Full wwPDB X-ray Structure Validation Report (i)

Dec 14, 2023 – 09:48 am GMT

PDB ID	:	2WQY
Title	:	Remodelling of carboxin binding to the Q-site of avian respiratory complex II
Authors	:	Ruprecht, J.; Iwata, S.; Cecchini, G.
Deposited on	:	2009-08-27
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

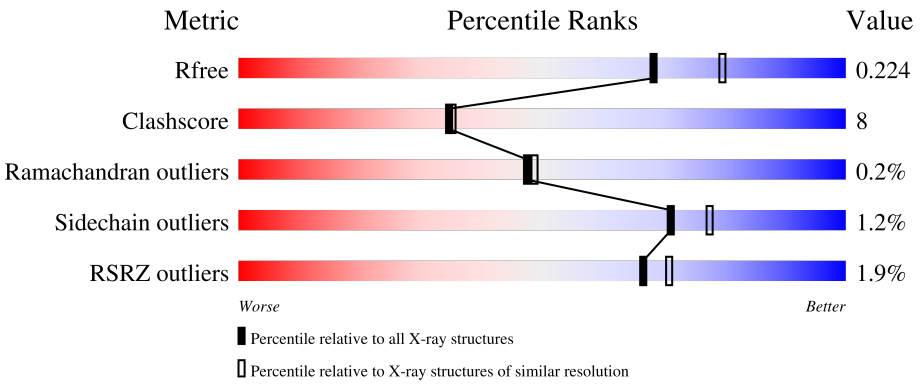
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	87% 12% •
1	N	621	85% 13% •
2	B	252	85% 9% • 5%
2	O	252	.% 86% 8% • 5%
3	C	141	3% 74% 23% ••

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Mol	Chain	Length	Quality of chain
3	P	141	7% 74% 24%
4	D	103	7% 81% 17%
4	Q	103	12% 81% 17%

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
13	GOL	P	208	-	-	-	X
14	BHG	C	142	X	-	-	-
14	BHG	P	204	X	-	-	-
17	PEE	D	109	-	-	-	X
17	PEE	Q	210	-	-	-	X
5	UNL	A	1003	-	-	X	-
5	UNL	A	1004	-	-	X	-
5	UNL	A	1005	-	-	-	X
5	UNL	A	1007	-	-	-	X
5	UNL	A	1008	-	-	-	X
5	UNL	A	1010	-	-	-	X
5	UNL	A	1011	-	-	-	X
5	UNL	A	1012	-	-	-	X
5	UNL	A	1015	-	-	-	X
5	UNL	A	1023	-	-	-	X
5	UNL	B	1005	-	-	X	-
5	UNL	B	1006	-	-	-	X
5	UNL	B	1007	-	-	-	X
5	UNL	B	1009	-	-	-	X
5	UNL	B	268	-	-	-	X
5	UNL	C	145	-	-	X	-
5	UNL	C	214	-	-	X	-
5	UNL	C	235	-	-	-	X
5	UNL	C	248	-	-	-	X
5	UNL	C	254	-	-	-	X
5	UNL	C	259	-	-	-	X
5	UNL	C	292	-	-	-	X
5	UNL	C	293	-	-	-	X
5	UNL	D	245	-	-	X	-
5	UNL	D	247	-	-	-	X
5	UNL	D	263	-	-	-	X
5	UNL	D	265	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	UNL	D	266	-	-	-	X
5	UNL	D	291	-	-	-	X
5	UNL	N	1003	-	-	X	-
5	UNL	N	1005	-	-	-	X
5	UNL	N	1006	-	-	-	X
5	UNL	N	1012	-	-	-	X
5	UNL	N	1014	-	-	-	X
5	UNL	N	1016	-	-	-	X
5	UNL	N	1018	-	-	-	X
5	UNL	N	1022	-	-	-	X
5	UNL	O	1005	-	-	X	-
5	UNL	O	276	-	-	-	X
5	UNL	P	211	-	-	X	X
5	UNL	P	224	-	-	-	X
5	UNL	P	274	-	-	-	X
5	UNL	Q	287	-	-	-	X
5	UNL	Q	288	-	-	-	X
9	OAA	A	1002	-	-	X	-
9	OAA	N	1002	-	X	X	-

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 19490 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
			Total	C	N	O	S			
1	A	613	4731	2959	844	899	29	0	0	0
1	N	612	4725	2956	843	897	29	0	0	0

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
			Total	C	N	O	S			
2	B	239	1918	1213	325	358	22	0	0	0
2	O	239	1918	1213	325	358	22	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	140	1078	708	179	187	4	0	0	0
3	P	140	1078	708	179	187	4	0	0	0

- Molecule 4 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B, SMALL SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	101	765	505	121	136	3	0	0	0
4	Q	101	765	505	121	136	3	0	0	0

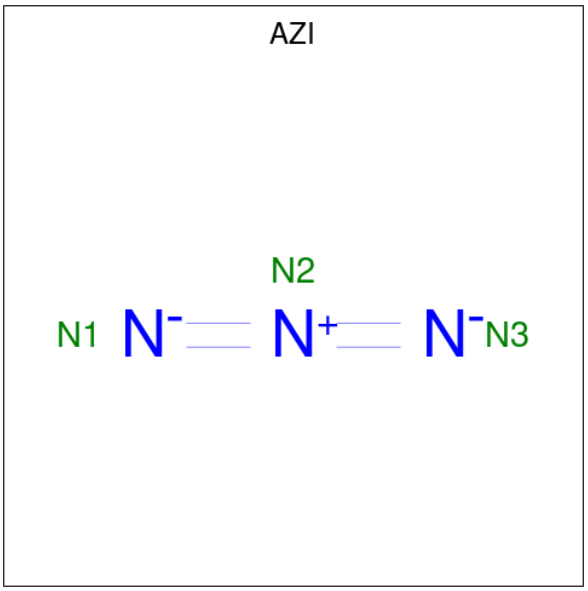
- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	21	29	19	10	0	0
5	B	10	14	9	5	0	0
5	C	15	22	13	9	0	0
5	D	9	9	9		0	0
5	N	21	24	20	4	0	0
5	O	6	10	5	5	0	0
5	P	7	11	6	5	0	0
5	Q	6	6	6		0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

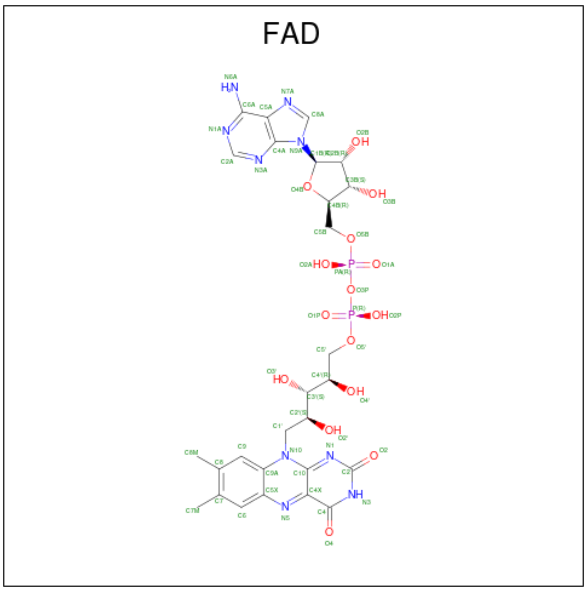
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
6	A	1	1	1	0	0
6	B	1	1	1	0	0
6	N	1	1	1	0	0
6	O	1	1	1	0	0

- Molecule 7 is AZIDE ION (three-letter code: AZI) (formula: N_3).



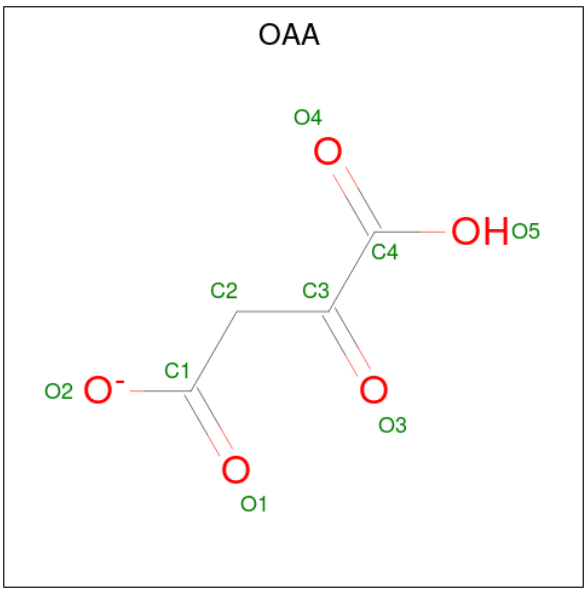
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	N		
7	A	1	3	3	0	0

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



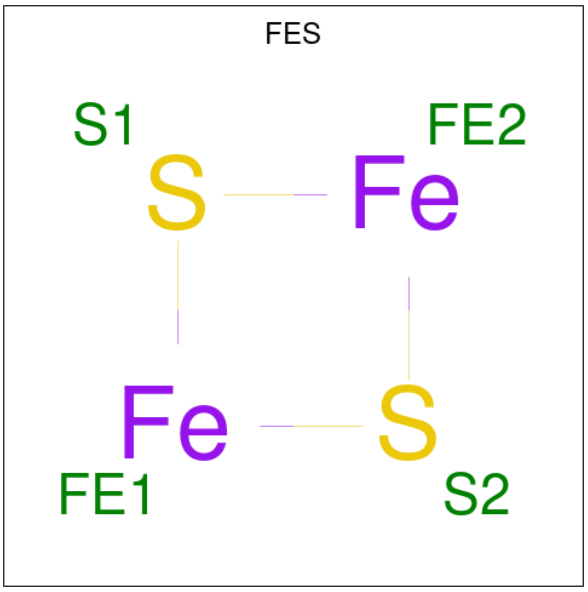
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	A	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
8	N	1	53	27	9	15	2	0	0

- Molecule 9 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).



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

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

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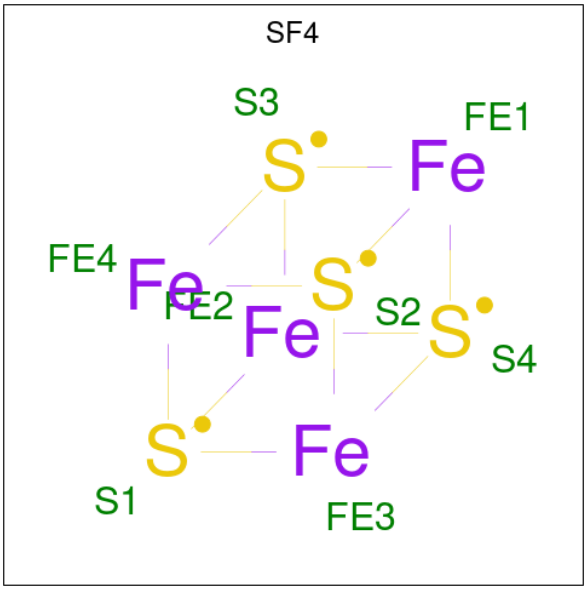
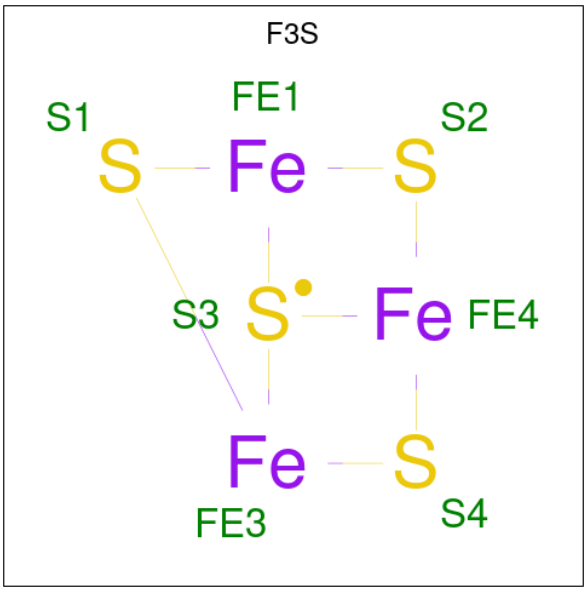
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
10	O	1	4	2	2	0	0

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



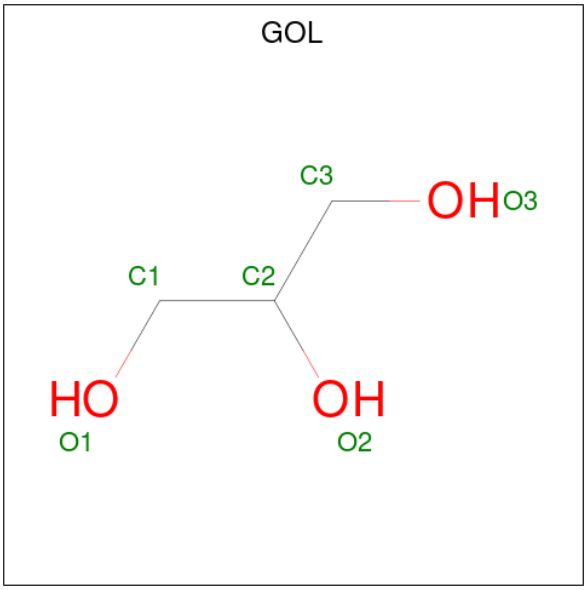
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
11	B	1	8	4	4	0	0
11	O	1	8	4	4	0	0

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



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

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



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

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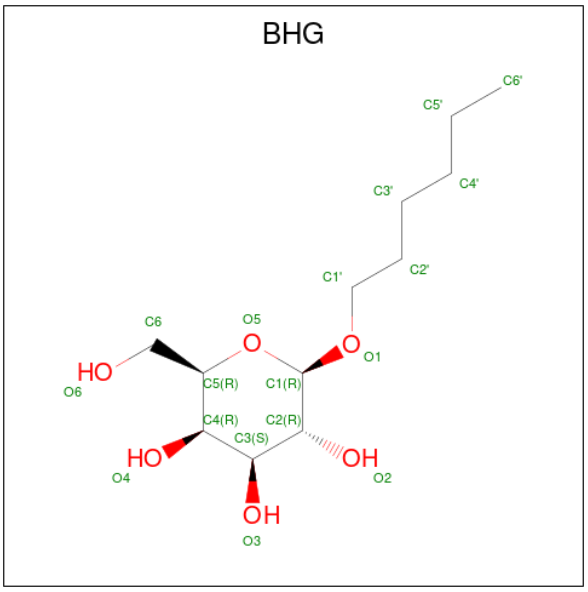
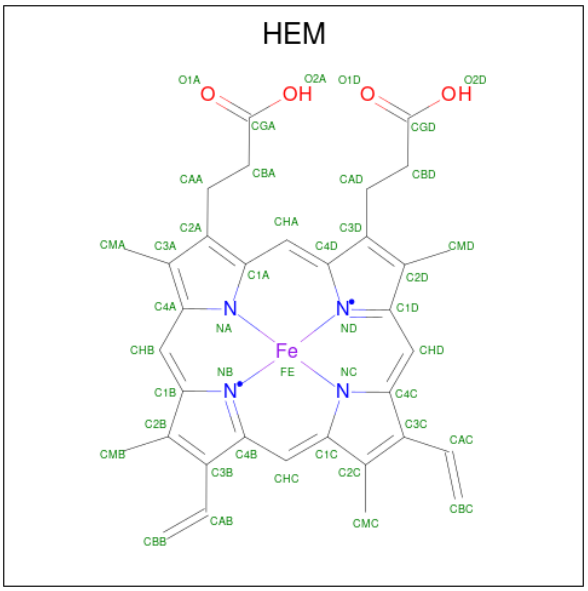
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
13	O	1	6	3	3	0	0
			Total	C	O		
13	P	1	6	3	3	0	0

- Molecule 14 is hexyl beta-D-galactopyranoside (three-letter code: BHG) (formula: $C_{12}H_{24}O_6$).



