



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 10:56 am GMT

PDB ID : 5A0Q
EMDB ID : EMD-2981
Title : Cryo-EM reveals the conformation of a substrate analogue in the human 20S proteasome core
Authors : daFonseca, P.C.A.; Morris, E.P.
Deposited on : 2015-04-22
Resolution : 3.50 Å(reported)
Based on initial model : 3UNE

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:

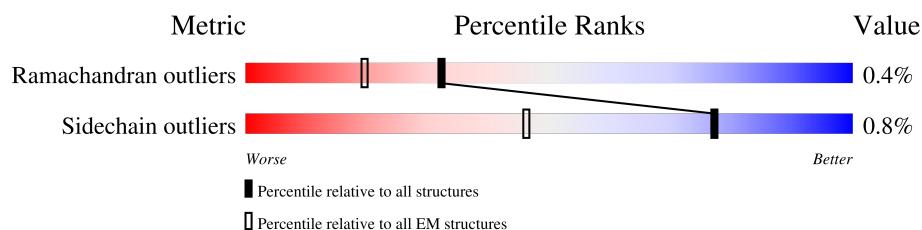
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	246	<div> <div>11%</div> <div>78%</div> <div>21%</div> </div>
1	O	246	<div> <div>11%</div> <div>78%</div> <div>21%</div> </div>
2	B	234	<div> <div>12%</div> <div>86%</div> <div>5%</div> <div>9%</div> </div>
2	P	234	<div> <div>12%</div> <div>86%</div> <div>5%</div> <div>9%</div> </div>
3	C	261	<div> <div>12%</div> <div>87%</div> <div>9%</div> </div>
3	Q	261	<div> <div>12%</div> <div>87%</div> <div>9%</div> </div>
4	D	248	<div> <div>16%</div> <div>85%</div> <div>14%</div> </div>
4	R	248	<div> <div>16%</div> <div>85%</div> <div>14%</div> </div>
5	E	241	<div> <div>14%</div> <div>86%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
5	S	241	
6	F	263	
6	T	263	
7	G	255	
7	U	255	
8	H	205	
8	V	205	
9	I	234	
9	W	234	
10	J	204	
10	X	204	
11	K	201	
11	Y	201	
12	L	204	
12	Z	204	
13	M	213	
13	a	213	
14	N	219	
14	b	219	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 43448 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
1	A	195	Total	C	N	O	S	0	0
			1514	963	254	284	13		
1	O	195	Total	C	N	O	S	0	0
			1514	963	254	284	13		

- Molecule 2 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	214	Total	C	N	O	S	0	0
			1671	1072	285	309	5		
2	P	214	Total	C	N	O	S	0	0
			1671	1072	285	309	5		

- Molecule 3 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	237	Total	C	N	O	S	0	0
			1860	1175	321	354	10		
3	Q	237	Total	C	N	O	S	0	0
			1860	1175	321	354	10		

- Molecule 4 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	214	Total	C	N	O	S	0	0
			1674	1056	300	313	5		
4	R	214	Total	C	N	O	S	0	0
			1674	1056	300	313	5		

- Molecule 5 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1643	1036	272	325	10		
5	S	215	Total	C	N	O	S	0	0
			1643	1036	272	325	10		

- Molecule 6 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	195	Total	C	N	O	S	0	0
			1535	969	278	278	10		
6	T	195	Total	C	N	O	S	0	0
			1535	969	278	278	10		

- Molecule 7 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	209	Total	C	N	O	S	0	0
			1626	1032	279	304	11		
7	U	209	Total	C	N	O	S	0	0
			1626	1032	279	304	11		

- Molecule 8 is a protein called PROTEASOME SUBUNIT BETA TYPE-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	183	Total	C	N	O	S	0	0
			1372	858	236	266	12		
8	V	183	Total	C	N	O	S	0	0
			1372	858	236	266	12		

- Molecule 9 is a protein called PROTEASOME SUBUNIT BETA TYPE-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	198	Total	C	N	O	S	0	0
			1490	939	251	288	12		
9	W	198	Total	C	N	O	S	0	0
			1490	939	251	288	12		

- Molecule 10 is a protein called PROTEASOME SUBUNIT BETA TYPE-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	176	Total	C	N	O	S	0	0
			1374	882	227	251	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	176	Total	C	N	O	S	0	0
			1374	882	227	251	14		

- Molecule 11 is a protein called PROTEASOME SUBUNIT BETA TYPE-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	189	Total	C	N	O	S	0	0
			1512	970	259	275	8		
11	Y	189	Total	C	N	O	S	0	0
			1512	970	259	275	8		

- Molecule 12 is a protein called PROTEASOME SUBUNIT BETA TYPE-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	192	Total	C	N	O	S	0	0
			1480	933	258	280	9		
12	Z	192	Total	C	N	O	S	0	0
			1480	933	258	280	9		

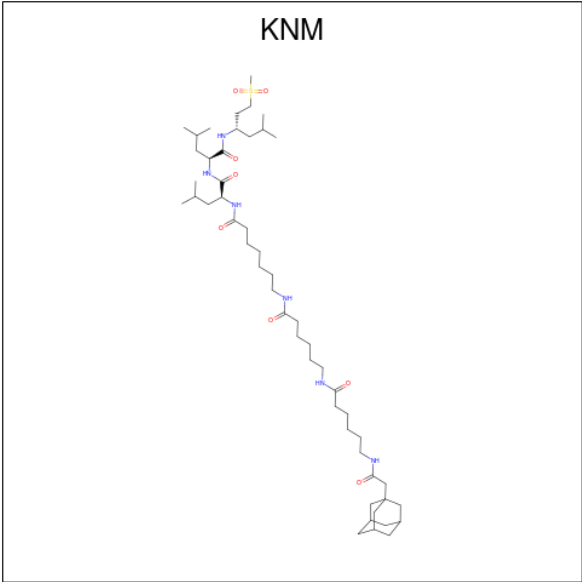
- Molecule 13 is a protein called PROTEASOME SUBUNIT BETA TYPE-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	190	Total	C	N	O	S	0	0
			1453	919	250	275	9		
13	a	190	Total	C	N	O	S	0	0
			1453	919	250	275	9		

- Molecule 14 is a protein called PROTEASOME SUBUNIT BETA TYPE-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	184	Total	C	N	O	S	0	0
			1428	905	245	267	11		
14	b	184	Total	C	N	O	S	0	0
			1428	905	245	267	11		

- Molecule 15 is ADA-(AHX)3-(LEU)3-VINYL SULFONE (three-letter code: KNM) (formula: C₅₁H₉₂N₆O₈S).

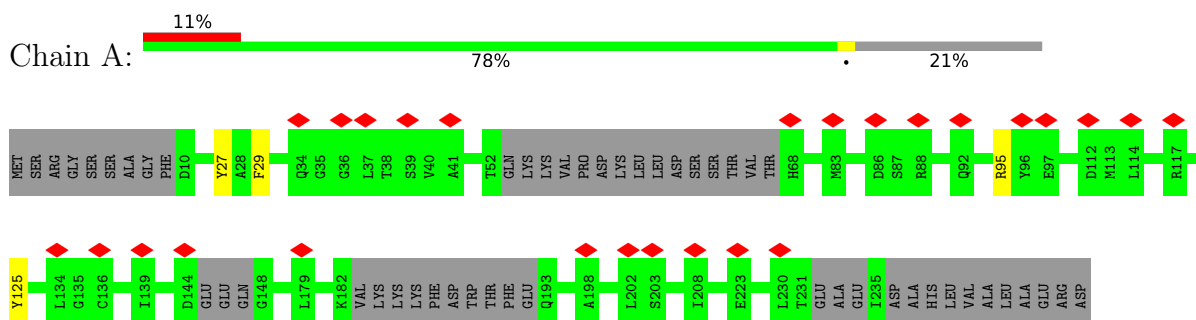


Mol	Chain	Residues	Atoms					AltConf
15	H	1	Total	C	N	O	S	0
			31	22	3	5	1	
15	I	1	Total	C	N	O	S	0
			30	22	3	4	1	
15	L	1	Total	C	N	O	S	0
			31	22	3	5	1	
15	V	1	Total	C	N	O	S	0
			31	22	3	5	1	
15	W	1	Total	C	N	O	S	0
			30	22	3	4	1	
15	Z	1	Total	C	N	O	S	0
			31	22	3	5	1	

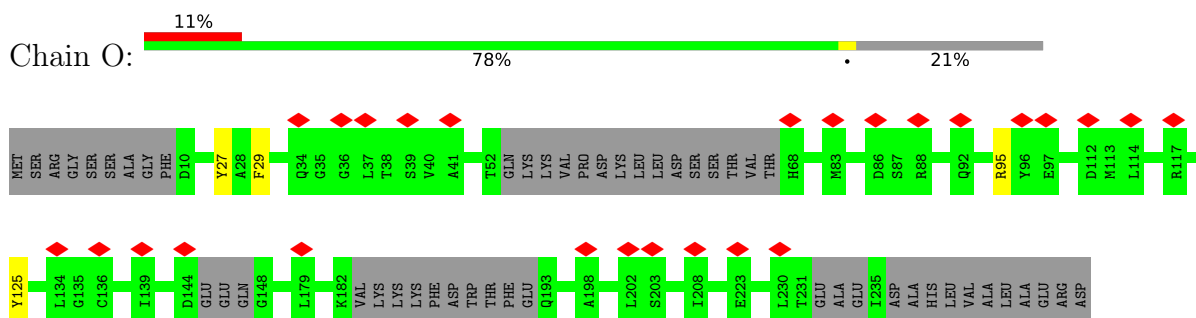
3 Residue-property plots

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

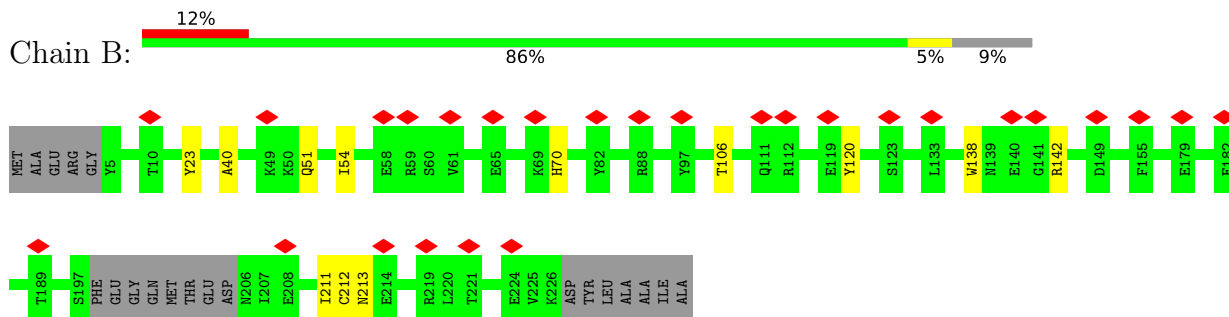
- Molecule 1: PROTEASOME SUBUNIT ALPHA TYPE-6



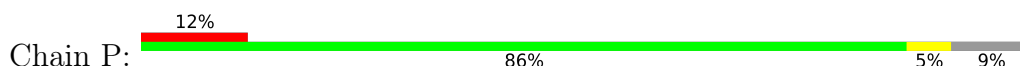
- Molecule 1: PROTEASOME SUBUNIT ALPHA TYPE-6

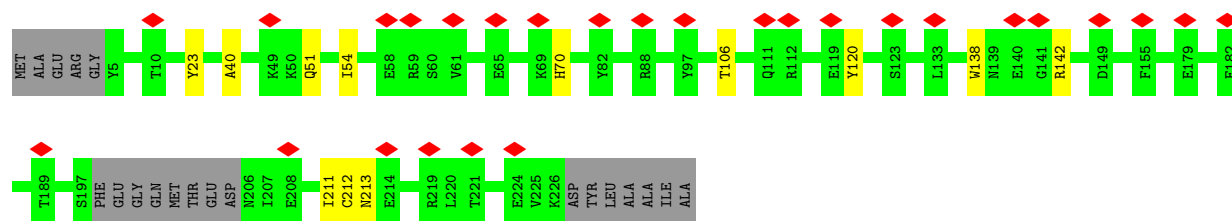


- Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE-2

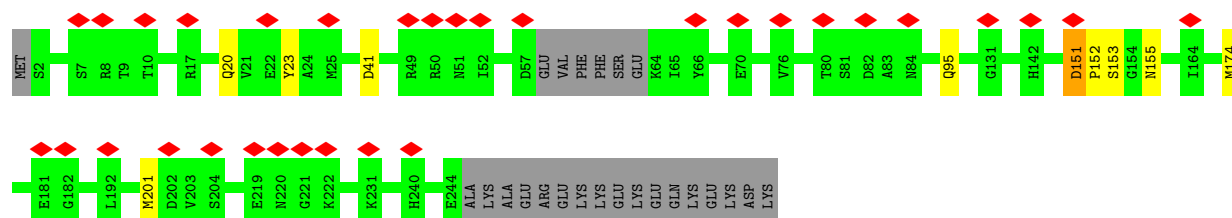
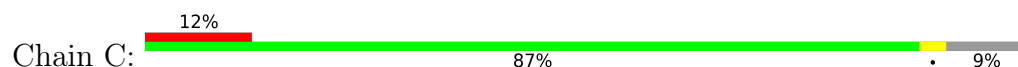


- Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE-2

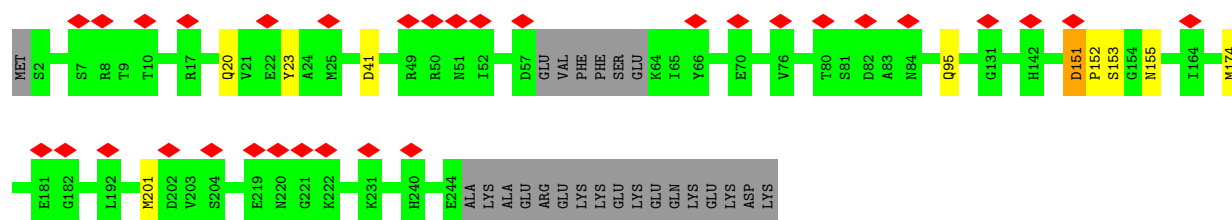
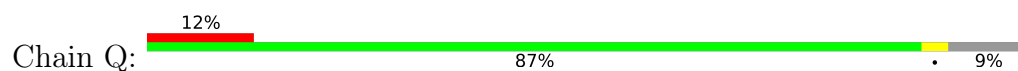




