



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:26 pm BST

PDB ID : 3AEF
Title : Crystal structure of porcine heart mitochondrial complex II with an empty quinone-binding pocket
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 : 2.80 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

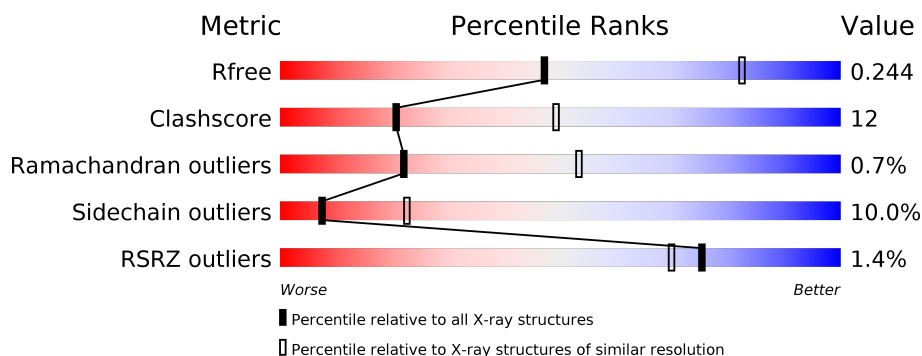
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 67%, yellow 67%, yellow 95%, orange 95%, orange 100%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 67% 28% .. </div> </div>
2	B	252	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 67%, yellow 67%, yellow 95%, orange 95%, orange 100%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 67% 25% • 5% </div> </div>
3	C	140	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, green 4%, green 71%, yellow 71%, yellow 95%, orange 95%, orange 100%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 4% 71% 24% .. </div> </div>
4	D	103	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 76%, yellow 76%, yellow 95%, orange 95%, orange 100%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 3% 76% 21% .. </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
10	EPH	D	1306	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 8642 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.

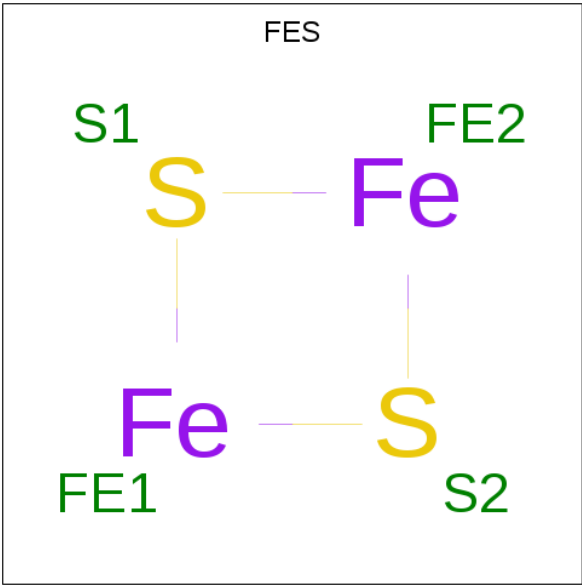
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			765	499	128	133	5			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



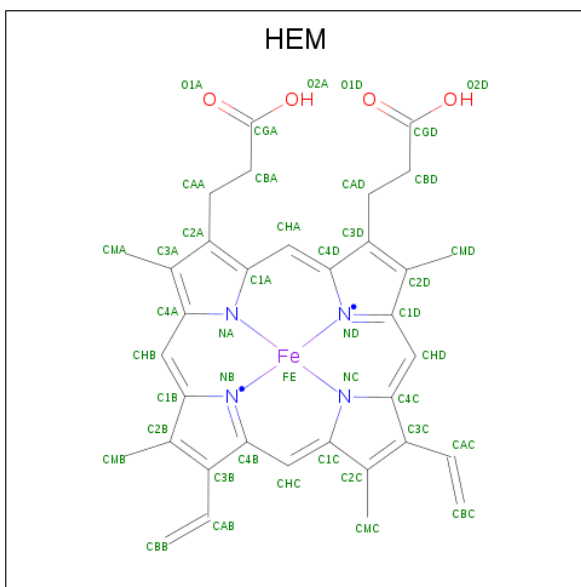
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



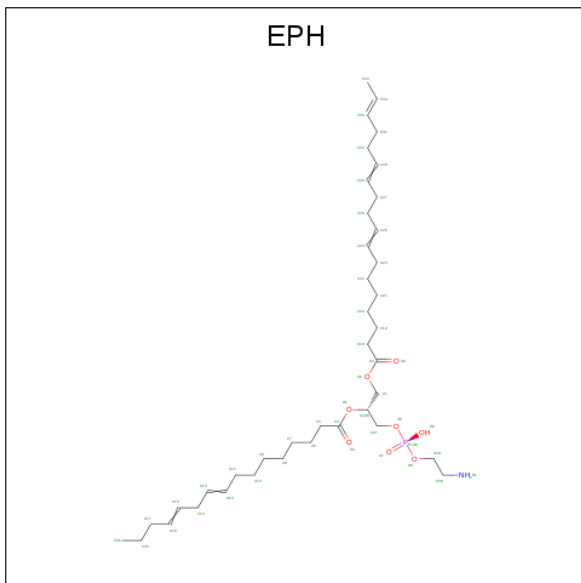
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 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
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 10 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
10	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

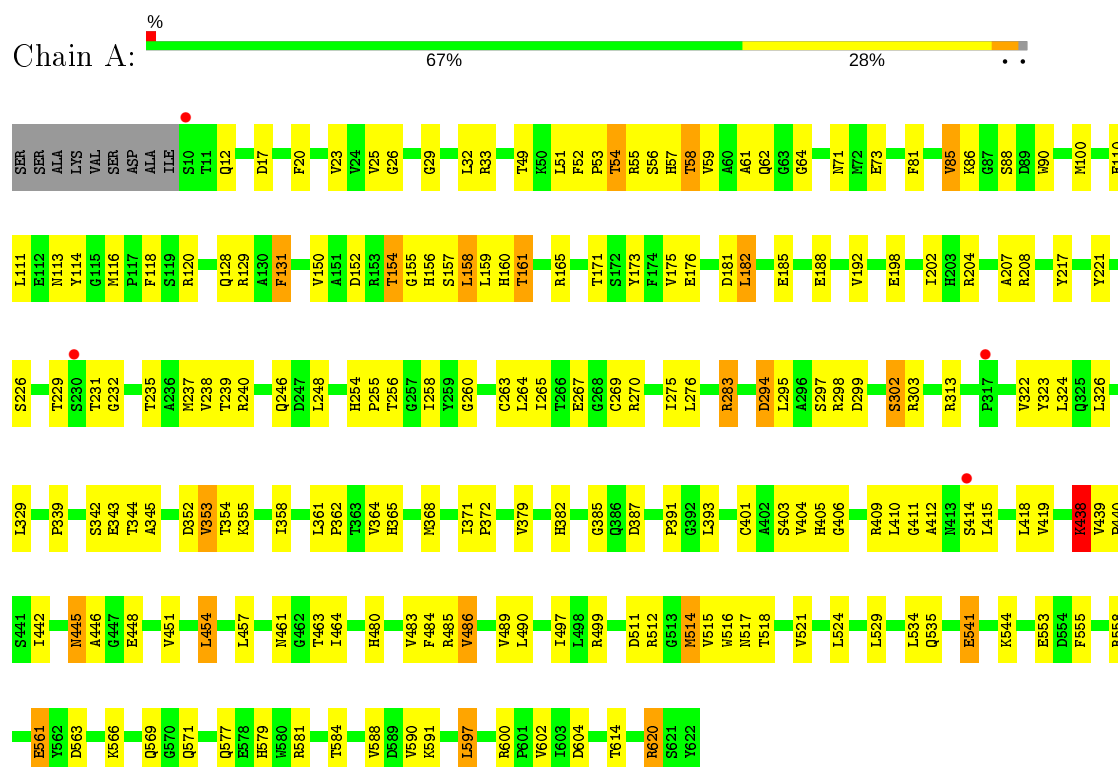
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total 2	O 2	0	0
11	B	1	Total 1	O 1	0	0