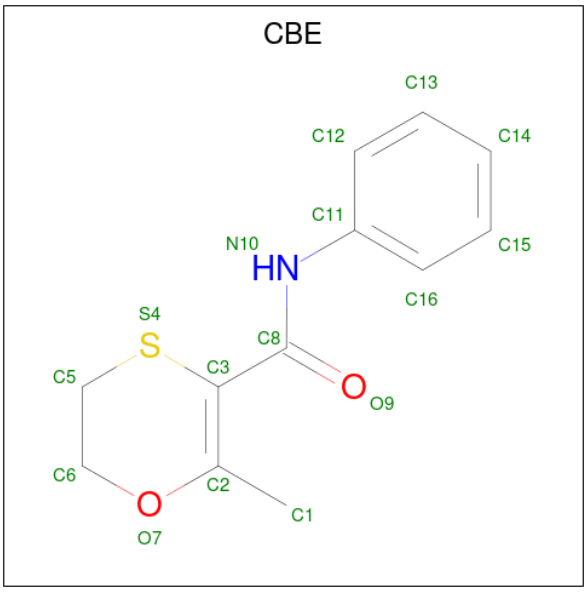
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
14	C	1	18	12	6	0	0
			Total	C	O		
14	P	1	18	12	6	0	0

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 16 is 2-METHYL-N-PHENYL-5,6-DIHYDRO-1,4-OXATHIINE-3-CARBOXAMIDE (three-letter code: CBE) (formula: $C_{12}H_{13}NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
16	C	1	16	12	1	2	1	0	0

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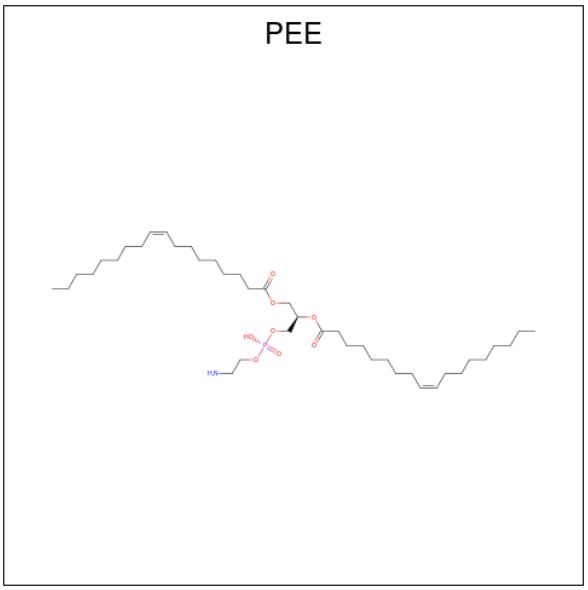
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
16	P	1	16	12	1	2	1	0	0

- Molecule 17 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
17	D	1	24	24	0	0
17	Q	1	24	24	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	A	548	548	548	0	0
18	B	297	297	297	0	0
18	C	102	102	102	0	0
18	D	60	60	60	0	0
18	N	558	558	558	0	0
18	O	287	287	287	0	0

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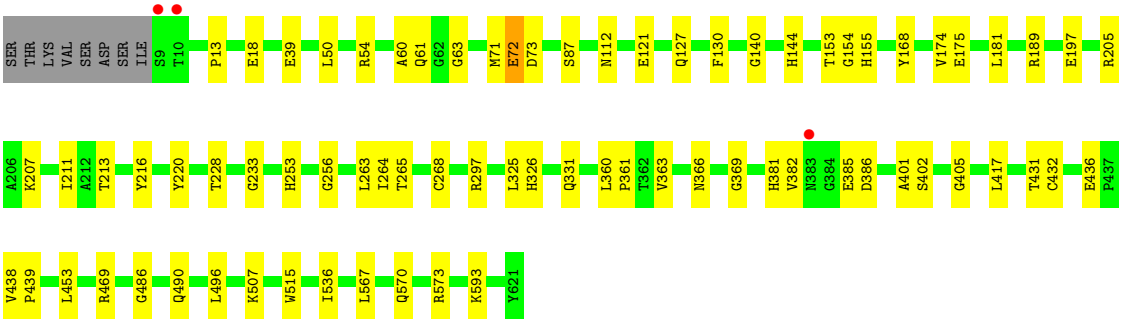
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	P	82	82	82	0	0
			Total	O		
18	Q	62	62	62	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

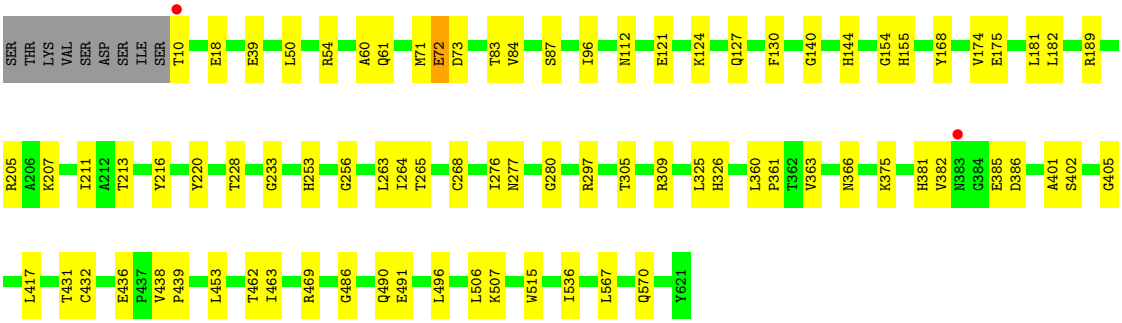
• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

Chain A:



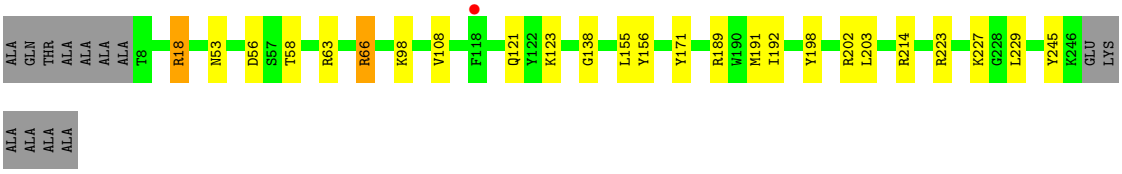
• Molecule 1: SUCCINATE DEHYDROGENASE FLAVOPROTEIN SUBUNIT

Chain N:



• Molecule 2: SUCCINATE DEHYDROGENASE IP SUBUNIT

Chain B:

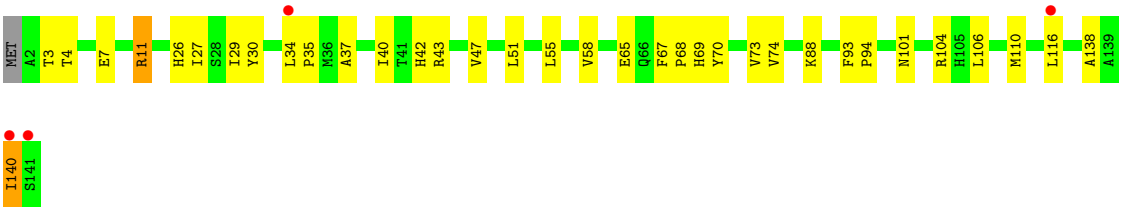


• Molecule 2: SUCCINATE DEHYDROGENASE IP SUBUNIT

Chain O:

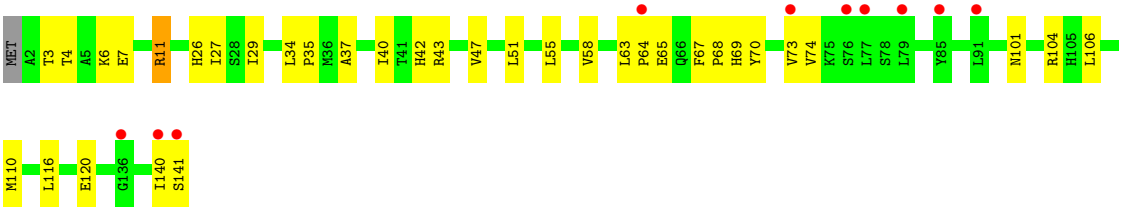
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT

Chain C:



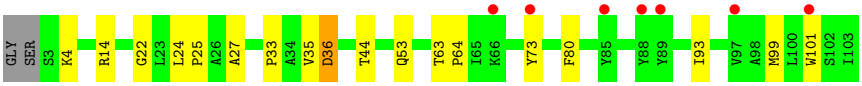
• Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT

Chain P:



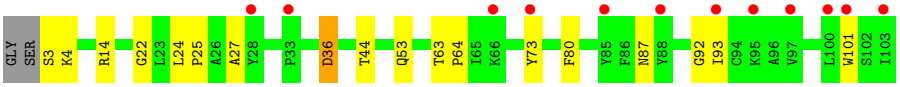
• Molecule 4: SUCCINATE DEHYDROGENASE CYTOCHROME B, SMALL SUBUNIT

Chain D:



• Molecule 4: SUCCINATE DEHYDROGENASE CYTOCHROME B, SMALL SUBUNIT

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	118.70Å 200.75Å 67.63Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	64.09 – 2.10 64.09 – 2.06	Depositor EDS
% Data completeness (in resolution range)	88.3 (64.09-2.10) 85.1 (64.09-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.62 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.184 , 0.223 0.184 , 0.224	Depositor DCC
R_{free} test set	8237 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 66.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.287 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19490	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: K, SF4, PEE, AZI, HEM, F3S, OAA, BHG, UNL, GOL, FAD, CBE, FES

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	0.65	0/4832	0.81	5/6543 (0.1%)
1	N	0.66	0/4826	0.81	5/6535 (0.1%)
2	B	0.66	0/1959	0.81	2/2641 (0.1%)
2	O	0.64	0/1959	0.80	2/2641 (0.1%)
3	C	0.51	0/1107	0.60	0/1506
3	P	0.49	0/1107	0.60	0/1506
4	D	0.44	0/788	0.60	0/1082
4	Q	0.43	0/788	0.59	0/1082
All	All	0.62	0/17366	0.77	14/23536 (0.1%)

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
3	C	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	18	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	N	469	ARG	NE-CZ-NH2	-7.86	116.37	120.30
2	O	18	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	A	469	ARG	NE-CZ-NH2	-6.79	116.91	120.30
2	O	18	ARG	NE-CZ-NH1	5.97	123.29	120.30
2	B	18	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	N	360	LEU	CA-CB-CG	5.82	128.68	115.30
1	A	360	LEU	CA-CB-CG	5.65	128.30	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	256	GLY	N-CA-C	-5.62	99.04	113.10
1	A	256	GLY	N-CA-C	-5.52	99.31	113.10
1	N	140	GLY	N-CA-C	5.23	126.18	113.10
1	A	140	GLY	N-CA-C	5.17	126.04	113.10
1	N	54	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	54	ARG	NE-CZ-NH1	5.11	122.86	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	30	TYR	Sidechain

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	4731	0	4614	57	0
1	N	4725	0	4609	65	0
2	B	1918	0	1910	27	0
2	O	1918	0	1909	27	0
3	C	1078	0	1118	35	0
3	P	1078	0	1118	36	0
4	D	765	0	761	19	0
4	Q	765	0	761	15	0
5	A	29	0	0	10	0
5	B	14	0	0	4	0
5	C	22	0	0	4	0
5	D	9	0	0	2	0
5	N	24	0	0	3	0
5	O	10	0	0	3	0
5	P	11	0	0	2	0
5	Q	6	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	3	0	0	0	0
8	A	53	0	29	4	0
8	N	53	0	29	4	0
9	A	9	0	2	6	0
9	N	9	0	2	5	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	0	0
13	C	6	0	8	1	0
13	O	6	0	8	2	0
13	P	6	0	8	0	0
14	C	18	0	24	0	0
14	P	18	0	24	0	0
15	C	41	0	24	1	0
15	P	41	0	24	0	0
16	C	16	0	13	3	0
16	P	16	0	13	3	0
17	D	24	0	40	0	0
17	Q	24	0	40	2	0
18	A	548	0	0	9	0
18	B	297	0	0	6	0
18	C	102	0	0	4	0
18	D	60	0	0	1	0
18	N	558	0	0	18	0
18	O	287	0	0	6	0
18	P	82	0	0	4	0
18	Q	62	0	0	1	0
All	All	19490	0	17096	286	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 8.

