



wwPDB EM Validation Summary Report ⓘ

Sep 20, 2025 – 07:26 am BST

PDB ID : 9IHF / pdb_00009ihf
EMDB ID : EMD-52870
Title : Nucleosome core particle bound by one monomer and one dimer of of DTT-reduced native myeloperoxidase
Authors : Raisch, T.; Burn, G.L.; Tacke, S.; Winkler, M.; Prumbaum, D.; Thee, S.; Zychlinsky, A.; Raunser, S.
Deposited on : 2025-02-21
Resolution : 3.16 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

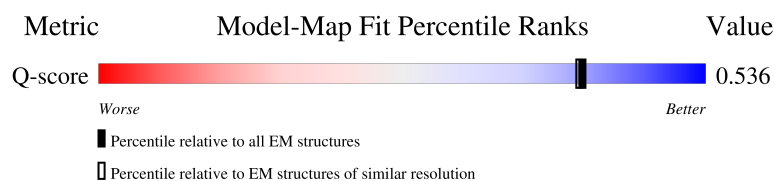
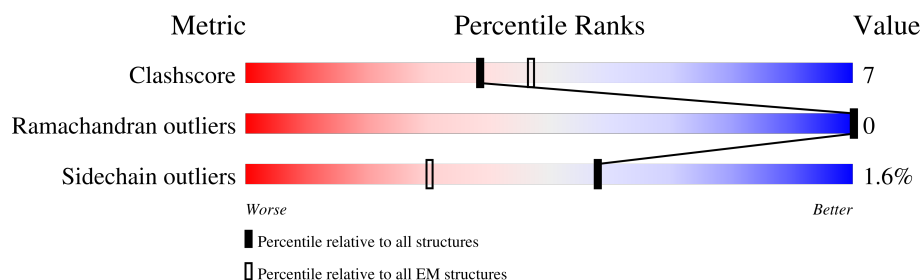
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14474 (2.66 - 3.66)

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	99	
1	E	99	
2	B	87	
2	F	87	

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Mol	Chain	Length	Quality of chain
3	C	111	
3	G	111	
4	D	96	
4	H	96	
5	I	147	
6	J	147	
7	K	108	
7	M	108	
7	O	108	
8	L	466	
8	N	466	
8	P	466	
9	Q	6	
10	R	5	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 25213 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	96	Total	C	N	O	S	0	0
			790	498	152	137	3		
1	E	95	Total	C	N	O	S	0	0
			784	495	150	136	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	conflict	UNP P84233
E	102	ALA	GLY	conflict	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	79	Total	C	N	O	S	0	0
			633	399	124	109	1		
2	F	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	108	Total	C	N	O	0	0
			834	525	165	144		
3	G	107	Total	C	N	O	0	0
			825	519	163	143		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	conflict	UNP P06897
G	99	ARG	GLY	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	94	Total	C	N	O	S	0	0
			735	463	132	138	2		
4	H	94	Total	C	N	O	S	0	0
			735	463	132	138	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	conflict	UNP P02281
H	29	THR	SER	conflict	UNP P02281

- Molecule 5 is a DNA chain called Widom-601 DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	133	Total	C	N	O	P	0	0
			2743	1298	514	798	133		

- Molecule 6 is a DNA chain called Widom-601 DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	133	Total	C	N	O	P	0	0
			2710	1287	492	798	133		

- Molecule 7 is a protein called Myeloperoxidase light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	100	Total	C	N	O	S	0	0
			806	511	143	148	4		
7	M	100	Total	C	N	O	S	0	0
			806	511	143	148	4		
7	O	100	Total	C	N	O	S	0	0
			806	511	143	148	4		

- Molecule 8 is a protein called Myeloperoxidase light chain.

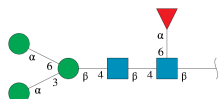
Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	457	Total	C	N	O	S	0	0
			3670	2316	677	652	25		
8	N	457	Total	C	N	O	S	0	0
			3670	2316	677	652	25		

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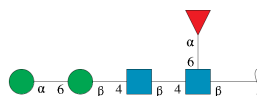
Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	457	Total	C	N	O	S	0	0
			3670	2316	677	652	25		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



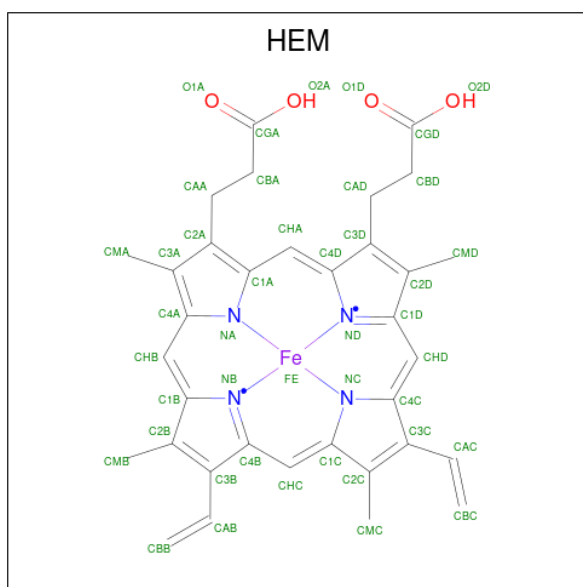
Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
10	R	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					AltConf
11	L	1	Total 43	C 34	Fe 1	N 4	O 4	0
11	N	1	Total 43	C 34	Fe 1	N 4	O 4	0
11	P	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

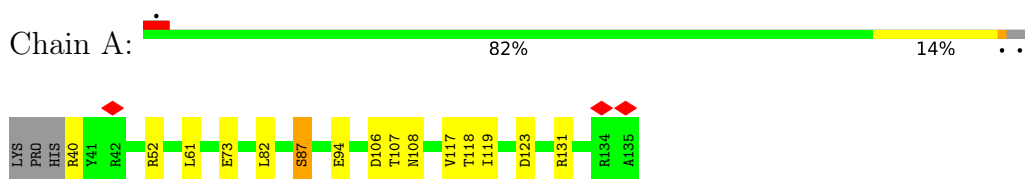


Mol	Chain	Residues	Atoms				AltConf
12	L	1	Total	C	N	O	0
			14	8	1	5	
12	L	1	Total	C	N	O	0
			14	8	1	5	
12	L	1	Total	C	N	O	0
			14	8	1	5	
12	N	1	Total	C	N	O	0
			14	8	1	5	
12	N	1	Total	C	N	O	0
			14	8	1	5	
12	P	1	Total	C	N	O	0
			14	8	1	5	
12	P	1	Total	C	N	O	0
			14	8	1	5	

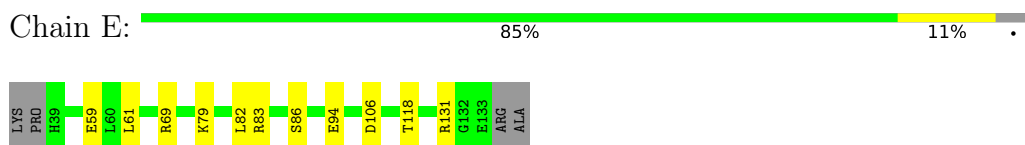
3 Residue-property plots [i](#)

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.