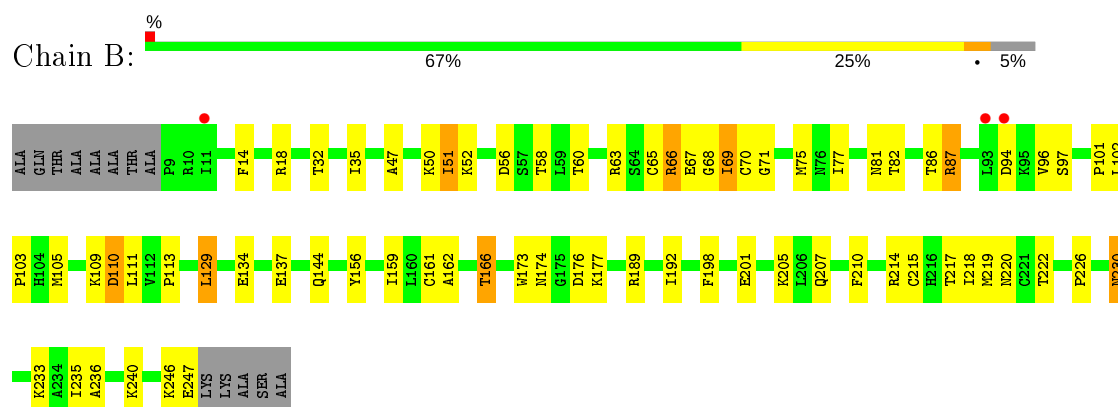
3 Residue-property plots

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.

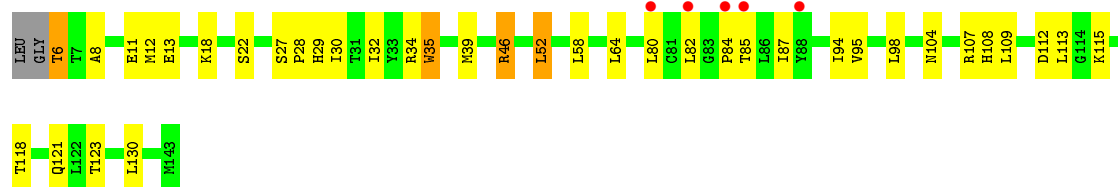
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial



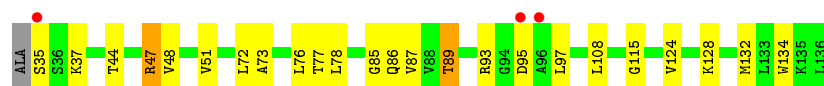
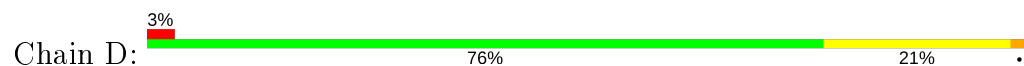
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



- Molecule 3: Succinate dehydrogenase cytochrome b560 subunit, mitochondrial



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.22Å 84.21Å 293.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.88 – 2.80 39.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	75.9 (39.88-2.80) 75.9 (39.88-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.202 , 0.251 0.200 , 0.244	Depositor DCC
R_{free} test set	1691 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8642	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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, 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	0.44	0/4828	0.63	3/6531 (0.0%)
2	B	0.46	0/1964	0.60	0/2648
3	C	0.43	0/1091	0.57	0/1483
4	D	0.44	0/784	0.62	0/1066
All	All	0.45	0/8667	0.61	3/11728 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	597	LEU	CA-CB-CG	5.10	127.02	115.30
1	A	454	LEU	CA-CB-CG	5.06	126.94	115.30

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	133	0
2	B	1922	0	1900	54	0
3	C	1064	0	1104	21	0
4	D	765	0	773	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	53	0	31	14	0
6	B	4	0	0	1	0
7	B	8	0	0	1	0
8	B	7	0	0	0	0
9	C	43	0	30	3	0
10	D	44	0	53	0	0
11	A	2	0	0	1	0
11	B	1	0	0	0	0
All	All	8642	0	8509	210	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 12.

