



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:10 pm BST

PDB ID : 3AEA
Title : Crystal structure of porcine heart mitochondrial complex II bound with N-(3-Dimethylaminomethyl-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 : 3.39 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

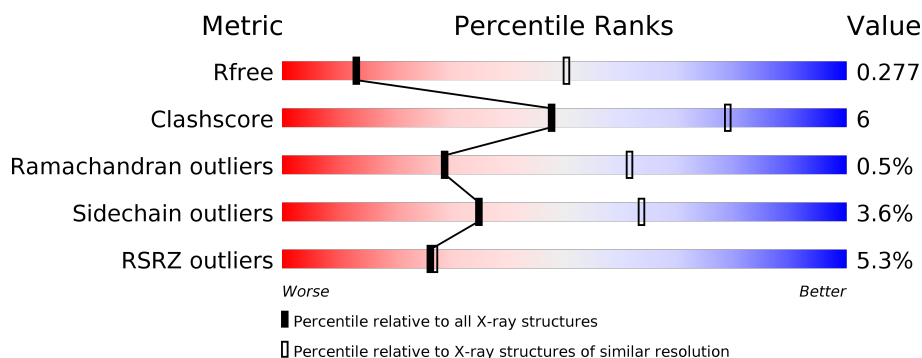
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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>8%</div> <div>79%</div> <div>18%</div> <div>••</div> </div>
2	B	252	<div> <div>4%</div> <div>81%</div> <div>12%</div> <div>• 5%</div> </div>
3	C	140	<div> <div>%</div> <div>92%</div> <div>6%</div> <div>•</div> </div>
4	D	103	<div> <div>%</div> <div>94%</div> <div>5%</div> <div>•</div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 8669 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.

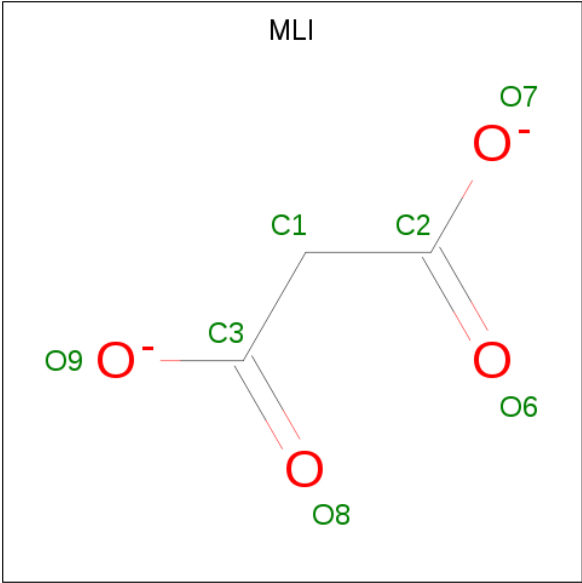
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			765	499	128	133	5			

- 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 MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



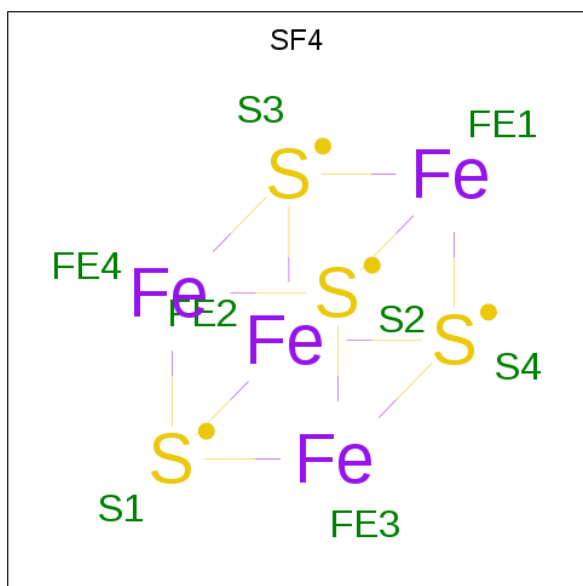
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



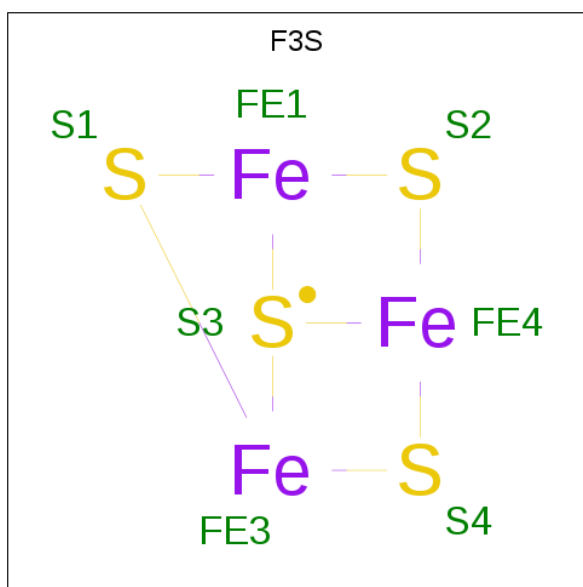
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		

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



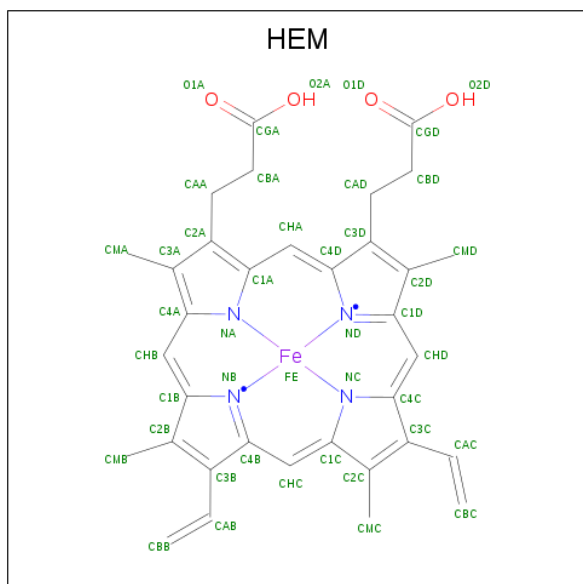
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



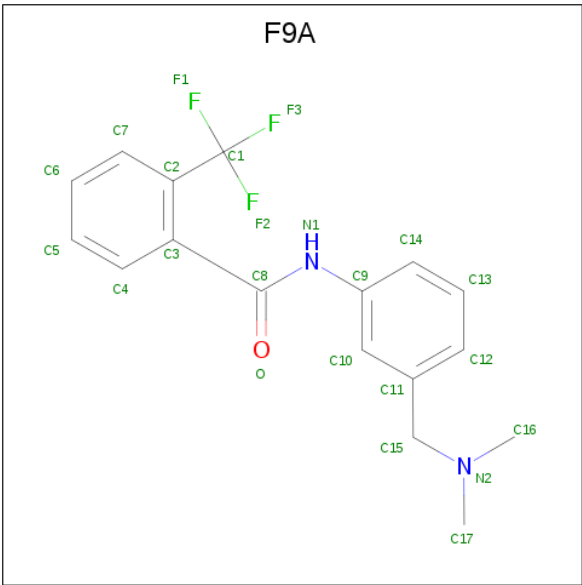
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		

