



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 03:54 AM EST

PDB ID : 3HCO
Title : Human ferrochelatase with Cd and protoporphyrin IX bound
Authors : Medlock, A.E.; Dailey, H.A.; Lanzilotta, W.N.
Deposited on : 2009-05-06
Resolution : 1.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

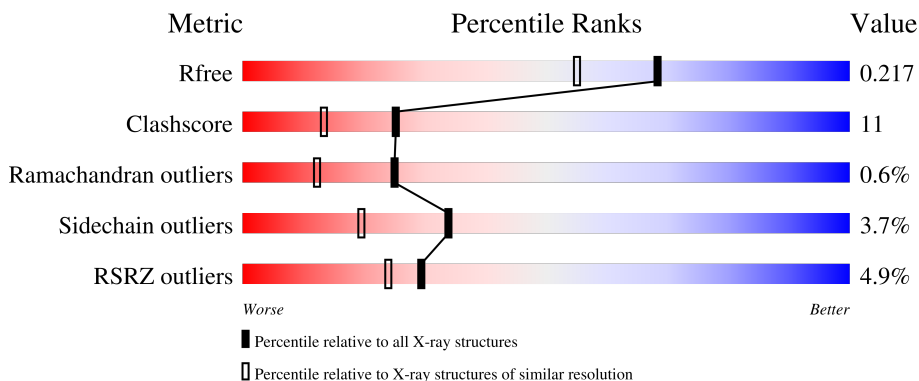
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	
1	B	359	

2 Entry composition [i](#)

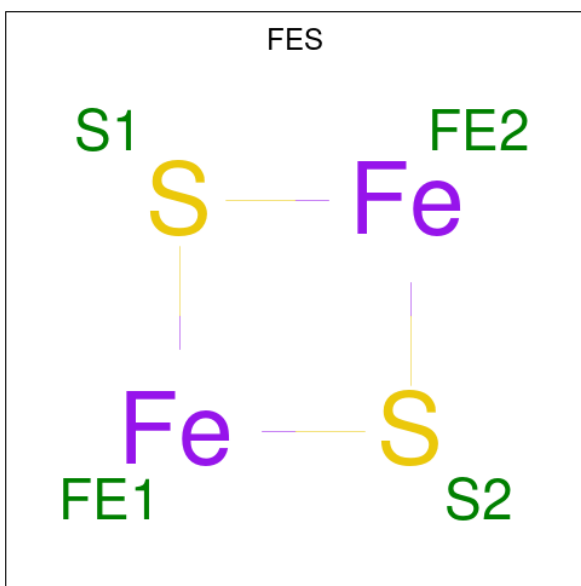
There are 9 unique types of molecules in this entry. The entry contains 6479 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	359	2923	1860	509	535	19	0	5	0
1	B	359	2917	1858	506	534	19	0	5	0

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



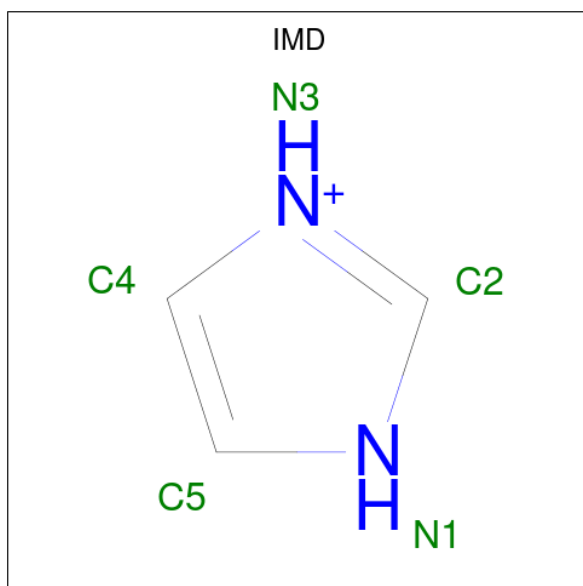
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	4	2	2	0	0
2	B	1	4	2	2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



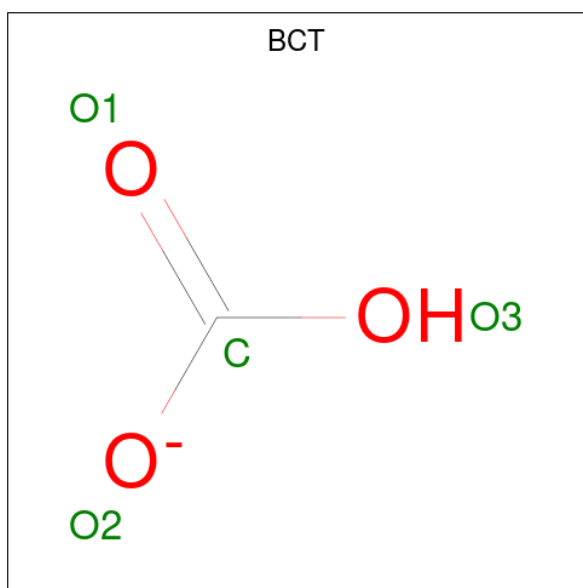
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		

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



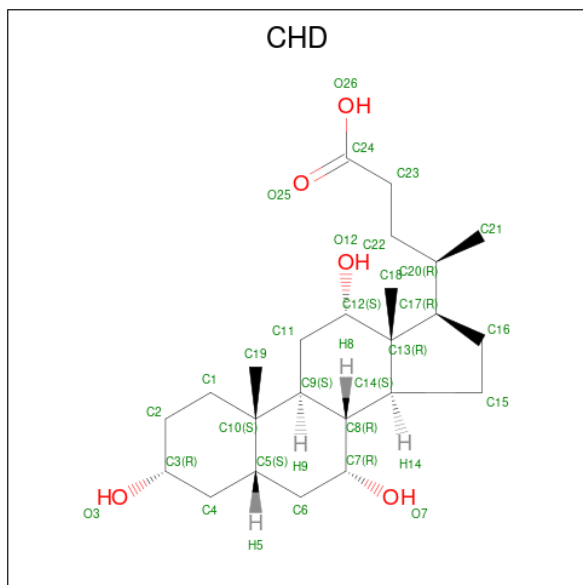
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 6 is CHOLIC ACID (three-letter code: CHD) (formula: $\text{C}_{24}\text{H}_{40}\text{O}_5$).



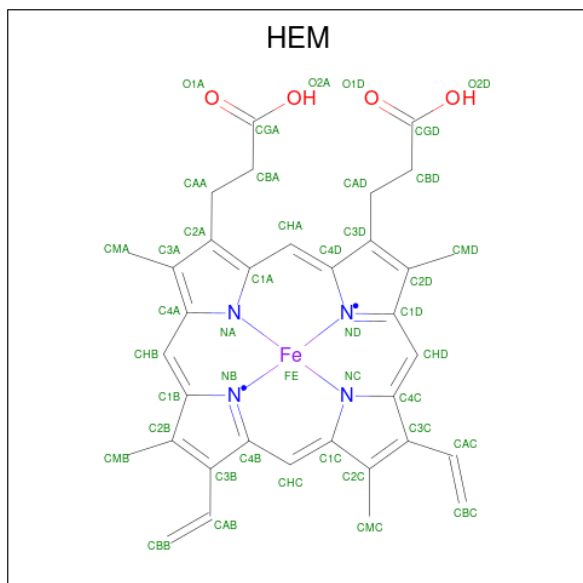
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			29	24	5		
6	A	1	Total	C	O	0	0
			29	24	5		

Continued on next page...

Continued from previous page...

