



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:54 PM UTC

PDB ID : 1KQF / pdb_00001kqf
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

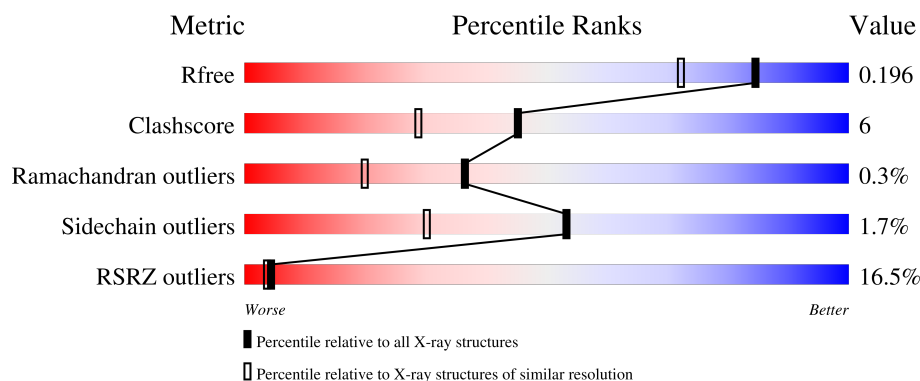
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1015	3% 85% 11% ..
2	B	294	14% 85% 13% ..
3	C	217	79% 65% 30% ..

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			

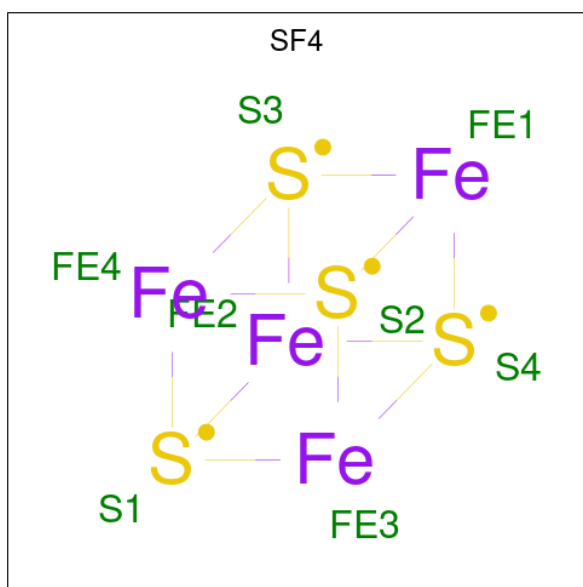
- Molecule 3 is a protein called FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, CYTOCHROME B556(FDN) SUBUNIT.

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 (CCD ID: 6MO) (formula: Mo).

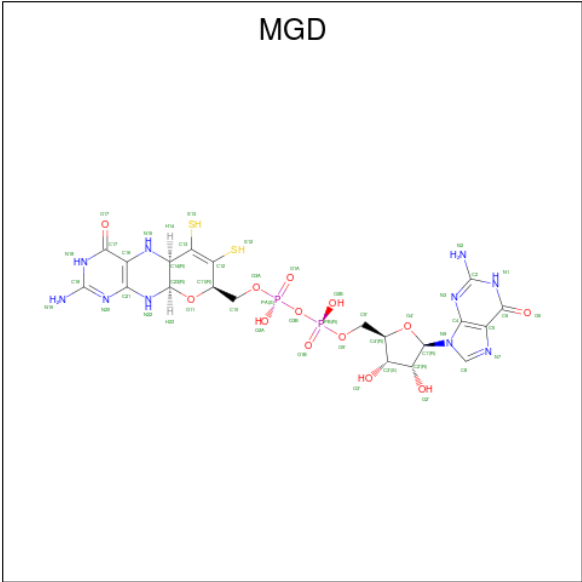
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mo	0	0
			1	1		

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



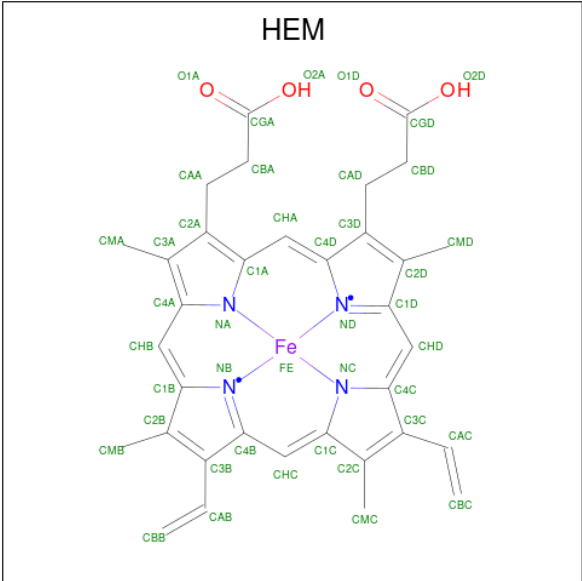
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		

- 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 (CCD ID: 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 (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



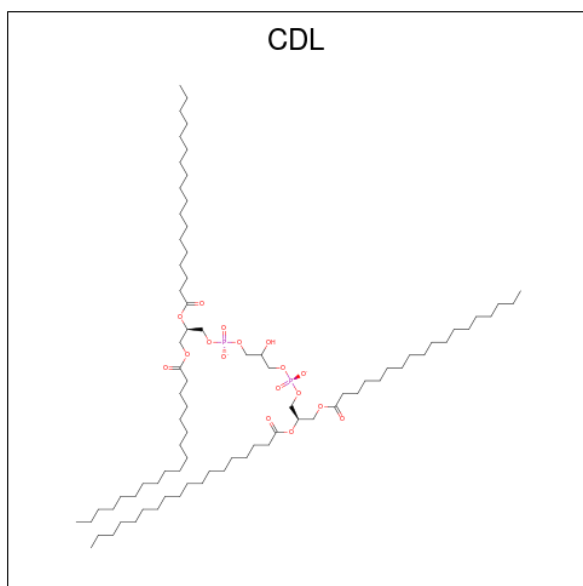
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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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 (CCD ID: 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		

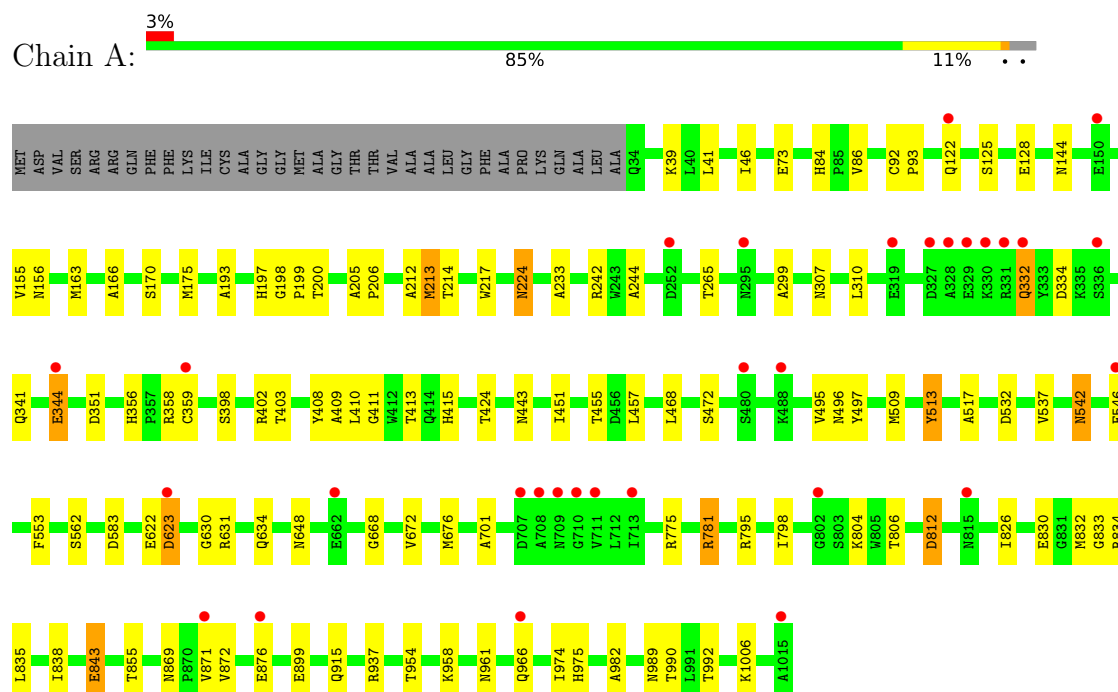
- Molecule 9 is water.

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		

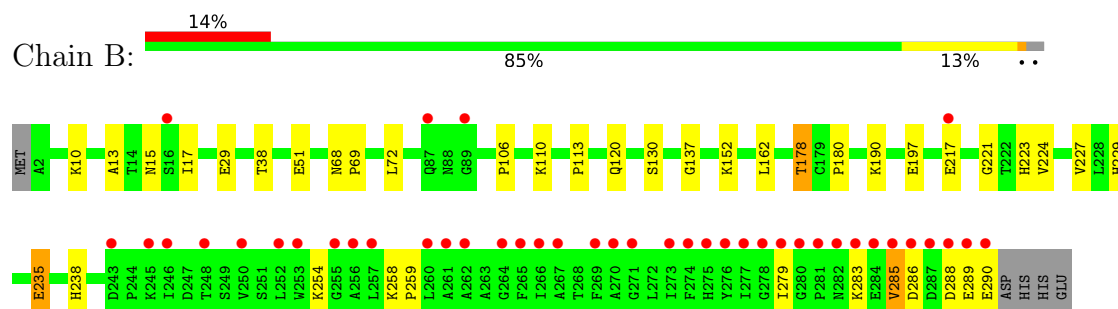
3 Residue-property plots

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.

