



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:21 AM UTC

PDB ID : 3SFD / pdb_00003sfd
Title : crystal structure of porcine mitochondrial respiratory complex II bound with oxaloacetate and pentachlorophenol
Authors : Zhou, Q.J.; Zhai, Y.J.; Liu, M.; Sun, F.
Deposited on : 2011-06-13
Resolution : 2.61 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

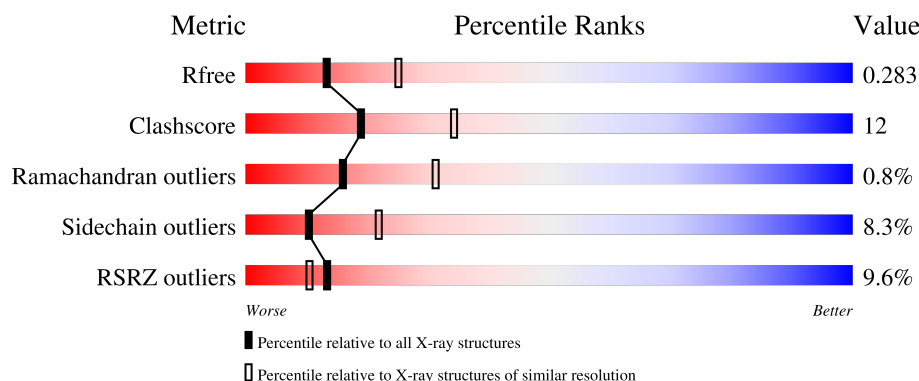
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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 $\leq 5\%$. 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	9% 69% 26% ..
2	B	252	8% 70% 21% 5%
3	C	140	16% 76% 19% ..
4	D	103	8% 73% 24% ..

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	OAA	A	701	-	-	X	-
9	F3S	B	304	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 8746 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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	252	VAL	ALA	SEE REMARK 999	UNP Q007T0

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

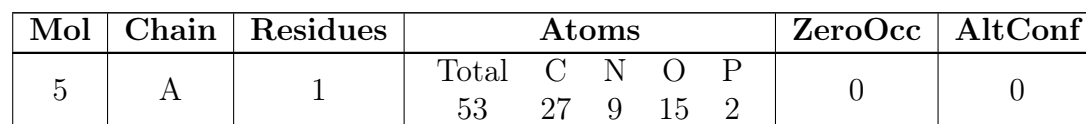
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	138	Total	C	N	O	S	0	0	0
			1064	695	179	183	7			

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

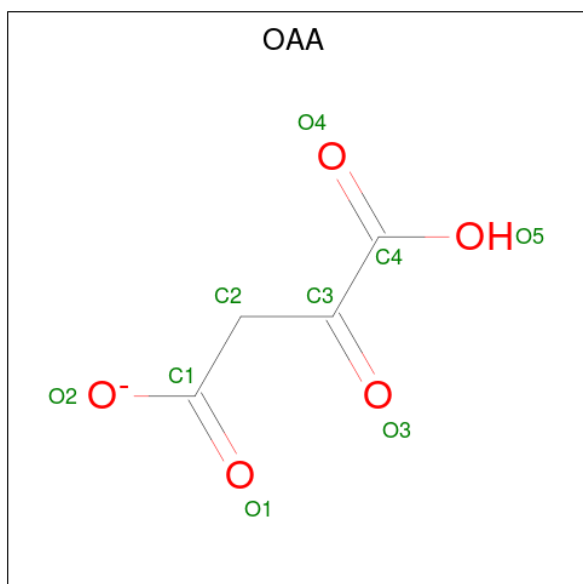
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			765	499	128	133	5			

There is a discrepancy between the modelled and reference sequences:

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

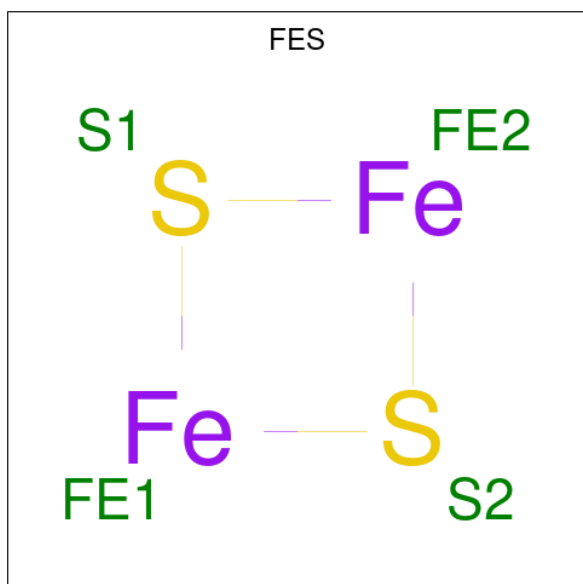


- Molecule 6 is OXALOACETATE ION (CCD ID: OAA) (formula: $\text{C}_4\text{H}_3\text{O}_5$).