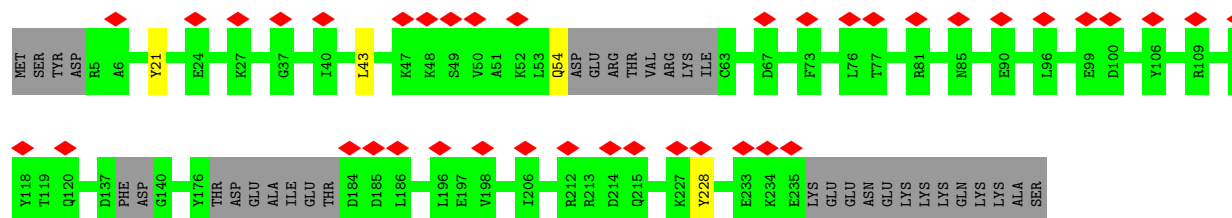
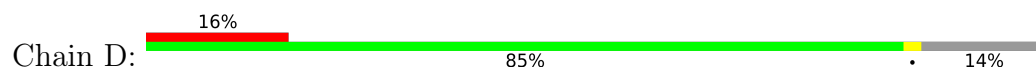
• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4



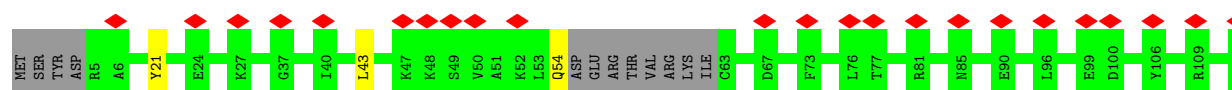
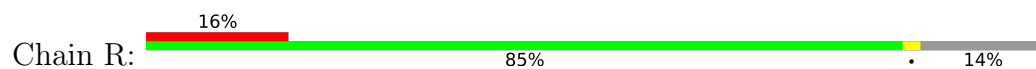
• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4

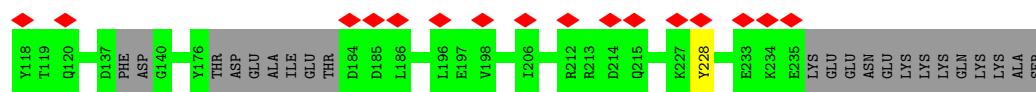


• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-7

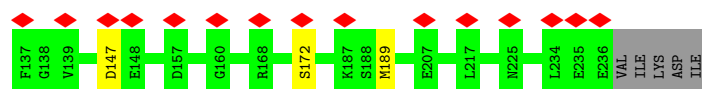
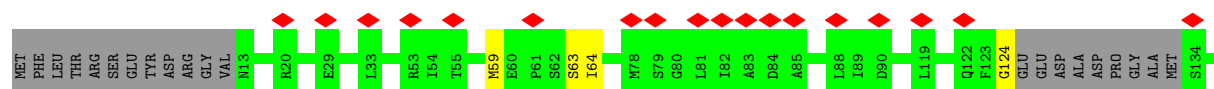
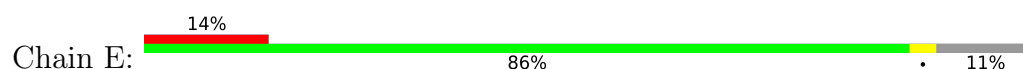


• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-7

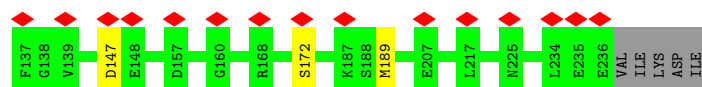
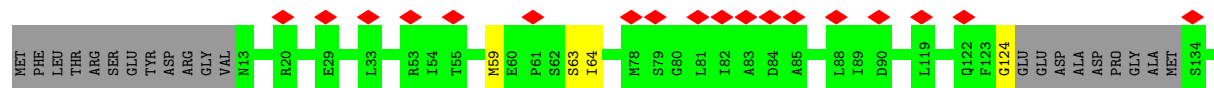
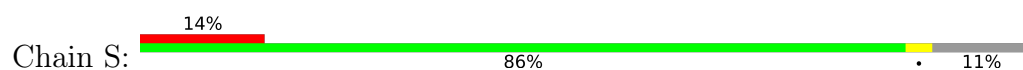




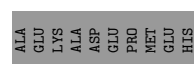
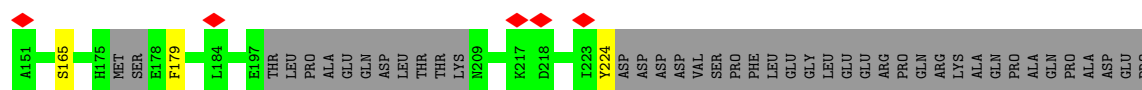
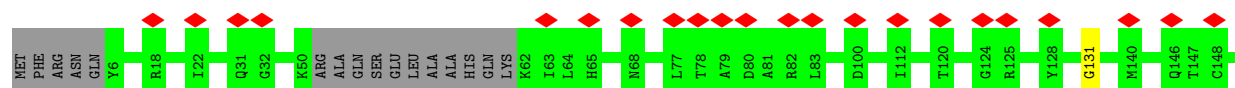
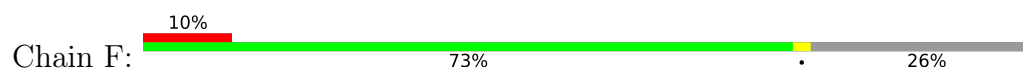
- Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-5



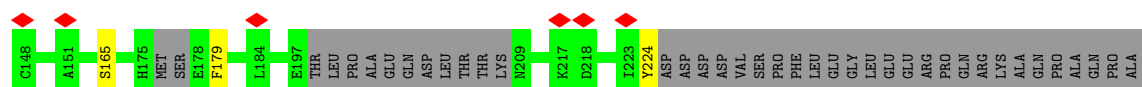
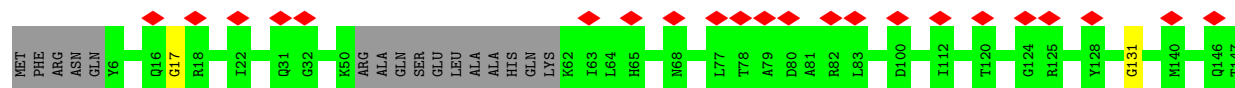
- Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-5



- Molecule 6: PROTEASOME SUBUNIT ALPHA TYPE-1



- Molecule 6: PROTEASOME SUBUNIT ALPHA TYPE-1



GLU
PRO
ALA
GLU
LYS
LYS
ASP
GLU
PRO
MET
GLU
HIS

• Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-3

Chain G: 13% 81% 18%

MET SER SER ILE GLY THR GLY TYR D8 L9 S10 Y25 T35 E50 LYS LEU VAL LEU SER LYS LEU LEU LEU LEU TYR TYR GLU GLU GLY SER ASN LYS ARG L66 D70 R71 A78 G79 L80 L81 L82 D83 A84 R85 D89 E93 N105 K109 D113 H120 S126

S141 V142 N143 D144 Y158 E175 M181 R187 V193 A194 I197 H201 ASP GLU VAL LYS ASP LYS A208 D230 E233 E234 A235 E236 K237 TYR ALA LYS LYS SER LEU LYS GLU ASP GLU SER ASP ASP ASN MET

• Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-3

Chain U: 13% 81% 18%

MET SER SER ILE GLY THR GLY TYR D8 L9 S10 Y25 T35 E50 LYS LEU VAL LEU SER LYS LEU LEU LEU LEU TYR TYR GLU GLU GLY SER ASN LYS ARG L66 D70 R71 A78 G79 L80 L81 L82 D83 A84 R85 D89 E93 N105 K109 D113 H120 S126

S141 V142 N143 D144 Y158 E175 M181 R187 V193 A194 I197 H201 ASP GLU VAL LYS ASP LYS A208 D230 E233 E234 A235 E236 K237 TYR ALA LYS LYS SER LEU LYS GLU ASP GLU SER ASP ASP ASN MET

• Molecule 8: PROTEASOME SUBUNIT BETA TYPE-6

Chain H: 13% 84% 11%

T1 F8 D9 G23 S24 Y25 N28 R29 V30 K33 L34 T35 P36 I37 R40 T41 F42 C43 S46 G47 D51 T52 Q53 Y61 E92 D93 L94 M95 A96 G97 W103 ASP PRO GLN GLY G109 M116 G129 S130 R144 E145 G146 F155 L176

L179 A180 E181 S182 V188 LEU LEU GLY ASP GLN ILE PRO LYS PHE ALA VAL P36 THR PRO PRO ALA

• Molecule 8: PROTEASOME SUBUNIT BETA TYPE-6

Chain V: 12% 84% 5% 11%

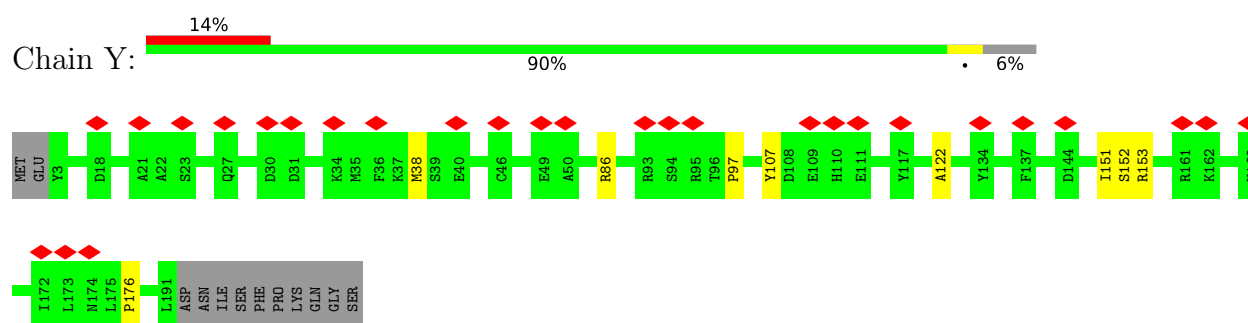
T1 Q7 F8 D9 G23 S24 Y25 N28 R29 V30 K33 L34 T35 P36 I37 R40 T41 F42 C43 S46 G47 D51 T52 Q53 Y61 E92 D93 L94 M95 A96 G97 W103 ASP PRO GLN GLY G109 M116 G129 S130 R144 E145 G146 F155

L176 L179 S182 V188 LEU LEU GLY ASP GLN ILE PRO LYS PHE ALA VAL P36 THR PRO PRO ALA

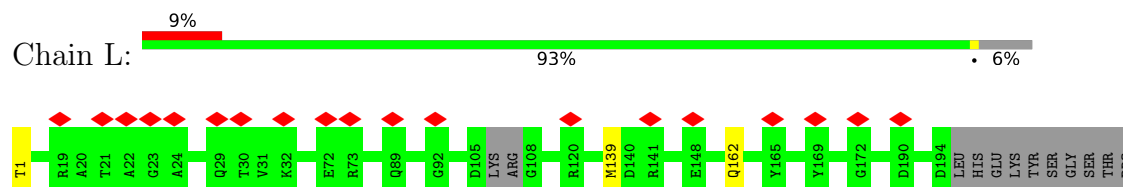
• Molecule 9: PROTEASOME SUBUNIT BETA TYPE-7

Chain I: 6% 81% 15%

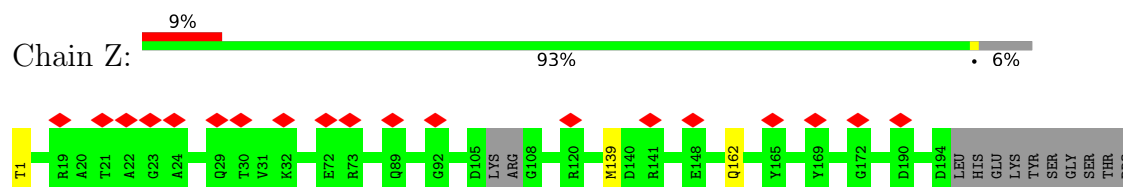




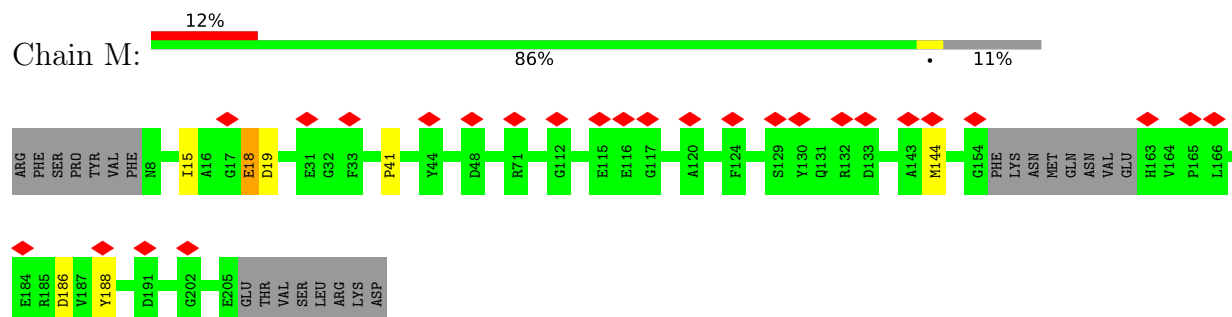
• Molecule 12: PROTEASOME SUBUNIT BETA TYPE-5