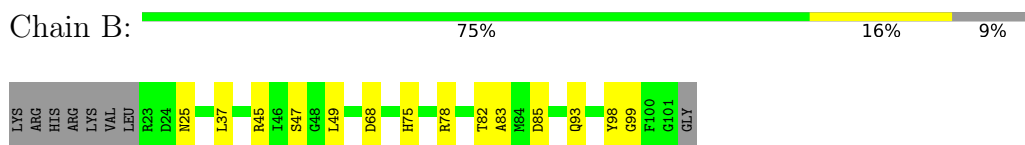
- Molecule 1: Histone H3.2



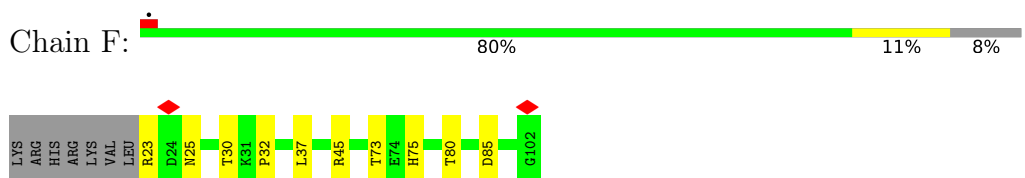
- Molecule 1: Histone H3.2



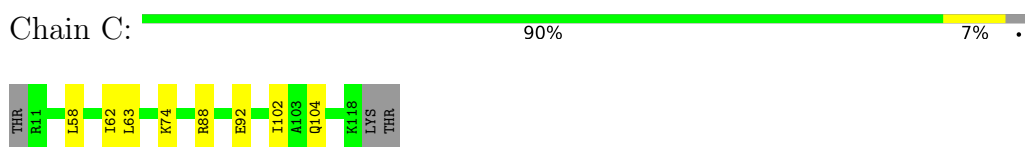
- Molecule 2: Histone H4



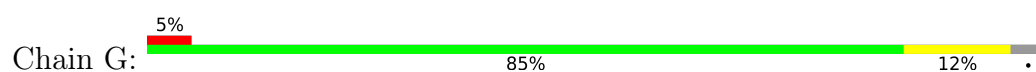
- Molecule 2: Histone H4



- Molecule 3: Histone H2A type 1



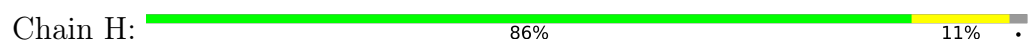
- Molecule 3: Histone H2A type 1



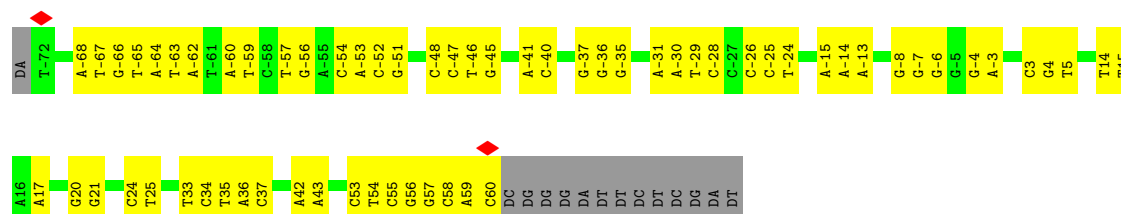
- Molecule 4: Histone H2B 1.1



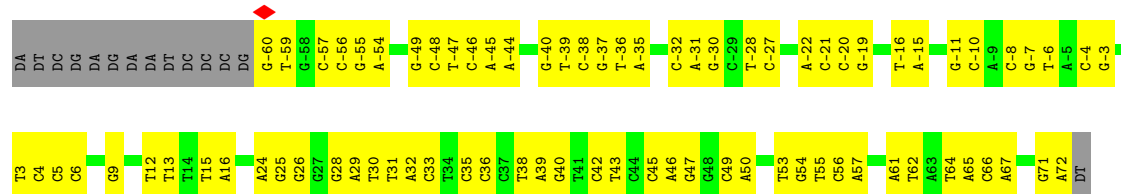
- Molecule 4: Histone H2B 1.1



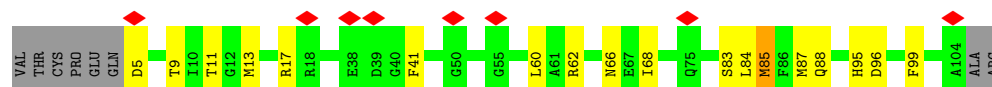
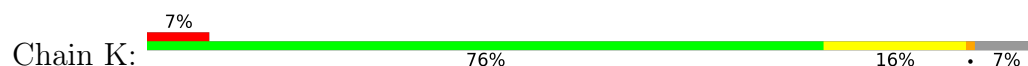
- Molecule 5: Widom-601 DNA (145-MER)




- Molecule 6: Widom-601 DNA (145-MER)



- Molecule 7: Myeloperoxidase light chain




- Molecule 7: Myeloperoxidase light chain

Chain M:  79% 13% 7%




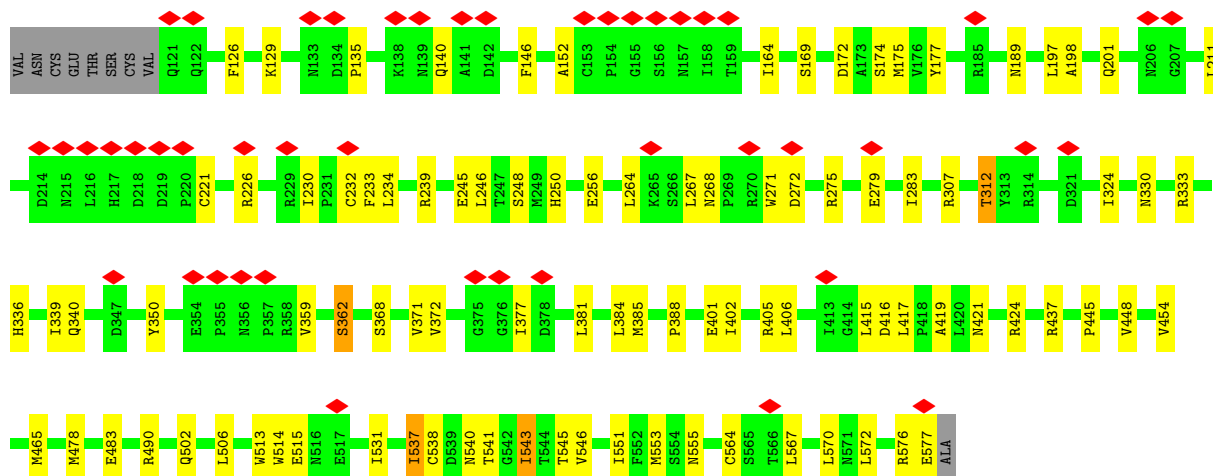
- Molecule 7: Myeloperoxidase light chain

Chain O:  75% 18% 7%




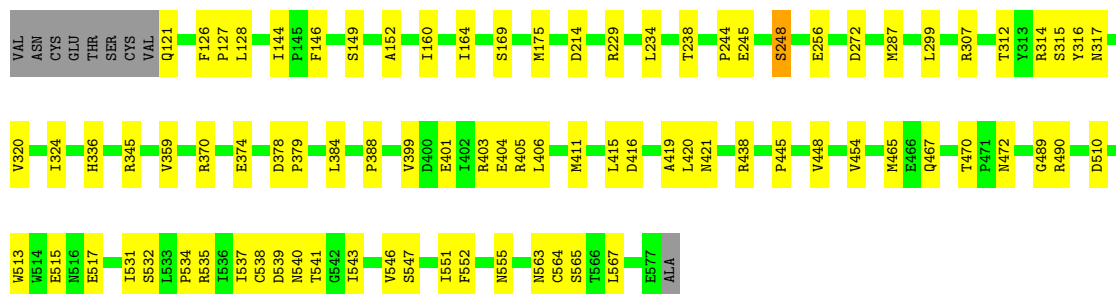
- Molecule 8: Myeloperoxidase light chain

Chain L:  10% 77% 20%




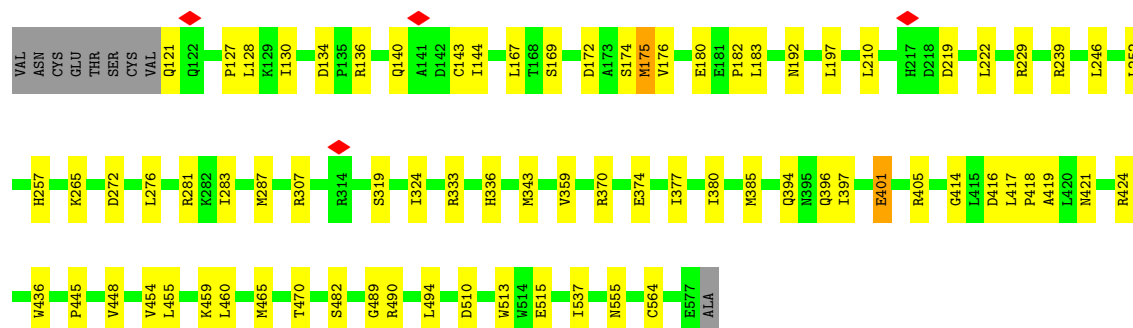
- Molecule 8: Myeloperoxidase light chain

Chain N:  80% 18% 2%



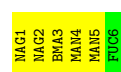
- Molecule 8: Myeloperoxidase light chain

Chain P:  82% 16% 2%



- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 17% 83%



- Molecule 10: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 20% 60% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53312	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70.3	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	42.159	Depositor
Minimum map value	-5.095	Depositor
Average map value	0.342	Depositor
Map value standard deviation	1.208	Depositor
Recommended contour level	5	Depositor
Map size (\AA)	272.0, 272.0, 272.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.68, 0.68, 0.68	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, HEM, NAG, FUC

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	0.11	0/800	0.18	0/1073
1	E	0.11	0/795	0.19	0/1067
2	B	0.14	0/640	0.21	0/857
2	F	0.12	0/645	0.20	0/862
3	C	0.12	0/844	0.22	0/1138
3	G	0.10	0/835	0.19	0/1127
4	D	0.12	0/746	0.22	0/1004
4	H	0.13	0/746	0.22	0/1004
5	I	0.17	0/3080	0.37	0/4756
6	J	0.18	0/3036	0.36	0/4679
7	K	0.13	0/830	0.34	0/1130
7	M	0.13	0/830	0.30	0/1130
7	O	0.11	0/830	0.32	0/1130
8	L	0.09	0/3756	0.24	0/5096
8	N	0.12	0/3756	0.24	0/5096
8	P	0.11	0/3756	0.25	0/5096
All	All	0.13	0/25925	0.28	0/36245

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	790	0	831	15	0
1	E	784	0	820	7	0
2	B	633	0	673	12	0
2	F	638	0	676	7	0
3	C	834	0	895	8	0
3	G	825	0	882	11	0
4	D	735	0	760	8	0
4	H	735	0	760	11	0
5	I	2743	0	1493	47	0
6	J	2710	0	1493	61	0
7	K	806	0	771	14	0
7	M	806	0	771	13	0
7	O	806	0	771	17	0
8	L	3670	0	3678	63	0
8	N	3670	0	3676	51	0
8	P	3670	0	3681	49	0
9	Q	71	0	61	0	0
10	R	60	0	52	2	0
11	L	43	0	30	5	0
11	N	43	0	30	2	0
11	P	43	0	30	6	0
12	L	42	0	39	1	0
12	N	28	0	26	0	0
12	P	28	0	26	0	0
All	All	25213	0	22925	341	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 341 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:OE1	2:B:25:ASN:ND2	2.20	0.75
11:L:601:HEM:HHC	11:L:601:HEM:HBB2	1.67	0.75
7:K:87:MET:HE1	11:L:601:HEM:HBB1	1.67	0.74
6:J:28:DG:H2''	6:J:29:DA:H5''	1.70	0.74
6:J:49:DC:H2'	6:J:50:DA:C8	2.24	0.72

