



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:53 am BST

PDB ID : 3AE3
Title : Crystal structure of porcine heart mitochondrial complex II bound with 2-Nitro-N-phenyl-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 : 3.35 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

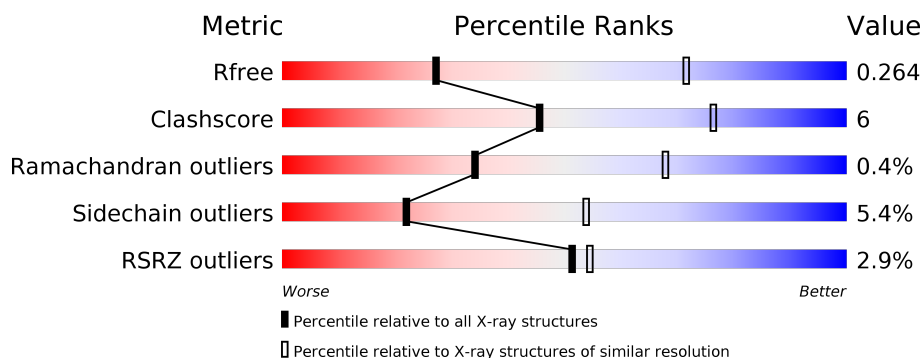
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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>3%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>..</div> </div> </div>
2	B	252	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>5%</div> </div> </div>
3	C	140	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
4	D	103	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	EPH	D	1306	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 8657 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.

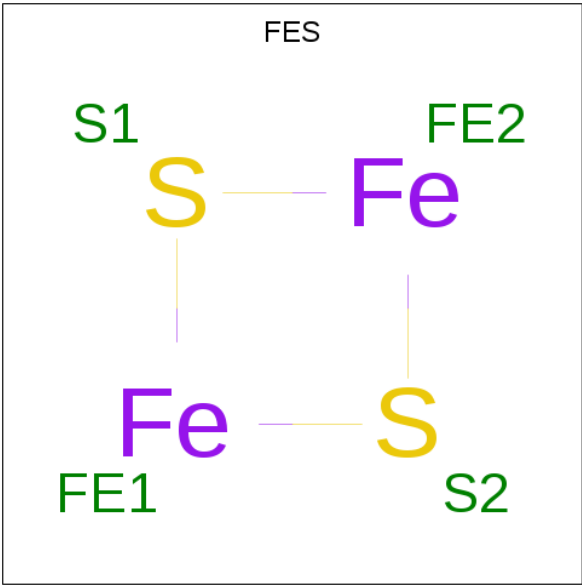
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			765	499	128	133	5			

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



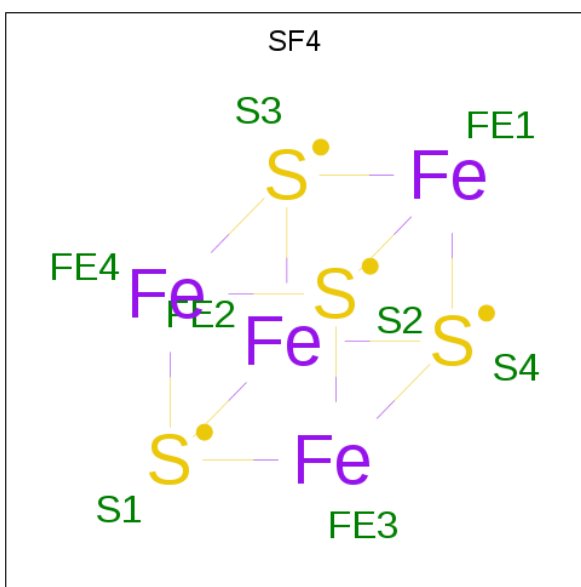
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



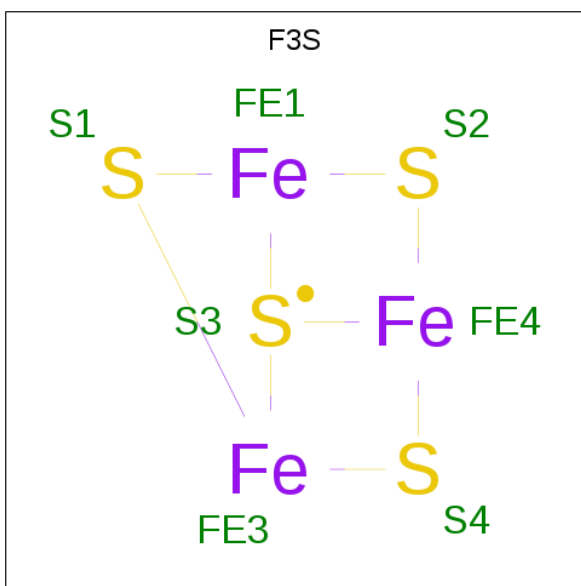
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		

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



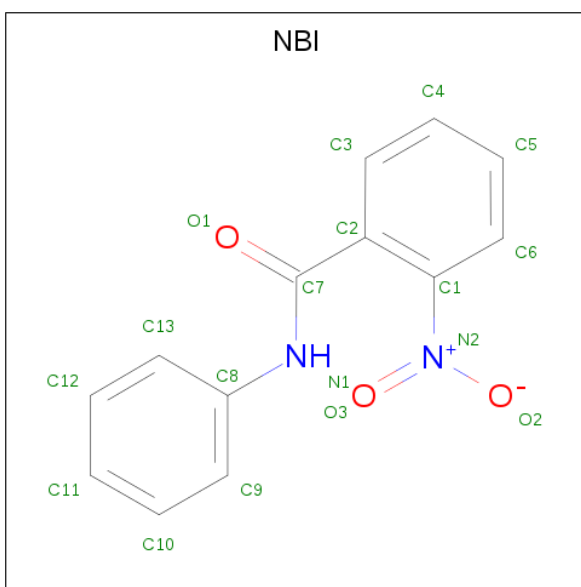
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		

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



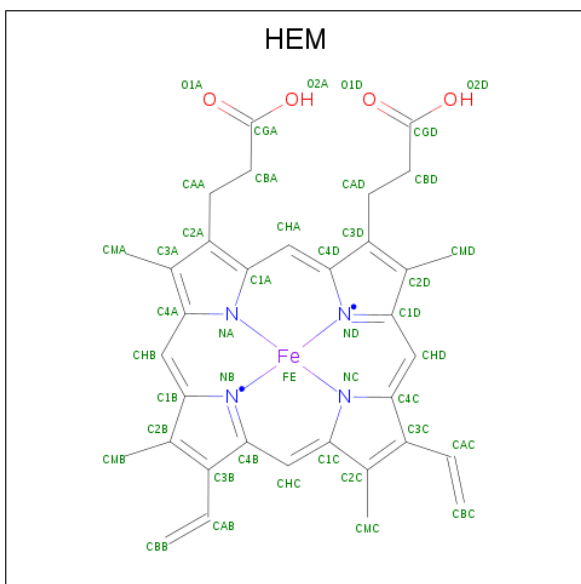
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is 2-nitro-N-phenylbenzamide (three-letter code: NBI) (formula: $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_3$).