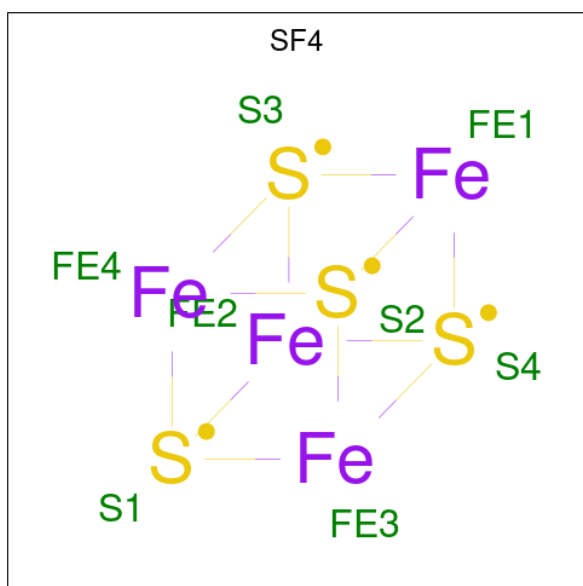
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



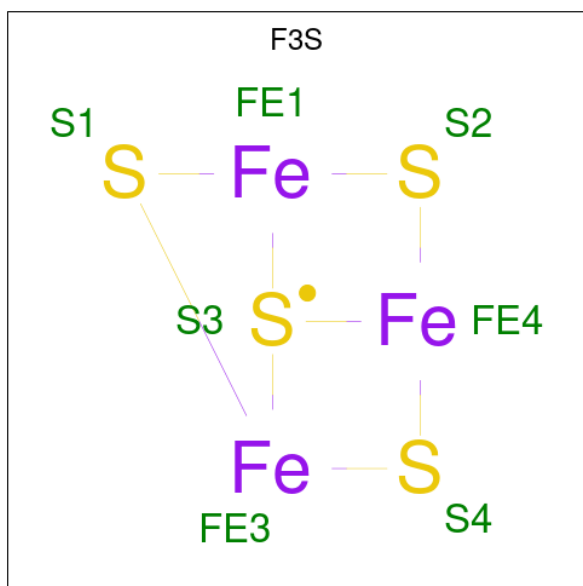
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



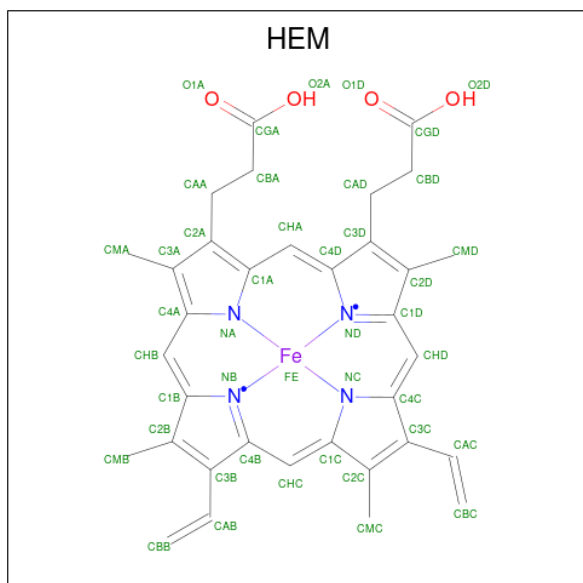
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



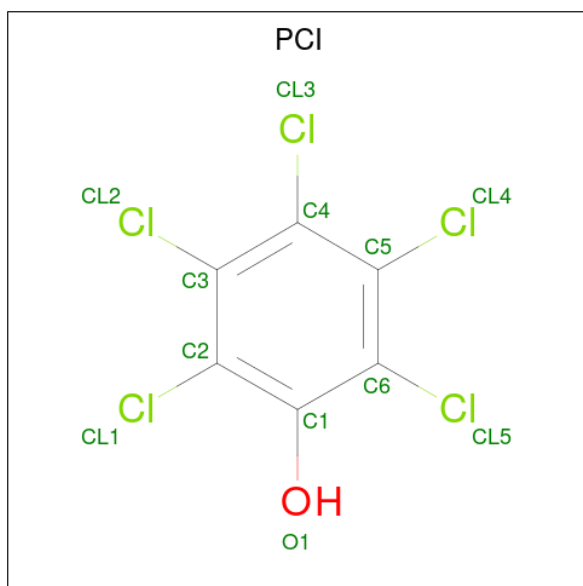
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- Molecule 11 is PENTACHLOROPHENOL (CCD ID: PCI) (formula: C_6HCl_5O).

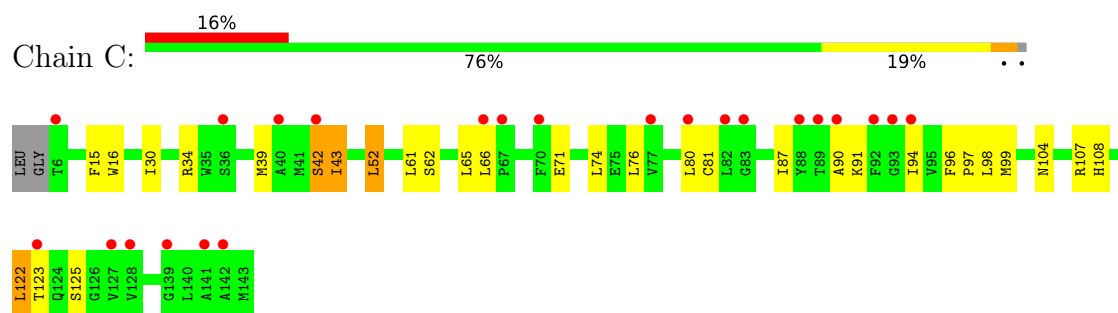


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	Cl	O		
			12	6	5	1		
							0	0

