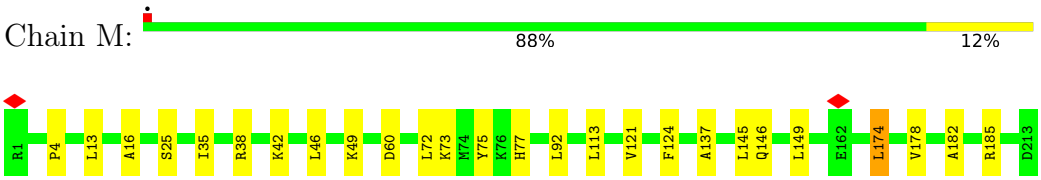
• Molecule 12: Proteasome subunit beta type-5

Chain Z:



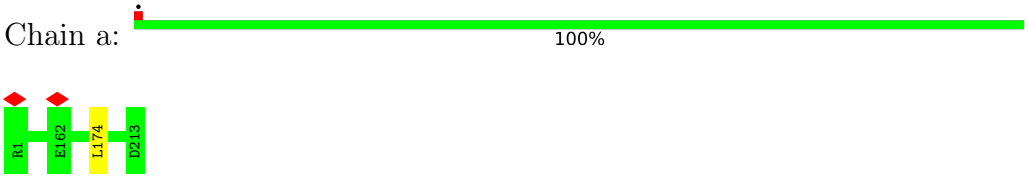
• Molecule 13: Proteasome subunit beta type-1

Chain M:



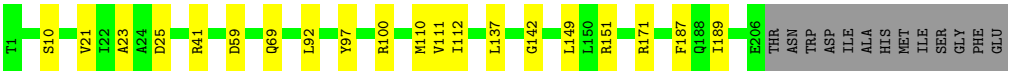
• Molecule 13: Proteasome subunit beta type-1

Chain a:



• Molecule 14: Proteasome subunit beta type-4

Chain N:

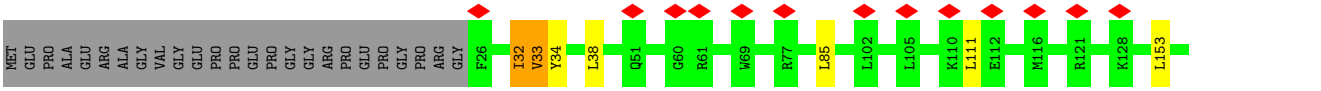


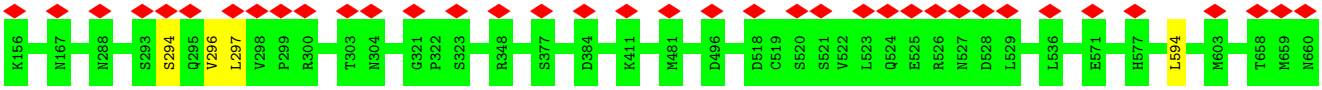
• Molecule 14: Proteasome subunit beta type-4

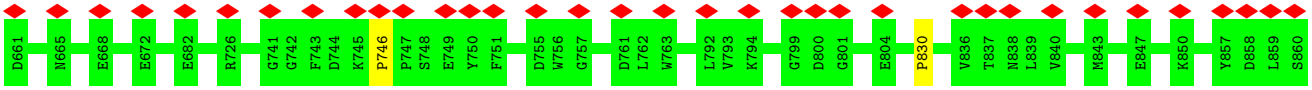
Chain b: 94% 6%

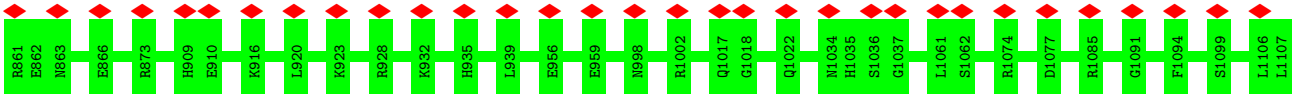
• Molecule 15: Proteasome activator complex subunit 4

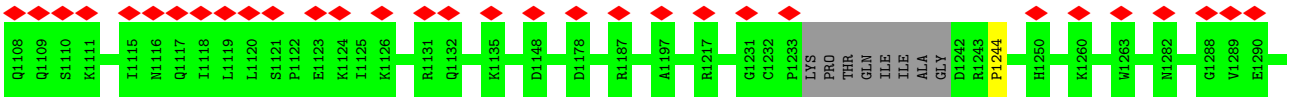
Chain c: 10% 95%

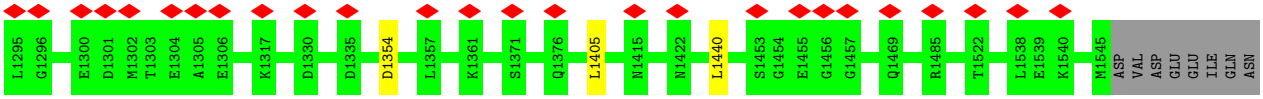


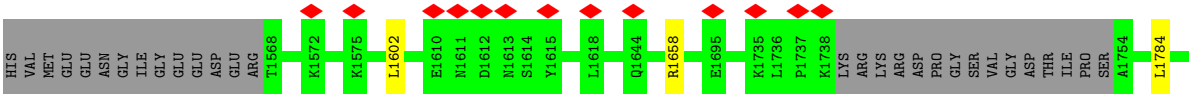


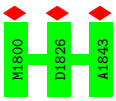






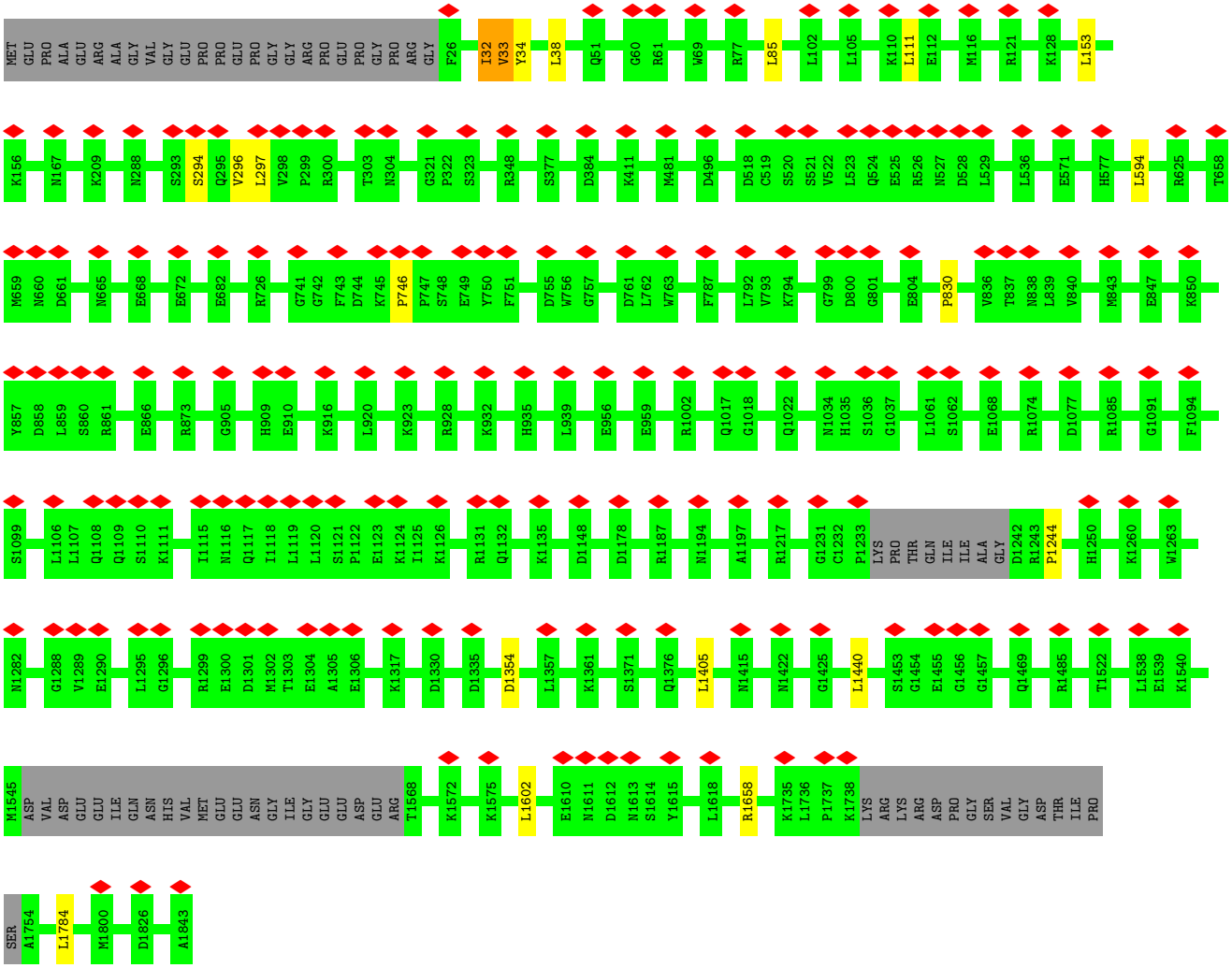






• Molecule 15: Proteasome activator complex subunit 4

Chain d: 10% 95%


MET GLU PRO ALA GLU ARG ALA GLY VAL GLY GLU PRO PRO GLU PRO GLY GLY ARG PRO GLU PRO GLY PRO ARG GLY F26 I32 V33 Y34 L38 Q51 G60 R61 W69 R77 L85 L102 L105 K110 L111 E112 M116 R121 K128 L153
K156 N167 K209 N288 S293 S294 Q295 V296 L297 V298 P299 R300 T303 N304 G321 P322 S323 R348 S377 D384 K411 M481 D496 D518 C519 S520 S521 V522 L523 Q524 E525 R526 N527 D528 L529 L536 E571 H577 L594 R625 T658
M659 N660 D661 N665 E668 E672 E682 R726 G741 G742 F743 D744 K745 P746 P747 S748 E749 Y750 F751 D755 W756 G757 D761 L762 W763 F787 L792 V793 K794 G799 D800 G801 E804 P830 V836 T837 N838 L839 V840 M843 E847 K850
Y857 D858 L859 S860 R861 E866 R873 G905 H909 E910 K916 L920 K923 R928 K932 H935 L939 E956 E959 R1002 Q1017 G1018 Q1022 N1034 H1035 S1036 G1037 L1061 S1062 E1068 R1074 D1077 R1085 G1091 F1094
S1099 L1106 L1107 Q1108 Q1109 S1110 K1111 T1115 N1116 Q1117 I1118 L1119 L1120 S1121 P1122 E1123 K1124 I1125 K1126 R1131 Q1132 K1135 D1148 D1178 R1187 N1194 A1197 R1217 G1231 C1232 P1233 LYS PRO THR GLN ILE ILE ALA GLY D1242 R1243 P1244 H1250 K1260 W1263
N1282 G1288 V1289 E1290 L1295 G1296 R1299 E1300 D1301 M1302 T1303 E1304 A1305 E1306 K1317 D1330 D1335 D1354 L1357 K1361 S1371 Q1376 L1405 N1415 N1422 G1425 L1440 S1453 G1454 E1455 G1456 G1457 Q1469 R1485 T1522 L1538 E1539 K1540
M1545 ASP VAL ASP GLU GLU ILE GLN ASN HIS VAL MET GLU GLU ASN GLY ILE GLY GLU GLU ASP GLU ARG T1568 K1572 K1575 L1602 E1610 N1611 D1612 N1613 S1614 Y1615 L1618 R1658 K1735 L1736 P1737 K1738 LYS ARG LYS ARG ASP PRO GLY SER VAL GLY ASP THR ILE PRO
SER A1754 L1784 M1800 D1826 A1843

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	20351	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	95000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	28.186	Depositor
Minimum map value	-16.724	Depositor
Average map value	0.017	Depositor
Map value standard deviation	1.004	Depositor
Recommended contour level	5.7	Depositor
Map size (Å)	466.56, 466.56, 466.56	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K0W, IHP

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	0.45	0/1697	0.57	0/2312
1	O	0.45	0/1697	0.57	0/2312
2	B	0.45	0/1615	0.56	0/2199
2	P	0.45	0/1615	0.56	0/2199
3	C	0.38	0/1440	0.56	0/1961
3	Q	0.38	0/1440	0.56	0/1961
4	D	0.40	1/1526 (0.1%)	0.59	0/2071
4	R	0.40	1/1526 (0.1%)	0.59	0/2071
5	E	0.39	0/1655	0.56	1/2252 (0.0%)
5	S	0.39	0/1655	0.56	1/2252 (0.0%)
6	F	0.41	0/1780	0.59	0/2415
6	T	0.41	0/1780	0.59	0/2415
7	G	0.45	0/1802	0.57	0/2446
7	U	0.45	0/1802	0.57	0/2446
8	H	0.47	0/1467	0.58	0/1989
8	V	0.47	0/1467	0.58	0/1989
9	I	0.45	0/1618	0.63	1/2202 (0.0%)
9	W	0.45	0/1618	0.63	1/2202 (0.0%)
10	J	0.47	1/1560 (0.1%)	0.57	0/2110
10	X	0.47	1/1560 (0.1%)	0.57	0/2110
11	K	0.45	0/1538	0.61	2/2087 (0.1%)
11	Y	0.45	0/1538	0.61	2/2087 (0.1%)
12	L	0.49	0/1534	0.59	0/2079
12	Z	0.49	0/1534	0.59	0/2079
13	M	0.45	0/1602	0.62	1/2166 (0.0%)
13	a	0.45	0/1602	0.62	1/2166 (0.0%)
14	N	0.48	0/1579	0.60	0/2143
14	b	0.48	0/1579	0.60	0/2143
15	c	0.36	0/13587	0.62	7/18538 (0.0%)
15	d	0.36	0/13587	0.62	7/18538 (0.0%)
All	All	0.41	4/72000 (0.0%)	0.60	24/97940 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1
6	T	0	1
10	J	0	1
10	X	0	1
11	K	0	1
11	Y	0	1
15	c	0	4
15	d	0	4
All	All	0	14

