



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 12:01 PM BST

PDB ID : 2H88
Title : Avian Mitochondrial Respiratory Complex II at 1.8 Angstrom Resolution
Authors : Huang, L.S.; Shen, J.T.; Wang, A.C.; Berry, E.A.
Deposited on : 2006-06-06
Resolution : 1.74 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 : 2.13.1
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) : 2.13.1

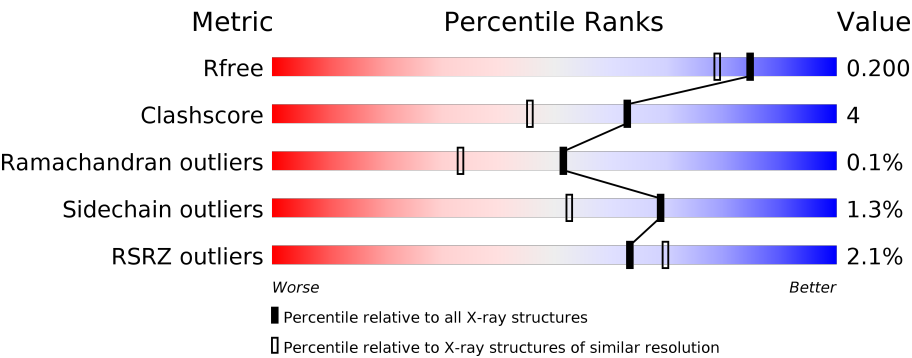
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	621	<div><div>%</div><div><div></div><div>90%</div><div>8%</div><div></div></div><div></div></div>
1	N	621	<div><div></div><div>91%</div><div>7%</div><div></div></div> <div></div>

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Mol	Chain	Length	Quality of chain
4	D	103	
4	Q	103	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	BHG	C	141	X	-	-	-
14	BHG	P	205	X	-	-	-
8	TEO	A	1002	X	-	-	-
8	TEO	N	1002	X	-	-	-
9	UNL	C	146	-	-	-	X
9	UNL	N	1007	-	-	X	-
9	UNL	O	1006	-	-	X	-
9	UNL	P	208	-	-	X	-
9	UNL	P	209	-	-	X	-
9	UNL	P	214	-	-	-	X
9	UNL	P	217	-	-	-	X
9	UNL	Q	212	-	-	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 19414 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 SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	0	0	0
			4726	2956	843	898	29			
1	N	612	Total	C	N	O	S	0	0	0
			4726	2956	843	898	29			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	ARG	CYS	conflict	UNP Q9YHT1
A	556	LEU	PHE	conflict	UNP Q9YHT1
A	560	GLU	ASP	conflict	UNP Q9YHT1
N	501	ARG	CYS	conflict	UNP Q9YHT1
N	556	LEU	PHE	conflict	UNP Q9YHT1
N	560	GLU	ASP	conflict	UNP Q9YHT1

- Molecule 2 is a protein called Succinate dehydrogenase Ip subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1916	1213	325	356	22			
2	O	239	Total	C	N	O	S	0	0	0
			1916	1213	325	356	22			

- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	139	Total	C	N	O	S	0	0	0
			1077	706	178	189	4			
3	P	139	Total	C	N	O	S	0	0	0
			1077	706	178	189	4			

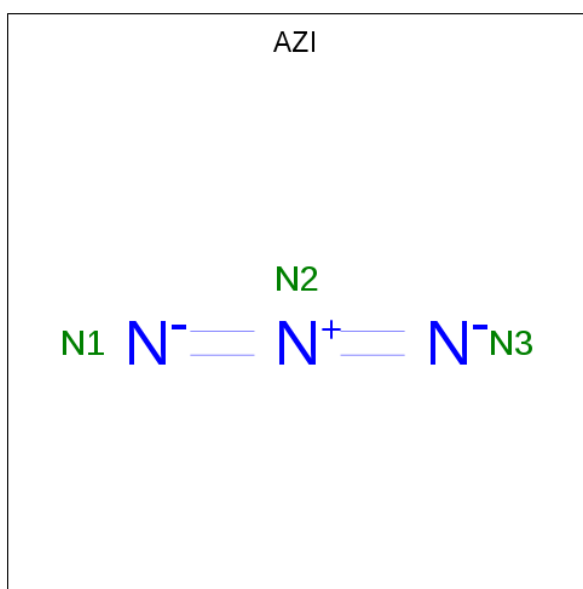
- Molecule 4 is a protein called Succinate dehydrogenase cytochrome B, small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	101	Total	C	N	O	S	0	0	0
			766	505	121	137	3			
4	Q	101	Total	C	N	O	S	0	0	0
			766	505	121	137	3			

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	O	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		
5	A	1	Total	K	0	0
			1	1		
5	N	1	Total	K	0	0
			1	1		

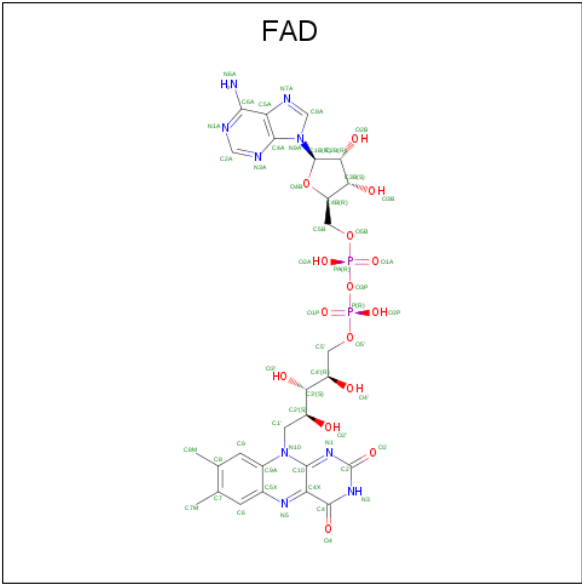
- Molecule 6 is AZIDE ION (three-letter code: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	N	0	0
			3	3		
6	N	1	Total	N	0	0
			3	3		

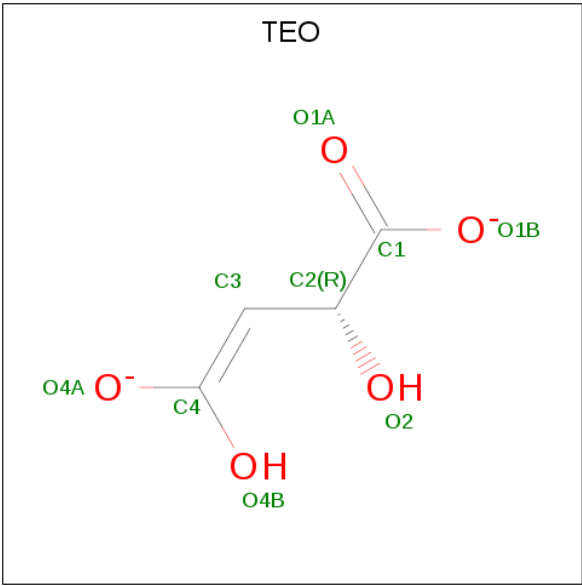
- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:

C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
7	N	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 8 is MALATE LIKE INTERMEDIATE (three-letter code: TEO) (formula: C₄H₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			9	4	5		

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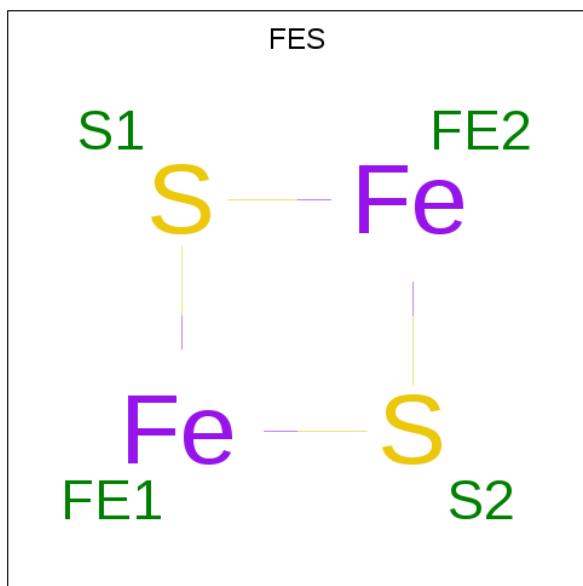
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	N	1	Total	C	O	0	0
			9	4	5		

- Molecule 9 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

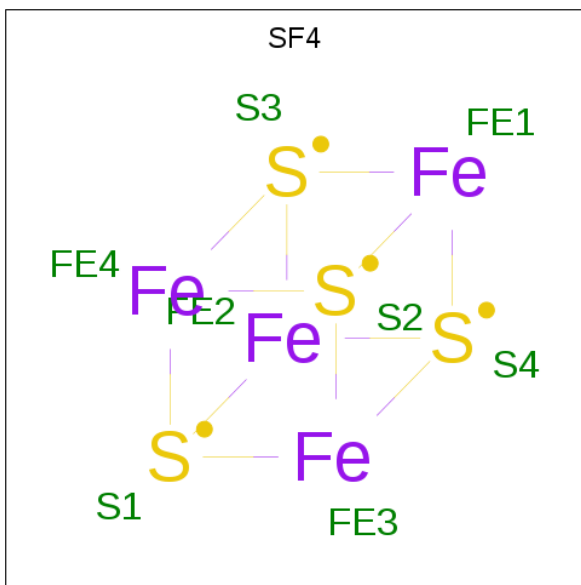
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	P	14	Total	C	O	0	0
			22	6	16		
9	Q	6	Total	C	O	0	0
			16	12	4		
9	D	11	Total	C	O	0	0
			32	21	11		
9	B	4	Total	O		0	0
			4	4			
9	C	9	Total	C	O	0	0
			16	6	10		
9	A	6	Total	O		0	0
			7	7			
9	N	10	Total	O		0	0
			11	11			
9	O	4	Total	O		0	0
			4	4			

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



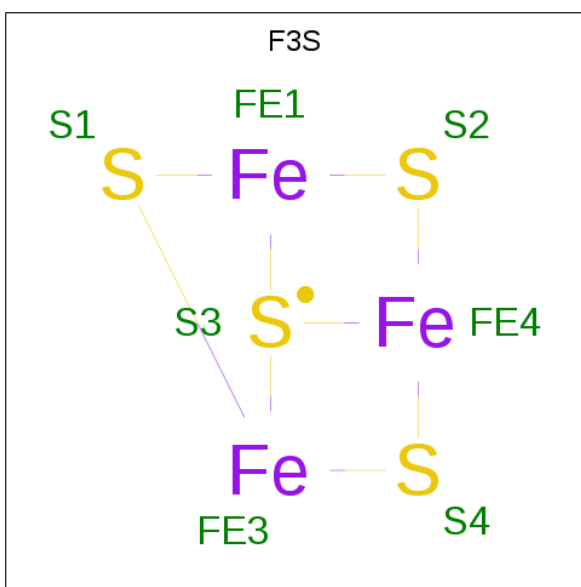
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			4	2	2		
10	O	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