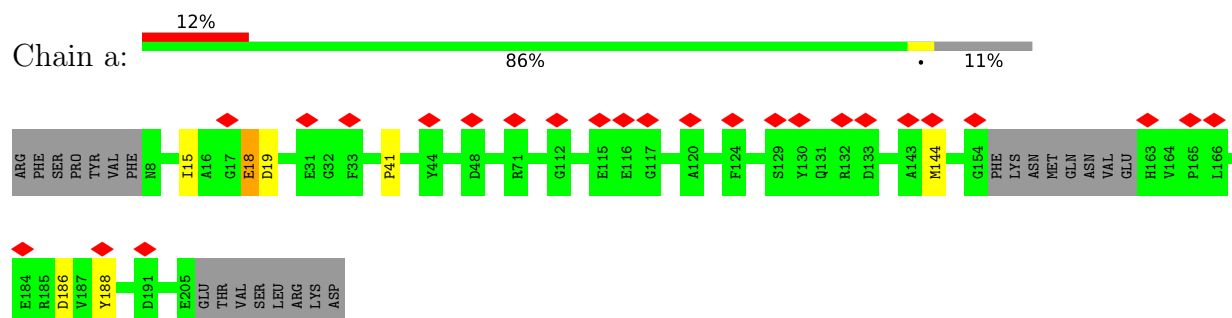
• Molecule 12: PROTEASOME SUBUNIT BETA TYPE-5



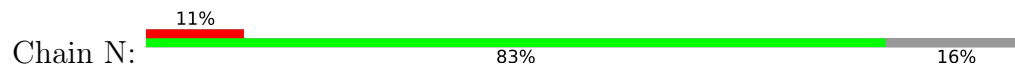
• Molecule 13: PROTEASOME SUBUNIT BETA TYPE-1

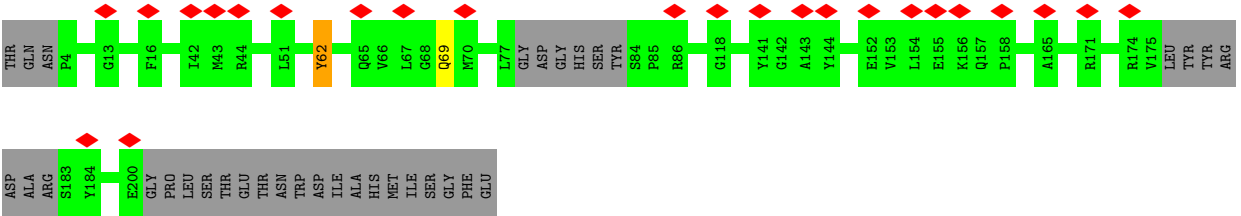


• Molecule 13: PROTEASOME SUBUNIT BETA TYPE-1

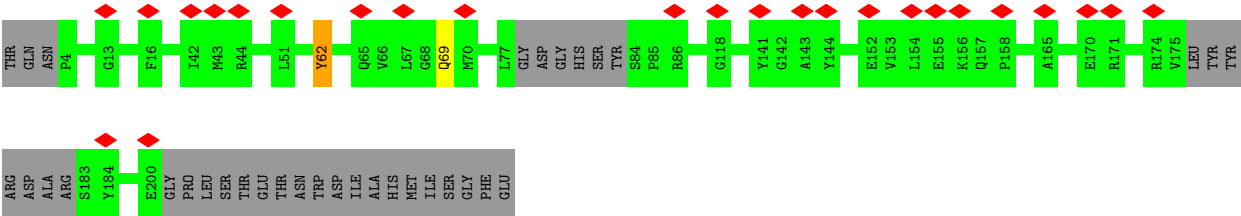
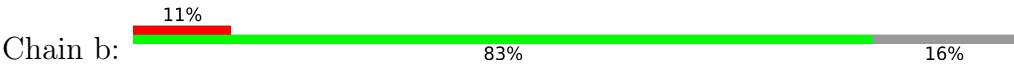


• Molecule 14: PROTEASOME SUBUNIT BETA TYPE-4





• Molecule 14: PROTEASOME SUBUNIT BETA TYPE-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	76500	Depositor
Resolution determination method	Not provided	
CTF correction method	FULL RECORDED IMAGE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4.8	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	134461	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	16.752	Depositor
Minimum map value	-13.472	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.2	Depositor
Map size (\AA)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.95	0/1537	1.10	5/2073 (0.2%)
1	O	0.95	0/1537	1.10	5/2073 (0.2%)
2	B	0.90	0/1707	1.05	5/2312 (0.2%)
2	P	0.90	0/1707	1.05	5/2312 (0.2%)
3	C	0.94	3/1887 (0.2%)	1.07	7/2542 (0.3%)
3	Q	0.94	3/1887 (0.2%)	1.07	7/2542 (0.3%)
4	D	1.00	1/1695 (0.1%)	1.09	2/2283 (0.1%)
4	R	1.00	1/1695 (0.1%)	1.09	2/2283 (0.1%)
5	E	0.82	0/1668	1.02	4/2252 (0.2%)
5	S	0.82	0/1668	1.02	4/2252 (0.2%)
6	F	0.99	0/1562	1.12	6/2105 (0.3%)
6	T	1.00	0/1562	1.19	7/2105 (0.3%)
7	G	0.97	0/1656	1.12	2/2232 (0.1%)
7	U	0.97	0/1656	1.12	2/2232 (0.1%)
8	H	1.05	1/1394 (0.1%)	1.16	7/1884 (0.4%)
8	V	1.04	1/1394 (0.1%)	1.16	7/1884 (0.4%)
9	I	0.96	2/1515 (0.1%)	1.14	4/2050 (0.2%)
9	W	0.96	2/1515 (0.1%)	1.14	4/2050 (0.2%)
10	J	0.92	1/1398 (0.1%)	1.07	3/1884 (0.2%)
10	X	0.92	1/1398 (0.1%)	1.07	3/1884 (0.2%)
11	K	0.87	0/1543	1.06	4/2088 (0.2%)
11	Y	0.87	0/1543	1.06	4/2088 (0.2%)
12	L	1.06	2/1508 (0.1%)	1.13	3/2038 (0.1%)
12	Z	1.06	2/1508 (0.1%)	1.13	3/2038 (0.1%)
13	M	0.91	0/1477	1.11	3/1990 (0.2%)
13	a	0.91	0/1477	1.11	3/1990 (0.2%)
14	N	0.91	1/1451 (0.1%)	1.08	2/1957 (0.1%)
14	b	0.91	1/1451 (0.1%)	1.08	2/1957 (0.1%)
All	All	0.95	22/43996 (0.1%)	1.10	115/59380 (0.2%)

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
1	A	0	1
1	O	0	1
5	E	0	1
5	S	0	1
7	G	0	1
7	U	0	1
9	I	0	2
9	W	0	2
10	J	0	1
10	X	0	1
11	K	0	1
11	Y	0	1
13	M	0	2
13	a	0	2
All	All	0	18

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1	THR	C-N	19.41	1.78	1.34
8	V	1	THR	C-N	19.41	1.78	1.34
9	I	123	PRO	N-CD	-7.63	1.37	1.47
9	W	123	PRO	N-CD	-7.63	1.37	1.47
12	L	1	THR	C-N	6.47	1.49	1.34
12	Z	1	THR	C-N	6.47	1.49	1.34
12	L	162	GLN	CD-OE1	6.09	1.37	1.24
12	Z	162	GLN	CD-OE1	6.09	1.37	1.24
4	D	54	GLN	CD-OE1	5.87	1.36	1.24
4	R	54	GLN	CD-OE1	5.85	1.36	1.24
10	J	168	GLN	CD-OE1	5.83	1.36	1.24
10	X	168	GLN	CD-OE1	5.83	1.36	1.24
3	C	20	GLN	CD-OE1	5.82	1.36	1.24
14	b	69	GLN	CD-OE1	5.82	1.36	1.24
3	Q	20	GLN	CD-OE1	5.80	1.36	1.24
14	N	69	GLN	CD-OE1	5.80	1.36	1.24
3	C	95	GLN	CD-OE1	5.71	1.36	1.24
3	Q	95	GLN	CD-OE1	5.71	1.36	1.24
3	Q	152	PRO	N-CD	5.12	1.55	1.47
3	C	152	PRO	N-CD	5.11	1.55	1.47
9	I	39	PRO	N-CD	5.10	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	39	PRO	N-CD	5.10	1.54	1.47

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	17	GLY	N-CA-C	15.39	151.57	113.10
8	H	47	GLY	N-CA-C	-9.29	89.87	113.10
8	V	47	GLY	N-CA-C	-9.29	89.87	113.10
11	Y	38	MET	CG-SD-CE	-8.17	87.13	100.20
11	K	38	MET	CG-SD-CE	-8.15	87.16	100.20
3	Q	153	SER	N-CA-C	-8.05	89.26	111.00
3	C	153	SER	N-CA-C	-8.04	89.28	111.00
2	B	120	TYR	CB-CG-CD2	-7.78	116.33	121.00
2	P	120	TYR	CB-CG-CD2	-7.78	116.33	121.00
7	G	25	TYR	CB-CG-CD2	-7.67	116.40	121.00
7	U	25	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	A	27	TYR	CB-CG-CD2	-7.65	116.41	121.00
1	O	27	TYR	CB-CG-CD2	-7.59	116.44	121.00
11	K	152	SER	N-CA-CB	7.55	121.83	110.50
11	Y	152	SER	N-CA-CB	7.55	121.83	110.50
1	A	27	TYR	CB-CG-CD1	7.50	125.50	121.00
1	O	27	TYR	CB-CG-CD1	7.50	125.50	121.00
9	I	119	THR	N-CA-C	-7.29	91.32	111.00
9	W	119	THR	N-CA-C	-7.29	91.32	111.00
2	B	120	TYR	CB-CG-CD1	7.24	125.34	121.00
2	P	120	TYR	CB-CG-CD1	7.24	125.34	121.00
12	L	1	THR	O-C-N	-7.23	111.12	122.70
12	Z	1	THR	O-C-N	-7.23	111.12	122.70
8	H	8	PHE	N-CA-C	7.23	130.51	111.00
2	P	23	TYR	CB-CG-CD2	-6.97	116.81	121.00
8	V	179	ILE	N-CA-C	-6.96	92.21	111.00
6	F	224	TYR	CB-CG-CD2	-6.95	116.83	121.00
6	T	224	TYR	CB-CG-CD2	-6.95	116.83	121.00
8	H	179	ILE	N-CA-C	-6.95	92.23	111.00
2	B	23	TYR	CB-CG-CD2	-6.90	116.86	121.00
5	E	59	MET	CG-SD-CE	-6.86	89.23	100.20
5	S	59	MET	CG-SD-CE	-6.86	89.23	100.20
9	I	119	THR	N-CA-CB	6.80	123.22	110.30
9	W	119	THR	N-CA-CB	6.80	123.22	110.30
8	V	7	GLN	CB-CA-C	-6.79	96.81	110.40
14	N	62	TYR	CB-CG-CD2	-6.78	116.93	121.00
14	b	62	TYR	CB-CG-CD2	-6.78	116.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	54	GLY	N-CA-C	-6.75	96.22	113.10
10	J	54	GLY	N-CA-C	-6.74	96.24	113.10
6	F	224	TYR	CB-CG-CD1	6.69	125.02	121.00
6	T	224	TYR	CB-CG-CD1	6.69	125.02	121.00
6	T	179	PHE	CB-CG-CD1	6.66	125.46	120.80
8	V	97	GLY	N-CA-C	-6.65	96.47	113.10
8	H	97	GLY	N-CA-C	-6.64	96.51	113.10
6	F	179	PHE	CB-CG-CD1	6.61	125.43	120.80
4	D	21	TYR	CB-CG-CD2	-6.52	117.09	121.00
4	R	21	TYR	CB-CG-CD2	-6.52	117.09	121.00
5	E	124	GLY	N-CA-C	-6.51	96.83	113.10
5	S	124	GLY	N-CA-C	-6.51	96.83	113.10
2	B	23	TYR	CB-CG-CD1	6.39	124.83	121.00
2	P	23	TYR	CB-CG-CD1	6.38	124.83	121.00
12	L	1	THR	C-N-CA	6.16	137.10	121.70
12	Z	1	THR	C-N-CA	6.16	137.10	121.70
8	H	61	TYR	CB-CG-CD2	-6.12	117.33	121.00
8	V	61	TYR	CB-CG-CD2	-6.12	117.33	121.00
14	N	62	TYR	CB-CG-CD1	6.11	124.67	121.00
14	b	62	TYR	CB-CG-CD1	6.11	124.67	121.00
9	W	189	TYR	N-CA-C	6.09	127.43	111.00
9	I	189	TYR	N-CA-C	6.08	127.42	111.00
10	J	100	GLY	C-N-CD	6.02	141.04	128.40
10	X	100	GLY	C-N-CD	5.99	140.97	128.40
12	Z	139	MET	CG-SD-CE	-5.91	90.75	100.20
12	L	139	MET	CG-SD-CE	-5.90	90.77	100.20
3	C	23	TYR	CB-CG-CD1	5.89	124.53	121.00
3	Q	23	TYR	CB-CG-CD1	5.89	124.53	121.00
7	G	25	TYR	CB-CG-CD1	5.86	124.52	121.00
7	U	25	TYR	CB-CG-CD1	5.86	124.52	121.00
9	I	38	SER	C-N-CD	5.79	140.57	128.40
9	W	38	SER	C-N-CD	5.79	140.57	128.40
3	C	151	ASP	C-N-CD	5.72	140.41	128.40
3	Q	151	ASP	C-N-CD	5.71	140.40	128.40
8	H	61	TYR	CB-CG-CD1	5.68	124.41	121.00
8	V	61	TYR	CB-CG-CD1	5.68	124.41	121.00
4	D	21	TYR	CB-CG-CD1	5.63	124.38	121.00
4	R	21	TYR	CB-CG-CD1	5.63	124.38	121.00
11	K	107	TYR	CB-CG-CD2	-5.57	117.66	121.00
11	Y	107	TYR	CB-CG-CD2	-5.54	117.68	121.00
6	T	179	PHE	CB-CG-CD2	-5.51	116.94	120.80
5	E	172	SER	N-CA-C	5.51	125.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	172	SER	N-CA-C	5.49	125.81	111.00
8	V	42	PHE	CB-CG-CD1	5.47	124.63	120.80
6	F	179	PHE	CB-CG-CD2	-5.47	116.97	120.80
8	H	42	PHE	CB-CG-CD1	5.44	124.61	120.80
10	X	8	GLY	N-CA-C	-5.44	99.50	113.10
10	J	8	GLY	N-CA-C	-5.44	99.51	113.10
3	C	201	MET	CG-SD-CE	-5.43	91.50	100.20
3	Q	201	MET	CG-SD-CE	-5.43	91.50	100.20
1	O	29	PHE	CB-CG-CD2	-5.40	117.02	120.80
1	A	29	PHE	CB-CG-CD2	-5.37	117.04	120.80
13	M	186	ASP	N-CA-C	-5.36	96.54	111.00
13	a	186	ASP	N-CA-C	-5.36	96.54	111.00
2	P	142	ARG	C-N-CD	-5.33	108.87	120.60
2	B	142	ARG	C-N-CD	-5.33	108.87	120.60
11	K	107	TYR	CB-CG-CD1	5.33	124.19	121.00
11	Y	107	TYR	CB-CG-CD1	5.33	124.19	121.00
3	C	23	TYR	CB-CG-CD2	-5.32	117.81	121.00
3	Q	23	TYR	CB-CG-CD2	-5.32	117.81	121.00
3	C	174	MET	CG-SD-CE	-5.30	91.72	100.20
3	Q	174	MET	CG-SD-CE	-5.29	91.75	100.20
13	M	19	ASP	CB-CG-OD2	5.22	123.00	118.30
13	a	19	ASP	CB-CG-OD2	5.22	123.00	118.30
6	F	131	GLY	N-CA-C	-5.19	100.13	113.10
6	T	131	GLY	N-CA-C	-5.19	100.13	113.10
3	Q	155	ASN	N-CA-C	-5.18	97.00	111.00
3	C	155	ASN	N-CA-C	-5.18	97.02	111.00
1	A	125	TYR	CB-CG-CD1	5.15	124.09	121.00
1	O	125	TYR	CB-CG-CD1	5.14	124.08	121.00
1	A	125	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	O	125	TYR	CB-CG-CD2	-5.12	117.93	121.00
6	F	165	SER	CB-CA-C	-5.09	100.44	110.10
6	T	165	SER	CB-CA-C	-5.09	100.44	110.10
13	M	144	MET	CG-SD-CE	-5.03	92.15	100.20
13	a	144	MET	CG-SD-CE	-5.03	92.16	100.20
5	E	64	ILE	N-CA-C	-5.00	97.50	111.00
5	S	64	ILE	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	95	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	E	147	ASP	Peptide
7	G	181	MET	Peptide
9	I	1	THR	Mainchain
9	I	111	TYR	Sidechain
10	J	16	LYS	Peptide
11	K	153	ARG	Sidechain
13	M	18	GLU	Peptide
13	M	188	TYR	Sidechain
1	O	95	ARG	Sidechain
5	S	147	ASP	Peptide
7	U	181	MET	Peptide
9	W	1	THR	Mainchain
9	W	111	TYR	Sidechain
10	X	16	LYS	Peptide
11	Y	153	ARG	Sidechain
13	a	18	GLU	Peptide
13	a	188	TYR	Sidechain