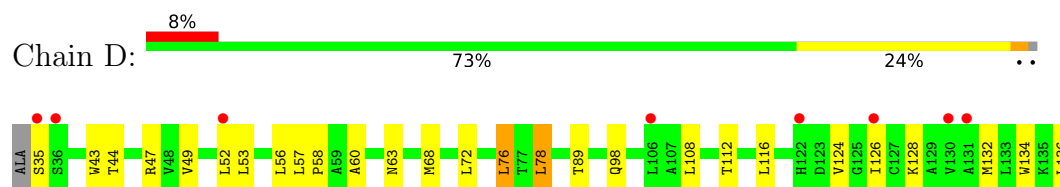
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	76	Total	O		
			76	76	0	0
12	B	30	Total	O		
			30	30	0	0
12	C	15	Total	O		
			15	15	0	0
12	D	9	Total	O		
			9	9	0	0

- 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	70.31Å 83.36Å 293.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.61 50.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	75.3 (50.00-2.61) 75.5 (50.00-2.61)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.57 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.242 , 0.286 0.242 , 0.283	Depositor DCC
R_{free} test set	2055 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8746	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: FES, HEM, F3S, PCI, FAD, OAA, SF4

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	0.48	0/4828	0.88	2/6531 (0.0%)
2	B	0.49	0/1964	0.87	4/2648 (0.2%)
3	C	0.49	0/1091	0.85	0/1483
4	D	0.46	0/784	0.94	0/1066
All	All	0.48	0/8667	0.88	6/11728 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	180	GLY	CA-C-N	7.21	126.47	118.97
2	B	180	GLY	C-N-CA	7.21	126.47	118.97
1	A	402	ALA	N-CA-C	-7.16	104.54	113.20
1	A	321	HIS	N-CA-C	5.52	116.35	108.74
2	B	102	LEU	CA-C-N	5.07	125.00	119.78
2	B	102	LEU	C-N-CA	5.07	125.00	119.78

