



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 03:00 PM UTC

PDB ID : 8XMW / pdb_00008xmw
EMDB ID : EMD-38490
Title : Local refinement of Hb-Hp bind to CD163
Authors : Xu, H.; Su, X.D.
Deposited on : 2023-12-28
Resolution : 2.94 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

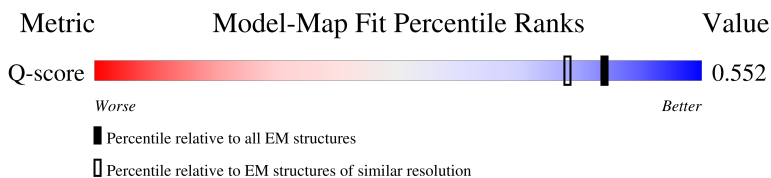
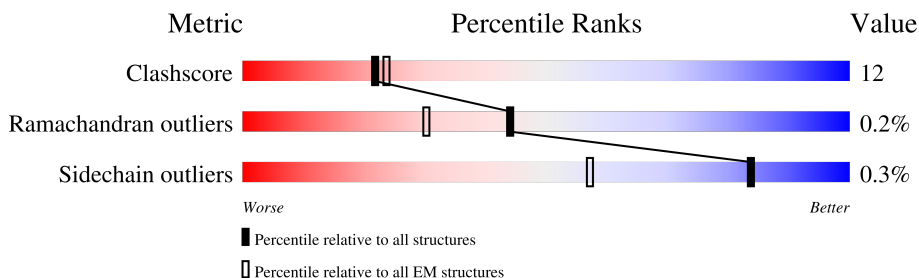
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 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	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13068 (2.44 - 3.44)

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	2	347	
2	D	1009	
2	G	1009	
3	A	142	

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Mol	Chain	Length	Quality of chain
4	B	147	74% 22%
5	C	2	100%
5	E	2	100%
5	F	2	50% 50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9538 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 Isoform 2 of Haptoglobin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	288	Total	C	N	O	S	0	0
			2263	1444	382	425	12		

- Molecule 2 is a protein called Scavenger receptor cysteine-rich type 1 protein M130.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	320	Total	C	N	O	S	0	0
			2442	1499	443	474	26		
2	G	320	Total	C	N	O	S	0	0
			2442	1499	443	474	26		

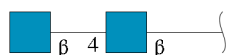
- Molecule 3 is a protein called Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	141	Total	C	N	O	S	0	0
			1068	685	187	193	3		

- Molecule 4 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	143	Total	C	N	O	S	0	0
			1091	703	189	196	3		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



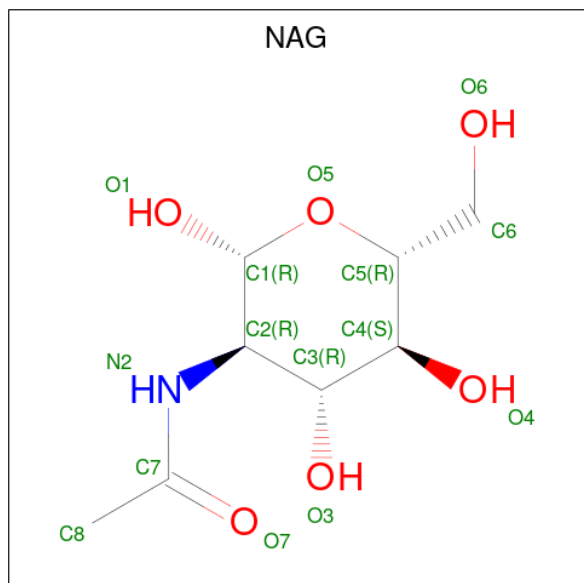
Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	2	Total	C	N	O		0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
6	2	1	Total	C	N	O	0
			14	8	1	5	
6	2	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	G	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	D	3	Total	Ca	0
			3	3	
7	G	3	Total	Ca	0
			3	3	

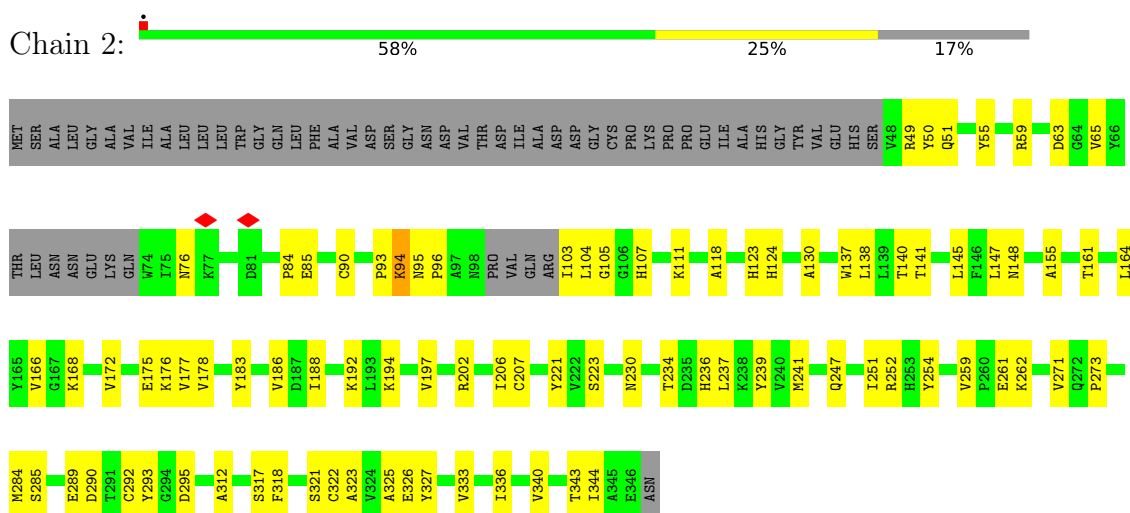
- # HEM

Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	B	1	Total 43	C 34	Fe 1	N 4	O 4	0

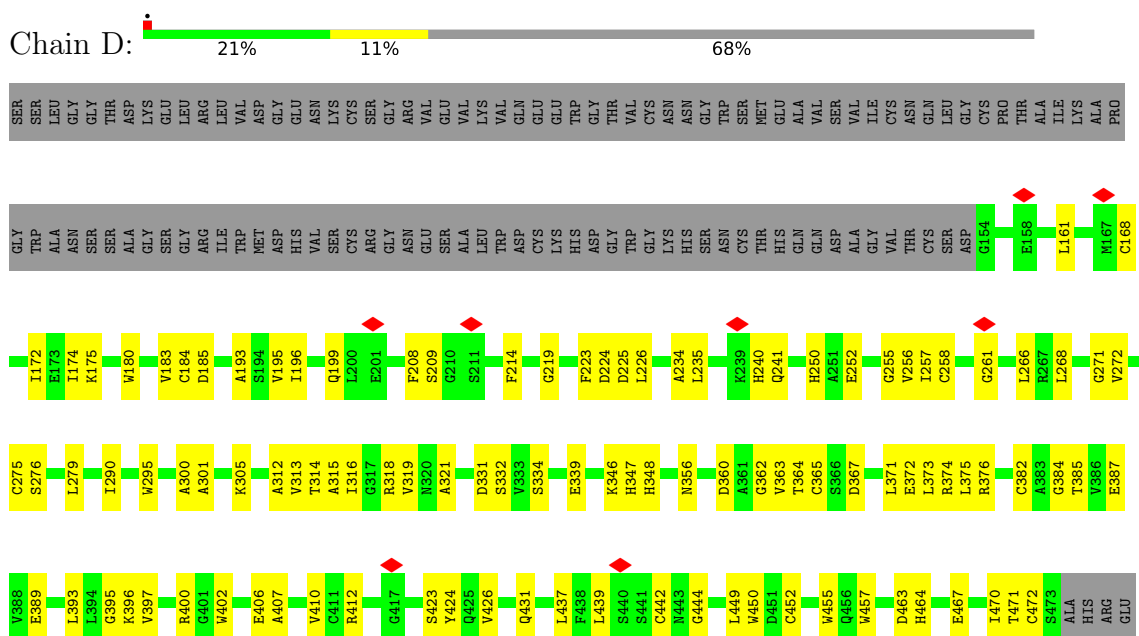
3 Residue-property plots

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: Isoform 2 of Haptoglobin



• Molecule 2: Scavenger receptor cysteine-rich type 1 protein M130

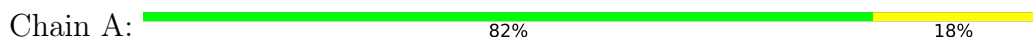


- Molecule 2: Scavenger receptor cysteine-rich type 1 protein M130

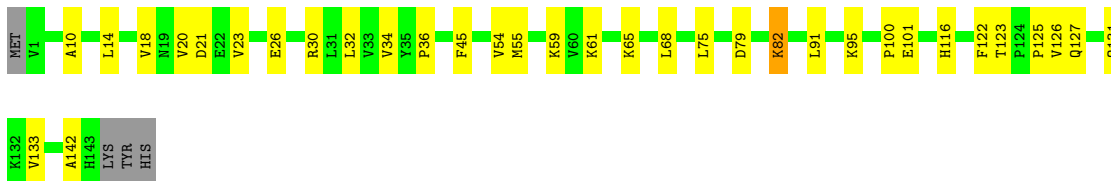
LEU	ALA	GLY	ASP	ALA	R400	G317	C168	SER
CYS	PRO	SER	ASP	ALA	R400	R318	C168	SER
GLN	ARG	ILE	SER	GLN	R403	R319	R171	TRP
GLN	PRO	CYS	ASP	GLN	E406	A320	I172	ASN
LEU	GLY	ASP	ASP	ASP	E406	A321	E173	GLY
LYS	THR	SER	SER	SER	R412	S322	V183	THR
CYS	THR	ASP	ASP	ASP	R412	R323	V183	ASP
GLY	CYS	PHE	PHE	PHE	R423	G324	R198	LYS
VAL	SER	SER	SER	SER	R423	I328	R199	GLU
ALA	HIS	LEU	LEU	ALA	R424	I328	R199	LEU
SER	ARG	GLU	GLU	GLU	I430	V333	V206	ARG
LEU	ARG	ALA	ALA	ALA	I430	V333	V206	LEU
THR	ASP	ALA	ALA	ALA	I437	V336	V206	VAL
PRO	GLY	SER	SER	SER	I437	V336	M213	TRP
GLY	VAL	VAL	VAL	VAL	G337	F214	F214	MET
GLY	VAL	LEU	LEU	LEU	G338	H338	G215	ASP
ALA	VAL	CYS	CYS	CYS	S441	S441	G215	HIS
ARG	CYS	ARG	ARG	ARG	C442	A341	F223	VAL
PHE	SER	GLU	GLU	GLU	C442	A341	F223	LYS
GLY	ARG	LEU	LEU	LEU	R443	Q344	D224	CYS
ANG	THR	GLN	GLN	GLN	R443	Q344	D224	SER
LYS	THR	CYS	CYS	CYS	R453	H347	L226	GLY
THR	GLY	THR	THR	THR	R453	H347	L226	ARG
ASN	GLY	THR	THR	THR	R454	H348	G230	ASN
GLY	ILE	THR	THR	THR	R455	E349	G230	VAL
GLN	ARG	VAL	VAL	VAL	Q456	E349	H240	GLU
ILE	LEU	VAL	VAL	VAL	Q457	H353	H240	SER
TRP	VAL	SER	SER	SER	R465	Y354	G242	ALA
ARG	ASN	ILE	ILE	ILE	R465	Y354	G242	LEU
GLY	GLY	LEU	LEU	LEU	R468	H357	K245	GLN
HIS	GLY	LEU	LEU	LEU	R468	H358	K245	ASP
MET	LYS	GLY	GLY	GLY	R471	R359	H246	GLY
PHE	THR	GLY	GLY	GLY	R471	R360	N247	THR
HIS	PRO	ALA	ALA	ALA	C472	A361	A251	GLY
CYS	CYS	HIS	HIS	HIS	C472	A361	A251	THR
THR	GLY	PHE	PHE	PHE	A473	G362	G362	VAL
GLY	GLY	GLY	GLY	GLY	ALA	V363	V256	VAL
ARG	GLY	GLY	GLY	GLY	ALA	V364	V256	CYS
THR	ARG	GLY	GLY	GLY	ARG	R364	I257	ASN
GLU	VAL	GLY	GLY	GLY	HIS	C365	I257	ASN
GLN	GLU	ASN	ASN	ASN	GLU	R366	C258	ASN
LEU	LEU	GLY	GLY	GLY	PRO	S367	S259	GLY
MET	LYS	GLN	GLN	GLN	ARG	D367		THR
GLY	THR	ILE	ILE	ILE	LEU	D370	L268	SER
THR	THR	ILE	ILE	ILE	LEU	D370	L268	MET
ASP	LEU	TRP	TRP	TRP	VAL	L371	D270	GLU
CYS	GLY	ALA	ALA	ALA	GLY	L371	D270	GLU
PRO	ALA	GLU	GLU	GLU	GLY	L375	G271	ALA
VAL	THR	GLU	GLU	GLU	ASP		V272	ALA
THR	GLY	PHE	PHE	PHE	ILE	C382	C275	SER
ALA	SER	GLN	GLN	GLN	PRO	A383	C275	ASP
LEU	LEU	CYS	CYS	CYS	CYS	G384	L279	ILE
GLY	CYS	GLY	GLY	GLY	THR	R385	L279	CYS
ALA	ASN	GLY	GLY	GLY	SER	V386	F283	ASN
SER	SER	HIS	HIS	HIS	ARG		F283	GLN
LEU	LEU	GLY	GLY	GLY	VAL	E389	T289	LEU
THR	THR	SER	SER	SER	GLU	E389	T289	GLY
CYS	PRO	ASP	ASP	ASP	VAL	R392	I290	ASP
PRO	ILE	GLY	GLY	GLY	VAL	R392	I290	PRO
SER	GLU	LEU	LEU	LEU	LYS	L393	F310	THR
GLU	GLU	SER	SER	SER	HIS	L394	T311	ALA
GLN	ASP	LEU	LEU	LEU	GLY	G395	L161	ILE
VAL	ALA	CYS	CYS	CYS</				