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

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

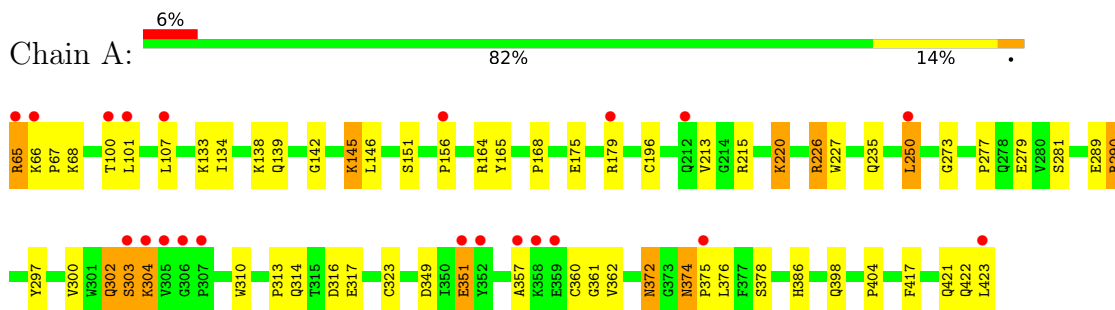
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	202	Total	O	0	0
			202	202		
9	B	191	Total	O	0	0
			191	191		

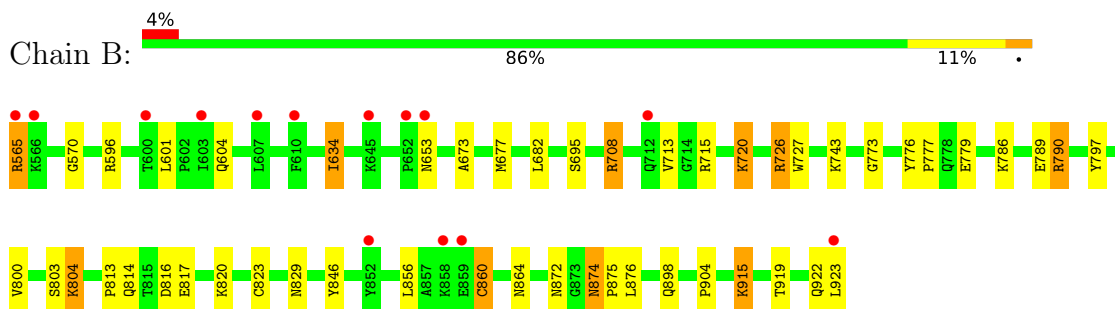
3 Residue-property plots [i](#)

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: Ferrochelatase, mitochondrial



- Molecule 1: Ferrochelatase, mitochondrial



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.27Å 92.83Å 109.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 1.80 47.18 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.19-1.80) 99.8 (47.18-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.210 , 0.252 0.215 , 0.217	Depositor DCC
R_{free} test set	4181 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtrriage
Anisotropy	0.056	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.8	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	0.95	EDS
Total number of atoms	6479	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 40.02 % 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 2.9125e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, BCT, HEM, IMD, CHD, GOL, 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	0.82	0/2999	0.84	3/4061 (0.1%)
1	B	0.81	0/3002	0.81	2/4066 (0.0%)
All	All	0.82	0/6001	0.83	5/8127 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	ARG	NE-CZ-NH1	13.61	127.11	120.30
1	B	726	ARG	NE-CZ-NH1	12.78	126.69	120.30
1	A	226	ARG	NE-CZ-NH2	-12.30	114.15	120.30
1	B	726	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	A	196	CYS	CA-CB-SG	-5.02	104.96	114.00

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	2923	0	2935	73	0
1	B	2917	0	2932	53	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	16	3	0
4	A	5	0	4	1	0
4	B	10	0	8	3	0
5	A	4	0	0	0	0
6	A	58	0	78	8	0
6	B	58	0	78	3	0
7	A	43	0	30	0	0
7	B	43	0	30	2	0
8	B	5	0	0	0	0
9	A	202	0	0	8	0
9	B	191	0	0	6	0
All	All	6479	0	6111	131	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 11.

