



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:52 pm BST

PDB ID : 3HCN  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

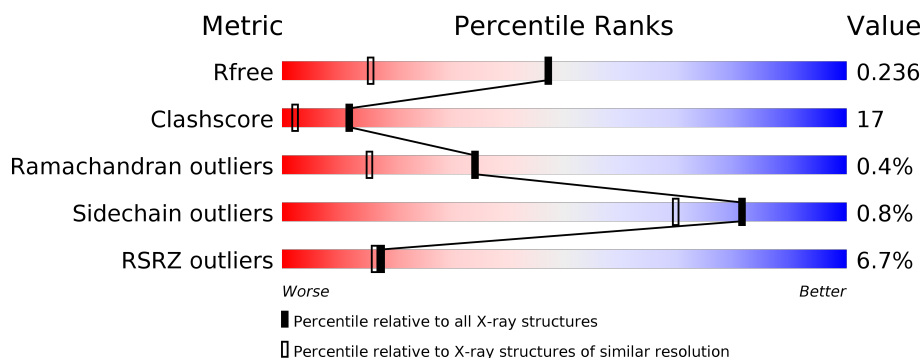
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>8%</div> <div>68%</div> <div>31%</div> </div>
1	B	359	<div> <div>6%</div> <div>71%</div> <div>29%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CHD	A	4	-	-	-	X

## 2 Entry composition [i](#)

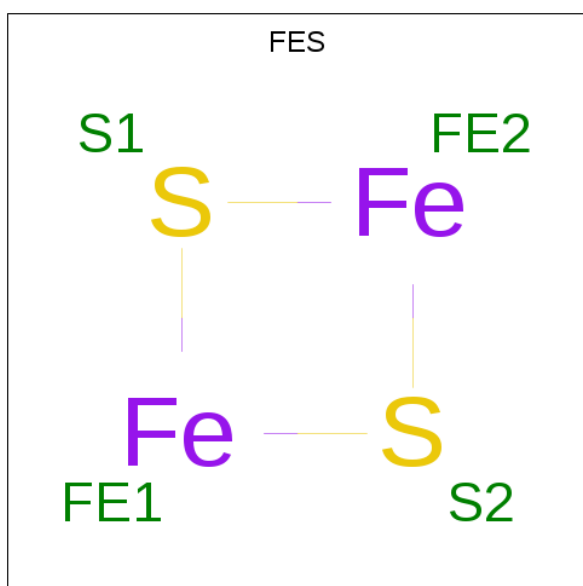
There are 9 unique types of molecules in this entry. The entry contains 7132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

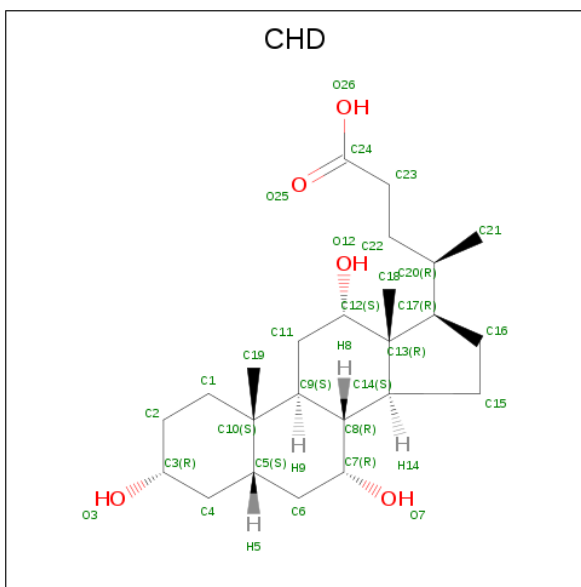
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	24	0
			3089	1955	543	570	21			
1	B	359	Total	C	N	O	S	0	12	0
			2994	1901	523	550	20			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



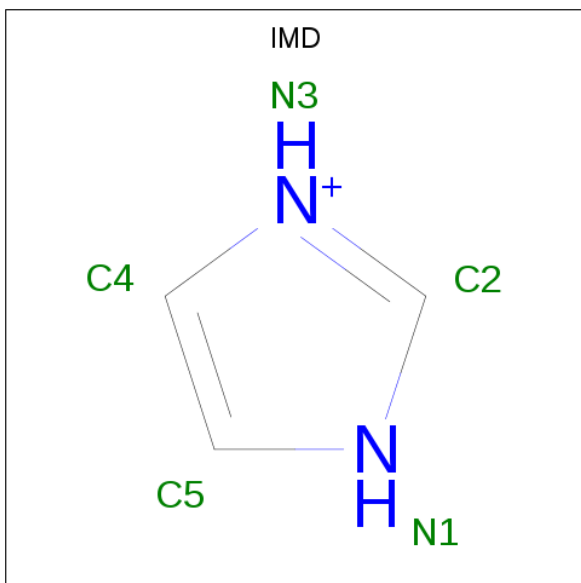
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

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



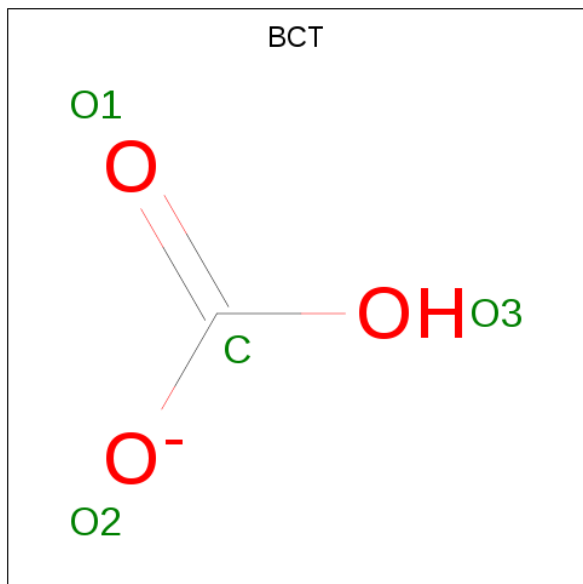
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			29	24	5		
3	A	1	Total	C	O	0	0
			29	24	5		
3	B	1	Total	C	O	0	0
			29	24	5		
3	B	1	Total	C	O	0	0
			29	24	5		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



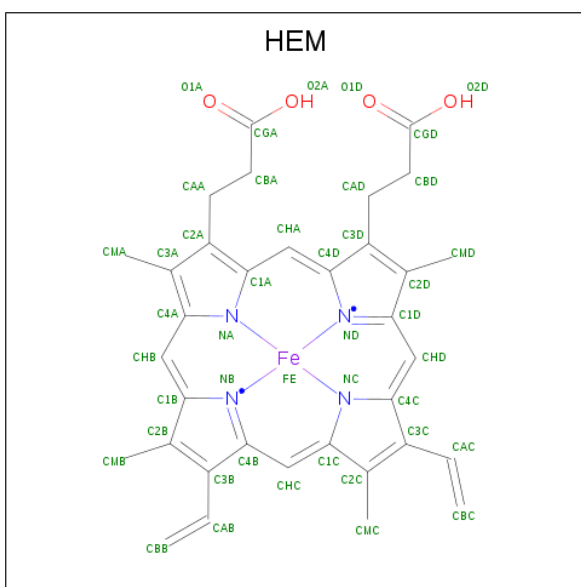
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



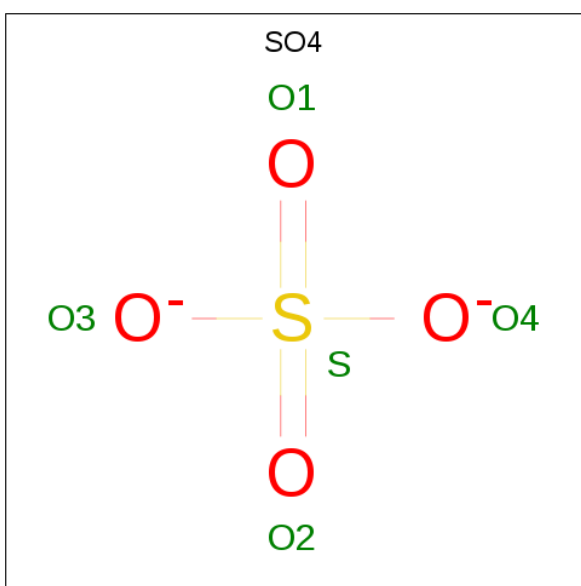
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: 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 (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).