All (210) 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	1.42	1.31
1:A:57:HIS:CE1	5:A:700:FAD:HM82	1.79	1.16
1:A:157:SER:O	1:A:161:THR:HG23	1.46	1.11
1:A:57:HIS:NE2	5:A:700:FAD:HM81	1.62	1.10
2:B:103:PRO:HD2	2:B:166:THR:HG23	1.33	1.08
2:B:67:GLU:HG2	2:B:69:ILE:HD11	1.56	0.86
2:B:103:PRO:HD2	2:B:166:THR:CG2	2.04	0.86
3:C:29:HIS:HD2	3:C:30:ILE:HG13	1.46	0.80
1:A:62:GLN:O	1:A:154:THR:HG23	1.81	0.80
1:A:563:ASP:H	1:A:571:GLN:HE22	1.31	0.78
1:A:59:VAL:HG13	1:A:159:LEU:HD23	1.65	0.77
4:D:72:LEU:O	4:D:76:LEU:HB2	1.88	0.74
1:A:353:VAL:HG12	1:A:358:ILE:HD11	1.69	0.74
1:A:57:HIS:CE1	1:A:226:SER:HA	2.23	0.73
1:A:56:SER:O	1:A:59:VAL:HG22	1.89	0.73
1:A:361:LEU:HD12	1:A:362:PRO:HD2	1.73	0.71
1:A:61:ALA:HB3	1:A:155:GLY:HA3	1.71	0.70
2:B:67:GLU:CG	2:B:69:ILE:HD11	2.21	0.70
2:B:101:PRO:HB3	2:B:111:LEU:HA	1.73	0.70
2:B:162:ALA:O	2:B:166:THR:HB	1.91	0.70
1:A:181:ASP:HA	1:A:237:MET:HG2	1.75	0.69
2:B:102:LEU:HD22	2:B:166:THR:HG21	1.74	0.69
2:B:81:ASN:ND2	2:B:166:THR:HG22	2.09	0.68
1:A:116:MET:HA	1:A:161:THR:HG21	1.76	0.67
1:A:298:ARG:O	1:A:302:SER:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ASP:OD2	1:A:354:THR:HG22	1.96	0.66
1:A:322:VAL:HG12	1:A:323:TYR:H	1.60	0.65
2:B:246:LYS:O	2:B:247:GLU:HB2	1.95	0.65
4:D:85:GLY:O	4:D:89:THR:HG22	1.97	0.65
1:A:322:VAL:HG12	1:A:323:TYR:N	2.12	0.64
2:B:198:PHE:HD2	2:B:201:GLU:HG3	1.63	0.64
1:A:516:TRP:HB3	2:B:60:THR:HG21	1.80	0.64
1:A:372:PRO:HA	1:A:401:CYS:O	1.98	0.64
1:A:463:THR:HG22	1:A:464:ILE:HG13	1.79	0.63
3:C:8:ALA:O	3:C:12:MET:HG3	1.98	0.63
1:A:275:ILE:HG23	1:A:283:ARG:HG3	1.83	0.61
1:A:405:HIS:CG	1:A:409:ARG:HG3	2.36	0.61
1:A:254:HIS:HD2	1:A:256:THR:H	1.47	0.60
1:A:497:ILE:HG22	1:A:534:LEU:HD22	1.82	0.60
1:A:387:ASP:OD2	1:A:600:ARG:NH1	2.35	0.60
3:C:46:ARG:HE	9:C:1305:HEM:CGD	2.15	0.60
2:B:173:TRP:HH2	3:C:30:ILE:HD11	1.66	0.60
1:A:405:HIS:ND1	1:A:409:ARG:HG3	2.18	0.59
4:D:85:GLY:O	4:D:89:THR:CG2	2.51	0.59
1:A:29:GLY:H	1:A:58:THR:HG21	1.69	0.58
1:A:265:ILE:HD13	1:A:358:ILE:HG21	1.84	0.58
1:A:111:LEU:HD11	1:A:419:VAL:HG21	1.84	0.58
1:A:442:ILE:HG13	1:A:446:ALA:CB	2.34	0.58
1:A:246:GLN:NE2	1:A:600:ARG:HE	2.02	0.58
1:A:157:SER:O	1:A:161:THR:CG2	2.38	0.57
1:A:353:VAL:CG1	1:A:358:ILE:HD11	2.34	0.57
2:B:66:ARG:CZ	2:B:66:ARG:HB3	2.35	0.57
2:B:102:LEU:HB3	2:B:166:THR:HG21	1.85	0.57
1:A:158:LEU:HD23	1:A:415:LEU:HD22	1.88	0.56
3:C:104:ASN:HD21	3:C:107:ARG:HH21	1.54	0.56
1:A:61:ALA:HA	5:A:700:FAD:C6	2.36	0.56
1:A:442:ILE:HG13	1:A:446:ALA:HB2	1.86	0.56
2:B:35:ILE:HD11	2:B:51:ILE:HG22	1.87	0.55
1:A:58:THR:CG2	5:A:700:FAD:O1A	2.54	0.55
1:A:90:TRP:HZ3	1:A:620:ARG:HB2	1.72	0.55
1:A:544:LYS:HG2	1:A:555:PHE:CE2	2.41	0.55
1:A:563:ASP:H	1:A:571:GLN:NE2	2.02	0.55
1:A:345:ALA:HB1	1:A:358:ILE:HD12	1.88	0.54
2:B:67:GLU:HG2	2:B:69:ILE:CD1	2.33	0.54
2:B:198:PHE:CD2	2:B:201:GLU:HG3	2.42	0.54
1:A:114:TYR:O	2:B:129:LEU:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:SER:HB2	1:A:406:GLY:HA3	1.90	0.54
2:B:65:CYS:HB3	2:B:70:CYS:HB3	1.90	0.53
1:A:239:THR:CG2	1:A:588:VAL:CG1	2.86	0.53
1:A:239:THR:HG21	1:A:588:VAL:CG1	2.39	0.53
2:B:18:ARG:HH22	2:B:58:THR:HB	1.72	0.53
2:B:65:CYS:SG	2:B:69:ILE:HD12	2.49	0.53
2:B:82:THR:HG21	2:B:87:ARG:HH12	1.74	0.53
1:A:118:PHE:HA	1:A:150:VAL:HG22	1.91	0.53
2:B:222:THR:OG1	2:B:230:ASN:ND2	2.42	0.52
1:A:49:THR:HG1	5:A:700:FAD:HO2A	1.55	0.52
1:A:581:ARG:NH2	1:A:604:ASP:OD2	2.42	0.51
2:B:68:GLY:HA2	6:B:302:FES:S1	2.51	0.51
1:A:61:ALA:HA	5:A:700:FAD:C5X	2.41	0.51
2:B:177:LYS:HE2	2:B:210:PHE:CD2	2.45	0.51
2:B:109:LYS:O	2:B:110:ASP:O	2.28	0.51
1:A:51:LEU:HD21	1:A:229:THR:HG21	1.93	0.51
3:C:35:TRP:CE3	3:C:35:TRP:HA	2.46	0.50
1:A:217:TYR:HB3	1:A:232:GLY:HA3	1.94	0.50
1:A:238:VAL:HG21	1:A:371:ILE:HG12	1.93	0.50
3:C:64:LEU:HG	4:D:115:GLY:HA2	1.94	0.50
2:B:71:GLY:HA3	2:B:159:ILE:HG22	1.94	0.50
1:A:382:HIS:NE2	1:A:385:GLY:HA2	2.27	0.49
3:C:35:TRP:HE3	3:C:35:TRP:HA	1.77	0.49
1:A:264:LEU:HB3	5:A:700:FAD:HM73	1.93	0.49
1:A:521:VAL:HA	1:A:524:LEU:HD12	1.94	0.49
2:B:103:PRO:CD	2:B:166:THR:HG23	2.23	0.49
3:C:29:HIS:CD2	3:C:30:ILE:H	2.30	0.49
1:A:248:LEU:HD12	1:A:535:GLN:CB	2.43	0.49
1:A:57:HIS:CE1	5:A:700:FAD:C8M	2.62	0.49
3:C:6:THR:HG23	3:C:11:GLU:OE2	2.12	0.49
1:A:561:GLU:OE2	1:A:581:ARG:NH1	2.45	0.49
1:A:248:LEU:HD12	1:A:535:GLN:HB2	1.95	0.49
2:B:111:LEU:O	2:B:113:PRO:HD3	2.13	0.49
2:B:226:PRO:HD2	7:B:303:SF4:S1	2.53	0.49
1:A:322:VAL:CG1	1:A:323:TYR:H	2.27	0.48
2:B:230:ASN:ND2	2:B:233:LYS:H	2.12	0.48
1:A:254:HIS:CE1	1:A:264:LEU:HD11	2.48	0.48
2:B:75:MET:HG3	2:B:77:ILE:HD11	1.96	0.48
1:A:58:THR:HG23	5:A:700:FAD:O1A	2.14	0.47
1:A:240:ARG:HG2	1:A:590:VAL:HG21	1.95	0.47
2:B:161:CYS:O	2:B:162:ALA:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HG22	5:A:700:FAD:O1A	2.15	0.47
1:A:152:ASP:OD2	1:A:339:PRO:HD2	2.15	0.47