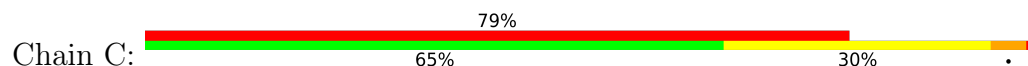
- Molecule 1: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, MAJOR SUBUNIT

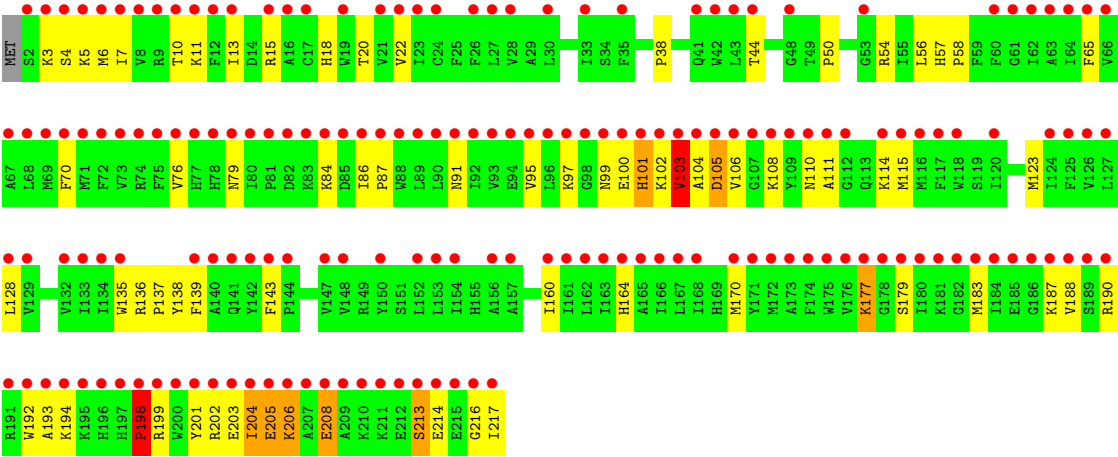


- Molecule 2: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, IRON-SULFUR SUBUNIT



- 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 40.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.9 (40.00-1.60) 94.1 (40.00-1.60)	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 0.182 , 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 , 53.1	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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.40	0/7910	1.01	50/10749 (0.5%)
2	B	0.40	0/2255	0.99	9/3056 (0.3%)
3	C	0.37	0/1840	1.06	17/2483 (0.7%)
All	All	0.40	0/12005	1.01	76/16288 (0.5%)

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	138	TYR	N-CA-C	11.97	123.87	111.07
1	A	975	HIS	N-CA-C	9.82	125.26	113.28
2	B	227	VAL	N-CA-C	-9.22	95.21	108.11
1	A	974	ILE	N-CA-C	9.05	119.96	111.91
1	A	334	ASP	N-CA-C	-8.91	94.79	108.96
1	A	992	THR	N-CA-C	8.16	121.34	110.08
3	C	104	ALA	N-CA-C	7.14	119.77	109.14
2	B	224	VAL	N-CA-C	-7.07	97.31	107.77
3	C	139	PHE	N-CA-C	7.06	122.79	114.04
1	A	915	GLN	CA-C-N	7.04	126.66	119.19
1	A	915	GLN	C-N-CA	7.04	126.66	119.19
1	A	562	SER	N-CA-C	7.02	121.93	113.23
1	A	166	ALA	N-CA-C	7.01	120.29	108.23
2	B	286	ASP	N-CA-C	-6.88	104.89	113.28
1	A	812	ASP	N-CA-C	-6.85	101.16	110.68
2	B	130	SER	N-CA-C	6.85	120.52	111.75
1	A	39	LYS	N-CA-C	6.76	121.12	113.01
3	C	56	LEU	N-CA-C	6.68	119.57	111.82
1	A	413	THR	N-CA-C	6.64	118.60	111.36
1	A	826	ILE	N-CA-C	6.63	121.62	113.00
1	A	537	VAL	N-CA-C	6.55	117.30	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	GLN	N-CA-C	-6.51	100.85	110.48
1	A	835	LEU	N-CA-C	-6.48	103.72	111.69
1	A	542	ASN	N-CA-C	-6.41	104.37	111.36
1	A	217	TRP	N-CA-C	6.41	118.84	111.02
3	C	76	VAL	N-CA-C	6.36	117.04	110.36
3	C	103	VAL	N-CA-C	6.31	120.98	113.22
1	A	144	ASN	N-CA-C	6.30	121.75	113.30
1	A	899	GLU	N-CA-C	6.29	120.22	112.54
1	A	982	ALA	N-CA-C	-6.29	102.41	110.53
2	B	221	GLY	N-CA-C	-6.27	105.27	112.29
1	A	623	ASP	N-CA-C	-6.15	100.89	110.42
3	C	143	PHE	CA-C-N	6.11	126.05	119.76
3	C	143	PHE	C-N-CA	6.11	126.05	119.76
1	A	170	SER	N-CA-C	6.04	117.83	110.41
2	B	178	THR	N-CA-C	6.01	118.79	111.82
1	A	410	LEU	N-CA-C	5.92	118.69	111.82
1	A	299	ALA	N-CA-C	5.89	118.18	111.11
1	A	532	ASP	N-CA-C	-5.84	106.32	113.50
3	C	70	PHE	N-CA-C	-5.81	105.02	111.36
1	A	468	LEU	N-CA-C	-5.81	102.17	110.59
1	A	224	ASN	N-CA-C	-5.75	106.43	113.50
1	A	233	ALA	N-CA-C	5.73	119.09	111.75
3	C	20	THR	N-CA-C	-5.69	104.69	111.69
3	C	179	SER	N-CA-C	5.67	117.54	111.36
1	A	214	THR	N-CA-C	5.65	119.35	112.23
3	C	213	SER	N-CA-C	-5.64	106.23	113.23
3	C	192	TRP	N-CA-C	-5.62	105.23	111.36
1	A	398	SER	N-CA-C	-5.60	106.41	113.18
1	A	974	ILE	CB-CA-C	-5.55	105.81	112.19
1	A	954	THR	N-CA-C	5.55	117.70	108.99
1	A	668	GLY	N-CA-C	-5.53	102.27	112.62
1	A	41	LEU	N-CA-C	5.53	118.83	111.75
1	A	244	ALA	N-CA-C	-5.53	105.27	112.23
1	A	781	ARG	N-CA-C	-5.52	105.42	111.82
1	A	212	ALA	N-CA-C	5.47	117.94	110.55
2	B	72	LEU	N-CA-C	-5.44	102.82	110.50
1	A	497	TYR	N-CA-C	5.44	119.01	112.38
1	A	701	ALA	N-CA-C	-5.44	100.43	109.46
1	A	455	THR	N-CA-C	-5.43	105.44	111.36
1	A	213	MET	N-CA-C	-5.43	102.01	110.10
3	C	106	VAL	N-CA-C	5.42	115.67	107.80
2	B	289	GLU	N-CA-C	-5.41	106.45	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	177	LYS	N-CA-C	5.40	117.86	110.24
1	A	990	THR	N-CA-C	-5.39	105.57	111.82
1	A	583	ASP	N-CA-CB	-5.38	106.21	111.27
1	A	472	SER	N-CA-C	-5.35	102.60	110.52
1	A	834	ARG	N-CA-C	5.29	117.38	108.96
1	A	833	GLY	N-CA-C	-5.23	101.95	111.15
1	A	843	GLU	N-CA-C	5.16	118.88	112.59
3	C	135	TRP	N-CA-C	5.15	116.66	108.67
1	A	513	TYR	N-CA-C	5.09	120.34	113.72
2	B	106	PRO	N-CA-C	5.04	118.42	110.50
1	A	1006	LYS	N-CA-C	5.04	119.42	113.28
1	A	265	THR	N-CA-C	-5.02	105.52	111.69
3	C	187	LYS	N-CA-C	5.01	117.91	109.95