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	153	TRP	C-N	-5.70	1.21	1.34
10	X	153	TRP	C-N	-5.69	1.21	1.34
4	D	99	GLU	C-N	-5.26	1.22	1.34
4	R	99	GLU	C-N	-5.23	1.22	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	d	1354	ASP	CB-CG-OD1	7.47	125.02	118.30
15	c	1354	ASP	CB-CG-OD1	7.43	124.98	118.30
15	c	111	LEU	CA-CB-CG	6.08	129.28	115.30
15	d	111	LEU	CA-CB-CG	6.06	129.24	115.30
15	c	1784	LEU	CA-CB-CG	5.91	128.90	115.30
15	d	1784	LEU	CA-CB-CG	5.91	128.90	115.30
15	d	38	LEU	CA-CB-CG	5.71	128.44	115.30
15	c	38	LEU	CA-CB-CG	5.71	128.43	115.30
11	K	103	LEU	CA-CB-CG	5.67	128.35	115.30
11	Y	103	LEU	CA-CB-CG	5.65	128.30	115.30
15	c	34	TYR	CB-CA-C	-5.36	99.68	110.40
15	c	594	LEU	CA-CB-CG	5.32	127.54	115.30
15	d	594	LEU	CA-CB-CG	5.32	127.54	115.30
15	d	34	TYR	CB-CA-C	-5.32	99.76	110.40
9	I	63	LEU	CA-CB-CG	5.32	127.53	115.30
9	W	63	LEU	CA-CB-CG	5.30	127.49	115.30
13	M	174	LEU	CA-CB-CG	5.27	127.41	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	174	LEU	CA-CB-CG	5.27	127.41	115.30
11	K	183	ILE	CG1-CB-CG2	-5.24	99.86	111.40
11	Y	183	ILE	CG1-CB-CG2	-5.24	99.88	111.40
15	d	85	LEU	CA-CB-CG	5.22	127.30	115.30
15	c	85	LEU	CA-CB-CG	5.20	127.26	115.30
5	S	3	LEU	CA-CB-CG	5.06	126.94	115.30
5	E	3	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	41	LYS	Peptide
10	J	29	ILE	Peptide
11	K	24	ASN	Peptide
6	T	41	LYS	Peptide
10	X	29	ILE	Peptide
11	Y	24	ASN	Peptide
15	c	1244	PRO	Peptide
15	c	294	SER	Peptide
15	c	296	VAL	Peptide
15	c	297	LEU	Peptide
15	d	1244	PRO	Peptide
15	d	294	SER	Peptide
15	d	296	VAL	Peptide
15	d	297	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1670	0	1579	18	0
1	O	1670	0	1579	19	0
2	B	1580	0	1542	7	0
2	P	1580	0	1542	7	0
3	C	1424	0	1338	11	0
3	Q	1424	0	1338	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1508	0	1491	19	0
4	R	1508	0	1491	17	0
5	E	1629	0	1551	13	0
5	S	1629	0	1551	13	0
6	F	1745	0	1706	16	0
6	T	1745	0	1706	15	0
7	G	1767	0	1686	11	0
7	U	1767	0	1686	12	0
8	H	1441	0	1396	11	0
8	V	1441	0	1396	10	0
9	I	1591	0	1565	9	0
9	W	1591	0	1565	14	0
10	J	1531	0	1541	10	0
10	X	1531	0	1541	9	0
11	K	1507	0	1488	24	0
11	Y	1507	0	1488	24	0
12	L	1503	0	1448	11	0
12	Z	1503	0	1448	12	0
13	M	1573	0	1549	17	0
13	a	1573	0	1549	0	0
14	N	1549	0	1511	19	0
14	b	1549	0	1511	0	0
15	c	13263	0	12819	0	0
15	d	13263	0	12819	0	0
16	c	36	0	6	0	0
16	d	36	0	6	0	0
17	c	44	0	0	0	0
17	d	44	0	0	0	0
All	All	70722	0	68432	317	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 4.

