



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:37 PM UTC

PDB ID : 7JZ6 / pdb_00007jz6
EMDB ID : EMD-22530
Title : The Cryo-EM structure of the Catalase-peroxidase from Escherichia coli
Authors : Su, C.-C.
Deposited on : 2020-09-01
Resolution : 2.53 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

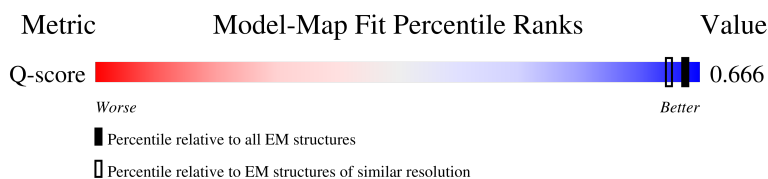
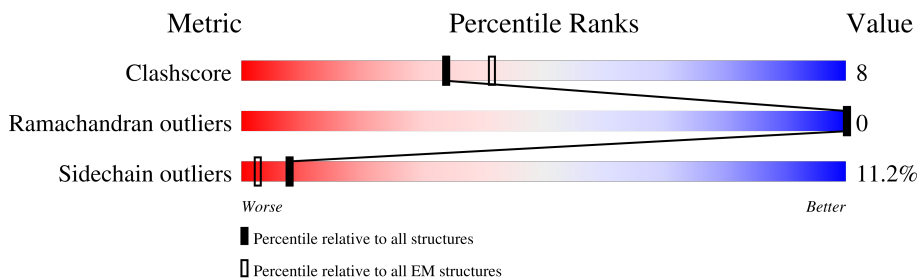
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.53 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	7309 (2.03 - 3.03)

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	726	13% 71% 17% • 9%
1	B	726	13% 71% 16% • 9%
1	C	726	13% 74% 14% • 9%
1	D	726	12% 71% 17% • 9%

2 Entry composition [i](#)

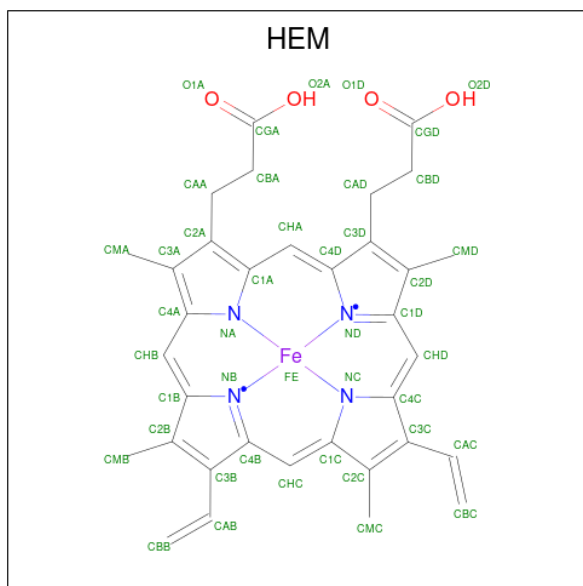
There are 3 unique types of molecules in this entry. The entry contains 20842 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catalase-peroxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	660	Total	C	N	O	S	0	0
			5154	3276	891	976	11		
1	B	662	Total	C	N	O	S	0	0
			5166	3282	894	979	11		
1	C	662	Total	C	N	O	S	0	0
			5166	3282	894	979	11		
1	D	662	Total	C	N	O	S	0	0
			5166	3282	894	979	11		

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

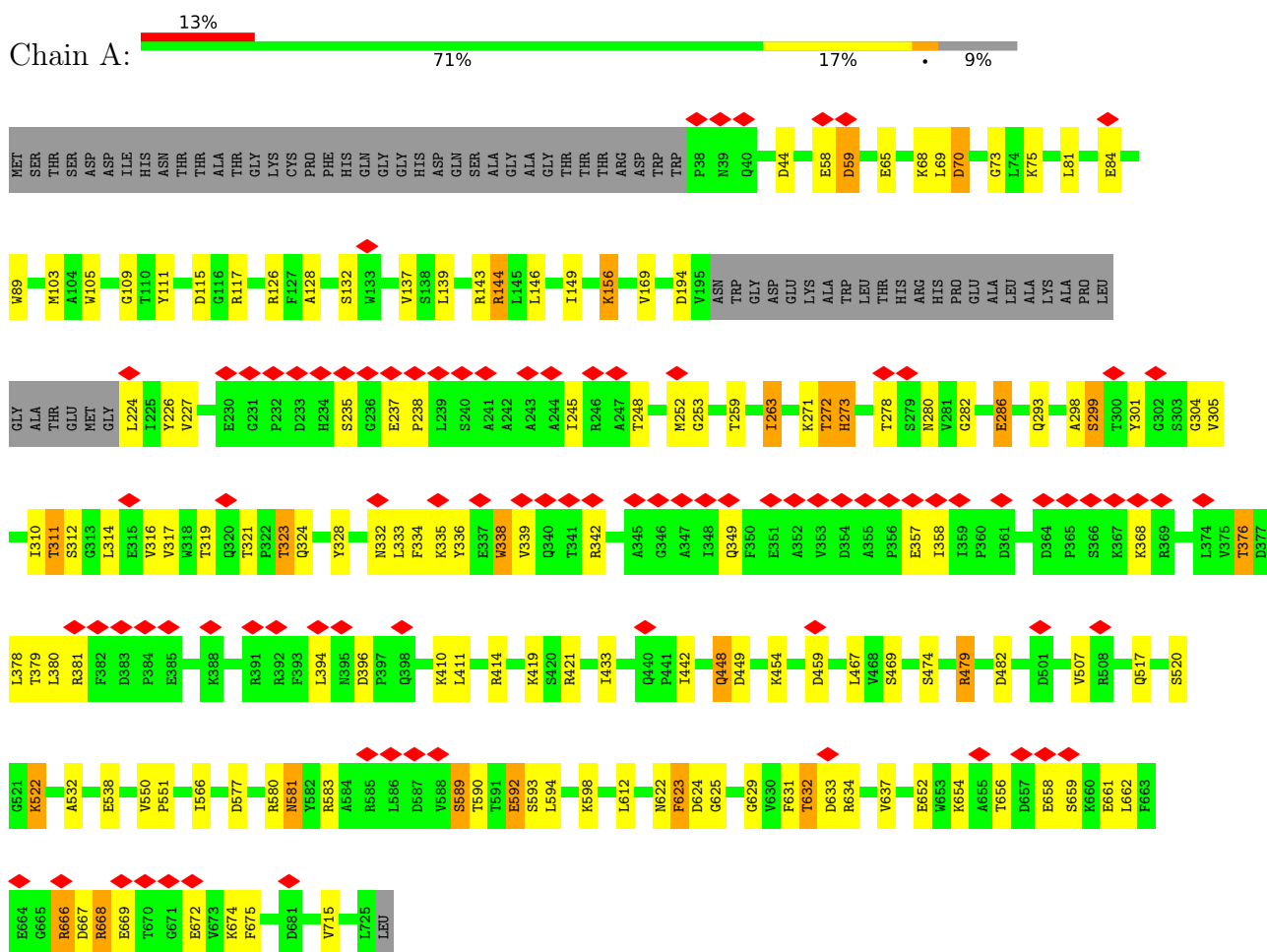
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	6	Total	O	0
			6	6	
3	B	4	Total	O	0
			4	4	
3	C	4	Total	O	0
			4	4	
3	D	4	Total	O	0
			4	4	

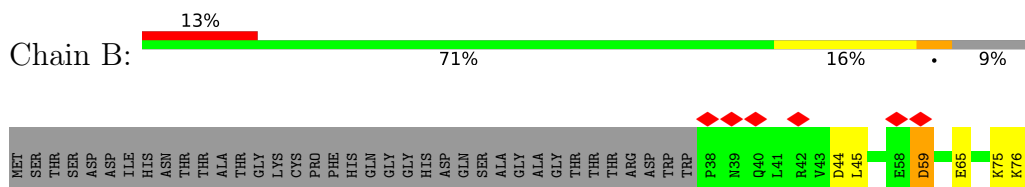
3 Residue-property plots

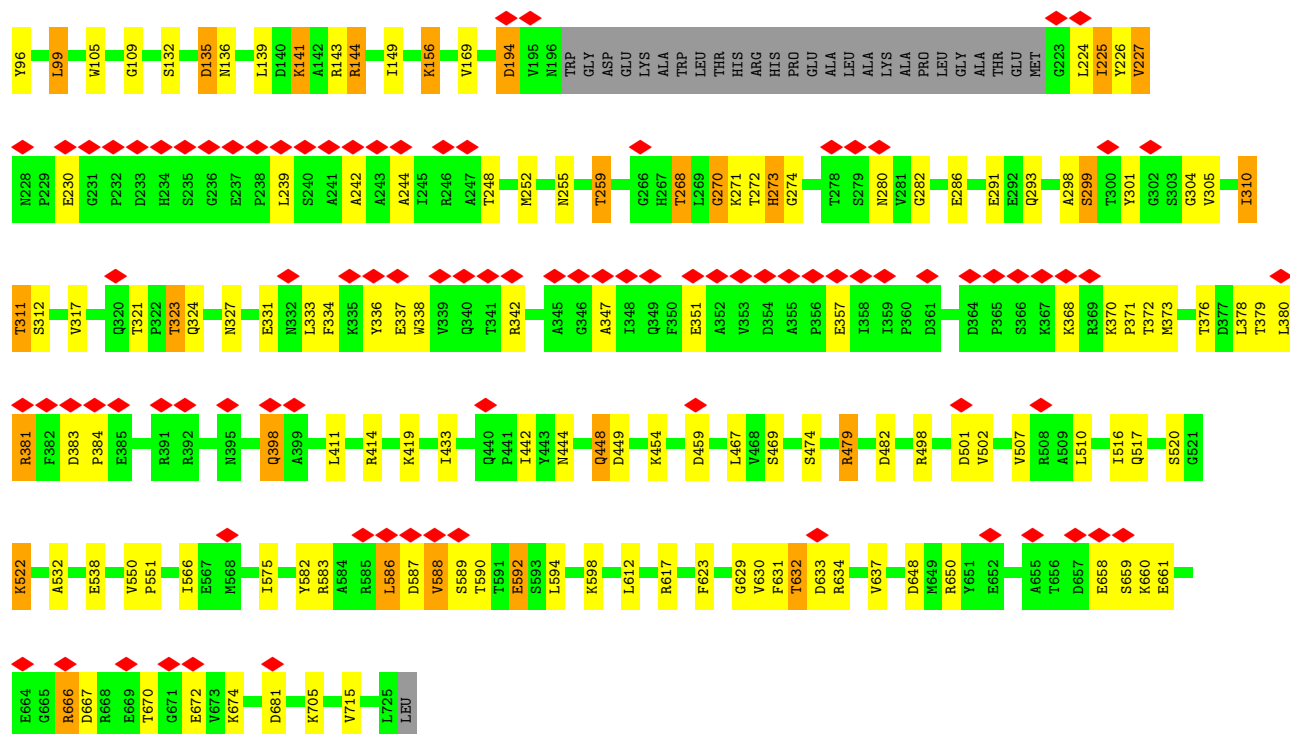
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Catalase-peroxidase

