Full wwPDB EM Validation Report ⓘ

Oct 24, 2022 – 06:52 PM EDT

PDB ID	:	8CVS
EMDB ID	:	EMD-27015
Title	:	Human PA200-20S proteasome with MG-132
Authors	:	Zhao, J.
Deposited on	:	2022-05-18
Resolution	:	3.10 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:

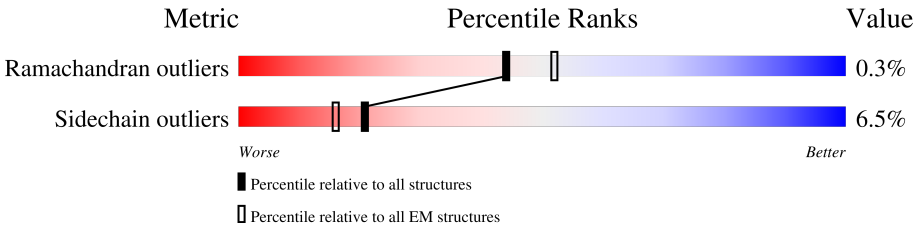
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)
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	234	87% 6% 7%
1	O	234	93% 5% •
2	B	261	• 82% 6% 12%
2	P	261	91% 5% 5%
3	C	248	• 82% 9% 9%
3	Q	248	94% • •
4	D	241	90% 5% 5%
4	R	241	• 94% • •
5	E	263	87% 5% 9%

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Mol	Chain	Length	Quality of chain
5	S	263	87% 10%
6	F	255	90% 5%
6	T	255	91% 6%
7	G	246	91% 5%
7	U	246	94% 5%
8	H	234	89% 5% 6%
8	V	234	87% 7% 6%
9	I	205	96%
9	W	205	94% 6%
10	J	201	91% 7%
10	X	201	92% 6%
11	K	204	93% 5%
11	Y	204	94%
12	L	241	85% 12%
12	Z	241	85% 12%
13	M	264	79% 18%
13	a	264	77% 5% 18%
14	N	205	96%
14	b	205	98%
15	c	1843	92% 6%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 61346 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-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	217	Total	C	N	O	S	0	0
			1665	1070	289	300	6		
1	O	230	Total	C	N	O	S	0	0
			1724	1117	296	306	5		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	230	Total	C	N	O	S	0	0
			1721	1089	295	328	9		
2	P	249	Total	C	N	O	S	0	0
			1874	1192	328	344	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	225	Total	C	N	O	S	0	0
			1666	1049	301	311	5		
3	Q	239	Total	C	N	O	S	0	0
			1781	1130	324	322	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	229	Total	C	N	O	S	0	0
			1711	1088	285	327	11		
4	R	235	Total	C	N	O	S	0	0
			1711	1089	294	318	10		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	240	Total	C	N	O	S	0	0
			1870	1178	340	340	12		
5	S	237	Total	C	N	O	S	0	0
			1784	1131	331	312	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	244	Total	C	N	O	S	0	0
			1867	1189	321	348	9		
6	T	240	Total	C	N	O	S	0	0
			1823	1162	317	333	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	238	Total	C	N	O	S	0	0
			1789	1145	304	327	13		
7	U	243	Total	C	N	O	S	0	0
			1840	1172	312	344	12		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	220	Total	C	N	O	S	0	0
			1617	1025	275	306	11		
8	V	221	Total	C	N	O	S	0	0
			1641	1038	278	314	11		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1562	1000	263	280	19		
9	W	204	Total	C	N	O	S	0	0
			1576	1008	264	285	19		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	196	Total	C	N	O	S	0	0
			1526	988	261	268	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	197	Total 1543	C 998	N 265	O 271	S 9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	201	Total 1545	C 980	N 274	O 282	S 9	0	0
11	Y	200	Total 1539	C 976	N 272	O 282	S 9	0	0

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	213	Total 1623	C 1032	N 280	O 301	S 10	0	0
12	Z	213	Total 1617	C 1032	N 281	O 294	S 10	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	216	Total 1671	C 1060	N 291	O 308	S 12	0	0
13	a	216	Total 1658	C 1053	N 290	O 303	S 12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total 1481	C 936	N 258	O 275	S 12	0	0
14	b	203	Total 1486	C 939	N 259	O 277	S 11	0	0

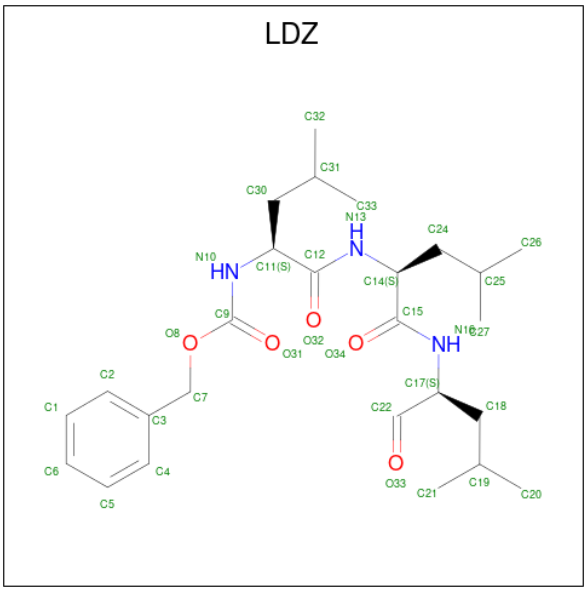
- Molecule 15 is a protein called Proteasome activator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	1802	Total 14159	C 9175	N 2444	O 2466	S 74	0	0

There are 3 discrepancies between the modelled and reference sequences:

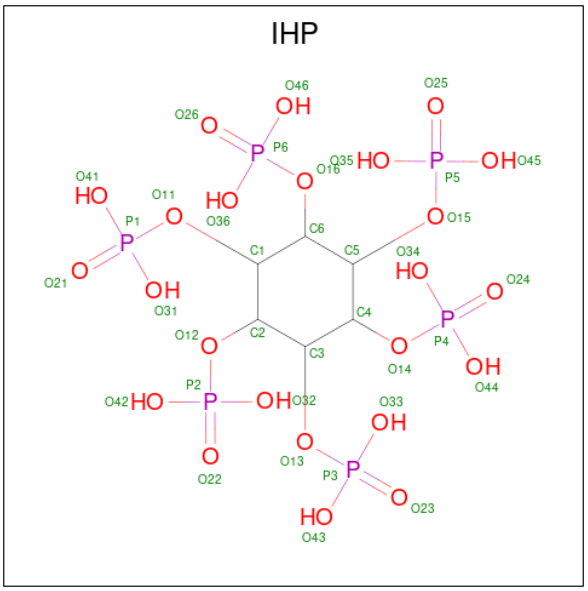
Chain	Residue	Modelled	Actual	Comment	Reference
c	821	ILE	LEU	conflict	UNP Q14997
c	822	LEU	ILE	conflict	UNP Q14997
c	1238	LEU	ILE	conflict	UNP Q14997

- Molecule 16 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-4-methyl-1-oxopentan-2-yl]-L-leucinamide (three-letter code: LDZ) (formula: $C_{26}H_{41}N_3O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
16	H	1	Total	C	N	O	0
			34	26	3	5	
16	K	1	Total	C	N	O	0
			34	26	3	5	
16	N	1	Total	C	N	O	0
			34	26	3	5	
16	V	1	Total	C	N	O	0
			34	26	3	5	
16	Y	1	Total	C	N	O	0
			34	26	3	5	
16	b	1	Total	C	N	O	0
			34	26	3	5	

- Molecule 17 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



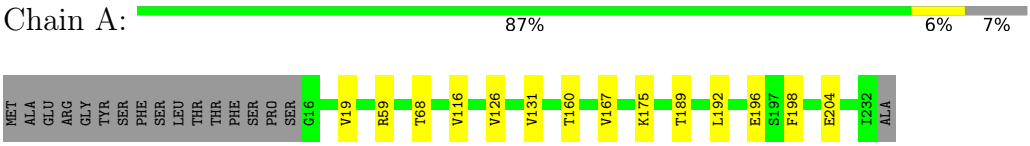
Mol	Chain	Residues	Atoms				AltConf
17	c	1	Total	C	O	P	0
			72	12	48	12	
17	c	1	Total	C	O	P	0
			72	12	48	12	

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.

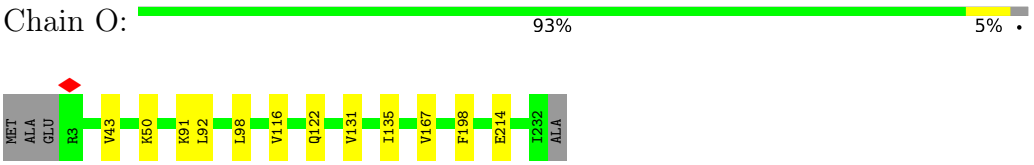
• Molecule 1: Proteasome subunit alpha type-2

Chain A:



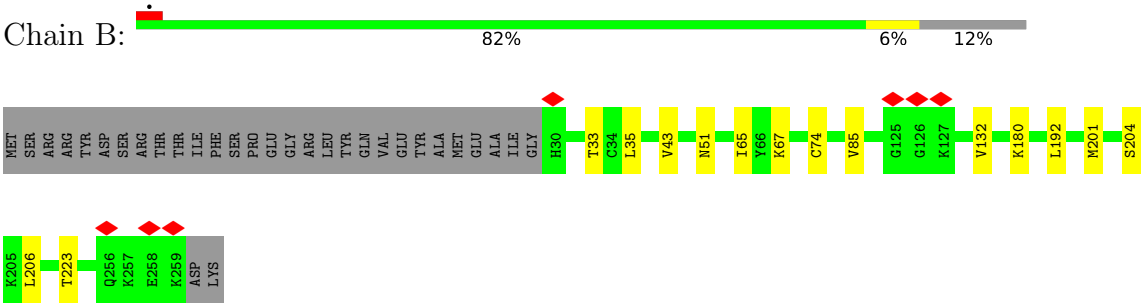
• Molecule 1: Proteasome subunit alpha type-2

Chain O:



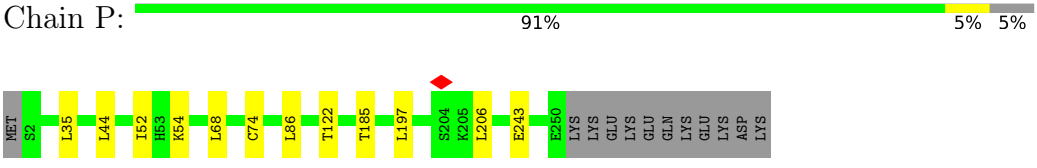
• Molecule 2: Proteasome subunit alpha type-4

Chain B:



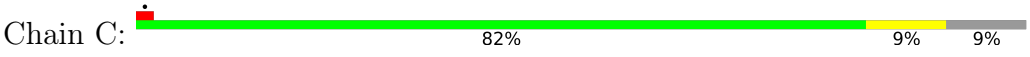
• Molecule 2: Proteasome subunit alpha type-4

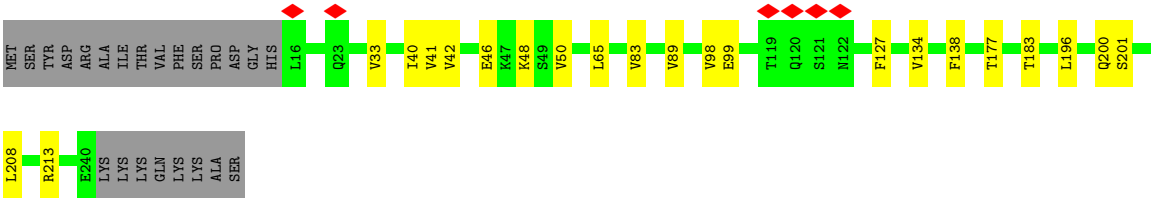
Chain P:



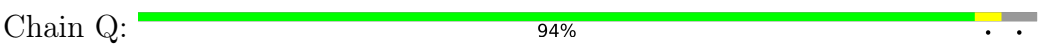
• Molecule 3: Proteasome subunit alpha type-7

Chain C:

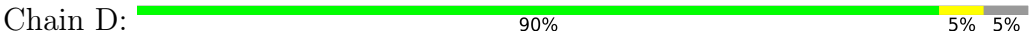


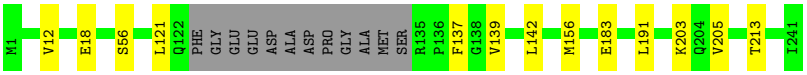


• Molecule 3: Proteasome subunit alpha type-7

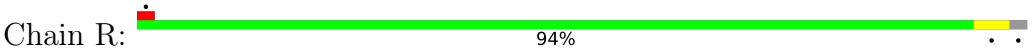


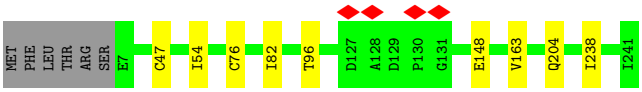
• Molecule 4: Proteasome subunit alpha type-5



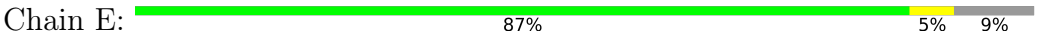


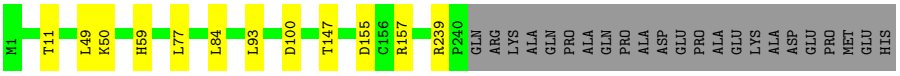
• Molecule 4: Proteasome subunit alpha type-5



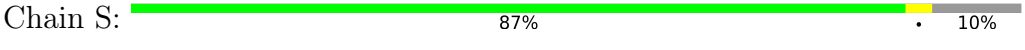


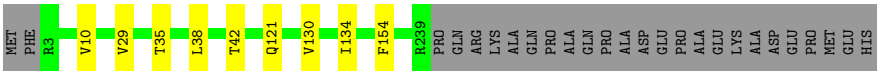
• Molecule 5: Proteasome subunit alpha type-1



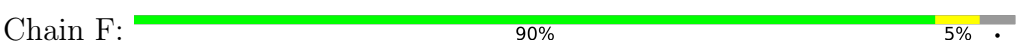


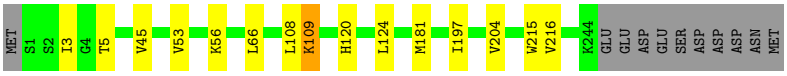
• Molecule 5: Proteasome subunit alpha type-1





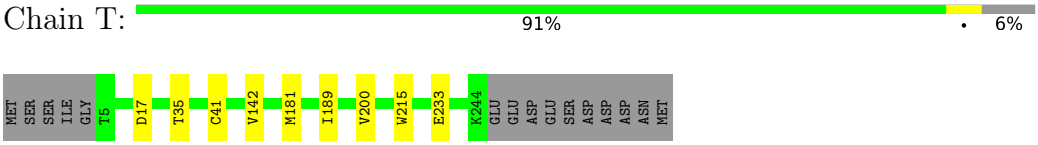
• Molecule 6: Proteasome subunit alpha type-3





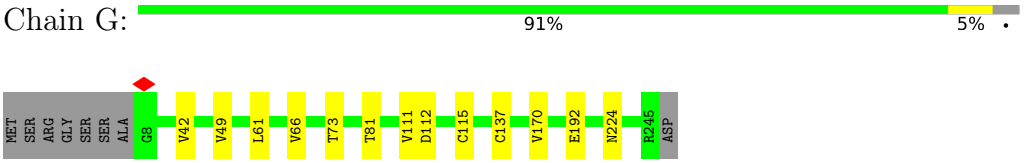
• Molecule 6: Proteasome subunit alpha type-3

Chain T:



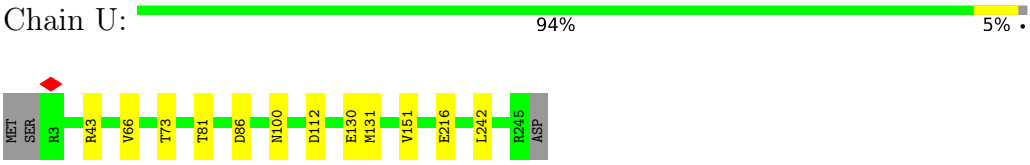
• Molecule 7: Proteasome subunit alpha type-6