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	94/99 (95%)	92 (98%)	2 (2%)	0	100	100
1	E	93/99 (94%)	92 (99%)	1 (1%)	0	100	100
2	B	77/87 (88%)	76 (99%)	1 (1%)	0	100	100
2	F	78/87 (90%)	77 (99%)	1 (1%)	0	100	100
3	C	106/111 (96%)	105 (99%)	1 (1%)	0	100	100
3	G	105/111 (95%)	104 (99%)	1 (1%)	0	100	100
4	D	92/96 (96%)	90 (98%)	2 (2%)	0	100	100
4	H	92/96 (96%)	90 (98%)	2 (2%)	0	100	100
7	K	98/108 (91%)	96 (98%)	2 (2%)	0	100	100
7	M	98/108 (91%)	95 (97%)	3 (3%)	0	100	100
7	O	98/108 (91%)	95 (97%)	3 (3%)	0	100	100
8	L	455/466 (98%)	446 (98%)	9 (2%)	0	100	100
8	N	455/466 (98%)	445 (98%)	10 (2%)	0	100	100
8	P	455/466 (98%)	441 (97%)	14 (3%)	0	100	100
All	All	2396/2508 (96%)	2344 (98%)	52 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	83/86 (96%)	82 (99%)	1 (1%)	67	82
1	E	83/86 (96%)	81 (98%)	2 (2%)	44	68
2	B	65/72 (90%)	64 (98%)	1 (2%)	60	78
2	F	65/72 (90%)	65 (100%)	0	100	100
3	C	85/88 (97%)	85 (100%)	0	100	100
3	G	84/88 (96%)	84 (100%)	0	100	100
4	D	80/82 (98%)	80 (100%)	0	100	100
4	H	80/82 (98%)	80 (100%)	0	100	100
7	K	86/93 (92%)	83 (96%)	3 (4%)	31	59
7	M	86/93 (92%)	84 (98%)	2 (2%)	45	69
7	O	86/93 (92%)	85 (99%)	1 (1%)	67	82
8	L	403/411 (98%)	394 (98%)	9 (2%)	47	70
8	N	403/411 (98%)	397 (98%)	6 (2%)	60	78
8	P	403/411 (98%)	395 (98%)	8 (2%)	50	72
All	All	2092/2168 (96%)	2059 (98%)	33 (2%)	58	77

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	P	192	ASN
8	P	210	LEU
8	P	564	CYS
8	L	362	SER
8	L	359	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
7	M	95	HIS
8	N	351	GLN
8	N	157	ASN
8	N	409	GLN
7	K	66	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 ⓘ

11 monosaccharides 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$
9	NAG	Q	1	8,9	14,14,15	0.78	0	17,19,21	1.36	2 (11%)
9	NAG	Q	2	9	14,14,15	0.73	0	17,19,21	1.04	1 (5%)
9	BMA	Q	3	9	11,11,12	0.83	0	15,15,17	2.36	4 (26%)
9	MAN	Q	4	9	11,11,12	0.73	0	15,15,17	1.20	1 (6%)
9	MAN	Q	5	9	11,11,12	0.71	0	15,15,17	1.27	1 (6%)
9	FUC	Q	6	9	10,10,11	0.80	0	14,14,16	1.11	0
10	NAG	R	1	8,10	14,14,15	1.06	1 (7%)	17,19,21	1.60	3 (17%)
10	NAG	R	2	10	14,14,15	0.81	0	17,19,21	1.04	0
10	BMA	R	3	10	11,11,12	0.84	0	15,15,17	2.24	5 (33%)
10	MAN	R	4	10	11,11,12	0.77	0	15,15,17	1.03	1 (6%)
10	FUC	R	5	10	10,10,11	0.85	0	14,14,16	0.91	0

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
9	NAG	Q	1	8,9	-	0/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	0/6/23/26	0/1/1/1
9	BMA	Q	3	9	-	2/2/19/22	0/1/1/1
9	MAN	Q	4	9	-	2/2/19/22	1/1/1/1
9	MAN	Q	5	9	-	2/2/19/22	1/1/1/1
9	FUC	Q	6	9	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	R	1	8,10	-	0/6/23/26	0/1/1/1
10	NAG	R	2	10	-	0/6/23/26	0/1/1/1
10	BMA	R	3	10	-	1/2/19/22	0/1/1/1
10	MAN	R	4	10	-	0/2/19/22	1/1/1/1
10	FUC	R	5	10	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	R	1	NAG	O5-C1	-2.36	1.39	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	3	BMA	C1-O5-C5	7.03	121.72	112.19
10	R	3	BMA	C1-O5-C5	6.72	121.30	112.19
9	Q	5	MAN	C1-O5-C5	3.90	117.47	112.19
9	Q	4	MAN	C1-O5-C5	3.67	117.16	112.19
9	Q	1	NAG	O5-C1-C2	-3.58	105.63	111.29

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	Q	5	MAN	C4-C5-C6-O6
9	Q	4	MAN	O5-C5-C6-O6
9	Q	3	BMA	O5-C5-C6-O6
9	Q	5	MAN	O5-C5-C6-O6
9	Q	3	BMA	C4-C5-C6-O6

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	Q	5	MAN	C1-C2-C3-C4-C5-O5
10	R	4	MAN	C1-C2-C3-C4-C5-O5
9	Q	4	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

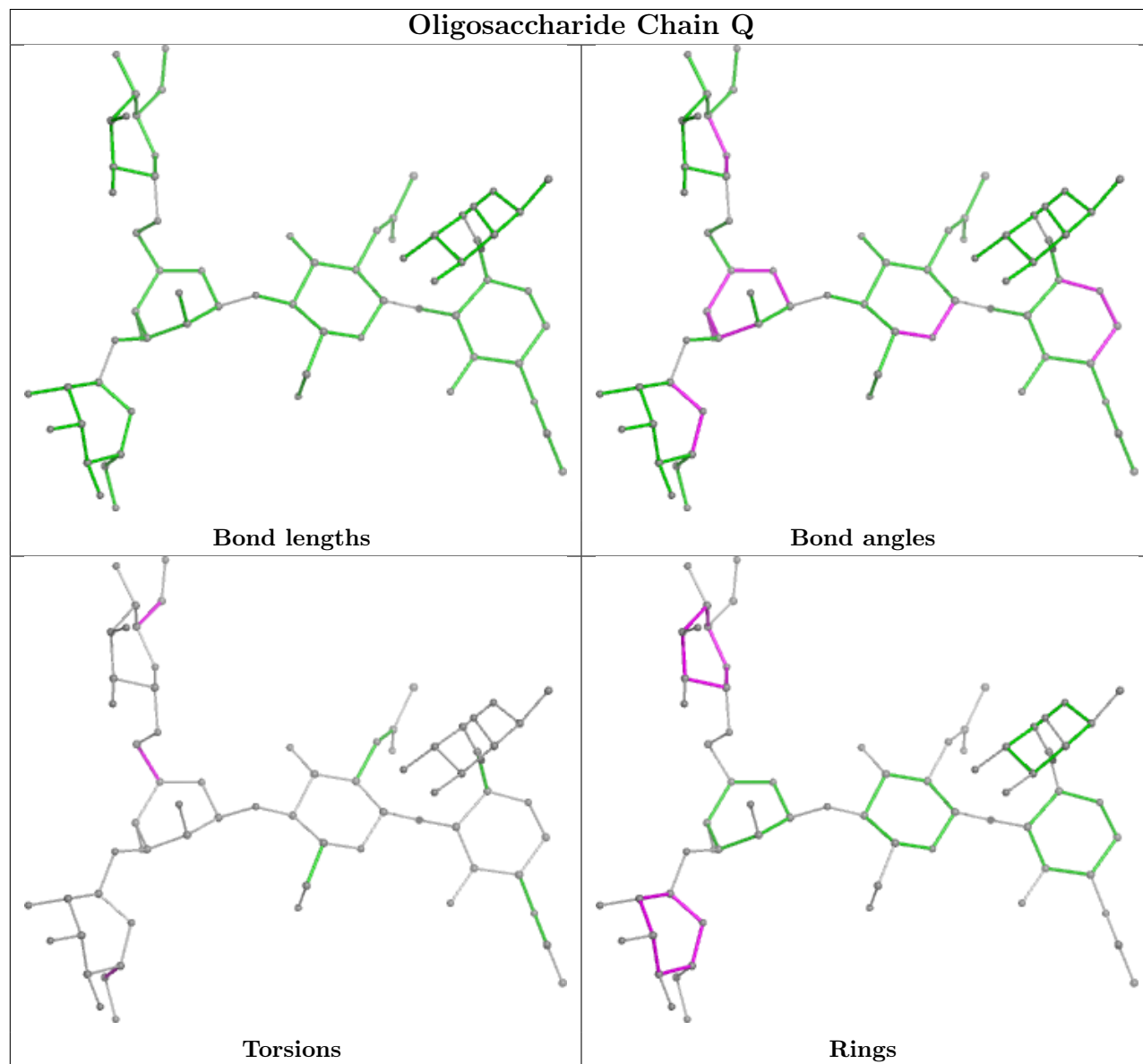
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	R	1	NAG	2	0

