



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:57 pm BST

PDB ID : 3ABV
Title : Crystal structure of porcine heart mitochondrial complex II bound with N-Bi
phenyl-3-yl-2-trifluoromethyl-benzamide
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A.; Sakamoto, K.; Mao, J.; Matsuoka, S.; Inoue, M.; Honma, T.; Tanaka, A.;
Kita, K.
Deposited on : 2009-12-22
Resolution : 3.24 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

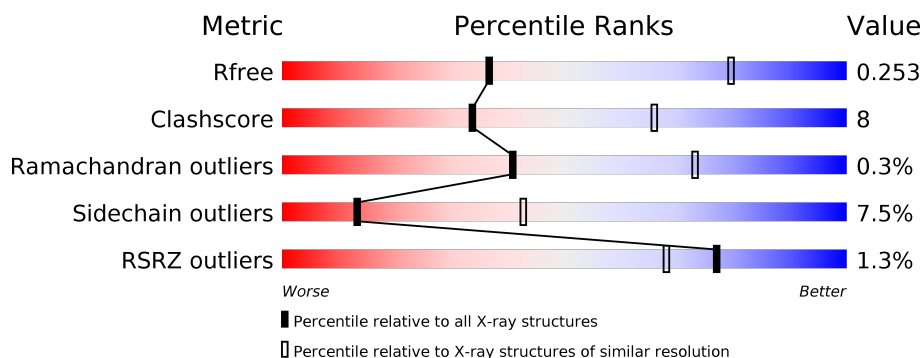
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	622	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>••</div> </div> </div>
2	B	252	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>• 5%</div> </div> </div>
3	C	140	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>••</div> </div> </div>
4	D	103	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>••</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MLI	A	701	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 8671 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
1	A	613	Total	C	N	O	S	0	0	0
			4729	2954	848	895	32			

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

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

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

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

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

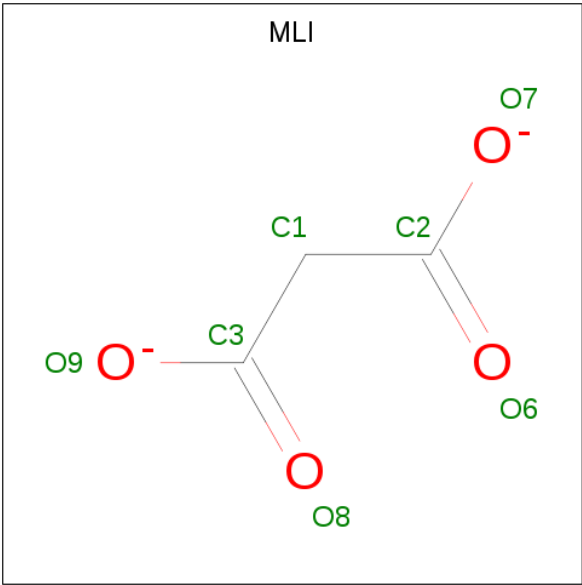
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			765	499	128	133	5			

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



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

- Molecule 6 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



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

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



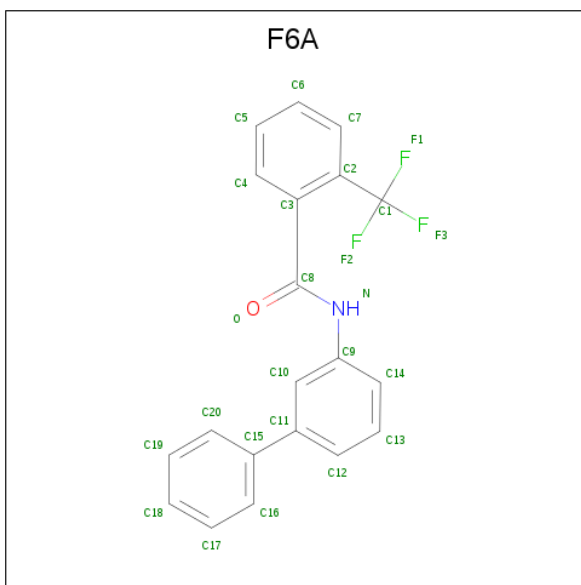
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



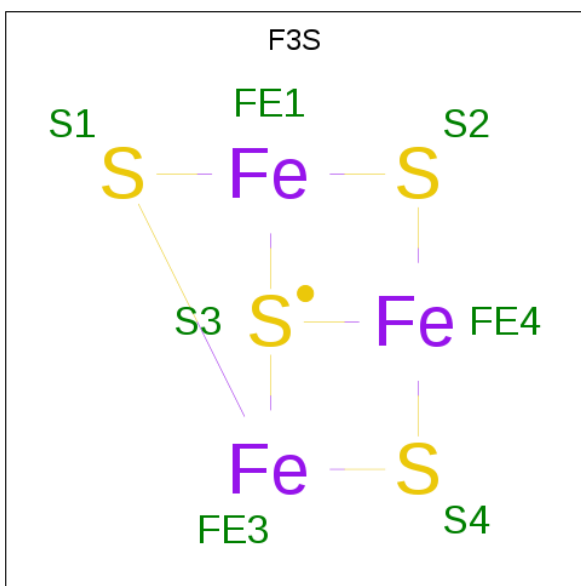
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is N-biphenyl-3-yl-2-(trifluoromethyl)benzamide (three-letter code: F6A) (formula: $\text{C}_{20}\text{H}_{14}\text{F}_3\text{NO}$).



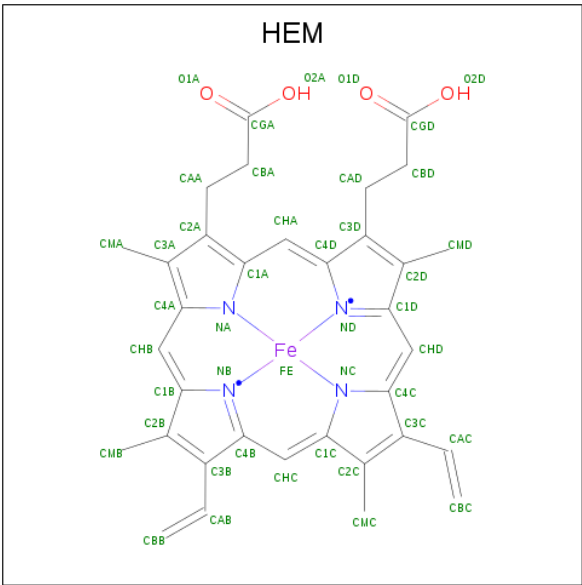
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	F	N	O	0	0
			25	20	3	1	1		

- Molecule 10 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



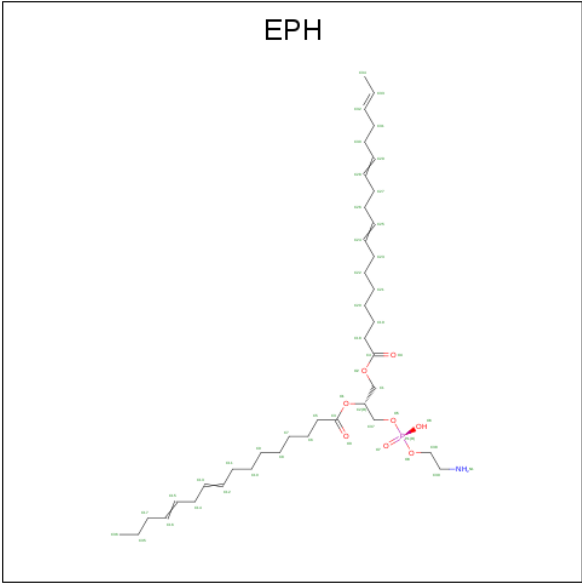
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