Chain G:



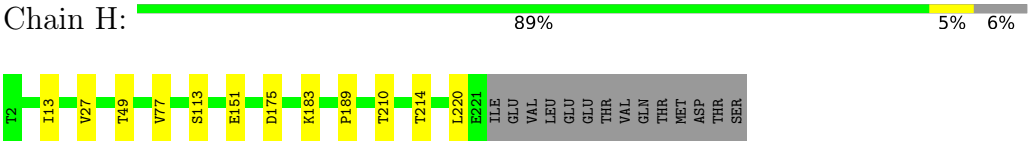
• Molecule 7: Proteasome subunit alpha type-6

Chain U:



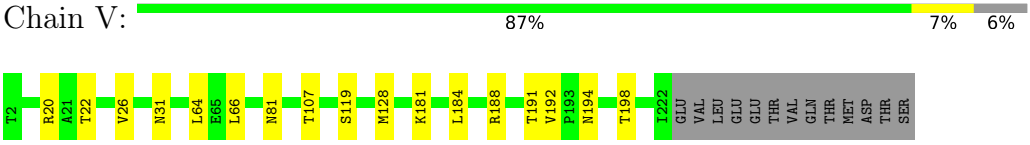
• Molecule 8: Proteasome subunit beta type-7

Chain H:



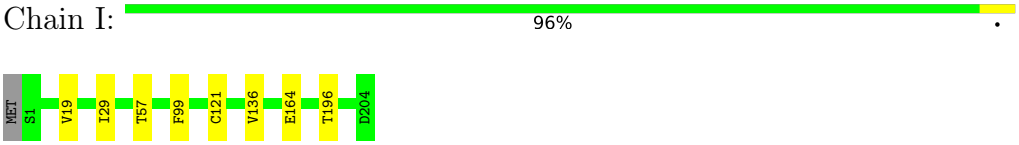
• Molecule 8: Proteasome subunit beta type-7

Chain V:



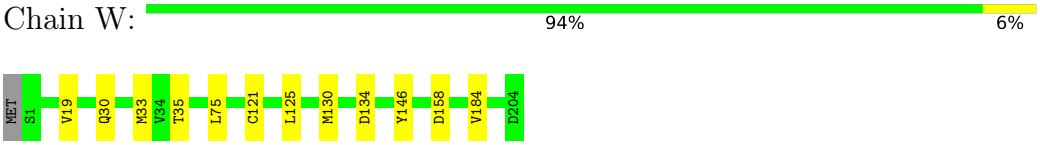
• Molecule 9: Proteasome subunit beta type-3

Chain I:



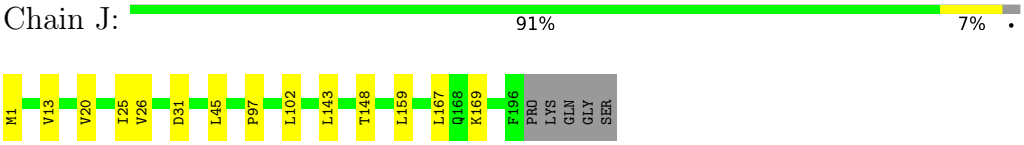
• Molecule 9: Proteasome subunit beta type-3

Chain W:



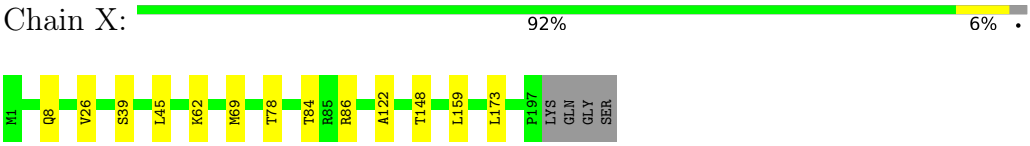
• Molecule 10: Proteasome subunit beta type-2

Chain J:



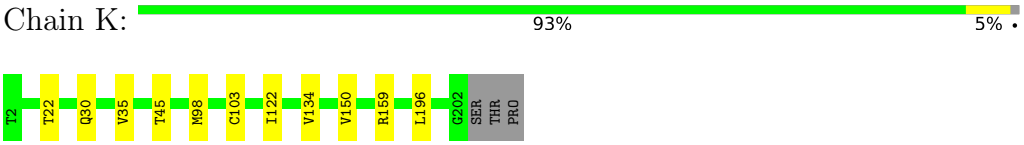
• Molecule 10: Proteasome subunit beta type-2

Chain X:



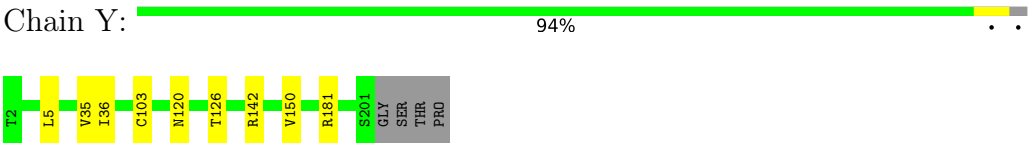
• Molecule 11: Proteasome subunit beta type-5

Chain K:



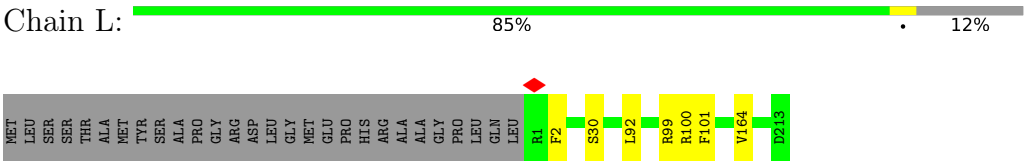
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



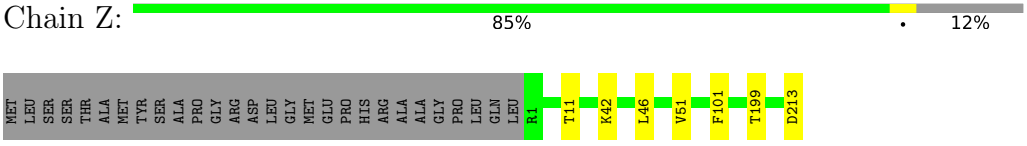
• Molecule 12: Proteasome subunit beta type-1

Chain L:



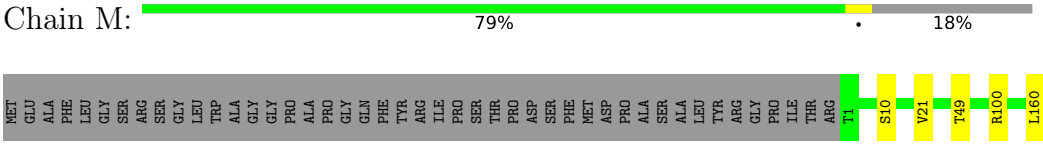
• Molecule 12: Proteasome subunit beta type-1

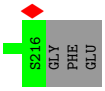
Chain Z:



• Molecule 13: Proteasome subunit beta type-4

Chain M:



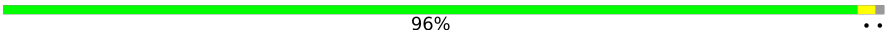


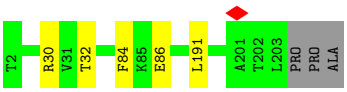
• Molecule 13: Proteasome subunit beta type-4

Chain a:

• Molecule 14: Proteasome subunit beta type-6

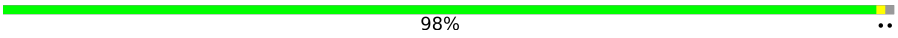
Chain N:

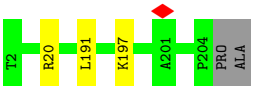




• Molecule 14: Proteasome subunit beta type-6

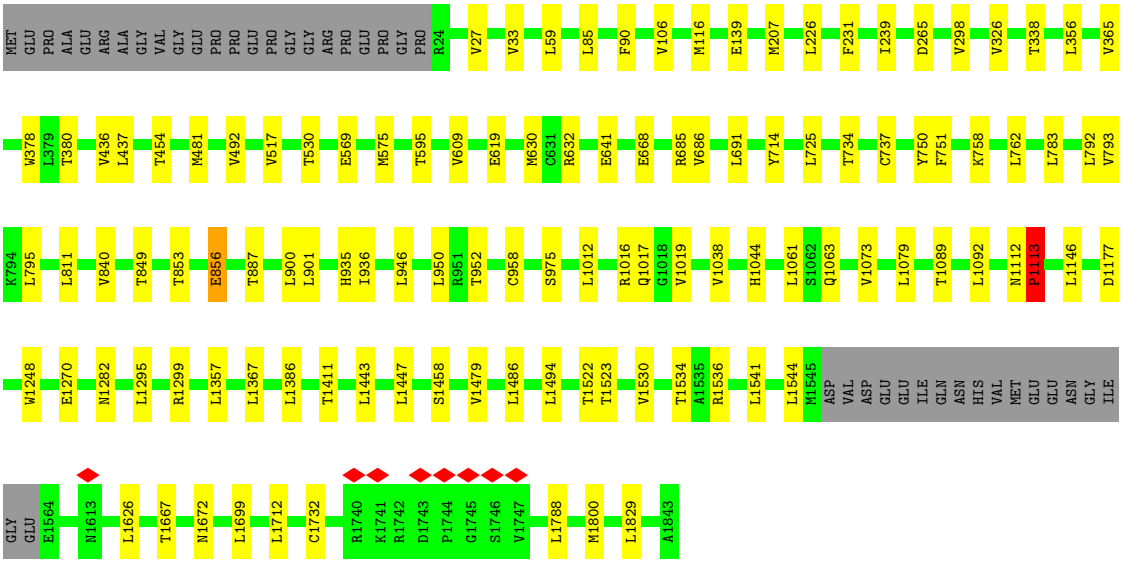
Chain b:





• Molecule 15: Proteasome activator complex subunit 4

Chain c:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70412	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.484	Depositor
Minimum map value	-0.690	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: LDZ, 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	0.57	0/1700	0.68	0/2306
1	O	0.59	0/1763	0.68	0/2400
2	B	0.59	0/1744	0.69	0/2359
2	P	0.59	0/1904	0.66	0/2579
3	C	0.60	0/1686	0.70	0/2287
3	Q	0.60	0/1807	0.68	0/2453
4	D	0.61	0/1737	0.69	0/2352
4	R	0.61	0/1738	0.66	0/2358
5	E	0.58	0/1906	0.70	0/2579
5	S	0.60	0/1818	0.69	0/2467
6	F	0.59	0/1902	0.70	1/2569 (0.0%)
6	T	0.60	0/1858	0.67	0/2512
7	G	0.58	0/1822	0.69	0/2476
7	U	0.59	0/1873	0.67	0/2542
8	H	0.58	0/1644	0.74	0/2234
8	V	0.58	0/1668	0.72	0/2263
9	I	0.56	0/1591	0.72	1/2148 (0.0%)
9	W	0.56	0/1605	0.73	0/2167
10	J	0.56	0/1558	0.68	0/2114
10	X	0.56	0/1576	0.69	0/2137
11	K	0.58	0/1576	0.69	0/2131
11	Y	0.57	0/1570	0.70	0/2125
12	L	0.58	0/1653	0.72	1/2230 (0.0%)
12	Z	0.59	0/1647	0.71	1/2223 (0.0%)
13	M	0.58	0/1704	0.70	0/2309
13	a	0.57	0/1691	0.69	0/2294
14	N	0.58	0/1507	0.68	0/2044
14	b	0.59	0/1513	0.70	0/2054
15	c	0.59	0/14498	0.68	2/19731 (0.0%)
All	All	0.59	0/62259	0.69	6/84443 (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
8	V	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c	1113	PRO	N-CA-CB	-6.77	95.15	102.60
15	c	1113	PRO	CA-N-CD	-5.80	103.38	111.50
9	I	99	PHE	CB-CA-C	5.57	121.55	110.40
12	Z	101	PHE	CB-CA-C	5.44	121.27	110.40
12	L	101	PHE	CB-CA-C	5.41	121.21	110.40
6	F	109	LYS	CB-CA-C	-5.15	100.10	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	V	188	ARG	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	215/234 (92%)	214 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	228/234 (97%)	225 (99%)	3 (1%)	0	100	100
2	B	228/261 (87%)	223 (98%)	4 (2%)	1 (0%)	34	69
2	P	247/261 (95%)	244 (99%)	2 (1%)	1 (0%)	34	69
3	C	223/248 (90%)	216 (97%)	6 (3%)	1 (0%)	34	69
3	Q	237/248 (96%)	237 (100%)	0	0	100	100
4	D	225/241 (93%)	221 (98%)	3 (1%)	1 (0%)	34	69
4	R	233/241 (97%)	232 (100%)	1 (0%)	0	100	100
5	E	238/263 (90%)	234 (98%)	3 (1%)	1 (0%)	34	69
5	S	235/263 (89%)	234 (100%)	1 (0%)	0	100	100
6	F	242/255 (95%)	240 (99%)	1 (0%)	1 (0%)	34	69
6	T	238/255 (93%)	238 (100%)	0	0	100	100
7	G	236/246 (96%)	234 (99%)	2 (1%)	0	100	100
7	U	241/246 (98%)	240 (100%)	1 (0%)	0	100	100
8	H	218/234 (93%)	213 (98%)	4 (2%)	1 (0%)	29	64
8	V	219/234 (94%)	215 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	196 (97%)	5 (2%)	1 (0%)	29	64
9	W	202/205 (98%)	196 (97%)	5 (2%)	1 (0%)	29	64
10	J	194/201 (96%)	192 (99%)	1 (0%)	1 (0%)	29	64
10	X	195/201 (97%)	192 (98%)	2 (1%)	1 (0%)	29	64
11	K	199/204 (98%)	198 (100%)	1 (0%)	0	100	100
11	Y	198/204 (97%)	198 (100%)	0	0	100	100
12	L	211/241 (88%)	209 (99%)	2 (1%)	0	100	100
12	Z	211/241 (88%)	208 (99%)	3 (1%)	0	100	100
13	M	214/264 (81%)	210 (98%)	4 (2%)	0	100	100
13	a	214/264 (81%)	210 (98%)	4 (2%)	0	100	100
14	N	200/205 (98%)	197 (98%)	3 (2%)	0	100	100
14	b	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
15	c	1798/1843 (98%)	1750 (97%)	39 (2%)	9 (0%)	29	64
All	All	7942/8447 (94%)	7814 (98%)	108 (1%)	20 (0%)	44	73

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	59	HIS
8	H	189	PRO
15	c	686	VAL
15	c	1113	PRO
2	B	67	LYS
6	F	109	LYS
10	X	122	ALA
15	c	1270	GLU
3	C	201	SER
4	D	12	VAL
15	c	668	GLU
15	c	758	LYS
15	c	856	GLU
15	c	1092	LEU
9	W	30	GLN
15	c	1112	ASN
15	c	1299	ARG
9	I	29	ILE
2	P	52	ILE
10	J	97	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	167/191 (87%)	153 (92%)	14 (8%)	11	38
1	O	162/191 (85%)	150 (93%)	12 (7%)	13	42
2	B	170/221 (77%)	156 (92%)	14 (8%)	11	38
2	P	181/221 (82%)	170 (94%)	11 (6%)	18	49
3	C	160/211 (76%)	139 (87%)	21 (13%)	4	17
3	Q	169/211 (80%)	162 (96%)	7 (4%)	30	64
4	D	179/203 (88%)	167 (93%)	12 (7%)	16	46
4	R	164/203 (81%)	155 (94%)	9 (6%)	21	53
5	E	195/224 (87%)	184 (94%)	11 (6%)	21	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	S	173/224 (77%)	164 (95%)	9 (5%)	23 55
6	F	184/212 (87%)	170 (92%)	14 (8%)	13 41
6	T	176/212 (83%)	167 (95%)	9 (5%)	24 56
7	G	181/210 (86%)	168 (93%)	13 (7%)	14 44
7	U	186/210 (89%)	174 (94%)	12 (6%)	17 47
8	H	166/195 (85%)	155 (93%)	11 (7%)	16 47
8	V	174/195 (89%)	158 (91%)	16 (9%)	9 33
9	I	164/174 (94%)	158 (96%)	6 (4%)	34 66
9	W	165/174 (95%)	154 (93%)	11 (7%)	16 46
10	J	151/171 (88%)	138 (91%)	13 (9%)	10 37
10	X	155/171 (91%)	143 (92%)	12 (8%)	13 41
11	K	146/159 (92%)	135 (92%)	11 (8%)	13 42
11	Y	145/159 (91%)	136 (94%)	9 (6%)	18 49
12	L	168/199 (84%)	162 (96%)	6 (4%)	35 67
12	Z	163/199 (82%)	157 (96%)	6 (4%)	34 66
13	M	170/215 (79%)	163 (96%)	7 (4%)	30 64
13	a	166/215 (77%)	153 (92%)	13 (8%)	12 40
14	N	143/159 (90%)	138 (96%)	5 (4%)	36 68
14	b	145/159 (91%)	142 (98%)	3 (2%)	53 79
15	c	1489/1673 (89%)	1383 (93%)	106 (7%)	14 44
All	All	6157/7161 (86%)	5754 (94%)	403 (6%)	21 47