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

- Molecule 8 is GLYCEROL (three-letter code: 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		



These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

Chain A:

8% 68% 31%

Items: R65, K66, P67, K68, T69, G70, I71, M76, G77, D87, R91, M99, T100, L101, P102, T103, Q104, H105, K106, L107, A108, P109, F110, K113, R114, R115, T116, Q120, F121, Q122, I134, W135, T136, S137, K138, Q139, G140, E141, P156, A173, M177, R184, Y191, P192, Q193, Y194, T100.

Chain B:

Node	Node	Node
R565	R715	R824
K566	K720	R825
P567	W721	K828
G570	I724	H841
I571	D725	D849
D587	R726	I850
R591	I734	E851
L601	Q735	Y852
P602	H740	S853
I603	K743	Q854
Q604	K743	V855
N605	L750	L856
K606	E751	A857
L607	K752	K858
A608	R753	E859
P609	P766	C860
F610	V769	G861
K613	R772	V862
R614	G773	E863
R615	V776	E869
T616	P777	N872
P617	K778	G873
Q620	E779	N874
I634	A782	P875
M635	Q785	L876
T636	K786	S891
S637	E789	N892
K638	R790	E893
Q639	Y797	L894
G640	R798	Q898
E641	L799	L899
K645	V800	T900
E649	S803	P904
N653	T804	L905
A673	W810	K915
M677	P813	Q921
D680	Q814	Q922
L682	T815	L923
E683	D816	
R684	E817	
Y710	K920	
N711	C926	
Q712		
V713		
C714		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.48 Å 92.96 Å 109.36 Å 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) 99.2 (47.13-1.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 1.60 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.214 , 0.236 0.214 , 0.236	Depositor DCC
$R_{free}$ test set	11011 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	0.647	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, CHD, IMD, FES, BCT, HEM, SO4

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	0.28	0/3161	0.56	1/4277 (0.0%)
1	B	0.28	0/3065	0.56	1/4147 (0.0%)
All	All	0.28	0/6226	0.56	2/8424 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ILE	N-CA-C	-5.78	95.40	111.00
1	B	724	ILE	N-CA-C	-5.47	96.23	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	126	0
1	B	2994	0	2991	103	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	220	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 17.

All (220) 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: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:853:SER:C	1:B:854[B]:GLN:CA	2.44	0.85
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:304[B]:LYS:O	1:A:304[B]:LYS:HD2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:A:290:ARG:HG2	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:HH11	1:B:790:ARG:HG2	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: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:B:734:ILE:HG21	1:B:786[B]:LYS:HG2	1.84	0.59
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: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:B:874:ASN:HD22	1:B:874:ASN:C	2.06	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:317[A]:GLU:HG2	1:B:905:LEU:HD11	1.87	0.56
1:A:306[B]:GLY:HA3	9:A:447:HOH:O	2.06	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: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:304[B]:LYS:HD2	1:A:304[B]:LYS:C	2.27	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:235:GLN:HG3	1:A:290:ARG:NH1	2.22	0.54
1:A:115:ARG:NE	6:A:424:HEM:O1A	2.41	0.54
1:A:250:LEU:HD23	1:A:250:LEU:O	2.08	0.53
1:A:286:LYS:HE2	1:B:786[A]:LYS:HZ3	1.73	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:854[A]:GLN:O	1:B:858:LYS:HG2	2.10	0.51
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:A:374:ASN:HD22	1:A:374:ASN:C	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:B:614:ARG:NH1	3:B:2:CHD:H42	2.28	0.49
1:A:277:PRO:CB	8:B:924[B]:GOL:H12	2.40	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: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:A:290:ARG:HG2	1:A:290:ARG:NH1	2.26	0.48
1:A:251[B]:GLU:HG2	1:A:252:LYS:HG2	1.96	0.48
1:A:65:ARG:HG3	1:A:65:ARG:HH11	1.78	0.48
1:B:858:LYS:HD3	9:B:1027:HOH:O	2.13	0.48
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:243:LYS:HZ3	1:A:369[B]:GLU:CD	2.17	0.47
1:B:713:VAL:HG13	1:B:715:ARG:H	1.80	0.47
1:B:817[A]:GLU:N	1:B:817[A]:GLU:OE2	2.47	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:740:HIS:HA	1:B:743[A]:LYS:HG2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:ILE:HD12	1:B:571:ILE:N	2.30	0.47
1:B:720:LYS:HZ3	1:B:923:LEU:CD1	2.28	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: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:NH1	1:B:790:ARG:HG2	2.30	0.46
1:B:874:ASN:HD22	1:B:875:PRO:CD	2.28	0.46
1:A:102:PRO:O	1:A:103:ILE:C	2.54	0.45
1:A:422:GLN:HG2	1:A:423:LEU:CD1	2.46	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:B:720:LYS:HZ3	1:B:923:LEU:HD11	1.82	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:250:LEU:HD23	1:A:250:LEU:C	2.38	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:286:LYS:NZ	1:B:789:GLU:OE2	2.50	0.44
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:243:LYS:NZ	1:A:369[B]:GLU:CD	2.70	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:891:SER:O	1:B:892:ASN:HB2	2.18	0.44
1:B:720:LYS:CD	1:B:923:LEU:HD22	2.47	0.44
1:B:602:PRO:O	1:B:603:ILE:C	2.55	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:THR:HA	1:A:415[B]:LYS:CE	2.48	0.43
1:A:71:ILE:HD12	1:A:71:ILE:N	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:HH11	1:A:215:ARG:HG2	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:C	1:A:304[A]:LYS:HG2	2.39	0.42
1:B:874:ASN:ND2	1:B:874:ASN:C	2.73	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:HH11	1:B:615:ARG:HG2	1.84	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: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:66:LYS:HG3	1:A:67:PRO:HD2	2.02	0.41
1:B:751:GLU:CD	1:B:751:GLU:H	2.23	0.41
1:A:76:MET:HG3	1:A:77:GLY:O	2.20	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: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
1:B:825:ARG:HH11	1:B:825:ARG:HG3	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%)	19	6
1	B	369/359 (103%)	362 (98%)	6 (2%)	1 (0%)	41	21
All	All	750/718 (104%)	734 (98%)	12 (2%)	4 (0%)	34	11