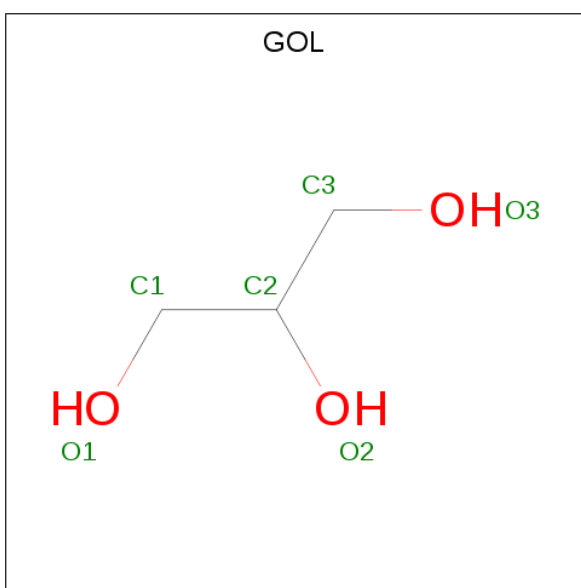
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			8	4	4		
11	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 12 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



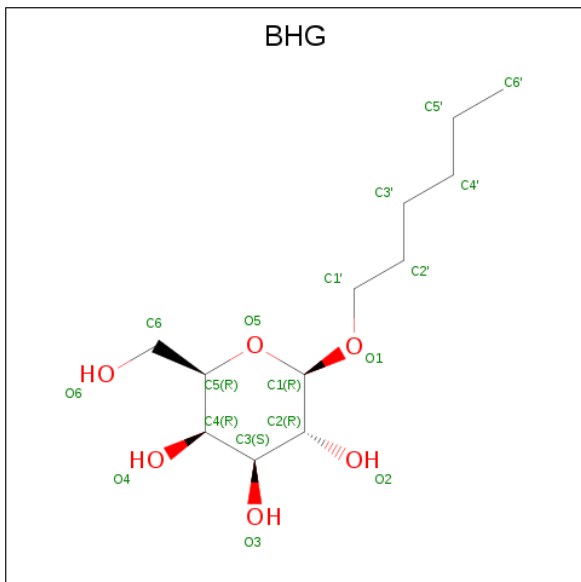
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	Fe	S	0	0
			7	3	4		
12	O	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



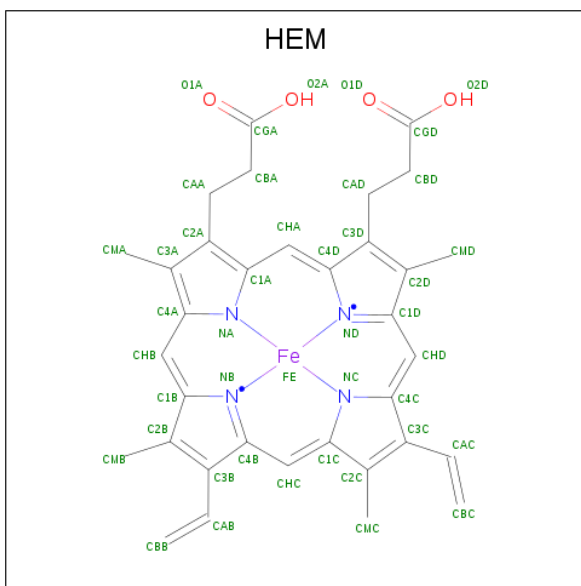
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			6	3	3		
13	O	1	Total	C	O	0	0
			6	3	3		

- Molecule 14 is hexyl beta-D-galactopyranoside (three-letter code: BHG) (formula: $\text{C}_{12}\text{H}_{24}\text{O}_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			18	12	6		
14	P	1	Total	C	O	0	0
			18	12	6		

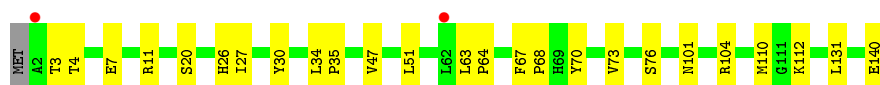
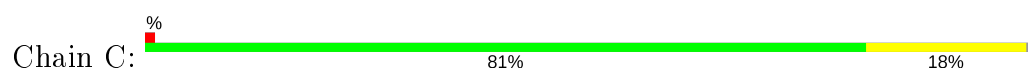
- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



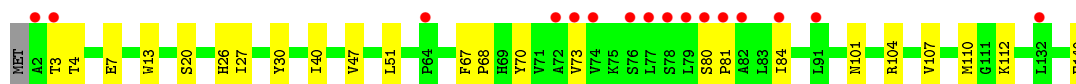
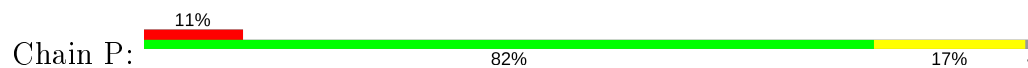
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total 41	C 32	Fe 1	N 4	O 4	0	0
15	P	1	Total 41	C 32	Fe 1	N 4	O 4	0	0

- Molecule 16 is water.

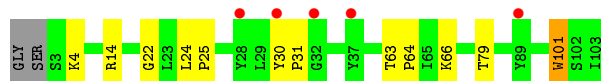
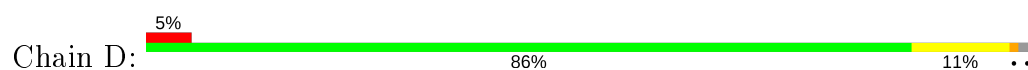
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	579	Total 579	O 579	0	0
16	B	296	Total 296	O 296	0	0
16	C	104	Total 104	O 104	0	0
16	D	51	Total 51	O 51	0	0
16	N	569	Total 569	O 569	0	0
16	O	281	Total 281	O 281	0	0
16	P	99	Total 99	O 99	0	0
16	Q	51	Total 51	O 51	0	0



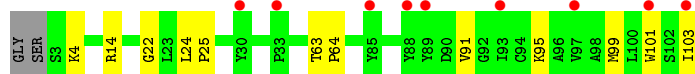
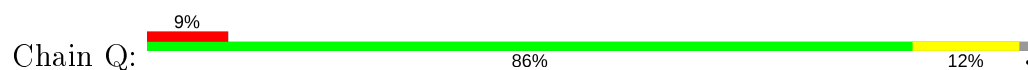
- Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT



- Molecule 4: Succinate dehydrogenase cytochrome B, small subunit



- Molecule 4: Succinate dehydrogenase cytochrome B, small subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.97Å 199.39Å 68.06Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	45.14 – 1.74 45.14 – 1.70	Depositor EDS
% Data completeness (in resolution range)	89.2 (45.14-1.74) 86.9 (45.14-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.178 , 0.206 0.174 , 0.200	Depositor DCC
R_{free} test set	15106 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.227 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19414	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: AZI, GOL, TEO, SF4, BHG, F3S, FES, HEM, UNL, K, FAD

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	0.99	1/4827 (0.0%)	0.86	2/6535 (0.0%)
1	N	1.01	1/4827 (0.0%)	0.87	1/6535 (0.0%)
2	B	0.99	2/1958 (0.1%)	0.83	0/2640
2	O	1.00	1/1958 (0.1%)	0.84	0/2640
3	C	0.73	0/1106	0.68	0/1503
3	P	0.73	0/1106	0.68	0/1503
4	D	0.60	0/789	0.64	0/1082
4	Q	0.54	0/789	0.62	0/1082
All	All	0.94	5/17360 (0.0%)	0.82	3/23520 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
3	C	0	1
3	P	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	84	ALA	CA-CB	6.40	1.65	1.52
2	B	142	TYR	CD1-CE1	6.09	1.48	1.39
1	A	103	ALA	CA-CB	5.94	1.65	1.52
2	B	84	ALA	CA-CB	5.23	1.63	1.52
1	N	148	CYS	CB-SG	5.16	1.91	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLY	N-CA-C	6.00	128.10	113.10
1	N	140	GLY	N-CA-C	5.91	127.87	113.10
1	A	318	LYS	CD-CE-NZ	5.25	123.78	111.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	TYR	Sidechain
3	C	30	TYR	Sidechain
1	N	172	TYR	Sidechain
3	P	30	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4726	0	4609	33	0
1	N	4726	0	4609	34	0
2	B	1916	0	1913	10	0
2	O	1916	0	1913	8	0
3	C	1077	0	1112	22	0
3	P	1077	0	1112	20	0
4	D	766	0	761	10	0
4	Q	766	0	761	10	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
6	A	3	0	0	0	0
6	N	3	0	0	0	0
7	A	53	0	30	3	0
7	N	53	0	30	3	0
8	A	9	0	2	3	0
8	N	9	0	2	1	0
9	A	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	4	0	0	1	0
9	C	16	0	0	0	0
9	D	32	0	0	1	0
9	N	11	0	0	3	0
9	O	4	0	0	2	0
9	P	22	0	0	4	0
9	Q	16	0	0	0	0
10	B	4	0	0	0	0
10	O	4	0	0	0	0
11	B	8	0	0	0	0
11	O	8	0	0	0	0
12	B	7	0	0	0	0
12	O	7	0	0	0	0
13	B	6	0	8	1	0
13	O	6	0	8	1	0
14	C	18	0	24	0	0
14	P	18	0	24	0	0
15	C	41	0	24	0	0
15	P	41	0	24	0	0
16	A	579	0	0	8	0
16	B	296	0	0	3	0
16	C	104	0	0	3	0
16	D	51	0	0	1	0
16	N	569	0	0	7	0
16	O	281	0	0	0	0
16	P	99	0	0	0	0
16	Q	51	0	0	0	0
All	All	19414	0	16966	146	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 4.