All (403) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	59	ARG
1	A	68	THR
1	A	116	VAL
1	A	126	VAL
1	A	131	VAL
1	A	160	THR
1	A	167	VAL
1	A	175	LYS
1	A	189	THR

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Mol	Chain	Res	Type
1	A	192	LEU
1	A	196	GLU
1	A	198	PHE
1	A	204	GLU
2	B	33	THR
2	B	35	LEU
2	B	43	VAL
2	B	51	ASN
2	B	65	ILE
2	B	74	CYS
2	B	85	VAL
2	B	132	VAL
2	B	180	LYS
2	B	192	LEU
2	B	201	MET
2	B	204	SER
2	B	206	LEU
2	B	223	THR
3	C	33	VAL
3	C	40	ILE
3	C	41	VAL
3	C	42	VAL
3	C	46	GLU
3	C	48	LYS
3	C	50	VAL
3	C	65	LEU
3	C	83	VAL
3	C	89	VAL
3	C	98	VAL
3	C	99	GLU
3	C	127	PHE
3	C	134	VAL
3	C	138	PHE
3	C	177	THR
3	C	183	THR
3	C	196	LEU
3	C	200	GLN
3	C	208	LEU
3	C	213	ARG
4	D	18	GLU
4	D	56	SER
4	D	121	LEU

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Mol	Chain	Res	Type
4	D	137	PHE
4	D	139	VAL
4	D	142	LEU
4	D	156	MET
4	D	183	GLU
4	D	191	LEU
4	D	203	LYS
4	D	205	VAL
4	D	213	THR
5	E	11	THR
5	E	49	LEU
5	E	50	LYS
5	E	77	LEU
5	E	84	LEU
5	E	93	LEU
5	E	100	ASP
5	E	147	THR
5	E	155	ASP
5	E	157	ARG
5	E	239	ARG
6	F	3	ILE
6	F	5	THR
6	F	45	VAL
6	F	53	VAL
6	F	56	LYS
6	F	66	LEU
6	F	108	LEU
6	F	120	HIS
6	F	124	LEU
6	F	181	MET
6	F	197	ILE
6	F	204	VAL
6	F	215	TRP
6	F	216	VAL
7	G	42	VAL
7	G	49	VAL
7	G	61	LEU
7	G	66	VAL
7	G	73	THR
7	G	81	THR
7	G	111	VAL
7	G	112	ASP

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Mol	Chain	Res	Type
7	G	115	CYS
7	G	137	CYS
7	G	170	VAL
7	G	192	GLU
7	G	224	ASN
8	H	13	ILE
8	H	27	VAL
8	H	49	THR
8	H	77	VAL
8	H	113	SER
8	H	151	GLU
8	H	175	ASP
8	H	183	LYS
8	H	210	THR
8	H	214	THR
8	H	220	LEU
9	I	19	VAL
9	I	57	THR
9	I	121	CYS
9	I	136	VAL
9	I	164	GLU
9	I	196	THR
10	J	1	MET
10	J	13	VAL
10	J	20	VAL
10	J	25	ILE
10	J	26	VAL
10	J	31	ASP
10	J	45	LEU
10	J	102	LEU
10	J	143	LEU
10	J	148	THR
10	J	159	LEU
10	J	167	LEU
10	J	169	LYS
11	K	22	THR
11	K	30	GLN
11	K	35	VAL
11	K	45	THR
11	K	98	MET
11	K	103	CYS
11	K	122	ILE

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Mol	Chain	Res	Type
11	K	134	VAL
11	K	150	VAL
11	K	159	ARG
11	K	196	LEU
12	L	2	PHE
12	L	30	SER
12	L	92	LEU
12	L	99	ARG
12	L	100	ARG
12	L	164	VAL
13	M	10	SER
13	M	21	VAL
13	M	49	THR
13	M	100	ARG
13	M	160	LEU
13	M	169	VAL
13	M	205	THR
14	N	30	ARG
14	N	32	THR
14	N	84	PHE
14	N	86	GLU
14	N	191	LEU
1	O	43	VAL
1	O	50	LYS
1	O	91	LYS
1	O	92	LEU
1	O	98	LEU
1	O	116	VAL
1	O	122	GLN
1	O	131	VAL
1	O	135	ILE
1	O	167	VAL
1	O	198	PHE
1	O	214	GLU
2	P	35	LEU
2	P	44	LEU
2	P	54	LYS
2	P	68	LEU
2	P	74	CYS
2	P	86	LEU
2	P	122	THR
2	P	185	THR

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Mol	Chain	Res	Type
2	P	197	LEU
2	P	206	LEU
2	P	243	GLU
3	Q	31	THR
3	Q	96	LEU
3	Q	129	ILE
3	Q	177	THR
3	Q	183	THR
3	Q	218	LYS
3	Q	219	ILE
4	R	47	CYS
4	R	54	ILE
4	R	76	CYS
4	R	82	ILE
4	R	96	THR
4	R	148	GLU
4	R	163	VAL
4	R	204	GLN
4	R	238	ILE
5	S	10	VAL
5	S	29	VAL
5	S	35	THR
5	S	38	LEU
5	S	42	THR
5	S	121	GLN
5	S	130	VAL
5	S	134	ILE
5	S	154	PHE
6	T	17	ASP
6	T	35	THR
6	T	41	CYS
6	T	142	VAL
6	T	181	MET
6	T	189	ILE
6	T	200	VAL
6	T	215	TRP
6	T	233	GLU
7	U	43	ARG
7	U	66	VAL
7	U	73	THR
7	U	81	THR
7	U	86	ASP

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Mol	Chain	Res	Type
7	U	100	ASN
7	U	112	ASP
7	U	130	GLU
7	U	131	MET
7	U	151	VAL
7	U	216	GLU
7	U	242	LEU
8	V	20	ARG
8	V	22	THR
8	V	26	VAL
8	V	31	ASN
8	V	64	LEU
8	V	66	LEU
8	V	81	ASN
8	V	107	THR
8	V	119	SER
8	V	128	MET
8	V	181	LYS
8	V	184	LEU
8	V	191	THR
8	V	192	VAL
8	V	194	ASN
8	V	198	THR
9	W	19	VAL
9	W	33	MET
9	W	35	THR
9	W	75	LEU
9	W	121	CYS
9	W	125	LEU
9	W	130	MET
9	W	134	ASP
9	W	146	TYR
9	W	158	ASP
9	W	184	VAL
10	X	8	GLN
10	X	26	VAL
10	X	39	SER
10	X	45	LEU
10	X	62	LYS
10	X	69	MET
10	X	78	THR
10	X	84	THR

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Mol	Chain	Res	Type
10	X	86	ARG
10	X	148	THR
10	X	159	LEU
10	X	173	LEU
11	Y	5	LEU
11	Y	35	VAL
11	Y	36	ILE
11	Y	103	CYS
11	Y	120	ASN
11	Y	126	THR
11	Y	142	ARG
11	Y	150	VAL
11	Y	181	ARG
12	Z	11	THR
12	Z	42	LYS
12	Z	46	LEU
12	Z	51	VAL
12	Z	199	THR
12	Z	213	ASP
13	a	14	VAL
13	a	21	VAL
13	a	25	ASP
13	a	30	TYR
13	a	76	LEU
13	a	92	LEU
13	a	94	ARG
13	a	100	ARG
13	a	137	LEU
13	a	155	GLU
13	a	169	VAL
13	a	191	THR
13	a	207	THR
14	b	20	ARG
14	b	191	LEU
14	b	197	LYS
15	c	27	VAL
15	c	33	VAL
15	c	59	LEU
15	c	85	LEU
15	c	90	PHE
15	c	106	VAL
15	c	116	MET

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Mol	Chain	Res	Type
15	c	139	GLU
15	c	207	MET
15	c	226	LEU
15	c	231	PHE
15	c	239	ILE
15	c	265	ASP
15	c	298	VAL
15	c	326	VAL
15	c	338	THR
15	c	356	LEU
15	c	365	VAL
15	c	378	TRP
15	c	380	THR
15	c	436	VAL
15	c	437	LEU
15	c	454	THR
15	c	481	MET
15	c	492	VAL
15	c	517	VAL
15	c	530	THR
15	c	569	GLU
15	c	575	MET
15	c	595	THR
15	c	609	VAL
15	c	619	GLU
15	c	630	MET
15	c	632	ARG
15	c	641	GLU
15	c	685	ARG
15	c	691	LEU
15	c	714	TYR
15	c	725	LEU
15	c	734	THR
15	c	737	CYS
15	c	750	TYR
15	c	751	PHE
15	c	762	LEU
15	c	783	LEU
15	c	792	LEU
15	c	793	VAL
15	c	795	LEU
15	c	811	LEU

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Mol	Chain	Res	Type
15	c	840	VAL
15	c	849	THR
15	c	853	THR
15	c	856	GLU
15	c	887	THR
15	c	900	LEU
15	c	901	LEU
15	c	935	HIS
15	c	936	ILE
15	c	946	LEU
15	c	950	LEU
15	c	952	THR
15	c	958	CYS
15	c	975	SER
15	c	1012	LEU
15	c	1016	ARG
15	c	1017	GLN
15	c	1019	VAL
15	c	1038	VAL
15	c	1044	HIS
15	c	1061	LEU
15	c	1063	GLN
15	c	1073	VAL
15	c	1079	LEU
15	c	1089	THR
15	c	1113	PRO
15	c	1146	LEU
15	c	1177	ASP
15	c	1248	TRP
15	c	1282	ASN
15	c	1295	LEU
15	c	1357	LEU
15	c	1367	LEU
15	c	1386	LEU
15	c	1411	THR
15	c	1443	LEU
15	c	1447	LEU
15	c	1458	SER
15	c	1479	VAL
15	c	1486	LEU
15	c	1494	LEU
15	c	1522	THR

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Mol	Chain	Res	Type
15	c	1523	THR
15	c	1530	VAL
15	c	1534	THR
15	c	1536	ARG
15	c	1541	LEU
15	c	1544	LEU
15	c	1626	LEU
15	c	1667	THR
15	c	1672	ASN
15	c	1699	LEU
15	c	1712	LEU
15	c	1732	CYS
15	c	1788	LEU
15	c	1800	MET
15	c	1829	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	95	GLN
1	A	118	GLN
1	A	147	GLN
2	B	51	ASN
2	B	53	HIS
2	B	109	GLN
3	C	54	GLN
3	C	146	GLN
3	C	200	GLN
4	D	152	GLN
4	D	224	GLN
5	E	5	GLN
5	E	8	ASN
5	E	16	GLN
5	E	31	GLN
6	F	72	HIS
6	F	221	ASN
7	G	100	ASN
7	G	193	GLN
8	H	173	ASN
8	H	194	ASN
9	I	39	GLN

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Mol	Chain	Res	Type
9	I	156	ASN
10	J	27	GLN
10	J	32	HIS
10	J	87	ASN
10	J	132	HIS
10	J	168	GLN
11	K	30	GLN
11	K	86	ASN
11	K	90	GLN
11	K	152	GLN
11	K	163	GLN
12	L	108	ASN
12	L	151	ASN
12	L	152	GLN
13	M	2	GLN
13	M	108	ASN
13	M	157	GLN
14	N	107	GLN
14	N	111	GLN
1	O	108	GLN
1	O	122	GLN
1	O	139	ASN
2	P	53	HIS
2	P	84	ASN
2	P	155	ASN
2	P	177	GLN
3	Q	92	GLN
4	R	152	GLN
5	S	31	GLN
5	S	43	HIS
5	S	60	GLN
5	S	121	GLN
6	T	97	ASN
6	T	147	GLN
6	T	221	ASN
7	U	100	ASN
7	U	150	GLN
8	V	31	ASN
8	V	117	HIS
8	V	166	ASN
9	W	39	GLN
9	W	172	ASN

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Mol	Chain	Res	Type
10	X	24	ASN
10	X	61	GLN
10	X	63	ASN
10	X	65	GLN
11	Y	120	ASN
11	Y	163	GLN
12	Z	157	ASN
12	Z	160	ASN
13	a	157	GLN
14	b	63	GLN
14	b	155	GLN
14	b	188	GLN
15	c	35	ASN
15	c	54	GLN
15	c	171	ASN
15	c	227	HIS
15	c	246	GLN
15	c	358	GLN
15	c	419	GLN
15	c	495	ASN
15	c	524	GLN
15	c	607	GLN
15	c	649	HIS
15	c	656	GLN
15	c	768	GLN
15	c	877	ASN
15	c	1022	GLN
15	c	1145	ASN
15	c	1214	GLN
15	c	1273	HIS
15	c	1282	ASN
15	c	1351	ASN
15	c	1415	ASN
15	c	1475	GLN
15	c	1521	ASN
15	c	1631	GLN
15	c	1714	GLN
15	c	1783	GLN

5.3.3 RNA

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)

8 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	$\#\|Z\| > 2$
16	LDZ	b	301	-	33,34,34	2.45	8 (24%)	42,44,44	1.15	2 (4%)
17	IHP	c	1901	-	36,36,36	0.83	0	54,60,60	1.47	7 (12%)
16	LDZ	Y	301	-	33,34,34	2.52	8 (24%)	42,44,44	1.35	6 (14%)
16	LDZ	K	301	-	33,34,34	2.46	8 (24%)	42,44,44	1.27	7 (16%)
16	LDZ	N	301	-	33,34,34	2.50	8 (24%)	42,44,44	1.47	8 (19%)
17	IHP	c	1902	-	36,36,36	0.77	0	54,60,60	1.28	4 (7%)
16	LDZ	H	301	-	33,34,34	2.49	8 (24%)	42,44,44	1.27	5 (11%)
16	LDZ	V	301	-	33,34,34	2.53	8 (24%)	42,44,44	1.66	10 (23%)

