



Full wwPDB EM Validation Report ⓘ

Jun 11, 2025 – 04:25 PM EDT

PDB ID : 9NB6 / pdb_00009nb6
EMDB ID : EMD-49218
Title : Cryo-EM structure of the CD163/Hp(1-1)Hb complex
Authors : Huang, C.-S.; White, J.B.R.; Degtjarik, O.; Mosyak, L.
Deposited on : 2025-02-13
Resolution : 3.30 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

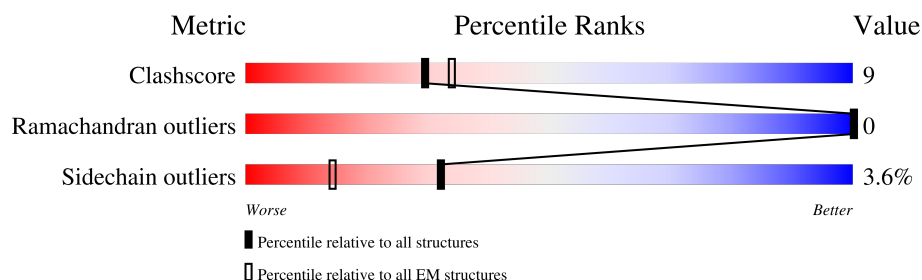
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1012	
1	B	1012	
1	C	1012	
2	D	142	
3	E	147	
4	F	347	
4	G	347	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24003 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 Scavenger receptor cysteine-rich type 1 protein M130.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	860	Total	C	N	O	S	0	0
			6504	3987	1181	1263	73		
1	B	858	Total	C	N	O	S	0	0
			6494	3982	1179	1260	73		
1	C	751	Total	C	N	O	S	0	0
			5684	3489	1029	1103	63		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1046	HIS	-	expression tag	UNP Q86VB7
A	1047	HIS	-	expression tag	UNP Q86VB7
A	1048	HIS	-	expression tag	UNP Q86VB7
A	1049	HIS	-	expression tag	UNP Q86VB7
A	1050	HIS	-	expression tag	UNP Q86VB7
A	1051	HIS	-	expression tag	UNP Q86VB7
A	1052	HIS	-	expression tag	UNP Q86VB7
A	1053	HIS	-	expression tag	UNP Q86VB7
B	1046	HIS	-	expression tag	UNP Q86VB7
B	1047	HIS	-	expression tag	UNP Q86VB7
B	1048	HIS	-	expression tag	UNP Q86VB7
B	1049	HIS	-	expression tag	UNP Q86VB7
B	1050	HIS	-	expression tag	UNP Q86VB7
B	1051	HIS	-	expression tag	UNP Q86VB7
B	1052	HIS	-	expression tag	UNP Q86VB7
B	1053	HIS	-	expression tag	UNP Q86VB7
C	1046	HIS	-	expression tag	UNP Q86VB7
C	1047	HIS	-	expression tag	UNP Q86VB7
C	1048	HIS	-	expression tag	UNP Q86VB7
C	1049	HIS	-	expression tag	UNP Q86VB7
C	1050	HIS	-	expression tag	UNP Q86VB7
C	1051	HIS	-	expression tag	UNP Q86VB7
C	1052	HIS	-	expression tag	UNP Q86VB7
C	1053	HIS	-	expression tag	UNP Q86VB7

- Molecule 2 is a protein called Hemoglobin subunit alpha.

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

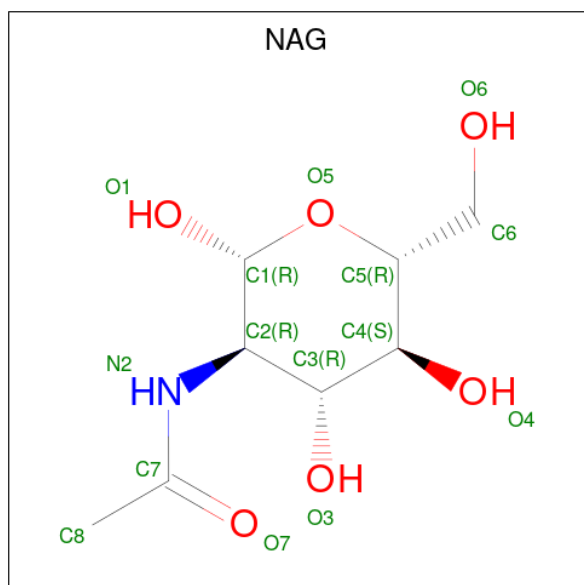
- Molecule 3 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	146	Total	C	N	O	S	0	0
			1122	724	195	200	3		

- Molecule 4 is a protein called Isoform 2 of Haptoglobin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	310	Total	C	N	O	S	0	0
			2437	1552	413	459	13		
4	G	56	Total	C	N	O	S	0	0
			455	287	79	86	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

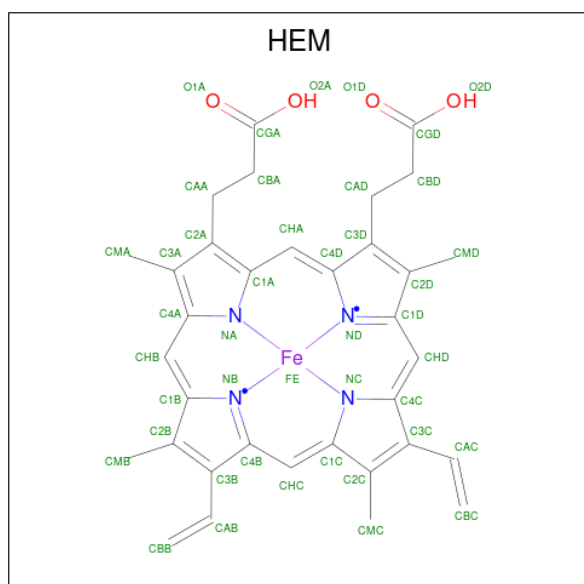
Continued from previous page...

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

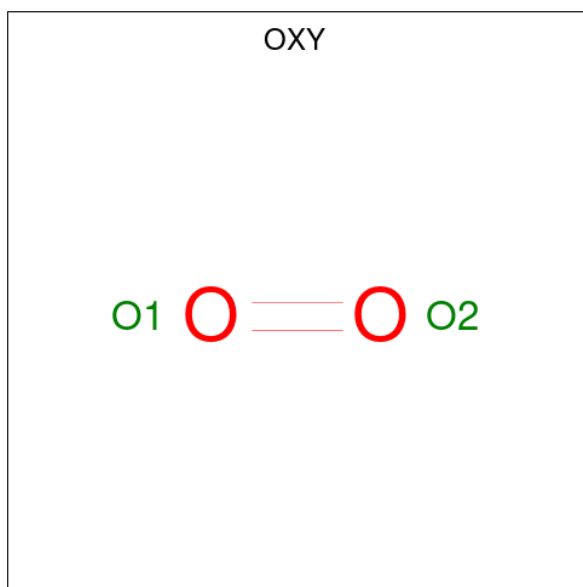
Mol	Chain	Residues	Atoms		AltConf
6	A	9	Total	Ca	0
			9	9	
6	B	8	Total	Ca	0
			8	8	
6	C	6	Total	Ca	0
			6	6	

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

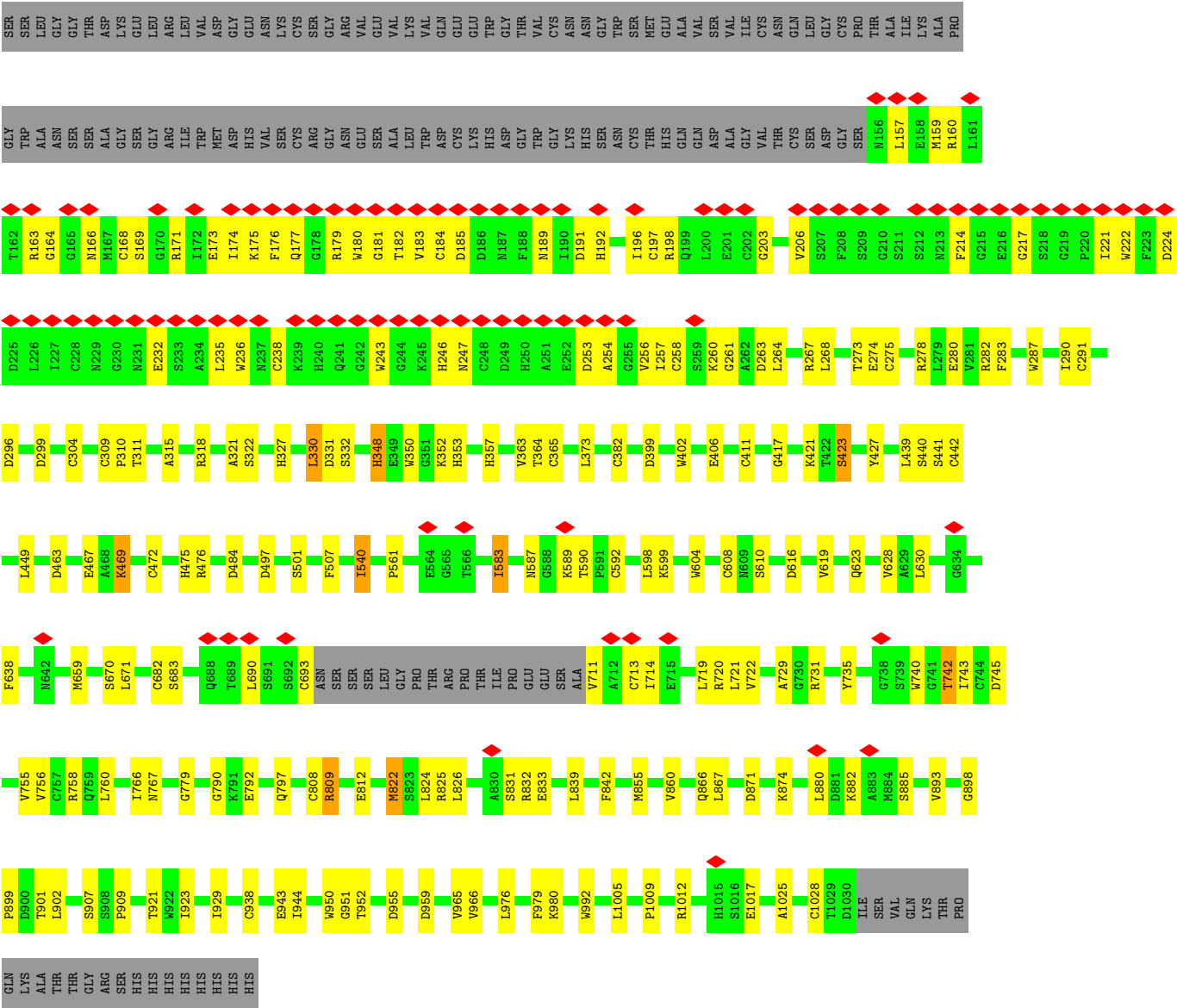


Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
7	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

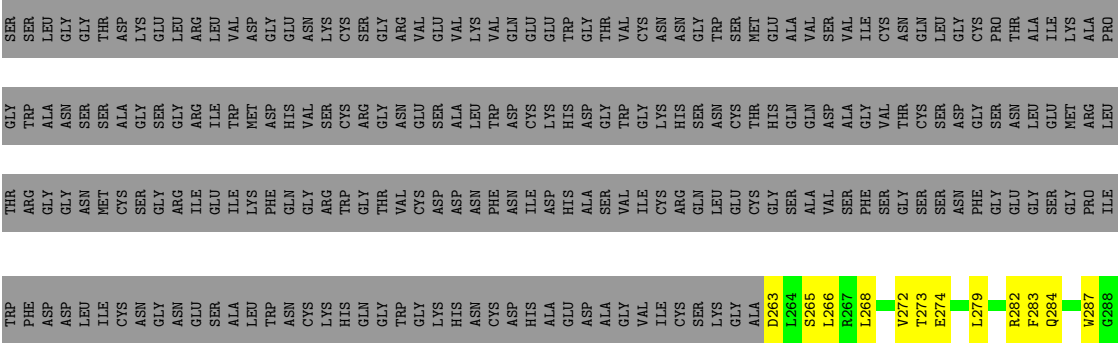
- Molecule 8 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂) (labeled as "Ligand of Interest" by depositor).

