



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:10 AM UTC

PDB ID : 3EJ6 / pdb_00003ej6
Title : Neurospora Crassa Catalase-3 Crystal Structure
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Deposited on : 2008-09-17
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

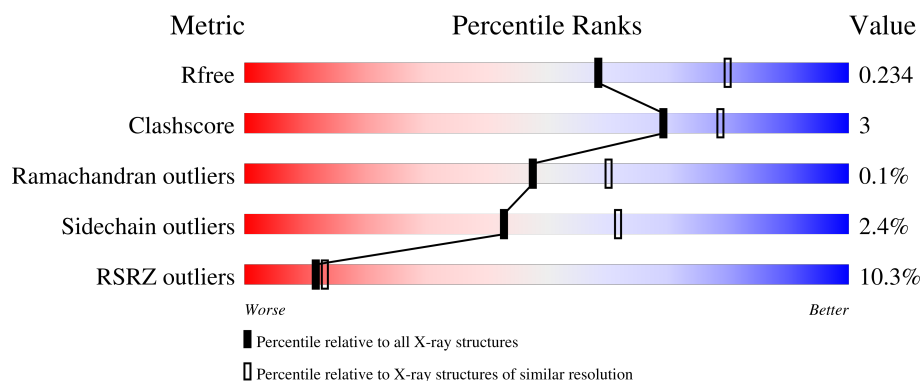
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	688	20% 87% 11%
1	B	688	7% 88% 10%
1	C	688	7% 90% 9%
1	D	688	6% 89% 10%

2 Entry composition [i](#)

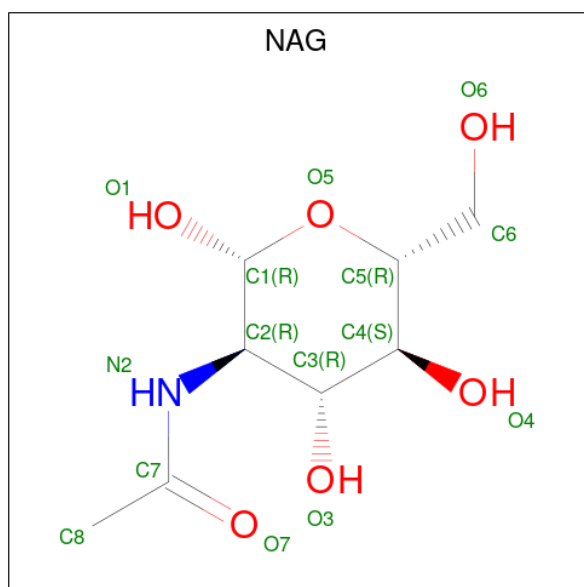
There are 4 unique types of molecules in this entry. The entry contains 23009 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	681	Total	C	N	O	S	47	0	0
			5340	3381	941	1012	6			
1	B	681	Total	C	N	O	S	72	0	0
			5340	3381	941	1012	6			
1	C	681	Total	C	N	O	S	83	0	0
			5340	3381	941	1012	6			
1	D	681	Total	C	N	O	S	64	0	0
			5340	3381	941	1012	6			

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



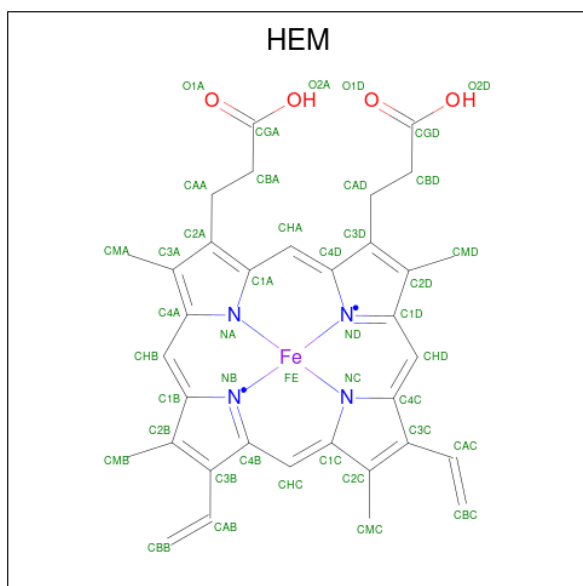
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

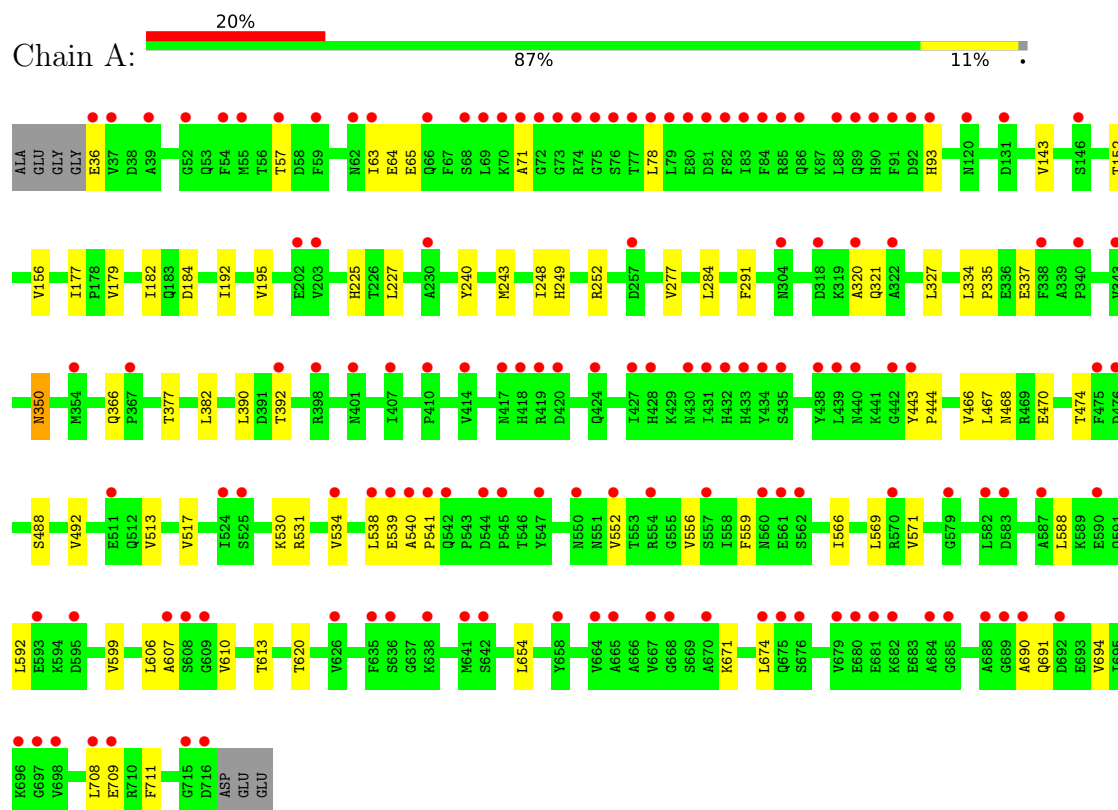
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	319	Total 319	O 319	0	0
4	B	336	Total 336	O 336	0	0
4	C	362	Total 362	O 362	0	0
4	D	348	Total 348	O 348	0	0

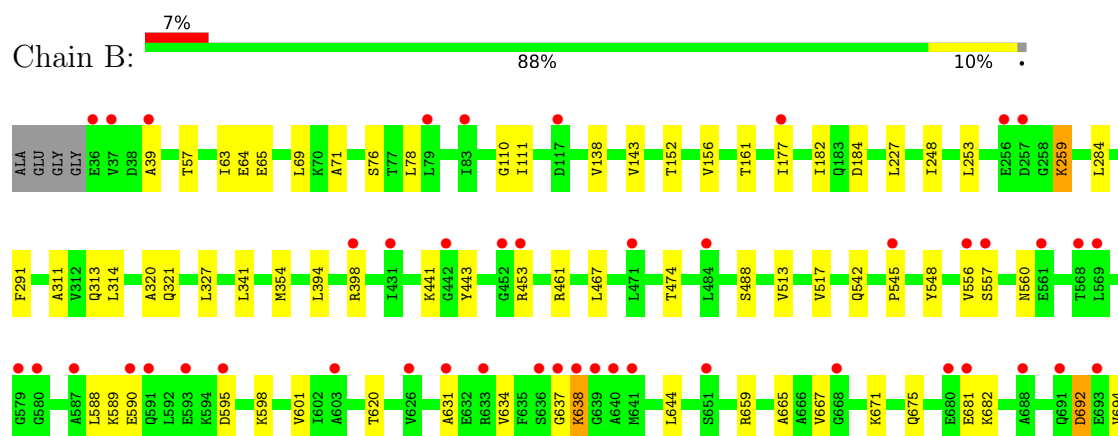
3 Residue-property plots [i](#)