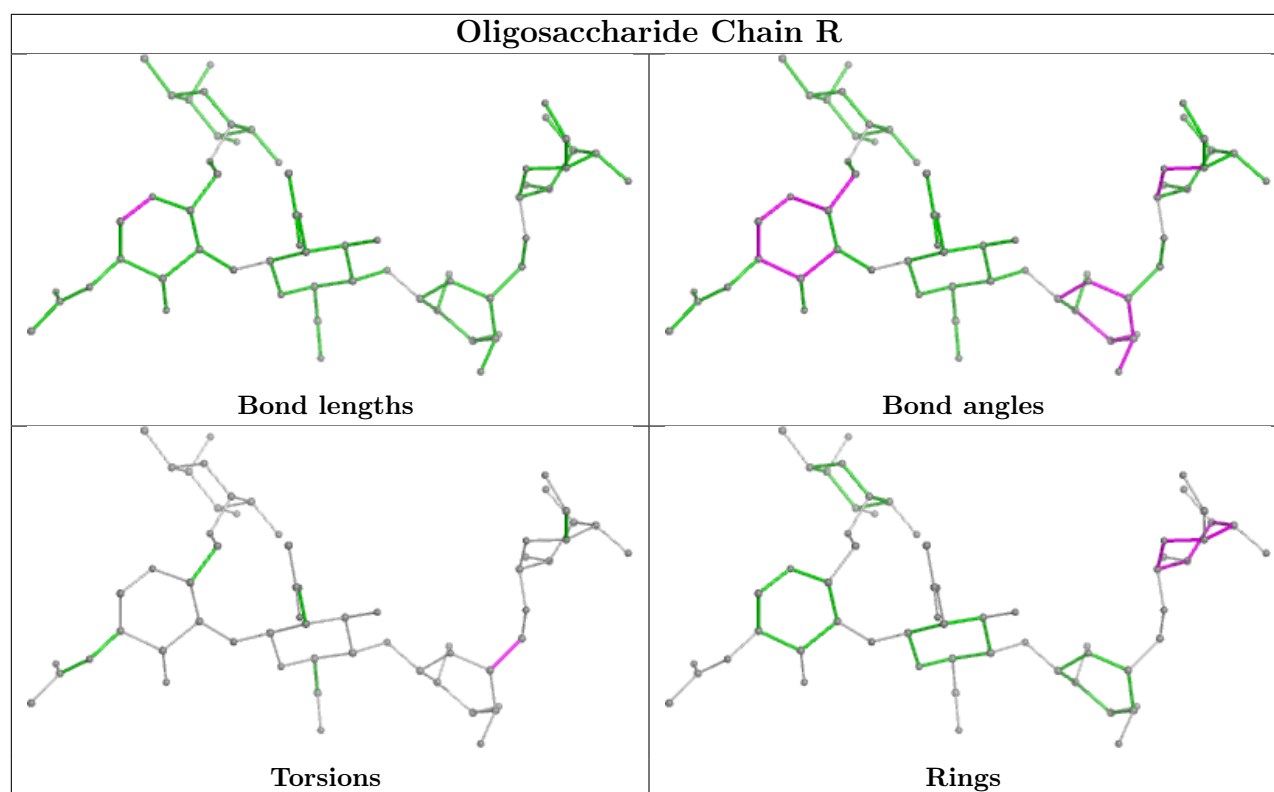
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	R	2	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

10 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
11	HEM	N	601	8	41,50,50	1.45	3 (7%)	45,82,82	1.50	7 (15%)
12	NAG	L	604	8	14,14,15	0.73	0	17,19,21	0.85	0
12	NAG	L	602	-	14,14,15	0.74	0	17,19,21	0.74	0
12	NAG	P	603	-	14,14,15	0.75	0	17,19,21	0.82	0
12	NAG	P	602	-	14,14,15	0.73	0	17,19,21	0.77	0
12	NAG	N	603	8	14,14,15	0.79	0	17,19,21	0.80	0
12	NAG	L	603	8	14,14,15	0.70	0	17,19,21	1.10	1 (5%)
12	NAG	N	602	-	14,14,15	0.74	0	17,19,21	0.76	0
11	HEM	P	601	8	41,50,50	1.48	3 (7%)	45,82,82	1.61	12 (26%)
11	HEM	L	601	8	41,50,50	1.44	4 (9%)	45,82,82	1.53	7 (15%)

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
11	HEM	N	601	8	-	2/12/54/54	-
12	NAG	L	604	8	-	0/6/23/26	0/1/1/1
12	NAG	L	602	-	-	0/6/23/26	0/1/1/1
12	NAG	P	603	-	-	2/6/23/26	0/1/1/1
12	NAG	P	602	-	-	0/6/23/26	0/1/1/1
12	NAG	N	603	8	-	1/6/23/26	0/1/1/1
12	NAG	L	603	8	-	2/6/23/26	0/1/1/1
12	NAG	N	602	-	-	0/6/23/26	0/1/1/1
11	HEM	P	601	8	-	7/12/54/54	-
11	HEM	L	601	8	-	6/12/54/54	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	601	HEM	C3C-C2C	-4.10	1.34	1.40
11	P	601	HEM	C3C-C2C	-4.02	1.34	1.40
11	L	601	HEM	C3C-C2C	-3.80	1.35	1.40
11	L	601	HEM	C3C-CAC	3.78	1.55	1.47
11	P	601	HEM	C3C-CAC	3.78	1.55	1.47

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	601	HEM	C1B-NB-C4B	3.16	108.34	105.07
11	L	601	HEM	C4D-ND-C1D	3.09	108.27	105.07
11	N	601	HEM	C3B-C2B-C1B	2.98	108.69	106.49
11	P	601	HEM	CAD-C3D-C4D	2.95	129.82	124.66
11	P	601	HEM	C1B-NB-C4B	2.94	108.11	105.07

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	L	601	HEM	C2A-CAA-CBA-CGA
11	P	601	HEM	C2D-C3D-CAD-CBD
11	P	601	HEM	C4D-C3D-CAD-CBD
12	L	603	NAG	C8-C7-N2-C2

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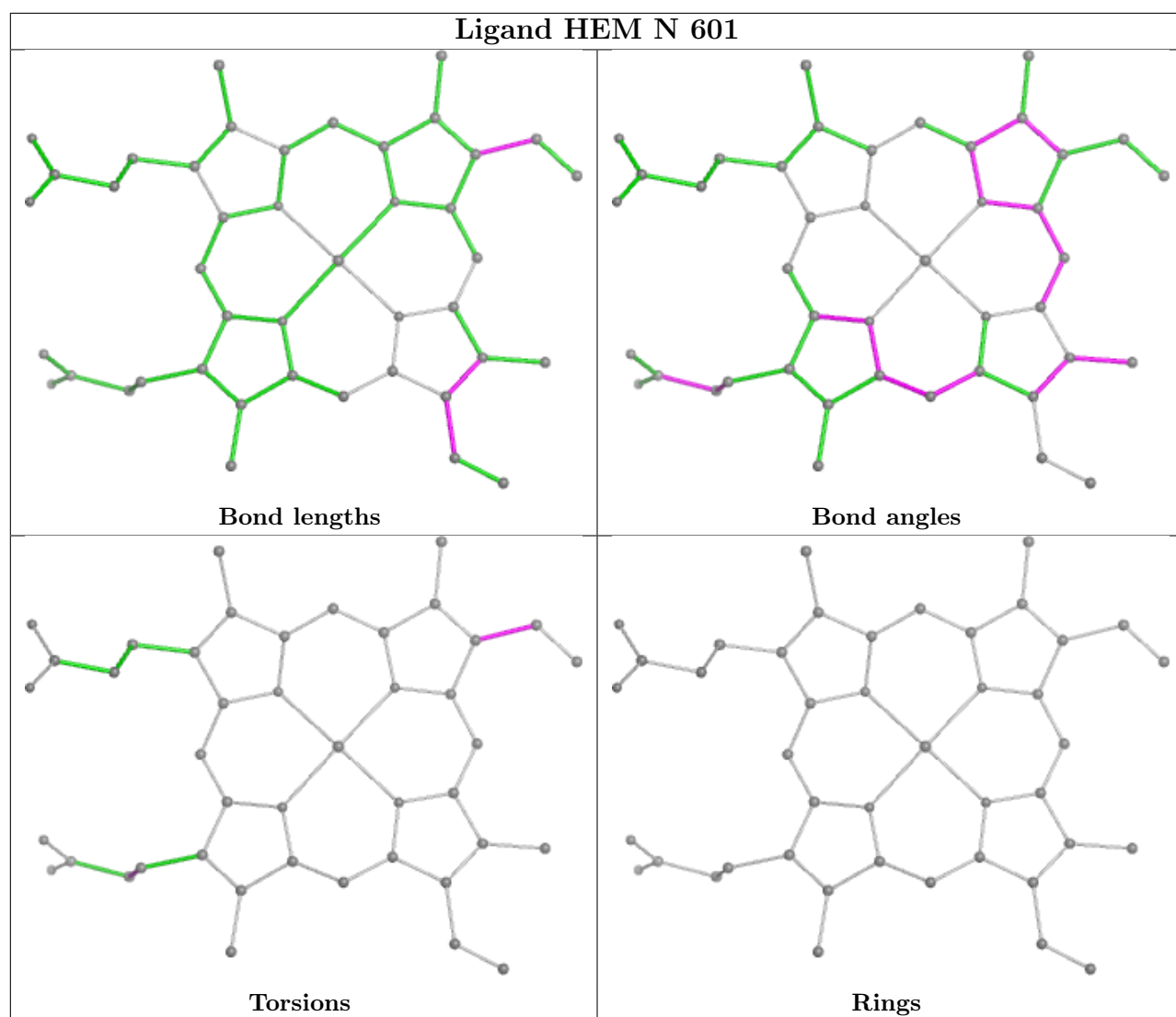
Mol	Chain	Res	Type	Atoms
12	L	603	NAG	O7-C7-N2-C2