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	186/246 (76%)	178 (96%)	8 (4%)	0	100	100
1	O	186/246 (76%)	178 (96%)	8 (4%)	0	100	100
2	B	210/234 (90%)	198 (94%)	10 (5%)	2 (1%)	13	46
2	P	210/234 (90%)	198 (94%)	10 (5%)	2 (1%)	13	46
3	C	233/261 (89%)	225 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	233/261 (89%)	225 (97%)	8 (3%)	0	100	100
4	D	206/248 (83%)	201 (98%)	5 (2%)	0	100	100
4	R	206/248 (83%)	201 (98%)	5 (2%)	0	100	100
5	E	211/241 (88%)	201 (95%)	9 (4%)	1 (0%)	25	59
5	S	211/241 (88%)	201 (95%)	9 (4%)	1 (0%)	25	59
6	F	187/263 (71%)	184 (98%)	3 (2%)	0	100	100
6	T	187/263 (71%)	185 (99%)	2 (1%)	0	100	100
7	G	203/255 (80%)	196 (97%)	7 (3%)	0	100	100
7	U	203/255 (80%)	196 (97%)	7 (3%)	0	100	100
8	H	179/205 (87%)	164 (92%)	13 (7%)	2 (1%)	12	45
8	V	179/205 (87%)	165 (92%)	12 (7%)	2 (1%)	12	45
9	I	194/234 (83%)	187 (96%)	6 (3%)	1 (0%)	25	59
9	W	194/234 (83%)	187 (96%)	6 (3%)	1 (0%)	25	59
10	J	168/204 (82%)	158 (94%)	10 (6%)	0	100	100
10	X	168/204 (82%)	158 (94%)	10 (6%)	0	100	100
11	K	187/201 (93%)	173 (92%)	10 (5%)	4 (2%)	5	32
11	Y	187/201 (93%)	173 (92%)	10 (5%)	4 (2%)	5	32
12	L	188/204 (92%)	182 (97%)	6 (3%)	0	100	100
12	Z	188/204 (92%)	182 (97%)	6 (3%)	0	100	100
13	M	186/213 (87%)	175 (94%)	10 (5%)	1 (0%)	25	59
13	a	186/213 (87%)	175 (94%)	10 (5%)	1 (0%)	25	59
14	N	178/219 (81%)	161 (90%)	17 (10%)	0	100	100
14	b	178/219 (81%)	161 (90%)	17 (10%)	0	100	100
All	All	5432/6456 (84%)	5168 (95%)	242 (4%)	22 (0%)	32	64

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	40	ALA
2	B	54	ILE
5	E	189	MET
8	H	8	PHE
11	K	122	ALA
11	K	151	ILE

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Mol	Chain	Res	Type
2	P	40	ALA
2	P	54	ILE
5	S	189	MET
8	V	8	PHE
11	Y	122	ALA
11	Y	151	ILE
8	H	28	ASN
11	K	176	PRO
8	V	28	ASN
11	Y	176	PRO
13	M	41	PRO
13	a	41	PRO
9	I	188	PRO
11	K	97	PRO
9	W	188	PRO
11	Y	97	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/210 (79%)	166 (100%)	0	100	100
1	O	166/210 (79%)	166 (100%)	0	100	100
2	B	177/191 (93%)	170 (96%)	7 (4%)	27	56
2	P	177/191 (93%)	170 (96%)	7 (4%)	27	56
3	C	199/221 (90%)	197 (99%)	2 (1%)	73	84
3	Q	199/221 (90%)	197 (99%)	2 (1%)	73	84
4	D	179/211 (85%)	177 (99%)	2 (1%)	70	83
4	R	179/211 (85%)	177 (99%)	2 (1%)	70	83
5	E	181/203 (89%)	180 (99%)	1 (1%)	84	91
5	S	181/203 (89%)	180 (99%)	1 (1%)	84	91
6	F	166/224 (74%)	166 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	166/224 (74%)	166 (100%)	0	100	100
7	G	170/212 (80%)	170 (100%)	0	100	100
7	U	170/212 (80%)	170 (100%)	0	100	100
8	H	142/159 (89%)	140 (99%)	2 (1%)	62	79
8	V	142/159 (89%)	140 (99%)	2 (1%)	62	79
9	I	162/195 (83%)	162 (100%)	0	100	100
9	W	162/195 (83%)	162 (100%)	0	100	100
10	J	149/173 (86%)	149 (100%)	0	100	100
10	X	149/173 (86%)	149 (100%)	0	100	100
11	K	160/171 (94%)	159 (99%)	1 (1%)	84	91
11	Y	160/171 (94%)	159 (99%)	1 (1%)	84	91
12	L	148/159 (93%)	148 (100%)	0	100	100
12	Z	148/159 (93%)	148 (100%)	0	100	100
13	M	155/178 (87%)	153 (99%)	2 (1%)	65	81
13	a	155/178 (87%)	153 (99%)	2 (1%)	65	81
14	N	152/181 (84%)	151 (99%)	1 (1%)	81	89
14	b	152/181 (84%)	151 (99%)	1 (1%)	81	89
All	All	4612/5376 (86%)	4576 (99%)	36 (1%)	77	88

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	51	GLN
2	B	70	HIS
2	B	106	THR
2	B	138	TRP
2	B	211	ILE
2	B	212	CYS
2	B	213	ASN
3	C	41	ASP
3	C	151	ASP
4	D	43	LEU
4	D	228	TYR
5	E	63	SER
8	H	9	ASP
8	H	176	LEU

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Mol	Chain	Res	Type
11	K	86	ARG
13	M	15	ILE
13	M	18	GLU
14	N	62	TYR
2	P	51	GLN
2	P	70	HIS
2	P	106	THR
2	P	138	TRP
2	P	211	ILE
2	P	212	CYS
2	P	213	ASN
3	Q	41	ASP
3	Q	151	ASP
4	R	43	LEU
4	R	228	TYR
5	S	63	SER
8	V	9	ASP
8	V	176	LEU
11	Y	86	ARG
13	a	15	ILE
13	a	18	GLU
14	b	62	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	51	GLN
2	B	62	HIS
2	B	87	HIS
2	B	206	ASN
2	B	213	ASN
3	C	84	ASN
5	E	224	GLN
7	G	22	GLN
7	G	105	ASN
8	H	38	HIS
10	J	64	GLN
10	J	161	HIS
10	J	187	HIS
11	K	101	ASN
11	K	186	ASN
11	K	189	HIS

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Mol	Chain	Res	Type
13	M	108	ASN
13	M	152	GLN
14	N	108	ASN
2	P	51	GLN
2	P	62	HIS
2	P	87	HIS
2	P	168	ASN
2	P	206	ASN
2	P	213	ASN
3	Q	84	ASN
4	R	146	GLN
4	R	154	HIS
5	S	224	GLN
7	U	22	GLN
7	U	105	ASN
8	V	38	HIS
9	W	80	ASN
10	X	64	GLN
10	X	161	HIS
10	X	187	HIS
11	Y	55	GLN
11	Y	101	ASN
11	Y	186	ASN
11	Y	189	HIS
13	a	108	ASN
13	a	152	GLN
14	b	108	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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
15	KNM	I	300	9	29,29,68	1.74	2 (6%)	36,39,91	1.20	2 (5%)
15	KNM	H	300	8	30,30,68	1.76	2 (6%)	39,41,91	0.94	2 (5%)
15	KNM	W	300	9	29,29,68	1.73	2 (6%)	36,39,91	1.20	2 (5%)
15	KNM	Z	300	12	30,30,68	1.75	2 (6%)	39,41,91	0.91	2 (5%)
15	KNM	V	300	8	30,30,68	1.76	2 (6%)	39,41,91	0.94	2 (5%)
15	KNM	L	300	12	30,30,68	1.75	2 (6%)	39,41,91	0.92	2 (5%)

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
15	KNM	I	300	9	-	20/37/37/98	-
15	KNM	H	300	8	-	27/38/38/98	-
15	KNM	W	300	9	-	20/37/37/98	-
15	KNM	Z	300	12	-	14/38/38/98	-
15	KNM	V	300	8	-	27/38/38/98	-
15	KNM	L	300	12	-	14/38/38/98	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	300	KNM	C16-S1	-9.19	1.66	1.78
15	V	300	KNM	C16-S1	-9.19	1.66	1.78
15	L	300	KNM	C16-S1	-8.97	1.66	1.78
15	Z	300	KNM	C16-S1	-8.95	1.66	1.78
15	I	300	KNM	C16-S1	-8.66	1.66	1.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	W	300	KNM	C16-S1	-8.60	1.67	1.78
15	L	300	KNM	C22-S1	-2.39	1.66	1.75
15	Z	300	KNM	C22-S1	-2.39	1.66	1.75
15	H	300	KNM	C22-S1	-2.37	1.66	1.75
15	V	300	KNM	C22-S1	-2.37	1.66	1.75
15	W	300	KNM	C22-S1	-2.35	1.66	1.75
15	I	300	KNM	C22-S1	-2.33	1.66	1.75

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	300	KNM	C1-N1-C3	4.42	122.36	114.16
15	I	300	KNM	C1-N1-C3	4.41	122.34	114.16
15	W	300	KNM	O5-S1-O4	-3.83	108.90	117.09
15	I	300	KNM	O5-S1-O4	-3.83	108.90	117.09
15	H	300	KNM	O5-S1-O4	-3.60	109.40	117.09
15	V	300	KNM	O5-S1-O4	-3.60	109.40	117.09
15	L	300	KNM	O5-S1-O4	-3.59	109.42	117.09
15	Z	300	KNM	O5-S1-O4	-3.59	109.42	117.09
15	L	300	KNM	C15-N3-C14	-2.41	119.36	123.20
15	Z	300	KNM	C15-N3-C14	-2.37	119.42	123.20
15	H	300	KNM	O5-S1-C16	2.35	109.99	108.34
15	V	300	KNM	O5-S1-C16	2.35	109.99	108.34

There are no chirality outliers.