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
16	LDZ	b	301	-	-	19/38/39/39	0/1/1/1
17	IHP	c	1901	-	-	5/30/54/54	0/1/1/1
16	LDZ	Y	301	-	-	13/38/39/39	0/1/1/1
16	LDZ	K	301	-	-	14/38/39/39	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LDZ	N	301	-	-	12/38/39/39	0/1/1/1
17	IHP	c	1902	-	-	2/30/54/54	0/1/1/1
16	LDZ	H	301	-	-	10/38/39/39	0/1/1/1
16	LDZ	V	301	-	-	23/38/39/39	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	301	LDZ	C15-N16	8.45	1.52	1.34
16	Y	301	LDZ	C15-N16	8.39	1.52	1.34
16	H	301	LDZ	C15-N16	8.27	1.52	1.34
16	N	301	LDZ	C15-N16	8.26	1.52	1.34
16	K	301	LDZ	C15-N16	8.26	1.52	1.34
16	b	301	LDZ	C15-N16	8.16	1.52	1.34
16	N	301	LDZ	C12-N13	6.49	1.48	1.34
16	V	301	LDZ	C12-N13	6.38	1.48	1.34
16	Y	301	LDZ	C12-N13	6.35	1.48	1.34
16	Y	301	LDZ	C9-N10	6.28	1.50	1.34
16	H	301	LDZ	C12-N13	6.26	1.47	1.34
16	H	301	LDZ	C9-N10	6.18	1.50	1.34
16	b	301	LDZ	C12-N13	6.16	1.47	1.34
16	K	301	LDZ	C12-N13	6.15	1.47	1.34
16	N	301	LDZ	C9-N10	6.15	1.49	1.34
16	V	301	LDZ	C9-N10	6.14	1.49	1.34
16	K	301	LDZ	C9-N10	6.08	1.49	1.34
16	b	301	LDZ	C9-N10	6.06	1.49	1.34
16	V	301	LDZ	O8-C9	4.30	1.43	1.35
16	Y	301	LDZ	O8-C9	4.17	1.43	1.35
16	H	301	LDZ	O8-C9	4.06	1.43	1.35
16	N	301	LDZ	O8-C9	3.93	1.42	1.35
16	b	301	LDZ	O8-C9	3.86	1.42	1.35
16	K	301	LDZ	O8-C9	3.85	1.42	1.35
16	V	301	LDZ	O34-C15	-2.79	1.17	1.23
16	N	301	LDZ	O34-C15	-2.74	1.17	1.23
16	N	301	LDZ	O31-C9	-2.71	1.16	1.21
16	b	301	LDZ	O31-C9	-2.71	1.16	1.21
16	K	301	LDZ	O31-C9	-2.70	1.16	1.21
16	Y	301	LDZ	O31-C9	-2.69	1.16	1.21
16	V	301	LDZ	O31-C9	-2.67	1.16	1.21
16	H	301	LDZ	O31-C9	-2.66	1.16	1.21
16	b	301	LDZ	O32-C12	-2.60	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	301	LDZ	O32-C12	-2.55	1.18	1.23
16	K	301	LDZ	O32-C12	-2.54	1.18	1.23
16	Y	301	LDZ	O34-C15	-2.51	1.18	1.23
16	N	301	LDZ	O32-C12	-2.51	1.18	1.23
16	H	301	LDZ	O34-C15	-2.50	1.18	1.23
16	b	301	LDZ	O34-C15	-2.47	1.18	1.23
16	V	301	LDZ	O32-C12	-2.46	1.18	1.23
16	H	301	LDZ	O32-C12	-2.44	1.18	1.23
16	K	301	LDZ	O34-C15	-2.43	1.18	1.23
16	K	301	LDZ	O8-C7	-2.25	1.41	1.45
16	b	301	LDZ	O8-C7	-2.22	1.41	1.45
16	N	301	LDZ	O8-C7	-2.12	1.41	1.45
16	Y	301	LDZ	O8-C7	-2.11	1.41	1.45
16	H	301	LDZ	O8-C7	-2.06	1.41	1.45
16	V	301	LDZ	O8-C7	-2.04	1.41	1.45

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	301	LDZ	O8-C9-N10	4.83	120.33	110.50
16	V	301	LDZ	C14-C15-N16	4.62	126.83	116.70
16	N	301	LDZ	O8-C9-N10	4.52	119.68	110.50
16	H	301	LDZ	O8-C9-N10	4.45	119.55	110.50
17	c	1901	IHP	C6-C5-C4	4.11	119.41	110.41
16	K	301	LDZ	O8-C9-N10	4.02	118.68	110.50
16	V	301	LDZ	O8-C9-N10	4.00	118.64	110.50
16	b	301	LDZ	O8-C9-N10	3.93	118.49	110.50
17	c	1902	IHP	C3-C2-C1	3.83	118.79	110.41
16	N	301	LDZ	C11-C12-N13	3.58	124.55	116.70
16	V	301	LDZ	O34-C15-N16	-3.54	116.37	122.93
17	c	1901	IHP	C5-C6-C1	3.47	118.01	110.41
16	Y	301	LDZ	O31-C9-N10	-3.09	119.78	124.85
16	K	301	LDZ	C14-C15-N16	2.98	123.24	116.70
17	c	1902	IHP	C6-C1-C2	2.95	116.86	110.41
16	V	301	LDZ	C11-C12-N13	2.93	123.12	116.70
16	H	301	LDZ	C17-N16-C15	-2.88	117.84	123.15
16	N	301	LDZ	O32-C12-N13	-2.82	117.71	122.93
16	H	301	LDZ	O31-C9-N10	-2.81	120.24	124.85
17	c	1901	IHP	O15-C5-C4	2.75	115.17	108.69
16	V	301	LDZ	O31-C9-N10	-2.74	120.35	124.85
17	c	1901	IHP	C5-C4-C3	2.69	116.30	110.41
17	c	1901	IHP	C6-C1-C2	2.65	116.20	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	c	1901	IHP	C3-C2-C1	2.64	116.19	110.41
16	K	301	LDZ	C15-C14-N13	-2.57	104.17	111.16
16	N	301	LDZ	O31-C9-N10	-2.56	120.65	124.85
16	b	301	LDZ	O31-C9-N10	-2.52	120.72	124.85
16	N	301	LDZ	C31-C30-C11	-2.45	108.68	115.43
17	c	1902	IHP	C5-C6-C1	2.41	115.69	110.41
16	N	301	LDZ	O8-C9-O31	-2.39	119.66	124.25
17	c	1902	IHP	C4-C3-C2	2.37	115.60	110.41
16	V	301	LDZ	O32-C12-N13	-2.36	118.55	122.93
16	K	301	LDZ	O34-C15-N16	-2.36	118.56	122.93
16	K	301	LDZ	C19-C18-C17	-2.31	109.56	115.34
16	Y	301	LDZ	O8-C9-O31	-2.27	119.89	124.25
16	K	301	LDZ	O31-C9-N10	-2.26	121.14	124.85
16	V	301	LDZ	C24-C14-N13	-2.26	105.37	110.58
16	N	301	LDZ	C15-C14-N13	-2.17	105.25	111.16
16	Y	301	LDZ	O33-C22-C17	-2.17	119.10	124.78
16	H	301	LDZ	O33-C22-C17	-2.15	119.14	124.78
16	V	301	LDZ	C31-C30-C11	-2.14	109.54	115.43
16	Y	301	LDZ	C19-C18-C17	-2.13	110.02	115.34
16	K	301	LDZ	O8-C9-O31	-2.13	120.17	124.25
16	V	301	LDZ	C15-C14-N13	-2.12	105.38	111.16
16	H	301	LDZ	O8-C9-O31	-2.11	120.21	124.25
17	c	1901	IHP	O13-C3-C4	2.05	113.53	108.69
16	N	301	LDZ	O33-C22-C17	-2.05	119.40	124.78
16	V	301	LDZ	C11-N10-C9	-2.05	115.91	120.90
16	Y	301	LDZ	C25-C24-C14	-2.01	109.91	115.43

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	H	301	LDZ	O31-C9-O8-C7
16	H	301	LDZ	N10-C9-O8-C7
16	K	301	LDZ	C30-C11-N10-C9
16	K	301	LDZ	N13-C14-C24-C25
16	K	301	LDZ	C18-C17-N16-C15
16	N	301	LDZ	O31-C9-O8-C7
16	N	301	LDZ	N10-C9-O8-C7
16	N	301	LDZ	O8-C9-N10-C11
16	N	301	LDZ	C18-C17-N16-C15
16	N	301	LDZ	C18-C17-C22-O33
16	V	301	LDZ	O31-C9-O8-C7

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Mol	Chain	Res	Type	Atoms
16	V	301	LDZ	N10-C9-O8-C7
16	V	301	LDZ	N13-C14-C24-C25
16	V	301	LDZ	C18-C17-N16-C15
16	Y	301	LDZ	O31-C9-O8-C7
16	Y	301	LDZ	N10-C9-O8-C7
16	Y	301	LDZ	C18-C17-N16-C15
16	Y	301	LDZ	C22-C17-C18-C19
16	b	301	LDZ	C22-C17-C18-C19
17	c	1901	IHP	C4-C5-O15-P5
16	N	301	LDZ	O31-C9-N10-C11
16	H	301	LDZ	O8-C9-N10-C11
16	Y	301	LDZ	N10-C11-C30-C31
16	K	301	LDZ	O31-C9-O8-C7
16	H	301	LDZ	O31-C9-N10-C11
16	K	301	LDZ	N10-C9-O8-C7
16	H	301	LDZ	C30-C11-N10-C9
16	H	301	LDZ	C3-C7-O8-C9
16	N	301	LDZ	N10-C11-C30-C31
16	V	301	LDZ	N10-C11-C30-C31
16	b	301	LDZ	N10-C11-C30-C31
16	b	301	LDZ	N13-C14-C24-C25
16	Y	301	LDZ	C24-C14-C15-O34
16	Y	301	LDZ	C24-C14-C15-N16
16	K	301	LDZ	C15-C14-C24-C25
16	V	301	LDZ	C12-C11-C30-C31
16	Y	301	LDZ	C12-C11-C30-C31
16	b	301	LDZ	C12-C11-C30-C31
16	b	301	LDZ	C15-C14-C24-C25
16	V	301	LDZ	C17-C18-C19-C20
16	V	301	LDZ	C17-C18-C19-C21
16	b	301	LDZ	C17-C18-C19-C21
16	Y	301	LDZ	N16-C17-C18-C19
16	b	301	LDZ	C12-C11-N10-C9
16	V	301	LDZ	C15-C14-C24-C25
16	N	301	LDZ	C11-C12-N13-C14
16	V	301	LDZ	C11-C12-N13-C14
16	V	301	LDZ	C14-C15-N16-C17
16	K	301	LDZ	O34-C15-N16-C17
16	N	301	LDZ	O32-C12-N13-C14
16	V	301	LDZ	O32-C12-N13-C14
16	V	301	LDZ	O34-C15-N16-C17
16	Y	301	LDZ	C15-C14-C24-C25

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Mol	Chain	Res	Type	Atoms
16	K	301	LDZ	C14-C15-N16-C17
16	Y	301	LDZ	N13-C14-C24-C25
16	b	301	LDZ	N16-C17-C18-C19
16	b	301	LDZ	C17-C18-C19-C20
16	N	301	LDZ	C12-C11-C30-C31
16	V	301	LDZ	C3-C7-O8-C9
16	b	301	LDZ	N13-C14-C15-N16
16	b	301	LDZ	N13-C14-C15-O34
16	V	301	LDZ	N10-C11-C12-O32
16	V	301	LDZ	N13-C14-C15-O34
16	N	301	LDZ	C17-C18-C19-C21
16	V	301	LDZ	N13-C14-C15-N16
16	V	301	LDZ	N10-C11-C12-N13
16	b	301	LDZ	C30-C11-C12-O32
16	N	301	LDZ	C17-C18-C19-C20
17	c	1901	IHP	C6-O16-P6-O46
17	c	1902	IHP	C2-O12-P2-O32
17	c	1902	IHP	C2-O12-P2-O42
16	V	301	LDZ	C30-C11-C12-O32
16	b	301	LDZ	C18-C17-N16-C15
16	H	301	LDZ	C12-C11-C30-C31
16	b	301	LDZ	C30-C11-C12-N13
16	H	301	LDZ	N10-C11-C30-C31
16	H	301	LDZ	N10-C11-C12-O32
16	K	301	LDZ	N16-C17-C18-C19
16	K	301	LDZ	C14-C24-C25-C27
16	V	301	LDZ	C30-C11-C12-N13
16	Y	301	LDZ	N10-C11-C12-O32
16	H	301	LDZ	N10-C11-C12-N13
16	V	301	LDZ	O8-C9-N10-C11
16	V	301	LDZ	O31-C9-N10-C11
16	b	301	LDZ	O8-C9-N10-C11
16	b	301	LDZ	O31-C9-N10-C11
16	Y	301	LDZ	N10-C11-C12-N13
17	c	1901	IHP	C1-O11-P1-O21
16	K	301	LDZ	O8-C9-N10-C11
16	K	301	LDZ	C14-C24-C25-C26
16	b	301	LDZ	N10-C11-C12-O32
17	c	1901	IHP	C1-O11-P1-O41
17	c	1901	IHP	C6-O16-P6-O36
16	b	301	LDZ	C24-C14-C15-O34
16	b	301	LDZ	C22-C17-N16-C15

Continued on next page...

Continued from previous page...

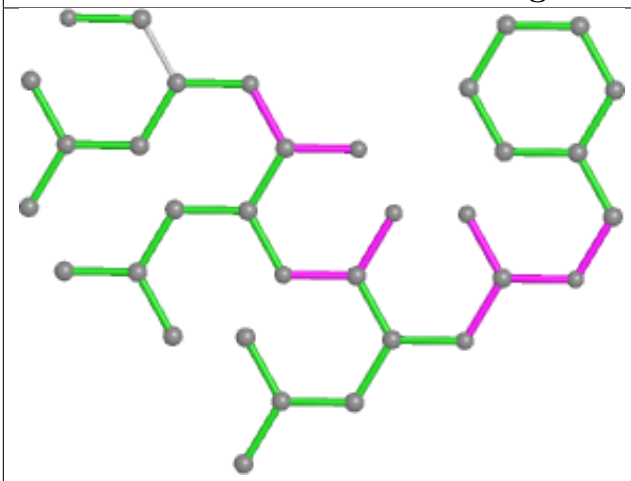
Mol	Chain	Res	Type	Atoms
16	K	301	LDZ	C17-C18-C19-C20
16	V	301	LDZ	C24-C14-C15-O34
16	K	301	LDZ	O31-C9-N10-C11

There are no ring outliers.

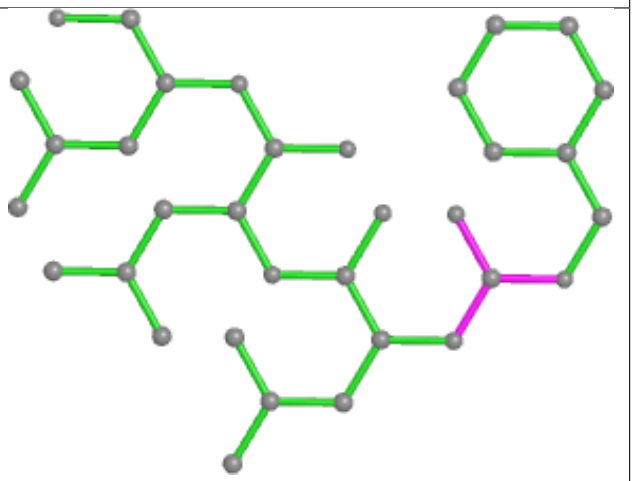
No monomer is involved in short contacts.

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.