All (131) 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:B:823[A]:CYS:SG	1:B:860:CYS:HB2	1.90	1.11
1:B:708:ARG:HH11	1:B:708:ARG:HG3	0.97	1.07
1:A:303[B]:SER:O	1:A:304[B]:LYS:CB	2.02	1.05
1:B:789[A]:GLU:OE1	9:B:315:HOH:O	1.78	1.00
1:B:720:LYS:HE3	1:B:923:LEU:HD22	1.43	0.99
1:A:303[B]:SER:O	1:A:304[B]:LYS:HB3	1.15	0.97
1:A:145:LYS:HD3	9:A:572:HOH:O	1.65	0.97
1:A:290:ARG:HH11	1:A:290:ARG:HG2	1.31	0.96
1:B:708:ARG:HG3	1:B:708:ARG:NH1	1.76	0.94
1:A:297:TYR:H	1:B:898:GLN:HE22	1.15	0.91
1:A:100:THR:HB	9:A:565:HOH:O	1.70	0.91
1:A:304[B]:LYS:HB2	1:A:310:TRP:CD2	2.05	0.91
1:A:134:ILE:H	1:A:134:ILE:HD12	1.36	0.89
1:B:708:ARG:HH11	1:B:708:ARG:CG	1.86	0.88
1:B:790:ARG:HG2	1:B:790:ARG:HH11	1.41	0.85
1:B:634:ILE:HD12	1:B:634:ILE:H	1.42	0.84
1:A:398:GLN:HE22	1:B:797:TYR:H	1.26	0.83
1:A:314:GLN:HB3	1:A:317:GLU:HG2	1.61	0.82
1:A:302[A]:GLN:NE2	9:A:475:HOH:O	2.01	0.81
1:A:304[A]:LYS:HE2	1:A:314:GLN:HE21	1.45	0.81
1:B:814[B]:GLN:HB2	1:B:817:GLU:HG2	1.63	0.81
1:A:100:THR:HG22	9:A:533:HOH:O	1.79	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLN:HG3	1:A:372:ASN:ND2	1.97	0.79
1:A:303[B]:SER:HA	1:A:314:GLN:HG3	1.65	0.79
6:A:4:CHD:H213	6:A:4:CHD:H183	1.64	0.79
1:A:101:LEU:HD21	6:A:4:CHD:H151	1.64	0.78
1:B:789[A]:GLU:HG3	9:B:261:HOH:O	1.84	0.77
1:A:303[A]:SER:O	4:A:424:IMD:H4	1.84	0.77
1:A:303[B]:SER:CA	1:A:314:GLN:HG3	2.17	0.75
1:B:634:ILE:HD12	1:B:634:ILE:N	2.03	0.74
1:A:250:LEU:H	1:A:250:LEU:HD23	1.54	0.72
1:B:720:LYS:CE	1:B:923:LEU:HD22	2.19	0.72
1:A:323[A]:CYS:SG	1:A:362:VAL:HB	2.30	0.72
1:A:290:ARG:HH11	1:A:290:ARG:CG	2.03	0.71
1:B:915:LYS:HE2	1:B:919:THR:HG21	1.72	0.71
1:B:634:ILE:H	1:B:634:ILE:CD1	2.03	0.70
1:A:303[B]:SER:HB2	1:A:314:GLN:HE21	1.56	0.70
1:A:303[B]:SER:HB2	1:A:314:GLN:NE2	2.07	0.69
1:B:803:SER:O	4:B:2:IMD:H4	1.93	0.69
1:B:814[A]:GLN:HG3	9:B:317:HOH:O	1.93	0.68
1:A:134:ILE:H	1:A:134:ILE:CD1	2.05	0.67
1:A:374:ASN:ND2	1:A:376:LEU:H	1.93	0.67
1:A:349:ASP:OD1	1:A:351:GLU:HG2	1.94	0.67
6:A:3:CHD:H183	6:A:3:CHD:H212	1.76	0.66
1:A:303[B]:SER:CB	1:A:314:GLN:HG3	2.26	0.65
1:B:790:ARG:HH11	1:B:790:ARG:CG	2.10	0.65
1:A:304[B]:LYS:HB2	1:A:310:TRP:CG	2.32	0.65
6:A:4:CHD:H183	6:A:4:CHD:C21	2.28	0.64
1:A:134:ILE:HD12	1:A:134:ILE:N	2.10	0.63
1:A:289:GLU:OE1	9:A:556:HOH:O	2.15	0.63
1:A:304[A]:LYS:HE2	1:A:314:GLN:NE2	2.14	0.62
1:A:304[A]:LYS:CE	1:A:314:GLN:HE21	2.11	0.62
1:A:142:GLY:HA2	1:A:145:LYS:HE3	1.81	0.62
1:B:601:LEU:HD21	6:B:924:CHD:H151	1.82	0.61
1:A:100:THR:CB	9:A:565:HOH:O	2.39	0.61
1:B:814[A]:GLN:OE1	1:B:816:ASP:HB2	2.01	0.60
1:A:226:ARG:HD3	1:A:279:GLU:OE2	2.01	0.59
1:B:565:ARG:N	1:B:565:ARG:HE	2.00	0.59
1:B:804:LYS:HE3	9:B:371:HOH:O	2.02	0.58
1:A:374:ASN:HD22	1:A:376:LEU:H	1.50	0.58
6:A:4:CHD:C21	6:A:4:CHD:C18	2.81	0.58
3:A:1[A]:GOL:H2	1:B:777:PRO:HB3	1.86	0.58
1:A:133:LYS:HE3	1:A:168:PRO:HD3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:922:GLN:O	1:B:923:LEU:HB2	2.03	0.56
1:A:300:VAL:HG12	1:A:313:PRO:HG2	1.88	0.56
1:B:713:VAL:HG23	1:B:715:ARG:HG2	1.86	0.56
9:A:534:HOH:O	1:B:786:LYS:HD2	2.06	0.55
1:A:213:VAL:HG23	1:A:215:ARG:HG2	1.87	0.55
1:A:139:GLN:HG3	1:A:372:ASN:HD22	1.69	0.55
1:A:422:GLN:O	1:A:423:LEU:HB2	2.07	0.54
1:A:277:PRO:HB3	3:A:1[B]:GOL:H2	1.88	0.54
1:A:303[B]:SER:OG	1:A:304[B]:LYS:N	2.37	0.54
1:A:139:GLN:NE2	1:A:378:SER:OG	2.41	0.53
1:A:297:TYR:N	1:B:898:GLN:HE22	1.96	0.53
1:B:874:ASN:ND2	1:B:876:LEU:H	2.08	0.52
1:B:915:LYS:HE2	1:B:919:THR:CG2	2.38	0.52
1:A:290:ARG:CG	1:A:290:ARG:NH1	2.67	0.51
1:B:800:VAL:HG12	1:B:813:PRO:HG2	1.91	0.51
1:A:302[B]:GLN:O	1:A:304[B]:LYS:N	2.43	0.51
1:B:789[A]:GLU:CG	9:B:261:HOH:O	2.50	0.51
1:A:398:GLN:HE22	1:B:797:TYR:N	2.03	0.51
1:A:357:ALA:O	1:A:361:GLY:HA2	2.11	0.51
1:A:290:ARG:HG2	1:A:290:ARG:NH1	2.11	0.51
1:A:175:GLU:O	1:A:179:ARG:HD3	2.10	0.51
1:A:145:LYS:HD2	1:A:146:LEU:N	2.26	0.50
1:A:164:ARG:HG3	1:A:165:TYR:CE2	2.45	0.50
1:B:874:ASN:C	1:B:874:ASN:HD22	2.15	0.50
1:B:922:GLN:HG2	1:B:923:LEU:HD13	1.94	0.50
1:B:726:ARG:HD3	1:B:779:GLU:OE2	2.12	0.50
1:B:790:ARG:CG	1:B:790:ARG:NH1	2.75	0.50
1:A:374:ASN:HD22	1:A:375:PRO:N	2.09	0.50
1:A:374:ASN:HD22	1:A:374:ASN:C	2.16	0.49
1:A:66:LYS:HG2	1:A:67:PRO:HD2	1.95	0.49
1:B:874:ASN:HD22	1:B:875:PRO:N	2.11	0.49
1:A:273:GLY:HA2	1:B:813:PRO:HG3	1.93	0.48
1:A:273:GLY:HA3	1:A:404:PRO:HD2	1.95	0.48
1:B:773:GLY:HA3	1:B:904:PRO:HD2	1.95	0.48
6:B:924:CHD:H212	6:B:924:CHD:H183	1.96	0.48
1:B:708:ARG:NH1	1:B:708:ARG:CG	2.55	0.47
1:A:281:SER:OG	3:A:1[B]:GOL:H31	2.14	0.47
1:A:303[B]:SER:HB2	1:A:314:GLN:HG3	1.97	0.47
1:B:601:LEU:HD12	1:B:604:GLN:HG3	1.97	0.47
4:B:3:IMD:H2	7:B:926:HEM:C4C	2.50	0.46
1:A:139:GLN:HE22	1:A:378:SER:N	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:PHE:O	1:A:421:GLN:HG2	2.14	0.46
1:B:823[A]:CYS:SG	1:B:860:CYS:CB	2.83	0.46
1:A:304[B]:LYS:HB2	1:A:310:TRP:CE3	2.49	0.45
6:A:3:CHD:H12A	6:A:3:CHD:H112	1.73	0.45
1:B:596:ARG:NH2	1:B:604:GLN:HB3	2.32	0.45
1:B:829:ASN:HD22	1:B:864:ASN:HB2	1.81	0.45
4:B:3:IMD:C2	7:B:926:HEM:NC	2.81	0.45
1:A:235:GLN:HG3	1:A:290:ARG:HH12	1.82	0.44
6:A:4:CHD:H112	6:A:4:CHD:H12A	1.78	0.44
1:A:65:ARG:HB2	1:A:156:PRO:HG3	1.99	0.44
1:A:314:GLN:OE1	1:A:316:ASP:HB2	2.18	0.44
1:A:313:PRO:HG3	1:B:773:GLY:HA2	2.00	0.44
1:B:570:GLY:HA3	1:B:682:LEU:HD13	2.00	0.43
1:B:673:ALA:O	1:B:677:MET:HG3	2.19	0.43
6:B:1:CHD:H12	6:B:1:CHD:H212	2.00	0.43
1:A:68:LYS:HB2	1:A:156:PRO:HD2	2.01	0.43
1:B:874:ASN:HD22	1:B:876:LEU:H	1.66	0.42
1:B:695:SER:HB2	1:B:776:TYR:HB2	2.01	0.42
1:A:372:ASN:HD22	1:A:372:ASN:HA	1.74	0.42
1:A:220:LYS:HE3	1:A:423:LEU:HD22	2.01	0.42
1:B:790:ARG:NH1	9:B:227:HOH:O	2.52	0.41
1:B:846:TYR:CD2	1:B:856:LEU:HD22	2.55	0.41
1:B:820:LYS:HA	1:B:856:LEU:HD11	2.02	0.41
6:A:4:CHD:H213	6:A:4:CHD:C18	2.41	0.41
1:A:304[A]:LYS:CE	1:A:314:GLN:NE2	2.78	0.41
1:A:179:ARG:NH1	9:A:449:HOH:O	2.54	0.41
1:A:151:SER:HB2	1:A:386:HIS:CD2	2.56	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	362/359 (101%)	347 (96%)	9 (2%)	6 (2%)	9	2
1	B	362/359 (101%)	353 (98%)	7 (2%)	2 (1%)	25	12
All	All	724/718 (101%)	700 (97%)	16 (2%)	8 (1%)	25	4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303[A]	SER
1	A	303[B]	SER
1	A	304[A]	LYS
1	A	304[B]	LYS
1	B	872[A]	ASN
1	B	872[B]	ASN
1	A	302[A]	GLN
1	A	302[B]	GLN

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/324 (102%)	317 (96%)	12 (4%)	35	20
1	B	329/324 (102%)	317 (96%)	12 (4%)	35	20
All	All	658/648 (102%)	634 (96%)	24 (4%)	34	20

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	107	LEU
1	A	138	LYS
1	A	145	LYS
1	A	220	LYS
1	A	227	TRP
1	A	250	LEU
1	A	290	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	351	GLU
1	A	360	CYS
1	A	372	ASN
1	A	374	ASN
1	B	565	ARG
1	B	634	ILE
1	B	653	ASN
1	B	708	ARG
1	B	720	LYS
1	B	727	TRP
1	B	743	LYS
1	B	790	ARG
1	B	804	LYS
1	B	860	CYS
1	B	874	ASN
1	B	915	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	247	HIS
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	622	GLN
1	B	829	ASN
1	B	864	ASN
1	B	874	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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	GOL	A	1[A]	-	5,5,5	0.46	0	5,5,5	1.05	0
2	FES	A	501	1	0,4,4	-	-	-		
3	GOL	A	1[B]	-	5,5,5	0.44	0	5,5,5	0.94	0
6	CHD	A	3	-	32,32,32	0.96	1 (3%)	51,51,51	1.95	15 (29%)
8	SO4	B	925	-	4,4,4	0.14	0	6,6,6	0.12	0
6	CHD	B	1	-	32,32,32	0.65	0	51,51,51	1.12	3 (5%)
4	IMD	A	424	7	3,5,5	0.27	0	4,5,5	0.39	0
5	BCT	A	425	7	2,3,3	0.78	0	2,3,3	0.76	0
7	HEM	A	426	4,5	41,50,50	1.97	7 (17%)	45,82,82	1.70	11 (24%)
7	HEM	B	926	4	41,50,50	1.84	7 (17%)	45,82,82	1.78	12 (26%)
4	IMD	B	3	7	3,5,5	0.49	0	4,5,5	0.26	0
4	IMD	B	2	7	3,5,5	0.24	0	4,5,5	0.25	0
6	CHD	A	4	-	32,32,32	0.79	1 (3%)	51,51,51	1.69	11 (21%)
2	FES	B	501	1	0,4,4	-	-	-		
6	CHD	B	924	-	32,32,32	0.67	0	51,51,51	1.44	5 (9%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1[A]	-	-	1/4/4/4	-
3	GOL	A	1[B]	-	-	1/4/4/4	-
6	CHD	A	3	-	-	8/9/74/74	0/4/4/4
2	FES	A	501	1	-	-	0/1/1/1
6	CHD	B	1	-	-	5/9/74/74	0/4/4/4
7	HEM	A	426	4,5	-	4/12/54/54	-
4	IMD	A	424	7	-	-	0/1/1/1
4	IMD	B	3	7	-	-	0/1/1/1
2	FES	B	501	1	-	-	0/1/1/1
4	IMD	B	2	7	-	-	0/1/1/1
6	CHD	A	4	-	-	8/9/74/74	0/4/4/4
7	HEM	B	926	4	-	4/12/54/54	-
6	CHD	B	924	-	-	8/9/74/74	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	426	HEM	C3D-C2D	7.93	1.53	1.36
7	B	926	HEM	C3D-C2D	7.64	1.53	1.36
6	A	3	CHD	C16-C15	4.21	1.65	1.54
7	A	426	HEM	C3C-C2C	-4.07	1.34	1.40
7	A	426	HEM	C3C-CAC	3.93	1.55	1.47
7	A	426	HEM	CAB-C3B	3.12	1.55	1.47
7	B	926	HEM	C3C-C2C	-3.10	1.36	1.40
7	A	426	HEM	C2C-C1C	2.97	1.49	1.42
7	B	926	HEM	CAA-C2A	2.85	1.56	1.52
7	B	926	HEM	C2C-C1C	2.67	1.48	1.42
7	B	926	HEM	CAB-C3B	2.54	1.54	1.47
7	B	926	HEM	CMB-C2B	2.50	1.56	1.50
7	A	426	HEM	CAA-C2A	2.42	1.55	1.52
7	B	926	HEM	C3C-CAC	2.37	1.52	1.47
7	A	426	HEM	CMB-C2B	2.25	1.55	1.50
6	A	4	CHD	C16-C15	2.25	1.60	1.54