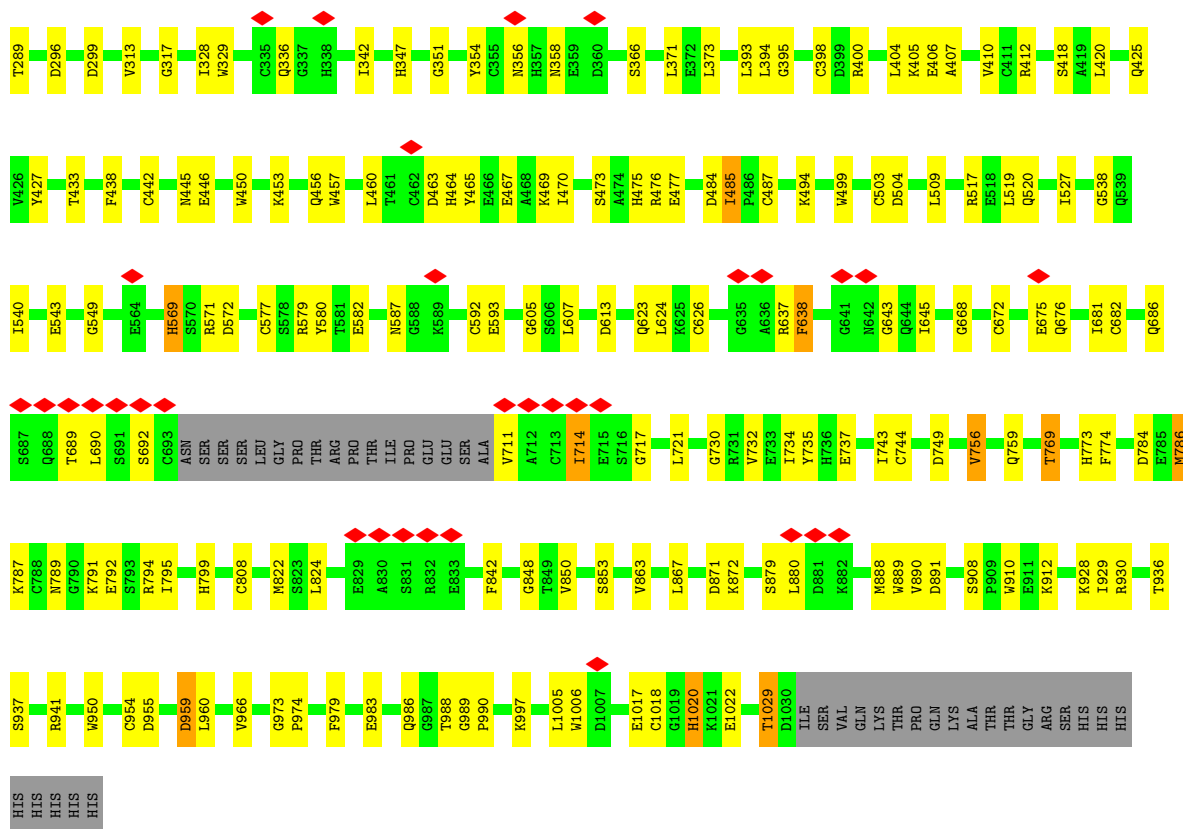


Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	O	0
			2	2	
8	E	1	Total	O	0
			2	2	



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





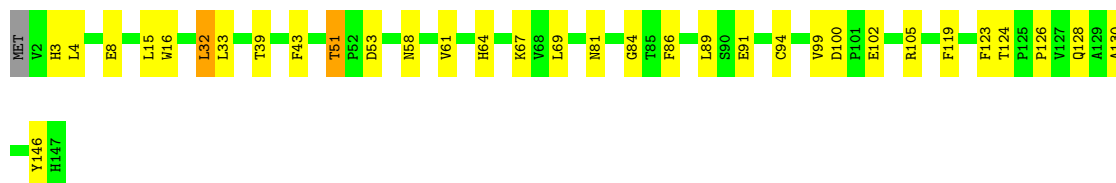
- Molecule 2: Hemoglobin subunit alpha

Chain D: 89% 10% .



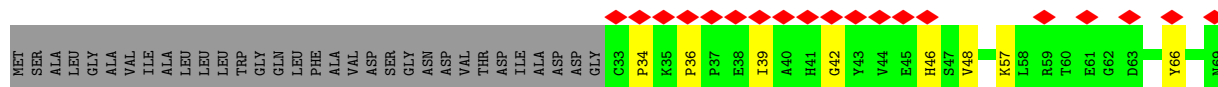
- Molecule 3: Hemoglobin subunit beta

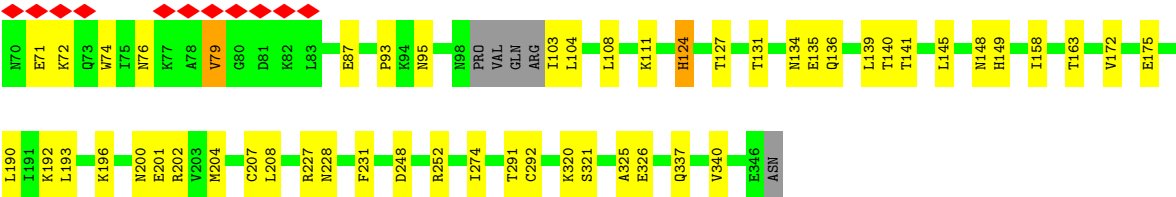
Chain E: 77% 21% ..



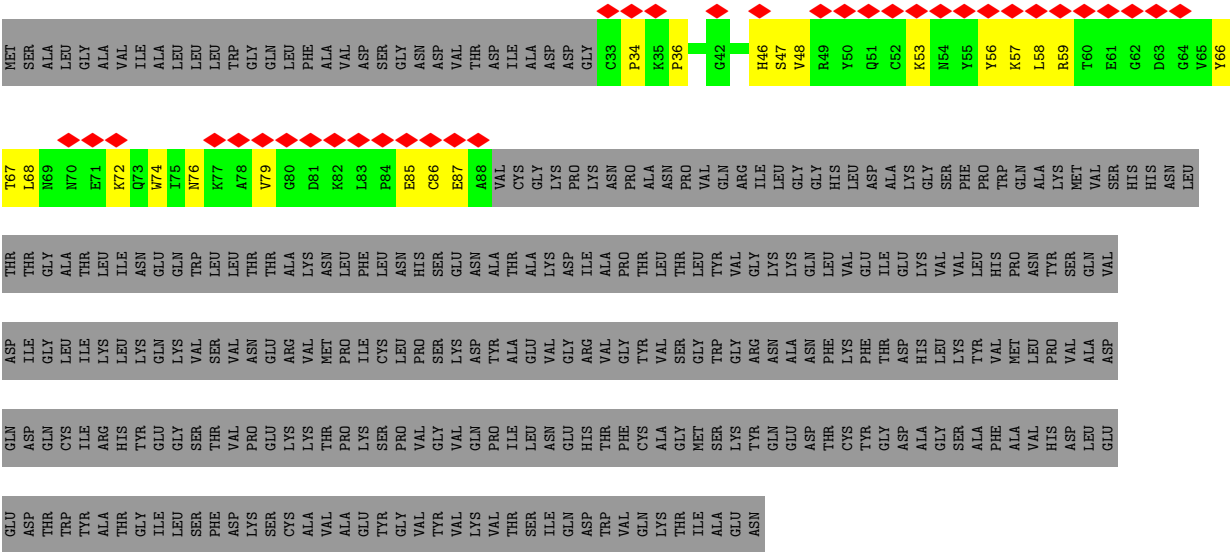
- Molecule 4: Isoform 2 of Haptoglobin

Chain F: 9% 72% 17% 11%





● Molecule 4: Isoform 2 of Haptoglobin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	245961	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.6	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	6.514	Depositor
Minimum map value	0.000	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	444.0, 444.0, 444.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	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, OXY, CA, NAG

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	0.10	0/6653	0.30	0/9008
1	B	0.11	0/6643	0.27	0/8995
1	C	0.13	0/5815	0.31	0/7880
2	D	0.09	0/1096	0.24	0/1491
3	E	0.11	0/1152	0.29	0/1566
4	F	0.12	0/2497	0.39	2/3391 (0.1%)
4	G	0.13	0/467	0.37	0/632
All	All	0.11	0/24323	0.30	2/32963 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	207	CYS	CA-C-N	10.86	137.18	120.68
4	F	207	CYS	C-N-CA	10.86	137.18	120.68

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	6504	0	6042	102	0
1	B	6494	0	6034	123	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5684	0	5298	119	0
2	D	1068	0	1070	9	0
3	E	1122	0	1115	22	0
4	F	2437	0	2391	38	0
4	G	455	0	433	16	0
5	A	42	0	39	0	0
5	B	42	0	39	0	0
5	C	42	0	39	2	0
6	A	9	0	0	0	0
6	B	8	0	0	0	0
6	C	6	0	0	0	0
7	D	43	0	30	2	0
7	E	43	0	30	5	0
8	D	2	0	0	0	0
8	E	2	0	0	1	0
All	All	24003	0	22560	419	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 9.