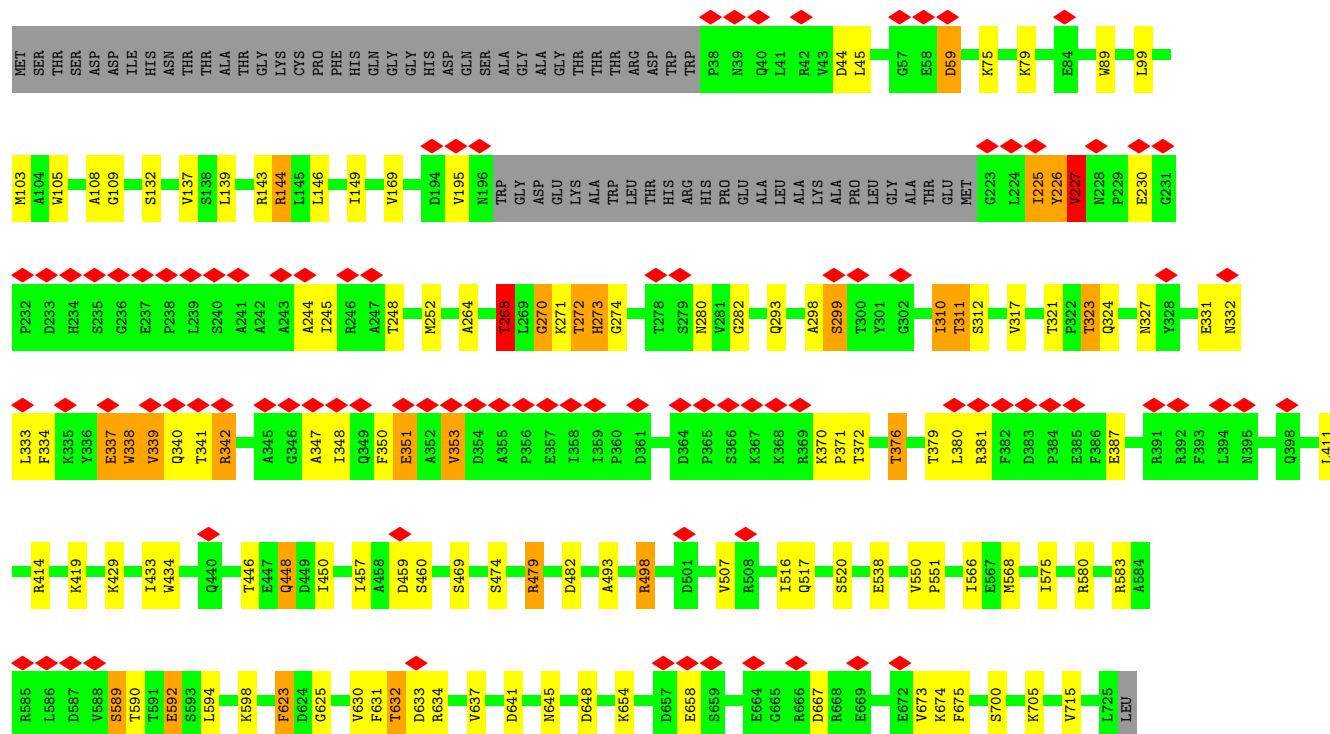
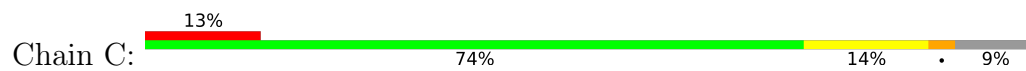


• Molecule 1: Catalase-peroxidase

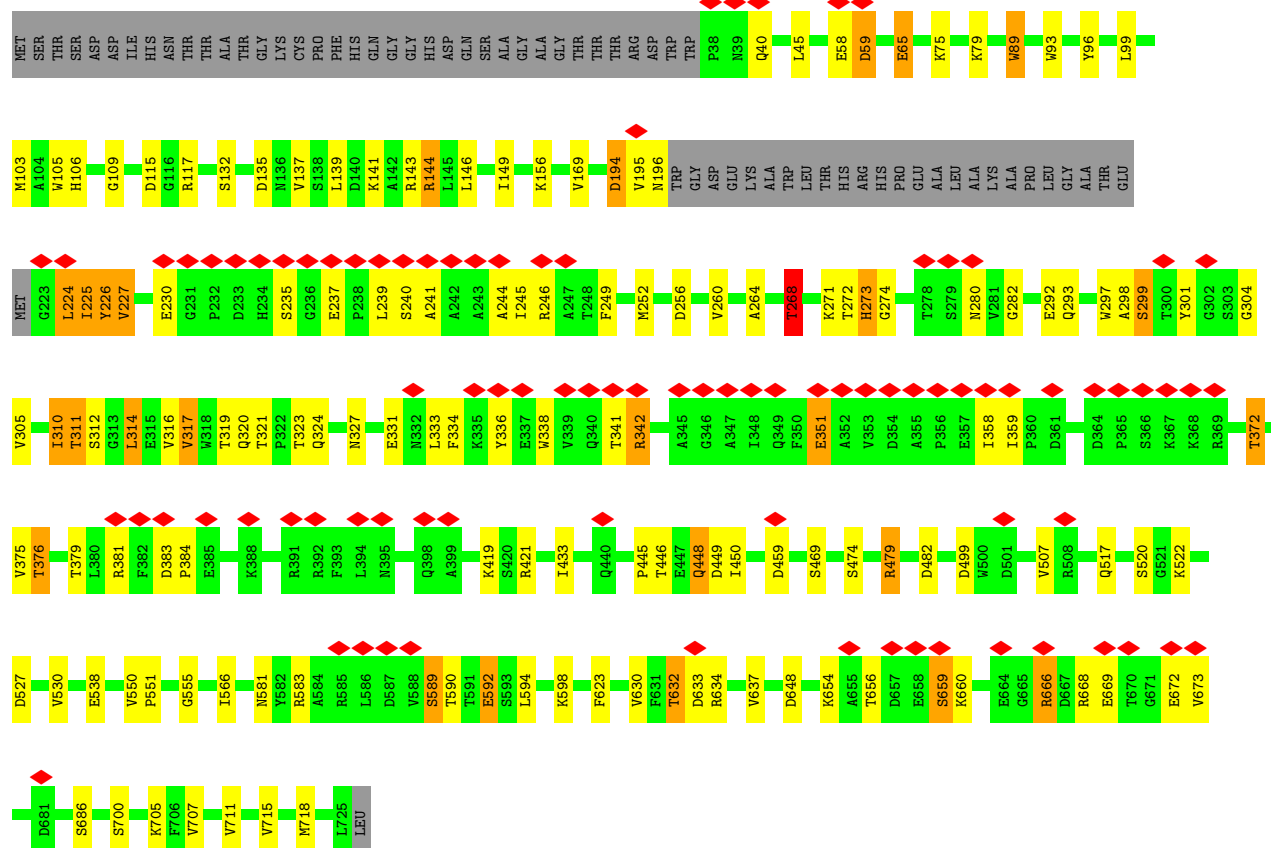




• Molecule 1: Catalase-peroxidase



• Molecule 1: Catalase-peroxidase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123643	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.688	Depositor
Minimum map value	-3.140	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.360	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	143.64, 117.72, 150.12001	wwPDB
Map dimensions	133, 109, 139	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: HEM

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	0.42	0/5283	0.61	4/7173 (0.1%)
1	B	0.44	1/5295 (0.0%)	0.67	7/7189 (0.1%)
1	C	0.44	2/5295 (0.0%)	0.63	7/7189 (0.1%)
1	D	0.42	0/5295	0.66	8/7189 (0.1%)
All	All	0.43	3/21168 (0.0%)	0.64	26/28740 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	227	VAL	C-O	-8.77	1.14	1.23
1	B	227	VAL	C-O	-8.23	1.14	1.23
1	C	89	TRP	C-O	-5.80	1.16	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	588	VAL	N-CA-C	16.70	126.23	110.53
1	D	225	ILE	N-CA-C	13.93	123.63	110.53
1	C	270	GLY	N-CA-C	8.90	127.58	111.02
1	B	270	GLY	N-CA-C	8.67	127.14	111.02
1	D	316	VAL	N-CA-C	8.09	119.44	108.11
1	D	240	SER	N-CA-C	7.57	119.53	111.28
1	B	268	THR	N-CA-C	-6.50	105.24	113.43
1	D	268	THR	N-CA-C	-6.31	106.21	114.04
1	C	273	HIS	N-CA-C	6.29	118.78	108.52
1	C	268	THR	N-CA-C	-6.28	105.52	113.43
1	D	273	HIS	N-CA-C	6.21	118.64	108.52
1	B	273	HIS	N-CA-C	6.00	118.19	108.41
1	C	227	VAL	CA-C-O	-5.95	115.74	121.63
1	B	501	ASP	N-CA-C	5.78	117.58	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	VAL	CA-C-O	-5.77	115.92	121.63
1	C	338	TRP	N-CA-C	5.53	118.48	109.24
1	A	273	HIS	N-CA-C	5.50	117.48	108.52
1	B	268	THR	CB-CA-C	5.40	118.72	109.65
1	C	268	THR	CB-CA-C	5.30	118.56	109.65
1	A	278	THR	OG1-CB-CG2	5.30	119.90	109.30
1	C	226	TYR	CA-CB-CG	5.29	123.42	113.90
1	D	226	TYR	CA-CB-CG	5.28	123.41	113.90
1	A	278	THR	CA-CB-CG2	5.14	119.24	110.50
1	A	70	ASP	N-CA-C	-5.13	98.33	107.98
1	D	89	TRP	CB-CA-C	5.09	117.95	110.87
1	D	239	LEU	N-CA-C	5.04	116.77	111.28

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	5154	0	5008	77	0
1	B	5166	0	5017	85	0
1	C	5166	0	5017	79	0
1	D	5166	0	5017	84	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0
2	C	43	0	30	3	0
2	D	43	0	30	8	0
3	A	6	0	0	2	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
All	All	20842	0	20179	334	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 8.