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 ⓘ

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	347/324 (107%)	342 (99%)	5 (1%)	67	47
1	B	336/324 (104%)	335 (100%)	1 (0%)	92	87
All	All	683/648 (105%)	677 (99%)	6 (1%)	81	65

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	TRP
1	A	255	GLU
1	A	304[A]	LYS
1	A	304[B]	LYS
1	A	374	ASN
1	B	874	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	HIS
1	A	235	GLN
1	A	247	HIS
1	A	329	ASN
1	A	364	ASN
1	A	374	ASN
1	A	386	HIS
1	A	398	GLN
1	A	421	GLN
1	B	653	ASN
1	B	735	GLN
1	B	747	HIS
1	B	829	ASN
1	B	872	ASN
1	B	874	ASN
1	B	892	ASN
1	B	898	GLN
1	B	921	GLN

### 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 carbohydrates 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	$\# Z  > 2$
3	CHD	A	4	-	29,32,32	1.59	7 (24%)	48,51,51	1.48	9 (18%)
5	BCT	A	1	6	0,3,3	0.00	-	0,3,3	0.00	-
6	HEM	B	926	4	27,50,50	1.77	7 (25%)	17,82,82	2.68	10 (58%)
8	GOL	B	924[B]	-	5,5,5	0.26	0	5,5,5	0.29	0
6	HEM	A	424	5,4	27,50,50	1.74	6 (22%)	17,82,82	2.68	9 (52%)
4	IMD	A	2	6	3,5,5	0.48	0	4,5,5	0.63	0
3	CHD	B	1	-	29,32,32	1.51	7 (24%)	48,51,51	1.37	7 (14%)
3	CHD	A	3	-	29,32,32	1.55	7 (24%)	48,51,51	1.39	7 (14%)
2	FES	A	501	1	0,4,4	0.00	-	-	-	-
4	IMD	B	925	6	3,5,5	0.64	0	4,5,5	0.56	0
7	SO4	A	425	-	4,4,4	0.27	0	6,6,6	0.05	0
4	IMD	B	3	6	3,5,5	0.46	0	4,5,5	0.50	0
3	CHD	B	2	-	29,32,32	1.58	6 (20%)	48,51,51	1.47	9 (18%)
2	FES	B	502	1	0,4,4	0.00	-	-	-	-
7	SO4	B	927	-	4,4,4	0.28	0	6,6,6	0.05	0
8	GOL	B	924[A]	-	5,5,5	0.27	0	5,5,5	0.30	0

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
3	CHD	A	4	-	-	0/7/74/74	0/4/4/4
6	HEM	B	926	4	-	0/6/54/54	-
2	FES	B	502	1	-	-	0/1/1/1
3	CHD	A	3	-	-	0/7/74/74	0/4/4/4
4	IMD	A	2	6	-	-	0/1/1/1
3	CHD	B	1	-	-	0/7/74/74	0/4/4/4
6	HEM	A	424	5,4	-	1/6/54/54	-
3	CHD	B	2	-	-	0/7/74/74	0/4/4/4
4	IMD	B	925	6	-	-	0/1/1/1
4	IMD	B	3	6	-	-	0/1/1/1
2	FES	A	501	1	-	-	0/1/1/1
8	GOL	B	924[B]	-	-	0/4/4/4	-
8	GOL	B	924[A]	-	-	0/4/4/4	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	424	HEM	C3C-CAC	-5.30	1.36	1.47
6	B	926	HEM	C3C-CAC	-5.03	1.37	1.47
6	A	424	HEM	C3B-C2B	4.01	1.45	1.40
6	B	926	HEM	C3B-C2B	3.39	1.45	1.40
6	B	926	HEM	C4A-CHB	-3.27	1.31	1.41
6	B	926	HEM	C4B-NB	3.12	1.42	1.36
6	A	424	HEM	C4A-CHB	-2.78	1.33	1.41
3	A	4	CHD	C18-C13	2.71	1.58	1.54
3	B	1	CHD	C11-C9	2.64	1.58	1.53
3	B	2	CHD	C18-C13	2.63	1.58	1.54
3	B	2	CHD	C20-C17	2.58	1.58	1.54
3	A	3	CHD	C18-C13	2.57	1.58	1.54
3	B	1	CHD	C18-C13	2.55	1.58	1.54
3	A	4	CHD	C20-C17	2.51	1.58	1.54
6	A	424	HEM	C4B-NB	2.47	1.41	1.36
3	A	3	CHD	C20-C17	2.44	1.58	1.54
3	A	3	CHD	C11-C9	2.43	1.57	1.53
6	B	926	HEM	C1A-NA	2.41	1.41	1.36
3	A	4	CHD	C11-C9	2.32	1.57	1.53
3	A	4	CHD	C6-C7	2.29	1.56	1.52
3	B	2	CHD	C6-C7	2.25	1.56	1.52
3	B	2	CHD	C8-C9	2.24	1.58	1.53
3	B	2	CHD	C11-C9	2.23	1.57	1.53
6	B	926	HEM	C1C-C2C	2.22	1.47	1.42
3	B	1	CHD	C6-C7	2.22	1.56	1.52
3	B	2	CHD	C6-C5	2.22	1.57	1.53
3	A	4	CHD	C8-C9	2.22	1.58	1.53
3	B	1	CHD	C6-C5	2.21	1.57	1.53
3	A	3	CHD	C6-C7	2.20	1.56	1.52
3	A	4	CHD	C6-C5	2.16	1.57	1.53
6	A	424	HEM	C1A-NA	2.15	1.40	1.36
3	A	3	CHD	C6-C5	2.13	1.57	1.53
3	A	3	CHD	C10-C9	2.13	1.60	1.56
3	B	1	CHD	C8-C9	2.12	1.58	1.53
3	A	3	CHD	C8-C9	2.08	1.57	1.53
6	A	424	HEM	C1C-C2C	2.08	1.47	1.42
6	B	926	HEM	C4D-C3D	2.05	1.47	1.42
3	B	1	CHD	C16-C17	2.05	1.58	1.54
3	A	4	CHD	C16-C17	2.03	1.58	1.54
3	B	1	CHD	C20-C17	2.01	1.57	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	926	HEM	C4C-C3C-C2C	-5.21	103.26	106.90
6	A	424	HEM	C4C-C3C-C2C	-5.06	103.36	106.90
6	A	424	HEM	CAA-CBA-CGA	4.06	119.48	112.67
3	B	1	CHD	C9-C11-C12	-4.05	108.95	114.30
6	B	926	HEM	CMA-C3A-C4A	-3.90	122.46	128.46
6	A	424	HEM	CMA-C3A-C4A	-3.83	122.58	128.46
6	B	926	HEM	CAA-CBA-CGA	3.81	119.06	112.67
3	A	3	CHD	C9-C11-C12	-3.62	109.52	114.30
6	B	926	HEM	C1D-C2D-C3D	-3.56	104.52	107.00
6	A	424	HEM	C1D-C2D-C3D	-3.54	104.54	107.00
6	A	424	HEM	C4A-C3A-C2A	3.47	109.41	107.00
3	A	4	CHD	C9-C11-C12	-3.39	109.83	114.30
6	B	926	HEM	C4A-C3A-C2A	3.30	109.29	107.00
3	B	2	CHD	C9-C11-C12	-3.29	109.95	114.30
6	A	424	HEM	CMD-C2D-C3D	3.23	131.02	124.94
6	B	926	HEM	CMD-C2D-C3D	3.15	130.88	124.94
3	B	2	CHD	C13-C17-C20	-2.89	116.05	119.50
3	B	2	CHD	C17-C13-C12	2.89	120.30	117.67
3	A	4	CHD	C13-C17-C20	-2.85	116.09	119.50
3	B	1	CHD	C16-C15-C14	-2.79	99.61	105.13
3	A	4	CHD	C11-C9-C10	-2.78	110.86	113.73
3	B	2	CHD	C13-C14-C8	-2.77	111.20	114.74
3	A	4	CHD	C17-C13-C12	2.76	120.19	117.67
6	A	424	HEM	CMB-C2B-C3B	2.75	129.83	124.68
3	A	4	CHD	C13-C14-C8	-2.74	111.23	114.74
3	A	3	CHD	C17-C13-C12	2.70	120.13	117.67
3	B	2	CHD	C11-C9-C10	-2.68	110.96	113.73
6	B	926	HEM	CMB-C2B-C3B	2.67	129.67	124.68
6	A	424	HEM	CMD-C2D-C1D	-2.62	124.44	128.46
3	A	3	CHD	C16-C15-C14	-2.52	100.13	105.13
6	B	926	HEM	CMD-C2D-C1D	-2.51	124.61	128.46
3	A	4	CHD	C16-C15-C14	-2.45	100.27	105.13
3	B	2	CHD	C16-C15-C14	-2.41	100.36	105.13
3	A	3	CHD	C11-C9-C10	-2.36	111.30	113.73
3	B	2	CHD	C23-C22-C20	-2.34	111.57	114.72
6	A	424	HEM	CBA-CAA-C2A	-2.33	108.18	112.49
3	A	3	CHD	C13-C14-C8	-2.30	111.80	114.74
3	B	1	CHD	C10-C9-C8	-2.28	109.37	111.82
3	A	4	CHD	C18-C13-C14	-2.27	107.66	111.21
3	A	4	CHD	C6-C5-C10	-2.25	110.27	112.66
3	B	2	CHD	C18-C13-C14	-2.25	107.69	111.21
3	A	4	CHD	C23-C22-C20	-2.25	111.69	114.72
3	B	1	CHD	C6-C5-C10	-2.23	110.29	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	926	HEM	C3B-C4B-NB	2.23	112.09	109.21
6	B	926	HEM	CBA-CAA-C2A	-2.19	108.45	112.49
3	A	3	CHD	C6-C5-C10	-2.17	110.35	112.66
3	B	1	CHD	C11-C9-C10	-2.17	111.49	113.73
3	B	2	CHD	C6-C5-C10	-2.15	110.38	112.66
3	B	1	CHD	C17-C13-C12	2.10	119.58	117.67
3	A	3	CHD	C10-C9-C8	-2.08	109.58	111.82
3	B	1	CHD	C18-C13-C14	-2.03	108.04	111.21