1:A:442:ILE:CG1	1:A:446:ALA:CB	2.92	0.47
1:A:490:LEU:HD13	1:A:541:GLU:HA	1.97	0.47
1:A:486:VAL:HG13	1:A:553:GLU:HB2	1.96	0.47
1:A:239:THR:CG2	1:A:588:VAL:HG13	2.44	0.47
1:A:198:GLU:O	1:A:515:VAL:HG13	2.15	0.46
1:A:26:GLY:HA2	5:A:700:FAD:H1B	1.96	0.46
1:A:81:PHE:O	1:A:85:VAL:HG12	2.16	0.46
1:A:71:ASN:H	1:A:128:GLN:NE2	2.14	0.46
1:A:86:LYS:O	1:A:620:ARG:HD2	2.16	0.46
2:B:218:ILE:O	2:B:219:MET:HB2	2.16	0.46
1:A:182:LEU:HD22	1:A:237:MET:HB3	1.97	0.46
1:A:270:ARG:HD3	1:A:276:LEU:HD13	1.98	0.46
3:C:18:LYS:O	3:C:22:SER:HB3	2.16	0.46
1:A:297:SER:HB3	1:A:299:ASP:OD1	2.16	0.45
1:A:246:GLN:HA	1:A:584:THR:O	2.16	0.45
3:C:52:LEU:HB3	9:C:1305:HEM:CAC	2.46	0.45
1:A:231:THR:HA	1:A:529:LEU:HD21	1.98	0.45
1:A:113:ASN:HD22	2:B:137:GLU:HA	1.81	0.45
1:A:604:ASP:O	1:A:614:THR:HG23	2.17	0.45
3:C:112:ASP:OD1	4:D:47:ARG:HD2	2.15	0.45
1:A:120:ARG:HD2	2:B:144:GLN:O	2.16	0.45
2:B:66:ARG:NH1	2:B:66:ARG:HB3	2.31	0.45
1:A:175:VAL:HG12	1:A:176:GLU:HG3	1.98	0.45
1:A:156:HIS:HE1	2:B:156:TYR:O	2.00	0.45
9:C:1305:HEM:HBA1	9:C:1305:HEM:HHA	1.99	0.45
1:A:185:GLU:OE2	1:A:442:ILE:HD12	2.17	0.44
4:D:124:VAL:HG13	4:D:128:LYS:HB3	1.99	0.44
1:A:414:SER:O	1:A:418:LEU:HD13	2.18	0.44
3:C:109:LEU:HD13	4:D:51:VAL:HG12	1.98	0.44
1:A:267:GLU:OE1	1:A:298:ARG:HD3	2.17	0.44
1:A:254:HIS:HB2	1:A:365:HIS:CG	2.52	0.44
1:A:264:LEU:CB	5:A:700:FAD:HM73	2.46	0.44
1:A:62:GLN:O	1:A:154:THR:CG2	2.60	0.43
1:A:100:MET:SD	1:A:404:VAL:HG21	2.58	0.43
2:B:174:ASN:ND2	4:D:93:ARG:HH11	2.16	0.43
1:A:202:ILE:HD13	1:A:451:VAL:HG22	1.99	0.43
1:A:445:ASN:O	1:A:448:GLU:HB2	2.18	0.43
2:B:236:ALA:O	2:B:240:LYS:HG3	2.17	0.43
4:D:86:GLN:HA	4:D:89:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PRO:HD2	1:A:298:ARG:HD2	1.99	0.43
1:A:518:THR:OG1	2:B:52:LYS:NZ	2.51	0.43
1:A:439:VAL:HA	1:A:440:PRO:HD3	1.88	0.43
1:A:581:ARG:HH22	1:A:604:ASP:CG	2.22	0.43
1:A:64:GLY:HA2	1:A:154:THR:HG21	2.00	0.43
2:B:230:ASN:CG	2:B:233:LYS:HB3	2.39	0.43
1:A:275:ILE:HD12	1:A:283:ARG:CZ	2.48	0.43
1:A:299:ASP:O	1:A:303:ARG:HB2	2.17	0.43
1:A:322:VAL:CG1	1:A:323:TYR:N	2.80	0.43
1:A:204:ARG:HH21	1:A:446:ALA:HB3	1.83	0.43
1:A:579:HIS:HD2	1:A:581:ARG:H	1.66	0.43
2:B:35:ILE:HD12	2:B:50:LYS:HE3	2.01	0.42
2:B:52:LYS:HA	2:B:56:ASP:O	2.19	0.42
2:B:176:ASP:CG	4:D:93:ARG:HH22	2.22	0.42
1:A:409:ARG:NH2	11:A:624:HOH:O	2.25	0.42
1:A:52:PHE:O	1:A:55:ARG:HG2	2.19	0.42
2:B:102:LEU:HA	2:B:103:PRO:HD3	1.92	0.42
1:A:33:ARG:NH2	1:A:110:GLU:OE1	2.48	0.42
1:A:379:VAL:HG21	1:A:393:LEU:HG	2.01	0.42
1:A:221:TYR:CG	1:A:364:VAL:HG21	2.54	0.42
1:A:59:VAL:HA	1:A:156:HIS:HA	2.02	0.42
4:D:73:ALA:O	4:D:77:THR:HG23	2.20	0.42
1:A:59:VAL:HG13	1:A:159:LEU:CD2	2.42	0.42
1:A:188:GLU:HG2	1:A:391:PRO:HB2	2.01	0.42
2:B:66:ARG:HH11	2:B:66:ARG:CG	2.32	0.42
3:C:118:THR:OG1	3:C:121:GLN:HG3	2.19	0.42
1:A:54:THR:HG21	1:A:160:HIS:CE1	2.54	0.42
2:B:207:GLN:NE2	4:D:37:LYS:HB2	2.34	0.42
1:A:411:GLY:O	1:A:412:ALA:HB3	2.19	0.42
3:C:104:ASN:ND2	3:C:107:ARG:HE	2.18	0.42
1:A:54:THR:CG2	1:A:54:THR:O	2.68	0.41
1:A:275:ILE:HD12	1:A:283:ARG:NE	2.36	0.41
1:A:438:LYS:HA	1:A:438:LYS:HE3	2.02	0.41
2:B:14:PHE:O	2:B:32:THR:HA	2.20	0.41
2:B:215:CYS:SG	2:B:235:ILE:HG21	2.59	0.41
1:A:342:SER:OG	1:A:353:VAL:HG21	2.20	0.41
2:B:47:ALA:O	2:B:51:ILE:HG23	2.21	0.41
1:A:511:ASP:HB3	1:A:517:ASN:OD1	2.20	0.41
1:A:52:PHE:CD1	1:A:53:PRO:HD2	2.56	0.41
4:D:128:LYS:O	4:D:132:MET:HG3	2.20	0.41
1:A:258:ILE:HG22	1:A:263:CYS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:MET:HA	1:A:514:MET:HE3	2.02	0.41
3:C:27:SER:HA	3:C:28:PRO:HD2	1.88	0.41
1:A:25:VAL:HG21	1:A:192:VAL:HG11	2.03	0.41
1:A:303:ARG:HG3	1:A:484:PHE:CZ	2.56	0.41
3:C:28:PRO:HB2	3:C:32:ILE:HG12	2.02	0.41
1:A:269:CYS:HB3	1:A:326:LEU:HD21	2.01	0.41
4:D:48:VAL:O	4:D:51:VAL:HG22	2.20	0.41
1:A:129:ARG:HA	1:A:129:ARG:HD2	1.87	0.41
1:A:480:HIS:HD2	1:A:489:VAL:O	2.04	0.41
1:A:52:PHE:CE2	1:A:54:THR:HB	2.56	0.41
1:A:20:PHE:O	1:A:207:ALA:HA	2.22	0.40
1:A:270:ARG:HD2	1:A:294:ASP:O	2.21	0.40
2:B:230:ASN:C	2:B:230:ASN:HD22	2.24	0.40
3:C:94:ILE:HD13	3:C:94:ILE:HA	1.95	0.40
1:A:131:PHE:CZ	1:A:267:GLU:HB3	2.55	0.40
5:A:700:FAD:H9	5:A:700:FAD:H1'1	1.82	0.40
1:A:171:THR:HB	1:A:173:TYR:CE1	2.56	0.40
2:B:220:ASN:HD21	3:C:39:MET:HE2	1.86	0.40
2:B:66:ARG:NH1	2:B:66:ARG:CB	2.85	0.40
3:C:46:ARG:NE	4:D:87:VAL:HG22	2.36	0.40
1:A:499:ARG:HB2	1:A:499:ARG:HE	1.69	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%)	570 (93%)	36 (6%)	5 (1%)	19 49
2	B	237/252 (94%)	219 (92%)	17 (7%)	1 (0%)	34 66
3	C	136/140 (97%)	129 (95%)	6 (4%)	1 (1%)	22 53
4	D	100/103 (97%)	94 (94%)	5 (5%)	1 (1%)	15 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1084/1117 (97%)	1012 (93%)	64 (6%)	8 (1%)	22	53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	110	ASP
1	A	260	GLY
1	A	283	ARG
4	D	95	ASP
1	A	438	LYS
1	A	569	GLN
3	C	84	PRO
1	A	483	VAL