All (286) 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)
5:B:1005:UNL:O5	5:B:1005:UNL:O6	1.55	1.25
5:A:1003:UNL:O6	5:A:1003:UNL:O5	1.54	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:1005:UNL:O6	5:O:1005:UNL:O5	1.54	1.24
5:A:1004:UNL:O6	5:A:1004:UNL:O5	1.55	1.23
5:P:211:UNL:O5	5:P:211:UNL:O1	1.57	1.22
5:C:214:UNL:O6	5:C:214:UNL:O5	1.56	1.22
5:C:145:UNL:O6	5:C:145:UNL:O5	1.55	1.22
5:O:1005:UNL:O5	5:O:1005:UNL:O1	1.57	1.22
5:C:145:UNL:O5	5:C:145:UNL:O1	1.57	1.22
5:P:211:UNL:O5	5:P:211:UNL:O6	1.55	1.22
5:N:1003:UNL:O5	5:N:1003:UNL:O1	1.58	1.21
5:N:1003:UNL:O5	5:N:1003:UNL:O6	1.56	1.21
5:A:1003:UNL:O5	5:A:1003:UNL:O1	1.57	1.20
5:B:1005:UNL:O5	5:B:1005:UNL:O1	1.57	1.18
5:A:1004:UNL:O5	5:A:1004:UNL:O1	1.59	1.16
5:C:214:UNL:O5	5:C:214:UNL:O1	1.59	1.15
2:O:66:ARG:HB2	2:O:66:ARG:HH11	1.22	1.03
2:B:66:ARG:HH11	2:B:66:ARG:HB2	1.24	1.02
1:N:189:ARG:HD3	1:N:439:PRO:HB2	1.42	1.01
1:A:189:ARG:HD3	1:A:439:PRO:HB2	1.43	1.00
1:A:112:ASN:HD22	2:B:138:GLY:H	1.13	0.95
1:N:280:GLY:HA2	18:N:2286:HOH:O	1.68	0.93
1:N:96:ILE:HG21	18:N:2096:HOH:O	1.68	0.91
1:N:112:ASN:HD22	2:O:138:GLY:H	1.22	0.86
5:A:1003:UNL:O5	5:A:1003:UNL:O4	1.94	0.85
5:O:1005:UNL:O5	5:O:1005:UNL:O3	1.95	0.85
1:A:297:ARG:HH22	9:A:1002:OAA:C2	1.92	0.82
1:N:96:ILE:HD13	18:N:2096:HOH:O	1.78	0.82
2:O:66:ARG:HH11	2:O:66:ARG:CB	1.94	0.79
2:B:66:ARG:HH11	2:B:66:ARG:CB	1.95	0.79
2:O:214:ARG:HH22	4:Q:53:GLN:HE22	1.31	0.79
1:A:507:LYS:HE3	18:A:2406:HOH:O	1.83	0.79
2:B:214:ARG:HH22	4:D:53:GLN:HE22	1.29	0.78
1:A:112:ASN:ND2	2:B:138:GLY:H	1.81	0.78
3:C:101:ASN:HD21	3:C:104:ARG:HH11	1.30	0.78
1:N:297:ARG:HH22	9:N:1002:OAA:C2	1.98	0.77
4:Q:24:LEU:HB2	4:Q:25:PRO:HD3	1.66	0.77
3:C:26:HIS:CD2	3:C:27:ILE:H	2.03	0.77
4:D:24:LEU:HB2	4:D:25:PRO:HD3	1.66	0.77
1:A:297:ARG:HH22	9:A:1002:OAA:H22	1.50	0.76
3:P:26:HIS:CD2	3:P:27:ILE:H	2.04	0.76
3:P:101:ASN:HD21	3:P:104:ARG:HH11	1.32	0.75
1:A:181:LEU:HD21	1:A:211:ILE:HD11	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PRO:HA	18:A:2003:HOH:O	1.87	0.74
3:P:7:GLU:O	3:P:11:ARG:HG2	1.88	0.74
3:P:3:THR:CG2	3:P:7:GLU:HB2	2.16	0.74
1:N:181:LEU:HD21	1:N:211:ILE:HD11	1.68	0.73
3:C:7:GLU:O	3:C:11:ARG:HG2	1.88	0.73
3:C:3:THR:CG2	3:C:7:GLU:HB2	2.18	0.72
3:P:141:SER:HB2	17:Q:210:PEE:H25	1.72	0.70
1:N:297:ARG:HH22	9:N:1002:OAA:H22	1.56	0.70
4:D:73:TYR:CD1	5:D:245:UNL:C2	2.75	0.69
1:N:112:ASN:ND2	2:O:138:GLY:H	1.91	0.67
1:A:593:LYS:HD2	5:A:1017:UNL:C2	2.25	0.67
2:O:18:ARG:NH2	2:O:56:ASP:OD2	2.28	0.67
1:A:216:TYR:H	1:A:366:ASN:ND2	1.93	0.67
1:A:486:GLY:O	1:A:490:GLN:HG3	1.96	0.66
1:N:486:GLY:O	1:N:490:GLN:HG3	1.96	0.65
1:A:18:GLU:OE1	1:A:438:VAL:HG11	1.96	0.65
1:N:277:ASN:O	18:N:2286:HOH:O	2.15	0.65
1:A:72:GLU:OE1	1:A:144:HIS:HD2	1.81	0.64
1:N:72:GLU:OE1	1:N:144:HIS:HD2	1.80	0.64
1:N:84:VAL:N	18:N:2096:HOH:O	2.30	0.64
2:B:18:ARG:NH2	2:B:56:ASP:OD2	2.31	0.64
3:C:43:ARG:CZ	16:C:144:CBE:H62	2.27	0.64
1:N:216:TYR:H	1:N:366:ASN:ND2	1.96	0.64
1:N:276:ILE:HB	18:N:2286:HOH:O	1.98	0.63
5:A:1003:UNL:O5	5:A:1003:UNL:O3	2.17	0.63
2:O:214:ARG:HH12	4:Q:53:GLN:NE2	1.97	0.62
1:N:60:ALA:HB3	1:N:154:GLY:HA3	1.82	0.62
1:N:121:GLU:HG2	18:N:2133:HOH:O	1.99	0.62
1:N:276:ILE:HD12	18:N:2286:HOH:O	1.99	0.62
3:C:37:ALA:O	3:C:40:ILE:HG12	2.00	0.61
3:P:37:ALA:O	3:P:40:ILE:HG12	2.01	0.61
2:B:214:ARG:HH12	4:D:53:GLN:NE2	1.98	0.60
1:A:573:ARG:HD3	18:A:2496:HOH:O	2.00	0.60
4:Q:63:THR:HB	4:Q:64:PRO:HD3	1.82	0.60
1:N:207:LYS:NZ	1:N:436:GLU:HB2	2.16	0.60
4:D:22:GLY:O	4:D:25:PRO:HD2	2.01	0.60
4:D:63:THR:HB	4:D:64:PRO:HD3	1.83	0.59
3:C:34:LEU:HB3	3:C:35:PRO:HD3	1.83	0.59
1:N:401:ALA:N	1:N:402:SER:HA	2.18	0.59
3:P:69:HIS:O	3:P:73:VAL:HG23	2.03	0.59
1:A:401:ALA:N	1:A:402:SER:HA	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:HIS:O	3:C:73:VAL:HG23	2.02	0.59
4:Q:22:GLY:O	4:Q:25:PRO:HD2	2.02	0.59
1:N:18:GLU:OE1	1:N:438:VAL:HG11	2.02	0.58
3:C:34:LEU:HD23	18:C:2089:HOH:O	2.04	0.58
13:O:1009:GOL:H32	18:O:2227:HOH:O	2.02	0.58
1:A:297:ARG:HH22	9:A:1002:OAA:C1	2.17	0.58
8:N:1001:FAD:C4	9:N:1002:OAA:H21	2.33	0.57
3:P:34:LEU:HB3	3:P:35:PRO:HD3	1.84	0.57
1:A:207:LYS:NZ	1:A:436:GLU:HB2	2.20	0.57
5:A:1003:UNL:O5	5:A:1003:UNL:O2	2.21	0.57
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.86	0.57
2:O:21:PRO:O	2:O:24:PRO:HD3	2.05	0.56
1:N:207:LYS:HZ1	1:N:436:GLU:HB2	1.71	0.56
16:P:202:CBE:O9	16:P:202:CBE:H16	2.04	0.56
1:A:112:ASN:HD22	2:B:138:GLY:N	1.93	0.56
16:C:144:CBE:O9	16:C:144:CBE:H16	2.04	0.56
3:P:4:THR:OG1	3:P:7:GLU:HG3	2.05	0.56
3:P:55:LEU:O	3:P:58:VAL:HG12	2.06	0.56
3:P:106:LEU:O	3:P:110:MET:HG3	2.05	0.56
5:A:1013:UNL:C2	18:A:2546:HOH:O	2.53	0.55
3:C:106:LEU:O	3:C:110:MET:HG3	2.06	0.55
1:A:417:LEU:HD21	8:A:1001:FAD:H5'2	1.88	0.55
8:A:1001:FAD:C4	9:A:1002:OAA:H21	2.36	0.55
1:N:491:GLU:HG3	5:N:1019:UNL:C2	2.36	0.55
1:N:112:ASN:HD22	2:O:138:GLY:N	2.00	0.55
1:N:263:LEU:HG	1:N:264:ILE:N	2.22	0.55
1:A:326:HIS:HD2	5:A:1021:UNL:C2	2.19	0.55
3:C:55:LEU:O	3:C:58:VAL:HG12	2.07	0.55
5:B:277:UNL:C2	18:B:2290:HOH:O	2.55	0.55
3:C:68:PRO:HA	4:D:99:MET:HE1	1.88	0.54
4:D:36:ASP:OD2	4:D:93:ILE:N	2.39	0.54
18:N:2260:HOH:O	2:O:66:ARG:HB3	2.07	0.54
1:A:263:LEU:HG	1:A:264:ILE:N	2.21	0.54
2:B:66:ARG:NH1	2:B:66:ARG:CG	2.71	0.54
3:C:101:ASN:ND2	3:C:104:ARG:HH11	2.04	0.54
1:N:507:LYS:HE3	18:N:2410:HOH:O	2.07	0.54
4:Q:3:SER:HA	18:Q:2003:HOH:O	2.08	0.54
4:Q:36:ASP:OD2	4:Q:93:ILE:N	2.41	0.54
3:C:42:HIS:HD2	3:C:101:ASN:HB3	1.73	0.54
2:O:198:TYR:O	2:O:202:ARG:HG3	2.08	0.54
2:O:223:ARG:HA	3:P:116:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:THR:OG1	3:C:7:GLU:HG3	2.06	0.53
1:A:297:ARG:NH2	9:A:1002:OAA:H22	2.21	0.53
3:P:47:VAL:O	3:P:51:LEU:HG	2.09	0.53
2:O:223:ARG:HD3	18:O:2265:HOH:O	2.09	0.53
1:A:331:GLN:HB3	18:A:2324:HOH:O	2.09	0.53
3:P:3:THR:HG22	3:P:7:GLU:HB2	1.89	0.53
1:N:297:ARG:HH22	9:N:1002:OAA:C1	2.21	0.52
2:B:66:ARG:HH11	2:B:66:ARG:CG	2.23	0.52
1:A:50:LEU:HD21	1:A:228:THR:HG21	1.91	0.52
3:C:47:VAL:O	3:C:51:LEU:HG	2.09	0.52
3:C:26:HIS:CG	3:C:27:ILE:H	2.27	0.52
2:O:66:ARG:HB2	2:O:66:ARG:NH1	2.07	0.52
3:P:42:HIS:HD2	3:P:101:ASN:HB3	1.74	0.52
3:C:3:THR:HG23	3:C:7:GLU:HB2	1.92	0.51
2:B:58:THR:HB	18:B:2084:HOH:O	2.09	0.51
2:O:66:ARG:NH1	2:O:66:ARG:CG	2.73	0.51
2:O:27:LYS:HD3	18:O:2030:HOH:O	2.09	0.51
1:N:155:HIS:HD2	18:O:2112:HOH:O	1.94	0.51
3:P:26:HIS:CG	3:P:27:ILE:H	2.29	0.51
1:N:50:LEU:HD21	1:N:228:THR:HG21	1.93	0.51
1:N:496:LEU:HD12	1:N:536:ILE:HG21	1.92	0.51
2:B:214:ARG:NH2	4:D:53:GLN:HE22	2.04	0.51
1:N:280:GLY:CA	18:N:2286:HOH:O	2.44	0.50
1:N:417:LEU:HD21	8:N:1001:FAD:H5'2	1.92	0.50
2:O:66:ARG:HH11	2:O:66:ARG:CG	2.23	0.50
4:Q:73:TYR:CD1	5:Q:288:UNL:C2	2.94	0.50
3:C:70:TYR:O	3:C:74:VAL:HG23	2.12	0.50
1:N:87:SER:HB2	1:N:405:GLY:HA3	1.93	0.50
3:P:3:THR:HG23	3:P:7:GLU:OE1	2.11	0.50
3:P:101:ASN:ND2	3:P:104:ARG:HH11	2.05	0.50
18:C:2021:HOH:O	3:P:40:ILE:HD11	2.11	0.49
2:B:223:ARG:HA	3:C:116:LEU:HD21	1.94	0.49
1:N:83:THR:C	18:N:2096:HOH:O	2.51	0.49
2:O:214:ARG:NH2	4:Q:53:GLN:HE22	2.06	0.49
1:A:87:SER:HB2	1:A:405:GLY:HA3	1.94	0.49
2:B:198:TYR:O	2:B:202:ARG:HG3	2.12	0.49
3:P:70:TYR:O	3:P:74:VAL:HG23	2.11	0.49
5:B:1005:UNL:O5	5:B:1005:UNL:O3	2.30	0.49
1:A:496:LEU:HD12	1:A:536:ILE:HG21	1.95	0.49
4:D:44:THR:HG21	4:D:80:PHE:HB2	1.95	0.49
1:N:326:HIS:HE1	18:N:2323:HOH:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:THR:HG22	3:C:7:GLU:HB2	1.91	0.49
3:P:3:THR:HG23	3:P:7:GLU:HB2	1.92	0.49
1:A:220:TYR:CG	1:A:363:VAL:HG21	2.48	0.48
1:N:83:THR:HB	18:N:2096:HOH:O	2.12	0.48
4:Q:44:THR:HG21	4:Q:80:PHE:HB2	1.95	0.48
1:N:431:THR:HG22	1:N:432:CYS:SG	2.53	0.48
3:C:3:THR:HG23	3:C:7:GLU:OE1	2.12	0.48
1:A:431:THR:HG22	1:A:432:CYS:SG	2.54	0.48
4:D:33:PRO:HG2	18:D:2022:HOH:O	2.13	0.48
1:A:155:HIS:HD2	18:B:2105:HOH:O	1.97	0.48
18:B:2141:HOH:O	4:D:4:LYS:HE3	2.14	0.48
1:A:61:GLN:OE1	1:A:265:THR:HB	2.14	0.48
1:A:369:GLY:HA2	18:A:2259:HOH:O	2.13	0.47
4:Q:27:ALA:HB1	17:Q:210:PEE:H63	1.96	0.47
1:A:205:ARG:NH2	1:A:438:VAL:HG13	2.29	0.47
1:A:453:LEU:C	1:A:453:LEU:HD23	2.35	0.47
3:P:67:PHE:HB3	3:P:68:PRO:HD3	1.96	0.47
1:N:205:ARG:NH2	1:N:438:VAL:HG13	2.29	0.47
2:O:155:LEU:CD1	2:O:192:ILE:HD11	2.45	0.47
2:B:245:TYR:O	4:D:4:LYS:NZ	2.48	0.47
1:N:253:HIS:NE2	1:N:263:LEU:HD11	2.29	0.47
1:N:515:TRP:CD1	2:O:108:VAL:HG11	2.50	0.47
3:C:67:PHE:HB3	3:C:68:PRO:HD3	1.96	0.47
2:O:245:TYR:O	4:Q:4:LYS:NZ	2.48	0.47
13:C:294:GOL:O3	4:D:93:ILE:HG23	2.15	0.47
1:N:61:GLN:OE1	1:N:265:THR:HB	2.15	0.47
1:N:174:VAL:HG12	1:N:175:GLU:HG3	1.97	0.47
1:A:515:TRP:CD1	2:B:108:VAL:HG11	2.50	0.46
4:D:73:TYR:CE1	5:D:245:UNL:C2	2.98	0.46
3:P:116:LEU:HD12	3:P:116:LEU:HA	1.81	0.46
2:B:155:LEU:HD11	2:B:192:ILE:HD11	1.98	0.46
2:B:214:ARG:HH12	4:D:53:GLN:HE21	1.64	0.46
2:O:155:LEU:HD11	2:O:192:ILE:HD11	1.98	0.46
1:A:253:HIS:NE2	1:A:263:LEU:HD11	2.31	0.46
3:C:88:LYS:NZ	3:C:140:ILE:HG12	2.30	0.46
2:B:66:ARG:HB2	2:B:66:ARG:NH1	2.09	0.46
3:P:43:ARG:CZ	16:P:202:CBE:H62	2.46	0.46
1:A:253:HIS:O	1:A:361:PRO:HA	2.16	0.46
3:C:68:PRO:HA	4:D:99:MET:CE	2.45	0.46
18:O:2042:HOH:O	3:P:6:LYS:HE2	2.15	0.46
1:N:124:LYS:NZ	18:N:2143:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:462:THR:HG21	18:N:2088:HOH:O	2.16	0.46
3:P:34:LEU:HD23	18:P:2074:HOH:O	2.16	0.46
16:C:144:CBE:O9	16:C:144:CBE:C16	2.63	0.45
3:C:65:GLU:HG3	3:C:69:HIS:CD2	2.51	0.45
1:N:375:LYS:HE2	18:N:2390:HOH:O	2.15	0.45
2:B:98:LYS:HE3	18:C:2025:HOH:O	2.16	0.45
1:N:453:LEU:C	1:N:453:LEU:HD23	2.37	0.45
2:O:104:HIS:O	13:O:1009:GOL:H12	2.17	0.45
1:A:197:GLU:HB2	18:A:2196:HOH:O	2.16	0.45
3:C:101:ASN:ND2	3:C:104:ARG:HD3	2.32	0.45
1:N:220:TYR:CG	1:N:363:VAL:HG21	2.52	0.45
1:A:381:HIS:ND1	1:A:386:ASP:OD1	2.46	0.45
2:O:191:MET:CE	2:O:203:LEU:HD21	2.46	0.45
1:N:381:HIS:ND1	1:N:386:ASP:OD1	2.47	0.44
2:B:155:LEU:CD1	2:B:192:ILE:HD11	2.46	0.44
2:B:121:GLN:NE2	2:B:171:TYR:OH	2.49	0.44
1:N:72:GLU:OE1	1:N:144:HIS:CD2	2.66	0.44
2:O:123:LYS:NZ	3:P:3:THR:O	2.47	0.44
3:P:63:LEU:HA	3:P:64:PRO:HD3	1.81	0.44
16:P:202:CBE:O9	16:P:202:CBE:C16	2.63	0.44
1:A:155:HIS:HE1	2:B:156:TYR:O	2.00	0.44
2:B:191:MET:CE	2:B:203:LEU:HD21	2.48	0.44
3:P:120:GLU:HG3	18:P:2075:HOH:O	2.18	0.44
1:A:174:VAL:HG12	1:A:175:GLU:HG3	2.00	0.44
3:C:116:LEU:HD12	3:C:116:LEU:HA	1.83	0.44
1:N:567:LEU:HD23	1:N:570:GLN:NE2	2.32	0.44
1:A:72:GLU:OE1	1:A:144:HIS:CD2	2.67	0.43
1:N:463:ILE:O	1:N:506:LEU:HA	2.18	0.43
3:P:65:GLU:HG3	3:P:69:HIS:CD2	2.53	0.43
1:A:567:LEU:HD23	1:A:570:GLN:NE2	2.33	0.43
1:N:60:ALA:HA	8:N:1001:FAD:N5	2.34	0.43
1:N:189:ARG:HH11	1:N:189:ARG:HG2	1.83	0.43
3:P:42:HIS:CD2	3:P:101:ASN:HB3	2.53	0.43
1:A:121:GLU:HG2	18:A:2126:HOH:O	2.18	0.43
1:A:213:THR:OG1	1:A:233:GLY:HA3	2.18	0.43
1:N:71:MET:HG2	1:N:127:GLN:HB2	2.00	0.43
3:C:42:HIS:CD2	3:C:101:ASN:HB3	2.53	0.43
1:N:155:HIS:CD2	18:O:2112:HOH:O	2.71	0.43
1:A:220:TYR:CD2	1:A:363:VAL:HG21	2.54	0.43
1:N:268:CYS:HB3	1:N:325:LEU:HD21	2.00	0.43
2:B:53:ASN:HA	18:B:2071:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:96:ILE:CG2	18:N:2096:HOH:O	2.46	0.43
1:N:297:ARG:NH2	9:N:1002:OAA:H22	2.28	0.43
1:A:268:CYS:HB3	1:A:325:LEU:HD21	2.00	0.43
2:O:214:ARG:HH12	4:Q:53:GLN:HE21	1.65	0.43
3:P:101:ASN:ND2	3:P:104:ARG:HD3	2.34	0.43
1:A:39:GLU:HB3	1:A:168:TYR:CE2	2.54	0.43
1:A:189:ARG:HG2	1:A:189:ARG:HH11	1.83	0.43
3:C:11:ARG:HG3	18:C:2006:HOH:O	2.18	0.43
1:A:189:ARG:NE	18:A:2392:HOH:O	2.30	0.42
4:D:53:GLN:NE2	4:D:53:GLN:HA	2.34	0.42
2:O:98:LYS:HE3	18:P:2021:HOH:O	2.18	0.42
4:Q:53:GLN:NE2	4:Q:53:GLN:HA	2.34	0.42
1:N:60:ALA:HA	8:N:1001:FAD:C5X	2.49	0.42
1:N:253:HIS:O	1:N:361:PRO:HA	2.18	0.42
1:A:60:ALA:HA	8:A:1001:FAD:C5X	2.50	0.42
3:C:29:ILE:C	3:C:29:ILE:HD12	2.40	0.42
3:C:43:ARG:HE	15:C:143:HEM:CGA	2.32	0.42
3:P:11:ARG:HG3	18:P:2007:HOH:O	2.19	0.41
1:A:297:ARG:HH22	9:A:1002:OAA:C3	2.34	0.41
2:B:123:LYS:NZ	3:C:3:THR:O	2.51	0.41
1:A:71:MET:HG2	1:A:127:GLN:HB2	2.01	0.41
1:N:382:VAL:O	1:N:385:GLU:HG3	2.20	0.41
3:P:55:LEU:HA	3:P:55:LEU:HD23	1.84	0.41
1:A:382:VAL:O	1:A:385:GLU:HG3	2.20	0.41
3:C:93:PHE:HB3	3:C:94:PRO:CD	2.50	0.41
3:P:29:ILE:HD12	3:P:29:ILE:C	2.41	0.41
1:N:39:GLU:HB3	1:N:168:TYR:CE2	2.56	0.41
1:N:213:THR:OG1	1:N:233:GLY:HA3	2.20	0.41
1:A:60:ALA:HA	8:A:1001:FAD:N5	2.35	0.41
1:A:207:LYS:HZ1	1:A:436:GLU:HB2	1.85	0.41
1:N:305:THR:O	1:N:309:ARG:HG3	2.20	0.41
3:P:55:LEU:HA	3:P:58:VAL:HG12	2.02	0.41
3:C:138:ALA:C	3:C:140:ILE:H	2.24	0.40
4:D:27:ALA:HA	4:D:35:VAL:HG11	2.04	0.40
1:N:182:LEU:HD23	1:N:182:LEU:HA	1.88	0.40
4:Q:87:ASN:HA	4:Q:92:GLY:HA2	2.04	0.40
1:A:63:GLY:HA2	1:A:153:THR:HG21	2.04	0.40
2:B:227:LYS:HE3	18:B:2273:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	611/621 (98%)	590 (97%)	21 (3%)	0	100	100
1	N	610/621 (98%)	590 (97%)	20 (3%)	0	100	100
2	B	237/252 (94%)	228 (96%)	8 (3%)	1 (0%)	34	32
2	O	237/252 (94%)	229 (97%)	7 (3%)	1 (0%)	34	32
3	C	138/141 (98%)	135 (98%)	2 (1%)	1 (1%)	22	18
3	P	138/141 (98%)	135 (98%)	2 (1%)	1 (1%)	22	18
4	D	99/103 (96%)	97 (98%)	2 (2%)	0	100	100
4	Q	99/103 (96%)	97 (98%)	2 (2%)	0	100	100
All	All	2169/2234 (97%)	2101 (97%)	64 (3%)	4 (0%)	47	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	66	ARG
2	O	66	ARG
3	C	140	ILE
3	P	140	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	498/506 (98%)	495 (99%)	3 (1%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	497/506 (98%)	493 (99%)	4 (1%)	81	86
2	B	214/219 (98%)	211 (99%)	3 (1%)	67	73
2	O	214/219 (98%)	211 (99%)	3 (1%)	67	73
3	C	118/119 (99%)	117 (99%)	1 (1%)	81	86
3	P	118/119 (99%)	117 (99%)	1 (1%)	81	86
4	D	78/79 (99%)	75 (96%)	3 (4%)	33	34
4	Q	78/79 (99%)	75 (96%)	3 (4%)	33	34
All	All	1815/1846 (98%)	1794 (99%)	21 (1%)	71	77