All (419) 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:C:453:LYS:HE3	1:C:453:LYS:HA	1.63	0.79
1:B:938:CYS:HB3	1:B:1028:CYS:HB2	1.66	0.78
4:F:48:VAL:HG12	4:G:47:SER:H	1.48	0.77
7:E:201:HEM:HHC	7:E:201:HEM:HBB2	1.68	0.75
1:B:192:HIS:HE1	1:B:235:LEU:HD21	1.53	0.74
1:B:439:LEU:HD11	1:B:449:LEU:HD11	1.69	0.72
1:B:352:LYS:O	1:B:353:HIS:ND1	2.24	0.70
1:B:955:ASP:HB2	1:B:980:LYS:HG2	1.73	0.69
1:B:184:CYS:HA	1:B:253:ASP:HA	1.74	0.69
1:B:871:ASP:OD2	1:B:950:TRP:NE1	2.26	0.69
3:E:124:THR:HG22	3:E:126:PRO:HD2	1.76	0.68
1:B:348:HIS:ND1	3:E:91:GLU:OE1	2.27	0.67
4:G:76:ASN:HB3	4:G:79:VAL:HG22	1.75	0.67
1:A:633:PRO:HB3	1:A:637:ARG:HH22	1.59	0.67
1:B:824:LEU:HD11	1:B:839:LEU:HD12	1.75	0.67
1:B:592:CYS:HB3	1:B:682:CYS:HB2	1.78	0.66
4:F:321:SER:HB2	4:F:325:ALA:HB3	1.77	0.66
1:B:185:ASP:HA	1:B:254:ALA:HB2	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:917:PRO:HA	1:A:920:GLU:HG3	1.76	0.65
1:A:860:VAL:HG13	1:A:923:ILE:HD11	1.79	0.65
1:A:647:ARG:NH1	1:A:907:SER:O	2.30	0.65
1:C:265:SER:HB3	1:C:282:ARG:HE	1.62	0.65
1:C:467:GLU:O	1:C:469:LYS:NZ	2.29	0.65
4:F:201:GLU:HG3	4:F:202:ARG:HG3	1.80	0.64
1:A:848:GLY:HA2	1:A:886:ILE:HD13	1.79	0.64
1:B:825:ARG:HH21	1:B:832:ARG:HD2	1.63	0.63
1:B:758:ARG:NH1	1:B:790:GLY:O	2.31	0.63
1:B:163:ARG:HG2	1:B:171:ARG:HE	1.64	0.63
7:E:201:HEM:HBC2	7:E:201:HEM:HHD	1.81	0.62
1:B:196:ILE:HG21	1:B:256:VAL:HG21	1.81	0.62
1:B:826:LEU:HD12	1:B:867:LEU:HD12	1.82	0.62
1:C:354:TYR:HB2	2:D:91:LYS:HD3	1.81	0.62
1:C:475:HIS:HD2	1:C:476:ARG:HG2	1.65	0.62
1:A:582:GLU:HG3	1:A:599:LYS:HB3	1.80	0.61
1:A:640:LYS:HD3	1:A:674:SER:HB2	1.82	0.61
1:B:177:GLN:HB2	1:B:179:ARG:HH21	1.66	0.61
1:C:593:GLU:HB2	1:C:681:ILE:HG23	1.81	0.61
1:C:973:GLY:HA3	1:C:1029:THR:HB	1.83	0.61
1:B:882:LYS:HE3	1:B:885:SER:HB2	1.83	0.60
1:B:1017:GLU:N	1:B:1017:GLU:OE2	2.34	0.60
1:A:462:CYS:HB2	1:A:465:TYR:HB2	1.84	0.60
4:F:76:ASN:HB3	4:F:79:VAL:HG22	1.84	0.60
1:A:187:ASN:ND2	1:A:225:ASP:OD1	2.33	0.60
1:B:183:VAL:O	1:B:254:ALA:N	2.31	0.59
1:B:278:ARG:NH1	1:B:322:SER:O	2.35	0.59
1:C:689:THR:OG1	1:C:690:LEU:N	2.34	0.59
1:A:517:ARG:HH22	1:A:550:HIS:HA	1.68	0.59
3:E:58:ASN:HB3	3:E:61:VAL:HG22	1.84	0.59
1:B:1009:PRO:HA	1:B:1012:ARG:HH22	1.68	0.58
4:F:36:PRO:HB3	4:G:48:VAL:HG21	1.83	0.58
1:A:421:LYS:HG2	1:A:423:SER:H	1.68	0.58
1:A:506:ASP:HB3	1:A:544:GLU:HA	1.85	0.58
1:B:719:LEU:HD13	1:B:756:VAL:HG13	1.85	0.58
1:C:400:ARG:HG3	1:C:465:TYR:CE2	2.38	0.58
1:A:568:SER:OG	1:A:571:ARG:NH1	2.36	0.58
1:A:216:GLU:OE2	4:F:252:ARG:NH2	2.35	0.58
7:D:201:HEM:HMB2	7:D:201:HEM:HBB2	1.86	0.57
3:E:102:GLU:OE1	4:F:228:ASN:ND2	2.38	0.57
1:B:267:ARG:HG2	1:B:280:GLU:HB2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:ASN:ND2	1:C:638:PHE:O	2.37	0.57
4:F:134:ASN:OD1	4:F:135:GLU:N	2.36	0.57
1:B:264:LEU:HD11	1:B:283:PHE:HD1	1.70	0.57
1:C:317:GLY:HA3	1:C:457:TRP:H	1.68	0.57
1:B:309:CYS:HB2	1:B:310:PRO:HD2	1.87	0.56
4:G:66:TYR:HB3	4:G:74:TRP:HB3	1.85	0.56
1:B:608:CYS:SG	1:B:610:SER:OG	2.59	0.56
1:A:583:ILE:HB	1:A:598:LEU:HD12	1.86	0.56
1:B:979:PHE:HB2	1:B:1025:ALA:HB3	1.88	0.56
2:D:76:ASP:OD1	2:D:79:ASN:ND2	2.38	0.56
4:F:145:LEU:HB3	4:F:158:ILE:HG21	1.87	0.56
4:F:149:HIS:HE1	4:F:158:ILE:HA	1.71	0.56
1:A:640:LYS:HA	1:A:677:VAL:HG11	1.88	0.56
1:A:781:ILE:HD12	1:A:781:ILE:H	1.71	0.56
1:B:497:ASP:N	1:B:497:ASP:OD1	2.35	0.56
1:B:929:ILE:HG12	1:B:944:ILE:HG22	1.88	0.56
1:A:809:ARG:NH1	1:C:1017:GLU:OE2	2.39	0.56
1:C:463:ASP:OD1	1:C:464:HIS:N	2.38	0.56
1:A:374:ARG:HE	1:A:376:ARG:HH12	1.52	0.56
3:E:16:TRP:HH2	3:E:69:LEU:HD22	1.70	0.56
1:A:161:LEU:HG	1:A:200:LEU:HD11	1.88	0.55
1:B:182:THR:H	1:B:221:ILE:HG12	1.72	0.55
1:B:826:LEU:HD21	1:B:923:ILE:HB	1.87	0.55
1:C:484:ASP:OD1	1:C:484:ASP:N	2.35	0.55
1:C:871:ASP:OD1	1:C:872:LYS:N	2.38	0.55
1:A:589:LYS:NZ	1:A:593:GLU:OE2	2.38	0.55
1:B:192:HIS:CE1	1:B:235:LEU:HD21	2.39	0.55
1:C:266:LEU:HD22	1:C:342:ILE:HD11	1.89	0.55
1:B:792:GLU:HG3	1:B:797:GLN:HB2	1.88	0.55
1:C:853:SER:OG	1:C:891:ASP:OD1	2.25	0.55
1:C:769:THR:HG23	1:C:773:HIS:HB3	1.89	0.55
1:C:966:VAL:HG22	1:C:1005:LEU:HD21	1.89	0.55
1:B:159:MET:HE1	1:B:235:LEU:HD22	1.89	0.55
1:A:995:GLU:O	1:A:997:LYS:NZ	2.38	0.54
1:B:224:ASP:HB3	1:B:246:HIS:HA	1.90	0.54
1:B:382:CYS:HB3	1:B:472:CYS:HB2	1.89	0.54
1:A:172:ILE:HD11	1:A:256:VAL:HG13	1.90	0.54
1:B:168:CYS:SG	1:B:260:LYS:HB3	2.48	0.54
1:C:263:ASP:OD2	1:C:282:ARG:NH1	2.41	0.54
1:A:599:LYS:HD2	1:A:604:TRP:CE2	2.43	0.54
1:C:476:ARG:NH2	1:C:543:GLU:OE1	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:95:ASN:HD22	4:F:111:LYS:HB3	1.72	0.54
1:A:480:LEU:HD21	1:A:515:LEU:HD21	1.89	0.54
2:D:32:ARG:NH2	3:E:123:PHE:O	2.40	0.54
1:A:838:ARG:NH1	1:A:920:GLU:OE1	2.42	0.53
1:A:689:THR:OG1	1:A:690:LEU:N	2.37	0.53
4:G:56:TYR:HB3	4:G:86:CYS:HB3	1.90	0.53
3:E:67:LYS:HD3	7:E:201:HEM:HBA2	1.91	0.53
1:C:519:LEU:O	1:C:520:GLN:NE2	2.42	0.53
1:C:959:ASP:N	1:C:959:ASP:OD1	2.40	0.53
4:F:66:TYR:HB3	4:F:74:TRP:HB3	1.91	0.53
1:C:405:LYS:HG3	1:C:406:GLU:OE2	2.09	0.53
3:E:16:TRP:CH2	3:E:69:LEU:HD22	2.43	0.53
4:F:103:ILE:HD13	4:F:291:THR:HG22	1.89	0.52
1:A:1017:GLU:O	1:B:809:ARG:NH1	2.43	0.52
7:D:201:HEM:HMC2	7:D:201:HEM:HBC2	1.90	0.52
1:C:889:TRP:HB3	1:C:910:TRP:HZ3	1.74	0.52
1:A:623:GLN:HB2	1:A:658:HIS:HD2	1.75	0.52
1:C:503:CYS:SG	1:C:504:ASP:N	2.82	0.52
1:A:268:LEU:HD21	1:A:363:VAL:HG12	1.92	0.52
1:A:273:THR:OG1	1:A:274:GLU:N	2.42	0.51
1:B:166:ASN:OD1	1:B:169:SER:N	2.39	0.51
1:B:169:SER:HB2	1:B:258:CYS:H	1.75	0.51
1:C:395:GLY:HA2	1:C:433:THR:HG21	1.92	0.51
1:B:735:TYR:HB2	1:B:740:TRP:CD2	2.46	0.51
1:B:463:ASP:OD1	1:B:463:ASP:N	2.39	0.51
1:C:273:THR:OG1	1:C:274:GLU:N	2.44	0.51
3:E:33:LEU:HD21	3:E:43:PHE:HD2	1.74	0.51
1:A:548:GLU:OE1	1:A:550:HIS:ND1	2.36	0.51
1:A:888:MET:SD	1:A:913:ARG:NH2	2.82	0.51
1:A:182:THR:HG21	1:A:253:ASP:HB3	1.93	0.51
1:A:370:ASP:N	1:A:370:ASP:OD1	2.41	0.51
1:B:951:GLY:HA3	1:B:992:TRP:CD1	2.46	0.51
1:C:438:PHE:HZ	1:C:460:LEU:HB2	1.75	0.51
1:C:373:LEU:HD21	1:C:410:VAL:HG13	1.92	0.51
1:B:221:ILE:HB	1:B:246:HIS:HB3	1.92	0.50
1:A:445:ASN:OD1	1:A:445:ASN:N	2.42	0.50
1:C:445:ASN:HB2	5:C:1102:NAG:H83	1.93	0.50
1:A:318:ARG:NH1	1:A:360:ASP:O	2.44	0.50
1:A:332:SER:O	1:A:332:SER:OG	2.25	0.50
1:C:296:ASP:OD1	1:C:299:ASP:N	2.38	0.50
1:A:166:ASN:OD1	1:A:167:MET:N	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:989:GLY:O	1:C:1020:HIS:NE2	2.37	0.50
1:A:158:GLU:HB3	1:A:175:LYS:HE2	1.94	0.50
1:C:759:GLN:HE21	1:C:794:ARG:HA	1.77	0.50
1:C:282:ARG:HB3	1:C:287:TRP:CD2	2.47	0.50
1:C:871:ASP:HB2	1:C:872:LYS:NZ	2.27	0.50
1:A:163:ARG:HH21	1:A:171:ARG:HH22	1.60	0.50
1:C:582:GLU:N	1:C:582:GLU:OE1	2.45	0.50
1:C:756:VAL:HG22	1:C:795:ILE:HD13	1.94	0.50
4:F:208:LEU:HD13	4:F:337:GLN:HG3	1.94	0.49
1:B:583:ILE:HG12	1:B:623:GLN:HE22	1.77	0.49
1:C:407:ALA:HB1	1:C:470:ILE:HD12	1.95	0.49
1:C:356:ASN:ND2	1:C:358:ASN:HB3	2.27	0.49
1:B:164:GLY:O	1:B:166:ASN:ND2	2.46	0.49
1:C:824:LEU:HB3	1:C:867:LEU:HD21	1.94	0.49
1:A:268:LEU:HD11	1:A:307:LEU:HD13	1.95	0.49
1:B:184:CYS:SG	1:B:185:ASP:N	2.85	0.49
1:B:273:THR:OG1	1:B:274:GLU:N	2.46	0.49
4:F:248:ASP:OD2	4:F:252:ARG:NH1	2.46	0.49
1:A:315:ALA:HB3	1:A:364:THR:HB	1.94	0.48
1:B:766:ILE:HG22	1:B:767:ASN:OD1	2.14	0.48
1:C:623:GLN:HG2	1:C:624:LEU:HD22	1.93	0.48
1:A:853:SER:OG	1:A:891:ASP:OD1	2.31	0.48
1:A:929:ILE:HD13	1:A:944:ILE:HG22	1.95	0.48
3:E:64:HIS:NE2	8:E:202:OXY:O2	2.46	0.48
4:F:39:ILE:HD11	4:F:42:GLY:HA3	1.95	0.48
1:B:171:ARG:HH11	1:B:217:GLY:HA2	1.79	0.48
1:C:356:ASN:HD21	1:C:358:ASN:HB3	1.79	0.48
1:C:438:PHE:CZ	1:C:460:LEU:HB2	2.48	0.48
1:B:206:VAL:HB	1:B:350:TRP:CD1	2.48	0.47
1:B:966:VAL:HG22	1:B:1005:LEU:HD11	1.95	0.47
1:A:219:GLY:O	1:A:250:HIS:NE2	2.31	0.47
1:B:157:LEU:HD12	1:B:236:TRP:HB3	1.96	0.47
1:B:742:THR:HG22	1:B:743:ILE:H	1.79	0.47
1:C:272:VAL:HG23	1:C:273:THR:HG22	1.95	0.47
1:C:734:ILE:HD11	1:C:743:ILE:HD11	1.95	0.47
1:B:315:ALA:HB3	1:B:364:THR:HB	1.96	0.47
1:A:747:SER:OG	1:A:786:MET:O	2.31	0.47
1:C:284:GLN:O	1:C:284:GLN:HG2	2.14	0.47
1:C:1018:CYS:SG	1:C:1022:GLU:HB2	2.54	0.47
4:F:74:TRP:CD1	4:G:36:PRO:HA	2.50	0.47
1:A:183:VAL:HG13	1:A:223:PHE:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:HIS:NE2	1:A:629:ALA:O	2.47	0.47
1:A:720:ARG:HG2	1:A:733:GLU:HB2	1.96	0.47
2:D:117:GLU:CD	2:D:117:GLU:H	2.22	0.47
1:A:319:VAL:HG11	1:A:457:TRP:CD1	2.50	0.47
1:B:264:LEU:HD11	1:B:283:PHE:CD1	2.50	0.47
4:F:131:THR:HG23	4:F:139:LEU:HB3	1.96	0.47
4:F:135:GLU:HB3	4:F:196:LYS:HD2	1.96	0.47
1:C:406:GLU:HB3	1:C:442:CYS:HB2	1.97	0.47
1:C:786:MET:HB3	1:C:786:MET:HE3	1.68	0.47
1:B:475:HIS:O	1:B:476:ARG:HD3	2.15	0.47
1:B:501:SER:HB2	1:B:540:ILE:HG23	1.97	0.47
1:B:719:LEU:HB2	1:B:760:LEU:HD21	1.97	0.47
1:C:477:GLU:HB3	1:C:494:LYS:HB3	1.96	0.47
1:B:173:GLU:HB3	1:B:180:TRP:HB3	1.96	0.46
1:C:517:ARG:NH2	1:C:549:GLY:O	2.48	0.46
1:C:928:LYS:HD2	1:C:1006:TRP:CZ2	2.50	0.46
1:C:929:ILE:HD11	1:C:1006:TRP:CZ3	2.49	0.46
1:C:371:LEU:HD23	1:C:450:TRP:CD2	2.51	0.46
1:C:425:GLN:HG2	1:C:427:TYR:CE1	2.50	0.46
1:C:675:GLU:HG2	1:C:676:GLN:HG2	1.98	0.46
3:E:99:VAL:O	3:E:146:TYR:OH	2.28	0.46
1:C:420:LEU:HD21	1:C:473:SER:HB3	1.97	0.46
1:A:962:ASP:HA	1:A:998:CYS:HB2	1.96	0.46
1:B:943:GLU:HG2	1:B:952:THR:HG22	1.96	0.46
2:D:119:THR:HG23	2:D:122:VAL:H	1.81	0.46
1:B:690:LEU:HD21	1:B:714:ILE:HG12	1.97	0.46
1:A:528:LEU:HD22	1:A:532:HIS:CD2	2.51	0.46
1:B:296:ASP:N	1:B:299:ASP:OD2	2.46	0.46
1:B:406:GLU:HG3	1:B:442:CYS:HB2	1.98	0.46
1:B:866:GLN:HG3	1:B:901:THR:HG22	1.97	0.46
1:B:722:VAL:HG22	1:B:731:ARG:HG2	1.97	0.46
1:B:224:ASP:HB2	1:B:247:ASN:H	1.80	0.46
1:C:997:LYS:HE3	1:C:997:LYS:HB2	1.81	0.46
1:B:191:ASP:OD1	1:B:191:ASP:N	2.43	0.46
1:C:329:TRP:HE3	1:C:351:GLY:HA2	1.81	0.46