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	129	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1922	0	1900	47	0
3	C	1064	0	1104	21	0
4	D	765	0	773	15	0
5	A	53	0	31	13	0
6	A	9	0	0	5	0
7	B	4	0	0	1	0
8	B	8	0	0	1	0
9	B	7	0	0	2	0
10	C	43	0	30	1	0
11	D	12	0	0	1	0
12	A	76	0	0	6	0
12	B	30	0	0	2	0
12	C	15	0	0	0	0
12	D	9	0	0	1	0
All	All	8746	0	8456	201	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (201) 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	1.21	1.48
1:A:57:HIS:CE1	5:A:700:FAD:HM82	1.91	1.04
1:A:72:MET:HE1	1:A:121:THR:HG21	1.47	0.96
1:A:58:THR:HG23	5:A:700:FAD:O1A	1.65	0.94
1:A:298:ARG:HH22	6:A:701:OAA:C1	1.86	0.89
1:A:373:THR:HG22	1:A:374:ASN:O	1.72	0.88
2:B:219:MET:HE2	9:B:304:F3S:S1	2.14	0.88
2:B:219:MET:HE1	2:B:232:GLY:HA3	1.55	0.86
1:A:64:GLY:HA2	1:A:154:THR:HG21	1.58	0.84
1:A:171:THR:HB	1:A:173:TYR:CE1	2.12	0.82
2:B:102:LEU:HD22	2:B:166:THR:HG21	1.61	0.82
1:A:72:MET:HE1	1:A:121:THR:CG2	2.10	0.82
1:A:303:ARG:HH11	1:A:303:ARG:HG2	1.44	0.81
1:A:152:ASP:HB2	1:A:339:PRO:HD2	1.64	0.80
2:B:164:CYS:SG	2:B:182:ALA:HB2	2.22	0.79
2:B:70:CYS:SG	2:B:72:SER:OG	2.46	0.73
1:A:29:GLY:H	1:A:58:THR:HG21	1.52	0.73
1:A:181:ASP:HA	1:A:237:MET:HG2	1.72	0.72
1:A:61:ALA:HB3	1:A:155:GLY:HA3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:SER:HB3	11:D:1:PCI:CL4	2.28	0.70
1:A:150:VAL:H	1:A:154:THR:HG23	1.54	0.70
1:A:299:ASP:O	1:A:303:ARG:HB2	1.92	0.69
1:A:58:THR:HG22	5:A:700:FAD:O4'	1.93	0.68
2:B:215:CYS:HA	9:B:304:F3S:S4	2.33	0.68
2:B:69:ILE:O	2:B:159:ILE:HD12	1.94	0.67
1:A:319:LYS:HA	12:A:696:HOH:O	1.95	0.66
3:C:61:LEU:O	3:C:65:LEU:HG	1.96	0.65
1:A:409:ARG:HH22	6:A:701:OAA:C1	2.09	0.65
1:A:222:PHE:HA	1:A:474:GLN:HE21	1.61	0.65
2:B:129:LEU:HD11	2:B:195:ARG:HB2	1.80	0.64
1:A:51:LEU:HD21	1:A:229:THR:HG21	1.80	0.64
1:A:113:ASN:HD22	2:B:138:GLY:H	1.45	0.64
2:B:52:LYS:HD2	2:B:57:SER:HA	1.80	0.63
1:A:171:THR:HB	1:A:173:TYR:HE1	1.62	0.63
1:A:130:ALA:HB2	1:A:145:HIS:HD2	1.62	0.63
1:A:104:ALA:HB3	1:A:105:PRO:HD3	1.82	0.62
4:D:60:ALA:HA	4:D:68:MET:HG2	1.82	0.61
2:B:219:MET:HG3	3:C:122:LEU:HD21	1.83	0.61
1:A:26:GLY:O	1:A:31:GLY:HA3	2.01	0.61
5:A:700:FAD:H8A	12:A:650:HOH:O	2.01	0.60
3:C:52:LEU:HD21	3:C:98:LEU:HA	1.84	0.60
1:A:414:SER:O	1:A:418:LEU:HD13	2.02	0.60
1:A:415:LEU:HG	5:A:700:FAD:C2	2.32	0.59
1:A:182:LEU:HD22	1:A:237:MET:HB3	1.85	0.59
2:B:230:ASN:ND2	2:B:233:LYS:H	1.99	0.59
1:A:86:LYS:O	1:A:620:ARG:HD2	2.03	0.58
2:B:35:ILE:HD11	2:B:51:ILE:HG22	1.85	0.58
1:A:361:LEU:HD12	1:A:362:PRO:HD2	1.84	0.58
1:A:113:ASN:ND2	2:B:138:GLY:H	2.01	0.58
3:C:91:LYS:HG3	4:D:134:TRP:CH2	2.37	0.58
2:B:176:ASP:HB3	3:C:16:TRP:CZ2	2.39	0.58
2:B:155:LEU:HD23	2:B:185:MET:HE2	1.86	0.57
1:A:303:ARG:O	1:A:307:LEU:HB2	2.05	0.57
1:A:150:VAL:H	1:A:154:THR:CG2	2.18	0.56
1:A:322:VAL:HG12	1:A:323:TYR:N	2.20	0.55
1:A:48:VAL:HG12	5:A:700:FAD:H2A	1.87	0.55
2:B:230:ASN:CG	2:B:233:LYS:HB3	2.32	0.55
1:A:486:VAL:HG13	1:A:553:GLU:HB2	1.89	0.55
2:B:103:PRO:HD2	2:B:166:THR:HG23	1.88	0.55
3:C:99:MET:HA	3:C:99:MET:HE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:HD13	1:A:237:MET:HE2	1.88	0.55
1:A:285:MET:HE2	1:A:301:VAL:HG22	1.87	0.55
1:A:130:ALA:HB2	1:A:145:HIS:CD2	2.42	0.54
1:A:52:PHE:HB3	1:A:55:ARG:HG2	1.88	0.54