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	65	0
2	B	2207	0	2140	21	0
3	C	1783	0	1836	59	0
4	A	1	0	0	0	0
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	17	2
9	B	399	0	0	6	0
9	C	93	0	0	10	0
All	All	13989	0	11620	139	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 (139) 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:830:GLU:HG3	1:A:832:MET:HE2	1.44	0.99
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
1:A:830:GLU:CG	1:A:832:MET:HE2	2.12	0.79
1:A:307:ASN:HB3	1:A:832:MET:HE3	1.65	0.79
3:C:202:ARG:O	3:C:206:LYS:HD2	1.83	0.78
3:C:101:HIS:HD2	3:C:102:LYS:H	1.33	0.76
1:A:830:GLU:HG3	1:A:832:MET:CE	2.16	0.75
3:C:15:ARG:HG2	3:C:183:MET:HE3	1.69	0.73
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:205:ALA:HB3	1:A:206:PRO:HD3	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:622:GLU:CD	1:A:648:ASN:HB2	2.21	0.65
1:A:937:ARG:NH2	9:A:1412:HOH:O	2.26	0.65
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:O	1:A:871:VAL:HG12	1.99	0.61
3:C:213:SER:HA	9:C:1896:HOH:O	2.00	0.61
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:216:GLY:O	3:C:217:ILE:C	2.45	0.59
3:C:190:ARG:O	3:C:194:LYS:HG3	2.02	0.59
1:A:310:LEU:HD22	1:A:832:MET:HE1	1.84	0.59
1:A:332:GLN:HG3	9:A:2386:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:199:ARG:O	3:C:203:GLU:HG2	2.06	0.55
1:A:224:ASN:HD21	1:A:795:ARG:HH22	1.54	0.55
2:B:68:ASN:HA	2:B:69:PRO:C	2.32	0.54
3:C:190:ARG:NH1	3:C:201:TYR:OH	2.36	0.54
1:A:84:HIS:HE1	1:A:634:GLN:OE1	1.90	0.54
1:A:344:GLU:CD	1:A:344:GLU:H	2.16	0.53
3:C:194:LYS:O	3:C:198:PRO:HG3	2.08	0.53
3:C:15:ARG:HA	3:C:183:MET:HE2	1.91	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:307:ASN:HB3	1:A:832:MET:CE	2.37	0.52
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:84:HIS:CD2	1:A:86:VAL:H	2.28	0.51
1:A:332:GLN:CG	9:A:2386:HOH:O	2.57	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:310:LEU:CD2	1:A:832:MET:HE1	2.40	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
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
3:C:123:MET:HA	3:C:123:MET:HE2	1.94	0.50
1:A:989:ASN:ND2	6:A:1018:MGD:H192	2.10	0.49
3:C:10:THR:HG21	3:C:183:MET:HE1	1.92	0.49
2:B:10:LYS:HB2	2:B:120:GLN:HB3	1.95	0.49
2:B:283:LYS:HD3	3:C:177:LYS:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:630:GLY:O	1:A:631:ARG:HB2	2.13	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: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
2:B:235:GLU:H	2:B:235:GLU:CD	2.24	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: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
1:A:958:LYS:NZ	9:A:2403:HOH:O	2.51	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:408:TYR:CD1	1:A:408:TYR:C	2.95	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
2:B:190:LYS:HD3	9:B:1161:HOH:O	2.18	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
3:C:160:ILE:O	3:C:164:HIS:HD2	2.01	0.43
1:A:359:CYS:CB	9:A:1672:HOH:O	2.43	0.43
2:B:38:THR:O	2:B:38:THR:HG22	2.17	0.43
2:B:217:GLU:HG2	9:B:1069:HOH:O	2.17	0.43
2:B:258:LYS:HB2	2:B:259:PRO:CD	2.48	0.43
1:A:344:GLU:CD	1:A:344:GLU:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:79:ASN:HD22	3:C:114:LYS:HA	1.85	0.41
3:C:105:ASP:HB3	9:C:1932:HOH:O	2.19	0.41
1:A:495:VAL:O	1:A:496:ASN:C	2.62	0.41
1:A:175:MET:HE2	1:A:457:LEU:HD22	2.03	0.41
1:A:804:LYS:HE3	1:A:806:THR:CG2	2.51	0.41
3:C:11:LYS:HG2	3:C:13:ILE:HG22	2.03	0.41
3:C:54:ARG:HD2	3:C:54:ARG:C	2.45	0.41
3:C:105:ASP:HB2	9:C:1672:HOH:O	2.20	0.41
1:A:155:VAL:O	1:A:156:ASN:C	2.64	0.40
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%)	43 24
2	B	287/294 (98%)	278 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	214/217 (99%)	206 (96%)	6 (3%)	2 (1%)	14	3
All	All	1480/1526 (97%)	1435 (97%)	41 (3%)	4 (0%)	36	20

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%)	810 (99%)	5 (1%)	78	66
2	B	238/243 (98%)	230 (97%)	8 (3%)	32	11
3	C	188/189 (100%)	180 (96%)	8 (4%)	26	7
All	All	1241/1269 (98%)	1220 (98%)	21 (2%)	53	30

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	GLN
1	A	344	GLU
1	A	424	THR
1	A	843	GLU
1	A	855	THR
2	B	51	GLU
2	B	113	PRO
2	B	162	LEU
2	B	178	THR
2	B	229	HIS
2	B	235	GLU

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Mol	Chain	Res	Type
2	B	285	VAL
2	B	290	GLU
3	C	101	HIS
3	C	103	VAL
3	C	105	ASP
3	C	137	PRO
3	C	198	PRO
3	C	204	ILE
3	C	205	GLU
3	C	206	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	122	GLN
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	522	ASN
1	A	542	ASN
1	A	596	HIS
1	A	665	GLN
1	A	749	GLN
1	A	752	ASN
1	A	865	ASN
1	A	966	GLN
1	A	989	ASN
2	B	155	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 oligosaccharides 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	A	1017	1	0,12,12	-	-	-		
7	HEM	C	809	3	50,50,50	1.63	12 (24%)	67,82,82	1.05	6 (8%)
7	HEM	C	810	3	50,50,50	1.48	9 (18%)	67,82,82	0.98	5 (7%)
6	MGD	A	1018	4	47,52,52	2.18	9 (19%)	58,81,81	2.33	16 (27%)
5	SF4	B	805	2	0,12,12	-	-	-		
5	SF4	B	807	2	0,12,12	-	-	-		
5	SF4	B	808	2	0,12,12	-	-	-		
6	MGD	A	1019	4	47,52,52	2.49	7 (14%)	58,81,81	1.80	10 (17%)
8	CDL	C	812	-	69,69,99	2.99	22 (31%)	75,81,111	2.64	16 (21%)
5	SF4	B	806	2	0,12,12	-	-	-		

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	A	1017	1	-	-	0/6/5/5
7	HEM	C	810	3	-	4/14/54/54	-
6	MGD	A	1018	4	-	6/22/66/66	0/6/6/6
5	SF4	B	805	2	-	-	0/6/5/5
5	SF4	B	806	2	-	-	0/6/5/5
5	SF4	B	807	2	-	-	0/6/5/5
5	SF4	B	808	2	-	-	0/6/5/5
6	MGD	A	1019	4	-	11/22/66/66	0/6/6/6
8	CDL	C	812	-	-	37/80/80/110	-
7	HEM	C	809	3	-	8/14/54/54	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	812	CDL	OB8-CB6	-14.83	1.12	1.45
6	A	1018	MGD	O3A-C10	-10.05	1.06	1.44
6	A	1019	MGD	O3A-C10	-9.85	1.07	1.44
8	C	812	CDL	OA6-CA5	9.71	1.61	1.34
8	C	812	CDL	OB6-CB5	7.64	1.55	1.34
6	A	1019	MGD	PB-O3B	7.18	1.67	1.59
6	A	1018	MGD	PB-O3B	6.39	1.66	1.59
8	C	812	CDL	C51-CB5	5.90	1.67	1.50
6	A	1019	MGD	C23-C14	-5.32	1.49	1.53
6	A	1019	MGD	O11-C23	-4.66	1.36	1.43
8	C	812	CDL	PA1-OA3	4.59	1.66	1.50
6	A	1019	MGD	C16-C21	4.22	1.45	1.38
7	C	809	HEM	CAB-C3B	4.07	1.58	1.47
7	C	810	HEM	CAC-C3C	3.88	1.57	1.47
8	C	812	CDL	C11-CA5	3.76	1.61	1.50
8	C	812	CDL	OA8-CA7	3.71	1.44	1.33
8	C	812	CDL	OB8-CB7	-3.54	1.23	1.33
6	A	1019	MGD	O5'-C5'	-3.33	1.32	1.44
7	C	810	HEM	CAB-C3B	3.32	1.56	1.47
7	C	810	HEM	CMC-C2C	3.07	1.57	1.50
8	C	812	CDL	C39-C38	-3.07	1.36	1.51
7	C	809	HEM	CAC-C3C	3.01	1.55	1.47
8	C	812	CDL	C79-C78	3.00	1.71	1.50
7	C	809	HEM	FE-NC	2.96	2.04	1.95
7	C	809	HEM	CMC-C2C	2.93	1.56	1.50
6	A	1018	MGD	C16-C21	2.89	1.43	1.38
8	C	812	CDL	PB2-OB4	2.88	1.68	1.55
8	C	812	CDL	PB2-OB3	2.84	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	812	CDL	C42-C41	-2.78	1.37	1.51
7	C	809	HEM	CBA-CAA	2.74	1.61	1.51
8	C	812	CDL	C12-C11	2.71	1.62	1.52
7	C	810	HEM	FE-NC	2.71	2.04	1.95
7	C	809	HEM	CMD-C2D	2.68	1.56	1.50
8	C	812	CDL	CB3-CB4	2.66	1.59	1.50
7	C	810	HEM	CMA-C3A	2.64	1.56	1.50
8	C	812	CDL	C19-C18	-2.62	1.35	1.51
6	A	1018	MGD	C23-N22	2.58	1.49	1.45
8	C	812	CDL	C52-C51	2.54	1.61	1.52
8	C	812	CDL	PA1-OA5	2.48	1.69	1.59
7	C	809	HEM	CMB-C2B	2.46	1.55	1.50
7	C	810	HEM	FE-NB	2.46	2.02	1.94
6	A	1018	MGD	O5'-C5'	-2.44	1.35	1.44
7	C	809	HEM	CAD-C3D	2.42	1.57	1.51
6	A	1018	MGD	C21-N22	2.41	1.38	1.35
8	C	812	CDL	OB9-CB7	2.39	1.29	1.22
7	C	809	HEM	CMA-C3A	2.36	1.55	1.50
6	A	1019	MGD	O11-C11	-2.34	1.39	1.43
6	A	1018	MGD	PB-O1B	-2.32	1.42	1.50
7	C	810	HEM	CMD-C2D	2.30	1.55	1.50
7	C	809	HEM	CBA-CGA	2.29	1.55	1.50
8	C	812	CDL	OB2-CB2	-2.22	1.36	1.44
7	C	809	HEM	FE-NB	2.18	2.01	1.94
6	A	1018	MGD	C10-C11	2.16	1.54	1.51
8	C	812	CDL	OB6-CB4	-2.12	1.41	1.46
7	C	810	HEM	CAD-C3D	2.10	1.56	1.51
6	A	1018	MGD	O2'-C2'	2.07	1.48	1.43
7	C	810	HEM	CMB-C2B	2.06	1.55	1.50
7	C	809	HEM	CAA-C2A	2.03	1.56	1.51
8	C	812	CDL	CA3-CA4	-2.01	1.44	1.50