ALA	THR	GLU	LYS	GLU	THR	GLU	VAL	SER	TRP	VAL
THR	GLY	ALA	GLU	TRP	THR	TRP	GLY	HIS	GLY	GLY
GLY	ARG	PHE	THR	ILE	THR	ILE	VAL	TRP	THR	CYS
SER	SER	GLY	GLY	CYS	ASP	GLY	ARG	GLY	CYS	GLY
ARG	GLY	GLN	ASP	ASP	ASN	GLN	GLN	ASN	ASP	GLN
GLN	THR	THR	LYS	LYS	LYS	GLY	GLY	CYS	TRP	GLN
SER	SER	PRO	GLY	ILE	ILE	ARG	CYS	ARG	ASP	THR
SER	ILE	ILE	LEU	LEU	LEU	ASP	ALA	HIS	LEU	LEU
	TRP	TRP	GLN	GLN	GLN	GLY	LYS	ASP	ASP	CYS
	LEU	ASN	GLY	GLY	GLY	GLY	LYS	ALA	HIS	ASN
	GLU	GLU	PRO	PRO	PRO	ILE	ASN	VAL	VAL	SER
	VAL	VAL	THR	THR	THR	ASN	ASN	VAL	VAL	SER
	CYS	CYS	LYS	LYS	CYS	PRO	CYS	ILE	CYS	LEU
	LYS	LYS	GLY	SER	SER	ALA	ALA	ARG	GLN	GLY
	ASN	ASN	ARG	ARG	ARG	ASP	LYS	PHE	GLY	THR
	GLU	GLU	VAL	VAL	VAL	LYS	ALA	MET	CYS	ARG
	SER	SER	GLU	GLU	ILE	ALA	ALA	SER	GLY	PRO
	LEU	LEU	TRP	TRP	TRP	MET	THR	ARG	GLU	THR
	TRP	TRP	HIS	HIS	ILE	ILE	VAL	GLU	ILE	ALA
	ASP	ASP	GLY	GLY	GLY	PRO	THR	THR	ASN	GLU
	CYS	CYS	GLY	GLY	GLY	MET	THR	SER	ALA	GLU
	PRO	PRO	SER	SER	SER	THR	VAL	GLU	THR	SER
	ALA	ALA	ALA	TRP	TRP	VAL	VAL	ALA	GLY	ALA
	ARG	ARG	ARG	THR	THR	ASN	ASN	SER	SER	VAL
	TRP	TRP	GLY	VAL	VAL	GLN	GLN	GLU	HIS	ALA
	HIS	HIS	ASP	ASP	ASP	CYS	CYS	GLY	GLY	ILE
	SER	SER	THR	THR	THR	PRO	PRO	ALA	GLU	THR
	GLU	GLU	GLU	SER	SER	LYS	LYS	CYS	GLY	SER
	CYS	CYS	GLY	TRP	TRP	ASP	ASP	ARG	THR	GLN
	LYS	LYS	LYS	ASP	ASP	THR	THR	TYR	LEU	ARG
	ASP	ASP	ALA	ALA	ALA	TRP	GLN	ASN	ASP	VAL
	ALA	ALA	VAL	VAL	VAL	CYS	CYS	GLY	GLU	GLY
	VAL	VAL	VAL	VAL	VAL	PRO	PRO	ALA	MET	GLY
	ASN	ASN	CYS	CYS	GLN	SER	SER	TRP	LYS	ARG
	THR	THR	GLN	GLN	GLN	PRO	PRO	THR	ASN	ALA
	ASP	ASP	ILE	ILE	GLY	GLU	GLU	GLY	LYS	ARG
	SER	SER	SER	SER	CYS	LYS	LYS	GLY	GLU	VAL
	VAL	VAL	GLN	GLN	GLY	ARG	ARG	SER	GLU	THR
	GLN	GLN	LYS	LYS	ALA	ALA	ALA	MET	ILE	ILE
	THR	THR	THR	THR	LEU	SER	SER	SER	TRP	THR
	PRO	PRO	PRO	PRO	LYS	PRO	PRO	GLU	GLN	CYS
	GLN	GLN	GLN	ALA	ALA	SER	SER	THR	CYS	THR

- Molecule 3: Hemoglobin subunit alpha



- Molecule 4: Hemoglobin subunit beta



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	432933	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.540	Depositor
Minimum map value	-2.556	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	2	0.21	0/2316	0.39	0/3142
2	D	0.16	0/2496	0.36	0/3374
2	G	0.20	0/2496	0.37	0/3374
3	A	0.23	0/1096	0.36	0/1491
4	B	0.19	0/1119	0.31	0/1522
All	All	0.19	0/9523	0.37	0/12903

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2263	0	2224	55	0
2	D	2442	0	2253	67	0
2	G	2442	0	2253	63	0
3	A	1068	0	1073	16	0
4	B	1091	0	1089	24	0
5	C	28	0	25	0	0
5	E	28	0	25	0	0
5	F	28	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	2	28	0	26	1	0
6	D	14	0	13	0	0
6	G	14	0	13	0	0
7	D	3	0	0	0	0
7	G	3	0	0	0	0
8	A	43	0	30	2	0
8	B	43	0	30	2	0
All	All	9538	0	9079	216	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 12.