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



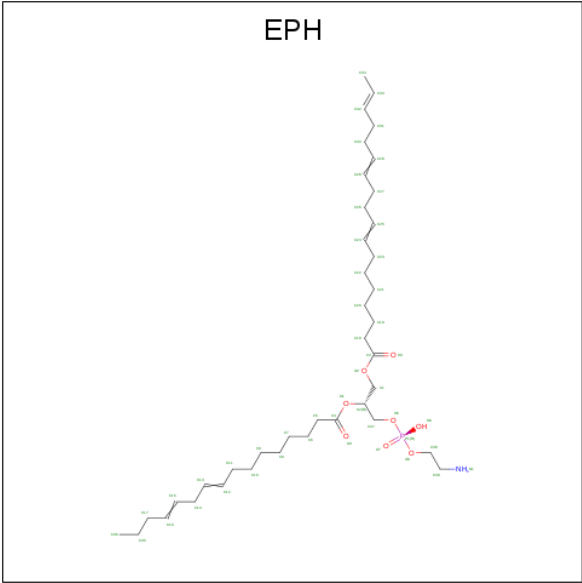
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 11 is N-{3-[(dimethylamino)methyl]phenyl}-2-(trifluoromethyl)benzamide (three-letter code: F9A) (formula: $C_{17}H_{17}F_3N_2O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	F	N	O	0	0
			23	17	3	2	1		

- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: C₃₉H₆₈NO₈P).

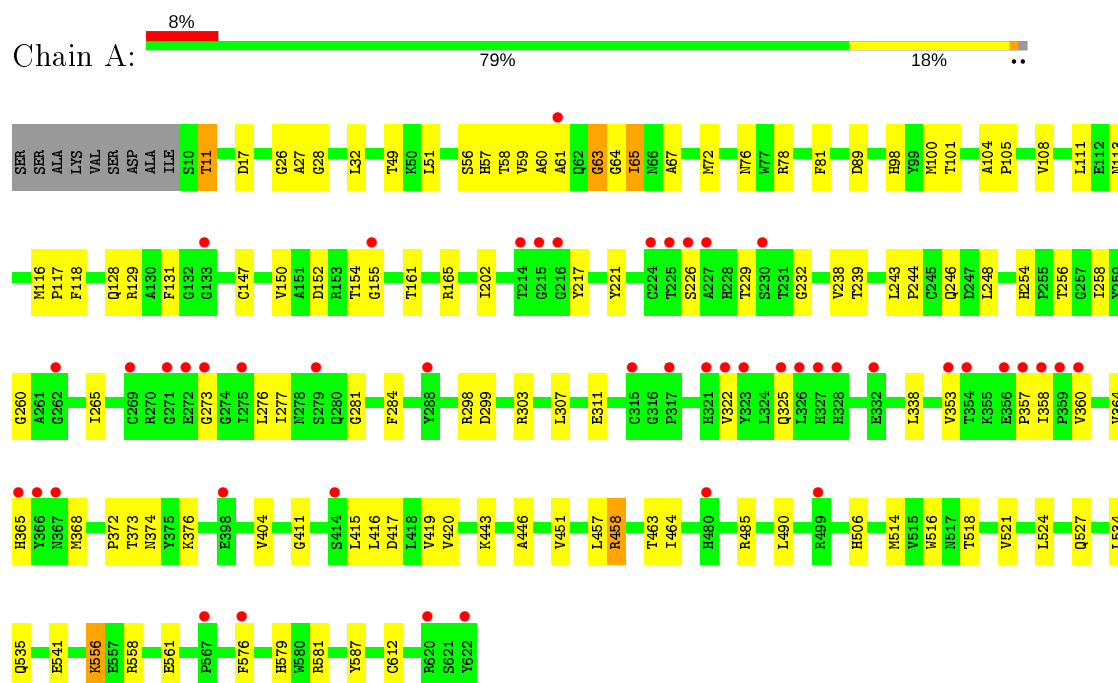


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

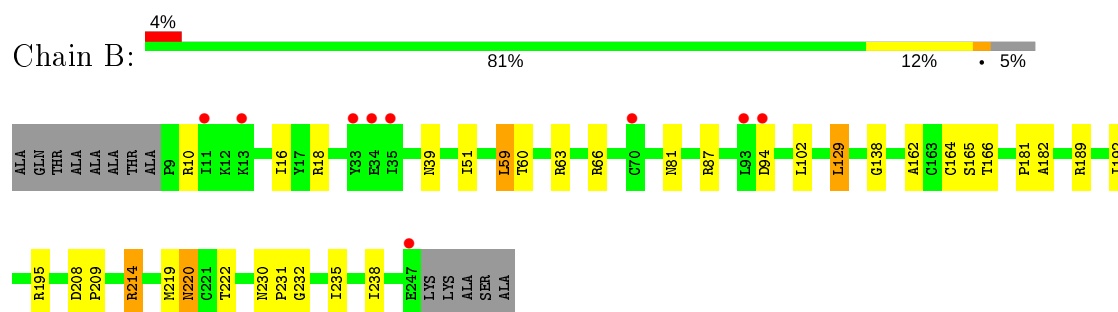
3 Residue-property plots [i](#)

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.

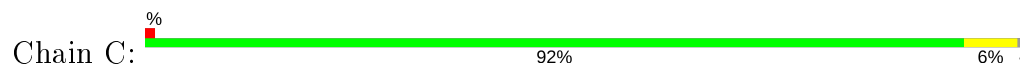
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial



- 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	71.50 Å 83.75 Å 294.96 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.77 – 3.39 43.77 – 3.39	Depositor EDS
% Data completeness (in resolution range)	98.2 (43.77-3.39) 98.2 (43.77-3.39)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.40 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.286 0.232 , 0.277	Depositor DCC
R_{free} test set	1271 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	100.0	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8669	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: F9A, SF4, MLI, 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	0.31	0/4828	0.49	1/6531 (0.0%)
2	B	0.31	0/1964	0.46	0/2648
3	C	0.31	0/1091	0.45	0/1483
4	D	0.29	0/784	0.43	0/1066
All	All	0.31	0/8667	0.47	1/11728 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	THR	CB-CA-C	-5.13	97.75	111.60

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	77	0
2	B	1922	0	1902	23	0
3	C	1064	0	1104	5	0
4	D	765	0	773	1	0
5	A	53	0	31	13	0
6	A	7	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
11	D	23	0	17	1	0
12	D	44	0	53	0	0
All	All	8669	0	8530	104	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 6.