All (317) 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)
14:N:23:ALA:HB2	14:N:189:ILE:HG12	1.71	0.70
14:N:21:VAL:CG2	14:N:189:ILE:CG2	2.75	0.65
14:N:21:VAL:CG2	14:N:189:ILE:HG23	2.27	0.64
14:N:21:VAL:HG23	14:N:189:ILE:CG2	2.28	0.64
13:M:145:LEU:HD21	13:M:182:ALA:HB2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:145:LEU:HD22	13:M:178:VAL:HG22	1.81	0.61
7:G:99:ARG:NH1	14:N:69:GLN:OE1	2.33	0.61
11:K:27:GLN:NE2	11:Y:169:LYS:O	2.34	0.60
6:F:117:GLN:NE2	7:G:83:ASP:OD1	2.34	0.60
1:O:158:GLY:O	2:P:83:ARG:NH2	2.34	0.60
11:K:169:LYS:O	11:Y:27:GLN:NE2	2.33	0.60
12:L:154:ASP:OD1	12:L:157:ARG:NH1	2.35	0.59
14:N:25:ASP:OD1	14:N:41:ARG:NH2	2.35	0.59
12:Z:154:ASP:OD1	12:Z:157:ARG:NH1	2.35	0.59
8:H:14:LEU:HD21	8:H:101:ALA:HB3	1.84	0.59
1:A:158:GLY:O	2:B:83:ARG:NH2	2.36	0.58
1:A:78:CYS:SG	1:A:79:VAL:N	2.77	0.58
10:J:121:CYS:SG	10:J:122:SER:N	2.77	0.58
8:V:14:LEU:HD21	8:V:101:ALA:HB3	1.84	0.58
12:Z:6:PHE:HE1	12:Z:156:ALA:HB2	1.68	0.58
12:L:6:PHE:HE1	12:L:156:ALA:HB2	1.68	0.57
3:Q:176:LYS:HG2	4:R:53:LEU:HD13	1.87	0.57
10:X:121:CYS:SG	10:X:122:SER:N	2.77	0.57
1:A:51:VAL:HG12	1:A:202:LEU:HD13	1.87	0.57
5:S:28:ILE:HA	5:S:31:ILE:HD12	1.86	0.57
14:N:21:VAL:HG23	14:N:189:ILE:HG23	1.87	0.57
1:O:78:CYS:SG	1:O:79:VAL:N	2.77	0.56
6:T:117:GLN:NE2	7:U:83:ASP:OD1	2.38	0.56
3:C:218:ARG:NH1	3:C:223:THR:OG1	2.38	0.56
3:C:176:LYS:HG2	4:D:53:LEU:HD13	1.86	0.56
5:E:28:ILE:HA	5:E:31:ILE:HD12	1.86	0.56
1:O:51:VAL:HG12	1:O:202:LEU:HD13	1.87	0.56
10:X:6:ASN:ND2	10:X:28:GLY:O	2.38	0.56
3:Q:218:ARG:NH1	3:Q:223:THR:OG1	2.38	0.56
4:R:208:LEU:HD23	4:R:220:LEU:HD12	1.89	0.55
11:Y:35:MET:HG2	11:Y:45:LEU:HG	1.88	0.55
14:N:92:LEU:HD23	14:N:112:ILE:HD11	1.89	0.55
11:K:35:MET:HG2	11:K:45:LEU:HG	1.88	0.55
6:F:215:VAL:HB	6:F:221:PHE:HD1	1.72	0.54
6:T:164:ARG:HH12	6:T:200:PRO:HG3	1.72	0.54
8:H:91:ARG:NH2	14:N:59:ASP:OD1	2.41	0.54
10:J:16:LYS:HB2	10:J:156:ASN:HA	1.90	0.54
13:M:4:PRO:HB2	14:N:100:ARG:HH11	1.72	0.54
9:I:163:ILE:HG12	9:I:170:GLY:HA2	1.90	0.54
4:D:208:LEU:HD23	4:D:220:LEU:HD12	1.89	0.54
6:T:215:VAL:HB	6:T:221:PHE:HD1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:164:ARG:HH12	6:F:200:PRO:HG3	1.72	0.53
6:T:45:VAL:HG22	6:T:214:ILE:HG12	1.90	0.53
4:R:146:GLN:HG3	4:R:161:ILE:HD11	1.91	0.53
4:D:146:GLN:OE1	4:D:159:ASN:ND2	2.32	0.53
4:D:146:GLN:HG3	4:D:161:ILE:HD11	1.91	0.53
10:X:16:LYS:HB2	10:X:156:ASN:HA	1.90	0.53
4:R:140:GLY:O	4:R:213:ARG:NH1	2.39	0.53
9:W:163:ILE:HG12	9:W:170:GLY:HA2	1.90	0.53
6:F:45:VAL:HG22	6:F:214:ILE:HG12	1.90	0.53
6:F:47:VAL:HG12	6:F:195:LEU:HD22	1.91	0.53
1:A:112:ASP:OD2	9:I:72:ARG:NH2	2.41	0.52
9:W:1:THR:N	9:W:168:GLY:O	2.42	0.52
11:K:14:LEU:HD21	11:K:160:LEU:HD22	1.92	0.52
10:J:61:THR:OG1	11:K:85:ARG:NH2	2.41	0.52
8:V:3:ILE:HD12	8:V:99:ILE:HG12	1.91	0.52
8:H:3:ILE:HD12	8:H:99:ILE:HG12	1.91	0.52
9:I:81:ARG:HA	9:I:84:LYS:HG2	1.92	0.52
6:T:47:VAL:HG12	6:T:195:LEU:HD22	1.91	0.52
6:F:46:LEU:HD13	6:F:73:SER:HB2	1.92	0.52
10:J:6:ASN:ND2	10:J:28:GLY:O	2.38	0.52
9:W:81:ARG:HA	9:W:84:LYS:HG2	1.92	0.52
13:M:137:ALA:HB3	13:M:146:GLN:HG2	1.90	0.51
1:A:11:ARG:O	1:A:24:GLN:NE2	2.37	0.51
11:Y:14:LEU:HD21	11:Y:160:LEU:HD22	1.92	0.51
1:O:112:ASP:OD2	9:W:72:ARG:NH2	2.41	0.51
7:U:68:ASN:OD1	7:U:224:HIS:ND1	2.36	0.51
13:M:92:LEU:HD23	13:M:124:PHE:HE2	1.75	0.51
2:P:92:LEU:HD13	2:P:112:ARG:HB3	1.92	0.51
3:C:200:THR:HG23	3:C:201:MET:HG2	1.93	0.51
13:M:13:LEU:HD11	13:M:149:LEU:HD11	1.92	0.51
2:B:92:LEU:HD13	2:B:112:ARG:HB3	1.92	0.50
1:O:11:ARG:O	1:O:24:GLN:NE2	2.37	0.50
3:Q:200:THR:HG23	3:Q:201:MET:HG2	1.93	0.50
6:T:46:LEU:HD13	6:T:73:SER:HB2	1.92	0.50
3:C:86:LEU:HD12	3:C:114:LEU:HD21	1.93	0.50
7:G:68:ASN:OD1	7:G:224:HIS:ND1	2.36	0.50
9:I:1:THR:N	9:I:168:GLY:O	2.42	0.50
6:T:81:ALA:HB2	6:T:130:VAL:HG21	1.93	0.50
11:Y:24:ASN:O	11:Y:26:VAL:N	2.45	0.50
6:F:72:ILE:HG22	6:F:134:ILE:HG12	1.93	0.50
6:F:81:ALA:HB2	6:F:130:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:24:ASN:O	11:K:26:VAL:N	2.45	0.50
5:S:146:VAL:HG11	5:S:222:PRO:HA	1.93	0.50
7:G:45:VAL:HG13	7:G:148:LEU:HD12	1.94	0.50
10:X:50:ILE:HG13	10:X:108:ILE:HG22	1.94	0.50
6:T:72:ILE:HG22	6:T:134:ILE:HG12	1.93	0.49
1:A:71:LYS:HG2	1:A:227:PHE:HD2	1.77	0.49
1:O:123:GLN:NE2	2:P:81:ASP:OD1	2.42	0.49
6:T:103:LEU:HD22	6:T:108:LEU:HB2	1.94	0.49
2:B:83:ARG:HA	2:B:86:VAL:HG12	1.94	0.49
1:O:141:ILE:HG22	1:O:151:VAL:HG22	1.94	0.49
4:D:132:LEU:HG	4:D:161:ILE:HD12	1.95	0.49
4:D:140:GLY:O	4:D:213:ARG:NH1	2.39	0.49
5:E:146:VAL:HG11	5:E:222:PRO:HA	1.93	0.49
1:A:141:ILE:HG22	1:A:151:VAL:HG22	1.94	0.49
4:D:168:VAL:HG13	4:D:194:ALA:HB1	1.94	0.49
8:V:55:VAL:HG13	8:V:86:MET:HG2	1.95	0.49
1:A:51:VAL:HG22	1:A:217:VAL:HG22	1.94	0.49
12:L:1:THR:HG21	12:L:46:ALA:HA	1.95	0.49
2:P:83:ARG:HA	2:P:86:VAL:HG12	1.94	0.49
3:Q:86:LEU:HD12	3:Q:114:LEU:HD21	1.93	0.49
8:H:55:VAL:HG13	8:H:86:MET:HG2	1.95	0.48
10:J:50:ILE:HG13	10:J:108:ILE:HG22	1.94	0.48
1:O:51:VAL:HG22	1:O:217:VAL:HG22	1.94	0.48
7:U:45:VAL:HG13	7:U:148:LEU:HD12	1.94	0.48
11:Y:92:LEU:HA	11:Y:97:PRO:HB3	1.95	0.48
1:A:123:GLN:NE2	2:B:81:ASP:OD1	2.42	0.48
4:R:132:LEU:HG	4:R:161:ILE:HD12	1.95	0.48
8:H:35:THR:OG1	8:H:43:CYS:SG	2.72	0.48
11:K:92:LEU:HA	11:K:97:PRO:HB3	1.95	0.48
12:L:103:GLY:HA2	12:L:179:VAL:HG11	1.95	0.48
1:O:71:LYS:HG2	1:O:227:PHE:HD2	1.77	0.48
4:R:168:VAL:HG13	4:R:194:ALA:HB1	1.94	0.48
8:V:35:THR:OG1	8:V:43:CYS:SG	2.72	0.48
5:S:88:LEU:HD22	5:S:116:VAL:HG13	1.95	0.48
12:Z:1:THR:HG21	12:Z:46:ALA:HA	1.95	0.48
9:W:44:CYS:HB2	9:W:99:VAL:HB	1.96	0.48
11:K:43:LEU:HD12	11:K:183:ILE:HD11	1.96	0.48
6:F:103:LEU:HD22	6:F:108:LEU:HB2	1.94	0.47
4:R:42:VAL:HG21	4:R:187:THR:HB	1.96	0.47
11:Y:43:LEU:HD12	11:Y:183:ILE:HD11	1.96	0.47
9:I:44:CYS:HB2	9:I:99:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:189:LYS:NZ	6:F:235:GLY:O	2.36	0.47
7:G:21:PHE:O	7:G:25:TYR:N	2.44	0.47
5:E:88:LEU:HD22	5:E:116:VAL:HG13	1.95	0.47
5:S:85:ALA:HB2	5:S:139:VAL:HG11	1.97	0.47
4:D:42:VAL:HG21	4:D:187:THR:HB	1.96	0.47
7:U:108:LEU:HD21	7:U:137:LEU:HB3	1.97	0.47
7:U:8:ASP:O	7:U:22:GLN:NE2	2.39	0.47
10:X:47:ARG:HD3	10:X:111:LEU:HD12	1.97	0.47
7:G:39:ILE:HD11	7:G:176:ILE:HG12	1.97	0.47
7:G:108:LEU:HD21	7:G:137:LEU:HB3	1.97	0.47
10:J:47:ARG:HD3	10:J:111:LEU:HD12	1.97	0.47
12:Z:103:GLY:HA2	12:Z:179:VAL:HG11	1.95	0.46
11:K:27:GLN:HB3	11:Y:172:ILE:HG22	1.98	0.46
7:U:163:CYS:SG	7:U:164:ALA:N	2.89	0.46
1:A:161:CYS:SG	1:A:162:GLY:N	2.88	0.46
8:V:124:SER:OG	8:V:143:TYR:OH	2.34	0.46
5:S:166:ASP:HB2	6:T:56:LEU:HB3	1.98	0.46
5:E:85:ALA:HB2	5:E:139:VAL:HG11	1.97	0.46
1:O:161:CYS:SG	1:O:162:GLY:N	2.88	0.46
5:S:14:THR:HG23	6:T:21:GLN:HE22	1.80	0.46
12:Z:97:MET:HG2	12:Z:98:GLY:H	1.80	0.46
7:G:163:CYS:SG	7:G:164:ALA:N	2.89	0.46
8:H:157:ALA:HB2	8:H:176:LEU:HD11	1.98	0.46
12:L:97:MET:HG2	12:L:98:GLY:H	1.81	0.46
2:P:33:PRO:HD2	2:P:48:GLU:HG3	1.97	0.46
4:R:146:GLN:OE1	4:R:159:ASN:ND2	2.32	0.46
12:Z:98:GLY:HA2	12:Z:115:ASP:HA	1.98	0.46
2:P:65:GLU:HG2	2:P:86:VAL:HG21	1.98	0.46
11:K:4:LEU:HD22	11:K:45:LEU:HD23	1.98	0.45
4:R:32:ALA:N	4:R:161:ILE:O	2.48	0.45
7:U:39:ILE:HD11	7:U:176:ILE:HG12	1.97	0.45
11:Y:4:LEU:HD22	11:Y:45:LEU:HD23	1.98	0.45
12:L:178:HIS:CE1	12:L:180:ARG:HB3	2.51	0.45
14:N:111:VAL:HG13	14:N:137:LEU:HD12	1.98	0.45
1:O:79:VAL:HG13	1:O:139:ILE:HB	1.97	0.45
7:U:21:PHE:O	7:U:25:TYR:N	2.44	0.45
12:Z:178:HIS:CE1	12:Z:180:ARG:HB3	2.51	0.45
2:B:33:PRO:HD2	2:B:48:GLU:HG3	1.97	0.45
5:E:14:THR:HG23	6:F:21:GLN:HE22	1.80	0.45
5:E:166:ASP:HB2	6:F:56:LEU:HB3	1.97	0.45
1:A:79:VAL:HG13	1:A:139:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLU:HG2	2:B:86:VAL:HG21	1.98	0.45
10:J:57:THR:O	11:K:85:ARG:NH2	2.50	0.45
12:L:98:GLY:HA2	12:L:115:ASP:HA	1.98	0.45
10:X:61:THR:OG1	11:Y:85:ARG:NH2	2.44	0.45
4:D:62:ILE:HD12	4:D:207:GLU:HG2	1.99	0.45
5:E:105:GLU:OE1	13:M:75:TYR:OH	2.32	0.45
4:R:65:LEU:HB2	4:R:69:VAL:HG13	1.98	0.45
13:M:46:LEU:HB3	13:M:72:LEU:HD11	1.97	0.45
13:M:185:ARG:NH1	9:W:27:ALA:O	2.38	0.45
13:M:35:ILE:O	14:N:151:ARG:NH2	2.35	0.45
9:W:45:GLY:HA3	9:W:52:THR:HG21	1.99	0.45
4:R:62:ILE:HD12	4:R:207:GLU:HG2	1.99	0.45
8:V:157:ALA:HB2	8:V:176:LEU:HD11	1.98	0.45
4:D:32:ALA:N	4:D:161:ILE:O	2.48	0.45
9:I:45:GLY:HA3	9:I:52:THR:HG21	1.99	0.45
11:K:86:ARG:NH1	11:K:90:ASP:OD2	2.50	0.45
14:N:171:ARG:NH2	9:W:140:ASP:OD2	2.50	0.45
11:Y:86:ARG:NH1	11:Y:90:ASP:OD2	2.50	0.45
6:T:49:LEU:HB2	6:T:195:LEU:HD11	2.00	0.44
10:X:57:THR:O	11:Y:85:ARG:NH2	2.50	0.44
5:E:10:ARG:HA	5:E:23:GLN:HE21	1.82	0.44
3:Q:194:ILE:H	3:Q:194:ILE:HG13	1.65	0.44
11:Y:4:LEU:HD22	11:Y:45:LEU:HB3	1.99	0.44
11:K:172:ILE:HG22	11:Y:27:GLN:HB3	1.99	0.44
5:S:10:ARG:HA	5:S:23:GLN:HE21	1.81	0.44
11:Y:102:LEU:O	11:Y:132:HIS:NE2	2.51	0.44
14:N:10:SER:OG	14:N:142:GLY:N	2.47	0.44
8:H:162:LEU:HD21	8:H:197:PHE:HD2	1.82	0.44
4:D:65:LEU:HB2	4:D:69:VAL:HG13	1.98	0.44
1:O:38:THR:HG21	1:O:171:LYS:HB2	2.00	0.44
1:A:38:THR:HG21	1:A:171:LYS:HB2	2.00	0.44
3:C:197:LEU:HA	3:C:200:THR:HG22	2.00	0.44
6:F:49:LEU:HB2	6:F:195:LEU:HD11	2.00	0.44
10:J:55:LEU:HG	10:J:57:THR:HG22	2.00	0.43
11:K:4:LEU:HD22	11:K:45:LEU:HB3	1.99	0.43
8:V:162:LEU:HD21	8:V:197:PHE:HD2	1.82	0.43
11:Y:11:ASP:OD1	11:Y:11:ASP:N	2.51	0.43
12:L:35:ILE:N	12:L:43:GLY:O	2.45	0.43
7:U:72:HIS:CE1	7:U:105:ASN:HB3	2.54	0.43
8:V:41:ILE:HG12	8:V:76:VAL:HG22	2.00	0.43
11:K:102:LEU:O	11:K:132:HIS:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:119:LEU:HB2	5:S:137:PHE:HZ	1.84	0.43
5:S:202:LEU:HA	5:S:205:VAL:HG22	2.00	0.43
10:X:34:VAL:HG12	10:X:35:THR:HG23	2.01	0.43
3:Q:158:GLY:O	4:R:55:ASP:N	2.51	0.43
5:S:193:GLU:O	5:S:197:SER:N	2.46	0.43
11:Y:34:LYS:HD3	11:Y:47:VAL:HG12	2.01	0.43
8:H:41:ILE:HG12	8:H:76:VAL:HG22	2.00	0.43
5:E:119:LEU:HB2	5:E:137:PHE:HZ	1.84	0.43
11:K:101:ASN:HB3	11:K:132:HIS:CE1	2.54	0.43
1:A:72:ILE:HG21	1:A:114:LEU:HD21	1.99	0.43
1:A:122:SER:HA	1:A:125:TYR:HD2	1.84	0.43
11:K:11:ASP:OD1	11:K:11:ASP:N	2.51	0.43
10:X:55:LEU:HG	10:X:57:THR:HG22	2.00	0.43
7:G:72:HIS:CE1	7:G:105:ASN:HB3	2.54	0.43
11:K:34:LYS:HD3	11:K:47:VAL:HG12	2.01	0.43
13:M:25:SER:HB2	13:M:42:LYS:HB2	2.00	0.43
1:O:122:SER:HA	1:O:125:TYR:HD2	1.84	0.43
3:Q:197:LEU:HA	3:Q:200:THR:HG22	2.00	0.43
5:E:202:LEU:HA	5:E:205:VAL:HG22	2.00	0.43
14:N:25:ASP:HA	14:N:187:PHE:HA	2.00	0.43
3:Q:46:ALA:HB1	3:Q:197:LEU:HD11	2.01	0.43
4:D:40:ILE:HG22	4:D:212:ARG:HA	2.01	0.42
1:O:72:ILE:HG21	1:O:114:LEU:HD21	1.99	0.42
4:R:40:ILE:HG22	4:R:212:ARG:HA	2.01	0.42
6:F:224:TYR:HD1	6:F:228:ASP:HB3	1.85	0.42
13:M:38:ARG:NH2	9:W:164:PHE:O	2.52	0.42
13:M:73:LYS:O	13:M:77:HIS:ND1	2.52	0.42
10:J:34:VAL:HG12	10:J:35:THR:HG23	2.01	0.42
8:V:179:ILE:HG12	8:V:184:VAL:HG22	2.01	0.42
13:M:174:LEU:HD23	9:W:202:TYR:CZ	2.55	0.42
1:O:17:SER:HB3	1:O:21:ARG:H	1.84	0.42
3:Q:76:VAL:HG12	3:Q:134:LEU:HG	2.02	0.42
11:Y:101:ASN:HB3	11:Y:132:HIS:CE1	2.54	0.42
8:H:179:ILE:HG12	8:H:184:VAL:HG22	2.01	0.42
6:F:83:LEU:HD23	6:F:128:TYR:HE1	1.85	0.42
11:K:31:ASP:N	11:K:31:ASP:OD1	2.52	0.42
3:Q:143:TYR:HB2	3:Q:146:GLN:NE2	2.35	0.42
6:T:224:TYR:HD1	6:T:228:ASP:HB3	1.85	0.42
11:K:42:ILE:HG22	11:K:106:GLY:HA3	2.02	0.42
11:Y:42:ILE:HG22	11:Y:106:GLY:HA3	2.02	0.42
3:C:46:ALA:HB1	3:C:197:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:53:GLN:HG2	1:O:202:LEU:HD21	2.02	0.42
3:Q:161:ALA:HB3	4:R:53:LEU:HD23	2.02	0.42
1:A:53:GLN:HG2	1:A:202:LEU:HD21	2.02	0.41
3:C:76:VAL:HG12	3:C:134:LEU:HG	2.02	0.41
4:D:188:ILE:HG21	4:D:228:TYR:CD1	2.56	0.41
12:L:18:SER:HB2	12:L:173:ALA:H	1.85	0.41
9:W:80:ASN:HD21	9:W:119:THR:HG21	1.85	0.41
11:Y:20:VAL:O	11:Y:34:LYS:NZ	2.41	0.41
1:A:116:LYS:HG3	2:B:83:ARG:HH11	1.85	0.41
13:M:60:ASP:OD1	14:N:97:TYR:OH	2.32	0.41
6:T:165:SER:OG	6:T:169:ARG:NH1	2.54	0.41
5:E:193:GLU:O	5:E:197:SER:N	2.46	0.41
14:N:149:LEU:HG	9:W:136:ALA:HB1	2.01	0.41
4:R:190:LEU:HD23	4:R:190:LEU:HA	1.88	0.41
11:Y:89:ALA:HA	11:Y:92:LEU:HD23	2.03	0.41
3:C:97:TYR:HH	11:K:67:TYR:HH	1.63	0.41
5:E:47:CYS:HA	5:E:219:THR:HG22	2.02	0.41
11:K:182:ILE:HG22	11:K:189:HIS:HB2	2.02	0.41
8:V:104:ASP:N	8:V:104:ASP:OD1	2.54	0.41
9:I:80:ASN:HD21	9:I:119:THR:HG21	1.85	0.41
7:U:41:CYS:SG	7:U:44:GLY:N	2.94	0.41
1:A:17:SER:HB3	1:A:21:ARG:H	1.84	0.41
8:H:104:ASP:OD1	8:H:104:ASP:N	2.54	0.41
1:O:116:LYS:HG3	2:P:83:ARG:HH11	1.85	0.41
4:D:190:LEU:HD23	4:D:190:LEU:HA	1.88	0.41
12:L:178:HIS:HE1	12:L:180:ARG:HB3	1.86	0.41
1:O:83:MET:HE3	7:U:14:PHE:HE1	1.85	0.41
11:K:44:LEU:HD12	11:K:104:LEU:HD12	2.03	0.41
13:M:49:LYS:HD2	13:M:113:LEU:HB2	2.03	0.41
6:T:83:LEU:HD23	6:T:128:TYR:HE1	1.85	0.41
7:U:160:TYR:HD2	7:U:163:CYS:HB2	1.85	0.41
12:Z:35:ILE:N	12:Z:43:GLY:O	2.45	0.41
3:C:158:GLY:O	4:D:55:ASP:N	2.51	0.41
3:C:161:ALA:HB3	4:D:53:LEU:HD23	2.02	0.41
1:O:13:ILE:HG13	1:O:15:ILE:HG12	2.03	0.41
11:Y:31:ASP:N	11:Y:31:ASP:OD1	2.52	0.41
11:Y:44:LEU:HD12	11:Y:104:LEU:HD12	2.03	0.41
12:Z:18:SER:HB2	12:Z:173:ALA:H	1.85	0.41
6:F:165:SER:OG	6:F:169:ARG:NH1	2.54	0.41
7:G:41:CYS:SG	7:G:44:GLY:N	2.94	0.41
9:I:112:SER:HB3	9:I:125:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:188:ILE:HG21	4:R:228:TYR:CD1	2.55	0.41
9:W:112:SER:HB3	9:W:125:VAL:HG11	2.03	0.41
7:G:160:TYR:HD2	7:G:163:CYS:HB2	1.85	0.40
14:N:41:ARG:HH11	14:N:41:ARG:HD2	1.76	0.40
14:N:92:LEU:HD21	14:N:110:MET:HG2	2.01	0.40
5:S:210:LEU:HA	5:S:214:ASN:HD21	1.86	0.40
12:Z:97:MET:HB3	12:Z:116:SER:HB3	2.03	0.40
1:A:13:ILE:HG13	1:A:15:ILE:HG12	2.03	0.40
3:C:143:TYR:HB2	3:C:146:GLN:NE2	2.35	0.40
8:H:124:SER:OG	8:H:143:TYR:OH	2.34	0.40
12:L:97:MET:HB3	12:L:116:SER:HB3	2.03	0.40
12:Z:178:HIS:HE1	12:Z:180:ARG:HB3	1.86	0.40
4:D:145:TYR:HD1	4:D:155:ALA:HA	1.87	0.40
5:E:38:ILE:HD12	5:E:202:LEU:HD12	2.02	0.40
13:M:16:ALA:HB2	13:M:121:VAL:HG23	2.03	0.40
5:S:38:ILE:HD12	5:S:202:LEU:HD12	2.02	0.40
5:S:47:CYS:HA	5:S:219:THR:HG22	2.02	0.40
9:W:59:ILE:HD12	9:W:82:MET:HB3	2.03	0.40
11:Y:182:ILE:HG22	11:Y:189:HIS:HB2	2.02	0.40
4:D:31:THR:HA	4:D:162:GLY:HA3	2.04	0.40
9:I:50:ALA:HB2	10:J:128:CYS:HB2	2.03	0.40
4:R:31:THR:HA	4:R:162:GLY:HA3	2.04	0.40
12:Z:4:LEU:HB3	12:Z:15:ALA:HB3	2.03	0.40
4:D:132:LEU:HD23	4:D:132:LEU:HA	2.12	0.40
11:K:89:ALA:HA	11:K:92:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	232/246 (94%)	218 (94%)	14 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	232/246 (94%)	218 (94%)	14 (6%)	0	100	100
2	B	212/234 (91%)	205 (97%)	7 (3%)	0	100	100
2	P	212/234 (91%)	205 (97%)	7 (3%)	0	100	100
3	C	203/261 (78%)	185 (91%)	18 (9%)	0	100	100
3	Q	203/261 (78%)	185 (91%)	18 (9%)	0	100	100
4	D	206/248 (83%)	190 (92%)	16 (8%)	0	100	100
4	R	206/248 (83%)	190 (92%)	16 (8%)	0	100	100
5	E	223/241 (92%)	202 (91%)	21 (9%)	0	100	100
5	S	223/241 (92%)	202 (91%)	21 (9%)	0	100	100
6	F	234/263 (89%)	222 (95%)	12 (5%)	0	100	100
6	T	234/263 (89%)	222 (95%)	12 (5%)	0	100	100
7	G	240/255 (94%)	228 (95%)	12 (5%)	0	100	100
7	U	240/255 (94%)	228 (95%)	12 (5%)	0	100	100
8	H	196/205 (96%)	191 (97%)	5 (3%)	0	100	100
8	V	196/205 (96%)	191 (97%)	5 (3%)	0	100	100
9	I	219/234 (94%)	206 (94%)	13 (6%)	0	100	100
9	W	219/234 (94%)	206 (94%)	13 (6%)	0	100	100
10	J	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
10	X	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
11	K	194/201 (96%)	181 (93%)	12 (6%)	1 (0%)	29	68
11	Y	194/201 (96%)	181 (93%)	12 (6%)	1 (0%)	29	68
12	L	198/204 (97%)	186 (94%)	12 (6%)	0	100	100
12	Z	198/204 (97%)	185 (93%)	13 (7%)	0	100	100
13	M	211/213 (99%)	201 (95%)	10 (5%)	0	100	100
13	a	211/213 (99%)	201 (95%)	10 (5%)	0	100	100
14	N	204/219 (93%)	191 (94%)	13 (6%)	0	100	100
14	b	204/219 (93%)	191 (94%)	13 (6%)	0	100	100
15	c	1765/1843 (96%)	1610 (91%)	151 (9%)	4 (0%)	47	82
15	d	1765/1843 (96%)	1611 (91%)	150 (8%)	4 (0%)	47	82
All	All	9478/10144 (93%)	8814 (93%)	654 (7%)	10 (0%)	54	85