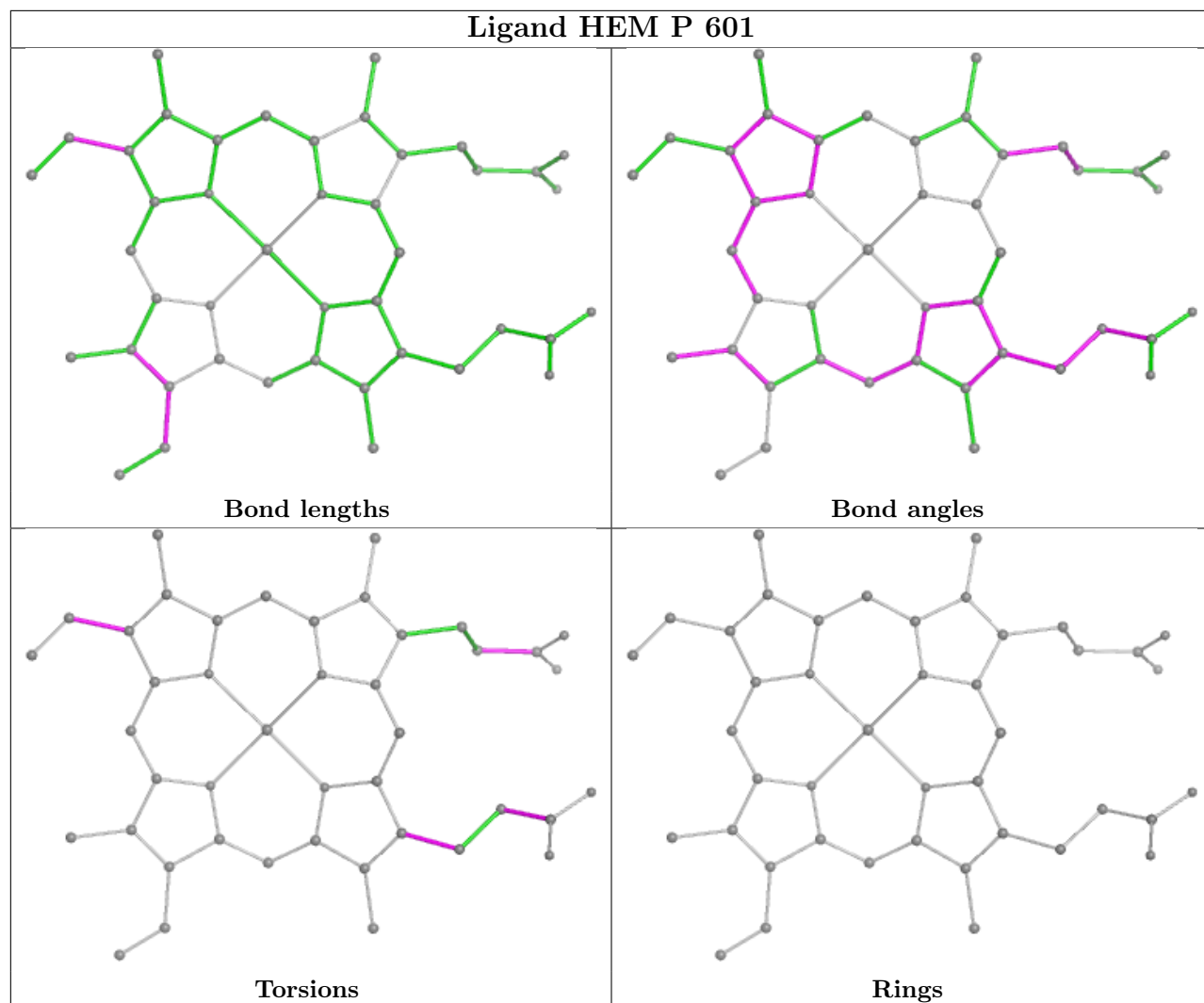
There are no ring outliers.

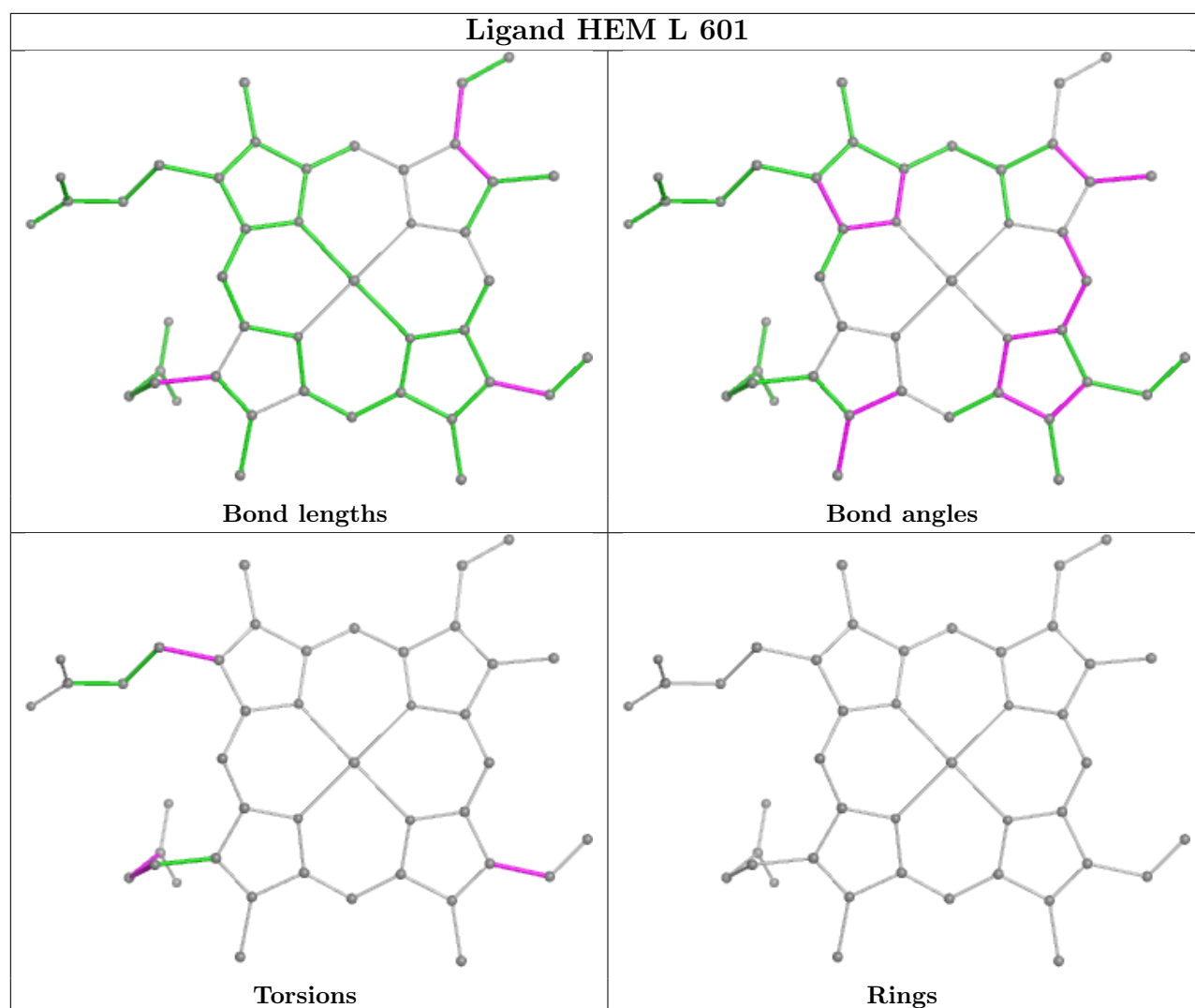
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	N	601	HEM	2	0
12	L	603	NAG	1	0
11	P	601	HEM	6	0
11	L	601	HEM	5	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

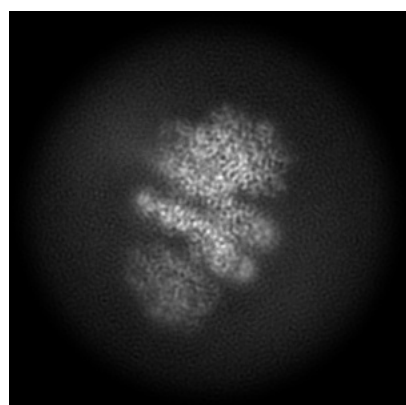
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52870. These allow visual inspection of the internal detail of the map and identification of artifacts.