All (146) 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)
9:O:1005:UNL:O1	9:O:1006:UNL:O1	1.69	1.09
1:N:13:PRO:O	9:N:1011:UNL:O1	1.75	1.04
9:B:1005:UNL:O1	9:B:1006:UNL:O1	1.84	0.96
4:Q:91:VAL:HG11	4:Q:99:MET:HE1	1.56	0.85
3:P:101:ASN:HD21	3:P:104:ARG:HH11	1.27	0.82
3:C:3:THR:HG22	3:C:7:GLU:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:3:THR:HG22	3:P:7:GLU:HB2	1.63	0.78
3:C:101:ASN:HD21	3:C:104:ARG:HH11	1.29	0.78
1:N:471:ASN:HB3	9:N:1007:UNL:O1	1.84	0.78
4:D:24:LEU:HB2	4:D:25:PRO:HD3	1.68	0.75
16:N:1533:HOH:O	2:O:88:LYS:HE2	1.86	0.75
4:Q:24:LEU:HB2	4:Q:25:PRO:HD3	1.67	0.74
3:C:26:HIS:CD2	3:C:27:ILE:H	2.05	0.74
1:N:205:ARG:NH2	1:N:440:SER:HA	2.02	0.74
1:A:207:LYS:NZ	1:A:436:GLU:OE1	2.21	0.74
1:N:205:ARG:HB3	16:N:1514:HOH:O	1.89	0.72
3:P:26:HIS:CD2	3:P:27:ILE:H	2.07	0.71
9:P:208:UNL:O1	9:P:209:UNL:O1	2.10	0.70
1:A:189:ARG:HD3	1:A:439:PRO:HB2	1.75	0.68
1:N:189:ARG:HD3	1:N:439:PRO:HB2	1.76	0.67
4:Q:22:GLY:O	4:Q:25:PRO:HD2	1.95	0.66
3:C:70:TYR:O	3:C:73:VAL:HG12	1.95	0.66
3:P:70:TYR:O	3:P:73:VAL:HG12	1.96	0.66
1:N:507:LYS:HE3	16:N:1170:HOH:O	1.95	0.66
1:N:471:ASN:CB	9:N:1007:UNL:O1	2.45	0.64
1:N:207:LYS:NZ	1:N:436:GLU:OE1	2.31	0.63
2:O:192:ILE:C	2:O:192:ILE:HD12	2.20	0.62
4:D:22:GLY:O	4:D:25:PRO:HD2	1.98	0.62
2:O:245:TYR:O	4:Q:4:LYS:NZ	2.32	0.62
1:A:387:LYS:HD3	16:A:2193:HOH:O	1.99	0.61
1:N:205:ARG:HH21	1:N:440:SER:HA	1.65	0.61
2:O:152:LEU:HD23	2:O:192:ILE:HD11	1.83	0.61
2:B:192:ILE:C	2:B:192:ILE:HD12	2.21	0.61
1:N:207:LYS:NZ	1:N:436:GLU:HB2	2.15	0.61
3:P:67:PHE:HB3	3:P:68:PRO:HD3	1.83	0.60
1:A:401:ALA:N	1:A:402:SER:HA	2.16	0.60
3:C:67:PHE:HB3	3:C:68:PRO:HD3	1.84	0.60
4:Q:95:LYS:HG3	4:Q:99:MET:CE	2.31	0.59
2:B:152:LEU:HD23	2:B:192:ILE:HD11	1.84	0.58
1:N:401:ALA:N	1:N:402:SER:HA	2.18	0.58
2:B:245:TYR:O	4:D:4:LYS:NZ	2.36	0.58
1:N:207:LYS:HZ1	1:N:436:GLU:HB2	1.70	0.57
1:A:507:LYS:HE3	16:A:2733:HOH:O	2.05	0.55
2:O:152:LEU:HD23	2:O:192:ILE:CD1	2.36	0.55
3:C:140:GLU:OXT	4:D:101:TRP:HD1	1.90	0.55
3:C:140:GLU:OXT	4:D:101:TRP:CD1	2.60	0.55
2:B:152:LEU:HD23	2:B:192:ILE:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:63:THR:HB	4:D:64:PRO:HD3	1.90	0.54
1:A:169:ASP:HB2	16:A:2502:HOH:O	2.07	0.54
4:Q:63:THR:HB	4:Q:64:PRO:HD3	1.90	0.54
3:P:101:ASN:ND2	3:P:104:ARG:HH11	2.03	0.53
3:C:110:MET:HE3	3:C:112:LYS:HD2	1.91	0.53
1:A:455:LYS:NZ	16:A:2885:HOH:O	2.41	0.53
4:Q:95:LYS:HG3	4:Q:99:MET:HE3	1.90	0.53
1:A:207:LYS:NZ	1:A:436:GLU:HB2	2.25	0.52
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.90	0.52
2:B:104:HIS:O	13:B:1009:GOL:H12	2.11	0.51
3:P:110:MET:HE3	3:P:112:LYS:HD2	1.92	0.51
3:P:4:THR:OG1	3:P:7:GLU:HG3	2.11	0.51
3:C:4:THR:OG1	3:C:7:GLU:HG3	2.10	0.51
1:A:593:LYS:HE3	16:A:2370:HOH:O	2.12	0.50
1:N:381:HIS:O	1:N:597:LYS:NZ	2.44	0.50
3:C:70:TYR:HA	3:C:73:VAL:HG12	1.93	0.50
3:P:70:TYR:HA	3:P:73:VAL:HG12	1.92	0.49
1:A:297:ARG:HH22	8:A:1002:TEO:C3	2.26	0.49
1:N:60:ALA:HB3	1:N:154:GLY:HA3	1.95	0.48
9:P:208:UNL:O1	9:P:209:UNL:O2	2.31	0.48
1:A:263:LEU:HG	1:A:264:ILE:N	2.28	0.48
1:A:220:TYR:CG	1:A:363:VAL:HG21	2.47	0.48
1:A:381:HIS:O	1:A:597:LYS:NZ	2.47	0.48
1:N:496:LEU:HD12	1:N:536:ILE:HG21	1.95	0.47
1:N:574:PRO:HD2	1:N:577:GLU:HB2	1.97	0.47
4:Q:95:LYS:HG3	4:Q:99:MET:HE2	1.96	0.47
3:C:3:THR:CG2	3:C:7:GLU:HB2	2.41	0.47
1:N:243:PRO:HB3	1:N:586:TYR:CZ	2.49	0.47
1:A:496:LEU:HD12	1:A:536:ILE:HG21	1.96	0.47
2:B:98:LYS:HE3	16:C:2230:HOH:O	2.15	0.47
1:N:263:LEU:HG	1:N:264:ILE:N	2.29	0.47
2:O:104:HIS:O	13:O:1009:GOL:H12	2.14	0.47
3:P:84:ILE:HD13	4:Q:103:ILE:HG22	1.97	0.47
1:N:121:GLU:HG2	16:N:1133:HOH:O	2.15	0.46
4:D:79:THR:HG21	9:D:107:UNL:C1	2.46	0.46
4:D:66:LYS:HG3	16:D:2127:HOH:O	2.16	0.46
4:Q:91:VAL:CG1	4:Q:99:MET:HE1	2.39	0.46
1:N:189:ARG:NH1	1:N:440:SER:O	2.38	0.46
1:A:297:ARG:HH22	8:A:1002:TEO:C4	2.30	0.45
1:A:11:GLN:HG3	16:A:2932:HOH:O	2.15	0.45
1:A:243:PRO:HB3	1:A:586:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:326:HIS:HD2	16:N:1422:HOH:O	1.99	0.45
3:C:101:ASN:ND2	3:C:104:ARG:HH11	2.05	0.45
3:C:70:TYR:O	3:C:73:VAL:CG1	2.64	0.45
1:N:414:LEU:HG	7:N:1001:FAD:C2	2.47	0.45
1:A:574:PRO:HD2	1:A:577:GLU:HB2	1.98	0.45
1:A:381:HIS:ND1	1:A:386:ASP:OD1	2.47	0.45
2:O:192:ILE:C	2:O:192:ILE:CD1	2.85	0.45
3:P:70:TYR:O	3:P:73:VAL:CG1	2.65	0.45
1:A:60:ALA:HA	7:A:1001:FAD:C5X	2.48	0.44
1:A:470:LEU:HD11	1:A:474:LYS:HE3	2.00	0.44
1:N:381:HIS:ND1	1:N:386:ASP:OD1	2.46	0.44
1:A:181:LEU:HD21	1:A:211:ILE:HD11	2.00	0.44
3:P:80:SER:HA	3:P:81:PRO:HD3	1.81	0.44
3:P:101:ASN:HD21	3:P:104:ARG:NH1	2.06	0.44
1:N:87:SER:HB2	1:N:405:GLY:HA3	1.98	0.44
1:N:60:ALA:HA	7:N:1001:FAD:C6	2.48	0.43
3:C:26:HIS:CG	3:C:27:ILE:H	2.37	0.43
1:N:60:ALA:HA	7:N:1001:FAD:C5X	2.47	0.43
1:N:507:LYS:HE2	1:N:509:PHE:CZ	2.53	0.43
9:O:1006:UNL:O1	9:P:208:UNL:O1	2.36	0.43
16:B:2845:HOH:O	4:D:4:LYS:CE	2.67	0.43
3:P:3:THR:CG2	3:P:7:GLU:HB2	2.41	0.43
2:B:95:LYS:NZ	16:B:2777:HOH:O	2.47	0.43
3:C:11:ARG:HD2	16:C:2556:HOH:O	2.18	0.43
3:C:63:LEU:HA	3:C:64:PRO:HD3	1.86	0.43
1:A:326:HIS:HE1	16:A:2021:HOH:O	2.01	0.42
1:N:297:ARG:HH22	8:N:1002:TEO:C3	2.32	0.42
3:P:140:GLU:HG3	3:P:140:GLU:OXT	2.19	0.42
3:C:131:LEU:HD23	3:C:131:LEU:HA	1.90	0.42
3:C:140:GLU:HG3	3:C:140:GLU:OXT	2.19	0.42
1:N:170:THR:HB	1:N:172:TYR:CE1	2.54	0.42
3:P:107:VAL:HA	3:P:110:MET:HE2	2.01	0.42
3:P:47:VAL:O	3:P:51:LEU:HG	2.20	0.42
1:A:87:SER:HB2	1:A:405:GLY:HA3	2.01	0.42
1:A:507:LYS:HE2	1:A:509:PHE:CZ	2.54	0.42
1:N:289:PRO:HD2	16:N:1215:HOH:O	2.19	0.42
2:B:192:ILE:C	2:B:192:ILE:CD1	2.87	0.42
3:C:34:LEU:HB3	3:C:35:PRO:HD3	2.01	0.42
1:N:326:HIS:HE1	16:N:1226:HOH:O	2.03	0.42
3:C:101:ASN:ND2	3:C:104:ARG:HD3	2.35	0.41
1:N:470:LEU:HD11	1:N:474:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:THR:HB	1:A:172:TYR:CE1	2.54	0.41
1:A:60:ALA:HA	7:A:1001:FAD:C6	2.49	0.41
3:C:47:VAL:O	3:C:51:LEU:HG	2.19	0.41
3:P:40:ILE:CG2	9:P:209:UNL:O2	2.69	0.41
2:B:102:LEU:HA	2:B:103:PRO:HD3	1.86	0.41
2:B:150:GLN:HG2	16:B:2054:HOH:O	2.19	0.41
3:C:76:SER:HB3	16:C:2741:HOH:O	2.20	0.41
1:N:181:LEU:HD21	1:N:211:ILE:HD11	2.03	0.41
1:A:354:LYS:NZ	16:A:2177:HOH:O	2.52	0.41
1:A:462:THR:O	1:A:462:THR:CG2	2.68	0.41
4:D:30:TYR:N	4:D:31:PRO:HD3	2.37	0.40
1:N:453:LEU:C	1:N:453:LEU:HD23	2.41	0.40
3:P:101:ASN:ND2	3:P:104:ARG:HD3	2.36	0.40
1:A:414:LEU:HG	7:A:1001:FAD:C2	2.52	0.40
1:A:253:HIS:O	1:A:361:PRO:HA	2.21	0.40
2:O:176:ASP:HB3	3:P:13:TRP:CZ2	2.57	0.40
1:A:297:ARG:HH22	8:A:1002:TEO:C2	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	610/621 (98%)	591 (97%)	19 (3%)	0	100	100
1	N	610/621 (98%)	591 (97%)	19 (3%)	0	100	100
2	B	237/252 (94%)	231 (98%)	5 (2%)	1 (0%)	34	17
2	O	237/252 (94%)	232 (98%)	4 (2%)	1 (0%)	34	17
3	C	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
3	P	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
4	D	99/103 (96%)	98 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	99/103 (96%)	98 (99%)	1 (1%)	0	100	100
All	All	2166/2232 (97%)	2113 (98%)	51 (2%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	66	ARG
2	O	66	ARG