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%)	453 (91%)	46 (9%)	9	27
2	B	214/220 (97%)	195 (91%)	19 (9%)	9	28
3	C	117/118 (99%)	99 (85%)	18 (15%)	2	8
4	D	76/76 (100%)	68 (90%)	8 (10%)	7	20
All	All	906/920 (98%)	815 (90%)	91 (10%)	7	22

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	17	ASP
1	A	23	VAL
1	A	32	LEU
1	A	54	THR
1	A	58	THR
1	A	73	GLU

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Mol	Chain	Res	Type
1	A	85	VAL
1	A	131	PHE
1	A	154	THR
1	A	158	LEU
1	A	161	THR
1	A	165	ARG
1	A	208	ARG
1	A	235	THR
1	A	294	ASP
1	A	295	LEU
1	A	302	SER
1	A	313	ARG
1	A	324	LEU
1	A	329	LEU
1	A	343	GLU
1	A	344	THR
1	A	353	VAL
1	A	355	LYS
1	A	368	MET
1	A	403	SER
1	A	410	LEU
1	A	438	LYS
1	A	445	ASN
1	A	454	LEU
1	A	457	LEU
1	A	461	ASN
1	A	485	ARG
1	A	486	VAL
1	A	512	ARG
1	A	514	MET
1	A	541	GLU
1	A	558	ARG
1	A	561	GLU
1	A	566	LYS
1	A	577	GLN
1	A	591	LYS
1	A	597	LEU
1	A	602	VAL
1	A	620	ARG
2	B	51	ILE
2	B	63	ARG
2	B	66	ARG

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Mol	Chain	Res	Type
2	B	69	ILE
2	B	86	THR
2	B	87	ARG
2	B	94	ASP
2	B	96	VAL
2	B	97	SER
2	B	105	MET
2	B	129	LEU
2	B	134	GLU
2	B	166	THR
2	B	189	ARG
2	B	192	ILE
2	B	205	LYS
2	B	214	ARG
2	B	217	THR
2	B	230	ASN
3	C	6	THR
3	C	13	GLU
3	C	34	ARG
3	C	35	TRP
3	C	46	ARG
3	C	52	LEU
3	C	58	LEU
3	C	80	LEU
3	C	82	LEU
3	C	85	THR
3	C	87	ILE
3	C	95	VAL
3	C	98	LEU
3	C	108	HIS
3	C	113	LEU
3	C	115	LYS
3	C	123	THR
3	C	130	LEU
4	D	35	SER
4	D	44	THR
4	D	47	ARG
4	D	78	LEU
4	D	89	THR
4	D	97	LEU
4	D	108	LEU
4	D	134	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	113	ASN
1	A	128	GLN
1	A	143	GLN
1	A	160	HIS
1	A	246	GLN
1	A	254	HIS
1	A	384	ASN
1	A	408	ASN
1	A	453	ASN
1	A	474	GLN
1	A	480	HIS
1	A	527	GLN
1	A	550	HIS
1	A	571	GLN
1	A	577	GLN
1	A	579	HIS
2	B	92	ASN
2	B	121	GLN
2	B	140	GLN
2	B	174	ASN
2	B	220	ASN
2	B	230	ASN
3	C	17	ASN
3	C	29	HIS
3	C	104	ASN
4	D	122	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 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
7	SF4	B	303	2	0,12,12	0.00	-	-		
5	FAD	A	700	1	51,58,58	1.36	6 (11%)	60,89,89	1.66	7 (11%)
6	FES	B	302	2	0,4,4	0.00	-	-		
8	F3S	B	304	2	0,9,9	0.00	-	-		
9	HEM	C	1305	3,4	27,50,50	2.14	6 (22%)	17,82,82	1.66	3 (17%)
10	EPH	D	1306	-	43,43,48	1.52	6 (13%)	45,48,53	1.33	4 (8%)

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
7	SF4	B	303	2	-	-	0/6/5/5
5	FAD	A	700	1	-	4/30/50/50	0/6/6/6
6	FES	B	302	2	-	-	0/1/1/1
8	F3S	B	304	2	-	-	0/3/3/3
9	HEM	C	1305	3,4	-	1/6/54/54	-
10	EPH	D	1306	-	1/1/4/14	26/47/47/52	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1305	HEM	C3D-C2D	5.25	1.53	1.37
9	C	1305	HEM	C3B-C2B	-4.51	1.34	1.40
10	D	1306	EPH	O1-C3	4.49	1.47	1.34
5	A	700	FAD	C10-N1	4.28	1.38	1.33
10	D	1306	EPH	O2-C4	4.14	1.45	1.33
5	A	700	FAD	C2A-N3A	4.07	1.38	1.32
9	C	1305	HEM	C3C-C2C	-3.88	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	1306	EPH	C25-C24	3.74	1.53	1.31
10	D	1306	EPH	C13-C12	3.72	1.53	1.31
10	D	1306	EPH	C29-C28	3.69	1.53	1.31
9	C	1305	HEM	C3C-CAC	3.64	1.55	1.47
5	A	700	FAD	C4X-N5	3.27	1.38	1.33
10	D	1306	EPH	C15-C16	3.20	1.53	1.29
9	C	1305	HEM	C3B-CAB	3.18	1.54	1.47
5	A	700	FAD	C4-N3	2.97	1.38	1.33
9	C	1305	HEM	CAA-C2A	2.57	1.55	1.52
5	A	700	FAD	C2A-N1A	2.56	1.38	1.33
5	A	700	FAD	C1'-N10	2.34	1.50	1.48