All (122) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	300	KNM	O1-C1-N1-C3
15	H	300	KNM	C2-C1-N1-C3
15	H	300	KNM	C3-C8-N2-C9
15	H	300	KNM	C17-C15-N3-C14
15	H	300	KNM	C21-C16-S1-O4
15	H	300	KNM	C21-C16-S1-O5
15	I	300	KNM	C2-C1-N1-C3
15	I	300	KNM	C4-C3-N1-C1
15	I	300	KNM	C8-C3-N1-C1
15	I	300	KNM	C3-C8-N2-C9
15	I	300	KNM	O3-C8-N2-C9
15	I	300	KNM	C21-C16-S1-O4
15	I	300	KNM	C21-C16-S1-O5
15	I	300	KNM	C21-C16-S1-C22

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Mol	Chain	Res	Type	Atoms
15	L	300	KNM	C11-C10-C9-N2
15	L	300	KNM	C21-C16-S1-O5
15	V	300	KNM	O1-C1-N1-C3
15	V	300	KNM	C2-C1-N1-C3
15	V	300	KNM	C3-C8-N2-C9
15	V	300	KNM	C17-C15-N3-C14
15	V	300	KNM	C21-C16-S1-O4
15	V	300	KNM	C21-C16-S1-O5
15	W	300	KNM	C2-C1-N1-C3
15	W	300	KNM	C4-C3-N1-C1
15	W	300	KNM	C8-C3-N1-C1
15	W	300	KNM	C3-C8-N2-C9
15	W	300	KNM	O3-C8-N2-C9
15	W	300	KNM	C21-C16-S1-O4
15	W	300	KNM	C21-C16-S1-O5
15	W	300	KNM	C21-C16-S1-C22
15	Z	300	KNM	C11-C10-C9-N2
15	Z	300	KNM	C21-C16-S1-O5
15	H	300	KNM	O3-C8-N2-C9
15	V	300	KNM	O3-C8-N2-C9
15	I	300	KNM	C11-C10-C9-C14
15	W	300	KNM	C11-C10-C9-C14
15	I	300	KNM	C11-C10-C9-N2
15	W	300	KNM	C11-C10-C9-N2
15	H	300	KNM	S1-C16-C21-C15
15	V	300	KNM	S1-C16-C21-C15
15	H	300	KNM	C11-C10-C9-N2
15	V	300	KNM	C11-C10-C9-N2
15	H	300	KNM	C11-C10-C9-C14
15	V	300	KNM	C11-C10-C9-C14
15	H	300	KNM	C4-C3-C8-O3
15	V	300	KNM	C4-C3-C8-O3
15	H	300	KNM	C4-C3-C8-N2
15	V	300	KNM	C4-C3-C8-N2
15	H	300	KNM	N3-C15-C21-C16
15	V	300	KNM	N3-C15-C21-C16
15	H	300	KNM	O2-C14-C9-C10
15	V	300	KNM	O2-C14-C9-C10
15	H	300	KNM	N3-C14-C9-C10
15	V	300	KNM	N3-C14-C9-C10
15	H	300	KNM	C3-C4-C5-C7
15	H	300	KNM	C9-C10-C11-C13

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Mol	Chain	Res	Type	Atoms
15	V	300	KNM	C3-C4-C5-C7
15	V	300	KNM	C9-C10-C11-C13
15	H	300	KNM	C9-C10-C11-C12
15	V	300	KNM	C9-C10-C11-C12
15	L	300	KNM	C3-C4-C5-C7
15	Z	300	KNM	C3-C4-C5-C7
15	I	300	KNM	C3-C4-C5-C6
15	W	300	KNM	C3-C4-C5-C6
15	L	300	KNM	O2-C14-N3-C15
15	Z	300	KNM	O2-C14-N3-C15
15	H	300	KNM	C3-C4-C5-C6
15	V	300	KNM	C3-C4-C5-C6
15	H	300	KNM	C10-C9-N2-C8
15	V	300	KNM	C10-C9-N2-C8
15	L	300	KNM	C3-C4-C5-C6
15	Z	300	KNM	C3-C4-C5-C6
15	H	300	KNM	C17-C15-C21-C16
15	V	300	KNM	C17-C15-C21-C16
15	I	300	KNM	C3-C4-C5-C7
15	W	300	KNM	C3-C4-C5-C7
15	L	300	KNM	C9-C14-N3-C15
15	Z	300	KNM	C9-C14-N3-C15
15	L	300	KNM	S1-C16-C21-C15
15	Z	300	KNM	S1-C16-C21-C15
15	I	300	KNM	O2-C14-N3-C15
15	W	300	KNM	O2-C14-N3-C15
15	H	300	KNM	C21-C15-C17-C18
15	V	300	KNM	C21-C15-C17-C18
15	H	300	KNM	N3-C15-C17-C18
15	V	300	KNM	N3-C15-C17-C18
15	L	300	KNM	C2-C1-N1-C3
15	I	300	KNM	C9-C14-N3-C15
15	W	300	KNM	C9-C14-N3-C15
15	Z	300	KNM	C2-C1-N1-C3
15	H	300	KNM	C14-C9-N2-C8
15	V	300	KNM	C14-C9-N2-C8
15	W	300	KNM	O2-C14-C9-N2
15	I	300	KNM	O2-C14-C9-N2
15	I	300	KNM	S1-C16-C21-C15
15	W	300	KNM	S1-C16-C21-C15
15	I	300	KNM	N3-C14-C9-N2
15	W	300	KNM	N3-C14-C9-N2

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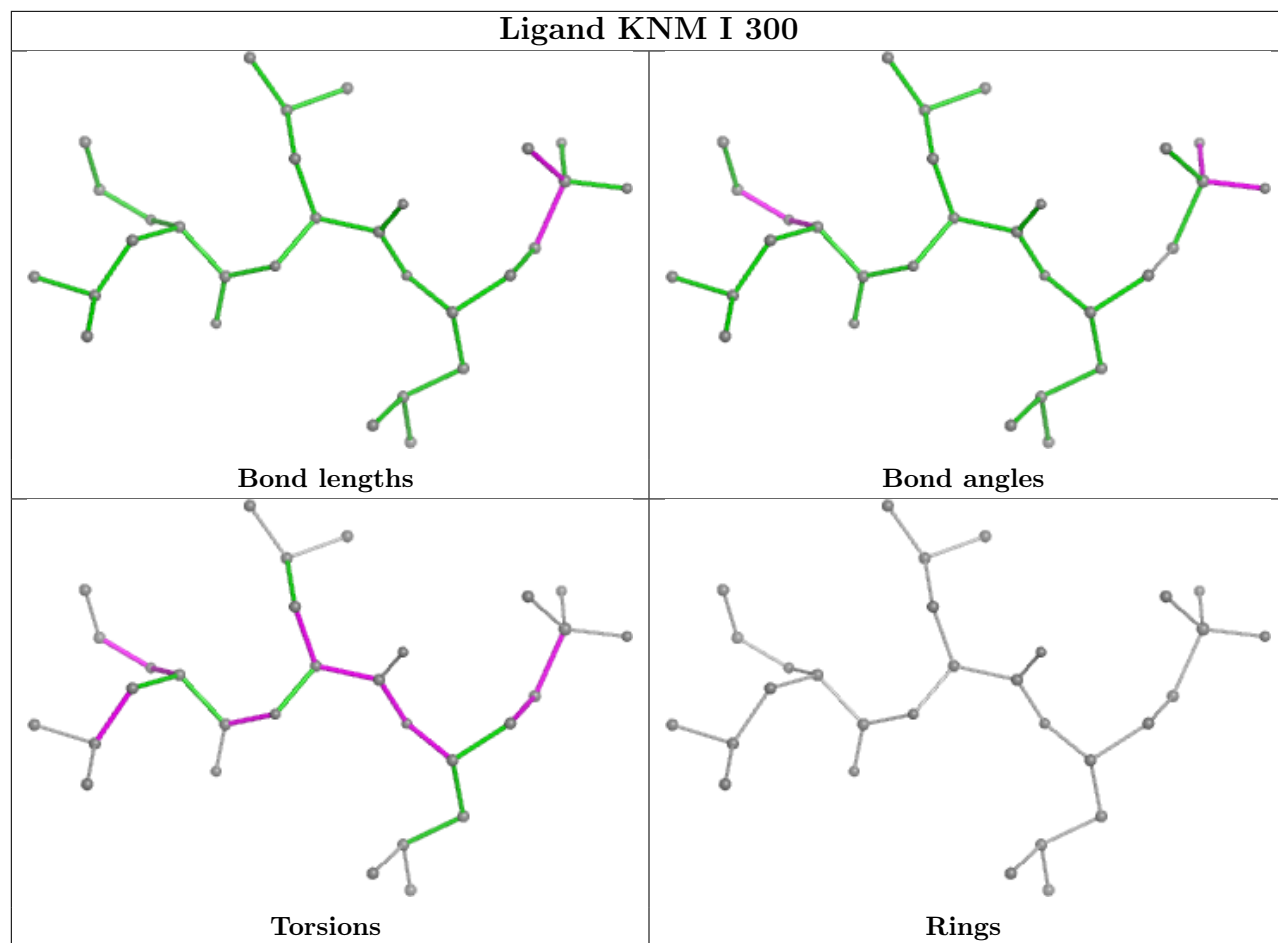
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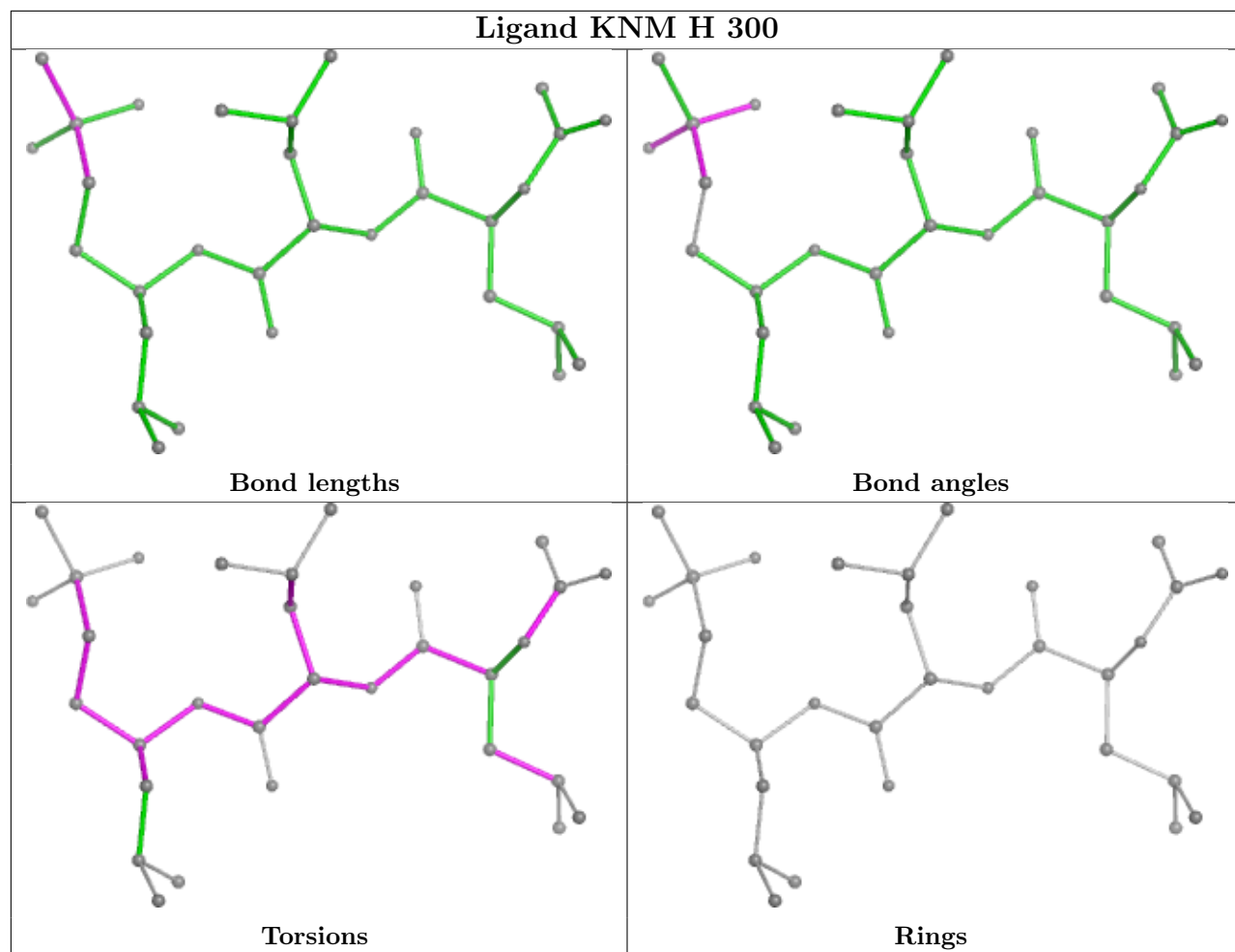
Mol	Chain	Res	Type	Atoms
15	L	300	KNM	O1-C1-N1-C3
15	Z	300	KNM	O1-C1-N1-C3
15	H	300	KNM	C21-C15-N3-C14
15	V	300	KNM	C21-C15-N3-C14
15	H	300	KNM	C21-C16-S1-C22
15	V	300	KNM	C21-C16-S1-C22
15	L	300	KNM	C15-C17-C18-C19
15	Z	300	KNM	C15-C17-C18-C19
15	L	300	KNM	C11-C10-C9-C14
15	Z	300	KNM	C11-C10-C9-C14
15	I	300	KNM	C17-C15-N3-C14
15	W	300	KNM	C17-C15-N3-C14
15	Z	300	KNM	O2-C14-C9-N2
15	L	300	KNM	O2-C14-C9-N2
15	I	300	KNM	O2-C14-C9-C10
15	W	300	KNM	O2-C14-C9-C10
15	H	300	KNM	O2-C14-N3-C15
15	V	300	KNM	O2-C14-N3-C15
15	Z	300	KNM	C9-C10-C11-C12
15	L	300	KNM	C9-C10-C11-C12
15	L	300	KNM	N3-C14-C9-N2
15	Z	300	KNM	N3-C14-C9-N2
15	I	300	KNM	C21-C15-N3-C14
15	W	300	KNM	C21-C15-N3-C14

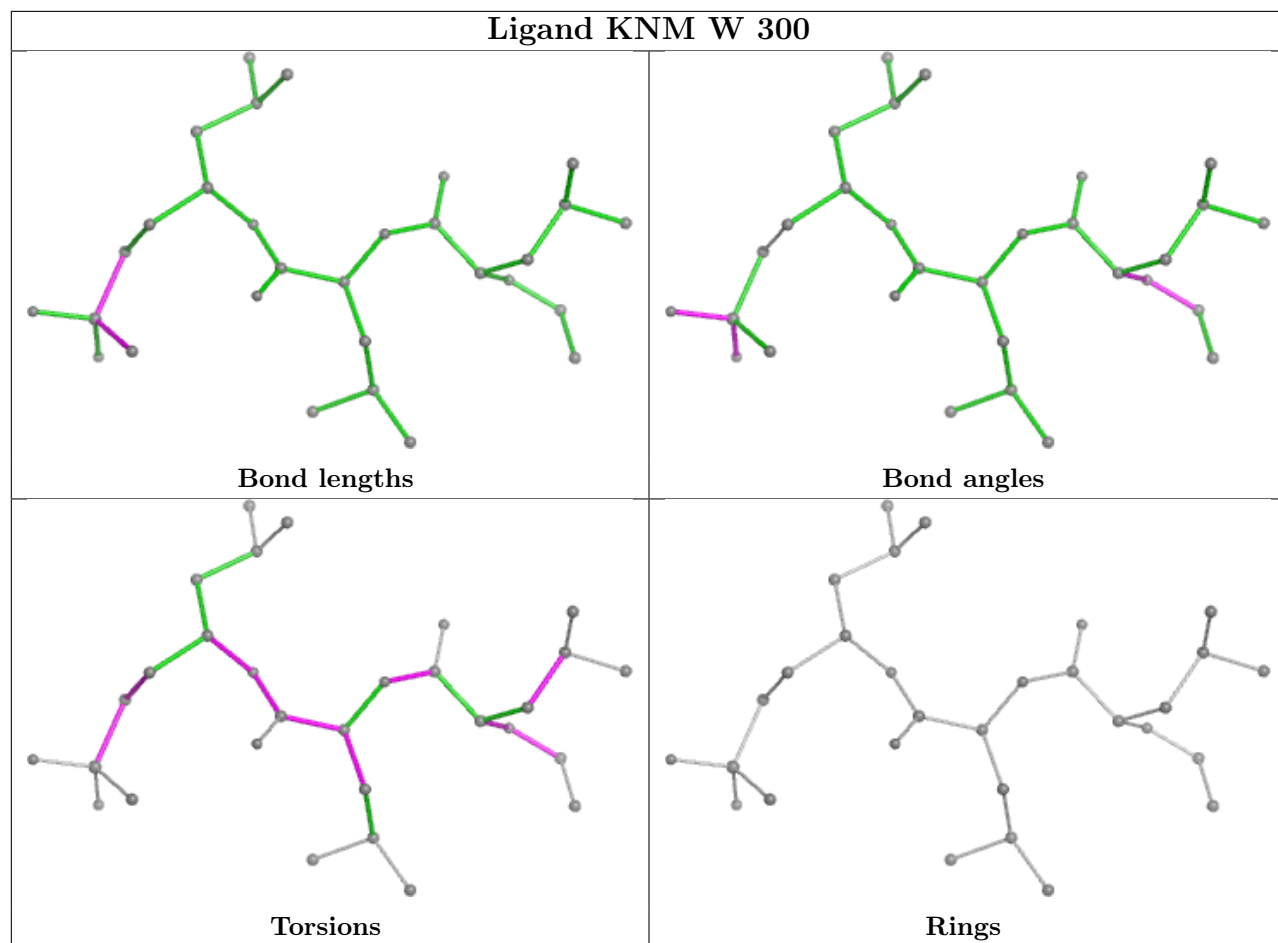
There are no ring outliers.