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

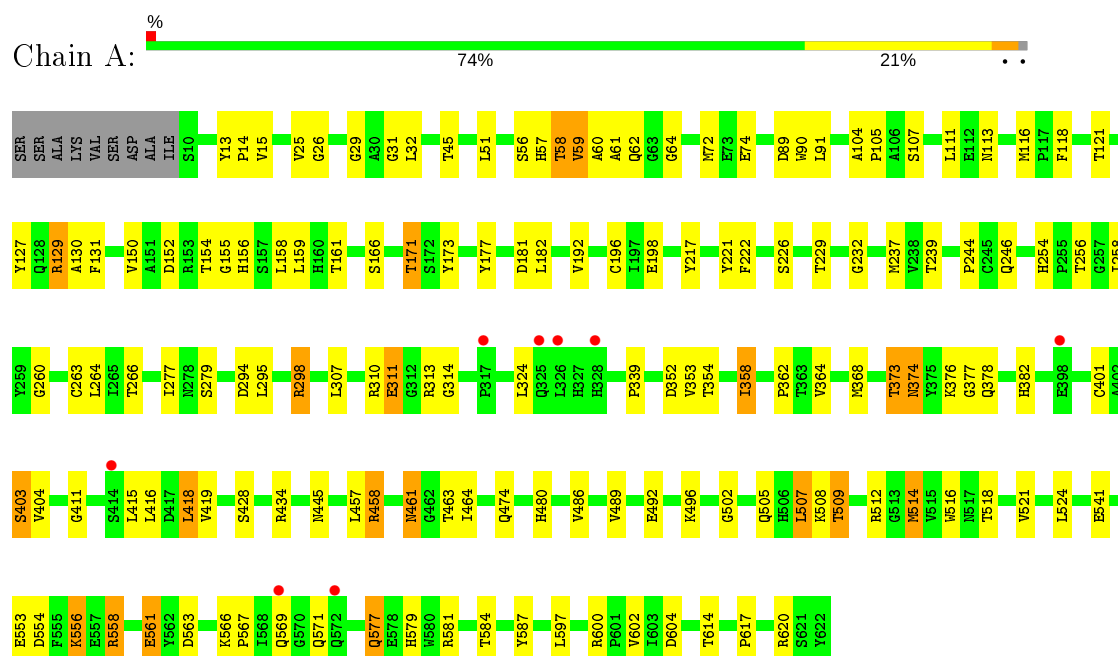


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

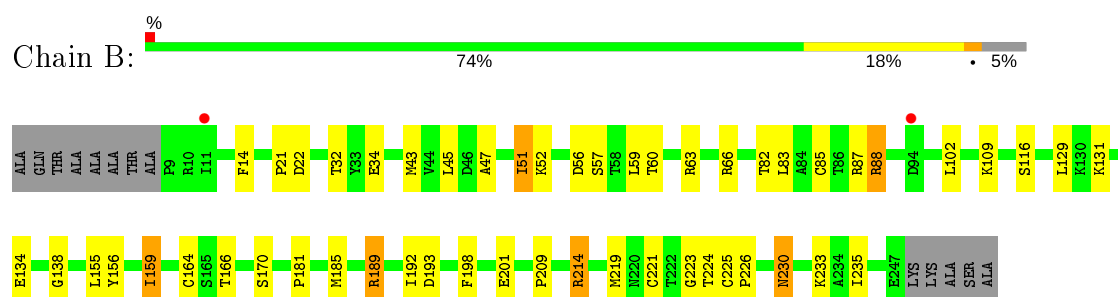
3 Residue-property plots

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

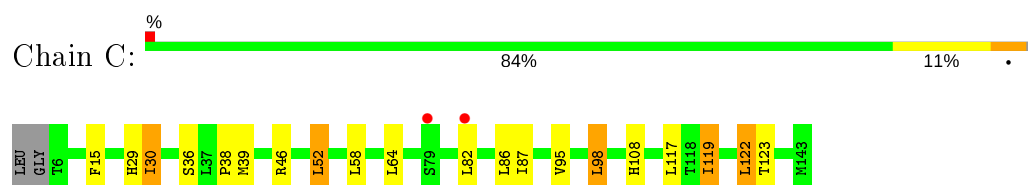
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial



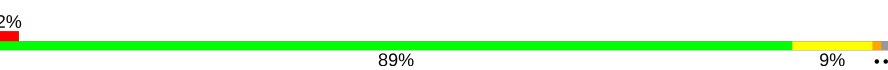
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



- Molecule 3: Succinate dehydrogenase cytochrome b560 subunit, mitochondrial



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

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.70 Å 84.17 Å 294.43 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.63 – 3.24 37.63 – 3.24	Depositor EDS
% Data completeness (in resolution range)	98.7 (37.63-3.24) 98.7 (37.63-3.24)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.53 (at 3.25 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.253 0.204 , 0.253	Depositor DCC
R_{free} test set	1474 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8671	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MLI, F6A, F3S, FES, EPH, HEM, 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	0.36	0/4828	0.55	0/6531
2	B	0.37	0/1964	0.54	0/2648
3	C	0.36	0/1091	0.50	0/1483
4	D	0.35	0/784	0.51	0/1066
All	All	0.36	0/8667	0.54	0/11728

There are no bond length outliers.

There are no bond angle outliers.