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	25	ILE
11	Y	25	ILE
15	c	32	ILE
15	c	33	VAL
15	d	32	ILE
15	d	33	VAL
15	c	746	PRO
15	d	746	PRO
15	c	830	PRO
15	d	830	PRO

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	A	157/210 (75%)	157 (100%)	0	100	100
1	O	157/210 (75%)	157 (100%)	0	100	100
2	B	147/191 (77%)	147 (100%)	0	100	100
2	P	147/191 (77%)	147 (100%)	0	100	100
3	C	117/221 (53%)	117 (100%)	0	100	100
3	Q	117/221 (53%)	117 (100%)	0	100	100
4	D	136/211 (64%)	136 (100%)	0	100	100
4	R	136/211 (64%)	136 (100%)	0	100	100
5	E	160/203 (79%)	160 (100%)	0	100	100
5	S	160/203 (79%)	160 (100%)	0	100	100
6	F	168/224 (75%)	167 (99%)	1 (1%)	86	95
6	T	168/224 (75%)	167 (99%)	1 (1%)	86	95
7	G	164/212 (77%)	164 (100%)	0	100	100
7	U	164/212 (77%)	164 (100%)	0	100	100
8	H	140/159 (88%)	140 (100%)	0	100	100
8	V	140/159 (88%)	140 (100%)	0	100	100
9	I	162/195 (83%)	161 (99%)	1 (1%)	86	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	162/195 (83%)	161 (99%)	1 (1%)	86	95
10	J	155/174 (89%)	154 (99%)	1 (1%)	86	95
10	X	155/174 (89%)	154 (99%)	1 (1%)	86	95
11	K	149/171 (87%)	149 (100%)	0	100	100
11	Y	149/171 (87%)	149 (100%)	0	100	100
12	L	139/159 (87%)	139 (100%)	0	100	100
12	Z	139/159 (87%)	139 (100%)	0	100	100
13	M	155/178 (87%)	155 (100%)	0	100	100
13	a	155/178 (87%)	155 (100%)	0	100	100
14	N	153/181 (84%)	153 (100%)	0	100	100
14	b	153/181 (84%)	153 (100%)	0	100	100
15	c	1271/1673 (76%)	1264 (99%)	7 (1%)	86	95
15	d	1271/1673 (76%)	1264 (99%)	7 (1%)	86	95
All	All	6746/8724 (77%)	6726 (100%)	20 (0%)	92	97

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	3	ARG
9	I	12	ILE
10	J	92	ASN
6	T	3	ARG
9	W	12	ILE
10	X	92	ASN
15	c	32	ILE
15	c	33	VAL
15	c	153	LEU
15	c	1405	LEU
15	c	1440	LEU
15	c	1602	LEU
15	c	1658	ARG
15	d	32	ILE
15	d	33	VAL
15	d	153	LEU
15	d	1405	LEU
15	d	1440	LEU
15	d	1602	LEU
15	d	1658	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	154	HIS
6	F	20	HIS
7	G	32	ASN
10	J	172	ASN
13	M	79	ASN
13	M	157	ASN
4	R	154	HIS
5	S	41	GLN
5	S	164	GLN
6	T	20	HIS
7	U	32	ASN
10	X	172	ASN
13	a	79	ASN
13	a	157	ASN
15	c	327	GLN
15	c	676	ASN
15	c	712	GLN
15	c	1165	HIS
15	c	1219	HIS
15	c	1392	HIS
15	d	327	GLN
15	d	676	ASN
15	d	712	GLN
15	d	1165	HIS
15	d	1219	HIS
15	d	1392	HIS
15	d	1796	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	K0W	c	1902	-	40,44,44	1.27	4 (10%)	66,74,74	1.25	7 (10%)
16	IHP	c	1901	-	36,36,36	1.59	4 (11%)	54,60,60	0.48	0
16	IHP	d	1901	-	36,36,36	1.61	4 (11%)	54,60,60	0.47	0
17	K0W	d	1902	-	40,44,44	1.27	4 (10%)	66,74,74	1.25	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	K0W	c	1902	-	-	8/42/66/66	0/1/1/1
16	IHP	c	1901	-	-	1/30/54/54	0/1/1/1
16	IHP	d	1901	-	-	1/30/54/54	0/1/1/1
17	K0W	d	1902	-	-	8/42/66/66	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	c	1901	IHP	P2-O22	3.41	1.61	1.50
16	d	1901	IHP	P2-O22	3.41	1.61	1.50
17	c	1902	K0W	PA3-O13	3.39	1.65	1.59
17	d	1902	K0W	PA3-O13	3.39	1.65	1.59
16	c	1901	IHP	P5-O25	3.39	1.61	1.50
16	d	1901	IHP	P5-O25	3.39	1.61	1.50
16	c	1901	IHP	P4-O24	3.38	1.61	1.50
16	d	1901	IHP	P4-O24	3.38	1.61	1.50
16	c	1901	IHP	P6-O26	3.37	1.61	1.50
16	d	1901	IHP	P6-O26	3.37	1.61	1.50
17	c	1902	K0W	PA6-O16	2.95	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	d	1902	K0W	PA6-O16	2.95	1.64	1.59
17	c	1902	K0W	PA4-O14	2.78	1.64	1.59
17	d	1902	K0W	PA4-O14	2.78	1.64	1.59
17	c	1902	K0W	PA2-O12	2.73	1.64	1.59
17	d	1902	K0W	PA2-O12	2.73	1.64	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	d	1902	K0W	O77-PA5-O15	3.42	109.39	102.48
17	c	1902	K0W	O77-PA5-O15	3.40	109.35	102.48
17	d	1902	K0W	C5-C6-C1	3.37	117.80	110.41
17	c	1902	K0W	C5-C6-C1	3.37	117.78	110.41
17	c	1902	K0W	C5-C4-C3	2.80	116.53	110.41
17	d	1902	K0W	C5-C4-C3	2.80	116.53	110.41
17	c	1902	K0W	PA1-O76-PB1	-2.69	123.61	132.83
17	d	1902	K0W	PA1-O76-PB1	-2.69	123.61	132.83
17	c	1902	K0W	C4-C3-C2	2.62	116.14	110.41
17	d	1902	K0W	C4-C3-C2	2.62	116.14	110.41
17	c	1902	K0W	O76-PA1-O11	2.58	107.70	102.48
17	d	1902	K0W	O76-PA1-O11	2.58	107.70	102.48
17	c	1902	K0W	C6-C1-C2	2.40	115.67	110.41
17	d	1902	K0W	C6-C1-C2	2.39	115.64	110.41