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	497/506 (98%)	493 (99%)	4 (1%)	81	72
1	N	497/506 (98%)	493 (99%)	4 (1%)	81	72
2	B	214/219 (98%)	210 (98%)	4 (2%)	57	36
2	O	214/219 (98%)	209 (98%)	5 (2%)	50	27
3	C	118/119 (99%)	117 (99%)	1 (1%)	81	72
3	P	118/119 (99%)	117 (99%)	1 (1%)	81	72
4	D	78/79 (99%)	76 (97%)	2 (3%)	46	22
4	Q	78/79 (99%)	76 (97%)	2 (3%)	46	22
All	All	1814/1846 (98%)	1791 (99%)	23 (1%)	69	52

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

Mol	Chain	Res	Type
1	A	48	THR
1	A	72	GLU
1	A	73	ASP
1	A	130	PHE
2	B	63	ARG
2	B	66	ARG

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Mol	Chain	Res	Type
2	B	67	GLU
2	B	189	ARG
3	C	20	SER
4	D	14	ARG
4	D	101	TRP
1	N	48	THR
1	N	72	GLU
1	N	73	ASP
1	N	130	PHE
2	O	63	ARG
2	O	66	ARG
2	O	67	GLU
2	O	189	ARG
2	O	217	THR
3	P	20	SER
4	Q	14	ARG
4	Q	101	TRP

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

Mol	Chain	Res	Type
1	A	326	HIS
1	A	534	GLN
2	B	121	GLN
2	B	137	GLN
3	C	26	HIS
3	C	66	GLN
3	C	101	ASN
1	N	326	HIS
1	N	534	GLN
2	O	121	GLN
2	O	137	GLN
3	P	26	HIS
3	P	66	GLN
3	P	101	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 86 ligands modelled in this entry, 64 are unknown and 4 are monoatomic - leaving 18 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
10	FES	B	1002	2	0,4,4	0.00	-	-		
13	GOL	O	1009	-	5,5,5	1.18	0	5,5,5	0.68	0
12	F3S	O	1004	2	0,9,9	0.00	-	-		
12	F3S	B	1004	2	0,9,9	0.00	-	-		
7	FAD	A	1001	1	51,58,58	2.15	19 (37%)	60,89,89	2.26	15 (25%)
14	BHG	C	141	-	18,18,18	1.79	4 (22%)	23,23,23	0.80	1 (4%)
10	FES	O	1002	2	0,4,4	0.00	-	-		
8	TEO	N	1002	-	1,8,8	0.49	0	0,10,10	0.00	-
6	AZI	A	623	-	0,2,2	0.00	-	0,1,1	0.00	-
11	SF4	B	1003	2	0,12,12	0.00	-	-		
7	FAD	N	1001	1	51,58,58	2.54	17 (33%)	60,89,89	2.33	15 (25%)
13	GOL	B	1009	-	5,5,5	1.16	0	5,5,5	0.53	0
11	SF4	O	1003	2	0,12,12	0.00	-	-		
6	AZI	N	623	-	0,2,2	0.00	-	0,1,1	0.00	-
15	HEM	P	201	3,4	26,48,50	2.04	9 (34%)	21,80,82	1.73	4 (19%)
15	HEM	C	142	3,4	26,48,50	2.03	6 (23%)	21,80,82	1.77	5 (23%)
8	TEO	A	1002	-	1,8,8	0.27	0	0,10,10	0.00	-
14	BHG	P	205	-	18,18,18	1.38	2 (11%)	23,23,23	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FES	B	1002	2	-	-	0/1/1/1
8	TEO	N	1002	-	1/1/3/4	2/2/8/8	-
12	F3S	B	1004	2	-	-	0/3/3/3
7	FAD	A	1001	1	-	10/30/50/50	0/6/6/6
14	BHG	C	141	-	1/1/5/5	1/9/29/29	0/1/1/1
10	FES	O	1002	2	-	-	0/1/1/1
12	F3S	O	1004	2	-	-	0/3/3/3
13	GOL	O	1009	-	-	4/4/4/4	-
11	SF4	B	1003	2	-	-	0/6/5/5
7	FAD	N	1001	1	-	9/30/50/50	0/6/6/6
13	GOL	B	1009	-	-	2/4/4/4	-
11	SF4	O	1003	2	-	-	0/6/5/5
15	HEM	P	201	3,4	-	0/6/50/54	-
15	HEM	C	142	3,4	-	0/6/50/54	-
8	TEO	A	1002	-	1/1/3/4	2/2/8/8	-
14	BHG	P	205	-	1/1/5/5	1/9/29/29	0/1/1/1

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	1001	FAD	C4X-C10	8.20	1.47	1.38
7	A	1001	FAD	C4X-N5	5.80	1.41	1.33
7	N	1001	FAD	C2A-N3A	5.63	1.41	1.32
7	A	1001	FAD	C10-N1	5.33	1.40	1.33
7	N	1001	FAD	C10-N1	5.22	1.40	1.33
7	A	1001	FAD	C4X-C10	5.04	1.43	1.38
14	C	141	BHG	O1-C1	4.77	1.48	1.40
15	C	142	HEM	C1A-NA	4.58	1.45	1.36
15	C	142	HEM	CAB-C3B	-4.57	1.42	1.51
7	N	1001	FAD	C2A-N1A	4.52	1.42	1.33
15	P	201	HEM	CAB-C3B	-4.50	1.42	1.51
15	P	201	HEM	CAA-C2A	4.44	1.58	1.52
7	N	1001	FAD	C4X-N5	4.41	1.39	1.33
7	N	1001	FAD	C5X-N5	4.31	1.42	1.35
7	N	1001	FAD	C2B-C1B	-4.28	1.47	1.53
14	P	205	BHG	O1-C1	3.82	1.46	1.40
7	N	1001	FAD	C4-C4X	3.78	1.47	1.41
7	A	1001	FAD	C2A-N3A	3.65	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1001	FAD	C2B-C1B	-3.48	1.48	1.53
15	C	142	HEM	C4B-NB	3.46	1.43	1.36
7	A	1001	FAD	PA-O2A	-3.38	1.39	1.55
15	P	201	HEM	C1A-NA	3.29	1.42	1.36
7	N	1001	FAD	C2-N3	3.26	1.44	1.38
7	N	1001	FAD	PA-O1A	-3.21	1.39	1.50
15	C	142	HEM	CAA-C2A	3.12	1.56	1.52
7	A	1001	FAD	PA-O1A	-3.10	1.39	1.50
7	A	1001	FAD	C4'-C3'	3.09	1.59	1.53
15	C	142	HEM	C1B-C2B	3.07	1.49	1.42
14	C	141	BHG	O5-C1	3.04	1.49	1.41
7	N	1001	FAD	C4'-C3'	3.04	1.59	1.53
7	A	1001	FAD	C4-C4X	3.00	1.46	1.41
7	N	1001	FAD	PA-O2A	-2.98	1.41	1.55
7	N	1001	FAD	O2'-C2'	2.90	1.49	1.43
7	N	1001	FAD	C1'-N10	2.86	1.51	1.48
15	P	201	HEM	C4B-NB	2.85	1.42	1.36
7	A	1001	FAD	O2'-C2'	2.83	1.49	1.43
7	N	1001	FAD	C2B-C3B	2.80	1.61	1.53
15	P	201	HEM	CAC-C3C	-2.72	1.45	1.51
7	A	1001	FAD	C2-N3	2.58	1.43	1.38
15	P	201	HEM	C4D-C3D	2.56	1.48	1.42
7	A	1001	FAD	C6-C7	2.53	1.44	1.37
14	P	205	BHG	C4-C5	2.52	1.58	1.53
14	C	141	BHG	C4-C5	2.49	1.58	1.53
7	A	1001	FAD	C2'-C3'	-2.45	1.48	1.53
14	C	141	BHG	C3-C2	2.44	1.58	1.52
15	P	201	HEM	C1B-C2B	2.33	1.47	1.42
15	P	201	HEM	C4C-C3C	2.33	1.47	1.42
7	A	1001	FAD	PA-O5B	-2.28	1.50	1.59
7	N	1001	FAD	C4-N3	2.26	1.37	1.33
7	A	1001	FAD	C5X-N5	2.25	1.39	1.35
7	A	1001	FAD	C4-N3	2.24	1.36	1.33
7	A	1001	FAD	C7M-C7	2.08	1.55	1.51
7	A	1001	FAD	C2A-N1A	2.08	1.37	1.33
15	P	201	HEM	C1C-C2C	2.07	1.47	1.42
15	C	142	HEM	C4D-C3D	2.06	1.47	1.42
7	N	1001	FAD	PA-O5B	-2.06	1.50	1.59
7	A	1001	FAD	C2B-C3B	2.04	1.58	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	1001	FAD	C4-N3-C2	9.11	122.83	115.14
7	A	1001	FAD	C4-N3-C2	8.52	122.34	115.14
7	N	1001	FAD	N3A-C2A-N1A	-6.43	118.62	128.68
7	A	1001	FAD	N3A-C2A-N1A	-6.29	118.84	128.68
7	N	1001	FAD	C4-C4X-C10	-5.62	116.23	119.95
7	A	1001	FAD	C4X-N5-C5X	5.58	122.34	116.77
7	A	1001	FAD	C4-C4X-C10	-5.27	116.46	119.95
7	N	1001	FAD	C4X-N5-C5X	4.83	121.60	116.77
7	A	1001	FAD	C4-C4X-N5	4.28	123.49	118.60
7	N	1001	FAD	C4-C4X-N5	4.19	123.39	118.60
7	N	1001	FAD	C4X-C10-N10	-3.89	116.31	120.30
15	C	142	HEM	CMD-C2D-C1D	-3.88	122.50	128.46
7	A	1001	FAD	C4X-C10-N10	-3.71	116.48	120.30
15	P	201	HEM	CMD-C2D-C1D	-3.61	122.91	128.46
15	C	142	HEM	CMD-C2D-C3D	3.40	131.35	124.94
15	P	201	HEM	CAC-C3C-C2C	3.23	131.01	124.69
7	N	1001	FAD	C4'-C3'-C2'	-3.21	106.69	113.36
15	P	201	HEM	CMD-C2D-C3D	3.20	130.97	124.94
7	A	1001	FAD	C4'-C3'-C2'	-3.11	106.89	113.36
15	C	142	HEM	CAC-C3C-C2C	3.08	130.71	124.69
7	A	1001	FAD	C1B-N9A-C4A	-3.01	121.36	126.64
7	N	1001	FAD	P-O3P-PA	2.99	143.08	132.83
7	N	1001	FAD	C4X-C4-N3	-2.91	119.44	123.43
7	N	1001	FAD	C1B-N9A-C4A	-2.90	121.55	126.64
15	P	201	HEM	C4C-C3C-C2C	-2.90	104.86	106.85
15	C	142	HEM	C4C-C3C-C2C	-2.76	104.95	106.85
7	A	1001	FAD	O5'-C5'-C4'	2.74	116.68	109.36
7	A	1001	FAD	P-O3P-PA	2.66	141.95	132.83
7	A	1001	FAD	C4X-C4-N3	-2.61	119.86	123.43
7	N	1001	FAD	O5'-C5'-C4'	2.60	116.31	109.36
7	A	1001	FAD	O2'-C2'-C3'	-2.49	103.05	109.10
7	N	1001	FAD	O2'-C2'-C3'	-2.48	103.07	109.10
7	N	1001	FAD	O3'-C3'-C2'	-2.47	102.84	108.81
14	C	141	BHG	C1'-O1-C1	2.30	117.65	113.84
7	A	1001	FAD	O3'-C3'-C2'	-2.19	103.52	108.81
7	N	1001	FAD	C9A-N10-C10	2.19	124.77	121.91
15	C	142	HEM	CAB-C3B-C4B	-2.06	125.29	128.46
7	N	1001	FAD	O2A-PA-O1A	2.05	122.39	112.24
7	A	1001	FAD	C8M-C8-C9	-2.05	115.45	120.34
7	A	1001	FAD	O2A-PA-O1A	2.01	122.20	112.24

