



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:03 PM UTC

PDB ID : 3HCN / pdb_00003hcn
Title : Hg and protoporphyrin bound Human Ferrochelatase
Authors : Medlock, A.E.; Dailey, H.A.; Lanzilotta, W.N.
Deposited on : 2009-05-06
Resolution : 1.60 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

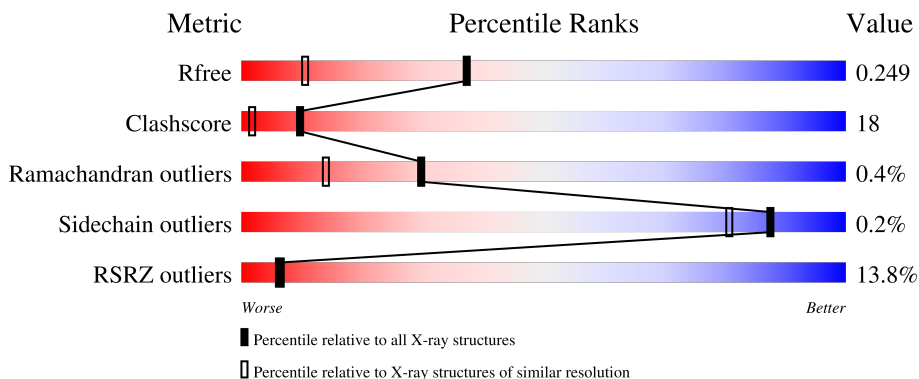
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	359	14% 67% 32% .
1	B	359	14% 69% 30%

2 Entry composition [i](#)

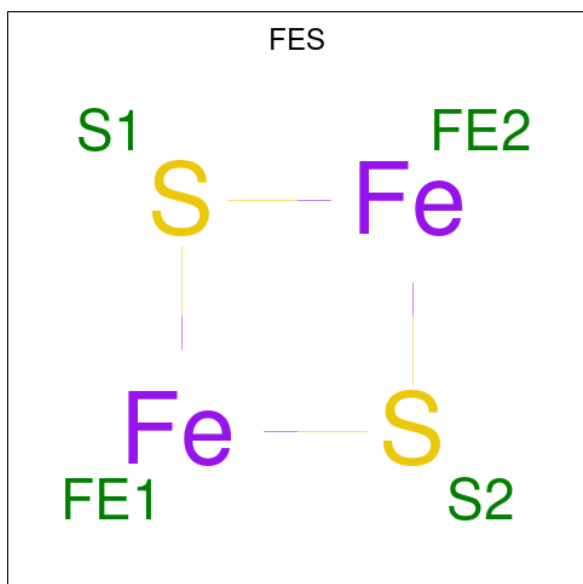
There are 9 unique types of molecules in this entry. The entry contains 7132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ferrochelatase, mitochondrial.

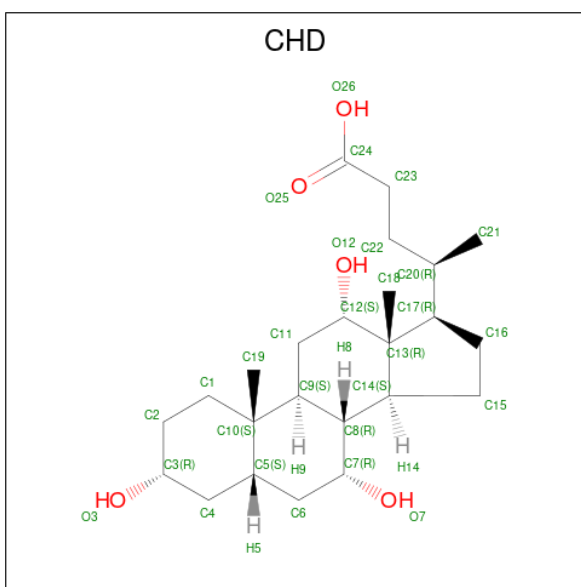
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	24	0
			3089	1955	543	570	21			
1	B	359	Total	C	N	O	S	0	12	0
			2994	1901	523	550	20			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



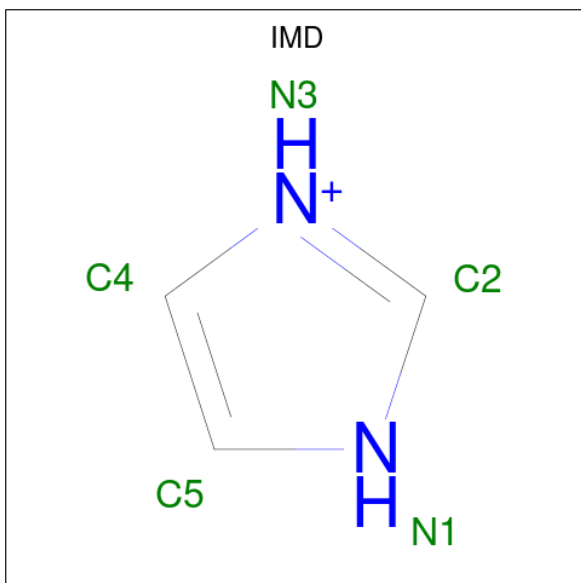
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is CHOLIC ACID (CCD ID: CHD) (formula: $\text{C}_{24}\text{H}_{40}\text{O}_5$).



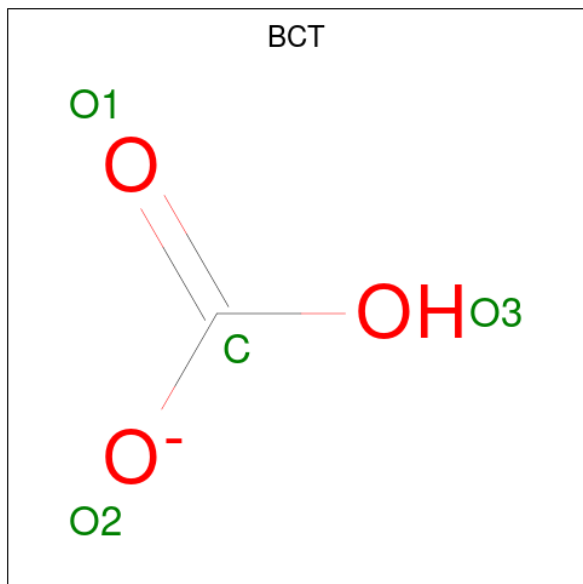
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			29	24	5		
3	A	1	Total	C	O	0	0
			29	24	5		
3	B	1	Total	C	O	0	0
			29	24	5		
3	B	1	Total	C	O	0	0
			29	24	5		

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



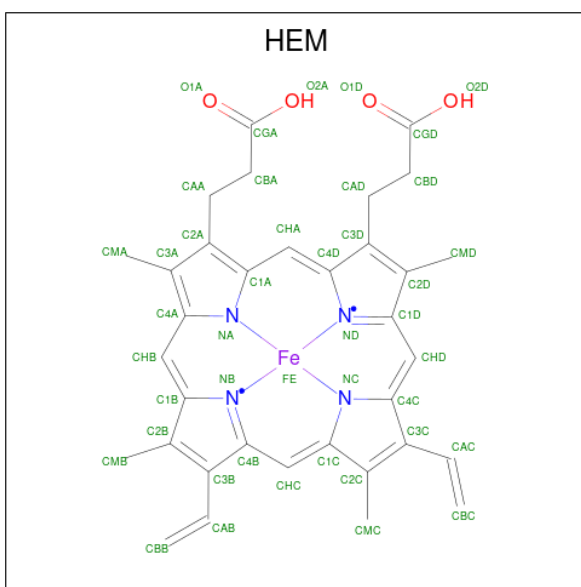
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



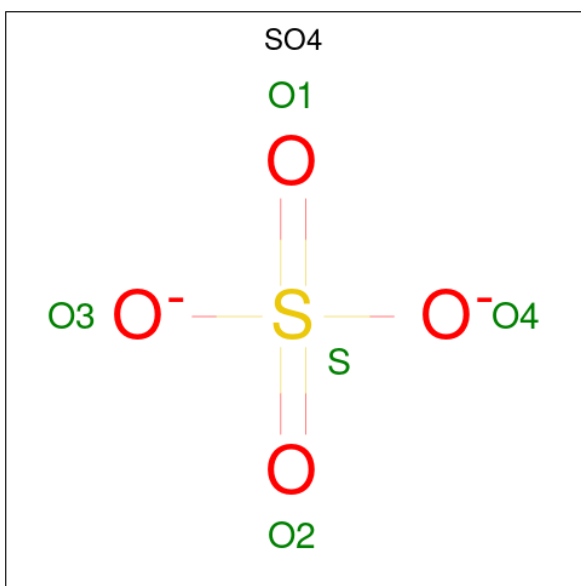
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



