Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2023 – 03:06 PM EDT

PDB ID	:	3AEG
Title	:	Crystal structure of porcine heart mitochondrial complex II bound with N-Bi phenyl-3-yl-2-iodo-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	:	3.27 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

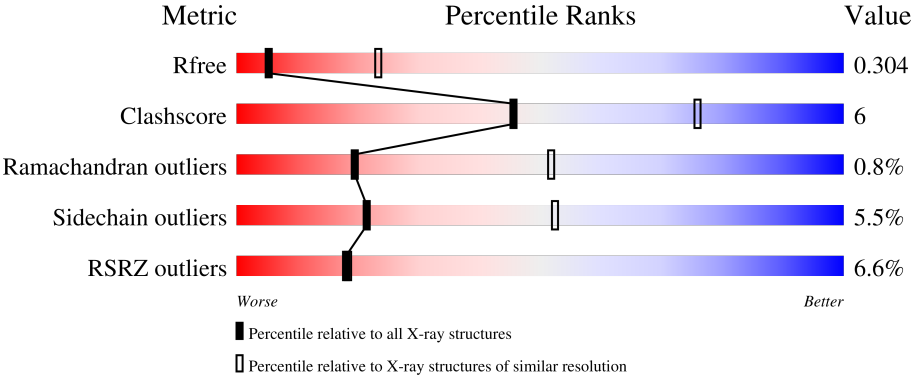
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.27 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	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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

Mol	Chain	Length	Quality of chain
1	A	622	8% 77% 20%
2	B	252	2% 79% 14% 5%
3	C	140	4% 85% 11%
4	D	103	11% 90% 8%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 8617 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

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

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

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

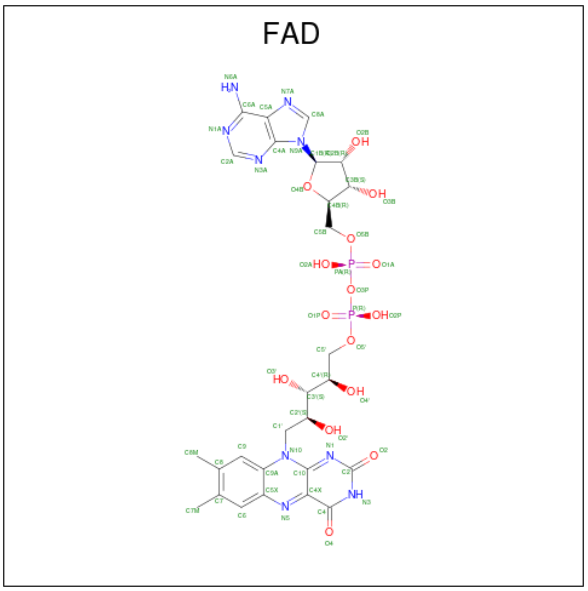
- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b560 subunit, mitochondrial.

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

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

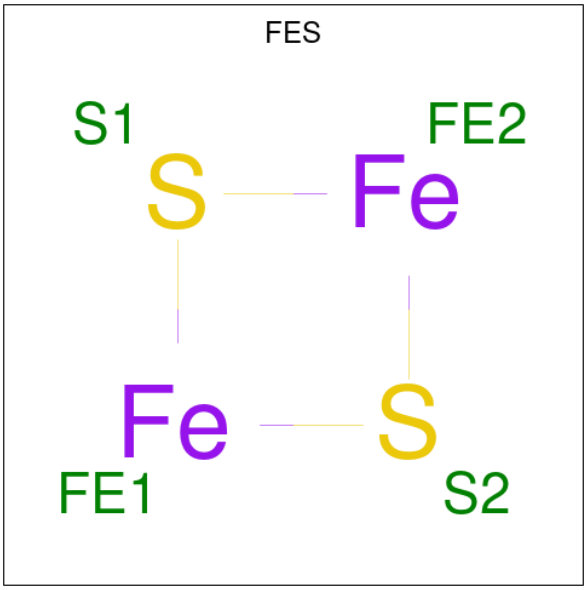
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	102	765	499	128	133	5	0	0	0

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



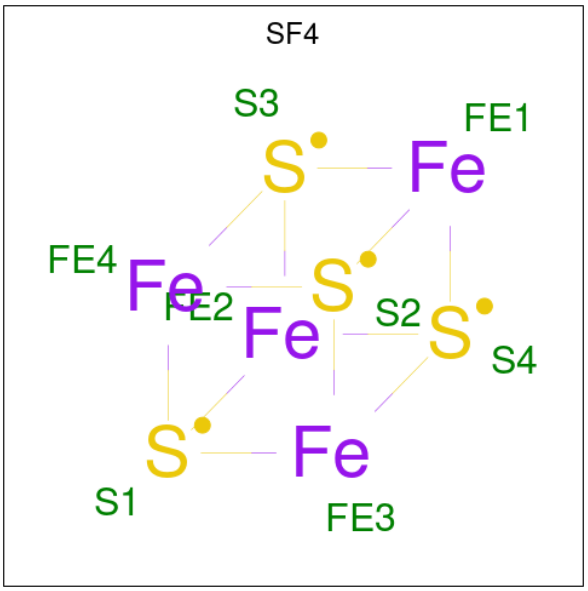
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	53	27	9	15	2	0	0

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



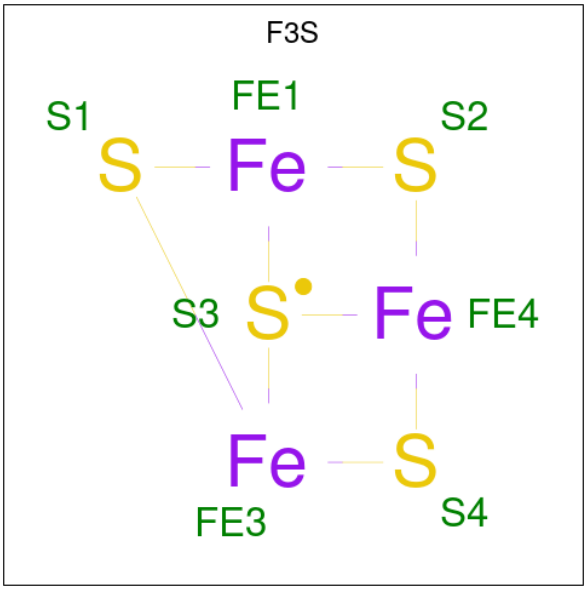
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
6	B	1	4	2	2	0	0

