



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:53 am BST

PDB ID : 1KQF
Title : FORMATE DEHYDROGENASE N FROM E. COLI
Authors : Jormakka, M.; Tornroth, S.; Byrne, B.; Iwata, S.
Deposited on : 2002-01-05
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 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

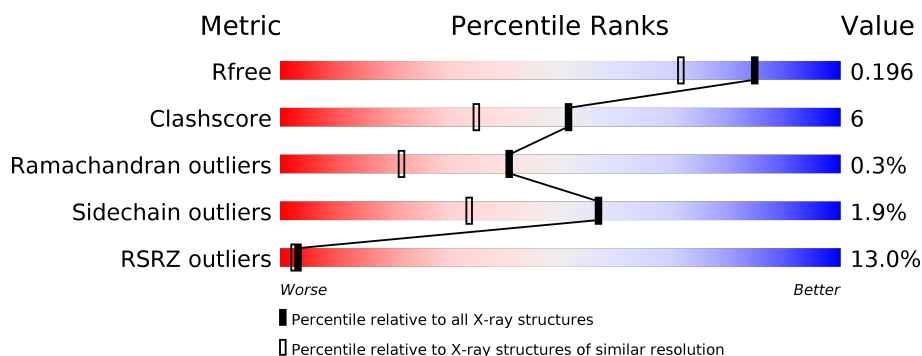
1 Overall quality at a glance

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 ≥ 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	1015	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 5px auto;"> 90% 7% </div> </div>
2	B	294	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 11%, orange 11%, yellow 11%, green 86%);"></div> <div style="display: flex; justify-content: space-between; width: 86%; margin: 5px auto;"> 86% 11% </div> </div>
3	C	217	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 69%, orange 69%, yellow 24%, green 72%);"></div> <div style="display: flex; justify-content: space-between; width: 72%; margin: 5px auto;"> 72% 24% </div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13989 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 FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, MAJOR SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	982	Total	C	N	O	S	Se	0	0	0
			7719	4872	1352	1457	37	1			

- Molecule 2 is a protein called FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	289	Total	C	N	O	S	0	0	0
			2207	1383	381	421	22			

- Molecule 3 is a protein called FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, CYTOCHROME B556(FDN) SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	216	Total	C	N	O	S	0	0	0
			1783	1192	301	276	14			

- Molecule 4 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo).

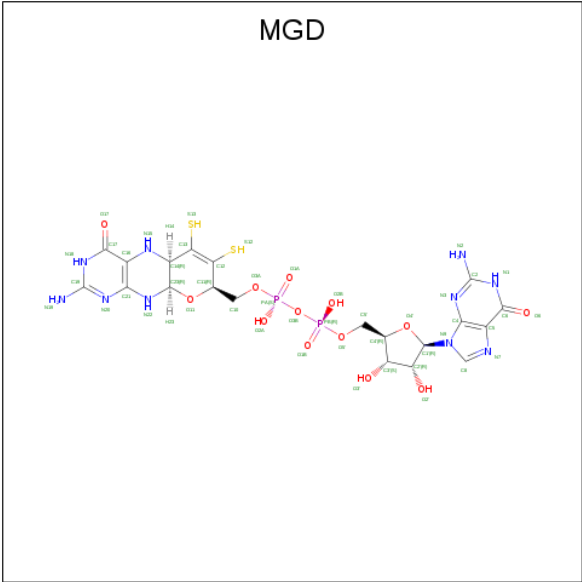
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mo	0	0
			1	1		

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



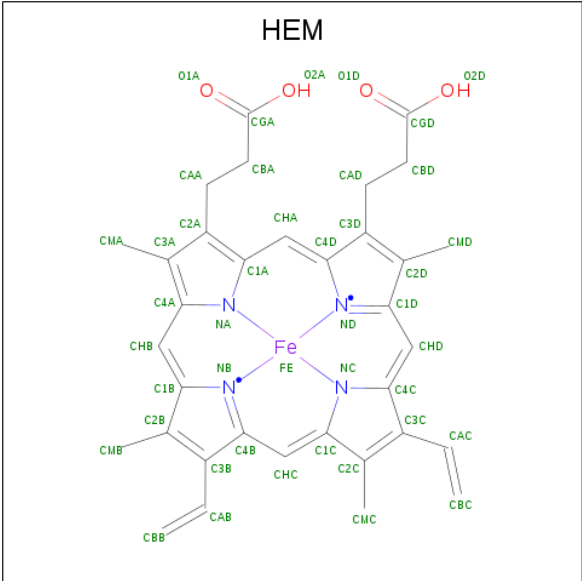
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 6 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



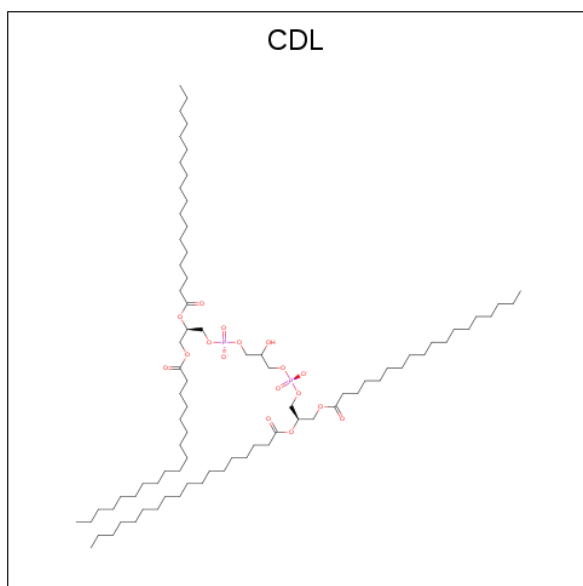
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 8 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	O	P	0	0
			70	51	17	2		

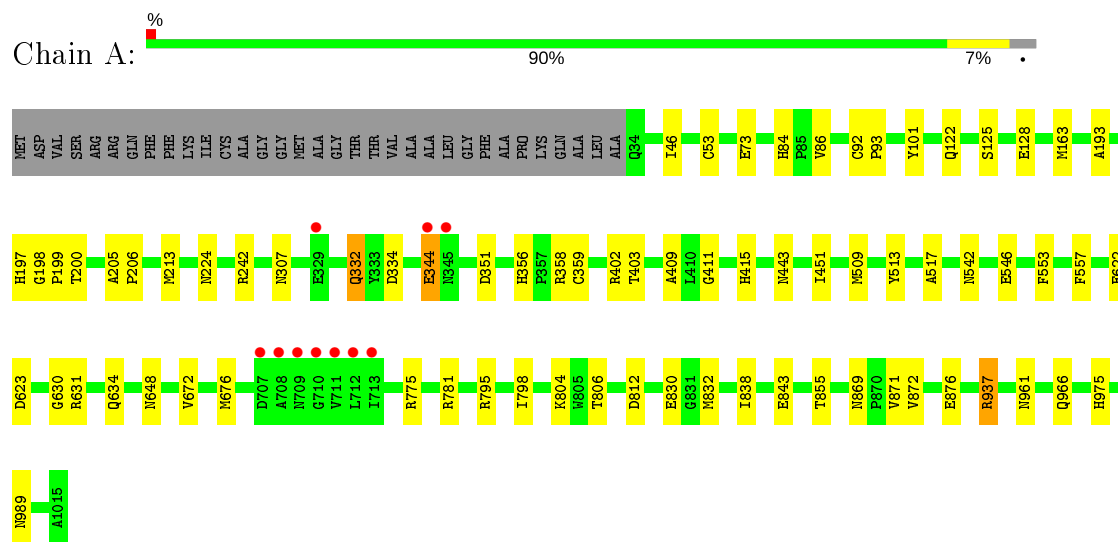
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1497	Total	O	0	0
			1497	1497		
9	B	399	Total	O	0	0
			399	399		
9	C	93	Total	O	0	0
			93	93		

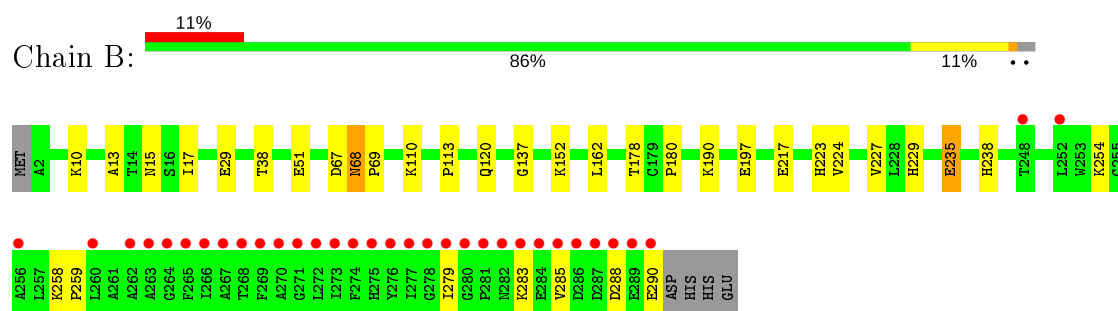
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

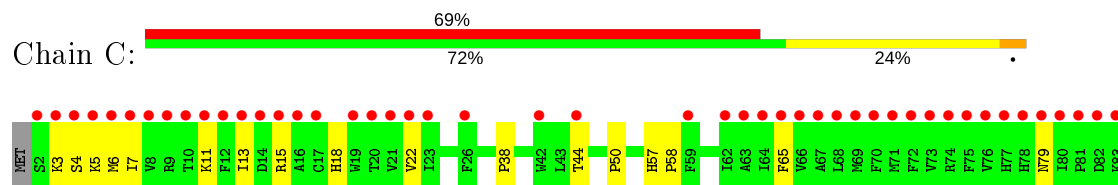
- Molecule 1: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, MAJOR SUBUNIT