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	105	0
2	B	1922	0	1900	32	0
3	C	1064	0	1104	13	0
4	D	765	0	773	4	0
5	A	53	0	31	11	0
6	A	7	0	2	2	0
7	B	4	0	0	0	0
8	B	8	0	0	0	0
9	B	25	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	7	0	0	0	0
11	C	43	0	30	3	0
12	D	44	0	53	1	0
All	All	8671	0	8525	145	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 (145) 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:HM82	1.20	1.46
1:A:61:ALA:HB3	1:A:155:GLY:HA3	1.30	1.10
2:B:102:LEU:HB3	2:B:166:THR:HG21	1.42	0.99
1:A:57:HIS:CE1	5:A:700:FAD:HM82	2.09	0.87
1:A:152:ASP:HB2	1:A:339:PRO:HD2	1.59	0.83
1:A:51:LEU:HD21	1:A:229:THR:HG21	1.65	0.78
1:A:563:ASP:H	1:A:571:GLN:HE22	1.31	0.76
1:A:181:ASP:HA	1:A:237:MET:HG2	1.70	0.74
1:A:486:VAL:HG12	1:A:553:GLU:HB2	1.71	0.72
1:A:56:SER:O	1:A:59:VAL:HG22	1.88	0.72
1:A:59:VAL:HG13	1:A:159:LEU:HD23	1.73	0.70
1:A:111:LEU:HD11	1:A:419:VAL:HG21	1.74	0.70
12:D:1306:EPH:H141	12:D:1306:EPH:H301	1.75	0.68
2:B:51:ILE:HD11	2:B:59:LEU:HD22	1.77	0.67
1:A:415:LEU:HG	5:A:700:FAD:C2	2.25	0.66
1:A:64:GLY:HA2	1:A:154:THR:HG21	1.77	0.66
1:A:57:HIS:O	1:A:59:VAL:N	2.29	0.65
1:A:61:ALA:HB3	1:A:155:GLY:CA	2.17	0.64
1:A:57:HIS:CE1	1:A:226:SER:HA	2.35	0.62
1:A:374:ASN:HB3	1:A:376:LYS:H	1.63	0.62
1:A:29:GLY:H	1:A:58:THR:HG21	1.65	0.62
2:B:181:PRO:HA	2:B:235:ILE:HD11	1.82	0.61
1:A:58:THR:HG22	5:A:700:FAD:O1A	2.01	0.61
4:D:72:LEU:O	4:D:76:LEU:HB2	2.01	0.60
2:B:198:PHE:HD2	2:B:201:GLU:HG3	1.66	0.60
1:A:57:HIS:NE2	5:A:700:FAD:HM81	2.14	0.58
1:A:492:GLU:O	1:A:496:LYS:HB2	2.04	0.56
1:A:129:ARG:HH11	1:A:130:ALA:H	1.51	0.56
1:A:279:SER:HB3	1:A:314:GLY:O	2.06	0.56
1:A:72:MET:CE	1:A:121:THR:HG21	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LEU:O	1:A:509:THR:HG21	2.05	0.55
1:A:72:MET:HE3	1:A:121:THR:HG21	1.89	0.55
1:A:579:HIS:HD2	1:A:581:ARG:H	1.54	0.55
1:A:518:THR:HA	1:A:521:VAL:HG22	1.88	0.55
2:B:116:SER:HB2	3:C:15:PHE:HD1	1.72	0.54
2:B:198:PHE:CD2	2:B:201:GLU:HG3	2.43	0.54
1:A:307:LEU:O	1:A:311:GLU:HG2	2.08	0.53
2:B:230:ASN:ND2	2:B:233:LYS:H	2.07	0.53
2:B:52:LYS:HA	2:B:56:ASP:O	2.09	0.53
1:A:254:HIS:HD2	1:A:256:THR:H	1.56	0.52
1:A:89:ASP:OD2	1:A:620:ARG:HD3	2.09	0.52
2:B:214:ARG:NH2	4:D:86:GLN:OE1	2.42	0.52
1:A:307:LEU:HD12	1:A:310:ARG:HD2	1.91	0.51
1:A:374:ASN:HB2	1:A:378:GLN:H	1.75	0.51
2:B:189:ARG:NH2	2:B:193:ASP:OD1	2.44	0.51
1:A:434:ARG:HE	1:A:434:ARG:HA	1.75	0.51
1:A:64:GLY:CA	1:A:154:THR:HG21	2.41	0.51
1:A:373:THR:HG23	1:A:377:GLY:HA2	1.93	0.51
1:A:57:HIS:C	1:A:59:VAL:N	2.63	0.50
1:A:221:TYR:CG	1:A:364:VAL:HG21	2.47	0.50
1:A:89:ASP:OD2	1:A:558:ARG:NH1	2.44	0.50
2:B:47:ALA:O	2:B:51:ILE:HG23	2.12	0.50
1:A:352:ASP:OD1	1:A:354:THR:HG22	2.11	0.49
1:A:566:LYS:HB2	1:A:567:PRO:HD2	1.94	0.49
1:A:25:VAL:HG21	1:A:192:VAL:HG11	1.95	0.49
3:C:64:LEU:HG	4:D:115:GLY:HA2	1.94	0.49
3:C:36:SER:HB2	3:C:38:PRO:HD2	1.95	0.49
1:A:60:ALA:HB1	5:A:700:FAD:HM72	1.95	0.49
1:A:104:ALA:HB3	1:A:105:PRO:HD3	1.94	0.49
1:A:166:SER:HB2	1:A:173:TYR:OH	2.13	0.49
1:A:244:PRO:HB3	1:A:587:TYR:CZ	2.48	0.48
1:A:104:ALA:HA	1:A:416:LEU:HD11	1.93	0.48
2:B:14:PHE:O	2:B:32:THR:HA	2.12	0.48
1:A:480:HIS:HD2	1:A:489:VAL:O	1.97	0.48
1:A:177:TYR:CE2	1:A:196:CYS:HB2	2.48	0.48
1:A:458:ARG:NH2	1:A:514:MET:HG2	2.28	0.48
1:A:581:ARG:HH22	1:A:604:ASP:CG	2.17	0.48
1:A:156:HIS:HE1	2:B:156:TYR:O	1.97	0.48
3:C:52:LEU:HD21	3:C:98:LEU:HA	1.94	0.48
1:A:58:THR:CG2	5:A:700:FAD:O1A	2.62	0.48
1:A:254:HIS:O	1:A:362:PRO:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ILE:O	1:A:507:LEU:HA	2.13	0.48
4:D:57:LEU:HB2	4:D:58:PRO:HD3	1.94	0.47
1:A:298:ARG:NH2	1:A:411:GLY:HA2	2.30	0.47
1:A:463:THR:HG23	1:A:464:ILE:HG13	1.97	0.47
1:A:264:LEU:HD22	5:A:700:FAD:C6	2.45	0.47
2:B:45:LEU:HD22	2:B:85:CYS:HB3	1.96	0.47
1:A:415:LEU:HA	1:A:418:LEU:HD22	1.96	0.46
2:B:209:PRO:O	2:B:214:ARG:NH1	2.49	0.46
1:A:373:THR:HG22	1:A:374:ASN:O	2.16	0.46
2:B:233:LYS:HA	3:C:117:LEU:HD13	1.98	0.46
1:A:118:PHE:HA	1:A:150:VAL:HG22	1.97	0.46
2:B:159:ILE:HA	2:B:159:ILE:HD13	1.77	0.46
1:A:561:GLU:OE2	1:A:581:ARG:NH1	2.48	0.46
1:A:113:ASN:ND2	2:B:138:GLY:H	2.14	0.45
1:A:57:HIS:CD2	5:A:700:FAD:C8M	2.93	0.45
1:A:116:MET:HA	1:A:161:THR:HG21	1.98	0.45
2:B:155:LEU:HD23	2:B:185:MET:HE2	1.98	0.45
1:A:604:ASP:O	1:A:614:THR:HG23	2.16	0.45
2:B:52:LYS:HD2	2:B:57:SER:HA	1.99	0.45
1:A:26:GLY:O	1:A:31:GLY:HA3	2.16	0.45
1:A:61:ALA:HA	5:A:700:FAD:N5	2.31	0.45
1:A:129:ARG:HA	1:A:129:ARG:HD2	1.49	0.45
1:A:91:LEU:HA	1:A:602:VAL:HG11	1.99	0.44
1:A:57:HIS:O	1:A:58:THR:C	2.56	0.44
2:B:230:ASN:HD22	2:B:230:ASN:C	2.21	0.44
3:C:29:HIS:HD2	3:C:30:ILE:HG23	1.82	0.44
2:B:21:PRO:HD2	2:B:109:LYS:HG3	1.98	0.44
1:A:461:ASN:HA	1:A:508:LYS:HD2	2.00	0.44
1:A:502:GLY:O	1:A:505:GLN:HG2	2.18	0.44
1:A:217:TYR:HB3	1:A:232:GLY:HA3	2.00	0.43
3:C:46:ARG:HE	11:C:1305:HEM:CGA	2.31	0.43
1:A:382:HIS:CE1	1:A:600:ARG:HB3	2.54	0.43
3:C:82:LEU:HB3	3:C:86:LEU:HD23	1.99	0.43
1:A:258:ILE:HG22	1:A:263:CYS:H	1.83	0.43
1:A:258:ILE:HG22	1:A:263:CYS:N	2.34	0.43
2:B:225:CYS:HA	2:B:226:PRO:HD3	1.90	0.43
1:A:521:VAL:HA	1:A:524:LEU:HD12	2.01	0.43
1:A:556:LYS:HD2	1:A:556:LYS:H	1.84	0.43
1:A:353:VAL:HG12	1:A:358:ILE:HD11	2.00	0.43
2:B:131:LYS:HB2	2:B:134:GLU:HG3	2.00	0.43
1:A:434:ARG:NE	1:A:434:ARG:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:HIS:C	1:A:59:VAL:H	2.21	0.43
1:A:266:THR:HA	6:A:701:MLI:O6	2.18	0.42
1:A:150:VAL:HB	1:A:154:THR:HA	2.01	0.42
5:A:700:FAD:H9	5:A:700:FAD:H1'1	1.81	0.42
1:A:90:TRP:HZ3	1:A:620:ARG:HB2	1.84	0.42
2:B:82:THR:HB	2:B:83:LEU:H	1.70	0.42
1:A:514:MET:H	2:B:22:ASP:CG	2.22	0.42
1:A:295:LEU:HD12	1:A:295:LEU:HA	1.90	0.42
1:A:90:TRP:CE2	1:A:617:PRO:HA	2.54	0.42
9:B:1201:F6A:C5	3:C:46:ARG:HG3	2.49	0.42
2:B:164:CYS:HB2	2:B:221:CYS:HB2	2.02	0.42
1:A:246:GLN:HA	1:A:584:THR:O	2.20	0.41
2:B:219:MET:HB3	3:C:122:LEU:HD21	2.03	0.41
1:A:401:CYS:C	1:A:403:SER:H	2.23	0.41
1:A:246:GLN:HE22	1:A:600:ARG:HE	1.69	0.41
1:A:298:ARG:HH22	6:A:701:MLI:C3	2.32	0.41
1:A:577:GLN:H	1:A:577:GLN:NE2	2.19	0.41
1:A:13:TYR:HA	1:A:14:PRO:HD3	1.93	0.41
1:A:62:GLN:O	1:A:154:THR:HG22	2.20	0.41
1:A:373:THR:CG2	1:A:377:GLY:HA2	2.50	0.41
1:A:45:THR:HB	1:A:171:THR:HG23	2.02	0.41
1:A:113:ASN:HD22	2:B:138:GLY:H	1.68	0.41
3:C:52:LEU:HB3	11:C:1305:HEM:CMB	2.51	0.41
3:C:52:LEU:HB3	11:C:1305:HEM:HMB1	2.02	0.41
1:A:373:THR:CG2	1:A:374:ASN:O	2.68	0.41
1:A:158:LEU:HD23	1:A:415:LEU:HD22	2.02	0.41
1:A:222:PHE:HA	1:A:474:GLN:HE21	1.85	0.41
1:A:458:ARG:HH21	1:A:514:MET:HG2	1.85	0.41
1:A:127:TYR:CZ	1:A:129:ARG:HD3	2.56	0.41
2:B:43:MET:HA	2:B:88:ARG:HA	2.02	0.41
1:A:182:LEU:HD12	1:A:237:MET:CE	2.50	0.40
1:A:516:TRP:HB3	2:B:60:THR:HG21	2.03	0.40
2:B:223:GLY:HA2	3:C:119:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	611/622 (98%)	573 (94%)	36 (6%)	2 (0%)	41	73
2	B	237/252 (94%)	220 (93%)	17 (7%)	0	100	100
3	C	136/140 (97%)	132 (97%)	4 (3%)	0	100	100
4	D	100/103 (97%)	96 (96%)	3 (3%)	1 (1%)	15	50
All	All	1084/1117 (97%)	1021 (94%)	60 (6%)	3 (0%)	41	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	569	GLN
1	A	260	GLY
4	D	95	ASP