All (216) 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)
1:2:252:ARG:HD3	2:G:251:ALA:HB2	1.55	0.88
2:D:407:ALA:HB1	2:D:470:ILE:HD13	1.59	0.83
2:G:272:VAL:HA	5:F:1:NAG:H62	1.66	0.78
1:2:123:HIS:HB2	1:2:161:THR:HG23	1.66	0.77
8:B:201:HEM:HH1	8:B:201:HEM:HHB2	1.68	0.74
2:D:372:GLU:HB2	2:D:389:GLU:HB2	1.71	0.72
1:2:254:TYR:OH	1:2:327:TYR:O	2.05	0.72
3:A:117:PHE:O	4:B:30:ARG:NH2	2.24	0.70
1:2:65:VAL:O	1:2:76:ASN:ND2	2.24	0.69
2:D:412:ARG:NH2	2:D:444:GLY:O	2.24	0.69
2:D:439:LEU:HD21	2:D:449:LEU:HD11	1.73	0.69
2:D:395:GLY:HA3	2:D:457:TRP:HH2	1.57	0.69
2:D:268:LEU:HD21	2:D:363:VAL:HG12	1.76	0.67
2:G:162:THR:HG22	2:G:163:ARG:HG3	1.75	0.67
1:2:340:VAL:O	1:2:344:ILE:HG12	1.93	0.67
2:G:313:VAL:HG21	2:G:371:LEU:HD11	1.77	0.67
3:A:27:GLU:OE1	3:A:112:HIS:NE2	2.26	0.66
2:D:318:ARG:HB2	2:D:321:ALA:HB3	1.77	0.66
2:D:374:ARG:HH22	2:D:389:GLU:HG3	1.60	0.66
1:2:49:ARG:NH1	1:2:51:GLN:OE1	2.30	0.65
1:2:221:TYR:CE1	1:2:241:MET:HG2	2.31	0.65
2:D:223:PHE:HB3	2:D:226:LEU:HD11	1.79	0.63
2:G:272:VAL:HG11	2:G:393:LEU:HB2	1.78	0.63
2:D:312:ALA:HB3	2:D:367:ASP:HA	1.81	0.63
2:G:268:LEU:HD21	2:G:363:VAL:HG22	1.81	0.63
3:A:122:HIS:CD2	4:B:34:VAL:HG21	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:178:VAL:HG11	1:2:343:THR:HG21	1.80	0.62
2:D:275:CYS:HB3	2:D:365:CYS:HB2	1.81	0.62
2:D:168:CYS:HB3	2:D:258:CYS:HB2	1.81	0.61
2:D:196:ILE:HD11	2:D:235:LEU:HD22	1.82	0.61
2:G:406:GLU:HG3	2:G:442:CYS:HB2	1.81	0.61
8:A:201:HEM:HBC2	8:A:201:HEM:HMC2	1.81	0.60
4:B:21:ASP:OD1	4:B:65:LYS:NZ	2.34	0.60
2:D:184:CYS:HB2	2:D:224:ASP:HA	1.83	0.60
2:G:359:GLU:OE2	3:A:11:LYS:NZ	2.36	0.59
2:G:171:ARG:NH1	2:G:173:GLU:OE2	2.35	0.58
4:B:26:GLU:OE2	4:B:30:ARG:NH1	2.37	0.58
2:D:396:LYS:HD2	2:D:467:GLU:OE2	2.04	0.58
1:2:230:ASN:ND2	4:B:101:GLU:OE2	2.31	0.57
2:G:198:ARG:NH2	2:G:230:GLY:O	2.26	0.57
3:A:114:PRO:O	4:B:116:HIS:NE2	2.37	0.57
2:D:374:ARG:NH1	2:D:387:GLU:OE2	2.39	0.56
2:G:183:VAL:HG13	2:G:223:PHE:HB2	1.88	0.56
2:D:375:LEU:O	2:D:376:ARG:NH1	2.40	0.55
1:2:103:ILE:N	1:2:295:ASP:OD2	2.40	0.54
2:D:406:GLU:HG2	2:D:439:LEU:HD23	1.90	0.54
1:2:175:GLU:HB2	1:2:194:LYS:HA	1.88	0.54
4:B:45:PHE:HA	4:B:59:LYS:HD2	1.89	0.54
1:2:223:SER:HB2	1:2:237:LEU:HD21	1.89	0.54
2:D:315:ALA:HB3	2:D:364:THR:HB	1.90	0.53
2:D:172:ILE:HD13	2:D:196:ILE:HG13	1.90	0.53
2:G:412:ARG:NH2	2:G:444:GLY:O	2.37	0.53
2:G:396:LYS:HE3	2:G:430:ILE:HD12	1.91	0.53
2:D:183:VAL:HG13	2:D:223:PHE:HB2	1.90	0.53
4:B:91:LEU:HA	4:B:95:LYS:HE2	1.91	0.53
2:G:272:VAL:HA	5:F:1:NAG:C6	2.38	0.53
1:2:333:VAL:HA	1:2:336:ILE:HG12	1.90	0.52
2:G:403:GLY:N	2:G:406:GLU:OE1	2.39	0.52
8:B:201:HEM:HMC2	8:B:201:HEM:HBC2	1.90	0.52
2:D:382:CYS:HB3	2:D:472:CYS:HB2	1.92	0.52
2:G:159:MET:HE3	2:G:199:GLN:HE22	1.74	0.52
2:D:240:HIS:O	2:D:241:GLN:HG3	2.10	0.51
2:G:225:ASP:O	2:G:240:HIS:HA	2.10	0.51
2:G:328:ILE:HB	2:G:353:HIS:CE1	2.45	0.51
2:D:168:CYS:HB2	2:D:261:GLY:HA3	1.93	0.51
2:D:397:VAL:HG22	2:D:437:LEU:HB3	1.92	0.51
1:2:50:TYR:HD2	1:2:84:PRO:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:331:ASP:OD1	2:D:332:SER:N	2.44	0.51
2:G:437:LEU:HD11	2:G:455:TRP:HE3	1.76	0.51
1:2:284:MET:HE2	1:2:326:GLU:HA	1.92	0.51
2:D:463:ASP:OD1	2:D:464:HIS:N	2.43	0.51
2:G:270:ASP:OD1	5:F:1:NAG:N2	2.36	0.51
2:G:242:GLY:HA3	2:G:245:LYS:HD3	1.91	0.51
2:D:318:ARG:NH1	2:D:360:ASP:O	2.43	0.51
2:G:400:ARG:HG3	2:G:465:TYR:CZ	2.46	0.51
1:2:124:HIS:HA	6:2:401:NAG:H82	1.93	0.50
2:G:440:SER:OG	2:G:453:LYS:O	2.27	0.50
1:2:234:THR:OG1	1:2:236:HIS:O	2.29	0.50
1:2:124:HIS:ND1	1:2:148:ASN:HB2	2.26	0.50
2:G:397:VAL:HB	2:G:468:ALA:HB3	1.93	0.50
3:A:31:ARG:NH1	4:B:127:GLN:OE1	2.31	0.50
4:B:75:LEU:HD21	4:B:133:VAL:HG11	1.93	0.50
2:G:289:THR:HG21	2:G:324:GLY:HA3	1.93	0.50
2:D:437:LEU:HD11	2:D:455:TRP:CE3	2.47	0.49
2:D:272:VAL:HG11	2:D:393:LEU:HB2	1.93	0.49
3:A:96:VAL:O	3:A:100:LEU:HG	2.12	0.49
1:2:321:SER:OG	1:2:325:ALA:O	2.31	0.49
2:G:241:GLN:NE2	2:G:245:LYS:O	2.45	0.49
2:G:316:ILE:HG13	2:G:456:GLN:HG2	1.94	0.48
2:D:193:ALA:HB2	2:D:208:PHE:HB3	1.94	0.48
2:G:318:ARG:HB2	2:G:321:ALA:HB3	1.94	0.48
2:D:219:GLY:H	2:D:250:HIS:HE2	1.62	0.48
2:G:375:LEU:HD12	2:G:382:CYS:HA	1.95	0.48
8:A:201:HEM:HMB1	8:A:201:HEM:HBB2	1.95	0.48
2:D:225:ASP:HB3	2:D:241:GLN:HG2	1.95	0.48
2:G:389:GLU:HB2	2:G:394:LEU:HD13	1.96	0.48
2:D:347:HIS:ND1	2:D:348:HIS:O	2.35	0.48
2:D:402:TRP:HH2	2:D:410:VAL:HG21	1.79	0.48
1:2:221:TYR:CD1	1:2:241:MET:HG2	2.49	0.47
1:2:95:ASN:ND2	1:2:111:LYS:O	2.48	0.47
1:2:166:VAL:HG21	1:2:197:VAL:HG21	1.97	0.47
2:G:366:SER:OG	2:G:370:ASP:OD1	2.22	0.47
4:B:123:THR:HB	4:B:125:PRO:HD2	1.95	0.47
2:D:313:VAL:HG11	2:D:371:LEU:HD11	1.96	0.47
2:G:172:ILE:HD11	2:G:256:VAL:HG13	1.96	0.47
1:2:271:VAL:HG23	1:2:318:PHE:HE1	1.78	0.47
1:2:285:SER:OG	1:2:289:GLU:HG2	2.14	0.47
2:G:290:ILE:O	2:G:361:ALA:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:18:VAL:HG13	4:B:23:VAL:HG21	1.97	0.47
1:2:188:ILE:HG13	1:2:336:ILE:HG21	1.96	0.47
2:G:392:ARG:HD2	2:G:392:ARG:O	2.14	0.47
1:2:137:TRP:CG	1:2:344:ILE:HD12	2.50	0.46
1:2:247:GLN:O	1:2:251:ILE:HD12	2.14	0.46
4:B:55:MET:O	4:B:61:LYS:NZ	2.40	0.46
1:2:273:PRO:HB3	1:2:318:PHE:CG	2.50	0.46
4:B:14:LEU:HD11	4:B:122:PHE:HD1	1.80	0.46
4:B:10:ALA:HB1	4:B:126:VAL:HG12	1.96	0.46
4:B:20:VAL:HA	4:B:68:LEU:HD23	1.97	0.46
2:D:423:SER:O	2:D:471:THR:OG1	2.32	0.46
2:G:437:LEU:HD12	2:G:456:GLN:O	2.15	0.46
3:A:42:TYR:CE1	3:A:93:VAL:HA	2.51	0.46
1:2:236:HIS:NE2	4:B:100:PRO:HG2	2.31	0.46
2:G:323:LYS:HB3	2:G:357:HIS:HB3	1.98	0.46
1:2:118:ALA:HB3	1:2:130:ALA:HB3	1.97	0.46
2:D:295:TRP:HD1	2:D:316:ILE:HB	1.81	0.46
3:A:35:SER:HB3	4:B:131:GLN:HG3	1.97	0.46
3:A:84:SER:OG	3:A:135:VAL:O	2.30	0.46
2:D:373:LEU:HB2	2:D:450:TRP:CZ2	2.51	0.46
2:G:384:GLY:HA2	2:G:424:TYR:CD2	2.51	0.46
1:2:93:PRO:HG2	1:2:96:PRO:HB3	1.98	0.45
2:D:437:LEU:HD11	2:D:455:TRP:HE3	1.81	0.45
1:2:104:LEU:HD22	1:2:323:ALA:HB2	1.99	0.45
2:G:226:LEU:HD23	2:G:240:HIS:HB3	1.98	0.45
1:2:168:LYS:HG2	1:2:202:ARG:HD2	1.98	0.45
2:D:319:VAL:HG12	2:D:457:TRP:CD1	2.51	0.45
2:G:213:ASN:HD22	2:G:349:GLU:HG2	1.81	0.45
2:D:300:ALA:HB1	2:D:363:VAL:HG23	1.99	0.45
3:A:16:LYS:HD3	3:A:116:GLU:HG2	1.98	0.45
2:G:333:VAL:HA	2:G:347:HIS:HB3	1.98	0.45
1:2:259:VAL:HG23	1:2:262:LYS:HB2	1.98	0.45
2:D:199:GLN:CD	2:D:234:ALA:HA	2.41	0.45
2:D:384:GLY:HA2	2:D:424:TYR:CD2	2.53	0.44
2:G:319:VAL:HA	2:G:457:TRP:O	2.16	0.44
2:G:336:GLN:HB2	2:G:338:HIS:ND1	2.33	0.44
1:2:206:ILE:HG21	1:2:312:ALA:HB2	1.99	0.44
2:D:442:CYS:HB2	2:D:452:CYS:HB2	1.57	0.44
2:D:185:ASP:OD1	2:D:252:GLU:HG3	2.18	0.44
2:D:175:LYS:HB2	2:D:180:TRP:CD2	2.52	0.44
2:G:275:CYS:HB3	2:G:365:CYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:138:SER:C	3:A:140:TYR:H	2.26	0.44
1:2:261:GLU:OE2	2:G:247:ASN:HB2	2.17	0.44
1:2:90:CYS:HB3	1:2:207:CYS:HB2	1.63	0.43
2:D:214:PHE:HZ	2:D:257:ILE:HG12	1.83	0.43
2:D:375:LEU:HA	2:D:385:THR:O	2.17	0.43
2:G:437:LEU:HD11	2:G:455:TRP:CE3	2.53	0.43
1:2:104:LEU:CD1	1:2:292:CYS:HB2	2.48	0.43
2:D:300:ALA:HB2	2:D:316:ILE:HG22	2.00	0.43
1:2:292:CYS:SG	1:2:293:TYR:N	2.89	0.43
2:D:301:ALA:HA	2:D:314:THR:HG21	2.00	0.43
1:2:105:GLY:HA3	1:2:289:GLU:OE1	2.19	0.43
1:2:124:HIS:CE1	1:2:148:ASN:HB2	2.54	0.43
4:B:100:PRO:HB3	4:B:142:ALA:HB1	2.00	0.43
1:2:107:HIS:HB2	1:2:239:TYR:O	2.18	0.43
1:2:138:LEU:HD22	1:2:164:LEU:HD21	2.01	0.43
1:2:141:THR:HG21	1:2:317:SER:HA	2.01	0.43
2:G:397:VAL:HG22	2:G:437:LEU:HD23	2.00	0.43
2:G:159:MET:HG2	2:G:199:GLN:NE2	2.34	0.43
2:G:328:ILE:O	2:G:353:HIS:NE2	2.29	0.43
1:2:284:MET:HG2	1:2:290:ASP:HB2	2.00	0.43
1:2:336:ILE:O	1:2:340:VAL:HG13	2.19	0.42
2:D:195:VAL:O	2:D:199:GLN:HG2	2.19	0.42
2:G:168:CYS:HB3	2:G:258:CYS:HB2	2.01	0.42
3:A:10:VAL:HG21	3:A:128:PHE:HB2	2.01	0.42
2:G:206:VAL:HG23	2:G:259:SER:HA	2.00	0.42
2:G:161:LEU:HA	2:G:171:ARG:O	2.19	0.42
2:D:315:ALA:O	2:D:364:THR:N	2.49	0.42
2:D:271:GLY:HA3	2:D:276:SER:O	2.20	0.42
2:G:423:SER:O	2:G:471:THR:OG1	2.29	0.42
3:A:119:PRO:HG2	4:B:55:MET:HG3	2.02	0.42
4:B:34:VAL:O	4:B:36:PRO:HD3	2.20	0.42
2:G:341:ALA:HB3	2:G:344:GLN:OE1	2.20	0.42
2:D:431:GLN:H	2:D:431:GLN:HG3	1.62	0.42
2:G:312:ALA:HB3	2:G:367:ASP:HA	2.01	0.42
4:B:32:LEU:HB2	4:B:54:VAL:HG11	2.01	0.42
1:2:55:TYR:HE1	1:2:94:LYS:HG3	1.85	0.41
1:2:183:TYR:HA	1:2:186:VAL:O	2.19	0.41
1:2:290:ASP:HB3	1:2:322:CYS:O	2.19	0.41
2:G:319:VAL:HG12	2:G:457:TRP:HD1	1.83	0.41
2:D:334:SER:N	2:D:346:LYS:O	2.46	0.41
2:G:257:ILE:HD13	2:G:283:PHE:HZ	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:305:LYS:NZ	2:D:339:GLU:O	2.43	0.41
1:2:59:ARG:HB3	1:2:85:GLU:O	2.21	0.41
2:D:279:LEU:HD23	2:D:290:ILE:HD12	2.01	0.41
2:G:319:VAL:HG12	2:G:457:TRP:CD1	2.55	0.41
2:D:161:LEU:HD21	2:D:256:VAL:HG13	2.01	0.41
2:G:310:PRO:HB3	2:G:367:ASP:HB3	2.01	0.41
2:D:400:ARG:HD2	4:B:79:ASP:HB3	2.02	0.41
1:2:140:THR:HG21	1:2:145:LEU:HD21	2.03	0.41
1:2:164:LEU:HB3	1:2:172:VAL:HG23	2.02	0.41
2:D:174:ILE:HD11	2:D:235:LEU:HD23	2.02	0.41
2:D:279:LEU:H	2:D:362:GLY:HA2	1.86	0.41
2:D:424:TYR:CE2	2:D:426:VAL:HA	2.56	0.41
2:G:171:ARG:HD3	2:G:215:GLY:O	2.20	0.41
2:G:224:ASP:HB3	2:G:241:GLN:HE21	1.86	0.41
2:G:279:LEU:HD12	2:G:279:LEU:HA	1.91	0.41
4:B:82:LYS:HE3	4:B:82:LYS:HB3	1.72	0.41
1:2:124:HIS:HE1	1:2:147:LEU:HB3	1.86	0.41
2:D:266:LEU:HD21	2:D:279:LEU:HD21	2.03	0.41
3:A:28:ALA:CB	3:A:105:LEU:HD23	2.51	0.41
2:G:375:LEU:HD23	2:G:386:VAL:HA	2.03	0.40
1:2:155:ALA:HB1	1:2:177:VAL:O	2.21	0.40
2:D:384:GLY:HA2	2:D:424:TYR:CG	2.56	0.40
2:D:356:ASN:OD1	2:D:356:ASN:N	2.53	0.40
2:G:354:TYR:CZ	3:A:7:LYS:HD2	2.55	0.40
1:2:176:LYS:HG2	1:2:192:LYS:HB3	2.04	0.40
2:D:209:SER:O	2:D:255:GLY:N	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	282/347 (81%)	260 (92%)	21 (7%)	1 (0%)	30	54
2	D	318/1009 (32%)	307 (96%)	11 (4%)	0	100	100
2	G	318/1009 (32%)	293 (92%)	24 (8%)	1 (0%)	36	59
3	A	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
4	B	141/147 (96%)	140 (99%)	1 (1%)	0	100	100
All	All	1198/2654 (45%)	1135 (95%)	61 (5%)	2 (0%)	44	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	63	ASP
2	G	240	HIS

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	2	246/294 (84%)	245 (100%)	1 (0%)	84	92
2	D	260/823 (32%)	260 (100%)	0	100	100
2	G	260/823 (32%)	260 (100%)	0	100	100
3	A	113/114 (99%)	112 (99%)	1 (1%)	70	82
4	B	115/119 (97%)	114 (99%)	1 (1%)	70	82
All	All	994/2173 (46%)	991 (100%)	3 (0%)	84	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	94	LYS
3	A	141	ARG
4	B	82	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	117	GLN
1	2	152	ASN
1	2	185	GLN
1	2	236	HIS
2	D	338	HIS
2	D	443	ASN
2	G	199	GLN
2	G	241	GLN
3	A	68	ASN
3	A	72	HIS
4	B	80	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 ⓘ