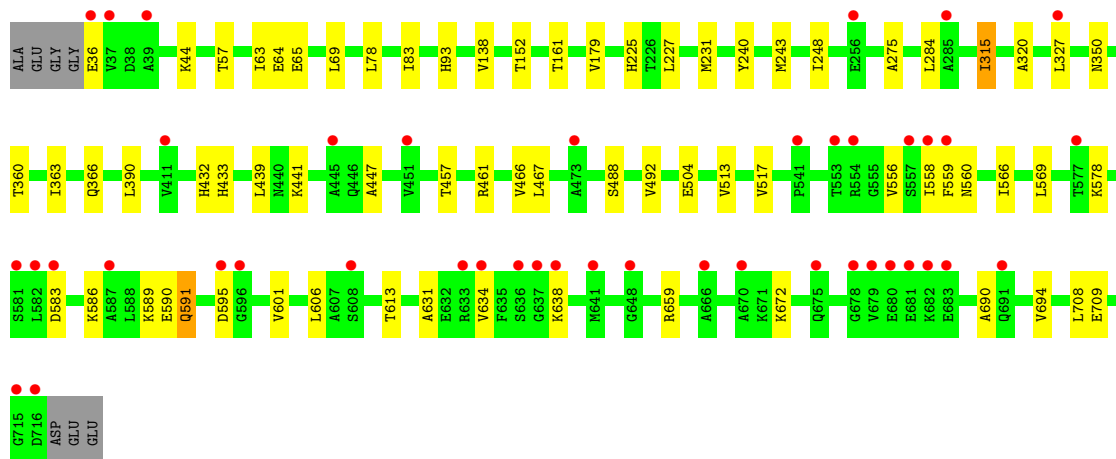
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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-3



• Molecule 1: Catalase-3





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.84Å 154.51Å 162.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.67 – 2.30 34.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.8 (34.67-2.30) 92.9 (34.67-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.242 0.235 , 0.234	Depositor DCC
R_{free} test set	13611 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23009	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.43	1/5473 (0.0%)	0.67	0/7424
1	B	0.45	3/5473 (0.1%)	0.71	5/7424 (0.1%)
1	C	0.47	3/5473 (0.1%)	0.69	6/7424 (0.1%)
1	D	0.45	2/5473 (0.0%)	0.70	6/7424 (0.1%)
All	All	0.45	9/21892 (0.0%)	0.69	17/29696 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	638	LYS	CA-CB	8.08	1.66	1.53
1	D	590	GLU	CA-CB	7.86	1.65	1.53
1	B	638	LYS	CA-CB	-6.92	1.41	1.53
1	C	259	LYS	CG-CD	-6.47	1.33	1.52
1	A	540	ALA	CA-CB	-6.21	1.46	1.53
1	D	44	LYS	CG-CD	-5.78	1.35	1.52
1	B	598	LYS	CG-CD	-5.58	1.35	1.52
1	C	700	GLU	CA-CB	5.21	1.61	1.53
1	B	259	LYS	CB-CG	5.11	1.67	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	583	ASP	CA-CB-CG	-10.79	101.81	112.60
1	D	591	GLN	OE1-CD-NE2	-10.23	112.37	122.60
1	B	542	GLN	OE1-CD-NE2	-9.83	112.77	122.60
1	B	638	LYS	N-CA-CB	7.23	120.59	109.97
1	D	591	GLN	CG-CD-NE2	6.88	126.71	116.40
1	B	542	GLN	CG-CD-NE2	6.65	126.37	116.40
1	C	595	ASP	CA-CB-CG	-6.38	106.22	112.60
1	B	259	LYS	CA-CB-CG	-6.17	101.76	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	692	ASP	N-CA-CB	-6.05	100.90	110.28
1	C	638	LYS	CB-CA-C	-6.02	100.61	110.85
1	C	675	GLN	CB-CA-C	-5.79	99.56	110.67
1	C	638	LYS	N-CA-CB	-5.61	101.85	110.16
1	D	586	LYS	CB-CG-CD	-5.42	98.82	111.30
1	D	44	LYS	CB-CG-CD	5.38	123.67	111.30
1	D	44	LYS	CG-CD-CE	5.22	123.32	111.30
1	C	713	VAL	N-CA-CB	5.20	121.89	111.91
1	C	713	VAL	CA-CB-CG1	5.15	119.15	110.40

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	5340	0	5155	45	0
1	B	5340	0	5153	39	0
1	C	5340	0	5154	35	0
1	D	5340	0	5154	37	0
2	A	14	0	13	0	0
2	B	42	0	39	0	0
2	C	28	0	26	0	0
2	D	28	0	26	0	0
3	A	43	0	30	2	0
3	B	43	0	30	1	0
3	C	43	0	30	2	0
3	D	43	0	30	1	0
4	A	319	0	0	0	0
4	B	336	0	0	0	0
4	C	362	0	0	0	0
4	D	348	0	0	0	0
All	All	23009	0	20840	145	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 3.