4:F:190:LEU:HD11	4:F:340:VAL:HG22	1.97	0.46
1:A:191:ASP:OD1	1:A:191:ASP:N	2.48	0.45
1:A:852:LYS:N	1:A:919:GLU:O	2.49	0.45
1:A:929:ILE:HD11	1:A:942:VAL:HG13	1.98	0.45
1:A:1023:ASP:OD1	1:A:1023:ASP:N	2.49	0.45
1:B:318:ARG:HG3	1:B:321:ALA:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:32:LEU:HD21	3:E:39:THR:HG21	1.99	0.45
1:A:612:TRP:CD1	1:A:678:ALA:HB1	2.51	0.45
1:A:914:LEU:H	1:A:914:LEU:HD12	1.81	0.45
1:B:720:ARG:HG3	1:B:740:TRP:CZ3	2.51	0.45
1:C:407:ALA:HB1	1:C:470:ILE:CD1	2.46	0.45
1:C:848:GLY:HA3	1:C:889:TRP:HD1	1.80	0.45
4:F:136:GLN:HB2	4:F:196:LYS:HD3	1.98	0.45
1:C:538:GLY:O	1:C:569:HIS:NE2	2.49	0.45
1:C:540:ILE:HD11	1:C:569:HIS:HA	1.99	0.45
3:E:51:THR:OG1	3:E:53:ASP:OD1	2.25	0.45
1:B:630:LEU:HD22	1:B:683:SER:HA	1.99	0.45
1:C:668:GLY:HA2	1:C:908:SER:O	2.17	0.45
1:B:235:LEU:HA	1:B:238:CYS:HB3	1.99	0.45
1:B:440:SER:OG	1:B:441:SER:N	2.50	0.45
1:C:850:VAL:HG13	1:C:890:VAL:HG13	1.97	0.45
3:E:81:ASN:O	3:E:84:GLY:N	2.49	0.45
1:A:954:CYS:SG	1:A:955:ASP:N	2.90	0.45
4:F:124:HIS:CE1	4:F:148:ASN:HB2	2.52	0.45
1:A:392:ARG:O	1:A:392:ARG:HG2	2.17	0.45
1:C:404:LEU:HD12	1:C:404:LEU:HA	1.86	0.45
1:A:375:LEU:HD21	1:A:470:ILE:HD11	1.99	0.44
1:B:263:ASP:OD1	1:B:263:ASP:N	2.44	0.44
1:C:475:HIS:O	1:C:476:ARG:HD3	2.16	0.44
1:C:929:ILE:HD11	1:C:1006:TRP:HZ3	1.82	0.44
2:D:32:ARG:HG2	3:E:128:GLN:NE2	2.31	0.44
3:E:86:PHE:HD1	3:E:89:LEU:HD12	1.82	0.44
4:F:34:PRO:HB3	4:G:72:LYS:HE2	1.98	0.44
4:F:57:LYS:NZ	4:F:87:GLU:OE2	2.46	0.44
1:A:266:LEU:HD12	1:A:281:VAL:HG22	1.99	0.44
1:B:421:LYS:HG2	1:B:423:SER:H	1.82	0.44
1:C:268:LEU:HD23	1:C:279:LEU:HD23	1.99	0.44
1:A:301:ALA:HA	1:A:314:THR:HG21	2.00	0.44
1:B:670:SER:HA	1:B:909:PRO:HB3	2.00	0.44
4:G:53:LYS:HE3	4:G:53:LYS:HB2	1.72	0.44
1:C:412:ARG:NH1	1:C:446:GLU:O	2.48	0.44
1:C:509:LEU:HD23	1:C:990:PRO:HG3	2.00	0.44
1:A:955:ASP:OD1	1:A:1022:GLU:HB3	2.18	0.44
1:C:272:VAL:HG12	5:C:1101:NAG:H62	2.00	0.44
4:G:59:ARG:CZ	4:G:85:GLU:HB3	2.47	0.44
1:B:232:GLU:HG3	1:B:238:CYS:HB2	1.99	0.44
1:C:930:ARG:HD3	1:C:950:TRP:CH2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:936:THR:OG1	1:C:937:SER:N	2.51	0.44
4:F:104:LEU:HD11	4:F:292:CYS:HB2	2.00	0.44
4:F:140:THR:OG1	4:F:141:THR:N	2.51	0.44
1:C:791:LYS:HB2	1:C:791:LYS:HE2	1.57	0.44
1:C:446:GLU:OE1	1:C:446:GLU:N	2.40	0.44
1:B:268:LEU:HD21	1:B:363:VAL:HG12	1.99	0.43
1:C:580:TYR:HD1	1:C:580:TYR:H	1.65	0.43
1:B:822:MET:HA	1:B:842:PHE:O	2.18	0.43
1:C:398:CYS:HB2	1:C:438:PHE:HB3	2.00	0.43
1:C:879:SER:OG	1:C:880:LEU:N	2.52	0.43
3:E:81:ASN:O	3:E:81:ASN:OD1	2.36	0.43
4:G:48:VAL:O	4:G:66:TYR:N	2.51	0.43
1:A:397:VAL:HG22	1:A:437:LEU:HB3	2.00	0.43
1:A:689:THR:HG1	1:A:690:LEU:H	1.66	0.43
1:C:717:GLY:HA2	1:C:735:TYR:HB3	2.00	0.43
1:B:197:CYS:HB3	1:B:203:GLY:O	2.19	0.43
1:B:740:TRP:O	1:B:779:GLY:HA3	2.18	0.43
4:F:95:ASN:ND2	4:F:111:LYS:O	2.52	0.43
1:A:889:TRP:HB3	1:A:910:TRP:CZ3	2.53	0.43
1:B:160:ARG:O	1:B:173:GLU:HB2	2.18	0.43
1:B:290:ILE:HG12	1:B:330:LEU:HB2	2.00	0.43
1:C:263:ASP:OD1	1:C:263:ASP:N	2.51	0.43
1:C:317:GLY:HA2	1:C:456:GLN:HE21	1.84	0.43
3:E:15:LEU:HB3	3:E:119:PHE:HE2	1.84	0.43
4:F:72:LYS:HG2	4:G:34:PRO:HG2	2.01	0.43
1:A:331:ASP:OD1	1:A:332:SER:N	2.52	0.43
1:C:289:THR:O	1:C:328:ILE:HA	2.19	0.43
1:C:485:ILE:H	1:C:485:ILE:HG13	1.65	0.43
1:C:732:VAL:HG11	1:C:743:ILE:HD12	2.00	0.43
1:C:789:ASN:OD1	1:C:792:GLU:HG3	2.18	0.43
1:A:732:VAL:HG23	1:A:815:GLY:HA2	1.99	0.43
1:B:157:LEU:HA	1:B:175:LYS:O	2.18	0.43
1:C:593:GLU:OE2	1:C:637:ARG:NH2	2.50	0.43
1:B:467:GLU:H	1:B:467:GLU:HG2	1.63	0.43
1:C:645:ILE:HG21	1:C:672:CYS:HB3	2.00	0.43
2:D:33:MET:HE2	2:D:33:MET:HB3	1.89	0.43
1:B:898:GLY:N	1:B:899:PRO:HD2	2.34	0.43
1:C:329:TRP:HA	1:C:351:GLY:HA2	2.00	0.43
4:G:59:ARG:HB2	4:G:87:GLU:HG2	2.01	0.43
1:B:745:ASP:OD2	1:B:812:GLU:HB3	2.19	0.42
1:C:572:ASP:OD1	1:C:572:ASP:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:912:LYS:HE2	1:C:912:LYS:HB2	1.87	0.42
4:F:175:GLU:OE1	4:F:192:LYS:NZ	2.38	0.42
1:A:503:CYS:SG	1:A:505:SER:OG	2.77	0.42
1:A:884:MET:HE1	1:A:886:ILE:HG23	2.02	0.42
1:A:953:VAL:HG23	1:A:993:LEU:HB2	2.00	0.42
1:B:159:MET:CE	1:B:235:LEU:HD22	2.48	0.42
1:B:198:ARG:HH22	1:B:203:GLY:HA2	1.84	0.42
1:B:260:LYS:HE3	1:B:260:LYS:HB2	1.75	0.42
1:B:275:CYS:HB3	1:B:365:CYS:HB2	2.01	0.42
1:B:484:ASP:OD1	1:B:484:ASP:N	2.51	0.42
3:E:3:HIS:HB2	3:E:4:LEU:HD12	2.00	0.42
3:E:8:GLU:HG2	3:E:130:ALA:HB2	2.01	0.42
1:A:440:SER:OG	1:A:441:SER:N	2.52	0.42
1:A:929:ILE:HG21	1:A:969:GLN:HB3	2.01	0.42
4:G:47:SER:HA	4:G:67:THR:HA	2.00	0.42
1:A:384:GLY:HA2	1:A:424:TYR:CD2	2.54	0.42
1:B:331:ASP:OD1	1:B:332:SER:N	2.53	0.42
1:B:587:ASN:OD1	1:B:638:PHE:HB3	2.20	0.42
1:B:599:LYS:HD2	1:B:604:TRP:CE2	2.54	0.42
1:B:671:LEU:HD12	1:B:909:PRO:HG2	2.02	0.42
1:B:755:VAL:HG23	1:B:790:GLY:HA2	2.02	0.42
1:C:848:GLY:HA3	1:C:889:TRP:CD1	2.53	0.42
4:F:172:VAL:HG11	4:F:193:LEU:HD13	2.01	0.42
1:A:503:CYS:SG	1:A:504:ASP:N	2.92	0.42
1:A:955:ASP:HB2	1:A:980:LYS:HB2	2.01	0.42
1:C:744:CYS:HB2	1:C:784:ASP:HA	2.01	0.42
1:C:822:MET:HA	1:C:842:PHE:O	2.20	0.42
4:G:57:LYS:HD2	4:G:58:LEU:H	1.85	0.42
1:B:671:LEU:HD12	1:B:671:LEU:H	1.85	0.42
1:C:418:SER:N	1:C:473:SER:OG	2.53	0.42
1:C:941:ARG:NH1	1:C:986:GLN:O	2.53	0.42
1:B:291:CYS:HB3	1:B:331:ASP:HA	2.01	0.42
4:F:227:ARG:HD3	4:F:231:PHE:O	2.19	0.42
1:B:176:PHE:HB3	1:B:222:TRP:CE2	2.55	0.42
1:B:304:CYS:HB3	1:B:311:THR:HG22	2.02	0.42
1:B:693:CYS:HB2	1:B:713:CYS:HB3	1.85	0.42
1:C:889:TRP:HB3	1:C:910:TRP:CZ3	2.51	0.42
2:D:39:THR:O	2:D:42:THR:OG1	2.37	0.42
1:A:822:MET:HA	1:A:842:PHE:O	2.19	0.42
1:B:874:LYS:HB2	1:B:874:LYS:HE3	1.86	0.42
1:C:605:GLY:HA2	1:C:643:GLY:HA3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:979:PHE:HB3	1:C:983:GLU:HB2	2.01	0.42
1:A:400:ARG:HG3	1:A:401:GLY:N	2.35	0.41
1:A:849:THR:HG23	1:A:888:MET:HB3	2.02	0.41
1:A:898:GLY:N	1:A:899:PRO:CD	2.83	0.41
1:A:973:GLY:HA3	1:A:1029:THR:HG23	2.02	0.41
1:B:174:ILE:H	1:B:181:GLY:H	1.67	0.41
1:B:411:CYS:HB3	1:B:417:GLY:O	2.19	0.41
1:B:831:SER:OG	1:B:833:GLU:O	2.36	0.41
1:C:592:CYS:HB3	1:C:682:CYS:CB	2.49	0.41
1:B:168:CYS:SG	1:B:261:GLY:N	2.93	0.41
1:B:282:ARG:HB2	1:B:287:TRP:CE3	2.55	0.41
1:C:313:VAL:HB	1:C:366:SER:HB3	2.02	0.41
1:C:487:CYS:HB3	1:C:577:CYS:HB2	2.02	0.41
1:C:954:CYS:SG	1:C:955:ASP:N	2.93	0.41
1:A:159:MET:HG3	1:A:160:ARG:N	2.35	0.41
1:B:469:LYS:H	1:B:469:LYS:HG2	1.76	0.41
1:B:619:VAL:HG12	1:B:659:MET:HG2	2.01	0.41
1:B:893:VAL:HA	1:B:907:SER:HB2	2.02	0.41
1:C:282:ARG:HB3	1:C:287:TRP:CE3	2.55	0.41
1:C:607:LEU:HD23	1:C:607:LEU:HA	1.84	0.41
4:F:149:HIS:HD1	4:F:158:ILE:HG12	1.85	0.41
7:E:201:HEM:HBC2	7:E:201:HEM:CHD	2.48	0.41
1:A:271:GLY:HA3	1:A:276:SER:O	2.20	0.41
1:C:690:LEU:HD23	1:C:714:ILE:HG12	2.02	0.41
1:A:931:LEU:HG	1:A:970:LEU:HD12	2.01	0.41
1:B:959:ASP:OD1	1:B:959:ASP:N	2.53	0.41
1:C:520:GLN:O	1:C:579:ARG:NE	2.53	0.41
1:C:592:CYS:O	1:C:682:CYS:HB2	2.20	0.41
1:C:692:SER:HA	1:C:714:ILE:H	1.85	0.41
1:C:824:LEU:HD21	1:C:863:VAL:HG13	2.01	0.41
1:A:866:GLN:HG3	1:A:901:THR:HG22	2.03	0.41
1:B:721:LEU:HA	1:B:731:ARG:O	2.20	0.41
1:C:871:ASP:OD2	1:C:950:TRP:NE1	2.52	0.41
1:A:842:PHE:HB2	1:A:847:TRP:CZ3	2.55	0.41
1:B:965:VAL:HG12	1:B:1005:LEU:HD12	2.02	0.41
1:C:463:ASP:OD1	1:C:463:ASP:C	2.63	0.41
3:E:100:ASP:HA	4:F:108:LEU:HD22	2.03	0.41
7:E:201:HEM:HHA	7:E:201:HEM:HBA1	2.03	0.41
1:A:232:GLU:HG3	1:A:234:ALA:O	2.21	0.41
1:A:890:VAL:HB	1:A:910:TRP:CZ3	2.55	0.41
1:A:945:TRP:HB2	1:A:950:TRP:CZ3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:TYR:HE1	1:B:561:PRO:HG3	1.86	0.41
1:B:589:LYS:H	1:B:589:LYS:HD2	1.85	0.41
4:F:227:ARG:HB3	4:F:231:PHE:HA	2.03	0.41
1:A:213:ASN:HD22	1:A:349:GLU:HG3	1.86	0.41
1:B:399:ASP:OD1	1:B:402:TRP:HB3	2.21	0.41
1:B:735:TYR:HB2	1:B:740:TRP:CE3	2.56	0.41
3:E:94:CYS:HB2	3:E:146:TYR:CE1	2.56	0.41
1:A:463:ASP:OD1	1:A:463:ASP:N	2.55	0.40
1:A:521:CYS:C	1:A:579:ARG:HG3	2.47	0.40
1:A:647:ARG:HD2	1:A:647:ARG:H	1.86	0.40
1:C:571:ARG:NH2	1:C:988:THR:HG22	2.36	0.40
1:C:686:GLN:N	1:C:686:GLN:OE1	2.53	0.40
1:C:974:PRO:O	1:C:1029:THR:OG1	2.34	0.40
1:A:554:LEU:HD23	1:A:554:LEU:HA	1.86	0.40
1:B:855:MET:HE2	1:B:921:THR:HG21	2.03	0.40
1:C:787:LYS:HD2	1:C:799:HIS:ND1	2.36	0.40
4:F:71:GLU:CD	4:F:71:GLU:H	2.29	0.40
4:F:93:PRO:HA	4:F:204:MET:HE1	2.02	0.40
1:A:218:SER:OG	1:A:219:GLY:N	2.55	0.40
1:B:616:ASP:N	1:B:616:ASP:OD1	2.55	0.40
1:C:494:LYS:HB2	1:C:499:TRP:CE3	2.56	0.40
2:D:2:VAL:HG12	4:F:326:GLU:HG2	2.03	0.40
4:G:68:LEU:HB2	4:G:74:TRP:CZ3	2.56	0.40
1:A:282:ARG:HB2	1:A:287:TRP:CE3	2.56	0.40
1:A:820:GLU:HA	1:A:843:TYR:HE1	1.86	0.40
1:B:860:VAL:HG13	1:B:923:ILE:HD12	2.04	0.40
4:F:46:HIS:CG	4:G:48:VAL:HG12	2.57	0.40
1:A:282:ARG:HB2	1:A:287:TRP:CZ3	2.55	0.40
1:A:714:ILE:H	1:A:714:ILE:HG13	1.76	0.40
1:A:888:MET:HB3	1:A:888:MET:HE2	1.87	0.40
1:B:721:LEU:HB3	1:B:729:ALA:C	2.47	0.40
1:C:721:LEU:HB3	1:C:730:GLY:HA3	2.03	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	A	856/1012 (85%)	833 (97%)	23 (3%)	0	100	100
1	B	854/1012 (84%)	833 (98%)	21 (2%)	0	100	100
1	C	747/1012 (74%)	723 (97%)	24 (3%)	0	100	100
2	D	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
3	E	144/147 (98%)	142 (99%)	2 (1%)	0	100	100
4	F	306/347 (88%)	295 (96%)	11 (4%)	0	100	100
4	G	54/347 (16%)	52 (96%)	2 (4%)	0	100	100
All	All	3100/4019 (77%)	3013 (97%)	87 (3%)	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	699/826 (85%)	670 (96%)	29 (4%)	26	54
1	B	698/826 (84%)	673 (96%)	25 (4%)	30	57
1	C	612/826 (74%)	587 (96%)	25 (4%)	26	54
2	D	113/114 (99%)	110 (97%)	3 (3%)	40	65
3	E	118/119 (99%)	115 (98%)	3 (2%)	42	67
4	F	266/294 (90%)	259 (97%)	7 (3%)	41	66
4	G	49/294 (17%)	48 (98%)	1 (2%)	50	71
All	All	2555/3299 (77%)	2462 (96%)	93 (4%)	32	57