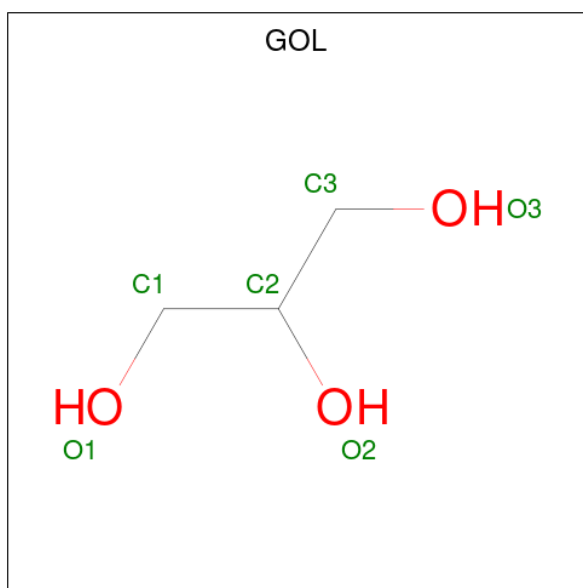
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 5	O 4	S 1	0	0
7	B	1	Total 5	O 4	S 1	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	1
			12	6	6		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	400	Total	O	0	0
			400	400		
9	B	398	Total	O	0	0
			398	398		

- Molecule 1: Ferrochelatase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.48Å 92.96Å 109.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.13 – 1.60 47.13 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.13-1.60) 98.0 (47.13-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 1.60Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.236 (Not available) , 0.249	Depositor DCC
R_{free} test set	11011 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtrriage
Anisotropy	0.647	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7132	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1232e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, HEM, SO4, GOL, BCT, CHD, FES

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	0.33	0/3161	0.81	3/4277 (0.1%)
1	B	0.33	0/3065	0.82	7/4147 (0.2%)
All	All	0.33	0/6226	0.82	10/8424 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	803	SER	N-CA-C	7.56	122.08	112.86
1	A	224	ILE	N-CA-C	-6.70	95.40	109.34
1	B	724	ILE	N-CA-C	-6.30	96.23	109.34
1	B	838	THR	N-CA-C	5.77	120.19	113.20
1	B	731	HIS	N-CA-C	5.76	118.30	111.33
1	B	774	ASP	CA-C-N	5.52	125.14	119.56
1	B	774	ASP	C-N-CA	5.52	125.14	119.56
1	A	338	THR	N-CA-C	5.48	119.83	113.20
1	B	802	GLN	N-CA-C	5.42	118.10	110.14
1	A	231	HIS	N-CA-C	5.09	117.49	111.33

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	3089	0	3073	128	0
1	B	2994	0	2991	105	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	58	0	78	3	0
3	B	58	0	78	5	0
4	A	5	0	4	1	0
4	B	10	0	8	1	0
5	A	4	0	0	0	0
6	A	43	0	30	2	0
6	B	43	0	30	1	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
8	B	12	0	16	4	0
9	A	400	0	0	16	0
9	B	398	0	0	7	0
All	All	7132	0	6308	225	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 18.