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	C	141	BHG	C4
14	P	205	BHG	C4
8	A	1002	TEO	C2
8	N	1002	TEO	C2

All (31) torsion outliers are listed below:

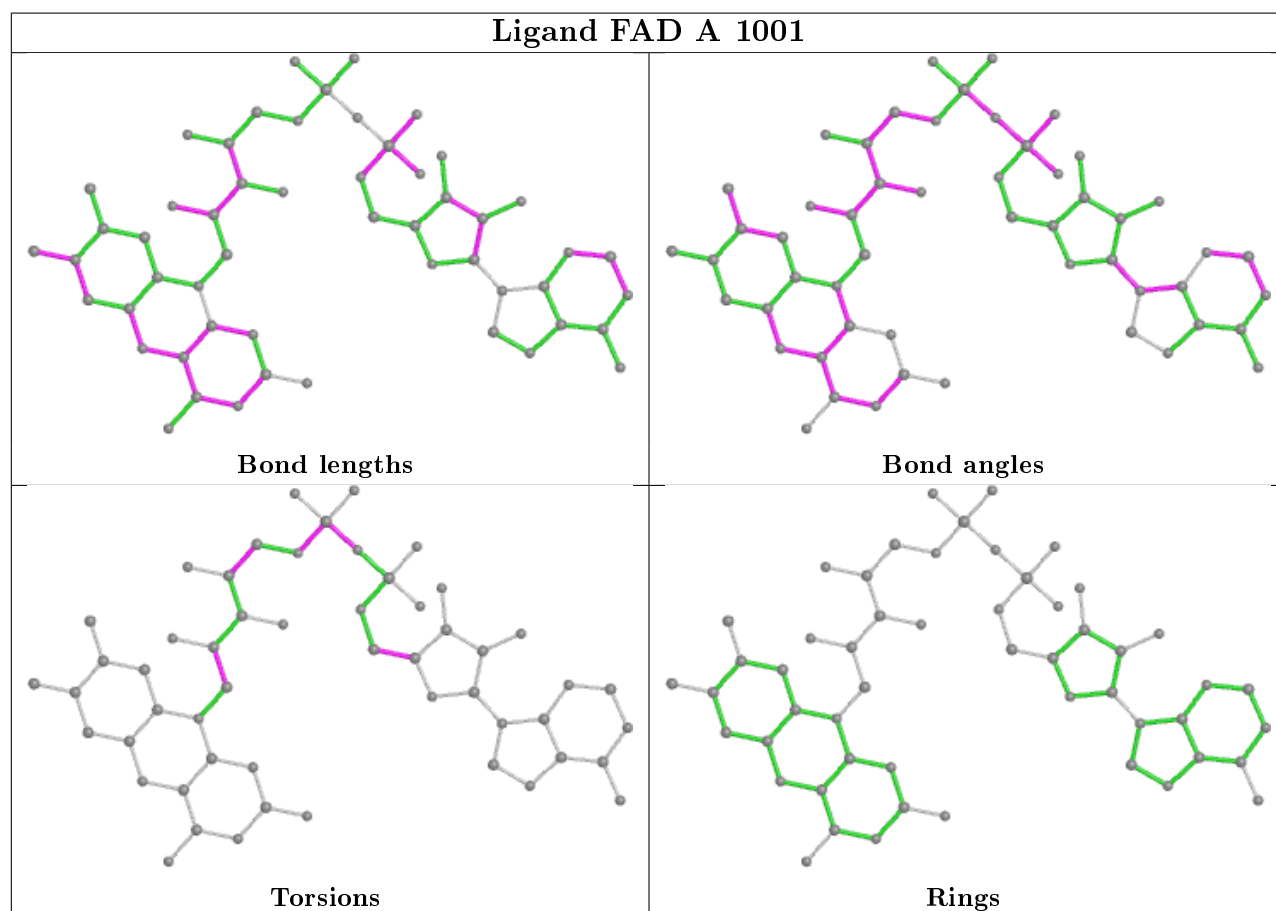
Mol	Chain	Res	Type	Atoms
8	A	1002	TEO	C1-C2-C3-C4
8	A	1002	TEO	O2-C2-C3-C4
7	A	1001	FAD	N10-C1'-C2'-O2'
7	A	1001	FAD	O4'-C4'-C5'-O5'
7	A	1001	FAD	C5'-O5'-P-O2P
8	N	1002	TEO	C1-C2-C3-C4
8	N	1002	TEO	O2-C2-C3-C4
7	N	1001	FAD	N10-C1'-C2'-O2'
7	N	1001	FAD	N10-C1'-C2'-C3'
7	N	1001	FAD	O4'-C4'-C5'-O5'
7	N	1001	FAD	C5'-O5'-P-O2P
13	O	1009	GOL	O1-C1-C2-C3
13	O	1009	GOL	C1-C2-C3-O3
13	B	1009	GOL	C1-C2-C3-O3
14	P	205	BHG	C3'-C4'-C5'-C6'
13	O	1009	GOL	O2-C2-C3-O3
7	A	1001	FAD	PA-O3P-P-O5'
7	N	1001	FAD	PA-O3P-P-O5'
13	B	1009	GOL	O2-C2-C3-O3
7	A	1001	FAD	C5'-O5'-P-O3P
7	N	1001	FAD	C5'-O5'-P-O3P
7	A	1001	FAD	C5'-O5'-P-O1P
7	A	1001	FAD	N10-C1'-C2'-C3'
7	A	1001	FAD	C3'-C4'-C5'-O5'
14	C	141	BHG	C2'-C3'-C4'-C5'
13	O	1009	GOL	O1-C1-C2-O2
7	A	1001	FAD	PA-O3P-P-O2P
7	N	1001	FAD	PA-O3P-P-O2P
7	N	1001	FAD	C5'-O5'-P-O1P
7	A	1001	FAD	O4B-C4B-C5B-O5B
7	N	1001	FAD	O4B-C4B-C5B-O5B

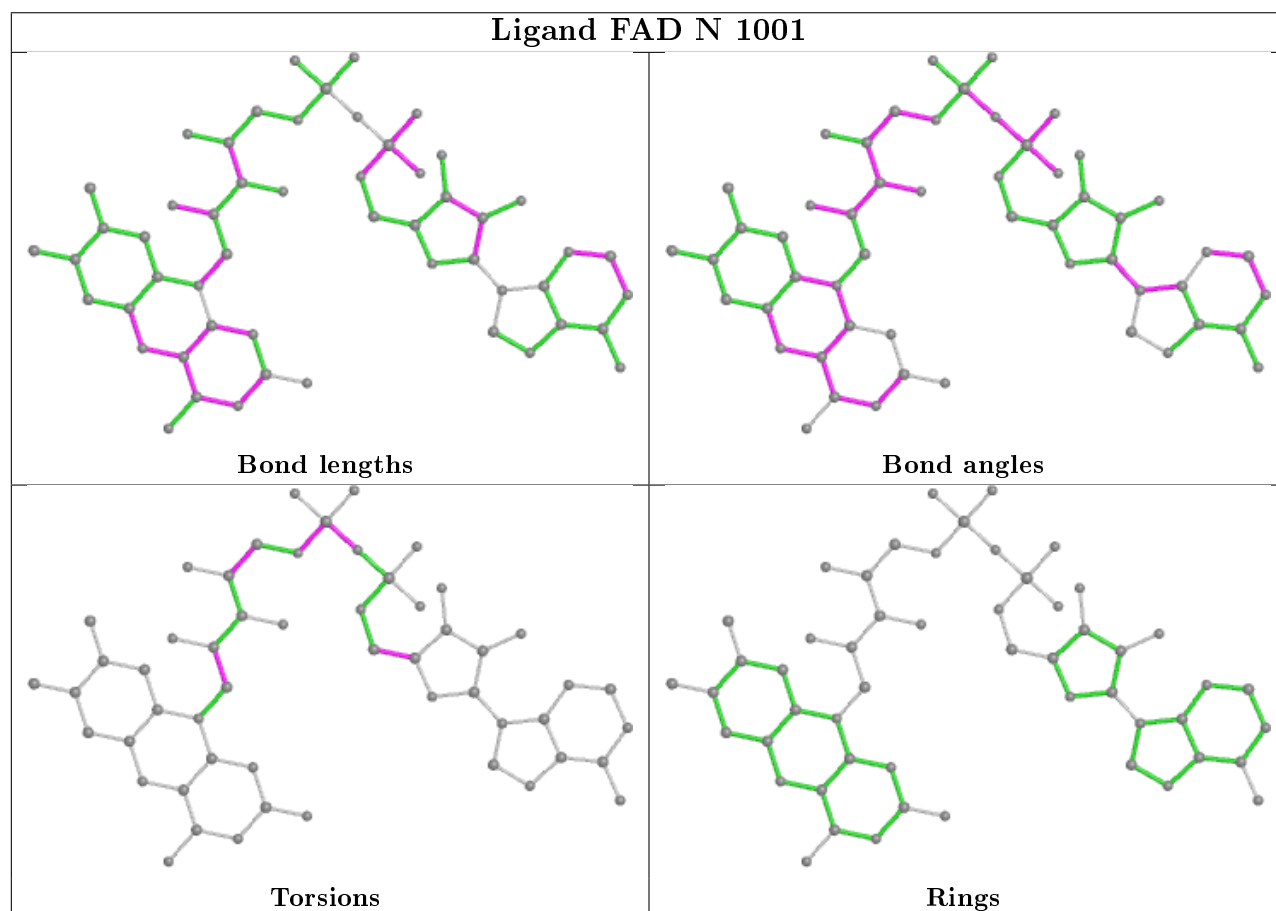
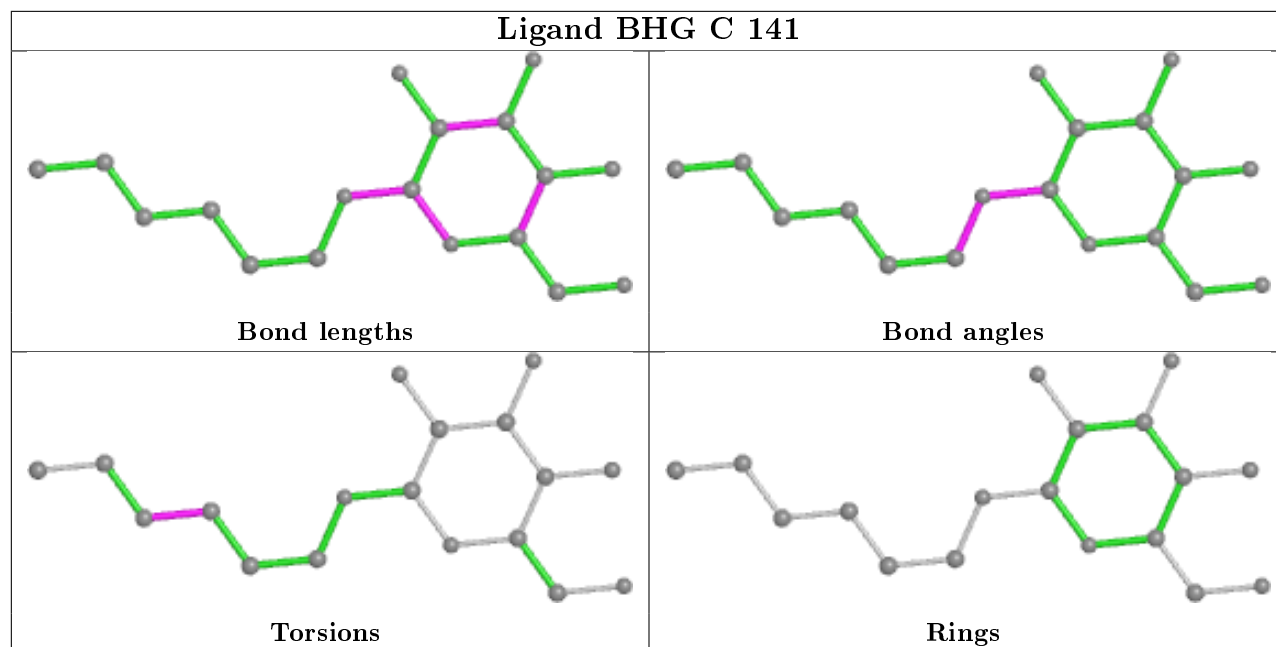
There are no ring outliers.