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	812	CDL	OB6-CB5-C51	13.81	141.36	111.48
6	A	1018	MGD	O11-C23-C14	8.99	114.96	108.96
8	C	812	CDL	CB6-OB8-CB7	-7.46	89.86	117.12
8	C	812	CDL	CA6-CA4-CA3	-7.23	94.93	111.78
8	C	812	CDL	C52-C51-CB5	-6.37	90.36	113.69
6	A	1019	MGD	C19-N20-C21	6.10	124.12	113.36
6	A	1018	MGD	C19-N20-C21	6.09	124.11	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	812	CDL	OB7-CB5-C51	-5.76	101.26	123.78
8	C	812	CDL	OA6-CA5-OA7	-5.23	111.48	123.70
6	A	1018	MGD	O4'-C1'-C2'	-5.00	95.92	106.62
6	A	1018	MGD	O11-C23-N22	4.70	112.87	108.61
6	A	1019	MGD	O11-C23-C14	4.28	111.82	108.96
6	A	1019	MGD	O4'-C1'-N9	-4.22	98.80	108.36
6	A	1018	MGD	O4'-C4'-C5'	4.18	122.74	109.33
6	A	1018	MGD	C23-C14-N15	3.68	111.48	107.87
8	C	812	CDL	CB6-CB4-CB3	-3.54	103.53	111.78
8	C	812	CDL	OA4-PA1-OA3	-3.25	97.33	112.44
7	C	809	HEM	CAD-C3D-C4D	-3.20	119.13	124.70
8	C	812	CDL	O1-C1-CA2	-3.16	98.79	109.70
6	A	1018	MGD	N2-C2-N3	3.14	125.80	119.67
6	A	1019	MGD	O5'-C5'-C4'	2.99	119.16	108.99
6	A	1019	MGD	PB-O5'-C5'	2.98	138.42	121.35
6	A	1018	MGD	O5'-C5'-C4'	2.96	119.06	108.99
6	A	1019	MGD	O2A-PA-O3B	-2.95	99.30	107.27
6	A	1018	MGD	PB-O5'-C5'	2.91	138.04	121.35
6	A	1018	MGD	C4'-O4'-C1'	-2.90	103.07	109.47
6	A	1019	MGD	N2-C2-N3	2.83	125.19	119.67
6	A	1018	MGD	N18-C19-N20	-2.77	118.25	123.32
8	C	812	CDL	OB6-CB5-OB7	-2.73	117.32	123.70
7	C	809	HEM	CAD-C3D-C2D	2.69	132.91	127.87
7	C	810	HEM	CMA-C3A-C2A	2.67	131.28	125.62
6	A	1019	MGD	O3B-PA-O1A	-2.62	102.82	110.70
8	C	812	CDL	OA7-CA5-C11	-2.57	113.73	123.78
7	C	810	HEM	O1D-CGD-CBD	-2.47	115.24	123.09
6	A	1018	MGD	O3A-C10-C11	2.43	114.58	108.58
6	A	1019	MGD	C17-C16-N15	2.35	122.66	116.27
6	A	1019	MGD	N18-C19-N20	-2.34	119.04	123.32
8	C	812	CDL	CA6-OA8-CA7	-2.24	108.93	117.12
6	A	1018	MGD	O4'-C1'-N9	-2.20	103.38	108.36
7	C	809	HEM	CMA-C3A-C2A	2.18	130.25	125.62
7	C	809	HEM	O1D-CGD-CBD	-2.15	116.26	123.09
7	C	810	HEM	O2D-CGD-O1D	2.15	128.86	123.33
7	C	810	HEM	CAD-CBD-CGD	2.08	119.18	113.67
8	C	812	CDL	CA4-OA6-CA5	-2.07	112.83	117.80
8	C	812	CDL	OA6-CA4-CA3	2.07	115.77	108.34
8	C	812	CDL	OB9-CB7-C71	-2.05	115.78	123.78
7	C	809	HEM	CAA-CBA-CGA	2.05	119.09	113.67
7	C	810	HEM	O1A-CGA-CBA	-2.04	116.61	123.09
7	C	809	HEM	CBC-CAC-C3C	-2.04	117.34	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1018	MGD	O2A-PA-O3B	-2.03	101.79	107.27
8	C	812	CDL	C40-C39-C38	2.03	124.61	114.37
6	A	1018	MGD	O6-C6-C5	-2.01	121.23	126.53
6	A	1018	MGD	C16-C17-N18	2.00	117.62	112.13

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1018	MGD	C10-O3A-PA-O3B
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-O3B
6	A	1019	MGD	C10-O3A-PA-O1A
7	C	809	HEM	C2C-C3C-CAC-CBC
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-OA2
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	CB2-OB2-PB2-OB5
8	C	812	CDL	CB3-OB5-PB2-OB2
8	C	812	CDL	CB3-OB5-PB2-OB3
8	C	812	CDL	CB3-OB5-PB2-OB4
8	C	812	CDL	OB9-CB7-OB8-CB6
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	O1-C1-CA2-OA2
8	C	812	CDL	CA5-C11-C12-C13
8	C	812	CDL	CA7-C31-C32-C33
8	C	812	CDL	C36-C37-C38-C39
8	C	812	CDL	CB2-C1-CA2-OA2
8	C	812	CDL	C51-CB5-OB6-CB4
8	C	812	CDL	OB7-CB5-OB6-CB4
7	C	809	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
7	C	809	HEM	C4C-C3C-CAC-CBC
8	C	812	CDL	C71-CB7-OB8-CB6
8	C	812	CDL	CB3-CB4-CB6-OB8
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	1018	MGD	PB-O3B-PA-O1A
8	C	812	CDL	C33-C34-C35-C36
8	C	812	CDL	C15-C16-C17-C18
8	C	812	CDL	OA5-CA3-CA4-CA6
8	C	812	CDL	OA5-CA3-CA4-OA6
6	A	1018	MGD	C10-O3A-PA-O2A
7	C	809	HEM	C4B-C3B-CAB-CBB
6	A	1019	MGD	C2'-C1'-N9-C8
7	C	810	HEM	C3D-CAD-CBD-CGD
7	C	809	HEM	CAD-CBD-CGD-O1D
6	A	1019	MGD	PB-O3B-PA-O1A
7	C	809	HEM	CAD-CBD-CGD-O2D
7	C	809	HEM	CAA-CBA-CGA-O2A
7	C	810	HEM	CAA-CBA-CGA-O1A
8	C	812	CDL	C41-C42-C43-C44
7	C	809	HEM	CAA-CBA-CGA-O1A
8	C	812	CDL	OB5-CB3-CB4-CB6
6	A	1019	MGD	C2'-C1'-N9-C4
7	C	810	HEM	CAA-CBA-CGA-O2A
8	C	812	CDL	C17-C18-C19-C20
8	C	812	CDL	OA7-CA5-OA6-CA4
8	C	812	CDL	C72-C71-CB7-OB8
8	C	812	CDL	C12-C11-CA5-OA7
7	C	810	HEM	C2B-C3B-CAB-CBB
6	A	1019	MGD	PB-O3B-PA-O2A