All (145) 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:248:ILE:HD12	3:C:4002:HEM:HMB1	1.64	0.79
1:A:654:LEU:HD21	1:A:674:LEU:HD23	1.65	0.78
1:B:248:ILE:HD12	3:B:4001:HEM:HMB1	1.66	0.76
1:A:248:ILE:HD12	3:A:4000:HEM:HMB1	1.66	0.76
1:C:71:ALA:HB2	1:C:78:LEU:HD21	1.72	0.72
1:A:467:LEU:HD22	1:D:78:LEU:HD11	1.73	0.70
1:C:152:THR:HG21	1:C:284:LEU:HD23	1.74	0.69
1:B:78:LEU:HD11	1:C:467:LEU:HD22	1.73	0.69
1:D:606:LEU:CD1	1:D:613:THR:HG23	2.24	0.68
1:B:467:LEU:HD22	1:C:78:LEU:HD11	1.74	0.67
1:D:152:THR:HG21	1:D:284:LEU:HD23	1.77	0.67
1:A:607:ALA:HB3	1:A:610:VAL:HG23	1.80	0.64
1:A:152:THR:HG21	1:A:284:LEU:HD23	1.81	0.62
1:A:320:ALA:HA	1:A:327:LEU:HD12	1.82	0.62
1:B:320:ALA:HA	1:B:327:LEU:HD12	1.84	0.60
1:A:571:VAL:HG11	1:A:592:LEU:HD21	1.84	0.59
1:B:71:ALA:HB2	1:B:78:LEU:HD21	1.84	0.58
1:A:531:ARG:O	1:A:534:VAL:HG12	2.03	0.58
1:C:606:LEU:CD1	1:C:613:THR:HG23	2.34	0.57
1:C:152:THR:HG21	1:C:284:LEU:CD2	2.33	0.57
1:B:138:VAL:HG22	1:B:161:THR:HG23	1.85	0.57
1:B:152:THR:HG21	1:B:284:LEU:HD23	1.86	0.57
1:B:57:THR:HG22	1:B:63:ILE:HD13	1.87	0.57
1:B:665:ALA:HB1	1:B:694:VAL:HG13	1.87	0.56
1:A:488:SER:HB2	1:A:556:VAL:HG21	1.90	0.54
1:C:320:ALA:HA	1:C:327:LEU:HD12	1.88	0.54
1:A:143:VAL:HG23	1:A:156:VAL:O	2.08	0.54
1:A:592:LEU:HD23	1:A:599:VAL:HG22	1.90	0.54
1:A:249:HIS:CD2	1:A:382:LEU:HD13	2.43	0.53
1:C:488:SER:HA	1:C:552:VAL:HG13	1.90	0.53
1:D:57:THR:CG2	1:D:63:ILE:HD13	2.39	0.53
1:D:152:THR:HG21	1:D:284:LEU:CD2	2.39	0.53
1:D:240:TYR:HA	1:D:243:MET:HE2	1.90	0.53
1:A:559:PHE:HB3	1:A:708:LEU:HD11	1.91	0.53
1:A:606:LEU:CD1	1:A:613:THR:HG23	2.39	0.52
1:D:138:VAL:HG22	1:D:161:THR:HG23	1.90	0.52
1:A:78:LEU:HD11	1:D:467:LEU:HD22	1.91	0.52
1:C:143:VAL:HG23	1:C:156:VAL:O	2.09	0.52
1:C:462:THR:HG22	1:D:466:VAL:HA	1.90	0.52
1:B:488:SER:HB2	1:B:556:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:ALA:HA	1:D:327:LEU:HD12	1.90	0.52
1:D:57:THR:HG22	1:D:63:ILE:HD13	1.92	0.52
1:A:57:THR:HG23	1:A:63:ILE:HD13	1.91	0.52
1:D:64:GLU:O	1:D:83:ILE:HG21	2.09	0.52
1:B:152:THR:HG21	1:B:284:LEU:CD2	2.40	0.51
1:B:57:THR:CG2	1:B:63:ILE:HD13	2.41	0.51
1:D:606:LEU:HD13	1:D:613:THR:HG23	1.92	0.51
1:B:667:VAL:HG22	1:B:694:VAL:HG21	1.93	0.51
1:B:284:LEU:HD21	1:B:291:PHE:CD2	2.46	0.50
1:A:492:VAL:HG11	1:A:708:LEU:HB3	1.93	0.50
1:A:57:THR:CG2	1:A:63:ILE:HD13	2.42	0.50
1:A:152:THR:HG21	1:A:284:LEU:CD2	2.42	0.50
1:A:240:TYR:HA	1:A:243:MET:HE2	1.93	0.50
1:A:592:LEU:HD23	1:A:599:VAL:CG2	2.42	0.49
1:B:143:VAL:HG23	1:B:156:VAL:O	2.12	0.49
1:B:354:MET:HA	1:B:354:MET:HE2	1.93	0.49
1:C:42:ARG:HD2	1:C:411:VAL:HG12	1.95	0.49
1:D:366:GLN:HE22	1:D:390:LEU:HD13	1.78	0.49
1:A:71:ALA:HB2	1:A:78:LEU:HD21	1.93	0.49
1:D:513:VAL:O	1:D:517:VAL:HG23	2.13	0.49
1:D:558:ILE:C	1:D:560:ASN:H	2.20	0.48
1:A:284:LEU:HD21	1:A:291:PHE:CD2	2.48	0.48
1:A:179:VAL:HG11	1:A:225:HIS:CE1	2.49	0.47
1:A:443:TYR:HA	1:A:444:PRO:C	2.40	0.47
1:A:321:GLN:NE2	1:A:474:THR:HG21	2.29	0.47
1:A:513:VAL:O	1:A:517:VAL:HG23	2.14	0.47
1:A:690:ALA:O	1:A:694:VAL:HG23	2.14	0.47
1:B:513:VAL:O	1:B:517:VAL:HG23	2.15	0.47
1:D:492:VAL:HG11	1:D:708:LEU:HB3	1.97	0.47
1:B:39:ALA:HB2	1:B:111:ILE:HD11	1.97	0.47
1:C:567:ALA:C	1:C:568:THR:HG23	2.39	0.47
1:D:488:SER:HB2	1:D:556:VAL:HG21	1.97	0.47
1:C:631:ALA:O	1:C:634:VAL:HG22	2.15	0.46
1:D:566:ILE:HB	1:D:569:LEU:HD12	1.97	0.46
1:D:231:MET:HE1	1:D:504:GLU:OE1	2.15	0.46
1:D:315:ILE:N	1:D:315:ILE:HD13	2.31	0.46
1:A:588:LEU:HD13	1:A:691:GLN:HG3	1.97	0.46
1:C:69:LEU:HG	1:C:78:LEU:HD12	1.97	0.46
1:C:252:ARG:NH1	1:C:377:THR:HG22	2.31	0.46
1:B:69:LEU:HG	1:B:78:LEU:HD12	1.97	0.46
1:B:321:GLN:NE2	1:B:474:THR:HG21	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:LEU:HG	1:D:78:LEU:HD12	1.97	0.46
1:A:607:ALA:HB3	1:A:610:VAL:CG2	2.45	0.46
1:B:156:VAL:HG22	1:B:177:ILE:HD12	1.97	0.46
1:B:589:LYS:HD2	1:B:601:VAL:HG23	1.98	0.46
1:A:466:VAL:HG23	1:B:461:ARG:O	2.16	0.46
1:D:360:THR:O	1:D:363:ILE:HG22	2.15	0.45
1:C:284:LEU:HD21	1:C:291:PHE:CD2	2.52	0.45
1:A:392:THR:HG21	3:A:4000:HEM:HBD1	1.99	0.45
1:A:566:ILE:HB	1:A:569:LEU:HD12	1.98	0.45
1:C:57:THR:CG2	1:C:63:ILE:HD13	2.47	0.45
1:D:492:VAL:HG11	1:D:708:LEU:HD22	1.98	0.45
1:B:39:ALA:HB2	1:B:111:ILE:CD1	2.48	0.44
1:C:57:THR:HG22	1:C:63:ILE:HD13	1.99	0.44
1:D:248:ILE:HD12	3:D:4003:HEM:HBB2	1.99	0.44
1:D:566:ILE:HD11	1:D:595:ASP:OD1	2.17	0.44
1:C:248:ILE:CD1	3:C:4002:HEM:HMB1	2.43	0.44
1:A:366:GLN:HE22	1:A:390:LEU:HD13	1.83	0.44
1:B:588:LEU:HD12	1:B:695:ILE:HD11	1.98	0.44
1:C:510:ASN:OD1	1:C:513:VAL:HG23	2.17	0.43
1:A:93:HIS:CE1	1:C:394:LEU:HD13	2.53	0.43
1:D:432:HIS:CE1	1:D:439:LEU:HB3	2.53	0.43
1:D:690:ALA:O	1:D:694:VAL:HG23	2.19	0.43
1:B:557:SER:HB3	1:B:560:ASN:HB2	1.99	0.43
1:A:192:ILE:HA	1:A:195:VAL:HG22	2.00	0.43
1:C:138:VAL:HG22	1:C:161:THR:HG23	1.99	0.43
1:B:441:LYS:O	1:B:443:TYR:CD1	2.71	0.43
1:A:284:LEU:HD13	1:A:620:THR:HB	2.01	0.43
1:D:63:ILE:HD12	1:D:83:ILE:HG23	2.00	0.43
1:C:138:VAL:CG2	1:C:349:LEU:HD21	2.48	0.43
1:B:644:LEU:HD23	1:C:502:ARG:NH1	2.34	0.43
1:A:182:ILE:HD12	1:A:184:ASP:O	2.18	0.42
1:B:631:ALA:O	1:B:634:VAL:HG22	2.19	0.42
1:C:457:THR:HG23	1:C:461:ARG:HH21	1.84	0.42
1:D:589:LYS:HD2	1:D:601:VAL:HG23	2.01	0.42
1:A:350:ASN:HD22	1:A:350:ASN:C	2.28	0.42
1:B:182:ILE:HD12	1:B:184:ASP:O	2.19	0.42
1:B:110:GLY:C	1:B:111:ILE:HD12	2.44	0.42
1:D:631:ALA:O	1:D:634:VAL:HG22	2.20	0.42
1:B:394:LEU:HD13	1:D:93:HIS:CE1	2.55	0.42
1:A:277:VAL:HG11	1:A:711:PHE:CZ	2.55	0.42
1:B:313:GLN:HG3	1:B:341:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ALA:HB3	1:D:559:PHE:CZ	2.56	0.41
1:B:64:GLU:HG2	1:D:447:ALA:O	2.21	0.41
1:C:156:VAL:HG22	1:C:177:ILE:HD12	2.02	0.41
1:A:78:LEU:HD22	1:B:76:SER:HB2	2.02	0.41
1:B:253:LEU:HD12	1:B:314:LEU:HD21	2.02	0.41
1:C:284:LEU:HD13	1:C:620:THR:HB	2.02	0.41
1:D:179:VAL:HG21	1:D:225:HIS:ND1	2.36	0.41
1:C:182:ILE:HD12	1:C:184:ASP:O	2.21	0.41
1:C:488:SER:HB2	1:C:556:VAL:HG21	2.02	0.41
1:C:677:ILE:HG13	1:C:679:VAL:HG23	2.03	0.41
1:B:284:LEU:HD13	1:B:620:THR:HB	2.03	0.41
1:C:239:SER:HA	1:C:292:HIS:CD2	2.56	0.41
1:C:513:VAL:O	1:C:517:VAL:HG23	2.21	0.41
1:D:492:VAL:HG21	1:D:708:LEU:HB3	2.03	0.41
1:B:311:ALA:HB1	1:B:341:LEU:HB3	2.03	0.40
1:B:545:PRO:HA	1:B:548:TYR:CD1	2.56	0.40
1:C:138:VAL:HG23	1:C:349:LEU:HD21	2.04	0.40
1:A:488:SER:HA	1:A:552:VAL:HG13	2.03	0.40
1:D:457:THR:HG23	1:D:461:ARG:HH21	1.85	0.40
1:A:156:VAL:HG22	1:A:177:ILE:HD12	2.04	0.40
1:A:252:ARG:NH1	1:A:377:THR:HG22	2.36	0.40
1:C:690:ALA:O	1:C:694:VAL:HG23	2.22	0.40
1:A:334:LEU:HD12	1:A:335:PRO:HD2	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 X-ray entries followed by that with respect to entries of similar resolution.