All (225) 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:A:304[B]:LYS:HE3	1:A:314:GLN:HE21	1.25	0.99
1:B:853:SER:C	1:B:854[B]:GLN:CA	2.44	0.90
1:A:297:TYR:H	1:B:898:GLN:HE22	1.14	0.89
1:A:398:GLN:HE22	1:B:797:TYR:H	1.20	0.89
1:A:323[B]:CYS:HB3	1:A:360[B]:CYS:SG	2.14	0.88
1:B:615:ARG:HD2	3:B:1:CHD:H231	1.59	0.84
1:A:101:LEU:HD21	3:A:3:CHD:H151	1.57	0.84
1:B:803:SER:O	4:B:925:IMD:H4	1.78	0.83
1:B:823[A]:CYS:HB3	1:B:860[A]:CYS:SG	2.19	0.82
1:B:609:PRO:O	1:B:613:LYS:HD3	1.79	0.80
1:A:178:GLU:HG2	1:A:219:MET:HE2	1.65	0.79
1:A:304[B]:LYS:HD2	1:A:304[B]:LYS:O	1.83	0.79
1:A:304[B]:LYS:CE	1:A:314:GLN:HE21	1.96	0.78
1:B:804:LYS:HE2	1:B:814[B]:GLN:NE2	1.98	0.77
1:A:220:LYS:HE3	1:A:423:LEU:HD22	1.67	0.77
1:A:235:GLN:HG3	1:A:290:ARG:HH12	1.50	0.76
1:A:87:ASP:HB3	1:A:91[A]:ARG:HH12	1.51	0.75
1:B:828:LYS:HB3	1:B:863:GLU:HG3	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:PRO:HB2	8:B:924[B]:GOL:H12	1.70	0.74
1:A:314:GLN:HB3	1:A:317[B]:GLU:HG2	1.70	0.74
1:A:122:GLN:HG3	9:A:706:HOH:O	1.87	0.73
1:B:635:TRP:O	1:B:639[A]:GLN:HG3	1.89	0.73
1:B:823[B]:CYS:SG	1:B:862:VAL:HG22	2.29	0.73
1:B:786[B]:LYS:HD3	9:B:361:HOH:O	1.89	0.72
1:B:634:ILE:O	1:B:638:LYS:HG2	1.89	0.72
1:B:608:ALA:HB3	1:B:609:PRO:HD3	1.71	0.72
1:A:101:LEU:HB2	1:A:104:GLN:HG3	1.71	0.71
1:B:601:LEU:HD21	3:B:1:CHD:H151	1.70	0.71
1:A:135:TRP:O	1:A:139[A]:GLN:HG3	1.91	0.70
1:A:323[A]:CYS:SG	1:A:360[A]:CYS:HB2	2.31	0.70
1:A:328:LYS:HB3	1:A:363:GLU:HG3	1.74	0.69
1:A:285:GLN:O	1:A:289[A]:GLU:HG3	1.91	0.69
1:A:303[A]:SER:O	1:A:304[A]:LYS:HG2	1.95	0.67
1:B:634:ILE:HG12	9:B:363:HOH:O	1.94	0.67
1:A:391:SER:OG	1:A:393[A]:GLU:HG2	1.94	0.67
1:A:290:ARG:HG2	1:A:290:ARG:HH11	1.60	0.66
1:A:220:LYS:HD2	1:A:423:LEU:HD13	1.76	0.66
1:A:304[B]:LYS:HE3	1:A:314:GLN:NE2	2.06	0.66
1:B:734:ILE:HG13	1:B:786[B]:LYS:HG2	1.78	0.66
1:B:637:SER:O	1:B:641:GLU:HG3	1.96	0.65
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.79	0.65
1:B:790:ARG:HG2	1:B:790:ARG:HH11	1.62	0.65
1:A:134:ILE:HG13	9:A:525:HOH:O	1.96	0.65
1:B:735:GLN:HG3	1:B:790:ARG:HH12	1.63	0.64
1:A:297:TYR:N	1:B:898:GLN:HE22	1.93	0.64
1:B:804:LYS:HE2	1:B:814[B]:GLN:HE22	1.61	0.63
1:A:304[A]:LYS:HD3	1:A:316:ASP:OD2	1.99	0.62
1:B:874:ASN:HD22	1:B:875:PRO:N	1.97	0.62
1:A:134:ILE:O	1:A:138:LYS:HG2	2.00	0.62
1:B:785:GLN:O	1:B:789:GLU:HG3	2.00	0.62
1:A:87:ASP:HB3	1:A:91[A]:ARG:NH1	2.15	0.61
1:B:874:ASN:HD22	1:B:874:ASN:C	2.06	0.61
1:B:823[B]:CYS:SG	1:B:860[B]:CYS:HB2	2.40	0.60
1:B:841:HIS:HB2	6:B:926:HEM:O1D	2.01	0.60
1:B:566[A]:LYS:CG	1:B:567:PRO:HD2	2.32	0.60
1:A:235:GLN:HA	1:A:290:ARG:NH1	2.17	0.60
1:A:306[A]:GLY:HA3	9:A:447:HOH:O	2.01	0.59
1:A:304[B]:LYS:HD2	1:A:304[B]:LYS:C	2.27	0.59
1:B:734:ILE:HG21	1:B:786[B]:LYS:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:VAL:HG12	1:A:313:PRO:HG2	1.85	0.59
1:A:308[A]:MET:SD	9:A:447:HOH:O	2.56	0.58
1:B:616:THR:O	1:B:620:GLN:HG3	2.03	0.58
1:A:235:GLN:HA	1:A:290:ARG:HH12	1.67	0.58
1:A:243:LYS:HZ3	1:A:369[B]:GLU:CD	2.11	0.58
1:A:302[B]:GLN:HB3	1:A:315:THR:OG1	2.03	0.58
1:B:566[A]:LYS:HG3	1:B:567:PRO:HD2	1.86	0.58
1:B:603:ILE:HG13	1:B:607:LEU:HG	1.86	0.57
1:A:308[A]:MET:HE3	3:A:3:CHD:H22	1.86	0.57
1:A:351:GLU:O	1:A:355:VAL:HG23	2.05	0.57
1:B:735:GLN:HA	1:B:790:ARG:NH1	2.19	0.56
1:A:306[B]:GLY:HA3	9:A:447:HOH:O	2.06	0.56
1:A:317[A]:GLU:HG2	1:B:905:LEU:HD11	1.87	0.56
1:A:339:SER:HB3	9:A:638:HOH:O	2.04	0.56
1:A:398:GLN:HE22	1:B:797:TYR:N	1.96	0.56
1:A:422:GLN:O	1:A:423:LEU:HB2	2.05	0.56
1:B:922:GLN:O	1:B:923:LEU:HB2	2.06	0.56
1:A:374:ASN:C	1:A:374:ASN:HD22	2.13	0.55
1:B:850:ILE:O	1:B:854[A]:GLN:HG2	2.06	0.55
1:A:308[A]:MET:SD	1:A:310:TRP:NE1	2.79	0.55
1:A:137:SER:O	1:A:141:GLU:HG3	2.07	0.55
1:B:874:ASN:ND2	1:B:876:LEU:H	2.05	0.54
1:A:302[B]:GLN:HB2	9:A:641:HOH:O	2.06	0.54
1:A:422:GLN:HG2	1:A:423:LEU:HD12	1.90	0.54
1:B:769:VAL:O	1:B:772:ARG:HG2	2.07	0.54
1:A:303[A]:SER:H	1:A:304[A]:LYS:HE3	1.72	0.54
1:B:856:LEU:HG	1:B:862:VAL:CG2	2.37	0.54
1:A:115:ARG:NE	6:A:424:HEM:O1A	2.41	0.54
1:A:235:GLN:HG3	1:A:290:ARG:NH1	2.22	0.54
1:A:250:LEU:O	1:A:250:LEU:HD23	2.08	0.53
1:B:720:LYS:HD3	1:B:923:LEU:HD22	1.89	0.53
1:A:357:ALA:O	1:A:361:GLY:HA2	2.09	0.53
1:B:587:ASP:HB3	1:B:591:ARG:HH12	1.74	0.53
1:A:341:HIS:HB2	6:A:424:HEM:O1D	2.09	0.53
1:B:820:LYS:HE2	1:B:824:GLU:OE2	2.09	0.53
1:A:225:ASP:HA	9:A:733:HOH:O	2.09	0.52
1:B:854[B]:GLN:O	1:B:858:LYS:HG2	2.09	0.52
1:A:374:ASN:HD22	1:A:375:PRO:CD	2.23	0.52
1:A:69:THR:HG23	1:A:184:ARG:HD2	1.90	0.52
1:B:678:GLU:HG2	1:B:719:MET:HE2	1.92	0.52
1:B:854[A]:GLN:O	1:B:858:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ALA:O	1:A:177:MET:HG3	2.11	0.51
1:B:601:LEU:HB2	1:B:604:GLN:HG3	1.92	0.51
1:B:800:VAL:HG12	1:B:813:PRO:HG2	1.93	0.51
1:A:357:ALA:HA	1:A:362:VAL:HG12	1.91	0.51
1:A:374:ASN:HD22	1:A:375:PRO:N	2.09	0.51
1:B:565:ARG:HG3	1:B:565:ARG:HH11	1.76	0.51
1:B:777:PRO:HB3	8:B:924[A]:GOL:H2	1.93	0.51
1:B:750:LEU:HA	1:B:753[A]:ARG:NH1	2.26	0.50
1:B:710:TYR:HA	1:B:713:VAL:HG12	1.93	0.50
1:A:235:GLN:CG	1:A:290:ARG:HH12	2.21	0.50
1:A:102:PRO:O	1:A:103:ILE:C	2.54	0.50
3:B:1:CHD:H161	3:B:2:CHD:H151	1.94	0.50
1:B:734:ILE:HG13	1:B:786[B]:LYS:CG	2.42	0.50
1:B:684:ARG:NH2	9:B:403:HOH:O	2.44	0.50
1:A:286:LYS:HE2	1:B:786[A]:LYS:NZ	2.27	0.49
1:A:235:GLN:HG3	1:A:290:ARG:HH22	1.77	0.49
1:B:776:TYR:HB3	1:B:777:PRO:HD3	1.94	0.49
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.95	0.49
1:A:250:LEU:HD23	1:A:250:LEU:C	2.38	0.49
9:A:436:HOH:O	1:B:786[A]:LYS:HE2	2.11	0.49
1:A:264:SER:HB3	1:A:303[A]:SER:HB3	1.94	0.49
1:B:673:ALA:O	1:B:677:MET:HG3	2.11	0.49
1:A:303[A]:SER:N	1:A:304[A]:LYS:HE3	2.27	0.49
1:A:277:PRO:CB	8:B:924[B]:GOL:H12	2.40	0.49
1:B:614:ARG:NH1	3:B:2:CHD:H42	2.28	0.49
1:B:720:LYS:HZ3	1:B:923:LEU:CD1	2.25	0.49
1:A:314:GLN:OE1	1:A:316:ASP:HB2	2.13	0.49
1:B:777:PRO:HB3	8:B:924[B]:GOL:H2	1.94	0.49
1:A:269:VAL:O	1:A:272:ARG:HG2	2.12	0.49
1:A:304[A]:LYS:HA	9:A:633:HOH:O	2.13	0.49
1:A:374:ASN:ND2	1:A:376:LEU:H	2.11	0.49
1:A:243:LYS:NZ	1:A:369[B]:GLU:CD	2.70	0.49
1:A:354[B]:GLN:CG	1:A:358:LYS:HE2	2.42	0.49
1:A:194:TYR:CD1	1:A:199[B]:THR:HG21	2.48	0.48
1:A:314:GLN:HB3	1:A:317[B]:GLU:CG	2.41	0.48
1:A:350:ILE:O	1:A:354[A]:GLN:HG3	2.13	0.48
1:B:602:PRO:O	1:B:603:ILE:C	2.55	0.48
1:A:290:ARG:HG2	1:A:290:ARG:NH1	2.26	0.48
1:A:65:ARG:HG3	1:A:65:ARG:HH11	1.78	0.48
1:A:251[B]:GLU:HG2	1:A:252:LYS:HG2	1.96	0.48
1:B:858:LYS:HD3	9:B:1027:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:HD3	1:A:279:GLU:OE2	2.13	0.47
1:A:323[A]:CYS:SG	1:A:362:VAL:HB	2.54	0.47
1:A:139[B]:GLN:HE21	1:A:373:GLY:HA2	1.78	0.47
1:A:263:HIS:HA	1:A:302[A]:GLN:HG2	1.97	0.47
1:A:304[B]:LYS:CE	1:A:314:GLN:NE2	2.73	0.47
1:B:614:ARG:HH12	3:B:2:CHD:H42	1.80	0.47
1:B:713:VAL:HG13	1:B:715:ARG:H	1.80	0.47
1:B:740:HIS:HA	1:B:743[A]:LYS:HG2	1.96	0.47
1:B:817[A]:GLU:OE2	1:B:817[A]:GLU:N	2.47	0.47
1:B:857:ALA:O	1:B:861:GLY:HA2	2.14	0.47
1:A:304[B]:LYS:HG2	9:A:602:HOH:O	2.15	0.47
1:A:345:LEU:HD11	1:A:352:TYR:CD2	2.50	0.47
1:B:571:ILE:N	1:B:571:ILE:HD12	2.30	0.47
1:A:303[A]:SER:C	1:A:304[A]:LYS:HG2	2.39	0.47
1:A:400:THR:HA	1:A:415[B]:LYS:HE2	1.97	0.46
1:A:369[B]:GLU:HG2	9:A:462:HOH:O	2.15	0.46
1:B:874:ASN:C	1:B:874:ASN:ND2	2.73	0.46
1:B:814[A]:GLN:HE21	1:B:816:ASP:HB2	1.80	0.46
1:B:726:ARG:HD3	1:B:779:GLU:OE2	2.14	0.46
1:A:350:ILE:HG12	9:A:430:HOH:O	2.15	0.46
1:B:790:ARG:HG2	1:B:790:ARG:NH1	2.30	0.46
1:B:720:LYS:HZ3	1:B:923:LEU:HD11	1.81	0.46
1:B:874:ASN:HD22	1:B:875:PRO:CD	2.28	0.46
1:A:422:GLN:HG2	1:A:423:LEU:CD1	2.46	0.45
1:B:751:GLU:H	1:B:751:GLU:CD	2.23	0.45
1:B:851:GLU:O	1:B:855:VAL:HG23	2.16	0.45
1:A:116:THR:O	1:A:120:GLN:HG3	2.16	0.45
1:B:849:ASP:OD1	1:B:851:GLU:HB3	2.16	0.45
1:A:374:ASN:HD22	1:A:375:PRO:HD2	1.80	0.45
1:B:900:THR:HA	1:B:915:LYS:HD2	1.98	0.45
1:A:76:MET:HB3	1:A:191:TYR:OH	2.17	0.45
1:B:616:THR:HB	1:B:617:PRO:HD3	1.98	0.45
1:B:740:HIS:CE1	1:B:869[B]:GLU:HG3	2.52	0.45
1:A:308[A]:MET:SD	1:A:310:TRP:CD1	3.10	0.45
1:A:394:LEU:HD21	1:A:423:LEU:OXT	2.16	0.45
1:A:415[B]:LYS:CE	1:A:419:THR:HG21	2.47	0.45
1:B:570:GLY:HA3	1:B:682:LEU:HD13	1.99	0.45
1:B:735:GLN:HA	1:B:790:ARG:HH12	1.80	0.45
1:B:823[A]:CYS:CB	1:B:860[A]:CYS:SG	3.01	0.44
1:A:415[B]:LYS:HD3	1:A:415[B]:LYS:C	2.42	0.44
1:A:286:LYS:NZ	1:B:789:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415[B]:LYS:NZ	1:A:419:THR:HG21	2.32	0.44
1:B:639[A]:GLN:NE2	9:B:1011:HOH:O	2.49	0.44
1:A:194:TYR:CD1	1:A:199[B]:THR:CG2	3.01	0.44
1:A:316:ASP:OD1	1:A:344:THR:HB	2.18	0.44
1:B:720:LYS:CD	1:B:923:LEU:HD22	2.47	0.44
1:B:891:SER:O	1:B:892:ASN:HB2	2.18	0.44
1:B:587:ASP:HB2	9:B:992:HOH:O	2.18	0.43
1:B:740:HIS:ND1	1:B:869[B]:GLU:HG3	2.34	0.43
1:A:99:MET:HB2	3:A:3:CHD:H62	2.00	0.43
1:B:645:LYS:O	1:B:649[A]:GLU:OE1	2.36	0.43
1:A:304[A]:LYS:HD2	9:A:641:HOH:O	2.18	0.43
1:A:400:THR:HA	1:A:415[B]:LYS:CE	2.48	0.43
1:A:71:ILE:N	1:A:71:ILE:HD12	2.34	0.42
1:A:417:PHE:O	1:A:421:GLN:HG2	2.20	0.42
1:A:274:ASP:HA	1:A:275:PRO:HD3	1.81	0.42
1:A:285:GLN:HG2	1:B:782:ALA:HB1	2.01	0.42
1:A:215:ARG:HG2	1:A:215:ARG:HH11	1.84	0.42
1:B:814[B]:GLN:HB2	1:B:817[B]:GLU:HG2	2.02	0.42
1:A:193:GLN:HG2	1:A:280:VAL:HA	2.02	0.42
1:A:303[A]:SER:O	1:A:305[A]:VAL:HG13	2.20	0.41
1:B:566[A]:LYS:HE2	1:B:680:ASP:O	2.20	0.41
1:B:615:ARG:HG2	1:B:615:ARG:HH11	1.84	0.41
1:A:371:LEU:O	1:A:372:ASN:C	2.63	0.41
1:B:721:TRP:H	1:B:921:GLN:NE2	2.18	0.41
1:A:289[A]:GLU:HG2	9:A:713:HOH:O	2.19	0.41
1:A:320:LYS:HE3	1:A:324:GLU:OE2	2.21	0.41
1:A:386:HIS:HD2	9:A:568:HOH:O	2.03	0.41
1:B:766:PRO:HG3	1:B:810:TRP:CZ2	2.55	0.41
1:A:194:TYR:HA	1:A:199[B]:THR:HG21	2.02	0.41
1:A:354[B]:GLN:HG3	1:A:358:LYS:HE2	2.02	0.41
1:A:66:LYS:HG3	1:A:67:PRO:HD2	2.02	0.41
1:A:232:LEU:HD12	1:A:380:ALA:HA	2.02	0.41
1:A:240:HIS:ND1	1:A:369[B]:GLU:HG3	2.35	0.41
1:A:76:MET:HG3	1:A:77:GLY:O	2.20	0.41
1:B:803:SER:O	1:B:804:LYS:C	2.62	0.41
1:A:296:PRO:HA	1:B:898:GLN:NE2	2.36	0.41
1:B:639[B]:GLN:HE21	1:B:873:GLY:HA2	1.86	0.41
1:B:751:GLU:CD	1:B:751:GLU:N	2.78	0.41
1:B:591:ARG:NH1	9:B:993:HOH:O	2.54	0.40
1:B:773:GLY:HA3	1:B:904:PRO:HD2	2.04	0.40
1:A:303[B]:SER:CB	4:A:2:IMD:HN3	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:825:ARG:HG3	1:B:825:ARG:HH11	1.87	0.40
1:B:894:LEU:HD21	1:B:923:LEU:O	2.22	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	381/359 (106%)	372 (98%)	6 (2%)	3 (1%)	16	5
1	B	369/359 (103%)	362 (98%)	6 (2%)	1 (0%)	36	20
All	All	750/718 (104%)	734 (98%)	12 (2%)	4 (0%)	30	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	ASN
1	B	872	ASN
1	A	303[A]	SER
1	A	303[B]	SER