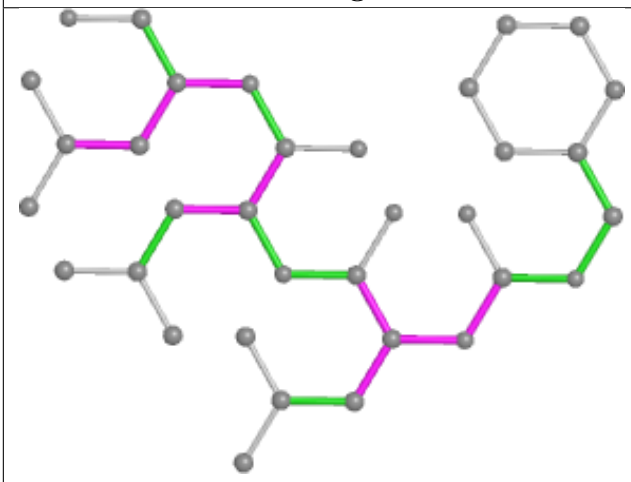
Ligand LDZ b 301



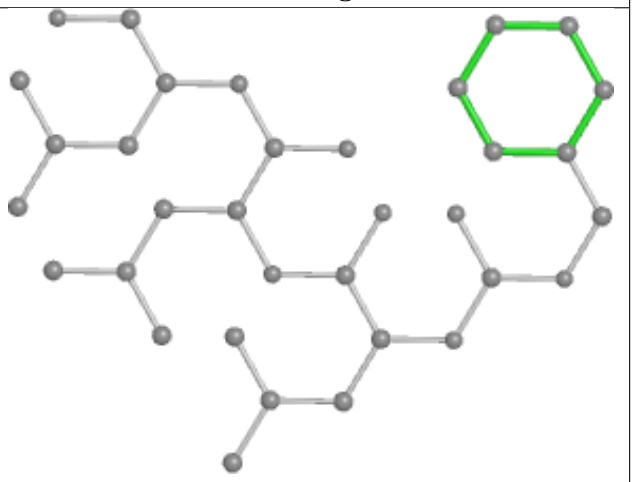
Bond lengths



Bond angles

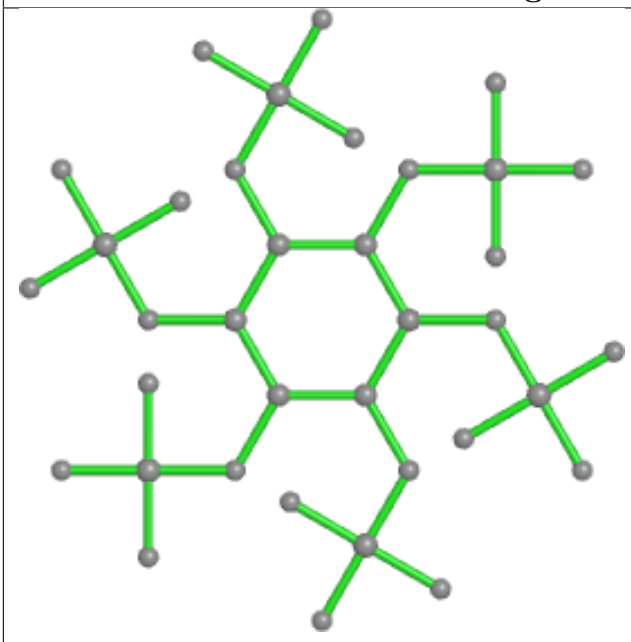


Torsions

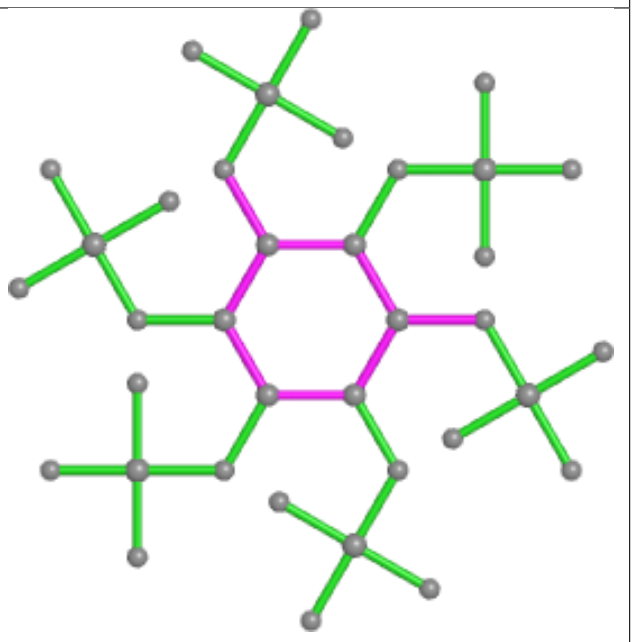


Rings

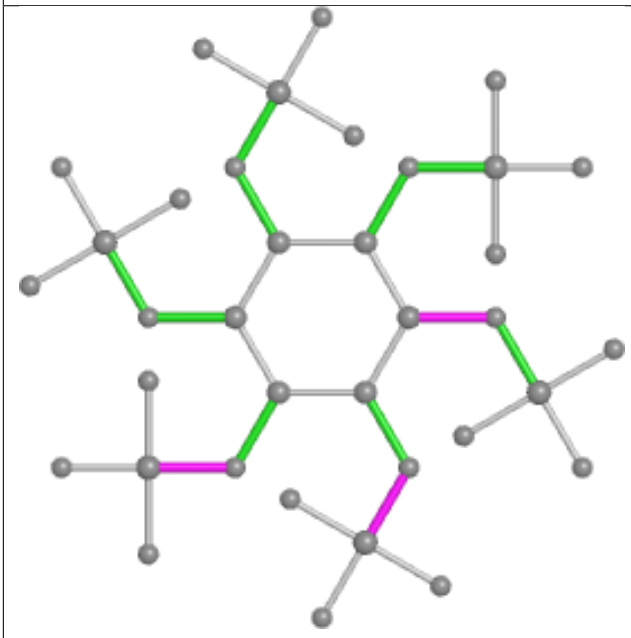
Ligand IHP c 1901



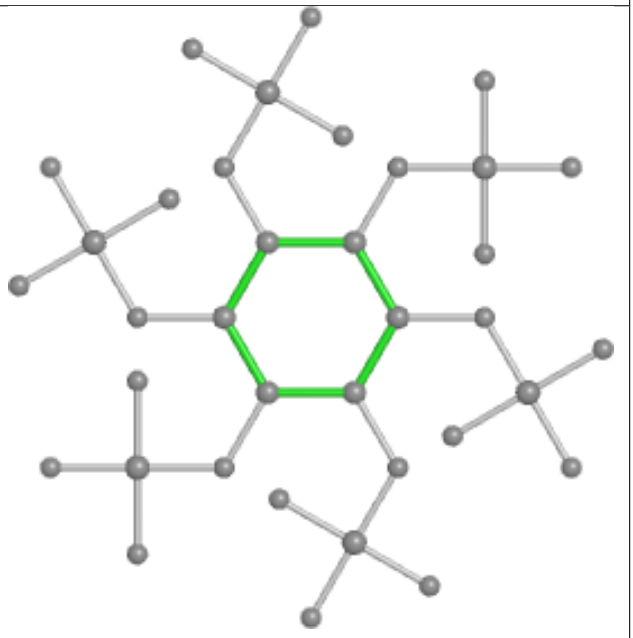
Bond lengths



Bond angles

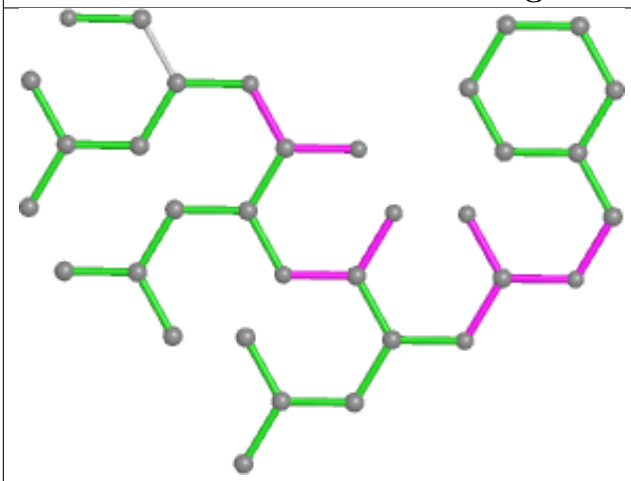


Torsions

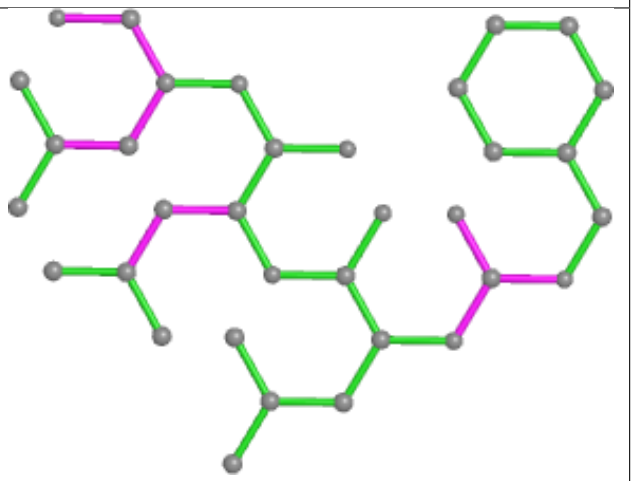


Rings

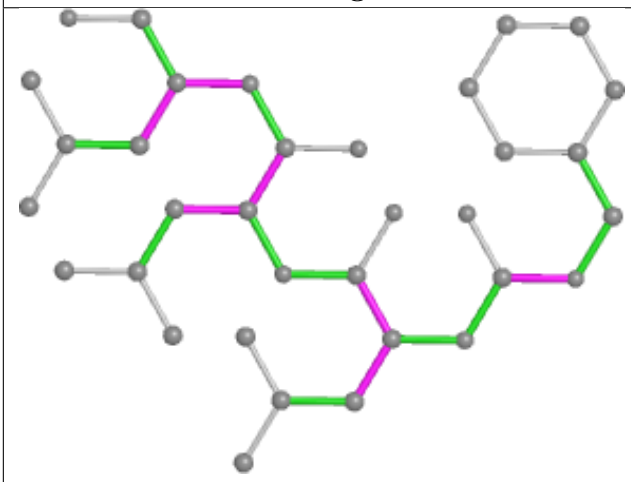
Ligand LDZ Y 301



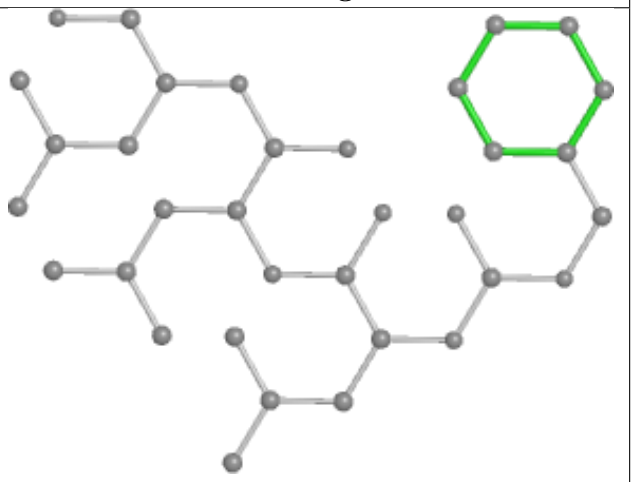
Bond lengths



Bond angles

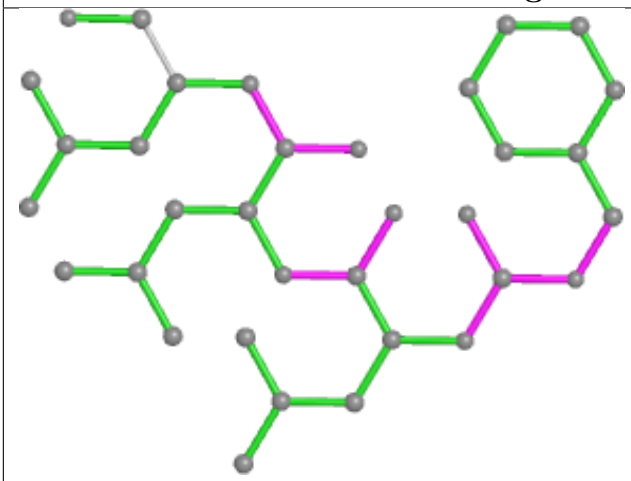


Torsions

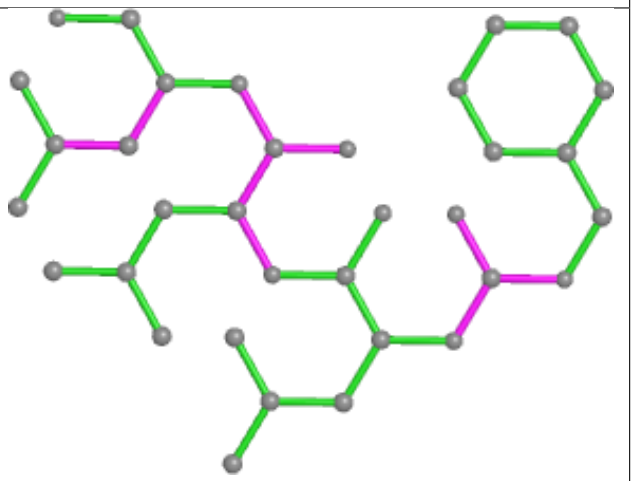


Rings

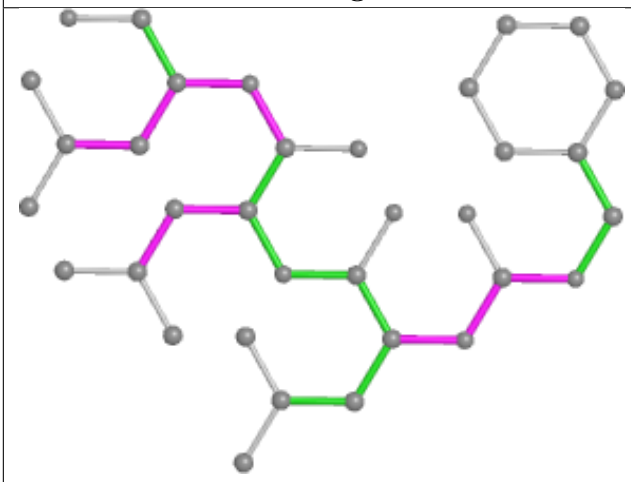
Ligand LDZ K 301



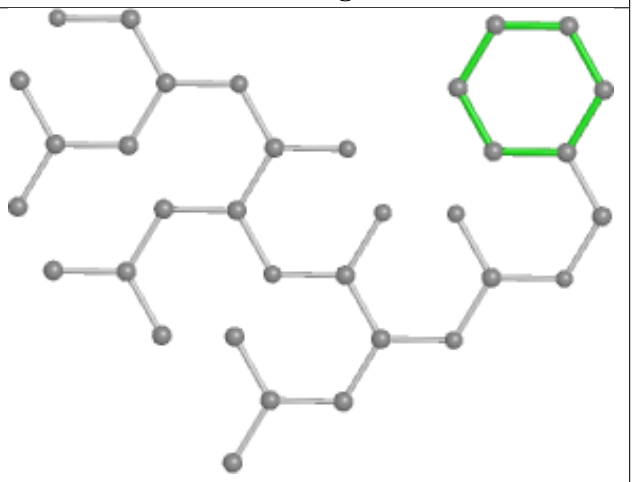
Bond lengths



Bond angles

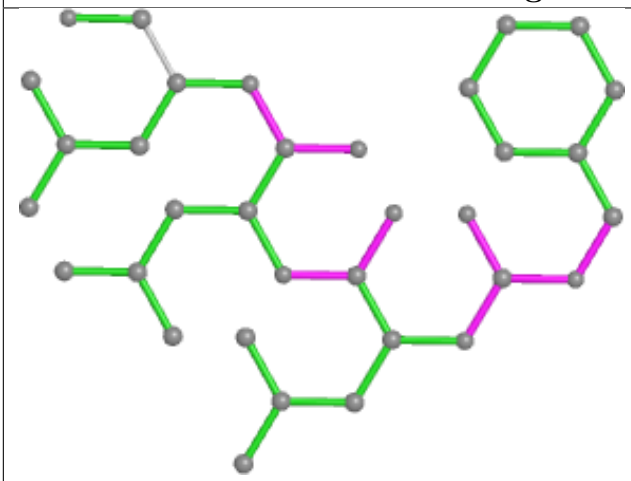


Torsions

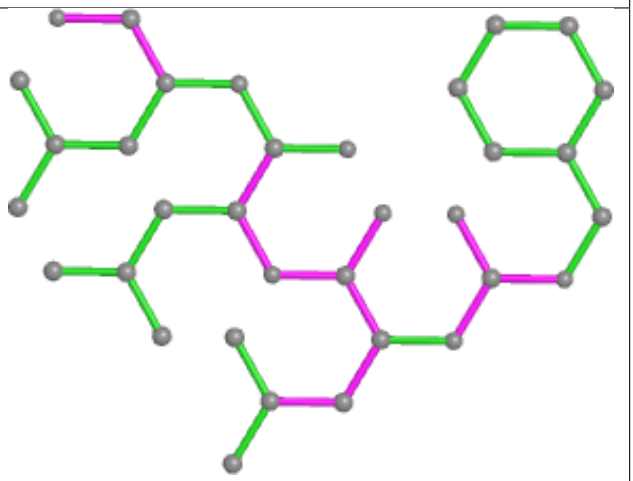


Rings