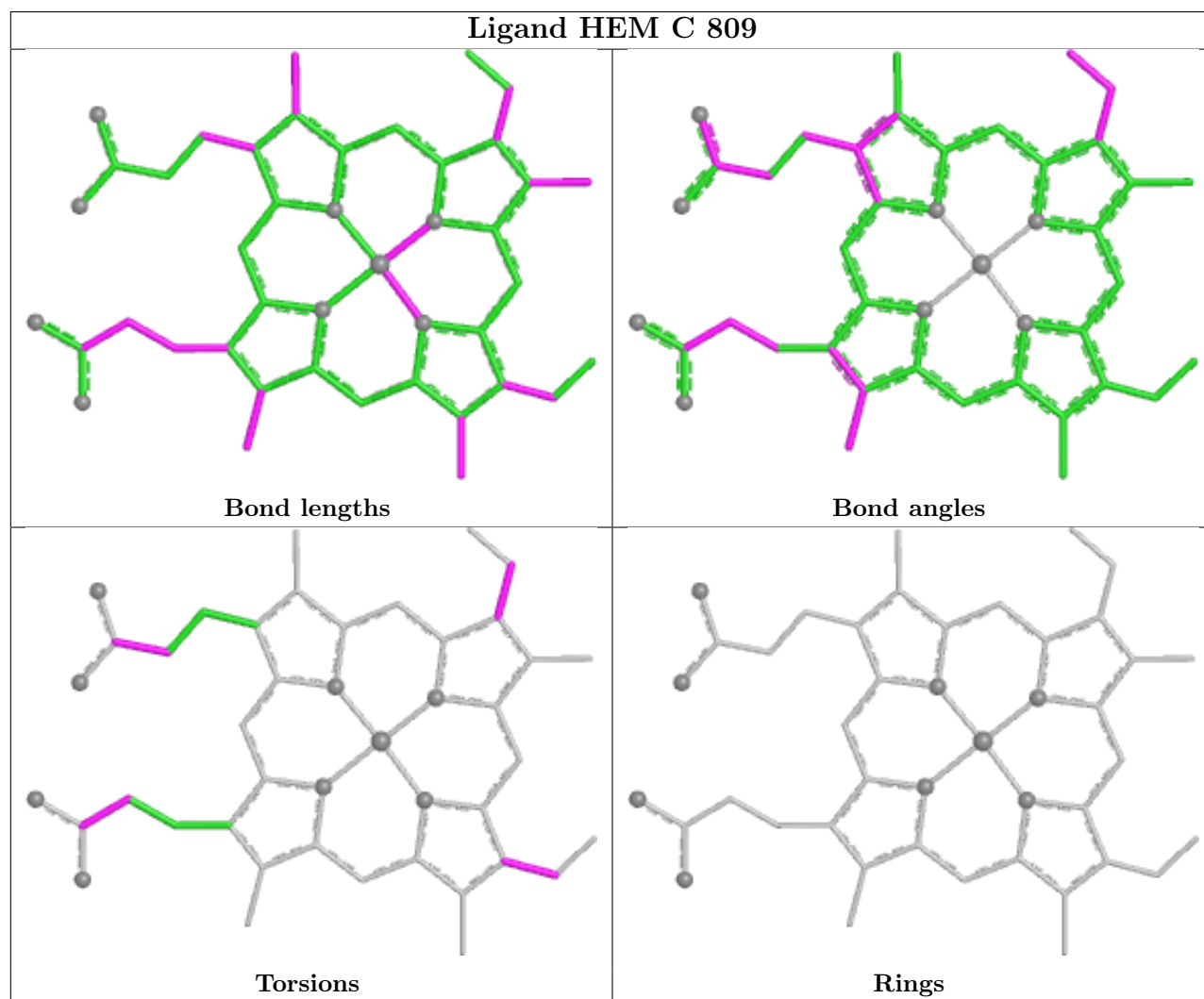
There are no ring outliers.

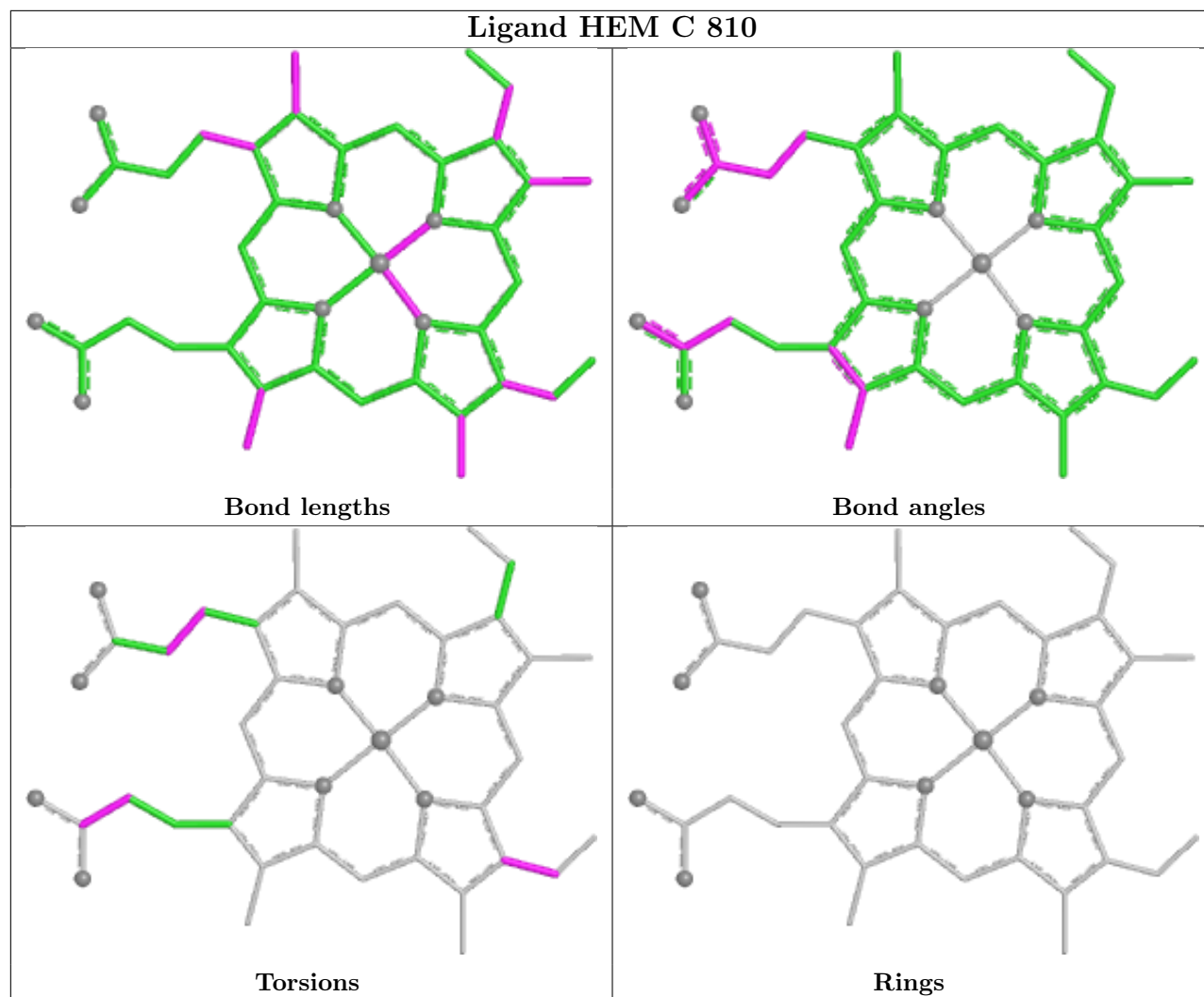
2 monomers are involved in 3 short contacts:

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

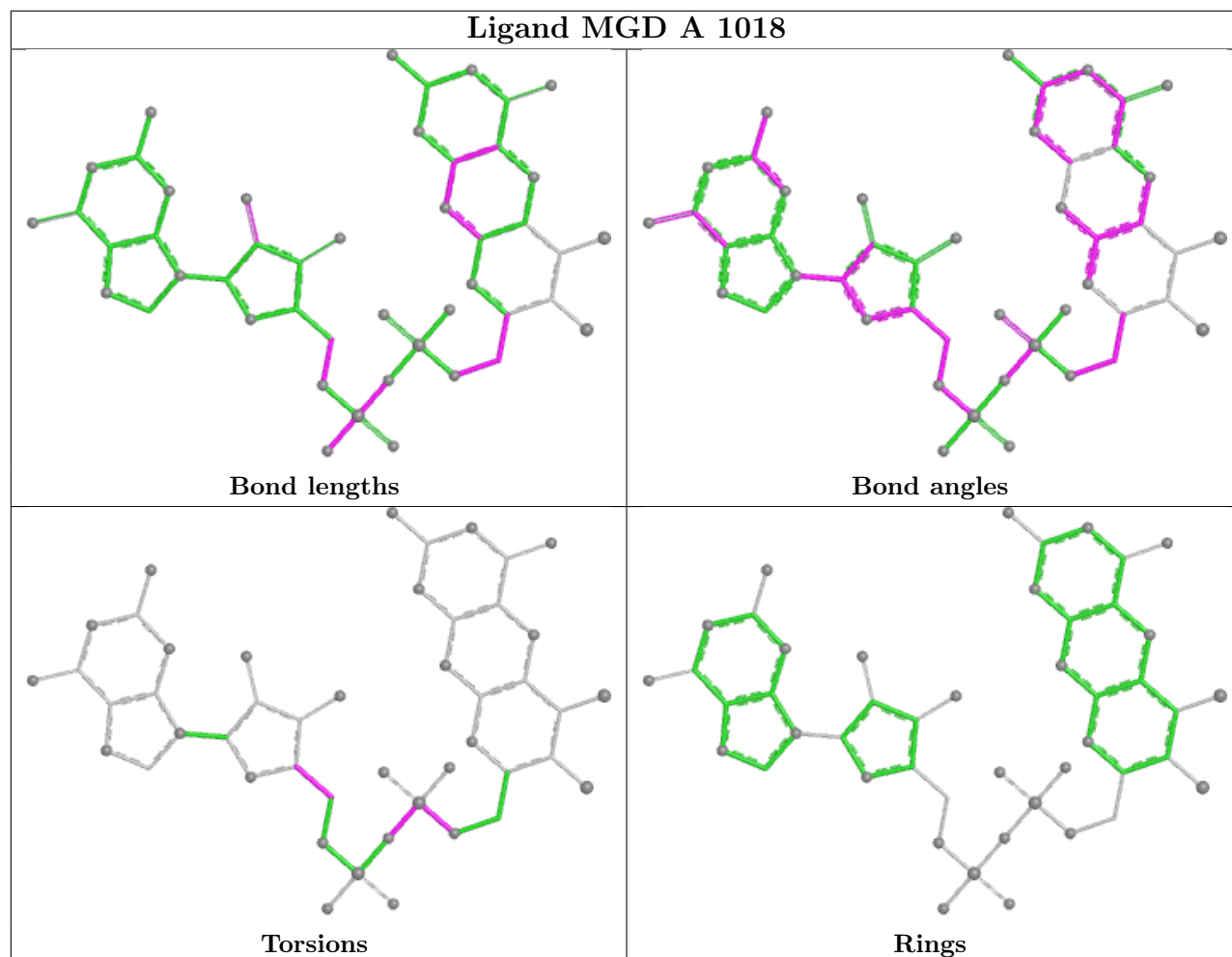
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