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	424	HEM	C2A-CAA-CBA-CGA

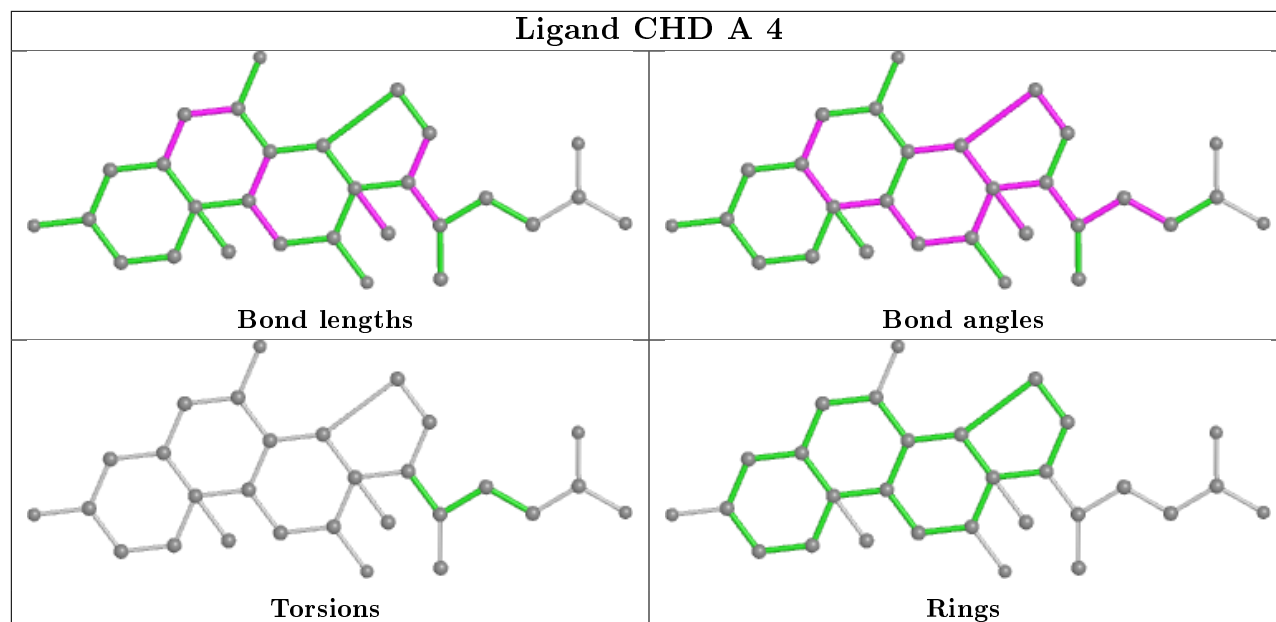
There are no ring outliers.

9 monomers are involved in 17 short contacts:

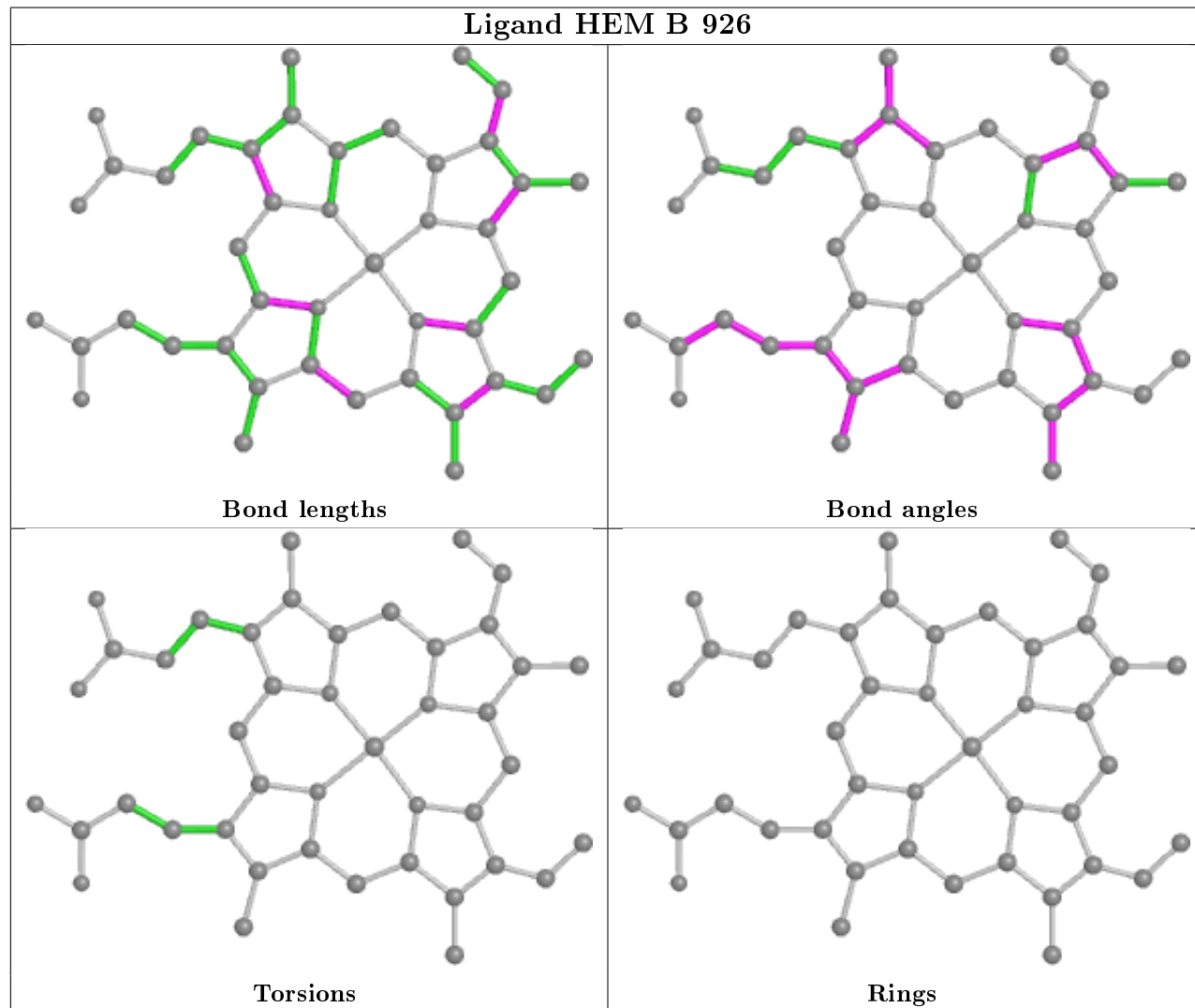
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	926	HEM	1	0
8	B	924[B]	GOL	3	0
6	A	424	HEM	2	0
4	A	2	IMD	1	0
3	B	1	CHD	3	0
3	A	3	CHD	3	0
4	B	925	IMD	1	0
3	B	2	CHD	3	0
8	B	924[A]	GOL	1	0

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

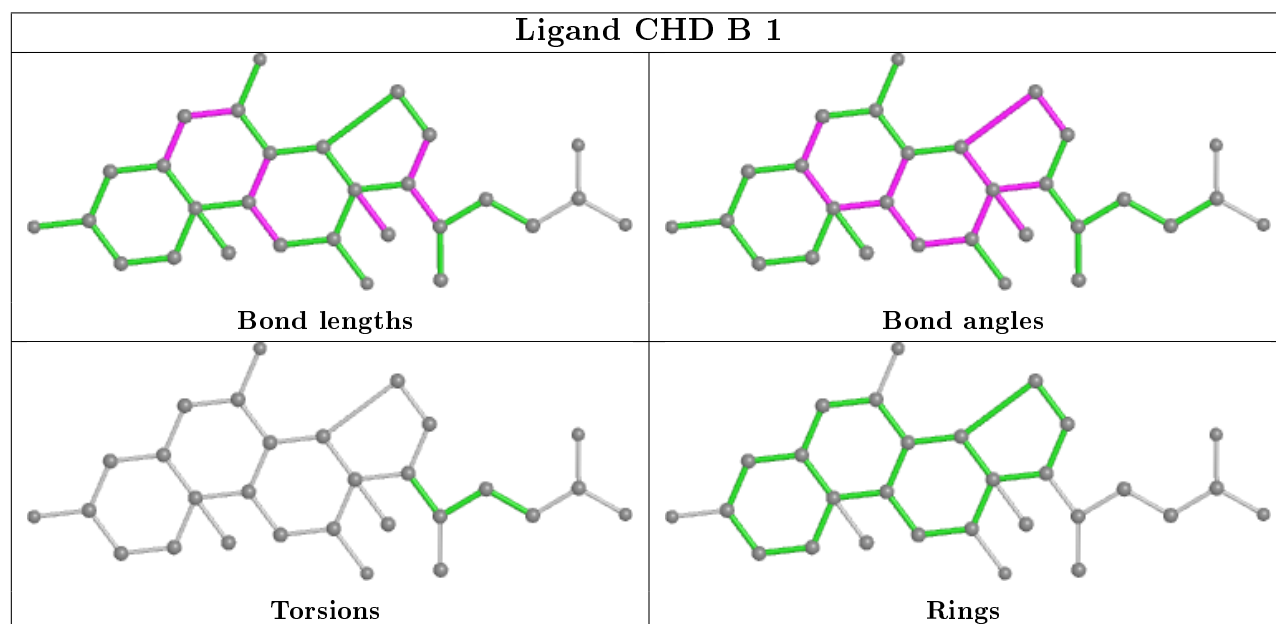
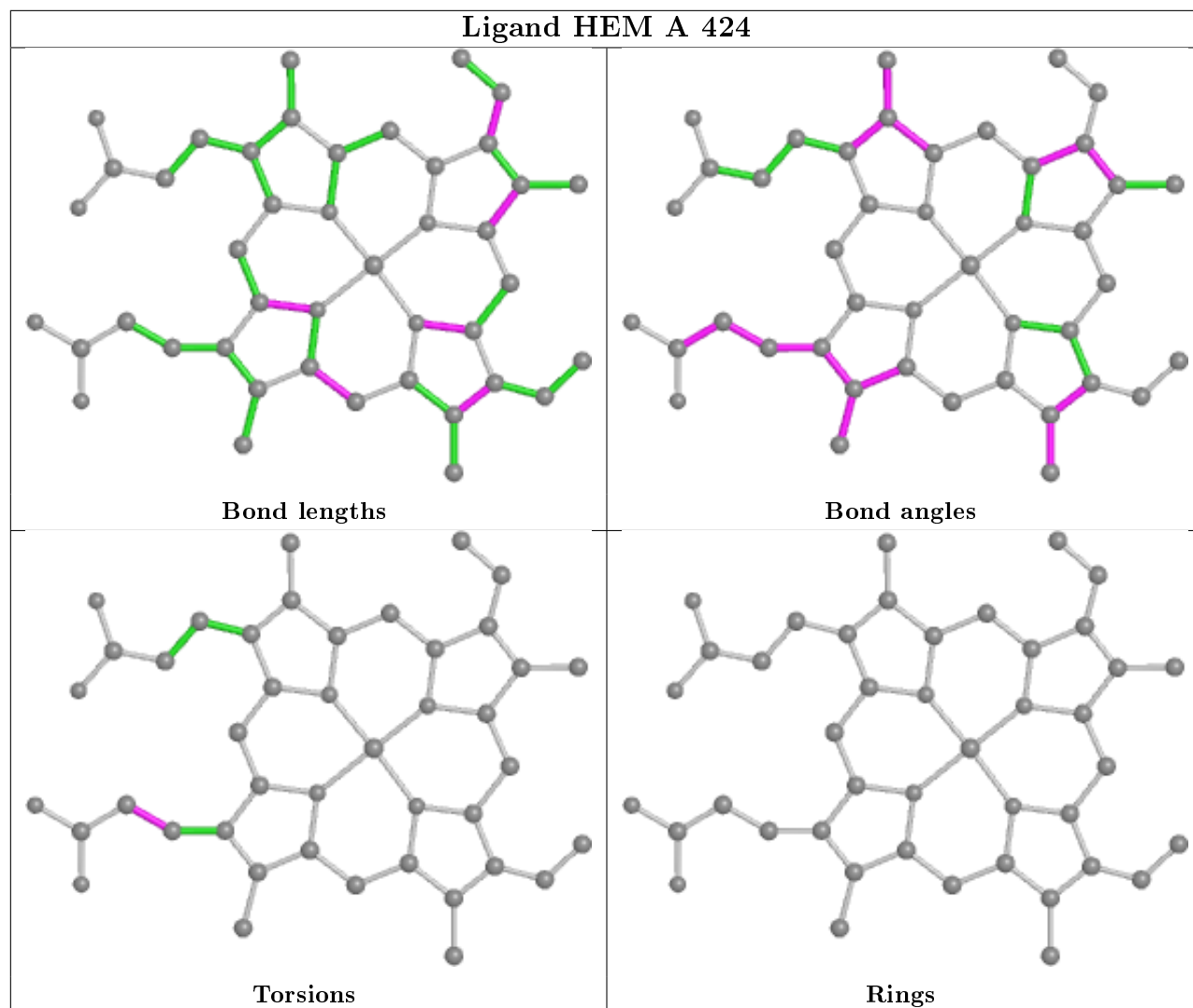
## Ligand CHD A 4