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4	CHD	C9-C8-C7	-5.45	105.36	111.88
7	B	926	HEM	CMC-C2C-C3C	5.16	134.34	124.68
6	A	3	CHD	C1-C10-C5	5.13	115.36	107.77
6	B	924	CHD	C21-C20-C22	-4.68	103.03	110.36
7	A	426	HEM	C4D-ND-C1D	4.58	109.80	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	426	HEM	CMC-C2C-C3C	4.45	133.01	124.68
6	A	3	CHD	C1-C10-C9	-4.19	104.76	111.35
6	A	3	CHD	C16-C17-C13	4.11	107.58	103.55
6	A	4	CHD	C1-C10-C5	3.95	113.61	107.77
7	B	926	HEM	C4B-CHC-C1C	3.79	127.55	122.56
6	B	924	CHD	C1-C10-C5	3.77	113.34	107.77
7	A	426	HEM	C4C-CHD-C1D	3.73	127.48	122.56
6	A	4	CHD	C16-C17-C13	3.67	107.15	103.55
6	A	3	CHD	C4-C3-C2	-3.58	106.28	110.55
6	A	3	CHD	C6-C5-C10	3.56	116.43	112.66
6	A	3	CHD	C9-C10-C5	3.39	113.33	108.58
6	A	3	CHD	C21-C20-C17	3.29	117.96	112.92
6	A	4	CHD	C21-C20-C17	3.09	117.66	112.92
7	B	926	HEM	C1B-NB-C4B	2.98	108.15	105.07
6	A	3	CHD	C2-C1-C10	2.96	117.85	112.78
7	B	926	HEM	C1D-C2D-C3D	-2.90	103.91	106.96
7	A	426	HEM	CHA-C4D-ND	2.84	127.89	124.38
6	A	3	CHD	C16-C15-C14	-2.84	99.50	105.13
6	B	924	CHD	C21-C20-C17	2.79	117.19	112.92
6	A	3	CHD	C14-C13-C12	2.75	109.97	107.40
6	A	3	CHD	C19-C10-C5	-2.67	105.83	110.36
7	B	926	HEM	C4C-CHD-C1D	2.66	126.07	122.56
6	A	4	CHD	C2-C1-C10	2.65	117.32	112.78
6	B	924	CHD	C1-C10-C9	-2.57	107.31	111.35
6	A	4	CHD	C1-C10-C9	-2.56	107.33	111.35
6	B	1	CHD	C1-C10-C5	2.52	111.49	107.77
6	B	1	CHD	C15-C14-C13	2.51	106.02	103.55
6	A	3	CHD	C17-C13-C12	-2.50	115.38	117.67
6	A	3	CHD	C10-C9-C8	2.48	114.49	111.82
7	B	926	HEM	CAA-CBA-CGA	-2.44	106.91	113.76
6	A	4	CHD	C17-C13-C12	-2.42	115.46	117.67
7	A	426	HEM	C1D-C2D-C3D	-2.38	104.45	106.96
6	B	924	CHD	C19-C10-C5	-2.36	106.36	110.36
7	B	926	HEM	CMA-C3A-C4A	-2.34	124.86	128.46
6	A	4	CHD	C11-C9-C8	2.33	114.29	110.88
6	A	4	CHD	C19-C10-C5	-2.32	106.43	110.36
7	A	426	HEM	CHC-C4B-NB	2.29	126.92	124.43
7	A	426	HEM	O2A-CGA-CBA	2.29	121.38	114.03
7	B	926	HEM	O2A-CGA-CBA	2.26	121.29	114.03
7	B	926	HEM	C2C-C3C-C4C	2.23	108.46	106.90
7	A	426	HEM	CHD-C1D-ND	2.21	126.84	124.43
6	B	1	CHD	C17-C13-C12	-2.18	115.67	117.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	426	HEM	O1A-CGA-CBA	-2.18	116.09	123.08
6	A	4	CHD	C4-C5-C10	2.17	114.96	112.66
7	A	426	HEM	C2C-C3C-C4C	2.15	108.40	106.90
6	A	4	CHD	C23-C22-C20	-2.13	110.62	114.52
7	B	926	HEM	C4B-C3B-C2B	2.13	108.81	107.11
6	A	3	CHD	C13-C17-C20	2.12	122.02	119.50
7	B	926	HEM	O1A-CGA-CBA	-2.07	116.42	123.08
7	B	926	HEM	O1D-CGD-CBD	-2.03	116.55	123.08
7	A	426	HEM	CAA-CBA-CGA	-2.02	108.09	113.76
6	A	3	CHD	C4-C5-C10	2.01	114.79	112.66

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	4	CHD	C16-C17-C20-C22
6	A	3	CHD	C13-C17-C20-C21
6	A	3	CHD	C13-C17-C20-C22
6	A	3	CHD	C16-C17-C20-C22
6	B	1	CHD	C20-C22-C23-C24
6	A	3	CHD	C17-C20-C22-C23
6	A	3	CHD	C16-C17-C20-C21
6	A	4	CHD	C13-C17-C20-C21
6	B	924	CHD	C16-C17-C20-C22
6	A	4	CHD	C17-C20-C22-C23
6	A	4	CHD	C21-C20-C22-C23
6	B	924	CHD	C21-C20-C22-C23
6	B	1	CHD	C17-C20-C22-C23
6	B	924	CHD	C17-C20-C22-C23
6	A	3	CHD	C21-C20-C22-C23
6	A	4	CHD	C16-C17-C20-C21
6	A	4	CHD	C13-C17-C20-C22
6	B	1	CHD	C21-C20-C22-C23
6	B	924	CHD	C13-C17-C20-C21
6	B	924	CHD	C13-C17-C20-C22
3	A	1[A]	GOL	O1-C1-C2-O2
3	A	1[B]	GOL	O2-C2-C3-O3
6	B	1	CHD	C22-C23-C24-O26
6	A	3	CHD	C22-C23-C24-O26
6	A	3	CHD	C22-C23-C24-O25
6	B	1	CHD	C22-C23-C24-O25
6	B	924	CHD	C16-C17-C20-C21

Continued on next page...

Continued from previous page...