6 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	$\# Z > 2$
5	NAG	C	1	1,5	14,14,15	0.25	0	17,19,21	0.48	0
5	NAG	C	2	5	14,14,15	0.20	0	17,19,21	0.40	0
5	NAG	E	1	5,2	14,14,15	0.30	0	17,19,21	0.48	0
5	NAG	E	2	5	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	F	1	5,2	14,14,15	0.91	0	17,19,21	0.97	0
5	NAG	F	2	5	14,14,15	0.57	0	17,19,21	0.67	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
5	NAG	C	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
5	NAG	E	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	NAG	F	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

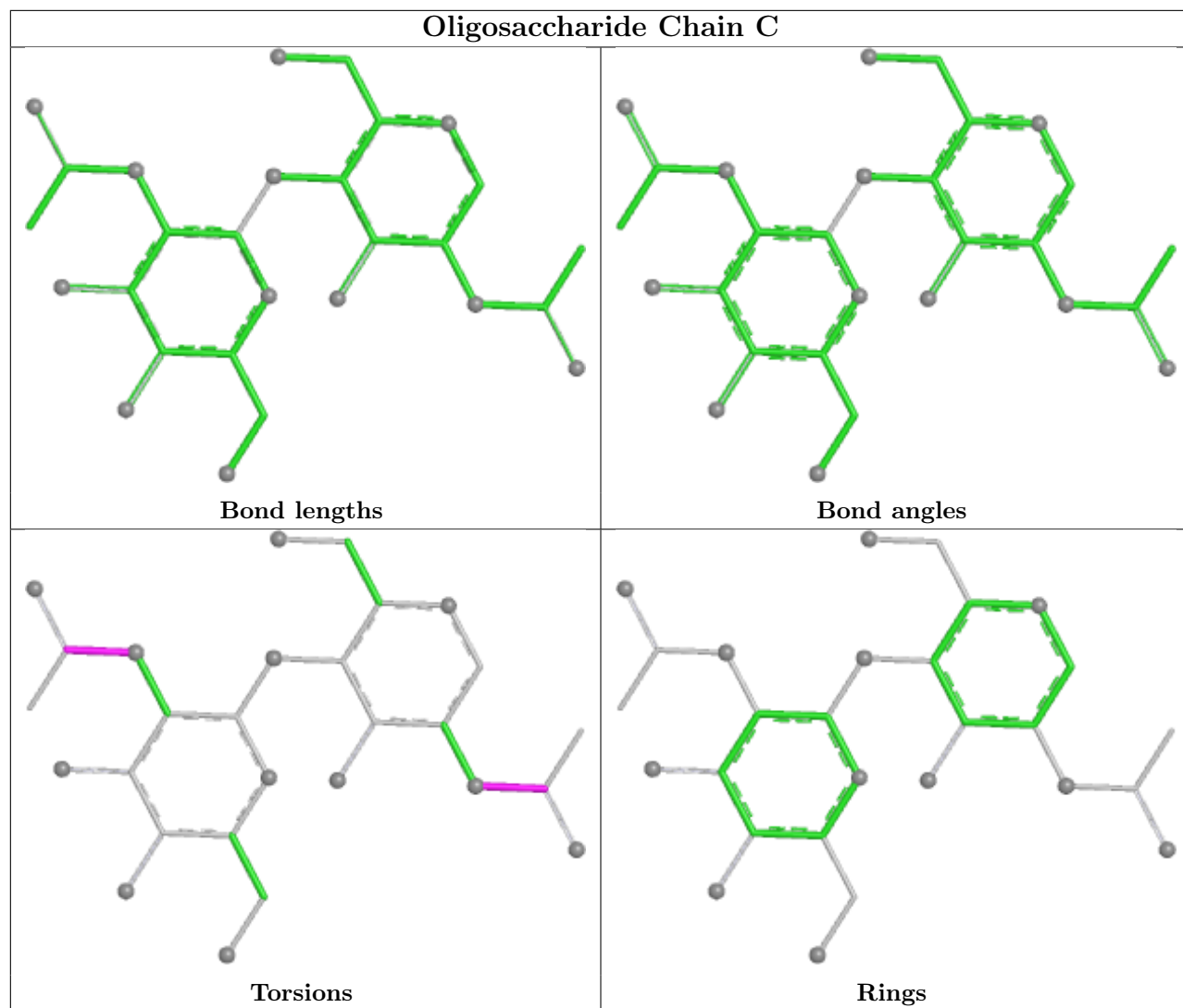
Mol	Chain	Res	Type	Atoms
5	F	2	NAG	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
5	F	1	NAG	C8-C7-N2-C2
5	C	1	NAG	C8-C7-N2-C2
5	C	1	NAG	O7-C7-N2-C2
5	C	2	NAG	C8-C7-N2-C2
5	C	2	NAG	O7-C7-N2-C2
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	F	1	NAG	O7-C7-N2-C2

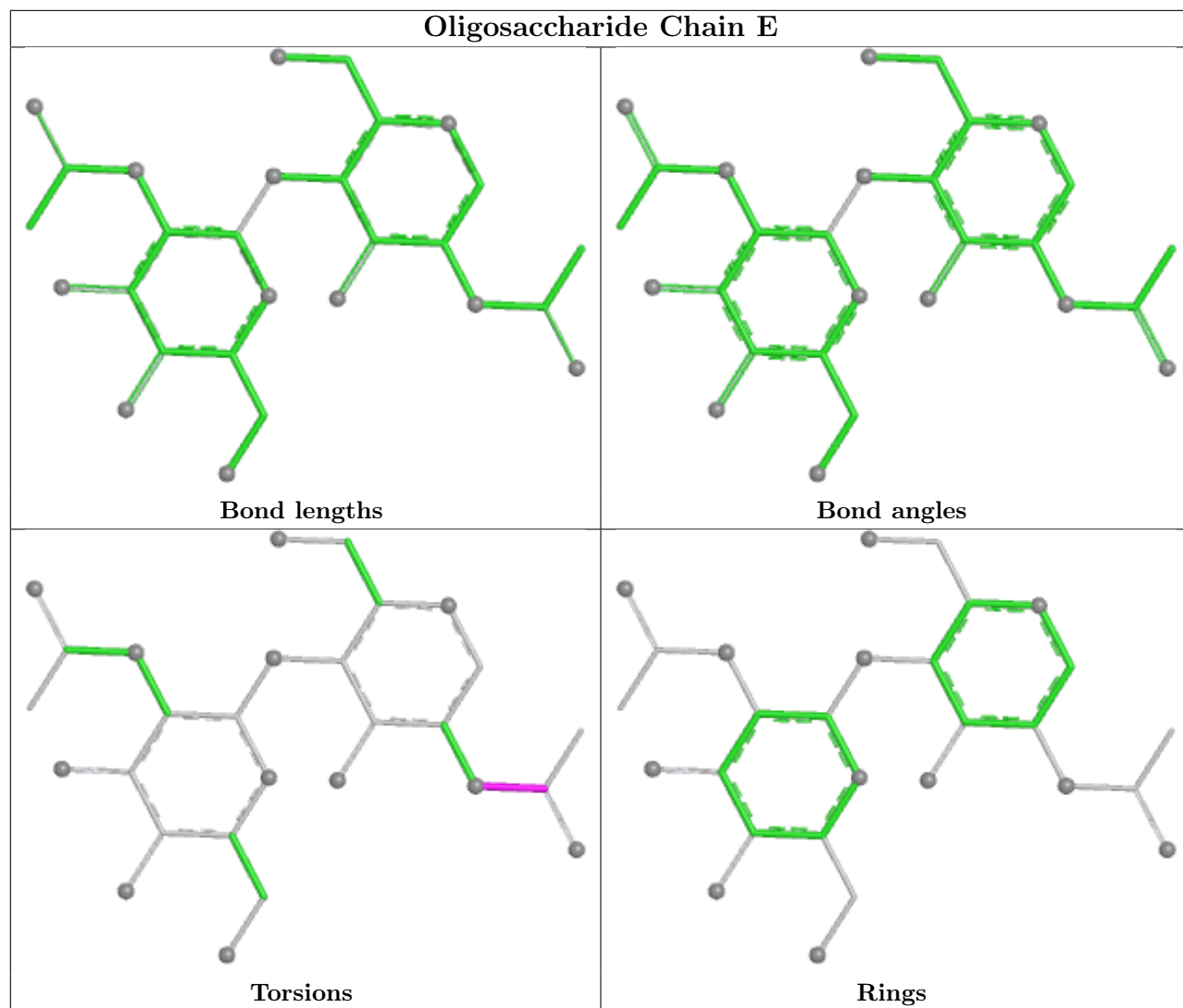
There are no ring outliers.

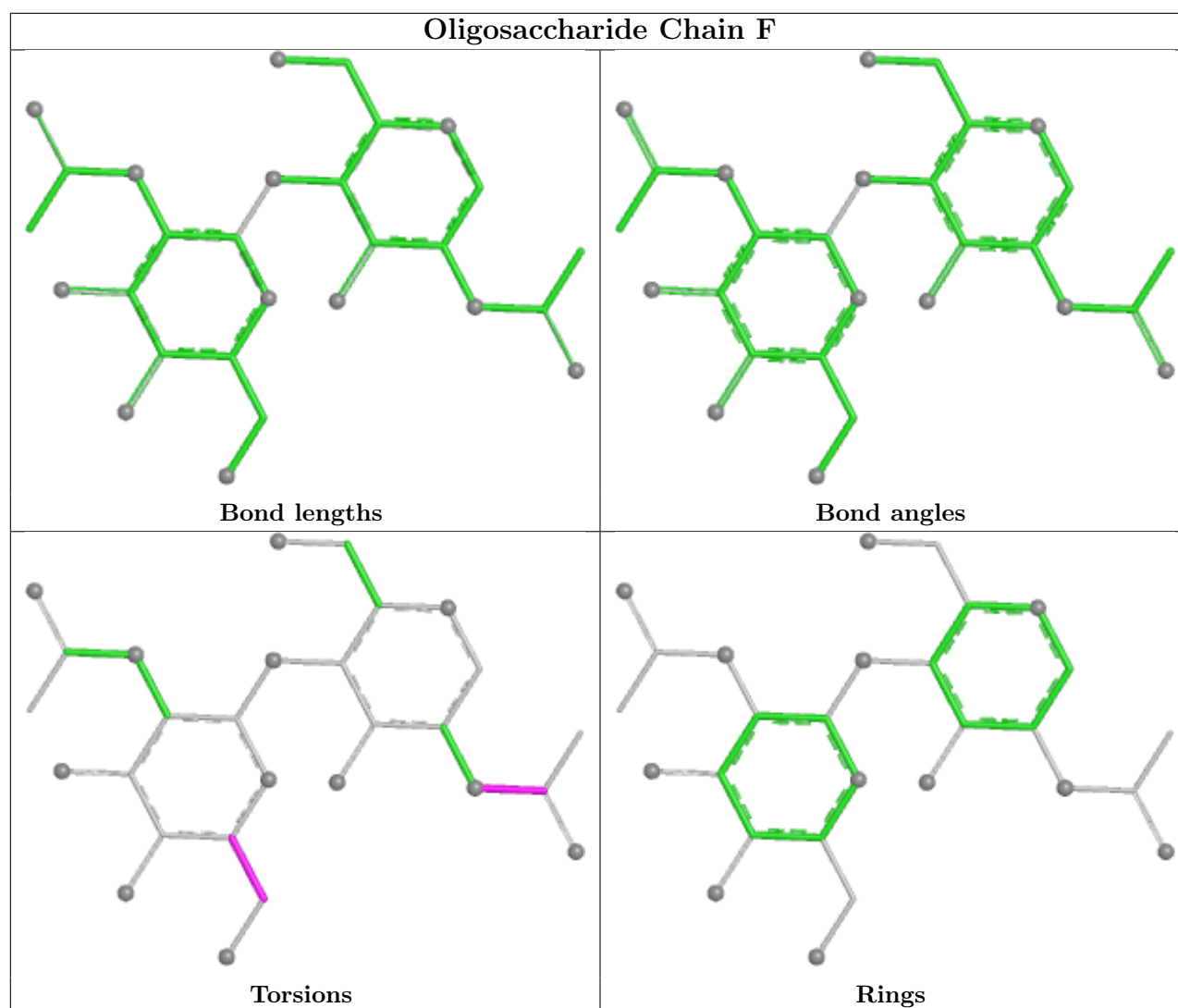
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	3	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](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
6	NAG	2	401	1	14,14,15	0.21	0	17,19,21	0.47	0
6	NAG	D	1101	2	14,14,15	0.26	0	17,19,21	0.42	0
8	HEM	B	201	4	50,50,50	1.38	6 (12%)	67,82,82	1.15	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	HEM	A	201	3	50,50,50	1.39	7 (14%)	67,82,82	1.09	5 (7%)
6	NAG	2	402	1	14,14,15	0.30	0	17,19,21	0.56	0
6	NAG	G	1101	2	14,14,15	0.20	0	17,19,21	0.43	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
6	NAG	2	401	1	-	2/6/23/26	0/1/1/1
6	NAG	D	1101	2	-	2/6/23/26	0/1/1/1
8	HEM	B	201	4	-	2/14/54/54	-
8	HEM	A	201	3	-	3/14/54/54	-
6	NAG	2	402	1	-	2/6/23/26	0/1/1/1
6	NAG	G	1101	2	-	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	201	HEM	FE-NB	3.43	2.05	1.94
8	A	201	HEM	FE-ND	3.22	2.04	1.94
8	B	201	HEM	FE-ND	3.19	2.04	1.94
8	A	201	HEM	FE-NA	3.05	2.05	1.95
8	A	201	HEM	CAB-C3B	3.05	1.55	1.47
8	B	201	HEM	CAC-C3C	3.04	1.55	1.47
8	A	201	HEM	CAC-C3C	2.98	1.55	1.47
8	B	201	HEM	CAB-C3B	2.94	1.55	1.47
8	A	201	HEM	FE-NB	2.93	2.03	1.94
8	A	201	HEM	FE-NC	2.92	2.04	1.95
8	B	201	HEM	FE-NA	2.53	2.03	1.95
8	B	201	HEM	FE-NC	2.50	2.03	1.95
8	A	201	HEM	C2A-C3A	-2.01	1.33	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	201	HEM	C3B-C2B-C1B	2.99	108.66	106.41
8	B	201	HEM	C1B-NB-C4B	2.48	108.14	105.21
8	A	201	HEM	C4D-ND-C1D	2.34	107.97	105.21
8	B	201	HEM	C3B-C4B-NB	-2.25	107.85	109.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	201	HEM	C2A-C1A-NA	-2.24	107.67	110.15
8	A	201	HEM	C3D-C4D-ND	-2.23	107.72	110.17
8	A	201	HEM	C3B-C2B-C1B	2.14	108.02	106.41
8	B	201	HEM	C2A-C1A-NA	-2.13	107.79	110.15
8	B	201	HEM	C4D-ND-C1D	2.11	107.71	105.21
8	A	201	HEM	C1B-NB-C4B	2.01	107.58	105.21