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	FAD	C4-N3-C2	6.10	120.29	115.14
5	A	700	FAD	N3A-C2A-N1A	-6.05	119.22	128.68
10	D	1306	EPH	O1-C3-C5	4.90	122.07	111.50
5	A	700	FAD	C4X-N5-C5X	4.69	121.46	116.77
9	C	1305	HEM	CAD-CBD-CGD	-3.78	106.33	112.67
5	A	700	FAD	C10-C4X-N5	-3.67	118.72	121.26
9	C	1305	HEM	C1D-C2D-C3D	-3.21	104.76	107.00
10	D	1306	EPH	O2-C4-C18	3.01	121.35	111.91
9	C	1305	HEM	CMA-C3A-C4A	-2.69	124.34	128.46
10	D	1306	EPH	O2-C4-O4	-2.67	116.84	123.59
10	D	1306	EPH	O1-C3-O3	-2.59	117.45	123.70
5	A	700	FAD	P-O3P-PA	-2.44	124.46	132.83
5	A	700	FAD	C4X-C4-N3	-2.30	120.29	123.43
5	A	700	FAD	C1'-N10-C10	2.17	120.35	118.41

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	D	1306	EPH	C2

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	700	FAD	PA-O3P-P-O5'
9	C	1305	HEM	C3D-CAD-CBD-CGD
10	D	1306	EPH	O1-C2-C37-O5
10	D	1306	EPH	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
10	D	1306	EPH	C37-O5-P1-O6
10	D	1306	EPH	O3-C3-O1-C2
10	D	1306	EPH	C5-C3-O1-C2
10	D	1306	EPH	C23-C24-C25-C26
10	D	1306	EPH	C27-C28-C29-C30
10	D	1306	EPH	C7-C8-C9-C10
10	D	1306	EPH	C19-C20-C21-C22
10	D	1306	EPH	C3-C5-C6-C7
10	D	1306	EPH	C1-C2-C37-O5
10	D	1306	EPH	C20-C21-C22-C23
10	D	1306	EPH	C18-C4-O2-C1
10	D	1306	EPH	O2-C1-C2-C37
10	D	1306	EPH	C5-C6-C7-C8
10	D	1306	EPH	C25-C26-C27-C28
10	D	1306	EPH	O4-C4-O2-C1
5	A	700	FAD	C5B-O5B-PA-O3P
10	D	1306	EPH	C37-O5-P1-O8
10	D	1306	EPH	C2-C37-O5-P1
10	D	1306	EPH	C37-O5-P1-O7
10	D	1306	EPH	C11-C10-C9-C8
10	D	1306	EPH	C18-C19-C20-C21
10	D	1306	EPH	O2-C1-C2-O1
5	A	700	FAD	O4B-C4B-C5B-O5B
10	D	1306	EPH	C13-C14-C15-C16
10	D	1306	EPH	C14-C15-C16-C17
5	A	700	FAD	O4'-C4'-C5'-O5'
10	D	1306	EPH	C24-C25-C26-C27

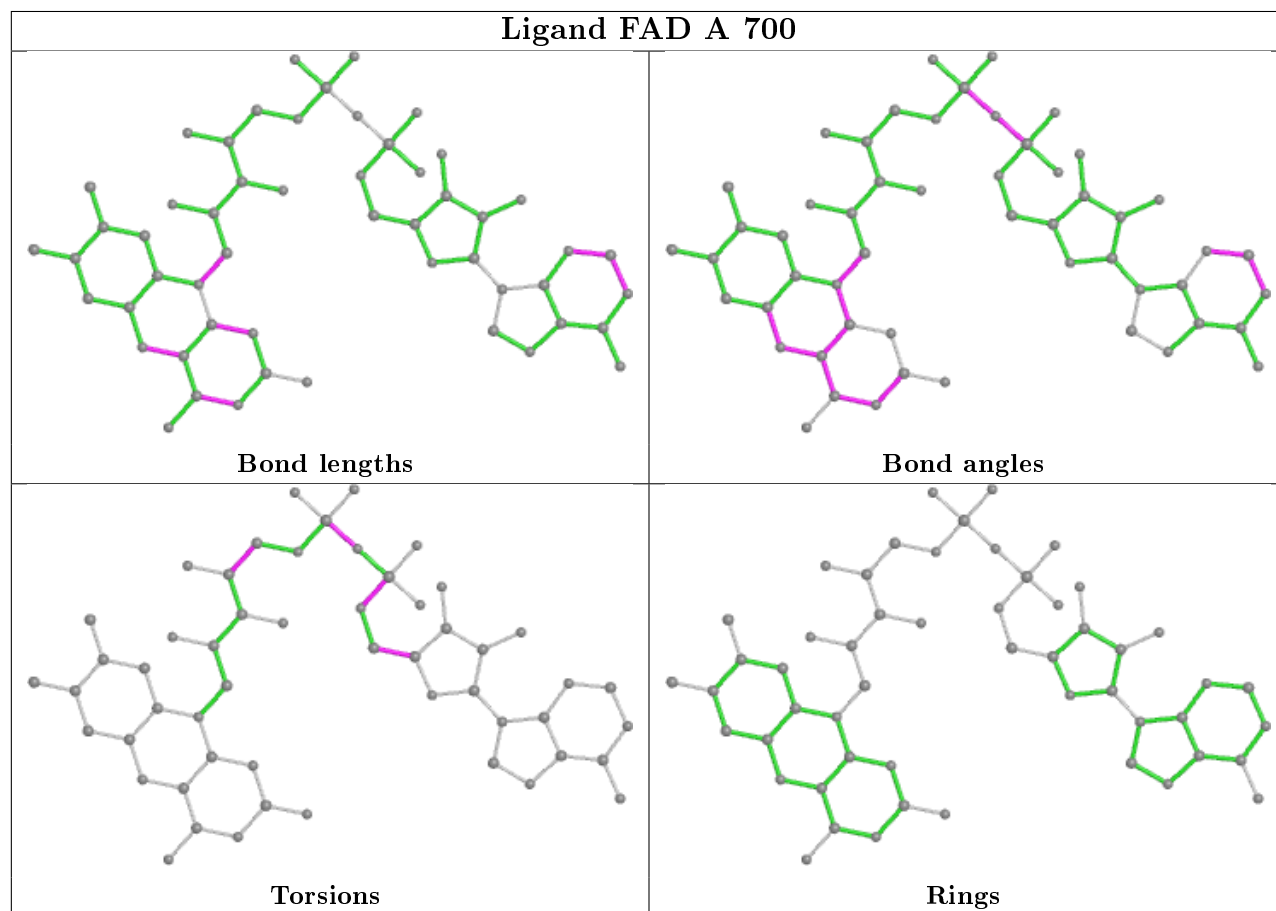
There are no ring outliers.