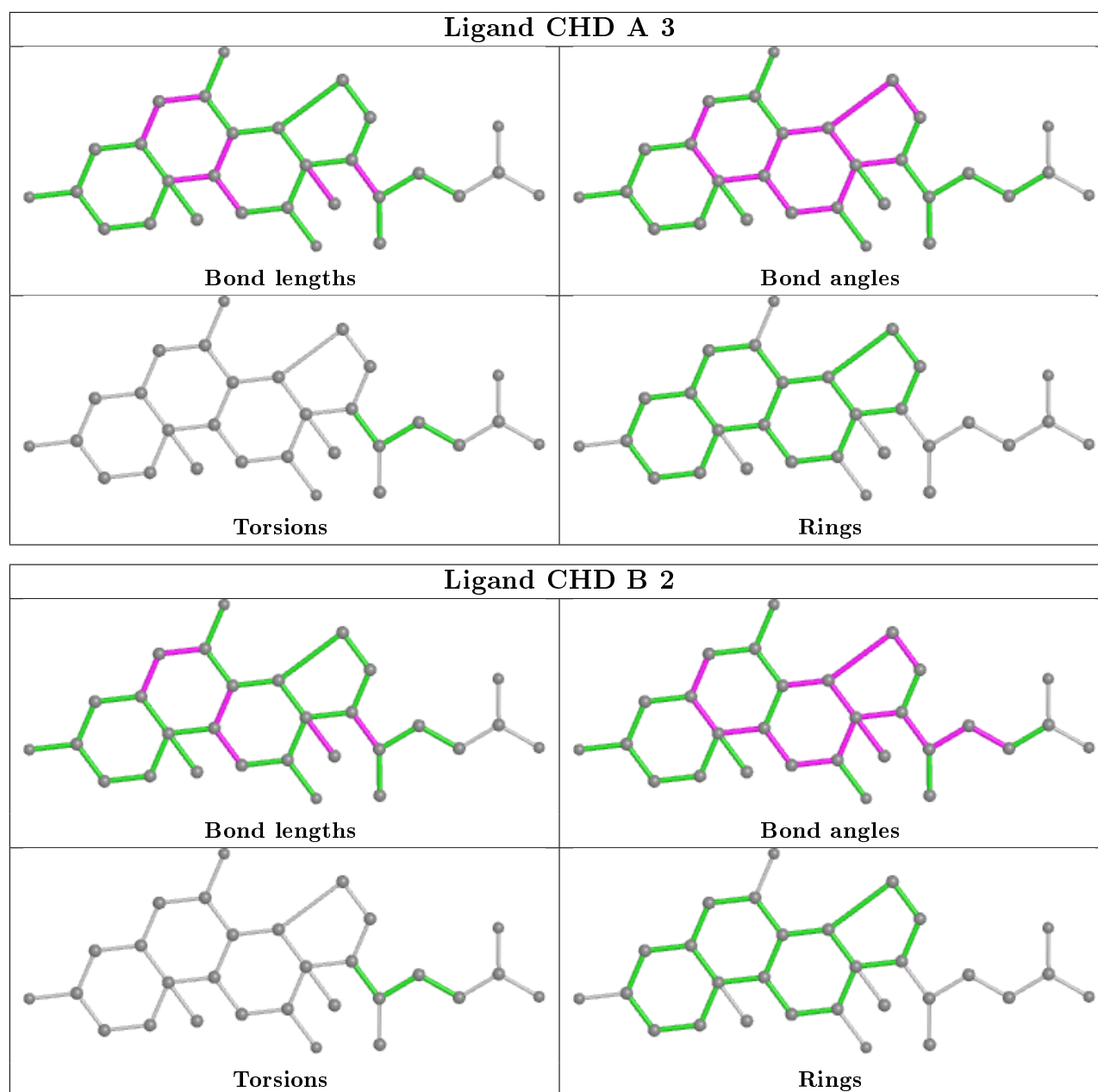


## Ligand HEM B 926









## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	359/359 (100%)	0.54	28 (7%)	13 11	7, 20, 39, 49	0
1	B	359/359 (100%)	0.51	20 (5%)	24 22	7, 21, 40, 49	0
All	All	718/718 (100%)	0.52	48 (6%)	17 16	7, 21, 40, 49	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305[A]	VAL	10.0
1	B	610	PHE	7.4
1	A	65	ARG	6.4
1	B	565	ARG	5.6
1	A	303[A]	SER	4.7
1	B	850	ILE	4.7
1	B	923	LEU	4.5
1	A	304[A]	LYS	4.3
1	A	110	PHE	4.1
1	A	423	LEU	4.1
1	B	603	ILE	4.1
1	A	350	ILE	3.7
1	B	607	LEU	3.3
1	A	113	LYS	3.2
1	B	614	ARG	3.2
1	A	307[A]	PRO	3.2
1	A	250	LEU	3.1
1	A	114	ARG	3.1
1	A	354[A]	GLN	3.1
1	B	566[A]	LYS	3.1
1	A	360[A]	CYS	3.0
1	A	66	LYS	3.0
1	A	351	GLU	3.0
1	A	359	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	212	GLN	3.0
1	A	308[A]	MET	2.9
1	B	606	LYS	2.9
1	A	306[A]	GLY	2.9
1	B	712	GLN	2.8
1	B	852	TYR	2.8
1	B	715	ARG	2.7
1	A	352	TYR	2.7
1	B	613	LYS	2.7
1	B	653	ASN	2.6
1	A	106	LYS	2.6
1	B	750	LEU	2.6
1	A	358	LYS	2.6
1	B	858	LYS	2.5
1	A	103	ILE	2.5
1	A	299	LEU	2.5
1	A	357	ALA	2.5
1	A	107	LEU	2.5
1	A	156	PRO	2.3
1	B	855	VAL	2.3
1	B	601	LEU	2.2
1	B	713	VAL	2.1
1	A	213	VAL	2.1
1	B	799	LEU	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](#)