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



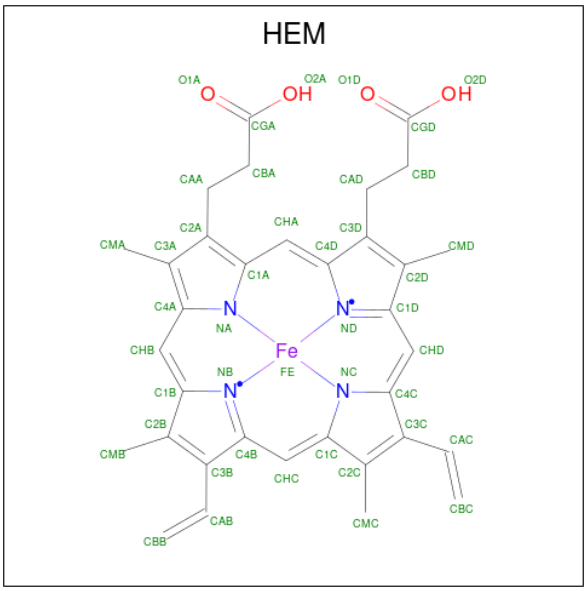
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	B	1	8	4	4	0	0

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



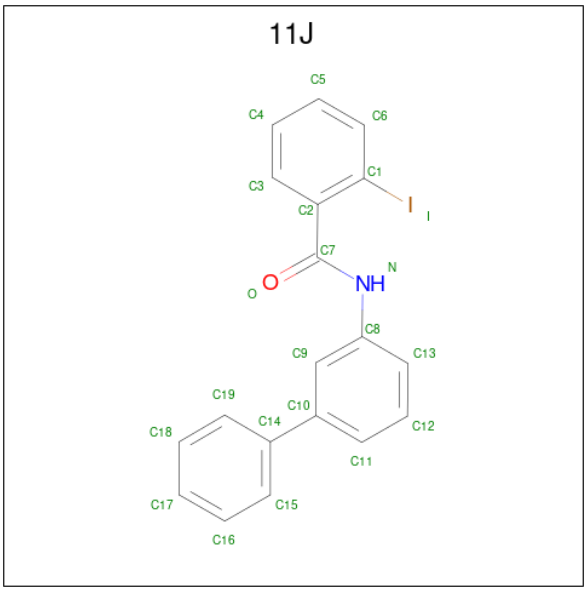
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	B	1	7	3	4	0	0

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 10 is N-biphenyl-3-yl-2-iodobenzamide (three-letter code: 11J) (formula: $C_{19}H_{14}INO$).



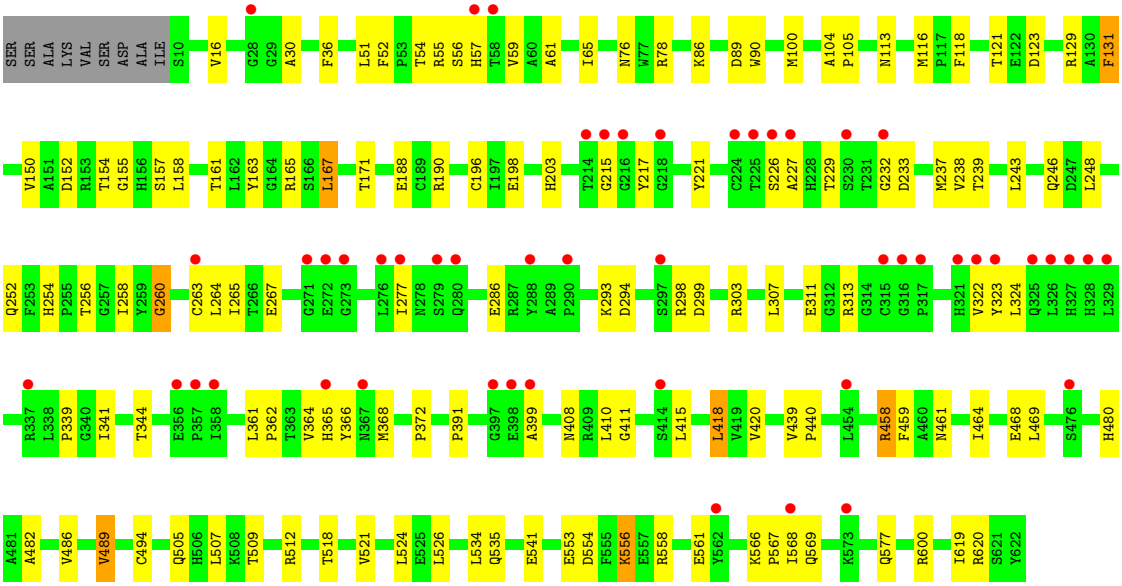
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	I	N	O		
10	C	1	22	19	1	1	1	0	0

3 Residue-property plots (i)

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

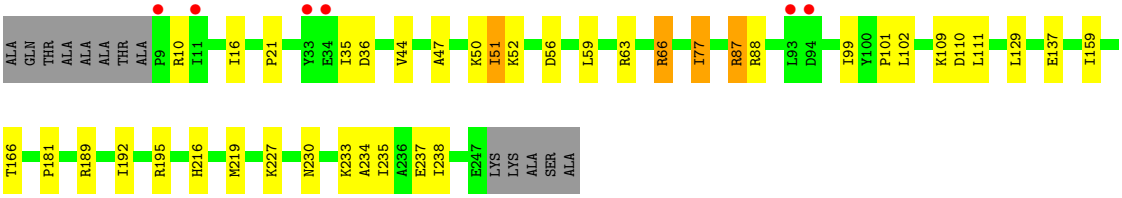
• Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain A:



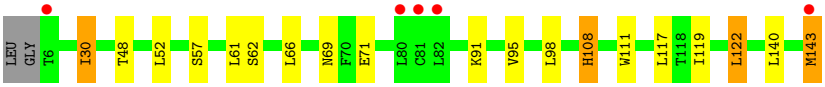
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain B:



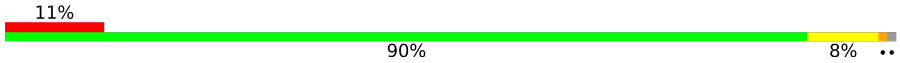
• Molecule 3: Succinate dehydrogenase cytochrome b560 subunit, mitochondrial