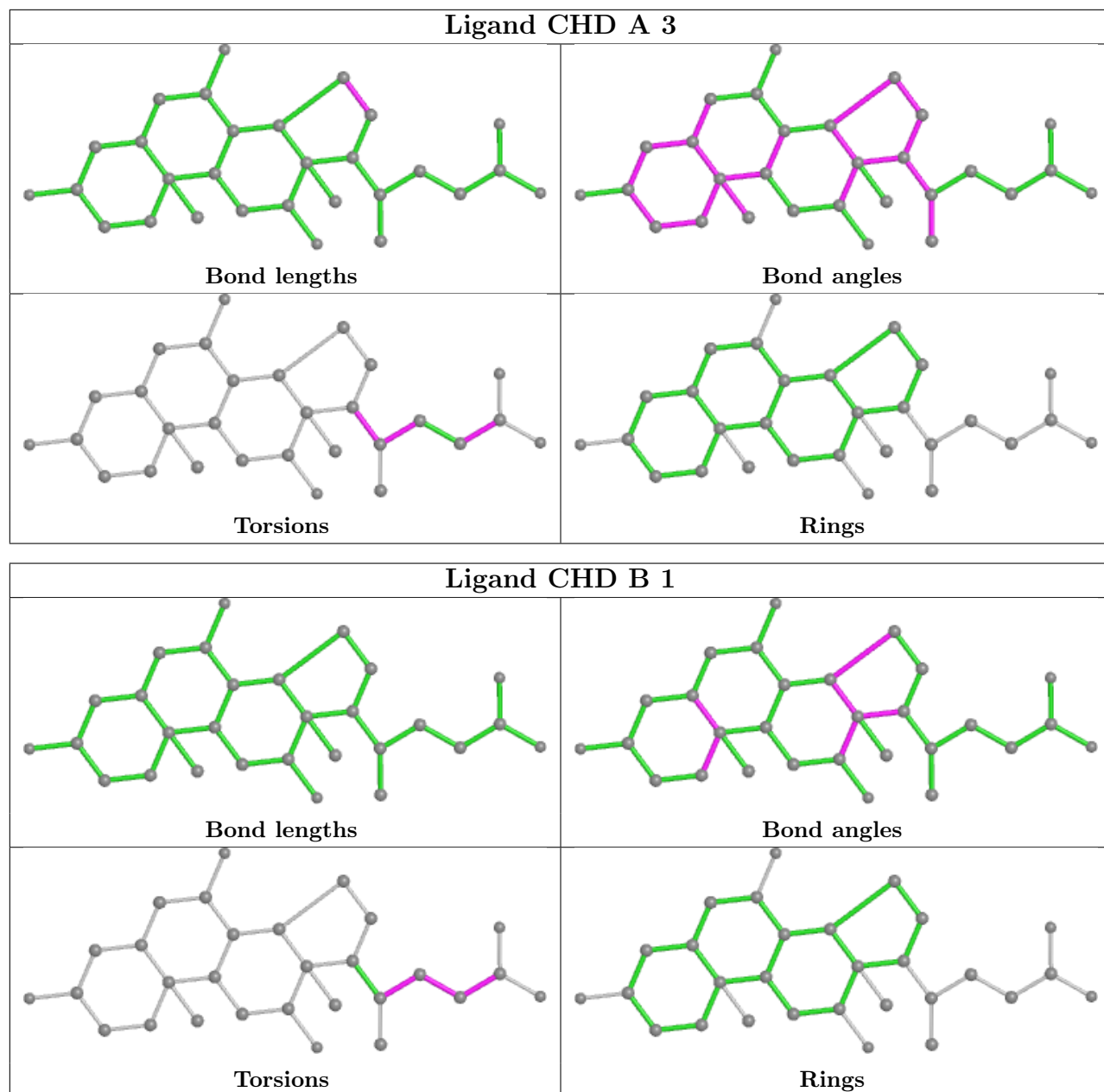
Mol	Chain	Res	Type	Atoms
7	A	426	HEM	CAD-CBD-CGD-O1D
7	B	926	HEM	CAD-CBD-CGD-O2D
7	B	926	HEM	CAD-CBD-CGD-O1D
7	A	426	HEM	CAD-CBD-CGD-O2D
7	A	426	HEM	CAA-CBA-CGA-O1A
6	B	924	CHD	C22-C23-C24-O26
7	B	926	HEM	CAA-CBA-CGA-O1A
6	B	924	CHD	C22-C23-C24-O25
6	A	4	CHD	C22-C23-C24-O26
6	A	4	CHD	C22-C23-C24-O25
7	B	926	HEM	CAA-CBA-CGA-O2A
7	A	426	HEM	CAA-CBA-CGA-O2A

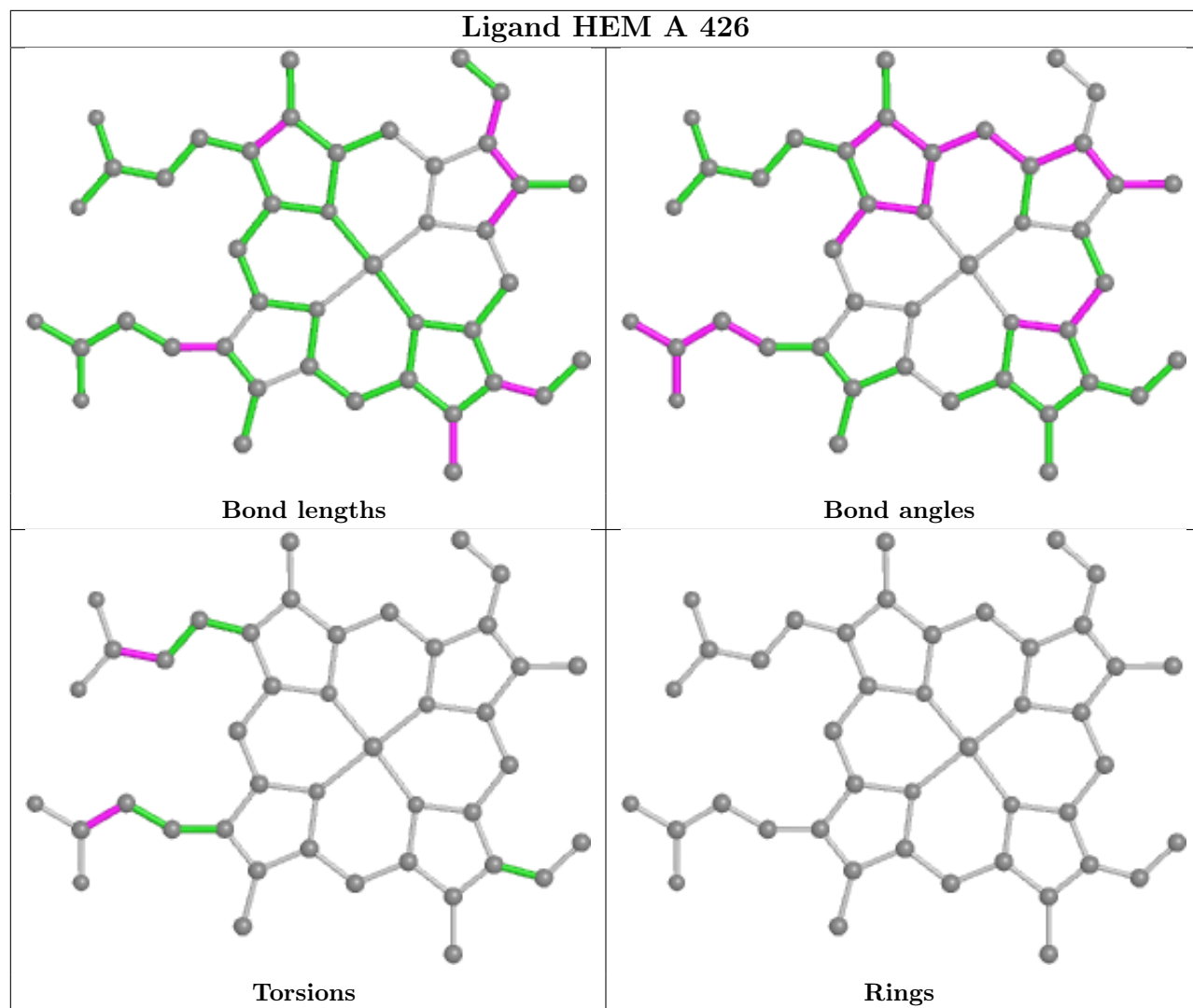
There are no ring outliers.