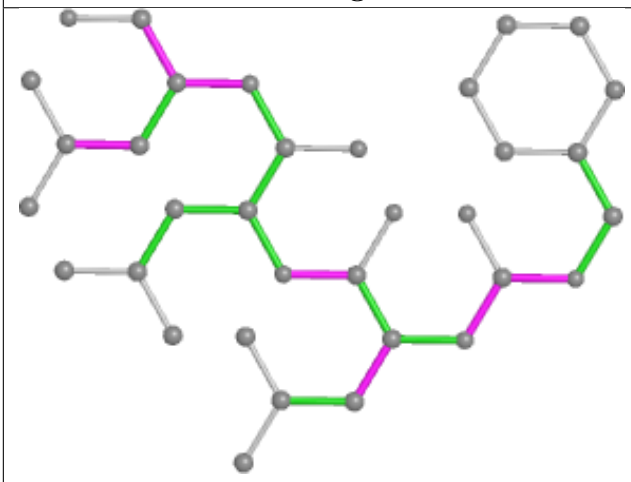
Ligand LDZ N 301



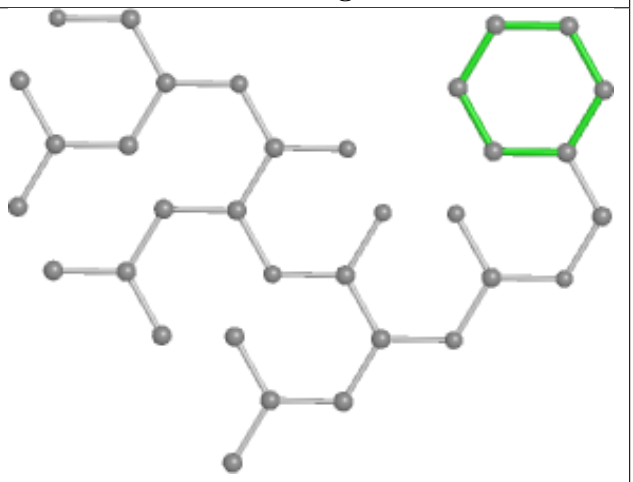
Bond lengths



Bond angles

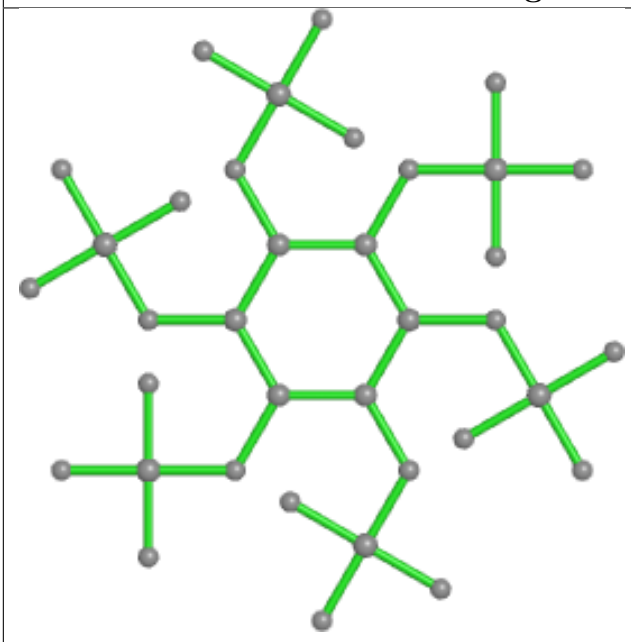


Torsions

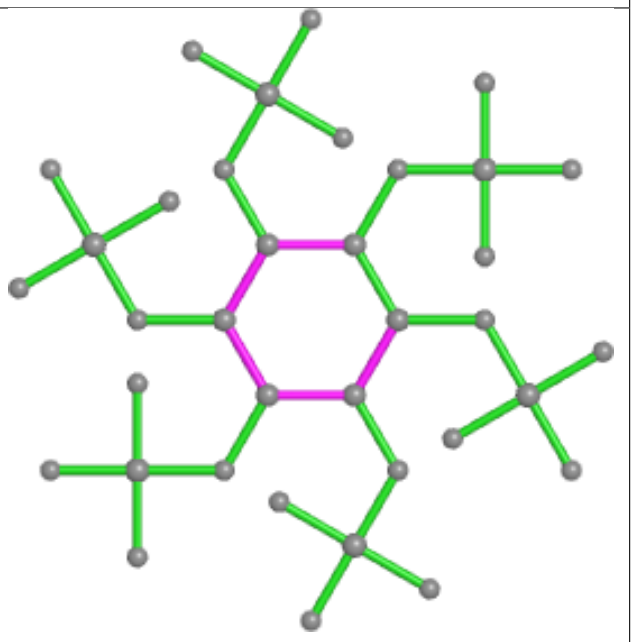


Rings

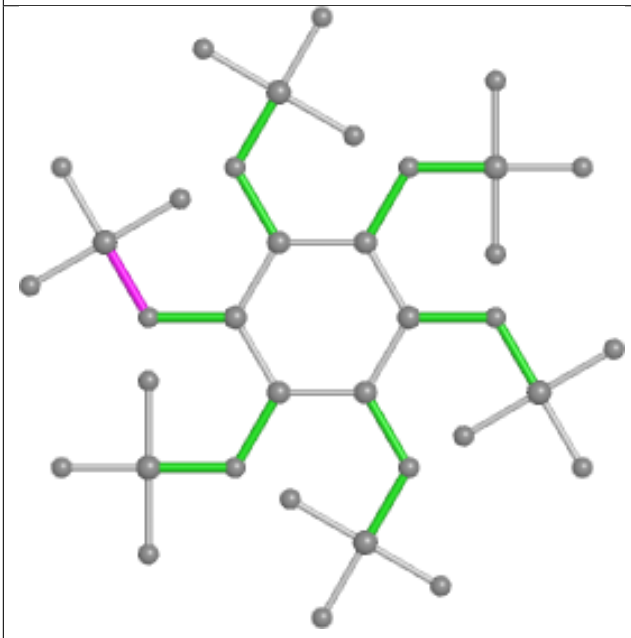
Ligand IHP c 1902



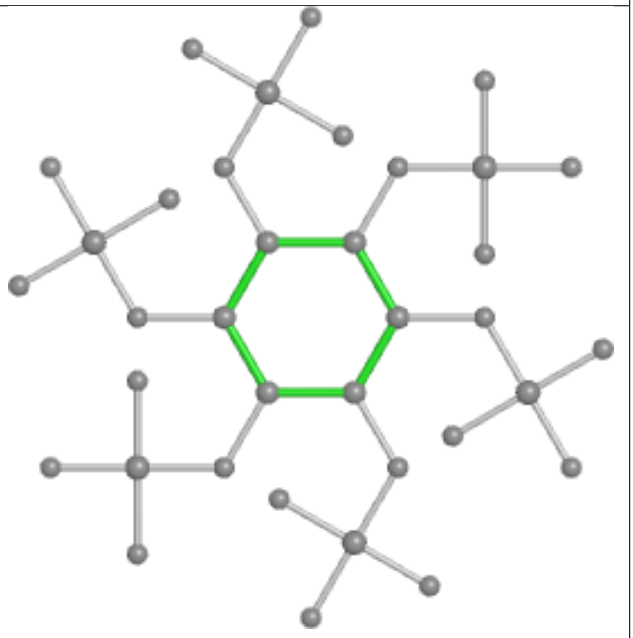
Bond lengths



Bond angles

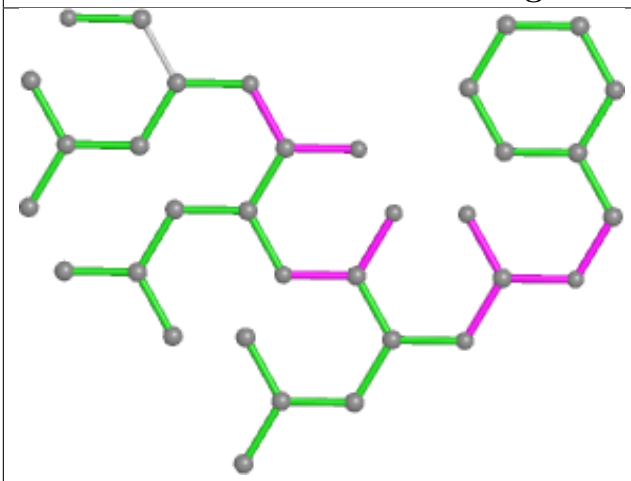


Torsions

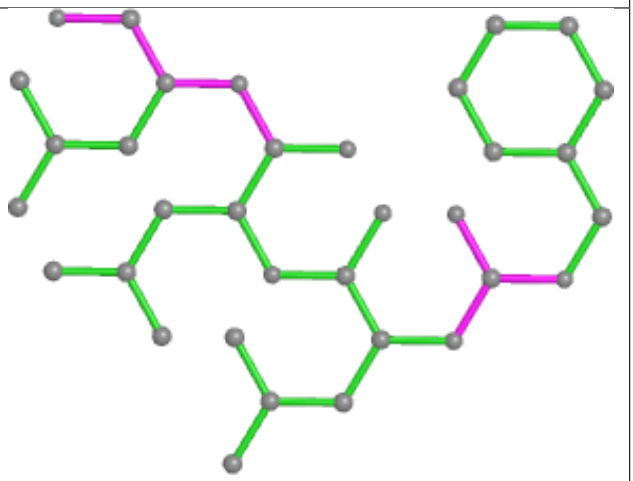


Rings

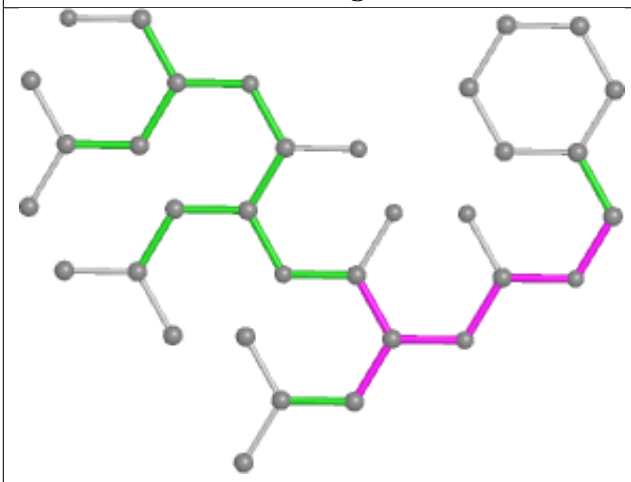
Ligand LDZ H 301



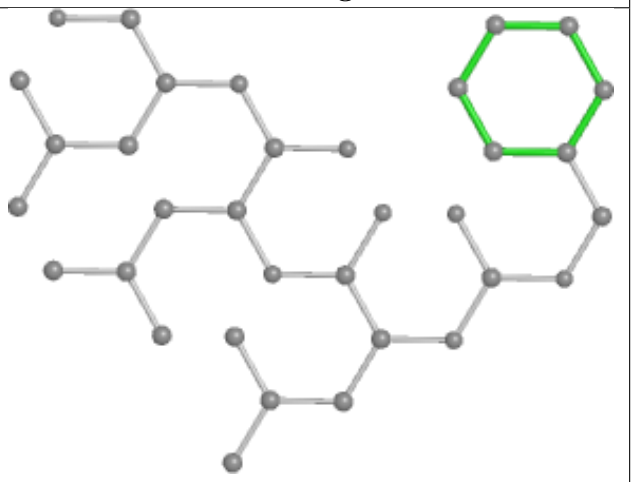
Bond lengths



Bond angles

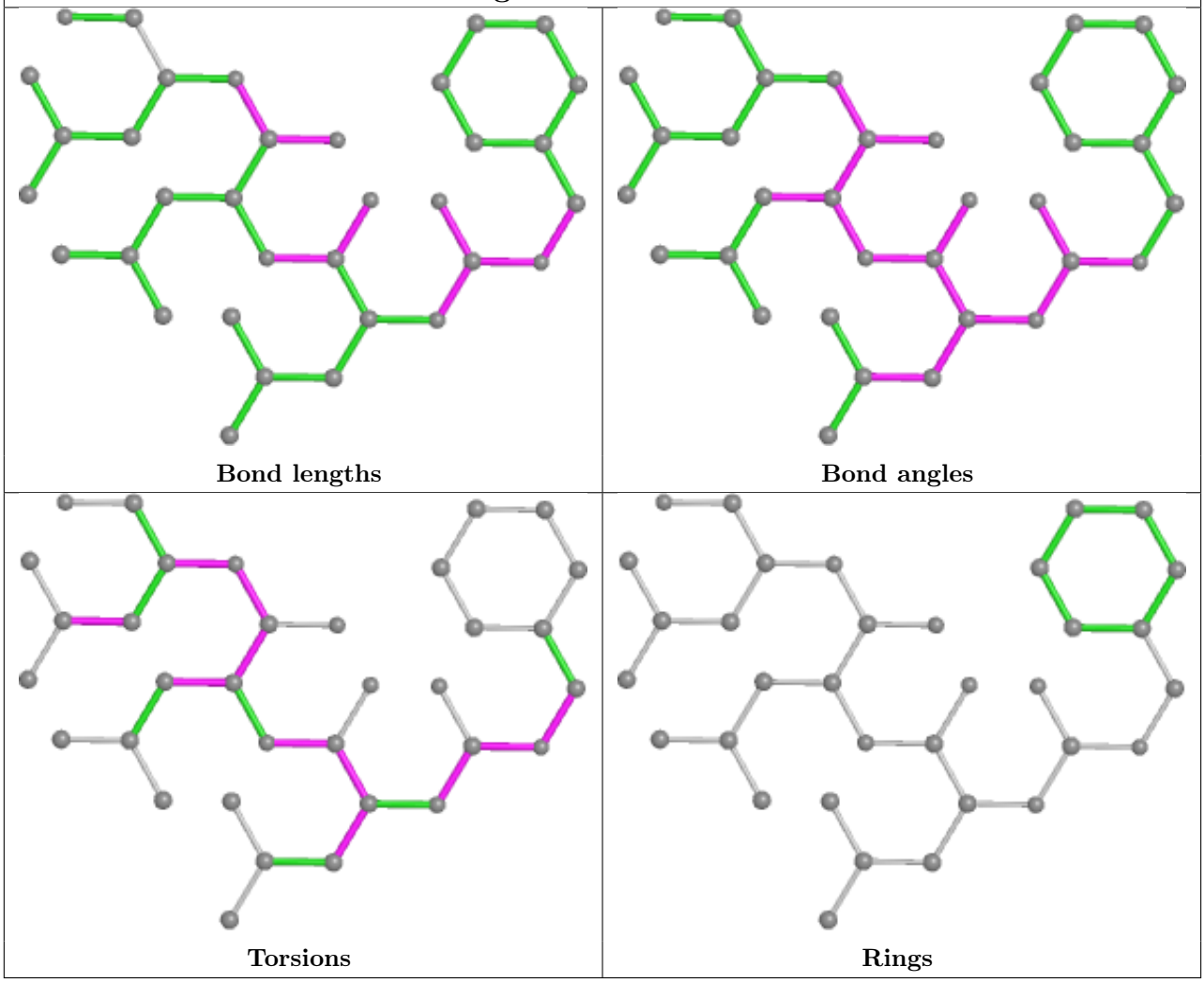


Torsions



Rings

Ligand LDZ V 301



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.

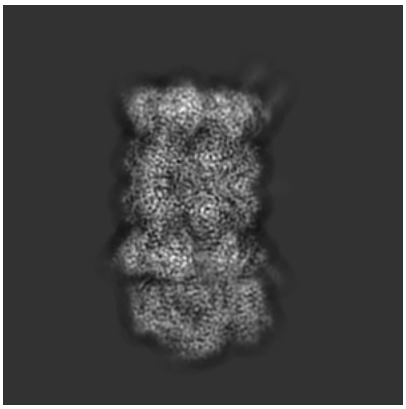
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27015. These allow visual inspection of the internal detail of the map and identification of artifacts.