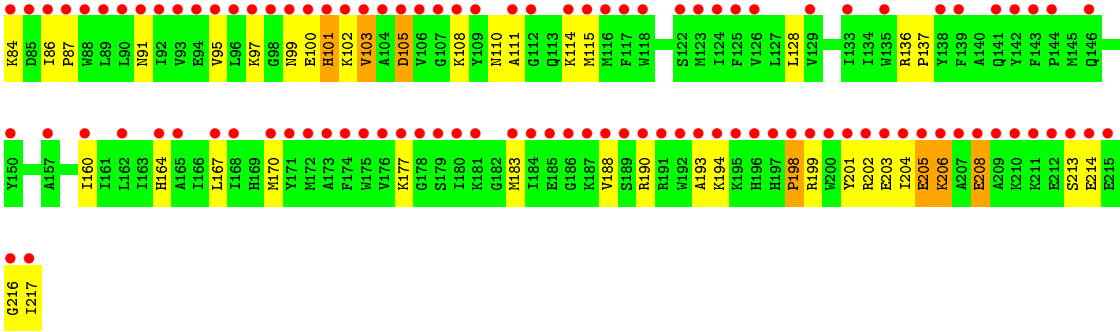


- Molecule 2: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, IRON-SULFUR SUBUNIT



- Molecule 3: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, CYTOCHROME B556(FDN) SUBUNIT





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	203.00Å 203.00Å 203.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.60 39.81 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.9 (40.00-1.60) 94.1 (39.81-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.60Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.177 , 0.195 0.183 , 0.196	Depositor DCC
R_{free} test set	3446 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13989	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6MO, MGD, CDL, SF4, SEC, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.34	0/7910	0.69	2/10749 (0.0%)
2	B	0.32	0/2255	0.68	2/3056 (0.1%)
3	C	0.33	0/1840	0.62	0/2483
All	All	0.33	0/12005	0.68	4/16288 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	334	ASP	N-CA-C	-6.00	94.79	111.00
2	B	227	VAL	N-CA-C	-5.85	95.21	111.00
1	A	975	HIS	N-CA-C	5.28	125.26	111.00
2	B	224	VAL	N-CA-C	-5.07	97.31	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	7719	0	7457	60	0
2	B	2207	0	2140	21	0
3	C	1783	0	1836	57	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	8	0	0	0	0
5	B	32	0	0	0	0
6	A	94	0	44	1	0
7	C	86	0	60	2	0
8	C	70	0	83	0	0
9	A	1497	0	0	16	2
9	B	399	0	0	6	0
9	C	93	0	0	10	0
All	All	13989	0	11620	132	2

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 6.

All (132) 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:359:CYS:HB3	9:A:1672:HOH:O	1.66	0.95
1:A:356:HIS:HD2	1:A:358:ARG:H	1.15	0.93
1:A:869:ASN:HB3	1:A:872:VAL:HG23	1.52	0.91
1:A:224:ASN:HD22	1:A:403:THR:H	1.16	0.88
1:A:622:GLU:OE1	1:A:648:ASN:HB2	1.73	0.86
3:C:15:ARG:HG2	3:C:183:MET:HE3	1.64	0.80
3:C:202:ARG:O	3:C:206:LYS:HD2	1.83	0.78
1:A:830:GLU:HG3	1:A:832:MET:CE	2.16	0.76
3:C:101:HIS:HD2	3:C:102:LYS:H	1.33	0.76
1:A:832:MET:SD	9:A:1601:HOH:O	2.47	0.73
2:B:152:LYS:HB3	9:B:1187:HOH:O	1.89	0.71
3:C:193:ALA:HB1	3:C:201:TYR:HB2	1.73	0.71
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.73	0.70
2:B:279:ILE:HD13	3:C:97:LYS:HA	1.74	0.70
1:A:197:HIS:HD2	1:A:200:THR:OG1	1.76	0.69
1:A:307:ASN:HB3	1:A:832:MET:HE1	1.75	0.69
1:A:205:ALA:HB3	1:A:206:PRO:HD3	1.74	0.68
1:A:830:GLU:HG3	1:A:832:MET:HE2	1.74	0.68
1:A:509:MET:SD	9:A:2296:HOH:O	2.52	0.68
2:B:197:GLU:HG3	9:B:1185:HOH:O	1.94	0.67
1:A:781:ARG:HA	1:A:798:ILE:HD11	1.76	0.66
3:C:84:LYS:HB3	9:C:1932:HOH:O	1.95	0.66
3:C:5:LYS:HG2	3:C:6:MET:SD	2.36	0.66
1:A:307:ASN:CB	1:A:832:MET:HE1	2.27	0.65
1:A:937:ARG:NH2	9:A:1412:HOH:O	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:HIS:CD2	3:C:102:LYS:HG3	2.32	0.64
1:A:351:ASP:HB3	9:A:1672:HOH:O	1.97	0.64
2:B:285:VAL:HG12	2:B:288:ASP:H	1.62	0.64
3:C:7:ILE:HG13	3:C:188:VAL:HG23	1.78	0.64
3:C:101:HIS:CD2	3:C:102:LYS:H	2.16	0.62
3:C:15:ARG:HA	3:C:183:MET:CE	2.30	0.62
1:A:871:VAL:HG12	1:A:871:VAL:O	1.99	0.61
3:C:213:SER:HA	9:C:1896:HOH:O	2.00	0.61
1:A:622:GLU:CD	1:A:648:ASN:HB2	2.21	0.60
3:C:198:PRO:HA	9:C:1844:HOH:O	2.00	0.59
3:C:86:ILE:HB	3:C:87:PRO:HD3	1.84	0.59
3:C:190:ARG:O	3:C:194:LYS:HG3	2.02	0.59
1:A:332:GLN:HG3	9:A:2386:HOH:O	2.02	0.59
1:A:869:ASN:HB3	1:A:872:VAL:CG2	2.31	0.59
3:C:204:ILE:O	3:C:208:GLU:HB2	2.02	0.58
2:B:137:GLY:HA3	3:C:136:ARG:HD2	1.84	0.58
3:C:201:TYR:HB3	9:C:1844:HOH:O	2.03	0.58
1:A:122:GLN:HG2	9:A:2086:HOH:O	2.05	0.56
3:C:202:ARG:HA	3:C:205:GLU:OE1	2.06	0.56
3:C:15:ARG:HA	3:C:183:MET:HE2	1.88	0.55
3:C:199:ARG:O	3:C:203:GLU:HG2	2.06	0.55
1:A:830:GLU:HG3	1:A:832:MET:HE3	1.88	0.55
1:A:224:ASN:HD21	1:A:795:ARG:HH22	1.54	0.55
3:C:216:GLY:O	3:C:217:ILE:C	2.45	0.55
3:C:190:ARG:NH1	3:C:201:TYR:OH	2.36	0.54
1:A:307:ASN:HB3	1:A:832:MET:CE	2.37	0.54
1:A:84:HIS:HE1	1:A:634:GLN:OE1	1.90	0.54
3:C:194:LYS:O	3:C:198:PRO:HG3	2.08	0.53
1:A:876:GLU:HG3	9:A:1903:HOH:O	2.08	0.53
3:C:101:HIS:HD2	3:C:102:LYS:N	2.04	0.53
1:A:224:ASN:HD22	1:A:403:THR:N	1.97	0.52
1:A:415:HIS:HD2	9:A:1099:HOH:O	1.92	0.52
3:C:11:LYS:HG2	3:C:13:ILE:H	1.75	0.52
2:B:238:HIS:HE1	9:B:932:HOH:O	1.93	0.52
3:C:217:ILE:HD12	9:C:1896:HOH:O	2.09	0.52
1:A:332:GLN:CG	9:A:2386:HOH:O	2.57	0.51
1:A:84:HIS:CD2	1:A:86:VAL:H	2.28	0.51
1:A:411:GLY:O	1:A:415:HIS:HE1	1.92	0.51
3:C:190:ARG:HD3	3:C:201:TYR:OH	2.11	0.51
1:A:961:ASN:OD1	1:A:966:GLN:OE1	2.28	0.51
2:B:29:GLU:OE1	2:B:223:HIS:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:MET:HG3	1:A:443:ASN:HA	1.92	0.51
1:A:73:GLU:HG3	9:A:1433:HOH:O	2.10	0.50
3:C:101:HIS:CD2	3:C:102:LYS:N	2.79	0.50
2:B:283:LYS:HD3	3:C:177:LYS:HB2	1.94	0.50
1:A:193:ALA:HA	1:A:451:ILE:HD11	1.94	0.50
1:A:125:SER:OG	1:A:128:GLU:HG3	2.12	0.50
1:A:92:CYS:CB	1:A:93:PRO:HD2	2.42	0.50
1:A:989:ASN:ND2	6:A:1018:MGD:H192	2.10	0.49
2:B:68:ASN:HA	2:B:69:PRO:C	2.32	0.49
1:A:630:GLY:O	1:A:631:ARG:HB2	2.13	0.49
2:B:10:LYS:HB2	2:B:120:GLN:HB3	1.95	0.49
1:A:344:GLU:H	1:A:344:GLU:CD	2.16	0.49
2:B:283:LYS:HD3	3:C:177:LYS:CB	2.43	0.48
3:C:44:THR:HB	3:C:50:PRO:HG3	1.95	0.48
3:C:170:MET:HG2	7:C:810:HEM:CAB	2.44	0.48
3:C:101:HIS:HD2	3:C:102:LYS:HG3	1.77	0.48
3:C:4:SER:OG	3:C:190:ARG:NH2	2.47	0.47
1:A:542:ASN:O	1:A:546:GLU:HG3	2.14	0.47
3:C:170:MET:HG2	7:C:810:HEM:HAB	1.95	0.47
3:C:108:LYS:HB3	9:C:1740:HOH:O	2.13	0.47
1:A:46:ILE:HD11	9:A:1544:HOH:O	2.14	0.47
1:A:832:MET:HE3	1:A:832:MET:HB2	1.55	0.47
1:A:163:MET:HG2	1:A:553:PHE:HB2	1.96	0.46
1:A:356:HIS:CD2	1:A:358:ARG:H	2.08	0.46
1:A:871:VAL:O	1:A:871:VAL:CG1	2.61	0.46
3:C:194:LYS:HA	9:C:1844:HOH:O	2.16	0.46
1:A:224:ASN:HD21	1:A:795:ARG:NH2	2.14	0.45
3:C:214:GLU:HA	3:C:214:GLU:OE1	2.16	0.45
1:A:198:GLY:N	1:A:199:PRO:CD	2.80	0.45
3:C:167:LEU:HA	3:C:170:MET:HE2	1.99	0.45
3:C:99:ASN:O	3:C:103:VAL:HG22	2.17	0.44
3:C:100:GLU:HB3	9:C:1107:HOH:O	2.16	0.44
1:A:513:TYR:HB2	1:A:517:ALA:HB2	1.99	0.44
3:C:11:LYS:HE2	3:C:13:ILE:HB	1.98	0.44
3:C:18:HIS:O	3:C:22:VAL:HG23	2.17	0.44
3:C:91:ASN:O	3:C:95:VAL:HG23	2.18	0.44
3:C:57:HIS:HB3	3:C:58:PRO:CD	2.48	0.44
1:A:623:ASP:HB3	9:A:1891:HOH:O	2.18	0.43
3:C:3:LYS:HD3	3:C:3:LYS:HA	1.83	0.43
1:A:634:GLN:HB3	9:A:1246:HOH:O	2.18	0.43
3:C:65:PHE:CZ	3:C:128:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:LYS:HD3	9:B:1161:HOH:O	2.18	0.43
3:C:160:ILE:O	3:C:164:HIS:HD2	2.01	0.43
2:B:13:ALA:HB1	3:C:38:PRO:CB	2.48	0.43
3:C:99:ASN:HB3	3:C:102:LYS:HD2	2.00	0.43
1:A:359:CYS:CB	9:A:1672:HOH:O	2.43	0.43
2:B:217:GLU:HG2	9:B:1069:HOH:O	2.17	0.43
2:B:38:THR:HG22	2:B:38:THR:O	2.17	0.43
2:B:258:LYS:HB2	2:B:259:PRO:CD	2.48	0.43
1:A:830:GLU:CG	1:A:832:MET:HE2	2.46	0.43
3:C:110:ASN:O	3:C:114:LYS:HG3	2.19	0.43
1:A:242:ARG:HB2	2:B:180:PRO:O	2.18	0.42
1:A:775:ARG:HD3	1:A:812:ASP:HA	2.01	0.42
2:B:235:GLU:HG3	9:B:1027:HOH:O	2.18	0.42
1:A:672:VAL:O	1:A:676:MET:HG2	2.19	0.42
1:A:224:ASN:ND2	1:A:402:ARG:HA	2.34	0.42
3:C:111:ALA:O	3:C:115:MET:HG3	2.19	0.42
2:B:15:ASN:OD1	2:B:17:ILE:HG12	2.20	0.42
3:C:105:ASP:HB3	9:C:1932:HOH:O	2.19	0.41
3:C:79:ASN:HD22	3:C:114:LYS:HA	1.85	0.41
2:B:235:GLU:H	2:B:235:GLU:CD	2.24	0.41
3:C:11:LYS:HG2	3:C:13:ILE:HG22	2.03	0.41
1:A:804:LYS:HE3	1:A:806:THR:CG2	2.51	0.41
3:C:105:ASP:HB2	9:C:1672:HOH:O	2.20	0.41
1:A:623:ASP:CB	9:A:1891:HOH:O	2.69	0.40
2:B:110:LYS:O	2:B:254:LYS:HE2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2324:HOH:O	9:A:2324:HOH:O[6_456]	1.12	1.08
9:A:1746:HOH:O	9:A:1746:HOH:O[6_456]	1.25	0.95