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.86Å 83.87Å 294.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.14 – 3.27 49.14 – 3.27	Depositor EDS
% Data completeness (in resolution range)	78.7 (49.14-3.27) 78.7 (49.14-3.27)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.25Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.244 , 0.312 0.243 , 0.304	Depositor DCC
R_{free} test set	1148 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	103.7	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8617	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, 11J, F3S, SF4, FES, HEM

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	0.48	0/6531
2	B	0.31	0/1964	0.47	0/2648
3	C	0.32	0/1091	0.46	0/1483
4	D	0.30	0/784	0.45	0/1066
All	All	0.31	0/8667	0.47	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	75	0
2	B	1922	0	1902	22	0
3	C	1064	0	1104	13	0
4	D	765	0	773	2	0
5	A	53	0	31	8	0
6	B	4	0	0	0	0
7	B	8	0	0	0	0
8	B	7	0	0	0	0
9	C	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	22	0	14	1	0
All	All	8617	0	8472	109	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 (109) 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	1.33	1.39
1:A:57:HIS:NE2	5:A:700:FAD:HM81	1.96	0.81
2:B:51:ILE:HD11	2:B:59:LEU:HD22	1.69	0.74
1:A:57:HIS:CE1	5:A:700:FAD:HM82	2.19	0.74
1:A:57:HIS:CE1	1:A:227:ALA:H	2.06	0.73
1:A:246:GLN:HE22	1:A:600:ARG:HE	1.39	0.70
1:A:246:GLN:NE2	1:A:600:ARG:HE	1.90	0.70
1:A:61:ALA:HB3	1:A:155:GLY:HA3	1.74	0.68
3:C:48:THR:O	3:C:52:LEU:HB2	1.96	0.65
2:B:102:LEU:HD22	2:B:166:THR:HG21	1.78	0.65
2:B:219:MET:HE3	3:C:117:LEU:HD22	1.78	0.65
1:A:415:LEU:HA	1:A:418:LEU:HD22	1.82	0.61
1:A:246:GLN:HB2	1:A:372:PRO:HG3	1.82	0.60
1:A:264:LEU:HD22	5:A:700:FAD:H6	1.85	0.58
1:A:52:PHE:HB3	1:A:55:ARG:HG3	1.86	0.58
1:A:464:ILE:O	1:A:507:LEU:HA	2.05	0.56
2:B:10:ARG:O	2:B:36:ASP:HA	2.06	0.56
1:A:566:LYS:HB2	1:A:567:PRO:HD2	1.89	0.55
3:C:140:LEU:HA	3:C:143:MET:HB2	1.87	0.55
1:A:116:MET:HA	1:A:161:THR:HG21	1.89	0.55
4:D:72:LEU:O	4:D:76:LEU:HB2	2.06	0.55
2:B:77:ILE:HG22	2:B:99:ILE:HG12	1.88	0.55
1:A:150:VAL:H	1:A:154:THR:HG22	1.71	0.55
2:B:181:PRO:HA	2:B:235:ILE:HD11	1.89	0.54
1:A:158:LEU:HD23	1:A:415:LEU:HD22	1.90	0.54
1:A:480:HIS:HD2	1:A:489:VAL:HG22	1.73	0.54
1:A:100:MET:HA	1:A:420:VAL:HG11	1.90	0.53
1:A:215:GLY:H	1:A:399:ALA:HB2	1.73	0.53
2:B:35:ILE:HD11	2:B:51:ILE:HG22	1.91	0.52
1:A:341:ILE:HA	1:A:344:THR:HG22	1.91	0.52
1:A:361:LEU:HD12	1:A:362:PRO:HD2	1.91	0.52
1:A:118:PHE:HA	1:A:150:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:CYS:SG	1:A:198:GLU:HB3	2.50	0.51
1:A:57:HIS:CD2	5:A:700:FAD:C8M	2.87	0.51
1:A:57:HIS:HE1	1:A:227:ALA:N	2.09	0.51
1:A:415:LEU:HG	5:A:700:FAD:C2	2.41	0.50
1:A:163:TYR:O	1:A:167:LEU:HD22	2.12	0.49
2:B:77:ILE:HG13	2:B:87:ARG:HG2	1.93	0.49
1:A:57:HIS:CE1	1:A:227:ALA:N	2.77	0.49
2:B:233:LYS:HD2	3:C:117:LEU:HD12	1.94	0.49
1:A:246:GLN:HE22	1:A:600:ARG:NE	2.09	0.48
1:A:486:VAL:HG12	1:A:553:GLU:HB2	1.94	0.48
2:B:52:LYS:HA	2:B:56:ASP:O	2.13	0.48
1:A:258:ILE:HG22	1:A:260:GLY:H	1.77	0.48
1:A:152:ASP:HB3	1:A:339:PRO:HD2	1.95	0.48
1:A:248:LEU:HD12	1:A:535:GLN:HB2	1.96	0.48
9:C:1305:HEM:HHA	9:C:1305:HEM:HBA2	1.96	0.48
3:C:57:SER:O	3:C:61:LEU:HB2	2.14	0.47
1:A:518:THR:HA	1:A:521:VAL:HG22	1.95	0.47
3:C:62:SER:HB2	3:C:66:LEU:HD12	1.95	0.47
1:A:298:ARG:HB2	1:A:408:ASN:HD21	1.80	0.47
1:A:57:HIS:CE1	1:A:226:SER:HA	2.49	0.47
1:A:113:ASN:HD22	2:B:137:GLU:HA	1.79	0.47
1:A:254:HIS:HD2	1:A:256:THR:H	1.63	0.47
2:B:234:ALA:O	2:B:238:ILE:HG13	2.15	0.47
1:A:365:HIS:HD2	1:A:366:TYR:HB2	1.79	0.47
1:A:418:LEU:HD21	5:A:700:FAD:O4'	2.15	0.47
3:C:52:LEU:HD21	3:C:98:LEU:HD23	1.96	0.47
2:B:159:ILE:HD11	2:B:227:LYS:HE2	1.97	0.46
2:B:47:ALA:O	2:B:51:ILE:HG23	2.15	0.46
1:A:217:TYR:HB3	1:A:232:GLY:HA3	1.96	0.46
2:B:129:LEU:HD11	2:B:195:ARG:HB2	1.97	0.46
1:A:30:ALA:HB2	1:A:418:LEU:HD12	1.98	0.46
1:A:150:VAL:HB	1:A:154:THR:HA	1.98	0.46
1:A:188:GLU:HG2	1:A:391:PRO:HG2	1.98	0.45
1:A:469:LEU:HD23	1:A:526:LEU:HD21	1.99	0.45
1:A:76:ASN:HD21	1:A:78:ARG:HD2	1.81	0.45
2:B:44:VAL:HG11	2:B:77:ILE:HG21	1.98	0.45
1:A:104:ALA:HB3	1:A:105:PRO:HD3	1.98	0.45
1:A:286:GLU:HG3	1:A:293:LYS:HE2	1.99	0.45
1:A:190:ARG:HD2	1:A:440:PRO:HB2	1.98	0.44
1:A:521:VAL:HA	1:A:524:LEU:HD12	1.99	0.44
2:B:101:PRO:HG3	2:B:111:LEU:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:ILE:H	3:C:30:ILE:HD13	1.83	0.44
3:C:91:LYS:O	3:C:95:VAL:HG23	2.18	0.44
1:A:61:ALA:HA	5:A:700:FAD:N5	2.33	0.44
1:A:86:LYS:O	1:A:620:ARG:HD3	2.18	0.43
1:A:90:TRP:HZ3	1:A:620:ARG:HB3	1.83	0.43
1:A:233:ASP:O	1:A:237:MET:HG3	2.18	0.43
1:A:258:ILE:HD13	1:A:263:CYS:HB2	2.01	0.43
1:A:494:CYS:SG	1:A:541:GLU:HG2	2.58	0.43
1:A:322:VAL:HG12	1:A:323:TYR:N	2.33	0.43
1:A:215:GLY:N	1:A:399:ALA:HB2	2.34	0.43
2:B:16:ILE:HG21	2:B:59:LEU:HD11	2.01	0.43
3:C:108:HIS:HA	3:C:111:TRP:CE3	2.53	0.43
1:A:221:TYR:CG	1:A:364:VAL:HG21	2.54	0.43
2:B:219:MET:HB3	3:C:122:LEU:HD21	2.01	0.43
1:A:299:ASP:O	1:A:303:ARG:HB2	2.19	0.42
3:C:69:ASN:HD21	3:C:71:GLU:HB2	1.83	0.42
1:A:415:LEU:HA	1:A:418:LEU:CD2	2.47	0.42
2:B:21:PRO:HD3	2:B:109:LYS:HG3	2.01	0.42
4:D:126:ILE:H	4:D:126:ILE:HG13	1.76	0.42
1:A:556:LYS:H	1:A:556:LYS:HD2	1.83	0.42
1:A:458:ARG:O	1:A:512:ARG:HG2	2.20	0.42
1:A:307:LEU:O	1:A:311:GLU:HG2	2.19	0.41
2:B:35:ILE:HD12	2:B:50:LYS:HD3	2.02	0.41
1:A:258:ILE:HG13	1:A:265:ILE:HD11	2.02	0.41
1:A:238:VAL:HG13	1:A:243:LEU:HB2	2.01	0.41
1:A:252:GLN:HB3	1:A:366:TYR:HB3	2.03	0.41
1:A:51:LEU:HD21	1:A:229:THR:HG21	2.02	0.41
1:A:16:VAL:HB	1:A:203:HIS:HD1	1.85	0.41
1:A:131:PHE:CE1	1:A:267:GLU:HB3	2.56	0.41
1:A:129:ARG:HD2	1:A:129:ARG:HA	1.97	0.40
1:A:410:LEU:HG	1:A:411:GLY:H	1.86	0.40
1:A:439:VAL:HA	1:A:440:PRO:HD3	1.93	0.40
2:B:216:HIS:CD2	10:C:1201:11J:H6	2.55	0.40
1:A:150:VAL:N	1:A:154:THR:HG22	2.35	0.40
3:C:119:ILE:HD13	3:C:119:ILE:HA	1.96	0.40
1:A:89:ASP:OD2	1:A:558:ARG:NH1	2.54	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%)	568 (93%)	38 (6%)	5 (1%)	19	52
2	B	237/252 (94%)	219 (92%)	16 (7%)	2 (1%)	19	52
3	C	136/140 (97%)	132 (97%)	4 (3%)	0	100	100
4	D	100/103 (97%)	94 (94%)	4 (4%)	2 (2%)	7	34
All	All	1084/1117 (97%)	1013 (94%)	62 (6%)	9 (1%)	19	52