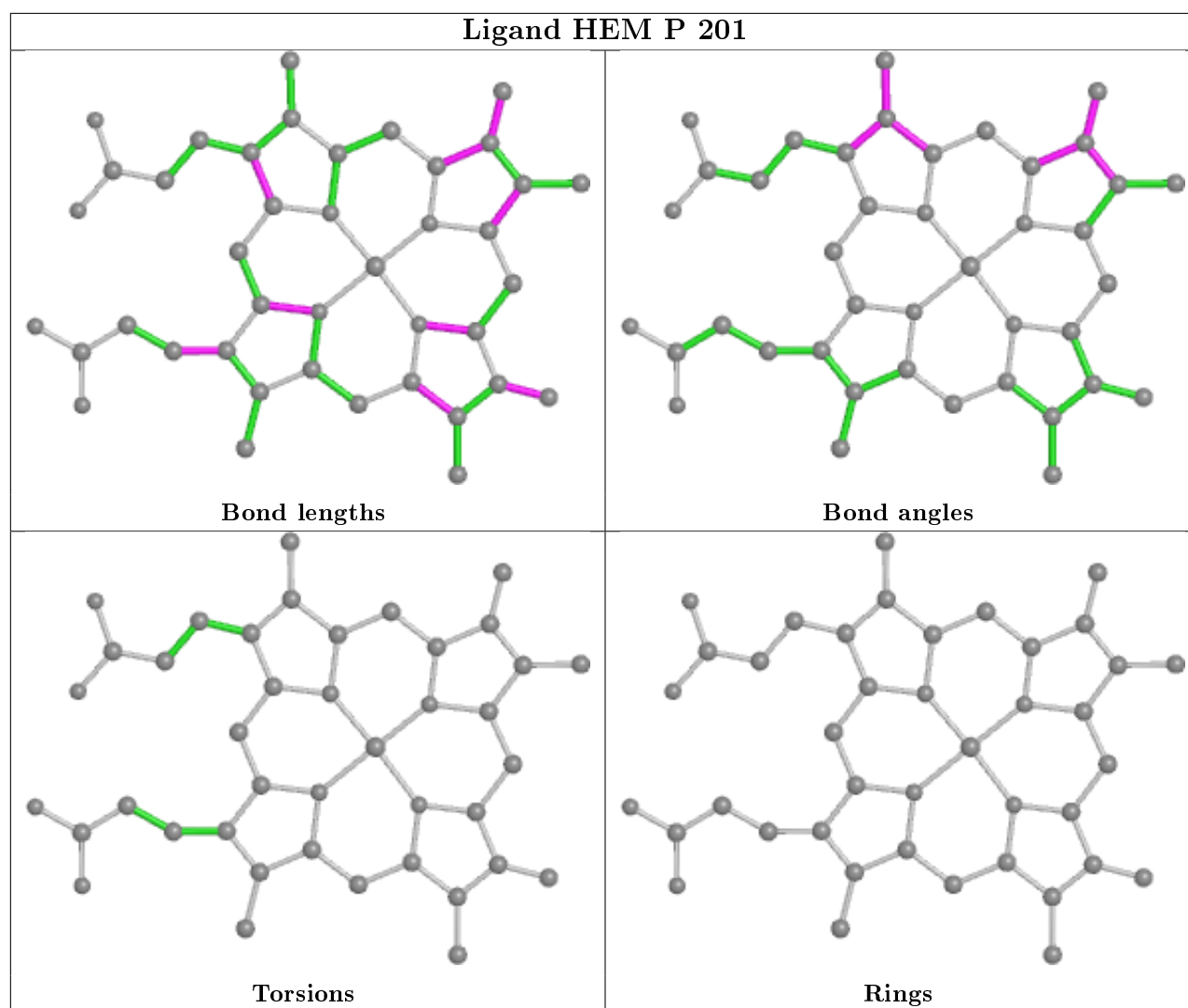
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	O	1009	GOL	1	0
7	A	1001	FAD	3	0
8	N	1002	TEO	1	0
7	N	1001	FAD	3	0
13	B	1009	GOL	1	0
8	A	1002	TEO	3	0

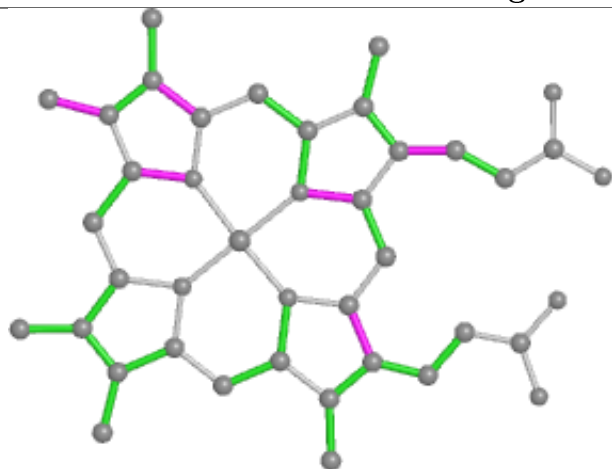
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



