Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 08:14 PM EDT

PDB ID	:	3AE1 / pdb_00003ae1
Title	:	Crystal structure of porcine heart mitochondrial complex II bound with N-Phenyl-2-(trifluoromethyl)-benzamide
Authors	:	Harada, S.; Sasaki, T.; Shindo, M.; Kido, Y.; Inaoka, D.K.; Omori, J.; Osanai, A.; Sakamoto, K.; Mao, J.; Matsuoka, S.; Inoue, M.; Honma, T.; Tanaka, A.; Kita, K.
Deposited on	:	2010-02-04
Resolution	:	3.14 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:

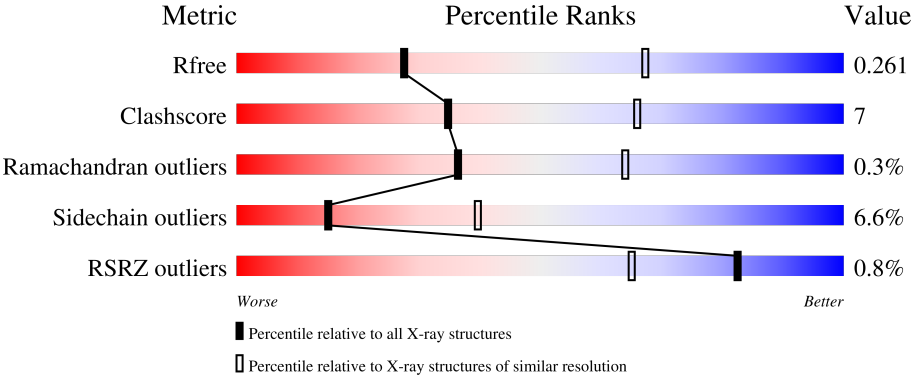
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.14 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	622	% 77% 18% • •
2	B	252	% 75% 17% • 5%
3	C	140	% 85% 11% • •
4	D	103	% 92% 7% •

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
12	EPH	D	1306	X	-	-	-
6	MLI	A	701	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 8665 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 [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	613	4729	2954	848	895	32	0	0	0

- Molecule 2 is a protein called Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	239	1922	1214	326	360	22	0	0	0

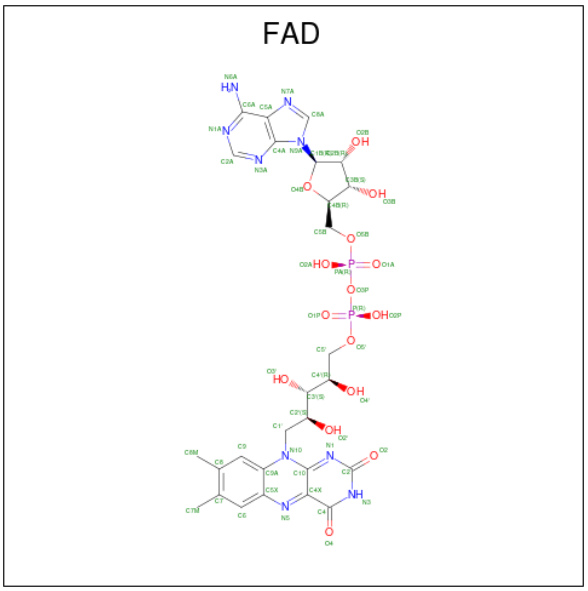
- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b560 subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	138	1064	695	179	183	7	0	0	0

- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

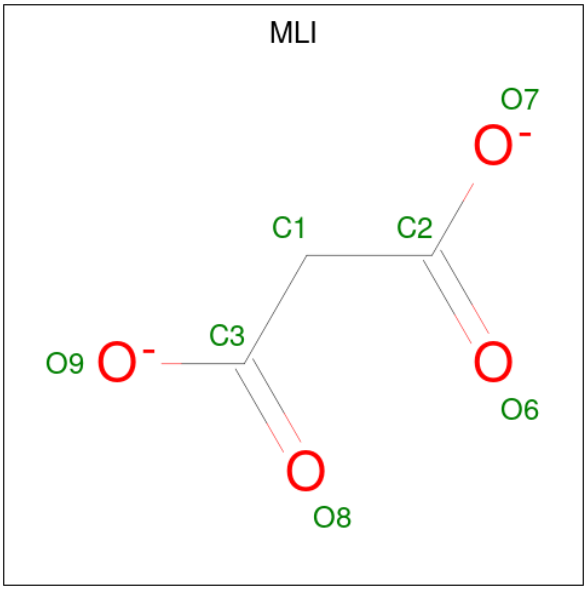
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	102	765	499	128	133	5	0	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



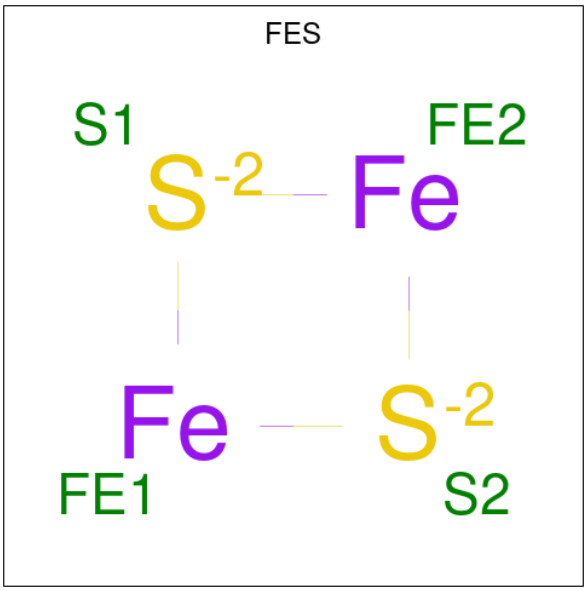
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	53	27	9	15	2	0	0

- Molecule 6 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



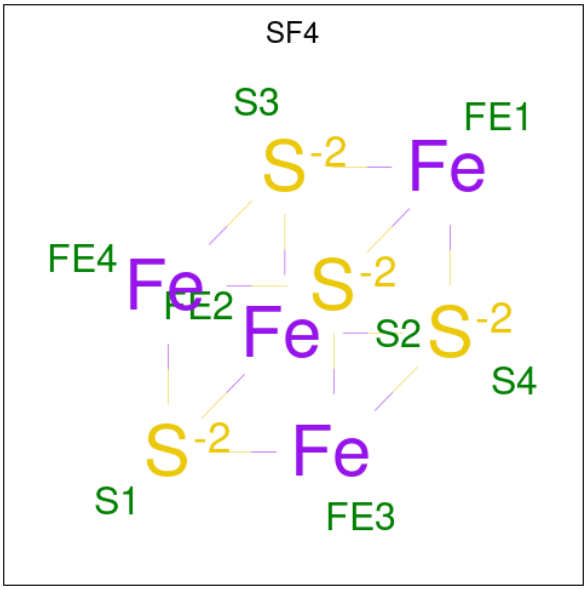
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	A	1	7	3	4		0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



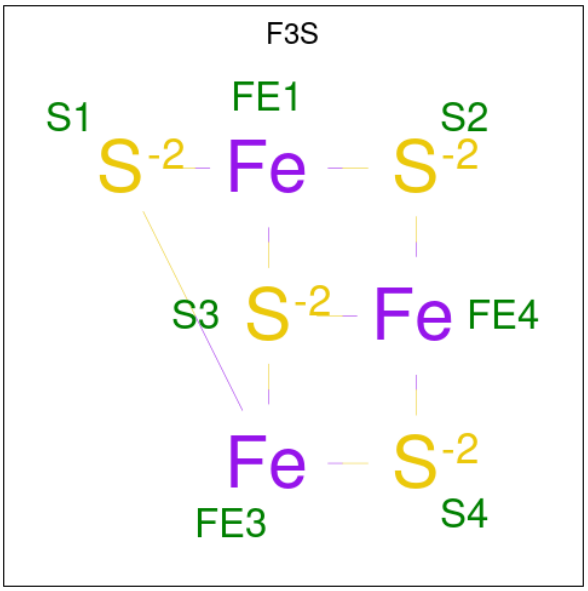
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	B	1	4	2	2	0	0