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	979/1015 (96%)	951 (97%)	26 (3%)	2 (0%)	47	26
2	B	287/294 (98%)	278 (97%)	9 (3%)	0	100	100
3	C	214/217 (99%)	206 (96%)	6 (3%)	2 (1%)	17	4
All	All	1480/1526 (97%)	1435 (97%)	41 (3%)	4 (0%)	41	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	208	GLU
1	A	409	ALA
1	A	838	ILE
3	C	198	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	815/837 (97%)	807 (99%)	8 (1%)	76	61
2	B	238/243 (98%)	229 (96%)	9 (4%)	33	10
3	C	188/189 (100%)	182 (97%)	6 (3%)	39	15
All	All	1241/1269 (98%)	1218 (98%)	23 (2%)	57	34

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	A	101	TYR
1	A	332	GLN
1	A	344	GLU
1	A	557	PHE
1	A	843	GLU

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Mol	Chain	Res	Type
1	A	855	THR
1	A	937	ARG
2	B	51	GLU
2	B	67	ASP
2	B	68	ASN
2	B	113	PRO
2	B	162	LEU
2	B	178	THR
2	B	229	HIS
2	B	235	GLU
2	B	290	GLU
3	C	101	HIS
3	C	103	VAL
3	C	105	ASP
3	C	137	PRO
3	C	205	GLU
3	C	206	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	191	ASN
1	A	197	HIS
1	A	224	ASN
1	A	332	GLN
1	A	341	GLN
1	A	356	HIS
1	A	362	ASN
1	A	415	HIS
1	A	479	GLN
1	A	689	GLN
1	A	865	ASN
1	A	966	GLN
1	A	989	ASN
2	B	185	HIS
2	B	223	HIS
2	B	238	HIS
3	C	79	ASN
3	C	101	HIS
3	C	164	HIS
3	C	196	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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	$\# Z > 2$
5	SF4	B	807	2	0,12,12	0.00	-	-		
5	SF4	B	808	2	0,12,12	0.00	-	-		
5	SF4	B	806	2	0,12,12	0.00	-	-		
7	HEM	C	810	3	27,50,50	2.07	8 (29%)	17,82,82	2.04	5 (29%)
6	MGD	A	1018	4	41,52,52	2.32	10 (24%)	43,81,81	3.31	23 (53%)
5	SF4	B	805	2	0,12,12	0.00	-	-		
5	SF4	A	1017	1	0,12,12	0.00	-	-		
7	HEM	C	809	3	27,50,50	2.18	9 (33%)	17,82,82	2.09	8 (47%)
8	CDL	C	812	-	69,69,99	2.93	21 (30%)	75,81,111	2.62	16 (21%)
6	MGD	A	1019	4	41,52,52	2.71	11 (26%)	43,81,81	2.85	18 (41%)

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
5	SF4	B	807	2	-	-	0/6/5/5
5	SF4	B	808	2	-	-	0/6/5/5
5	SF4	B	806	2	-	-	0/6/5/5
6	MGD	A	1018	4	-	6/18/66/66	0/6/6/6
7	HEM	C	810	3	-	0/6/54/54	-
5	SF4	B	805	2	-	-	0/6/5/5
5	SF4	A	1017	1	-	-	0/6/5/5
7	HEM	C	809	3	-	0/6/54/54	-
8	CDL	C	812	-	-	38/80/80/110	-
6	MGD	A	1019	4	-	8/18/66/66	0/6/6/6