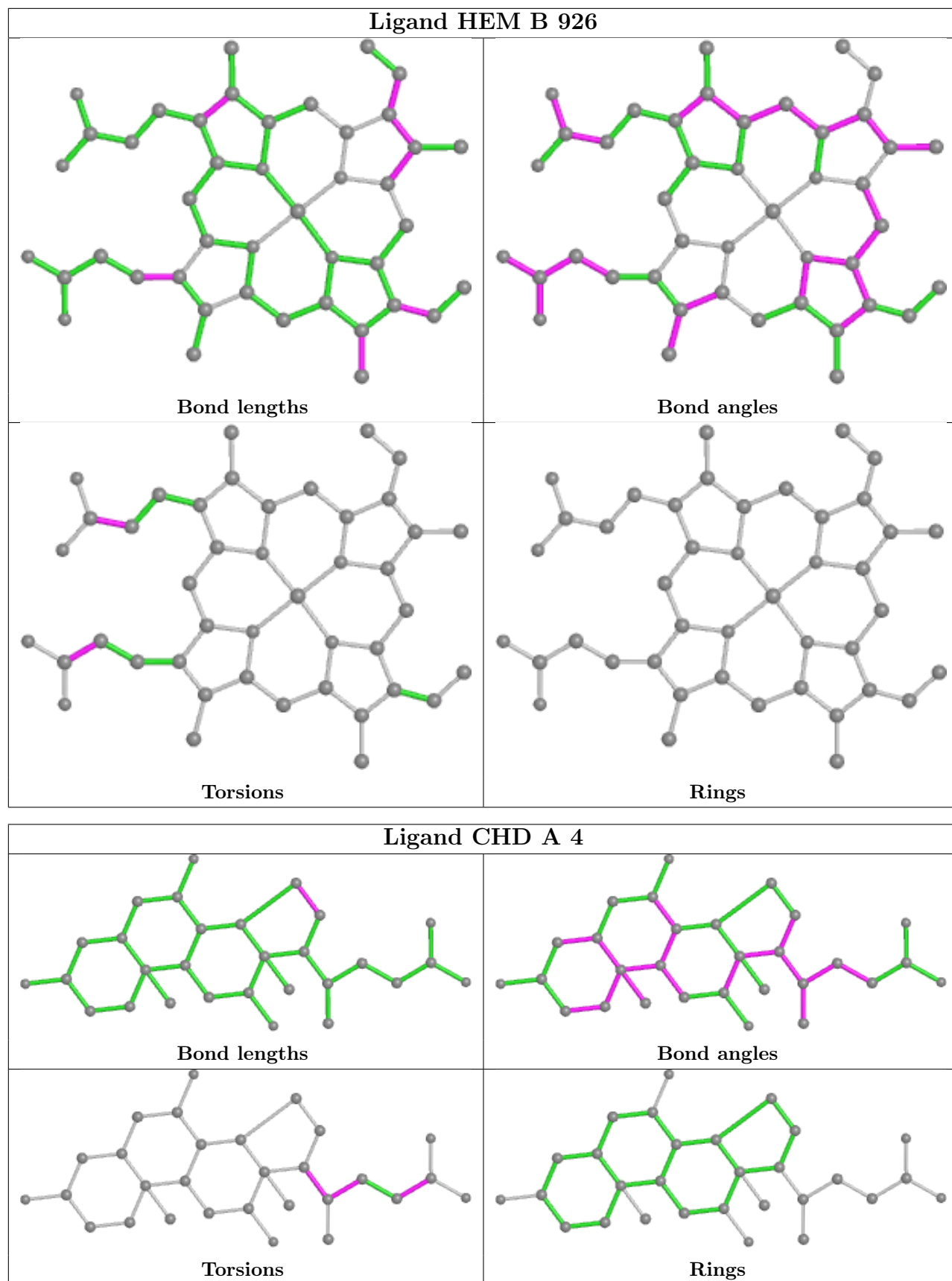
10 monomers are involved in 18 short contacts:

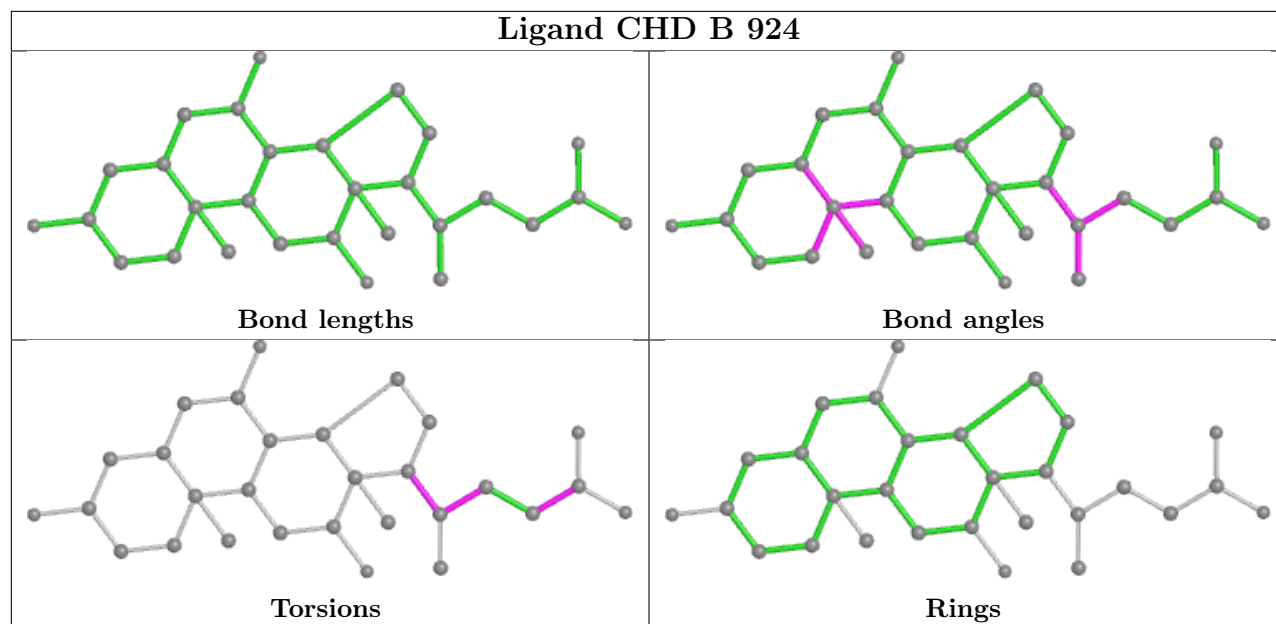
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1[A]	GOL	1	0
3	A	1[B]	GOL	2	0
6	A	3	CHD	2	0
6	B	1	CHD	1	0
4	A	424	IMD	1	0
7	B	926	HEM	2	0
4	B	3	IMD	2	0
4	B	2	IMD	1	0
6	A	4	CHD	6	0
6	B	924	CHD	2	0

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.









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%)	0.31	21 (5%) 23 18	6, 22, 44, 53	0
1	B	359/359 (100%)	0.30	14 (3%) 39 33	7, 24, 44, 54	0
All	All	718/718 (100%)	0.31	35 (4%) 29 24	6, 23, 44, 54	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	607	LEU	4.7
1	A	65	ARG	4.7
1	B	610	PHE	4.5
1	A	306	GLY	4.3
1	B	565	ARG	3.7
1	A	305	VAL	3.6
1	A	423	LEU	3.4
1	A	307	PRO	3.3
1	A	352	TYR	3.1
1	A	107	LEU	3.1
1	B	603	ILE	3.1
1	A	357	ALA	3.1
1	A	303[A]	SER	3.0
1	A	359	GLU	2.9
1	B	852	TYR	2.9
1	B	653	ASN	2.8
1	A	250	LEU	2.8
1	A	66	LYS	2.8
1	A	212	GLN	2.8
1	B	566	LYS	2.7
1	B	923	LEU	2.7
1	A	358	LYS	2.6
1	B	712	GLN	2.6
1	A	100	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	101	LEU	2.4
1	A	156	PRO	2.3
1	B	652	PRO	2.3
1	B	858	LYS	2.3
1	B	600	THR	2.2
1	B	645	LYS	2.2
1	B	859	GLU	2.2
1	A	375	PRO	2.1
1	A	304[A]	LYS	2.1
1	A	179	ARG	2.0
1	A	351	GLU	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 monosaccharides 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.