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



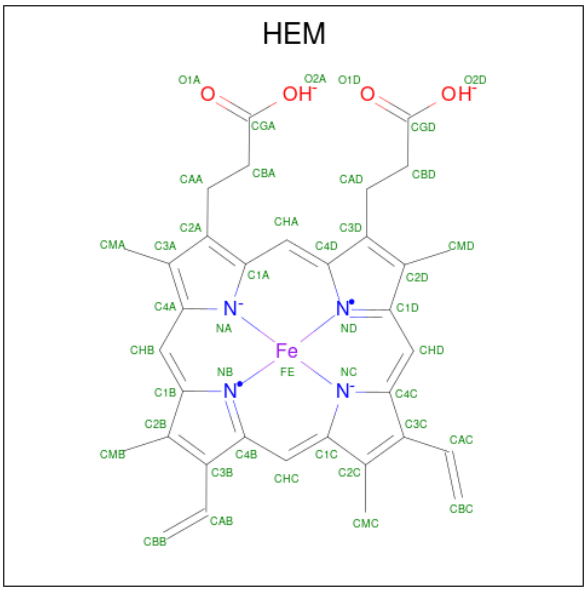
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	B	1	8	4	4	0	0

- Molecule 9 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



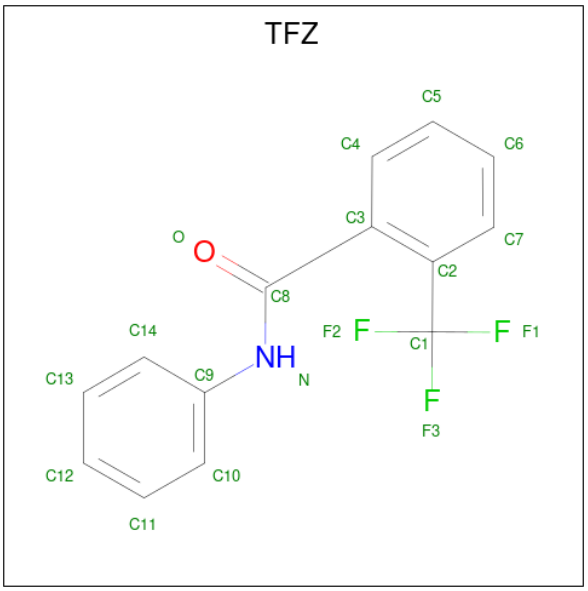
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	B	1	7	3	4	0	0

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



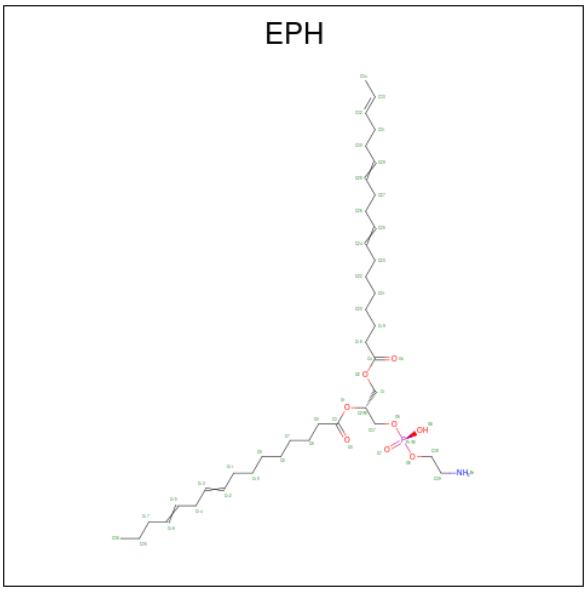
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
10	C	1	43	34	1	4	4	0	0

- Molecule 11 is N-phenyl-2-(trifluoromethyl)benzamide (CCD ID: TFZ) (formula: $C_{14}H_{10}F_3NO$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
11	C	1	19	14	3	1	1	0	0

- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (CCD ID: EPH) (formula: $C_{39}H_{68}NO_8P$).



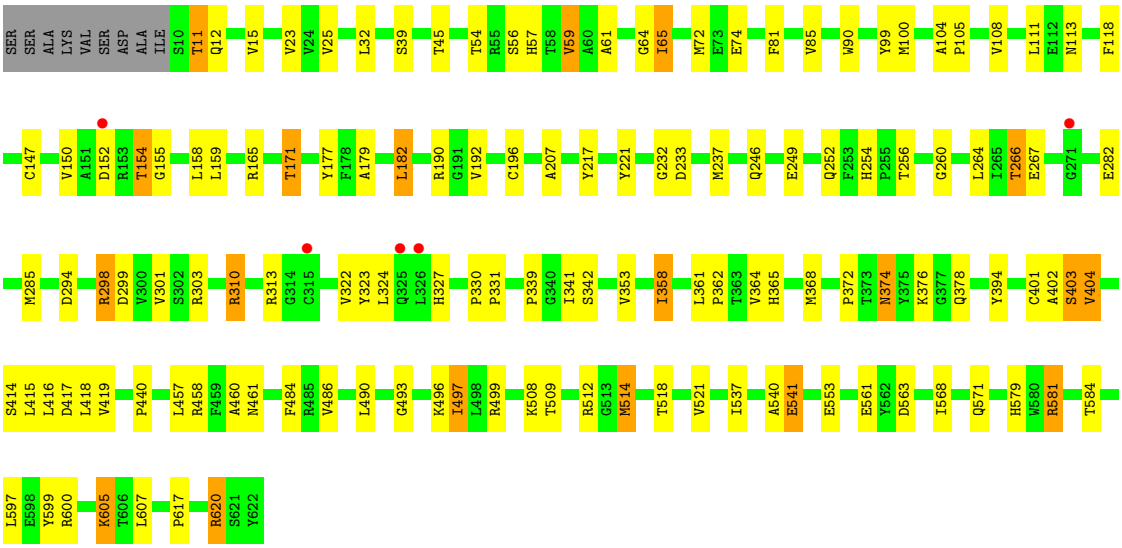
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	D	1	44	34	1	8	1	0	0

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.

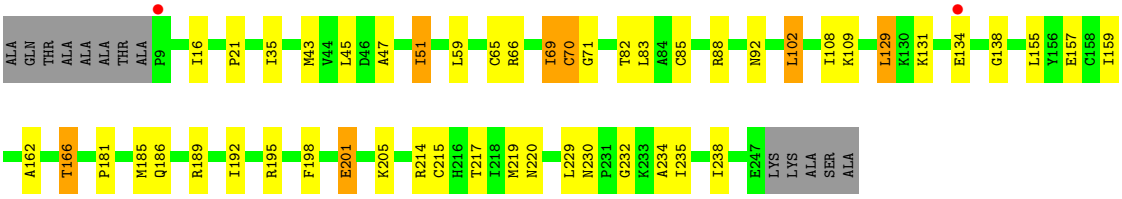
• Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain A:



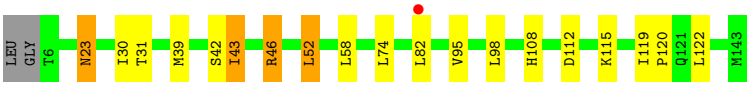
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain B:



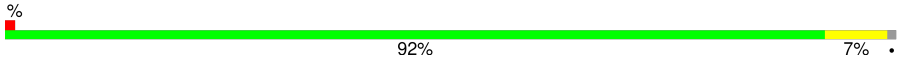
• Molecule 3: Succinate dehydrogenase cytochrome b560 subunit, mitochondrial

Chain C:



• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.47Å 84.06Å 294.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.62 – 3.14 47.62 – 3.14	Depositor EDS
% Data completeness (in resolution range)	95.3 (47.62-3.14) 95.3 (47.62-3.14)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 3.12Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0102	Depositor
R, R_{free}	0.220 , 0.268 0.220 , 0.261	Depositor DCC
R_{free} test set	1536 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	77.5	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8665	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: HEM, SF4, MLI, F3S, FES, EPH, TFZ, 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	0.43	0/4828	0.82	4/6531 (0.1%)
2	B	0.42	0/1964	0.80	2/2648 (0.1%)
3	C	0.46	0/1091	0.85	0/1483
4	D	0.40	0/784	0.85	0/1066
All	All	0.43	0/8667	0.82	6/11728 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	12	GLN	N-CA-C	-11.76	99.46	114.04
1	A	11	THR	CB-CA-C	-7.64	98.78	111.23
1	A	402	ALA	N-CA-C	-6.82	104.95	113.20
2	B	102	LEU	CA-C-N	6.32	126.34	119.89
2	B	102	LEU	C-N-CA	6.32	126.34	119.89
1	A	266	THR	N-CA-C	5.00	116.74	110.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4729	0	4618	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1922	0	1901	30	0
3	C	1064	0	1104	12	0
4	D	765	0	773	4	0
5	A	53	0	31	10	0
6	A	7	0	2	3	0
7	B	4	0	0	0	0
8	B	8	0	0	0	0
9	B	7	0	0	1	0
10	C	43	0	30	1	0
11	C	19	0	10	3	0
12	D	44	0	53	0	0
All	All	8665	0	8522	127	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 7.

All (127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:HIS:NE2	5:A:700:FAD:HM81	1.38	1.35
1:A:57:HIS:NE2	5:A:700:FAD:C8M	1.91	1.32
1:A:61:ALA:HB3	1:A:155:GLY:HA3	1.39	1.04
2:B:102:LEU:HB3	2:B:166:THR:HG21	1.50	0.94
1:A:57:HIS:NE2	5:A:700:FAD:HM83	1.85	0.89
1:A:57:HIS:CE1	5:A:700:FAD:HM81	2.11	0.83
2:B:219:MET:HE1	2:B:232:GLY:HA3	1.59	0.83
1:A:11:THR:HG22	1:A:11:THR:O	1.79	0.80
1:A:486:VAL:HG12	1:A:553:GLU:HB2	1.70	0.73
1:A:59:VAL:HG13	1:A:159:LEU:HD23	1.71	0.72
4:D:72:LEU:O	4:D:76:LEU:HB2	1.91	0.70
3:C:52:LEU:HB3	10:C:1305:HEM:HAC	1.73	0.69
1:A:104:ALA:HB3	1:A:105:PRO:HD3	1.76	0.68
1:A:415:LEU:HG	5:A:700:FAD:C2	2.24	0.67
1:A:310:ARG:HG2	1:A:310:ARG:HH11	1.59	0.66
1:A:64:GLY:HA2	1:A:154:THR:HG21	1.76	0.66
1:A:150:VAL:H	1:A:154:THR:HB	1.62	0.65
1:A:374:ASN:HB3	1:A:376:LYS:H	1.61	0.64
3:C:23:ASN:HD22	3:C:23:ASN:H	1.44	0.64
1:A:56:SER:O	1:A:59:VAL:HG22	1.97	0.64
1:A:57:HIS:CD2	5:A:700:FAD:HM83	2.34	0.62
1:A:457:LEU:O	1:A:509:THR:HG21	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:HD2	1:A:440:PRO:HB2	1.84	0.59
2:B:215:CYS:HA	9:B:304:F3S:S4	2.45	0.57
1:A:246:GLN:HB2	1:A:372:PRO:HG3	1.87	0.57
1:A:620:ARG:O	1:A:620:ARG:HG3	2.06	0.56
1:A:458:ARG:NH2	1:A:514:MET:HG2	2.21	0.56
1:A:518:THR:HA	1:A:521:VAL:HG22	1.87	0.56
1:A:605:LYS:O	1:A:605:LYS:HE3	2.06	0.55
1:A:254:HIS:HD2	1:A:256:THR:H	1.54	0.55
1:A:61:ALA:HA	5:A:700:FAD:N5	2.23	0.54
2:B:35:ILE:HD11	2:B:51:ILE:HG22	1.89	0.54
2:B:51:ILE:HD11	2:B:59:LEU:HD22	1.89	0.54
2:B:198:PHE:CD2	2:B:201:GLU:HG3	2.43	0.54
3:C:46:ARG:HD3	4:D:87:VAL:HG22	1.89	0.54
3:C:42:SER:O	11:C:1201:TFZ:H10	2.09	0.53
2:B:155:LEU:HD23	2:B:185:MET:HE2	1.91	0.53
2:B:129:LEU:HD21	2:B:195:ARG:HB2	1.91	0.52
1:A:579:HIS:HD2	1:A:581:ARG:H	1.54	0.52
1:A:150:VAL:HB	1:A:154:THR:HA	1.92	0.52
2:B:69:ILE:O	2:B:70:CYS:C	2.52	0.52
1:A:158:LEU:HD23	1:A:415:LEU:HD22	1.92	0.52
2:B:230:ASN:HD22	2:B:230:ASN:C	2.17	0.52
1:A:150:VAL:HG12	1:A:150:VAL:O	2.10	0.51
1:A:57:HIS:NE2	5:A:700:FAD:C8	2.68	0.50
1:A:217:TYR:HB3	1:A:232:GLY:HA3	1.92	0.50
3:C:52:LEU:HD21	3:C:98:LEU:HA	1.94	0.50
1:A:64:GLY:HA3	1:A:147:CYS:SG	2.52	0.49
1:A:353:VAL:HG12	1:A:358:ILE:HD11	1.93	0.49
3:C:39:MET:HG2	11:C:1201:TFZ:H6	1.94	0.49
1:A:401:CYS:C	1:A:403:SER:H	2.21	0.49
2:B:65:CYS:O	2:B:66:ARG:HG3	2.13	0.49
1:A:111:LEU:HD11	1:A:419:VAL:HG21	1.94	0.48
1:A:267:GLU:OE1	1:A:298:ARG:HD3	2.13	0.48
1:A:57:HIS:CD2	5:A:700:FAD:C8M	2.84	0.48
2:B:219:MET:CE	2:B:232:GLY:HA3	2.39	0.48
1:A:310:ARG:HH11	1:A:310:ARG:CG	2.26	0.48
1:A:461:ASN:HD22	1:A:508:LYS:HE3	1.78	0.48
1:A:11:THR:O	1:A:11:THR:CG2	2.51	0.48
1:A:266:THR:HA	6:A:701:MLI:O8	2.14	0.48
2:B:235:ILE:HA	2:B:238:ILE:HD12	1.96	0.48
2:B:21:PRO:HD3	2:B:109:LYS:HG3	1.95	0.47
1:A:509:THR:HG23	1:A:512:ARG:HH12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:HD12	1:A:108:VAL:HG22	1.96	0.47
3:C:42:SER:C	11:C:1201:TFZ:H10	2.39	0.47
3:C:112:ASP:OD1	4:D:47:ARG:HD2	2.15	0.47
1:A:179:ALA:N	5:A:700:FAD:N1A	2.46	0.46
1:A:496:LYS:HG3	1:A:499:ARG:HH22	1.80	0.46
2:B:131:LYS:HB2	2:B:134:GLU:HG3	1.97	0.46
1:A:81:PHE:O	1:A:85:VAL:HG12	2.15	0.46
1:A:414:SER:HA	1:A:417:ASP:HB3	1.97	0.46
2:B:69:ILE:O	2:B:71:GLY:N	2.48	0.46
1:A:104:ALA:HA	1:A:416:LEU:HD11	1.96	0.46
1:A:497:ILE:HG21	1:A:537:ILE:HG21	1.98	0.46
1:A:361:LEU:HD12	1:A:362:PRO:HD2	1.98	0.46
1:A:414:SER:O	1:A:418:LEU:HD13	2.15	0.46
1:A:299:ASP:O	1:A:303:ARG:HB2	2.16	0.46
3:C:119:ILE:N	3:C:120:PRO:HD2	2.31	0.46
2:B:43:MET:HA	2:B:88:ARG:HA	1.97	0.45
1:A:285:MET:HE2	1:A:301:VAL:HG22	1.98	0.45
1:A:25:VAL:HG21	1:A:192:VAL:HG11	1.98	0.45
1:A:39:SER:OG	1:A:171:THR:HG23	2.16	0.45
3:C:74:LEU:HD22	4:D:136:LEU:HD13	1.99	0.45
1:A:45:THR:HB	1:A:171:THR:HG22	1.99	0.45
3:C:43:ILE:H	3:C:43:ILE:HG13	1.52	0.44
1:A:254:HIS:O	1:A:362:PRO:HA	2.17	0.44
1:A:90:TRP:HZ3	1:A:620:ARG:HB3	1.83	0.44
1:A:246:GLN:HE22	1:A:600:ARG:HE	1.64	0.44
1:A:99:TYR:HB2	1:A:607:LEU:HD11	1.98	0.44
1:A:584:THR:HA	1:A:599:TYR:CD2	2.53	0.43
1:A:378:GLN:HG2	1:A:394:TYR:CE2	2.54	0.43
1:A:113:ASN:HD22	2:B:138:GLY:H	1.65	0.43
3:C:82:LEU:HD23	3:C:82:LEU:H	1.83	0.43
1:A:100:MET:SD	1:A:404:VAL:HG11	2.58	0.43
1:A:113:ASN:ND2	2:B:138:GLY:H	2.17	0.43
1:A:182:LEU:HD13	1:A:237:MET:HB3	1.99	0.43
1:A:493:GLY:O	1:A:497:ILE:HB	2.18	0.43
1:A:563:ASP:H	1:A:571:GLN:NE2	2.17	0.43
1:A:221:TYR:CG	1:A:364:VAL:HG21	2.54	0.42
1:A:254:HIS:HB2	1:A:365:HIS:HB2	2.01	0.42
2:B:181:PRO:HA	2:B:235:ILE:HD11	2.00	0.42
1:A:249:GLU:HB2	1:A:540:ALA:HB2	2.01	0.42
2:B:16:ILE:HG21	2:B:59:LEU:HD11	2.01	0.42
1:A:490:LEU:HD13	1:A:541:GLU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:ALA:O	2:B:166:THR:OG1	2.25	0.42
1:A:152:ASP:HB2	1:A:339:PRO:HD2	2.01	0.42
1:A:264:LEU:HD21	6:A:701:MLI:O8	2.20	0.42
2:B:21:PRO:HG3	2:B:108:ILE:O	2.19	0.42
1:A:90:TRP:CE2	1:A:617:PRO:HA	2.55	0.42
1:A:233:ASP:O	1:A:237:MET:HG3	2.20	0.42
1:A:118:PHE:HA	1:A:150:VAL:HG22	2.02	0.41
2:B:45:LEU:HD22	2:B:85:CYS:HB3	2.02	0.41
2:B:47:ALA:O	2:B:51:ILE:HG23	2.21	0.41
1:A:563:ASP:HB3	1:A:571:GLN:HE22	1.85	0.41
2:B:157:GLU:HB2	2:B:229:LEU:HD21	2.03	0.41
1:A:23:VAL:HG23	1:A:207:ALA:HB3	2.02	0.41
2:B:82:THR:HB	2:B:83:LEU:H	1.73	0.41
2:B:70:CYS:SG	2:B:71:GLY:N	2.94	0.41
1:A:303:ARG:HG3	1:A:484:PHE:CZ	2.55	0.41
1:A:341:ILE:HG13	1:A:342:SER:N	2.35	0.41
1:A:514:MET:HA	1:A:514:MET:HE2	2.03	0.41
1:A:330:PRO:HA	1:A:331:PRO:HD3	1.92	0.40
2:B:198:PHE:HD2	2:B:201:GLU:HG3	1.86	0.40
1:A:322:VAL:CG1	1:A:323:TYR:N	2.84	0.40
1:A:177:TYR:CE2	1:A:196:CYS:HB2	2.56	0.40
2:B:234:ALA:O	2:B:238:ILE:HG13	2.22	0.40
1:A:298:ARG:HH22	6:A:701:MLI:C2	2.34	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	611/622 (98%)	580 (95%)	29 (5%)	2 (0%)	36 64
2	B	237/252 (94%)	221 (93%)	15 (6%)	1 (0%)	30 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	136/140 (97%)	133 (98%)	3 (2%)	0	100	100
4	D	100/103 (97%)	97 (97%)	3 (3%)	0	100	100
All	All	1084/1117 (97%)	1031 (95%)	50 (5%)	3 (0%)	36	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	70	CYS
1	A	460	ALA
1	A	260	GLY

