



wwPDB EM Validation Summary Report ⓘ

Aug 27, 2026 – 04:42 am BST

PDB ID : 9FMU / pdb_00009fmu
EMDB ID : EMD-50570
Title : Cryo-EM structure of human CD163 SRCR1-9 in complex with haptoglobin-hemoglobin
Authors : Andersen, C.B.F.; Kollman, J.M.
Deposited on : 2024-06-07
Resolution : 4.46 Å(reported)

This is a wwPDB EM Validation Summary 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.50

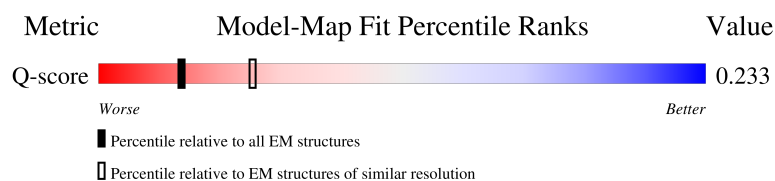
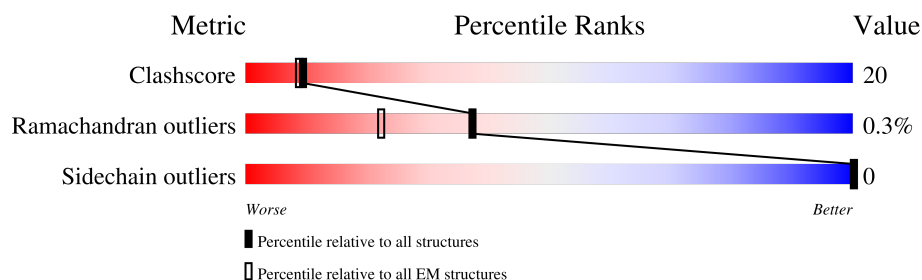
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.46 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	3001 (3.96 - 4.96)

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	142	
2	B	147	
3	C	347	
4	D	1036	

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Mol	Chain	Length	Quality of chain
4	E	1036	48%41%21%38%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14763 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 Hemopressin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	141	Total	C	N	O	S	0	0
			1069	685	187	194	3		

- Molecule 2 is a protein called Spinorphin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	146	Total	C	N	O	S	0	0
			1123	724	195	201	3		

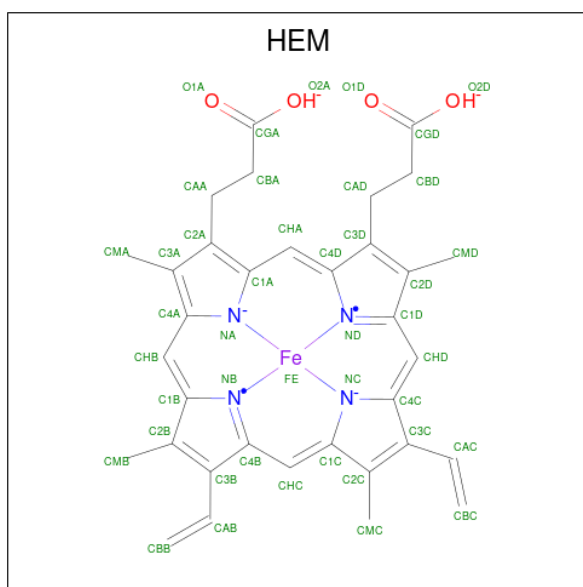
- Molecule 3 is a protein called Isoform 2 of Haptoglobin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	254	Total	C	N	O	S	0	0
			1982	1265	334	373	10		

- Molecule 4 is a protein called Scavenger receptor cysteine-rich type 1 protein M130.

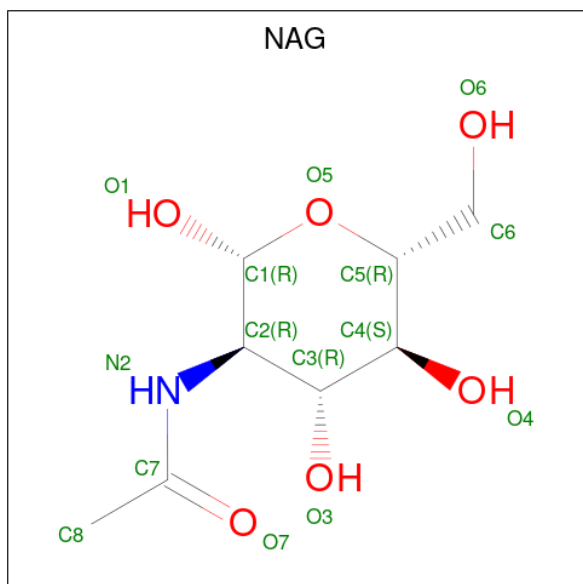
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	738	Total	C	N	O	S	0	0
			5585	3433	1009	1081	62		
4	E	640	Total	C	N	O	S	0	0
			4845	2977	880	935	53		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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

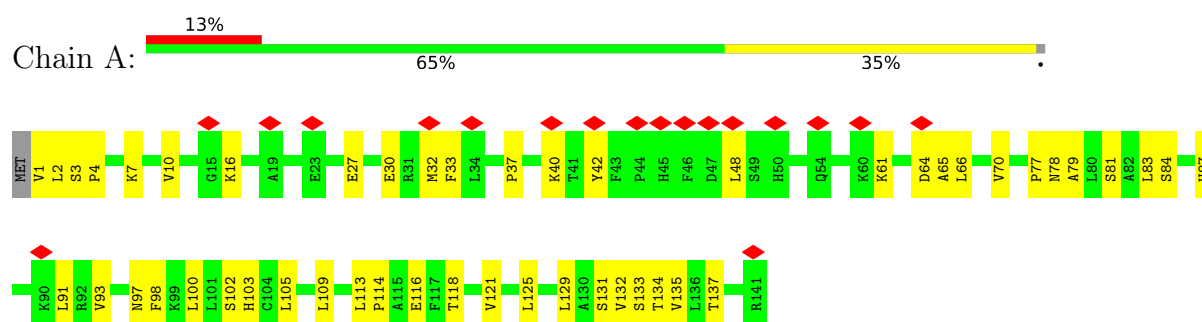
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	D	2	Total	Ca	0
			2	2	
7	E	1	Total	Ca	0
			1	1	

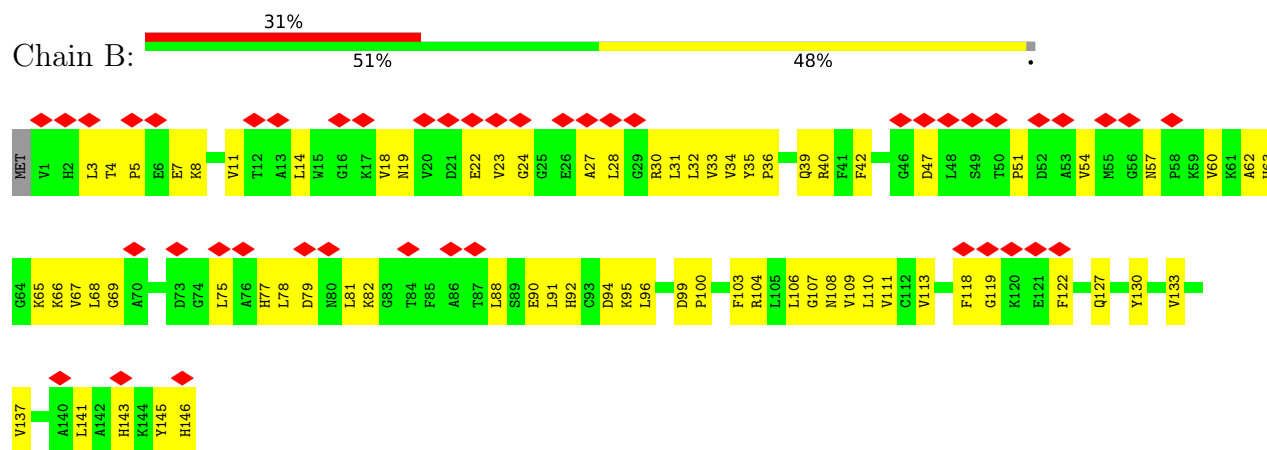
3 Residue-property plots [i](#)

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.