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/506 (99%)	460 (92%)	39 (8%)	12	41
2	B	214/220 (97%)	200 (94%)	14 (6%)	17	49
3	C	117/118 (99%)	106 (91%)	11 (9%)	8	31
4	D	76/76 (100%)	72 (95%)	4 (5%)	22	56
All	All	906/920 (98%)	838 (92%)	68 (8%)	13	43

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	32	LEU
1	A	58	THR
1	A	59	VAL
1	A	74	GLU
1	A	107	SER
1	A	129	ARG
1	A	131	PHE
1	A	171	THR
1	A	198	GLU
1	A	239	THR
1	A	277	ILE
1	A	294	ASP
1	A	298	ARG
1	A	311	GLU
1	A	313	ARG
1	A	324	LEU
1	A	358	ILE
1	A	368	MET
1	A	373	THR
1	A	374	ASN
1	A	403	SER
1	A	404	VAL
1	A	418	LEU
1	A	428	SER
1	A	445	ASN
1	A	458	ARG
1	A	461	ASN
1	A	507	LEU
1	A	509	THR
1	A	512	ARG
1	A	514	MET
1	A	541	GLU
1	A	554	ASP
1	A	556	LYS
1	A	558	ARG
1	A	561	GLU
1	A	577	GLN
1	A	597	LEU
2	B	34	GLU
2	B	51	ILE
2	B	63	ARG
2	B	66	ARG

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Mol	Chain	Res	Type
2	B	87	ARG
2	B	88	ARG
2	B	129	LEU
2	B	159	ILE
2	B	170	SER
2	B	189	ARG
2	B	192	ILE
2	B	214	ARG
2	B	224	THR
2	B	230	ASN
3	C	30	ILE
3	C	39	MET
3	C	52	LEU
3	C	58	LEU
3	C	87	ILE
3	C	95	VAL
3	C	98	LEU
3	C	108	HIS
3	C	119	ILE
3	C	122	LEU
3	C	123	THR
4	D	76	LEU
4	D	78	LEU
4	D	134	TRP
4	D	136	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	113	ASN
1	A	128	GLN
1	A	246	GLN
1	A	254	HIS
1	A	327	HIS
1	A	384	ASN
1	A	445	ASN
1	A	453	ASN
1	A	461	ASN
1	A	480	HIS
1	A	527	GLN
1	A	550	HIS

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Mol	Chain	Res	Type
1	A	571	GLN
1	A	577	GLN
1	A	579	HIS
2	B	121	GLN
2	B	174	ASN
2	B	220	ASN
2	B	230	ASN
3	C	29	HIS
3	C	104	ASN