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	499/506 (99%)	466 (93%)	33 (7%)	15	40
2	B	214/220 (97%)	200 (94%)	14 (6%)	15	40
3	C	117/118 (99%)	106 (91%)	11 (9%)	8	28
4	D	76/76 (100%)	74 (97%)	2 (3%)	40	64
All	All	906/920 (98%)	846 (93%)	60 (7%)	15	40

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	32	LEU
1	A	54	THR
1	A	59	VAL
1	A	65	ILE
1	A	72	MET
1	A	74	GLU
1	A	154	THR
1	A	165	ARG

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Mol	Chain	Res	Type
1	A	171	THR
1	A	182	LEU
1	A	252	GLN
1	A	282	GLU
1	A	294	ASP
1	A	298	ARG
1	A	310	ARG
1	A	313	ARG
1	A	324	LEU
1	A	327	HIS
1	A	358	ILE
1	A	368	MET
1	A	374	ASN
1	A	403	SER
1	A	404	VAL
1	A	497	ILE
1	A	514	MET
1	A	541	GLU
1	A	561	GLU
1	A	568	ILE
1	A	581	ARG
1	A	597	LEU
1	A	605	LYS
1	A	620	ARG
2	B	51	ILE
2	B	69	ILE
2	B	92	ASN
2	B	129	LEU
2	B	159	ILE
2	B	166	THR
2	B	186	GLN
2	B	189	ARG
2	B	192	ILE
2	B	201	GLU
2	B	205	LYS
2	B	214	ARG
2	B	217	THR
2	B	220	ASN
3	C	23	ASN
3	C	30	ILE
3	C	31	THR
3	C	43	ILE

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Mol	Chain	Res	Type
3	C	46	ARG
3	C	52	LEU
3	C	58	LEU
3	C	95	VAL
3	C	108	HIS
3	C	115	LYS
3	C	122	LEU
4	D	78	LEU
4	D	124	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	62	GLN
1	A	113	ASN
1	A	128	GLN
1	A	143	GLN
1	A	246	GLN
1	A	254	HIS
1	A	325	GLN
1	A	374	ASN
1	A	378	GLN
1	A	382	HIS
1	A	384	ASN
1	A	386	GLN
1	A	408	ASN
1	A	445	ASN
1	A	453	ASN
1	A	461	ASN
1	A	478	GLN
1	A	527	GLN
1	A	550	HIS
1	A	569	GLN
1	A	571	GLN
1	A	579	HIS
1	A	608	ASN
2	B	121	GLN
2	B	220	ASN
2	B	230	ASN
3	C	17	ASN
3	C	23	ASN

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Mol	Chain	Res	Type
3	C	104	ASN
4	D	42	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	TFZ	C	1201	-	20,20,20	1.66	2 (10%)	28,28,28	0.99	2 (7%)
10	HEM	C	1305	4,3	50,50,50	1.88	11 (22%)	67,82,82	1.34	5 (7%)
12	EPH	D	1306	-	43,43,48	1.58	7 (16%)	46,48,53	1.28	3 (6%)
6	MLI	A	701	-	6,6,6	1.16	0	7,7,7	1.08	0
8	SF4	B	303	2	0,12,12	-	-	-		
9	F3S	B	304	2	0,9,9	-	-	-		
7	FES	B	302	2	0,4,4	-	-	-		
5	FAD	A	700	-	58,58,58	1.14	6 (10%)	85,89,89	1.63	17 (20%)