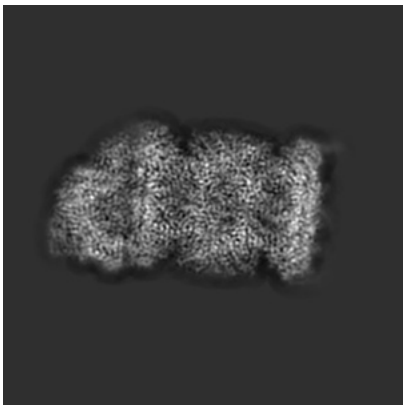
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

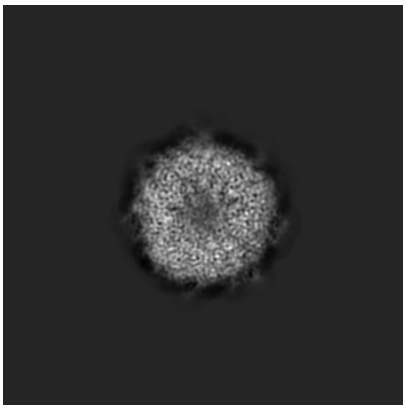
6.1.1 Primary map



X

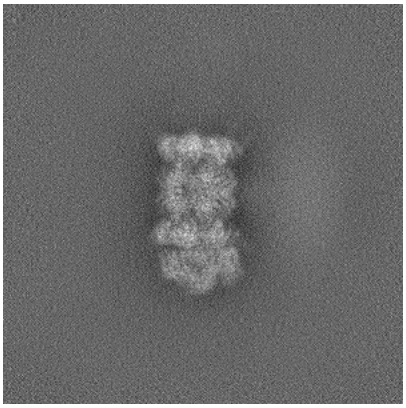


Y

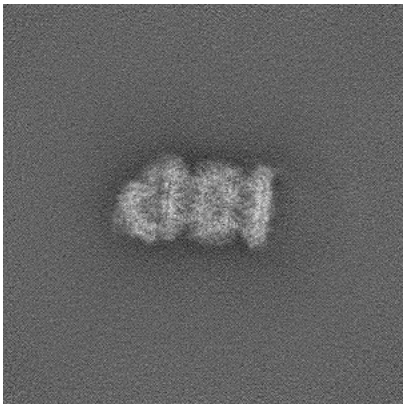


Z

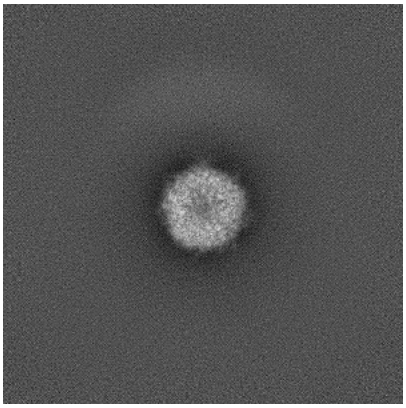
6.1.2 Raw map



X



Y



Z

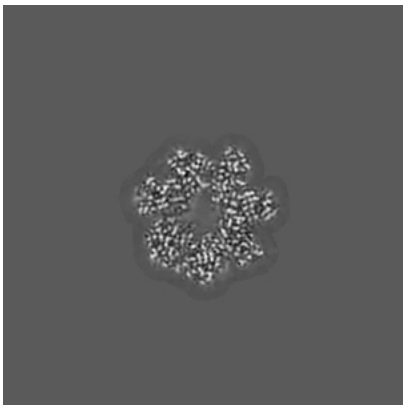
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

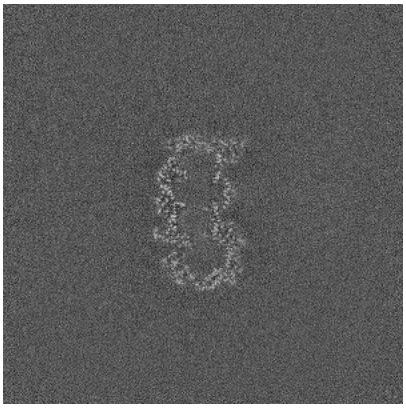
X Index: 150

Y Index: 150

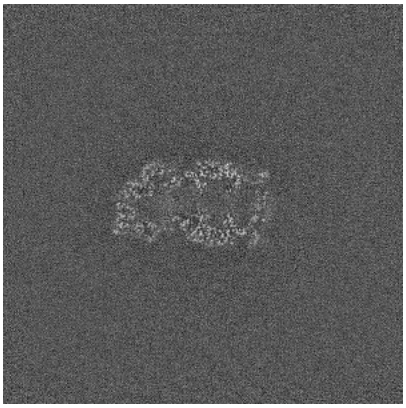


Z Index: 150

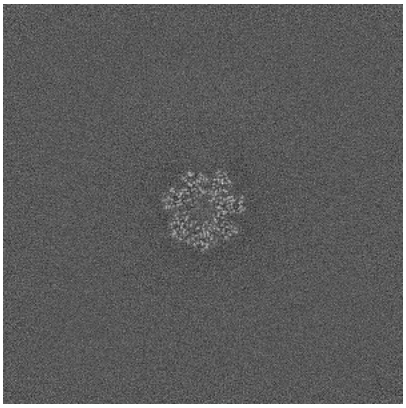
6.2.2 Raw map



X Index: 256



Y Index: 256

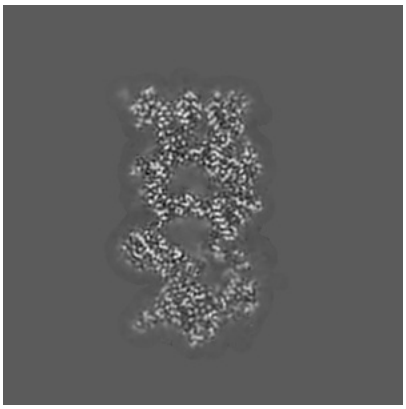


Z Index: 256

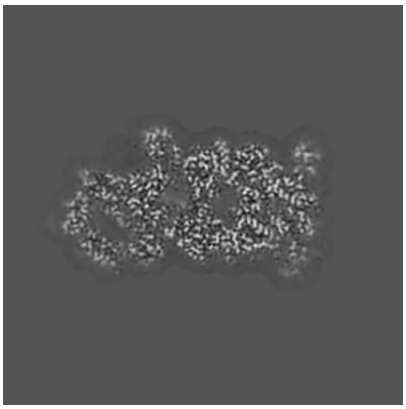
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

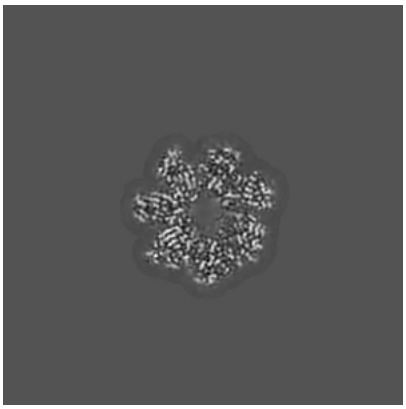
6.3.1 Primary map



X Index: 170

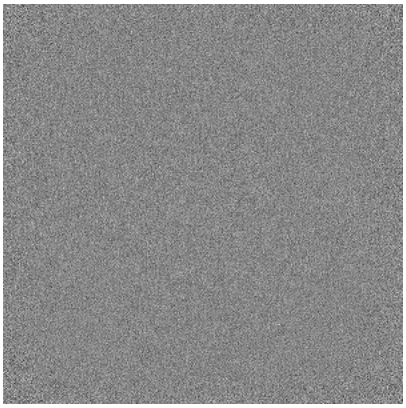


Y Index: 121

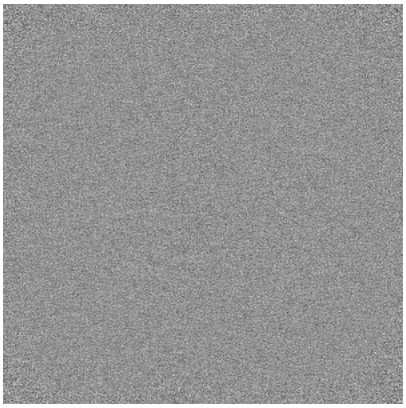


Z Index: 180

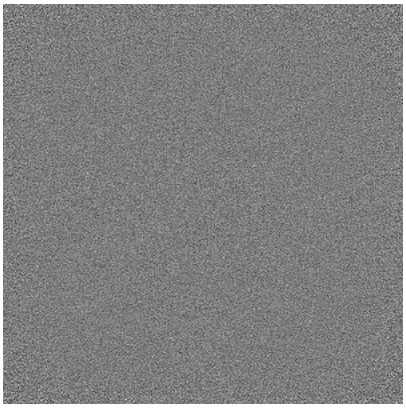
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

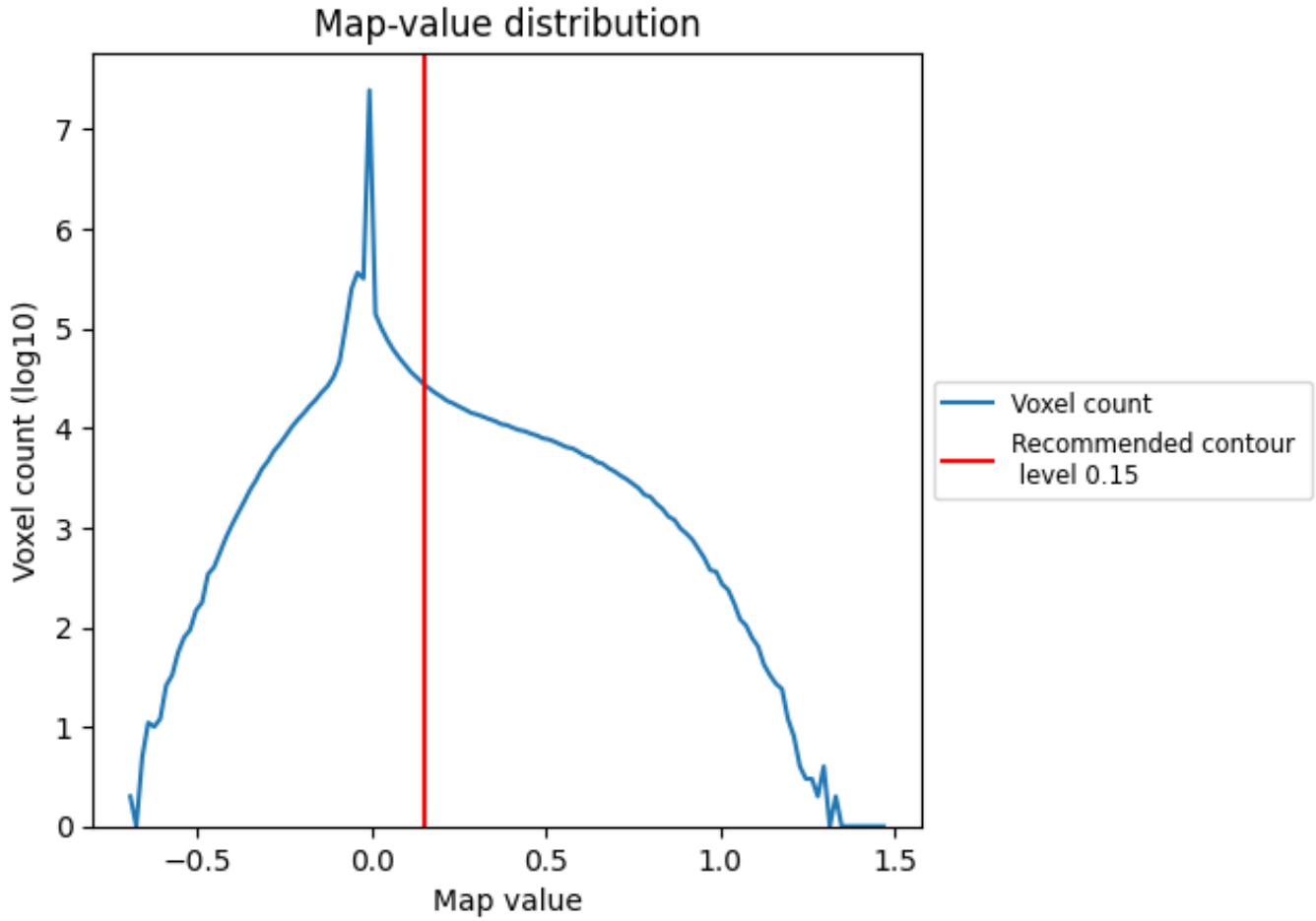
6.5 Mask visualisation (i)

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

7 Map analysis

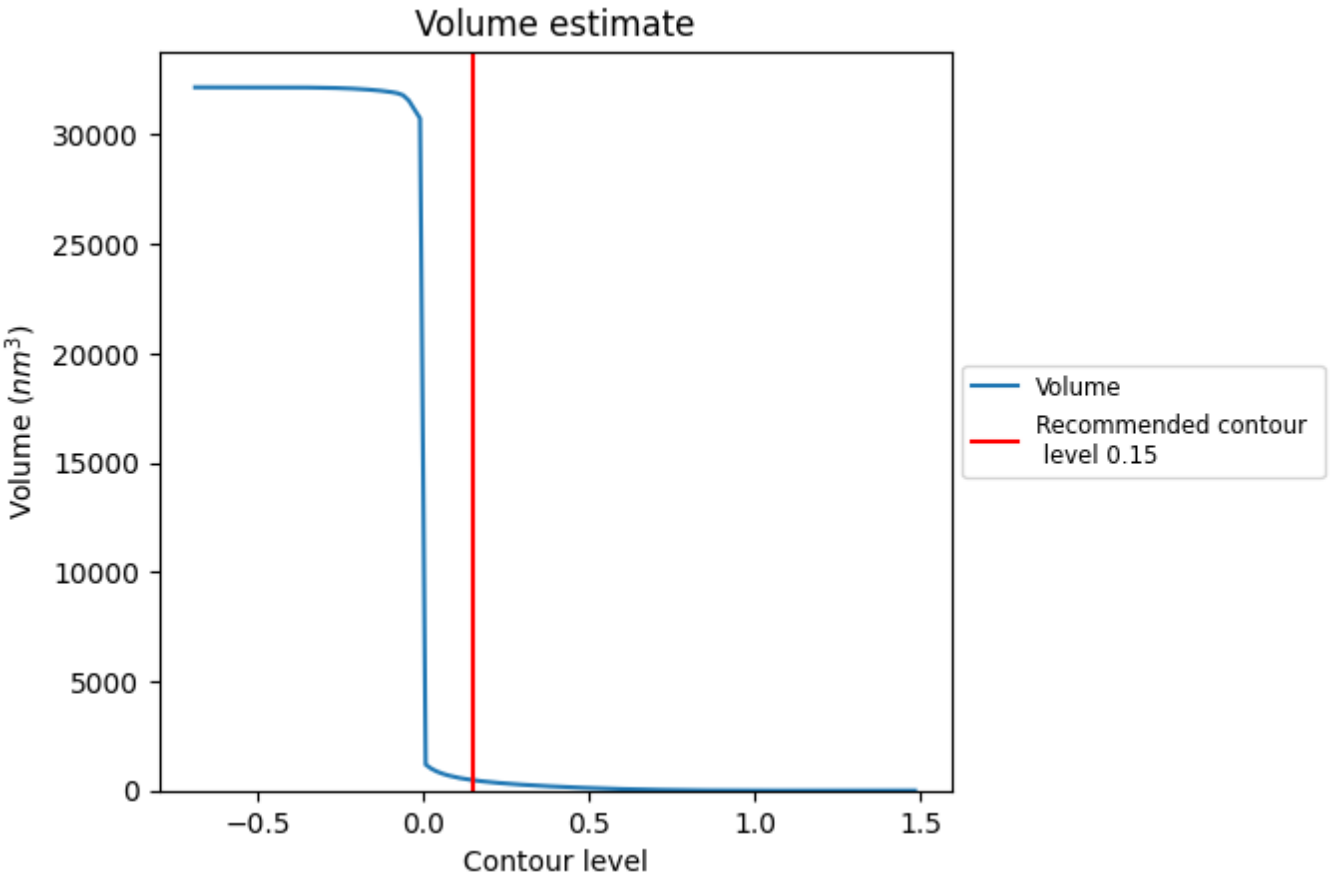
This section contains the results of statistical analysis of the map.

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.