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	c	1901	IHP	C1-O11-P1-O21
16	d	1901	IHP	C1-O11-P1-O21
17	c	1902	K0W	C4-C3-O13-PA3
17	c	1902	K0W	C2-O12-PA2-O22
17	d	1902	K0W	C4-C3-O13-PA3
17	d	1902	K0W	C2-O12-PA2-O22
17	c	1902	K0W	C6-O11-PA1-O76
17	d	1902	K0W	C6-O11-PA1-O76
17	c	1902	K0W	C3-O13-PA3-O23
17	d	1902	K0W	C3-O13-PA3-O23
17	c	1902	K0W	C2-C3-O13-PA3
17	d	1902	K0W	C2-C3-O13-PA3
17	c	1902	K0W	C4-O14-PA4-O44
17	d	1902	K0W	C4-O14-PA4-O44

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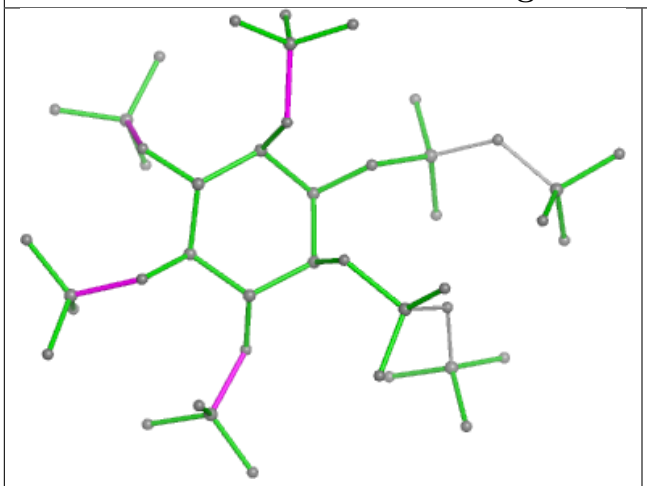
Mol	Chain	Res	Type	Atoms
17	c	1902	K0W	C2-O12-PA2-O32
17	c	1902	K0W	C3-O13-PA3-O43
17	d	1902	K0W	C2-O12-PA2-O32
17	d	1902	K0W	C3-O13-PA3-O43

There are no ring outliers.

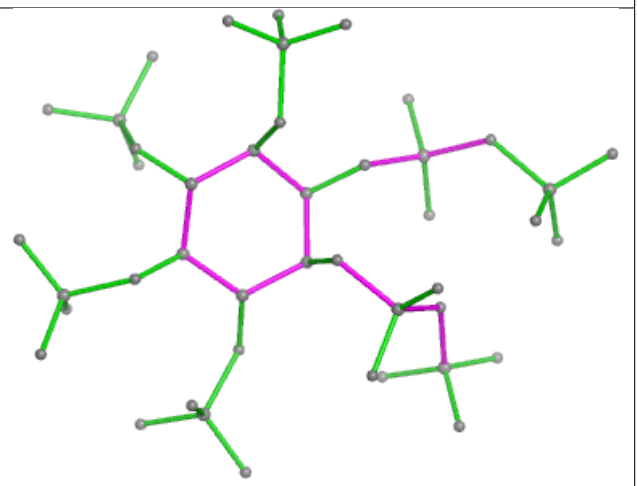
No monomer is involved in short contacts.