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 carbohydrates 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	$\# Z > 2$
5	FAD	A	700	1	51,58,58	1.42	7 (13%)	60,89,89	1.68	10 (16%)
12	EPH	D	1306	-	43,43,48	1.60	7 (16%)	45,48,53	1.20	2 (4%)
8	SF4	B	303	2	0,12,12	0.00	-	-		
6	MLI	A	701	-	0,6,6	0.00	-	0,7,7	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	F6A	B	1201	-	27,27,27	1.26	2 (7%)	38,38,38	0.81	1 (2%)
7	FES	B	302	2	0,4,4	0.00	-	-		
11	HEM	C	1305	3,4	27,50,50	2.19	6 (22%)	17,82,82	1.35	3 (17%)
10	F3S	B	304	2	0,9,9	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	A	700	1	-	6/30/50/50	0/6/6/6
12	EPH	D	1306	-	-	28/47/47/52	-
8	SF4	B	303	2	-	-	0/6/5/5
6	MLI	A	701	-	-	0/0/4/4	-
9	F6A	B	1201	-	-	2/18/18/18	0/3/3/3
7	FES	B	302	2	-	-	0/1/1/1
11	HEM	C	1305	3,4	-	0/6/54/54	-
10	F3S	B	304	2	-	-	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1305	HEM	C3D-C2D	5.41	1.53	1.37
9	B	1201	F6A	C3-C2	5.40	1.49	1.40
11	C	1305	HEM	C3C-C2C	-4.81	1.33	1.40
12	D	1306	EPH	O1-C3	4.62	1.47	1.34
12	D	1306	EPH	O2-C4	4.44	1.46	1.33
11	C	1305	HEM	C3B-C2B	-4.32	1.34	1.40
5	A	700	FAD	C10-N1	4.31	1.38	1.33
5	A	700	FAD	C2A-N3A	4.11	1.38	1.32
5	A	700	FAD	C4X-N5	4.04	1.39	1.33
12	D	1306	EPH	C13-C12	3.76	1.53	1.31
12	D	1306	EPH	C29-C28	3.67	1.53	1.31
12	D	1306	EPH	C25-C24	3.66	1.53	1.31
11	C	1305	HEM	C3C-CAC	3.41	1.54	1.47
5	A	700	FAD	C4-N3	3.36	1.38	1.33
11	C	1305	HEM	C3B-CAB	3.31	1.54	1.47
12	D	1306	EPH	C15-C16	3.18	1.53	1.29
9	B	1201	F6A	C9-N	-2.85	1.35	1.41
5	A	700	FAD	C2A-N1A	2.69	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	1306	EPH	P1-O7	2.59	1.60	1.50
5	A	700	FAD	C1'-N10	2.42	1.50	1.48
5	A	700	FAD	C5X-N5	2.30	1.39	1.35
11	C	1305	HEM	CAA-C2A	2.02	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	FAD	N3A-C2A-N1A	-5.88	119.48	128.68
5	A	700	FAD	C4-N3-C2	5.50	119.79	115.14
5	A	700	FAD	C4X-N5-C5X	4.41	121.17	116.77
12	D	1306	EPH	O1-C3-C5	4.33	120.83	111.50
5	A	700	FAD	C10-C4X-N5	-3.87	118.58	121.26
9	B	1201	F6A	F2-C1-C2	-3.18	107.16	112.70
5	A	700	FAD	C4-C4X-N5	3.09	122.13	118.60
5	A	700	FAD	P-O3P-PA	-2.86	123.01	132.83
12	D	1306	EPH	O2-C4-C18	2.63	120.16	111.91
5	A	700	FAD	C5X-C9A-N10	2.52	119.54	117.72
11	C	1305	HEM	C1D-C2D-C3D	-2.43	105.31	107.00
5	A	700	FAD	C4X-C4-N3	-2.19	120.44	123.43
5	A	700	FAD	C4'-C3'-C2'	-2.19	108.81	113.36
11	C	1305	HEM	CAD-CBD-CGD	-2.13	109.10	112.67
5	A	700	FAD	C1'-C2'-C3'	2.11	115.68	109.79
11	C	1305	HEM	CAA-CBA-CGA	-2.00	109.31	112.67

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	700	FAD	N10-C1'-C2'-O2'
5	A	700	FAD	C5'-O5'-P-O1P
5	A	700	FAD	C5'-O5'-P-O2P
12	D	1306	EPH	O2-C1-C2-O1
12	D	1306	EPH	C28-C29-C30-C31
12	D	1306	EPH	C37-O5-P1-O7
12	D	1306	EPH	C37-O5-P1-O8
12	D	1306	EPH	C14-C15-C16-C17
12	D	1306	EPH	O8-C38-C39-N1
9	B	1201	F6A	C3-C8-N-C9
12	D	1306	EPH	C23-C24-C25-C26
12	D	1306	EPH	C27-C28-C29-C30
9	B	1201	F6A	O-C8-N-C9

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Mol	Chain	Res	Type	Atoms
12	D	1306	EPH	C4-C18-C19-C20
12	D	1306	EPH	C11-C12-C13-C14
12	D	1306	EPH	C7-C8-C9-C10
12	D	1306	EPH	C11-C10-C9-C8
12	D	1306	EPH	C20-C21-C22-C23
12	D	1306	EPH	C18-C4-O2-C1
12	D	1306	EPH	O2-C1-C2-C37
12	D	1306	EPH	C12-C13-C14-C15
5	A	700	FAD	PA-O3P-P-O5'
12	D	1306	EPH	C25-C26-C27-C28
12	D	1306	EPH	O1-C2-C37-O5
12	D	1306	EPH	O4-C4-O2-C1
12	D	1306	EPH	C3-C5-C6-C7
12	D	1306	EPH	C21-C22-C23-C24
12	D	1306	EPH	C1-C2-C37-O5
12	D	1306	EPH	C6-C7-C8-C9
12	D	1306	EPH	C9-C10-C11-C12
12	D	1306	EPH	C13-C14-C15-C16
12	D	1306	EPH	C24-C25-C26-C27
5	A	700	FAD	C5'-O5'-P-O3P
5	A	700	FAD	O4B-C4B-C5B-O5B
12	D	1306	EPH	C38-O8-P1-O7
12	D	1306	EPH	C2-C37-O5-P1