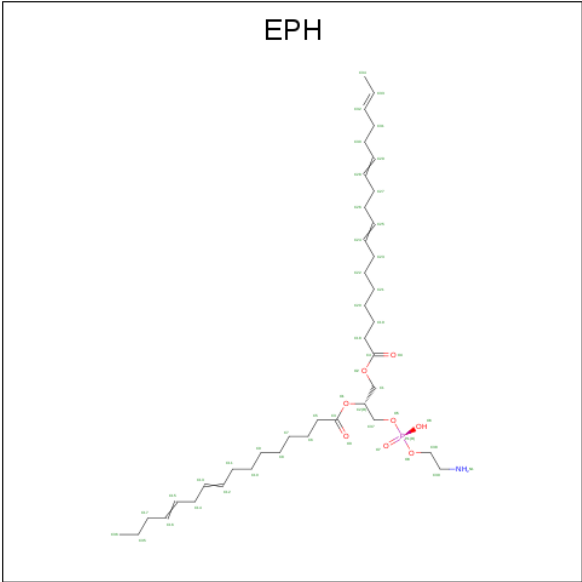
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			18	13	2	3		

- 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	0	0
			43	34	1	4	4		

- Molecule 11 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: $C_{39}H_{68}NO_8P$).

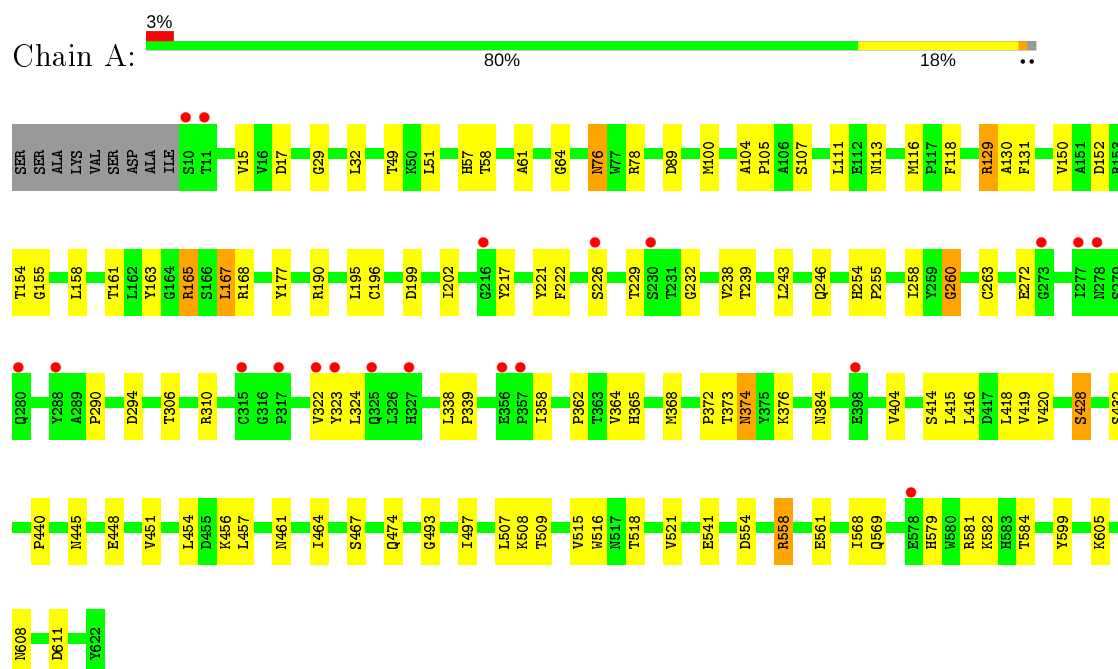


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

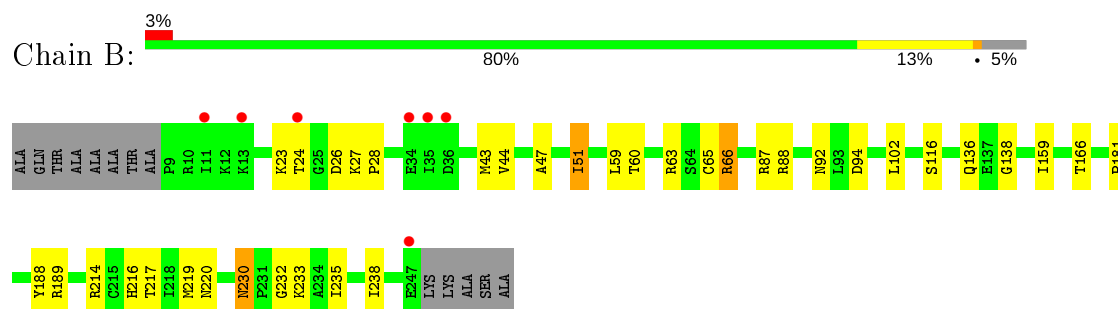
3 Residue-property plots

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

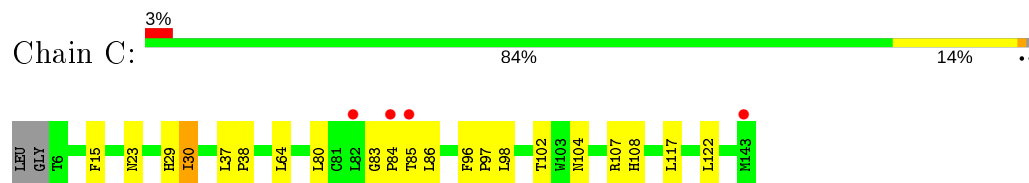
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial