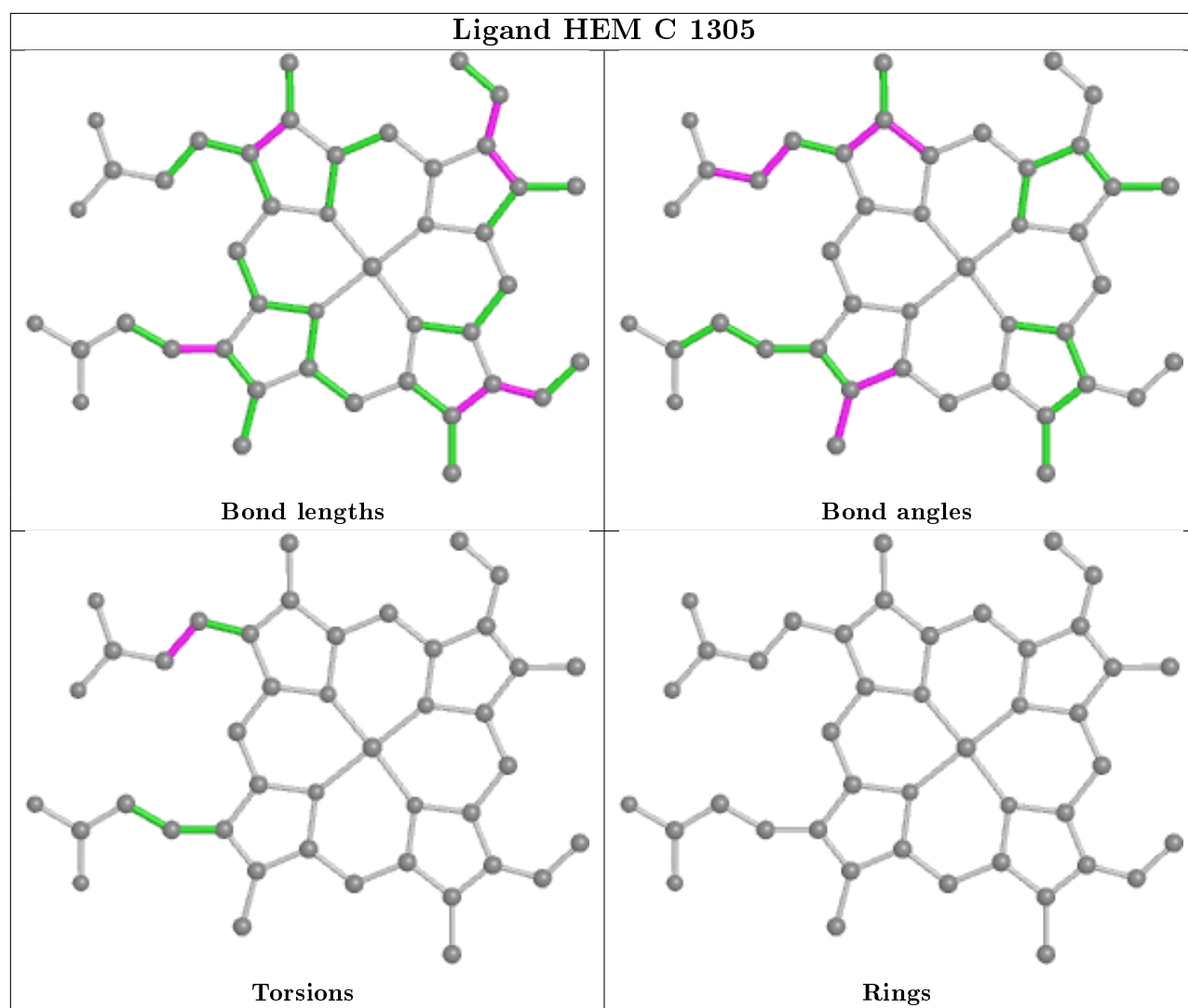
4 monomers are involved in 19 short contacts:

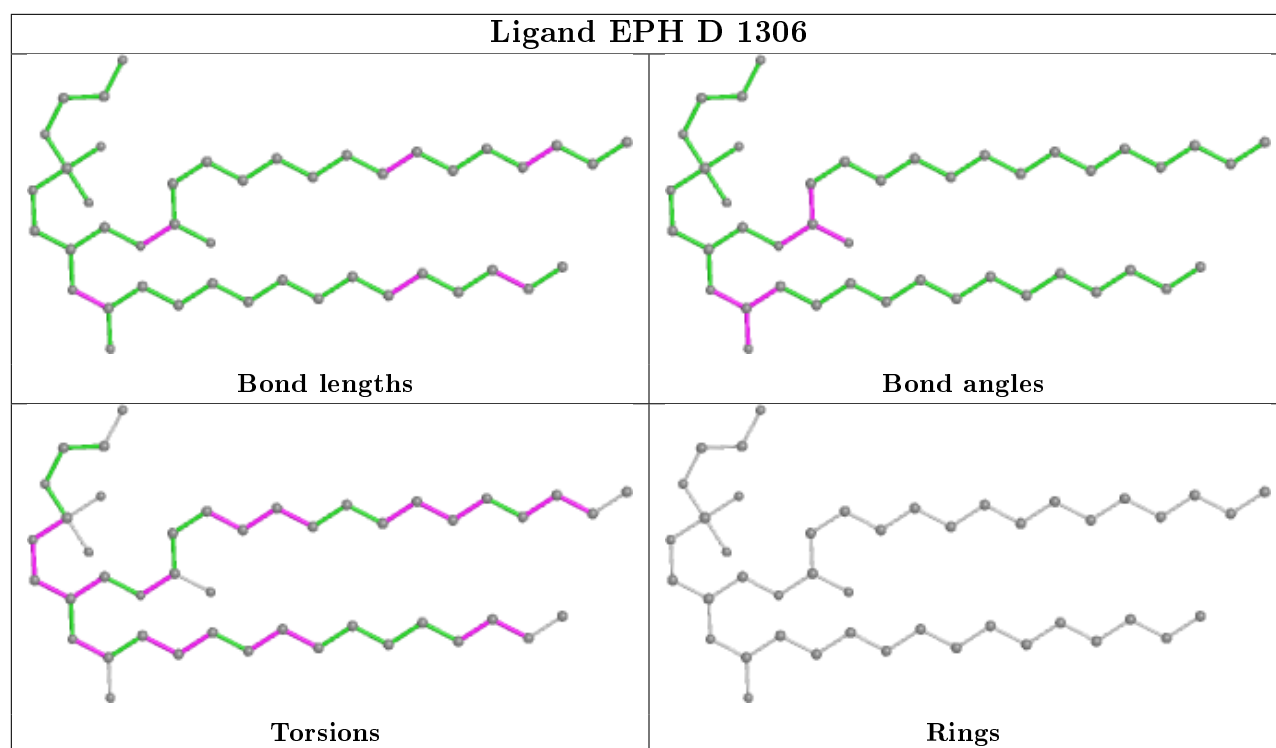
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	303	SF4	1	0
5	A	700	FAD	14	0
6	B	302	FES	1	0
9	C	1305	HEM	3	0

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.







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%)	-0.21	4 (0%) 87 84	31, 51, 79, 94	0
2	B	239/252 (94%)	-0.33	3 (1%) 77 72	33, 46, 78, 90	0
3	C	138/140 (98%)	-0.20	5 (3%) 42 32	33, 57, 94, 103	0
4	D	102/103 (99%)	-0.38	3 (2%) 51 41	38, 54, 76, 101	0
All	All	1092/1117 (97%)	-0.25	15 (1%) 75 70	31, 51, 81, 103	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	35	SER	5.0
4	D	95	ASP	3.7
1	A	317	PRO	3.0
3	C	82	LEU	2.9
2	B	11	ILE	2.8
2	B	94	ASP	2.4
1	A	10	SER	2.3
3	C	88	TYR	2.3
3	C	80	LEU	2.3
3	C	84	PRO	2.2
1	A	414	SER	2.2
2	B	93	LEU	2.2
3	C	85	THR	2.1
1	A	230	SER	2.1
4	D	96	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