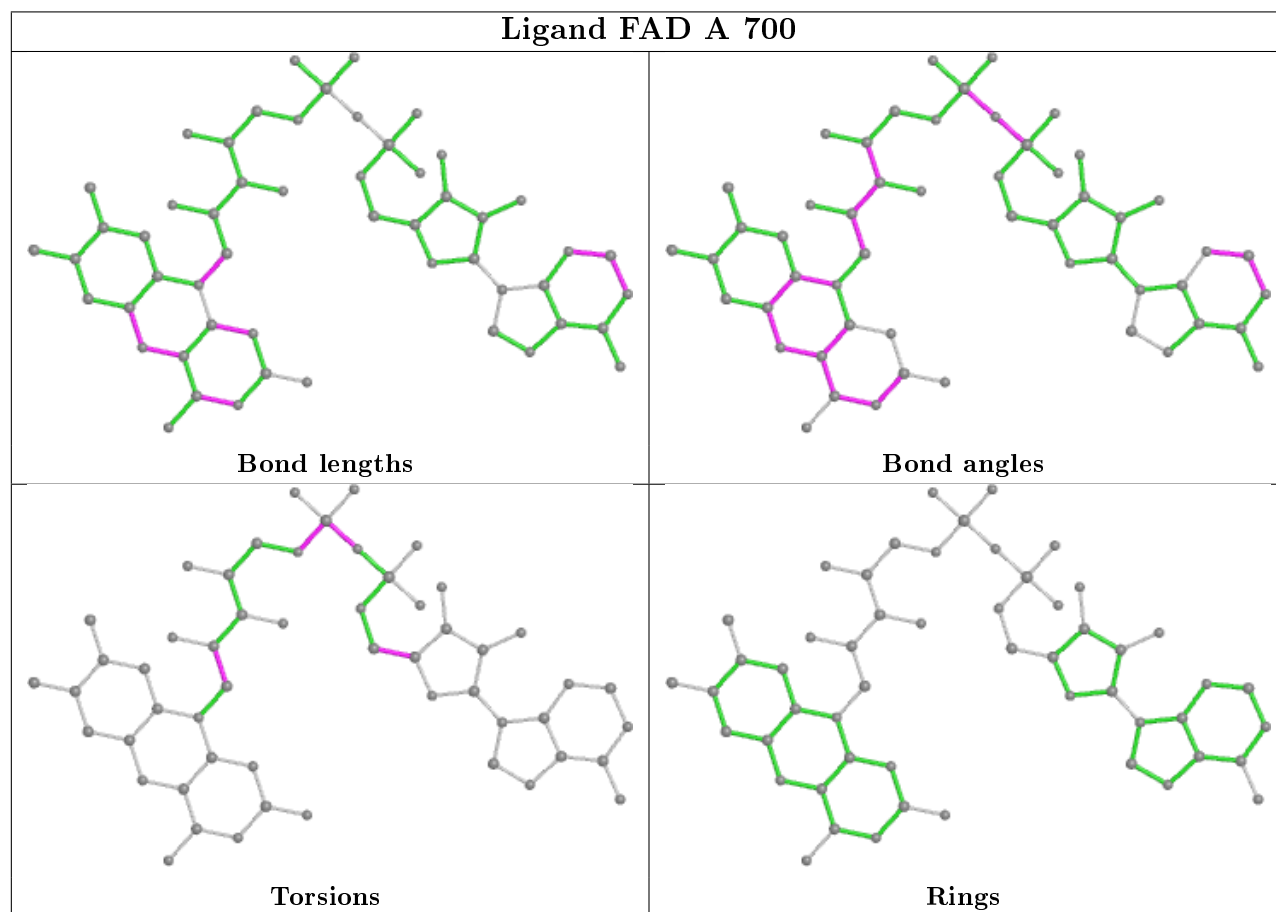
There are no ring outliers.

5 monomers are involved in 18 short contacts:

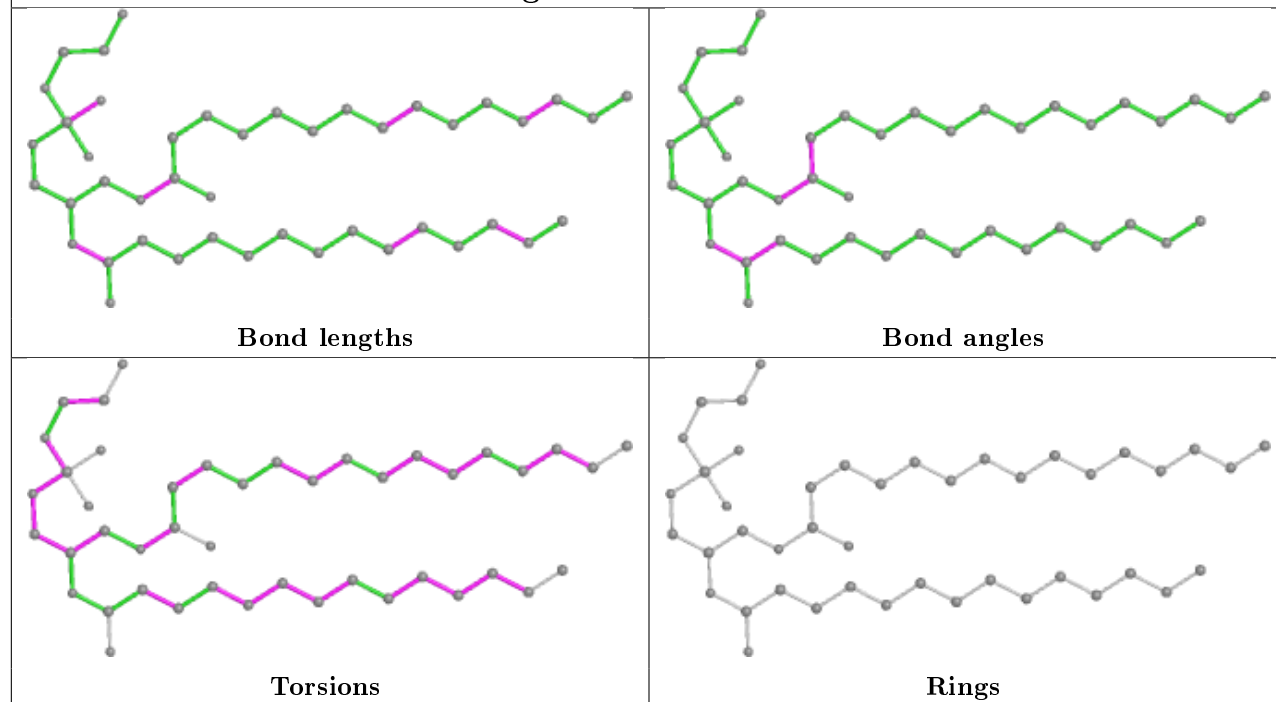
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	700	FAD	11	0
12	D	1306	EPH	1	0
6	A	701	MLI	2	0
9	B	1201	F6A	1	0
11	C	1305	HEM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