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	ILE
1	A	292	ASP
1	A	296	ASP
1	A	333	VAL
1	A	334	SER
1	A	342	ILE
1	A	343	TRP
1	A	363	VAL
1	A	365	CYS
1	A	370	ASP
1	A	371	LEU
1	A	388	VAL
1	A	439	LEU
1	A	442	CYS
1	A	464	HIS
1	A	507	PHE
1	A	525	VAL
1	A	527	ILE
1	A	589	LYS
1	A	630	LEU
1	A	671	LEU
1	A	823	SER
1	A	886	ILE
1	A	902	LEU
1	A	927	ASN
1	A	986	GLN
1	A	996	VAL
1	A	1020	HIS
1	A	1028	CYS
1	B	189	ASN
1	B	214	PHE
1	B	243	TRP
1	B	257	ILE
1	B	327	HIS
1	B	330	LEU
1	B	348	HIS
1	B	357	HIS
1	B	373	LEU
1	B	423	SER
1	B	469	LYS
1	B	507	PHE
1	B	540	ILE
1	B	583	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	590	THR
1	B	598	LEU
1	B	628	VAL
1	B	711	VAL
1	B	742	THR
1	B	808	CYS
1	B	809	ARG
1	B	822	MET
1	B	880	LEU
1	B	902	LEU
1	B	976	LEU
1	C	283	PHE
1	C	336	GLN
1	C	347	HIS
1	C	393	LEU
1	C	394	LEU
1	C	485	ILE
1	C	527	ILE
1	C	569	HIS
1	C	613	ASP
1	C	626	CYS
1	C	638	PHE
1	C	711	VAL
1	C	714	ILE
1	C	737	GLU
1	C	749	ASP
1	C	756	VAL
1	C	769	THR
1	C	774	PHE
1	C	786	MET
1	C	808	CYS
1	C	888	MET
1	C	959	ASP
1	C	960	LEU
1	C	1020	HIS
1	C	1029	THR
2	D	48	ASP
2	D	53	SER
2	D	140	LYS
3	E	32	LEU
3	E	51	THR
3	E	105	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	79	VAL
4	F	124	HIS
4	F	127	THR
4	F	163	THR
4	F	200	ASN
4	F	274	ILE
4	F	320	LYS
4	G	46	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	A	454	ASN
1	A	553	HIS
1	A	688	GLN
1	A	801	HIS
1	B	199	GLN
1	B	213	ASN
1	B	336	GLN
1	B	347	HIS
1	B	797	GLN
1	C	336	GLN
1	C	520	GLN
1	C	773	HIS
1	C	1015	HIS
2	D	98	ASN
4	F	69	ASN
4	F	95	ASN
4	F	200	ASN
4	F	272	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 23 are monoatomic - leaving 13 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
5	NAG	C	1102	1	14,14,15	0.73	0	17,19,21	0.80	0
5	NAG	A	1101	1	14,14,15	0.80	0	17,19,21	0.85	0
5	NAG	B	1101	1	14,14,15	0.78	0	17,19,21	0.95	1 (5%)
5	NAG	C	1103	1	14,14,15	0.71	0	17,19,21	0.78	0
5	NAG	A	1102	1	14,14,15	0.72	0	17,19,21	0.77	0
5	NAG	A	1103	1	14,14,15	0.70	0	17,19,21	0.76	0
5	NAG	B	1103	1	14,14,15	0.72	0	17,19,21	0.78	0
8	OXY	D	202	-	1,1,1	0.16	0	-	-	-
7	HEM	E	201	3	42,50,50	1.57	4 (9%)	46,82,82	1.50	7 (15%)
8	OXY	E	202	-	1,1,1	0.17	0	-	-	-
5	NAG	B	1102	1	14,14,15	0.71	0	17,19,21	0.77	0
7	HEM	D	201	2	42,50,50	1.49	6 (14%)	46,82,82	1.30	6 (13%)
5	NAG	C	1101	1	14,14,15	0.70	0	17,19,21	0.84	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1102	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1101	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1101	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1103	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1102	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1103	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1103	1	-	0/6/23/26	0/1/1/1
7	HEM	E	201	3	-	4/12/54/54	-
5	NAG	B	1102	1	-	0/6/23/26	0/1/1/1
7	HEM	D	201	2	-	0/12/54/54	-
5	NAG	C	1101	1	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	201	HEM	C3C-C2C	-4.97	1.33	1.40
7	D	201	HEM	C3C-C2C	-3.90	1.35	1.40
7	D	201	HEM	C3C-CAC	3.47	1.55	1.47
7	E	201	HEM	C3C-CAC	3.31	1.55	1.47
7	E	201	HEM	C3C-C4C	3.21	1.46	1.41
7	D	201	HEM	CAB-C3B	3.11	1.55	1.47
7	E	201	HEM	CAB-C3B	2.98	1.55	1.47
7	D	201	HEM	C3C-C4C	2.62	1.45	1.41
7	D	201	HEM	CMB-C2B	2.05	1.55	1.50
7	D	201	HEM	CMD-C2D	2.02	1.54	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	201	HEM	C3B-C2B-C1B	3.04	108.69	106.41
7	E	201	HEM	C4C-CHD-C1D	2.91	126.40	122.56
7	E	201	HEM	C4B-CHC-C1C	2.70	126.12	122.56
7	E	201	HEM	C1B-NB-C4B	2.45	108.11	105.21
7	E	201	HEM	C4D-ND-C1D	2.40	108.05	105.21
7	D	201	HEM	C4D-ND-C1D	2.33	107.97	105.21
7	E	201	HEM	C3B-C4B-NB	-2.19	107.89	109.47
7	D	201	HEM	C1B-NB-C4B	2.15	107.76	105.21
5	B	1101	NAG	O5-C1-C2	-2.13	108.00	111.29
7	E	201	HEM	C3D-C4D-ND	-2.12	107.84	110.17
7	D	201	HEM	C3D-C4D-ND	-2.11	107.86	110.17
7	D	201	HEM	C4B-CHC-C1C	2.09	125.31	122.56
7	D	201	HEM	CMC-C2C-C3C	2.09	128.86	124.68
5	C	1101	NAG	O5-C1-C2	-2.08	108.08	111.29
7	D	201	HEM	C3B-C2B-C1B	2.07	107.96	106.41