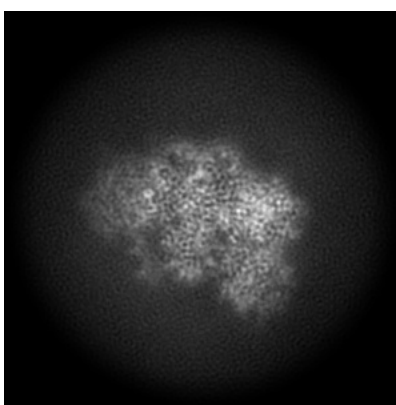
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

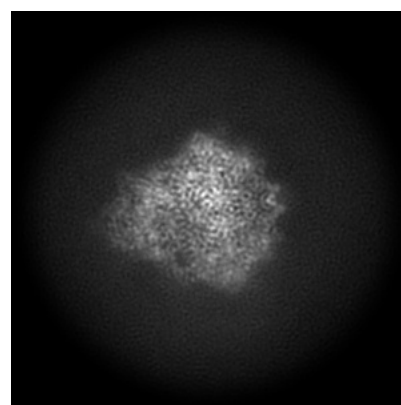
6.1.1 Primary map



X



Y

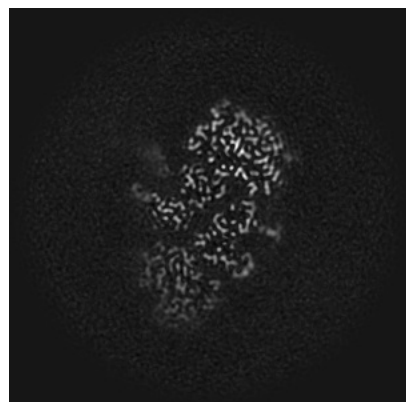


Z

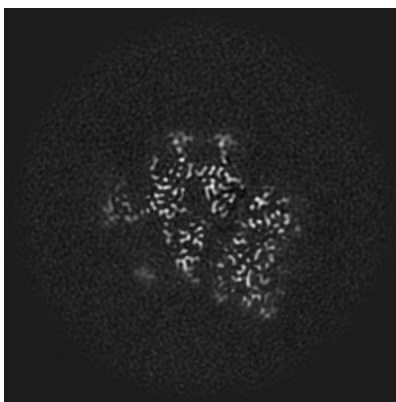
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

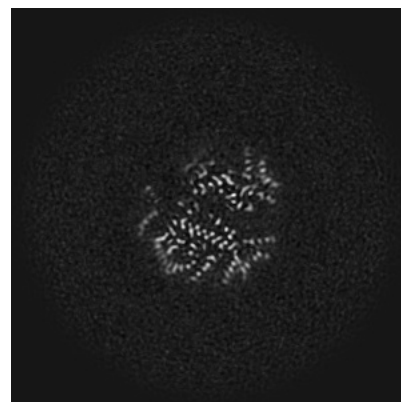
6.2.1 Primary map



X Index: 200



Y Index: 200

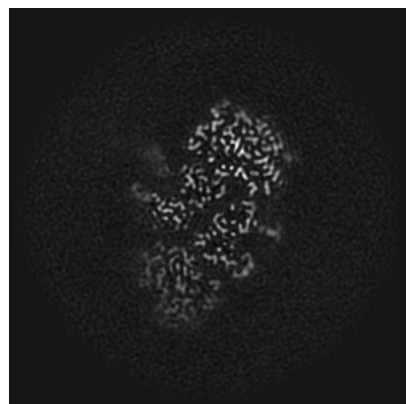


Z Index: 200

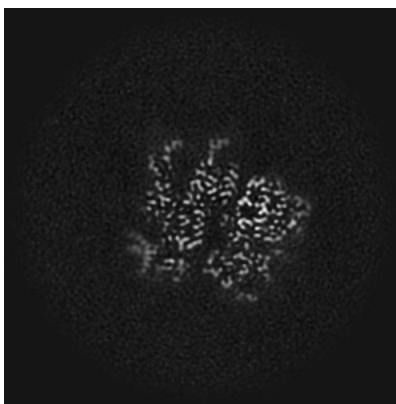
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

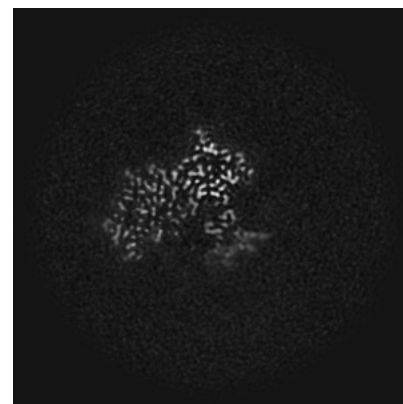
6.3.1 Primary map



X Index: 200



Y Index: 219

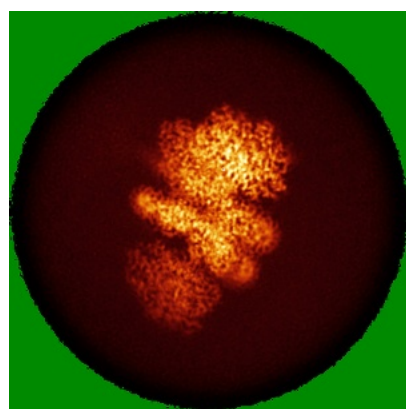


Z Index: 241

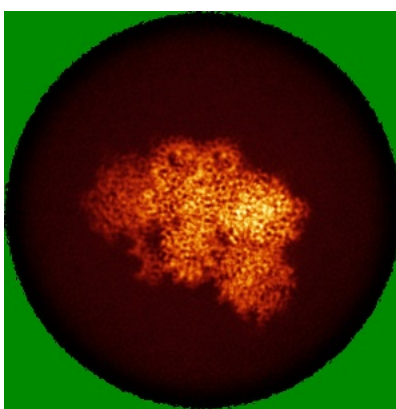
The images above show the largest variance slices of the map in three orthogonal directions.

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

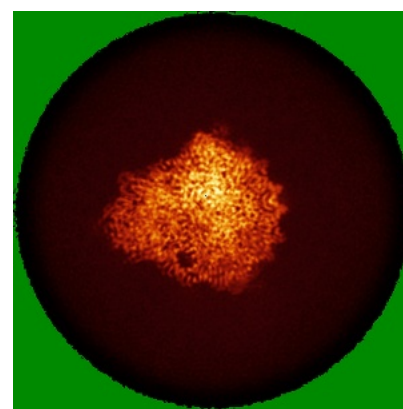
6.4.1 Primary map



X



Y

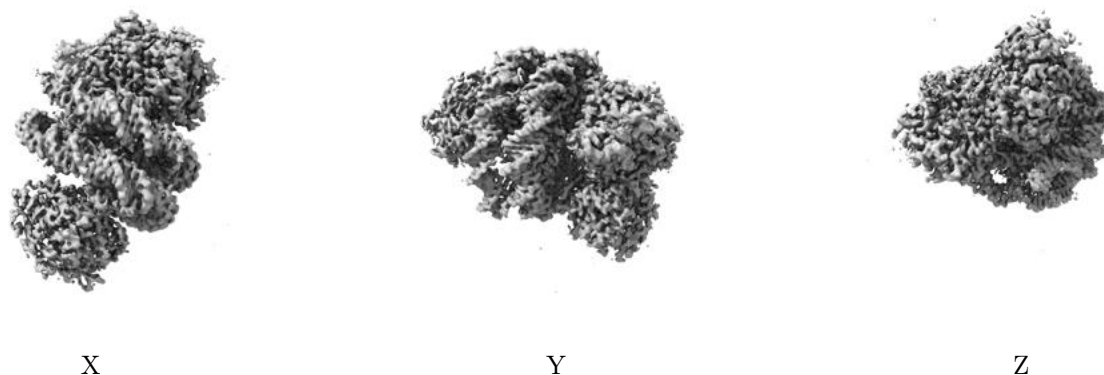


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

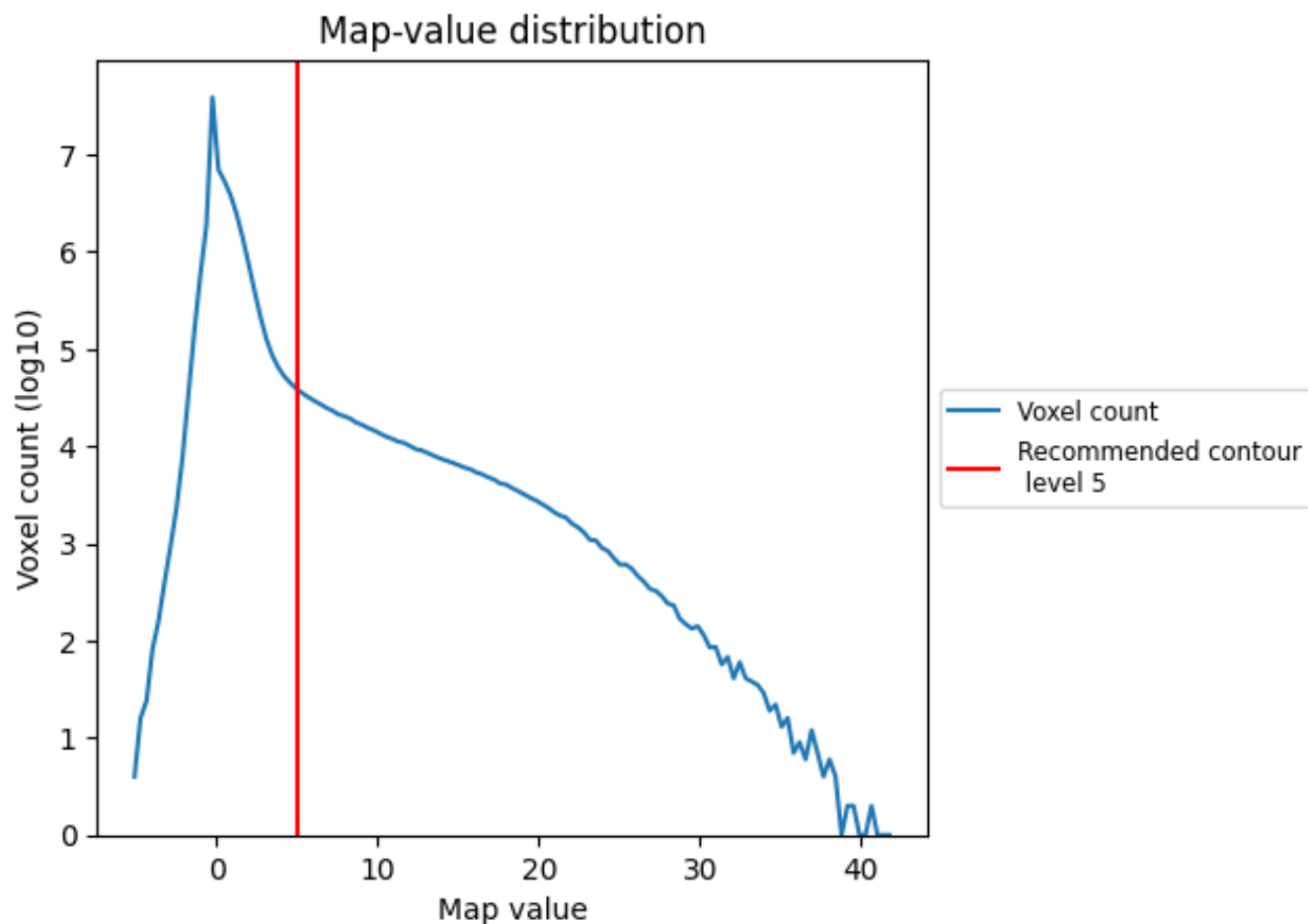
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