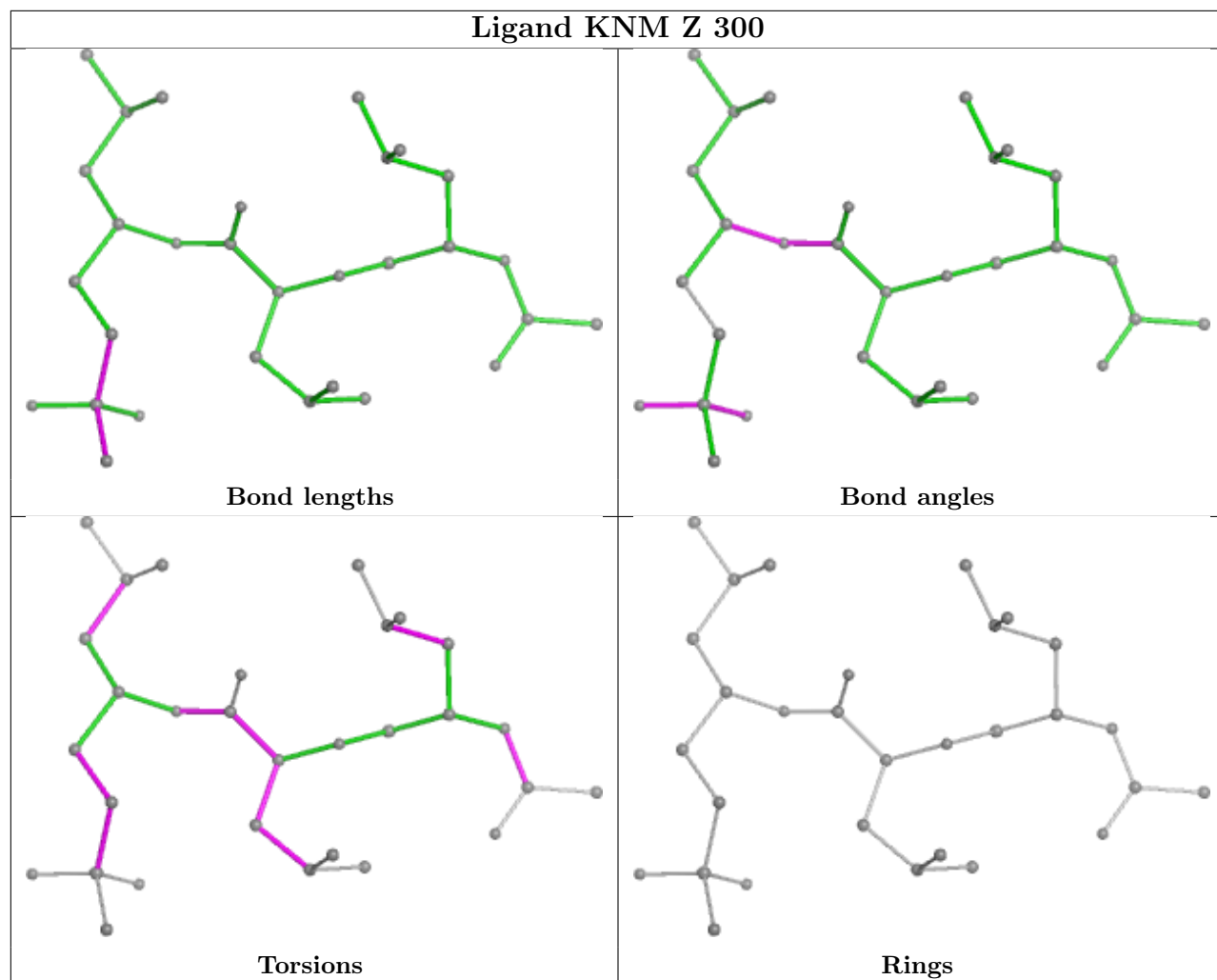
No monomer is involved in short contacts.

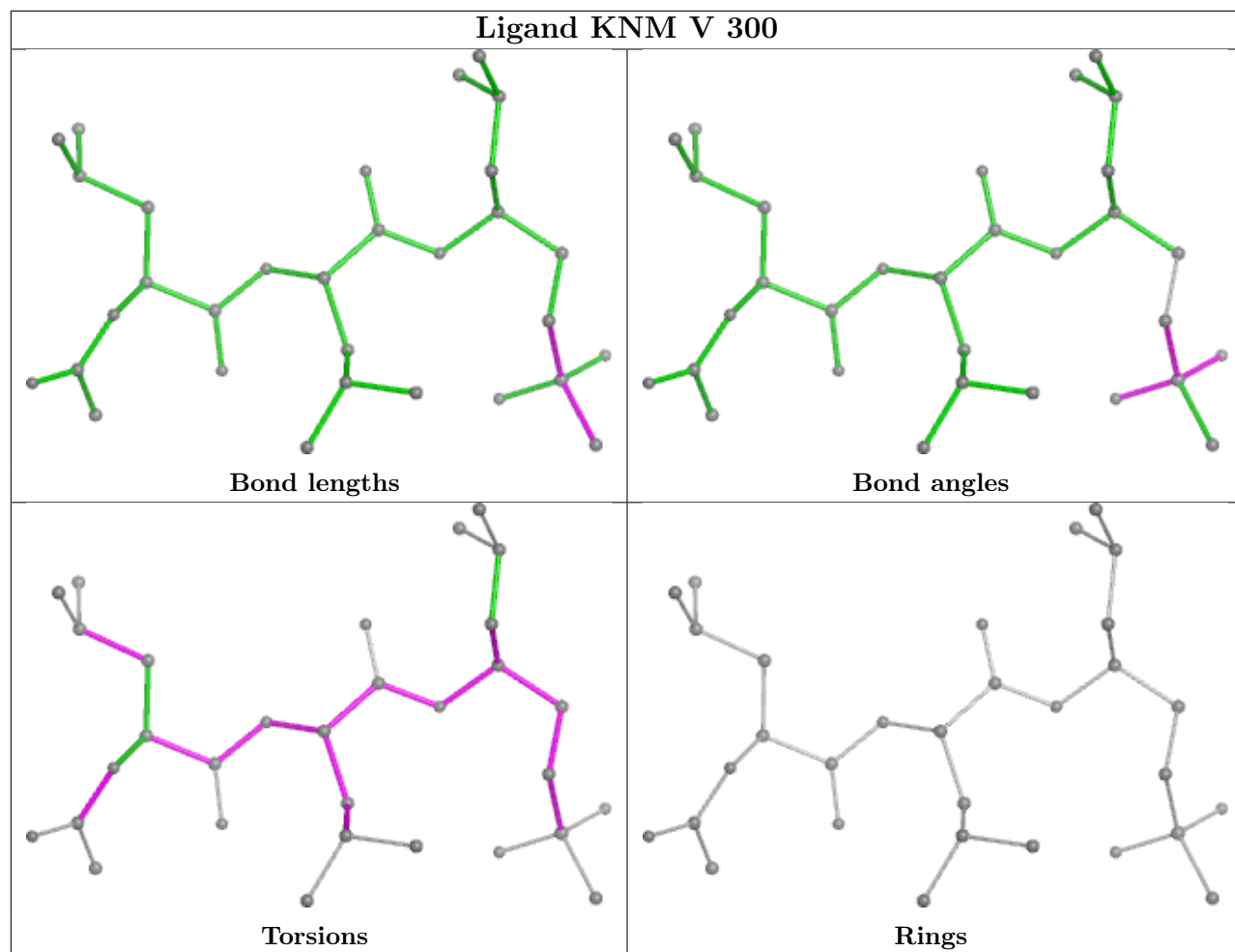
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

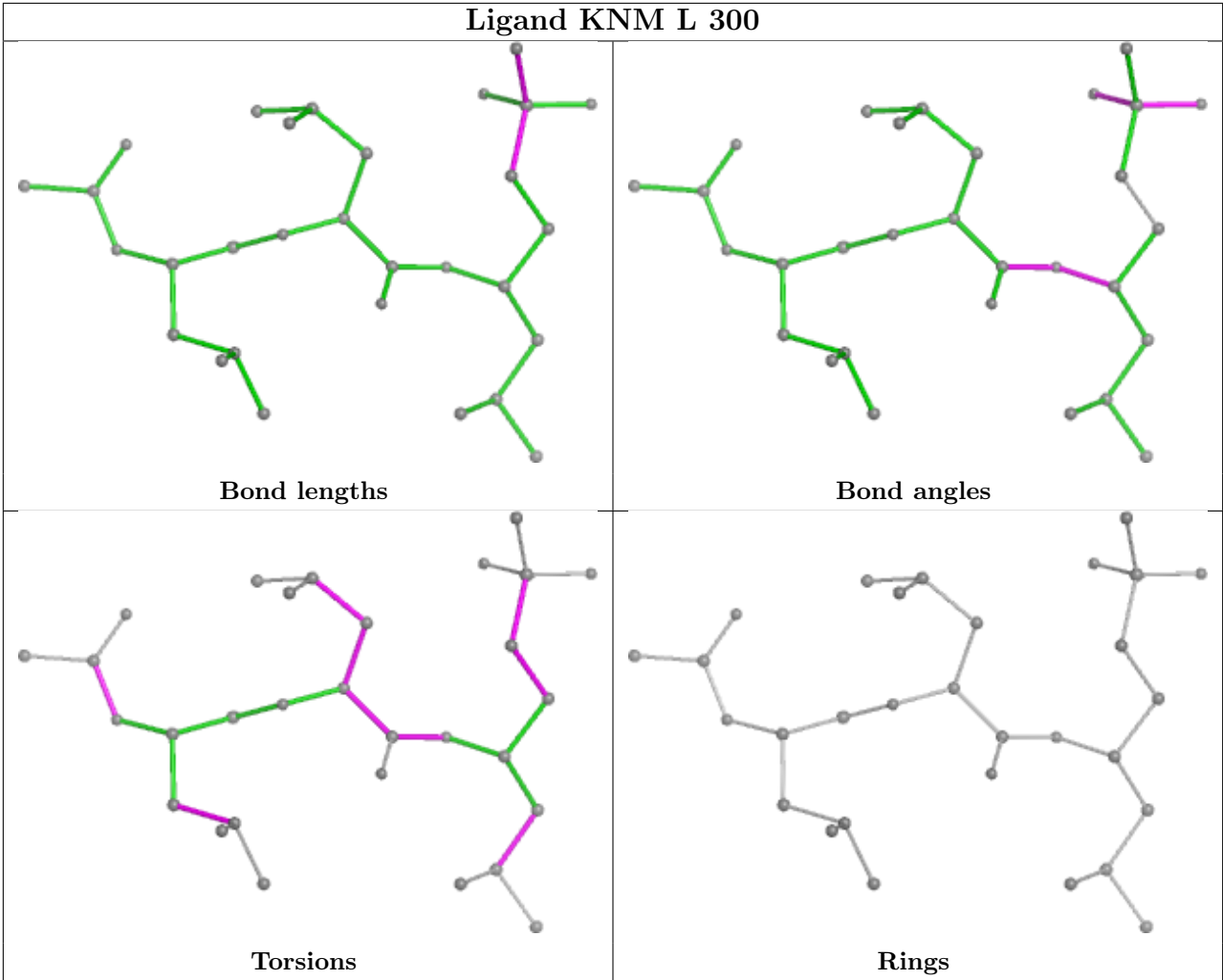












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	1
8	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	1:THR	C	2:THR	N	1.78
1	V	1:THR	C	2:THR	N	1.78

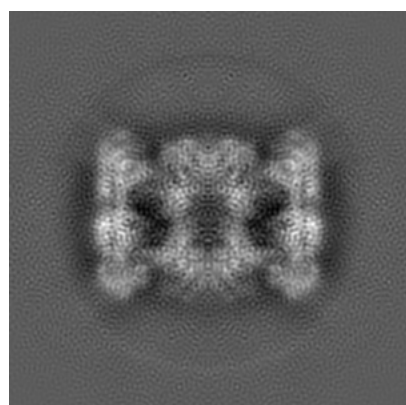
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2981. These allow visual inspection of the internal detail of the map and identification of artifacts.