All (334) 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:D:226:TYR:HE1	1:D:252:MET:SD	1.13	1.72
1:B:226:TYR:HE1	1:B:252:MET:SD	1.17	1.62
1:C:226:TYR:HE1	1:C:252:MET:SD	1.26	1.55
1:D:226:TYR:CE1	1:D:252:MET:SD	2.05	1.50
1:A:226:TYR:HE1	1:A:252:MET:SD	1.32	1.48
1:B:226:TYR:CE1	1:B:252:MET:SD	2.08	1.46
1:C:226:TYR:CE1	1:C:252:MET:SD	2.17	1.37
1:A:226:TYR:CE1	1:A:252:MET:SD	2.17	1.37
1:C:109:GLY:O	1:C:252:MET:HE1	1.42	1.17
1:B:109:GLY:O	1:B:252:MET:HE1	1.52	1.09
1:D:109:GLY:O	1:D:252:MET:HE1	1.60	1.00
1:C:105:TRP:CZ3	1:C:226:TYR:OH	2.07	0.94
1:A:323:THR:OG1	1:A:324:GLN:OE1	1.87	0.93
1:C:323:THR:OG1	1:C:324:GLN:OE1	1.87	0.91
1:B:589:SER:HB3	1:B:594:LEU:HD21	1.53	0.91
1:D:105:TRP:CZ3	1:D:226:TYR:OH	2.14	0.90
1:D:323:THR:OG1	1:D:324:GLN:OE1	1.89	0.90
1:B:105:TRP:CZ3	1:B:226:TYR:OH	2.11	0.90
1:B:323:THR:OG1	1:B:324:GLN:OE1	1.90	0.89
1:C:109:GLY:O	1:C:252:MET:CE	2.24	0.85
1:C:339:VAL:HG13	1:C:351:GLU:HG3	1.61	0.81
1:C:105:TRP:HZ3	1:C:226:TYR:OH	1.60	0.81
1:B:109:GLY:O	1:B:252:MET:CE	2.29	0.80
1:A:68:LYS:HB2	1:A:156:LYS:HD3	1.63	0.80
1:B:105:TRP:HZ3	1:B:226:TYR:OH	1.64	0.79
1:D:109:GLY:O	1:D:252:MET:CE	2.33	0.77
1:C:225:ILE:HD13	1:C:225:ILE:N	1.99	0.76
1:C:340:GLN:HE21	1:C:348:ILE:HG23	1.49	0.76
1:D:105:TRP:HZ3	1:D:226:TYR:OH	1.63	0.76
1:C:273:HIS:HB2	1:C:311:THR:HG23	1.69	0.74
1:A:144:ARG:NH1	1:A:293:GLN:O	2.20	0.73
1:D:246:ARG:NH2	1:D:256:ASP:OD1	2.22	0.73
1:A:273:HIS:HB2	1:A:311:THR:HG23	1.70	0.72
1:B:398:GLN:N	1:B:398:GLN:OE1	2.23	0.72
2:A:1001:HEM:O2A	3:A:1101:HOH:O	2.08	0.71
1:B:225:ILE:N	1:B:225:ILE:HD13	2.05	0.70
1:C:339:VAL:HG12	1:C:351:GLU:O	1.92	0.69
1:B:273:HIS:HB2	1:B:311:THR:HG23	1.74	0.69
1:A:109:GLY:C	1:A:252:MET:HE1	2.17	0.69
1:A:105:TRP:CZ3	1:A:226:TYR:OH	2.45	0.68
1:A:226:TYR:CZ	1:A:252:MET:SD	2.83	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:HIS:HB2	1:D:311:THR:HG23	1.74	0.68
1:D:583:ARG:NH1	1:D:589:SER:O	2.27	0.68
1:D:135:ASP:OD2	1:D:224:LEU:HD23	1.94	0.67
1:A:259:THR:O	1:A:263:ILE:HG13	1.95	0.66
1:C:59:ASP:N	1:C:59:ASP:OD1	2.29	0.66
1:C:334:PHE:HA	1:C:381:ARG:HH22	1.60	0.66
2:D:1001:HEM:HMC1	2:D:1001:HEM:HBC2	1.80	0.63
1:C:333:LEU:O	1:C:338:TRP:HZ3	1.82	0.62
1:B:59:ASP:OD1	1:B:59:ASP:N	2.33	0.62
1:B:589:SER:HB3	1:B:594:LEU:CD2	2.29	0.61
1:C:340:GLN:HE21	1:C:348:ILE:CG2	2.12	0.61
2:B:1001:HEM:HMC1	2:B:1001:HEM:HBC2	1.81	0.61
1:C:195:VAL:HG23	1:C:195:VAL:O	2.00	0.61
1:C:333:LEU:O	1:C:338:TRP:CZ3	2.53	0.61
2:C:1001:HEM:HMC1	2:C:1001:HEM:HBC2	1.81	0.61
1:C:339:VAL:CG1	1:C:351:GLU:HG3	2.31	0.61
2:A:1001:HEM:HMC1	2:A:1001:HEM:HBC2	1.82	0.61
1:C:333:LEU:HA	1:C:338:TRP:CH2	2.35	0.61
1:A:280:ASN:O	1:A:299:SER:HA	2.01	0.61
1:B:271:LYS:NZ	1:B:272:THR:O	2.33	0.60
1:D:144:ARG:NH1	1:D:293:GLN:O	2.34	0.60
1:D:230:GLU:O	1:D:375:VAL:HG21	2.00	0.60
1:A:68:LYS:HB2	1:A:156:LYS:CD	2.31	0.60
1:A:245:ILE:HD11	1:A:376:THR:HG22	1.84	0.60
1:B:144:ARG:NH1	1:B:293:GLN:O	2.34	0.60
1:A:479:ARG:NH2	1:A:482:ASP:OD2	2.35	0.59
1:A:658:GLU:N	1:A:658:GLU:OE1	2.35	0.59
1:A:273:HIS:HB2	1:A:311:THR:CG2	2.32	0.59
1:B:583:ARG:NH1	1:B:589:SER:O	2.36	0.59
1:B:502:VAL:HG22	1:B:582:TYR:CD1	2.38	0.58
1:A:70:ASP:OD2	1:A:73:GLY:HA3	2.03	0.58
1:B:224:LEU:C	1:B:225:ILE:HD13	2.28	0.58
1:B:226:TYR:O	1:B:248:THR:HG21	2.03	0.58
1:B:282:GLY:N	1:B:298:ALA:O	2.33	0.58
1:D:479:ARG:NH2	1:D:482:ASP:OD2	2.36	0.58
1:A:589:SER:OG	1:A:590:THR:N	2.36	0.58
1:A:321:THR:O	1:A:323:THR:N	2.37	0.57
1:D:334:PHE:HA	1:D:381:ARG:HH11	1.68	0.57
1:B:502:VAL:HG22	1:B:582:TYR:CG	2.39	0.57
1:A:105:TRP:HZ3	1:A:226:TYR:OH	1.88	0.57
1:C:144:ARG:NH1	1:C:293:GLN:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:ARG:NH2	1:C:482:ASP:OD2	2.36	0.57
1:C:517:GLN:O	1:C:520:SER:O	2.23	0.57
1:B:479:ARG:NH2	1:B:482:ASP:OD2	2.37	0.57
1:A:111:TYR:O	1:A:252:MET:HE3	2.06	0.56
1:D:517:GLN:O	1:D:520:SER:O	2.23	0.56
1:C:274:GLY:HA2	1:C:310:ILE:HG23	1.88	0.56
1:C:538:GLU:HG3	1:C:550:VAL:HG23	1.88	0.56
1:B:517:GLN:O	1:B:520:SER:O	2.23	0.56
1:C:321:THR:O	1:C:323:THR:N	2.39	0.56
1:B:321:THR:O	1:B:323:THR:N	2.39	0.55
1:A:667:ASP:OD1	1:A:669:GLU:N	2.34	0.55
1:B:274:GLY:HA2	1:B:310:ILE:HG23	1.89	0.55
1:A:538:GLU:HG3	1:A:550:VAL:HG23	1.89	0.55
1:D:273:HIS:HB2	1:D:311:THR:CG2	2.36	0.55
1:C:273:HIS:HB2	1:C:311:THR:CG2	2.36	0.54
1:D:589:SER:OG	1:D:590:THR:N	2.39	0.54
1:C:282:GLY:N	1:C:298:ALA:O	2.36	0.54
1:D:321:THR:O	1:D:323:THR:N	2.41	0.54
1:B:502:VAL:HG22	1:B:582:TYR:CD2	2.41	0.54
1:D:311:THR:OG1	1:D:312:SER:N	2.38	0.54
1:B:273:HIS:HB2	1:B:311:THR:CG2	2.36	0.54
1:C:551:PRO:HD2	1:C:715:VAL:HG21	1.90	0.54
1:B:538:GLU:HG3	1:B:550:VAL:HG23	1.90	0.53
1:C:311:THR:OG1	1:C:312:SER:N	2.37	0.53
1:A:226:TYR:O	1:A:248:THR:HG21	2.09	0.53
1:A:517:GLN:O	1:A:520:SER:O	2.26	0.53
1:C:589:SER:OG	1:C:590:THR:N	2.41	0.53
1:D:59:ASP:OD1	1:D:59:ASP:N	2.40	0.53
1:B:242:ALA:HA	1:B:379:THR:HG21	1.91	0.53
1:D:274:GLY:HA2	1:D:310:ILE:HG23	1.91	0.53
1:A:674:LYS:HD3	1:A:675:PHE:CZ	2.44	0.53
1:C:339:VAL:CG1	1:C:351:GLU:O	2.57	0.53
1:B:502:VAL:HG22	1:B:582:TYR:CE1	2.45	0.52
1:D:551:PRO:HD2	1:D:715:VAL:HG21	1.91	0.52
1:A:311:THR:OG1	1:A:312:SER:N	2.41	0.52
1:D:538:GLU:HG3	1:D:550:VAL:HG23	1.91	0.52
1:A:551:PRO:HD2	1:A:715:VAL:HG21	1.91	0.52
1:A:59:ASP:N	1:A:59:ASP:OD1	2.42	0.52
1:B:551:PRO:HD2	1:B:715:VAL:HG21	1.92	0.52
1:A:590:THR:OG1	1:A:593:SER:OG	2.21	0.52
1:B:502:VAL:CG2	1:B:582:TYR:CE2	2.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:LEU:HD23	1:A:532:ALA:HB1	1.92	0.51
1:D:137:VAL:HG23	1:D:297:TRP:CG	2.45	0.51
1:C:137:VAL:HG22	1:C:137:VAL:O	2.08	0.51
1:B:89:TRP:CZ3	1:B:305:VAL:HG12	2.45	0.51
1:D:89:TRP:CZ3	1:D:305:VAL:HG12	2.47	0.50
1:D:226:TYR:CE1	1:D:252:MET:CE	2.93	0.50
1:C:339:VAL:CG1	1:C:353:VAL:HB	2.41	0.50
1:A:109:GLY:O	1:A:252:MET:HE1	2.10	0.50
1:A:111:TYR:HB3	1:A:252:MET:HE2	1.92	0.50
1:B:194:ASP:OD1	1:B:194:ASP:N	2.44	0.50
1:C:333:LEU:HA	1:C:338:TRP:HH2	1.76	0.50
2:D:1001:HEM:HBC2	2:D:1001:HEM:CMC	2.42	0.49
1:C:583:ARG:NH1	1:C:589:SER:O	2.44	0.49
1:B:333:LEU:HA	1:B:338:TRP:CH2	2.47	0.49
1:B:498:ARG:CZ	1:B:510:LEU:HD13	2.42	0.49
1:C:674:LYS:HD3	1:C:675:PHE:CZ	2.48	0.49
1:B:357:GLU:HB3	1:B:368:LYS:HB2	1.95	0.49
1:D:135:ASP:CG	1:D:224:LEU:HD23	2.37	0.48
1:D:117:ARG:HD3	1:D:194:ASP:HB2	1.94	0.48
2:A:1001:HEM:HBC2	2:A:1001:HEM:CMC	2.43	0.48
1:B:502:VAL:HG22	1:B:582:TYR:CE2	2.48	0.48
1:B:135:ASP:OD2	1:B:225:ILE:HG12	2.14	0.48
1:A:282:GLY:N	1:A:298:ALA:O	2.35	0.48
1:A:411:LEU:HD12	1:A:414:ARG:NH1	2.28	0.48
1:D:282:GLY:N	1:D:298:ALA:O	2.37	0.48
2:C:1001:HEM:HBC2	2:C:1001:HEM:CMC	2.43	0.48
1:C:340:GLN:NE2	1:C:348:ILE:CG2	2.77	0.47
2:B:1001:HEM:HBC2	2:B:1001:HEM:CMC	2.43	0.47
1:B:502:VAL:CG2	1:B:582:TYR:CD2	2.98	0.47
1:C:380:LEU:HD23	1:C:380:LEU:H	1.80	0.47
1:D:93:TRP:CH2	1:D:317:VAL:HG11	2.49	0.47
1:B:89:TRP:CE3	1:B:305:VAL:HG12	2.50	0.47
1:B:502:VAL:HG22	1:B:582:TYR:CZ	2.49	0.47
1:C:381:ARG:HG2	1:C:381:ARG:HH21	1.79	0.47
1:C:446:THR:O	1:C:450:ILE:HG12	2.15	0.47
1:A:271:LYS:NZ	1:A:272:THR:O	2.48	0.47
1:C:227:VAL:HG12	1:C:244:ALA:HB1	1.97	0.47
1:D:446:THR:O	1:D:450:ILE:HG12	2.14	0.47
1:A:301:TYR:O	1:A:304:GLY:N	2.45	0.47
1:A:253:GLY:O	1:A:410:LYS:NZ	2.47	0.46
1:C:583:ARG:HE	1:C:594:LEU:HD11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:666:ARG:HA	1:D:672:GLU:O	2.15	0.46
1:C:448:GLN:NE2	1:C:448:GLN:HA	2.30	0.46
1:C:632:THR:OG1	1:C:633:ASP:N	2.48	0.46
1:A:115:ASP:N	1:A:115:ASP:OD1	2.48	0.46
1:C:341:THR:OG1	1:C:342:ARG:N	2.44	0.46
1:D:312:SER:HB3	2:D:1001:HEM:HBA1	1.97	0.46
1:D:292:GLU:HA	1:D:292:GLU:OE2	2.16	0.46