4:D:89:THR:HA	4:D:98:GLN:HE22	1.73	0.54
1:A:463:THR:HG22	1:A:506:HIS:HB3	1.90	0.54
1:A:463:THR:HG23	1:A:464:ILE:HG13	1.90	0.53
2:B:219:MET:HE1	2:B:232:GLY:CA	2.34	0.53
3:C:107:ARG:HD2	3:C:125:SER:HB2	1.91	0.53
3:C:87:ILE:O	3:C:91:LYS:HB2	2.08	0.53
1:A:254:HIS:HB2	1:A:365:HIS:HB2	1.90	0.53
1:A:298:ARG:NH2	6:A:701:OAA:C1	2.66	0.52
2:B:83:LEU:HB2	2:B:86:THR:HG22	1.92	0.52
4:D:47:ARG:NH1	12:D:6:HOH:O	2.41	0.52
1:A:52:PHE:O	1:A:53:PRO:C	2.53	0.52
1:A:563:ASP:HB3	1:A:571:GLN:HE22	1.75	0.51
1:A:45:THR:HB	1:A:171:THR:HG23	1.93	0.50
1:A:323:TYR:HD2	1:A:357:PRO:HB2	1.76	0.50
1:A:405:HIS:ND1	1:A:409:ARG:HG3	2.26	0.50
2:B:51:ILE:HD11	2:B:59:LEU:HD22	1.93	0.50
1:A:258:ILE:HG22	1:A:263:CYS:H	1.76	0.50
1:A:303:ARG:HG2	1:A:303:ARG:NH1	2.22	0.50
1:A:453:ASN:HD21	1:A:527:GLN:HE22	1.59	0.50
1:A:346:MET:O	1:A:350:GLY:N	2.35	0.50
1:A:568:ILE:O	1:A:569:GLN:HB2	2.12	0.50
1:A:288:TYR:HE2	1:A:307:LEU:HD23	1.75	0.49
2:B:76:ASN:HB3	2:B:100:TYR:HB2	1.94	0.49
2:B:230:ASN:ND2	2:B:233:LYS:HB3	2.27	0.49
3:C:74:LEU:HD12	4:D:132:MET:HE2	1.93	0.49
1:A:254:HIS:HB2	1:A:365:HIS:CB	2.42	0.49
1:A:117:PRO:HA	12:A:629:HOH:O	2.12	0.49
2:B:198:PHE:HD2	2:B:201:GLU:HG3	1.78	0.49
1:A:248:LEU:HD12	1:A:535:GLN:HB2	1.93	0.49
1:A:445:ASN:O	1:A:448:GLU:HB2	2.13	0.49
1:A:374:ASN:OD1	1:A:378:GLN:NE2	2.40	0.48
1:A:265:ILE:HD13	1:A:360:VAL:HG12	1.95	0.48
2:B:230:ASN:HD22	2:B:230:ASN:C	2.20	0.48
1:A:66:ASN:HB3	1:A:80:HIS:CE1	2.48	0.48
1:A:88:SER:HB2	1:A:406:GLY:HA3	1.95	0.48
2:B:23:LYS:HB3	2:B:26:ASP:HB2	1.95	0.48
2:B:79:GLY:HA3	3:C:34:ARG:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLN:HG2	1:A:394:TYR:CE2	2.49	0.48
2:B:222:THR:OG1	2:B:230:ASN:ND2	2.47	0.48
1:A:248:LEU:O	1:A:536:THR:HG23	2.14	0.47
2:B:47:ALA:O	2:B:51:ILE:HG23	2.14	0.47
2:B:155:LEU:HD13	2:B:189:ARG:HA	1.96	0.47
1:A:410:LEU:O	1:A:413:ASN:HB2	2.14	0.47
1:A:264:LEU:HD22	5:A:700:FAD:C6	2.44	0.47
3:C:90:ALA:O	3:C:94:ILE:HG12	2.15	0.47
1:A:492:GLU:O	1:A:496:LYS:HB2	2.14	0.47
12:B:262:HOH:O	4:D:35:SER:HB3	2.15	0.46
1:A:29:GLY:HA3	1:A:418:LEU:HD23	1.97	0.46
2:B:232:GLY:HA2	2:B:235:ILE:HD12	1.96	0.46
1:A:303:ARG:HH11	1:A:303:ARG:CG	2.22	0.46
1:A:72:MET:HE3	1:A:128:GLN:H	1.79	0.46
1:A:493:GLY:O	1:A:497:ILE:HG12	2.15	0.46
1:A:292:ALA:HB3	1:A:622:TYR:HB3	1.97	0.46
4:D:57:LEU:HB2	4:D:58:PRO:HD3	1.97	0.46
1:A:246:GLN:HE22	1:A:600:ARG:HE	1.64	0.46
1:A:480:HIS:HD2	1:A:489:VAL:O	1.99	0.46
1:A:217:TYR:HB3	1:A:232:GLY:HA3	1.97	0.46
1:A:401:CYS:C	1:A:403:SER:H	2.23	0.46
2:B:226:PRO:HD2	8:B:303:SF4:S1	2.56	0.46
1:A:485:ARG:NE	12:A:673:HOH:O	2.48	0.45
3:C:104:ASN:ND2	3:C:107:ARG:HE	2.14	0.45
1:A:120:ARG:HG3	2:B:144:GLN:O	2.15	0.45
1:A:310:ARG:HA	12:A:684:HOH:O	2.15	0.45
2:B:116:SER:HB2	3:C:15:PHE:HD1	1.80	0.45
1:A:10:SER:C	1:A:12:GLN:H	2.24	0.45
1:A:52:PHE:CE2	1:A:54:THR:HB	2.50	0.45
2:B:65:CYS:O	2:B:66:ARG:HG3	2.16	0.45
2:B:38:ASN:HB2	12:B:264:HOH:O	2.16	0.45
2:B:70:CYS:SG	2:B:72:SER:CB	3.04	0.45
1:A:322:VAL:HG12	1:A:323:TYR:H	1.81	0.45
1:A:97:ILE:HA	1:A:404:VAL:HG23	1.98	0.45
1:A:458:ARG:NH2	1:A:514:MET:HG2	2.32	0.45
4:D:72:LEU:HB3	4:D:126:ILE:HD11	1.98	0.45
1:A:84:THR:HA	1:A:410:LEU:HD22	1.99	0.45
1:A:458:ARG:HH22	1:A:514:MET:HG2	1.81	0.45
1:A:190:ARG:CD	1:A:440:PRO:HB2	2.47	0.44
1:A:36:PHE:O	1:A:40:GLU:HB2	2.17	0.44