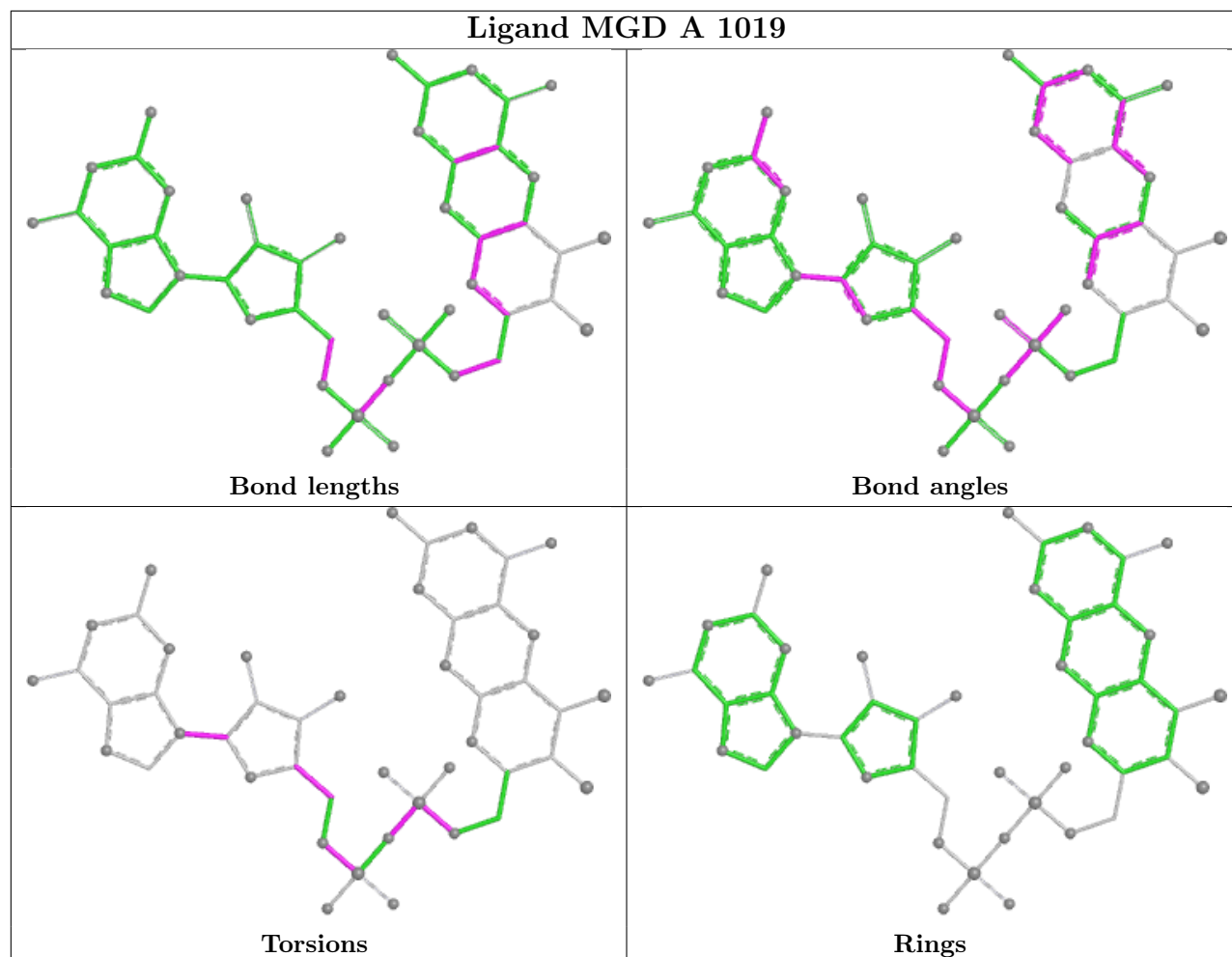




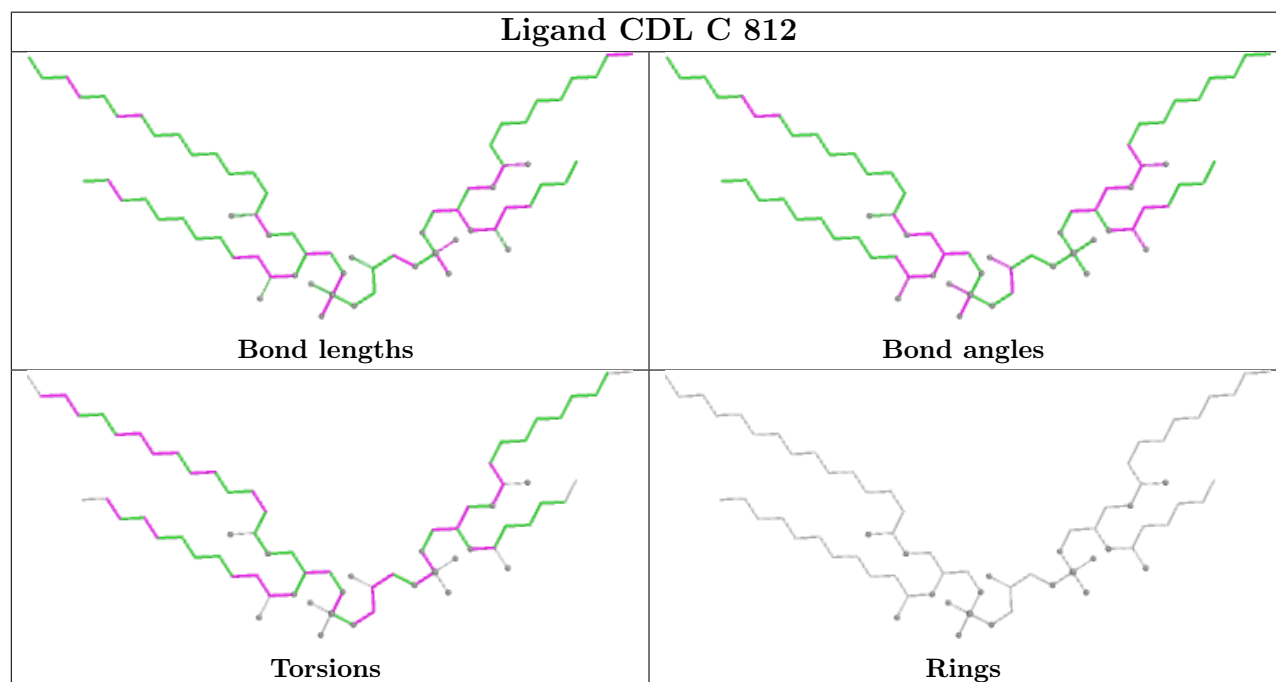
Ligand MGD A 1018



Ligand MGD A 1019



Ligand CDL C 812



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%)	-0.01	31 (3%) 50 53	11, 18, 30, 56	0
2	B	289/294 (98%)	0.46	42 (14%) 6 5	11, 18, 52, 67	0
3	C	216/217 (99%)	3.11	172 (79%) 0 0	30, 49, 63, 65	0
All	All	1486/1526 (97%)	0.54	245 (16%) 4 4	11, 19, 54, 67	0