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	2	402	NAG	O5-C5-C6-O6
6	2	402	NAG	C4-C5-C6-O6
6	D	1101	NAG	C4-C5-C6-O6
6	D	1101	NAG	O5-C5-C6-O6
6	2	401	NAG	O5-C5-C6-O6
8	B	201	HEM	C4B-C3B-CAB-CBB
8	A	201	HEM	C1A-C2A-CAA-CBA
8	A	201	HEM	C2A-CAA-CBA-CGA
8	B	201	HEM	C3D-CAD-CBD-CGD
6	2	401	NAG	C4-C5-C6-O6
8	A	201	HEM	C3A-C2A-CAA-CBA

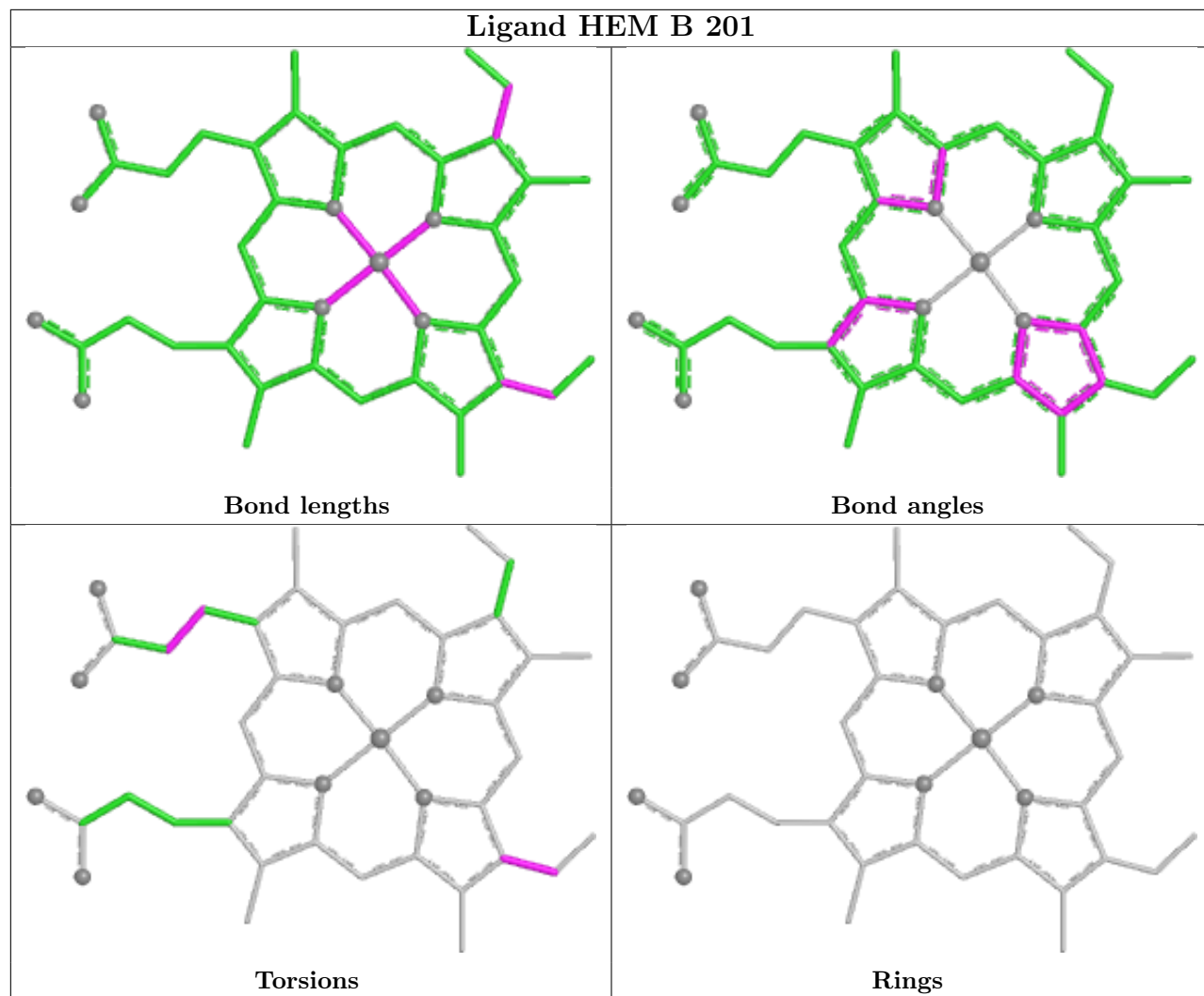
There are no ring outliers.

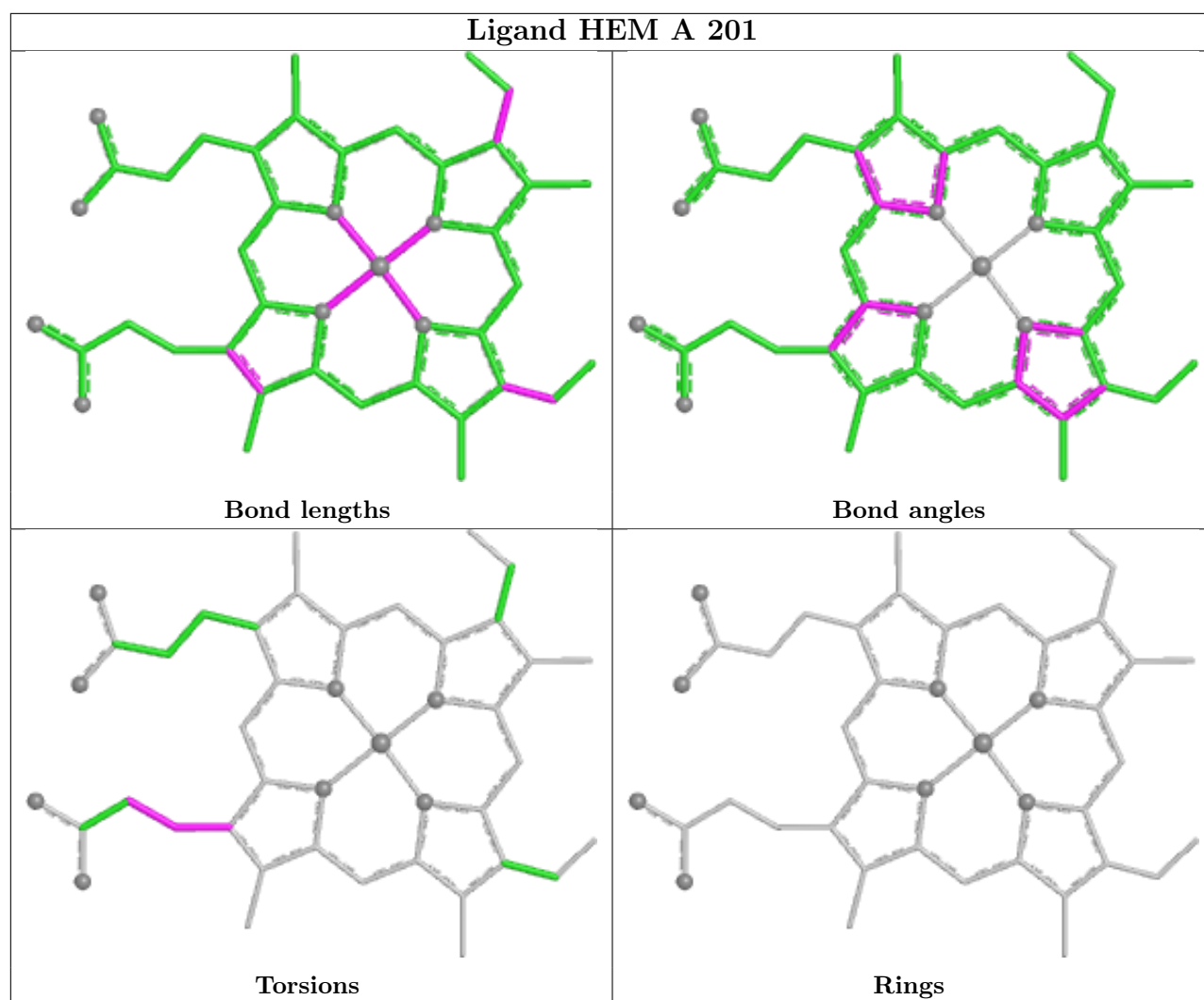
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	2	401	NAG	1	0
8	B	201	HEM	2	0
8	A	201	HEM	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 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.

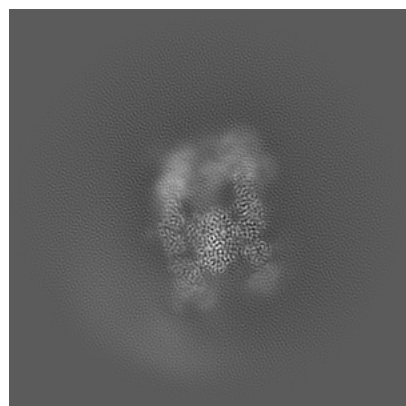
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38490. These allow visual inspection of the internal detail of the map and identification of artifacts.