1:A:322:VAL:CG1	1:A:323:TYR:N	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LEU:CB	5:A:700:FAD:HM72	2.47	0.44
1:A:322:VAL:CG1	1:A:323:TYR:H	2.31	0.44
1:A:563:ASP:H	1:A:571:GLN:NE2	2.16	0.44
1:A:581:ARG:HH22	1:A:604:ASP:CG	2.26	0.44
1:A:264:LEU:HB2	5:A:700:FAD:HM72	2.00	0.44
1:A:59:VAL:HB	1:A:159:LEU:HD23	1.98	0.44
1:A:415:LEU:O	1:A:419:VAL:HG23	2.18	0.44
1:A:52:PHE:CD1	1:A:53:PRO:HD2	2.53	0.43
3:C:43:ILE:H	3:C:43:ILE:HG13	1.42	0.43
3:C:52:LEU:HB3	10:C:1305:HEM:HAC	2.00	0.43
1:A:52:PHE:CD2	1:A:54:THR:HB	2.53	0.43
2:B:102:LEU:HA	2:B:103:PRO:HD3	1.78	0.43
1:A:615:VAL:HA	1:A:616:PRO:HD3	1.88	0.43
1:A:516:TRP:HB3	2:B:60:THR:HG21	2.01	0.43
2:B:66:ARG:HA	2:B:85:CYS:HB2	2.00	0.43
4:D:49:VAL:HG11	4:D:78:LEU:HD13	2.00	0.43
1:A:26:GLY:HA2	5:A:700:FAD:H1B	2.00	0.43
4:D:124:VAL:HG13	4:D:128:LYS:CG	2.49	0.43
1:A:514:MET:HA	1:A:514:MET:CE	2.49	0.43
4:D:53:LEU:HD11	4:D:76:LEU:CD1	2.49	0.43
1:A:76:ASN:HA	12:A:657:HOH:O	2.19	0.42
1:A:550:HIS:CE1	1:A:552:ARG:HG2	2.54	0.42
1:A:559:VAL:HB	1:A:580:TRP:HB2	1.99	0.42
1:A:264:LEU:HD13	1:A:365:HIS:CE1	2.54	0.42
4:D:43:TRP:O	4:D:47:ARG:HG2	2.19	0.42
1:A:72:MET:H	1:A:128:GLN:HE21	1.67	0.42
2:B:68:GLY:HA2	7:B:302:FES:S1	2.59	0.42
1:A:91:LEU:O	1:A:583:HIS:CE1	2.72	0.42
1:A:239:THR:CG2	1:A:588:VAL:HG13	2.49	0.42
2:B:198:PHE:CD2	2:B:201:GLU:HG3	2.54	0.42
2:B:65:CYS:SG	2:B:68:GLY:N	2.92	0.42
1:A:63:GLY:N	6:A:701:OAA:O5	2.52	0.42
1:A:254:HIS:HB2	1:A:365:HIS:CG	2.55	0.42
3:C:52:LEU:CD1	3:C:97:PRO:HB2	2.50	0.42
1:A:149:CYS:HA	1:A:154:THR:CG2	2.50	0.42
1:A:485:ARG:HB3	1:A:490:LEU:HD11	2.02	0.42
1:A:100:MET:SD	1:A:404:VAL:HG21	2.60	0.42
2:B:102:LEU:HD22	2:B:166:THR:CG2	2.41	0.42
1:A:264:LEU:HD22	5:A:700:FAD:H6	2.01	0.41
2:B:66:ARG:HD2	2:B:66:ARG:O	2.20	0.41
1:A:198:GLU:O	1:A:515:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:124:VAL:HG13	4:D:128:LYS:HG2	2.02	0.41
1:A:81:PHE:O	1:A:85:VAL:HG12	2.20	0.41
1:A:116:MET:HA	1:A:161:THR:HG21	2.02	0.41
1:A:346:MET:HA	1:A:351:VAL:H	1.85	0.41
1:A:374:ASN:HB3	1:A:376:LYS:H	1.84	0.41
1:A:409:ARG:NH2	6:A:701:OAA:O1	2.54	0.41
3:C:96:PHE:HB3	3:C:97:PRO:CD	2.51	0.41
1:A:351:VAL:HG13	1:A:356:GLU:HG3	2.02	0.41
3:C:62:SER:HB2	3:C:66:LEU:HD12	2.02	0.40
4:D:112:THR:O	4:D:116:LEU:HG	2.21	0.40
1:A:57:HIS:NE2	5:A:700:FAD:C8	2.82	0.40
1:A:330:PRO:HA	1:A:331:PRO:HD3	1.96	0.40
2:B:220:ASN:HD21	3:C:39:MET:HE2	1.86	0.40
1:A:345:ALA:O	1:A:349:ALA:HB3	2.20	0.40
1:A:575:PRO:HG2	1:A:578:GLU:HB2	2.02	0.40
3:C:71:GLU:HG2	4:D:132:MET:HE1	2.02	0.40
1:A:254:HIS:CD2	1:A:256:THR:H	2.39	0.40
2:B:71:GLY:HA3	2:B:159:ILE:CG2	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%)	559 (92%)	46 (8%)	6 (1%)	12	26
2	B	237/252 (94%)	217 (92%)	17 (7%)	3 (1%)	9	19
3	C	136/140 (97%)	130 (96%)	6 (4%)	0	100	100
4	D	100/103 (97%)	97 (97%)	3 (3%)	0	100	100
All	All	1084/1117 (97%)	1003 (92%)	72 (7%)	9 (1%)	16	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	ASN
1	A	151	ALA
1	A	569	GLN
2	B	24	THR
2	B	74	ALA
1	A	317	PRO
2	B	73	CYS
1	A	286	GLU
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%)	458 (92%)	41 (8%)	10	22
2	B	214/221 (97%)	198 (92%)	16 (8%)	12	26
3	C	117/118 (99%)	107 (92%)	10 (8%)	10	21
4	D	76/76 (100%)	68 (90%)	8 (10%)	6	13
All	All	906/921 (98%)	831 (92%)	75 (8%)	10	22