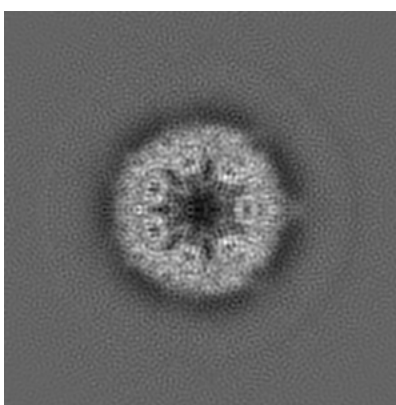
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

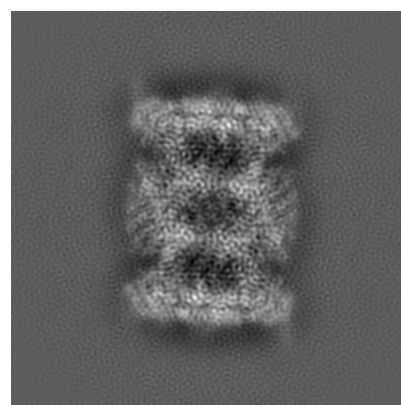
6.1.1 Primary map



X



Y

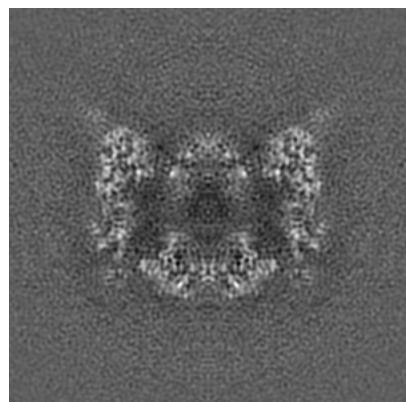


Z

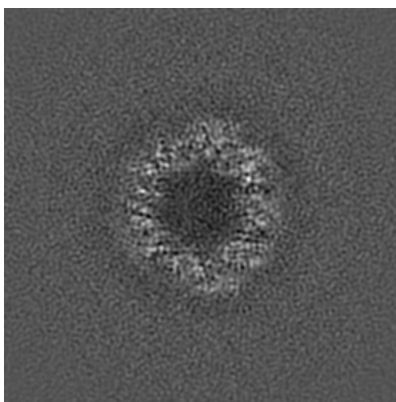
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

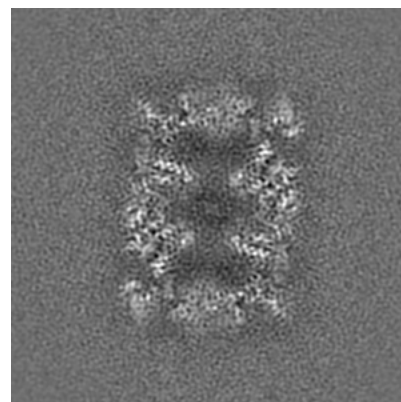
6.2.1 Primary map



X Index: 128



Y Index: 128

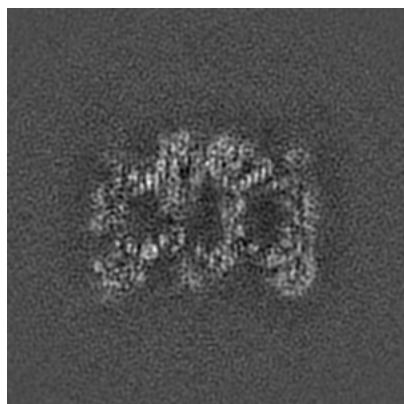


Z Index: 128

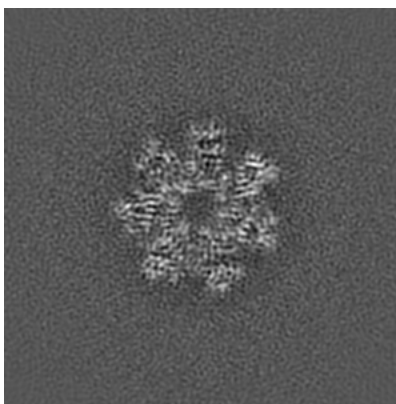
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

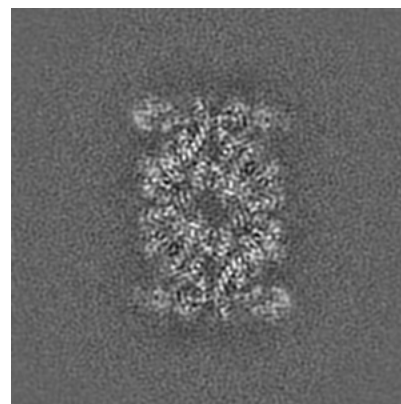
6.3.1 Primary map



X Index: 146



Y Index: 145

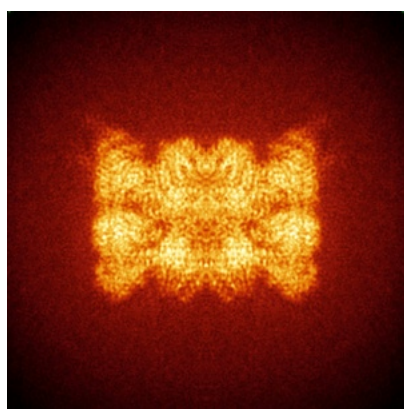


Z Index: 100

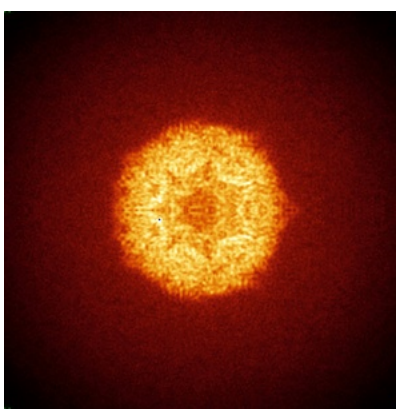
The images above show the largest variance slices of the map in three orthogonal directions.

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

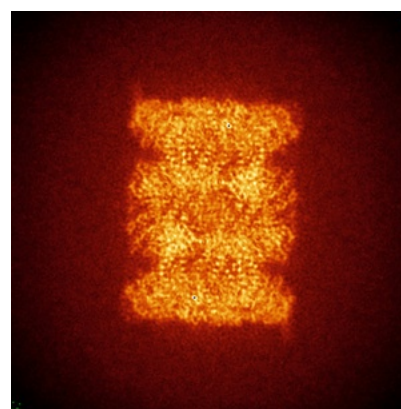
6.4.1 Primary map



X



Y

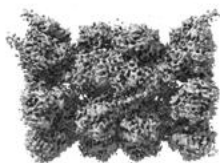


Z

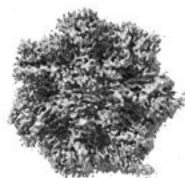
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

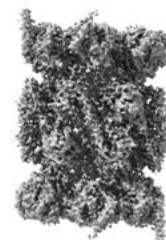
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

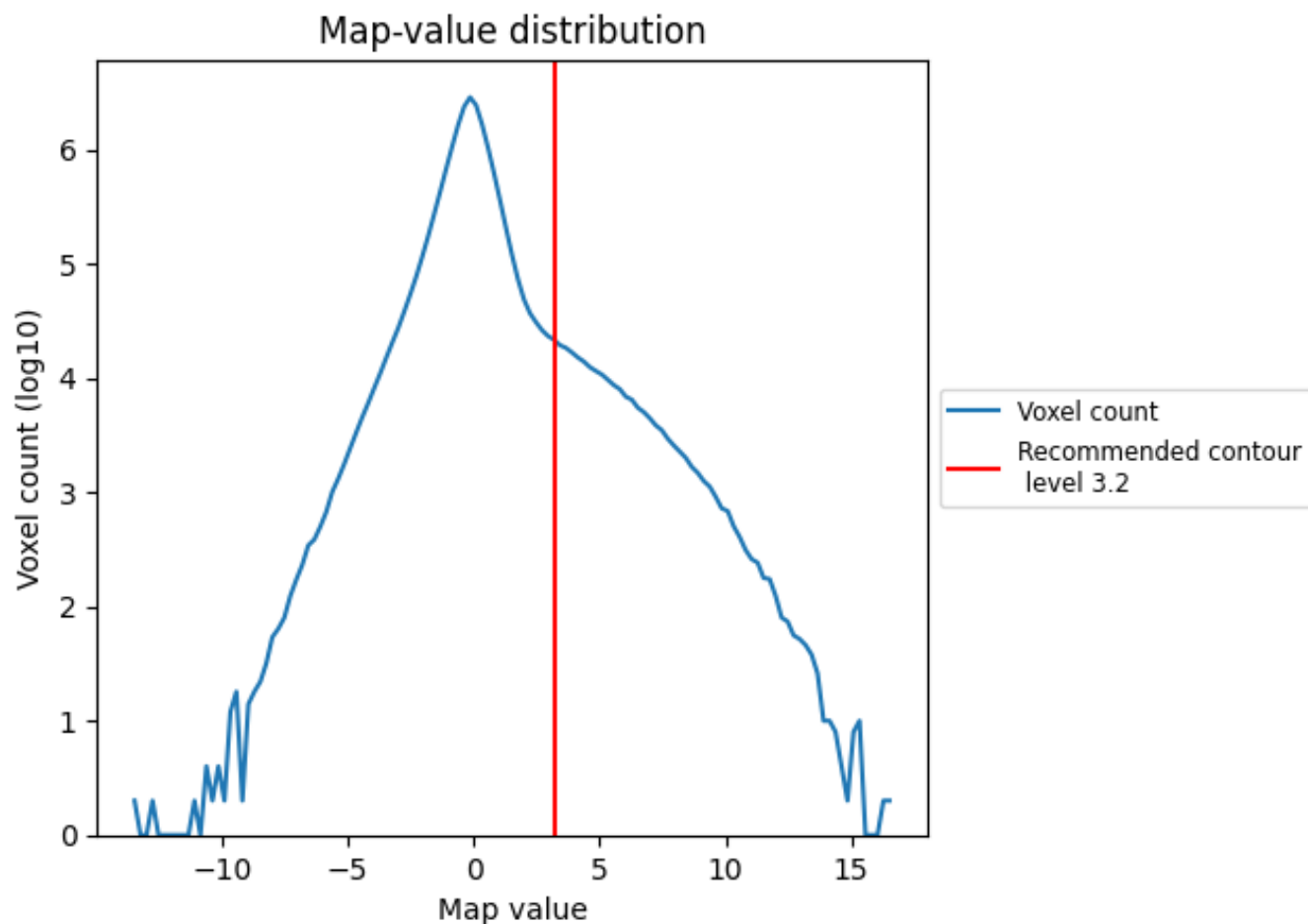
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

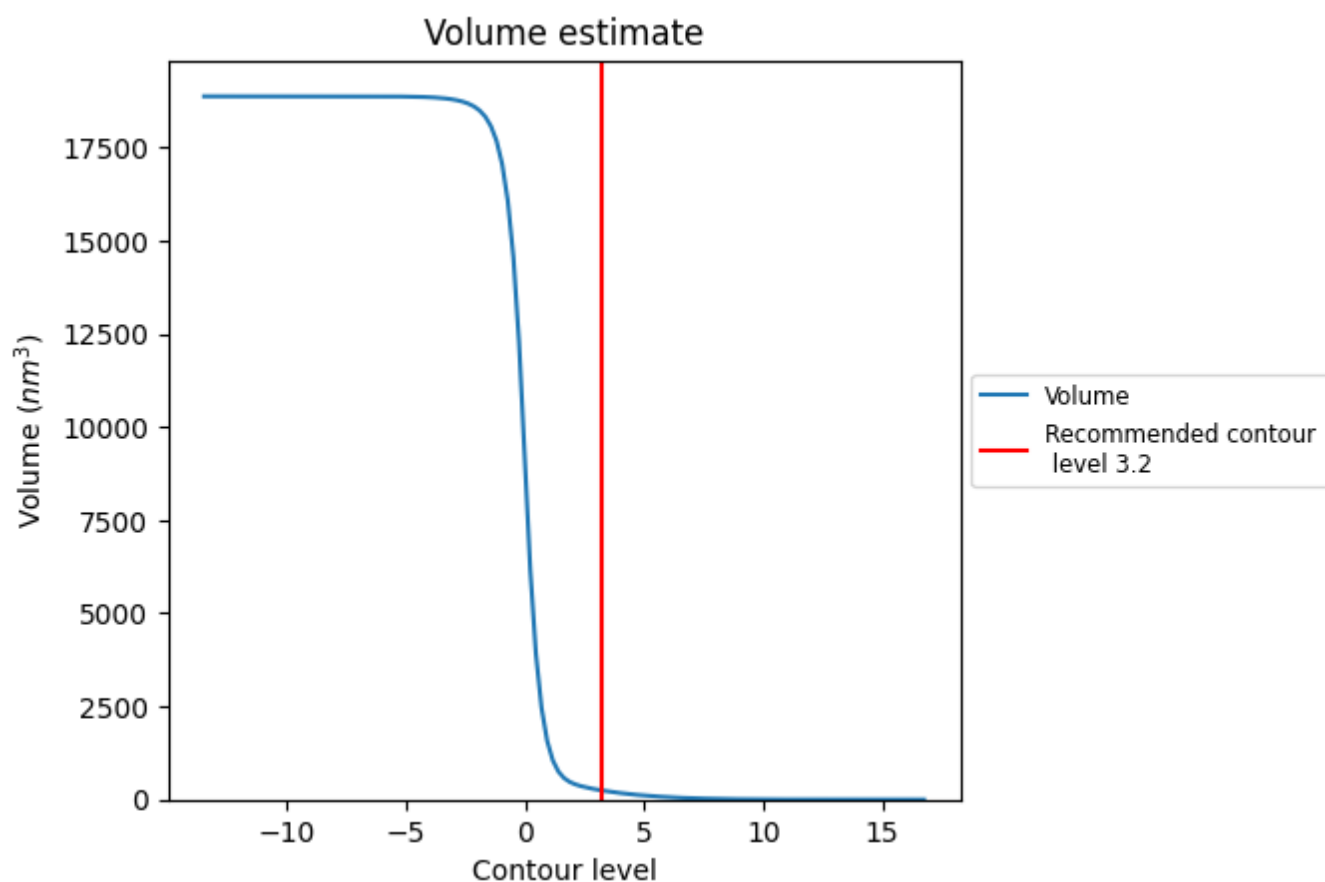
This section contains the results of statistical analysis of the map.