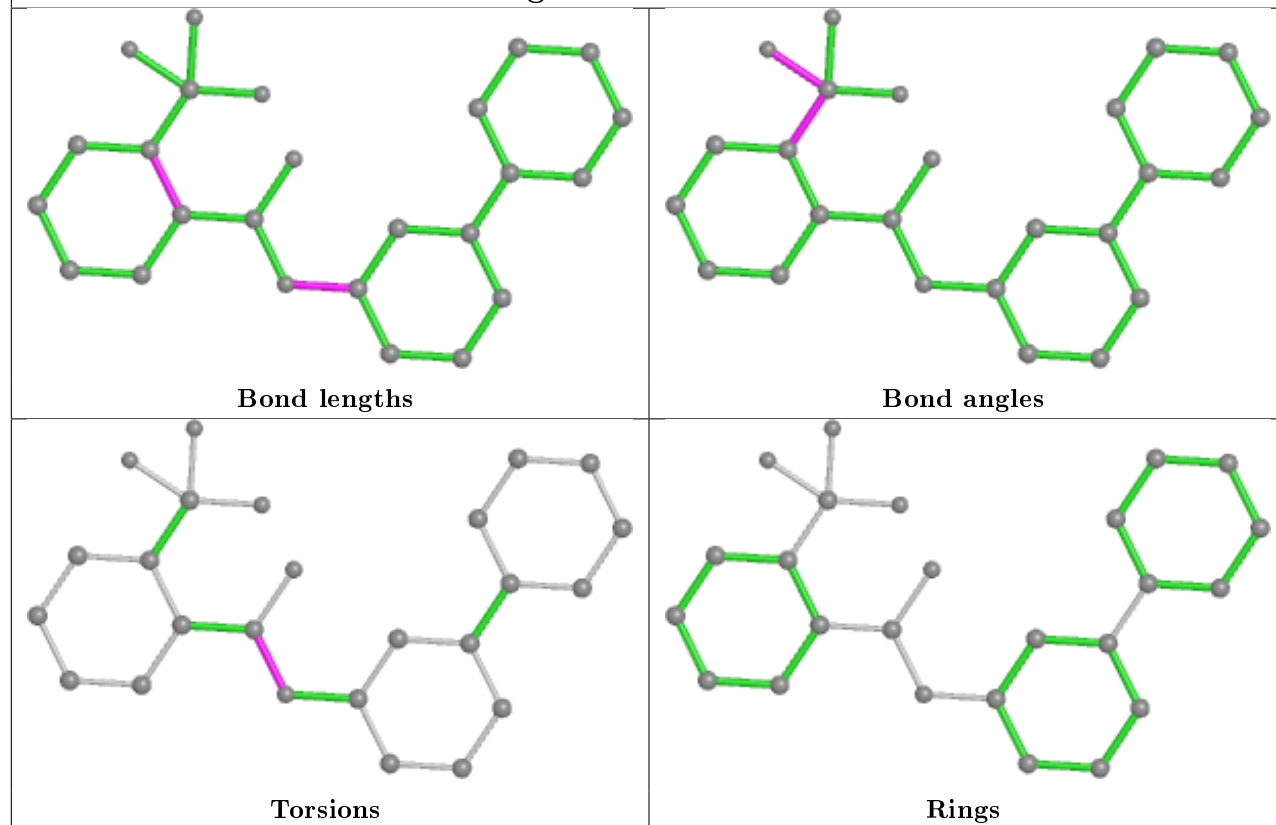
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

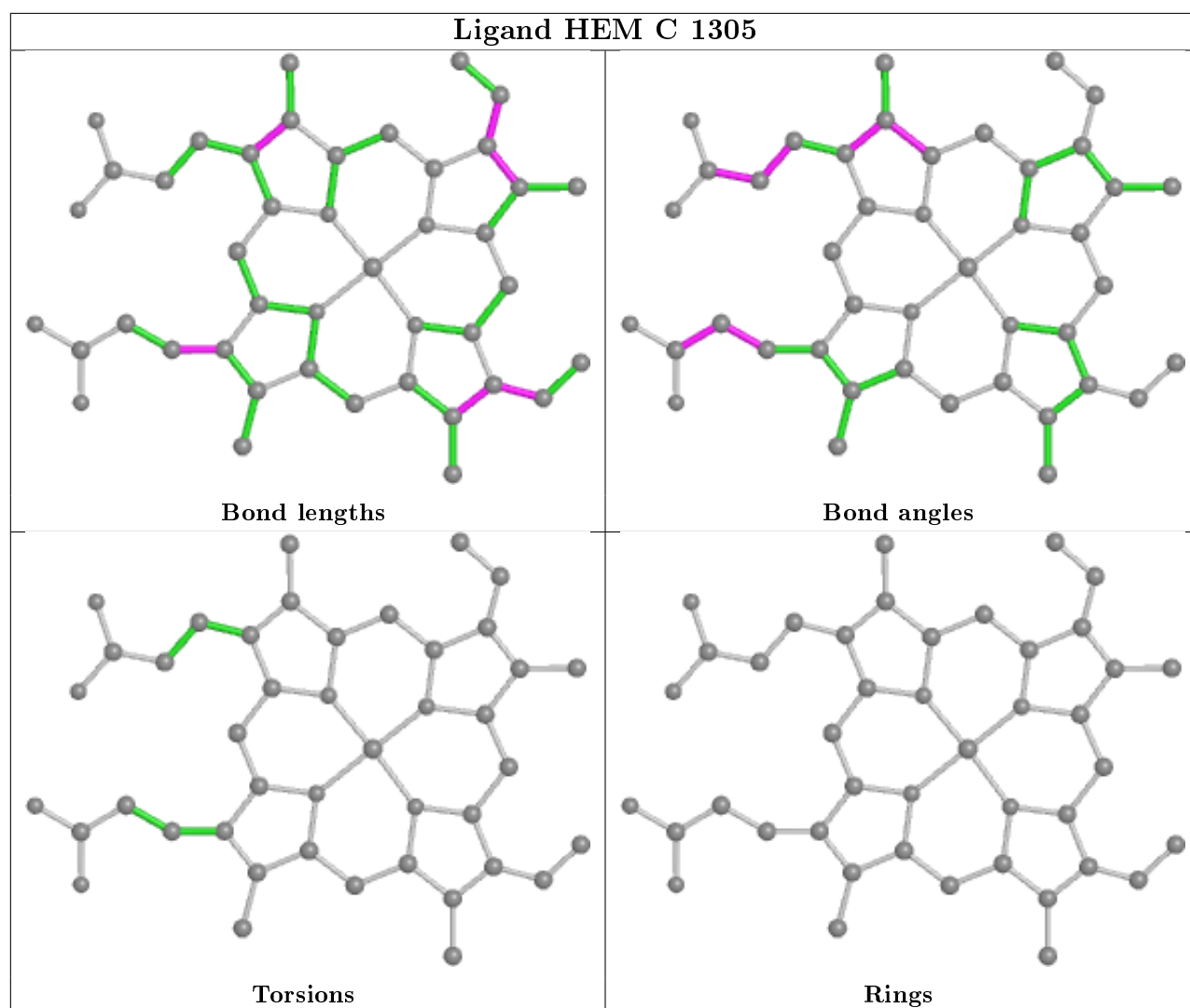


Ligand EPH D 1306



Ligand F6A B 1201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	613/622 (98%)	-0.20	8 (1%) 77 68	47, 68, 100, 126	0
2	B	239/252 (94%)	-0.22	2 (0%) 86 80	46, 62, 100, 114	0
3	C	138/140 (98%)	-0.29	2 (1%) 75 66	50, 69, 110, 120	0
4	D	102/103 (99%)	-0.39	2 (1%) 65 54	49, 67, 114, 120	1 (0%)
All	All	1092/1117 (97%)	-0.23	14 (1%) 77 68	46, 66, 104, 126	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	35	SER	7.0
1	A	572	GLN	3.1
1	A	325	GLN	2.6
2	B	94	ASP	2.5
2	B	11	ILE	2.4
3	C	82	LEU	2.3
1	A	317	PRO	2.3
1	A	328	HIS	2.2
4	D	95	ASP	2.2
1	A	569	GLN	2.1
1	A	326	LEU	2.1
1	A	414	SER	2.1
3	C	79	SER	2.1
1	A	398	GLU	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