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	32	LEU
1	A	54	THR
1	A	59	VAL
1	A	65	ILE
1	A	128	GLN
1	A	154	THR
1	A	157	SER
1	A	158	LEU
1	A	165	ARG
1	A	167	LEU
1	A	170	ASP
1	A	171	THR

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Mol	Chain	Res	Type
1	A	182	LEU
1	A	238	VAL
1	A	258	ILE
1	A	277	ILE
1	A	298	ARG
1	A	303	ARG
1	A	311	GLU
1	A	315	CYS
1	A	318	GLU
1	A	332	GLU
1	A	344	THR
1	A	358	ILE
1	A	368	MET
1	A	374	ASN
1	A	403	SER
1	A	419	VAL
1	A	438	LYS
1	A	448	GLU
1	A	453	ASN
1	A	486	VAL
1	A	488	SER
1	A	505	GLN
1	A	514	MET
1	A	521	VAL
1	A	561	GLU
1	A	568	ILE
1	A	588	VAL
1	A	590	VAL
2	B	51	ILE
2	B	63	ARG
2	B	69	ILE
2	B	96	VAL
2	B	105	MET
2	B	129	LEU
2	B	146	ILE
2	B	147	GLU
2	B	159	ILE
2	B	166	THR
2	B	189	ARG
2	B	192	ILE
2	B	201	GLU
2	B	205	LYS