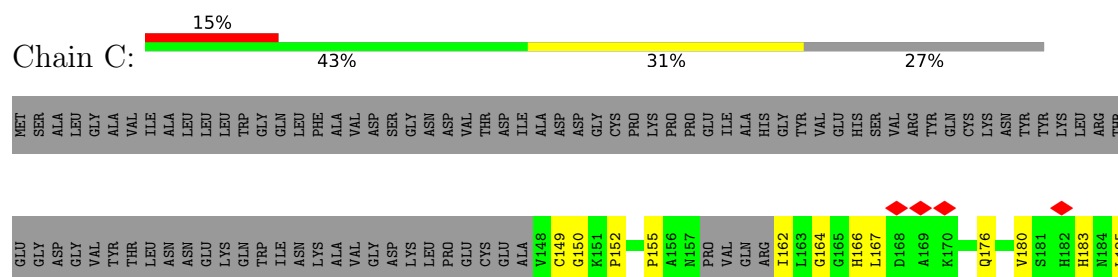
• Molecule 1: Hemopressin



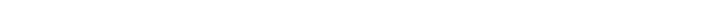
• Molecule 2: Spinorphin

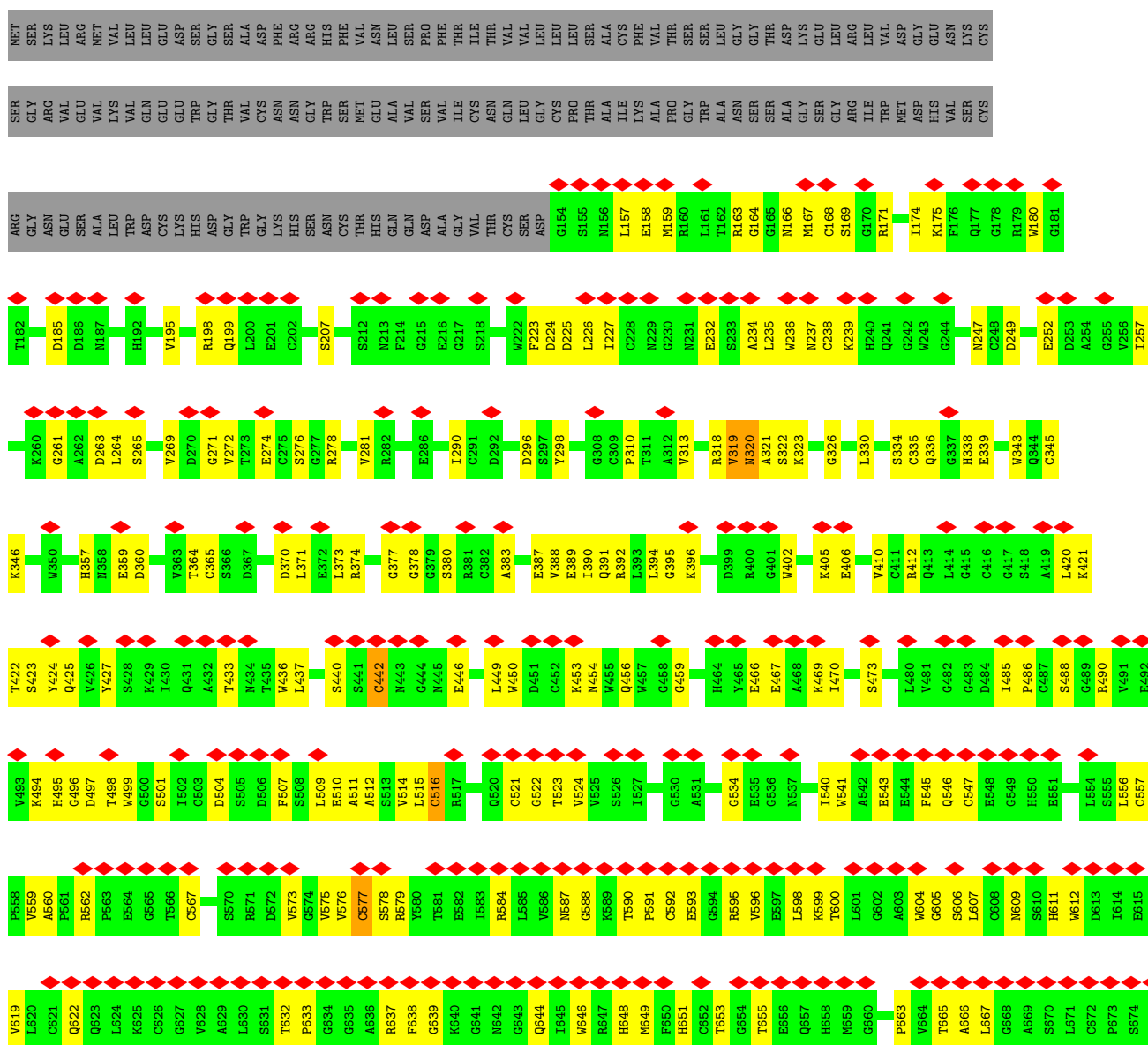


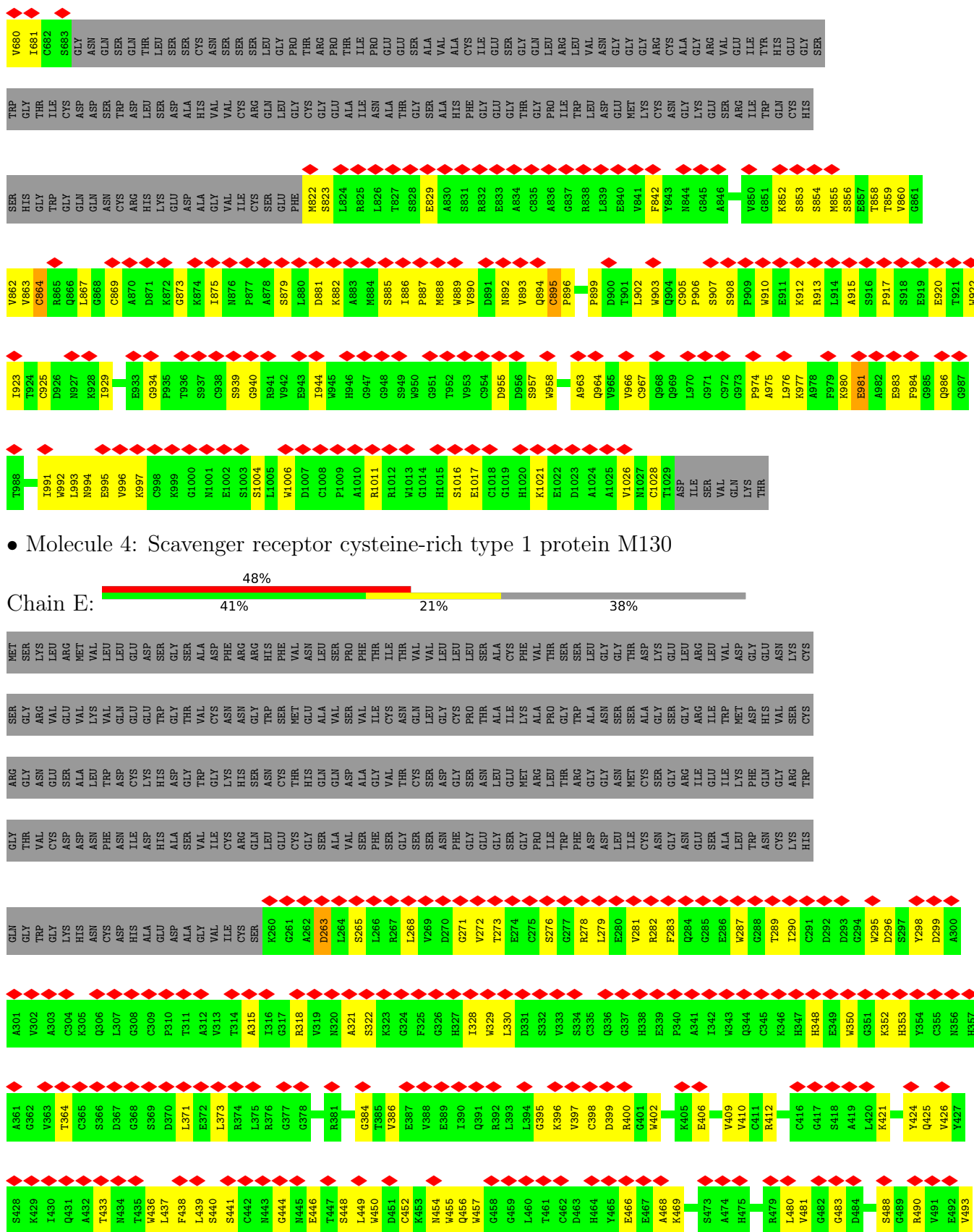
• Molecule 3: Isoform 2 of Haptoglobin



- Molecule 4: Scavenger receptor cysteine-rich type 1 protein M130

Chain D:  38% 44% 27% 29%





GLY	THR	ASN	L867	N807	D745	N885	L624	E564	K494
GLY	GLY	LYS	G868	C508	D746	Q886	K625	G565	H495
PRO	ARG	ILE	G869	R809	S747	Q887	G626	S566	D496
ILE	LEU	LEU	A870	H810	W748	Q888	G627	C567	G497
TRP	GLN	GLN	D871	K911	D749	T889	V628	C568	T498
LEU	GLU	GLU	K872	E912	L750	L890	A629	H699	W499
ASN	PRO	GLY	G873	D913	S751	SER	L630	S570	G500
VAL	THR	THR	K874	A814	D752	CYS	S631	R571	S501
LYS	SER	LYS	G875	G815	A753	ASN	T632	D572	I502
CYS	CYS	LYS	I875	V816	H754	SER	P633	G573	D504
LYS	SER	LYS	N876	I817	V755	SER	G634	G574	S505
GLY	GLY	ASN	P877	C818	W758	LEU	G635	V575	D506
ASN	ARG	VAL	A878	S819	Q759	GLY	A636	V576	F507
GLU	GLU	GLU	S879	E820	L760	PRO	R637	C577	S508
SER	SER	ILE	L880	F821	L761	THR	F638	S578	L509
LEU	LEU	TRP	D881	M822	G761	ARG	G639	R579	A512
TRP	TRP	HIS	K882	S823	G762	PRO	K640	T581	C516
ASP	GLY	GLY	A883	L824	G763	THR	G641	I582	R517
CYS	GLY	PRO	M884	R825	E764	ILE	N642	I583	C516
PRO	SER	SER	G885	L826	A765	GLU	G643	R584	R517
ALA	TRP	ALA	T827	G827	I766	GLU	Q644	L585	Q520
ARG	GLY	ARG	I886	R828	N767	SER	I645	V586	C521
TRP	VAL	VAL	P887	E829	A768	ALA	W646	N587	G522
GLY	CYS	CYS	M888	A830	T769	VAL	R647	G588	C521
HIS	ASP	ASP	W889	S831	A772	ALA	H648	C589	G522
SER	ASP	SER	D891	R832	H773	ILE	G649	K589	L528
GLU	SER	TRP	N892	E833	F774	GLU	M649	T590	G529
CYS	TRP	ASP	G893	A834	G775	SER	F650	P591	G530
HIS	LEU	LYS	V893	C835	E776	GLY	H651	C592	A531
LYS	ASP	ASP	Q894	C836	G777	Q718	C652	E593	H532
GLU	ASP	ALA	C895	A836	T778	L719	T653	G594	F533
ALA	GLN	ALA	P896	R837	G779	R720	G654	R595	G534
ALA	VAL	VAL	K897	R838	G780	L721	T655	V596	E535
VAL	VAL	CYS	G898	L839	P780	T722	G656	E597	G536
ASN	CYS	ASN	P899	E840	I781	N723	E657	L598	N537
CYS	GLN	GLN	D900	W841	W782	G724	Q657	K599	G538
THR	GLN	LEU	T901	F942	L783	G725	H658	T600	Q539
ASP	LEU	GLY	L902	V943	D784	G726	M659	L601	I540
ILE	GLY	CYS	W903	N844	E785	R727	G660	G602	V541
SER	VAL	PRO	Q904	G845	W786	C728	D661	A603	A542
VAL	GLN	ALA	C905	A846	K787	A729	C662	W604	E543
LYS	LYS	LEU	P906	W847	G788	G730	P663	G605	F543
THR	LYS	ALA	S907	G848	N789	R731	V664	S606	E544
	ALA	PHE	S908	T949	G790	V732	T665	L607	F545
	LYS	LYS	P909	V850	K791	E733	A666	C508	Q546
	GLU	ALA	W910	G851	E792	I734	L667	N609	C547
	ALA	ALA	E911	K952	G793	V735	G668	S610	E548
	PHE	GLY	K912	S853	S793	E737	A669	H611	G549
	GLY	GLN	R913	S854	R794	G738	S670	W612	H550
			L914	M855	I795	S739	L671	D613	E551
			A915	S856	W796	W740	P673	I614	S552
			S916	E857	Q797	G741	G674	E615	L556
			P917	T858	C798	T742	S674	D616	C557
			S918	V859	C799	I743	G675	H617	P558
			V860	V860	S800	G744	Q676	H618	V559
			E919	G861	S801	I743	Q676	V619	A560
			E920	V862	H801	G744	V677	L620	P561
			V863	V863	G802	C744	A678	G521	R562
			T921	R865	W803	G804	G682	Q622	P563
			W922	C864	G804	Q805	G682	Q621	
			I923	R865	Q805	Q806	G684	Q623	
			T924	C866	Q806	Q806			
			C925						
			D926						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38511	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 ($e^-/\text{\AA}^2$)	90	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.315	Depositor
Minimum map value	-1.605	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	1	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, NAG, 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	A	0.24	0/1097	0.71	0/1491
2	B	0.30	0/1153	0.75	0/1566
3	C	0.25	0/2029	0.64	1/2756 (0.0%)
4	D	0.23	0/5714	0.74	13/7740 (0.2%)
4	E	0.21	0/4955	0.68	4/6712 (0.1%)
All	All	0.23	0/14948	0.71	18/20265 (0.1%)

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
4	D	0	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	557	CYS	CA-CB-SG	9.18	135.51	114.40
4	E	547	CYS	CA-CB-SG	7.73	132.19	114.40
4	D	547	CYS	CA-CB-SG	7.62	131.94	114.40
4	D	516	CYS	CA-CB-SG	6.69	129.79	114.40
4	D	547	CYS	CB-CA-C	6.19	120.92	109.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	442	CYS	Peptide

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	1069	0	1072	41	0
2	B	1123	0	1118	68	0
3	C	1982	0	1955	87	0
4	D	5585	0	5214	218	0
4	E	4845	0	4541	173	0
5	A	43	0	30	6	0
5	B	43	0	30	5	0
6	C	28	0	26	0	0
6	D	28	0	26	2	0
6	E	14	0	13	0	0
7	D	2	0	0	0	0
7	E	1	0	0	0	0
All	All	14763	0	14025	578	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 20.