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 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/324 (107%)	346 (100%)	1 (0%)	86	78
1	B	336/324 (104%)	336 (100%)	0	100	100
All	All	683/648 (105%)	682 (100%)	1 (0%)	87	81

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	GLU

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	120	GLN
1	A	235	GLN
1	A	329	ASN
1	A	364	ASN
1	A	372	ASN
1	A	374	ASN
1	A	386	HIS
1	A	398	GLN
1	A	421	GLN
1	B	620	GLN
1	B	653	ASN
1	B	735	GLN
1	B	802	GLN
1	B	872	ASN
1	B	874	ASN
1	B	890	GLN
1	B	892	ASN
1	B	898	GLN
1	B	921	GLN

5.3.3 RNA ⓘ

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](#)

16 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$
7	SO4	B	927	-	4,4,4	0.39	0	6,6,6	0.07	0
6	HEM	B	926	4	50,50,50	1.75	11 (22%)	67,82,82	1.47	10 (14%)
4	IMD	B	925	6	5,5,5	0.43	0	5,5,5	0.36	0
6	HEM	A	424	5,4	50,50,50	1.94	16 (32%)	67,82,82	1.46	12 (17%)
2	FES	B	502	1	0,4,4	-	-	-	-	-
5	BCT	A	1	6	3,3,3	0.47	0	2,3,3	0.11	0
3	CHD	A	4	-	32,32,32	1.56	8 (25%)	51,51,51	1.45	8 (15%)
8	GOL	B	924[B]	-	5,5,5	0.27	0	5,5,5	0.32	0
3	CHD	A	3	-	32,32,32	1.53	9 (28%)	51,51,51	1.38	7 (13%)
2	FES	A	501	1	0,4,4	-	-	-	-	-
3	CHD	B	1	-	32,32,32	1.49	8 (25%)	51,51,51	1.36	7 (13%)
7	SO4	A	425	-	4,4,4	0.38	0	6,6,6	0.07	0
4	IMD	B	3	6	5,5,5	0.29	0	5,5,5	0.34	0
8	GOL	B	924[A]	-	5,5,5	0.27	0	5,5,5	0.33	0
4	IMD	A	2	6	5,5,5	0.37	0	5,5,5	0.49	0
3	CHD	B	2	-	32,32,32	1.55	7 (21%)	51,51,51	1.44	8 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	B	926	4	-	8/14/54/54	-
6	HEM	A	424	5,4	-	7/14/54/54	-
4	IMD	B	925	6	-	-	0/1/1/1
2	FES	B	502	1	-	-	0/1/1/1
3	CHD	A	4	-	-	0/9/74/74	0/4/4/4
8	GOL	B	924[B]	-	-	0/4/4/4	-
3	CHD	A	3	-	-	0/9/74/74	0/4/4/4
2	FES	A	501	1	-	-	0/1/1/1
3	CHD	B	1	-	-	0/9/74/74	0/4/4/4
4	IMD	B	3	6	-	-	0/1/1/1
8	GOL	B	924[A]	-	-	0/4/4/4	-
4	IMD	A	2	6	-	-	0/1/1/1
3	CHD	B	2	-	-	0/9/74/74	0/4/4/4