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
11	TFZ	C	1201	-	-	2/14/14/14	0/2/2/2
12	EPH	D	1306	-	1/1/4/14	23/47/47/52	-
6	MLI	A	701	-	-	2/4/4/4	-
9	F3S	B	304	2	-	-	0/3/3/3
10	HEM	C	1305	4,3	-	9/14/54/54	-
8	SF4	B	303	2	-	-	0/6/5/5
7	FES	B	302	2	-	-	0/1/1/1
5	FAD	A	700	-	-	10/34/50/50	0/6/6/6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1305	HEM	C3D-C2D	7.81	1.53	1.36
11	C	1201	TFZ	C3-C2	6.65	1.51	1.40
12	D	1306	EPH	O1-C3	4.53	1.47	1.34
10	C	1305	HEM	FE-ND	4.48	2.08	1.94
12	D	1306	EPH	O2-C4	4.34	1.46	1.33
5	A	700	FAD	C4X-N5	3.84	1.39	1.30
12	D	1306	EPH	C25-C24	3.74	1.52	1.31
12	D	1306	EPH	C29-C28	3.73	1.52	1.31
12	D	1306	EPH	C13-C12	3.72	1.52	1.31
10	C	1305	HEM	FE-NB	3.69	2.06	1.94
10	C	1305	HEM	FE-NC	3.44	2.06	1.95
12	D	1306	EPH	C15-C16	3.21	1.52	1.29
10	C	1305	HEM	FE-NA	3.18	2.05	1.95
10	C	1305	HEM	CAC-C3C	2.85	1.55	1.47
10	C	1305	HEM	CAB-C3B	2.83	1.54	1.47
5	A	700	FAD	C10-N1	2.76	1.38	1.33
5	A	700	FAD	C2A-N1A	2.75	1.38	1.33
11	C	1201	TFZ	C9-N	-2.60	1.36	1.41
12	D	1306	EPH	P1-O7	2.58	1.59	1.50
5	A	700	FAD	C2A-N3A	2.44	1.38	1.33
10	C	1305	HEM	CMA-C3A	2.23	1.55	1.50
10	C	1305	HEM	CMB-C2B	2.22	1.55	1.50
10	C	1305	HEM	CMD-C2D	2.13	1.55	1.50
10	C	1305	HEM	CMC-C2C	2.09	1.55	1.50
5	A	700	FAD	C8A-N7A	2.08	1.35	1.31
5	A	700	FAD	P-O3P	2.08	1.61	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	700	FAD	N3A-C2A-N1A	-5.93	119.61	128.58
10	C	1305	HEM	C4D-ND-C1D	5.53	111.75	105.21
12	D	1306	EPH	O1-C3-C5	4.38	120.95	111.48
5	A	700	FAD	C5A-C4A-N3A	-4.18	120.95	126.72
5	A	700	FAD	N9A-C8A-N7A	-3.81	108.53	113.94
5	A	700	FAD	C2A-N3A-C4A	3.40	120.14	111.83
5	A	700	FAD	C5A-N7A-C8A	3.35	108.72	103.45
5	A	700	FAD	C4-N3-C2	-3.18	119.99	125.64
10	C	1305	HEM	CAD-CBD-CGD	-3.11	105.43	113.67
5	A	700	FAD	C4'-C3'-C2'	-2.98	108.61	113.57
5	A	700	FAD	C4X-C4-N3	2.84	120.47	113.25
12	D	1306	EPH	O2-C4-C18	2.78	120.31	111.83
5	A	700	FAD	C9A-C5X-N5	-2.73	119.55	122.45
5	A	700	FAD	C10-C4X-N5	-2.71	119.27	124.81
5	A	700	FAD	N3A-C4A-N9A	2.68	131.72	127.17
12	D	1306	EPH	C30-C29-C28	-2.53	111.17	126.42
5	A	700	FAD	C4X-C10-N10	2.53	120.11	116.48
10	C	1305	HEM	CAD-C3D-C4D	2.52	129.08	124.70
5	A	700	FAD	C4A-C5A-N7A	-2.48	107.75	110.58
11	C	1201	TFZ	C1-C2-C3	2.42	125.15	121.96
5	A	700	FAD	C4-C4X-N5	2.37	121.49	118.21
5	A	700	FAD	O4-C4-C4X	-2.28	120.52	126.53
10	C	1305	HEM	C1B-NB-C4B	2.22	107.84	105.21
10	C	1305	HEM	C3B-C4B-NB	-2.14	107.93	109.47
5	A	700	FAD	C5X-C9A-N10	2.08	119.85	117.97
5	A	700	FAD	C4X-C10-N1	-2.06	119.54	124.59
11	C	1201	TFZ	F3-C1-C2	-2.05	109.00	112.65

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	D	1306	EPH	C2

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	700	FAD	N10-C1'-C2'-O2'
5	A	700	FAD	N10-C1'-C2'-C3'
5	A	700	FAD	PA-O3P-P-O5'
10	C	1305	HEM	C2B-C3B-CAB-CBB
10	C	1305	HEM	C4B-C3B-CAB-CBB
10	C	1305	HEM	C2C-C3C-CAC-CBC
12	D	1306	EPH	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
12	D	1306	EPH	C37-O5-P1-O6
12	D	1306	EPH	C37-O5-P1-O7
12	D	1306	EPH	C37-O5-P1-O8
12	D	1306	EPH	C5-C3-O1-C2
12	D	1306	EPH	C38-O8-P1-O5
12	D	1306	EPH	O8-C38-C39-N1
11	C	1201	TFZ	C3-C8-N-C9
12	D	1306	EPH	O3-C3-O1-C2
11	C	1201	TFZ	O-C8-N-C9
12	D	1306	EPH	C18-C4-O2-C1
12	D	1306	EPH	O4-C4-O2-C1
12	D	1306	EPH	C3-C5-C6-C7
5	A	700	FAD	C2'-C3'-C4'-C5'
12	D	1306	EPH	C19-C20-C21-C22
12	D	1306	EPH	C4-C18-C19-C20
10	C	1305	HEM	C4C-C3C-CAC-CBC
12	D	1306	EPH	C9-C10-C11-C12
12	D	1306	EPH	O2-C1-C2-C37
12	D	1306	EPH	C11-C10-C9-C8
5	A	700	FAD	O3'-C3'-C4'-C5'
12	D	1306	EPH	C18-C19-C20-C21
12	D	1306	EPH	C7-C8-C9-C10
5	A	700	FAD	C2'-C3'-C4'-O4'
5	A	700	FAD	P-O3P-PA-O1A
12	D	1306	EPH	C6-C7-C8-C9
5	A	700	FAD	O3'-C3'-C4'-O4'
6	A	701	MLI	C3-C1-C2-O7
5	A	700	FAD	O4B-C4B-C5B-O5B
6	A	701	MLI	C3-C1-C2-O6
12	D	1306	EPH	C1-C2-O1-C3
10	C	1305	HEM	CAD-CBD-CGD-O1D
10	C	1305	HEM	C3D-CAD-CBD-CGD
10	C	1305	HEM	CAD-CBD-CGD-O2D
10	C	1305	HEM	CAA-CBA-CGA-O1A
12	D	1306	EPH	C24-C25-C26-C27
10	C	1305	HEM	CAA-CBA-CGA-O2A
12	D	1306	EPH	C28-C29-C30-C31
12	D	1306	EPH	C20-C21-C22-C23
5	A	700	FAD	P-O3P-PA-O2A