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

Mol	Chain	Res	Type
1	A	72	GLU
1	A	73	ASP
1	A	130	PHE
2	B	63	ARG
2	B	189	ARG
2	B	229	LEU
3	C	11	ARG
4	D	14	ARG
4	D	36	ASP
4	D	101	TRP
1	N	10	THR
1	N	72	GLU
1	N	73	ASP
1	N	130	PHE
2	O	63	ARG
2	O	189	ARG
2	O	229	LEU
3	P	11	ARG
4	Q	14	ARG
4	Q	36	ASP
4	Q	101	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN

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Mol	Chain	Res	Type
1	A	112	ASN
1	A	144	HIS
1	A	155	HIS
1	A	185	ASN
1	A	326	HIS
1	A	366	ASN
1	A	383	ASN
1	A	534	GLN
1	A	571	GLN
2	B	121	GLN
3	C	26	HIS
3	C	42	HIS
3	C	69	HIS
3	C	101	ASN
4	D	9	HIS
4	D	53	GLN
1	N	43	ASN
1	N	112	ASN
1	N	144	HIS
1	N	155	HIS
1	N	185	ASN
1	N	366	ASN
1	N	383	ASN
1	N	534	GLN
1	N	571	GLN
2	O	121	GLN
3	P	26	HIS
3	P	42	HIS
3	P	69	HIS
3	P	101	ASN
4	Q	9	HIS
4	Q	53	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 122 ligands modelled in this entry, 95 are unknown and 4 are monoatomic - leaving 23 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	$\#\|Z\| > 2$
15	HEM	C	143	4,3	40,48,50	1.43	4 (10%)	46,80,82	1.50	8 (17%)
11	SF4	B	1003	2	0,12,12	-	-	-		
13	GOL	C	294	-	5,5,5	1.21	0	5,5,5	0.59	0
13	GOL	P	208	-	5,5,5	1.27	0	5,5,5	0.61	0
16	CBE	P	202	-	16,17,17	1.06	1 (6%)	16,22,22	1.86	2 (12%)
9	OAA	A	1002	-	8,8,8	5.49	3 (37%)	9,10,10	1.80	3 (33%)
14	BHG	P	204	-	18,18,18	1.58	3 (16%)	23,23,23	0.68	0
14	BHG	C	142	-	18,18,18	1.92	5 (27%)	23,23,23	0.76	0
9	OAA	N	1002	-	8,8,8	6.00	4 (50%)	9,10,10	1.83	3 (33%)
12	F3S	O	1004	2	0,9,9	-	-	-		
13	GOL	O	1009	-	5,5,5	1.05	0	5,5,5	0.58	0
8	FAD	A	1001	1	53,58,58	2.00	15 (28%)	68,89,89	1.73	17 (25%)
16	CBE	C	144	-	16,17,17	1.07	1 (6%)	16,22,22	1.86	2 (12%)
8	FAD	N	1001	1	53,58,58	2.09	17 (32%)	68,89,89	1.72	14 (20%)
11	SF4	O	1003	2	0,12,12	-	-	-		
10	FES	B	1002	2	0,4,4	-	-	-		
13	GOL	B	1010	-	5,5,5	1.09	0	5,5,5	0.52	0
17	PEE	D	109	-	22,22,50	1.49	4 (18%)	18,20,55	1.04	2 (11%)
7	AZI	A	623	-	0,2,2	-	-	0,1,1	-	-
17	PEE	Q	210	-	22,22,50	1.47	4 (18%)	18,20,55	1.04	2 (11%)
15	HEM	P	201	4,3	40,48,50	1.55	6 (15%)	46,80,82	1.44	6 (13%)
10	FES	O	1002	2	0,4,4	-	-	-		
12	F3S	B	1004	2	0,9,9	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	HEM	C	143	4,3	-	3/10/50/54	-
11	SF4	B	1003	2	-	-	0/6/5/5
13	GOL	C	294	-	-	2/4/4/4	-
13	GOL	P	208	-	-	2/4/4/4	-
16	CBE	P	202	-	-	2/6/19/19	0/1/2/2
9	OAA	A	1002	-	-	4/8/8/8	-
14	BHG	P	204	-	1/1/5/5	2/9/29/29	0/1/1/1
14	BHG	C	142	-	1/1/5/5	3/9/29/29	0/1/1/1
9	OAA	N	1002	-	-	4/8/8/8	-
12	F3S	O	1004	2	-	-	0/3/3/3
13	GOL	O	1009	-	-	4/4/4/4	-
8	FAD	A	1001	1	-	9/30/50/50	0/6/6/6
16	CBE	C	144	-	-	2/6/19/19	0/1/2/2
8	FAD	N	1001	1	-	10/30/50/50	0/6/6/6
11	SF4	O	1003	2	-	-	0/6/5/5
10	FES	B	1002	2	-	-	0/1/1/1
13	GOL	B	1010	-	-	1/4/4/4	-
17	PEE	D	109	-	-	10/18/18/54	-
17	PEE	Q	210	-	-	14/18/18/54	-
15	HEM	P	201	4,3	-	3/10/50/54	-
10	FES	O	1002	2	-	-	0/1/1/1
12	F3S	B	1004	2	-	-	0/3/3/3