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	217	ILE	9.1
3	C	204	ILE	7.9
3	C	106	VAL	7.8
2	B	286	ASP	6.9
3	C	192	TRP	6.9
2	B	287	ASP	6.8
3	C	207	ALA	6.8
2	B	285	VAL	6.7
3	C	92	ILE	6.2
2	B	288	ASP	6.0
3	C	105	ASP	5.9
2	B	289	GLU	5.9
3	C	188	VAL	5.9
3	C	209	ALA	5.9
3	C	88	TRP	5.8
3	C	216	GLY	5.7
2	B	269	PHE	5.7
3	C	201	TYR	5.7
3	C	96	LEU	5.5
3	C	7	ILE	5.5
3	C	86	ILE	5.4
3	C	200	TRP	5.3
3	C	73	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
3	C	8	VAL	5.2
3	C	81	PRO	5.1
3	C	104	ALA	5.1
3	C	90	LEU	5.0
3	C	80	ILE	5.0
3	C	193	ALA	5.0
2	B	290	GLU	4.9
3	C	210	LYS	4.9
3	C	76	VAL	4.9
2	B	274	PHE	4.8
3	C	101	HIS	4.7
2	B	267	ALA	4.7
3	C	93	VAL	4.7
3	C	87	PRO	4.7
3	C	176	VAL	4.6
3	C	6	MET	4.6
3	C	111	ALA	4.6
3	C	103	VAL	4.6
3	C	184	ILE	4.6
2	B	284	GLU	4.5
2	B	279	ILE	4.5
3	C	213	SER	4.4
3	C	5	LYS	4.4
3	C	212	GLU	4.3
3	C	89	LEU	4.3
1	A	708	ALA	4.2
3	C	196	HIS	4.2
3	C	180	ILE	4.2
2	B	283	LYS	4.2
3	C	3	LYS	4.2
3	C	84	LYS	4.2
3	C	13	ILE	4.2
3	C	2	SER	4.1
3	C	109	TYR	4.1
3	C	70	PHE	4.1
3	C	95	VAL	4.1
3	C	198	PRO	4.1
3	C	75	PHE	4.1
3	C	4	SER	4.1
3	C	189	SER	4.1
3	C	83	LYS	4.1
3	C	175	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
3	C	12	PHE	4.0
2	B	281	PRO	4.0
3	C	205	GLU	3.9
3	C	214	GLU	3.9
2	B	273	ILE	3.9
3	C	107	GLY	3.9
3	C	211	LYS	3.9
3	C	78	HIS	3.9
3	C	16	ALA	3.8
3	C	102	LYS	3.8
3	C	171	TYR	3.8
3	C	206	LYS	3.8
3	C	197	HIS	3.8
3	C	168	ILE	3.8
1	A	710	GLY	3.8
3	C	19	TRP	3.7
3	C	181	LYS	3.7
3	C	62	ILE	3.7
3	C	42	TRP	3.7
3	C	202	ARG	3.7
2	B	277	ILE	3.7
3	C	215	GLU	3.6
3	C	118	TRP	3.6
3	C	174	PHE	3.6
3	C	199	ARG	3.6
1	A	1015	ALA	3.6
3	C	67	ALA	3.5
3	C	68	LEU	3.5
3	C	77	HIS	3.5
3	C	173	ALA	3.5
1	A	332	GLN	3.5
2	B	275	HIS	3.5
3	C	91	ASN	3.4
3	C	115	MET	3.4
2	B	260	LEU	3.4
1	A	330	LYS	3.4
2	B	252	LEU	3.4
2	B	250	VAL	3.4
3	C	21	VAL	3.3
3	C	117	PHE	3.3
3	C	182	GLY	3.3
3	C	23	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	329	GLU	3.2
3	C	194	LYS	3.2
3	C	208	GLU	3.2
3	C	97	LYS	3.2
3	C	66	VAL	3.2
3	C	124	ILE	3.2
3	C	126	VAL	3.2
3	C	150	TYR	3.1
2	B	89	GLY	3.1
3	C	165	ALA	3.1
1	A	295	ASN	3.1
3	C	191	ARG	3.1
3	C	142	TYR	3.1
2	B	266	ILE	3.1
1	A	707	ASP	3.1
1	A	344	GLU	3.1
3	C	132	VAL	3.0
3	C	9	ARG	3.0
3	C	154	ILE	3.0
3	C	22	VAL	3.0
3	C	183	MET	3.0
2	B	278	GLY	3.0
2	B	265	PHE	3.0
3	C	143	PHE	3.0
3	C	114	LYS	2.9
3	C	100	GLU	2.9
1	A	713	ILE	2.9
3	C	26	PHE	2.9
2	B	276	TYR	2.9
3	C	116	MET	2.9
3	C	120	ILE	2.9
3	C	163	ILE	2.9
3	C	203	GLU	2.9
2	B	282	ASN	2.9
2	B	256	ALA	2.8
3	C	85	ASP	2.8
3	C	98	GLY	2.8
3	C	133	ILE	2.8
3	C	112	GLY	2.8
3	C	186	GLY	2.8
3	C	72	PHE	2.8
3	C	152	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	170	MET	2.8
3	C	44	THR	2.8
3	C	190	ARG	2.7
3	C	11	LYS	2.7
3	C	108	LYS	2.7
1	A	709	ASN	2.7
2	B	262	ALA	2.7
3	C	195	LYS	2.7
3	C	82	ASP	2.7
3	C	148	VAL	2.7
3	C	162	LEU	2.7
3	C	167	LEU	2.7
3	C	64	ILE	2.7
3	C	71	MET	2.7
2	B	270	ALA	2.7
1	A	319	GLU	2.7
3	C	178	GLY	2.7
1	A	966	GLN	2.6
2	B	87	GLN	2.6
3	C	65	PHE	2.6
3	C	99	ASN	2.6
2	B	264	GLY	2.6
2	B	271	GLY	2.6
3	C	69	MET	2.6
2	B	217	GLU	2.6
2	B	280	GLY	2.6
3	C	10	THR	2.6
3	C	129	VAL	2.6
1	A	876	GLU	2.6
2	B	243	ASP	2.6
2	B	245	LYS	2.5
3	C	153	LEU	2.5
3	C	187	LYS	2.5
3	C	28	VAL	2.5
3	C	74	ARG	2.5
3	C	48	GLY	2.5
3	C	179	SER	2.5
1	A	815	ASN	2.5
3	C	79	ASN	2.5
3	C	125	PHE	2.5
3	C	134	ILE	2.5
3	C	147	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	160	ILE	2.5
1	A	252	ASP	2.4
1	A	623	ASP	2.4
3	C	17	CYS	2.4
3	C	35	PHE	2.4
3	C	60	PHE	2.4
3	C	94	GLU	2.4
3	C	53	GLY	2.4
3	C	161	ILE	2.4
3	C	177	LYS	2.4
3	C	30	LEU	2.4
3	C	157	ALA	2.4
1	A	359	CYS	2.4
3	C	135	TRP	2.4
3	C	110	ASN	2.3
1	A	802	GLY	2.3
1	A	327	ASP	2.3
2	B	261	ALA	2.3
3	C	27	LEU	2.3
3	C	33	ILE	2.3
3	C	172	MET	2.3
3	C	141	GLN	2.3
1	A	150	GLU	2.2
1	A	711	VAL	2.2
1	A	871	VAL	2.2
3	C	63	ALA	2.2
3	C	43	LEU	2.2
2	B	255	GLY	2.2
3	C	61	GLY	2.2
3	C	15	ARG	2.2
1	A	328	ALA	2.2
3	C	156	ALA	2.2
1	A	662	GLU	2.2
3	C	41	GLN	2.1
1	A	331	ARG	2.1
3	C	164	HIS	2.1
3	C	128	LEU	2.1
1	A	488	LYS	2.1
1	A	336	SER	2.1
1	A	122	GLN	2.1
2	B	246	ILE	2.1
2	B	257	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	127	LEU	2.1
1	A	546	GLU	2.1
2	B	16	SER	2.1
3	C	139	PHE	2.1
3	C	166	ILE	2.1
3	C	185	GLU	2.1
3	C	144	PRO	2.1
2	B	253	TRP	2.1
2	B	248	THR	2.0
3	C	140	ALA	2.0
1	A	480	SER	2.0
3	C	24	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

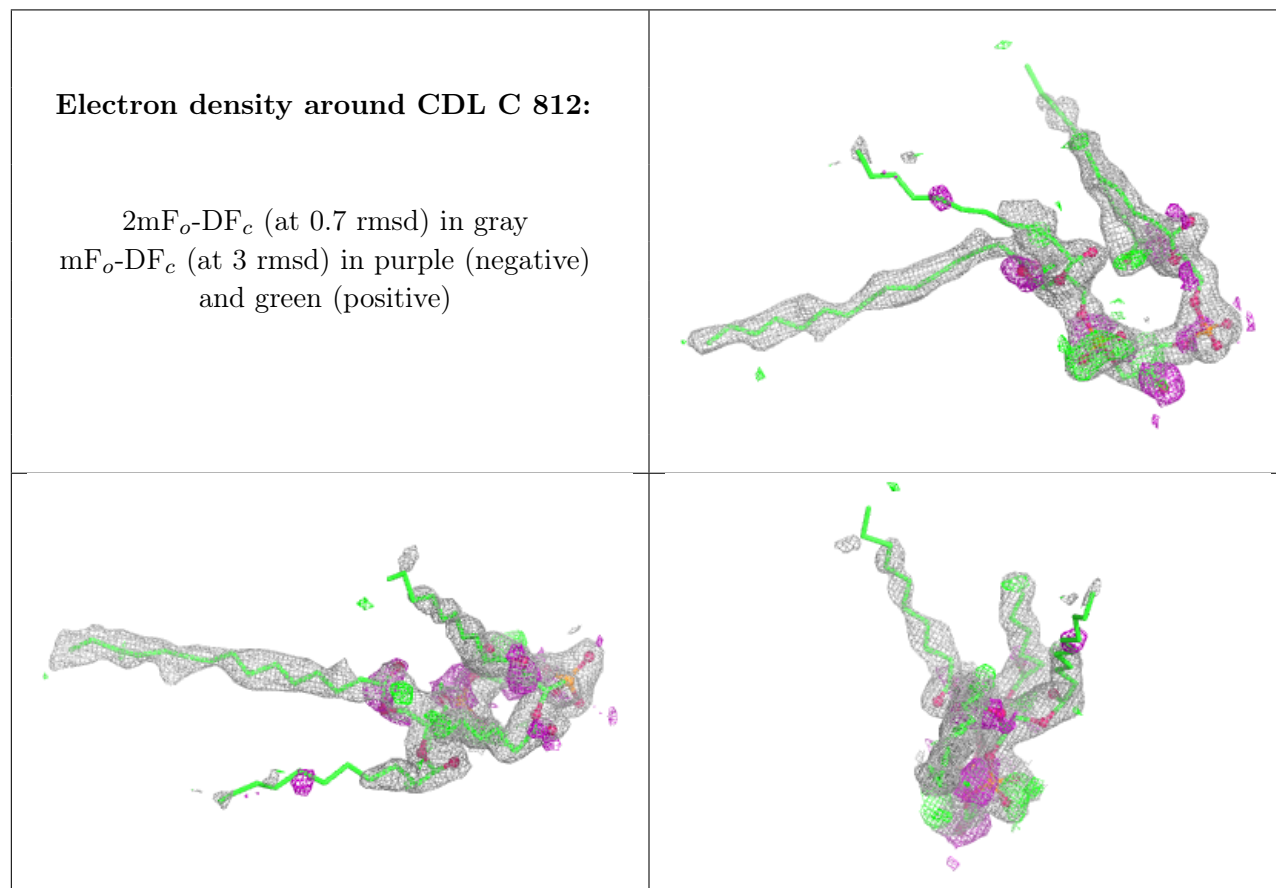
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