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	110	ASP
1	A	56	SER
1	A	568	ILE
1	A	569	GLN
2	B	66	ARG
4	D	126	ILE
1	A	482	ALA
1	A	260	GLY
4	D	36	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/506 (99%)	468 (94%)	31 (6%)	18	48
2	B	214/220 (97%)	204 (95%)	10 (5%)	26	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	117/118 (99%)	113 (97%)	4 (3%)	37	65
4	D	76/76 (100%)	71 (93%)	5 (7%)	16	46
All	All	906/920 (98%)	856 (94%)	50 (6%)	21	52

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	PHE
1	A	54	THR
1	A	59	VAL
1	A	65	ILE
1	A	121	THR
1	A	123	ASP
1	A	131	PHE
1	A	157	SER
1	A	165	ARG
1	A	167	LEU
1	A	171	THR
1	A	239	THR
1	A	277	ILE
1	A	294	ASP
1	A	313	ARG
1	A	324	LEU
1	A	368	MET
1	A	418	LEU
1	A	458	ARG
1	A	459	PHE
1	A	461	ASN
1	A	468	GLU
1	A	489	VAL
1	A	505	GLN
1	A	509	THR
1	A	534	LEU
1	A	554	ASP
1	A	556	LYS
1	A	561	GLU
1	A	577	GLN
1	A	619	ILE
2	B	51	ILE
2	B	63	ARG
2	B	66	ARG

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Mol	Chain	Res	Type
2	B	77	ILE
2	B	87	ARG
2	B	88	ARG
2	B	189	ARG
2	B	192	ILE
2	B	230	ASN
2	B	237	GLU
3	C	30	ILE
3	C	108	HIS
3	C	122	LEU
3	C	143	MET
4	D	78	LEU
4	D	97	LEU
4	D	102	LYS
4	D	134	TRP
4	D	136	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	113	ASN
1	A	128	GLN
1	A	246	GLN
1	A	321	HIS
1	A	365	HIS
1	A	378	GLN
1	A	384	ASN
1	A	408	ASN
1	A	461	ASN
1	A	474	GLN
1	A	480	HIS
1	A	550	HIS
1	A	577	GLN
2	B	31	GLN
2	B	39	ASN
2	B	121	GLN
2	B	220	ASN
2	B	230	ASN
3	C	17	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
8	F3S	B	304	2	0,9,9	-	-	-		
6	FES	B	302	2	0,4,4	-	-	-		
10	11J	C	1201	-	23,24,24	1.08	2 (8%)	28,32,32	0.57	0
7	SF4	B	303	2	0,12,12	-	-	-		
9	HEM	C	1305	3,4	41,50,50	2.01	8 (19%)	45,82,82	1.72	5 (11%)
5	FAD	A	700	1	53,58,58	1.17	4 (7%)	68,89,89	1.38	9 (13%)