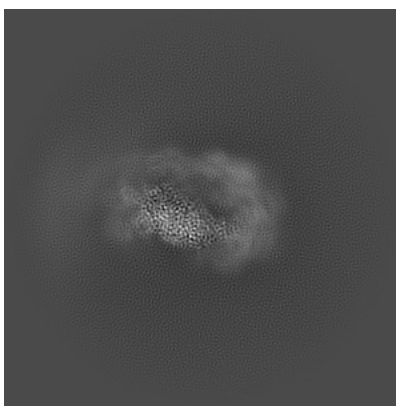
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

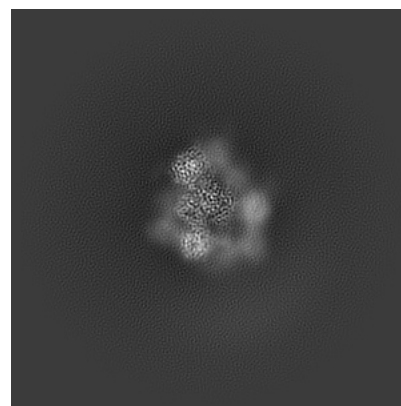
6.1.1 Primary map



X

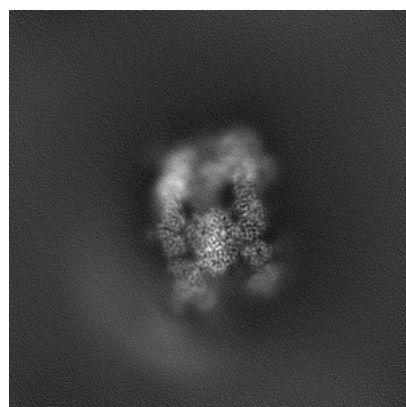


Y

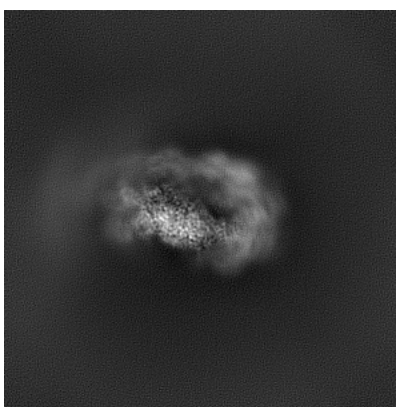


Z

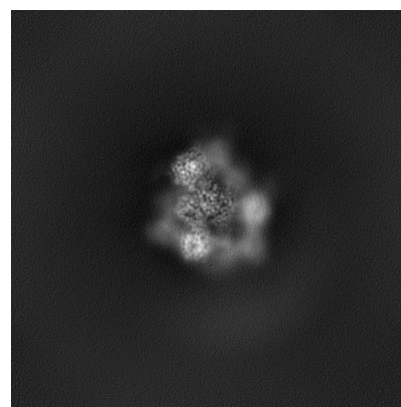
6.1.2 Raw map



X



Y

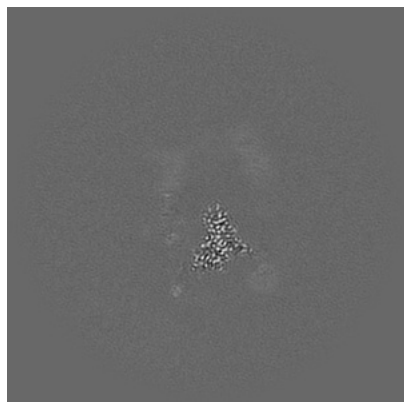


Z

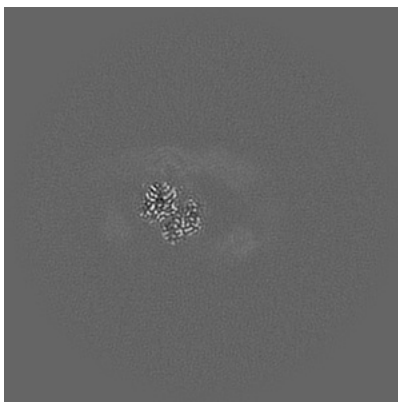
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 180

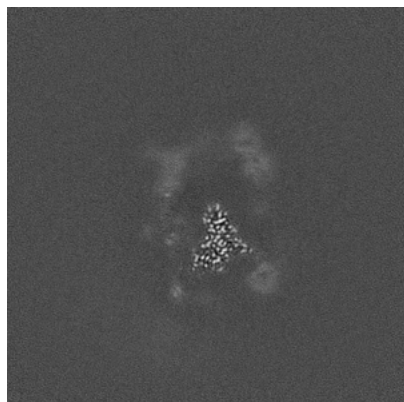


Y Index: 180

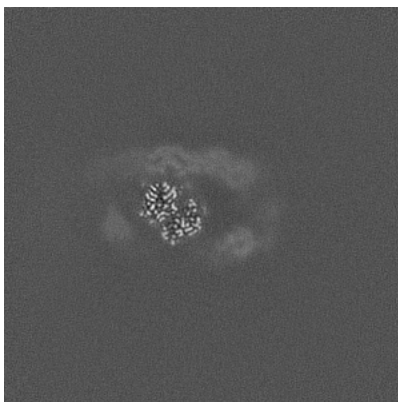


Z Index: 180

6.2.2 Raw map



X Index: 180



Y Index: 180

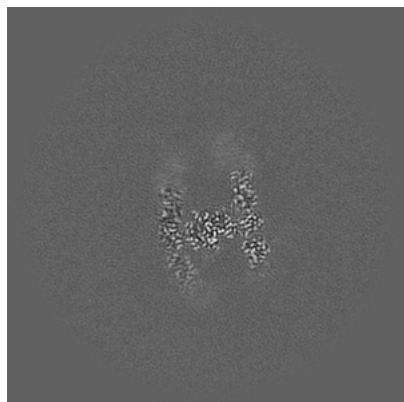


Z Index: 180

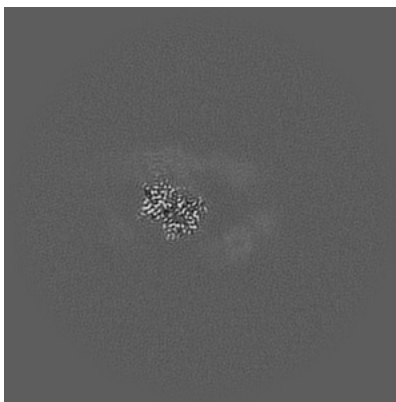
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

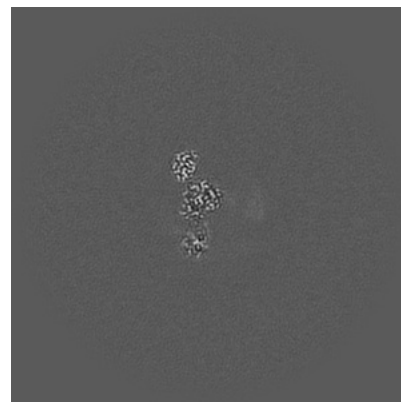
6.3.1 Primary map



X Index: 163

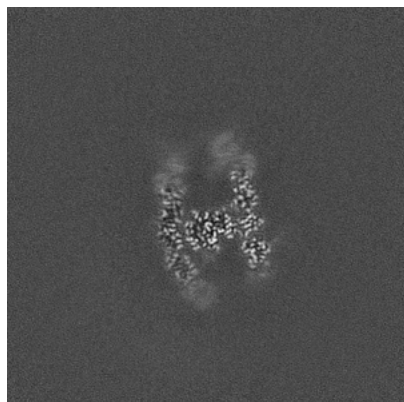


Y Index: 186

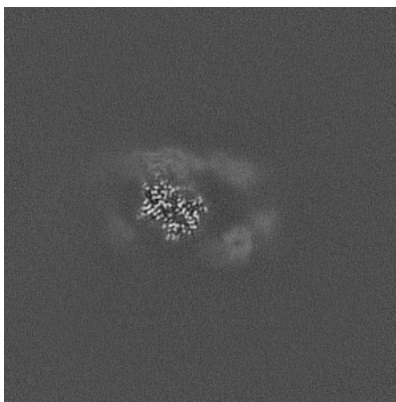


Z Index: 167

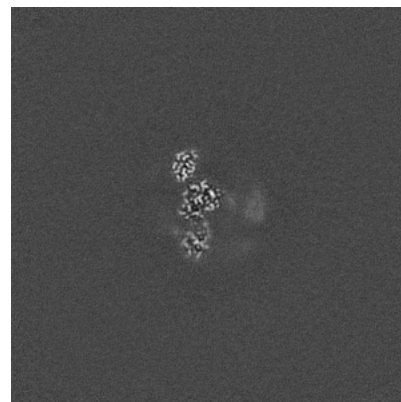
6.3.2 Raw map



X Index: 163



Y Index: 186

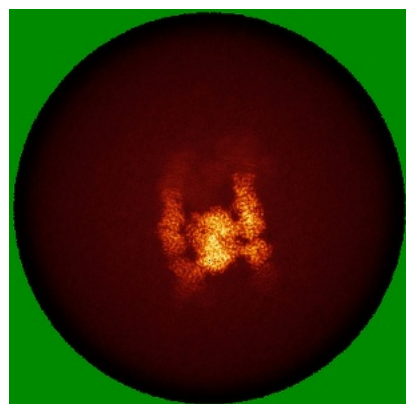


Z Index: 167

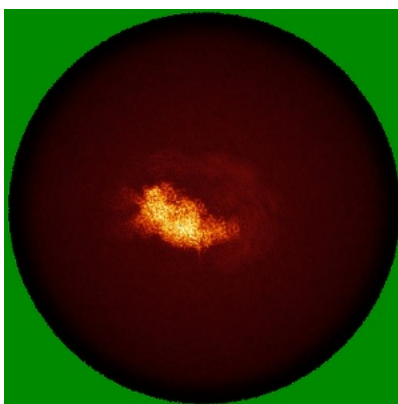
The images above show the largest variance slices of the map in three orthogonal directions.

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

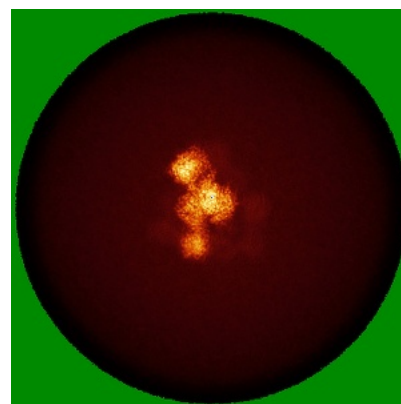
6.4.1 Primary map



X

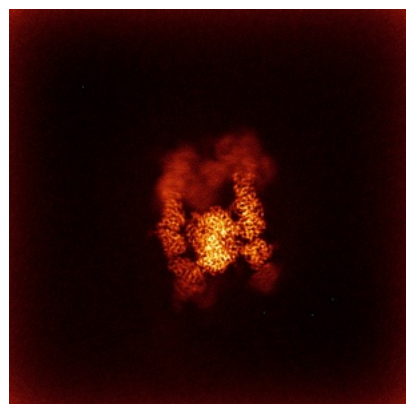


Y

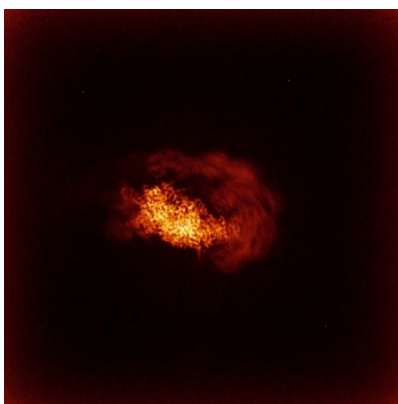


Z

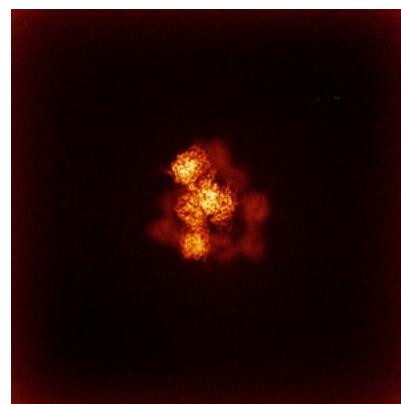
6.4.2 Raw map



X



Y

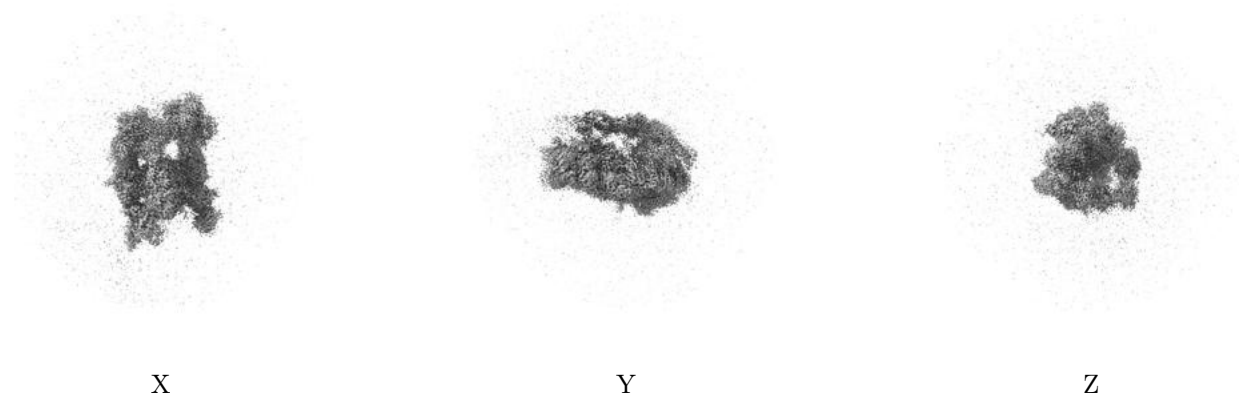


Z

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

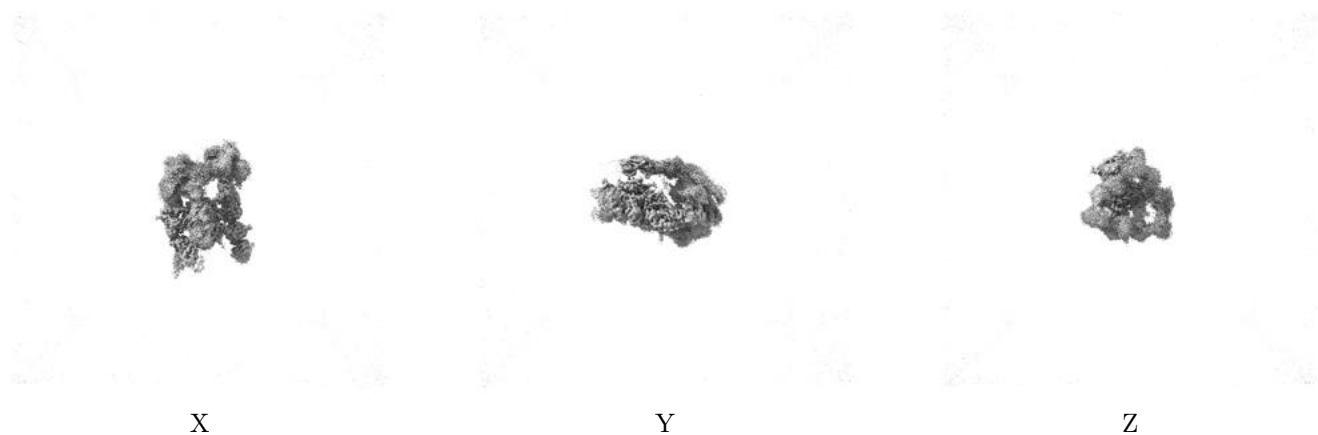
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