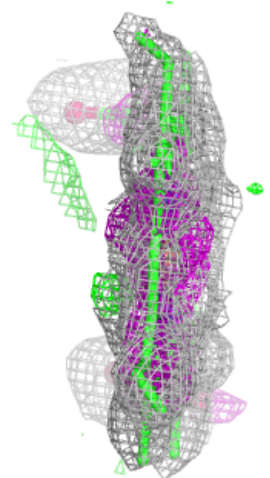
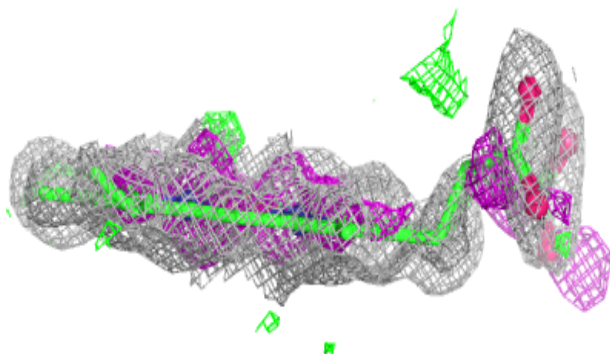
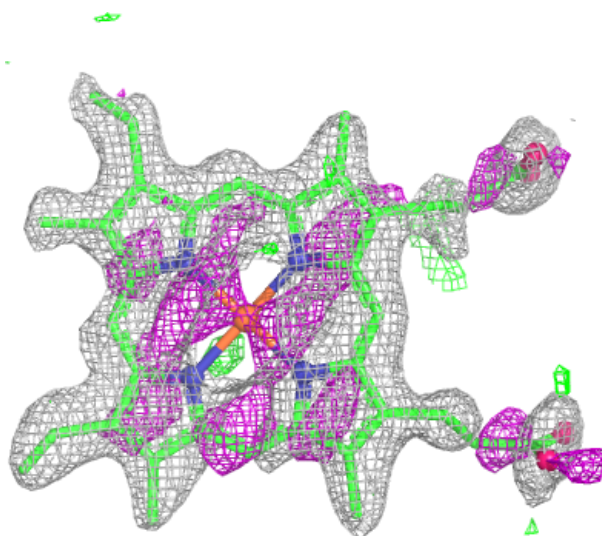
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CDL	C	812	70/100	0.75	0.25	44,56,61,61	0
7	HEM	C	810	43/43	0.86	0.18	44,45,48,49	0
7	HEM	C	809	43/43	0.92	0.13	29,33,35,37	0
6	MGD	A	1019	47/47	0.95	0.08	11,14,16,18	0
6	MGD	A	1018	47/47	0.96	0.07	11,13,14,15	0
5	SF4	B	808	8/8	0.98	0.05	16,18,19,19	0
5	SF4	A	1017	8/8	0.99	0.04	11,12,12,12	0
5	SF4	B	805	8/8	0.99	0.04	12,13,13,14	0
5	SF4	B	806	8/8	0.99	0.04	12,13,13,13	0
5	SF4	B	807	8/8	0.99	0.04	14,15,16,16	0
4	6MO	A	1016	1/1	0.99	0.03	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.



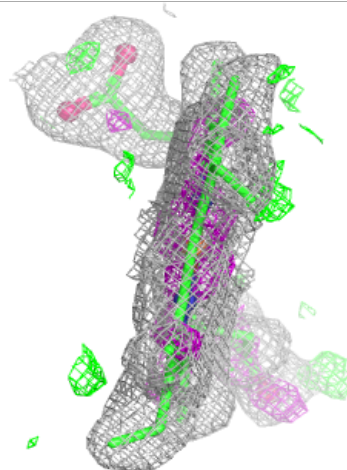
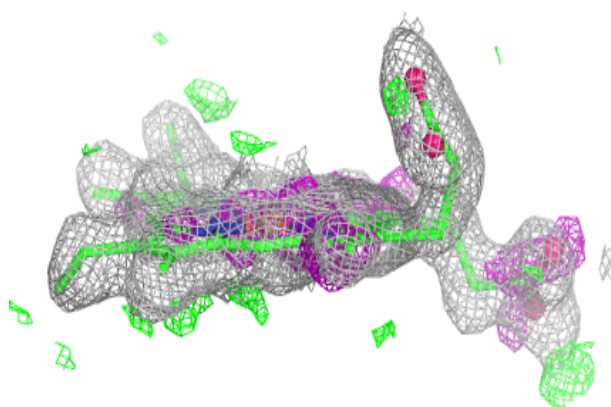
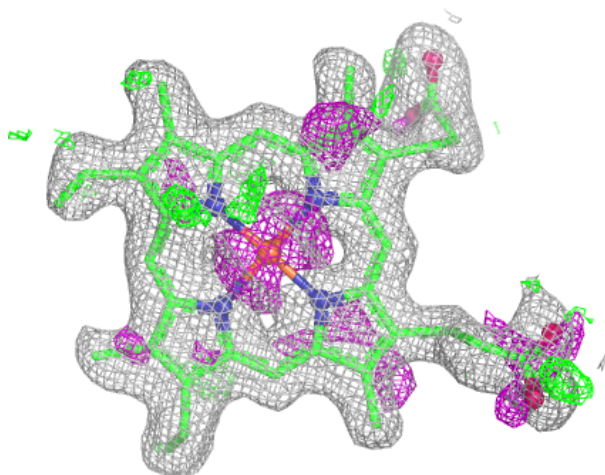
Electron density around HEM C 810:

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



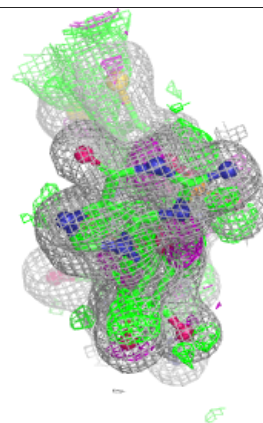
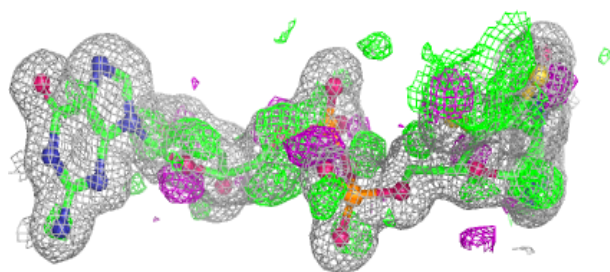
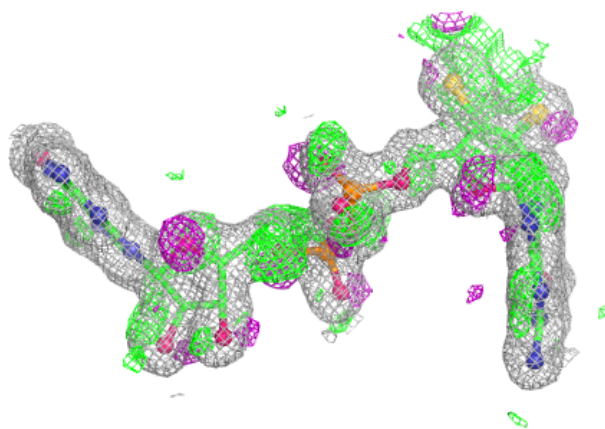
Electron density around HEM C 809:

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

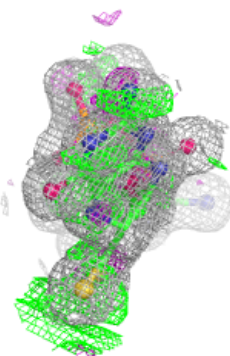
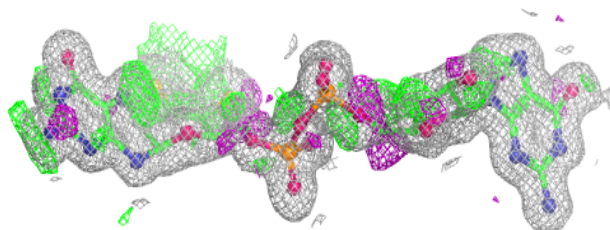
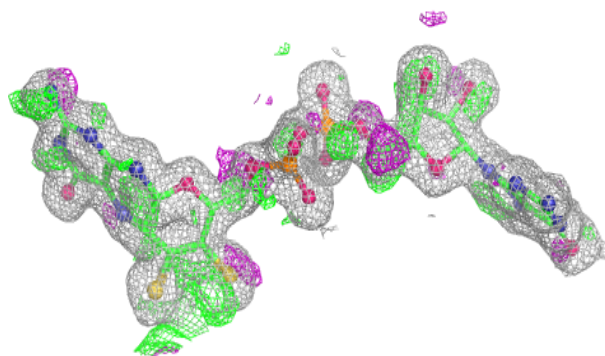


Electron density around MGD A 1019:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.