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



- Molecule 3: Succinate dehydrogenase cytochrome b560 subunit, mitochondrial



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

Chain D:  91% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.51Å 84.50Å 295.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.44 – 3.35 48.44 – 3.35	Depositor EDS
% Data completeness (in resolution range)	85.1 (48.44-3.35) 85.1 (48.44-3.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.261 0.216 , 0.264	Depositor DCC
R_{free} test set	1144 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	78.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.8	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	0.91	EDS
Total number of atoms	8657	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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, NBI, 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	0.32	0/4828	0.49	0/6531
2	B	0.31	0/1964	0.46	0/2648
3	C	0.33	0/1091	0.48	0/1483
4	D	0.30	0/784	0.45	0/1066
All	All	0.32	0/8667	0.48	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	81	0
2	B	1922	0	1900	20	0
3	C	1064	0	1104	8	0
4	D	765	0	773	3	0
5	A	53	0	31	17	0
6	B	4	0	0	0	0
7	B	8	0	0	0	0
8	B	7	0	0	0	0
9	B	18	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	43	0	30	1	0
11	D	44	0	53	0	0
All	All	8657	0	8519	108	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 (108) 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:CE1	5:A:700:FAD:HM82	1.51	1.43
1:A:57:HIS:NE2	5:A:700:FAD:HM82	1.47	1.28
1:A:57:HIS:CE1	5:A:700:FAD:C8M	2.39	1.04
1:A:415:LEU:HG	5:A:700:FAD:C2	2.03	0.88
1:A:57:HIS:HE1	5:A:700:FAD:HM82	1.38	0.87
1:A:57:HIS:O	1:A:57:HIS:CD2	2.30	0.85
1:A:57:HIS:NE2	5:A:700:FAD:HM81	1.94	0.83
1:A:58:THR:HG22	5:A:700:FAD:O4'	1.80	0.81
1:A:61:ALA:HB3	1:A:155:GLY:HA3	1.67	0.76
2:B:102:LEU:HB3	2:B:166:THR:HG21	1.70	0.73
1:A:57:HIS:O	1:A:57:HIS:CG	2.45	0.70
1:A:111:LEU:HD11	1:A:419:VAL:HG21	1.74	0.70
1:A:58:THR:HG23	5:A:700:FAD:O1A	1.93	0.68
1:A:57:HIS:NE2	5:A:700:FAD:C8	2.56	0.68
1:A:57:HIS:CE1	1:A:226:SER:HA	2.33	0.63
2:B:51:ILE:HD11	2:B:59:LEU:HD22	1.82	0.60
1:A:246:GLN:HB2	1:A:372:PRO:HG3	1.83	0.60
1:A:374:ASN:HB3	1:A:376:LYS:H	1.66	0.59
4:D:53:LEU:HD11	4:D:76:LEU:HD22	1.84	0.59
1:A:258:ILE:HD12	1:A:263:CYS:HB2	1.85	0.59
1:A:418:LEU:HD21	5:A:700:FAD:H4'	1.85	0.58
2:B:219:MET:HE2	2:B:232:GLY:HA3	1.85	0.57
1:A:113:ASN:ND2	2:B:138:GLY:H	2.03	0.57
1:A:415:LEU:HG	5:A:700:FAD:O2	2.04	0.57
1:A:217:TYR:HB3	1:A:232:GLY:HA3	1.86	0.56
1:A:89:ASP:OD2	1:A:558:ARG:NH1	2.39	0.55
1:A:61:ALA:HA	5:A:700:FAD:N5	2.22	0.54
2:B:23:LYS:HB3	2:B:26:ASP:HB2	1.88	0.54
1:A:57:HIS:HE1	1:A:226:SER:HA	1.71	0.54
1:A:568:ILE:HG13	1:A:569:GLN:N	2.22	0.54
1:A:246:GLN:HA	1:A:584:THR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG12	1:A:323:TYR:H	1.74	0.53
1:A:51:LEU:HD21	1:A:229:THR:HG21	1.90	0.52
1:A:61:ALA:HA	5:A:700:FAD:C5X	2.40	0.52
1:A:61:ALA:HB1	5:A:700:FAD:C4X	2.41	0.51
1:A:165:ARG:HE	1:A:168:ARG:HH11	1.59	0.51
1:A:568:ILE:HG13	1:A:569:GLN:H	1.77	0.50
1:A:29:GLY:H	1:A:58:THR:HG21	1.75	0.50
1:A:415:LEU:HA	1:A:418:LEU:HD22	1.92	0.50
2:B:233:LYS:HA	3:C:117:LEU:HD13	1.93	0.50
4:D:72:LEU:HD13	4:D:76:LEU:HD23	1.94	0.50
1:A:49:THR:OG1	5:A:700:FAD:O2B	2.26	0.49
1:A:104:ALA:HB3	1:A:105:PRO:HD3	1.94	0.49
1:A:129:ARG:HG3	1:A:130:ALA:N	2.27	0.49