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
8	F3S	B	304	2	-	-	0/3/3/3
6	FES	B	302	2	-	-	0/1/1/1
10	11J	C	1201	-	-	2/8/12/12	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	B	303	2	-	-	0/6/5/5
9	HEM	C	1305	3,4	-	10/12/54/54	-
5	FAD	A	700	1	-	10/30/50/50	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1305	HEM	C3D-C2D	8.08	1.53	1.36
9	C	1305	HEM	C3C-C2C	-4.32	1.34	1.40
5	A	700	FAD	C4X-N5	4.21	1.38	1.30
5	A	700	FAD	C2A-N3A	4.01	1.38	1.32
9	C	1305	HEM	C3C-CAC	3.56	1.55	1.47
9	C	1305	HEM	CAB-C3B	2.83	1.55	1.47
9	C	1305	HEM	CAA-C2A	2.76	1.56	1.52
5	A	700	FAD	C10-N1	2.72	1.38	1.33
10	C	1201	11J	C8-N	-2.66	1.36	1.41
9	C	1305	HEM	FE-ND	2.63	2.09	1.96
5	A	700	FAD	C2A-N1A	2.56	1.38	1.33
10	C	1201	11J	C2-C1	2.49	1.49	1.39
9	C	1305	HEM	CMB-C2B	2.16	1.55	1.50
9	C	1305	HEM	FE-NB	2.04	2.07	1.96

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	1305	HEM	C4D-ND-C1D	6.61	111.90	105.07
5	A	700	FAD	N3A-C2A-N1A	-5.77	119.66	128.68
9	C	1305	HEM	C4C-CHD-C1D	3.67	127.40	122.56
9	C	1305	HEM	C4B-CHC-C1C	3.25	126.85	122.56
5	A	700	FAD	C4-N3-C2	-3.14	119.84	125.64
9	C	1305	HEM	C1B-NB-C4B	3.03	108.20	105.07
5	A	700	FAD	C4X-C4-N3	2.81	120.33	113.19
5	A	700	FAD	P-O3P-PA	-2.57	124.02	132.83
5	A	700	FAD	O4-C4-C4X	-2.52	119.92	126.60
5	A	700	FAD	C10-C4X-N5	-2.41	119.75	124.86
5	A	700	FAD	C4X-C10-N10	2.40	119.98	116.48
5	A	700	FAD	C9A-C5X-N5	-2.27	119.96	122.43
5	A	700	FAD	C4X-C10-N1	-2.27	119.47	124.73
9	C	1305	HEM	CAD-C3D-C4D	2.25	128.59	124.66

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	700	FAD	N10-C1'-C2'-O2'
5	A	700	FAD	N10-C1'-C2'-C3'
5	A	700	FAD	C1'-C2'-C3'-O3'
5	A	700	FAD	C1'-C2'-C3'-C4'
5	A	700	FAD	O2'-C2'-C3'-O3'
5	A	700	FAD	O2'-C2'-C3'-C4'
5	A	700	FAD	C3'-C4'-C5'-O5'
5	A	700	FAD	O4'-C4'-C5'-O5'
9	C	1305	HEM	C1A-C2A-CAA-CBA
9	C	1305	HEM	C3A-C2A-CAA-CBA
9	C	1305	HEM	C2A-CAA-CBA-CGA
9	C	1305	HEM	C2B-C3B-CAB-CBB
9	C	1305	HEM	C4B-C3B-CAB-CBB
9	C	1305	HEM	C3D-CAD-CBD-CGD
10	C	1201	11J	O-C7-N-C8
10	C	1201	11J	C2-C7-N-C8
5	A	700	FAD	PA-O3P-P-O5'
9	C	1305	HEM	C4D-C3D-CAD-CBD
9	C	1305	HEM	C2D-C3D-CAD-CBD
9	C	1305	HEM	CAA-CBA-CGA-O2A
9	C	1305	HEM	CAA-CBA-CGA-O1A
5	A	700	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

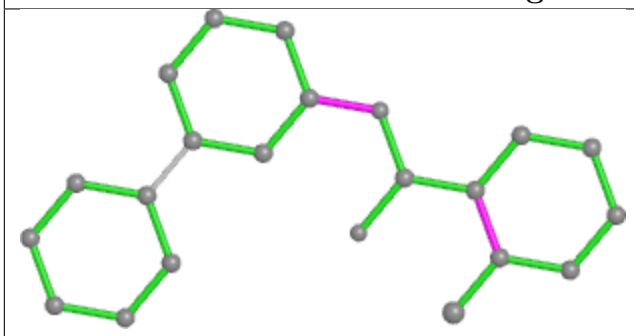
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1201	11J	1	0
9	C	1305	HEM	1	0
5	A	700	FAD	8	0

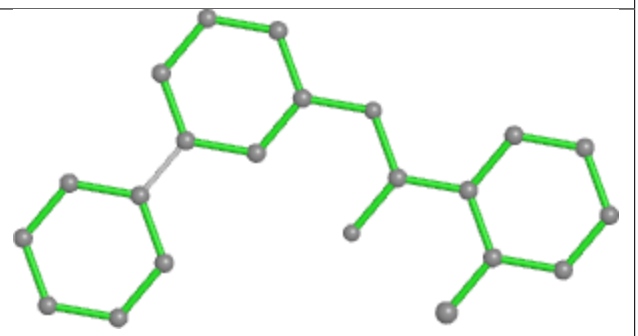
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