The worst 5 of 578 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)
4:D:590:THR:HG22	4:D:593:GLU:HG2	1.50	0.93
4:D:986:GLN:HE22	4:D:1021:LYS:HA	1.33	0.92
4:D:421:LYS:HG2	4:D:423:SER:H	1.40	0.85
3:C:349:ASP:OD1	3:C:350:THR:N	2.12	0.82
1:A:102:SER:HB2	1:A:129:LEU:HD13	1.62	0.82

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	139/142 (98%)	129 (93%)	10 (7%)	0	100	100
2	B	144/147 (98%)	139 (96%)	5 (4%)	0	100	100
3	C	250/347 (72%)	234 (94%)	16 (6%)	0	100	100
4	D	734/1036 (71%)	704 (96%)	27 (4%)	3 (0%)	30	67
4	E	636/1036 (61%)	609 (96%)	24 (4%)	3 (0%)	24	63
All	All	1903/2708 (70%)	1815 (95%)	82 (4%)	6 (0%)	37	71

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	686	GLN
4	D	263	ASP
4	D	320	ASN
4	D	422	THR
4	E	263	ASP

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	113/114 (99%)	113 (100%)	0	100	100
2	B	118/119 (99%)	118 (100%)	0	100	100
3	C	217/294 (74%)	217 (100%)	0	100	100
4	D	602/849 (71%)	602 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	521/849 (61%)	521 (100%)	0	100	100
All	All	1571/2225 (71%)	1571 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	876	ASN
4	E	347	HIS
4	D	986	GLN
4	E	539	GLN
4	D	231	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 ⓘ

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	C	1002	3	14,14,15	0.75	0	17,19,21	0.77	0
6	NAG	C	1001	3	14,14,15	0.76	0	17,19,21	0.80	0
6	NAG	D	2004	4	14,14,15	0.67	0	17,19,21	1.11	2 (11%)
6	NAG	E	1102	4	14,14,15	0.79	0	17,19,21	0.75	0
6	NAG	D	2003	4	14,14,15	0.74	0	17,19,21	0.91	0
5	HEM	B	201	2	50,50,50	1.43	6 (12%)	66,82,82	1.20	5 (7%)
5	HEM	A	201	1	50,50,50	1.31	6 (12%)	66,82,82	1.03	3 (4%)

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	C	1002	3	-	0/6/23/26	0/1/1/1
6	NAG	C	1001	3	-	0/6/23/26	0/1/1/1
6	NAG	D	2004	4	-	2/6/23/26	0/1/1/1
6	NAG	E	1102	4	-	2/6/23/26	0/1/1/1
6	NAG	D	2003	4	-	2/6/23/26	0/1/1/1
5	HEM	B	201	2	-	3/14/54/54	-
5	HEM	A	201	1	-	3/14/54/54	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	201	HEM	FE-ND	4.13	2.07	1.94
5	B	201	HEM	FE-NB	3.38	2.05	1.94
5	A	201	HEM	CAC-C3C	2.95	1.55	1.47
5	B	201	HEM	CAC-C3C	2.94	1.55	1.47
5	A	201	HEM	CAB-C3B	2.89	1.55	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	201	HEM	CMB-C2B-C1B	2.93	129.50	125.04
5	B	201	HEM	CAD-CBD-CGD	-2.62	107.97	113.60
5	B	201	HEM	C1B-NB-C4B	2.61	107.77	105.07
6	D	2004	NAG	O5-C1-C2	-2.49	107.36	111.29
5	A	201	HEM	C4D-ND-C1D	2.45	107.60	105.07

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

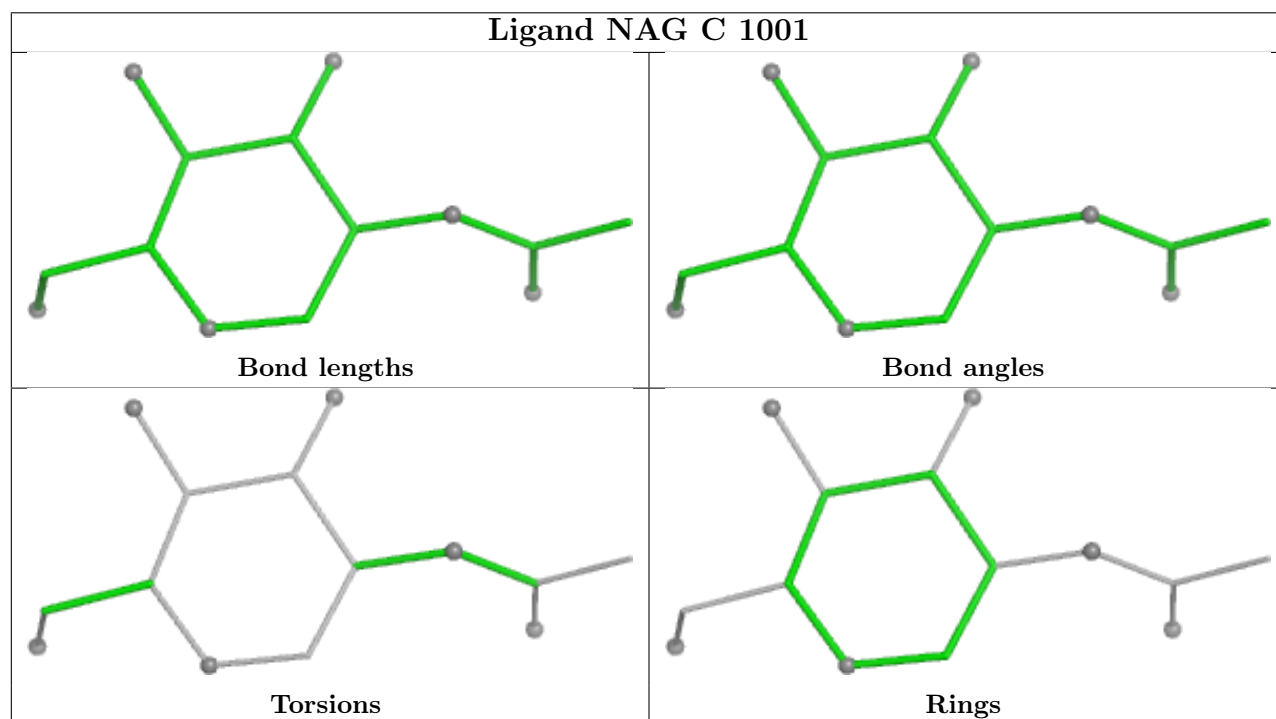
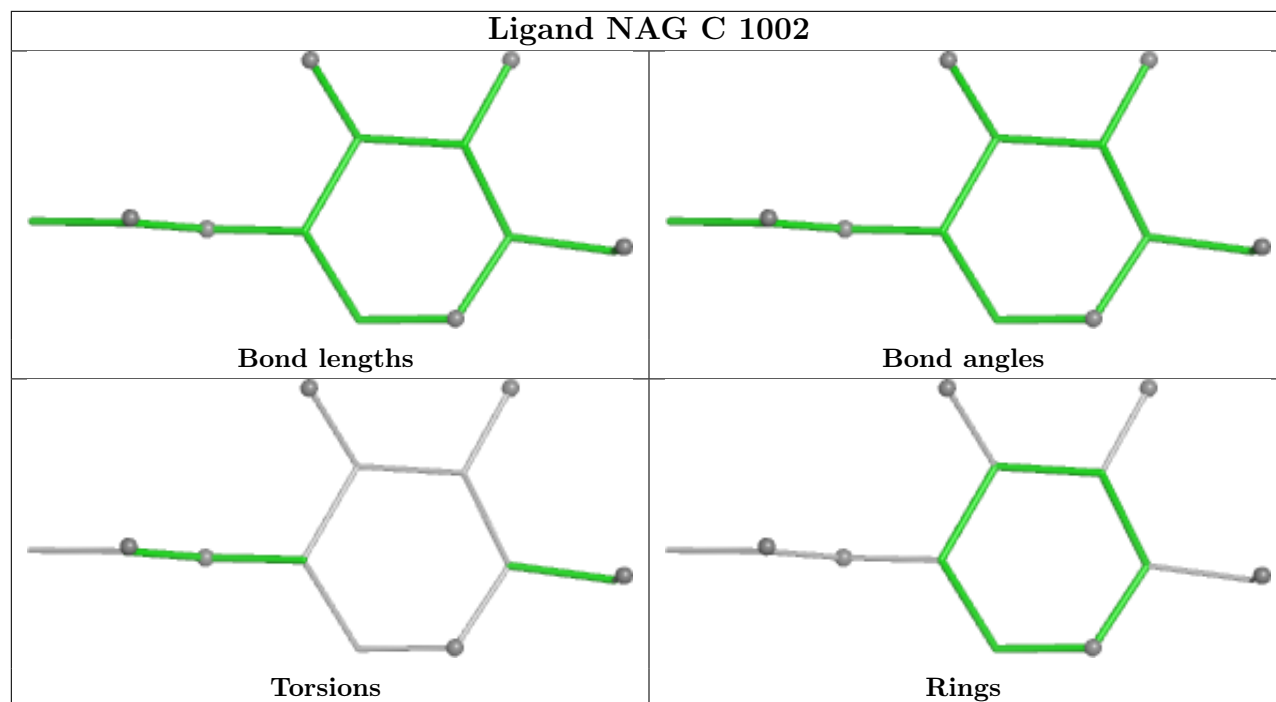
Mol	Chain	Res	Type	Atoms
6	D	2003	NAG	C8-C7-N2-C2
6	D	2003	NAG	O7-C7-N2-C2
6	D	2004	NAG	C8-C7-N2-C2
6	D	2004	NAG	O7-C7-N2-C2
6	E	1102	NAG	C8-C7-N2-C2