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	424	HEM	C3B-C2B	4.31	1.45	1.37
6	A	424	HEM	C1B-NB	-3.98	1.33	1.40
6	A	424	HEM	CAC-C3C	-3.92	1.36	1.47
6	B	926	HEM	C3B-C2B	3.89	1.45	1.37
6	B	926	HEM	CAC-C3C	-3.71	1.37	1.47
6	B	926	HEM	C1B-NB	-3.47	1.34	1.40
6	A	424	HEM	C3C-C4C	3.39	1.51	1.46
6	B	926	HEM	O2A-CGA	-3.36	1.19	1.30
6	B	926	HEM	C3C-C4C	3.35	1.51	1.46
6	B	926	HEM	CHB-C4A	-3.35	1.31	1.39
6	A	424	HEM	C4C-NC	-3.26	1.33	1.39
6	A	424	HEM	O2A-CGA	-3.23	1.20	1.30
6	A	424	HEM	FE-NB	3.03	2.04	1.94
6	A	424	HEM	FE-NA	3.01	2.05	1.95
6	A	424	HEM	FE-ND	2.98	2.04	1.94
6	A	424	HEM	C1D-C2D	2.87	1.50	1.44
6	B	926	HEM	C1D-C2D	2.85	1.50	1.44
6	A	424	HEM	FE-NC	2.84	2.04	1.95
3	A	4	CHD	C18-C13	2.81	1.58	1.54
6	A	424	HEM	CHB-C4A	-2.75	1.33	1.39
3	B	2	CHD	C18-C13	2.72	1.58	1.54
3	B	1	CHD	C11-C9	2.70	1.58	1.53
3	A	3	CHD	C18-C13	2.66	1.58	1.54
3	B	1	CHD	C18-C13	2.65	1.58	1.54
3	B	2	CHD	C20-C17	2.64	1.58	1.54
6	B	926	HEM	C4C-NC	-2.63	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4	CHD	C20-C17	2.57	1.58	1.54
3	A	3	CHD	C20-C17	2.51	1.58	1.54
3	A	3	CHD	C11-C9	2.49	1.57	1.53
3	A	4	CHD	C11-C9	2.38	1.57	1.53
6	B	926	HEM	C3C-C2C	2.33	1.41	1.37
6	A	424	HEM	C3C-C2C	2.29	1.41	1.37
3	B	2	CHD	C11-C9	2.28	1.57	1.53
6	A	424	HEM	C1D-ND	-2.28	1.34	1.38
3	B	2	CHD	C8-C9	2.27	1.58	1.53
3	A	3	CHD	C10-C9	2.26	1.60	1.56
3	A	4	CHD	C8-C9	2.25	1.58	1.53
3	B	2	CHD	C6-C5	2.25	1.57	1.53
3	B	1	CHD	C6-C5	2.24	1.57	1.53
6	B	926	HEM	CBD-CGD	-2.23	1.45	1.50
6	A	424	HEM	CBD-CGD	-2.20	1.45	1.50
3	A	4	CHD	C6-C5	2.18	1.57	1.53
3	A	3	CHD	C6-C5	2.16	1.57	1.53
3	B	1	CHD	C8-C9	2.15	1.58	1.53
3	A	4	CHD	C6-C7	2.12	1.56	1.52
3	A	3	CHD	C8-C9	2.11	1.57	1.53
3	B	2	CHD	C10-C9	2.11	1.59	1.56
3	B	1	CHD	C16-C17	2.08	1.58	1.54
3	B	2	CHD	C6-C7	2.08	1.56	1.52
3	B	1	CHD	C20-C17	2.07	1.57	1.54
6	B	926	HEM	CMA-C3A	2.06	1.55	1.50
3	B	1	CHD	C10-C9	2.06	1.59	1.56
3	B	1	CHD	C6-C7	2.06	1.56	1.52
3	A	4	CHD	C16-C17	2.05	1.58	1.54
3	A	3	CHD	C6-C7	2.04	1.56	1.52
6	A	424	HEM	CMA-C3A	2.03	1.54	1.50
3	A	3	CHD	C16-C17	2.03	1.58	1.54
3	A	3	CHD	C4-C3	2.02	1.55	1.52
3	A	4	CHD	C4-C3	2.01	1.55	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	926	HEM	C2B-C1B-NB	4.33	114.82	109.84
6	B	926	HEM	C4C-C3C-C2C	-4.10	103.26	106.81
3	B	1	CHD	C9-C11-C12	-4.08	108.95	114.29
6	A	424	HEM	C4C-C3C-C2C	-3.98	103.36	106.81
3	A	3	CHD	C9-C11-C12	-3.65	109.52	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	926	HEM	C3B-C4B-NB	3.65	112.09	109.47
3	A	4	CHD	C9-C11-C12	-3.42	109.83	114.29
6	A	424	HEM	C2B-C1B-NB	3.40	113.74	109.84
3	B	2	CHD	C9-C11-C12	-3.32	109.95	114.29
3	B	2	CHD	C17-C13-C12	2.93	120.30	117.67
6	A	424	HEM	C3B-C2B-C1B	-2.91	104.22	106.41
3	B	2	CHD	C13-C17-C20	-2.84	116.05	119.48
6	A	424	HEM	C3B-C4B-NB	2.83	111.50	109.47
3	B	1	CHD	C16-C15-C14	-2.83	99.61	105.14
6	A	424	HEM	C4D-ND-C1D	2.81	108.53	105.21
3	A	4	CHD	C17-C13-C12	2.80	120.19	117.67
3	A	4	CHD	C11-C9-C10	-2.80	110.86	113.70
3	A	4	CHD	C13-C17-C20	-2.80	116.09	119.48
3	B	2	CHD	C13-C14-C8	-2.78	111.20	114.72
6	B	926	HEM	C3B-C2B-C1B	-2.77	104.33	106.41
3	A	4	CHD	C13-C14-C8	-2.75	111.23	114.72
3	A	3	CHD	C17-C13-C12	2.74	120.13	117.67
3	B	2	CHD	C11-C9-C10	-2.70	110.96	113.70
6	B	926	HEM	CBC-CAC-C3C	2.62	140.61	127.53
6	A	424	HEM	CHC-C1C-NC	2.57	127.25	124.45
3	A	3	CHD	C16-C15-C14	-2.56	100.13	105.14
3	A	4	CHD	C16-C15-C14	-2.49	100.27	105.14
6	A	424	HEM	CBC-CAC-C3C	2.48	139.93	127.53
6	B	926	HEM	CHC-C1C-NC	2.48	127.16	124.45
3	B	2	CHD	C16-C15-C14	-2.45	100.36	105.14
6	B	926	HEM	C4B-C3B-C2B	-2.44	105.03	107.28
3	A	3	CHD	C11-C9-C10	-2.37	111.30	113.70
6	B	926	HEM	C1D-C2D-C3D	-2.34	104.52	106.98
6	A	424	HEM	C1D-C2D-C3D	-2.32	104.54	106.98
3	A	3	CHD	C13-C14-C8	-2.30	111.80	114.72
6	A	424	HEM	C4B-C3B-C2B	-2.30	105.17	107.28
6	A	424	HEM	C4A-C3A-C2A	2.26	109.41	106.82
3	A	4	CHD	C18-C13-C14	-2.26	107.66	111.20
3	A	4	CHD	C6-C5-C10	-2.25	110.27	112.66
3	B	2	CHD	C18-C13-C14	-2.24	107.69	111.20
3	B	1	CHD	C6-C5-C10	-2.23	110.29	112.66
6	A	424	HEM	CAA-C2A-C1A	2.22	129.28	124.94
3	B	1	CHD	C10-C9-C8	-2.21	109.37	111.84
6	A	424	HEM	CAA-CBA-CGA	2.19	119.48	113.67
3	B	1	CHD	C11-C9-C10	-2.18	111.49	113.70
3	A	3	CHD	C6-C5-C10	-2.17	110.35	112.66
6	B	926	HEM	C4A-C3A-C2A	2.16	109.29	106.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	CHD	C6-C5-C10	-2.14	110.38	112.66
3	B	1	CHD	C17-C13-C12	2.13	119.58	117.67
6	B	926	HEM	CAA-CBA-CGA	2.03	119.06	113.67
3	A	3	CHD	C10-C9-C8	-2.02	109.58	111.84
3	B	1	CHD	C18-C13-C14	-2.02	108.04	111.20

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	424	HEM	C2A-CAA-CBA-CGA
6	A	424	HEM	C2B-C3B-CAB-CBB
6	A	424	HEM	C2C-C3C-CAC-CBC
6	B	926	HEM	C2B-C3B-CAB-CBB
6	B	926	HEM	C2C-C3C-CAC-CBC
6	B	926	HEM	C4C-C3C-CAC-CBC
6	A	424	HEM	CAD-CBD-CGD-O1D
6	A	424	HEM	CAD-CBD-CGD-O2D
6	B	926	HEM	CAD-CBD-CGD-O2D
6	B	926	HEM	CAA-CBA-CGA-O2A
6	B	926	HEM	CAD-CBD-CGD-O1D
6	A	424	HEM	C4B-C3B-CAB-CBB
6	A	424	HEM	C4C-C3C-CAC-CBC
6	B	926	HEM	C4B-C3B-CAB-CBB
6	B	926	HEM	CAA-CBA-CGA-O1A

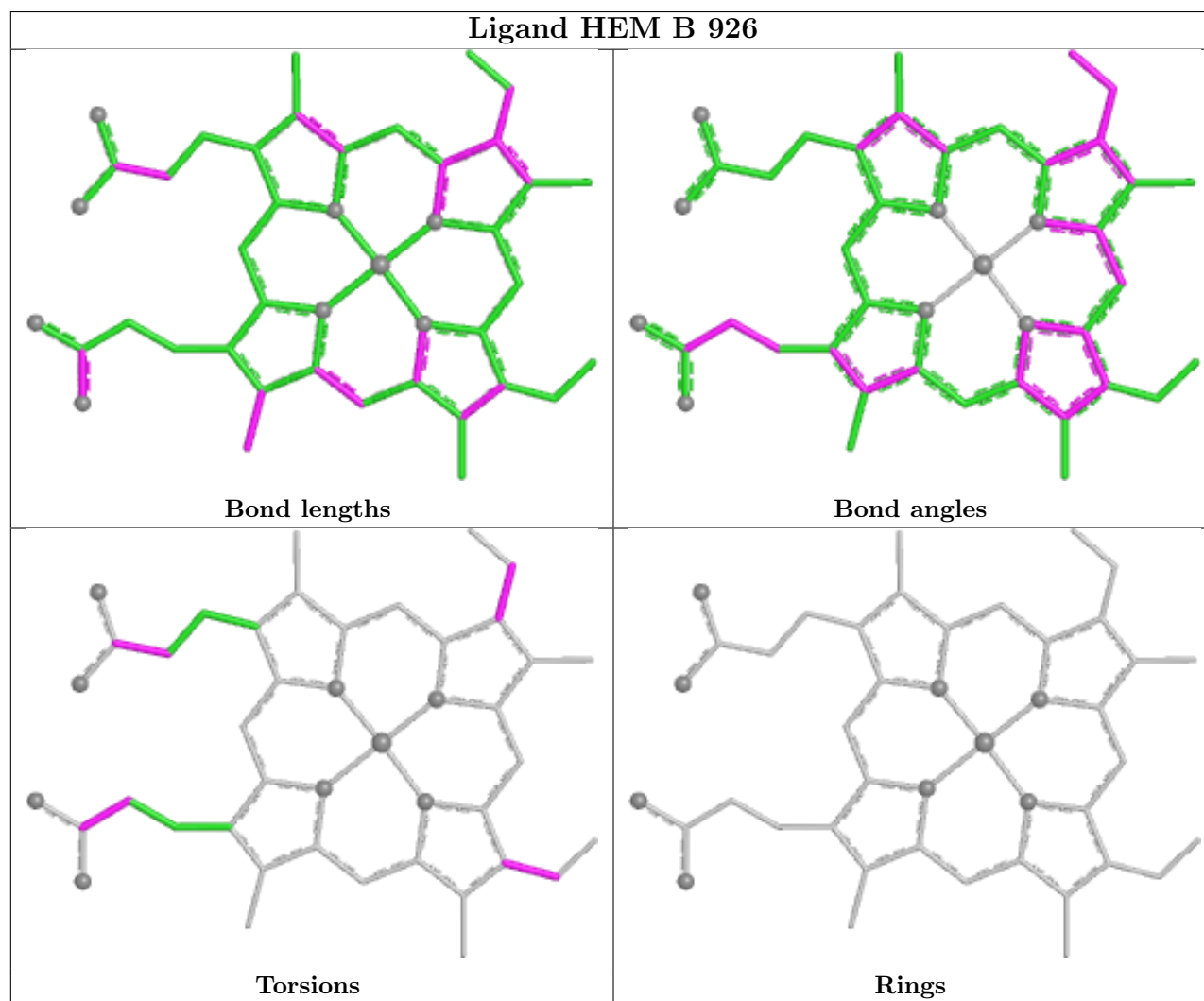
There are no ring outliers.