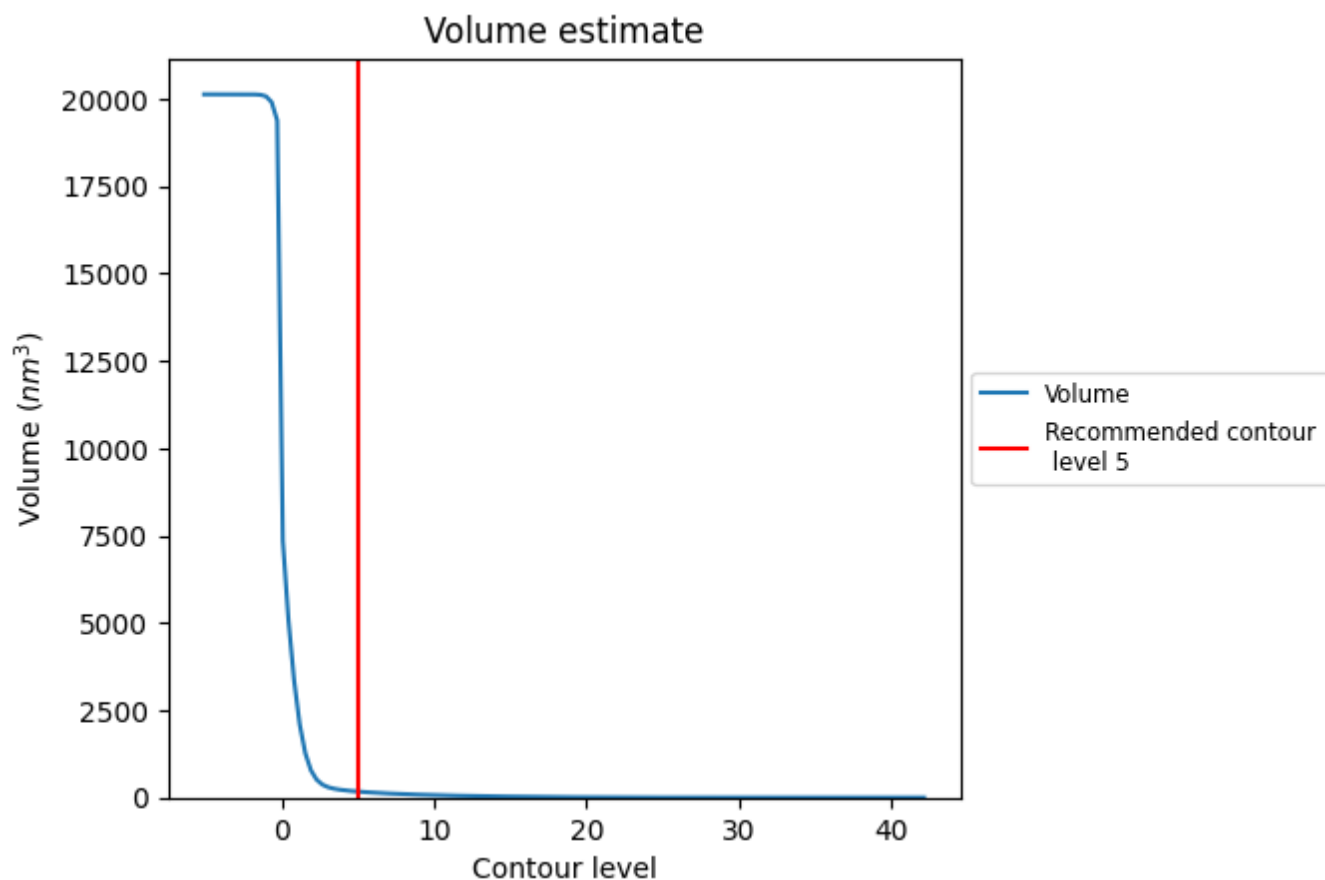
This section contains the results of statistical analysis of the map.

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.

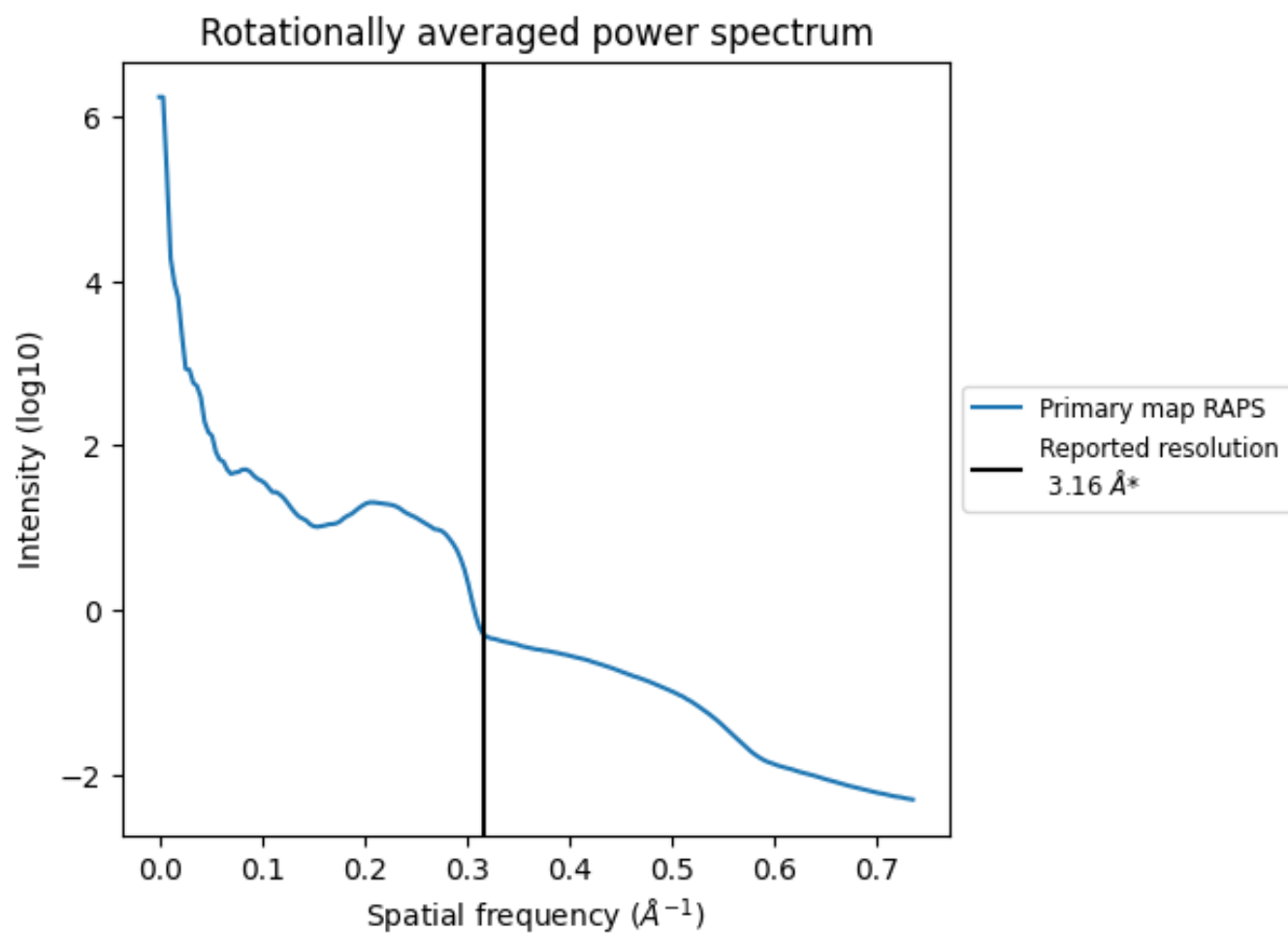
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 171 nm^3 ; this corresponds to an approximate mass of 155 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 0.316 Å⁻¹

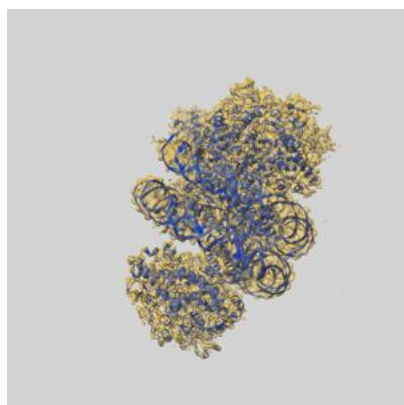
8 Fourier-Shell correlation

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

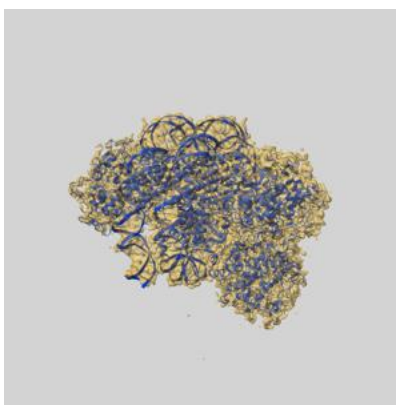
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52870 and PDB model 9IHF. Per-residue inclusion information can be found in section [3](#) on page [9](#).