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	679/688 (99%)	652 (96%)	26 (4%)	1 (0%)	48 60
1	B	679/688 (99%)	657 (97%)	21 (3%)	1 (0%)	48 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	679/688 (99%)	659 (97%)	20 (3%)	0	100	100
1	D	679/688 (99%)	645 (95%)	34 (5%)	0	100	100
All	All	2716/2752 (99%)	2613 (96%)	101 (4%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	637	GLY
1	A	541	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	559/563 (99%)	546 (98%)	13 (2%)	44	63
1	B	559/563 (99%)	543 (97%)	16 (3%)	37	55
1	C	559/563 (99%)	547 (98%)	12 (2%)	47	66
1	D	559/563 (99%)	546 (98%)	13 (2%)	44	63
All	All	2236/2252 (99%)	2182 (98%)	54 (2%)	43	62

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	64	GLU
1	A	65	GLU
1	A	227	LEU
1	A	337	GLU
1	A	350	ASN
1	A	468	ASN
1	A	470	GLU
1	A	530	LYS
1	A	538	LEU

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Mol	Chain	Res	Type
1	A	539	GLU
1	A	671	LYS
1	A	709	GLU
1	B	65	GLU
1	B	227	LEU
1	B	259	LYS
1	B	398	ARG
1	B	453	ARG
1	B	590	GLU
1	B	595	ASP
1	B	638	LYS
1	B	659	ARG
1	B	671	LYS
1	B	675	GLN
1	B	681	GLU
1	B	682	LYS
1	B	692	ASP
1	B	696	LYS
1	B	709	GLU
1	C	65	GLU
1	C	227	LEU
1	C	337	GLU
1	C	398	ARG
1	C	441	LYS
1	C	530	LYS
1	C	594	LYS
1	C	629	GLU
1	C	638	LYS
1	C	682	LYS
1	C	696	LYS
1	C	709	GLU
1	D	36	GLU
1	D	65	GLU
1	D	227	LEU
1	D	315	ILE
1	D	350	ASN
1	D	433	HIS
1	D	441	LYS
1	D	578	LYS
1	D	591	GLN
1	D	638	LYS
1	D	659	ARG

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Mol	Chain	Res	Type
1	D	672	LYS
1	D	709	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	89	GLN
1	A	133	GLN
1	A	304	ASN
1	A	313	GLN
1	A	321	GLN
1	A	350	ASN
1	A	362	GLN
1	A	366	GLN
1	A	393	GLN
1	A	449	GLN
1	A	510	ASN
1	A	512	GLN
1	A	516	ASN
1	A	522	ASN
1	A	526	ASN
1	A	691	GLN
1	B	53	GLN
1	B	89	GLN
1	B	133	GLN
1	B	169	ASN
1	B	220	GLN
1	B	304	ASN
1	B	321	GLN
1	B	362	GLN
1	B	366	GLN
1	B	393	GLN
1	B	512	GLN
1	B	516	ASN
1	B	526	ASN
1	C	53	GLN
1	C	66	GLN
1	C	89	GLN
1	C	266	HIS
1	C	294	GLN
1	C	362	GLN

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Mol	Chain	Res	Type
1	C	366	GLN
1	C	449	GLN
1	C	512	GLN
1	C	516	ASN
1	D	53	GLN
1	D	89	GLN
1	D	133	GLN
1	D	220	GLN
1	D	350	ASN
1	D	366	GLN
1	D	417	ASN
1	D	449	GLN
1	D	512	GLN
1	D	516	ASN
1	D	520	GLN
1	D	526	ASN
1	D	560	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](#)

12 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	NAG	B	5007	1	14,14,15	0.42	0	17,19,21	1.24	2 (11%)
3	HEM	C	4002	1	50,50,50	1.86	8 (16%)	67,82,82	1.41	5 (7%)
2	NAG	A	5002	1	14,14,15	0.52	0	17,19,21	0.56	0
3	HEM	B	4001	1	50,50,50	1.90	8 (16%)	67,82,82	1.38	5 (7%)
2	NAG	B	5006	1	14,14,15	0.51	0	17,19,21	0.74	0
2	NAG	C	5008	1	14,14,15	0.53	0	17,19,21	0.69	0
2	NAG	C	5009	1	14,14,15	0.60	0	17,19,21	0.71	0
2	NAG	D	5014	1	14,14,15	0.48	0	17,19,21	0.83	0
3	HEM	D	4003	1	50,50,50	1.93	10 (20%)	67,82,82	1.35	4 (5%)
2	NAG	B	5005	1	14,14,15	0.54	0	17,19,21	0.83	0
2	NAG	D	5013	1	14,14,15	0.59	0	17,19,21	0.65	0
3	HEM	A	4000	1,4	50,50,50	1.88	8 (16%)	67,82,82	1.42	5 (7%)

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	NAG	B	5007	1	-	0/6/23/26	0/1/1/1
3	HEM	C	4002	1	-	7/14/54/54	-
2	NAG	A	5002	1	-	4/6/23/26	0/1/1/1
3	HEM	B	4001	1	-	4/14/54/54	-
2	NAG	B	5006	1	-	3/6/23/26	0/1/1/1
2	NAG	C	5008	1	-	2/6/23/26	0/1/1/1
2	NAG	C	5009	1	-	0/6/23/26	0/1/1/1
2	NAG	D	5014	1	-	4/6/23/26	0/1/1/1
3	HEM	D	4003	1	-	6/14/54/54	-
2	NAG	B	5005	1	-	2/6/23/26	0/1/1/1
2	NAG	D	5013	1	-	0/6/23/26	0/1/1/1
3	HEM	A	4000	1,4	-	6/14/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4001	HEM	C3D-C2D	7.88	1.53	1.36
3	D	4003	HEM	C3D-C2D	7.86	1.53	1.36
3	A	4000	HEM	C3D-C2D	7.84	1.53	1.36
3	C	4002	HEM	C3D-C2D	7.83	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4003	HEM	FE-NB	4.81	2.09	1.94
3	D	4003	HEM	FE-ND	4.55	2.08	1.94
3	B	4001	HEM	FE-ND	4.55	2.08	1.94
3	B	4001	HEM	FE-NB	4.33	2.08	1.94
3	C	4002	HEM	FE-ND	4.33	2.08	1.94
3	A	4000	HEM	FE-ND	4.29	2.08	1.94
3	A	4000	HEM	FE-NB	4.21	2.07	1.94
3	C	4002	HEM	FE-NB	3.92	2.07	1.94
3	D	4003	HEM	FE-NC	3.79	2.07	1.95
3	B	4001	HEM	FE-NC	3.61	2.07	1.95
3	A	4000	HEM	FE-NC	3.43	2.06	1.95
3	C	4002	HEM	FE-NA	3.36	2.06	1.95
3	D	4003	HEM	FE-NA	3.34	2.06	1.95
3	A	4000	HEM	FE-NA	3.33	2.06	1.95
3	C	4002	HEM	FE-NC	3.19	2.05	1.95
3	B	4001	HEM	FE-NA	3.04	2.05	1.95
3	B	4001	HEM	CAB-C3B	2.89	1.55	1.47
3	C	4002	HEM	CAC-C3C	2.85	1.55	1.47
3	B	4001	HEM	CAC-C3C	2.82	1.54	1.47
3	A	4000	HEM	CAC-C3C	2.81	1.54	1.47
3	D	4003	HEM	CAC-C3C	2.79	1.54	1.47
3	C	4002	HEM	CAB-C3B	2.79	1.54	1.47
3	D	4003	HEM	CAB-C3B	2.78	1.54	1.47
3	A	4000	HEM	CAB-C3B	2.77	1.54	1.47
3	A	4000	HEM	CMD-C2D	2.05	1.55	1.50
3	B	4001	HEM	CMB-C2B	2.03	1.54	1.50
3	D	4003	HEM	CMD-C2D	2.02	1.54	1.50
3	D	4003	HEM	CMA-C3A	2.02	1.54	1.50
3	D	4003	HEM	CMB-C2B	2.02	1.54	1.50
3	C	4002	HEM	CMD-C2D	2.01	1.54	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4001	HEM	C4D-ND-C1D	5.72	111.98	105.21
3	D	4003	HEM	C4D-ND-C1D	5.65	111.89	105.21
3	A	4000	HEM	C4D-ND-C1D	5.63	111.88	105.21
3	C	4002	HEM	C4D-ND-C1D	5.57	111.81	105.21
2	B	5007	NAG	C1-O5-C5	3.92	117.43	112.19
3	C	4002	HEM	C3B-C4B-NB	-2.61	107.60	109.47
3	C	4002	HEM	C1B-NB-C4B	2.51	108.18	105.21
3	A	4000	HEM	C1B-NB-C4B	2.51	108.18	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4000	HEM	C3B-C4B-NB	-2.49	107.68	109.47
3	A	4000	HEM	C2A-C1A-NA	-2.47	107.41	110.15
3	A	4000	HEM	C3B-C2B-C1B	2.47	108.27	106.41
3	C	4002	HEM	C3B-C2B-C1B	2.44	108.24	106.41
3	B	4001	HEM	C2A-C1A-NA	-2.42	107.47	110.15
3	C	4002	HEM	C2A-C1A-NA	-2.37	107.52	110.15
3	B	4001	HEM	C1B-NB-C4B	2.35	107.99	105.21
3	B	4001	HEM	C3B-C2B-C1B	2.33	108.16	106.41
3	D	4003	HEM	C2A-C1A-NA	-2.33	107.57	110.15
3	D	4003	HEM	C1B-NB-C4B	2.24	107.86	105.21
3	D	4003	HEM	C3B-C2B-C1B	2.12	108.00	106.41
3	B	4001	HEM	C3B-C4B-NB	-2.09	107.97	109.47
2	B	5007	NAG	O5-C5-C6	2.02	111.59	107.66