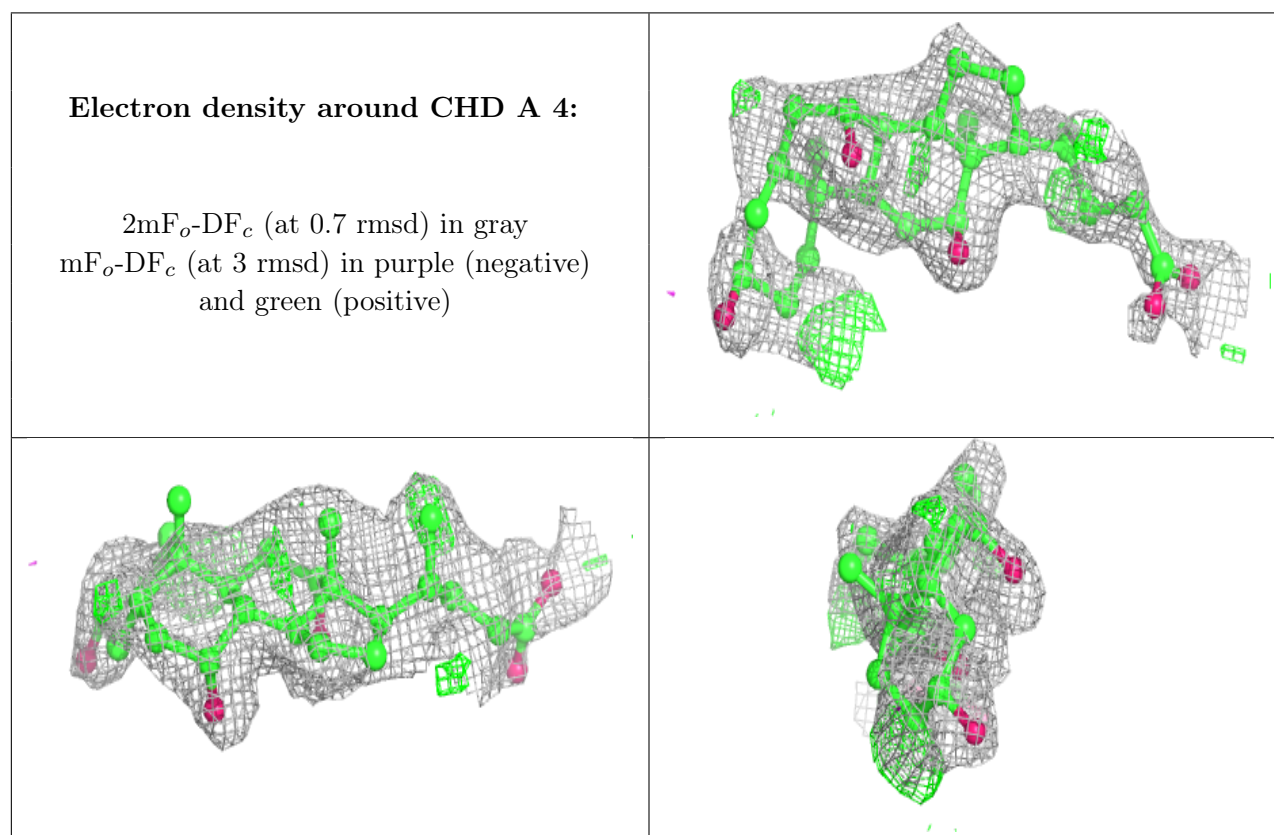
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CHD	A	4	29/29	0.67	0.25	64,68,71,72	0
6	CHD	A	3	29/29	0.68	0.35	103,104,107,107	0
6	CHD	B	924	29/29	0.77	0.21	36,38,55,57	0
6	CHD	B	1	29/29	0.81	0.27	54,55,66,67	0
4	IMD	A	424	5/5	0.90	0.15	20,21,22,25	0
5	BCT	A	425	4/4	0.91	0.18	39,41,42,42	0
4	IMD	B	3	5/5	0.93	0.12	28,29,30,31	0
8	SO4	B	925	5/5	0.93	0.19	65,66,67,67	0
3	GOL	A	1[A]	6/6	0.95	0.20	7,10,11,12	6
3	GOL	A	1[B]	6/6	0.95	0.20	8,9,12,13	6
7	HEM	B	926	43/43	0.97	0.10	11,17,24,30	0
4	IMD	B	2	5/5	0.97	0.09	22,22,22,24	0

Continued on next page...

Continued from previous page...

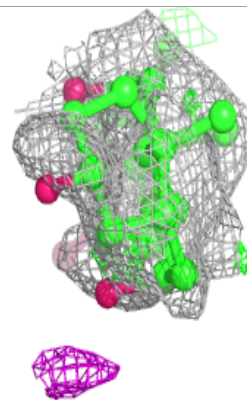
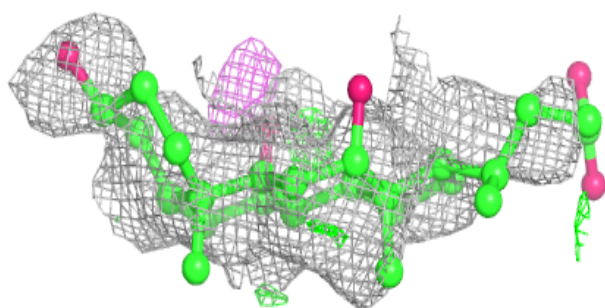
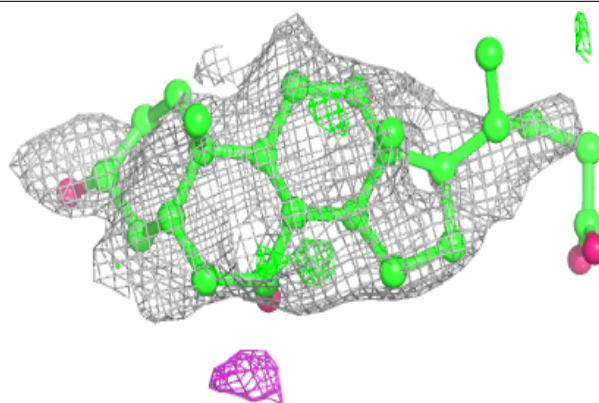
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	HEM	A	426	43/43	0.98	0.10	11,17,23,27	0
2	FES	A	501	4/4	0.98	0.08	16,18,18,22	0
2	FES	B	501	4/4	0.98	0.08	17,19,19,21	0

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.

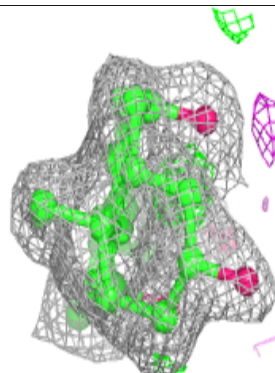
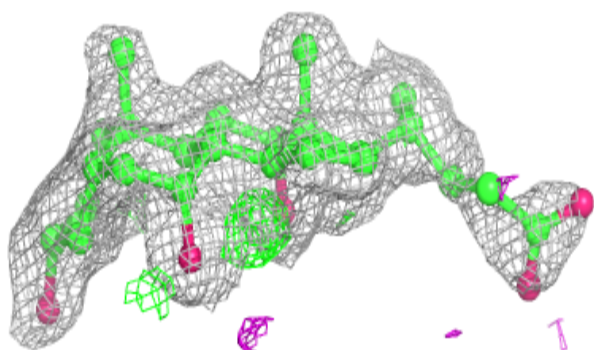
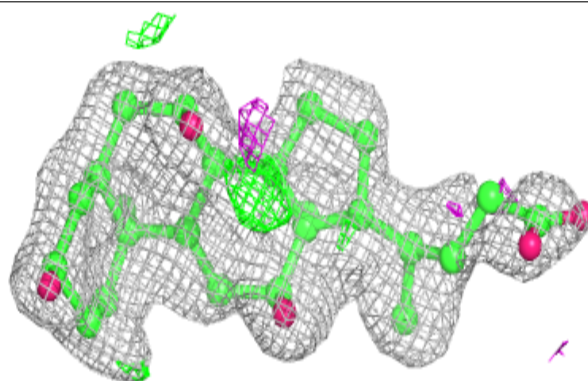