There are no chirality outliers.

All (8) torsion outliers are listed below:

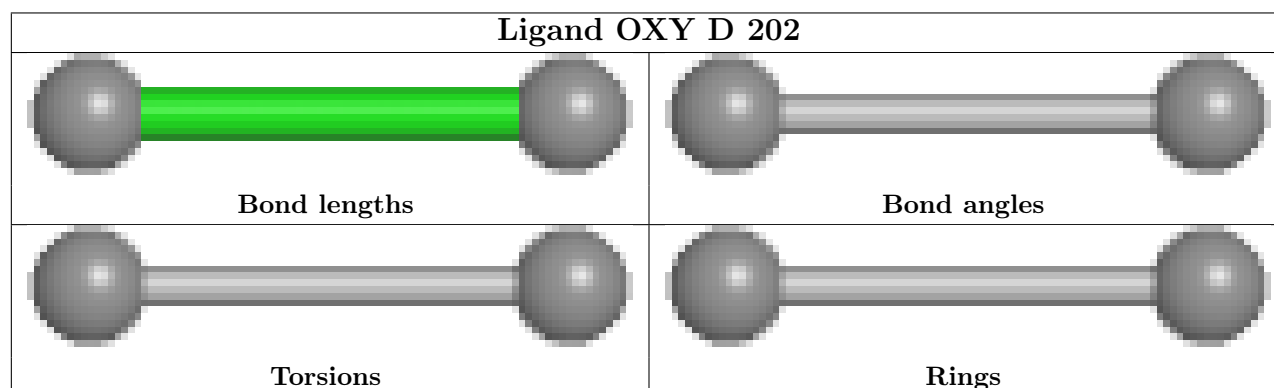
Mol	Chain	Res	Type	Atoms
5	B	1101	NAG	C8-C7-N2-C2
5	B	1101	NAG	O7-C7-N2-C2
5	C	1102	NAG	C8-C7-N2-C2
5	C	1102	NAG	O7-C7-N2-C2
7	E	201	HEM	C3A-C2A-CAA-CBA
7	E	201	HEM	C1A-C2A-CAA-CBA
7	E	201	HEM	C4B-C3B-CAB-CBB
7	E	201	HEM	CAA-CBA-CGA-O2A

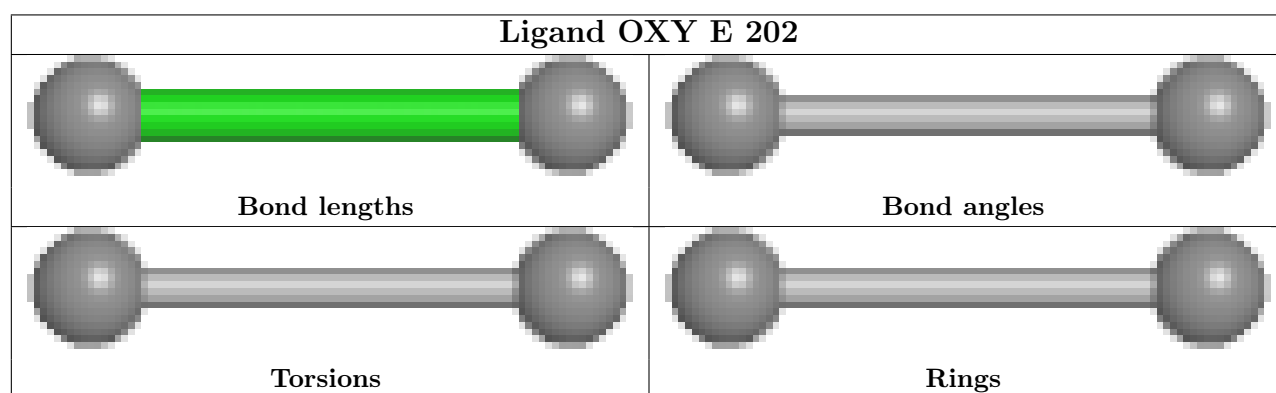
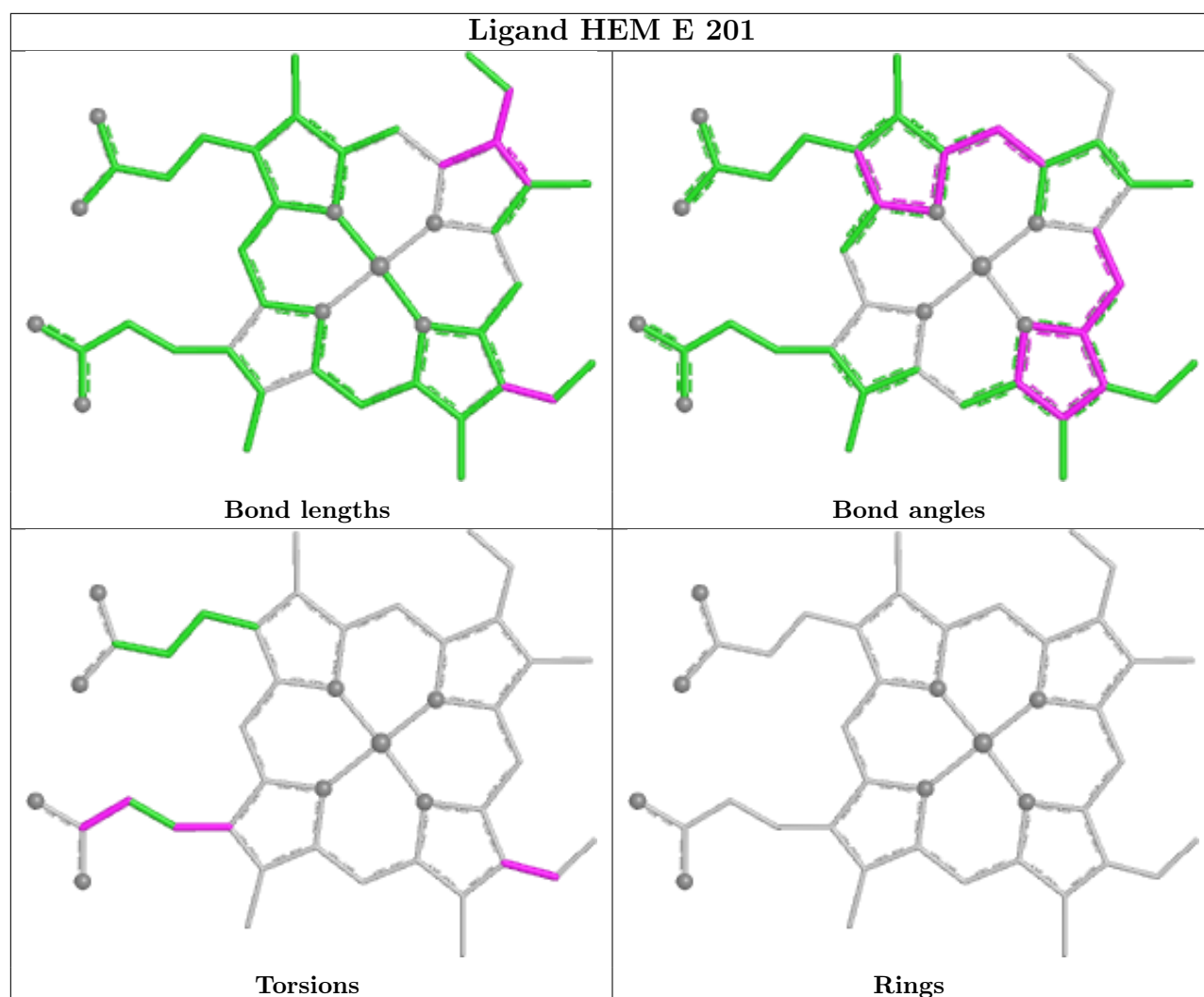
There are no ring outliers.

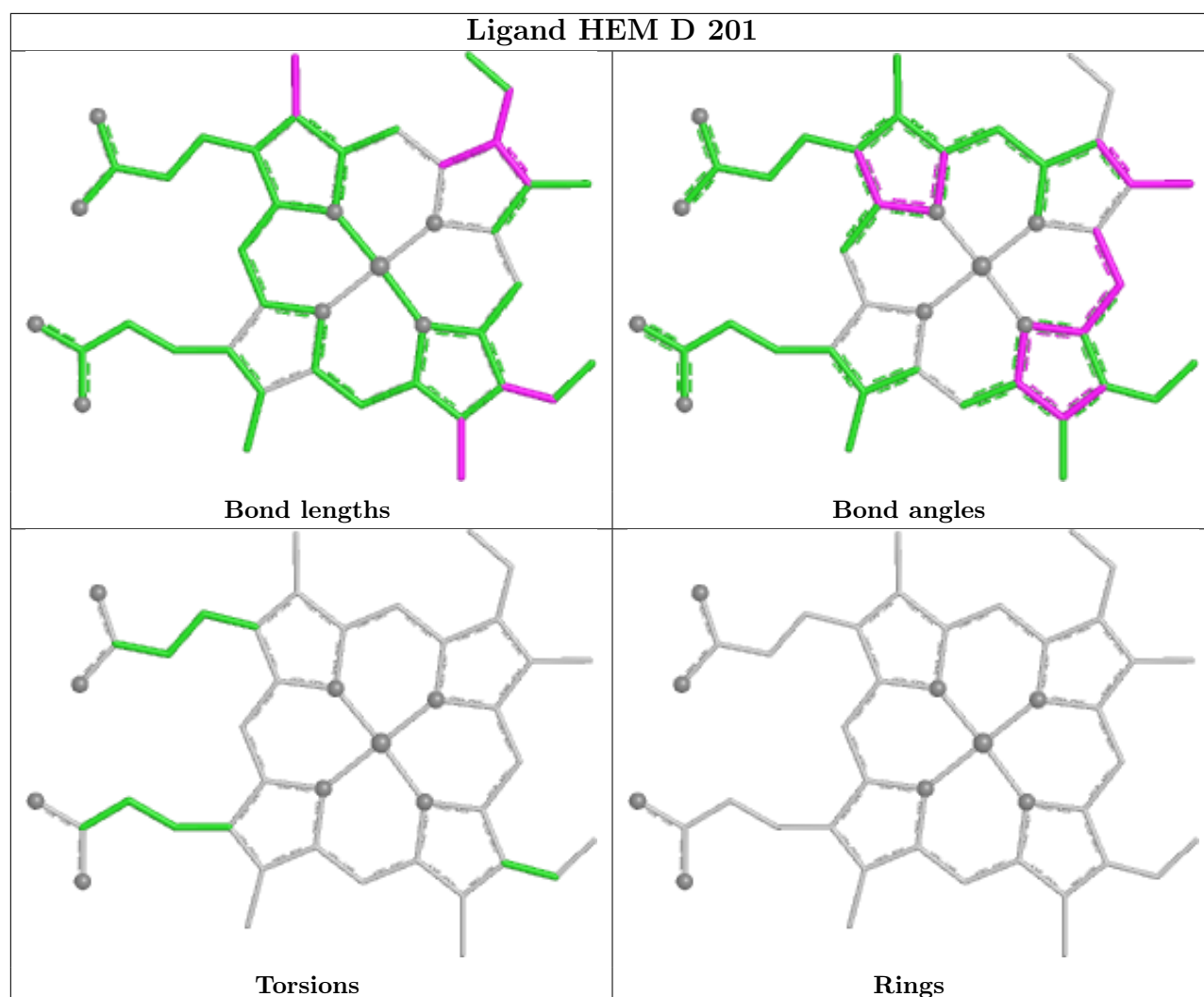
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1102	NAG	1	0
7	E	201	HEM	5	0
8	E	202	OXY	1	0
7	D	201	HEM	2	0
5	C	1101	NAG	1	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.

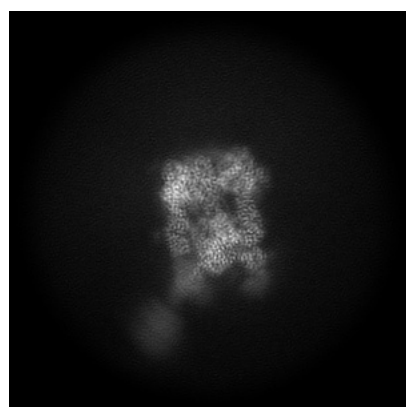
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49218. These allow visual inspection of the internal detail of the map and identification of artifacts.