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

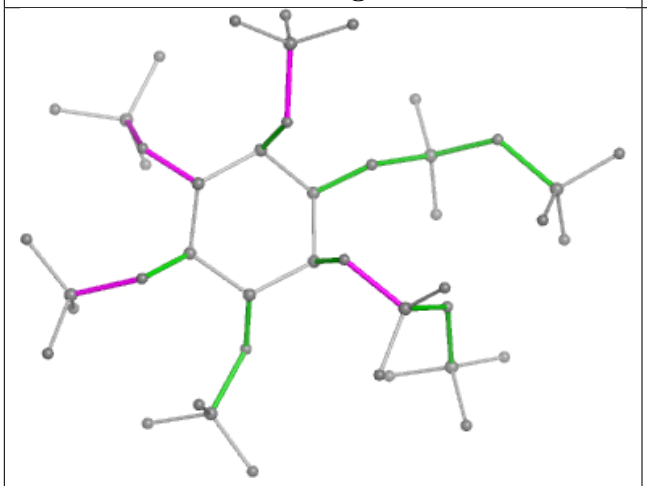
Ligand K0W c 1902



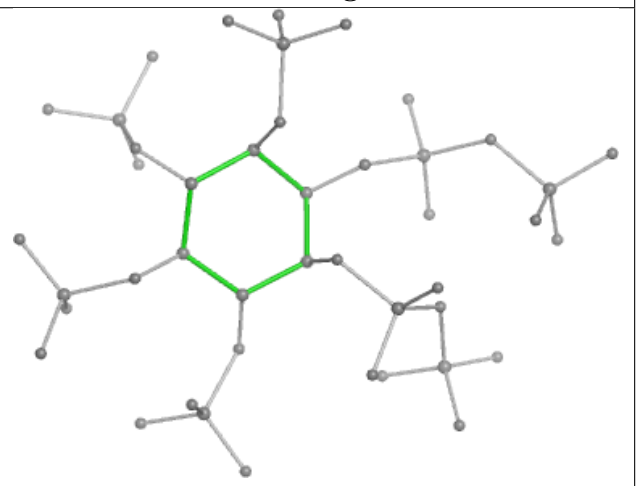
Bond lengths



Bond angles

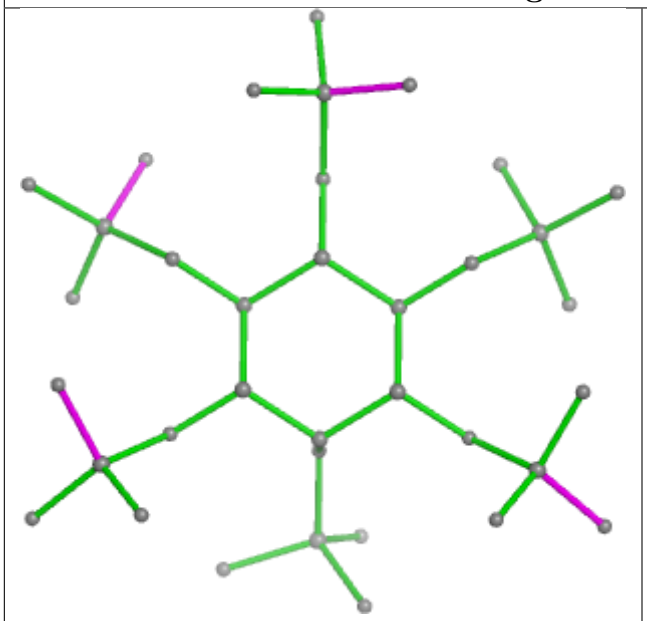


Torsions

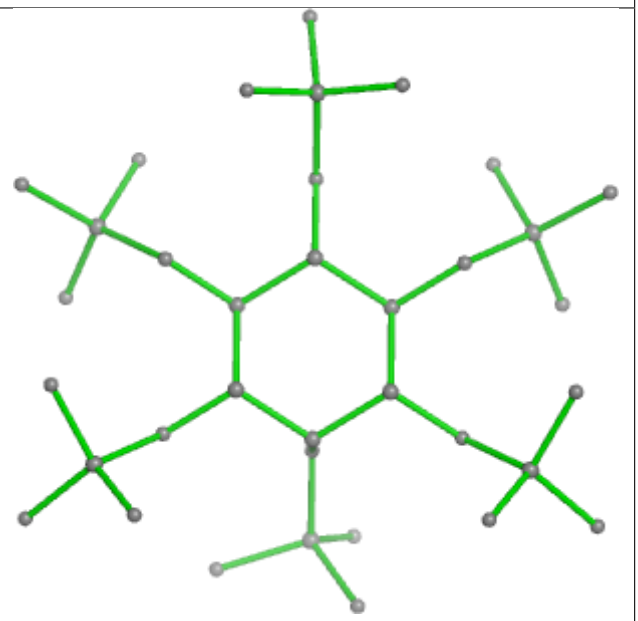


Rings

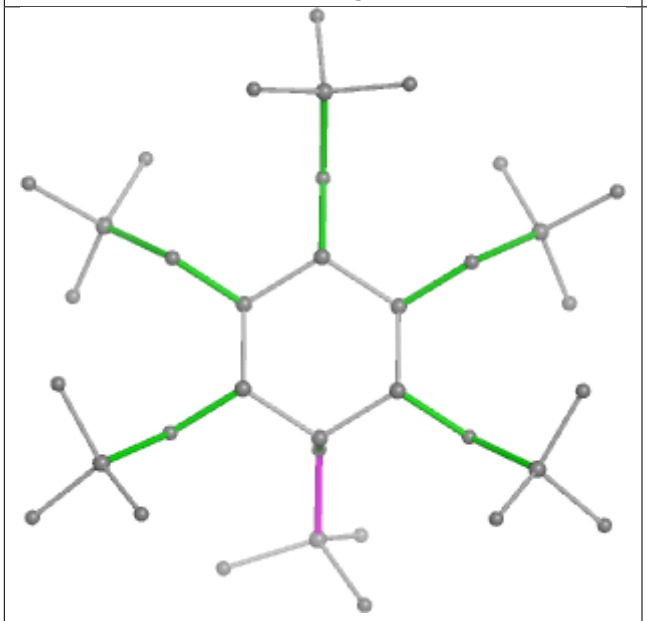
Ligand IHP c 1901



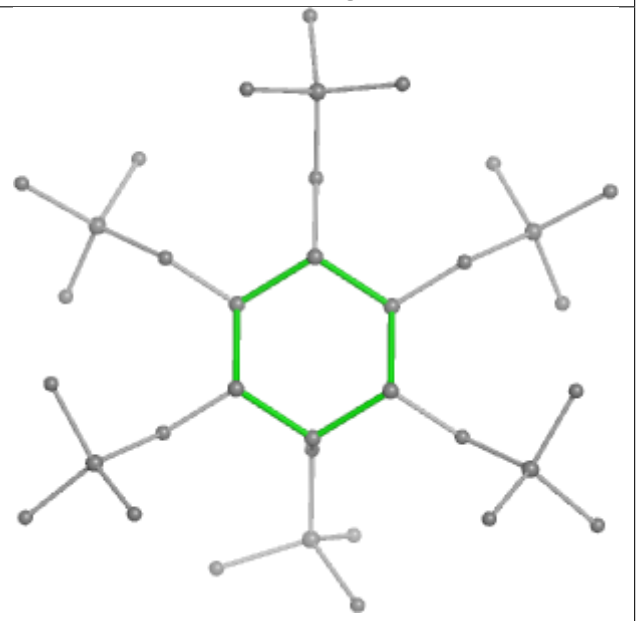
Bond lengths



Bond angles

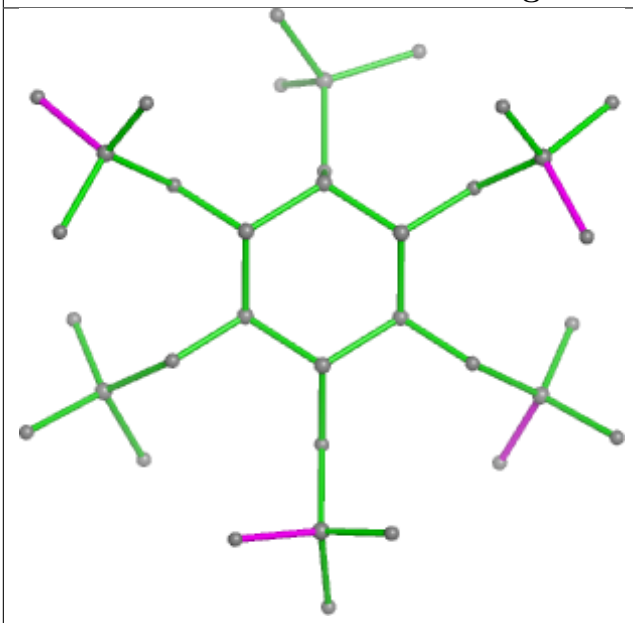


Torsions

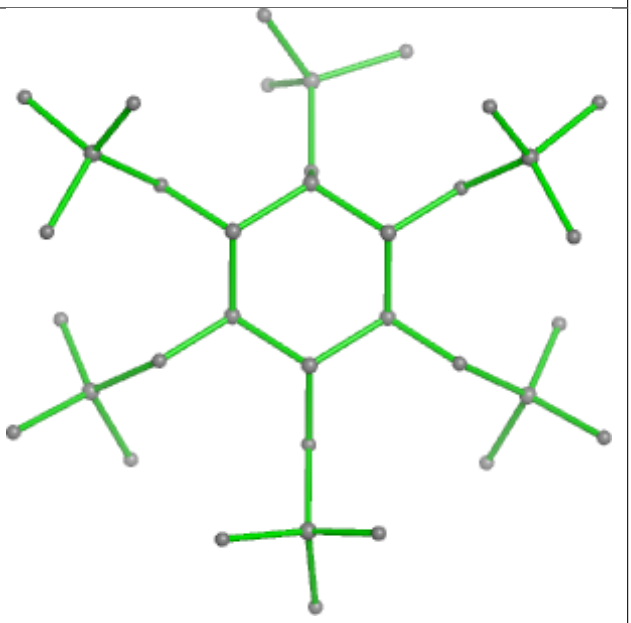


Rings

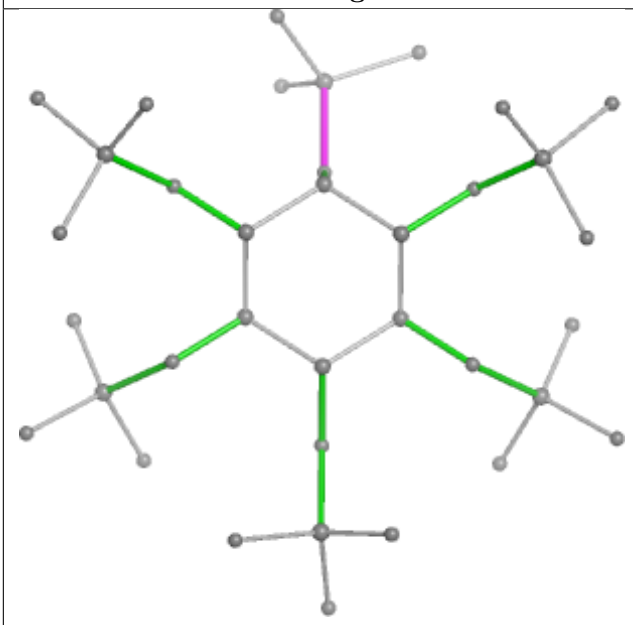
Ligand IHP d 1901



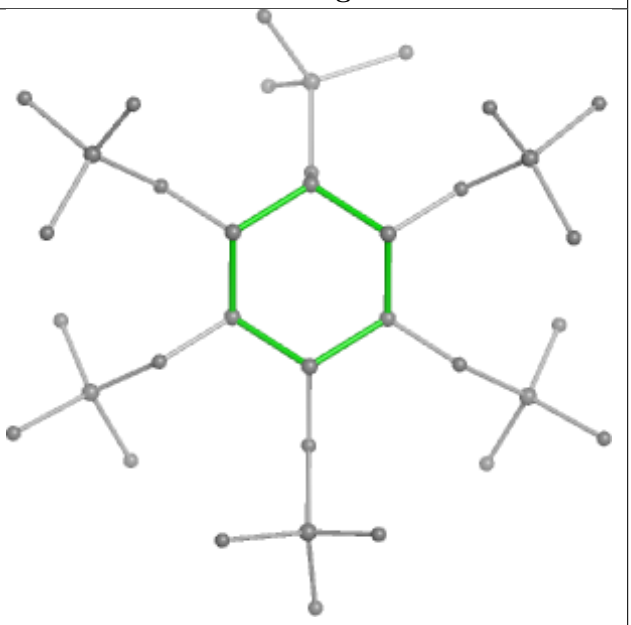
Bond lengths



Bond angles

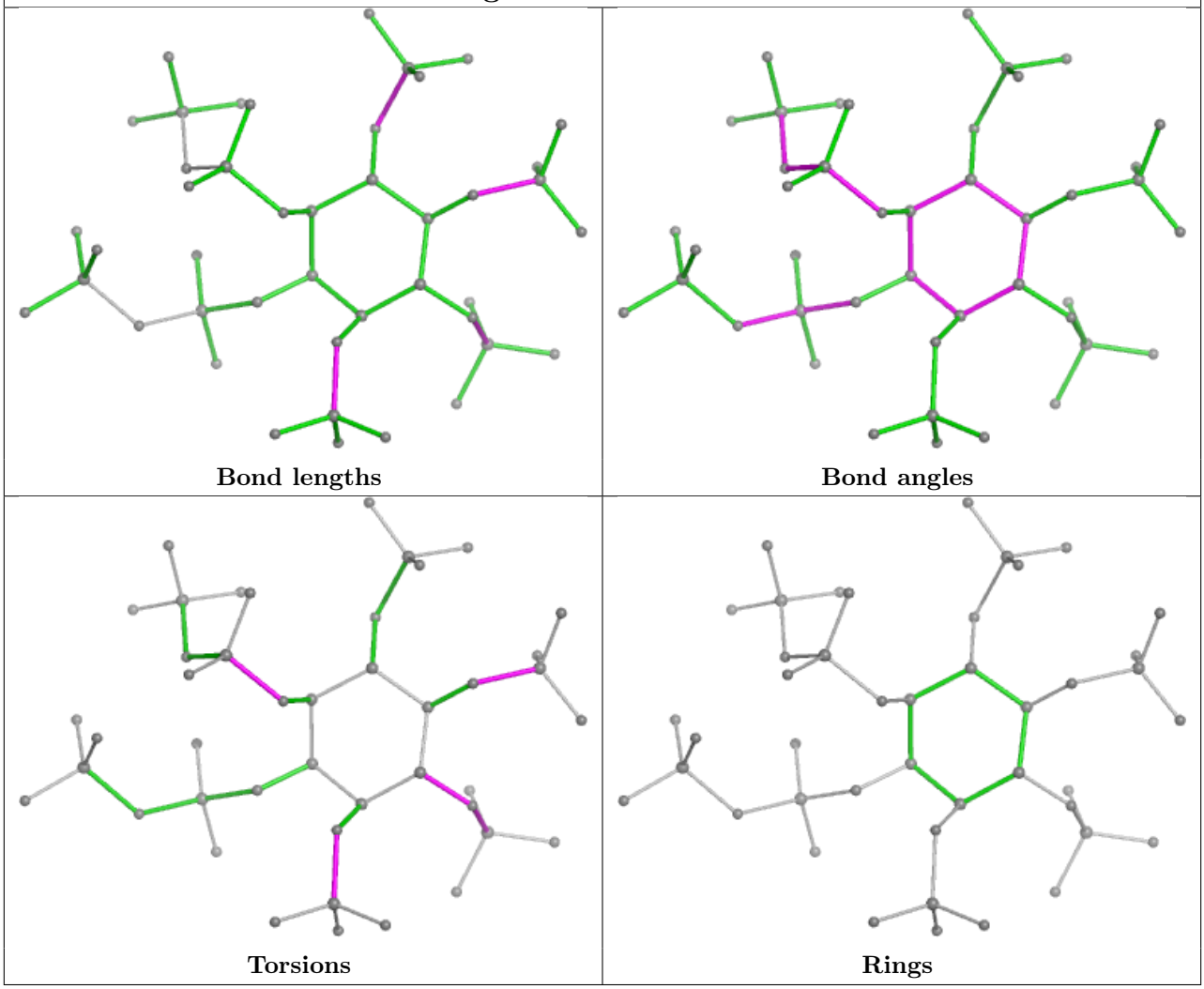


Torsions



Rings

Ligand K0W d 1902



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

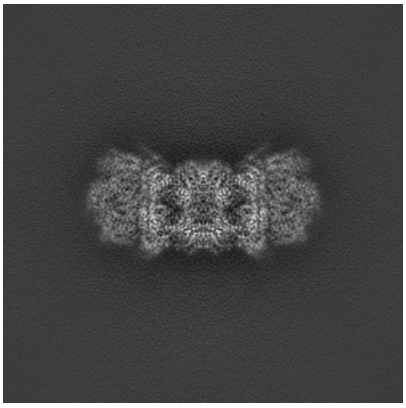
6 Map visualisation (i)

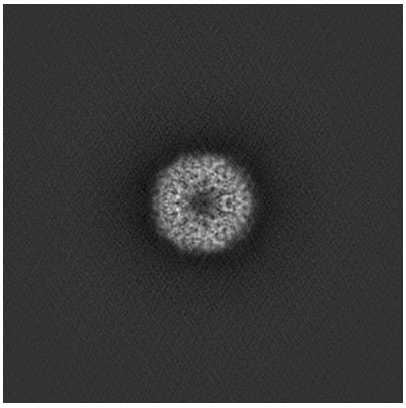
This section contains visualisations of the EMDB entry EMD-4860. These allow visual inspection of the internal detail of the map and identification of artifacts.

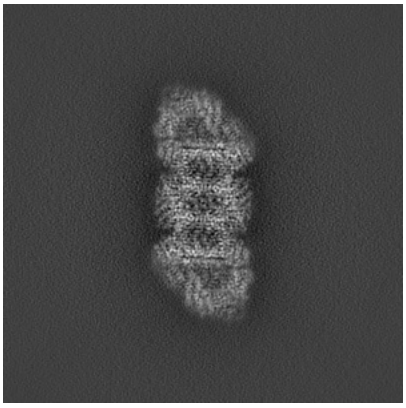
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

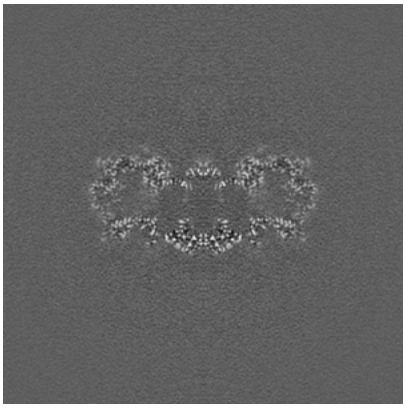

Y

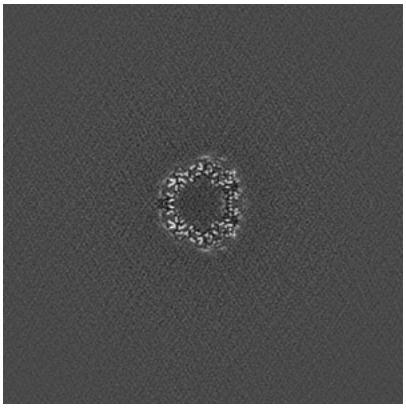

Z

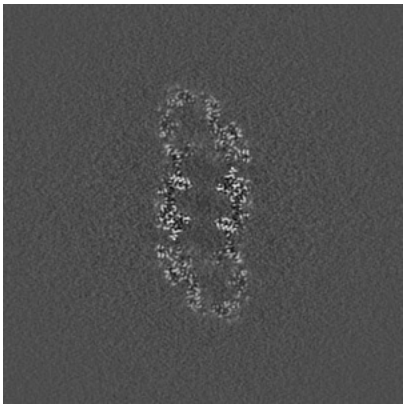
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 288

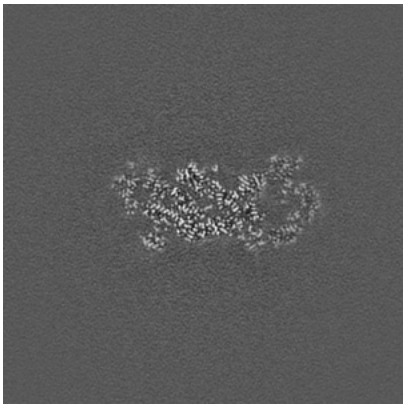

Y Index: 288

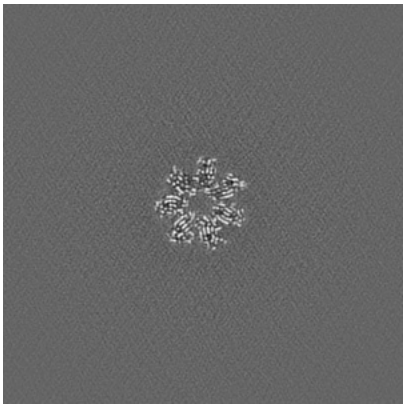

Z Index: 288

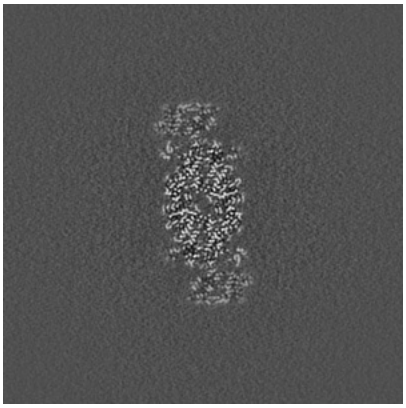
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 253

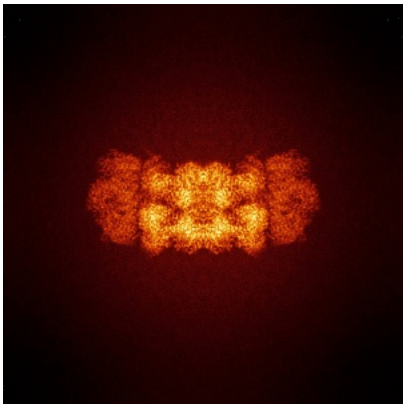

Y Index: 312

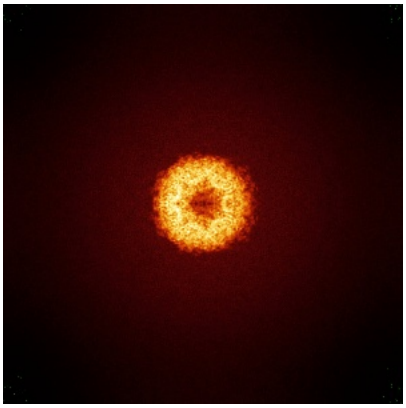

Z Index: 252

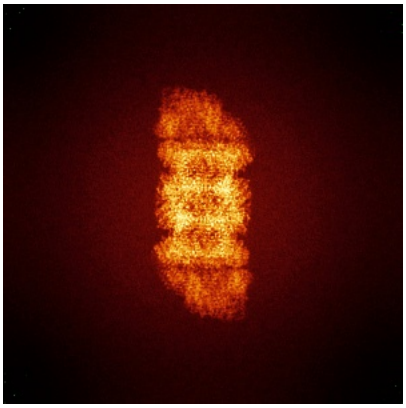
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