All (104) 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	1.30	1.37
1:A:61:ALA:HB3	1:A:155:GLY:HA3	1.51	0.93
1:A:57:HIS:CE1	5:A:700:FAD:HM82	2.13	0.84
1:A:113:ASN:HD22	2:B:138:GLY:H	1.32	0.78
2:B:220:ASN:HD21	3:C:39:MET:HG3	1.55	0.71
3:C:52:LEU:HB3	10:C:1305:HEM:HAC	1.75	0.69
1:A:61:ALA:HA	5:A:700:FAD:N5	2.08	0.68
1:A:57:HIS:NE2	5:A:700:FAD:C8	2.58	0.66
1:A:246:GLN:HB2	1:A:372:PRO:HG3	1.78	0.64
2:B:181:PRO:HA	2:B:235:ILE:HD11	1.80	0.64
1:A:11:THR:O	1:A:11:THR:HG22	1.98	0.62
4:D:72:LEU:O	4:D:76:LEU:HB2	1.98	0.62
1:A:58:THR:HA	5:A:700:FAD:O4'	2.00	0.62
1:A:57:HIS:O	1:A:59:VAL:N	2.32	0.62
1:A:64:GLY:HA2	1:A:154:THR:HG21	1.80	0.61
2:B:165:SER:HA	2:B:181:PRO:HG2	1.82	0.61
1:A:57:HIS:O	1:A:60:ALA:N	2.28	0.59
1:A:49:THR:HA	5:A:700:FAD:N3A	2.17	0.59
1:A:217:TYR:HB3	1:A:232:GLY:HA3	1.85	0.58
1:A:116:MET:HA	1:A:161:THR:HG21	1.87	0.57
1:A:556:LYS:HD2	1:A:556:LYS:H	1.69	0.57
1:A:258:ILE:HD11	1:A:265:ILE:HG23	1.86	0.57
2:B:102:LEU:HD22	2:B:166:THR:HG21	1.85	0.57
1:A:57:HIS:O	1:A:58:THR:C	2.43	0.57
1:A:27:ALA:H	5:A:700:FAD:H4B	1.70	0.57
1:A:51:LEU:HD21	1:A:229:THR:HG21	1.87	0.56
1:A:118:PHE:HA	1:A:150:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:HIS:HD2	1:A:256:THR:H	1.54	0.55
1:A:57:HIS:C	1:A:59:VAL:N	2.57	0.55
1:A:254:HIS:HB2	1:A:365:HIS:HB2	1.89	0.55
1:A:516:TRP:HB3	2:B:60:THR:HG21	1.88	0.55
2:B:222:THR:HG22	2:B:231:PRO:HD2	1.89	0.55
1:A:111:LEU:HD11	1:A:419:VAL:HG21	1.89	0.55
2:B:219:MET:CE	2:B:232:GLY:HA3	2.37	0.54
1:A:415:LEU:HG	5:A:700:FAD:C2	2.39	0.53
2:B:162:ALA:O	2:B:166:THR:HG22	2.08	0.53
1:A:518:THR:HA	1:A:521:VAL:HG22	1.89	0.52
3:C:62:SER:HB2	3:C:66:LEU:HD12	1.93	0.51
1:A:524:LEU:HA	1:A:527:GLN:HE21	1.77	0.50
1:A:104:ALA:HB3	1:A:105:PRO:HD3	1.94	0.50
1:A:81:PHE:HA	1:A:101:THR:HG21	1.94	0.49
1:A:104:ALA:HA	1:A:416:LEU:HD11	1.93	0.49
1:A:152:ASP:HB2	1:A:338:LEU:HA	1.95	0.49
1:A:57:HIS:CE1	1:A:226:SER:HA	2.48	0.49
1:A:485:ARG:HD2	1:A:490:LEU:HD21	1.95	0.49
2:B:219:MET:HE1	2:B:232:GLY:HA3	1.95	0.48
2:B:18:ARG:HD3	2:B:59:LEU:HD12	1.96	0.48
1:A:579:HIS:HD2	1:A:581:ARG:H	1.61	0.48
3:C:52:LEU:HD21	3:C:98:LEU:HA	1.96	0.48
1:A:254:HIS:HB2	1:A:365:HIS:CB	2.44	0.47
1:A:298:ARG:NH2	1:A:411:GLY:HA2	2.29	0.47
1:A:458:ARG:NH2	1:A:514:MET:HG2	2.29	0.47
1:A:65:ILE:HD12	1:A:108:VAL:HG22	1.95	0.47
1:A:374:ASN:HB3	1:A:376:LYS:H	1.80	0.47
2:B:129:LEU:HD21	2:B:195:ARG:HB2	1.96	0.47
2:B:102:LEU:HB3	2:B:166:THR:HG21	1.98	0.46
2:B:214:ARG:NE	2:B:214:ARG:HA	2.29	0.46
2:B:235:ILE:HA	2:B:238:ILE:HD12	1.97	0.46
11:D:1201:F9A:O	11:D:1201:F9A:H14	2.16	0.46
1:A:100:MET:HA	1:A:420:VAL:HG11	1.97	0.46
1:A:443:LYS:HB2	1:A:446:ALA:HB2	1.96	0.46
1:A:353:VAL:HG12	1:A:358:ILE:HD11	1.97	0.46
1:A:28:GLY:HA3	5:A:700:FAD:O1P	2.15	0.46
1:A:67:ALA:HB2	1:A:108:VAL:HG21	1.97	0.46
1:A:49:THR:OG1	5:A:700:FAD:O2B	2.22	0.45
1:A:129:ARG:O	1:A:147:CYS:HB3	2.17	0.45
1:A:63:GLY:N	5:A:700:FAD:O4	2.50	0.45
2:B:208:ASP:HB2	2:B:209:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:THR:HG22	1:A:360:VAL:HG21	1.99	0.45
1:A:248:LEU:HD12	1:A:535:GLN:HB2	1.98	0.45
3:C:46:ARG:HE	10:C:1305:HEM:CGD	2.30	0.44
2:B:81:ASN:ND2	2:B:166:THR:HG23	2.33	0.44
1:A:238:VAL:HG13	1:A:243:LEU:HB2	2.01	0.43
2:B:222:THR:HG21	2:B:230:ASN:OD1	2.19	0.43
1:A:221:TYR:CG	1:A:364:VAL:HG21	2.54	0.43
2:B:219:MET:HE2	2:B:232:GLY:HA3	2.01	0.43
1:A:202:ILE:HD13	1:A:451:VAL:HG22	2.00	0.43
1:A:117:PRO:O	1:A:150:VAL:HG13	2.19	0.42
1:A:56:SER:O	1:A:57:HIS:C	2.56	0.42
1:A:463:THR:HG23	1:A:464:ILE:HG13	2.00	0.42
2:B:16:ILE:HG21	2:B:59:LEU:HD11	2.01	0.42
1:A:113:ASN:ND2	2:B:138:GLY:H	2.08	0.42
1:A:373:THR:HG22	1:A:374:ASN:O	2.20	0.42
1:A:64:GLY:CA	1:A:154:THR:HG21	2.49	0.41
1:A:254:HIS:CD2	1:A:256:THR:H	2.38	0.41
1:A:129:ARG:HA	1:A:129:ARG:HD2	1.80	0.41
1:A:277:ILE:HG23	1:A:281:GLY:HA2	2.02	0.41
1:A:325:GLN:HG3	1:A:357:PRO:HB3	2.01	0.41
1:A:576:PHE:HA	1:A:579:HIS:CE1	2.55	0.41
2:B:181:PRO:HG3	9:B:304:F3S:S3	2.59	0.41
1:A:244:PRO:HB3	1:A:587:TYR:CZ	2.56	0.41
5:A:700:FAD:H9	5:A:700:FAD:H1'1	1.81	0.41
1:A:89:ASP:OD2	1:A:558:ARG:NH1	2.54	0.41
1:A:76:ASN:HD21	1:A:78:ARG:HD2	1.85	0.41
1:A:72:MET:HG2	1:A:128:GLN:HB2	2.03	0.40
1:A:265:ILE:HD11	1:A:360:VAL:HG11	2.03	0.40
2:B:164:CYS:SG	2:B:182:ALA:HB2	2.61	0.40
1:A:463:THR:HG22	1:A:506:HIS:HB3	2.03	0.40
1:A:98:HIS:CE1	1:A:612:CYS:HB3	2.56	0.40
1:A:26:GLY:HA2	5:A:700:FAD:O4B	2.20	0.40
1:A:276:LEU:HB3	1:A:284:PHE:CE2	2.57	0.40
1:A:299:ASP:O	1:A:303:ARG:HB2	2.22	0.40
1:A:150:VAL:HB	1:A:154:THR:HA	2.02	0.40
1:A:307:LEU:O	1:A:311:GLU:HG2	2.22	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%)	572 (94%)	35 (6%)	4 (1%)	22	55
2	B	237/252 (94%)	220 (93%)	16 (7%)	1 (0%)	34	67
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%)	1022 (94%)	57 (5%)	5 (0%)	29	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	GLY
1	A	273	GLY
1	A	322	VAL
2	B	59	LEU
1	A	63	GLY