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	812	CDL	OB8-CB6	-14.51	1.12	1.45
6	A	1018	MGD	O3A-C10	-9.94	1.06	1.44
6	A	1019	MGD	O3A-C10	-9.74	1.07	1.44
8	C	812	CDL	OA6-CA5	9.73	1.61	1.34
8	C	812	CDL	OB6-CB5	7.65	1.55	1.34
8	C	812	CDL	C51-CB5	5.86	1.67	1.50
6	A	1019	MGD	C17-N18	5.47	1.42	1.33
6	A	1019	MGD	C23-C14	-5.32	1.49	1.53
6	A	1018	MGD	C17-N18	5.22	1.42	1.33
6	A	1018	MGD	C6-N1	5.14	1.42	1.33
6	A	1019	MGD	C6-N1	5.09	1.41	1.33
7	C	809	HEM	C3B-CAB	5.06	1.58	1.47
6	A	1019	MGD	O11-C23	-4.86	1.36	1.43
7	C	810	HEM	C3C-CAC	4.85	1.57	1.47
8	C	812	CDL	PA1-OA3	4.46	1.66	1.50
7	C	810	HEM	C3B-CAB	4.07	1.56	1.47
7	C	810	HEM	C3B-C2B	-4.03	1.34	1.40
8	C	812	CDL	C11-CA5	3.73	1.61	1.50
7	C	809	HEM	C3C-CAC	3.72	1.55	1.47
8	C	812	CDL	OA8-CA7	3.70	1.44	1.33
7	C	809	HEM	C3C-C2C	-3.70	1.35	1.40
8	C	812	CDL	OB8-CB7	-3.51	1.23	1.33
6	A	1019	MGD	O11-C11	-3.48	1.39	1.43
6	A	1019	MGD	C17-C16	3.45	1.46	1.41
6	A	1019	MGD	O5'-C5'	-3.32	1.32	1.44
7	C	809	HEM	C3B-C2B	-3.29	1.35	1.40
6	A	1019	MGD	O4'-C1'	3.28	1.45	1.41
7	C	809	HEM	CAA-C2A	3.08	1.56	1.52
7	C	809	HEM	CAD-C3D	3.04	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1018	MGD	C17-C16	2.95	1.45	1.41
8	C	812	CDL	PB2-OB4	2.85	1.68	1.55
7	C	810	HEM	C3C-C2C	-2.76	1.36	1.40
8	C	812	CDL	PB2-OB3	2.75	1.60	1.50
8	C	812	CDL	CB3-CB4	2.75	1.59	1.50
8	C	812	CDL	C12-C11	2.70	1.62	1.52
8	C	812	CDL	C39-C38	-2.69	1.36	1.51
8	C	812	CDL	C79-C78	2.65	1.71	1.49
7	C	810	HEM	CAD-C3D	2.57	1.56	1.52
8	C	812	CDL	C52-C51	2.52	1.61	1.52
6	A	1018	MGD	O5'-C5'	-2.44	1.35	1.44
8	C	812	CDL	C42-C41	-2.43	1.37	1.51
8	C	812	CDL	PA1-OA5	2.42	1.69	1.59
6	A	1018	MGD	C23-N22	2.41	1.49	1.44
8	C	812	CDL	OB9-CB7	2.39	1.29	1.22
6	A	1018	MGD	C2-N1	2.35	1.39	1.35
6	A	1019	MGD	C16-C21	2.35	1.45	1.41
7	C	810	HEM	CMC-C2C	2.31	1.57	1.51
6	A	1018	MGD	PB-O1B	-2.29	1.42	1.50
8	C	812	CDL	C19-C18	-2.28	1.35	1.51
6	A	1019	MGD	C2-N1	2.26	1.39	1.35
8	C	812	CDL	OB2-CB2	-2.23	1.36	1.44
7	C	809	HEM	CMD-C2D	2.22	1.56	1.51
7	C	809	HEM	CMC-C2C	2.19	1.56	1.51
7	C	810	HEM	CMA-C3A	2.18	1.56	1.51
6	A	1018	MGD	O2'-C2'	2.16	1.48	1.43
6	A	1018	MGD	C10-C11	2.11	1.54	1.52
7	C	810	HEM	CAA-C2A	2.06	1.55	1.52
8	C	812	CDL	CA3-CA4	-2.02	1.44	1.50
7	C	809	HEM	C1D-ND	2.01	1.40	1.36

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	812	CDL	OB6-CB5-C51	13.86	141.36	111.50
6	A	1018	MGD	O11-C23-C14	8.99	114.96	108.96
6	A	1018	MGD	O4'-C1'-C2'	-7.53	95.92	106.93
8	C	812	CDL	CB6-OB8-CB7	-7.36	89.86	117.12
8	C	812	CDL	CA6-CA4-CA3	-7.13	94.93	111.79
8	C	812	CDL	C52-C51-CB5	-6.40	90.36	113.62
6	A	1019	MGD	C21-N22-C23	-6.38	111.17	123.67
8	C	812	CDL	OB7-CB5-C51	-5.76	101.26	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1019	MGD	C5-C6-N1	-5.26	116.24	123.43
6	A	1019	MGD	N3-C2-N1	-5.17	120.33	127.22
6	A	1018	MGD	N3-C2-N1	-5.13	120.38	127.22
8	C	812	CDL	OA6-CA5-OA7	-5.06	111.48	123.70
6	A	1019	MGD	C6-N1-C2	4.97	123.83	115.93
6	A	1018	MGD	N2-C2-N3	4.91	125.80	117.79
6	A	1018	MGD	C5-C6-N1	-4.89	116.75	123.43
6	A	1018	MGD	C16-C21-N22	4.88	122.59	118.13
6	A	1019	MGD	C16-C21-N22	4.76	122.49	118.13
6	A	1018	MGD	C6-C5-C4	-4.62	116.39	120.80
6	A	1018	MGD	N18-C19-N20	-4.57	118.25	125.42
6	A	1018	MGD	C6-N1-C2	4.57	123.19	115.93
6	A	1019	MGD	C6-C5-C4	-4.56	116.44	120.80
6	A	1019	MGD	N2-C2-N3	4.54	125.19	117.79
6	A	1019	MGD	O11-C23-C14	4.28	111.82	108.96
6	A	1019	MGD	C19-N20-C21	4.27	124.12	114.54
6	A	1018	MGD	C19-N20-C21	4.27	124.11	114.54
6	A	1019	MGD	C17-C16-N15	4.22	122.66	119.12
6	A	1018	MGD	O11-C23-N22	4.19	112.87	108.57
6	A	1019	MGD	N18-C19-N20	-4.07	119.04	125.42
6	A	1018	MGD	O4'-C4'-C5'	4.06	122.74	109.37
6	A	1018	MGD	C21-N22-C23	-4.03	115.78	123.67
6	A	1018	MGD	C17-N18-C19	4.02	122.31	115.93
7	C	810	HEM	CAD-CBD-CGD	3.88	119.18	112.67
7	C	809	HEM	CAA-CBA-CGA	3.83	119.09	112.67
7	C	810	HEM	CMA-C3A-C4A	-3.82	122.59	128.46
6	A	1019	MGD	C17-N18-C19	3.69	121.79	115.93
7	C	809	HEM	CMA-C3A-C4A	-3.61	122.91	128.46
8	C	812	CDL	CB6-CB4-CB3	-3.49	103.53	111.79
6	A	1018	MGD	C17-C16-C21	3.47	117.65	114.57
7	C	810	HEM	CMA-C3A-C2A	3.36	131.28	124.94
7	C	810	HEM	CMB-C2B-C3B	3.11	130.50	124.68
6	A	1018	MGD	N19-C19-N20	3.09	122.05	117.25
8	C	812	CDL	O1-C1-CA2	-3.07	98.79	109.56
8	C	812	CDL	OA4-PA1-OA3	-3.02	97.33	112.24
6	A	1018	MGD	C23-C14-C13	-2.99	103.82	110.53
6	A	1019	MGD	O5'-C5'-C4'	2.96	119.16	108.99
6	A	1018	MGD	O5'-C5'-C4'	2.93	119.06	108.99
7	C	809	HEM	CMB-C2B-C3B	2.92	130.15	124.68
7	C	810	HEM	CMC-C2C-C3C	2.92	130.14	124.68
6	A	1019	MGD	PB-O5'-C5'	2.85	138.42	121.68
6	A	1019	MGD	C23-C14-C13	-2.85	104.14	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	809	HEM	CMA-C3A-C2A	2.81	130.25	124.94
6	A	1018	MGD	PB-O5'-C5'	2.79	138.04	121.68
8	C	812	CDL	OB6-CB5-OB7	-2.64	117.32	123.70
7	C	809	HEM	CBD-CAD-C3D	2.58	117.22	112.48
8	C	812	CDL	OA7-CA5-C11	-2.56	113.73	123.73
6	A	1019	MGD	C17-C16-C21	2.53	116.82	114.57
6	A	1019	MGD	C16-C17-N18	-2.29	117.51	124.01
6	A	1018	MGD	C16-C17-N18	-2.25	117.62	124.01
7	C	809	HEM	CMC-C2C-C3C	2.22	128.83	124.68
8	C	812	CDL	CA6-OA8-CA7	-2.21	108.93	117.12
6	A	1018	MGD	N2-C2-N1	-2.21	113.81	117.25
7	C	809	HEM	CMD-C2D-C1D	-2.20	125.08	128.46
6	A	1018	MGD	C17-C16-N15	2.15	120.93	119.12
7	C	809	HEM	CMD-C2D-C3D	2.13	128.96	124.94
6	A	1019	MGD	PA-O3B-PB	2.07	139.93	132.83
8	C	812	CDL	OB9-CB7-C71	-2.04	115.78	123.73
8	C	812	CDL	OA6-CA4-CA3	2.03	115.77	108.40
6	A	1018	MGD	C4-C5-N7	2.03	111.51	109.40
8	C	812	CDL	CA4-OA6-CA5	-2.02	112.83	117.79
8	C	812	CDL	C40-C39-C38	2.01	124.61	114.42

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	812	CDL	O1-C1-CB2-OB2
8	C	812	CDL	CA2-C1-CB2-OB2
8	C	812	CDL	C1-CA2-OA2-PA1
8	C	812	CDL	CA3-OA5-PA1-OA3
8	C	812	CDL	CA3-OA5-PA1-OA4
8	C	812	CDL	C11-CA5-OA6-CA4
8	C	812	CDL	CB2-OB2-PB2-OB3
8	C	812	CDL	CB3-OB5-PB2-OB2
8	C	812	CDL	CB3-OB5-PB2-OB3
8	C	812	CDL	CB3-OB5-PB2-OB4
6	A	1018	MGD	C10-O3A-PA-O1A
6	A	1018	MGD	O4'-C4'-C5'-O5'
6	A	1019	MGD	C5'-O5'-PB-O1B
6	A	1019	MGD	C5'-O5'-PB-O2B
6	A	1019	MGD	C5'-O5'-PB-O3B
6	A	1019	MGD	C10-O3A-PA-O1A
8	C	812	CDL	OB9-CB7-OB8-CB6