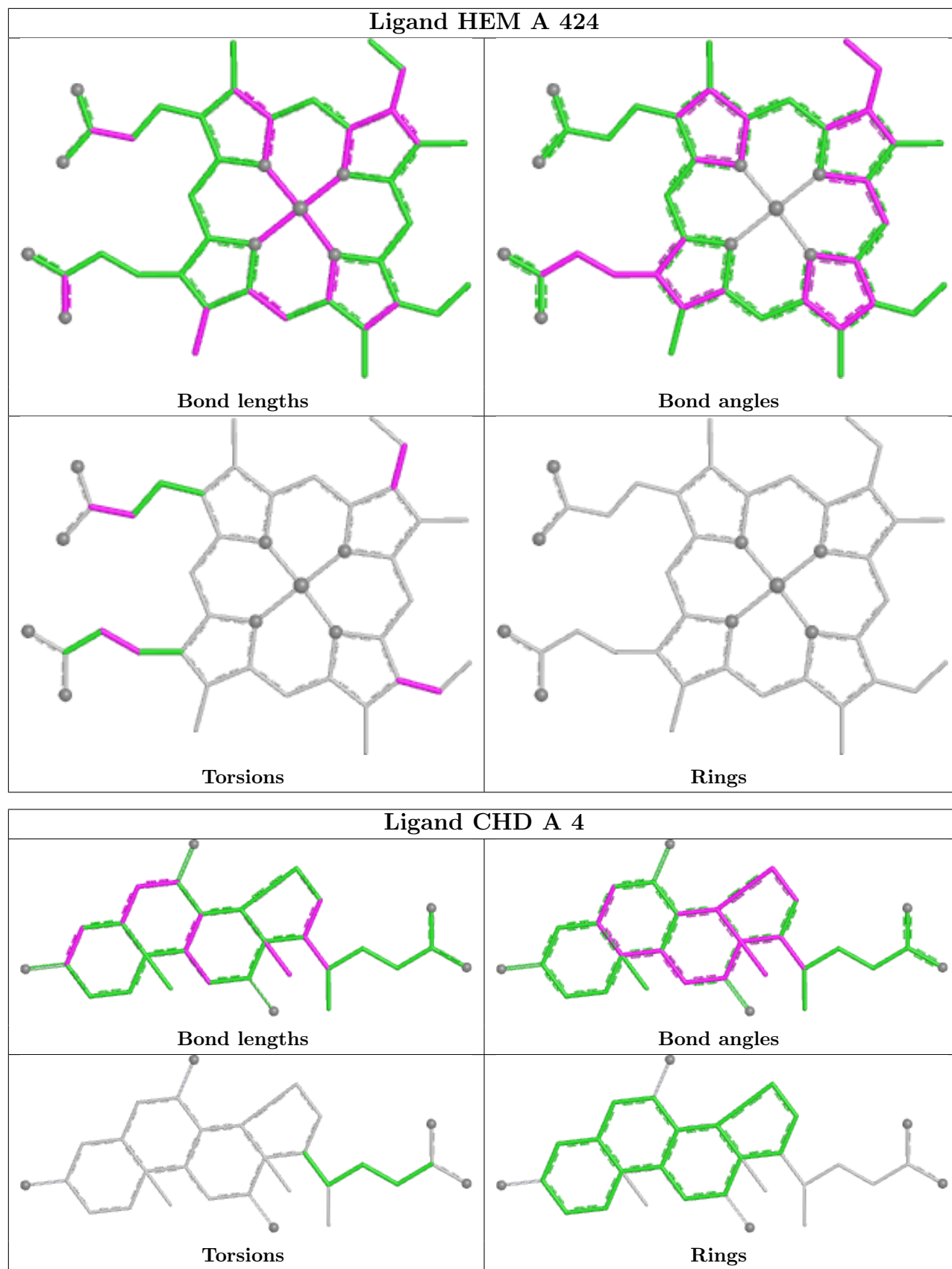
9 monomers are involved in 17 short contacts:

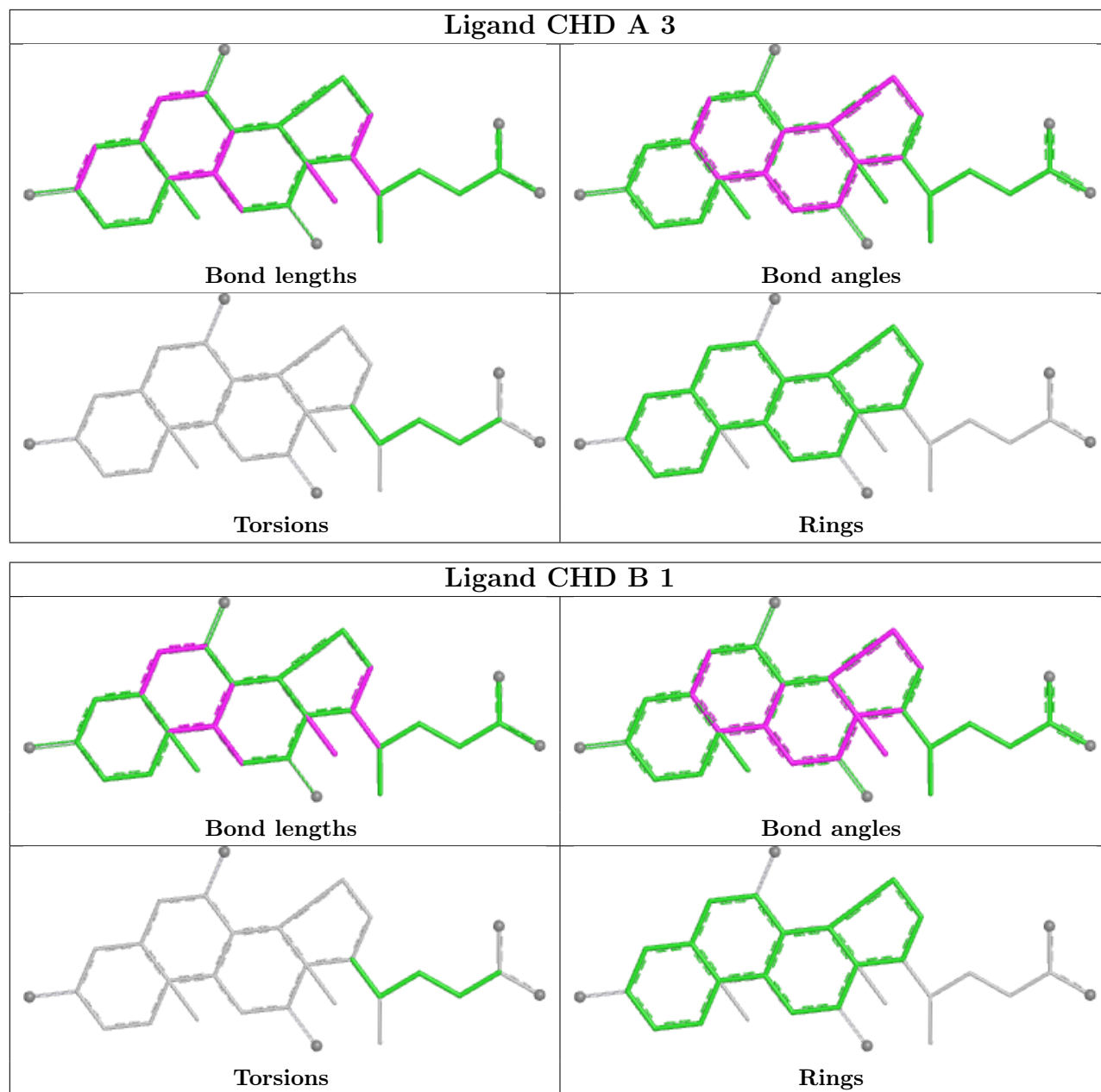
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	926	HEM	1	0
4	B	925	IMD	1	0
6	A	424	HEM	2	0
8	B	924[B]	GOL	3	0
3	A	3	CHD	3	0
3	B	1	CHD	3	0
8	B	924[A]	GOL	1	0
4	A	2	IMD	1	0
3	B	2	CHD	3	0