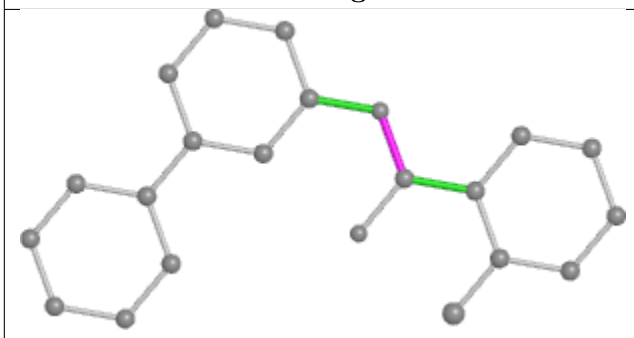
Ligand 11J C 1201



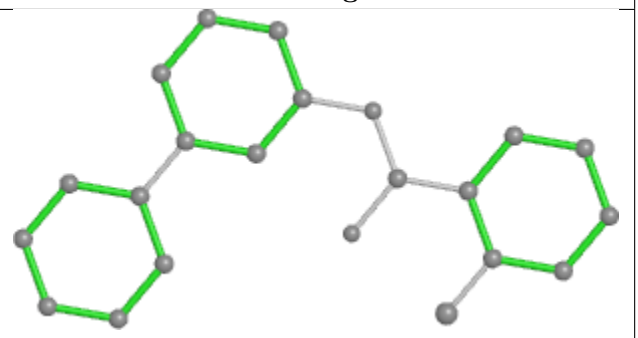
Bond lengths



Bond angles

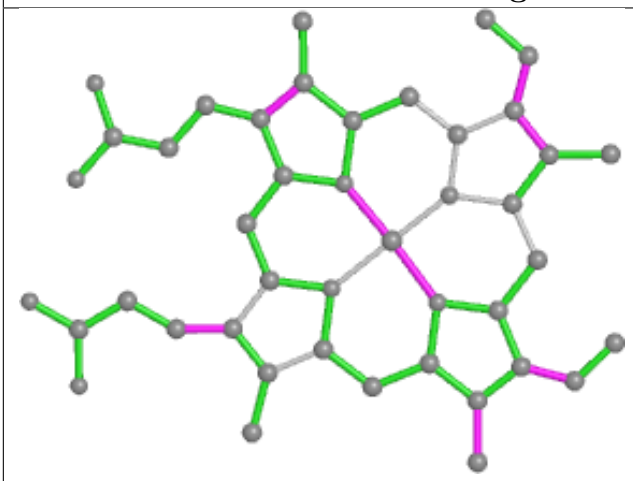


Torsions

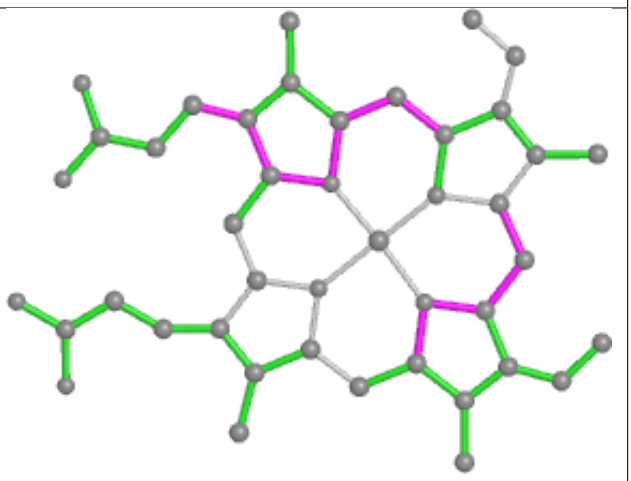


Rings

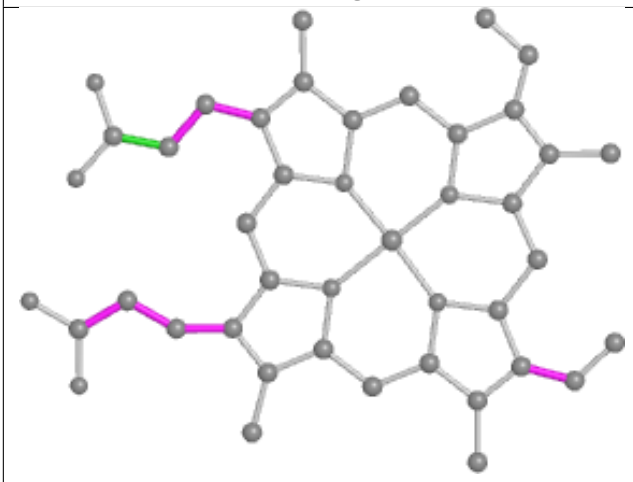
Ligand HEM C 1305



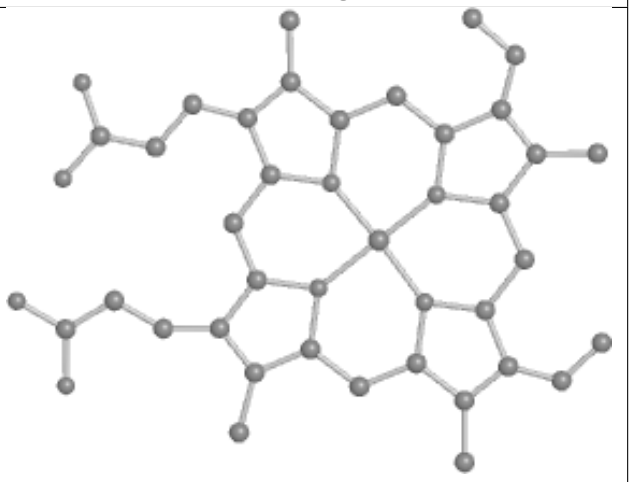
Bond lengths



Bond angles

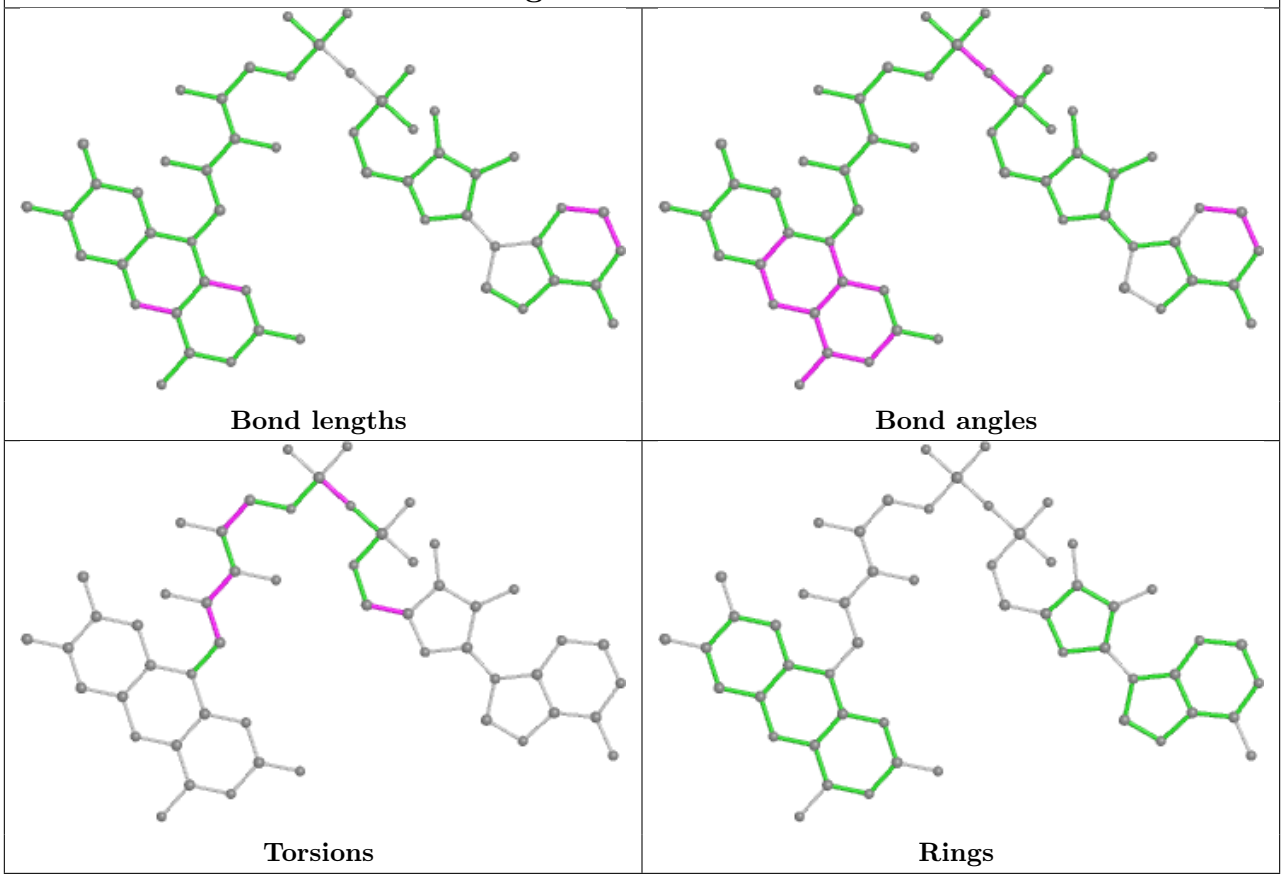


Torsions



Rings

Ligand FAD A 700



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	613/622 (98%)	0.40	50 (8%)	11	11	86, 112, 166, 186	0
2	B	239/252 (94%)	0.31	6 (2%)	57	53	83, 103, 129, 142	0
3	C	138/140 (98%)	0.07	5 (3%)	42	40	88, 109, 133, 142	0
4	D	102/103 (99%)	0.38	11 (10%)	5	5	97, 110, 131, 138	0
All	All	1092/1117 (97%)	0.34	72 (6%)	18	18	83, 109, 157, 186	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	PRO	4.9
1	A	230	SER	4.6
1	A	272	GLU	4.3
1	A	317	PRO	4.0
1	A	288	TYR	3.9
1	A	322	VAL	3.9
1	A	398	GLU	3.8
1	A	216	GLY	3.8
2	B	11	ILE	3.7
1	A	358	ILE	3.7
4	D	62	LEU	3.7
1	A	326	LEU	3.5
1	A	57	HIS	3.5
2	B	93	LEU	3.5
1	A	328	HIS	3.5
4	D	61	TYR	3.4
4	D	64	PRO	3.4