1:B:334:PHE:HA	1:B:381:ARG:HH11	1.80	0.46
1:A:411:LEU:HD12	1:A:414:ARG:CZ	2.46	0.46
1:B:589:SER:OG	1:B:590:THR:N	2.47	0.46
1:D:227:VAL:HG23	2:D:1001:HEM:HMB1	1.97	0.46
1:D:583:ARG:HD2	1:D:594:LEU:HD12	1.99	0.46
1:A:238:PRO:O	1:A:379:THR:OG1	2.27	0.45
1:D:235:SER:O	1:D:237:GLU:N	2.45	0.45
1:D:319:THR:O	1:D:359:ILE:HG12	2.16	0.45
1:B:65:GLU:O	1:B:156:LYS:HG2	2.16	0.45
1:B:312:SER:OG	2:B:1001:HEM:O1A	2.25	0.45
1:D:590:THR:O	1:D:594:LEU:HG	2.17	0.45
1:B:291:GLU:OE1	1:B:291:GLU:N	2.39	0.45
1:C:339:VAL:HG12	1:C:353:VAL:HB	1.98	0.45
1:D:264:ALA:O	1:D:268:THR:CG2	2.65	0.45
1:D:194:ASP:O	1:D:196:ASN:N	2.50	0.45
1:A:589:SER:HB3	1:A:594:LEU:HD21	1.98	0.45
1:D:103:MET:HE1	1:D:146:LEU:HD11	1.98	0.45
1:D:530:VAL:HG13	1:D:718:MET:SD	2.56	0.45
1:A:666:ARG:HA	1:A:672:GLU:O	2.16	0.45
1:C:271:LYS:NZ	1:C:272:THR:O	2.50	0.45
1:A:139:LEU:O	1:A:143:ARG:HG3	2.17	0.45
1:B:659:SER:O	1:B:661:GLU:N	2.50	0.45
1:C:103:MET:HE1	1:C:146:LEU:HD11	1.99	0.45
1:B:632:THR:OG1	1:B:633:ASP:N	2.49	0.44
1:D:93:TRP:HH2	1:D:317:VAL:CG1	2.31	0.44
1:A:592:GLU:CD	1:A:592:GLU:H	2.25	0.44
1:D:241:ALA:HB3	1:D:379:THR:OG1	2.16	0.44
1:B:226:TYR:CZ	1:B:252:MET:SD	2.97	0.44
1:D:336:TYR:O	1:D:338:TRP:CZ3	2.71	0.44
1:A:65:GLU:O	1:A:156:LYS:HG2	2.16	0.44
1:A:632:THR:OG1	1:A:633:ASP:N	2.50	0.44
1:B:380:LEU:O	1:B:381:ARG:HB3	2.17	0.44
1:A:319:THR:HG22	1:A:328:TYR:HB2	2.00	0.44
1:C:493:ALA:O	1:C:498:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:TYR:CE1	1:B:252:MET:CE	2.98	0.44
1:D:106:HIS:CD2	1:D:225:ILE:HD12	2.52	0.44
1:B:351:GLU:HA	1:B:372:THR:HA	1.98	0.44
1:D:449:ASP:CG	1:D:522:LYS:HG2	2.42	0.44
1:B:449:ASP:CG	1:B:522:LYS:HG2	2.43	0.44
1:D:194:ASP:O	1:D:195:VAL:C	2.61	0.44
1:D:383:ASP:O	1:D:384:PRO:C	2.61	0.44
1:A:103:MET:HE1	1:A:146:LEU:HD11	2.00	0.44
1:C:327:ASN:O	1:C:331:GLU:HG3	2.17	0.44
1:C:332:ASN:O	1:C:338:TRP:HH2	2.01	0.44
1:C:337:GLU:OE1	1:C:337:GLU:HA	2.18	0.44
1:D:448:GLN:NE2	1:D:448:GLN:HA	2.31	0.44
1:C:139:LEU:O	1:C:143:ARG:HG3	2.17	0.43
1:D:327:ASN:O	1:D:331:GLU:HG3	2.17	0.43
1:C:379:THR:C	1:C:381:ARG:H	2.24	0.43
1:A:333:LEU:O	1:A:338:TRP:HZ3	2.01	0.43
1:B:327:ASN:O	1:B:331:GLU:HG3	2.18	0.43
1:C:339:VAL:CG2	1:C:340:GLN:N	2.81	0.43
1:D:89:TRP:O	1:D:96:TYR:OH	2.22	0.43
1:D:527:ASP:OD2	1:D:555:GLY:N	2.44	0.43
1:B:333:LEU:O	1:B:338:TRP:HZ3	2.01	0.43
1:B:592:GLU:H	1:B:592:GLU:CD	2.25	0.43
1:D:312:SER:HB3	2:D:1001:HEM:CBA	2.48	0.43
1:D:333:LEU:HA	1:D:338:TRP:CH2	2.54	0.43
1:B:617:ARG:NE	1:B:681:ASP:OD1	2.47	0.43
1:A:623:PHE:C	1:A:625:GLY:H	2.25	0.43
1:A:667:ASP:OD1	1:A:669:GLU:HB3	2.19	0.43
1:A:117:ARG:HD3	1:A:194:ASP:O	2.18	0.43
1:B:381:ARG:O	1:B:381:ARG:HG3	2.19	0.43
1:C:590:THR:O	1:C:594:LEU:HG	2.19	0.43
1:A:333:LEU:HA	1:A:338:TRP:CH2	2.54	0.43
1:A:577:ASP:OD2	1:A:580:ARG:NE	2.49	0.43
1:B:272:THR:HG22	2:B:1001:HEM:HAA1	2.01	0.43
1:D:272:THR:OG1	1:D:314:LEU:O	2.23	0.43
1:B:136:ASN:OD1	1:B:136:ASN:N	2.51	0.43
1:B:666:ARG:HA	1:B:672:GLU:O	2.19	0.43
1:C:226:TYR:O	1:C:248:THR:HG21	2.19	0.43
1:D:301:TYR:O	1:D:304:GLY:N	2.48	0.43
1:A:448:GLN:NE2	1:A:448:GLN:HA	2.34	0.43
1:B:311:THR:OG1	1:B:312:SER:N	2.48	0.43
1:C:264:ALA:O	1:C:268:THR:CG2	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:659:SER:OG	1:D:660:LYS:N	2.51	0.43
1:A:656:THR:OG1	1:A:662:LEU:HD23	2.19	0.42
1:A:659:SER:O	1:A:661:GLU:N	2.51	0.42
1:B:448:GLN:NE2	1:B:448:GLN:HA	2.32	0.42
1:B:336:TYR:O	1:B:338:TRP:CZ3	2.72	0.42
1:B:467:LEU:HD23	1:B:532:ALA:HB1	2.00	0.42
1:B:648:ASP:C	1:B:650:ARG:H	2.27	0.42
1:C:339:VAL:HG22	1:C:340:GLN:N	2.33	0.42
1:D:245:ILE:HD11	1:D:376:THR:HG22	2.02	0.42
1:D:592:GLU:CD	1:D:592:GLU:H	2.25	0.42
1:D:632:THR:OG1	1:D:633:ASP:N	2.52	0.42
1:B:270:GLY:O	1:B:271:LYS:HB3	2.20	0.42
1:C:342:ARG:HA	1:C:347:ALA:O	2.20	0.42
1:C:592:GLU:CD	1:C:592:GLU:H	2.26	0.42
1:A:227:VAL:HG23	2:A:1001:HEM:HMB1	2.01	0.42
1:D:445:PRO:HB2	1:D:450:ILE:HD11	2.01	0.42
1:A:111:TYR:N	1:A:252:MET:HE3	2.34	0.42
1:A:235:SER:O	1:A:237:GLU:N	2.47	0.42
1:A:273:HIS:HE1	2:A:1001:HEM:O2D	2.03	0.42
1:B:383:ASP:O	1:B:384:PRO:C	2.62	0.42
1:D:280:ASN:O	1:D:299:SER:HA	2.20	0.42
1:C:245:ILE:HD11	1:C:376:THR:HG22	2.01	0.42
1:D:341:THR:OG1	1:D:342:ARG:N	2.48	0.42
1:A:652:GLU:HB2	1:A:668:ARG:HG3	2.01	0.42
1:B:76:LYS:HA	1:B:79:LYS:HD3	2.01	0.42
1:A:111:TYR:HB3	1:A:252:MET:CE	2.49	0.41
1:B:338:TRP:CZ2	1:B:373:MET:HG3	2.55	0.41
1:D:139:LEU:O	1:D:143:ARG:HG3	2.20	0.41
1:D:89:TRP:HZ3	1:D:305:VAL:HG12	1.85	0.41
1:A:449:ASP:CG	1:A:522:LYS:HG2	2.46	0.41
1:A:581:ASN:HB2	1:A:622:ASN:OD1	2.21	0.41
1:A:590:THR:O	1:A:594:LEU:HG	2.20	0.41
1:C:589:SER:HB3	1:C:594:LEU:HD21	2.02	0.41
1:C:623:PHE:C	1:C:625:GLY:H	2.27	0.41
1:A:128:ALA:HB2	1:A:286:GLU:OE2	2.21	0.41
1:B:301:TYR:O	1:B:304:GLY:N	2.50	0.41
1:C:270:GLY:O	1:C:271:LYS:HB3	2.21	0.41
1:C:321:THR:O	1:C:321:THR:OG1	2.38	0.41
1:C:457:ILE:O	1:C:460:SER:OG	2.30	0.41
1:D:449:ASP:OD1	1:D:522:LYS:HG2	2.20	0.41
1:C:411:LEU:HD12	1:C:414:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:TRP:HH2	1:D:317:VAL:HG11	1.85	0.41
1:D:707:VAL:O	1:D:711:VAL:HG23	2.21	0.41
1:D:227:VAL:HG12	1:D:244:ALA:HB1	2.03	0.41
1:D:246:ARG:NH1	1:D:383:ASP:OD2	2.54	0.41
1:D:333:LEU:O	1:D:338:TRP:CZ3	2.74	0.41
1:D:376:THR:HG21	2:D:1001:HEM:HBB2	2.02	0.41
1:A:81:LEU:HA	1:A:84:GLU:OE2	2.20	0.41
1:B:96:TYR:O	1:B:99:LEU:HB3	2.21	0.41
1:B:141:LYS:HD3	1:B:141:LYS:N	2.34	0.41
1:B:370:LYS:O	1:B:371:PRO:C	2.64	0.41
1:B:411:LEU:HD12	1:B:414:ARG:CZ	2.51	0.41
1:D:321:THR:C	1:D:323:THR:H	2.28	0.41
1:A:89:TRP:CZ3	1:A:305:VAL:HG12	2.56	0.41
1:A:316:VAL:HG23	1:A:349:GLN:OE1	2.21	0.41
1:A:336:TYR:O	1:A:338:TRP:CZ3	2.74	0.41
1:B:629:GLY:HA2	1:B:631:PHE:CE1	2.55	0.41
1:C:137:VAL:HG13	1:C:311:THR:OG1	2.21	0.41
1:C:280:ASN:O	1:C:299:SER:HA	2.21	0.41
1:C:434:TRP:HA	1:C:568:MET:HE2	2.03	0.41
1:A:357:GLU:HB3	1:A:368:LYS:CB	2.51	0.41
1:B:230:GLU:OE2	1:B:347:ALA:HB1	2.21	0.41
1:C:339:VAL:O	1:C:350:PHE:HA	2.21	0.41
1:C:583:ARG:HE	1:C:594:LEU:CD1	2.33	0.41
1:D:65:GLU:O	1:D:156:LYS:HG2	2.21	0.41
1:D:256:ASP:O	1:D:260:VAL:HG23	2.21	0.41
1:D:312:SER:CB	2:D:1001:HEM:O1A	2.69	0.41
1:A:652:GLU:OE1	1:A:652:GLU:HA	2.21	0.40
1:B:280:ASN:O	1:B:299:SER:HA	2.20	0.40
1:C:631:PHE:HB3	1:C:645:ASN:HB2	2.04	0.40
1:D:93:TRP:CZ3	1:D:271:LYS:HD2	2.56	0.40
1:D:115:ASP:OD1	1:D:115:ASP:N	2.54	0.40
1:A:629:GLY:HA2	1:A:631:PHE:CE1	2.55	0.40
1:B:99:LEU:HD12	1:B:99:LEU:O	2.21	0.40
1:B:227:VAL:HG12	1:B:244:ALA:HB1	2.03	0.40
1:C:273:HIS:HE1	2:C:1001:HEM:O2D	2.03	0.40
1:D:245:ILE:HG23	1:D:249:PHE:CD1	2.57	0.40
1:D:312:SER:HB3	2:D:1001:HEM:O1A	2.20	0.40
1:B:586:LEU:HA	1:B:586:LEU:HD12	1.87	0.40
1:A:376:THR:HB	3:A:1106:HOH:O	2.20	0.40
1:B:273:HIS:HE1	2:B:1001:HEM:O2D	2.04	0.40
1:C:370:LYS:O	1:C:371:PRO:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:PHE:HA	1:A:381:ARG:HE	1.85	0.40
1:B:139:LEU:O	1:B:143:ARG:HG3	2.22	0.40
1:B:255:ASN:O	1:B:259:THR:OG1	2.38	0.40
1:C:108:ALA:O	1:C:414:ARG:NH1	2.51	0.40
1:C:334:PHE:HA	1:C:381:ARG:NH2	2.32	0.40
1:D:351:GLU:HA	1:D:372:THR:HA	2.02	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	656/726 (90%)	607 (92%)	49 (8%)	0	100	100
1	B	658/726 (91%)	609 (93%)	49 (7%)	0	100	100
1	C	658/726 (91%)	602 (92%)	56 (8%)	0	100	100
1	D	658/726 (91%)	606 (92%)	52 (8%)	0	100	100
All	All	2630/2904 (91%)	2424 (92%)	206 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	534/584 (91%)	474 (89%)	60 (11%)	6	11
1	B	535/584 (92%)	473 (88%)	62 (12%)	5	10
1	C	535/584 (92%)	477 (89%)	58 (11%)	6	12
1	D	535/584 (92%)	476 (89%)	59 (11%)	6	11
All	All	2139/2336 (92%)	1900 (89%)	239 (11%)	8	11