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5002	NAG	C8-C7-N2-C2
2	A	5002	NAG	O7-C7-N2-C2
2	B	5006	NAG	C1-C2-N2-C7
2	D	5014	NAG	C1-C2-N2-C7
3	B	4001	HEM	C2C-C3C-CAC-CBC
2	A	5002	NAG	O5-C5-C6-O6
2	A	5002	NAG	C4-C5-C6-O6
2	D	5014	NAG	O5-C5-C6-O6
2	B	5006	NAG	C8-C7-N2-C2
2	D	5014	NAG	C4-C5-C6-O6
2	B	5006	NAG	O7-C7-N2-C2
3	A	4000	HEM	C2B-C3B-CAB-CBB
3	A	4000	HEM	C2C-C3C-CAC-CBC
3	C	4002	HEM	C2B-C3B-CAB-CBB
3	C	4002	HEM	C2C-C3C-CAC-CBC
3	D	4003	HEM	C2C-C3C-CAC-CBC
3	B	4001	HEM	C4C-C3C-CAC-CBC
3	C	4002	HEM	C4C-C3C-CAC-CBC
3	D	4003	HEM	C4C-C3C-CAC-CBC
3	A	4000	HEM	C4C-C3C-CAC-CBC
3	C	4002	HEM	C4B-C3B-CAB-CBB
2	B	5005	NAG	C3-C2-N2-C7
3	A	4000	HEM	C4B-C3B-CAB-CBB
3	D	4003	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
3	B	4001	HEM	CAA-CBA-CGA-O2A
3	B	4001	HEM	CAA-CBA-CGA-O1A
2	B	5005	NAG	C1-C2-N2-C7
3	D	4003	HEM	CAA-CBA-CGA-O1A
3	C	4002	HEM	CAA-CBA-CGA-O2A
3	A	4000	HEM	CAA-CBA-CGA-O2A
3	C	4002	HEM	CAA-CBA-CGA-O1A
2	D	5014	NAG	C3-C2-N2-C7
3	A	4000	HEM	CAA-CBA-CGA-O1A
3	D	4003	HEM	C2B-C3B-CAB-CBB
3	D	4003	HEM	C4B-C3B-CAB-CBB
2	C	5008	NAG	C8-C7-N2-C2
3	C	4002	HEM	CAD-CBD-CGD-O2D
2	C	5008	NAG	O7-C7-N2-C2

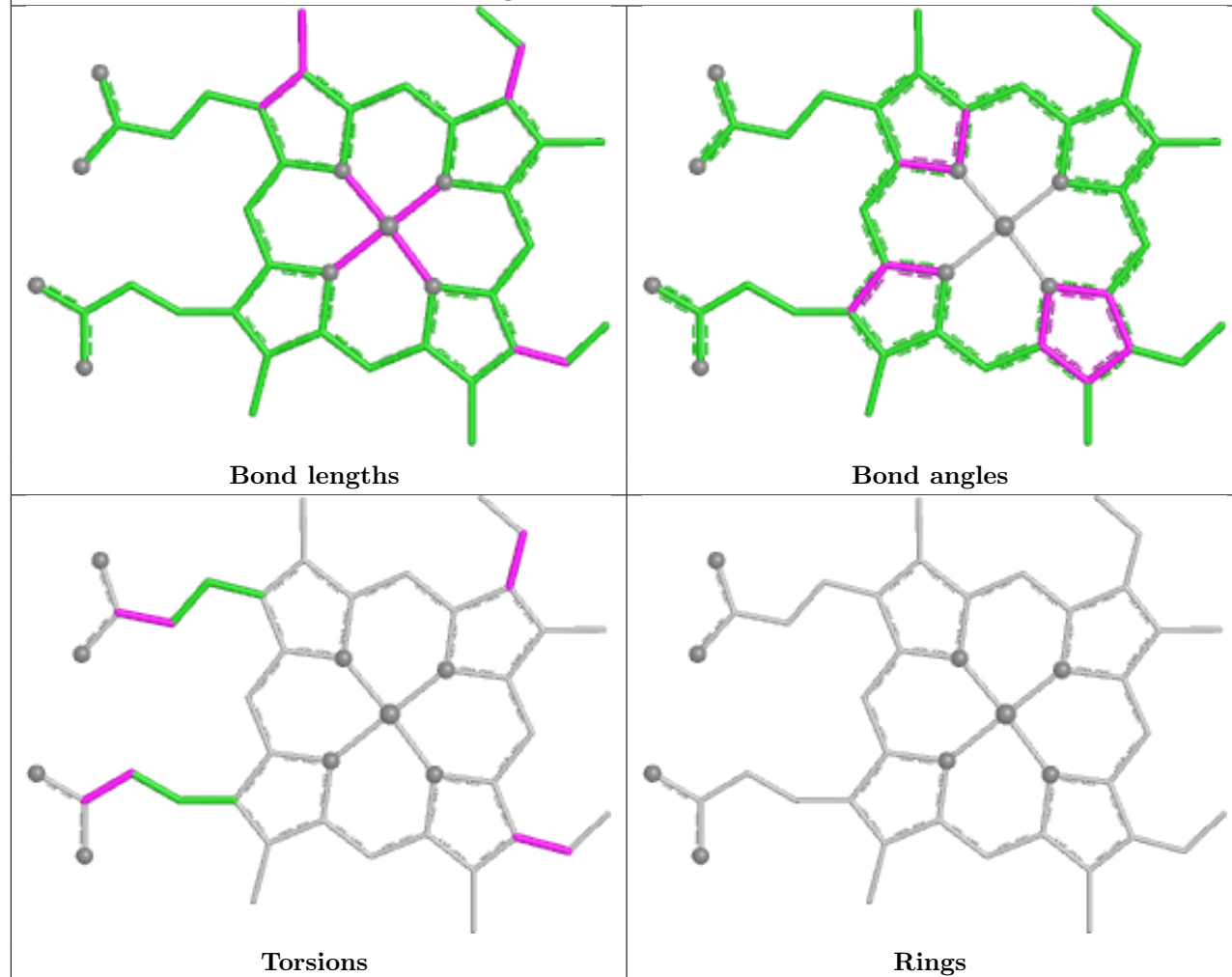
There are no ring outliers.

4 monomers are involved in 6 short contacts:

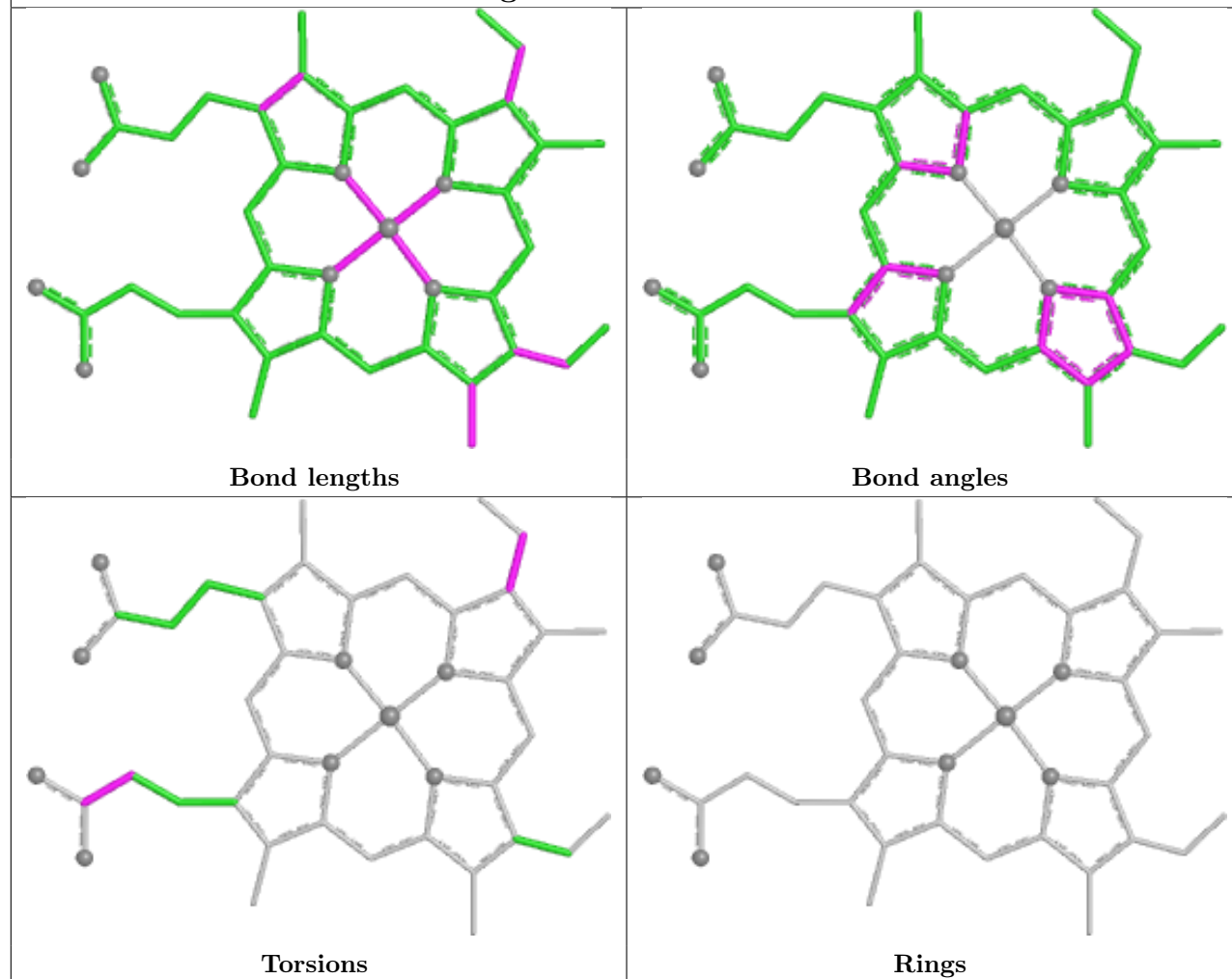
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4002	HEM	2	0
3	B	4001	HEM	1	0
3	D	4003	HEM	1	0
3	A	4000	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