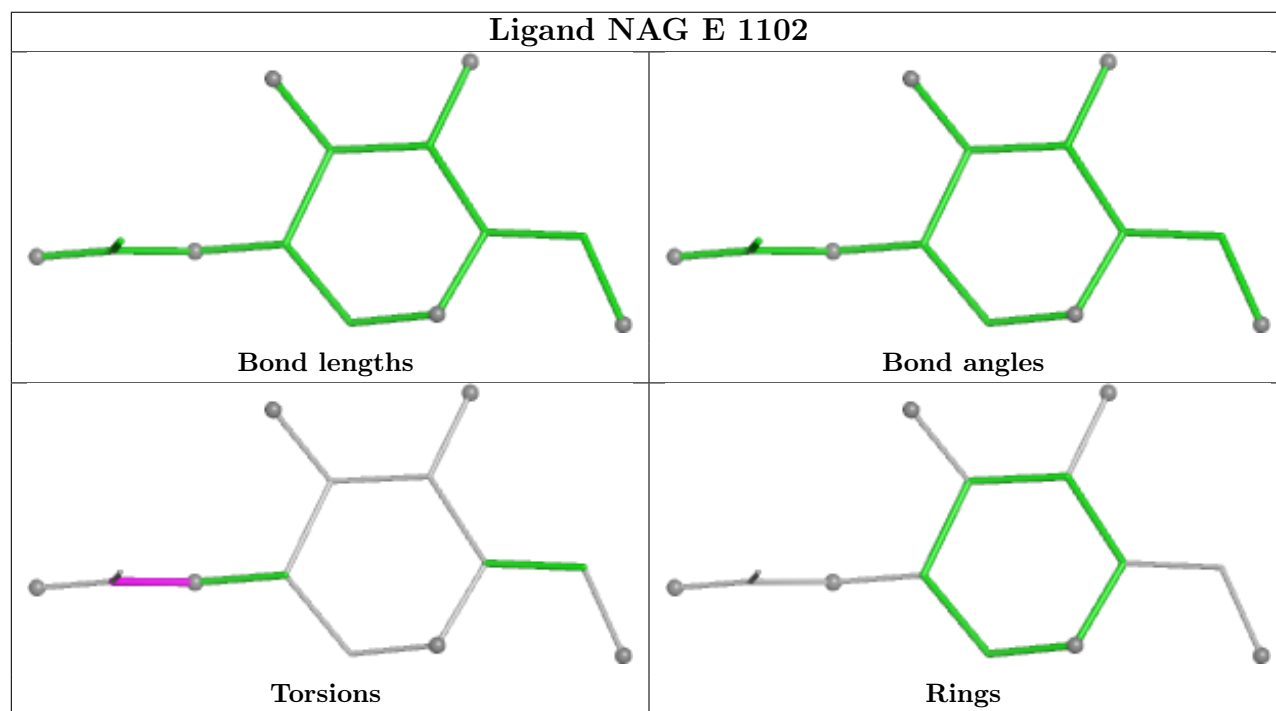
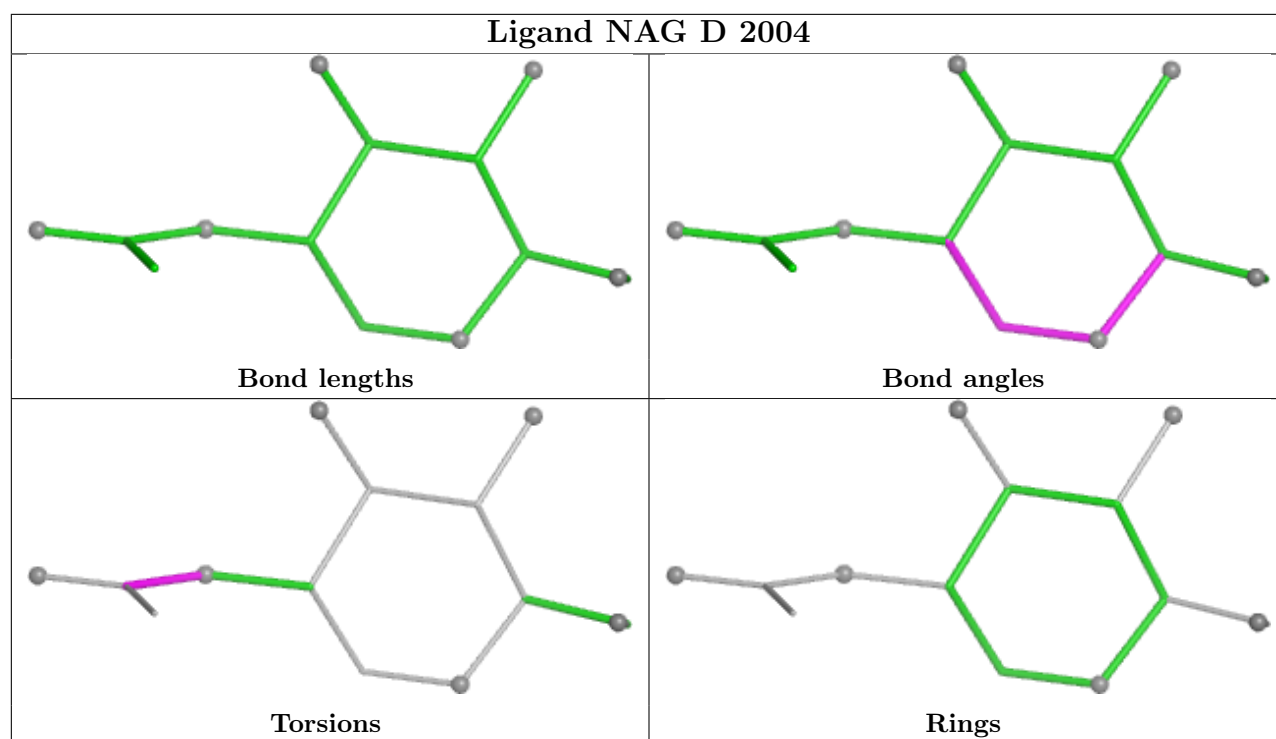
There are no ring outliers.

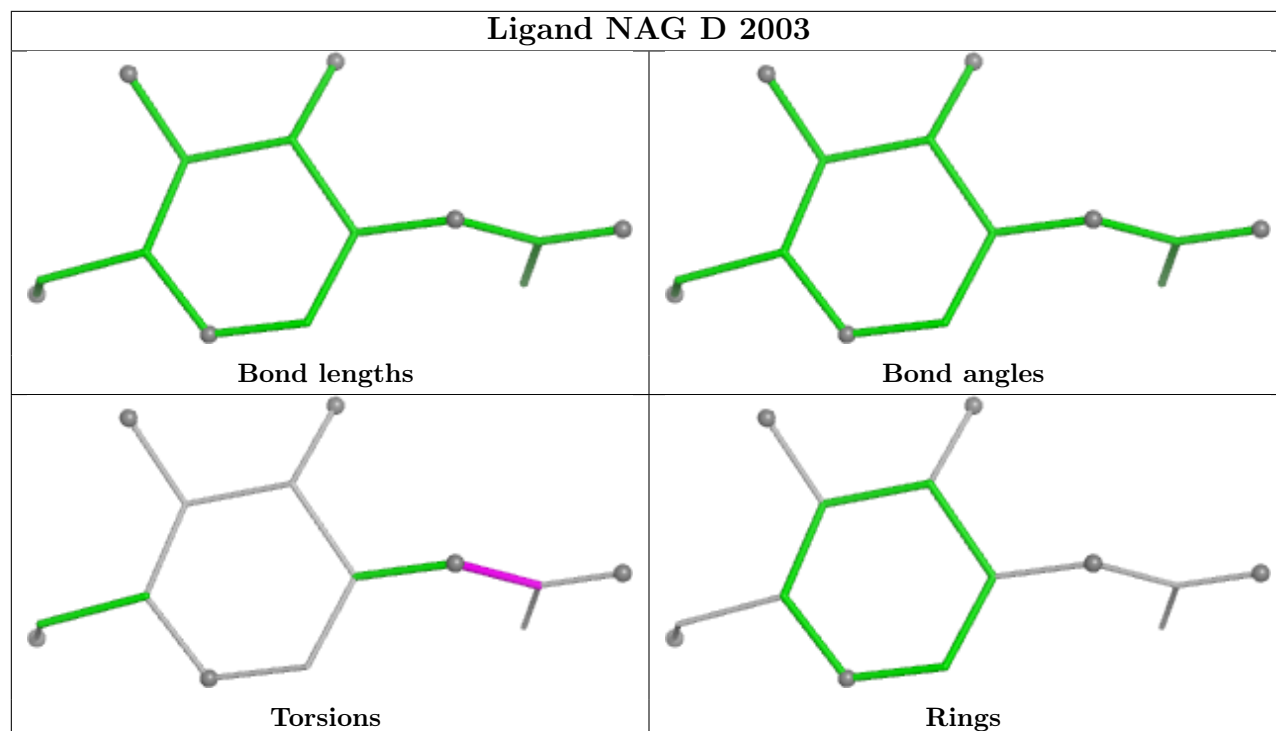
3 monomers are involved in 13 short contacts:

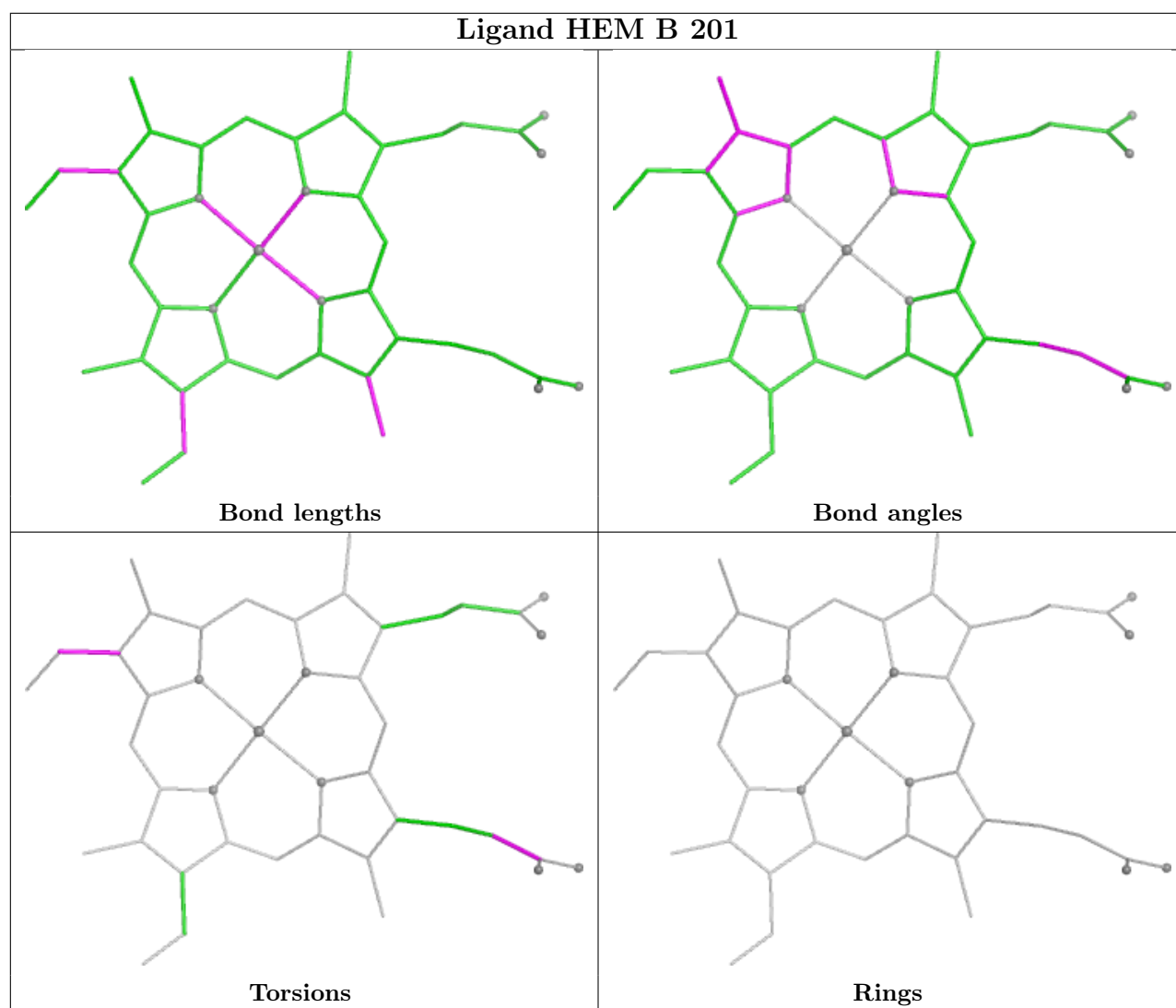
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	2004	NAG	2	0
5	B	201	HEM	5	0
5	A	201	HEM	6	0