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASP
1	A	58	GLU
1	A	59	ASP
1	A	69	LEU
1	A	75	LYS
1	A	126	ARG
1	A	132	SER
1	A	137	VAL
1	A	144	ARG
1	A	149	ILE
1	A	156	LYS
1	A	169	VAL
1	A	224	LEU
1	A	263	ILE
1	A	272	THR
1	A	286	GLU
1	A	299	SER
1	A	310	ILE
1	A	311	THR
1	A	314	LEU
1	A	317	VAL
1	A	323	THR
1	A	332	ASN
1	A	335	LYS
1	A	338	TRP
1	A	339	VAL
1	A	342	ARG
1	A	358	ILE
1	A	376	THR
1	A	378	LEU
1	A	380	LEU
1	A	394	LEU
1	A	396	ASP

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Mol	Chain	Res	Type
1	A	419	LYS
1	A	421	ARG
1	A	433	ILE
1	A	442	ILE
1	A	448	GLN
1	A	454	LYS
1	A	459	ASP
1	A	469	SER
1	A	474	SER
1	A	479	ARG
1	A	507	VAL
1	A	522	LYS
1	A	566	ILE
1	A	581	ASN
1	A	583	ARG
1	A	589	SER
1	A	592	GLU
1	A	598	LYS
1	A	612	LEU
1	A	623	PHE
1	A	624	ASP
1	A	632	THR
1	A	634	ARG
1	A	637	VAL
1	A	654	LYS
1	A	666	ARG
1	A	668	ARG
1	B	44	ASP
1	B	45	LEU
1	B	59	ASP
1	B	75	LYS
1	B	99	LEU
1	B	132	SER
1	B	135	ASP
1	B	141	LYS
1	B	144	ARG
1	B	149	ILE
1	B	156	LYS
1	B	169	VAL
1	B	194	ASP
1	B	225	ILE
1	B	239	LEU

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Mol	Chain	Res	Type
1	B	259	THR
1	B	268	THR
1	B	286	GLU
1	B	299	SER
1	B	310	ILE
1	B	311	THR
1	B	317	VAL
1	B	323	THR
1	B	337	GLU
1	B	342	ARG
1	B	376	THR
1	B	378	LEU
1	B	381	ARG
1	B	398	GLN
1	B	419	LYS
1	B	433	ILE
1	B	442	ILE
1	B	444	ASN
1	B	448	GLN
1	B	454	LYS
1	B	459	ASP
1	B	469	SER
1	B	474	SER
1	B	479	ARG
1	B	507	VAL
1	B	516	ILE
1	B	522	LYS
1	B	566	ILE
1	B	575	ILE
1	B	586	LEU
1	B	587	ASP
1	B	588	VAL
1	B	592	GLU
1	B	598	LYS
1	B	612	LEU
1	B	623	PHE
1	B	630	VAL
1	B	632	THR
1	B	634	ARG
1	B	637	VAL
1	B	658	GLU
1	B	660	LYS

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Mol	Chain	Res	Type
1	B	666	ARG
1	B	667	ASP
1	B	670	THR
1	B	674	LYS
1	B	705	LYS
1	C	44	ASP
1	C	45	LEU
1	C	59	ASP
1	C	75	LYS
1	C	79	LYS
1	C	99	LEU
1	C	132	SER
1	C	144	ARG
1	C	149	ILE
1	C	169	VAL
1	C	225	ILE
1	C	227	VAL
1	C	230	GLU
1	C	268	THR
1	C	272	THR
1	C	299	SER
1	C	310	ILE
1	C	311	THR
1	C	317	VAL
1	C	323	THR
1	C	337	GLU
1	C	339	VAL
1	C	342	ARG
1	C	351	GLU
1	C	353	VAL
1	C	372	THR
1	C	376	THR
1	C	387	GLU
1	C	419	LYS
1	C	429	LYS
1	C	433	ILE
1	C	448	GLN
1	C	459	ASP
1	C	469	SER
1	C	474	SER
1	C	479	ARG
1	C	498	ARG

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Mol	Chain	Res	Type
1	C	507	VAL
1	C	516	ILE
1	C	566	ILE
1	C	575	ILE
1	C	580	ARG
1	C	589	SER
1	C	592	GLU
1	C	598	LYS
1	C	623	PHE
1	C	630	VAL
1	C	632	THR
1	C	634	ARG
1	C	637	VAL
1	C	641	ASP
1	C	648	ASP
1	C	654	LYS
1	C	658	GLU
1	C	667	ASP
1	C	673	VAL
1	C	700	SER
1	C	705	LYS
1	D	40	GLN
1	D	45	LEU
1	D	58	GLU
1	D	59	ASP
1	D	65	GLU
1	D	75	LYS
1	D	79	LYS
1	D	99	LEU
1	D	132	SER
1	D	141	LYS
1	D	144	ARG
1	D	149	ILE
1	D	169	VAL
1	D	194	ASP
1	D	224	LEU
1	D	227	VAL
1	D	268	THR
1	D	299	SER
1	D	310	ILE
1	D	311	THR
1	D	314	LEU

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Mol	Chain	Res	Type
1	D	317	VAL
1	D	320	GLN
1	D	342	ARG
1	D	351	GLU
1	D	358	ILE
1	D	372	THR
1	D	376	THR
1	D	419	LYS
1	D	421	ARG
1	D	433	ILE
1	D	448	GLN
1	D	459	ASP
1	D	469	SER
1	D	474	SER
1	D	479	ARG
1	D	499	ASP
1	D	507	VAL
1	D	566	ILE
1	D	581	ASN
1	D	589	SER
1	D	592	GLU
1	D	598	LYS
1	D	623	PHE
1	D	630	VAL
1	D	632	THR
1	D	634	ARG
1	D	637	VAL
1	D	648	ASP
1	D	654	LYS
1	D	656	THR
1	D	659	SER
1	D	666	ARG
1	D	668	ARG
1	D	669	GLU
1	D	673	VAL
1	D	686	SER
1	D	700	SER
1	D	705	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	703	HIS
1	B	49	HIS
1	B	327	ASN
1	B	581	ASN
1	B	645	ASN
1	C	49	HIS
1	C	173	ASN
1	C	340	GLN
1	C	645	ASN
1	C	703	HIS
1	D	49	HIS
1	D	581	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	C	1001	1	50,50,50	1.46	5 (10%)	67,82,82	1.14	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	1001	1	50,50,50	1.47	6 (12%)	67,82,82	1.16	6 (8%)
2	HEM	A	1001	1	50,50,50	1.47	6 (12%)	67,82,82	1.14	4 (5%)
2	HEM	D	1001	1	50,50,50	1.46	6 (12%)	67,82,82	1.16	6 (8%)

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
2	HEM	C	1001	1	-	2/14/54/54	-
2	HEM	B	1001	1	-	2/14/54/54	-
2	HEM	A	1001	1	-	2/14/54/54	-
2	HEM	D	1001	1	-	2/14/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	HEM	FE-NB	4.47	2.08	1.94
2	C	1001	HEM	FE-NB	4.28	2.08	1.94
2	B	1001	HEM	FE-NB	4.26	2.08	1.94
2	D	1001	HEM	FE-NB	4.25	2.08	1.94
2	A	1001	HEM	FE-ND	3.96	2.07	1.94
2	C	1001	HEM	FE-ND	3.94	2.07	1.94
2	D	1001	HEM	FE-ND	3.94	2.07	1.94
2	B	1001	HEM	FE-ND	3.85	2.06	1.94
2	D	1001	HEM	FE-NA	3.64	2.07	1.95
2	B	1001	HEM	FE-NA	3.64	2.07	1.95
2	C	1001	HEM	FE-NA	3.62	2.07	1.95
2	A	1001	HEM	FE-NA	3.54	2.06	1.95
2	A	1001	HEM	CAB-C3B	2.97	1.55	1.47
2	B	1001	HEM	CAB-C3B	2.96	1.55	1.47
2	D	1001	HEM	CAB-C3B	2.96	1.55	1.47
2	C	1001	HEM	CAB-C3B	2.95	1.55	1.47
2	C	1001	HEM	CAC-C3C	2.91	1.55	1.47
2	B	1001	HEM	CAC-C3C	2.90	1.55	1.47
2	A	1001	HEM	CAC-C3C	2.87	1.55	1.47
2	D	1001	HEM	CAC-C3C	2.84	1.55	1.47
2	B	1001	HEM	C2A-C3A	-2.04	1.33	1.38
2	A	1001	HEM	C2A-C3A	-2.03	1.33	1.38
2	D	1001	HEM	C2A-C3A	-2.03	1.33	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	HEM	C1B-NB-C4B	2.71	108.41	105.21
2	C	1001	HEM	C1B-NB-C4B	2.70	108.41	105.21
2	A	1001	HEM	CHC-C1C-NC	2.69	127.38	124.45
2	A	1001	HEM	C1B-NB-C4B	2.63	108.32	105.21
2	B	1001	HEM	CHC-C1C-NC	2.62	127.30	124.45
2	B	1001	HEM	C1B-NB-C4B	2.59	108.27	105.21
2	C	1001	HEM	CHC-C1C-NC	2.55	127.23	124.45
2	D	1001	HEM	CHC-C1C-NC	2.53	127.21	124.45
2	D	1001	HEM	C3B-C2B-C1B	2.36	108.18	106.41
2	D	1001	HEM	CHD-C4C-NC	2.17	126.81	124.45
2	A	1001	HEM	C4D-ND-C1D	2.15	107.75	105.21
2	D	1001	HEM	C2B-C1B-NB	-2.14	107.39	109.84
2	B	1001	HEM	C3B-C2B-C1B	2.12	108.00	106.41
2	B	1001	HEM	C4D-ND-C1D	2.11	107.70	105.21
2	A	1001	HEM	CHD-C4C-NC	2.10	126.74	124.45
2	C	1001	HEM	CHD-C4C-NC	2.10	126.74	124.45
2	C	1001	HEM	C4D-ND-C1D	2.07	107.66	105.21
2	C	1001	HEM	C3B-C2B-C1B	2.06	107.96	106.41
2	D	1001	HEM	C4D-ND-C1D	2.05	107.63	105.21
2	B	1001	HEM	C2B-C1B-NB	-2.03	107.51	109.84
2	C	1001	HEM	C2B-C1B-NB	-2.01	107.53	109.84
2	B	1001	HEM	CHD-C4C-NC	2.00	126.63	124.45

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	HEM	CAA-CBA-CGA-O2A
2	C	1001	HEM	CAA-CBA-CGA-O2A
2	D	1001	HEM	CAA-CBA-CGA-O2A
2	B	1001	HEM	CAA-CBA-CGA-O2A
2	B	1001	HEM	CAA-CBA-CGA-O1A
2	A	1001	HEM	CAA-CBA-CGA-O1A
2	D	1001	HEM	CAA-CBA-CGA-O1A
2	C	1001	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

4 monomers are involved in 21 short contacts:

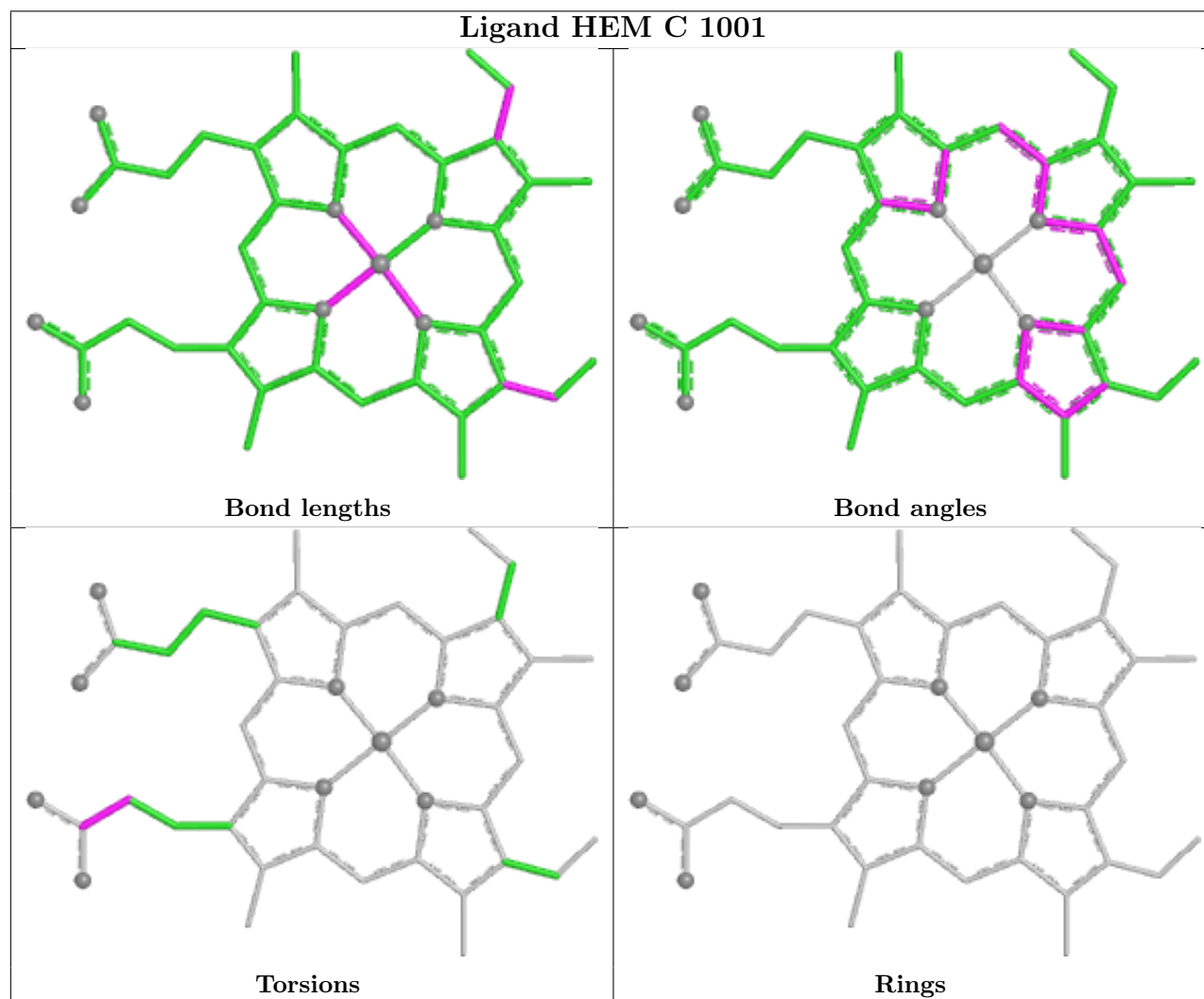
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	HEM	3	0