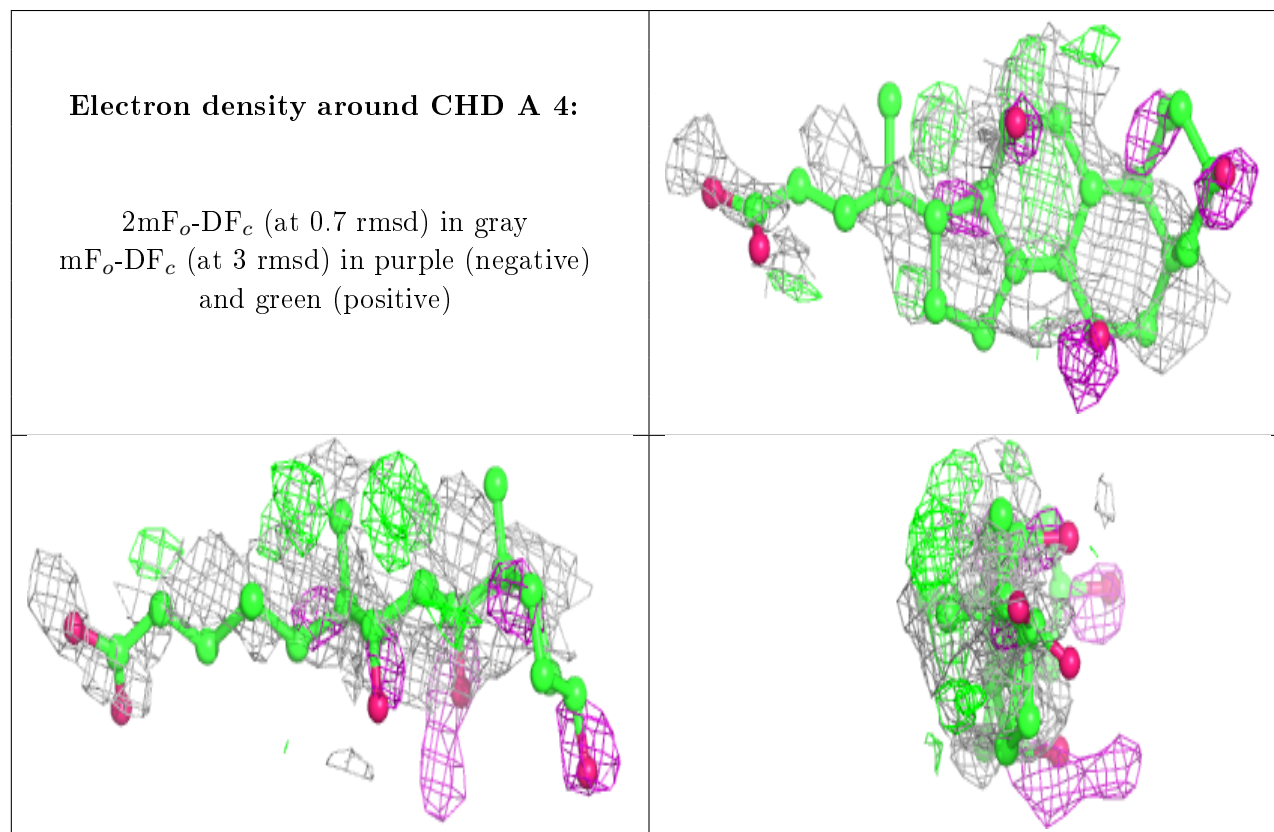
There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> 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.

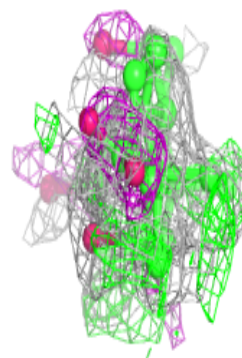
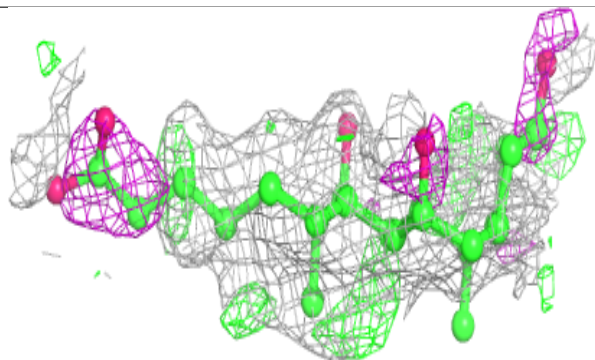
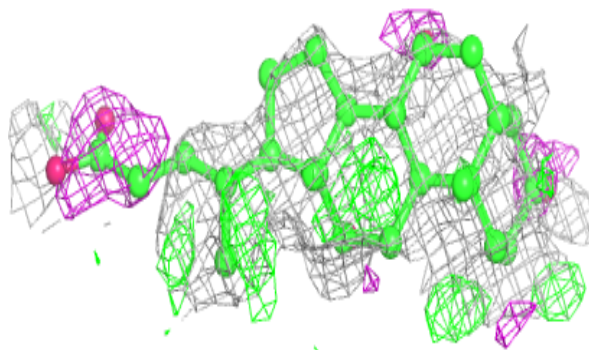
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CHD	A	4	29/29	0.31	0.56	57,57,60,60	0
3	CHD	A	3	29/29	0.47	0.38	47,48,54,55	0
3	CHD	B	1	29/29	0.66	0.18	31,34,47,49	0
3	CHD	B	2	29/29	0.71	0.27	47,48,57,58	0
8	GOL	B	924[B]	6/6	0.82	0.29	18,20,21,21	6
8	GOL	B	924[A]	6/6	0.82	0.29	16,16,18,19	6
5	BCT	A	1	4/4	0.84	0.19	44,45,45,46	0
4	IMD	A	2	5/5	0.87	0.13	25,25,26,27	0
4	IMD	B	925	5/5	0.90	0.09	18,19,20,20	0
7	SO4	A	425	5/5	0.90	0.29	60,61,61,61	0
4	IMD	B	3	5/5	0.91	0.12	20,21,22,22	0
7	SO4	B	927	5/5	0.93	0.22	58,58,59,59	0
6	HEM	A	424	43/43	0.96	0.12	12,16,24,29	0
6	HEM	B	926	43/43	0.96	0.12	13,17,24,27	0
2	FES	A	501	4/4	0.98	0.08	14,15,15,17	0
2	FES	B	502	4/4	0.98	0.08	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.