2:B:43:MET:HA	2:B:88:ARG:HA	1.94	0.49
1:A:516:TRP:HB3	2:B:60:THR:HG21	1.94	0.49
1:A:118:PHE:HA	1:A:150:VAL:HG22	1.94	0.49
1:A:322:VAL:HG12	1:A:323:TYR:N	2.27	0.49
3:C:96:PHE:HB3	3:C:97:PRO:HD3	1.95	0.49
1:A:113:ASN:HD22	2:B:138:GLY:H	1.61	0.49
1:A:152:ASP:HB2	1:A:338:LEU:HA	1.95	0.48
3:C:104:ASN:ND2	3:C:107:ARG:HE	2.10	0.48
1:A:464:ILE:O	1:A:507:LEU:HA	2.14	0.48
1:A:518:THR:HA	1:A:521:VAL:HG22	1.95	0.48
1:A:190:ARG:HD2	1:A:440:PRO:HB2	1.96	0.48
1:A:222:PHE:HA	1:A:474:GLN:HE21	1.78	0.47
1:A:461:ASN:HD22	1:A:508:LYS:HE3	1.79	0.47
1:A:238:VAL:HG13	1:A:243:LEU:HB2	1.94	0.47
2:B:65:CYS:O	2:B:66:ARG:HG3	2.14	0.47
2:B:219:MET:CE	2:B:232:GLY:HA3	2.44	0.47
1:A:306:THR:O	1:A:310:ARG:HG2	2.14	0.47
1:A:152:ASP:HB2	1:A:339:PRO:HD2	1.96	0.47
1:A:445:ASN:O	1:A:448:GLU:HG3	2.15	0.47
2:B:116:SER:HB2	3:C:15:PHE:HD1	1.80	0.47
1:A:163:TYR:O	1:A:167:LEU:HD22	2.15	0.47
1:A:428:SER:O	1:A:432:SER:HB2	2.16	0.46
1:A:493:GLY:O	1:A:497:ILE:HG12	2.16	0.46
1:A:100:MET:HA	1:A:420:VAL:HG11	1.97	0.46
1:A:195:LEU:HD22	1:A:454:LEU:HD21	1.98	0.45
2:B:181:PRO:HA	2:B:235:ILE:HD11	1.98	0.45
1:A:129:ARG:HA	1:A:129:ARG:NE	2.31	0.45
1:A:199:ASP:HA	1:A:515:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:GLN:HE21	2:B:136:GLN:HA	1.81	0.45
2:B:47:ALA:O	2:B:51:ILE:HG23	2.17	0.45
2:B:44:VAL:HG23	2:B:87:ARG:O	2.15	0.45
3:C:37:LEU:N	3:C:38:PRO:HD2	2.32	0.45
1:A:582:LYS:HD3	1:A:599:TYR:HB3	1.98	0.45
1:A:177:TYR:CE2	1:A:196:CYS:HB2	2.52	0.44
1:A:129:ARG:HD2	1:A:272:GLU:OE2	2.16	0.44
1:A:64:GLY:HA2	1:A:154:THR:HG21	2.00	0.44
1:A:202:ILE:HD13	1:A:451:VAL:HG22	1.99	0.44
3:C:102:THR:HG23	10:C:1305:HEM:HAB	2.00	0.44
1:A:608:ASN:HD22	1:A:611:ASP:HB2	1.83	0.43
1:A:116:MET:HA	1:A:161:THR:HG21	2.01	0.43
1:A:221:TYR:CG	1:A:364:VAL:HG21	2.54	0.43
1:A:254:HIS:HB2	1:A:365:HIS:CB	2.49	0.43
1:A:373:THR:HG22	1:A:374:ASN:O	2.19	0.43
1:A:579:HIS:HD2	1:A:581:ARG:H	1.68	0.42
1:A:76:ASN:HD21	1:A:78:ARG:HD2	1.85	0.42
1:A:457:LEU:O	1:A:509:THR:HG21	2.19	0.42
2:B:188:TYR:HB2	2:B:238:ILE:HD11	2.01	0.42
2:B:230:ASN:HD22	2:B:230:ASN:C	2.23	0.41
4:D:68:MET:O	4:D:72:LEU:HB2	2.19	0.41
1:A:104:ALA:HA	1:A:416:LEU:HD11	2.01	0.41
1:A:254:HIS:HA	1:A:255:PRO:HD3	1.94	0.41
1:A:272:GLU:HG3	1:A:338:LEU:HD11	2.03	0.41
5:A:700:FAD:H9	5:A:700:FAD:H1'1	1.81	0.41
2:B:27:LYS:HA	2:B:28:PRO:HD3	1.97	0.41
3:C:29:HIS:HD2	3:C:30:ILE:HG23	1.86	0.41
3:C:83:GLY:HA2	3:C:84:PRO:HD3	1.94	0.41
1:A:254:HIS:HB2	1:A:365:HIS:HB2	2.02	0.41
2:B:216:HIS:CD2	9:B:1201:NBI:H6	2.56	0.41
1:A:258:ILE:HG22	1:A:260:GLY:H	1.85	0.40
1:A:254:HIS:O	1:A:362:PRO:HA	2.21	0.40
1:A:414:SER:O	1:A:418:LEU:HD13	2.21	0.40
1:A:582:LYS:HD3	1:A:599:TYR:CB	2.51	0.40
1:A:158:LEU:HD22	1:A:415:LEU:HD22	2.04	0.40
1:A:61:ALA:HA	5:A:700:FAD:C6	2.52	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%)	562 (92%)	46 (8%)	3 (0%)	29	63
2	B	237/252 (94%)	217 (92%)	19 (8%)	1 (0%)	34	68
3	C	136/140 (97%)	131 (96%)	5 (4%)	0	100	100
4	D	100/103 (97%)	97 (97%)	3 (3%)	0	100	100
All	All	1084/1117 (97%)	1007 (93%)	73 (7%)	4 (0%)	34	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	ASN
1	A	290	PRO
2	B	24	THR
1	A	260	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%)	475 (95%)	24 (5%)	25	57
2	B	214/220 (97%)	203 (95%)	11 (5%)	24	55
3	C	117/118 (99%)	108 (92%)	9 (8%)	13	41
4	D	76/76 (100%)	71 (93%)	5 (7%)	16	47
All	All	906/920 (98%)	857 (95%)	49 (5%)	22	54