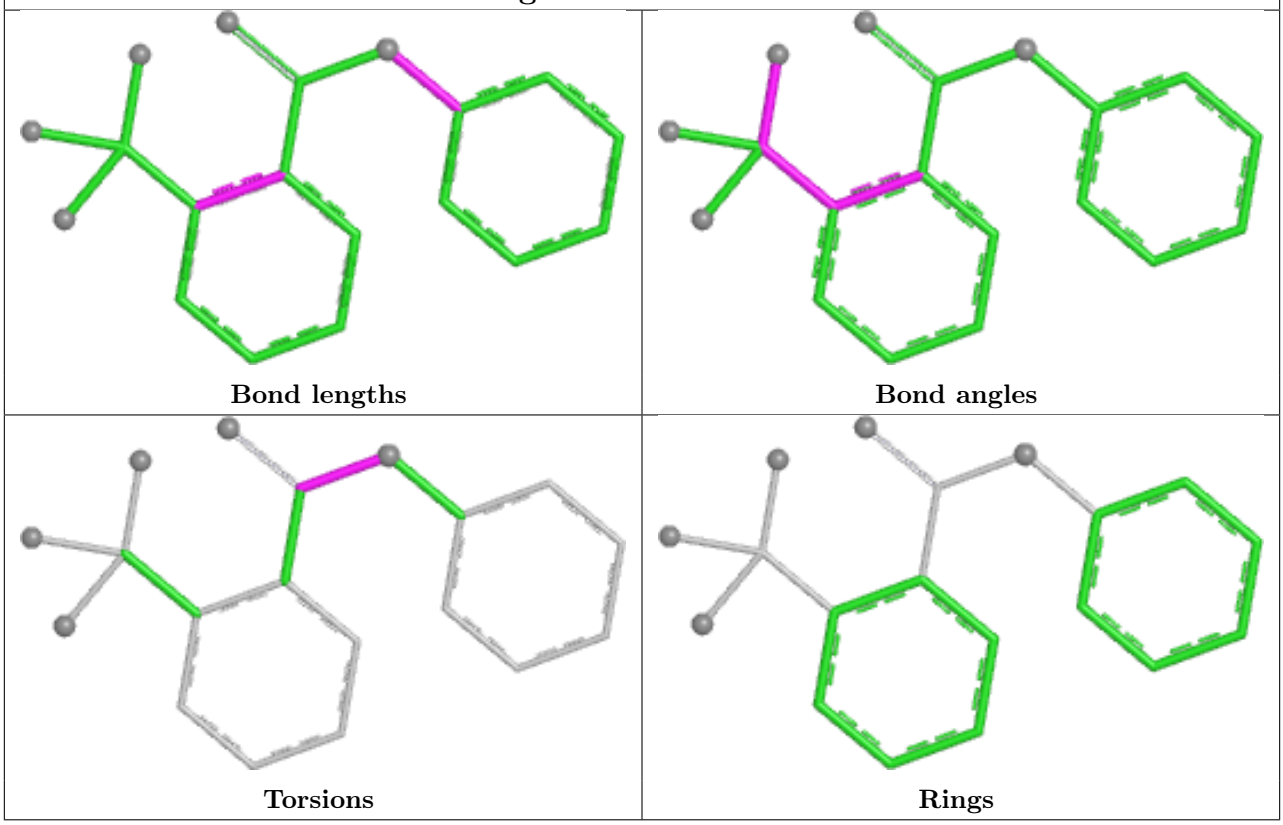
There are no ring outliers.

5 monomers are involved in 18 short contacts:

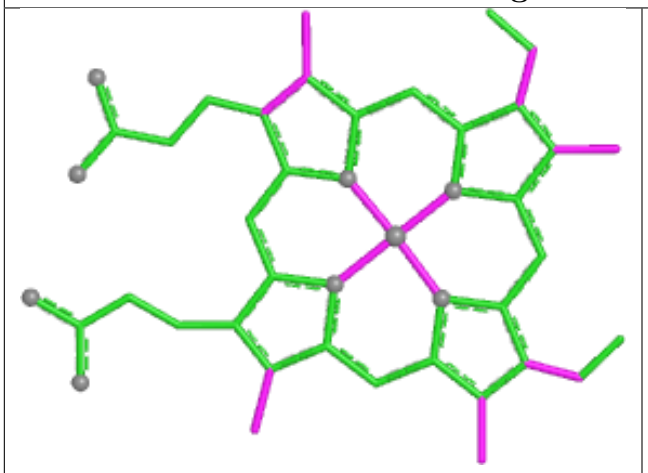
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	1201	TFZ	3	0
10	C	1305	HEM	1	0
6	A	701	MLI	3	0
9	B	304	F3S	1	0
5	A	700	FAD	10	0

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.