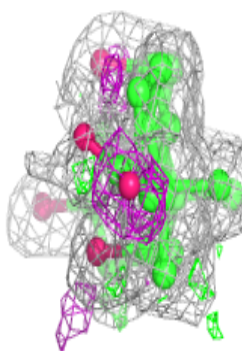
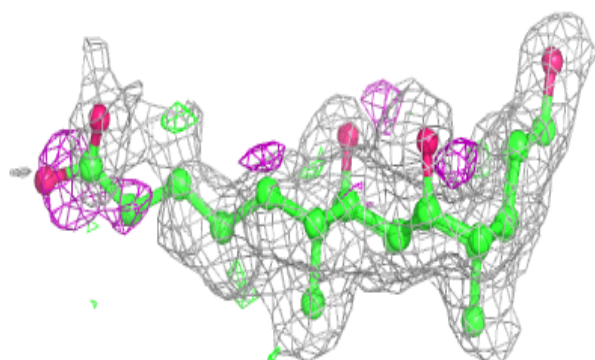
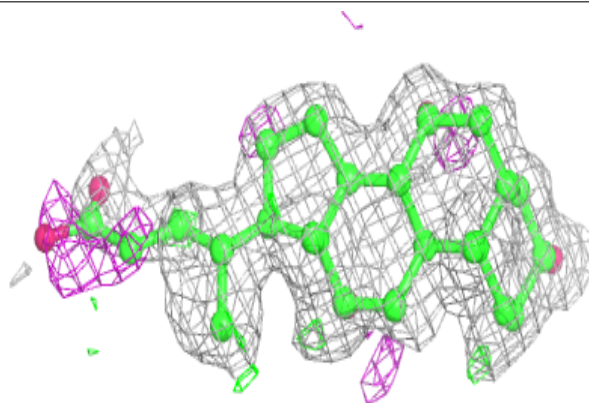


**Electron density around CHD A 3:**

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

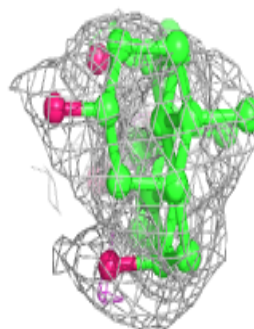
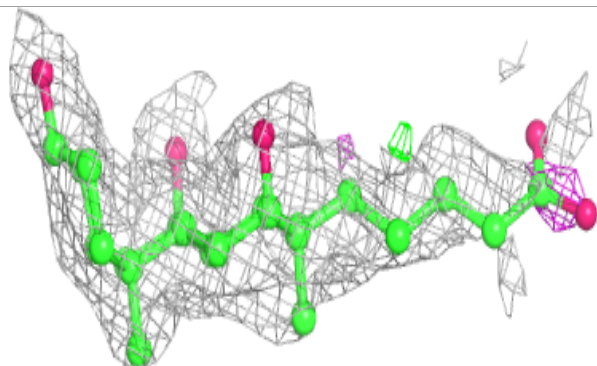
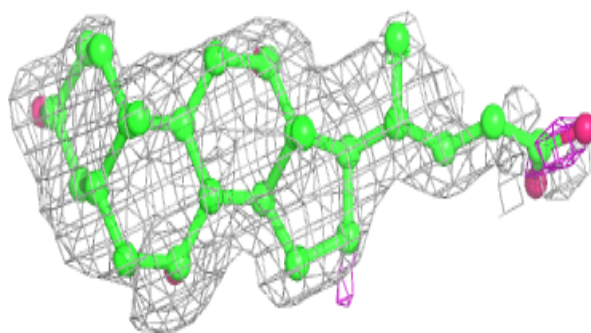
**Electron density around CHD B 1:**

$2mF_o-DF_c$  (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:**

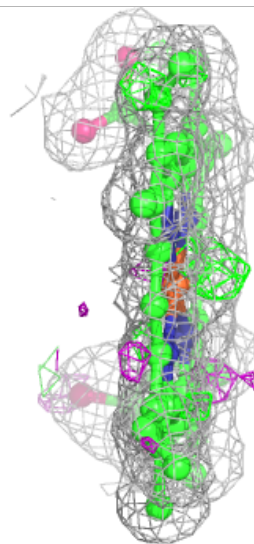
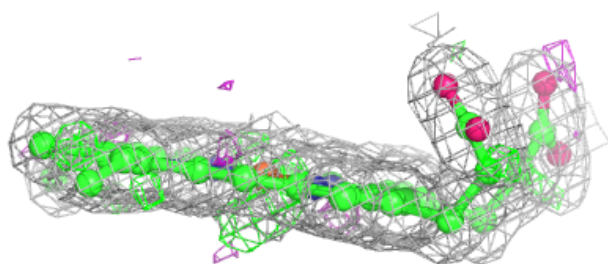
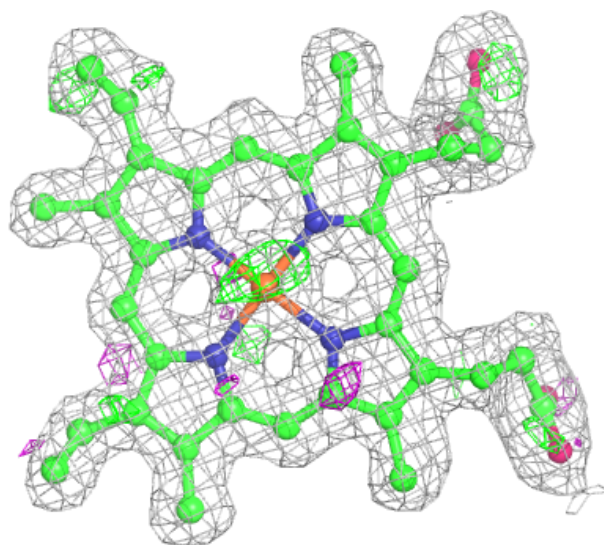
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM A 424:**

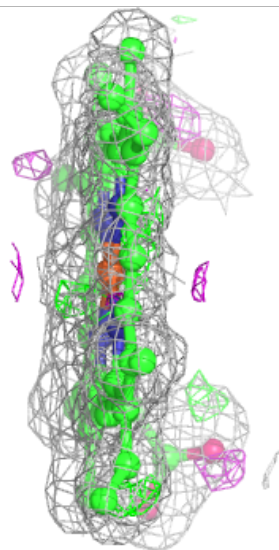
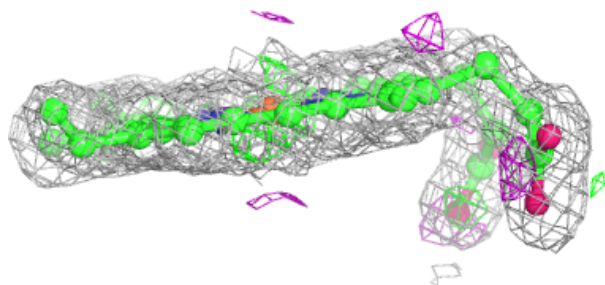
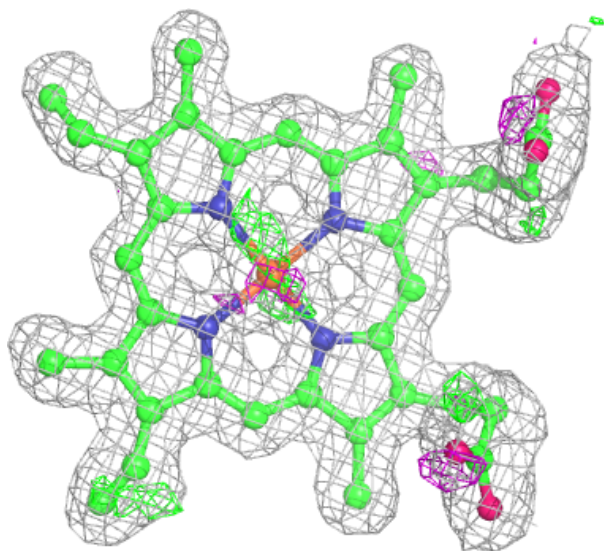
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**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.