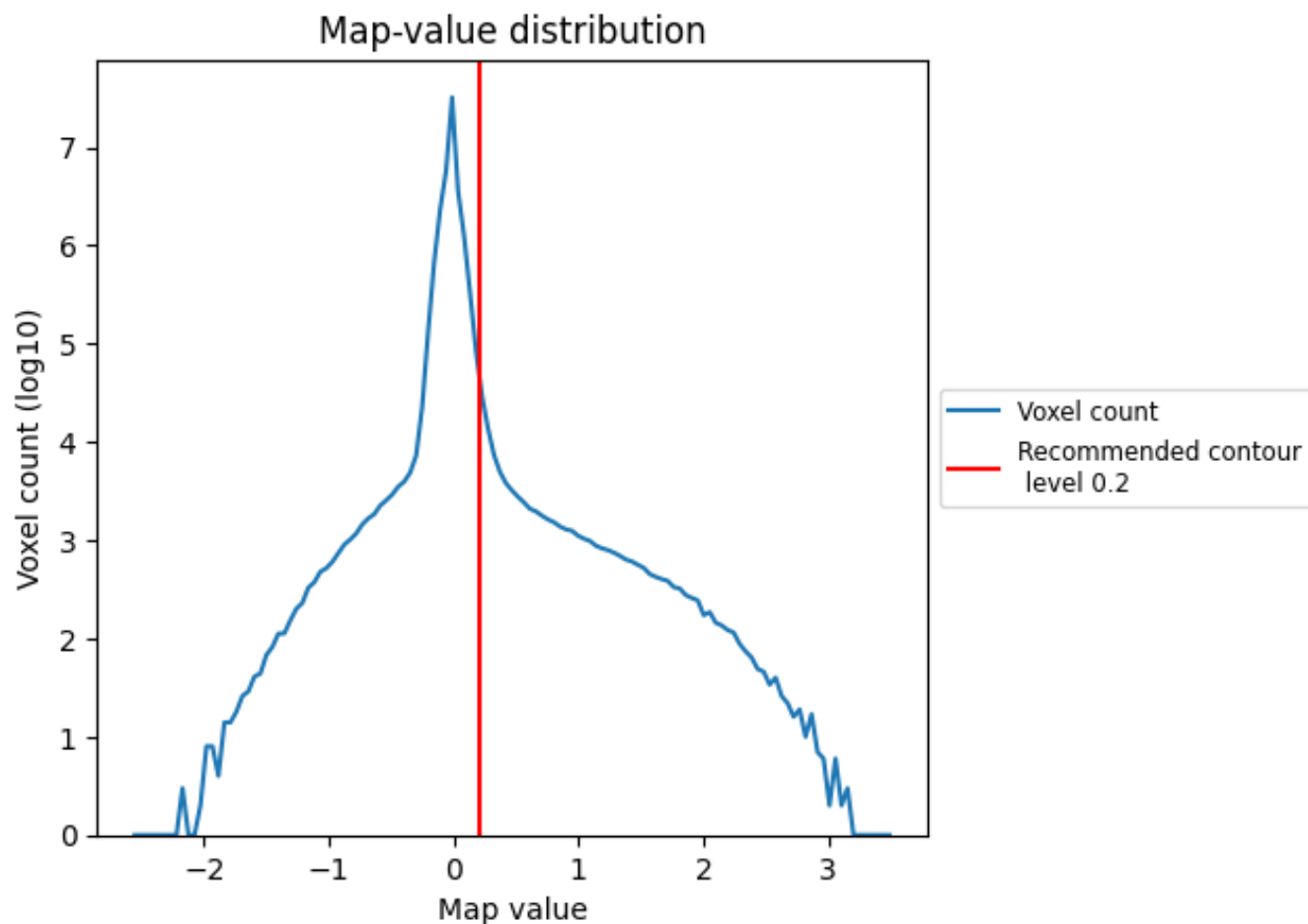
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

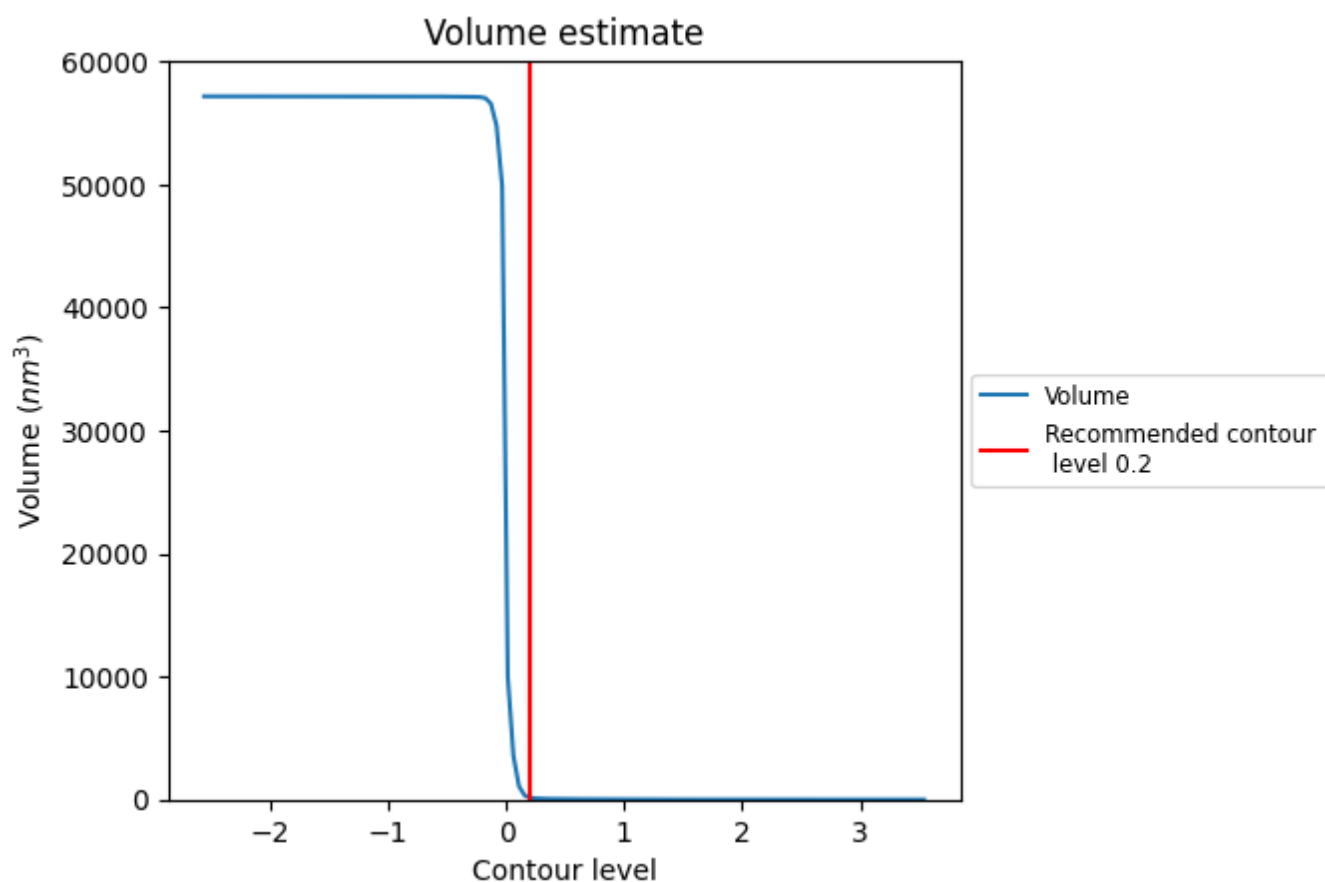
This section contains the results of statistical analysis of the map.

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.

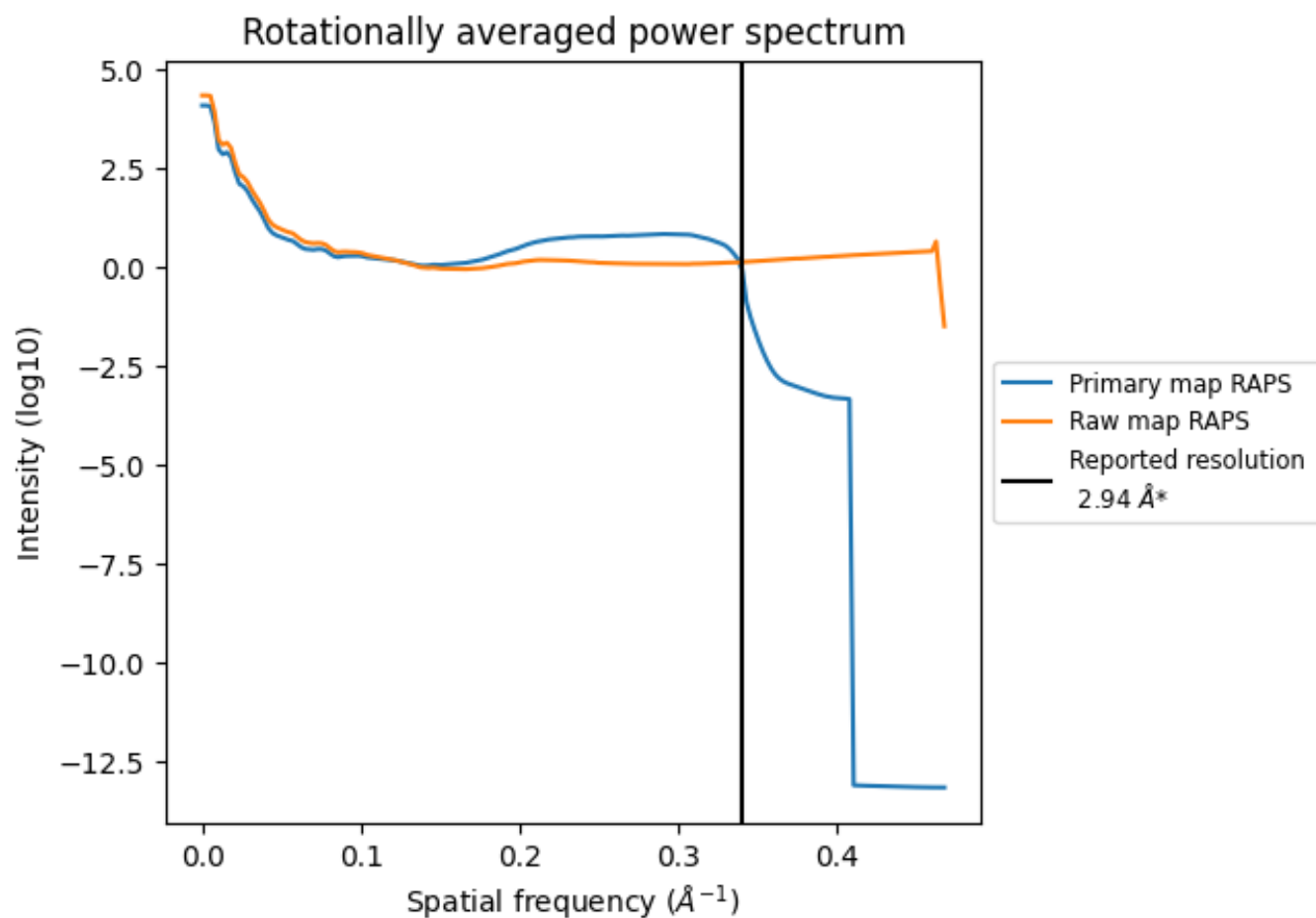
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 172 nm³; 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 ⓘ