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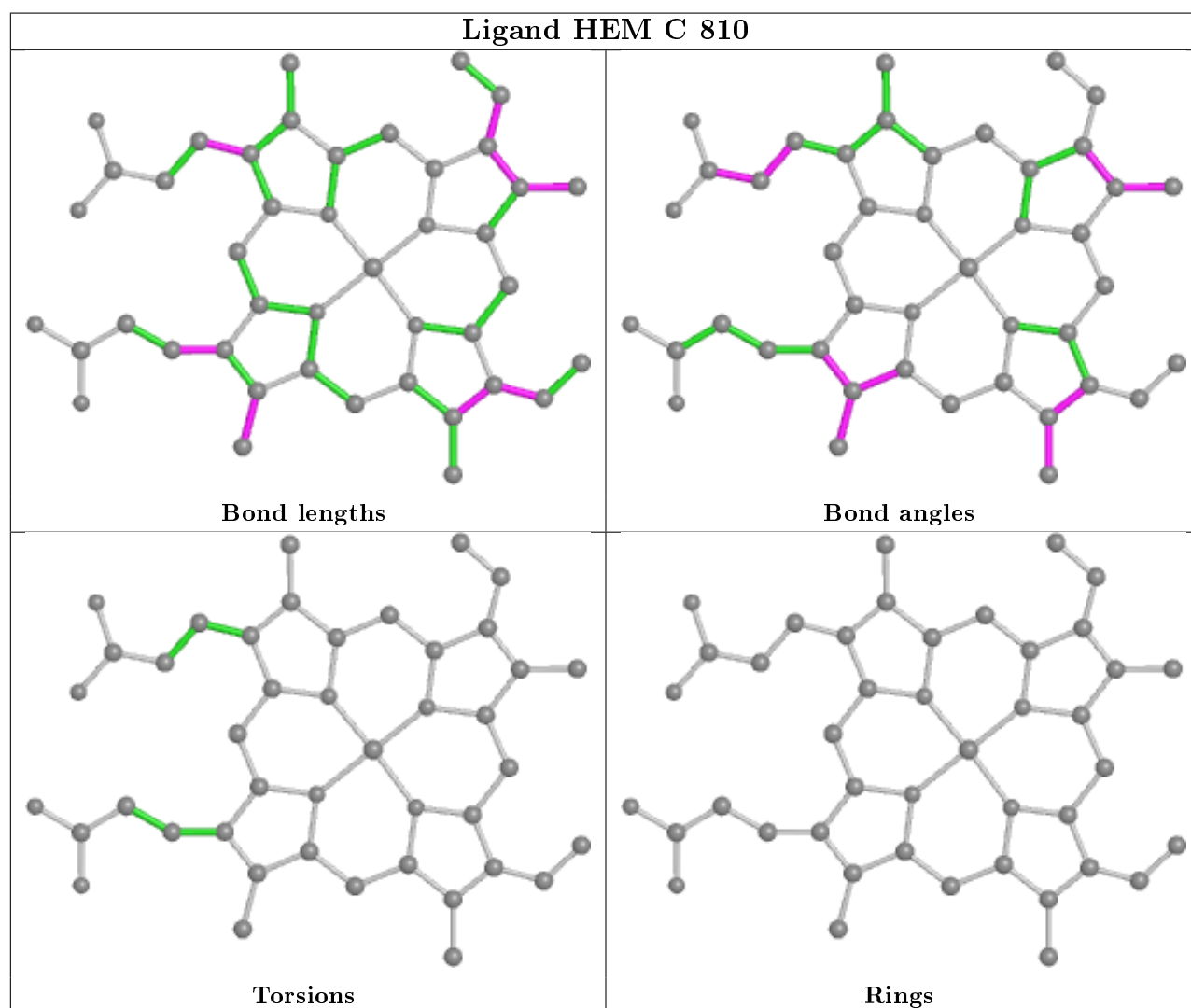
Mol	Chain	Res	Type	Atoms
6	A	1018	MGD	C3'-C4'-C5'-O5'
6	A	1019	MGD	O4'-C4'-C5'-O5'
6	A	1019	MGD	C3'-C4'-C5'-O5'
8	C	812	CDL	CA5-C11-C12-C13
8	C	812	CDL	O1-C1-CA2-OA2
8	C	812	CDL	CA3-OA5-PA1-OA2
8	C	812	CDL	CB2-OB2-PB2-OB5
8	C	812	CDL	C36-C37-C38-C39
8	C	812	CDL	CA7-C31-C32-C33
8	C	812	CDL	CB2-C1-CA2-OA2
8	C	812	CDL	OB7-CB5-OB6-CB4
8	C	812	CDL	C51-CB5-OB6-CB4
8	C	812	CDL	CB3-CB4-CB6-OB8
8	C	812	CDL	C71-CB7-OB8-CB6
8	C	812	CDL	OB5-CB3-CB4-OB6
8	C	812	CDL	OB6-CB4-CB6-OB8
8	C	812	CDL	C40-C41-C42-C43
8	C	812	CDL	C35-C36-C37-C38
8	C	812	CDL	C37-C38-C39-C40
6	A	1019	MGD	C10-O3A-PA-O3B
8	C	812	CDL	C33-C34-C35-C36
8	C	812	CDL	C15-C16-C17-C18
6	A	1018	MGD	PB-O3B-PA-O1A
6	A	1018	MGD	C10-O3A-PA-O2A
8	C	812	CDL	OA5-CA3-CA4-CA6
8	C	812	CDL	OA5-CA3-CA4-OA6
8	C	812	CDL	CA2-OA2-PA1-OA5
6	A	1019	MGD	PB-O3B-PA-O1A
8	C	812	CDL	C41-C42-C43-C44
8	C	812	CDL	OB5-CB3-CB4-CB6
8	C	812	CDL	OA7-CA5-OA6-CA4
8	C	812	CDL	C72-C71-CB7-OB8
6	A	1018	MGD	C10-O3A-PA-O3B
8	C	812	CDL	C17-C18-C19-C20
8	C	812	CDL	C12-C11-CA5-OA7

There are no ring outliers.

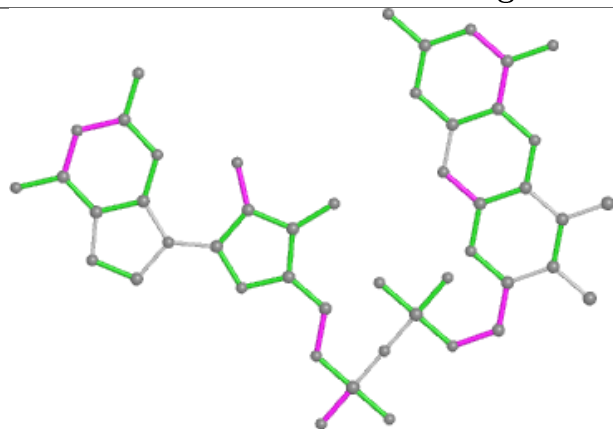
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	810	HEM	2	0
6	A	1018	MGD	1	0

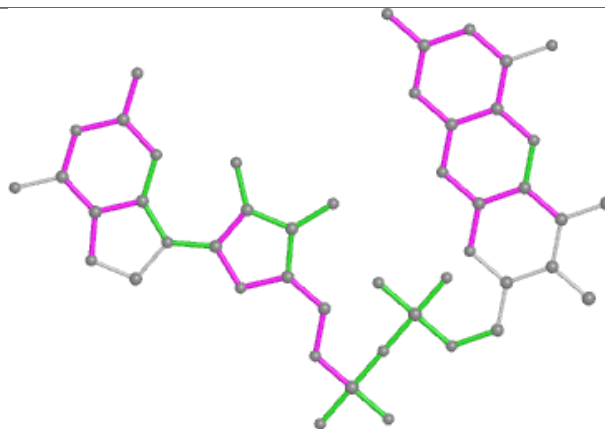
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