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	1002	OAA	O3-C3	13.90	1.51	1.23
9	A	1002	OAA	O3-C3	12.07	1.47	1.23
9	A	1002	OAA	C2-C1	-8.44	1.38	1.51
9	N	1002	OAA	C2-C1	-7.29	1.39	1.51
8	A	1001	FAD	C4X-N5	5.68	1.41	1.30
8	N	1001	FAD	C4X-N5	5.48	1.41	1.30
14	C	142	BHG	O1-C1	5.32	1.49	1.40
15	P	201	HEM	CAB-C3B	-5.32	1.39	1.50
9	N	1002	OAA	C3-C4	-5.23	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	143	HEM	CAB-C3B	-5.10	1.40	1.50
8	A	1001	FAD	C2A-N3A	4.57	1.39	1.32
8	N	1001	FAD	C10-N10	4.49	1.47	1.37
8	A	1001	FAD	C10-N10	4.34	1.46	1.37
8	N	1001	FAD	PA-O1A	-4.24	1.35	1.50
14	P	204	BHG	O1-C1	4.21	1.47	1.40
17	D	109	PEE	C39-C38	4.01	1.55	1.31
8	N	1001	FAD	C2A-N3A	3.93	1.38	1.32
8	A	1001	FAD	PA-O2A	-3.91	1.37	1.55
8	A	1001	FAD	PA-O1A	-3.90	1.37	1.50
17	Q	210	PEE	C39-C38	3.90	1.54	1.31
15	P	201	HEM	CAC-C3C	-3.84	1.42	1.51
8	N	1001	FAD	C6-C5X	3.81	1.46	1.40
17	D	109	PEE	C18-C19	3.79	1.53	1.31
8	N	1001	FAD	PA-O2A	-3.79	1.37	1.55
9	A	1002	OAA	C3-C4	-3.78	1.48	1.53
17	Q	210	PEE	C18-C19	3.59	1.52	1.31
8	A	1001	FAD	C6-C7	3.46	1.44	1.39
8	N	1001	FAD	C9-C9A	3.39	1.45	1.39
15	C	143	HEM	CAC-C3C	-3.37	1.43	1.51
14	C	142	BHG	O5-C1	3.25	1.50	1.41
8	N	1001	FAD	C6-C7	3.22	1.44	1.39
8	N	1001	FAD	C2B-C1B	-3.11	1.49	1.53
8	N	1001	FAD	C2-N3	3.06	1.46	1.39
8	N	1001	FAD	C8-C7	3.05	1.48	1.40
8	A	1001	FAD	C6-C5X	2.92	1.44	1.40
14	P	204	BHG	O5-C1	2.89	1.49	1.41
8	N	1001	FAD	C2A-N1A	2.82	1.39	1.33
8	A	1001	FAD	C8-C7	2.81	1.47	1.40
16	C	144	CBE	C11-N10	-2.78	1.36	1.41
16	P	202	CBE	C11-N10	-2.77	1.36	1.41
8	A	1001	FAD	C9A-C5X	2.75	1.45	1.41
17	Q	210	PEE	C17-C18	-2.68	1.35	1.50
8	A	1001	FAD	C2-N3	2.67	1.45	1.39
8	N	1001	FAD	C4'-C3'	2.62	1.58	1.53
8	A	1001	FAD	C10-N1	2.56	1.38	1.33
8	A	1001	FAD	C2A-N1A	2.51	1.38	1.33
8	N	1001	FAD	C10-N1	2.49	1.38	1.33
17	D	109	PEE	C17-C18	-2.48	1.36	1.50
15	P	201	HEM	C1A-NA	2.42	1.41	1.36
14	C	142	BHG	C4-C5	2.41	1.58	1.53
14	P	204	BHG	C4-C5	2.39	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	201	HEM	CMD-C2D	2.39	1.55	1.50
8	A	1001	FAD	C9-C8	2.38	1.43	1.39
9	N	1002	OAA	O4-C4	2.37	1.28	1.22
8	N	1001	FAD	C4A-N3A	2.33	1.38	1.35
14	C	142	BHG	C3-C2	2.28	1.58	1.52
17	Q	210	PEE	C21-C20	-2.26	1.34	1.49
8	N	1001	FAD	P-O5'	-2.23	1.50	1.59
17	D	109	PEE	C21-C20	-2.21	1.34	1.49
15	C	143	HEM	C1A-NA	2.18	1.40	1.36
14	C	142	BHG	O5-C5	2.15	1.49	1.44
15	P	201	HEM	C4D-ND	-2.08	1.36	1.40
8	N	1001	FAD	C8A-N7A	-2.07	1.31	1.34
15	C	143	HEM	CMD-C2D	2.04	1.55	1.50
8	A	1001	FAD	C2B-C1B	-2.03	1.50	1.53
15	P	201	HEM	CAA-C2A	2.03	1.55	1.52
8	A	1001	FAD	C5A-N7A	-2.00	1.32	1.39

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1001	FAD	N3A-C2A-N1A	-5.99	119.32	128.68
8	N	1001	FAD	N3A-C2A-N1A	-5.85	119.54	128.68
16	C	144	CBE	O7-C2-C1	5.61	116.08	109.32
16	P	202	CBE	O7-C2-C1	5.61	116.07	109.32
15	P	201	HEM	C4B-CHC-C1C	4.76	128.84	122.56
15	C	143	HEM	C4B-CHC-C1C	4.68	128.74	122.56
8	A	1001	FAD	C4-C4X-N5	4.18	124.17	118.23
8	N	1001	FAD	C4-C4X-N5	4.16	124.15	118.23
8	A	1001	FAD	C5X-N5-C4X	3.57	124.02	118.07
8	N	1001	FAD	C5X-N5-C4X	3.52	123.93	118.07
16	P	202	CBE	C11-N10-C8	-3.31	121.79	127.53
16	C	144	CBE	C11-N10-C8	-3.29	121.81	127.53
8	N	1001	FAD	C10-N1-C2	3.14	123.17	116.90
17	Q	210	PEE	C21-C20-C19	3.08	126.79	112.71
17	D	109	PEE	C21-C20-C19	3.03	126.58	112.71
8	A	1001	FAD	C4-N3-C2	-3.00	120.09	125.64
8	N	1001	FAD	C4-N3-C2	-2.99	120.12	125.64
9	A	1002	OAA	O4-C4-C3	-2.96	117.77	121.72
15	C	143	HEM	CAD-C3D-C2D	-2.92	122.43	127.88
8	A	1001	FAD	P-O3P-PA	2.90	142.78	132.83
15	C	143	HEM	C4C-CHD-C1D	2.87	126.35	122.56
9	N	1002	OAA	O3-C3-C4	-2.87	115.28	119.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1001	FAD	C10-N1-C2	2.85	122.61	116.90
15	P	201	HEM	C4C-CHD-C1D	2.84	126.30	122.56
8	N	1001	FAD	C10-C4X-N5	-2.82	118.86	124.86
8	N	1001	FAD	P-O3P-PA	2.82	142.51	132.83
8	N	1001	FAD	C1B-N9A-C4A	-2.79	121.73	126.64
17	D	109	PEE	C16-C17-C18	2.76	128.23	112.43
9	N	1002	OAA	O4-C4-C3	-2.74	118.06	121.72
8	A	1001	FAD	C10-C4X-N5	-2.72	119.09	124.86
8	A	1001	FAD	C1B-N9A-C4A	-2.72	121.86	126.64
15	C	143	HEM	C1D-C2D-C3D	-2.69	104.13	106.96
9	A	1002	OAA	O3-C3-C4	-2.68	115.54	119.43
8	A	1001	FAD	O5'-C5'-C4'	2.68	116.52	109.36
17	Q	210	PEE	C16-C17-C18	2.67	127.75	112.43
8	A	1001	FAD	C1'-C2'-C3'	2.67	117.25	109.79
8	A	1001	FAD	C4X-C4-N3	2.65	119.93	113.19
15	P	201	HEM	CAD-C3D-C2D	-2.65	122.94	127.88
8	N	1001	FAD	O5'-C5'-C4'	2.62	116.34	109.36
15	C	143	HEM	C4C-C3C-C2C	-2.56	105.09	106.85
15	P	201	HEM	CHA-C4D-ND	-2.55	121.23	124.38
8	N	1001	FAD	C1'-C2'-C3'	2.50	116.77	109.79
8	N	1001	FAD	C4X-C4-N3	2.46	119.43	113.19
15	C	143	HEM	CAD-C3D-C4D	2.43	128.90	124.66
15	P	201	HEM	C1D-C2D-C3D	-2.41	104.42	106.96
8	A	1001	FAD	C4'-C3'-C2'	-2.37	108.44	113.36
9	A	1002	OAA	O5-C4-C3	2.36	120.42	113.97
15	C	143	HEM	CHA-C4D-ND	-2.35	121.48	124.38
8	N	1001	FAD	C4'-C3'-C2'	-2.33	108.51	113.36
15	P	201	HEM	CAD-C3D-C4D	2.29	128.66	124.66
8	N	1001	FAD	C7M-C7-C6	-2.26	115.31	119.49
9	N	1002	OAA	O5-C4-C3	2.18	119.94	113.97
8	A	1001	FAD	C7M-C7-C6	-2.18	115.46	119.49
8	A	1001	FAD	O3'-C3'-C2'	-2.17	103.57	108.81
8	A	1001	FAD	C8M-C8-C7	2.16	125.17	120.74
8	A	1001	FAD	C9A-C5X-N5	-2.15	120.10	122.43
15	C	143	HEM	C2D-C1D-ND	2.13	112.44	109.88
8	N	1001	FAD	C8M-C8-C7	2.05	124.93	120.74
8	A	1001	FAD	C8M-C8-C9	-2.00	115.79	119.49

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	C	142	BHG	C4

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Mol	Chain	Res	Type	Atom
14	P	204	BHG	C4

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1001	FAD	N10-C1'-C2'-O2'
8	A	1001	FAD	N10-C1'-C2'-C3'
8	A	1001	FAD	O4'-C4'-C5'-O5'
8	A	1001	FAD	C5'-O5'-P-O1P
8	A	1001	FAD	C5'-O5'-P-O2P
8	N	1001	FAD	N10-C1'-C2'-O2'
8	N	1001	FAD	N10-C1'-C2'-C3'
8	N	1001	FAD	O4'-C4'-C5'-O5'
8	N	1001	FAD	C5'-O5'-P-O1P
8	N	1001	FAD	C5'-O5'-P-O2P
8	N	1001	FAD	PA-O3P-P-O5'
9	A	1002	OAA	O3-C3-C4-O4
9	A	1002	OAA	O3-C3-C4-O5
9	A	1002	OAA	C2-C3-C4-O5
9	N	1002	OAA	O3-C3-C4-O4
9	N	1002	OAA	O3-C3-C4-O5
9	N	1002	OAA	C2-C3-C4-O4
9	N	1002	OAA	C2-C3-C4-O5
13	C	294	GOL	C1-C2-C3-O3
17	D	109	PEE	C18-C19-C20-C21
17	D	109	PEE	C17-C18-C19-C20
17	Q	210	PEE	C17-C18-C19-C20
14	C	142	BHG	C2'-C3'-C4'-C5'
17	D	109	PEE	C32-C33-C34-C35
17	Q	210	PEE	C11-C12-C13-C14
17	Q	210	PEE	C32-C33-C34-C35
17	Q	210	PEE	C13-C14-C15-C16
13	B	1010	GOL	C1-C2-C3-O3
13	O	1009	GOL	O1-C1-C2-C3
13	O	1009	GOL	C1-C2-C3-O3
13	P	208	GOL	C1-C2-C3-O3
17	Q	210	PEE	C12-C13-C14-C15
14	C	142	BHG	C1'-C2'-C3'-C4'
17	D	109	PEE	C33-C34-C35-C36
13	C	294	GOL	O2-C2-C3-O3
13	O	1009	GOL	O2-C2-C3-O3
17	D	109	PEE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
17	Q	210	PEE	C35-C36-C37-C38
8	A	1001	FAD	C3'-C4'-C5'-O5'
8	N	1001	FAD	C3'-C4'-C5'-O5'
17	Q	210	PEE	C14-C15-C16-C17
17	Q	210	PEE	C15-C16-C17-C18
17	Q	210	PEE	C30-C31-C32-C33
16	C	144	CBE	C2-C3-C8-O9
16	P	202	CBE	C2-C3-C8-O9
16	C	144	CBE	C2-C3-C8-N10
16	P	202	CBE	C2-C3-C8-N10
17	Q	210	PEE	C33-C34-C35-C36
14	C	142	BHG	C3'-C4'-C5'-C6'
17	D	109	PEE	C34-C35-C36-C37
17	Q	210	PEE	C34-C35-C36-C37
14	P	204	BHG	C2'-C3'-C4'-C5'
8	A	1001	FAD	PA-O3P-P-O5'
17	Q	210	PEE	C38-C39-C40-C41
17	D	109	PEE	C31-C32-C33-C34
13	P	208	GOL	O2-C2-C3-O3
9	A	1002	OAA	C2-C3-C4-O4
15	C	143	HEM	C2A-CAA-CBA-CGA
15	P	201	HEM	C2A-CAA-CBA-CGA
13	O	1009	GOL	O1-C1-C2-O2
17	D	109	PEE	C10-C11-C12-C13
17	D	109	PEE	C12-C13-C14-C15
15	P	201	HEM	CAD-CBD-CGD-O2D
17	Q	210	PEE	C37-C38-C39-C40
17	D	109	PEE	C15-C16-C17-C18
15	C	143	HEM	CAD-CBD-CGD-O2D
8	A	1001	FAD	O4B-C4B-C5B-O5B
15	C	143	HEM	CAD-CBD-CGD-O1D
17	Q	210	PEE	C16-C17-C18-C19
15	P	201	HEM	CAD-CBD-CGD-O1D
8	A	1001	FAD	C5'-O5'-P-O3P
8	N	1001	FAD	C5'-O5'-P-O3P
14	P	204	BHG	C1'-C2'-C3'-C4'
8	N	1001	FAD	O4B-C4B-C5B-O5B
8	N	1001	FAD	PA-O3P-P-O1P

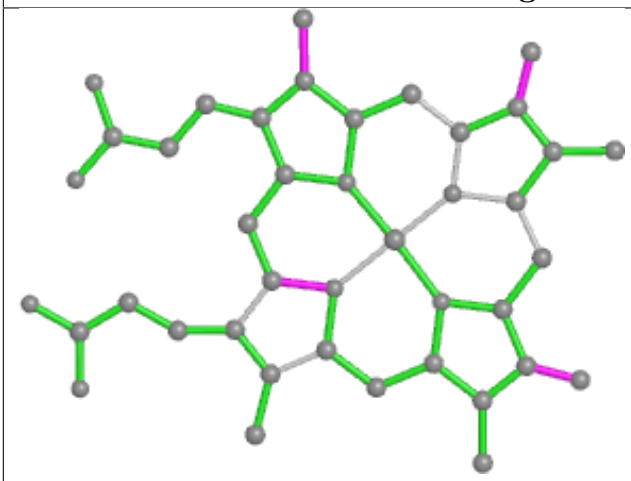
There are no ring outliers.