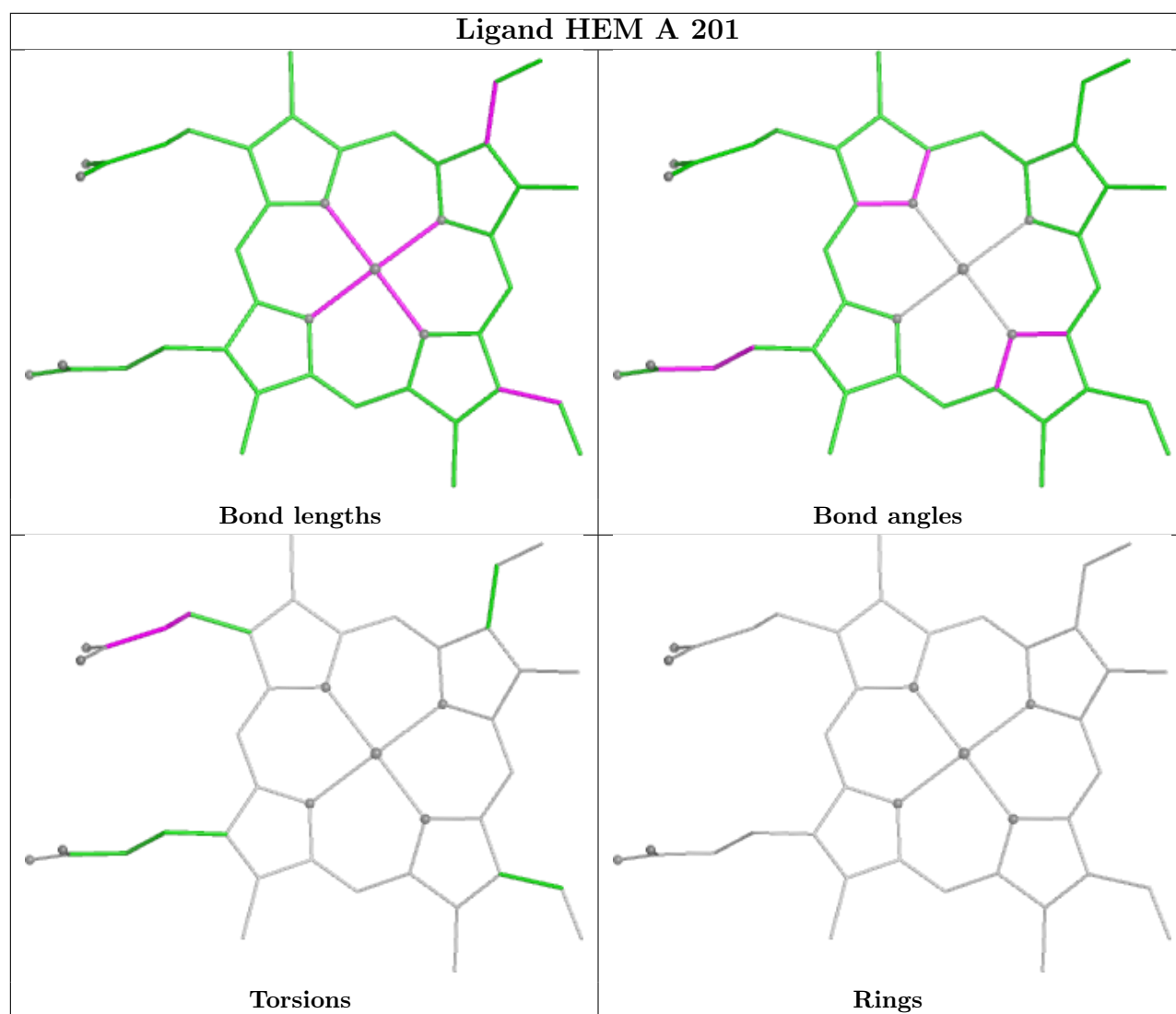
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

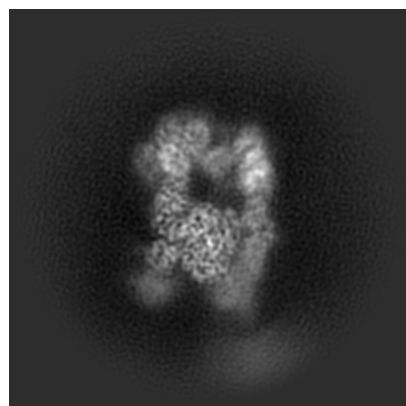
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50570. These allow visual inspection of the internal detail of the map and identification of artifacts.

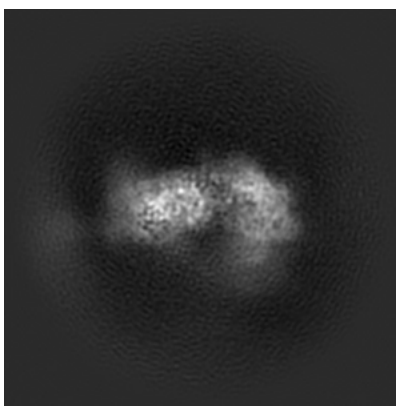
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

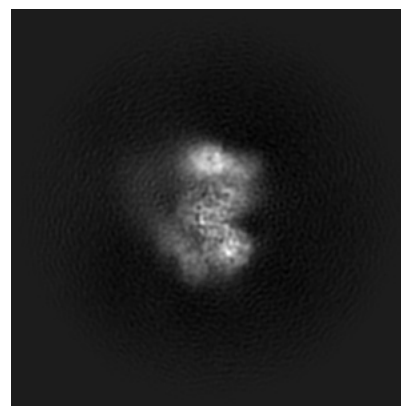
6.1.1 Primary map



X

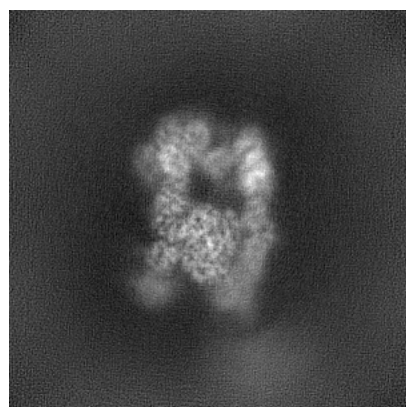


Y

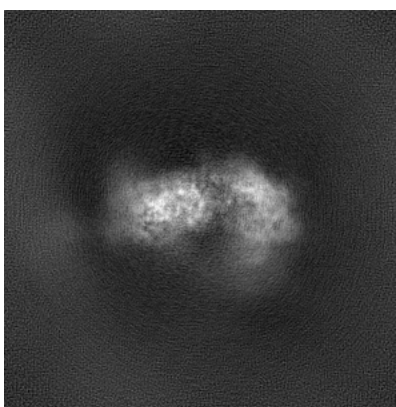


Z

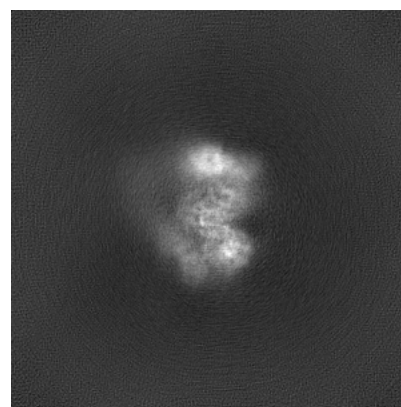
6.1.2 Raw map



X



Y

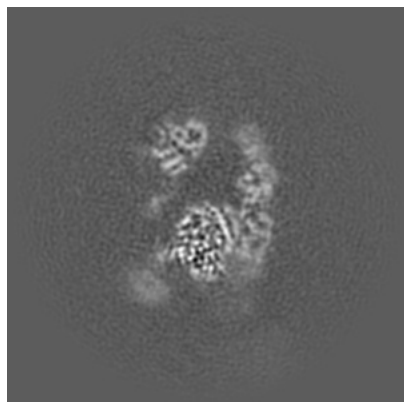


Z

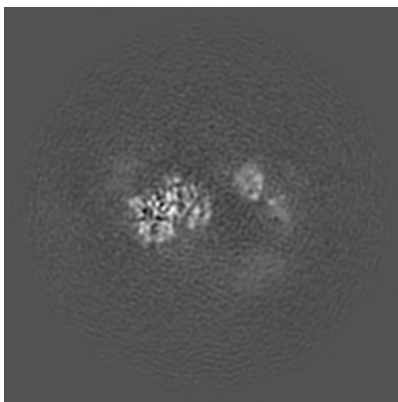
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