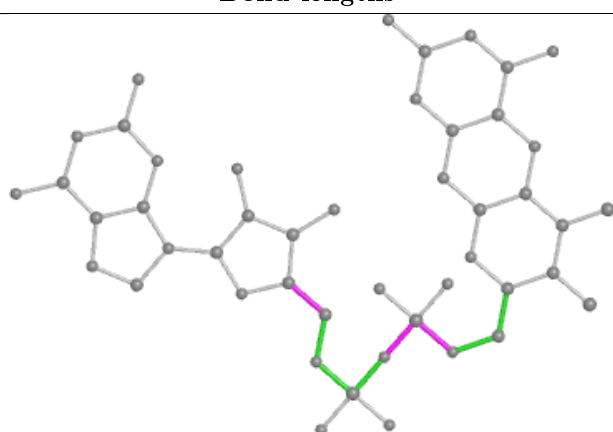
Ligand MGD A 1018



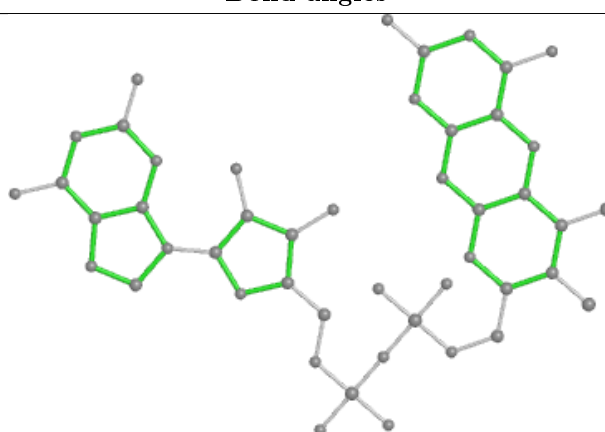
Bond lengths



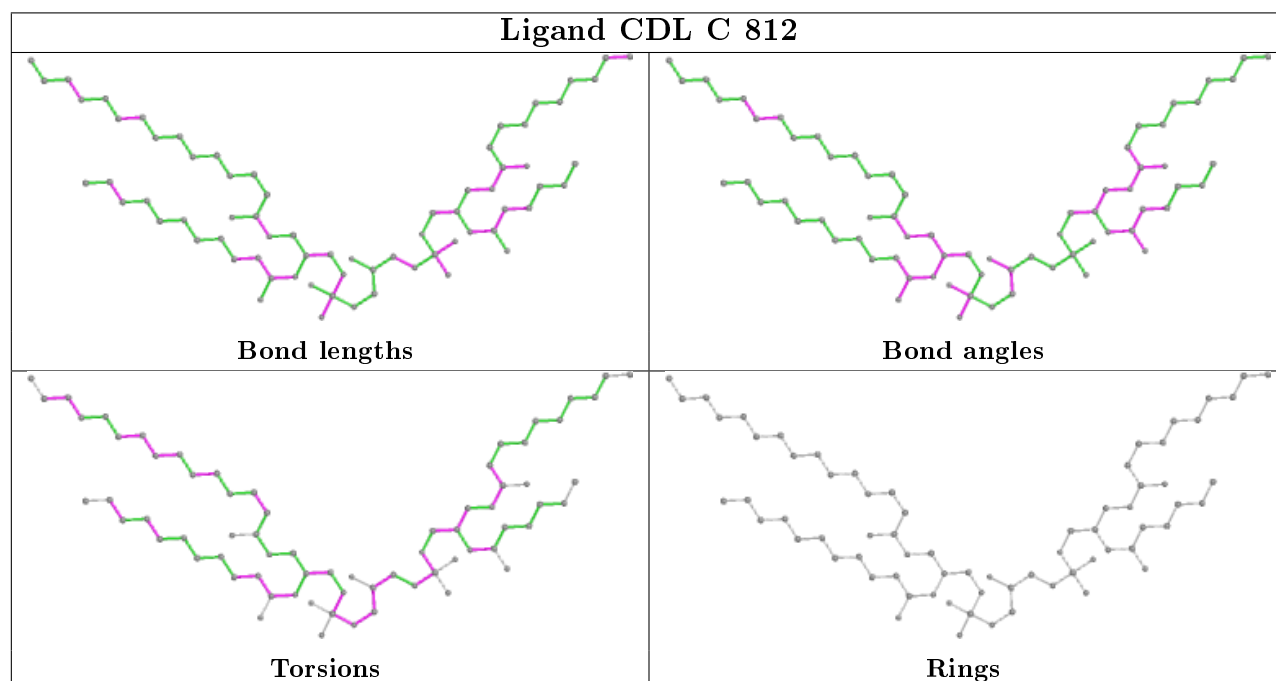
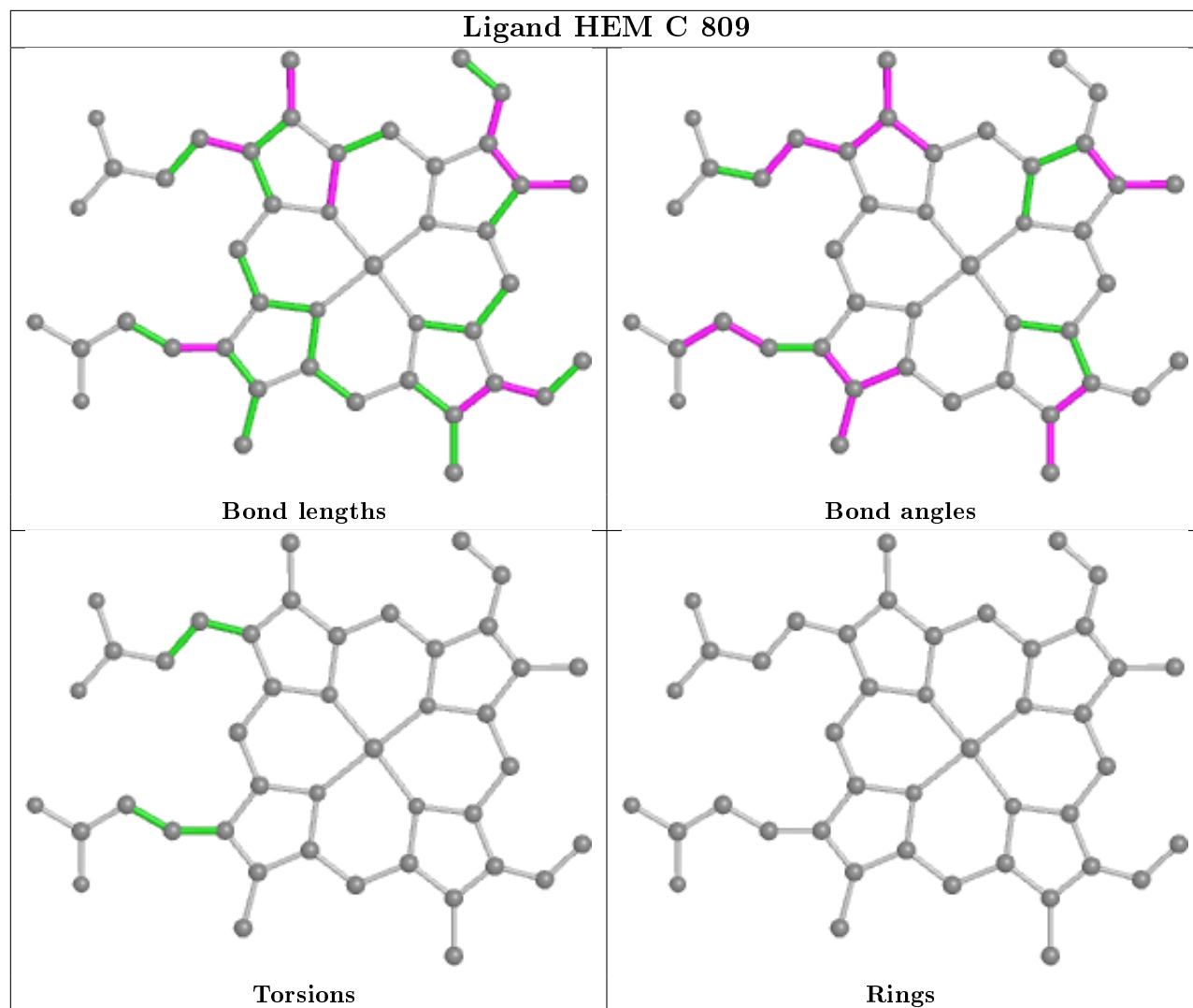
Bond angles