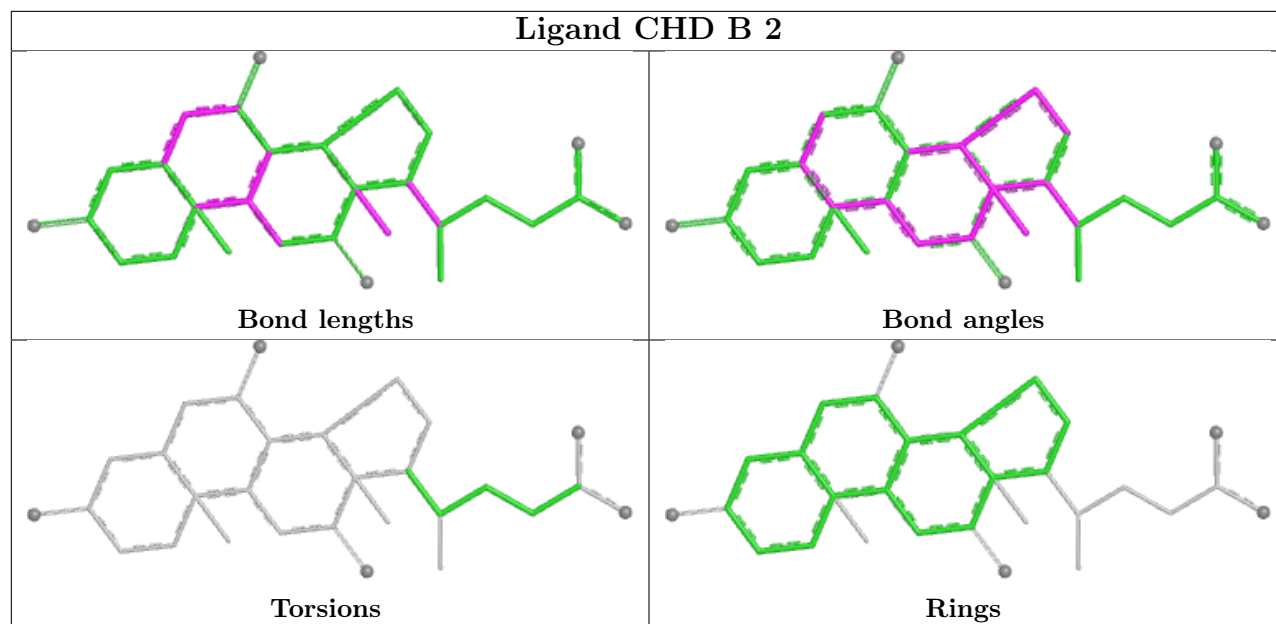
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for 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 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	359/359 (100%)	0.80	50 (13%)	6 6	5, 20, 38, 49	24 (6%)
1	B	359/359 (100%)	0.86	49 (13%)	7 6	7, 21, 40, 49	12 (3%)
All	All	718/718 (100%)	0.83	99 (13%)	6 6	5, 20, 39, 49	36 (5%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305[A]	VAL	10.8
1	A	304[A]	LYS	7.4
1	B	850	ILE	5.7
1	B	610	PHE	5.5
1	B	923	LEU	5.3
1	A	308[A]	MET	5.0
1	B	713	VAL	5.0
1	A	213	VAL	4.9
1	B	860[A]	CYS	4.7
1	A	253[A]	ARG	4.6
1	A	303[A]	SER	4.5
1	B	565	ARG	4.2
1	B	856	LEU	4.0
1	A	350	ILE	3.9
1	B	566[A]	LYS	3.8
1	A	212	GLN	3.8
1	B	858	LYS	3.7
1	A	423	LEU	3.6
1	B	753[A]	ARG	3.6
1	A	307[A]	PRO	3.6
1	A	354[A]	GLN	3.5
1	A	250	LEU	3.4
1	A	302[A]	GLN	3.4
1	A	356	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	360[A]	CYS	3.3
1	B	855	VAL	3.3
1	A	357	ALA	3.2
1	B	608	ALA	3.2
1	A	113	LYS	3.2
1	A	306[A]	GLY	3.2
1	B	612	ALA	3.2
1	B	712	GLN	3.1
1	B	854[A]	GLN	3.1
1	B	862	VAL	3.1
1	B	853	SER	3.1
1	B	682	LEU	3.1
1	B	614	ARG	3.0
1	A	328	LYS	3.0
1	B	715	ARG	2.9
1	A	65	ARG	2.9
1	B	684	ARG	2.9
1	A	359	GLU	2.8
1	A	110	PHE	2.8
1	B	656	PRO	2.8
1	A	220	LYS	2.8
1	A	107	LEU	2.8
1	B	857	ALA	2.7
1	B	649[A]	GLU	2.7
1	B	650	LEU	2.7
1	B	611	ILE	2.7
1	A	358	LYS	2.7
1	A	361	GLY	2.7
1	B	861	GLY	2.7
1	B	613	LYS	2.7
1	B	750	LEU	2.7
1	B	852	TYR	2.7
1	B	653	ASN	2.6
1	B	718	THR	2.6
1	A	348	LEU	2.6
1	A	352	TYR	2.6
1	A	375	PRO	2.6
1	A	372	ASN	2.5
1	A	217	PRO	2.5
1	B	607	LEU	2.5
1	B	848	LEU	2.4
1	B	912	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	355	VAL	2.4
1	A	362	VAL	2.4
1	A	351	GLU	2.4
1	B	751	GLU	2.4
1	B	859	GLU	2.4
1	B	681	GLY	2.4
1	B	609	PRO	2.4
1	B	601	LEU	2.4
1	A	218	THR	2.4
1	B	603	ILE	2.4
1	A	211	ASN	2.3
1	A	96	ARG	2.3
1	A	216	LYS	2.3
1	A	353	SER	2.3
1	B	587	ASP	2.3
1	A	249	PRO	2.3
1	A	346	TYR	2.3
1	A	134	ILE	2.3
1	A	179	ARG	2.2
1	A	374	ASN	2.2
1	B	652	PRO	2.2
1	A	252	LYS	2.2
1	B	828	LYS	2.2
1	B	680	ASP	2.1
1	A	215	ARG	2.1
1	A	371	LEU	2.1
1	A	254	SER	2.1
1	A	66	LYS	2.1
1	B	817[A]	GLU	2.0
1	B	839	SER	2.0
1	B	634	ILE	2.0
1	A	247	HIS	2.0
1	B	645	LYS	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

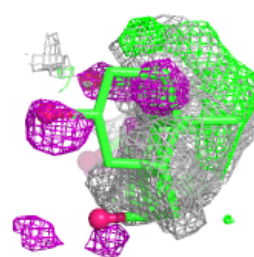
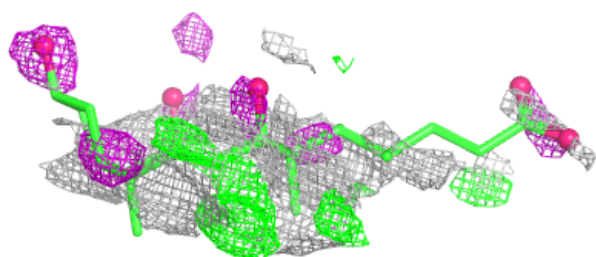
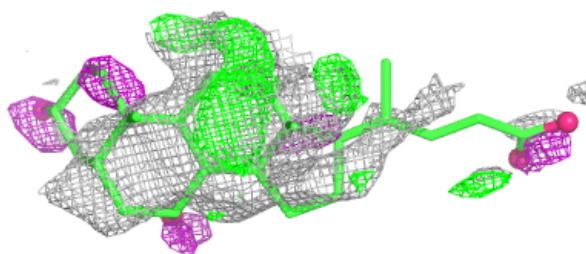
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CHD	A	4	29/29	0.28	0.25	57,57,60,60	0
3	CHD	A	3	29/29	0.48	0.26	47,48,54,55	0
7	SO4	A	425	5/5	0.61	0.16	60,61,61,61	0
5	BCT	A	1	4/4	0.76	0.24	44,45,45,46	0
3	CHD	B	1	29/29	0.76	0.18	31,34,47,49	0
3	CHD	B	2	29/29	0.77	0.17	47,48,57,58	0
7	SO4	B	927	5/5	0.79	0.12	58,58,59,59	0
8	GOL	B	924[A]	6/6	0.83	0.15	16,16,18,19	6
8	GOL	B	924[B]	6/6	0.83	0.15	18,20,21,21	6
4	IMD	B	3	5/5	0.89	0.12	20,21,22,22	0
4	IMD	A	2	5/5	0.89	0.12	25,25,26,27	0
4	IMD	B	925	5/5	0.92	0.09	18,19,20,20	0
6	HEM	A	424	43/43	0.97	0.09	12,16,24,29	0
6	HEM	B	926	43/43	0.97	0.10	13,17,24,27	0
2	FES	A	501	4/4	0.98	0.05	14,15,15,17	0
2	FES	B	502	4/4	0.98	0.05	15,15,15,17	0