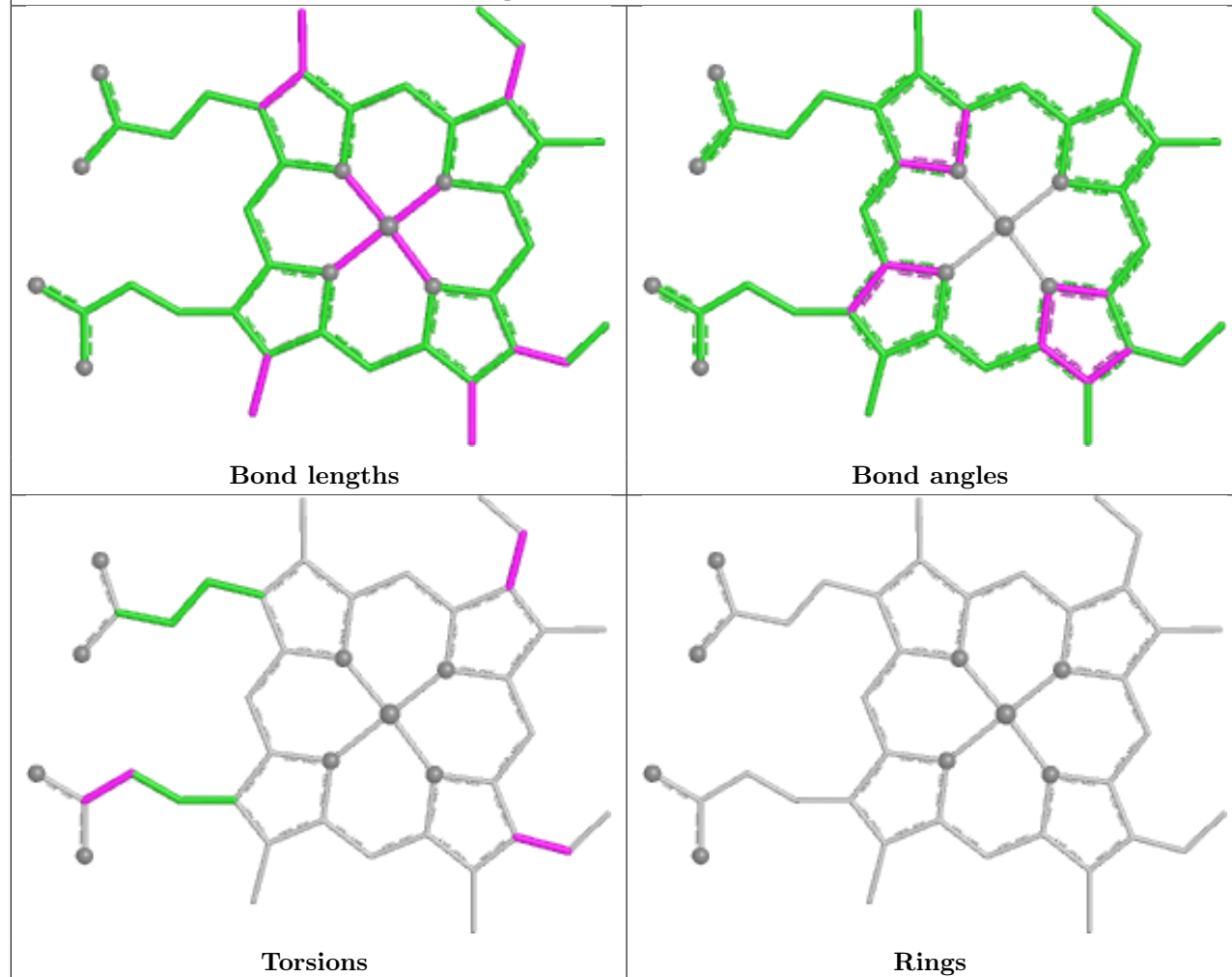
Ligand HEM C 4002

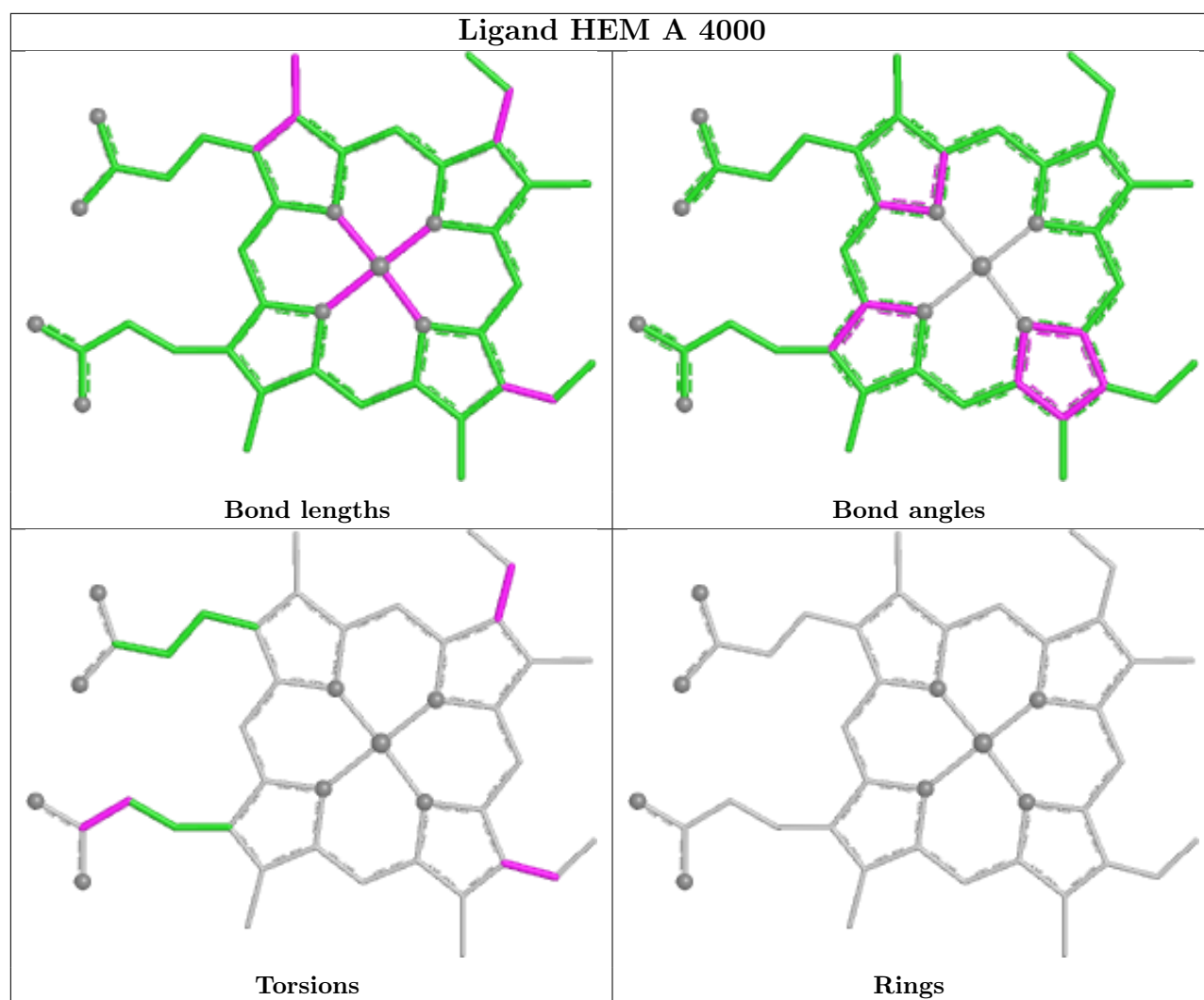


Ligand HEM B 4001



Ligand HEM D 4003





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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	681/688 (98%)	1.37	140 (20%) 2 3	10, 23, 23, 24	13 (1%)
1	B	681/688 (98%)	0.98	48 (7%) 22 24	10, 23, 23, 24	20 (2%)
1	C	681/688 (98%)	0.97	49 (7%) 21 23	10, 23, 23, 24	22 (3%)
1	D	681/688 (98%)	0.94	43 (6%) 26 28	10, 23, 23, 25	16 (2%)
All	All	2724/2752 (98%)	1.07	280 (10%) 12 13	10, 23, 23, 25	71 (2%)