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.

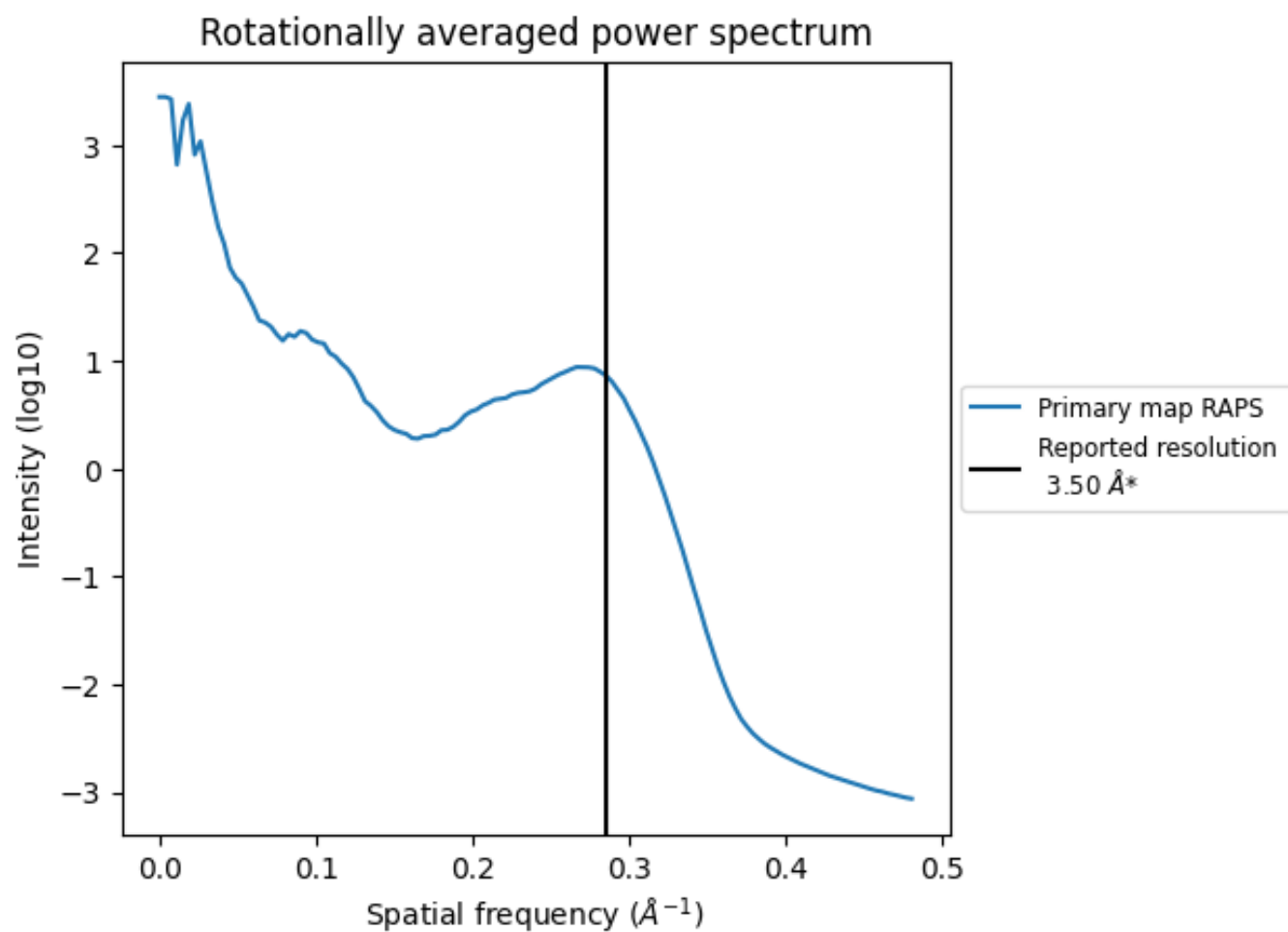
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 249 nm³; this corresponds to an approximate mass of 225 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

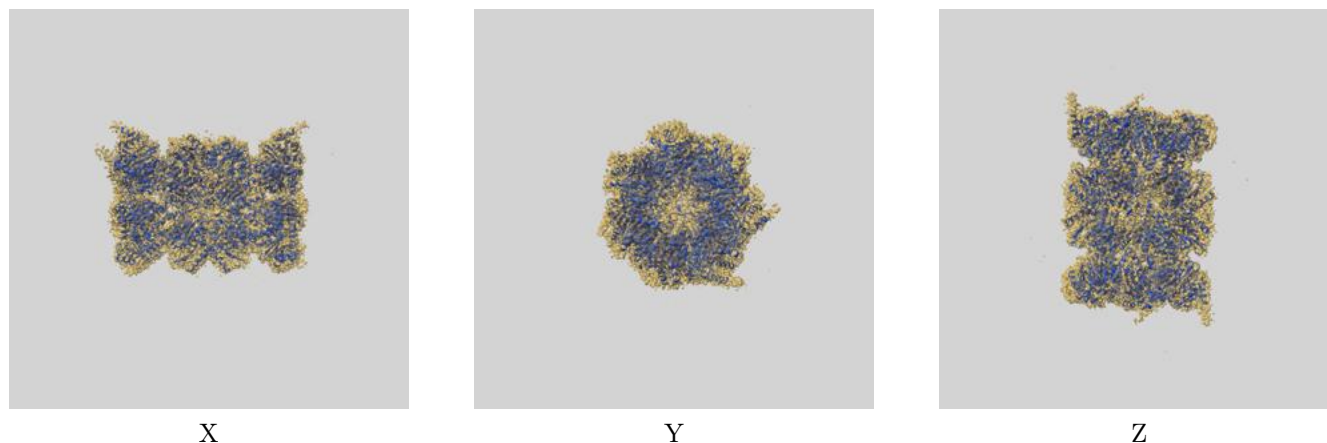
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

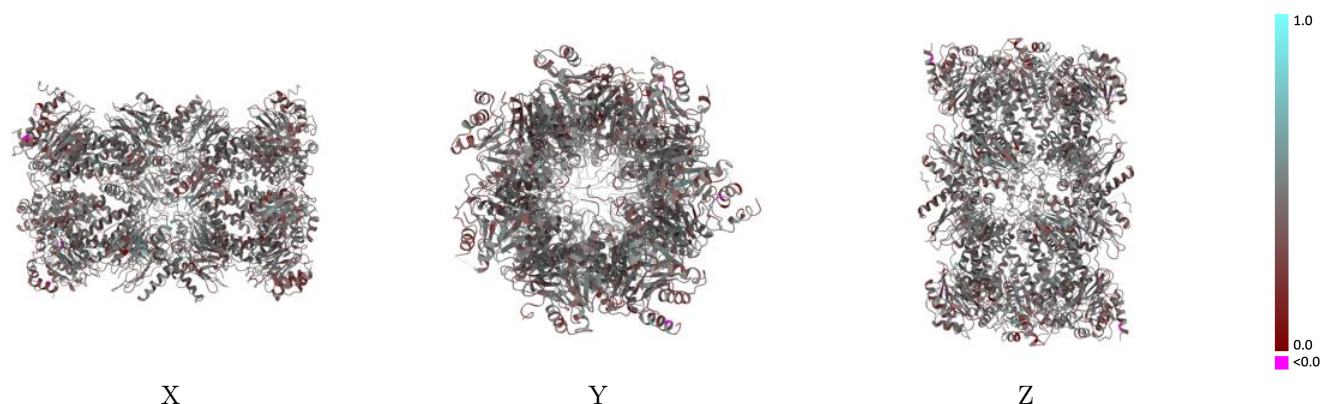
This section contains information regarding the fit between EMDB map EMD-2981 and PDB model 5A0Q. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



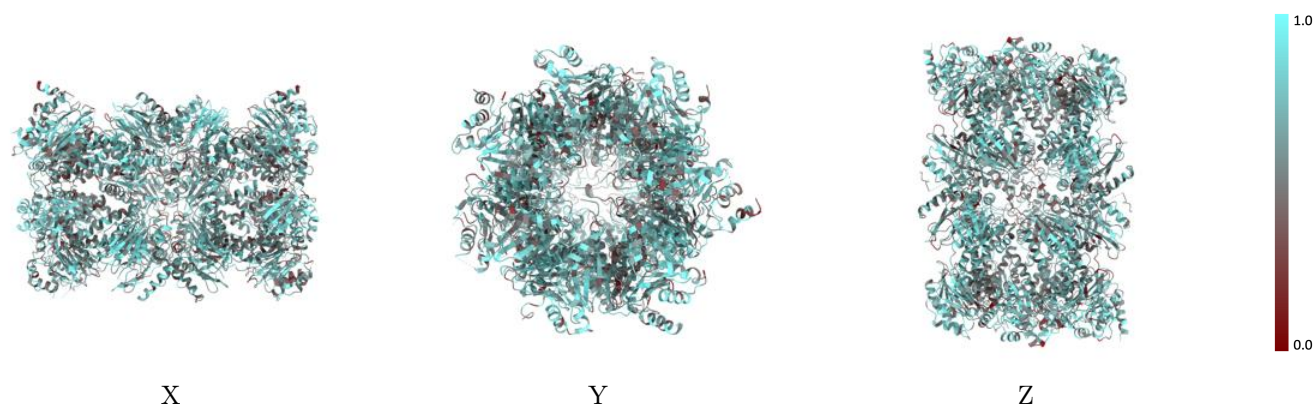
The images above show the 3D surface view of the map at the recommended contour level 3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



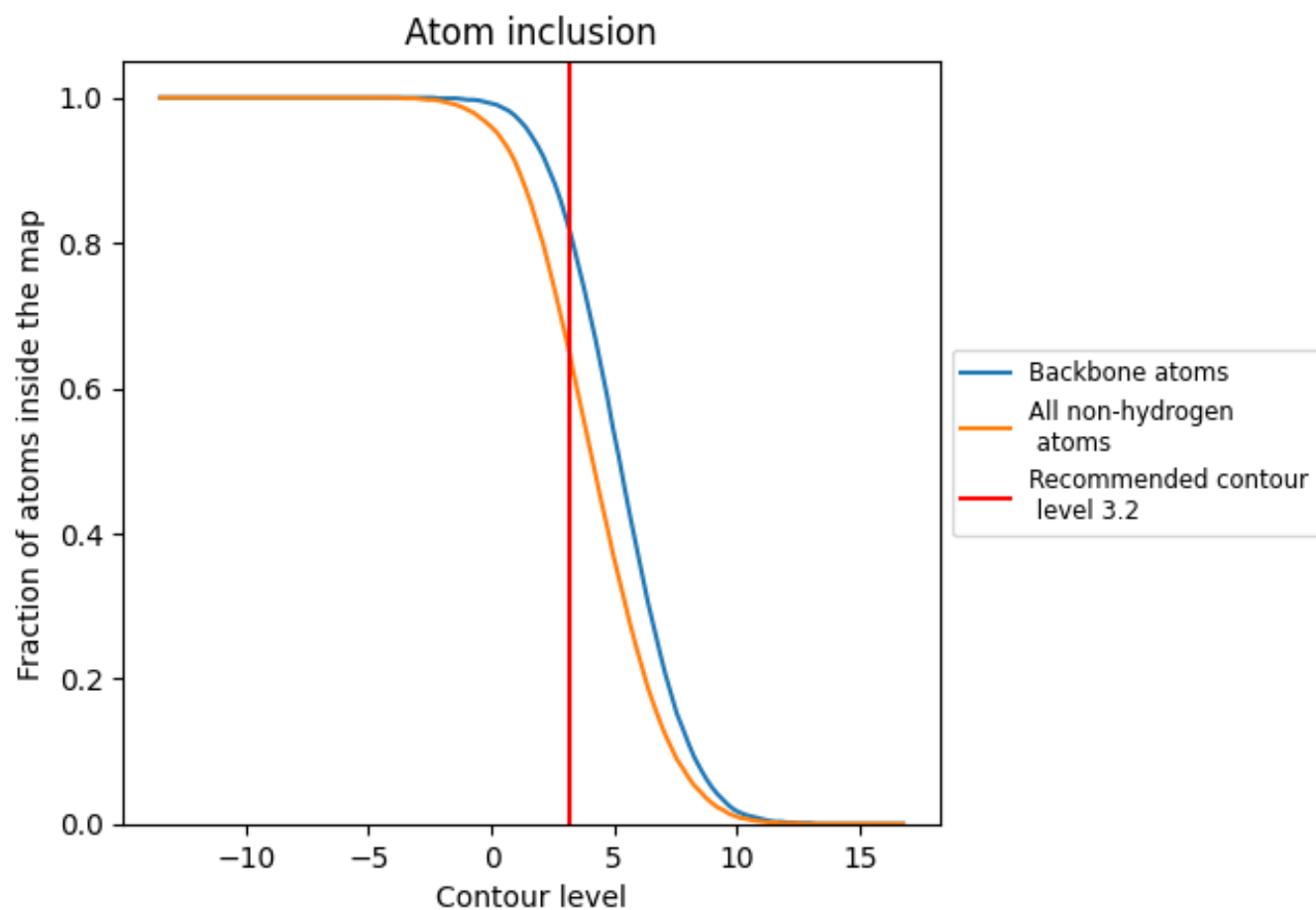
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.2).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 64% 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 (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6450	 0.4260
A	 0.6340	 0.4310
B	 0.6690	 0.4240
C	 0.6450	 0.4180
D	 0.6260	 0.4200
E	 0.6460	 0.4120
F	 0.6400	 0.4210
G	 0.6330	 0.4180
H	 0.6440	 0.4290
I	 0.6710	 0.4400
J	 0.6060	 0.4300
K	 0.6340	 0.4310
L	 0.6980	 0.4420
M	 0.6280	 0.4300
N	 0.6470	 0.4250
O	 0.6350	 0.4290
P	 0.6690	 0.4240
Q	 0.6440	 0.4210
R	 0.6260	 0.4170
S	 0.6460	 0.4120
T	 0.6400	 0.4250
U	 0.6330	 0.4150
V	 0.6430	 0.4320
W	 0.6700	 0.4400
X	 0.6060	 0.4290
Y	 0.6350	 0.4300
Z	 0.6980	 0.4420
a	 0.6290	 0.4250
b	 0.6460	 0.4270