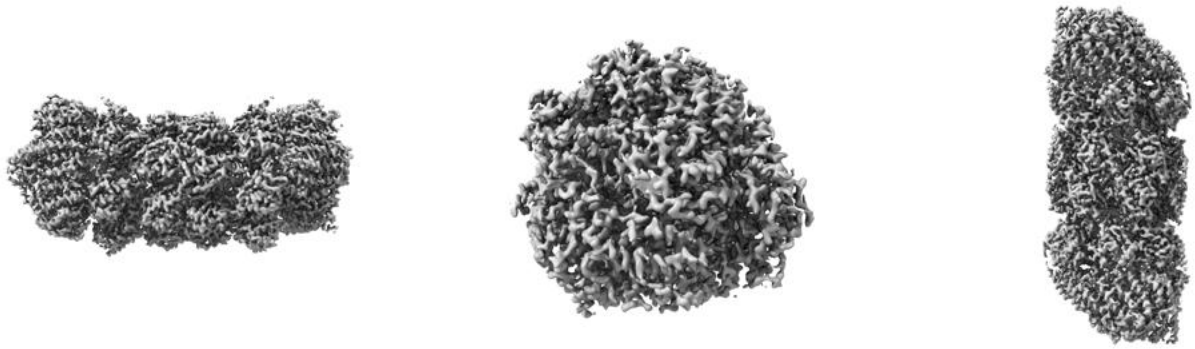

Y


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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

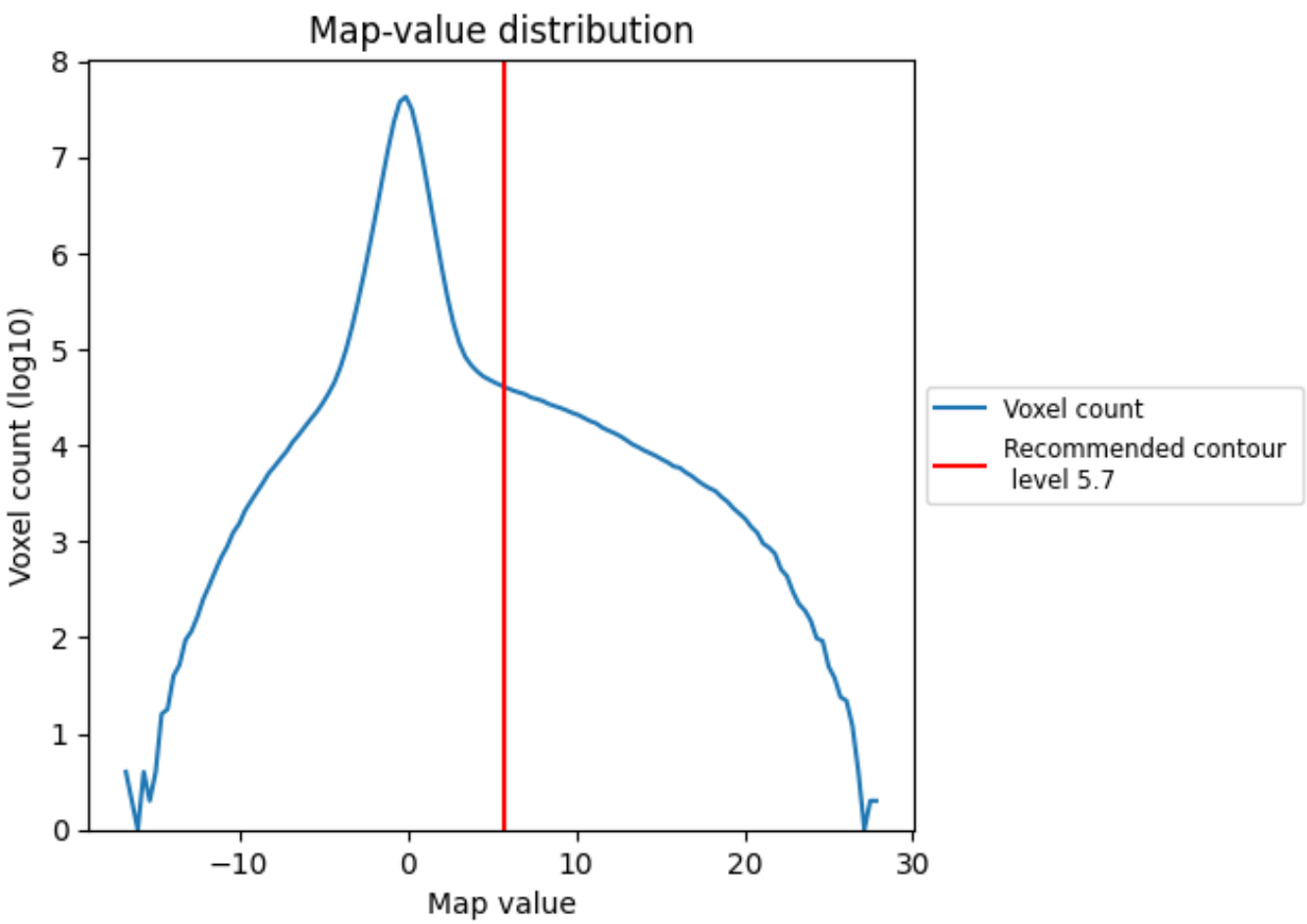
6.6 Mask visualisation (i)

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

7 Map analysis (i)

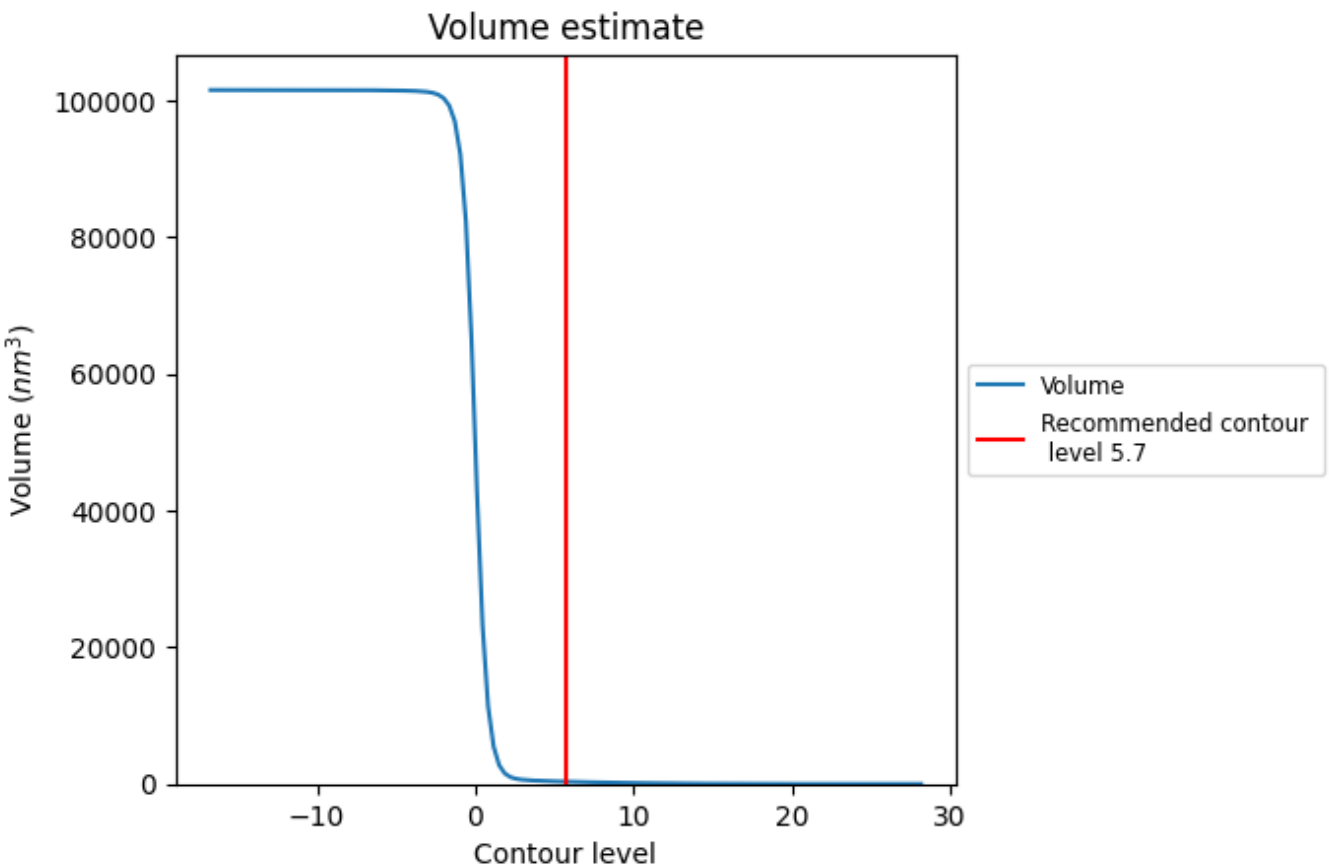
This section contains the results of statistical analysis of the map.

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.

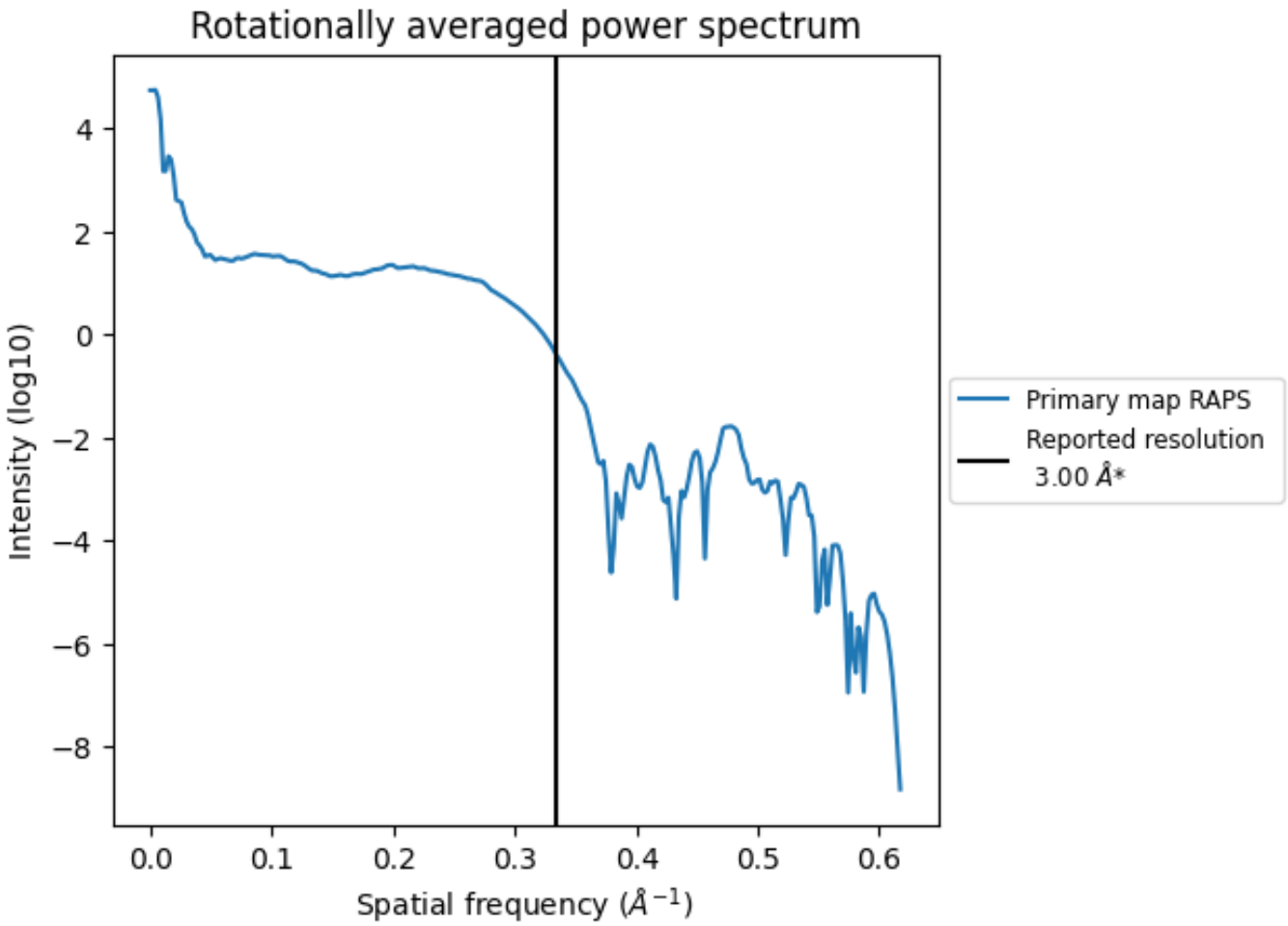
7.2 Volume estimate (i)



The volume at the recommended contour level is 340 nm^3; this corresponds to an approximate mass of 307 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)