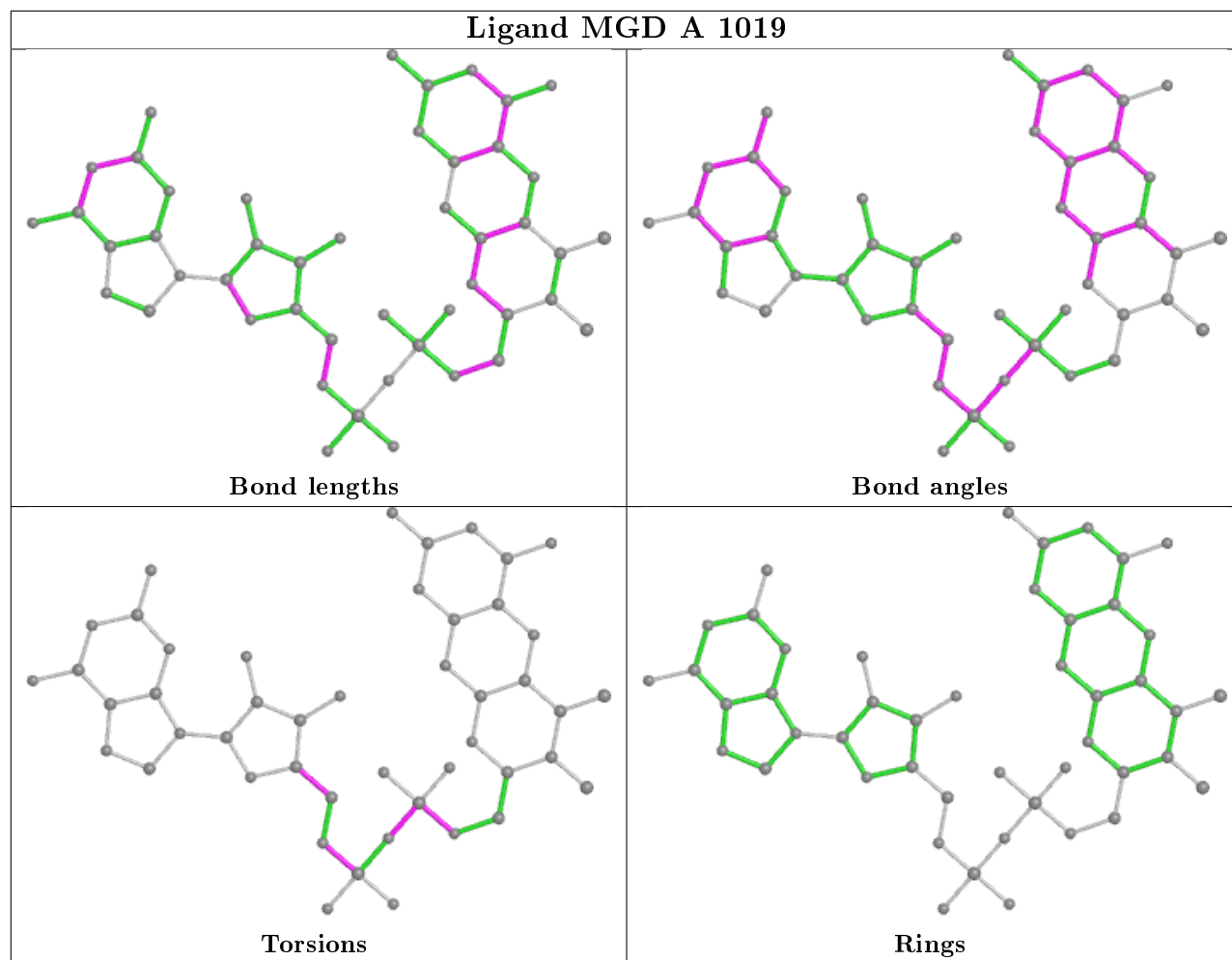


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	981/1015 (96%)	-0.20	10 (1%) 82 82	11, 18, 30, 56	0
2	B	289/294 (98%)	0.47	33 (11%) 5 4	11, 18, 52, 67	0
3	C	216/217 (99%)	3.97	150 (69%) 0 0	30, 49, 63, 65	0
All	All	1486/1526 (97%)	0.54	193 (12%) 3 2	11, 19, 54, 67	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	217	ILE	18.4
3	C	207	ALA	14.5
2	B	285	VAL	13.5
3	C	209	ALA	12.2
3	C	216	GLY	12.1
2	B	287	ASP	12.0
3	C	2	SER	11.8
2	B	289	GLU	11.1
2	B	288	ASP	11.1
2	B	286	ASP	11.1
3	C	204	ILE	11.0
3	C	192	TRP	10.7
3	C	211	LYS	10.5
3	C	212	GLU	10.5
3	C	105	ASP	10.3
3	C	90	LEU	10.3
3	C	201	TYR	10.1
3	C	210	LYS	10.1
3	C	213	SER	10.0
2	B	290	GLU	10.0
3	C	86	ILE	10.0
3	C	80	ILE	9.8
3	C	89	LEU	9.7

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Mol	Chain	Res	Type	RSRZ
3	C	214	GLU	9.5
3	C	92	ILE	9.1
3	C	93	VAL	9.0
3	C	103	VAL	8.8
3	C	101	HIS	8.7
3	C	5	LYS	8.6
3	C	3	LYS	8.5
3	C	7	ILE	8.3
3	C	215	GLU	8.2
3	C	6	MET	7.9
3	C	73	VAL	7.9
3	C	206	LYS	7.8
3	C	88	TRP	7.8
3	C	96	LEU	7.7
3	C	4	SER	7.7
3	C	188	VAL	7.4
3	C	106	VAL	7.3
3	C	200	TRP	7.2
3	C	142	TYR	7.2
3	C	81	PRO	7.0
3	C	70	PHE	6.9
3	C	83	LYS	6.9
3	C	77	HIS	6.8
3	C	91	ASN	6.7
3	C	75	PHE	6.5
3	C	118	TRP	6.5
3	C	13	ILE	6.5
3	C	205	GLU	6.2
3	C	208	GLU	6.2
3	C	97	LYS	6.2
3	C	175	TRP	6.1
3	C	102	LYS	6.1
2	B	269	PHE	6.1
3	C	104	ALA	6.1
2	B	260	LEU	6.0
2	B	274	PHE	6.0
3	C	191	ARG	6.0
1	A	709	ASN	5.9
1	A	708	ALA	5.8
3	C	194	LYS	5.6
2	B	284	GLU	5.6
3	C	202	ARG	5.6

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Mol	Chain	Res	Type	RSRZ
3	C	171	TYR	5.5
2	B	279	ILE	5.4
3	C	109	TYR	5.4
3	C	193	ALA	5.4
3	C	87	PRO	5.2
3	C	94	GLU	5.1
3	C	8	VAL	5.1
2	B	267	ALA	5.1
3	C	12	PHE	5.1
2	B	283	LYS	5.0
2	B	278	GLY	5.0
3	C	196	HIS	4.9
3	C	99	ASN	4.9
3	C	78	HIS	4.9
3	C	76	VAL	4.8
3	C	197	HIS	4.8
3	C	150	TYR	4.8
3	C	19	TRP	4.7
3	C	176	VAL	4.7
3	C	98	GLY	4.7
3	C	85	ASP	4.7
3	C	186	GLY	4.6
3	C	72	PHE	4.6
3	C	74	ARG	4.6
3	C	174	PHE	4.6
3	C	189	SER	4.6
3	C	203	GLU	4.6
3	C	190	ARG	4.5
3	C	198	PRO	4.5
3	C	100	GLU	4.5
3	C	82	ASP	4.4
2	B	252	LEU	4.4
1	A	711	VAL	4.4
3	C	180	ILE	4.4
3	C	95	VAL	4.3
2	B	271	GLY	4.1
2	B	281	PRO	4.1
3	C	26	PHE	4.0
3	C	69	MET	4.0
3	C	199	ARG	4.0
3	C	115	MET	3.9
3	C	181	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
3	C	143	PHE	3.9
3	C	66	VAL	3.8
3	C	138	TYR	3.7
3	C	112	GLY	3.7
3	C	65	PHE	3.7
3	C	84	LYS	3.6
3	C	14	ASP	3.6
3	C	117	PHE	3.6
3	C	139	PHE	3.5
3	C	42	TRP	3.5
3	C	111	ALA	3.5
1	A	344	GLU	3.5
2	B	282	ASN	3.5
3	C	11	LYS	3.5
3	C	178	GLY	3.5
2	B	256	ALA	3.5
3	C	107	GLY	3.4
2	B	276	TYR	3.4
2	B	266	ILE	3.4
3	C	17	CYS	3.3
3	C	172	MET	3.3
2	B	277	ILE	3.3
1	A	329	GLU	3.3
3	C	10	THR	3.2
3	C	141	GLN	3.2
3	C	125	PHE	3.1
2	B	265	PHE	3.1
3	C	179	SER	3.1
3	C	71	MET	3.0
3	C	184	ILE	3.0
3	C	16	ALA	3.0
3	C	173	ALA	3.0
3	C	170	MET	3.0
3	C	185	GLU	3.0
3	C	187	LYS	3.0
3	C	68	LEU	2.9
3	C	23	ILE	2.9
1	A	710	GLY	2.9
2	B	273	ILE	2.9
2	B	272	LEU	2.8
2	B	280	GLY	2.8
3	C	146	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	64	ILE	2.8
3	C	195	LYS	2.8
3	C	135	TRP	2.8
3	C	122	SER	2.8
3	C	108	LYS	2.8
3	C	22	VAL	2.8
3	C	144	PRO	2.7
3	C	114	LYS	2.7
3	C	62	ILE	2.7
1	A	713	ILE	2.7
3	C	67	ALA	2.6
3	C	157	ALA	2.6
1	A	712	LEU	2.6
2	B	270	ALA	2.6
3	C	183	MET	2.6
3	C	177	LYS	2.6
3	C	126	VAL	2.6
2	B	275	HIS	2.5
3	C	165	ALA	2.5
3	C	133	ILE	2.5
2	B	268	THR	2.5
3	C	15	ARG	2.5
2	B	262	ALA	2.4
1	A	345	ASN	2.4
3	C	9	ARG	2.4
3	C	162	LEU	2.4
3	C	167	LEU	2.4
2	B	248	THR	2.4
1	A	707	ASP	2.4
3	C	20	THR	2.3
3	C	59	PHE	2.3
3	C	124	ILE	2.3
3	C	160	ILE	2.3
2	B	263	ALA	2.2
3	C	129	VAL	2.2
3	C	123	MET	2.2
2	B	264	GLY	2.2
3	C	79	ASN	2.2
3	C	63	ALA	2.1
3	C	164	HIS	2.0
3	C	44	THR	2.0
3	C	168	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	116	MET	2.0
3	C	21	VAL	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](#)