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%)	484 (97%)	15 (3%)	41	68
2	B	214/220 (97%)	202 (94%)	12 (6%)	21	51
3	C	117/118 (99%)	114 (97%)	3 (3%)	46	72
4	D	76/76 (100%)	73 (96%)	3 (4%)	32	61
All	All	906/920 (98%)	873 (96%)	33 (4%)	35	63

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	32	LEU
1	A	65	ILE
1	A	131	PHE
1	A	165	ARG
1	A	239	THR
1	A	368	MET
1	A	404	VAL
1	A	417	ASP
1	A	457	LEU
1	A	458	ARG
1	A	534	LEU
1	A	541	GLU
1	A	556	LYS
1	A	561	GLU
2	B	10	ARG
2	B	39	ASN
2	B	51	ILE
2	B	63	ARG
2	B	66	ARG
2	B	87	ARG
2	B	94	ASP
2	B	129	LEU
2	B	189	ARG
2	B	192	ILE
2	B	214	ARG
2	B	220	ASN
3	C	30	ILE
3	C	82	LEU
3	C	123	THR
4	D	78	LEU
4	D	108	LEU
4	D	134	TRP

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	143	GLN
1	A	156	HIS

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Mol	Chain	Res	Type
1	A	186	ASN
1	A	246	GLN
1	A	254	HIS
1	A	374	ASN
1	A	378	GLN
1	A	384	ASN
1	A	408	ASN
1	A	461	ASN
1	A	474	GLN
1	A	550	HIS
1	A	579	HIS
2	B	92	ASN
2	B	121	GLN
2	B	174	ASN
2	B	220	ASN
3	C	29	HIS
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 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	$\# Z > 2$
12	EPH	D	1306	-	43,43,48	1.55	7 (16%)	45,48,53	1.12	2 (4%)
7	FES	B	302	2	0,4,4	0.00	-	-		
8	SF4	B	303	2	0,12,12	0.00	-	-		
11	F9A	D	1201	-	24,24,24	1.35	2 (8%)	34,34,34	1.50	4 (11%)
6	MLI	A	701	-	0,6,6	0.00	-	0,7,7	0.00	-
10	HEM	C	1305	3,4	27,50,50	2.17	6 (22%)	17,82,82	1.36	2 (11%)
9	F3S	B	304	2	0,9,9	0.00	-	-		
5	FAD	A	700	1	51,58,58	1.42	6 (11%)	60,89,89	1.69	11 (18%)

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
12	EPH	D	1306	-	-	27/47/47/52	-
9	F3S	B	304	2	-	-	0/3/3/3
8	SF4	B	303	2	-	-	0/6/5/5
11	F9A	D	1201	-	-	1/18/18/18	0/2/2/2
6	MLI	A	701	-	-	0/0/4/4	-
10	HEM	C	1305	3,4	-	1/6/54/54	-
7	FES	B	302	2	-	-	0/1/1/1
5	FAD	A	700	1	-	3/30/50/50	0/6/6/6

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	1201	F9A	C3-C2	5.75	1.50	1.40
10	C	1305	HEM	C3D-C2D	5.52	1.54	1.37
5	A	700	FAD	C10-N1	4.54	1.39	1.33
12	D	1306	EPH	O2-C4	4.44	1.46	1.33
10	C	1305	HEM	C3B-C2B	-4.44	1.34	1.40
12	D	1306	EPH	O1-C3	4.38	1.46	1.34
10	C	1305	HEM	C3C-C2C	-4.31	1.34	1.40
5	A	700	FAD	C4X-N5	3.89	1.38	1.33
5	A	700	FAD	C2A-N3A	3.83	1.38	1.32
12	D	1306	EPH	C25-C24	3.66	1.53	1.31
12	D	1306	EPH	C29-C28	3.66	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	1306	EPH	C13-C12	3.64	1.52	1.31
10	C	1305	HEM	C3C-CAC	3.47	1.54	1.47
10	C	1305	HEM	C3B-CAB	3.40	1.54	1.47
5	A	700	FAD	C4-N3	3.34	1.38	1.33
12	D	1306	EPH	C15-C16	3.13	1.53	1.29
5	A	700	FAD	C1'-N10	2.95	1.51	1.48
11	D	1201	F9A	C9-N1	-2.78	1.36	1.41
5	A	700	FAD	C2A-N1A	2.65	1.38	1.33
12	D	1306	EPH	P1-O7	2.41	1.59	1.50
10	C	1305	HEM	CAA-C2A	2.18	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	FAD	N3A-C2A-N1A	-5.83	119.57	128.68
5	A	700	FAD	C4-N3-C2	5.65	119.92	115.14
11	D	1201	F9A	C16-N2-C15	4.65	120.30	110.69
11	D	1201	F9A	C17-N2-C15	4.32	119.61	110.69
11	D	1201	F9A	C17-N2-C16	4.01	120.09	109.73
5	A	700	FAD	C5X-C9A-N10	3.93	120.57	117.72
5	A	700	FAD	C4X-N5-C5X	3.86	120.63	116.77
12	D	1306	EPH	O1-C3-C5	3.58	119.22	111.50
5	A	700	FAD	C1'-N10-C9A	-2.87	116.03	118.29
12	D	1306	EPH	O2-C4-C18	2.67	120.28	111.91
5	A	700	FAD	C3B-C2B-C1B	2.59	104.88	100.98
5	A	700	FAD	C10-C4X-N5	-2.51	119.52	121.26
5	A	700	FAD	P-O3P-PA	-2.37	124.69	132.83
10	C	1305	HEM	CAA-CBA-CGA	-2.36	108.72	112.67
11	D	1201	F9A	F2-C1-C2	-2.30	108.70	112.70
10	C	1305	HEM	C1D-C2D-C3D	-2.21	105.46	107.00
5	A	700	FAD	C4X-C4-N3	-2.19	120.43	123.43
5	A	700	FAD	C4-C4X-N5	2.19	121.10	118.60
5	A	700	FAD	C9A-N10-C10	-2.00	119.29	121.91