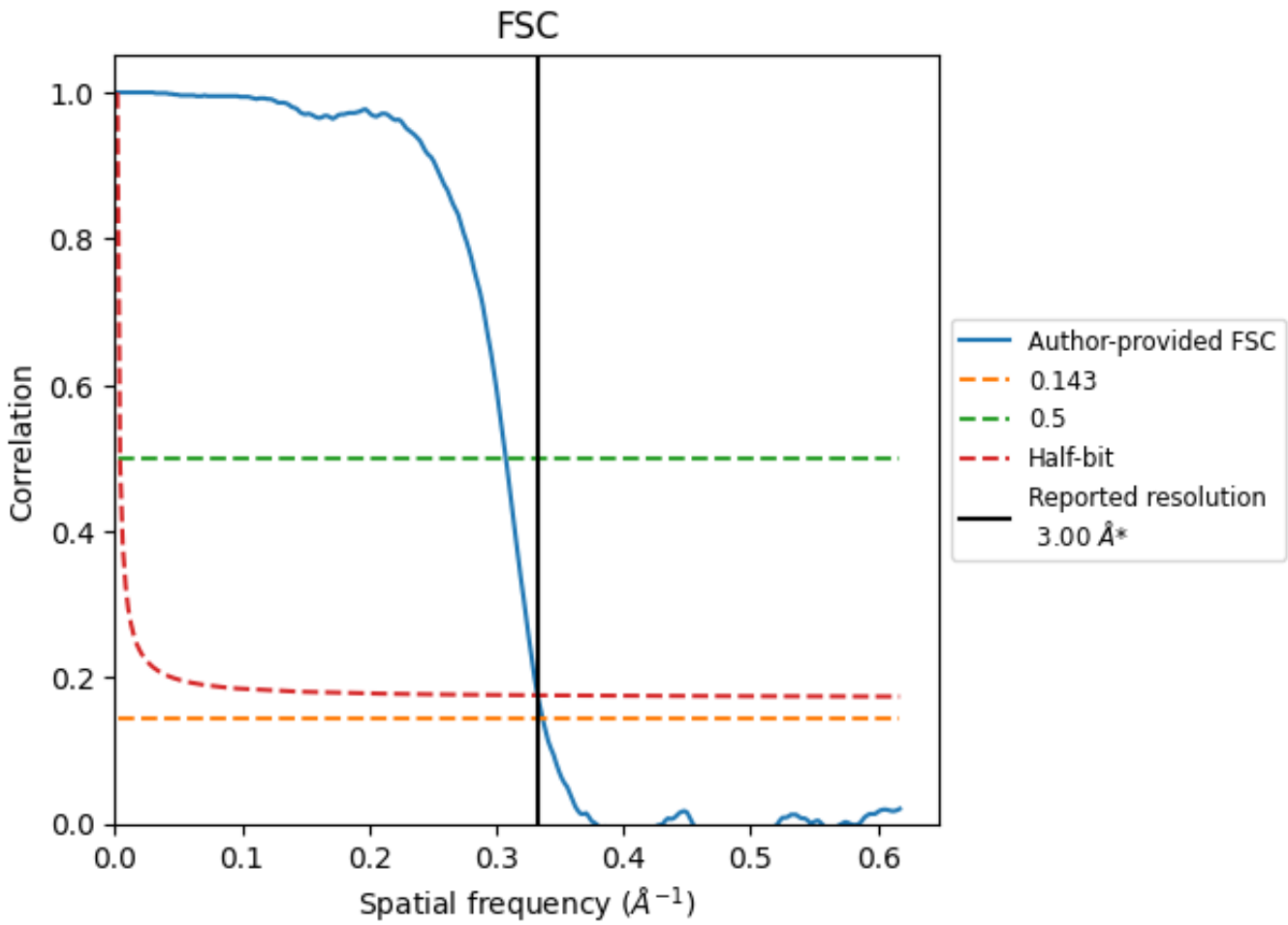


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

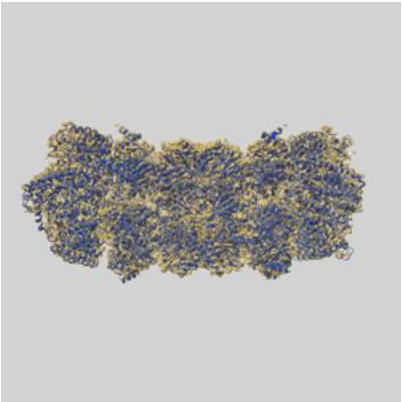
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.97	3.25	3.01
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

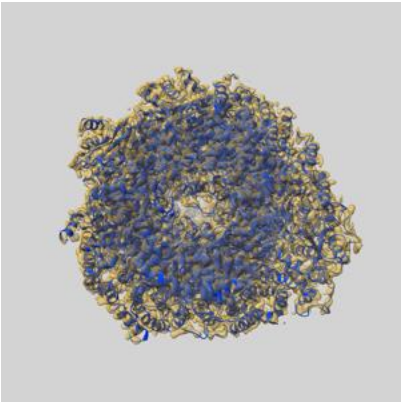
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4860 and PDB model 6REY. Per-residue inclusion information can be found in section 3 on page 9.

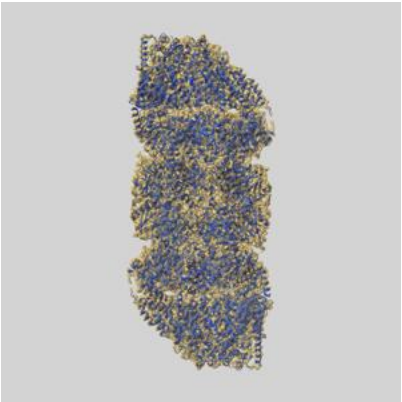
9.1 Map-model overlay (i)



X



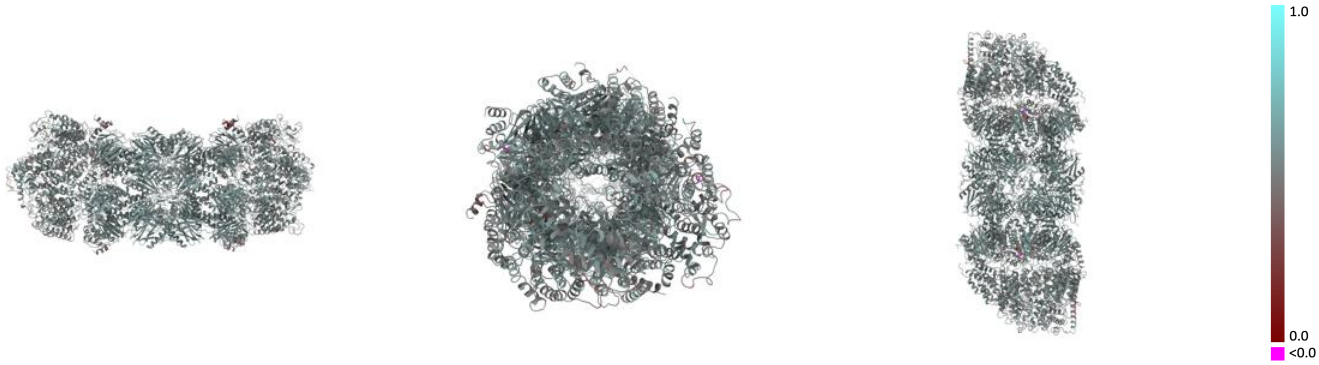
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.7 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.

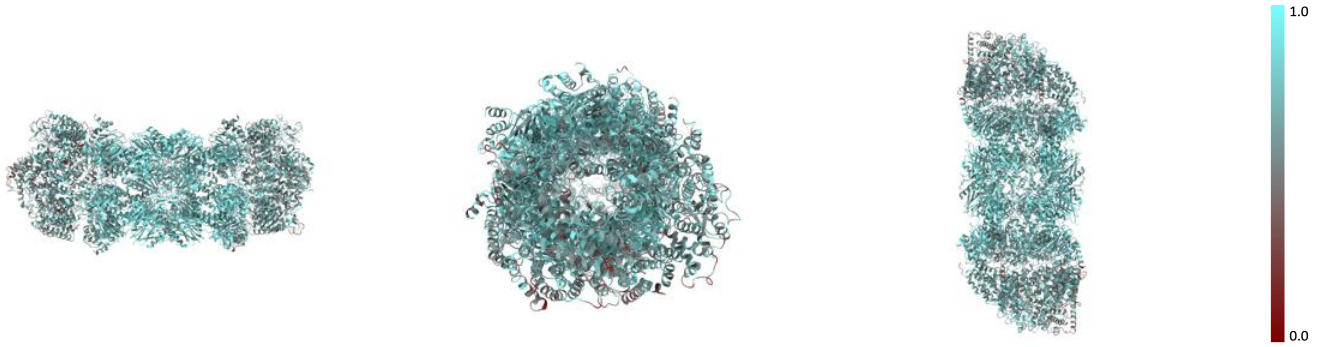
9.2 Q-score mapped to coordinate model (i)



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.

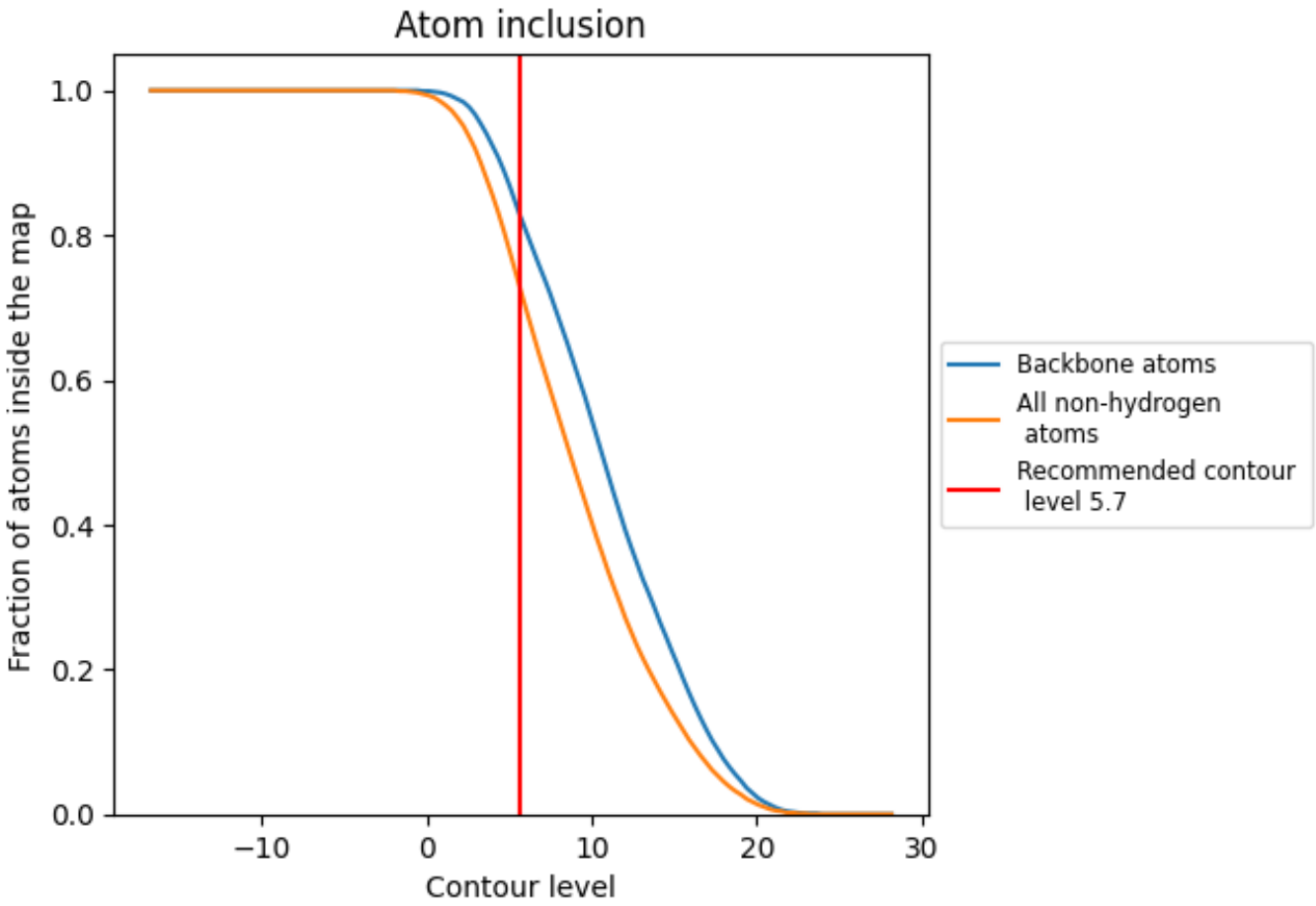
9.3 Atom inclusion mapped to coordinate model (i)



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 (5.7).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (5.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7230	0.5310
A	0.7520	0.5370
B	0.7840	0.5480
C	0.7350	0.5240
D	0.6820	0.5060
E	0.7210	0.5300
F	0.7920	0.5420
G	0.7780	0.5400
H	0.8160	0.5540
I	0.8210	0.5510
J	0.8220	0.5540
K	0.8160	0.5480
L	0.8220	0.5460
M	0.8000	0.5500
N	0.8400	0.5550
O	0.7530	0.5350
P	0.7870	0.5470
Q	0.7350	0.5210
R	0.6820	0.5080
S	0.7210	0.5290
T	0.7910	0.5400
U	0.7750	0.5390
V	0.8180	0.5540
W	0.8210	0.5510
X	0.8200	0.5540
Y	0.8170	0.5470
Z	0.8220	0.5470
a	0.7970	0.5480
b	0.8370	0.5550
c	0.6220	0.5140
d	0.6220	0.5140