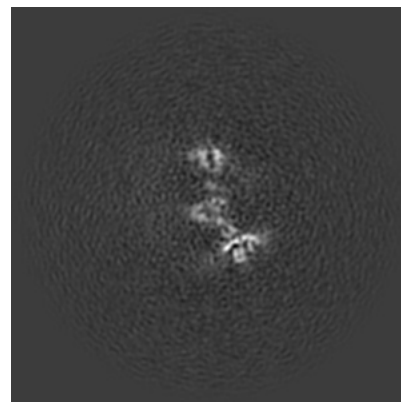
6.2.1 Primary map



X Index: 160

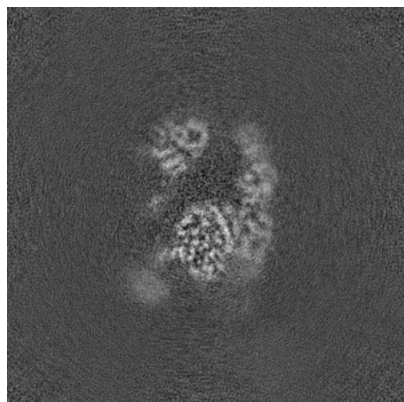


Y Index: 160

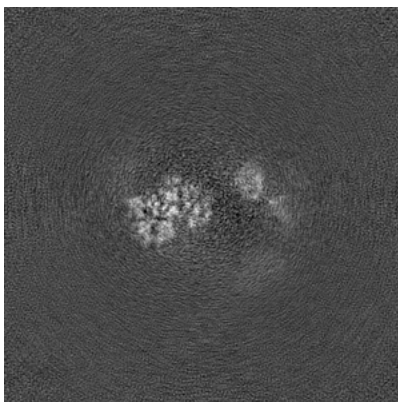


Z Index: 160

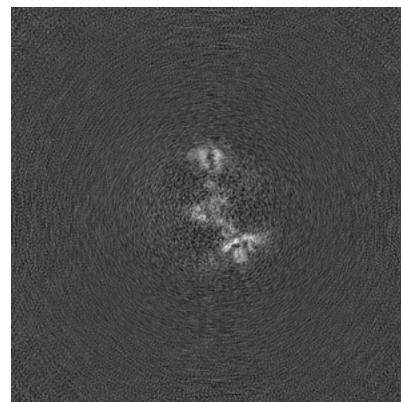
6.2.2 Raw map



X Index: 160



Y Index: 160

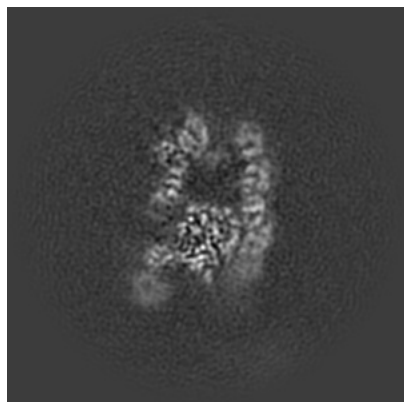


Z Index: 160

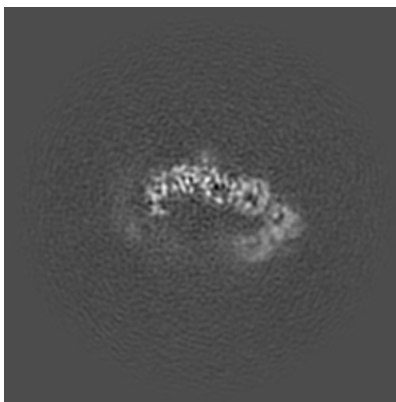
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

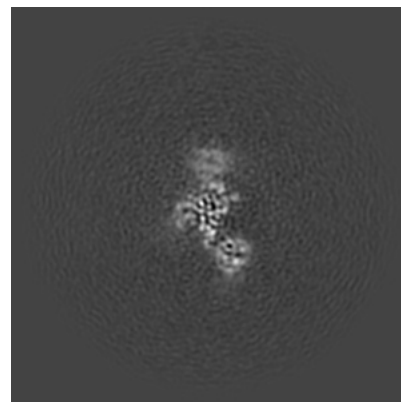
6.3.1 Primary map



X Index: 165

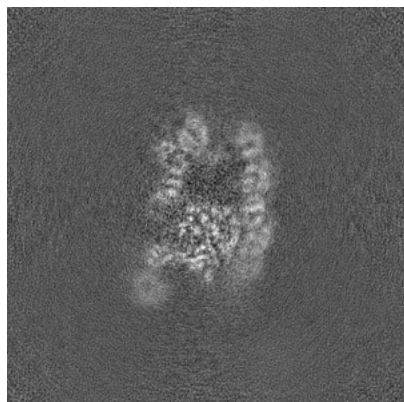


Y Index: 131

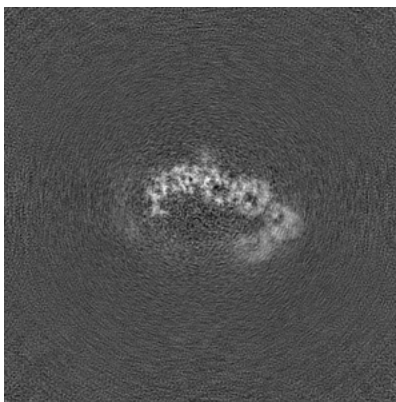


Z Index: 126

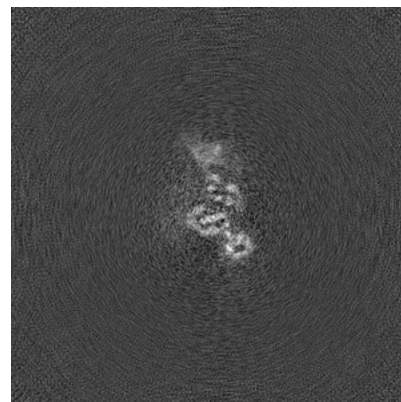
6.3.2 Raw map



X Index: 165



Y Index: 131

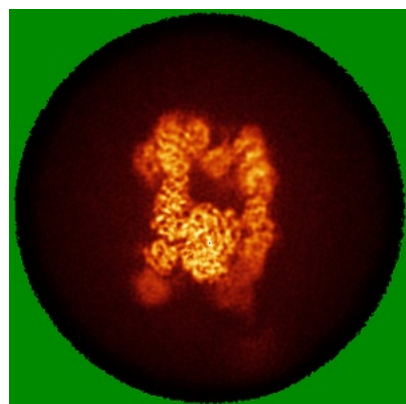


Z Index: 140

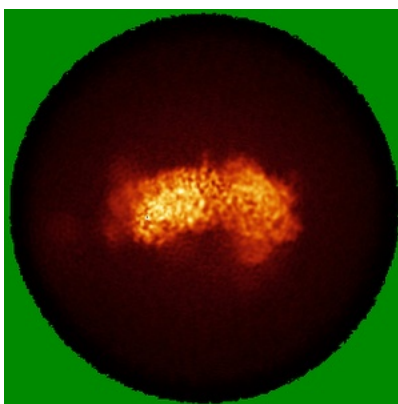
The images above show the largest variance slices of the map in three orthogonal directions.

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

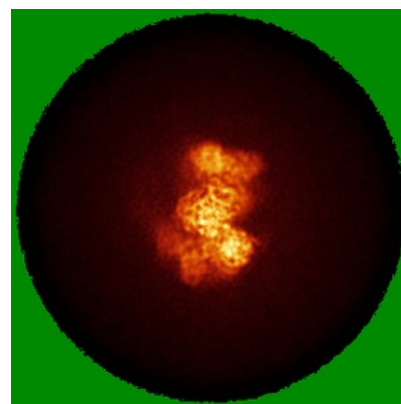
6.4.1 Primary map



X

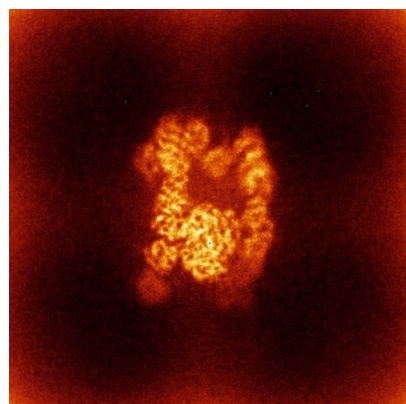


Y

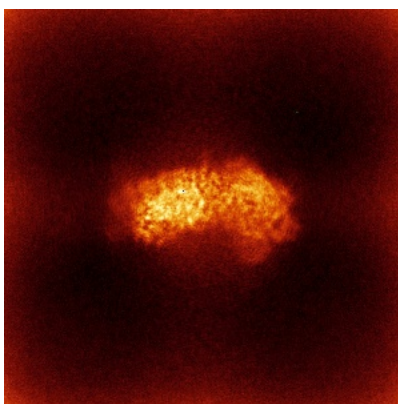


Z

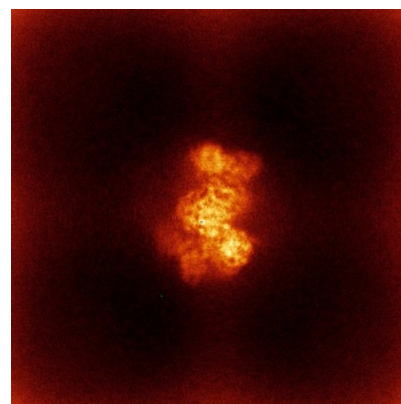
6.4.2 Raw map



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.

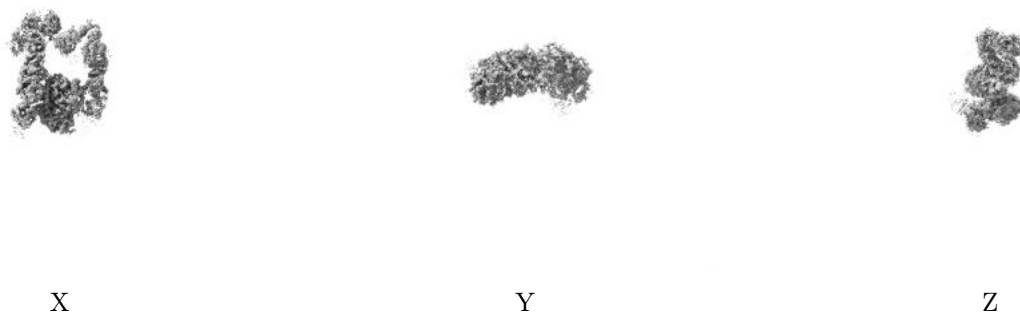
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. 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.

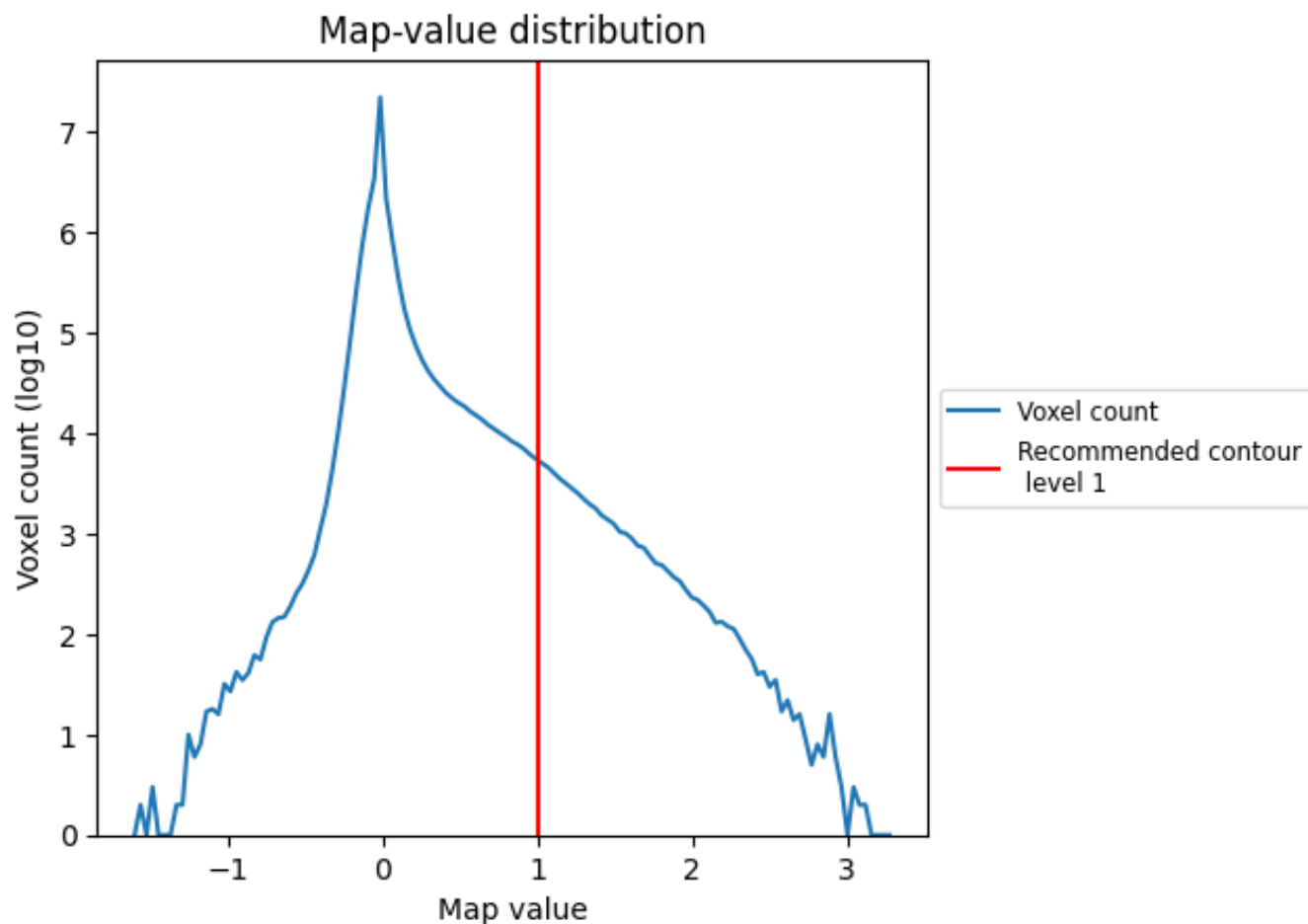
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