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	D	1306	EPH	C25-C26-C27-C28
12	D	1306	EPH	C28-C29-C30-C31
12	D	1306	EPH	C37-O5-P1-O6
12	D	1306	EPH	C37-O5-P1-O7

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Mol	Chain	Res	Type	Atoms
12	D	1306	EPH	C12-C13-C14-C15
12	D	1306	EPH	O8-C38-C39-N1
10	C	1305	HEM	C3D-CAD-CBD-CGD
5	A	700	FAD	N10-C1'-C2'-O2'
5	A	700	FAD	N10-C1'-C2'-C3'
12	D	1306	EPH	C18-C4-O2-C1
11	D	1201	F9A	C11-C15-N2-C17
12	D	1306	EPH	O4-C4-O2-C1
12	D	1306	EPH	C23-C24-C25-C26
12	D	1306	EPH	C37-O5-P1-O8
12	D	1306	EPH	C38-O8-P1-O5
12	D	1306	EPH	C18-C19-C20-C21
12	D	1306	EPH	C4-C18-C19-C20
12	D	1306	EPH	C3-C5-C6-C7
12	D	1306	EPH	C9-C10-C11-C12
12	D	1306	EPH	C21-C22-C23-C24
12	D	1306	EPH	C11-C10-C9-C8
12	D	1306	EPH	C13-C14-C15-C16
12	D	1306	EPH	C6-C7-C8-C9
12	D	1306	EPH	C14-C15-C16-C17
12	D	1306	EPH	C38-O8-P1-O7
12	D	1306	EPH	C20-C21-C22-C23
5	A	700	FAD	O4B-C4B-C5B-O5B
12	D	1306	EPH	C1-C2-C37-O5
12	D	1306	EPH	C24-C25-C26-C27
12	D	1306	EPH	O1-C3-C5-C6
12	D	1306	EPH	C26-C27-C28-C29
12	D	1306	EPH	O3-C3-C5-C6

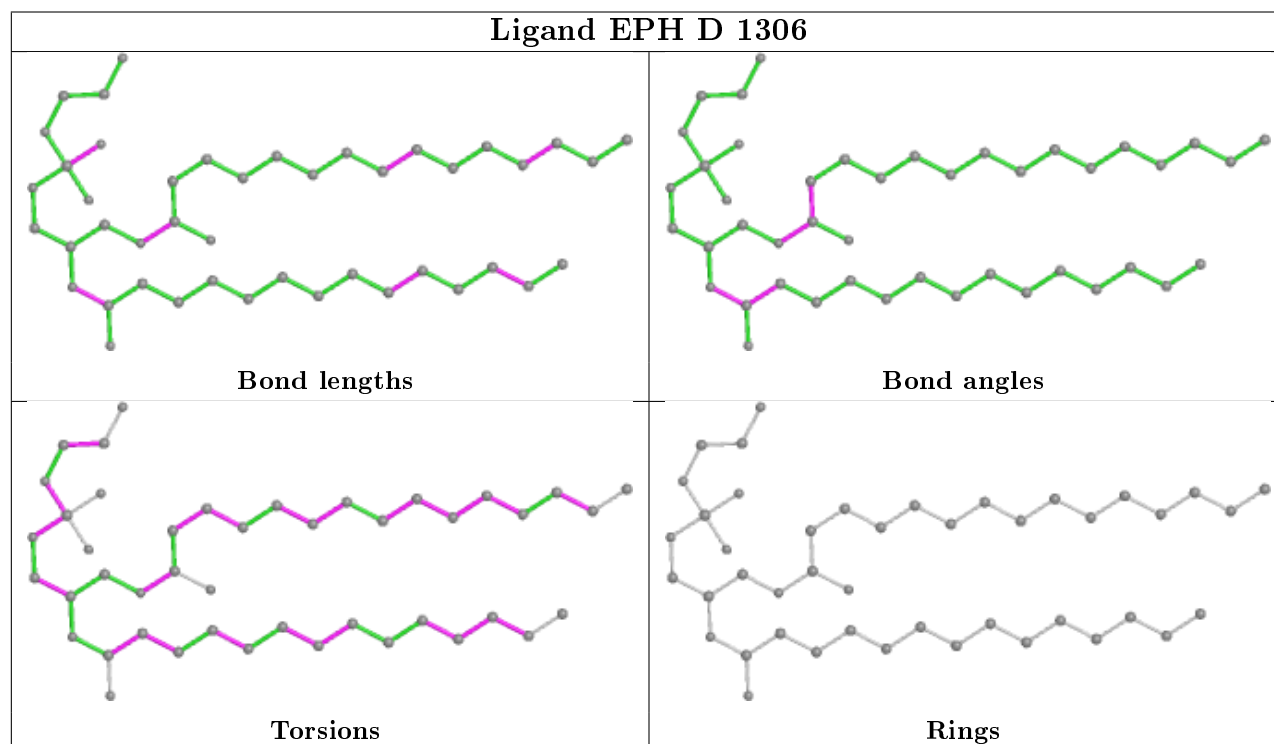
There are no ring outliers.