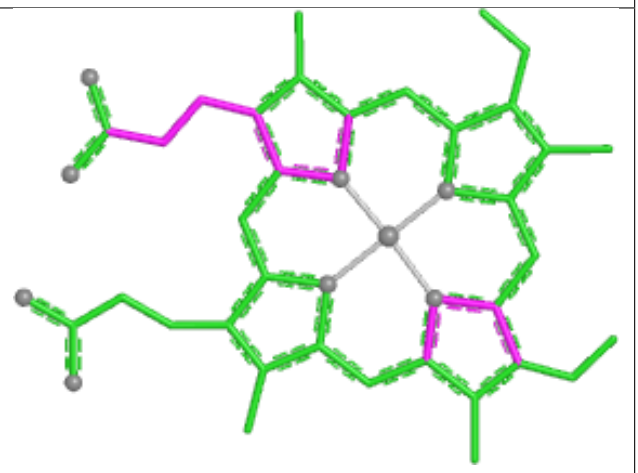
Ligand TFZ C 1201



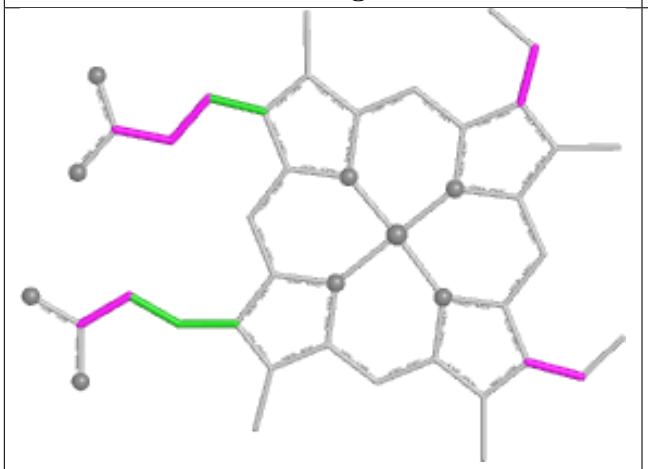
Ligand HEM C 1305



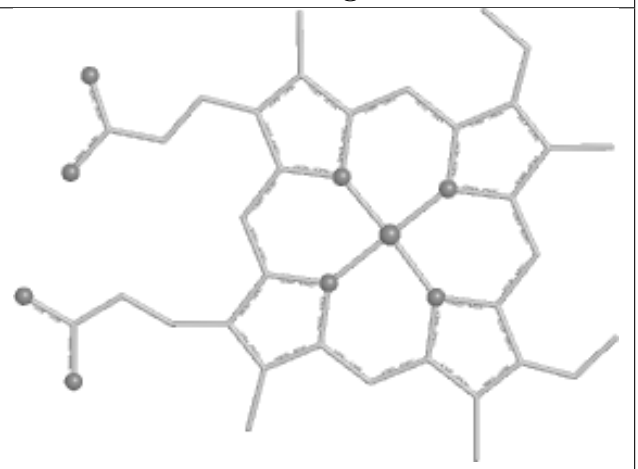
Bond lengths



Bond angles

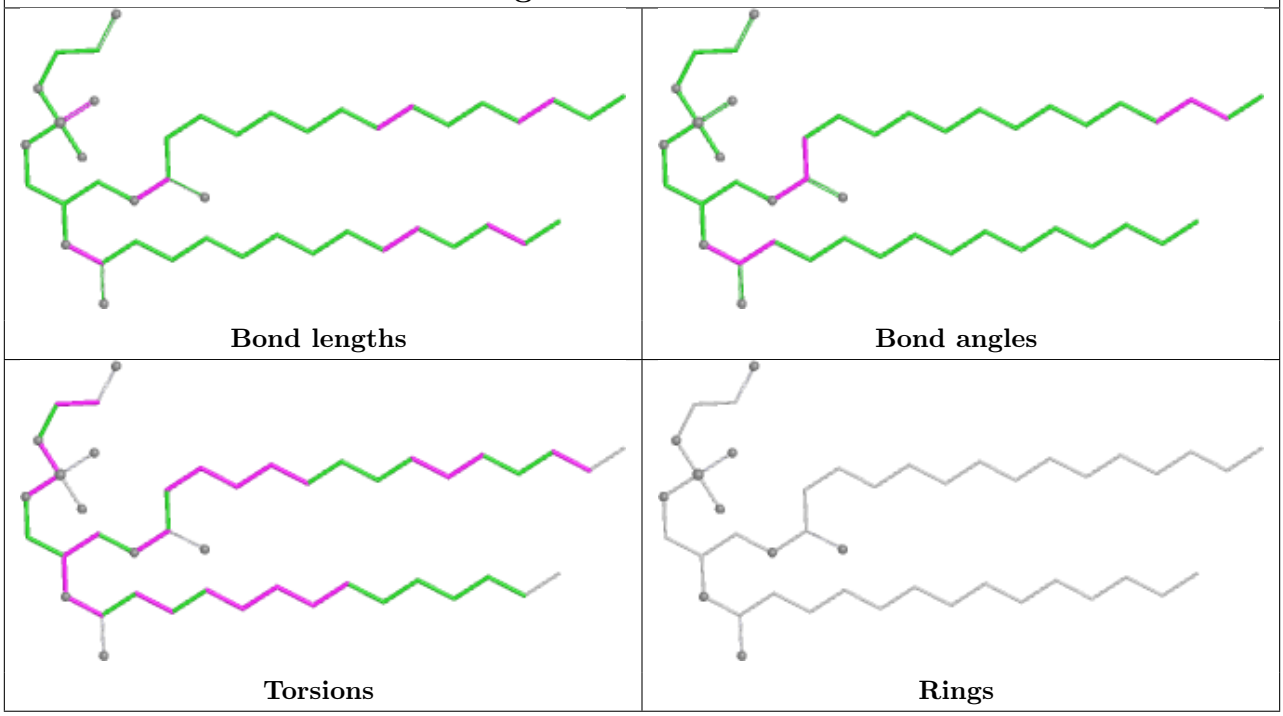


Torsions

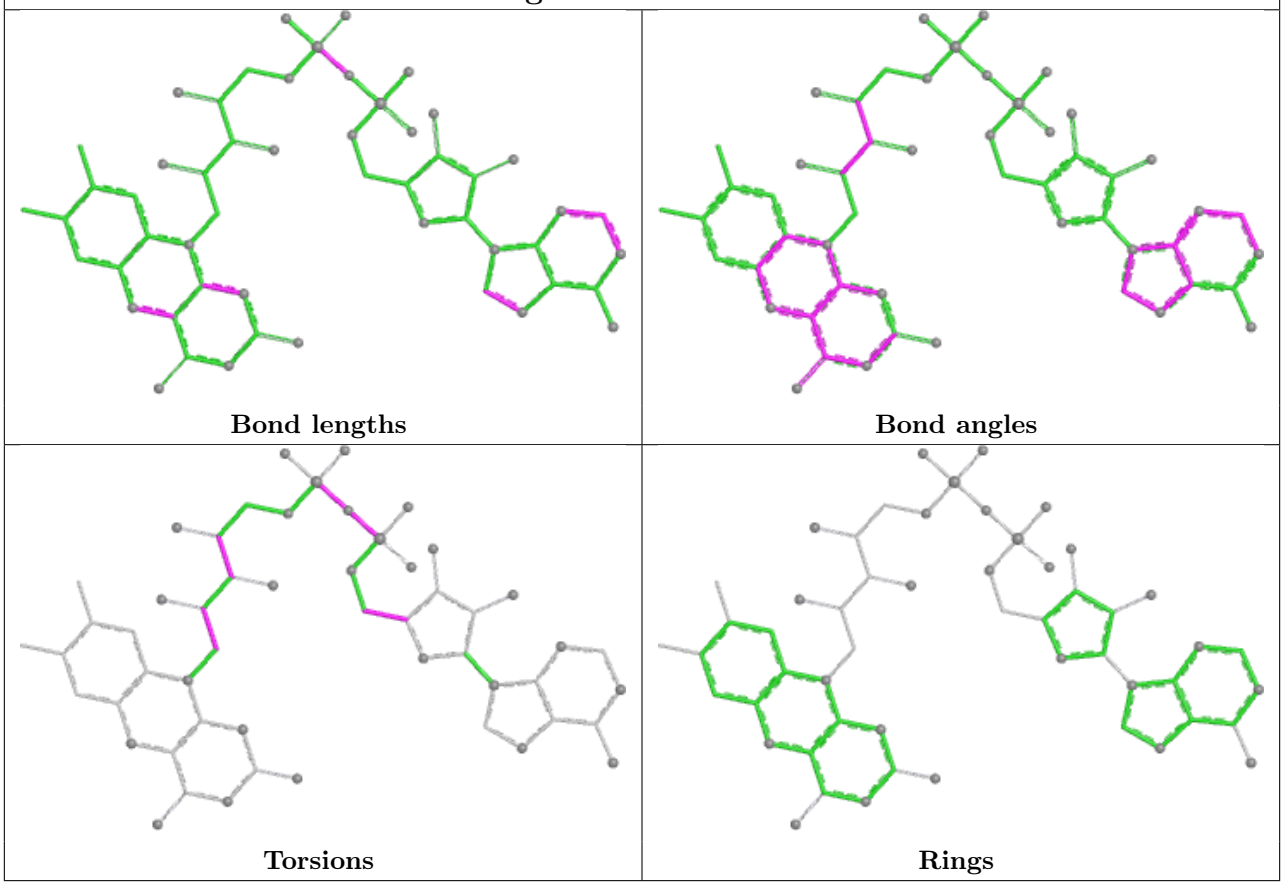


Rings

Ligand EPH D 1306



Ligand FAD A 700



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	613/622 (98%)	0.09	5 (0%)	82	65	57, 78, 109, 132	0
2	B	239/252 (94%)	0.09	2 (0%)	82	65	58, 73, 109, 131	0
3	C	138/140 (98%)	0.05	1 (0%)	84	68	66, 85, 128, 138	0
4	D	102/103 (99%)	0.04	1 (0%)	79	61	67, 83, 105, 118	0
All	All	1092/1117 (97%)	0.08	9 (0%)	82	65	57, 79, 112, 138	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	35	SER	4.6
2	B	9	PRO	3.3
3	C	82	LEU	3.2
2	B	134	GLU	2.7
1	A	271	GLY	2.4
1	A	152	ASP	2.3
1	A	315	CYS	2.1
1	A	326	LEU	2.0
1	A	325	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

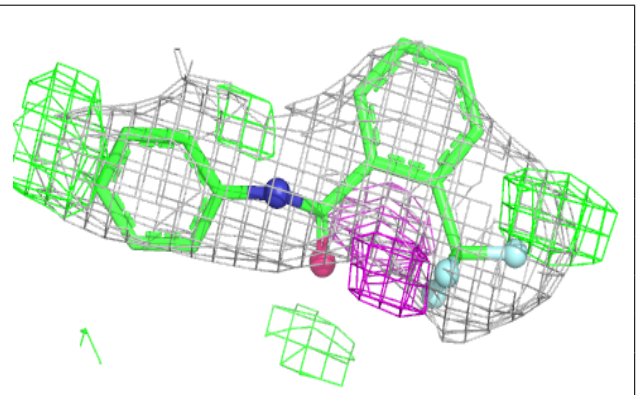
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