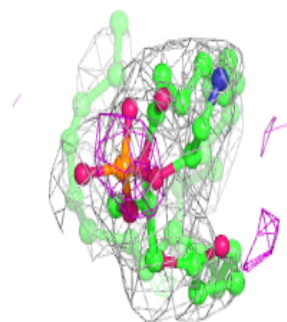
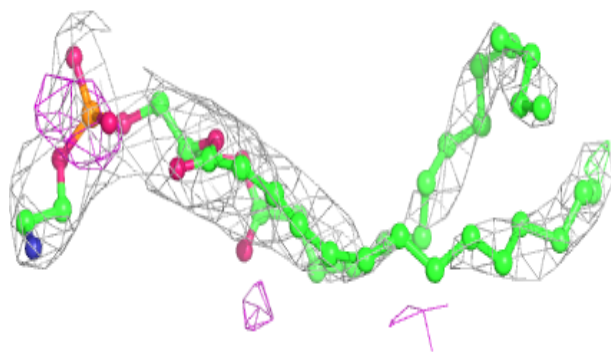
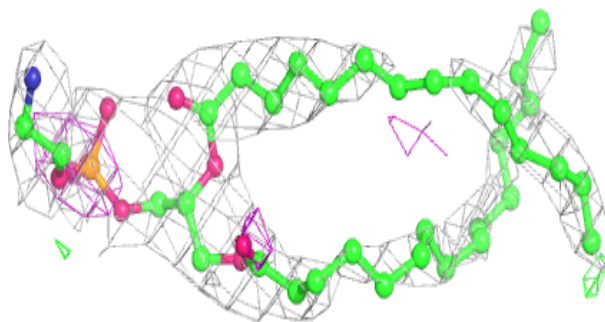
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	EPH	D	1306	44/49	0.88	0.40	75,88,102,102	0
6	MLI	A	701	7/7	0.94	0.28	92,93,93,93	0
5	FAD	A	700	53/53	0.95	0.31	52,56,58,58	0
9	F6A	B	1201	25/25	0.95	0.24	60,60,64,64	0
11	HEM	C	1305	43/43	0.97	0.20	50,51,56,59	0
10	F3S	B	304	7/7	0.99	0.14	66,66,67,67	0
8	SF4	B	303	8/8	1.00	0.14	47,48,49,49	0
7	FES	B	302	4/4	1.00	0.15	47,47,48,48	0

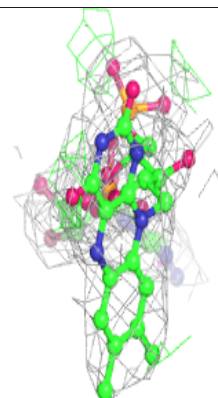
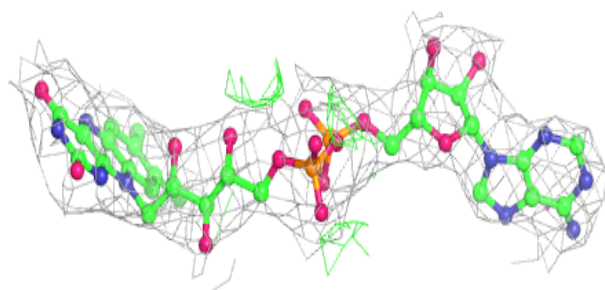
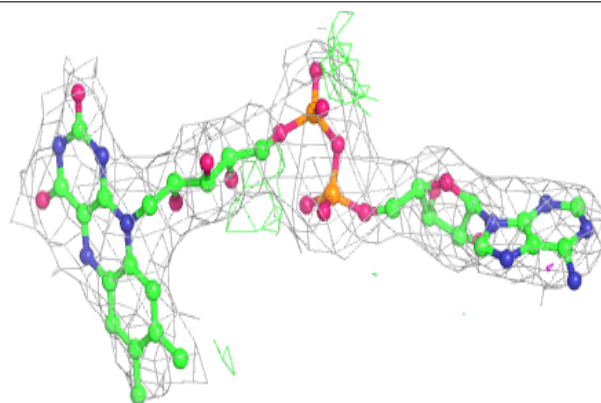
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

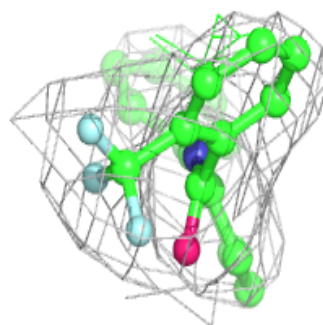
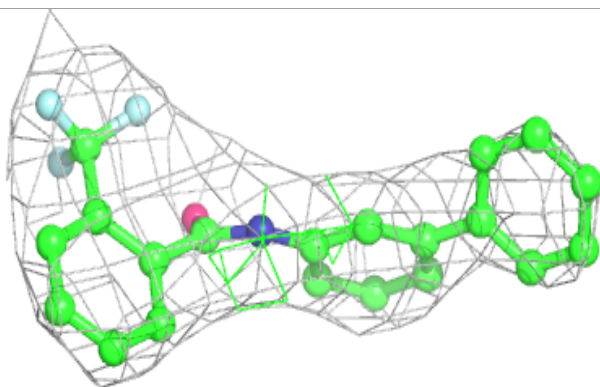
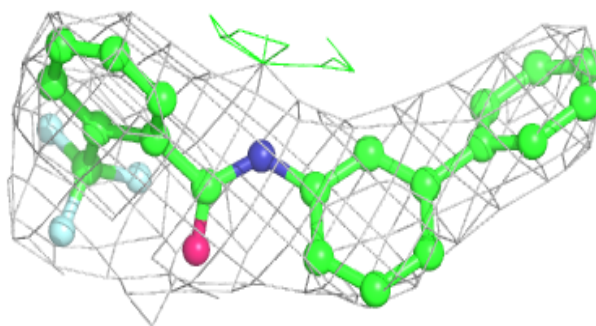
**Electron density around FAD A 700:**

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



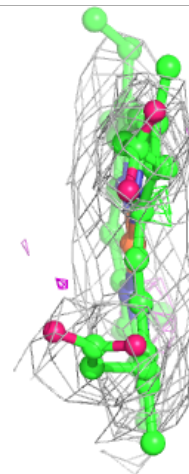
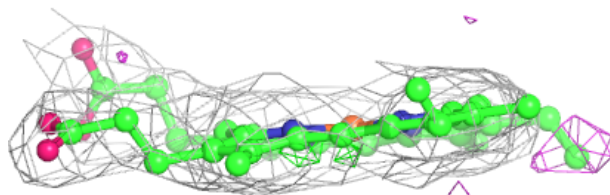
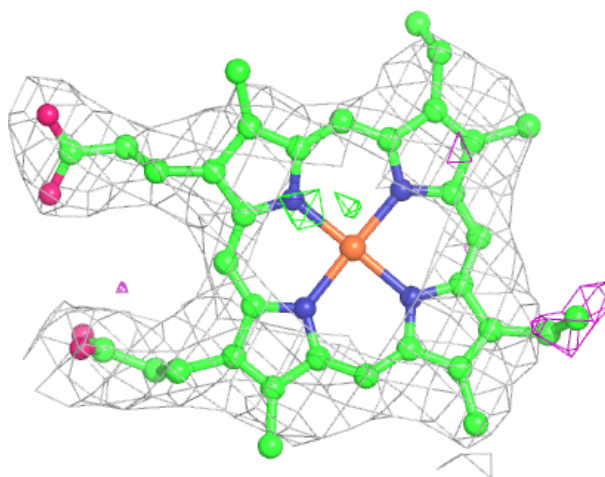
Electron density around F6A B 1201:

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



Electron density around 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.