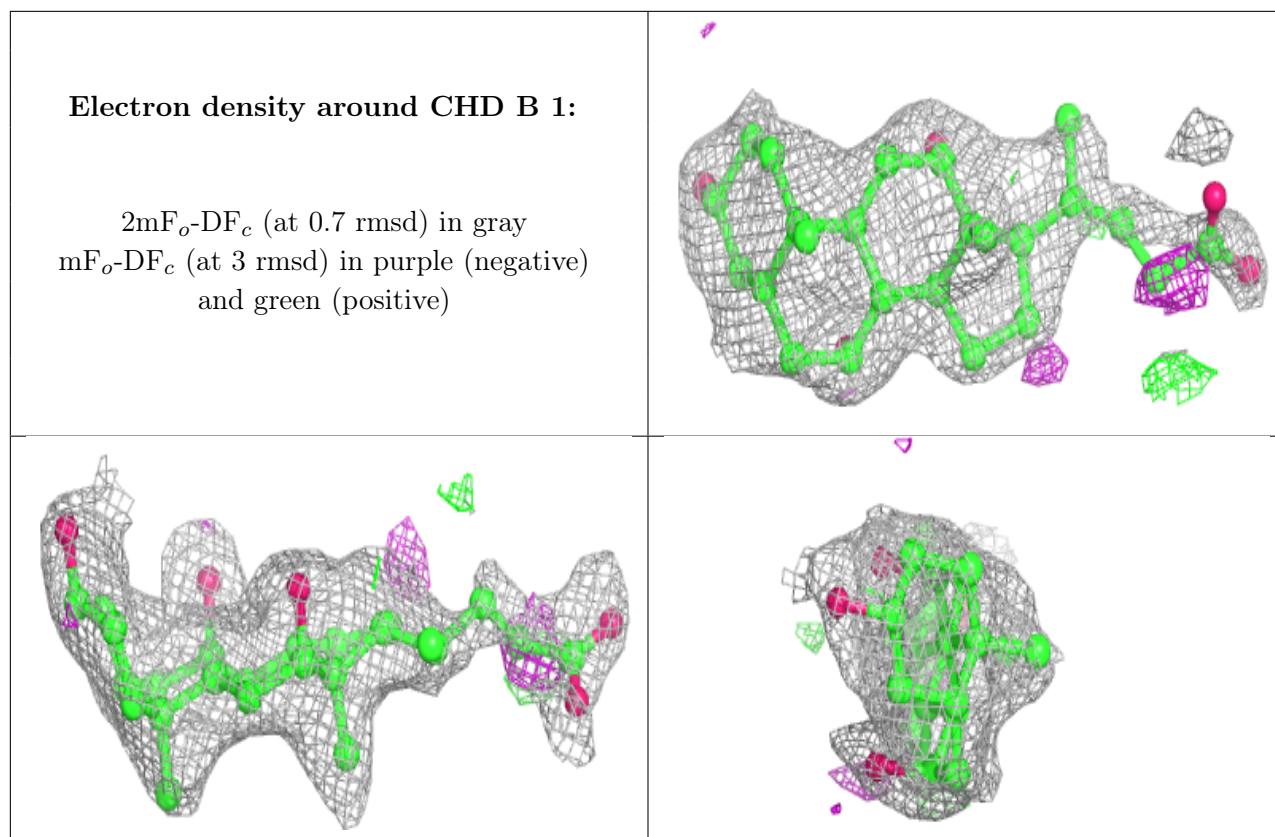
Electron density around CHD A 3:

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

**Electron density around CHD B 924:**

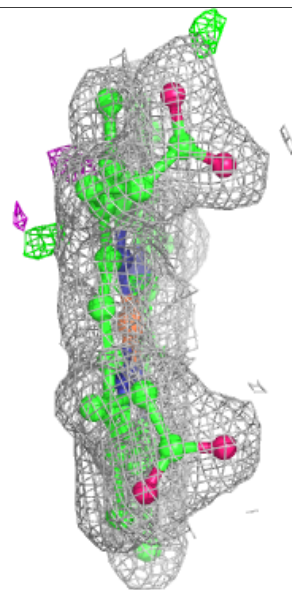
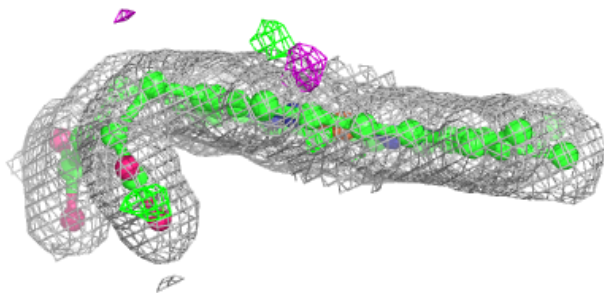
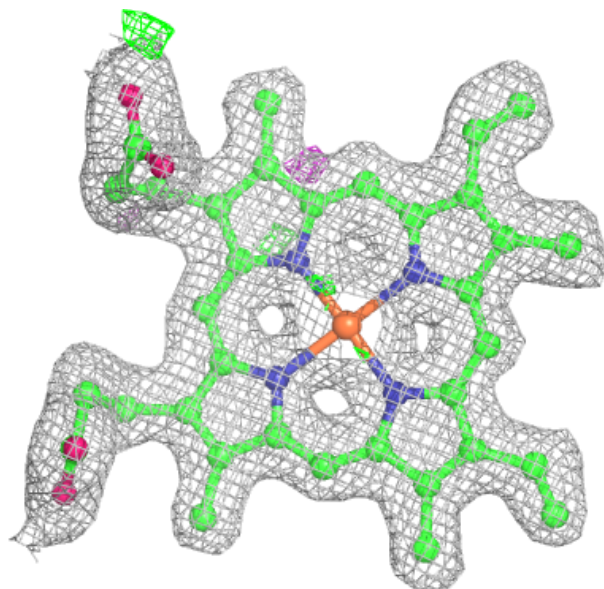
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

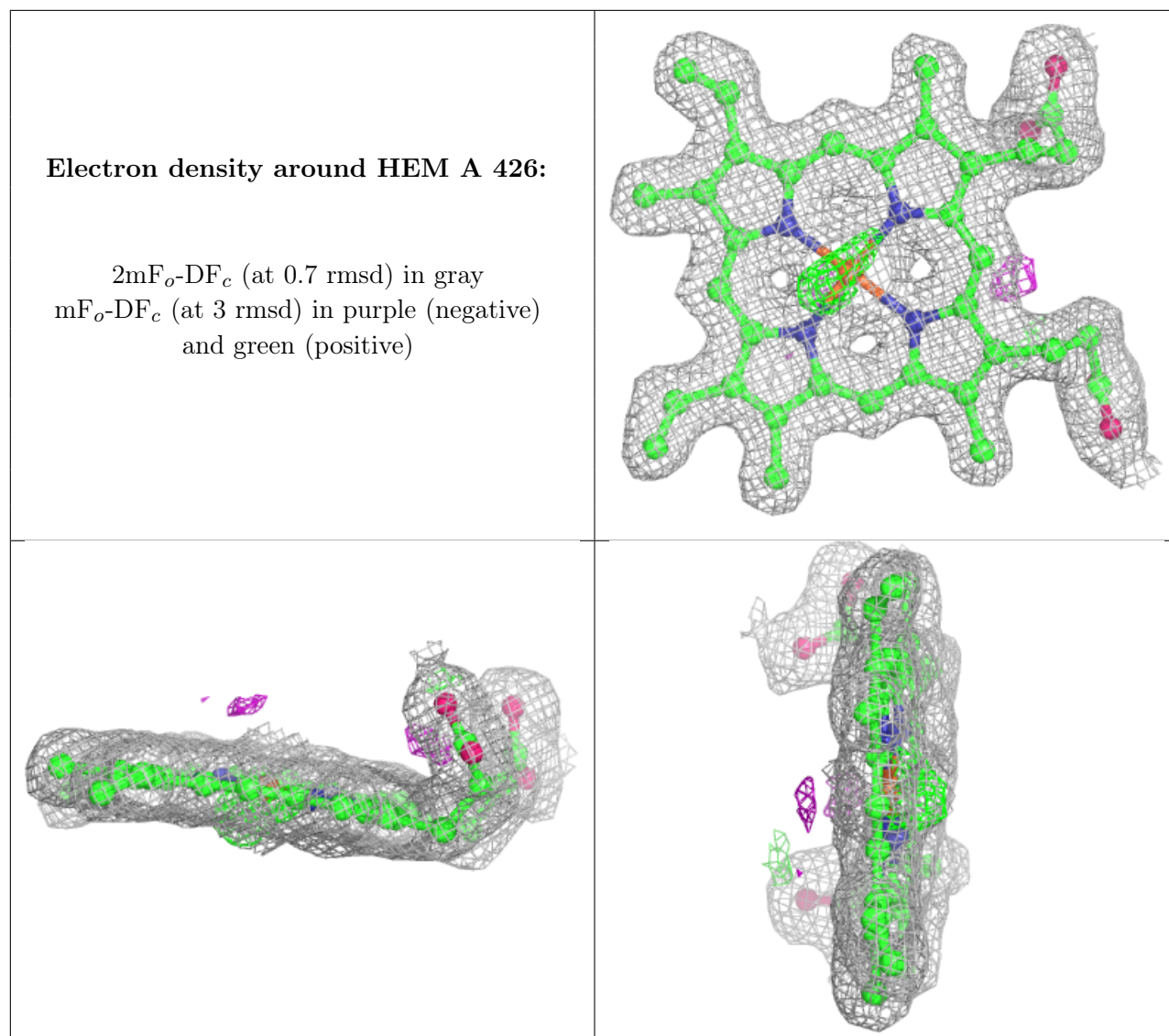




Electron density around HEM B 926:

$2mF_o-DF_c$ (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.