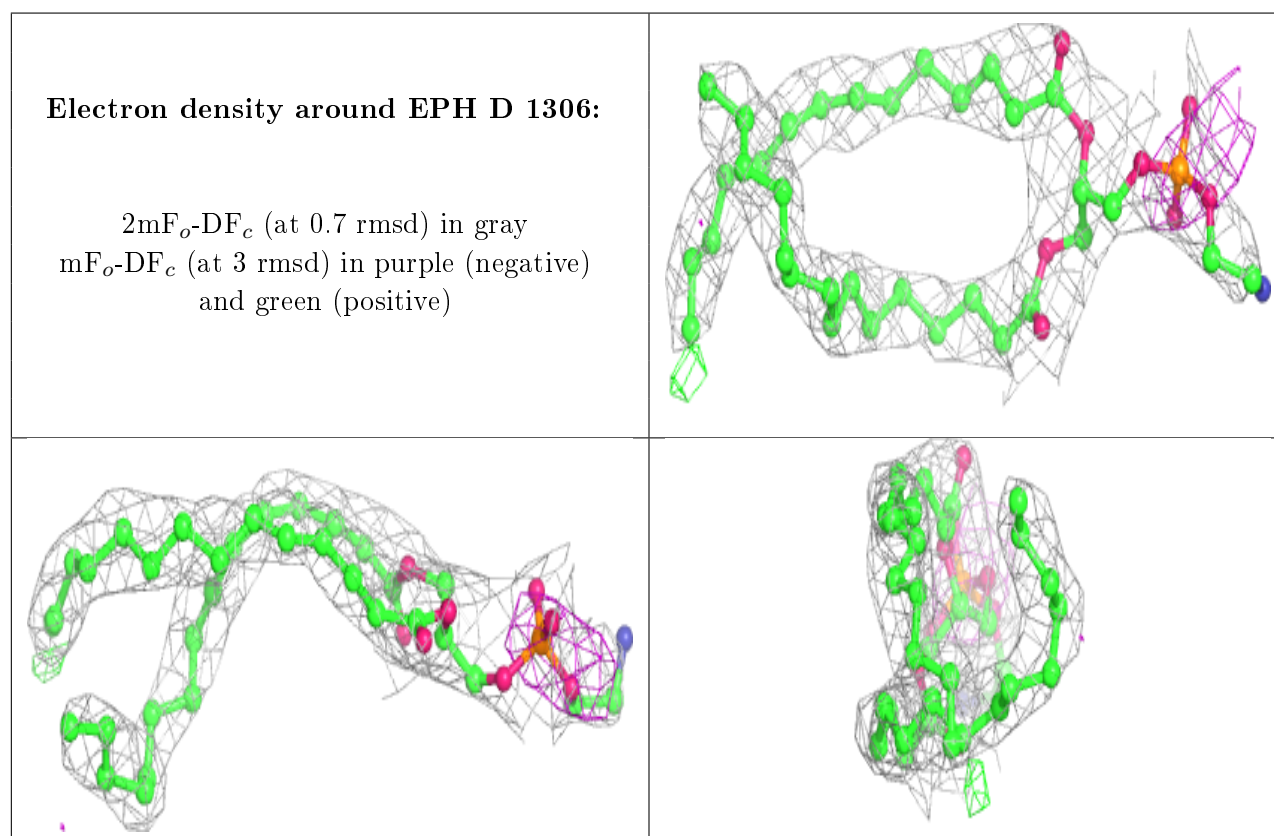
There are no carbohydrates in this entry.

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.

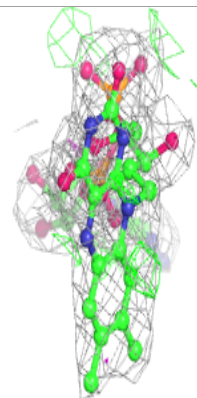
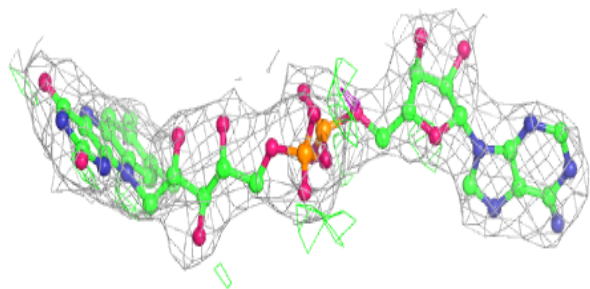
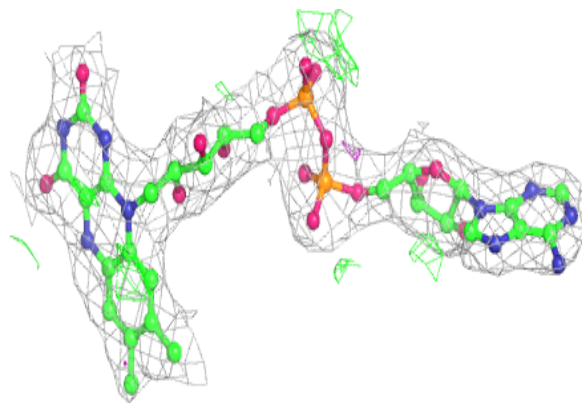
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	EPH	D	1306	44/49	0.86	0.26	52,71,96,97	0
5	FAD	A	700	53/53	0.97	0.26	35,40,43,43	0
9	HEM	C	1305	43/43	0.98	0.16	40,43,51,54	0
8	F3S	B	304	7/7	0.99	0.11	35,35,37,40	0
6	FES	B	302	4/4	1.00	0.16	39,43,44,44	0
7	SF4	B	303	8/8	1.00	0.12	32,34,35,36	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.



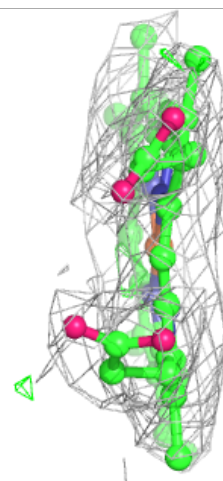
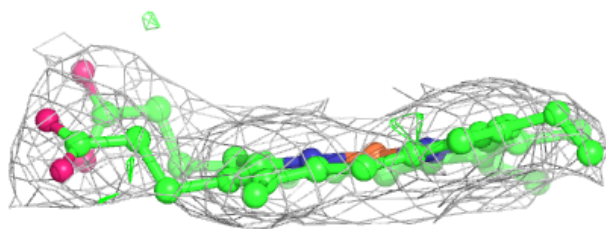
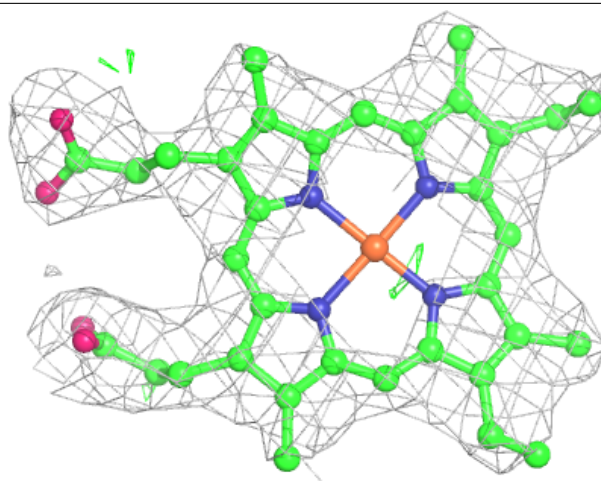
Electron density around FAD A 700:

$2mF_o-DF_c$ (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.