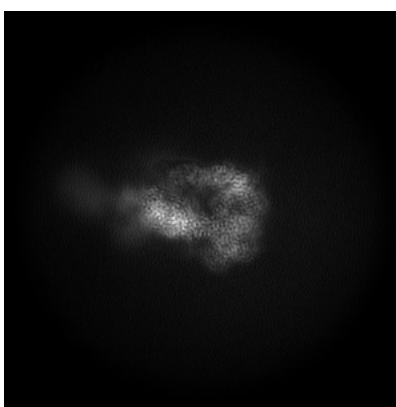
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

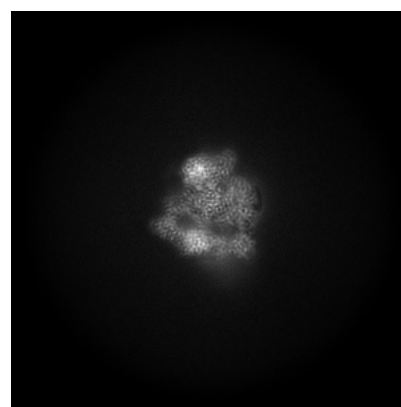
6.1.1 Primary map



X



Y



Z

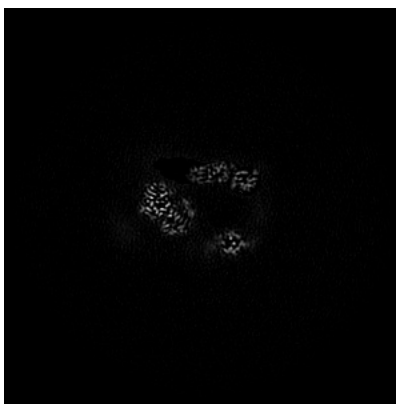
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

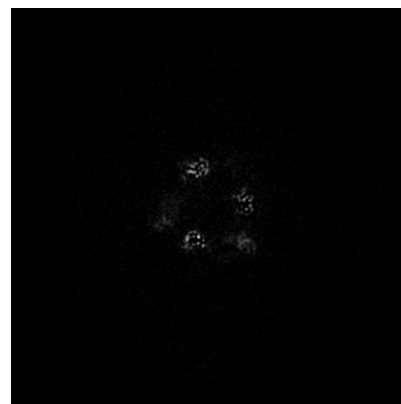
6.2.1 Primary map



X Index: 200



Y Index: 200

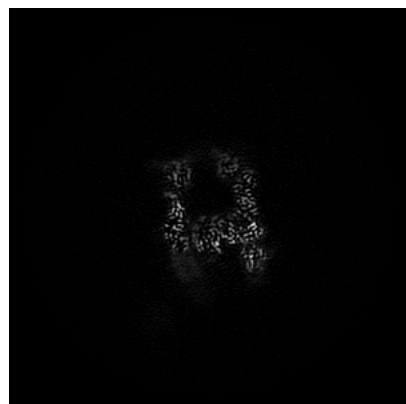


Z Index: 200

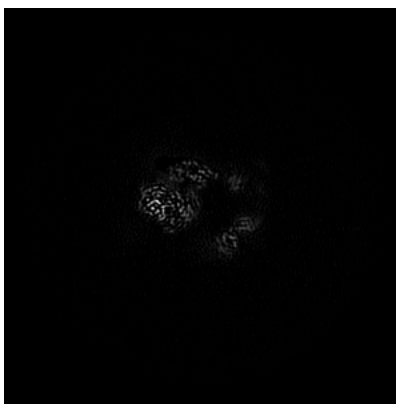
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

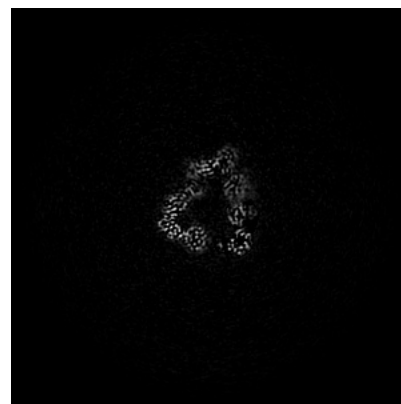
6.3.1 Primary map



X Index: 188



Y Index: 210

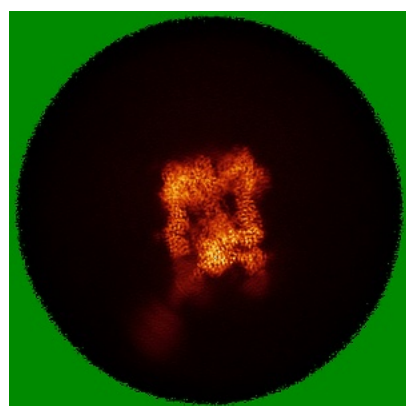


Z Index: 231

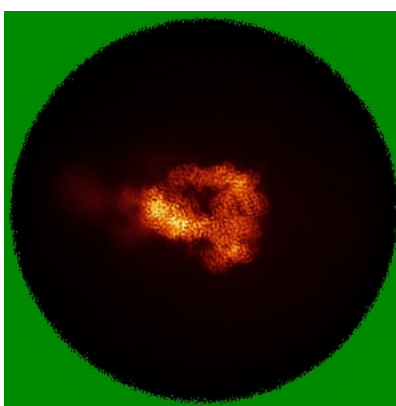
The images above show the largest variance slices of the map in three orthogonal directions.

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

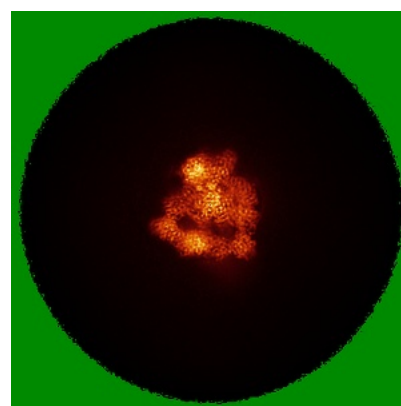
6.4.1 Primary map



X



Y



Z

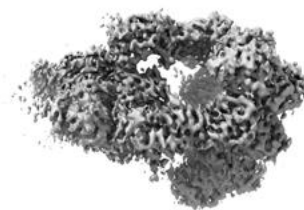
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

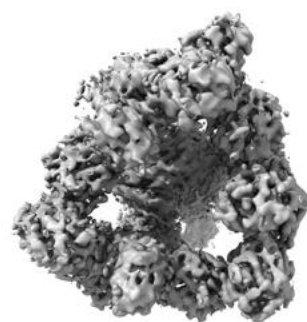
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

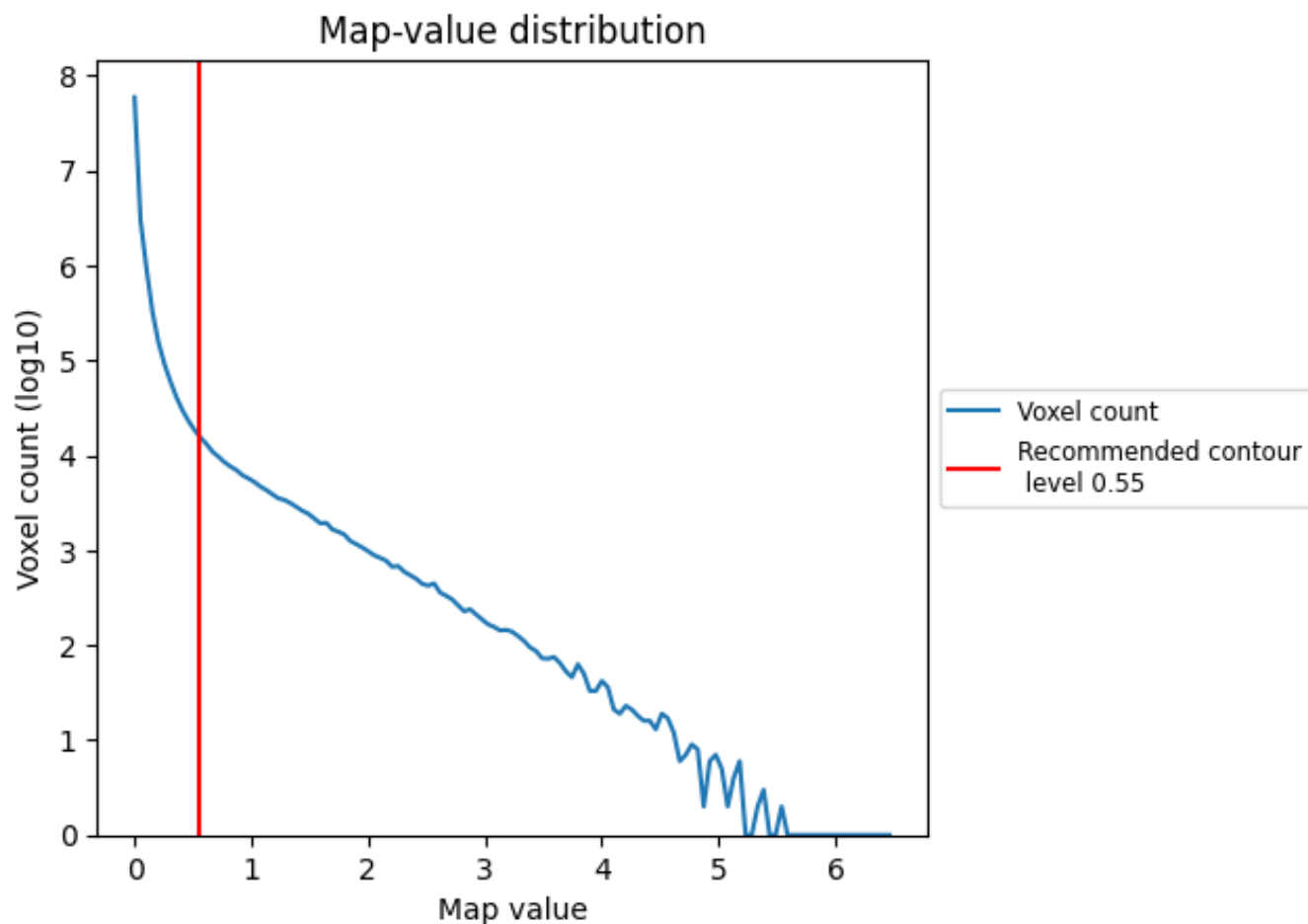
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

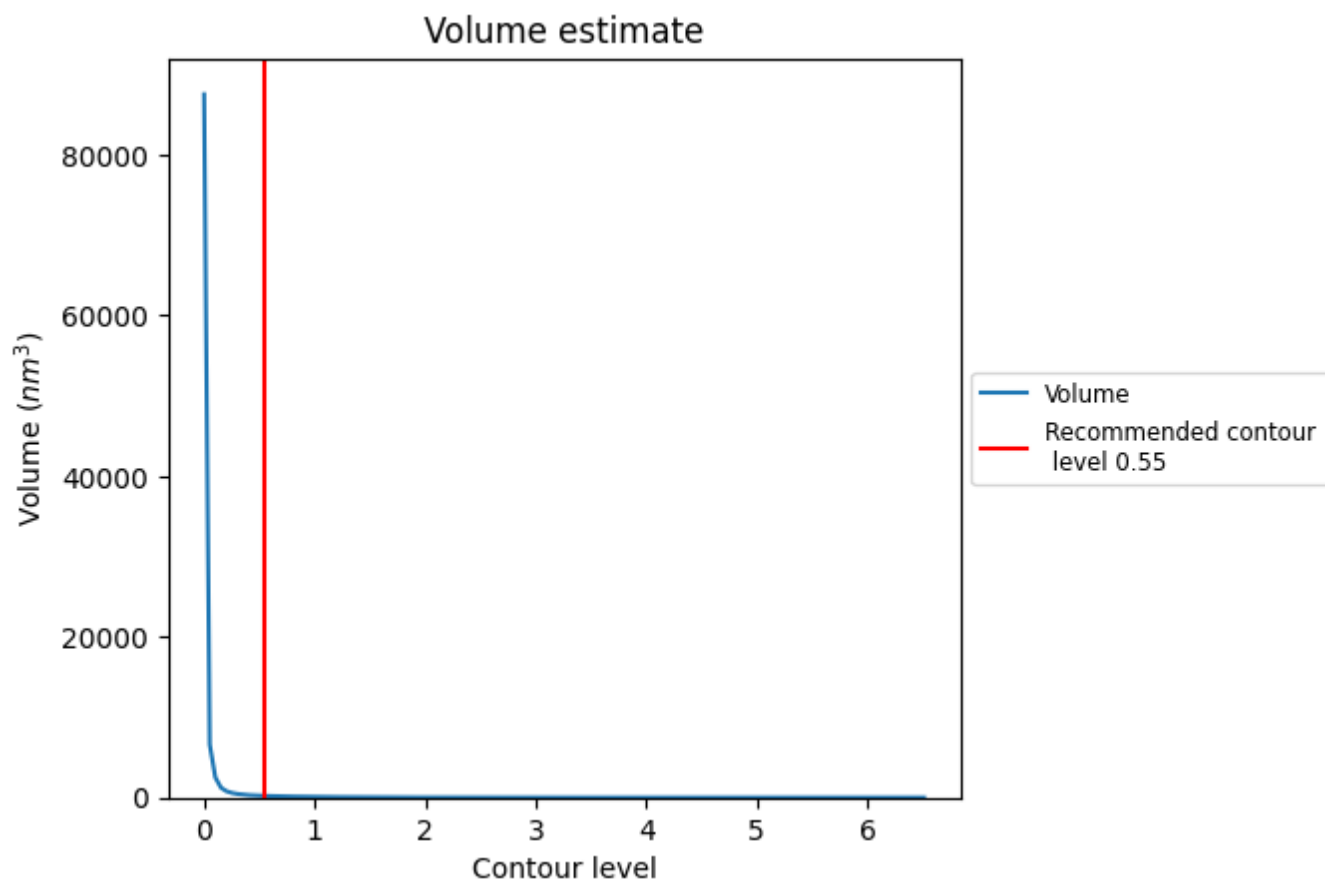
This section contains the results of statistical analysis of the map.

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.