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	715	GLY	8.0
1	A	36	GLU	7.4
1	C	36	GLU	7.1
1	B	36	GLU	7.0
1	D	36	GLU	7.0
1	C	37	VAL	6.6
1	D	37	VAL	6.3
1	B	37	VAL	6.3
1	C	715	GLY	6.2
1	B	680	GLU	5.7
1	A	37	VAL	5.7
1	A	716	ASP	5.7
1	D	716	ASP	5.6
1	B	716	ASP	5.5
1	A	540	ALA	5.3
1	C	716	ASP	5.2
1	A	541	PRO	5.1
1	D	681	GLU	4.6
1	B	579	GLY	4.5
1	D	680	GLU	4.5
1	C	540	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	636	SER	4.1
1	A	69	LEU	4.1
1	D	636	SER	4.1
1	A	88	LEU	4.0
1	D	638	LYS	3.9
1	A	83	ILE	3.8
1	C	641	MET	3.8
1	A	582	LEU	3.8
1	A	608	SER	3.8
1	B	688	ALA	3.7
1	A	680	GLU	3.6
1	D	39	ALA	3.6
1	A	84	PHE	3.6
1	D	641	MET	3.6
1	A	552	VAL	3.6
1	D	715	GLY	3.5
1	D	583	ASP	3.5
1	D	678	GLY	3.5
1	A	431	ILE	3.4
1	A	670	ALA	3.4
1	A	78	LEU	3.4
1	A	75	GLY	3.4
1	A	542	GLN	3.4
1	A	354	MET	3.3
1	A	79	LEU	3.3
1	B	580	GLY	3.3
1	C	680	GLU	3.3
1	A	579	GLY	3.2
1	D	595	ASP	3.2
1	A	432	HIS	3.2
1	A	120	ASN	3.2
1	D	581	SER	3.2
1	A	715	GLY	3.1
1	A	675	GLN	3.1
1	A	554	ARG	3.1
1	A	560	ASN	3.1
1	B	593	GLU	3.0
1	C	72	GLY	3.0
1	C	560	ASN	3.0
1	A	90	HIS	3.0
1	B	595	ASP	3.0
1	D	637	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	59	PHE	3.0
1	A	545	PRO	3.0
1	D	473	ALA	3.0
1	A	76	SER	3.0
1	B	442	GLY	3.0
1	D	682	LYS	3.0
1	A	72	GLY	3.0
1	A	73	GLY	3.0
1	A	692	ASP	3.0
1	C	684	ALA	2.9
1	A	434	TYR	2.9
1	A	539	GLU	2.9
1	B	641	MET	2.9
1	A	475	PHE	2.9
1	A	70	LYS	2.9
1	A	557	SER	2.9
1	B	637	GLY	2.9
1	A	91	PHE	2.9
1	C	83	ILE	2.9
1	A	538	LEU	2.9
1	C	542	GLN	2.9
1	A	709	GLU	2.9
1	A	68	SER	2.8
1	A	668	GLY	2.8
1	C	579	GLY	2.8
1	A	82	PHE	2.8
1	A	131	ASP	2.8
1	C	545	PRO	2.8
1	A	54	PHE	2.8
1	B	638	LYS	2.8
1	A	63	ILE	2.8
1	A	93	HIS	2.8
1	A	525	SER	2.8
1	A	66	GLN	2.8
1	C	681	GLU	2.8
1	D	670	ALA	2.8
1	A	338	PHE	2.8
1	B	257	ASP	2.8
1	A	626	VAL	2.8
1	A	257	ASP	2.7
1	D	648	GLY	2.7
1	B	693	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	679	VAL	2.7
1	D	411	VAL	2.7
1	A	392	THR	2.7
1	A	665	ALA	2.7
1	B	631	ALA	2.7
1	C	544	ASP	2.7
1	A	562	SER	2.7
1	D	608	SER	2.7
1	A	85	ARG	2.7
1	A	439	LEU	2.7
1	C	607	ALA	2.7
1	D	587	ALA	2.7
1	A	443	TYR	2.7
1	A	92	ASP	2.7
1	C	561	GLU	2.7
1	A	685	GLY	2.7
1	A	641	MET	2.6
1	A	80	GLU	2.6
1	A	561	GLU	2.6
1	C	398	ARG	2.6
1	C	580	GLY	2.6
1	A	322	ALA	2.6
1	A	62	ASN	2.6
1	A	340	PRO	2.6
1	A	146	SER	2.6
1	A	674	LEU	2.6
1	B	561	GLU	2.6
1	D	554	ARG	2.6
1	C	690	ALA	2.6
1	B	651	SER	2.6
1	A	418	HIS	2.6
1	D	675	GLN	2.5
1	A	57	THR	2.5
1	A	428	HIS	2.5
1	C	713	VAL	2.5
1	A	590	GLU	2.5
1	A	550	ASN	2.5
1	A	595	ASP	2.5
1	A	696	LYS	2.5
1	B	545	PRO	2.5
1	D	596	GLY	2.5
1	A	77	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	664	VAL	2.5
1	D	666	ALA	2.5
1	A	636	SER	2.5
1	B	681	GLU	2.5
1	A	440	ASN	2.5
1	A	71	ALA	2.5
1	D	445	ALA	2.5
1	A	442	GLY	2.5
1	B	639	GLY	2.5
1	D	634	VAL	2.4
1	C	88	LEU	2.4
1	B	691	GLN	2.4
1	A	684	ALA	2.4
1	B	587	ALA	2.4
1	C	637	GLY	2.4
1	D	633	ARG	2.4
1	A	318	ASP	2.4
1	A	401	ASN	2.4
1	A	607	ALA	2.4
1	C	447	ALA	2.4
1	A	435	SER	2.4
1	B	471	LEU	2.4
1	C	69	LEU	2.4
1	A	89	GLN	2.4
1	A	688	ALA	2.4
1	B	452	GLY	2.4
1	C	56	THR	2.4
1	C	582	LEU	2.4
1	A	74	ARG	2.4
1	A	419	ARG	2.4
1	C	45	GLU	2.4
1	D	541	PRO	2.3
1	A	52	GLY	2.3
1	C	473	ALA	2.3
1	A	667	VAL	2.3
1	A	424	GLN	2.3
1	C	471	LEU	2.3
1	D	683	GLU	2.3
1	A	81	ASP	2.3
1	A	367	PRO	2.3
1	A	689	GLY	2.3
1	C	73	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	557	SER	2.3
1	A	433	HIS	2.3
1	A	635	PHE	2.3
1	B	256	GLU	2.3
1	A	304	ASN	2.3
1	C	697	GLY	2.3
1	A	39	ALA	2.3
1	A	230	ALA	2.3
1	A	320	ALA	2.3
1	B	453	ARG	2.3
1	D	256	GLU	2.3
1	B	79	LEU	2.3
1	C	489	LEU	2.3
1	A	587	ALA	2.3
1	B	484	LEU	2.2
1	C	467	LEU	2.2
1	A	410	PRO	2.2
1	B	398	ARG	2.2
1	A	690	ALA	2.2
1	C	129	ALA	2.2
1	A	86	GLN	2.2
1	B	557	SER	2.2
1	C	608	SER	2.2
1	A	343	VAL	2.2
1	D	451	VAL	2.2
1	A	420	ASP	2.2
1	A	544	ASP	2.2
1	C	696	LYS	2.2
1	B	568	THR	2.2
1	A	427	ILE	2.2
1	B	431	ILE	2.2
1	A	534	VAL	2.2
1	B	668	GLY	2.2
1	B	590	GLU	2.2
1	A	682	LYS	2.2
1	B	603	ALA	2.2
1	A	676	SER	2.2
1	C	581	SER	2.2
1	C	676	SER	2.2
1	D	327	LEU	2.2
1	D	558	ILE	2.2
1	A	583	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	411	VAL	2.2
1	C	82	PHE	2.2
1	B	640	ALA	2.2
1	C	636	SER	2.2
1	D	285	ALA	2.2
1	A	438	TYR	2.1
1	A	570	ARG	2.1
1	B	83	ILE	2.1
1	B	569	LEU	2.1
1	A	697	GLY	2.1
1	D	577	THR	2.1
1	A	55	MET	2.1
1	A	638	LYS	2.1
1	A	202	GLU	2.1
1	A	681	GLU	2.1
1	A	203	VAL	2.1
1	B	633	ARG	2.1
1	A	642	SER	2.1
1	D	582	LEU	2.1
1	A	417	ASN	2.1
1	A	547	TYR	2.1
1	C	476	ASP	2.1
1	A	414	VAL	2.1
1	B	556	VAL	2.1
1	D	559	PHE	2.1
1	A	609	GLY	2.1
1	C	77	THR	2.1
1	A	511	GLU	2.1
1	A	524	ILE	2.1
1	B	117	ASP	2.1
1	A	593	GLU	2.0
1	B	39	ALA	2.0
1	C	445	ALA	2.0
1	A	430	ASN	2.0
1	A	476	ASP	2.0
1	A	708	LEU	2.0
1	C	166	ASP	2.0
1	A	658	TYR	2.0
1	A	698	VAL	2.0
1	B	626	VAL	2.0
1	D	679	VAL	2.0
1	D	553	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	557	SER	2.0
1	B	591	GLN	2.0
1	C	90	HIS	2.0
1	D	691	GLN	2.0
1	A	398	ARG	2.0
1	A	407	ILE	2.0
1	B	177	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