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	17	ASP
1	A	32	LEU
1	A	76	ASN
1	A	107	SER
1	A	129	ARG
1	A	131	PHE
1	A	165	ARG
1	A	167	LEU
1	A	239	THR
1	A	294	ASP
1	A	324	LEU
1	A	358	ILE
1	A	368	MET
1	A	384	ASN
1	A	404	VAL
1	A	428	SER
1	A	456	LYS
1	A	467	SER
1	A	541	GLU
1	A	554	ASP
1	A	558	ARG
1	A	561	GLU
1	A	605	LYS
2	B	51	ILE
2	B	63	ARG
2	B	66	ARG
2	B	92	ASN
2	B	94	ASP
2	B	159	ILE
2	B	189	ARG
2	B	214	ARG
2	B	217	THR
2	B	220	ASN
2	B	230	ASN
3	C	23	ASN
3	C	30	ILE
3	C	64	LEU
3	C	80	LEU
3	C	85	THR
3	C	86	LEU
3	C	98	LEU

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Mol	Chain	Res	Type
3	C	108	HIS
3	C	122	LEU
4	D	52	LEU
4	D	63	ASN
4	D	72	LEU
4	D	108	LEU
4	D	134	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	44	ASN
1	A	113	ASN
1	A	128	GLN
1	A	143	GLN
1	A	156	HIS
1	A	246	GLN
1	A	254	HIS
1	A	384	ASN
1	A	408	ASN
1	A	453	ASN
1	A	461	ASN
1	A	474	GLN
1	A	491	GLN
1	A	527	GLN
1	A	550	HIS
1	A	571	GLN
1	A	579	HIS
1	A	608	ASN
2	B	92	ASN
2	B	121	GLN
2	B	136	GLN
2	B	174	ASN
2	B	220	ASN
2	B	230	ASN
3	C	23	ASN
3	C	29	HIS
3	C	104	ASN
4	D	63	ASN

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 ⓘ

7 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$
9	NBI	B	1201	-	18,19,19	1.41	3 (16%)	22,25,25	0.88	1 (4%)
5	FAD	A	700	1	51,58,58	1.40	7 (13%)	60,89,89	1.60	8 (13%)
11	EPH	D	1306	-	43,43,48	1.73	8 (18%)	45,48,53	1.19	3 (6%)
7	SF4	B	303	2	0,12,12	0.00	-	-		
10	HEM	C	1305	3,4	27,50,50	2.13	6 (22%)	17,82,82	1.47	3 (17%)
6	FES	B	302	2	0,4,4	0.00	-	-		
8	F3S	B	304	2	0,9,9	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NBI	B	1201	-	-	4/10/12/12	0/2/2/2
5	FAD	A	700	1	-	5/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	EPH	D	1306	-	1/1/4/14	33/47/47/52	-
7	SF4	B	303	2	-	-	0/6/5/5
10	HEM	C	1305	3,4	-	1/6/54/54	-
6	FES	B	302	2	-	-	0/1/1/1
8	F3S	B	304	2	-	-	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1305	HEM	C3D-C2D	5.53	1.54	1.37
11	D	1306	EPH	P1-O6	5.05	1.79	1.55
5	A	700	FAD	C10-N1	4.57	1.39	1.33
11	D	1306	EPH	O2-C4	4.42	1.46	1.33
11	D	1306	EPH	O1-C3	4.42	1.46	1.34
10	C	1305	HEM	C3B-C2B	-4.18	1.34	1.40
10	C	1305	HEM	C3C-C2C	-4.12	1.34	1.40
5	A	700	FAD	C2A-N3A	3.87	1.38	1.32
5	A	700	FAD	C4X-N5	3.79	1.38	1.33
9	B	1201	NBI	C2-C1	3.72	1.49	1.41
11	D	1306	EPH	C13-C12	3.67	1.53	1.31
11	D	1306	EPH	C25-C24	3.65	1.52	1.31
11	D	1306	EPH	C29-C28	3.65	1.52	1.31
10	C	1305	HEM	C3C-CAC	3.54	1.55	1.47
5	A	700	FAD	C4-N3	3.36	1.38	1.33
10	C	1305	HEM	C3B-CAB	3.28	1.54	1.47
11	D	1306	EPH	C15-C16	3.13	1.53	1.29
9	B	1201	NBI	C8-N1	-3.11	1.35	1.41
9	B	1201	NBI	C1-N2	-2.95	1.40	1.45
5	A	700	FAD	C1'-N10	2.56	1.50	1.48
11	D	1306	EPH	P1-O7	2.51	1.59	1.50
5	A	700	FAD	C2A-N1A	2.49	1.38	1.33
10	C	1305	HEM	CAA-C2A	2.29	1.55	1.52
5	A	700	FAD	C5X-N5	2.09	1.38	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	FAD	N3A-C2A-N1A	-5.86	119.52	128.68
5	A	700	FAD	C4-N3-C2	5.79	120.03	115.14
11	D	1306	EPH	O1-C3-C5	3.76	119.59	111.50
5	A	700	FAD	C4X-N5-C5X	3.75	120.51	116.77
11	D	1306	EPH	O2-C4-C18	3.14	121.76	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1201	NBI	C6-C1-N2	3.04	119.73	116.47
5	A	700	FAD	C5X-C9A-N10	3.00	119.89	117.72
10	C	1305	HEM	CAA-CBA-CGA	-2.98	107.67	112.67
10	C	1305	HEM	CMA-C3A-C4A	-2.56	124.53	128.46
5	A	700	FAD	P-O3P-PA	-2.21	125.24	132.83
5	A	700	FAD	C10-C4X-N5	-2.14	119.78	121.26
5	A	700	FAD	C1'-N10-C9A	2.10	119.95	118.29
11	D	1306	EPH	O2-C4-O4	-2.07	118.38	123.59
10	C	1305	HEM	C1D-C2D-C3D	-2.03	105.58	107.00
5	A	700	FAD	C4X-C4-N3	-2.02	120.66	123.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	D	1306	EPH	C2

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	1201	NBI	C2-C1-N2-O3
9	B	1201	NBI	C6-C1-N2-O3
5	A	700	FAD	N10-C1'-C2'-O2'
5	A	700	FAD	N10-C1'-C2'-C3'
11	D	1306	EPH	C5-C3-O1-C2
11	D	1306	EPH	C38-O8-P1-O7
11	D	1306	EPH	O8-C38-C39-N1
10	C	1305	HEM	C3D-CAD-CBD-CGD
11	D	1306	EPH	O3-C3-O1-C2
11	D	1306	EPH	C18-C4-O2-C1
11	D	1306	EPH	C23-C24-C25-C26
11	D	1306	EPH	O4-C4-O2-C1
9	B	1201	NBI	C9-C8-N1-C7
9	B	1201	NBI	C13-C8-N1-C7
11	D	1306	EPH	C38-O8-P1-O5
11	D	1306	EPH	C7-C8-C9-C10
11	D	1306	EPH	C3-C5-C6-C7
11	D	1306	EPH	C4-C18-C19-C20
11	D	1306	EPH	C20-C21-C22-C23
11	D	1306	EPH	C27-C28-C29-C30
5	A	700	FAD	O4B-C4B-C5B-O5B
11	D	1306	EPH	C13-C14-C15-C16
11	D	1306	EPH	C2-C37-O5-P1