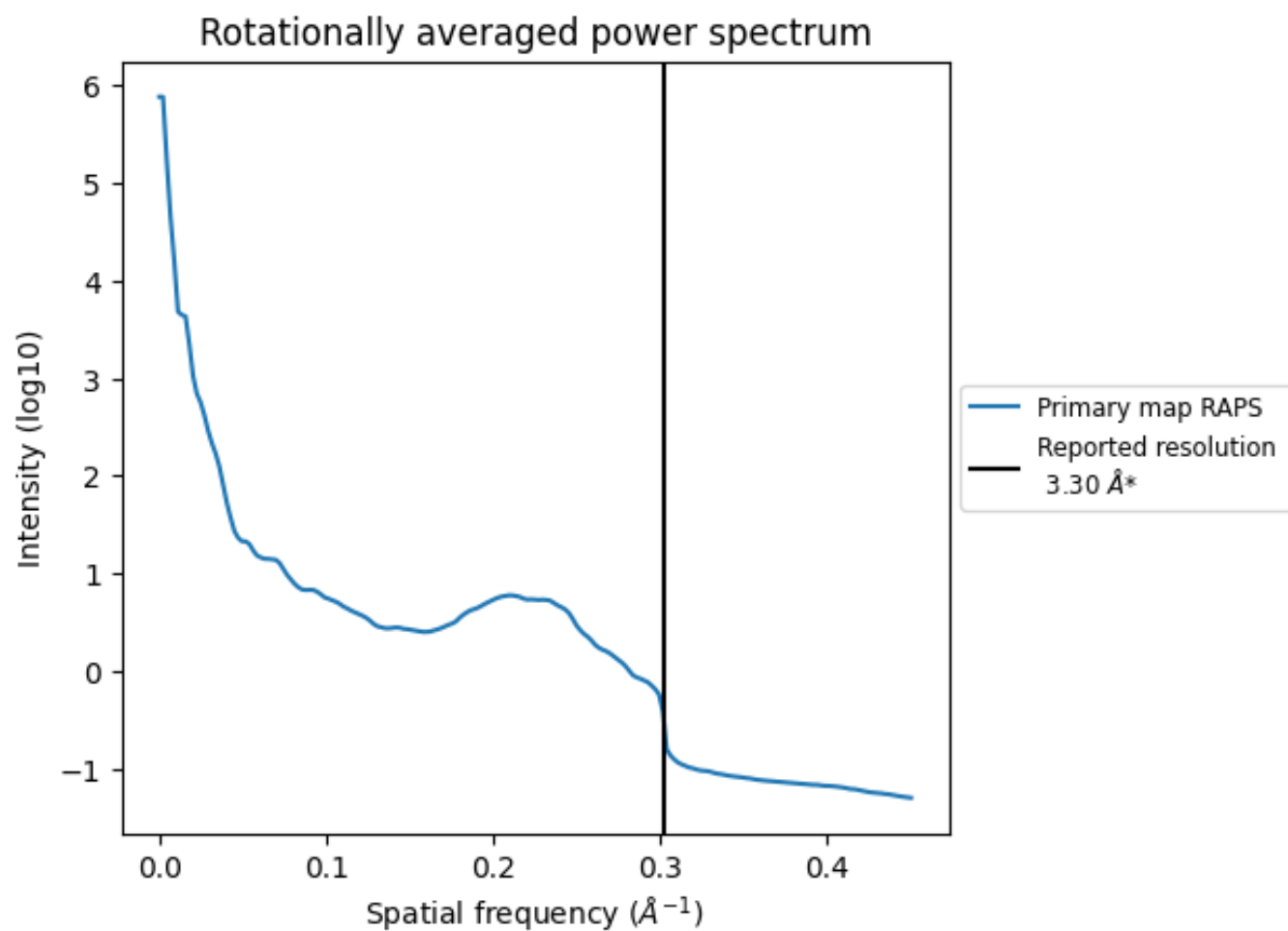
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 207 nm³; this corresponds to an approximate mass of 187 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 0.303 Å⁻¹

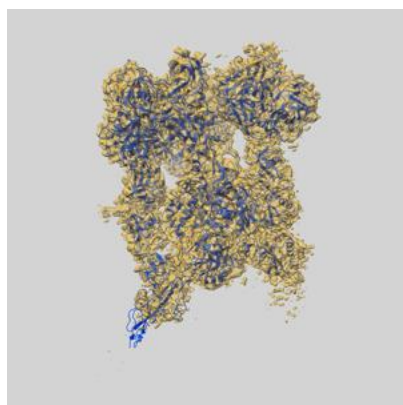
8 Fourier-Shell correlation

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

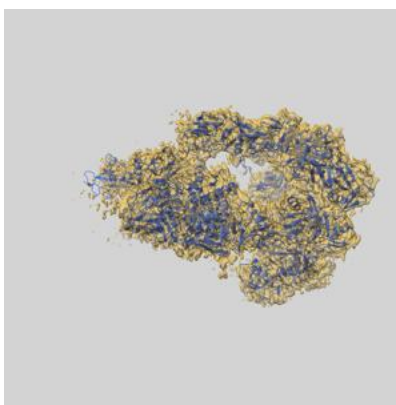
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49218 and PDB model 9NB6. Per-residue inclusion information can be found in section [3](#) on page [7](#).

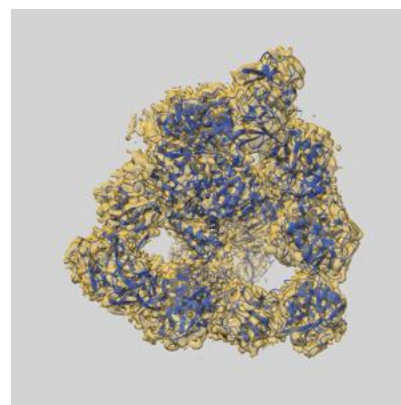
9.1 Map-model overlay [i](#)



X



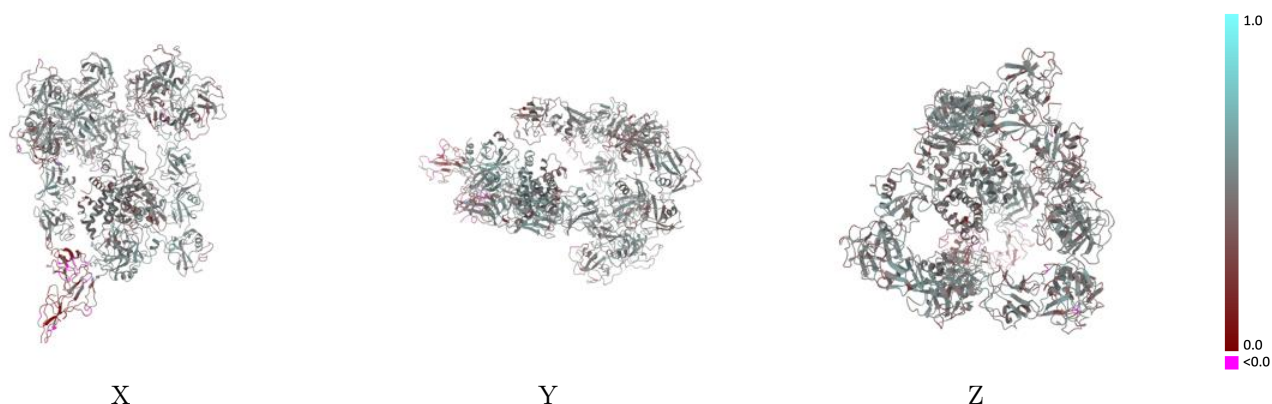
Y



Z

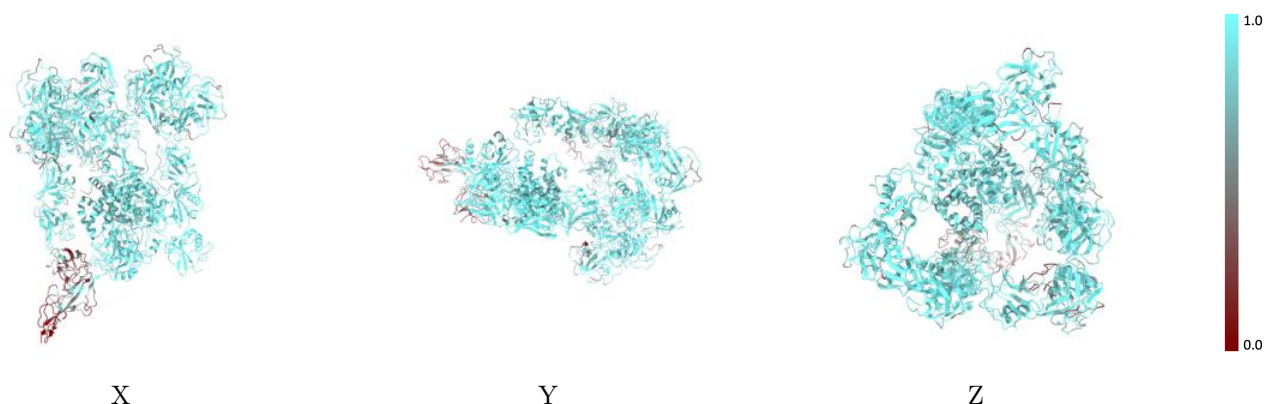
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



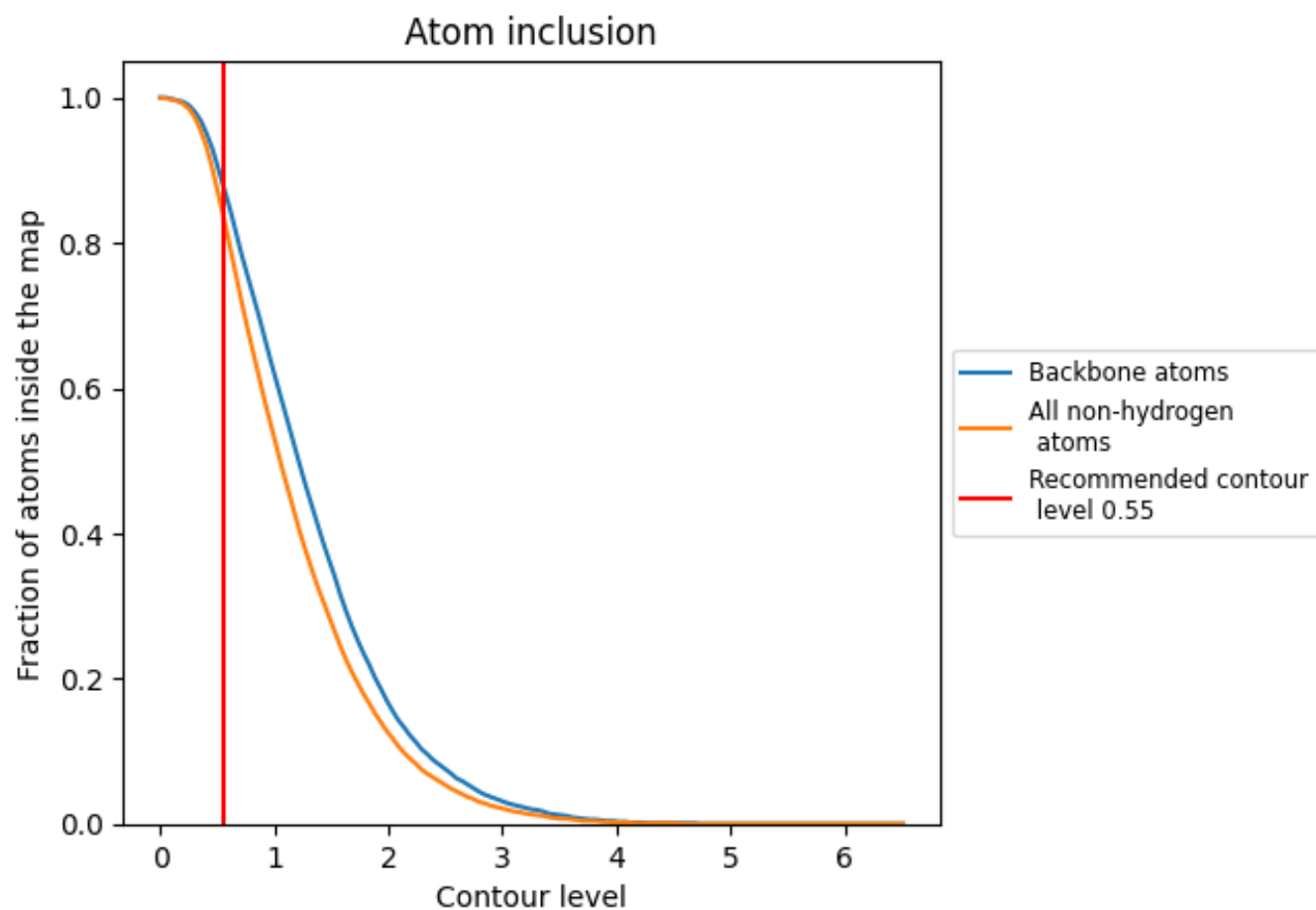
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8390	<div><div></div></div> 0.4580
A	<div><div></div></div> 0.8940	<div><div></div></div> 0.4720
B	<div><div></div></div> 0.8160	<div><div></div></div> 0.4460
C	<div><div></div></div> 0.8160	<div><div></div></div> 0.4540
D	<div><div></div></div> 0.9510	<div><div></div></div> 0.5120
E	<div><div></div></div> 0.8730	<div><div></div></div> 0.4530
F	<div><div></div></div> 0.8440	<div><div></div></div> 0.4820
G	<div><div></div></div> 0.2880	<div><div></div></div> 0.2220

1.0

0.0

<0.0