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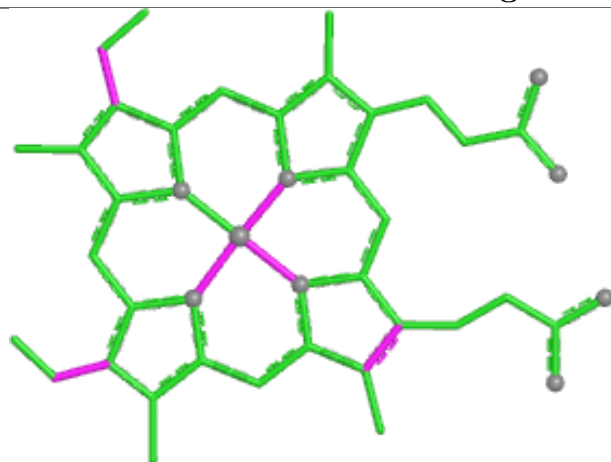
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	HEM	5	0
2	A	1001	HEM	5	0
2	D	1001	HEM	8	0

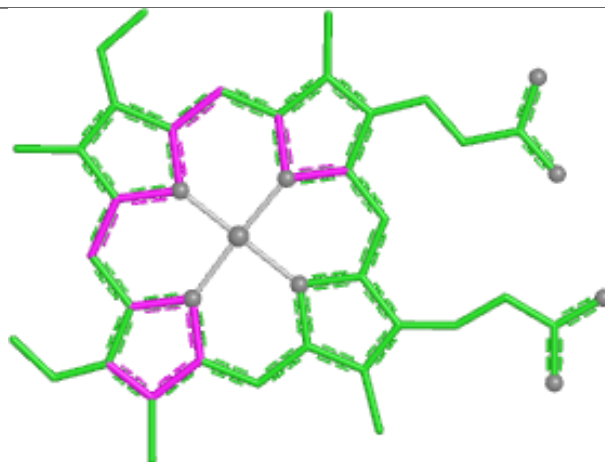
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



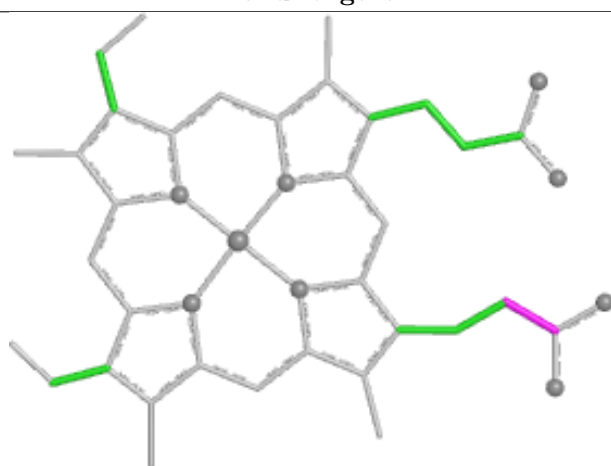
Ligand HEM B 1001



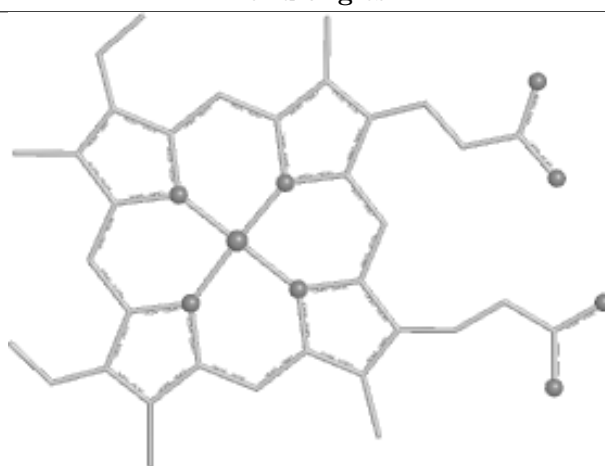
Bond lengths



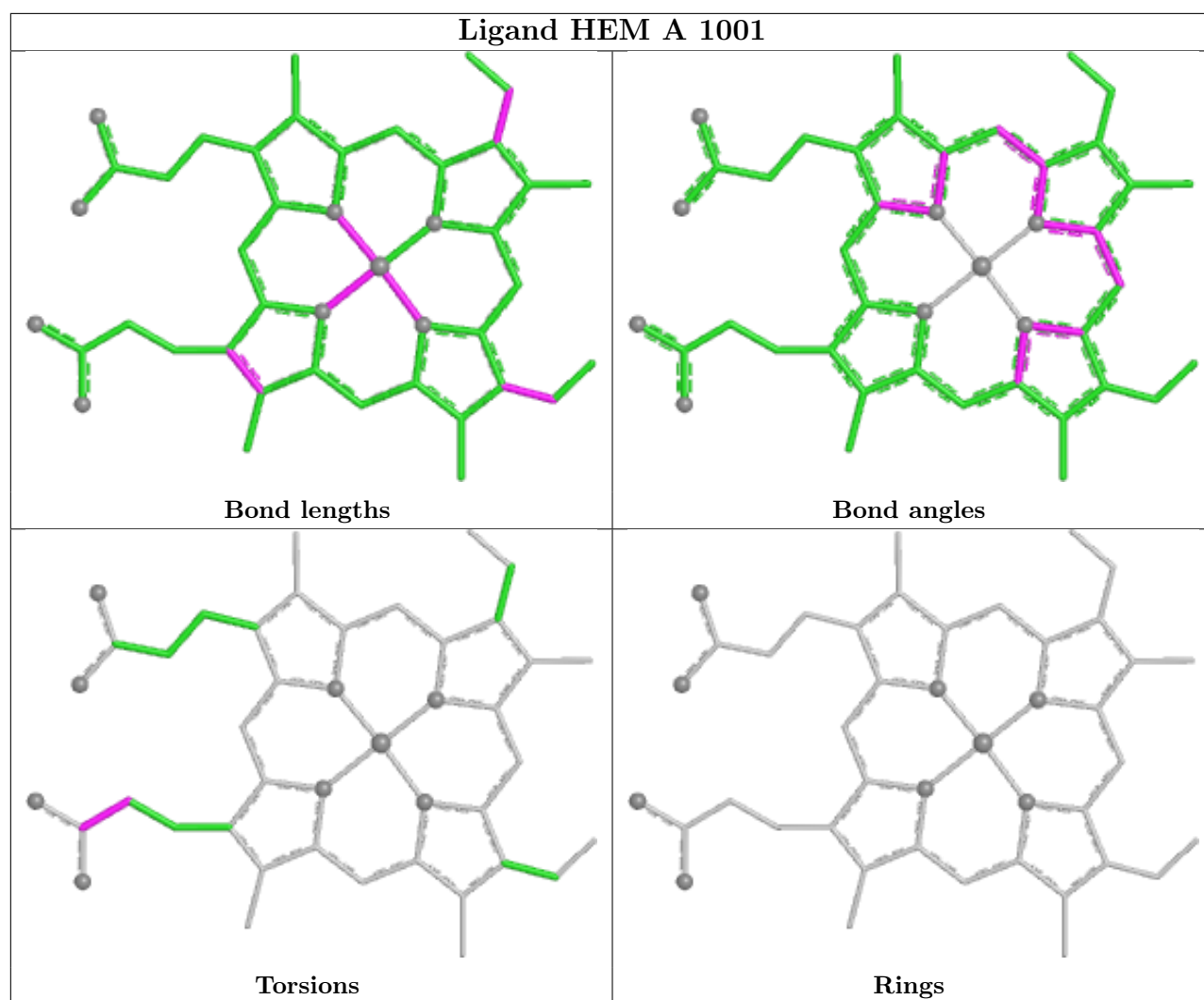
Bond angles

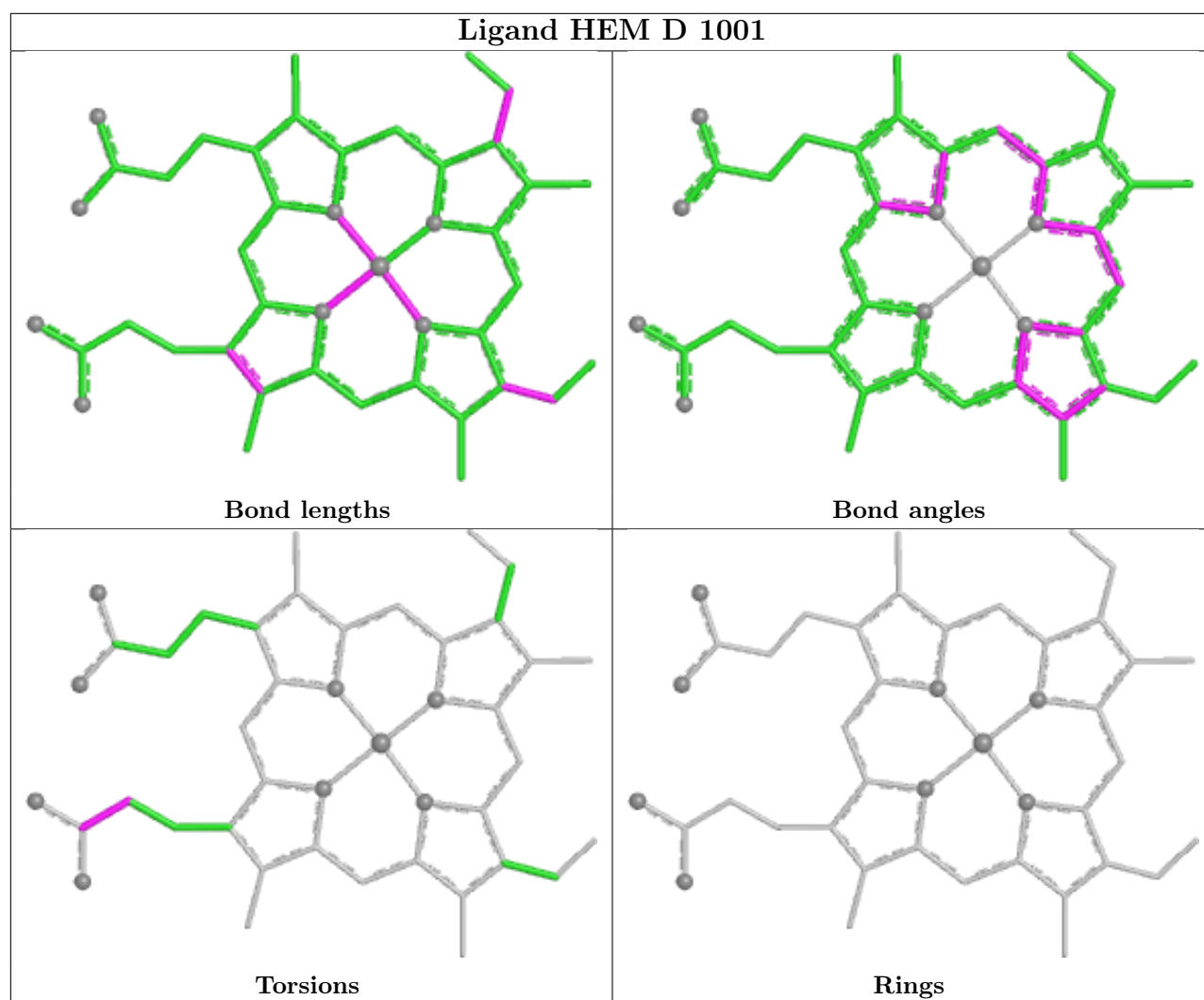


Torsions



Rings





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.