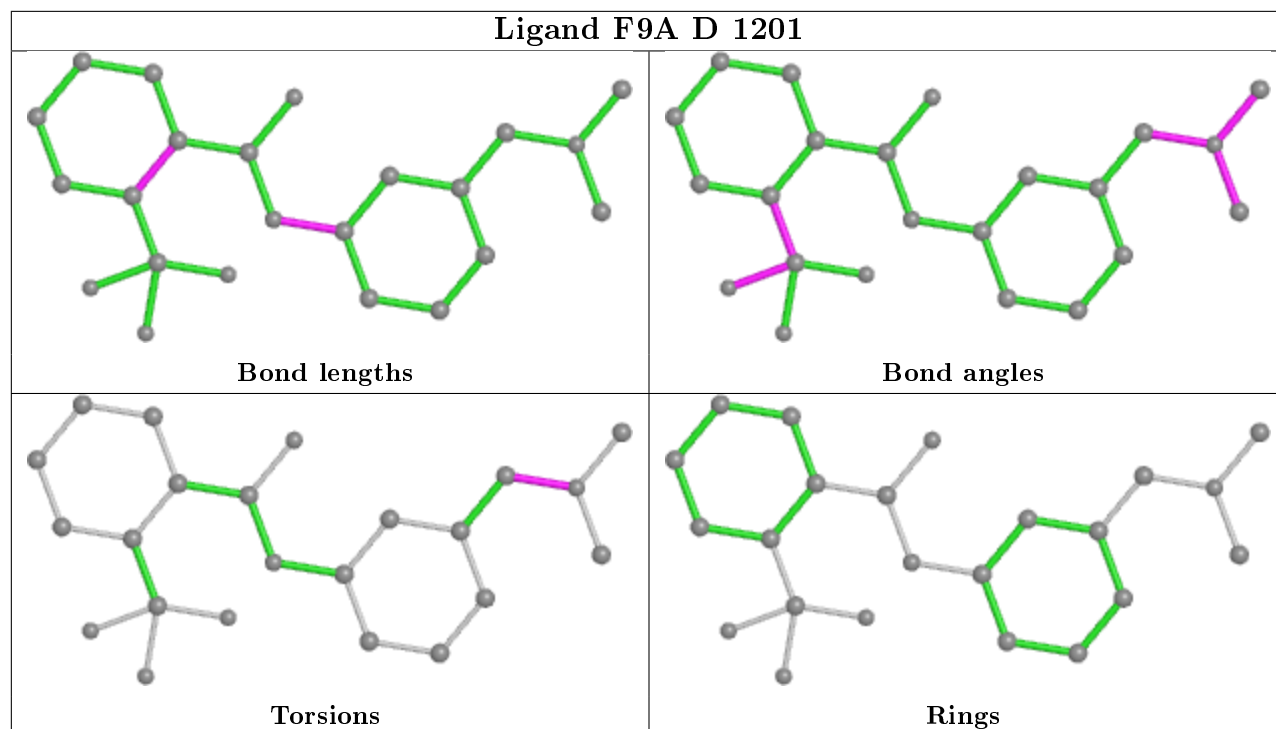
4 monomers are involved in 17 short contacts:

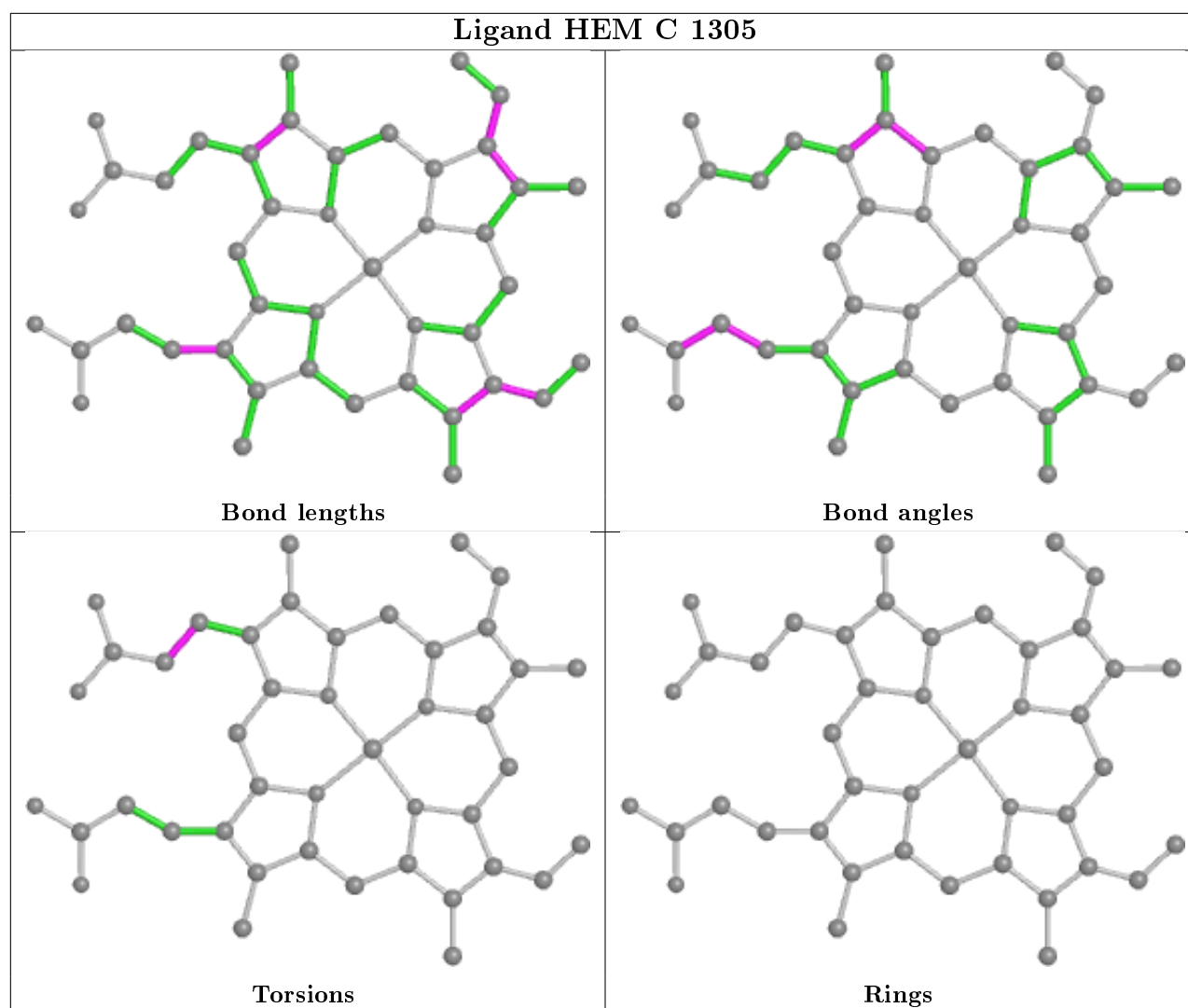
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	1201	F9A	1	0
10	C	1305	HEM	2	0
9	B	304	F3S	1	0
5	A	700	FAD	13	0