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Mol	Chain	Res	Type	Atoms
5	A	700	FAD	PA-O3P-P-O5'
11	D	1306	EPH	C28-C29-C30-C31
11	D	1306	EPH	C14-C15-C16-C17
11	D	1306	EPH	C25-C26-C27-C28
11	D	1306	EPH	C21-C22-C23-C24
11	D	1306	EPH	C11-C10-C9-C8
11	D	1306	EPH	C37-O5-P1-O6
11	D	1306	EPH	C38-O8-P1-O6
11	D	1306	EPH	O2-C1-C2-O1
11	D	1306	EPH	C19-C18-C4-O2
11	D	1306	EPH	C1-C2-O1-C3
11	D	1306	EPH	O2-C1-C2-C37
11	D	1306	EPH	C5-C6-C7-C8
11	D	1306	EPH	C12-C13-C14-C15
11	D	1306	EPH	C24-C25-C26-C27
5	A	700	FAD	C3B-C4B-C5B-O5B
11	D	1306	EPH	C22-C23-C24-C25
11	D	1306	EPH	C37-O5-P1-O8
11	D	1306	EPH	C39-C38-O8-P1
11	D	1306	EPH	C9-C10-C11-C12

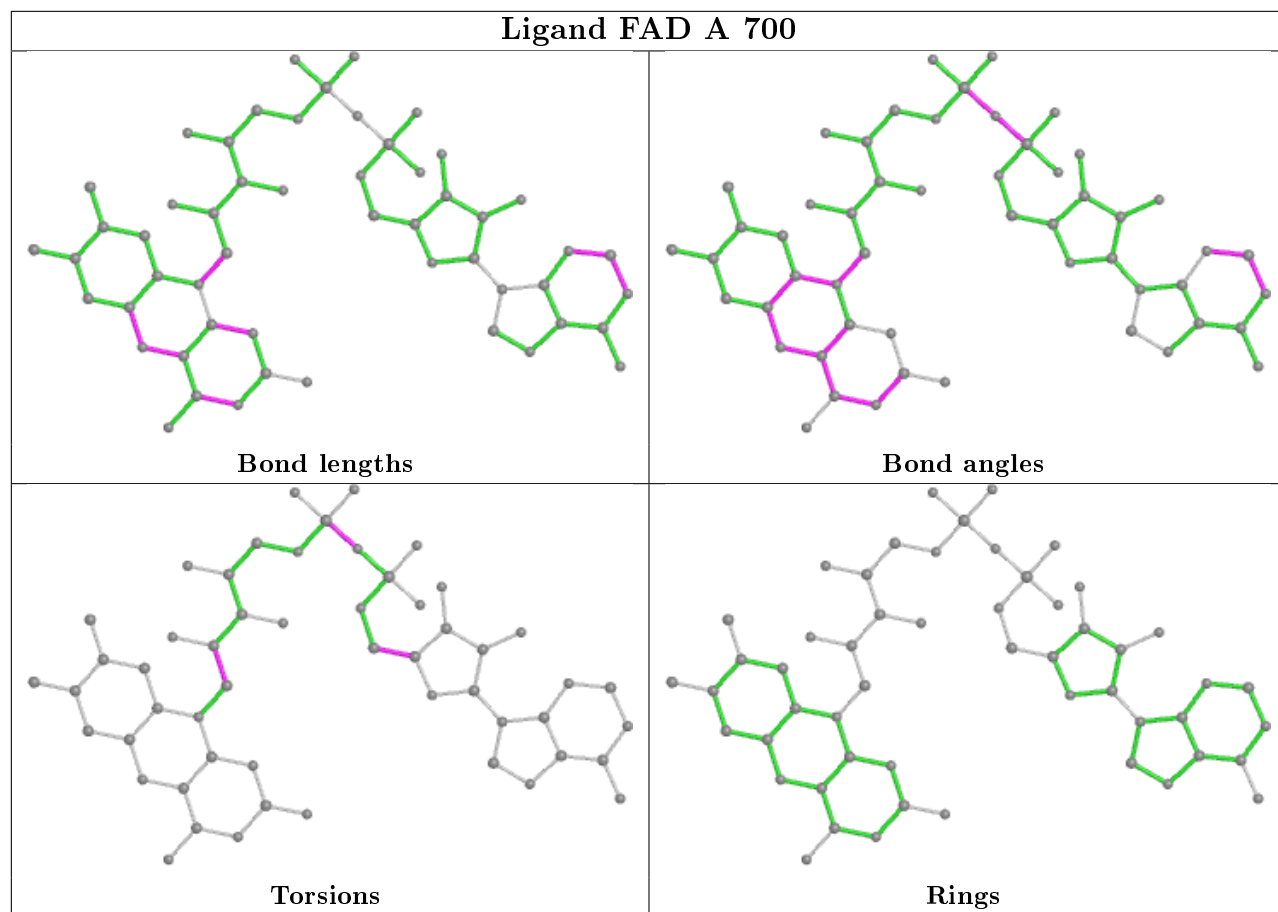
There are no ring outliers.

3 monomers are involved in 19 short contacts:

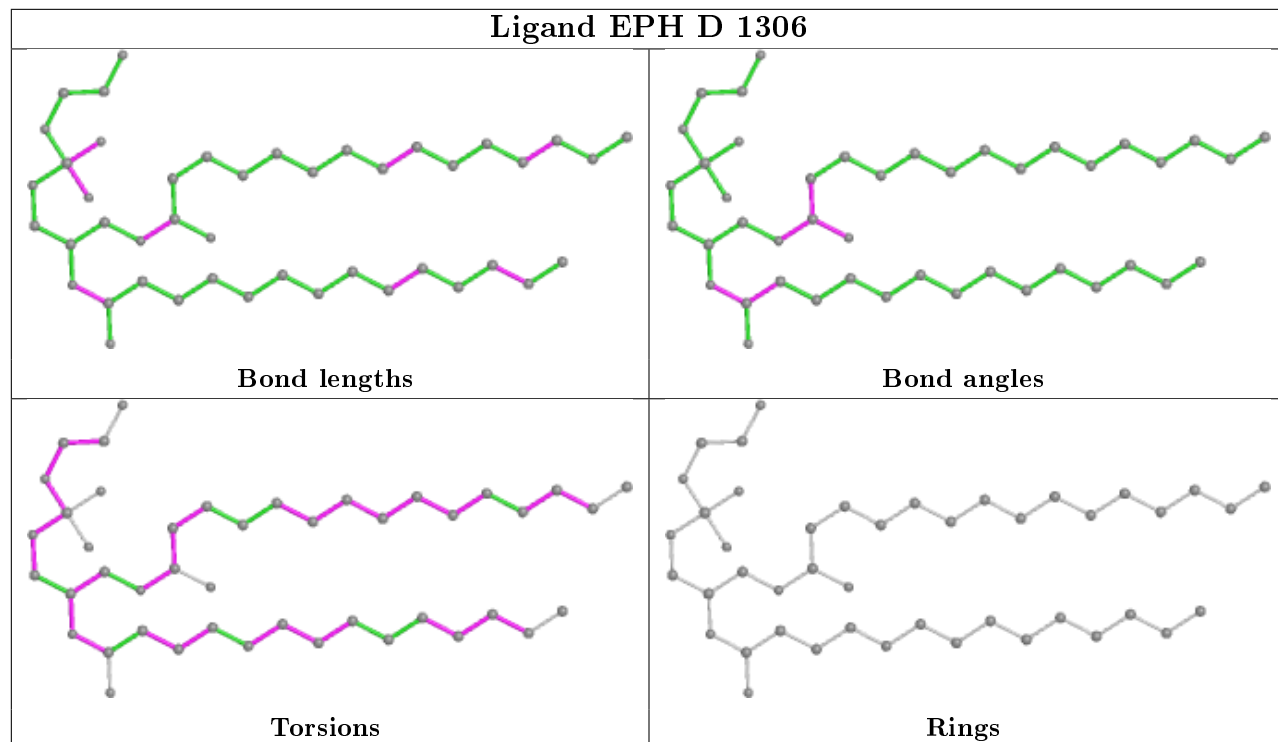
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1201	NBI	1	0
5	A	700	FAD	17	0
10	C	1305	HEM	1	0