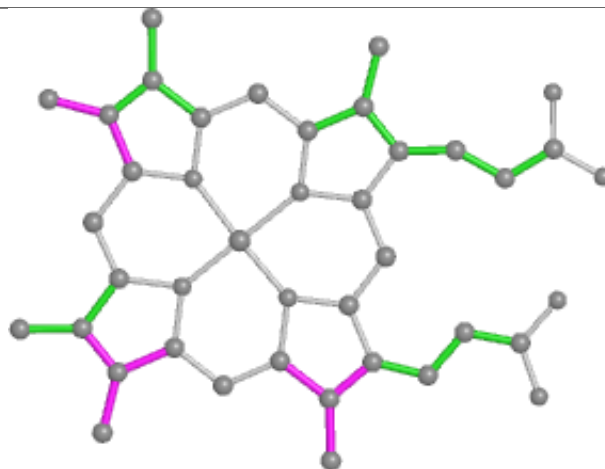




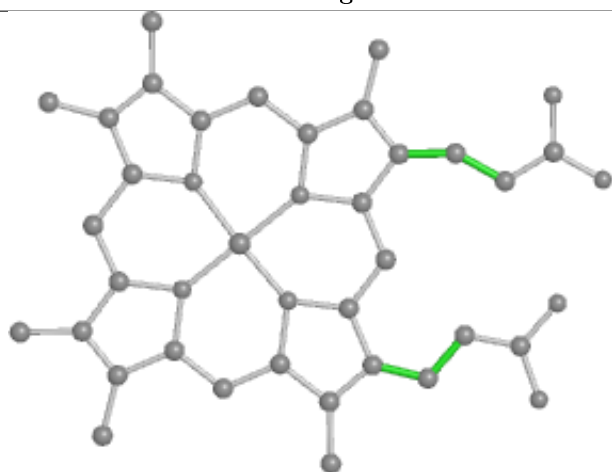
Ligand HEM C 142



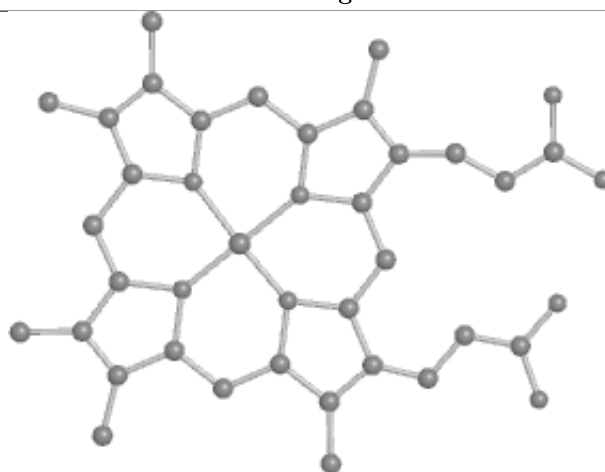
Bond lengths



Bond angles

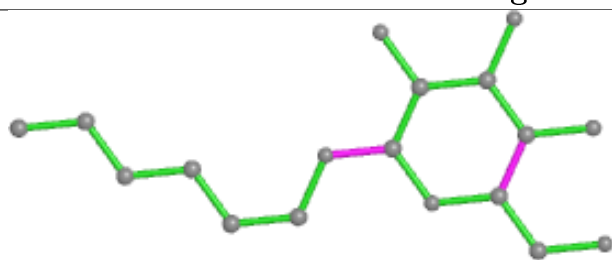


Torsions

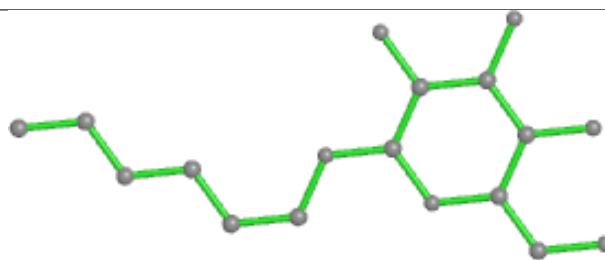


Rings

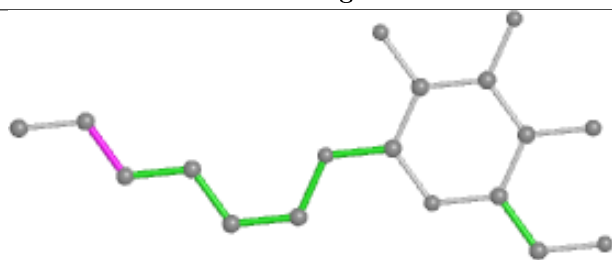
Ligand BHG P 205



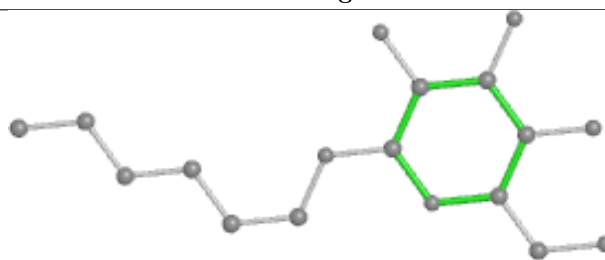
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	612/621 (98%)	-0.40	6 (0%) 82 87	14, 23, 45, 74	0
1	N	612/621 (98%)	-0.41	3 (0%) 91 93	12, 22, 43, 69	0
2	B	239/252 (94%)	-0.48	2 (0%) 86 90	15, 24, 41, 70	0
2	O	239/252 (94%)	-0.45	3 (1%) 77 82	14, 23, 37, 69	0
3	C	139/140 (99%)	-0.17	2 (1%) 75 81	21, 35, 50, 61	0
3	P	139/140 (99%)	0.32	16 (11%) 4 6	21, 37, 81, 92	0
4	D	101/103 (98%)	0.11	5 (4%) 28 33	26, 42, 58, 66	0
4	Q	101/103 (98%)	0.49	9 (8%) 9 12	27, 47, 69, 79	0
All	All	2182/2232 (97%)	-0.29	46 (2%) 63 70	12, 25, 54, 92	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	79	LEU	6.5
3	P	78	SER	4.6
1	A	10	THR	4.5
3	P	64	PRO	4.3
4	Q	88	TYR	4.1
2	O	8	THR	3.9
4	Q	85	TYR	3.8
3	P	74	VAL	3.8
3	P	76	SER	3.6
4	Q	103	ILE	3.5
2	B	8	THR	3.5
3	P	77	LEU	3.4
4	Q	33	PRO	3.4
1	A	568	GLN	3.3
4	D	32	GLY	3.1
3	P	2	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	30	TYR	2.9
4	Q	93	ILE	2.9
3	P	73	VAL	2.8
3	P	81	PRO	2.8
1	N	10	THR	2.7
3	C	62	LEU	2.7
1	N	568	GLN	2.7
2	O	246	LYS	2.6
1	A	566	PRO	2.6
3	P	132	LEU	2.6
3	P	3	THR	2.5
1	A	13	PRO	2.5
3	P	84	ILE	2.5
3	P	82	ALA	2.5
4	Q	30	TYR	2.4
4	Q	89	TYR	2.4
1	N	185	ASN	2.4
1	A	567	LEU	2.3
3	C	2	ALA	2.3
1	A	571	GLN	2.3
3	P	72	ALA	2.2
3	P	91	LEU	2.2
4	Q	101	TRP	2.2
2	O	245	TYR	2.2
2	B	246	LYS	2.2
4	D	37	TYR	2.2
4	D	89	TYR	2.1
4	Q	97	VAL	2.1
3	P	80	SER	2.1
4	D	28	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	UNL	P	217	1/-	-0.03	0.43	113,113,113,113	0
9	UNL	N	1003	2/-	0.32	0.39	114,114,114,114	0
9	UNL	D	108	1/-	0.46	0.14	63,63,63,63	0
9	UNL	D	252	1/-	0.49	0.12	73,73,73,73	0
9	UNL	O	1008	1/-	0.50	0.20	63,63,63,63	0
9	UNL	C	143	2/-	0.54	0.17	65,65,65,65	0
9	UNL	P	214	4/-	0.60	0.76	94,94,94,95	0
9	UNL	A	1007	2/-	0.62	0.33	65,65,65,66	0
9	UNL	Q	212	7/-	0.63	0.51	74,75,76,76	0
9	UNL	B	1008	1/-	0.64	0.20	69,69,69,69	0
9	UNL	P	215	4/-	0.65	0.17	74,74,75,76	0
9	UNL	D	249	1/-	0.65	0.31	72,72,72,72	0
9	UNL	Q	256	1/-	0.66	0.20	84,84,84,84	0
9	UNL	P	231	1/-	0.67	0.21	74,74,74,74	0
9	UNL	D	254	1/-	0.68	0.10	67,67,67,67	0
9	UNL	O	1007	1/-	0.68	0.16	59,59,59,59	0
9	UNL	Q	219	1/-	0.74	0.12	60,60,60,60	0
9	UNL	A	1006	1/-	0.74	0.35	63,63,63,63	0
9	UNL	D	250	1/-	0.75	0.12	73,73,73,73	0
9	UNL	B	1006	1/-	0.76	0.10	60,60,60,60	0
9	UNL	C	146	4/-	0.76	0.46	108,109,109,109	0
9	UNL	N	1005	1/-	0.77	0.25	76,76,76,76	0
9	UNL	P	220	2/-	0.77	0.28	81,81,81,81	0
9	UNL	N	1008	1/-	0.77	0.15	65,65,65,65	0
9	UNL	C	238	1/-	0.77	0.10	59,59,59,59	0
9	UNL	A	1005	1/-	0.78	0.13	63,63,63,63	0
9	UNL	A	1004	1/-	0.78	0.23	61,61,61,61	0
9	UNL	N	1010	1/-	0.79	0.11	60,60,60,60	0
9	UNL	D	116	10/-	0.79	0.22	65,66,69,69	0
9	UNL	B	1007	1/-	0.79	0.19	61,61,61,61	0
9	UNL	P	242	1/-	0.81	0.17	57,57,57,57	0
9	UNL	D	253	1/-	0.81	0.15	72,72,72,72	0
9	UNL	P	230	1/-	0.81	0.18	69,69,69,69	0
9	UNL	P	241	1/-	0.81	0.23	59,59,59,59	0
9	UNL	O	1006	1/-	0.82	0.13	54,54,54,54	0
6	AZI	N	623	3/3	0.82	0.09	68,68,70,71	0
9	UNL	P	209	2/-	0.82	0.15	49,49,49,49	0

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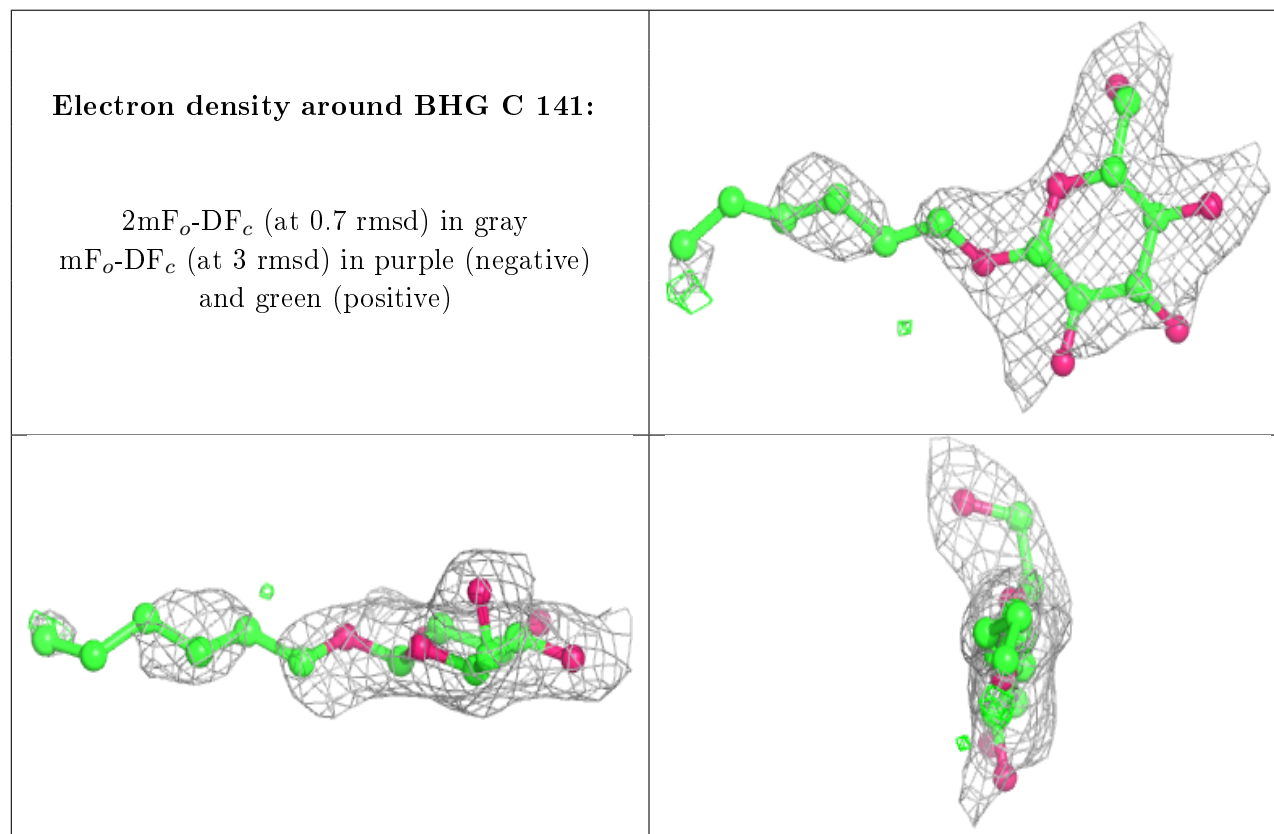
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	UNL	A	1008	1/-	0.84	0.25	64,64,64,64	0
9	UNL	C	237	1/-	0.84	0.14	66,66,66,66	0
9	UNL	C	144	1/-	0.84	0.21	62,62,62,62	0
9	UNL	P	240	1/-	0.85	0.12	56,56,56,56	0
9	UNL	N	1009	1/-	0.85	0.17	54,54,54,54	0
9	UNL	C	147	1/-	0.85	0.14	59,59,59,59	0
14	BHG	C	141	18/18	0.86	0.16	48,70,75,75	0
9	UNL	D	251	1/-	0.86	0.10	73,73,73,73	0
9	UNL	Q	213	5/-	0.86	0.19	74,74,74,74	0
9	UNL	P	216	1/-	0.87	0.19	53,53,53,53	0
9	UNL	A	1003	1/-	0.88	0.25	69,69,69,69	0
9	UNL	C	149	1/-	0.88	0.17	81,81,81,81	0
9	UNL	Q	228	1/-	0.88	0.11	64,64,64,64	0
9	UNL	N	1004	1/-	0.89	0.14	60,60,60,60	0
9	UNL	N	1011	1/-	0.89	0.13	37,37,37,37	0
9	UNL	P	229	1/-	0.89	0.11	54,54,54,54	0
9	UNL	N	1006	1/-	0.90	0.14	54,54,54,54	0
6	AZI	A	623	3/3	0.90	0.11	62,62,63,64	0
9	UNL	C	145	4/-	0.91	0.20	100,100,100,100	0
9	UNL	P	232	1/-	0.91	0.29	61,61,61,61	0
9	UNL	D	107	6/-	0.92	0.29	66,68,69,70	0
9	UNL	N	1012	1/-	0.92	0.12	53,53,53,53	0
9	UNL	D	114	8/-	0.93	0.16	61,63,64,65	0
13	GOL	O	1009	6/6	0.94	0.10	35,40,41,43	0
9	UNL	P	208	1/-	0.94	0.09	44,44,44,44	0
13	GOL	B	1009	6/6	0.94	0.09	33,36,38,38	0
14	BHG	P	205	18/18	0.95	0.12	36,42,59,61	0
9	UNL	Q	218	1/-	0.95	0.11	53,53,53,53	0
9	UNL	N	1007	1/-	0.95	0.18	44,44,44,44	0
9	UNL	C	148	1/-	0.96	0.14	56,56,56,56	0
9	UNL	B	1005	1/-	0.96	0.07	39,39,39,39	0
8	TEO	N	1002	9/9	0.97	0.06	17,18,19,20	1
15	HEM	P	201	41/43	0.97	0.11	28,33,50,53	0
9	UNL	D	119	1/-	0.97	0.18	63,63,63,63	0
9	UNL	O	1005	1/-	0.98	0.10	35,35,35,35	0
5	K	A	622	1/1	0.98	0.07	24,24,24,24	0
5	K	N	622	1/1	0.98	0.07	25,25,25,25	0
7	FAD	N	1001	53/53	0.98	0.08	11,14,18,21	0
7	FAD	A	1001	53/53	0.98	0.07	12,14,18,22	0
15	HEM	C	142	41/43	0.98	0.09	27,32,49,52	0
12	F3S	O	1004	7/7	0.99	0.09	19,20,21,22	0
5	K	O	253	1/1	0.99	0.06	39,39,39,39	0