4	D	126	ILE	3.3
3	C	82	LEU	3.2
1	A	276	LEU	3.2
1	A	215	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	399	ALA	3.1
4	D	131	ALA	3.1
1	A	226	SER	3.1
1	A	315	CYS	3.0
4	D	60	ALA	3.0
1	A	279	SER	2.9
1	A	290	PRO	2.9
1	A	397	GLY	2.9
1	A	321	HIS	2.8
1	A	327	HIS	2.8
1	A	365	HIS	2.7
1	A	214	THR	2.7
3	C	6	THR	2.7
1	A	224	CYS	2.6
1	A	414	SER	2.6
1	A	367	ASN	2.6
1	A	325	GLN	2.6
1	A	263	CYS	2.6
1	A	271	GLY	2.5
1	A	280	GLN	2.5
2	B	34	GLU	2.5
1	A	58	THR	2.5
1	A	573	LYS	2.5
1	A	273	GLY	2.5
4	D	35	SER	2.5
2	B	33	TYR	2.4
1	A	323	TYR	2.4
1	A	356	GLU	2.3
1	A	225	THR	2.3
4	D	136	LEU	2.3
1	A	277	ILE	2.3
1	A	329	LEU	2.2
3	C	81	CYS	2.2
4	D	63	ASN	2.2
1	A	218	GLY	2.2
1	A	454	LEU	2.2
1	A	227	ALA	2.2
3	C	80	LEU	2.2
1	A	476	SER	2.2
1	A	568	ILE	2.2
1	A	232	GLY	2.2
1	A	28	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	66	SER	2.1
1	A	562	TYR	2.1
2	B	94	ASP	2.1
3	C	143	MET	2.1
4	D	127	CYS	2.1
2	B	9	PRO	2.1
1	A	337	ARG	2.0
1	A	297	SER	2.0
1	A	316	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

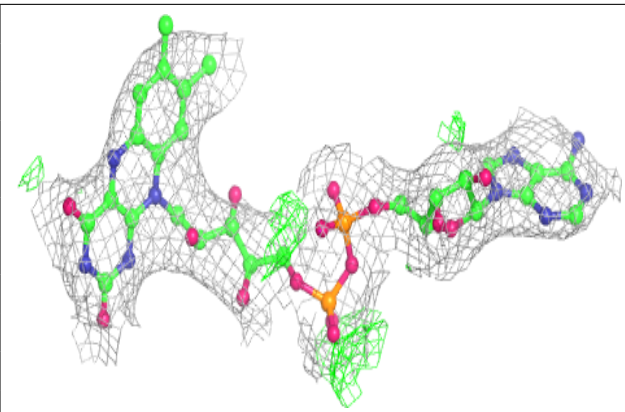
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