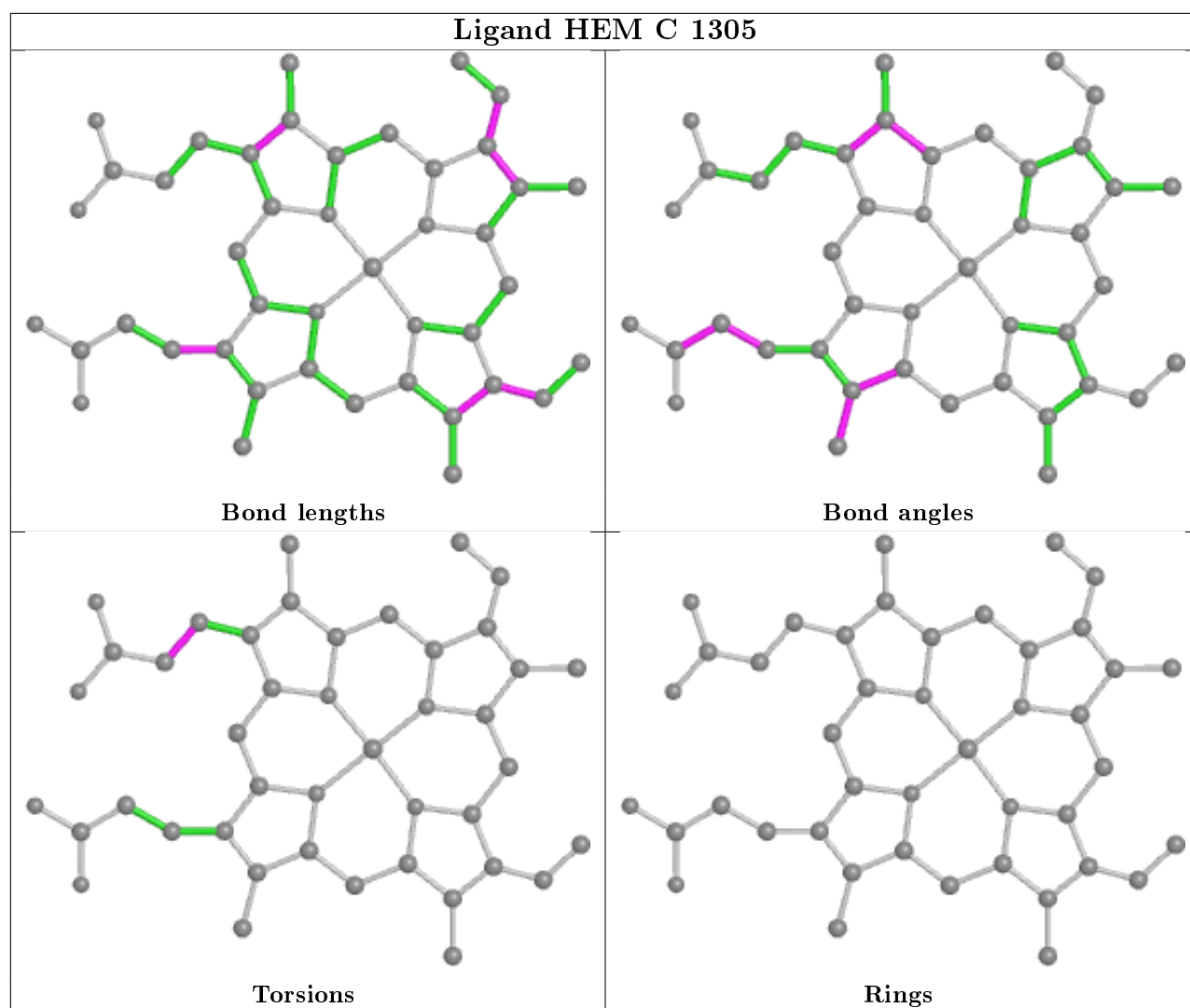
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FAD A 700



Ligand EPH D 1306





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%)	0.10	20 (3%) 46 48	57, 82, 137, 161	0
2	B	239/252 (94%)	0.05	7 (2%) 51 54	54, 75, 112, 136	0
3	C	138/140 (98%)	-0.02	4 (2%) 51 54	67, 84, 140, 157	0
4	D	102/103 (99%)	-0.20	1 (0%) 82 86	68, 86, 114, 128	0
All	All	1092/1117 (97%)	0.05	32 (2%) 51 54	54, 81, 129, 161	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	TYR	5.1
1	A	277	ILE	4.6
4	D	35	SER	4.5
1	A	10	SER	3.8
3	C	85	THR	3.7
2	B	11	ILE	3.6
1	A	325	GLN	3.6
1	A	357	PRO	3.0
1	A	280	GLN	2.9
1	A	317	PRO	2.9
1	A	322	VAL	2.9
3	C	84	PRO	2.8
1	A	315	CYS	2.8
1	A	230	SER	2.7
1	A	226	SER	2.6
2	B	35	ILE	2.6
1	A	273	GLY	2.6
1	A	327	HIS	2.5
2	B	34	GLU	2.5
3	C	82	LEU	2.5
3	C	143	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	216	GLY	2.5
2	B	24	THR	2.4
1	A	11	THR	2.3
1	A	278	ASN	2.3
2	B	247	GLU	2.3
2	B	13	LYS	2.2
1	A	398	GLU	2.2
1	A	356	GLU	2.1
1	A	578	GLU	2.1
2	B	36	ASP	2.1
1	A	288	TYR	2.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