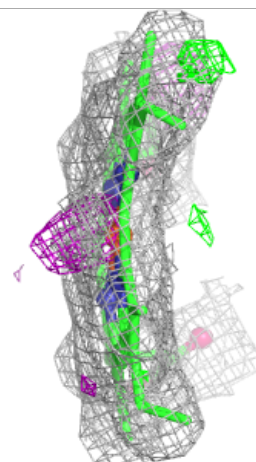
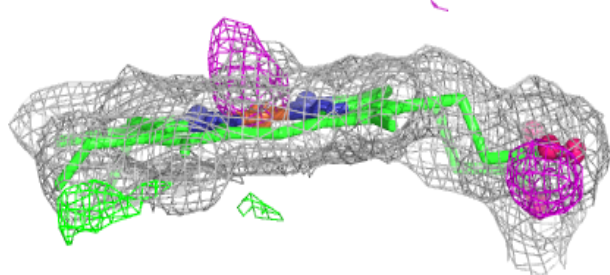
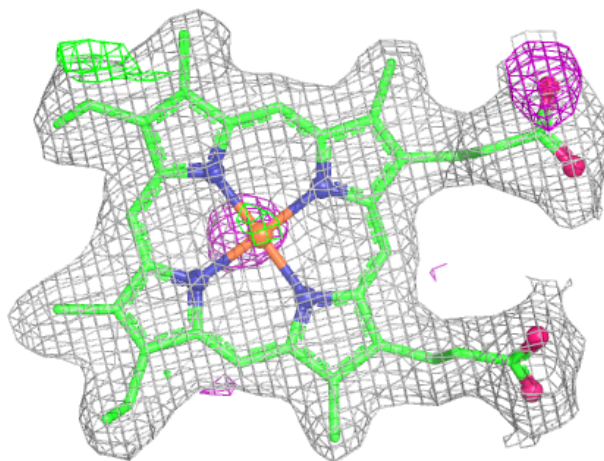
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	5007	14/15	0.39	0.21	24,24,24,24	0
2	NAG	A	5002	14/15	0.59	0.16	23,24,24,24	0
2	NAG	C	5009	14/15	0.62	0.16	24,24,24,24	0
2	NAG	D	5014	14/15	0.62	0.17	23,23,23,23	0
2	NAG	D	5013	14/15	0.65	0.15	24,24,25,25	0
2	NAG	C	5008	14/15	0.67	0.15	23,23,23,23	0
2	NAG	B	5005	14/15	0.68	0.14	23,24,24,24	0
2	NAG	B	5006	14/15	0.71	0.21	23,23,23,23	0
3	HEM	A	4000	43/43	0.92	0.11	22,22,22,22	0
3	HEM	D	4003	43/43	0.92	0.12	22,22,22,22	0
3	HEM	C	4002	43/43	0.93	0.12	22,22,23,23	0
3	HEM	B	4001	43/43	0.94	0.10	22,22,22,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

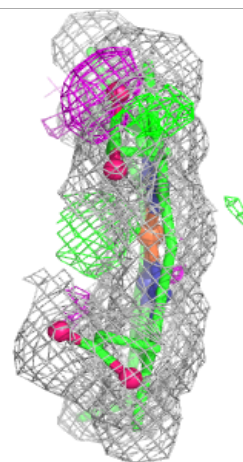
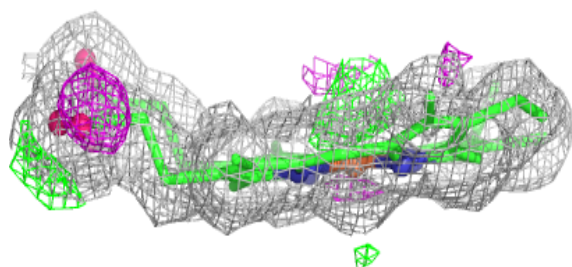
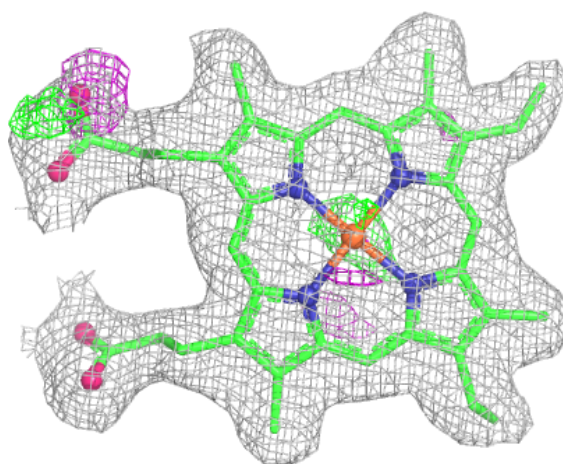
Electron density around HEM A 4000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



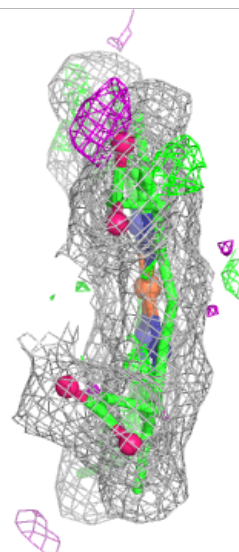
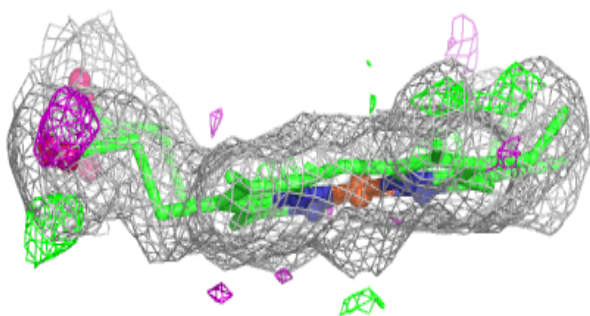
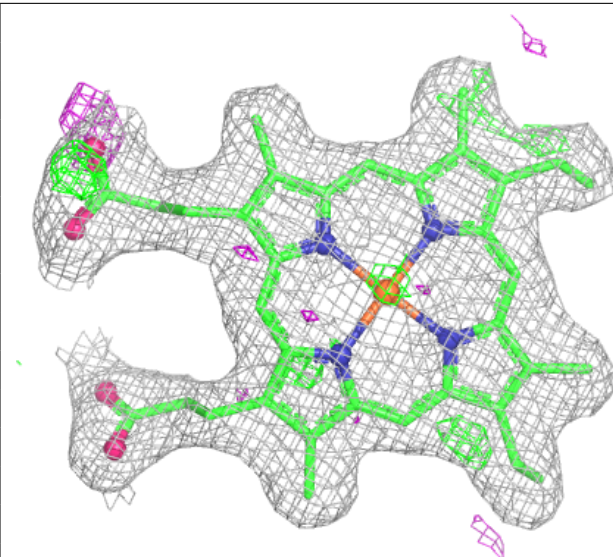
Electron density around HEM D 4003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



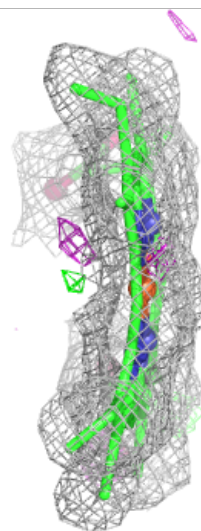
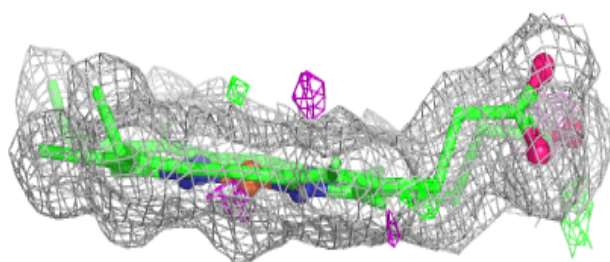
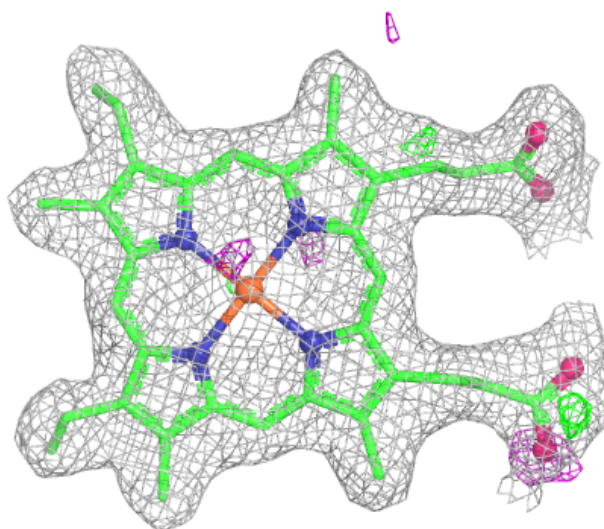
Electron density around HEM C 4002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 4001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.