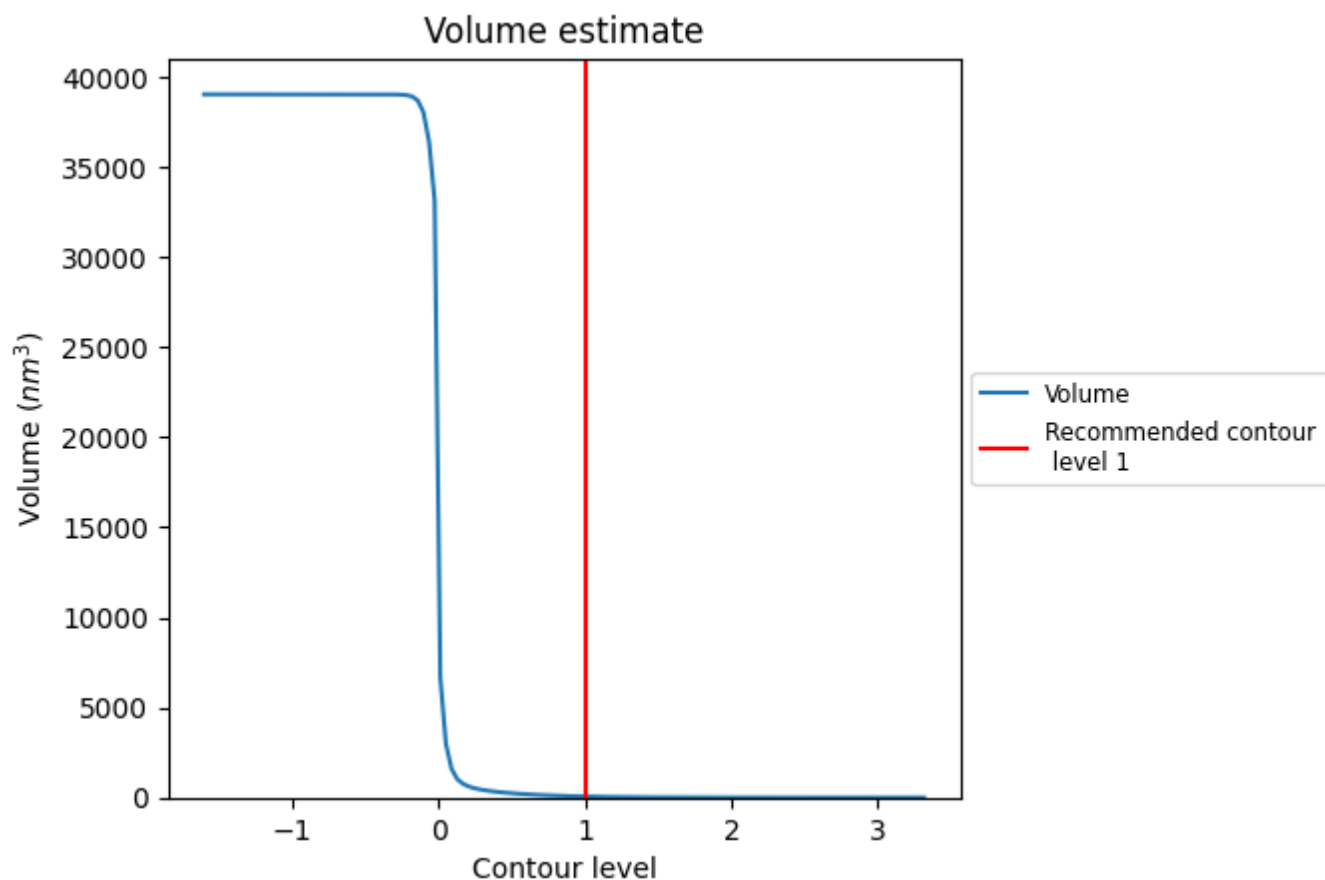
This section contains the results of statistical analysis of the map.

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.

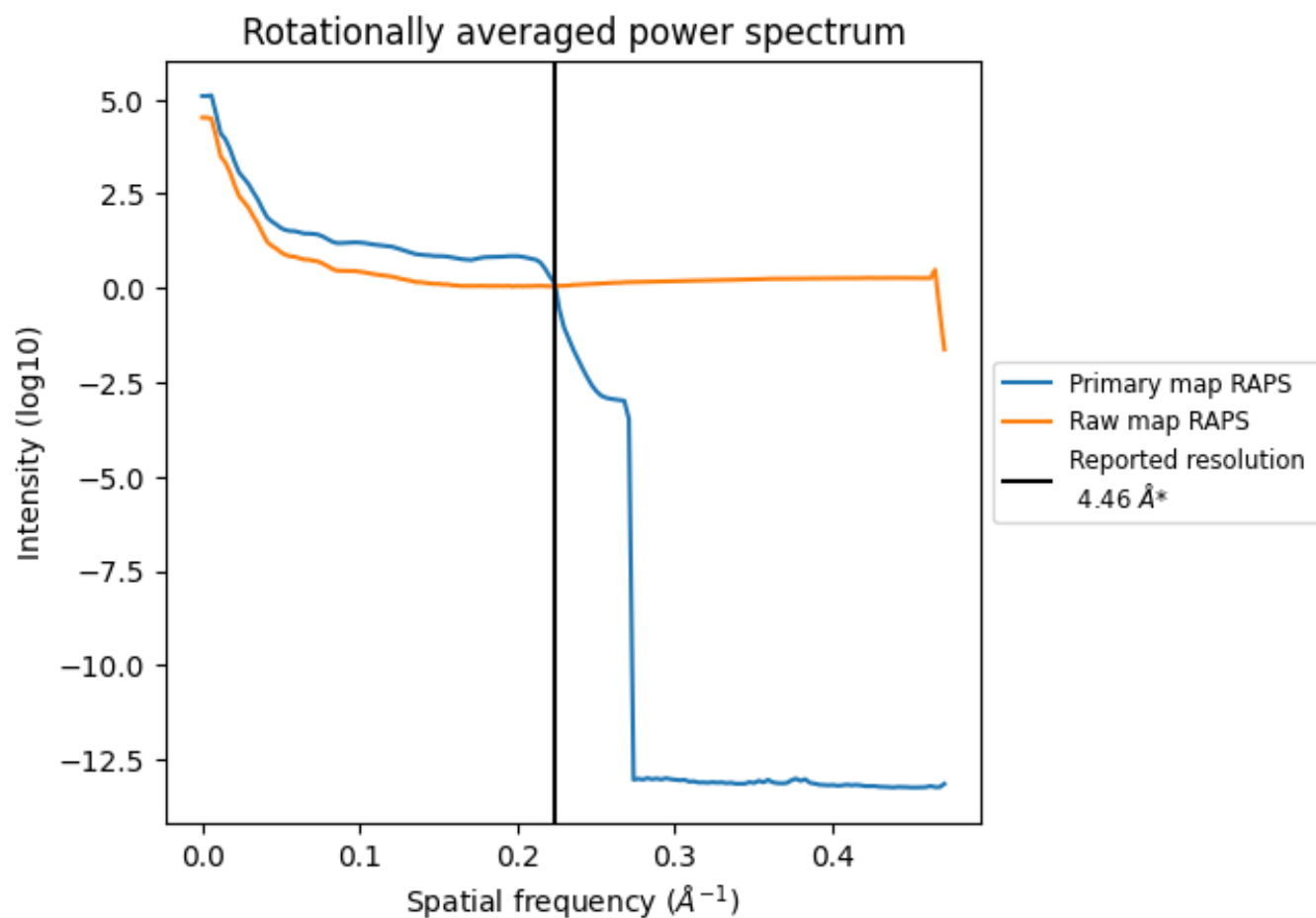
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 59 nm³; this corresponds to an approximate mass of 53 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 ⓘ