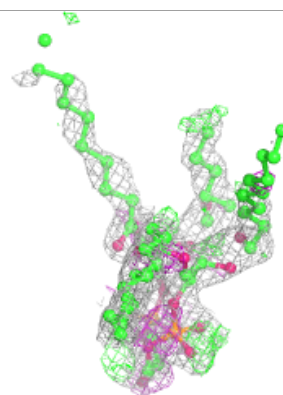
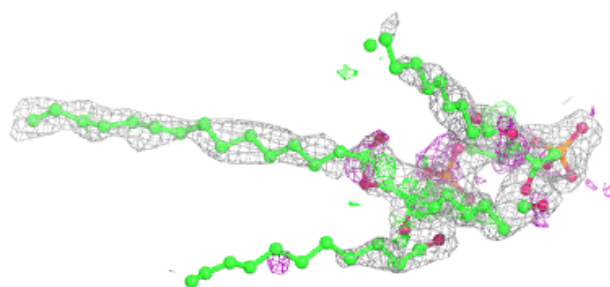
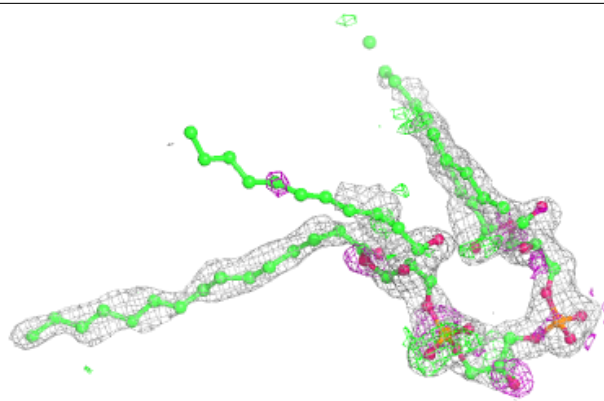
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	CDL	C	812	70/100	0.76	0.26	44,56,61,61	0
7	HEM	C	810	43/43	0.87	0.25	44,45,48,49	0
7	HEM	C	809	43/43	0.92	0.15	29,33,35,37	0
6	MGD	A	1018	47/47	0.96	0.11	11,13,14,15	0
6	MGD	A	1019	47/47	0.96	0.12	11,14,16,18	0
5	SF4	B	807	8/8	0.98	0.08	14,15,16,16	0
5	SF4	B	808	8/8	0.98	0.07	16,18,19,19	0
5	SF4	A	1017	8/8	0.99	0.10	11,12,12,12	0
5	SF4	B	806	8/8	0.99	0.09	12,13,13,13	0
5	SF4	B	805	8/8	0.99	0.09	12,13,13,14	0
4	6MO	A	1016	1/1	0.99	0.09	16,16,16,16	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.

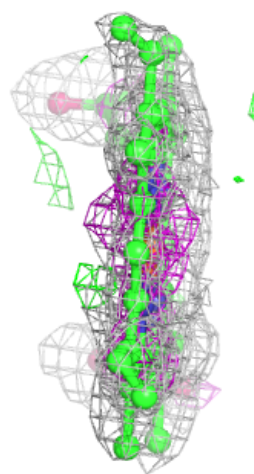
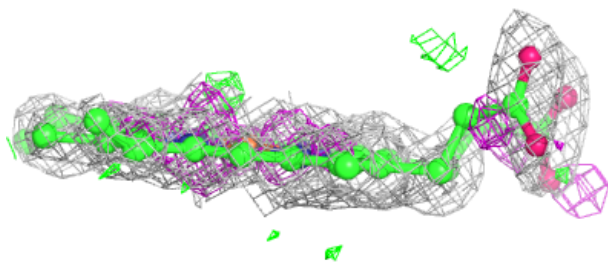
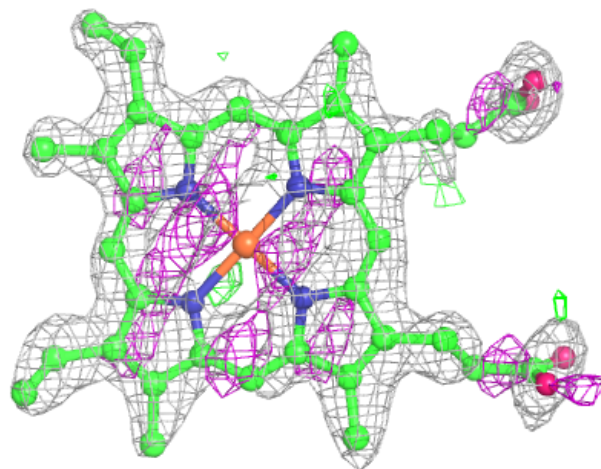
Electron density around CDL C 812:

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



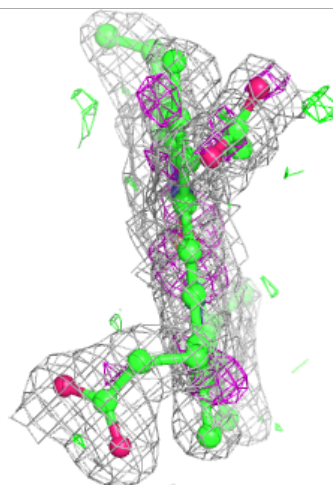
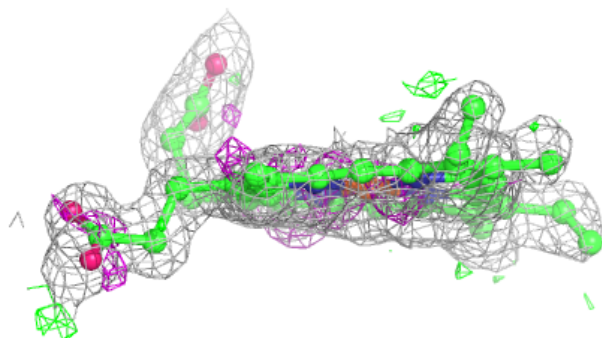
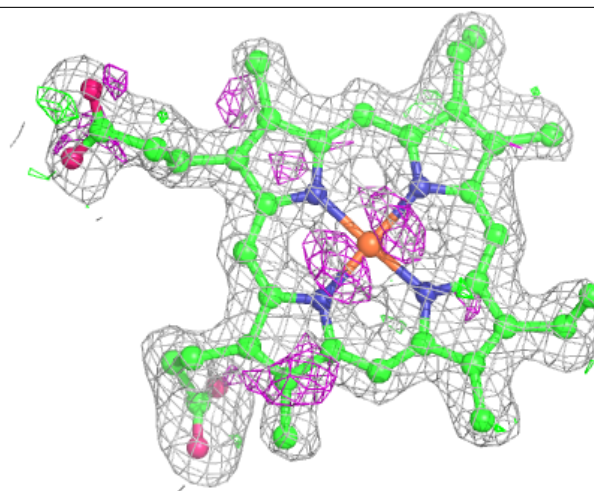
Electron density around HEM C 810:

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



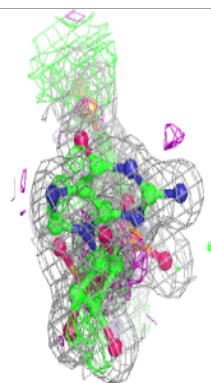
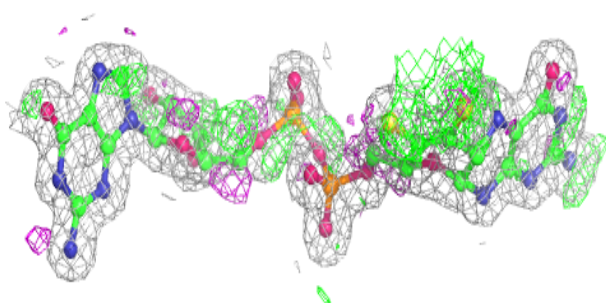
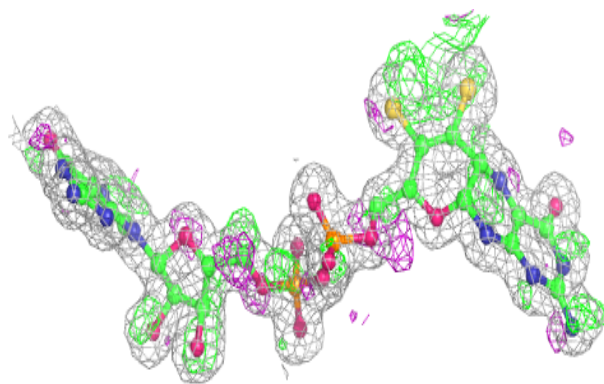
Electron density around HEM C 809:

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

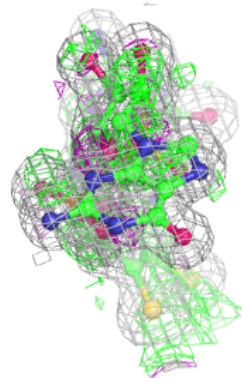
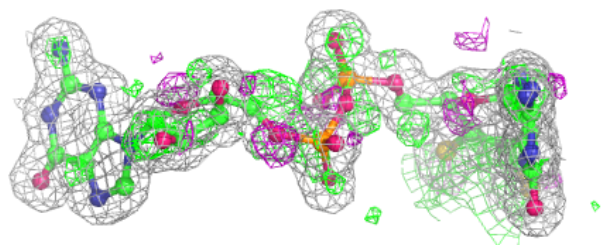
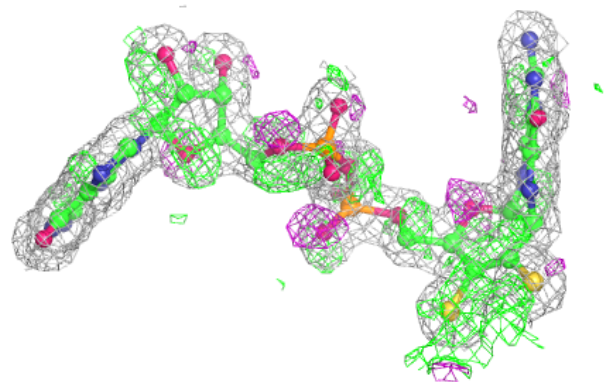


Electron density around MGD A 1018:

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

**Electron density around MGD A 1019:**

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



6.5 Other polymers

There are no such residues in this entry.