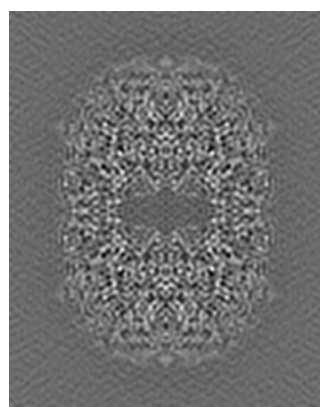
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22530. These allow visual inspection of the internal detail of the map and identification of artifacts.

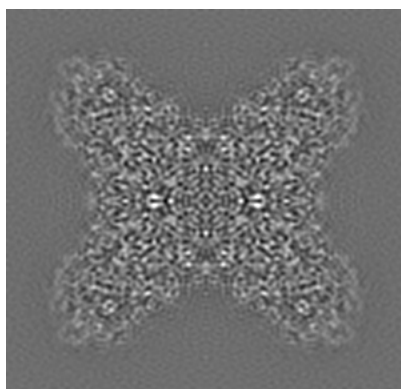
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

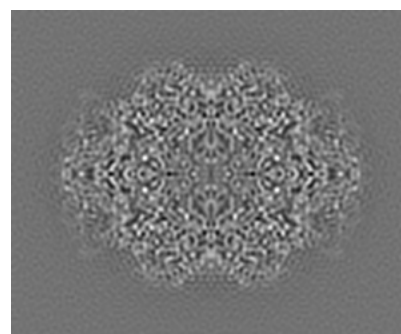
6.1.1 Primary map



X



Y

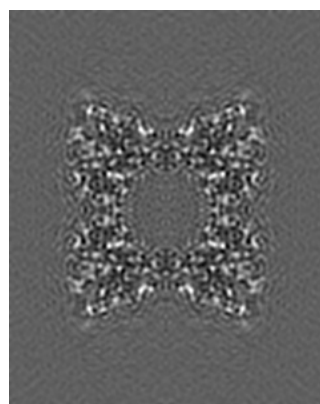


Z

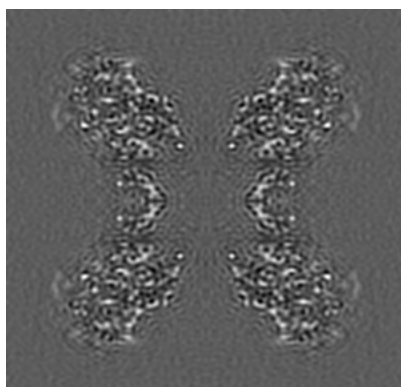
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

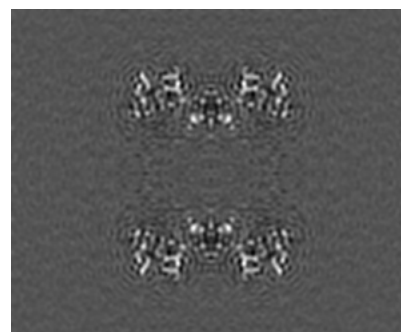
6.2.1 Primary map



X Index: 66



Y Index: 54

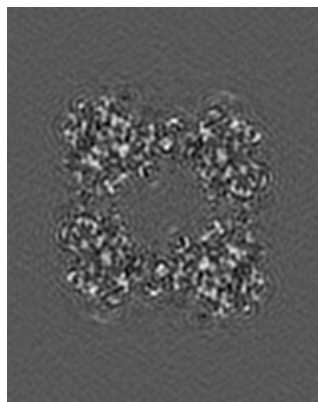


Z Index: 69

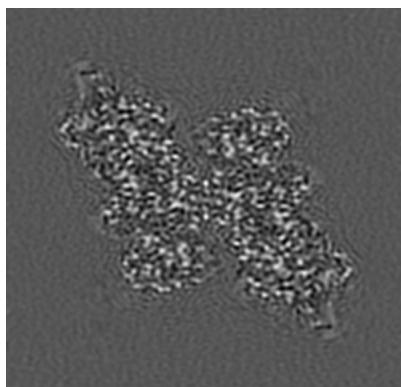
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

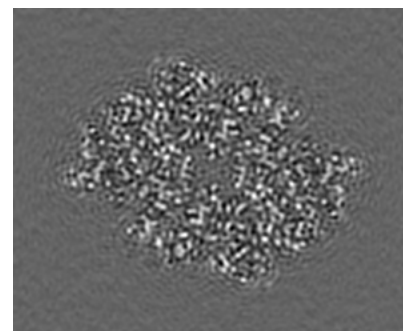
6.3.1 Primary map



X Index: 58



Y Index: 36

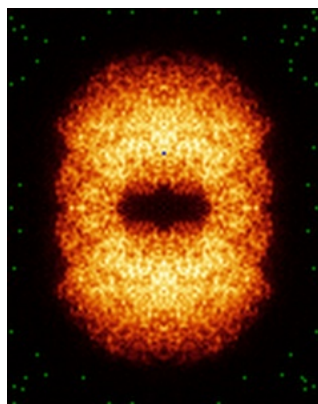


Z Index: 41

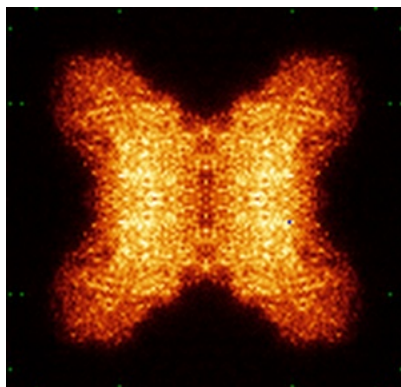
The images above show the largest variance slices of the map in three orthogonal directions.

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

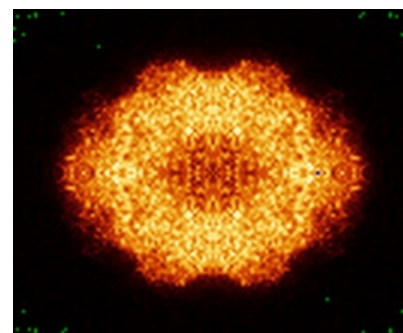
6.4.1 Primary map



X



Y

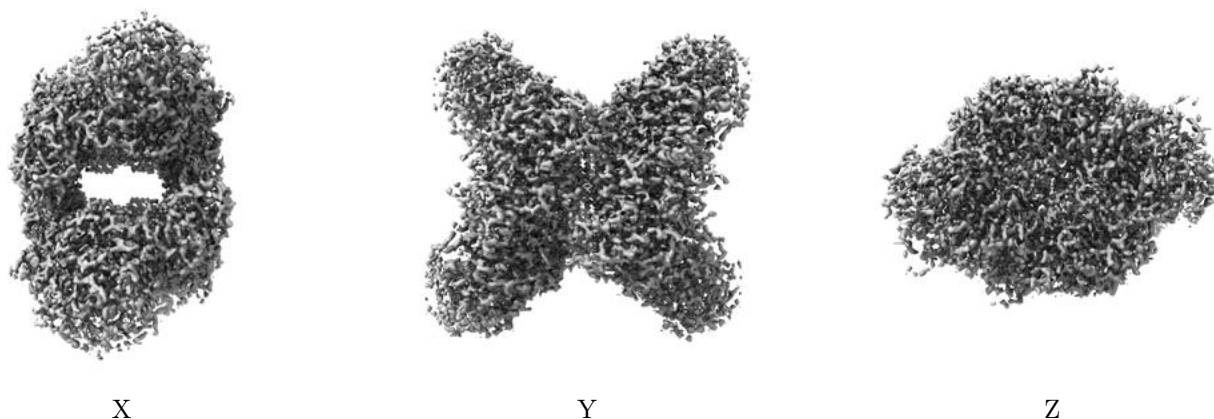


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

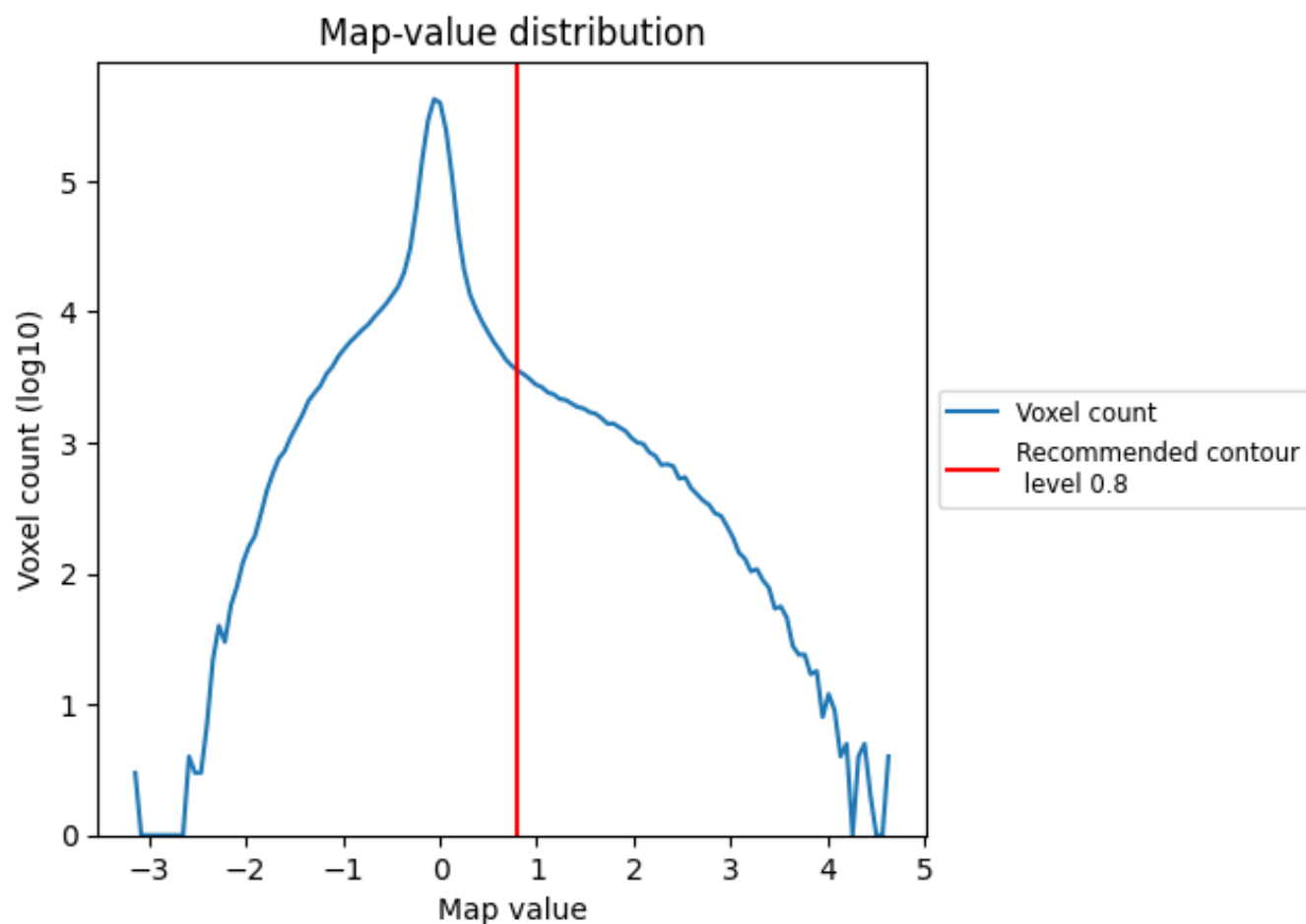
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