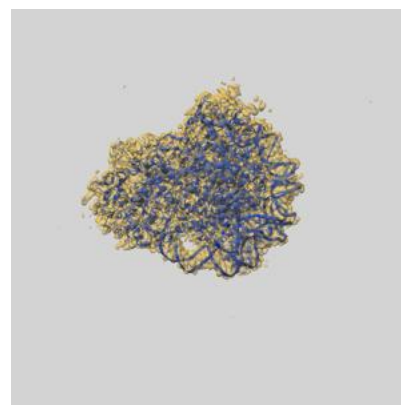
9.1 Map-model overlay [i](#)



X



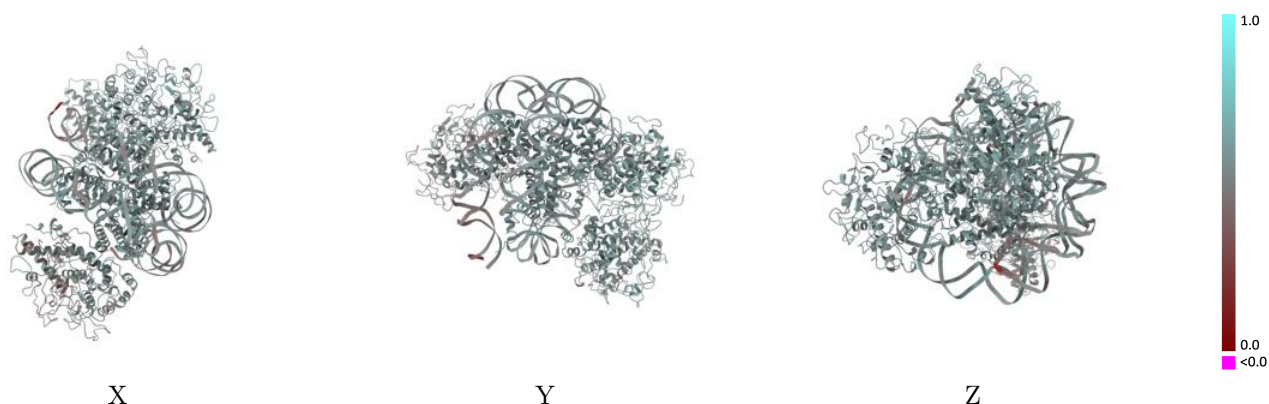
Y



Z

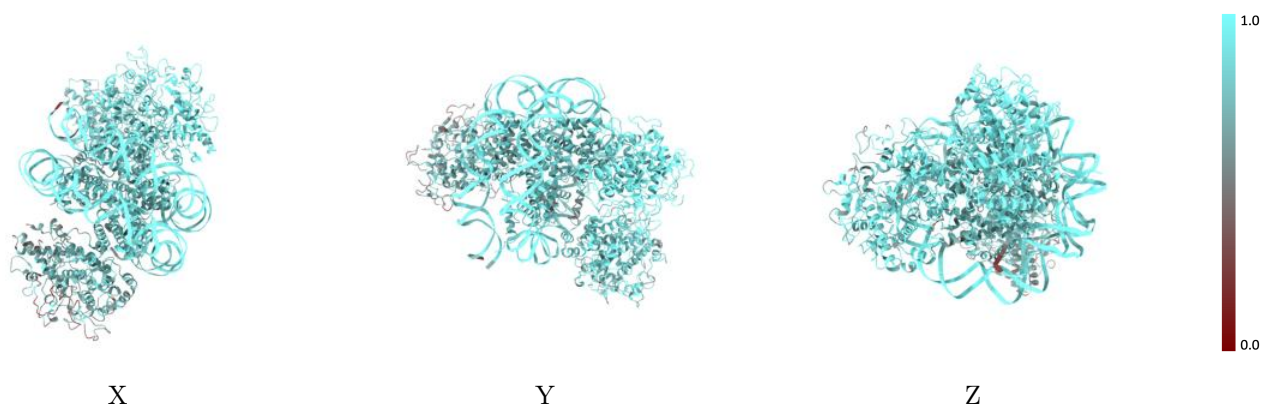
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



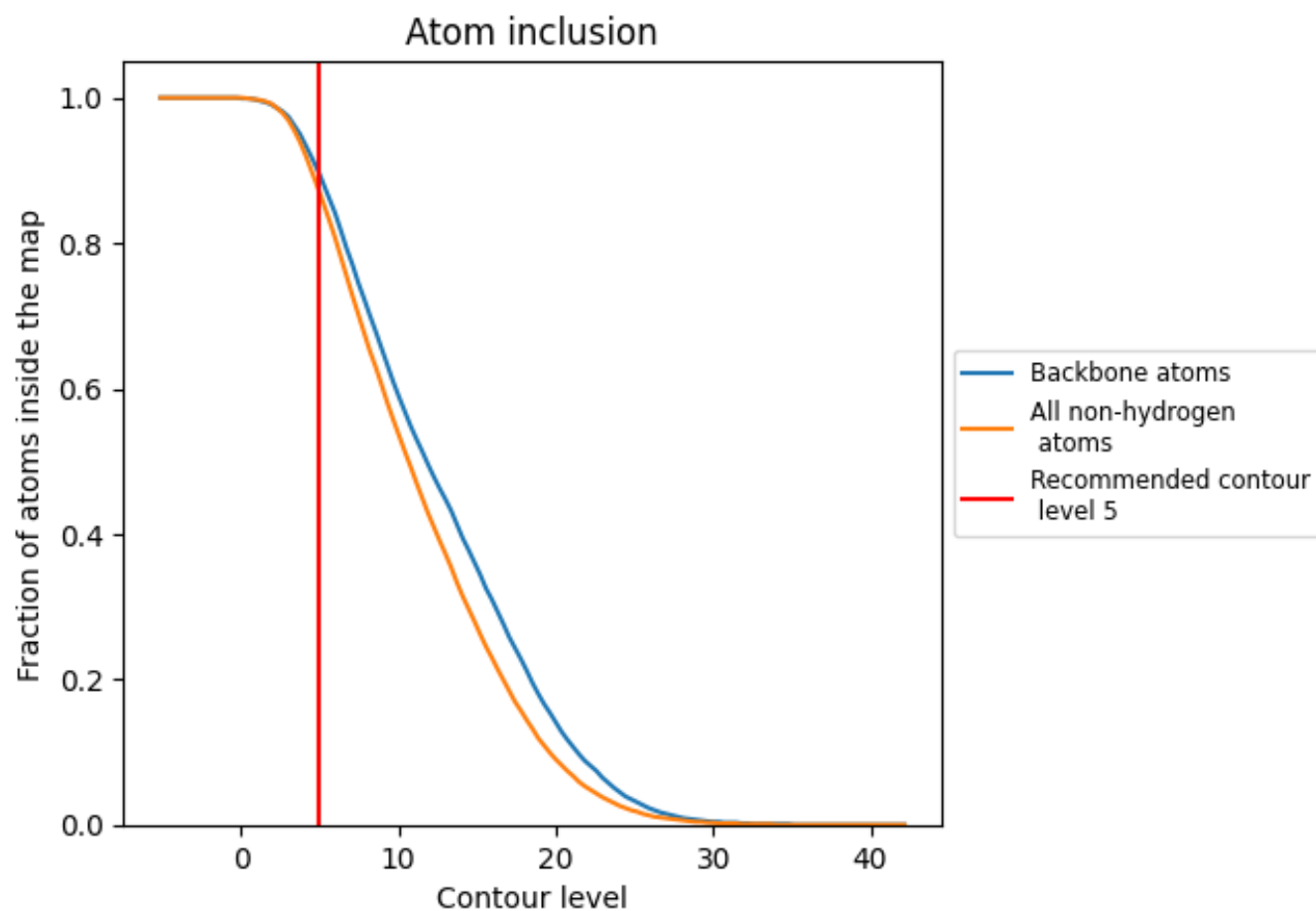
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8700	<div></div> 0.5360
A	<div></div> 0.8430	<div></div> 0.5670
B	<div></div> 0.9060	<div></div> 0.5760
C	<div></div> 0.8760	<div></div> 0.5680
D	<div></div> 0.8690	<div></div> 0.5510
E	<div></div> 0.8860	<div></div> 0.5720
F	<div></div> 0.8900	<div></div> 0.5790
G	<div></div> 0.8450	<div></div> 0.5630
H	<div></div> 0.8730	<div></div> 0.5560
I	<div></div> 0.9230	<div></div> 0.5060
J	<div></div> 0.9250	<div></div> 0.5000
K	<div></div> 0.7010	<div></div> 0.4870
L	<div></div> 0.7050	<div></div> 0.4970
M	<div></div> 0.9600	<div></div> 0.5690
N	<div></div> 0.9580	<div></div> 0.5630
O	<div></div> 0.9010	<div></div> 0.5590
P	<div></div> 0.8750	<div></div> 0.5470
Q	<div></div> 0.8870	<div></div> 0.5230
R	<div></div> 0.8830	<div></div> 0.5580

1.0
0.0
<0.0