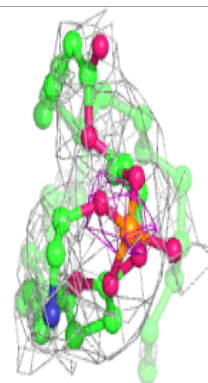
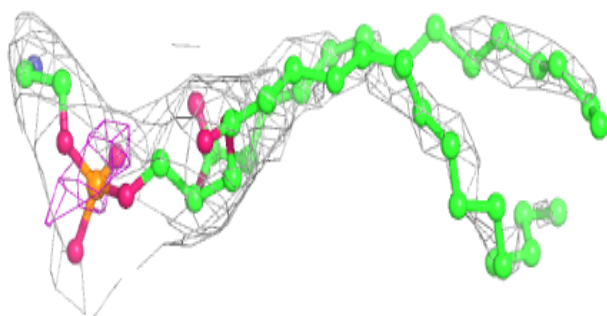
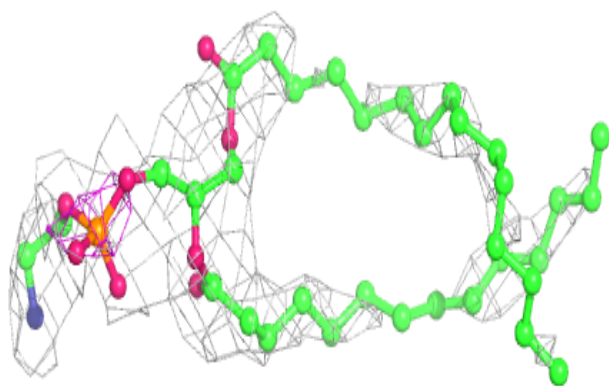
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	EPH	D	1306	44/49	0.90	0.59	105,110,116,116	0
5	FAD	A	700	53/53	0.92	0.33	64,66,70,70	0
9	NBI	B	1201	18/18	0.96	0.32	86,86,87,87	0
10	HEM	C	1305	43/43	0.97	0.24	74,75,77,78	0
6	FES	B	302	4/4	0.99	0.21	58,58,58,59	0
7	SF4	B	303	8/8	1.00	0.17	56,56,56,57	0
8	F3S	B	304	7/7	1.00	0.14	61,61,62,62	0

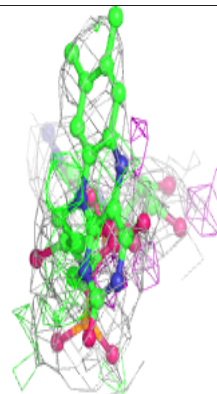
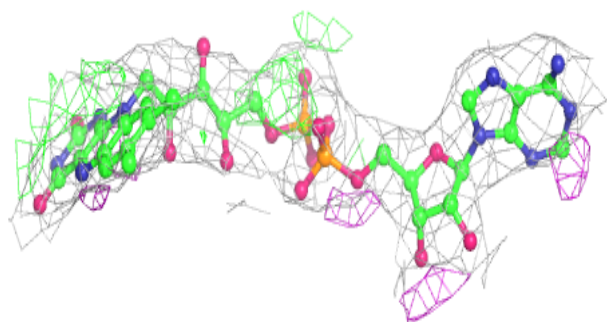
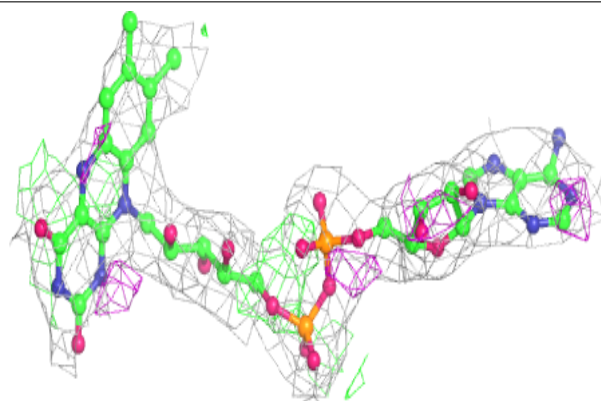
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

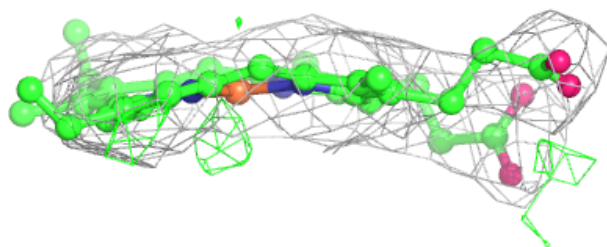
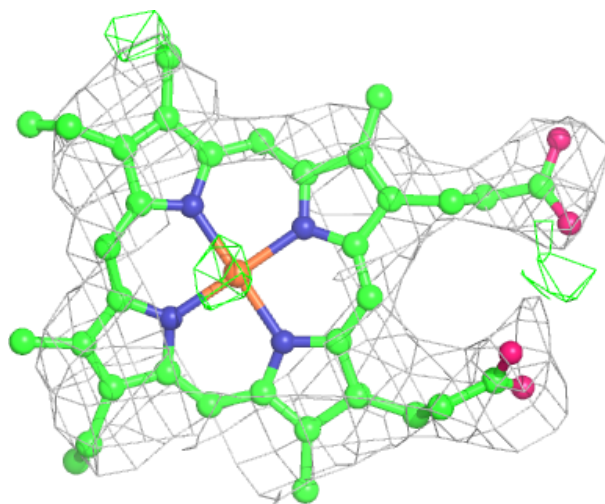
**Electron density around FAD A 700:**

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



Electron density around 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.