10 monomers are involved in 29 short contacts:

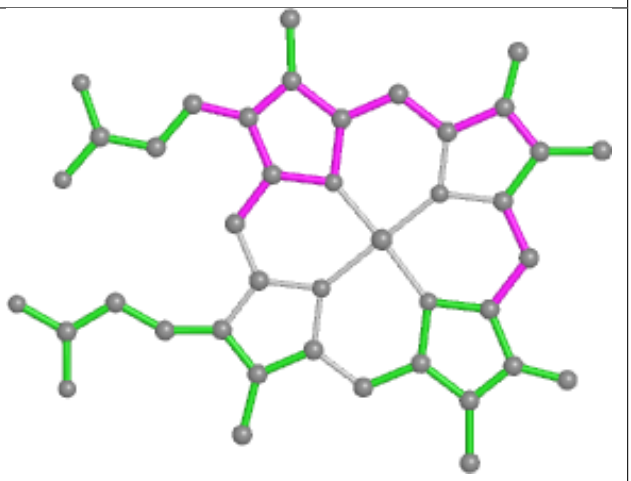
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	143	HEM	1	0
13	C	294	GOL	1	0
16	P	202	CBE	3	0
9	A	1002	OAA	6	0
9	N	1002	OAA	5	0
13	O	1009	GOL	2	0
8	A	1001	FAD	4	0
16	C	144	CBE	3	0
8	N	1001	FAD	4	0
17	Q	210	PEE	2	0