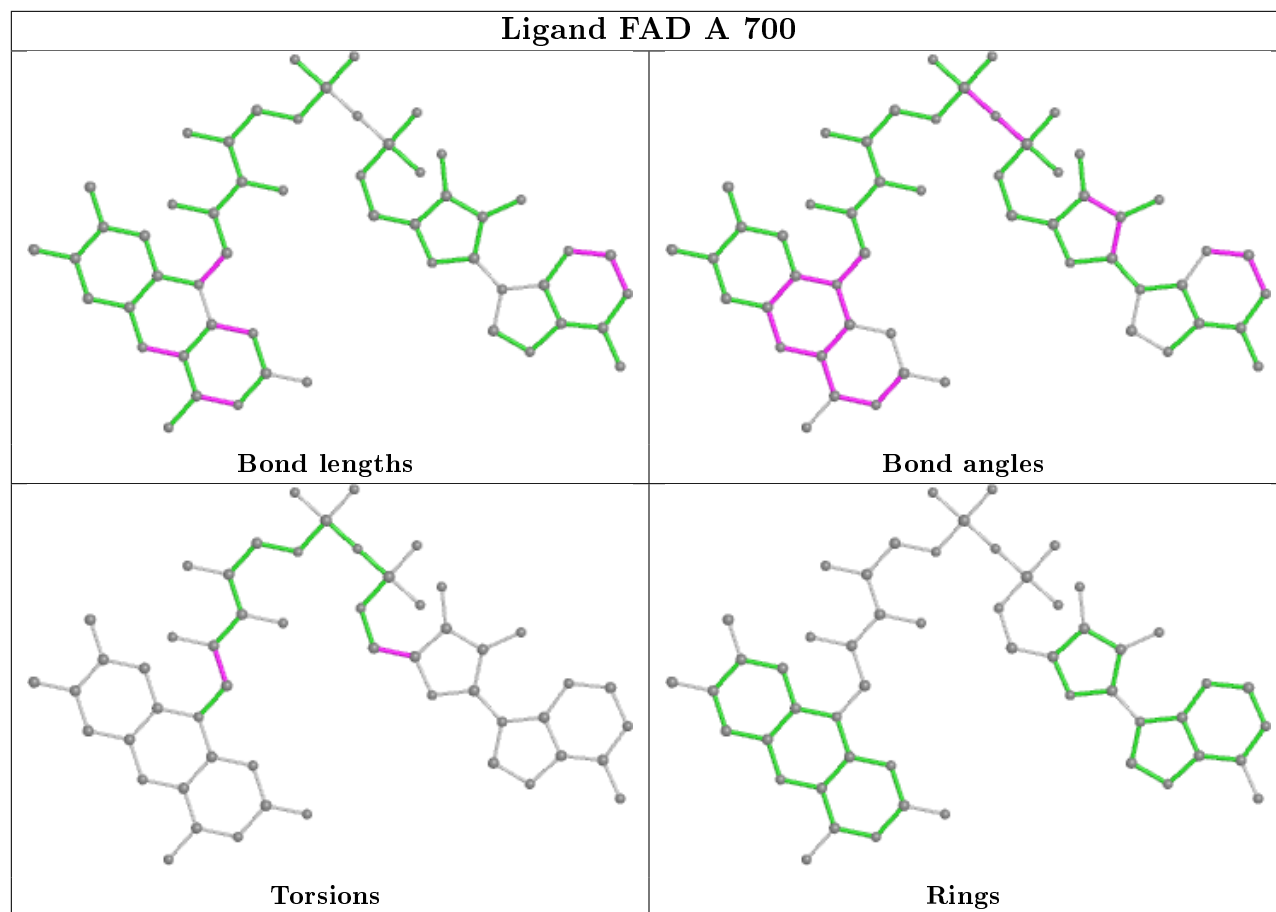
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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%)	0.38	47 (7%) 13 15	61, 107, 192, 211	0
2	B	239/252 (94%)	0.24	9 (3%) 40 39	75, 98, 136, 164	0
3	C	138/140 (98%)	-0.03	1 (0%) 87 87	90, 107, 161, 176	0
4	D	102/103 (99%)	-0.09	1 (0%) 82 81	89, 110, 138, 154	0
All	All	1092/1117 (97%)	0.25	58 (5%) 26 27	61, 106, 184, 211	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	35	SER	8.6
1	A	326	LEU	7.1
1	A	357	PRO	6.3
1	A	323	TYR	6.1
1	A	325	GLN	6.0
1	A	327	HIS	5.2
1	A	359	PRO	5.1
1	A	322	VAL	5.0
1	A	133	GLY	4.4
1	A	288	TYR	4.4
1	A	398	GLU	4.1
1	A	328	HIS	4.0
1	A	226	SER	3.8
1	A	315	CYS	3.7
1	A	230	SER	3.6
2	B	11	ILE	3.6
1	A	414	SER	3.5
1	A	275	ILE	3.5
1	A	271	GLY	3.5
1	A	356	GLU	3.4
1	A	61	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	622	TYR	3.4
1	A	262	GLY	3.3
1	A	215	GLY	3.3
1	A	358	ILE	3.2
1	A	227	ALA	3.2
1	A	155	GLY	3.1
2	B	34	GLU	3.1
2	B	70	CYS	3.1
1	A	272	GLU	3.0
1	A	367	ASN	3.0
2	B	94	ASP	3.0
1	A	273	GLY	2.9
1	A	576	PHE	2.8
1	A	214	THR	2.8
1	A	366	TYR	2.7
1	A	354	THR	2.7
2	B	35	ILE	2.7
1	A	480	HIS	2.6
1	A	216	GLY	2.6
1	A	353	VAL	2.5
1	A	321	HIS	2.5
1	A	620	ARG	2.5
3	C	84	PRO	2.5
2	B	93	LEU	2.5
1	A	317	PRO	2.5
1	A	332	GLU	2.4
1	A	224	CYS	2.4
2	B	247	GLU	2.3
1	A	365	HIS	2.2
2	B	13	LYS	2.2
1	A	360	VAL	2.2
2	B	33	TYR	2.1
1	A	567	PRO	2.1
1	A	279	SER	2.1
1	A	225	THR	2.0
1	A	269	CYS	2.0
1	A	499	ARG	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