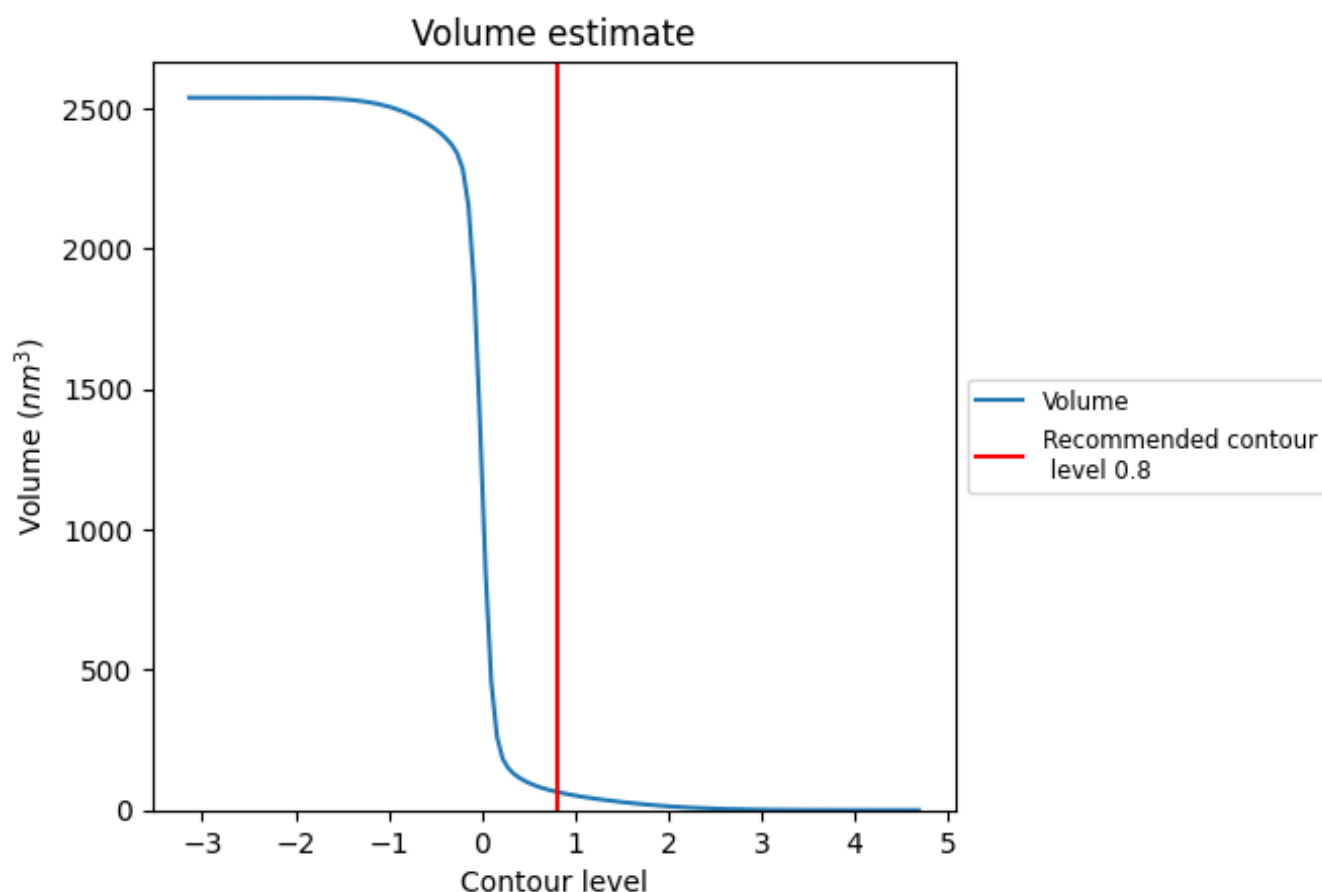
This section contains the results of statistical analysis of the map.

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 66 nm³; this corresponds to an approximate mass of 59 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

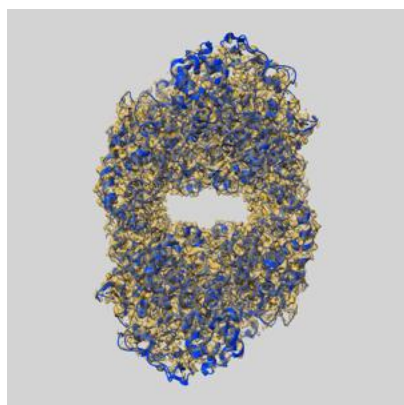
8 Fourier-Shell correlation ⓘ

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

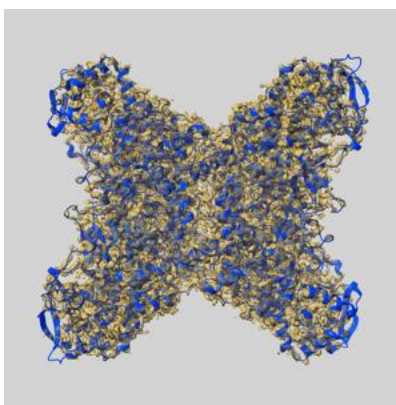
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22530 and PDB model 7JZ6. Per-residue inclusion information can be found in section 3 on page 5.

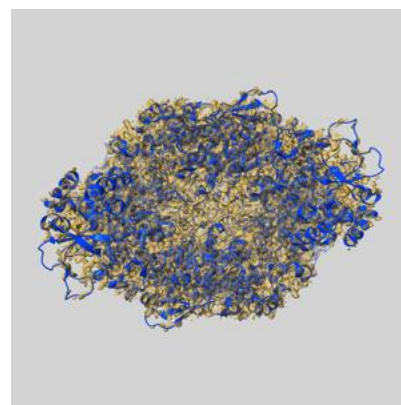
9.1 Map-model overlay [i](#)



X



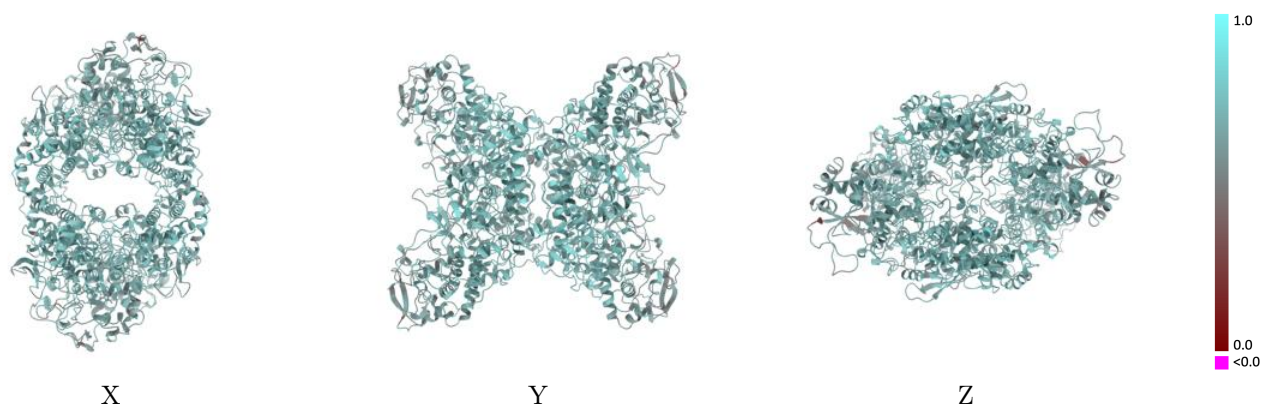
Y



Z

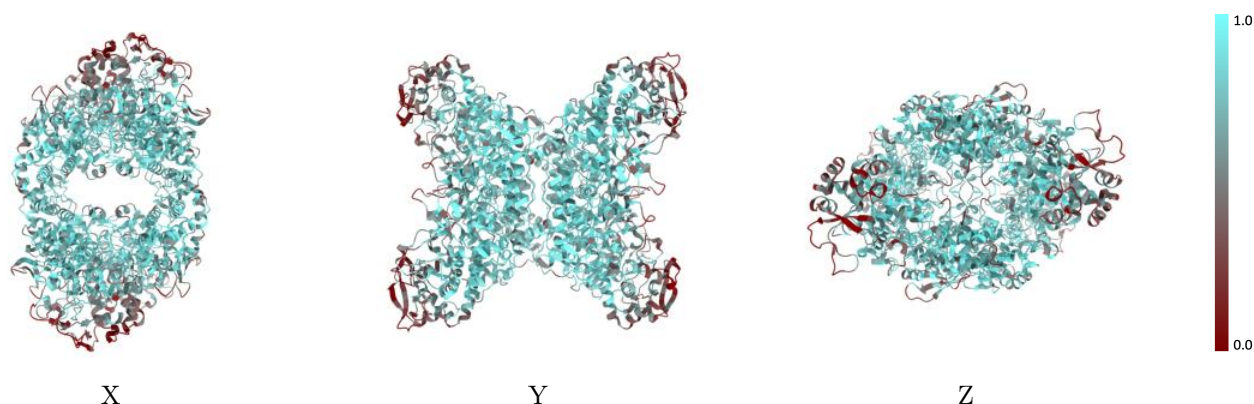
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



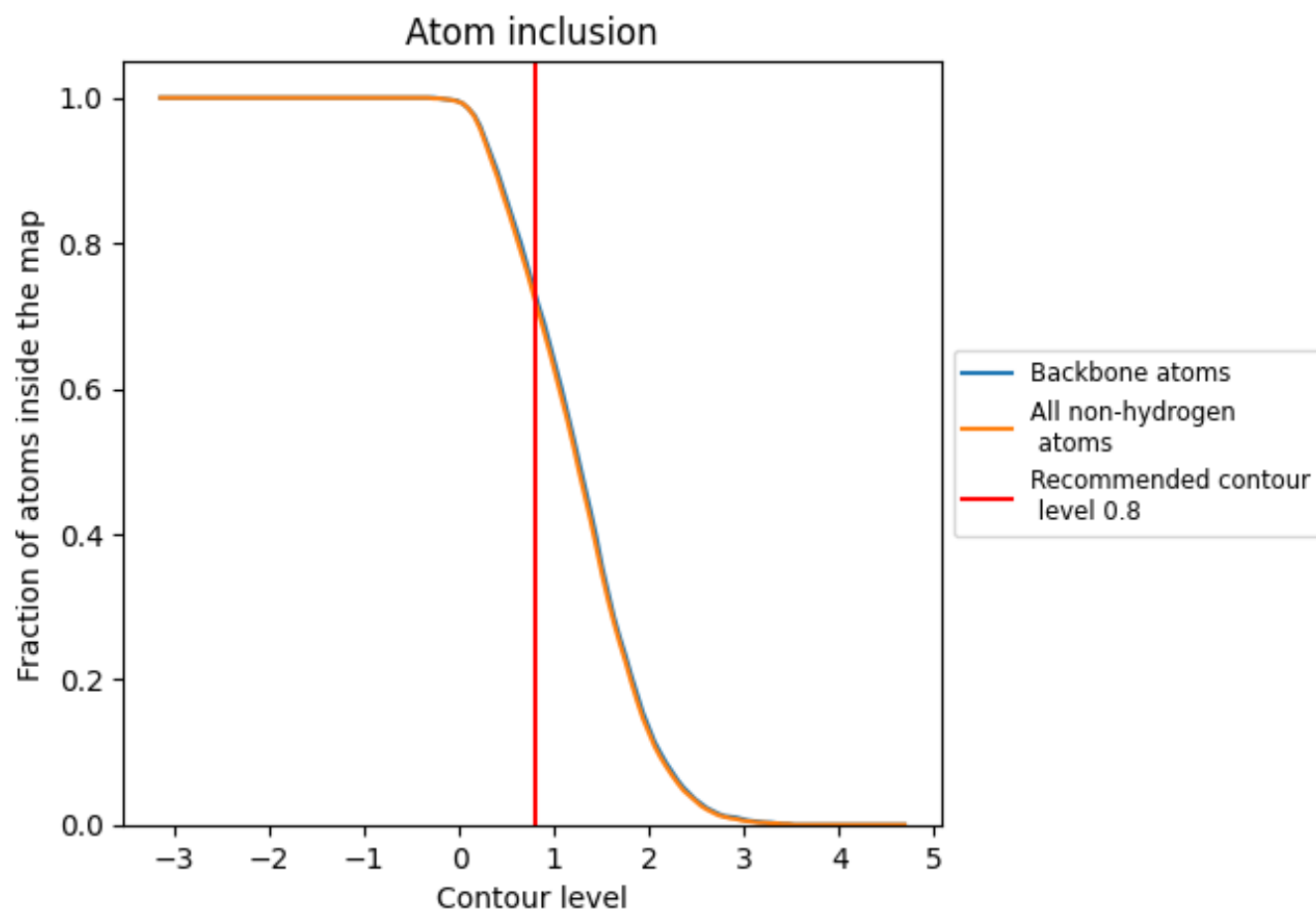
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 72% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.6660
A	0.7250	0.6670
B	0.7210	0.6660
C	0.7220	0.6650
D	0.7220	0.6670