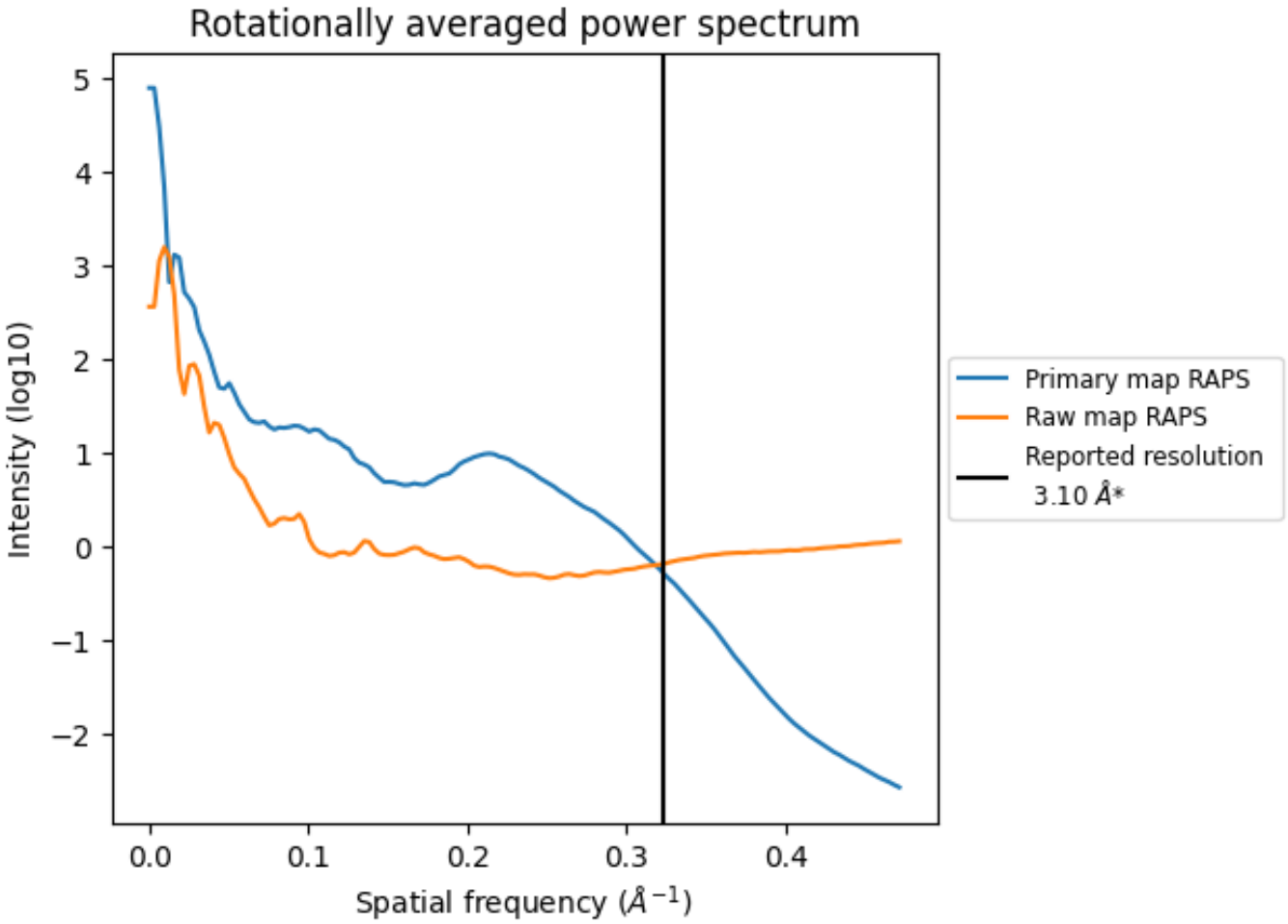
7.2 Volume estimate



The volume at the recommended contour level is 474 nm^3; this corresponds to an approximate mass of 428 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)

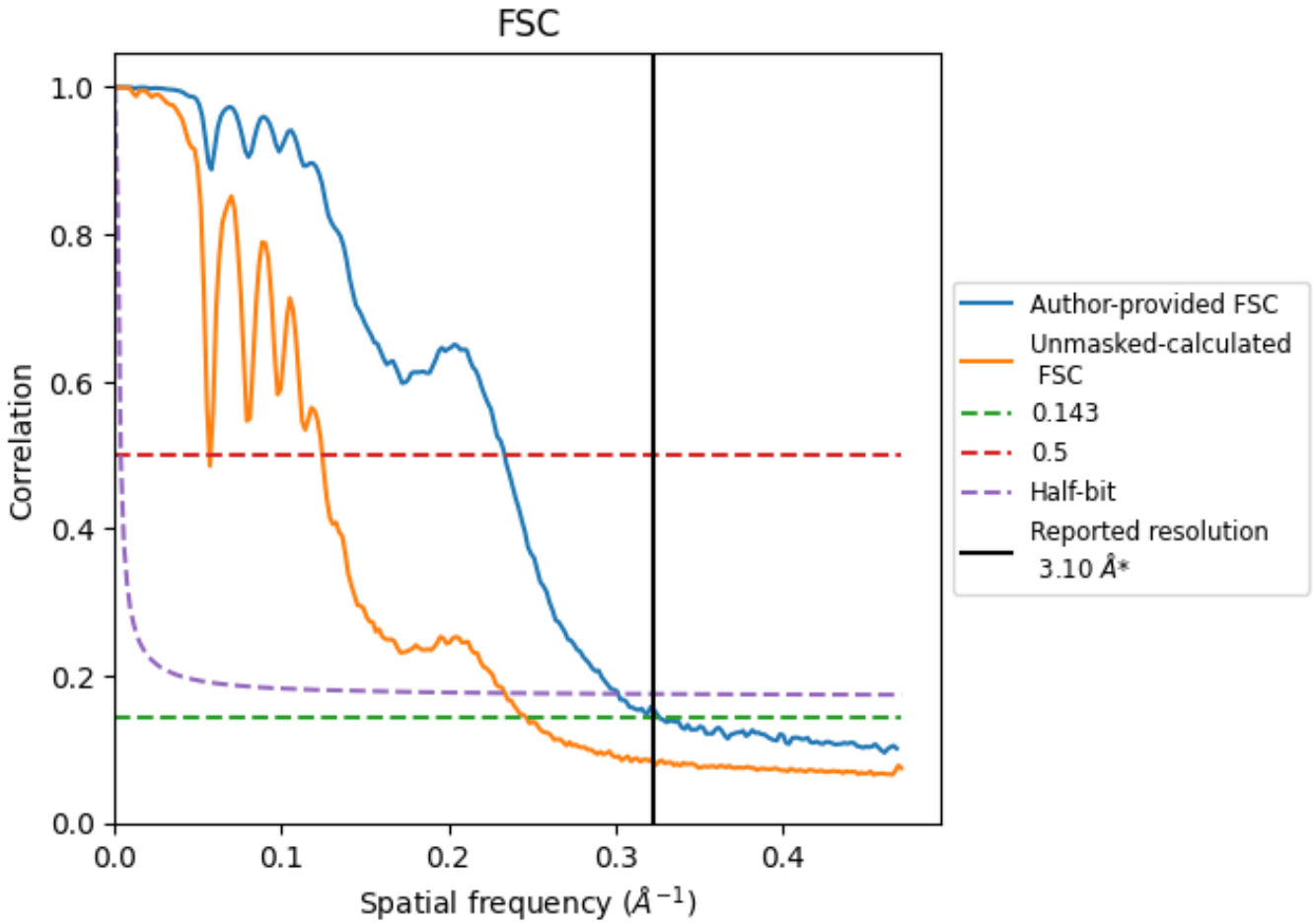


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

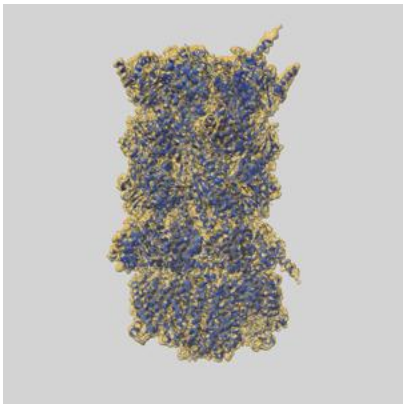
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	4.28	3.31
Unmasked-calculated*	4.05	17.61	4.27

*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 4.05 differs from the reported value 3.1 by more than 10 %

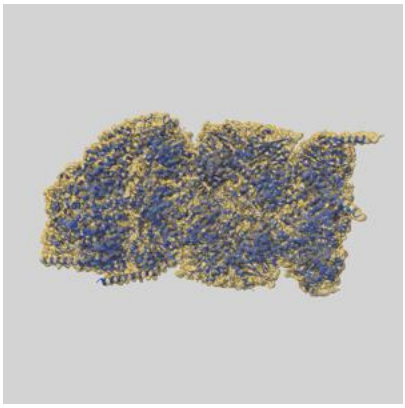
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27015 and PDB model 8CVS. Per-residue inclusion information can be found in section 3 on page 9.

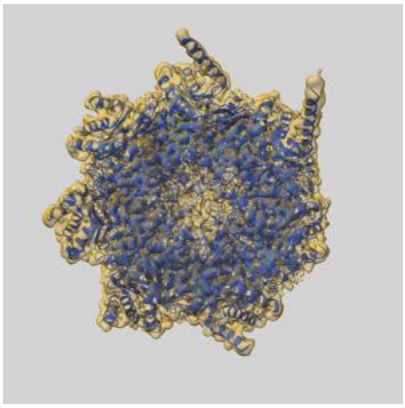
9.1 Map-model overlay



X



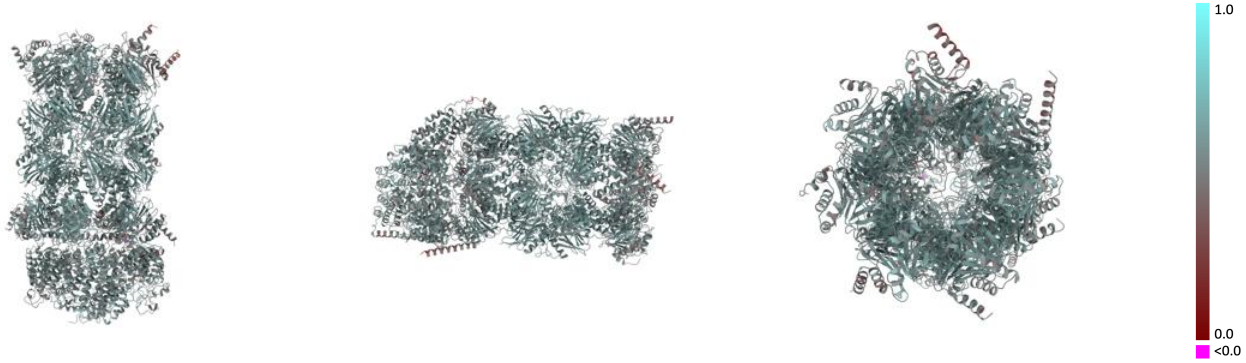
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

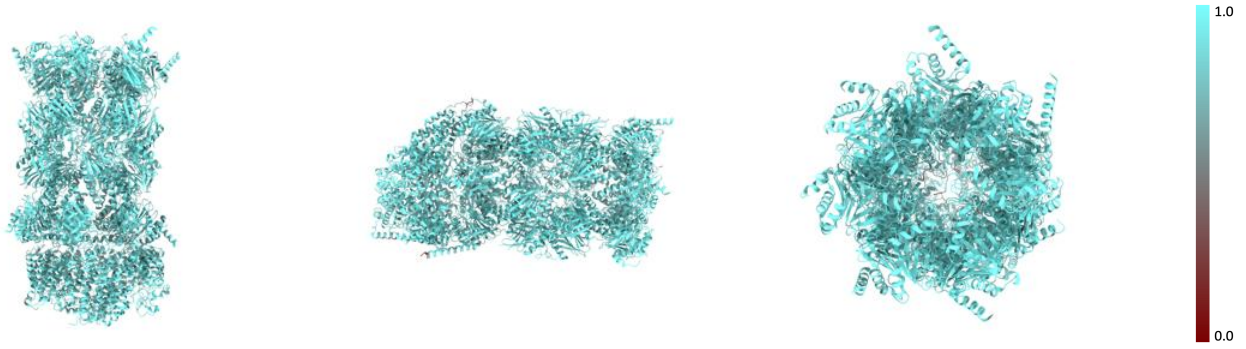
9.2 Q-score mapped to coordinate model



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.

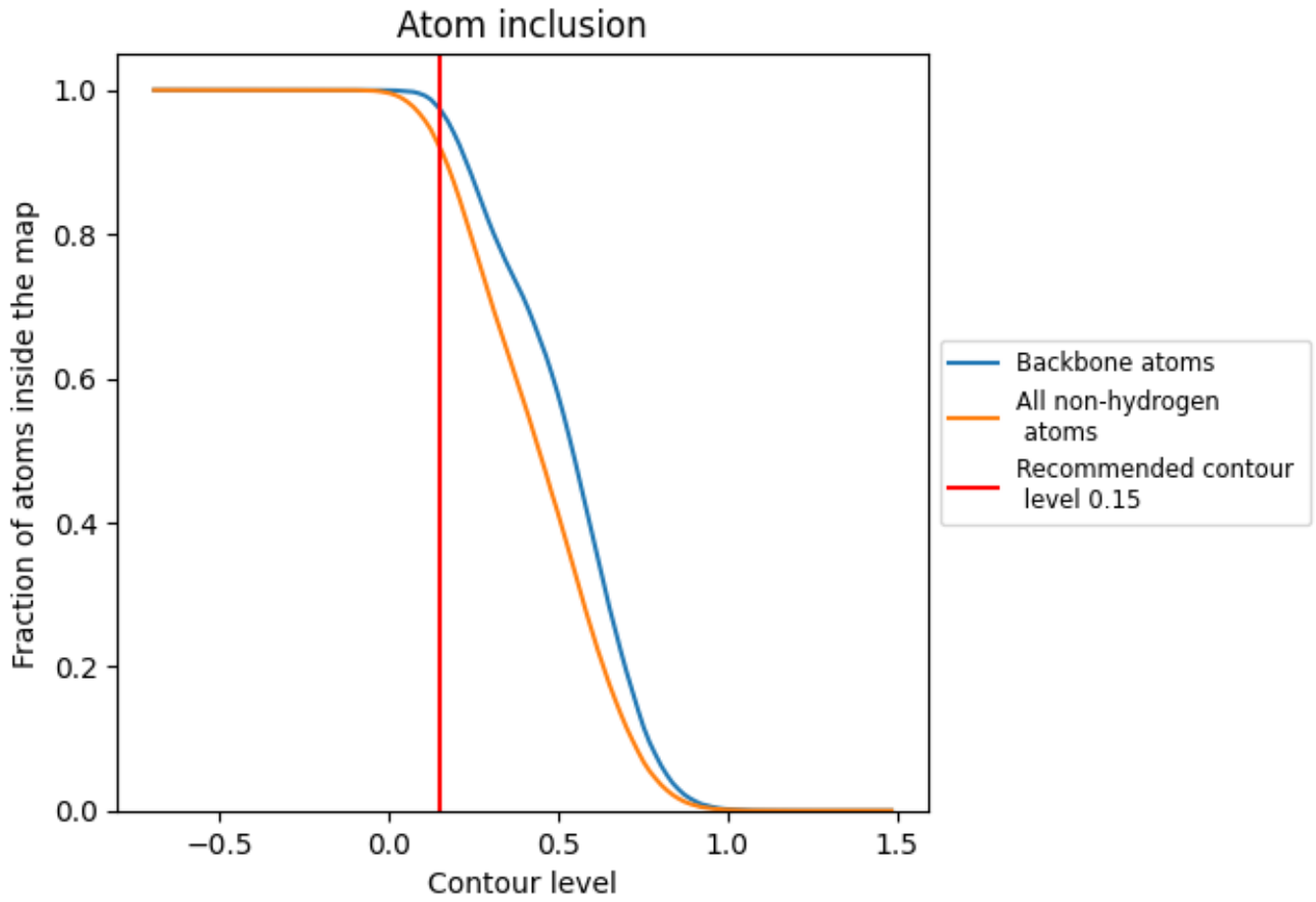
9.3 Atom inclusion mapped to coordinate model



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9224	0.5590
A	0.9258	0.5670
B	0.8628	0.5260
C	0.8661	0.5230
D	0.8927	0.5460
E	0.9233	0.5630
F	0.9261	0.5620
G	0.9386	0.5670
H	0.9422	0.5870
I	0.9491	0.5860
J	0.9444	0.5880
K	0.9457	0.5840
L	0.9528	0.5860
M	0.9458	0.5870
N	0.9494	0.5890
O	0.9402	0.5590
P	0.9206	0.5410
Q	0.8993	0.5070
R	0.9127	0.5400
S	0.9397	0.5430
T	0.9315	0.5510
U	0.9298	0.5500
V	0.9497	0.5780
W	0.9470	0.5890
X	0.9456	0.5860
Y	0.9508	0.5870
Z	0.9419	0.5810
a	0.9510	0.5880
b	0.9388	0.5850
c	0.8968	0.5380