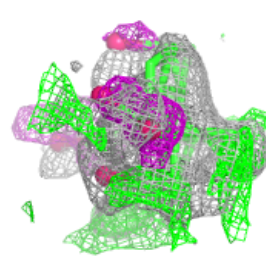
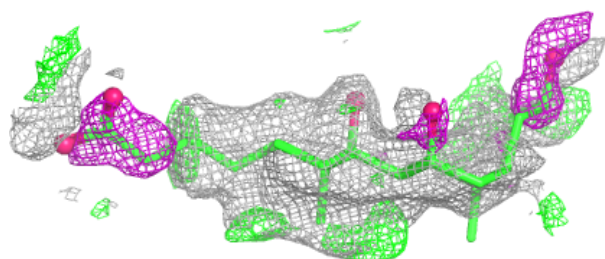
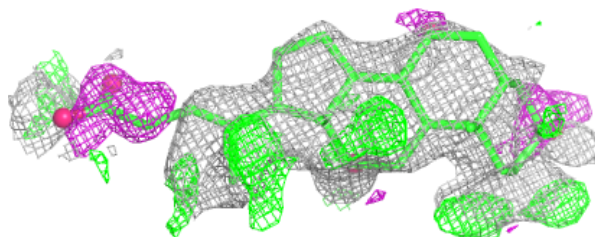
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD A 4:

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

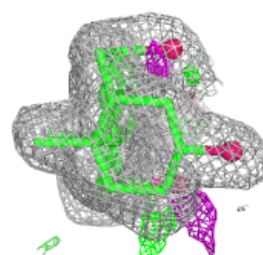
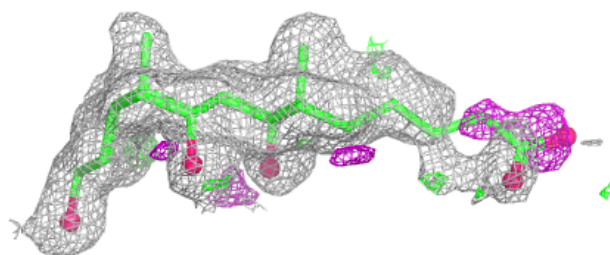
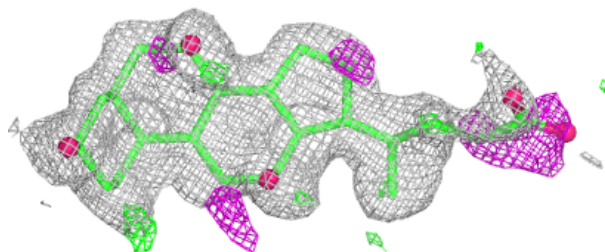
**Electron density around CHD A 3:**

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

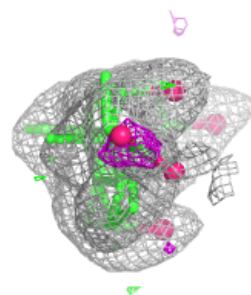
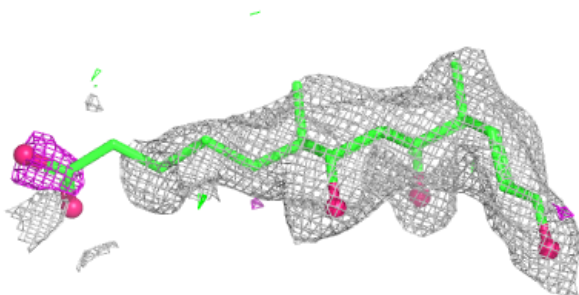
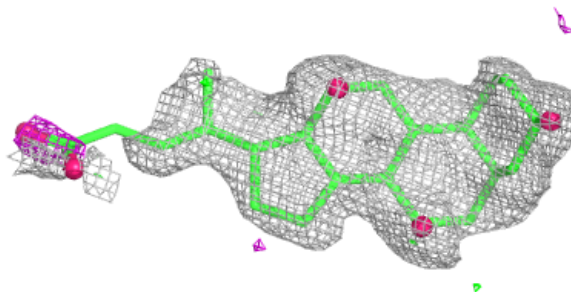


Electron density around CHD B 1:

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

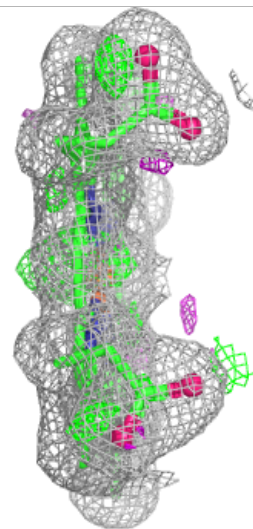
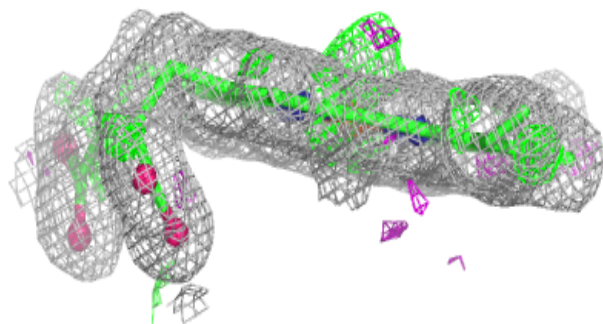
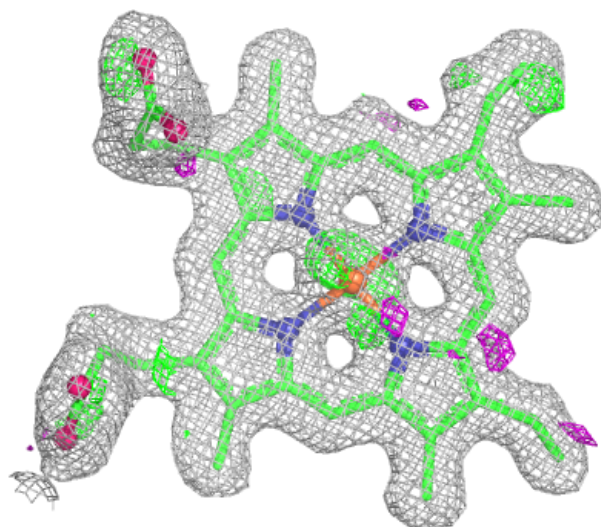
**Electron density around CHD B 2:**

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



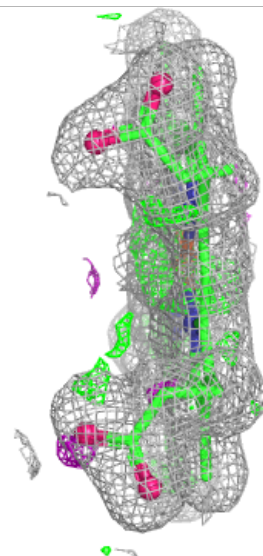
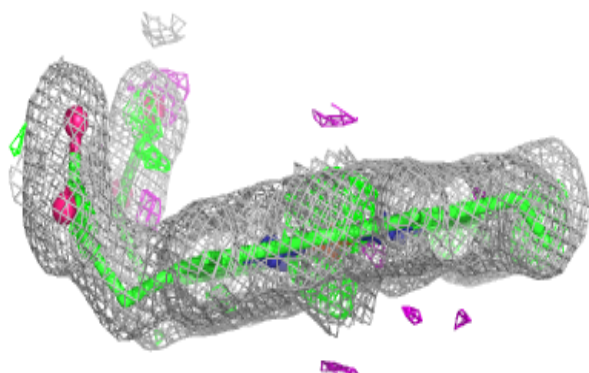
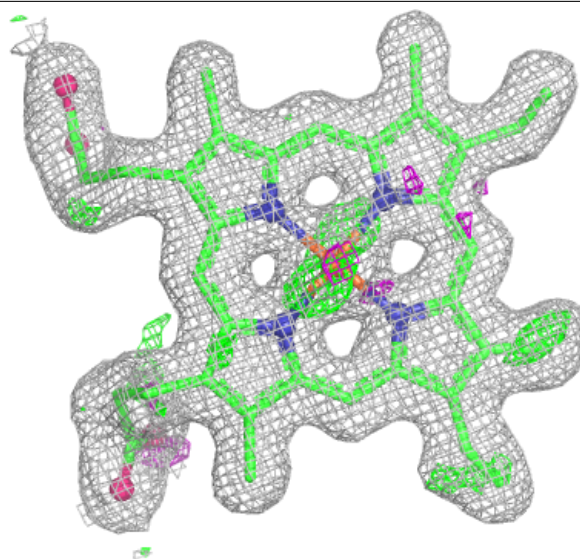
Electron density around HEM A 424:

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



Electron density around HEM B 926:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.