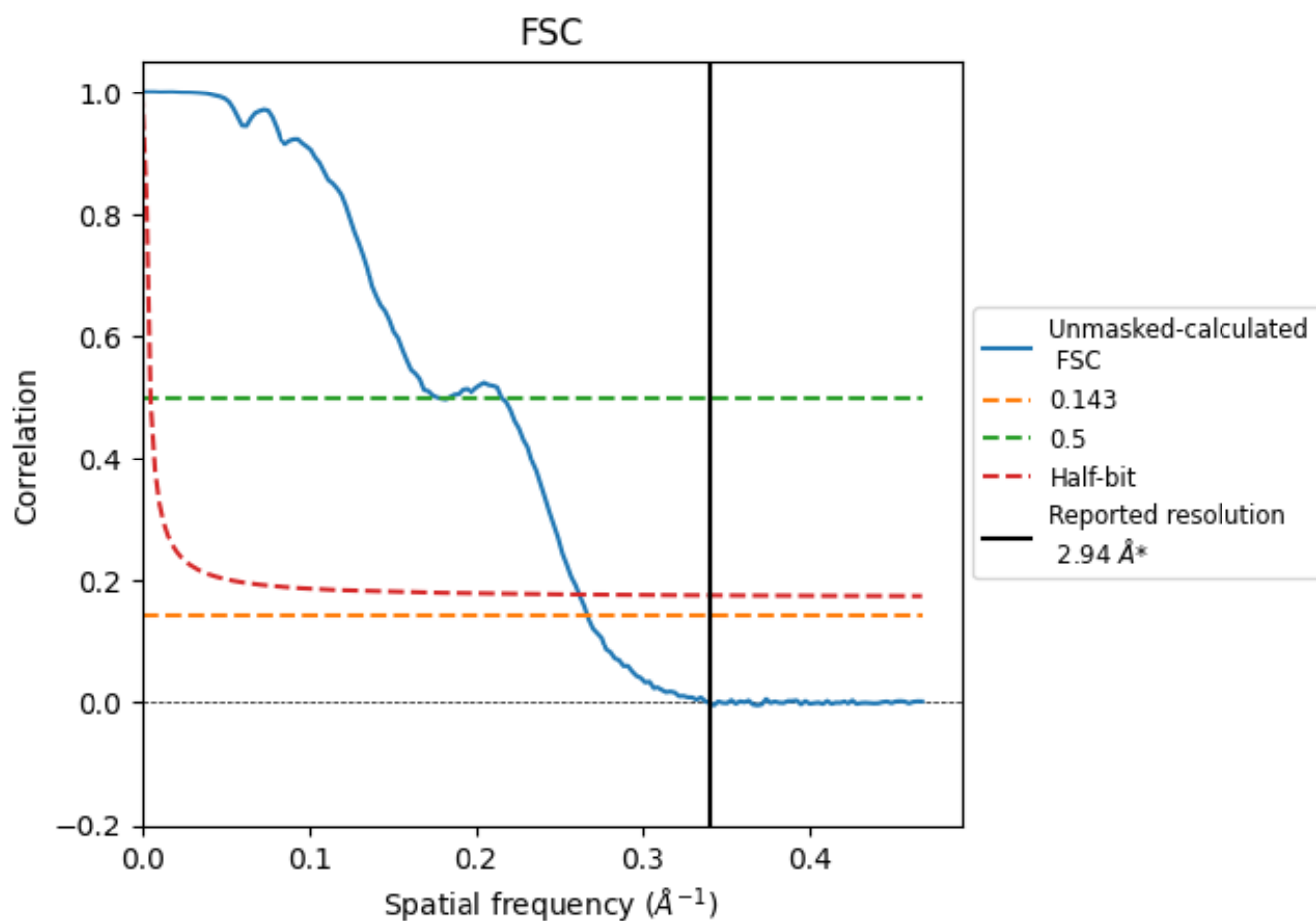


*Reported resolution corresponds to spatial frequency of 0.340 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.340 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

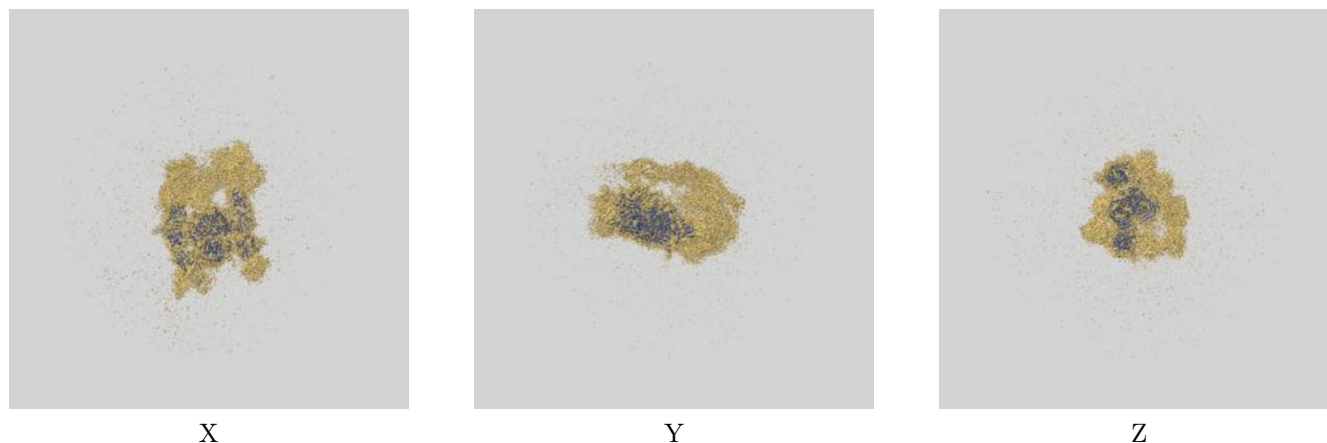
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.75	5.67	3.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 2.94 by more than 10 %

9 Map-model fit [i](#)

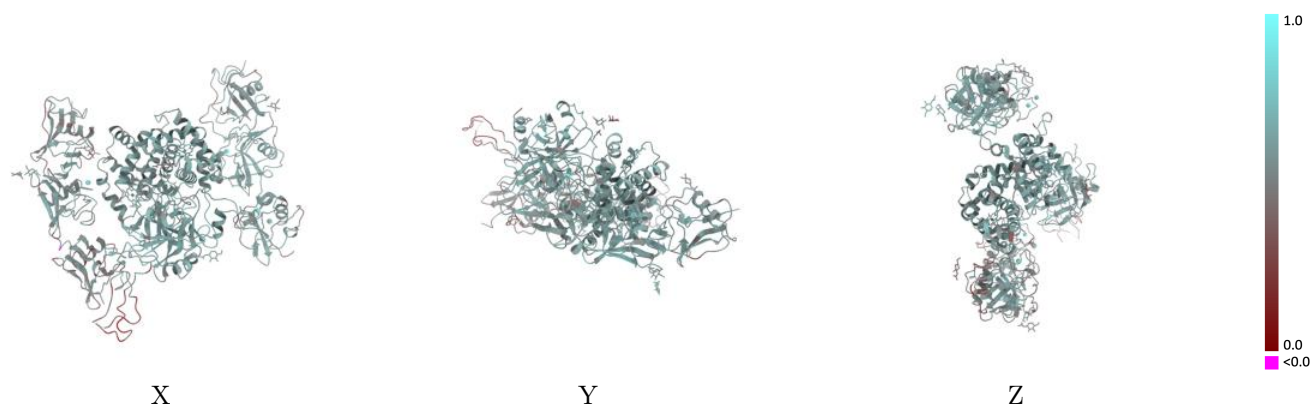
This section contains information regarding the fit between EMDB map EMD-38490 and PDB model 8XMW. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



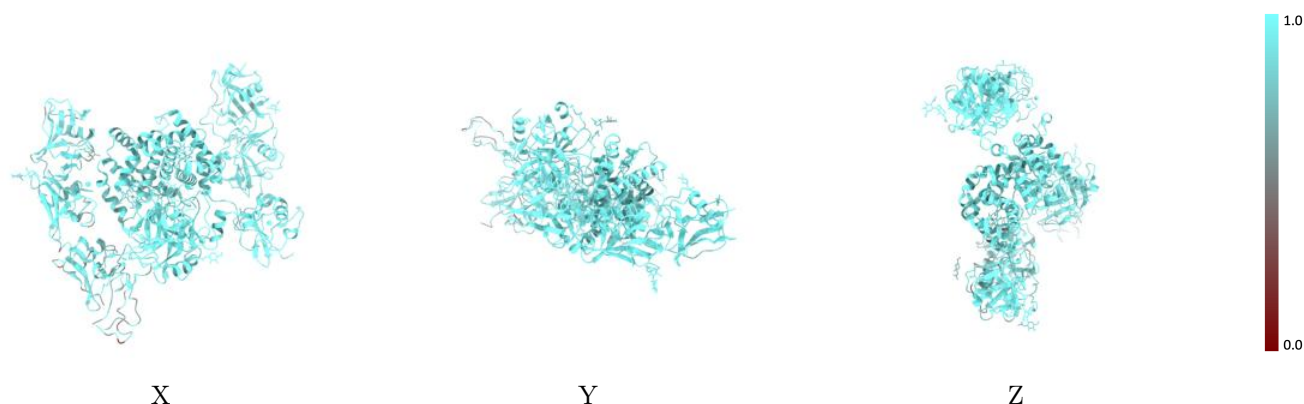
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



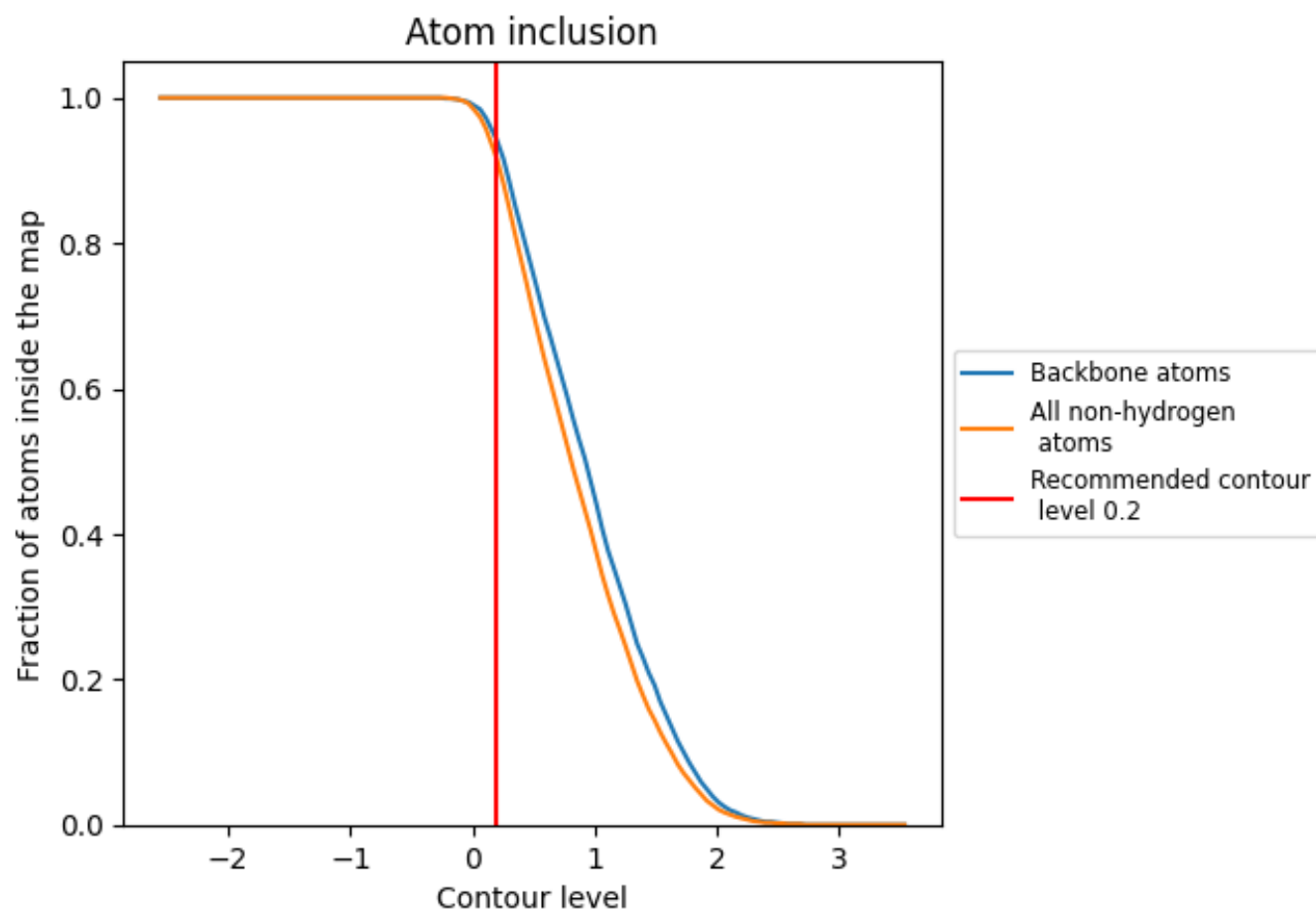
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9160	0.5520
2	0.9210	0.5630
A	0.9630	0.5970
B	0.9410	0.5860
C	0.8210	0.4280
D	0.8590	0.4970
E	0.8930	0.5180
F	0.9640	0.5930
G	0.9370	0.5630

1.0

0.0

<0.0