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

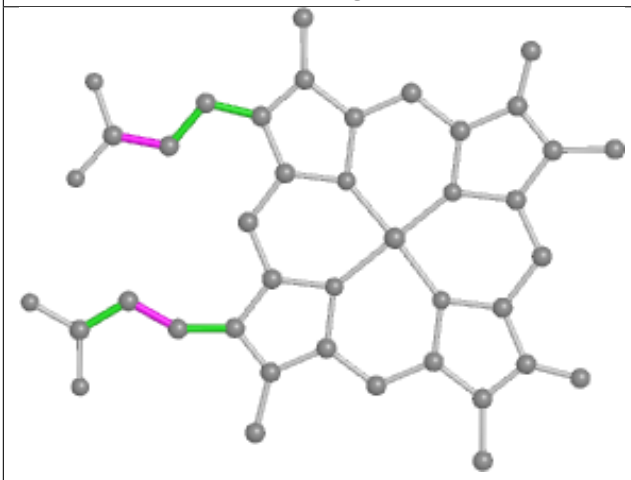
Ligand HEM C 143



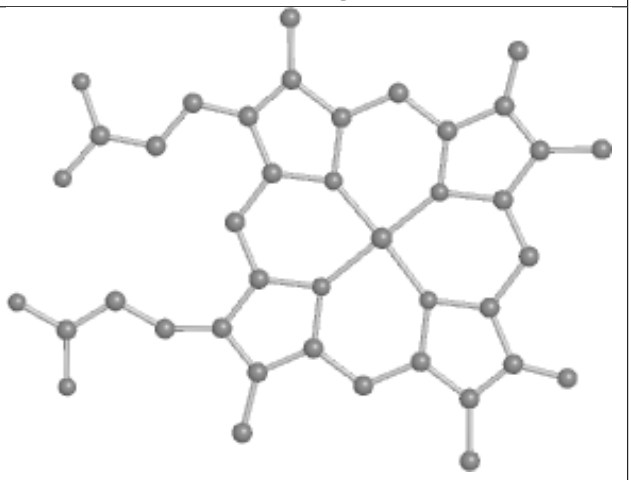
Bond lengths



Bond angles

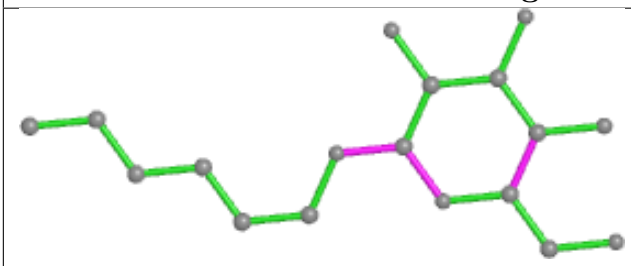


Torsions

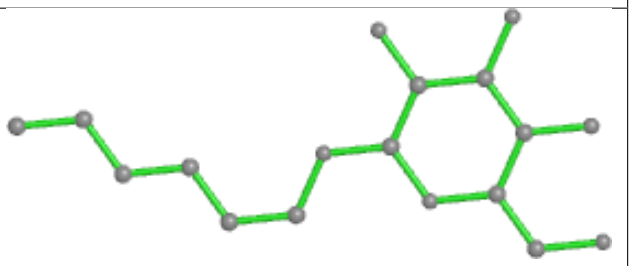


Rings

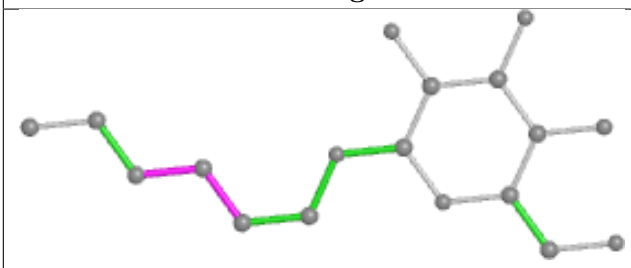
Ligand BHG P 204



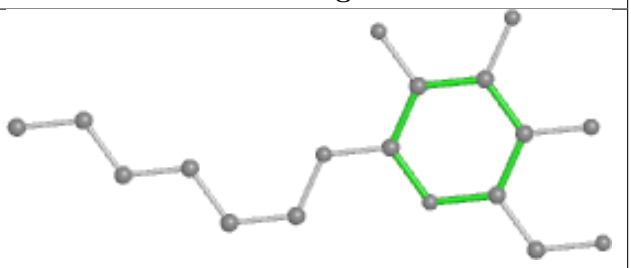
Bond lengths



Bond angles

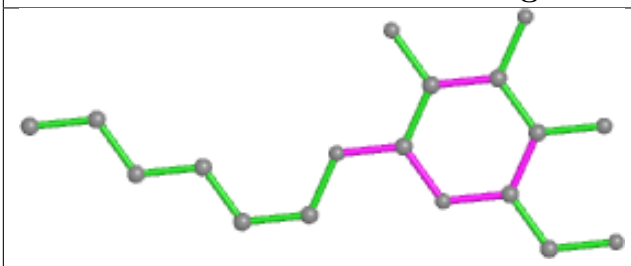


Torsions

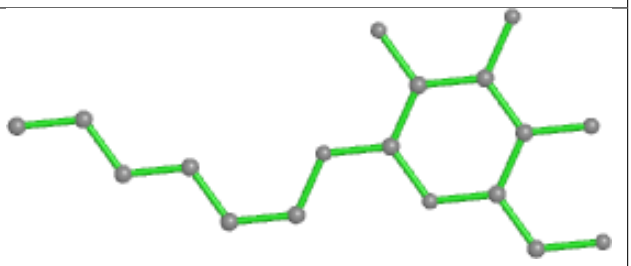


Rings

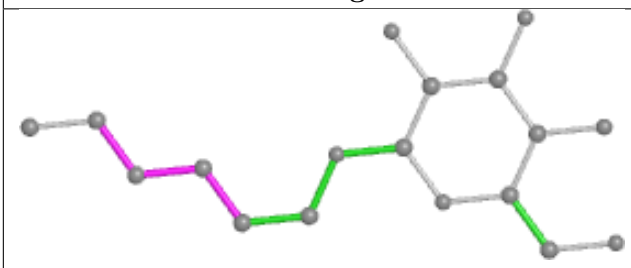
Ligand BHG C 142



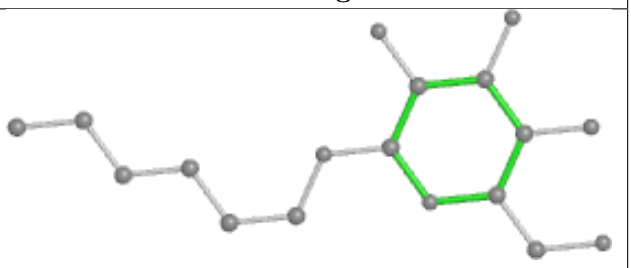
Bond lengths



Bond angles

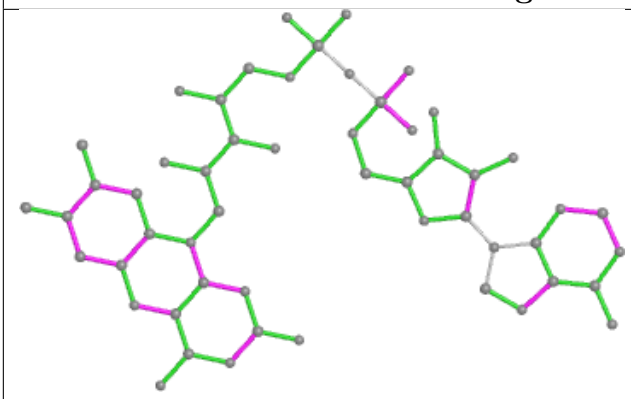


Torsions

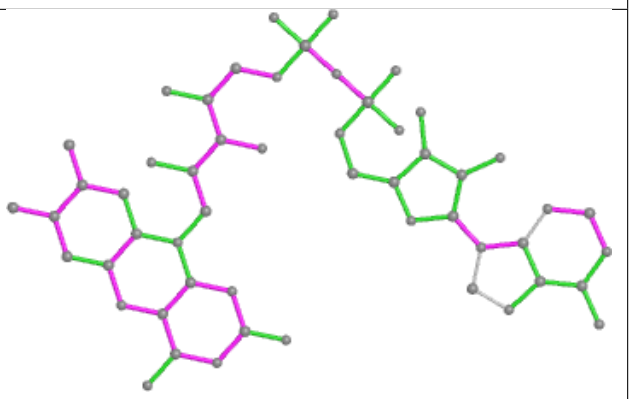


Rings

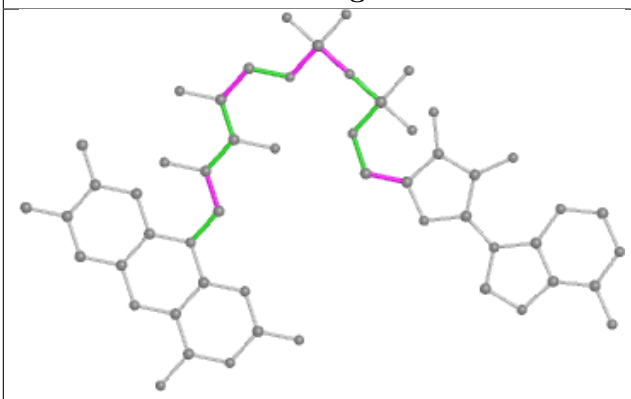
Ligand FAD A 1001



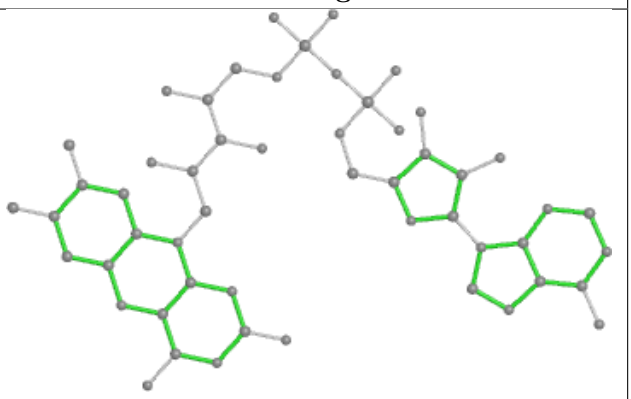
Bond lengths



Bond angles

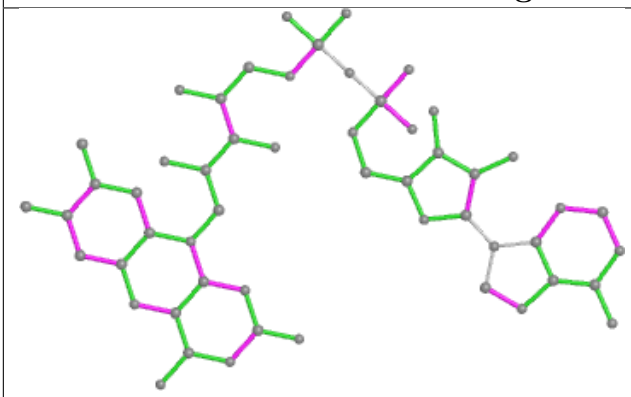


Torsions

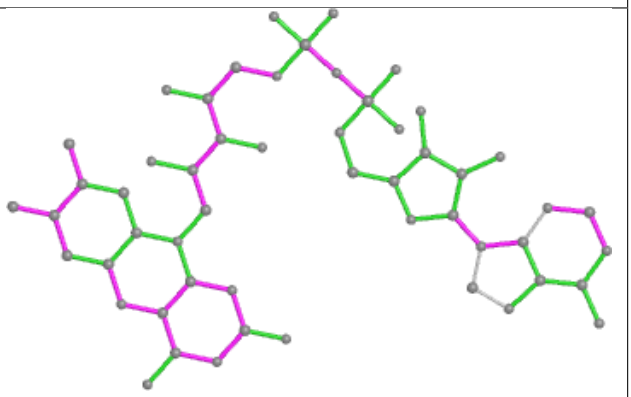


Rings

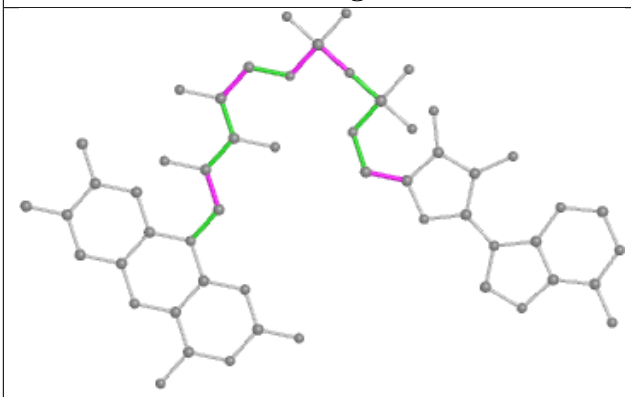
Ligand FAD N 1001



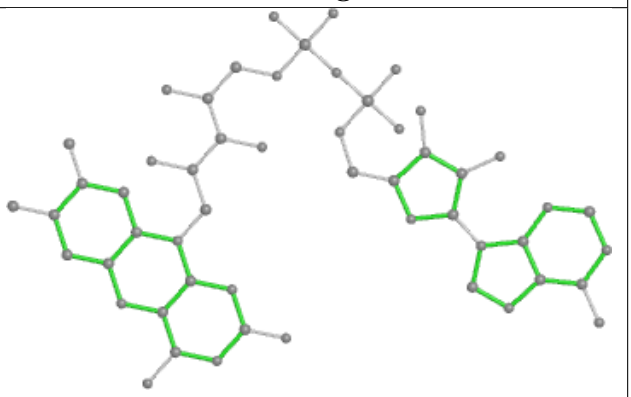
Bond lengths



Bond angles



Torsions



Rings

Ligand PEE D 109

Bond lengths

Bond angles

Torsions

Rings

Ligand PEE Q 210

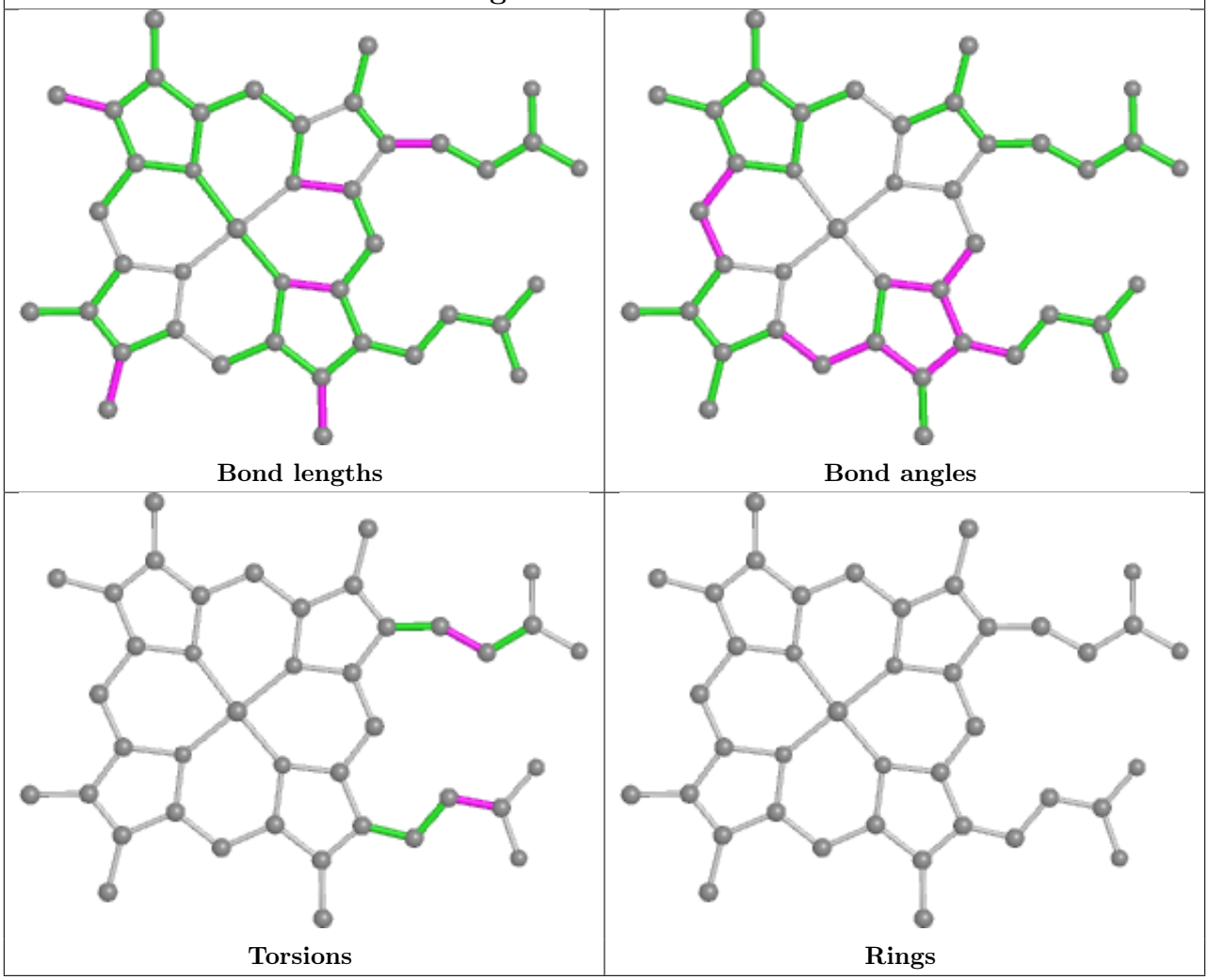
Bond lengths

Bond angles

Torsions

Rings

Ligand HEM P 201



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	613/621 (98%)	-0.13	3 (0%)	91	92	11, 23, 45, 85	0
1	N	612/621 (98%)	-0.11	2 (0%)	94	94	10, 22, 42, 81	0
2	B	239/252 (94%)	-0.16	1 (0%)	92	93	14, 22, 38, 67	0
2	O	239/252 (94%)	-0.16	2 (0%)	86	88	13, 22, 37, 68	0
3	C	140/141 (99%)	0.15	4 (2%)	51	57	19, 34, 52, 75	0
3	P	140/141 (99%)	0.47	10 (7%)	16	20	18, 37, 77, 87	0
4	D	101/103 (98%)	0.43	7 (6%)	16	21	21, 41, 59, 62	0
4	Q	101/103 (98%)	0.64	12 (11%)	4	5	26, 47, 67, 75	0
All	All	2185/2234 (97%)	-0.01	41 (1%)	66	71	10, 24, 53, 87	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	10	THR	9.6
3	P	141	SER	7.4
3	P	140	ILE	6.9
3	C	140	ILE	6.3
1	A	9	SER	5.5
4	Q	103	ILE	5.1
4	Q	93	ILE	5.0
3	C	141	SER	4.9
4	Q	101	TRP	4.8
4	Q	73	TYR	4.6
1	A	10	THR	4.4
4	D	73	TYR	4.2
2	O	245	TYR	3.9
4	Q	28	TYR	3.8
2	O	246	LYS	3.3
3	P	76	SER	3.2

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Mol	Chain	Res	Type	RSRZ
4	D	89	TYR	3.1
4	Q	88	TYR	3.1
4	Q	100	LEU	2.9
4	D	85	TYR	2.9
1	A	383	ASN	2.8
4	D	97	VAL	2.8
3	C	116	LEU	2.7
3	P	73	VAL	2.7
3	P	85	TYR	2.6
3	C	34	LEU	2.6
1	N	383	ASN	2.6
3	P	136	GLY	2.5
3	P	64	PRO	2.5
2	B	118	PHE	2.5
4	Q	33	PRO	2.4
3	P	79	LEU	2.4
4	D	66	LYS	2.3
4	D	101	TRP	2.2
4	Q	95	LYS	2.2
4	Q	85	TYR	2.2
4	Q	66	LYS	2.2
4	D	88	TYR	2.2
3	P	77	LEU	2.1
4	Q	97	VAL	2.1
3	P	91	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	UNL	N	1005	1/-	-0.09	1.74	76,76,76,76	0
5	UNL	B	1007	1/-	0.11	0.89	74,74,74,74	0
5	UNL	N	1012	1/-	0.14	1.01	94,94,94,94	0
5	UNL	Q	287	1/-	0.16	0.77	75,75,75,75	0
5	UNL	C	259	1/-	0.20	0.49	64,64,64,64	0
5	UNL	B	1006	1/-	0.25	1.25	76,76,76,76	0
5	UNL	N	1014	1/-	0.32	0.61	76,76,76,76	0
5	UNL	A	1005	1/-	0.33	1.31	66,66,66,66	0
13	GOL	P	208	6/6	0.35	1.64	155,156,156,157	0
5	UNL	N	1022	1/-	0.42	0.65	72,72,72,72	0
5	UNL	O	276	1/-	0.46	0.45	65,65,65,65	0
5	UNL	A	1022	1/-	0.47	0.35	51,51,51,51	0
5	UNL	P	211	5/-	0.47	0.96	119,119,120,121	0
5	UNL	D	265	1/-	0.50	1.14	103,103,103,103	0
5	UNL	N	1016	1/-	0.53	0.40	62,62,62,62	0
5	UNL	B	1005	5/-	0.53	0.39	92,93,93,94	0
5	UNL	D	266	1/-	0.54	0.56	62,62,62,62	0
5	UNL	P	224	1/-	0.55	0.66	71,71,71,71	0
5	UNL	N	1006	1/-	0.58	0.53	52,52,52,52	0
5	UNL	A	1007	1/-	0.60	0.56	66,66,66,66	0
17	PEE	Q	210	24/51	0.60	0.56	70,82,95,95	0
5	UNL	N	1018	1/-	0.61	0.48	46,46,46,46	0
5	UNL	B	1009	1/-	0.61	0.62	73,73,73,73	0
5	UNL	C	235	1/-	0.63	0.52	71,71,71,71	0
5	UNL	D	247	1/-	0.64	0.41	68,68,68,68	0
5	UNL	A	1015	1/-	0.64	1.04	69,69,69,69	0
5	UNL	C	248	1/-	0.64	0.70	57,57,57,57	0
17	PEE	D	109	24/51	0.64	0.41	48,64,74,75	0
5	UNL	C	214	5/-	0.64	0.37	90,91,92,93	0
5	UNL	N	1023	1/-	0.65	0.32	45,45,45,45	0
5	UNL	A	1003	6/-	0.65	0.26	135,136,136,137	0
5	UNL	C	254	1/-	0.67	0.45	55,55,55,55	0
5	UNL	A	1010	1/-	0.67	0.66	67,67,67,67	0
5	UNL	A	1023	1/-	0.69	0.45	53,53,53,53	0
5	UNL	C	292	1/-	0.69	0.57	64,64,64,64	0
5	UNL	O	1005	5/-	0.71	0.37	146,146,147,147	0
5	UNL	D	291	1/-	0.72	0.42	58,58,58,58	0
5	UNL	B	277	1/-	0.73	0.23	46,46,46,46	0
5	UNL	B	268	1/-	0.74	0.49	51,51,51,51	0
5	UNL	A	1004	4/-	0.75	0.21	55,60,60,61	0
5	UNL	N	1021	1/-	0.75	0.29	42,42,42,42	0
5	UNL	A	1013	1/-	0.75	0.27	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	UNL	C	293	1/-	0.76	0.50	62,62,62,62	0
5	UNL	N	1013	1/-	0.76	0.30	57,57,57,57	0
5	UNL	N	1009	1/-	0.76	0.32	50,50,50,50	0
5	UNL	P	274	1/-	0.76	0.52	56,56,56,56	0
5	UNL	A	1012	1/-	0.77	0.69	69,69,69,69	0
5	UNL	D	263	1/-	0.77	0.51	53,53,53,53	0
5	UNL	A	1011	1/-	0.77	0.44	55,55,55,55	0
5	UNL	P	285	1/-	0.77	0.35	50,50,50,50	0
5	UNL	O	282	1/-	0.78	0.28	52,52,52,52	0
5	UNL	A	1008	1/-	0.78	1.01	62,62,62,62	0
5	UNL	Q	288	1/-	0.79	0.45	44,44,44,44	0
5	UNL	N	1007	1/-	0.79	0.38	59,59,59,59	0
5	UNL	B	280	1/-	0.80	0.40	53,53,53,53	0
5	UNL	D	262	1/-	0.81	0.47	59,59,59,59	0
14	BHG	C	142	18/18	0.81	0.37	49,67,79,79	0
5	UNL	Q	237	1/-	0.81	0.38	47,47,47,47	0
7	AZI	A	623	3/3	0.81	0.19	56,56,64,64	0
5	UNL	C	251	1/-	0.82	0.49	53,53,53,53	0
5	UNL	P	233	1/-	0.82	0.40	44,44,44,44	0
5	UNL	A	1014	1/-	0.83	0.47	47,47,47,47	0
5	UNL	A	1009	1/-	0.83	0.30	50,50,50,50	0
5	UNL	B	258	1/-	0.83	0.37	57,57,57,57	0
5	UNL	O	1006	1/-	0.83	0.48	66,66,66,66	0
5	UNL	O	1007	1/-	0.83	0.31	69,69,69,69	0
5	UNL	A	1016	1/-	0.83	0.62	50,50,50,50	0
5	UNL	C	289	1/-	0.84	0.33	57,57,57,57	0
13	GOL	C	294	6/6	0.84	0.64	132,132,133,133	0
5	UNL	Q	221	1/-	0.85	0.49	56,56,56,56	0
5	UNL	A	1021	1/-	0.85	0.31	37,37,37,37	0
5	UNL	B	297	1/-	0.85	0.26	51,51,51,51	0
5	UNL	O	1008	1/-	0.85	0.29	47,47,47,47	0
5	UNL	C	145	4/-	0.85	0.11	70,70,70,70	0
5	UNL	P	218	1/-	0.86	0.44	57,57,57,57	0
5	UNL	B	1008	1/-	0.86	0.69	61,61,61,61	0
5	UNL	C	267	1/-	0.86	0.47	52,52,52,52	0
5	UNL	N	1020	1/-	0.87	0.27	56,56,56,56	0
5	UNL	C	256	1/-	0.87	0.47	61,61,61,61	0
5	UNL	P	236	1/-	0.87	0.45	53,53,53,53	0
5	UNL	N	1008	1/-	0.88	0.38	39,39,39,39	0
5	UNL	N	1003	4/-	0.88	0.15	57,58,59,59	0
5	UNL	N	1010	1/-	0.89	0.44	63,63,63,63	0
5	UNL	C	240	1/-	0.89	0.38	45,45,45,45	0