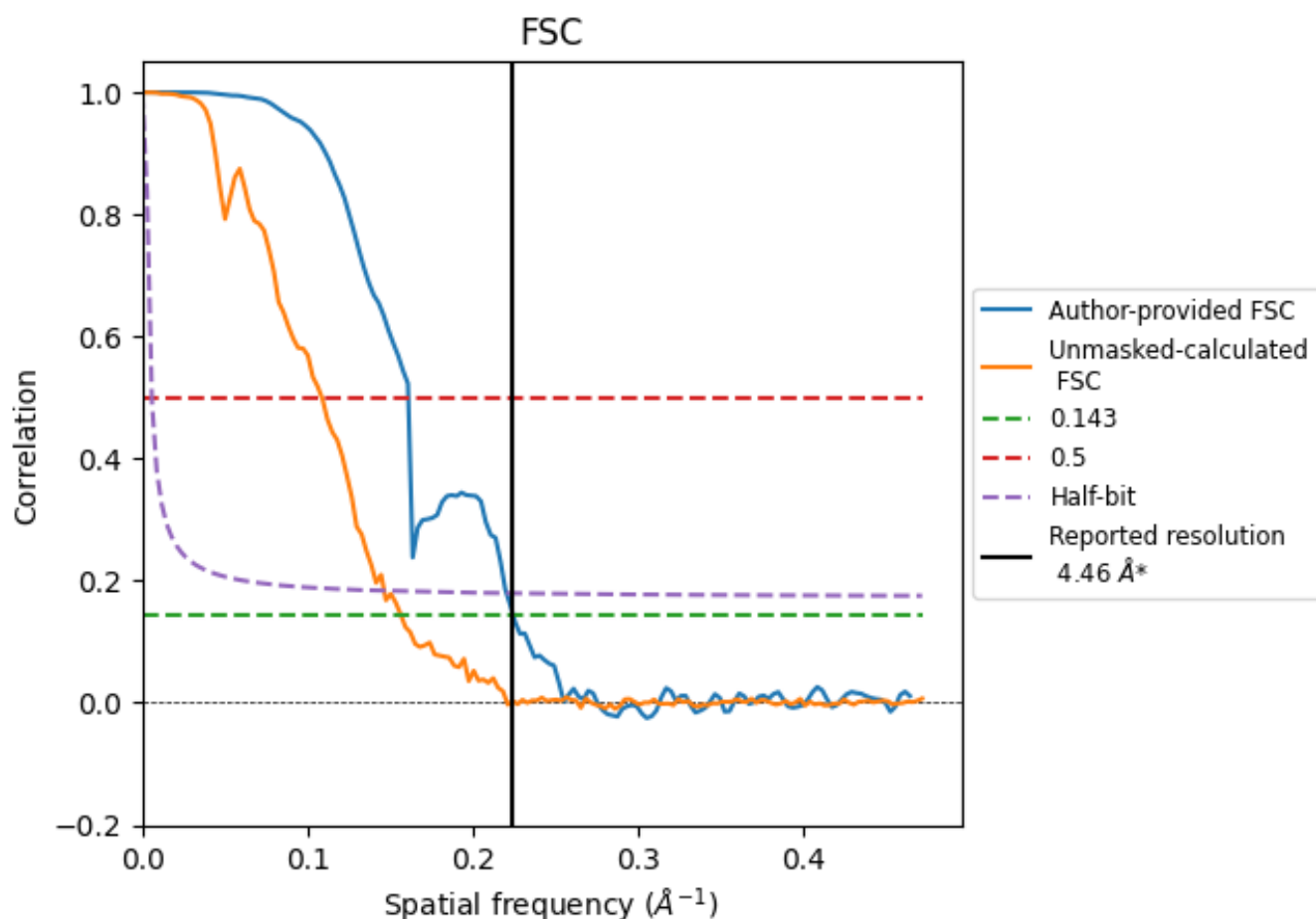


*Reported resolution corresponds to spatial frequency of 0.224 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.224 Å⁻¹

8.2 Resolution estimates [i](#)

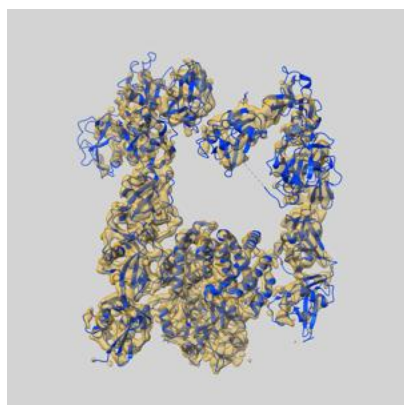
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.46	-	-
Author-provided FSC curve	4.46	6.22	4.54
Unmasked-calculated*	6.39	9.20	6.84

*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 6.39 differs from the reported value 4.46 by more than 10 %

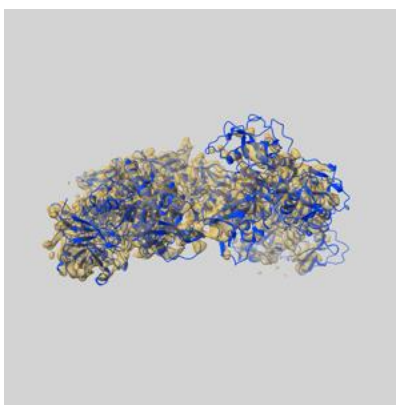
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50570 and PDB model 9FMU. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

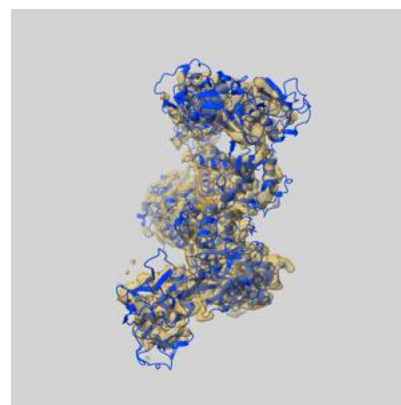
9.1 Map-model overlay [i](#)



X



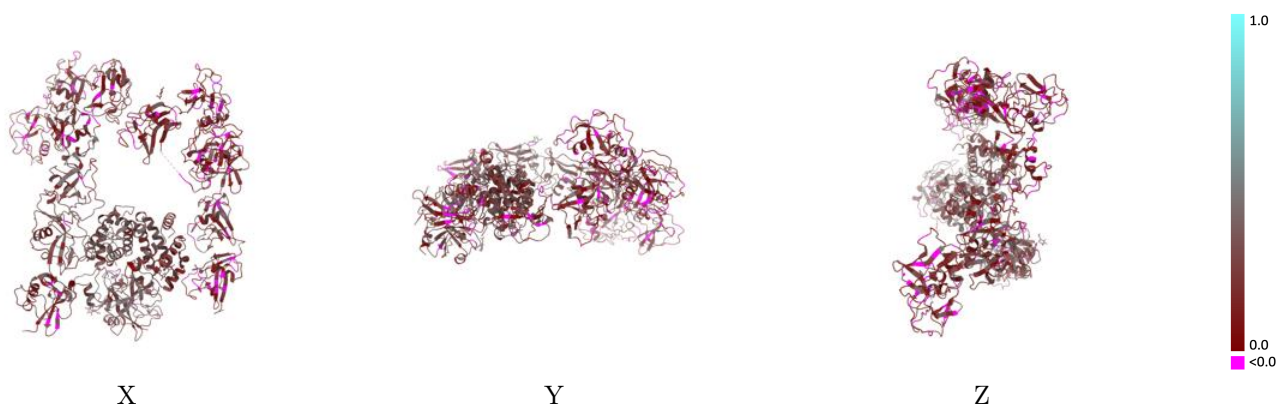
Y



Z

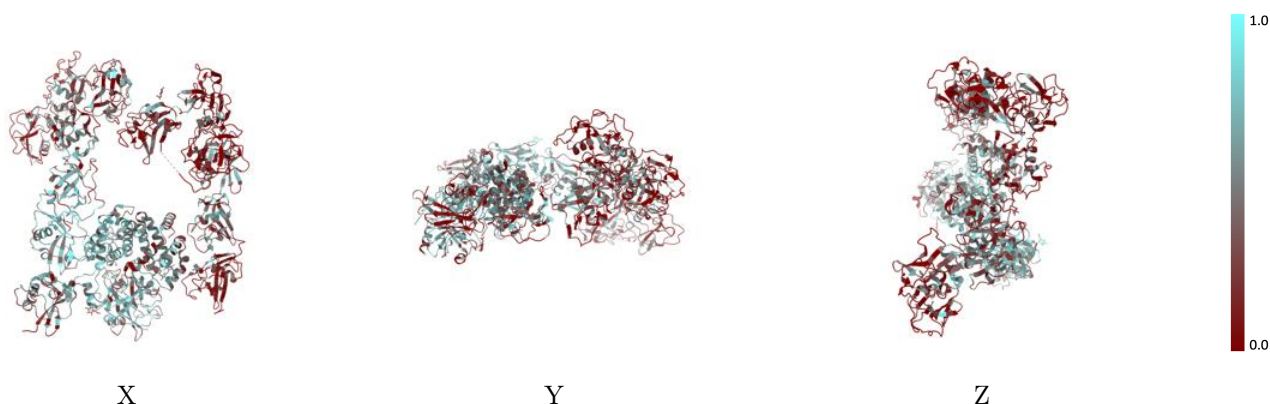
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



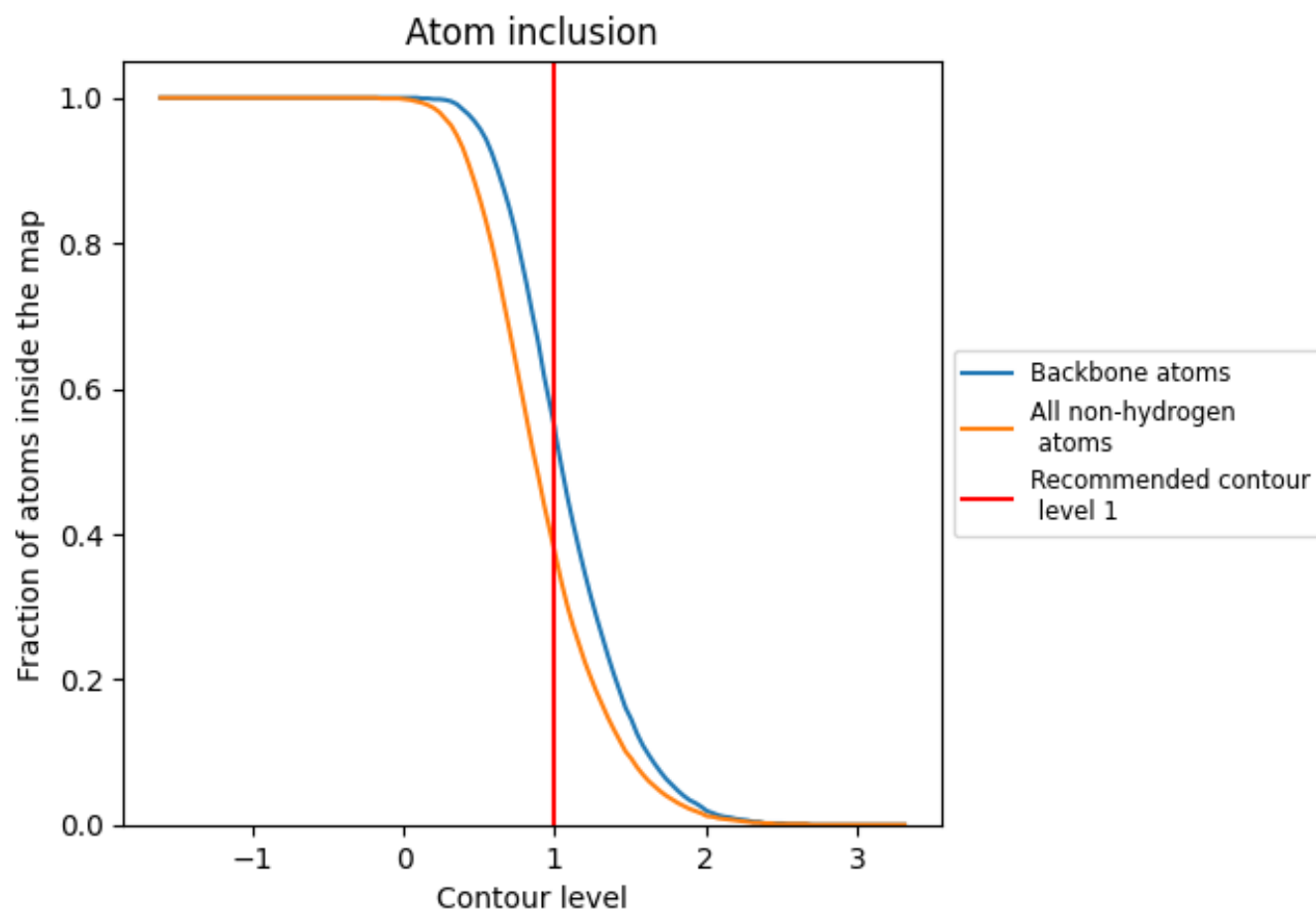
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 38% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3760	0.2330
A	0.5970	0.3190
B	0.4940	0.2800
C	0.5670	0.3160
D	0.3820	0.2330
E	0.2110	0.1660