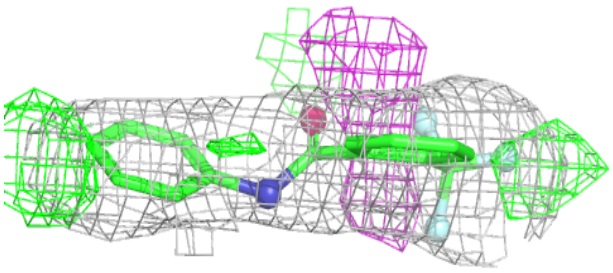
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	TFZ	C	1201	19/19	0.78	0.23	108,108,109,109	0
6	MLI	A	701	7/7	0.86	0.17	87,87,88,88	0
12	EPH	D	1306	44/49	0.87	0.21	115,121,127,127	0
5	FAD	A	700	53/53	0.91	0.14	62,63,68,69	0
10	HEM	C	1305	43/43	0.96	0.12	76,77,79,79	0
9	F3S	B	304	7/7	0.98	0.05	68,68,68,69	0
8	SF4	B	303	8/8	0.99	0.03	53,54,55,55	0
7	FES	B	302	4/4	1.00	0.03	58,58,59,60	0

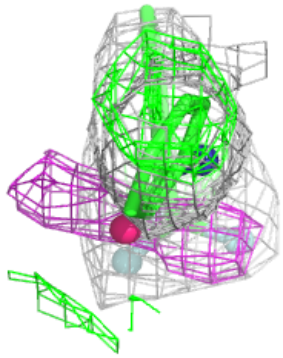
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TFZ C 1201:

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

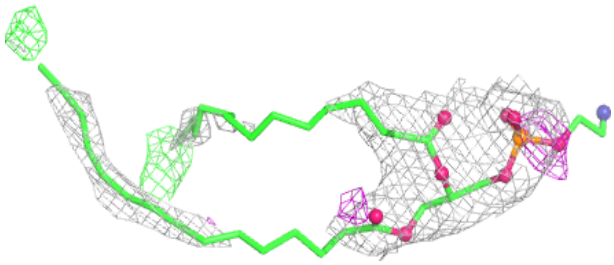


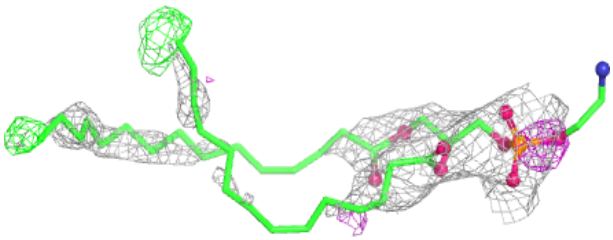


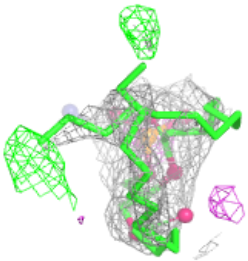


Electron density around EPH D 1306:

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

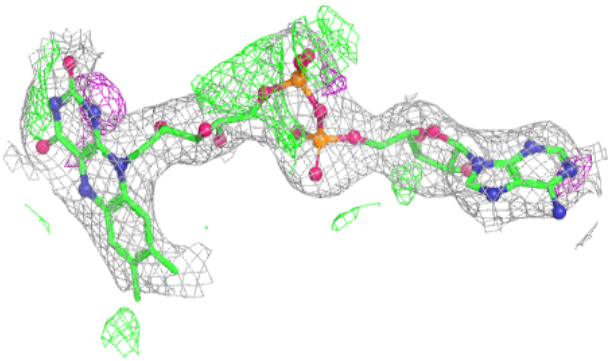


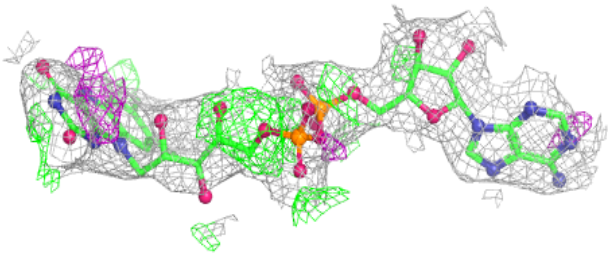


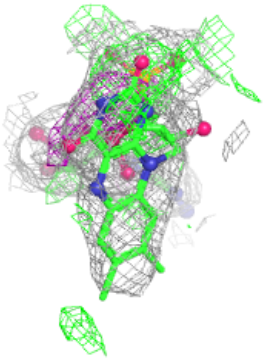


Electron density around FAD A 700:

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

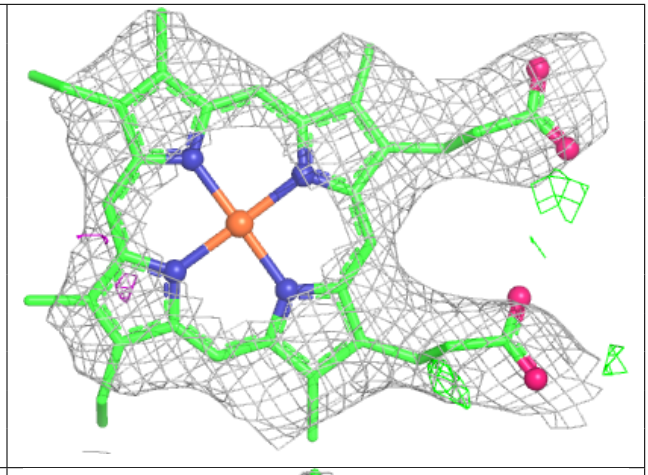


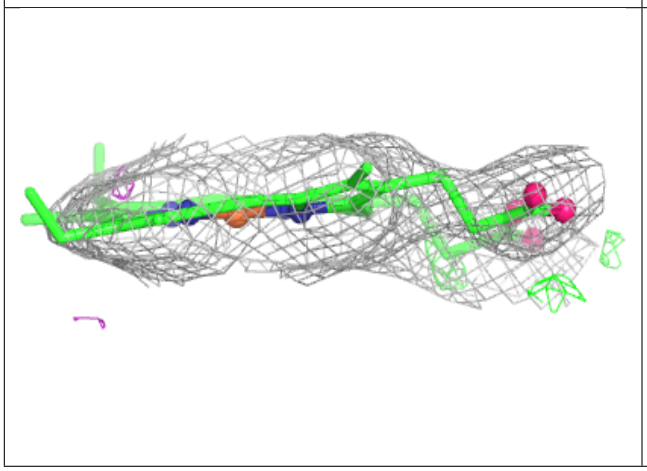


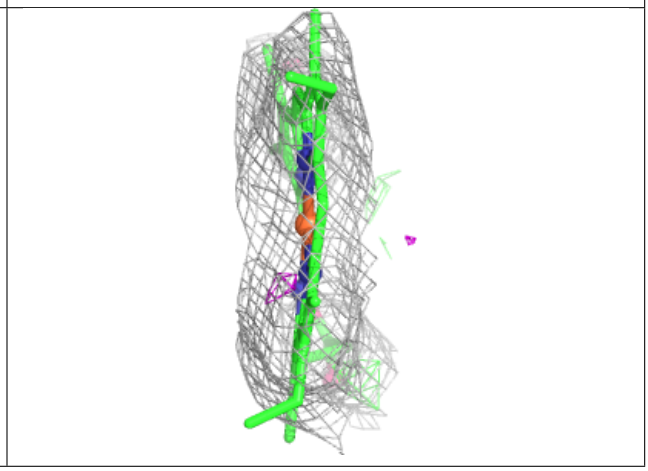


Electron density around HEM C 1305:

$2mF_o$-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.