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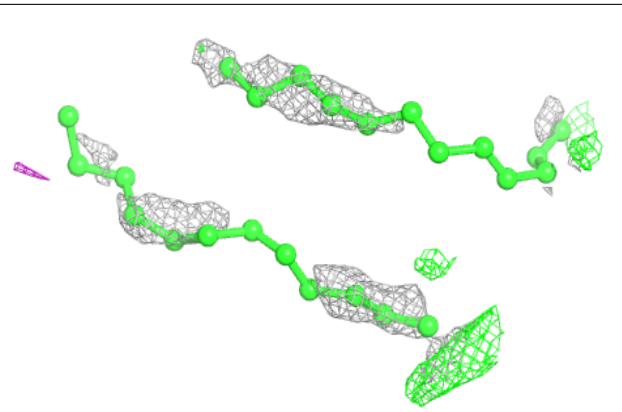
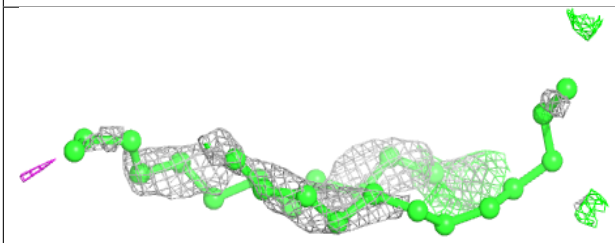
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	UNL	Q	234	1/-	0.89	0.61	53,53,53,53	0
5	UNL	C	241	1/-	0.90	0.31	61,61,61,61	0
5	UNL	N	1019	1/-	0.90	0.46	49,49,49,49	0
13	GOL	O	1009	6/6	0.90	0.20	29,30,33,33	0
5	UNL	D	245	1/-	0.90	0.45	58,58,58,58	0
5	UNL	C	272	1/-	0.90	0.43	54,54,54,54	0
5	UNL	N	1011	1/-	0.90	0.30	38,38,38,38	0
5	UNL	N	1017	1/-	0.90	0.25	30,30,30,30	0
5	UNL	D	250	1/-	0.91	0.43	53,53,53,53	0
5	UNL	N	1004	1/-	0.91	0.33	45,45,45,45	0
5	UNL	A	1017	1/-	0.91	0.18	48,48,48,48	0
5	UNL	N	1015	1/-	0.92	0.46	42,42,42,42	0
5	UNL	D	255	1/-	0.92	0.23	35,35,35,35	0
5	UNL	Q	219	1/-	0.92	0.34	45,45,45,45	0
14	BHG	P	204	18/18	0.92	0.17	38,45,58,59	0
5	UNL	A	1018	1/-	0.92	0.41	45,45,45,45	0
5	UNL	A	1006	1/-	0.92	0.29	47,47,47,47	0
5	UNL	A	1020	1/-	0.93	0.30	34,34,34,34	0
5	UNL	A	1019	1/-	0.93	0.28	37,37,37,37	0
13	GOL	B	1010	6/6	0.95	0.15	26,29,32,32	0
16	CBE	C	144	16/16	0.95	0.17	28,32,37,39	0
6	K	O	253	1/1	0.96	0.08	39,39,39,39	0
16	CBE	P	202	16/16	0.96	0.12	25,30,35,35	0
9	OAA	A	1002	9/9	0.96	0.11	19,21,24,26	0
9	OAA	N	1002	9/9	0.96	0.12	13,17,22,23	0
8	FAD	A	1001	53/53	0.97	0.12	9,14,22,25	0
8	FAD	N	1001	53/53	0.97	0.12	4,13,21,24	0
15	HEM	C	143	41/43	0.97	0.13	23,32,40,49	0
15	HEM	P	201	41/43	0.97	0.13	29,32,43,48	0
10	FES	B	1002	4/4	0.99	0.11	14,16,16,17	0
10	FES	O	1002	4/4	0.99	0.10	14,16,16,19	0
11	SF4	B	1003	8/8	0.99	0.10	16,17,19,21	0
11	SF4	O	1003	8/8	0.99	0.11	14,18,20,20	0
12	F3S	B	1004	7/7	0.99	0.11	17,19,20,25	0
12	F3S	O	1004	7/7	0.99	0.13	15,20,22,22	0
6	K	A	622	1/1	0.99	0.09	24,24,24,24	0
6	K	B	253	1/1	0.99	0.06	38,38,38,38	0
6	K	N	622	1/1	0.99	0.09	19,19,19,19	0

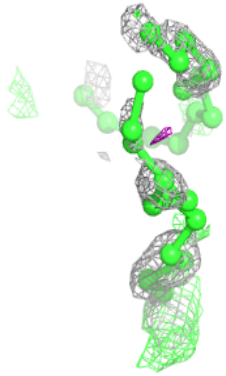
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PEE Q 210:

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

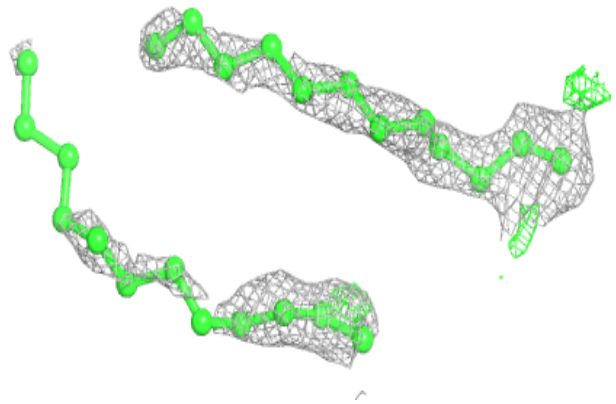


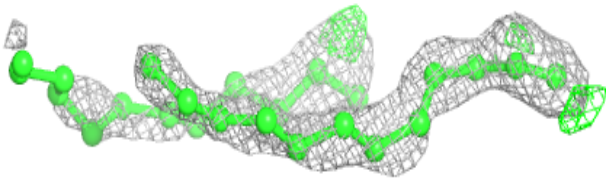


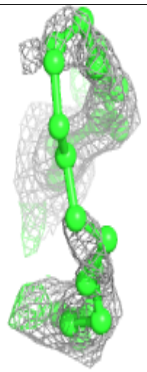


Electron density around PEE D 109:

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

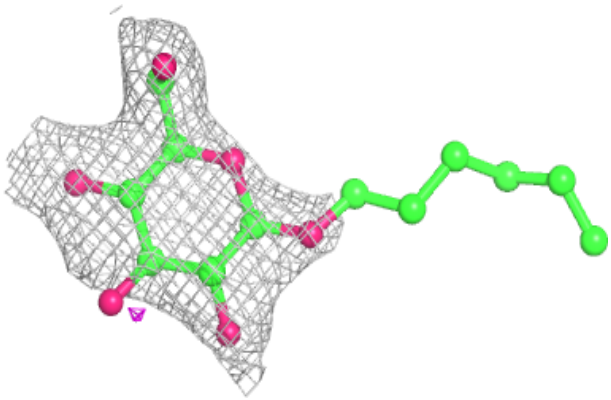


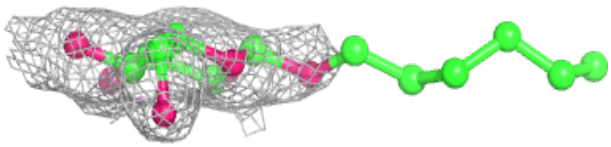


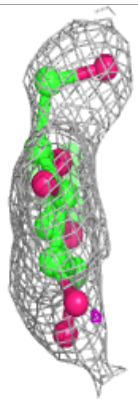


Electron density around BHG C 142:

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

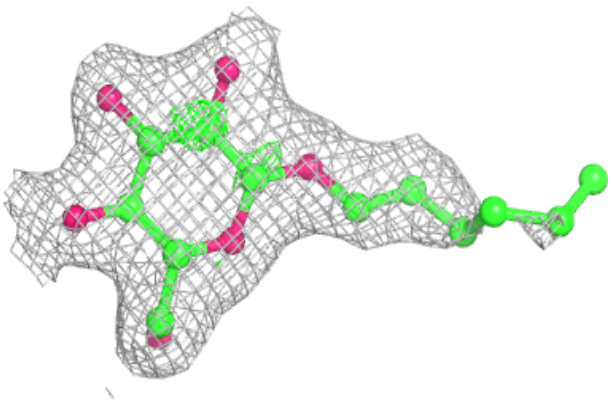


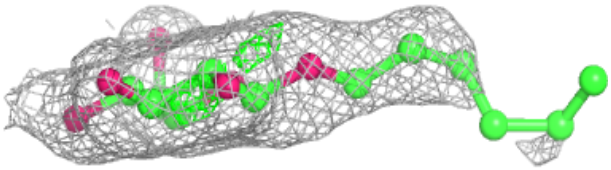


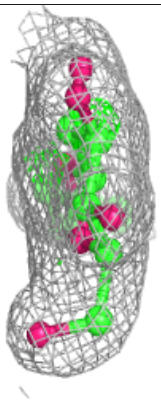


Electron density around BHG P 204:

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

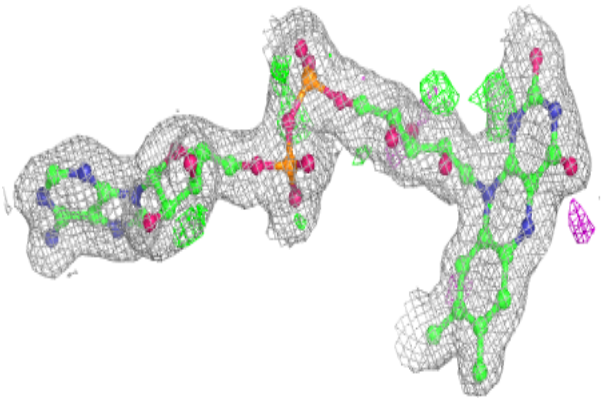


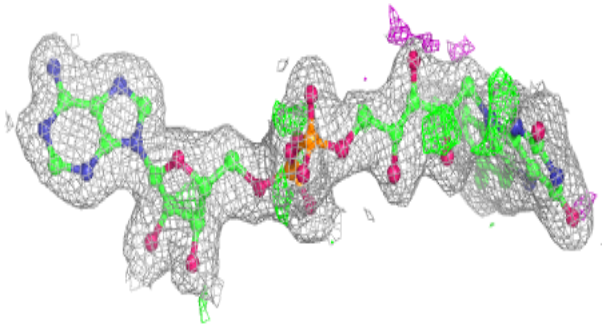


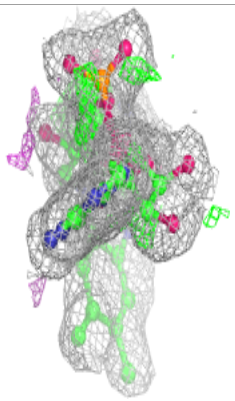


Electron density around FAD A 1001:

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

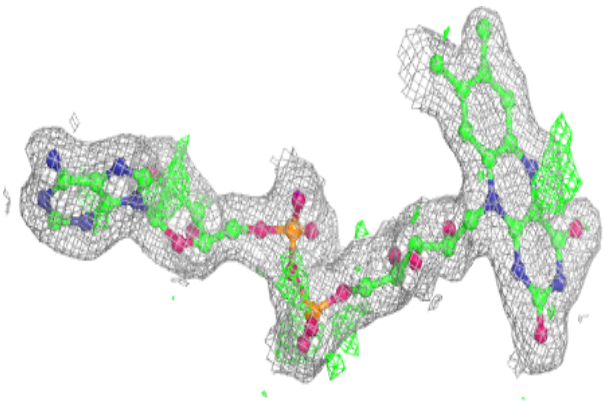


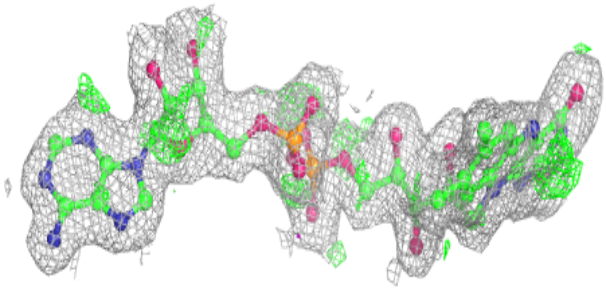


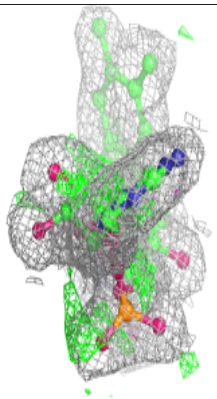


Electron density around FAD N 1001:

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

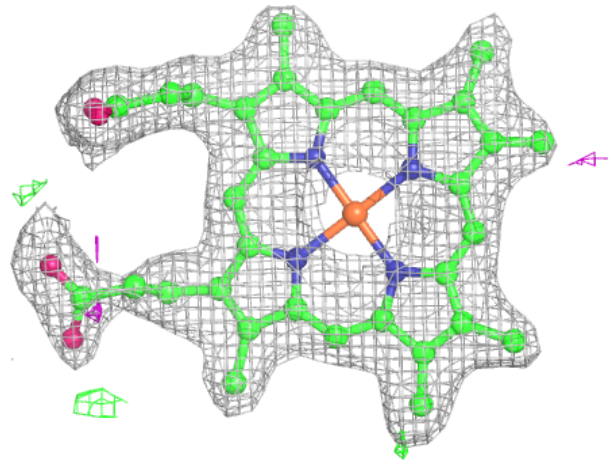


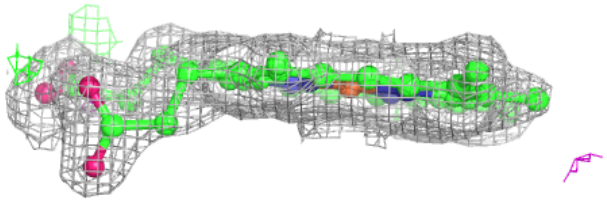


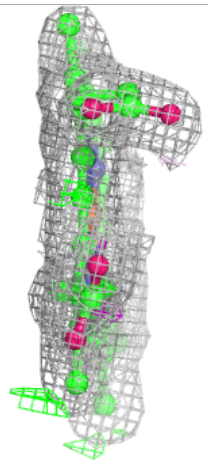


Electron density around HEM C 143:

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

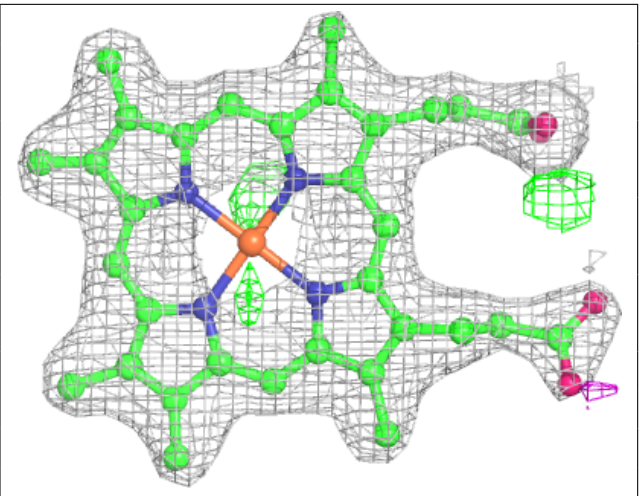


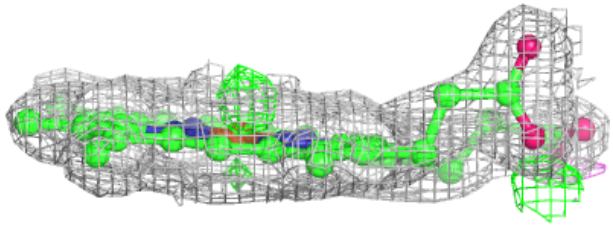


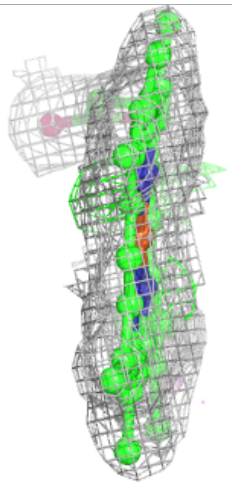


Electron density around HEM P 201:

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







6.5 Other polymers (i)

There are no such residues in this entry.