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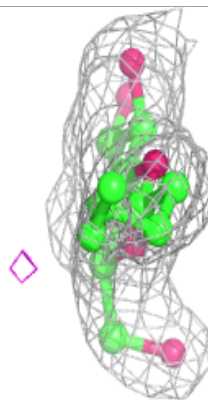
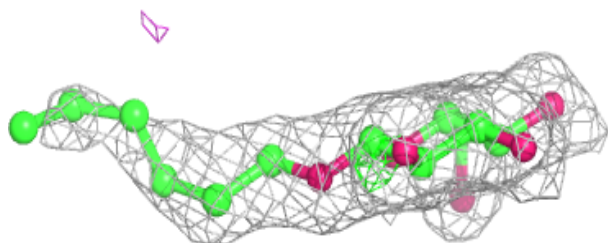
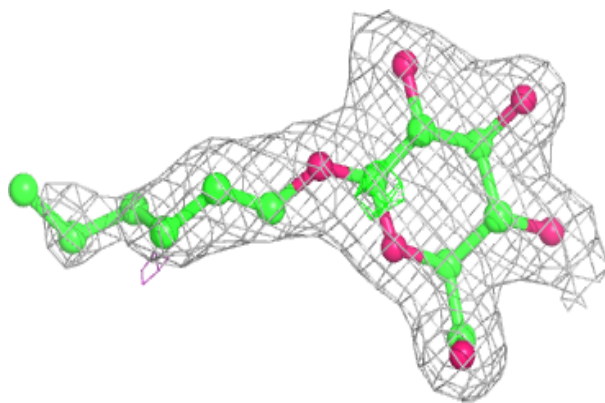
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	TEO	A	1002	9/9	0.99	0.06	18,20,23,24	1
5	K	B	253	1/1	0.99	0.06	38,38,38,38	0
12	F3S	B	1004	7/7	0.99	0.08	18,20,21,22	0
10	FES	O	1002	4/4	1.00	0.09	13,14,14,15	0
10	FES	B	1002	4/4	1.00	0.08	14,16,16,16	0
11	SF4	O	1003	8/8	1.00	0.09	16,17,18,18	0
11	SF4	B	1003	8/8	1.00	0.08	17,19,19,19	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.



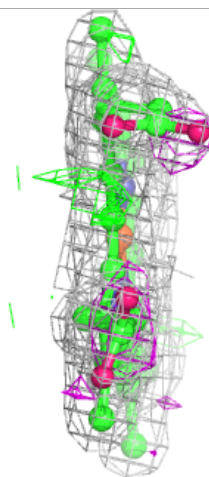
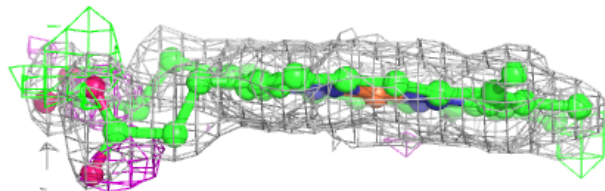
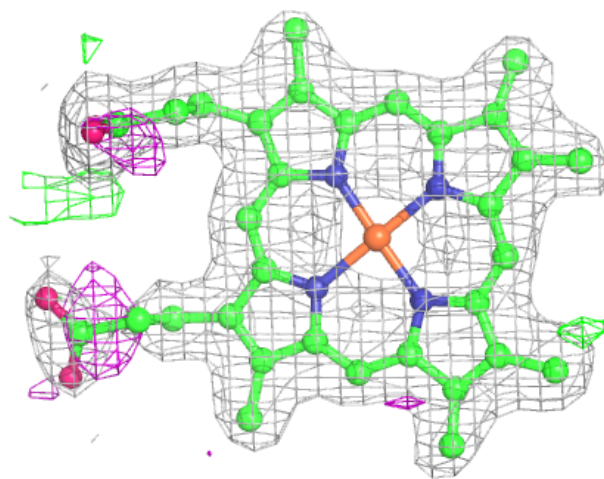
Electron density around BHG P 205:

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



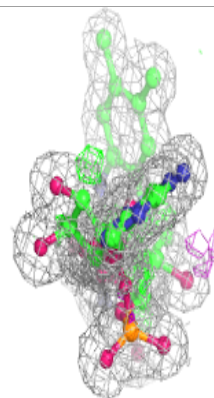
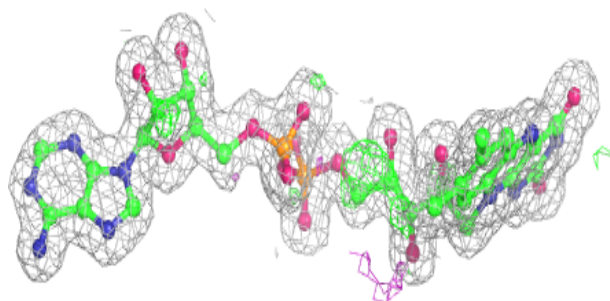
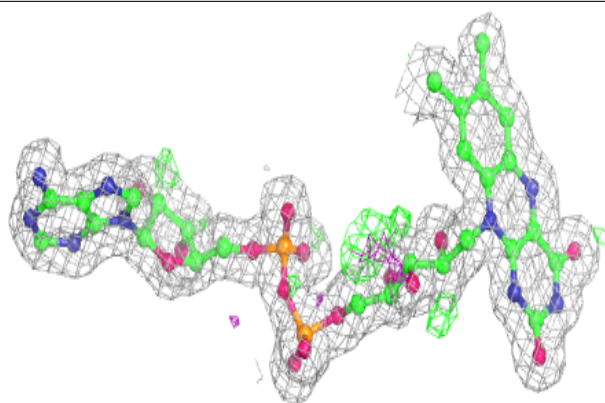
Electron density around HEM P 201:

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

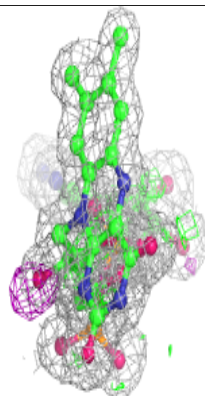
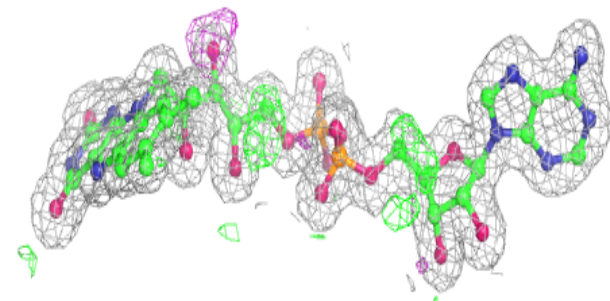
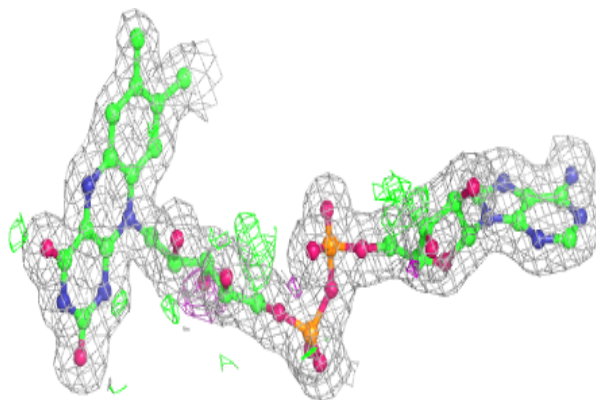


Electron density around FAD N 1001:

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

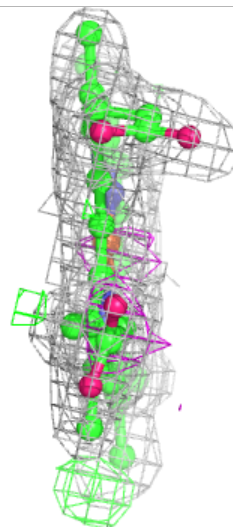
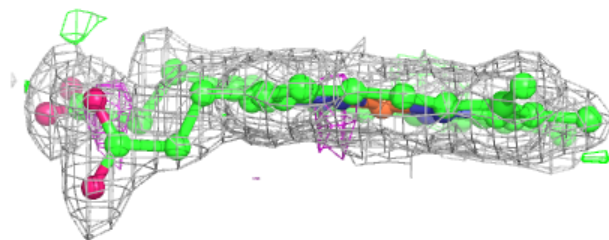
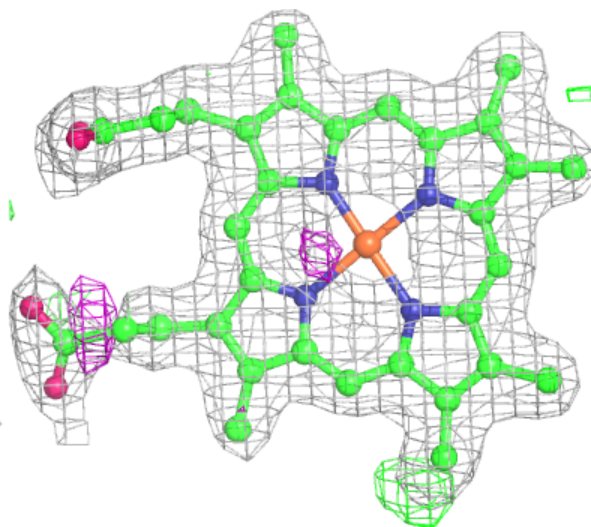
**Electron density around FAD A 1001:**

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



Electron density around HEM C 142:

$2mF_o-DF_c$ (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.