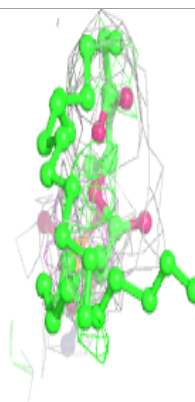
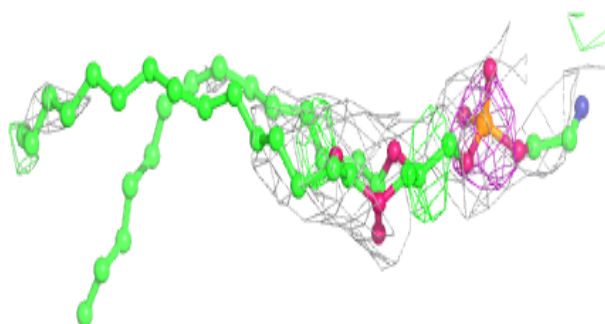
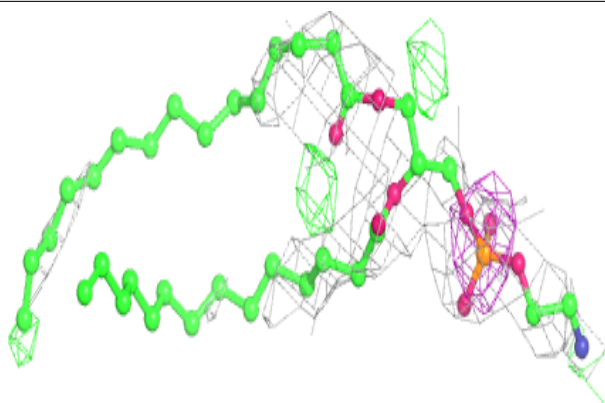
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.81	0.55	140,147,153,153	0
6	MLI	A	701	7/7	0.84	0.41	177,177,177,177	0
5	FAD	A	700	53/53	0.85	0.42	82,82,87,87	0
11	F9A	D	1201	23/23	0.93	0.25	103,103,105,105	0
10	HEM	C	1305	43/43	0.97	0.24	95,95,97,98	0
9	F3S	B	304	7/7	0.98	0.18	95,96,96,96	0
7	FES	B	302	4/4	0.99	0.27	79,80,80,80	0
8	SF4	B	303	8/8	1.00	0.20	75,76,76,76	0

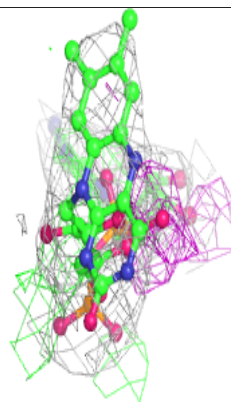
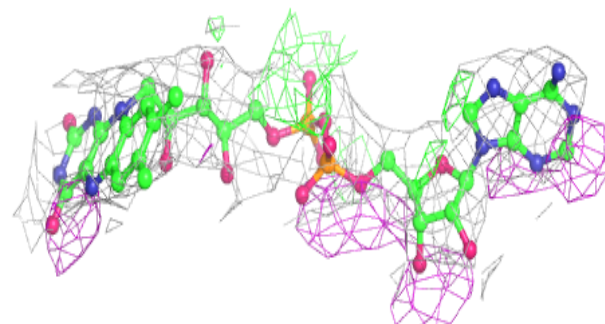
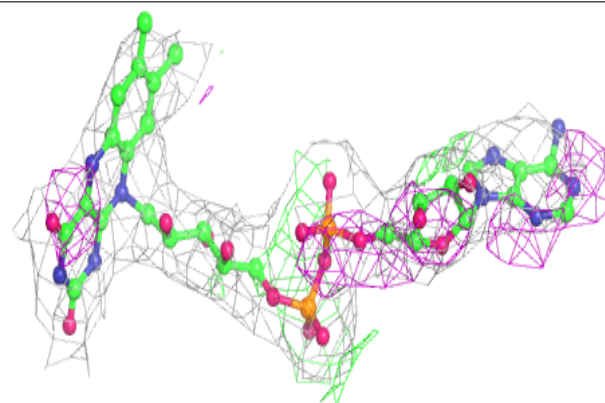
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

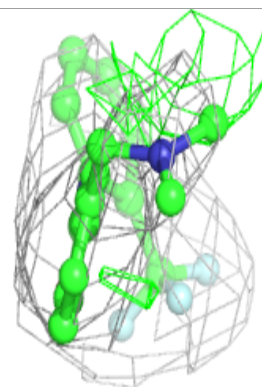
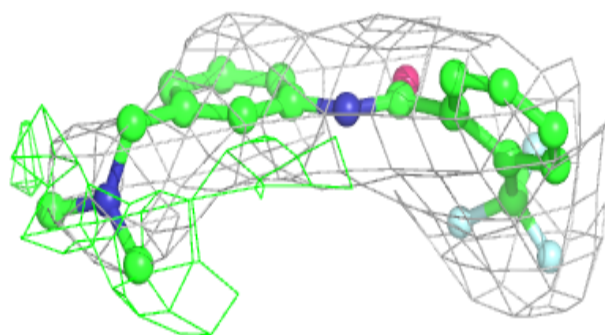
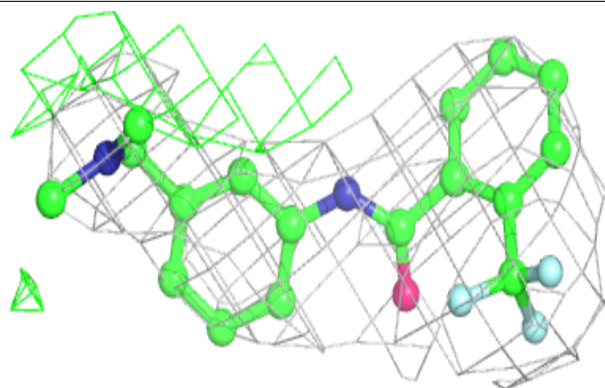
**Electron density around FAD A 700:**

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



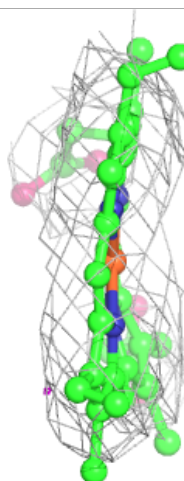
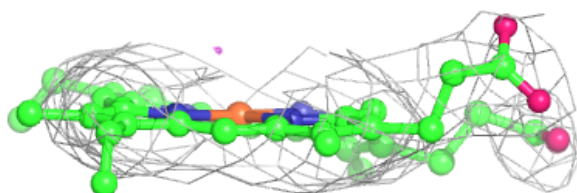
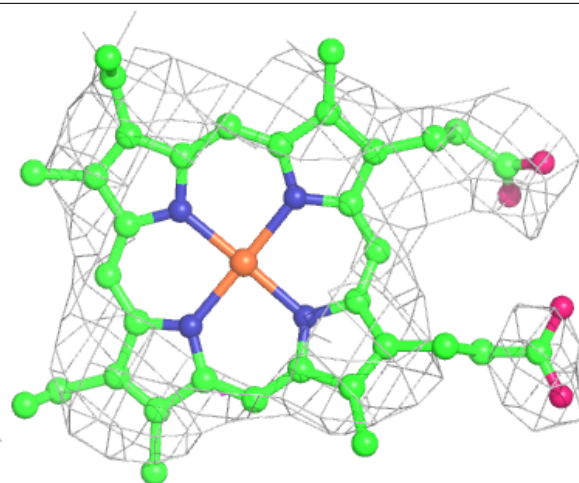
Electron density around F9A D 1201:

$2mF_o - DF_c$ (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.