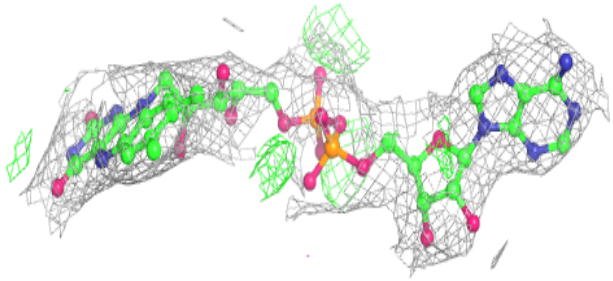
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FAD	A	700	53/53	0.91	0.45	94,96,99,100	0
9	HEM	C	1305	43/43	0.97	0.26	87,87,89,90	0
8	F3S	B	304	7/7	0.98	0.19	102,102,102,103	0
6	FES	B	302	4/4	0.98	0.23	94,94,94,95	0
7	SF4	B	303	8/8	0.99	0.20	84,84,85,85	0
10	11J	C	1201	22/22	0.99	0.27	100,100,101,103	0

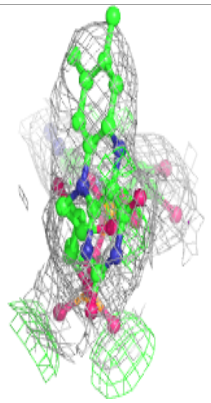
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

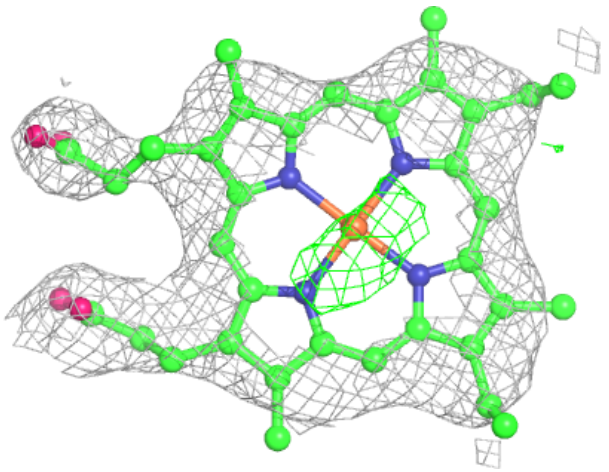


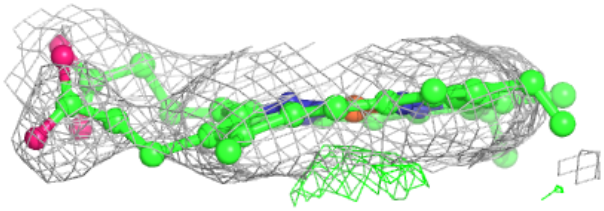


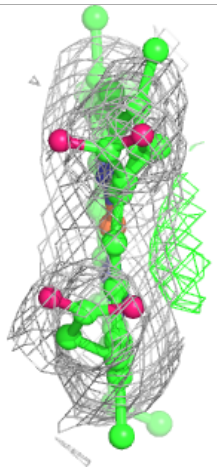


Electron density around HEM C 1305:

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

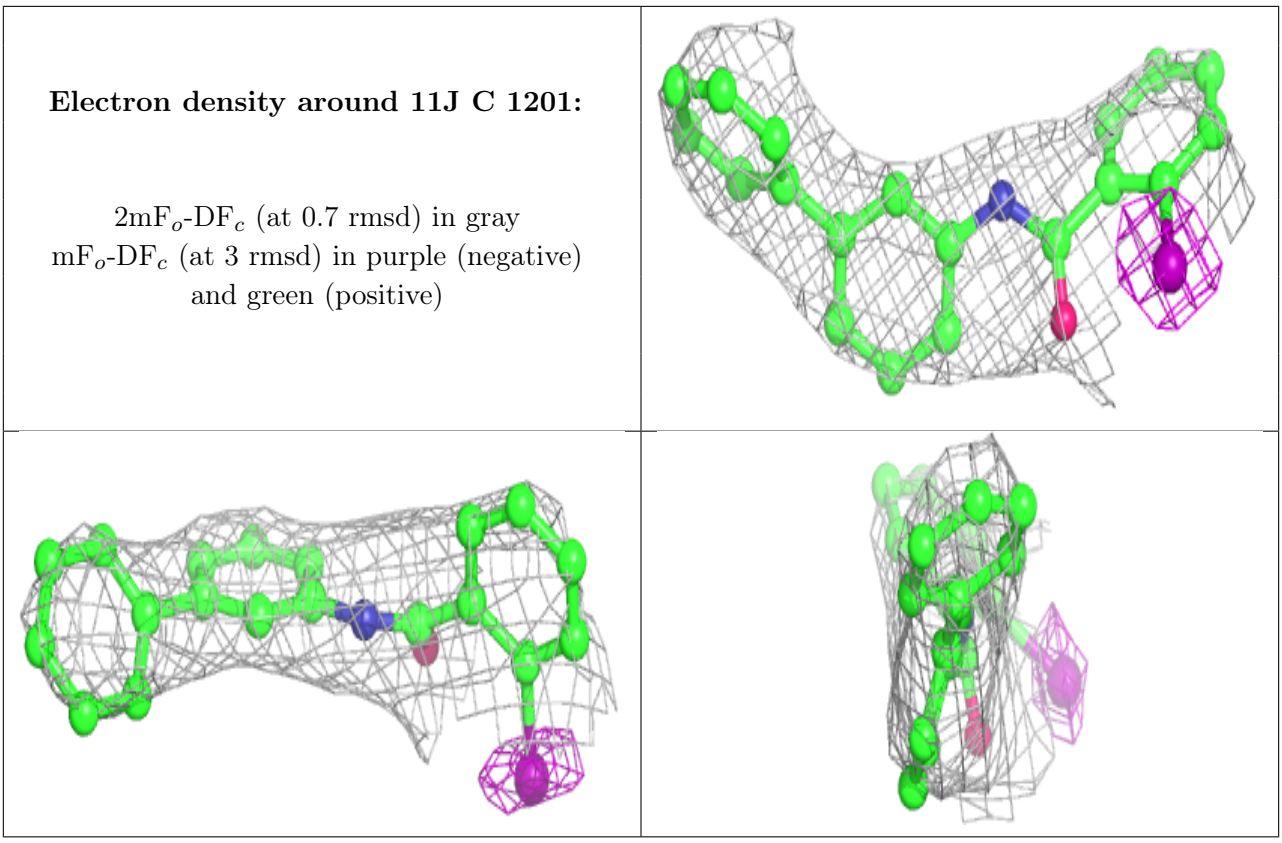






Electron density around 11J C 1201:

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



6.5 Other polymers (i)

There are no such residues in this entry.