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Mol	Chain	Res	Type
2	B	214	ARG
2	B	217	THR
3	C	30	ILE
3	C	42	SER
3	C	43	ILE
3	C	52	LEU
3	C	76	LEU
3	C	80	LEU
3	C	81	CYS
3	C	108	HIS
3	C	122	LEU
3	C	123	THR
4	D	44	THR
4	D	52	LEU
4	D	56	LEU
4	D	63	ASN
4	D	76	LEU
4	D	78	LEU
4	D	108	LEU
4	D	136	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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	160	HIS
1	A	246	GLN
1	A	325	GLN
1	A	327	HIS
1	A	384	ASN
1	A	386	GLN
1	A	453	ASN
1	A	474	GLN
1	A	480	HIS
1	A	527	GLN
1	A	550	HIS
1	A	571	GLN

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Mol	Chain	Res	Type
1	A	579	HIS
2	B	39	ASN
2	B	92	ASN
2	B	121	GLN
2	B	174	ASN
2	B	220	ASN
2	B	230	ASN
3	C	17	ASN
3	C	23	ASN
3	C	29	HIS
4	D	42	HIS
4	D	63	ASN
4	D	98	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
7	FES	B	302	2	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FAD	A	700	1	58,58,58	1.46	9 (15%)	85,89,89	1.64	19 (22%)
10	HEM	C	1305	3,4	50,50,50	2.88	27 (54%)	67,82,82	2.16	19 (28%)
6	OAA	A	701	-	8,8,8	6.63	5 (62%)	8,10,10	1.18	1 (12%)
9	F3S	B	304	2	0,9,9	-	-	-	-	-
8	SF4	B	303	2	0,12,12	-	-	-	-	-
11	PCI	D	1	-	12,12,12	2.07	5 (41%)	18,18,18	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FES	B	302	2	-	-	0/1/1/1
5	FAD	A	700	1	-	7/34/50/50	0/6/6/6
10	HEM	C	1305	3,4	-	7/14/54/54	-
6	OAA	A	701	-	-	4/8/8/8	-
9	F3S	B	304	2	-	-	0/3/3/3
8	SF4	B	303	2	-	-	0/6/5/5
11	PCI	D	1	-	-	-	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	OAA	C2-C1	-15.74	1.26	1.51
6	A	701	OAA	C2-C3	-6.52	1.26	1.51
6	A	701	OAA	C3-C4	-5.26	1.45	1.53
10	C	1305	HEM	CHC-C1C	5.23	1.48	1.38
10	C	1305	HEM	C3C-C2C	5.18	1.47	1.37
5	A	700	FAD	C9A-C5X	5.02	1.49	1.41
10	C	1305	HEM	C3B-C2B	4.97	1.47	1.37
6	A	701	OAA	O3-C3	4.94	1.33	1.23
10	C	1305	HEM	CHD-C4C	4.93	1.48	1.38
10	C	1305	HEM	FE-ND	4.89	2.09	1.94
10	C	1305	HEM	CHB-C1B	4.87	1.48	1.38
10	C	1305	HEM	FE-NA	4.83	2.11	1.95
10	C	1305	HEM	FE-NB	4.79	2.09	1.94
10	C	1305	HEM	FE-NC	4.56	2.10	1.95
10	C	1305	HEM	CHA-C4D	4.47	1.47	1.38
10	C	1305	HEM	CHC-C4B	4.01	1.48	1.39
10	C	1305	HEM	CHD-C1D	3.89	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1305	HEM	CHA-C1A	3.82	1.48	1.39
10	C	1305	HEM	CHB-C4A	3.70	1.47	1.39
11	D	1	PCI	C4-CL3	3.63	1.80	1.72
10	C	1305	HEM	C2A-C3A	3.61	1.48	1.38
5	A	700	FAD	C8-C7	3.54	1.49	1.40
10	C	1305	HEM	C4D-C3D	-3.43	1.39	1.45
10	C	1305	HEM	C4D-ND	-3.38	1.34	1.40
11	D	1	PCI	C6-CL5	3.26	1.79	1.72
5	A	700	FAD	C5A-C6A	3.15	1.49	1.41
10	C	1305	HEM	C3B-C4B	-3.05	1.39	1.44
5	A	700	FAD	PA-O3P	2.92	1.62	1.59
11	D	1	PCI	C3-CL2	2.89	1.79	1.72
11	D	1	PCI	C5-CL4	2.87	1.78	1.72
5	A	700	FAD	P-O3P	2.74	1.62	1.59
11	D	1	PCI	C2-CL1	2.72	1.78	1.72
5	A	700	FAD	C10-N10	2.69	1.43	1.37
5	A	700	FAD	C8A-N7A	2.63	1.36	1.31
10	C	1305	HEM	C1A-NA	-2.53	1.34	1.39
10	C	1305	HEM	C1B-NB	-2.51	1.35	1.40
5	A	700	FAD	C5X-N5	-2.47	1.34	1.39
10	C	1305	HEM	C1D-ND	-2.43	1.34	1.38
10	C	1305	HEM	C1B-C2B	-2.42	1.39	1.44
10	C	1305	HEM	C1D-C2D	-2.41	1.39	1.44
10	C	1305	HEM	C1C-C2C	2.32	1.49	1.45
10	C	1305	HEM	C1A-C2A	2.20	1.49	1.44
10	C	1305	HEM	C4C-NC	-2.18	1.35	1.39
6	A	701	OAA	O5-C4	-2.15	1.24	1.30
5	A	700	FAD	C4-N3	-2.14	1.34	1.38
10	C	1305	HEM	C4B-NB	-2.06	1.34	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1305	HEM	C3B-C2B-C1B	-6.88	101.24	106.41
10	C	1305	HEM	C3C-C2C-C1C	-6.14	101.24	107.05
5	A	700	FAD	C5A-C4A-N3A	-4.71	120.23	126.72
10	C	1305	HEM	C2B-C1B-NB	4.71	115.25	109.84
5	A	700	FAD	N3A-C2A-N1A	-4.45	121.85	128.58
10	C	1305	HEM	C3A-C4A-NA	4.19	116.85	110.14
10	C	1305	HEM	C3D-C4D-ND	4.06	114.63	110.17
5	A	700	FAD	O4B-C1B-N9A	3.98	115.74	108.09
10	C	1305	HEM	C3B-C4B-NB	3.87	112.24	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	FAD	C2A-N3A-C4A	3.85	121.24	111.83
10	C	1305	HEM	C2D-C1D-ND	3.38	113.81	109.90
10	C	1305	HEM	C1A-C2A-C3A	-3.19	101.94	106.87
10	C	1305	HEM	C2A-C1A-NA	3.15	113.65	110.15
10	C	1305	HEM	CMB-C2B-C1B	3.00	129.73	125.03
5	A	700	FAD	N9A-C8A-N7A	-2.98	109.71	113.94
10	C	1305	HEM	CMC-C2C-C1C	2.96	129.95	124.73
5	A	700	FAD	C4'-C3'-C2'	-2.96	108.65	113.57
10	C	1305	HEM	CHC-C1C-NC	-2.91	121.28	124.45
5	A	700	FAD	C4X-C10-N10	2.90	120.63	116.48
10	C	1305	HEM	C2C-C1C-NC	2.85	114.92	109.64
5	A	700	FAD	C4A-C5A-N7A	-2.83	107.34	110.58
5	A	700	FAD	C4X-C4-N3	2.67	120.05	113.25
10	C	1305	HEM	C4A-C3A-C2A	-2.58	103.86	106.82
5	A	700	FAD	C4X-C10-N1	-2.55	118.33	124.59
5	A	700	FAD	N3A-C4A-N9A	2.50	131.42	127.17
5	A	700	FAD	C5X-N5-C4X	2.45	122.06	118.09
5	A	700	FAD	C10-N1-C2	2.44	122.14	116.85
5	A	700	FAD	C4-N3-C2	-2.43	121.32	125.64
5	A	700	FAD	C1'-C2'-C3'	2.42	116.23	109.66
10	C	1305	HEM	CHD-C1D-ND	-2.35	121.90	124.42
5	A	700	FAD	C5A-C4A-N9A	2.32	108.34	105.81
5	A	700	FAD	C5A-N7A-C8A	2.32	107.10	103.45
10	C	1305	HEM	C4D-ND-C1D	-2.27	102.52	105.21
5	A	700	FAD	O4-C4-C4X	-2.24	120.62	126.53
5	A	700	FAD	C9A-C5X-N5	-2.17	120.15	122.45
6	A	701	OAA	O4-C4-C3	-2.17	119.11	121.81
10	C	1305	HEM	CHA-C4D-ND	-2.17	121.69	124.37
10	C	1305	HEM	CHC-C4B-NB	-2.16	122.10	124.42
10	C	1305	HEM	CAA-CBA-CGA	-2.00	108.36	113.67

There are no chirality outliers.

All (18) 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	O4'-C4'-C5'-O5'
6	A	701	OAA	C2-C3-C4-O4
6	A	701	OAA	C2-C3-C4-O5
10	C	1305	HEM	C2C-C3C-CAC-CBC
10	C	1305	HEM	C4C-C3C-CAC-CBC

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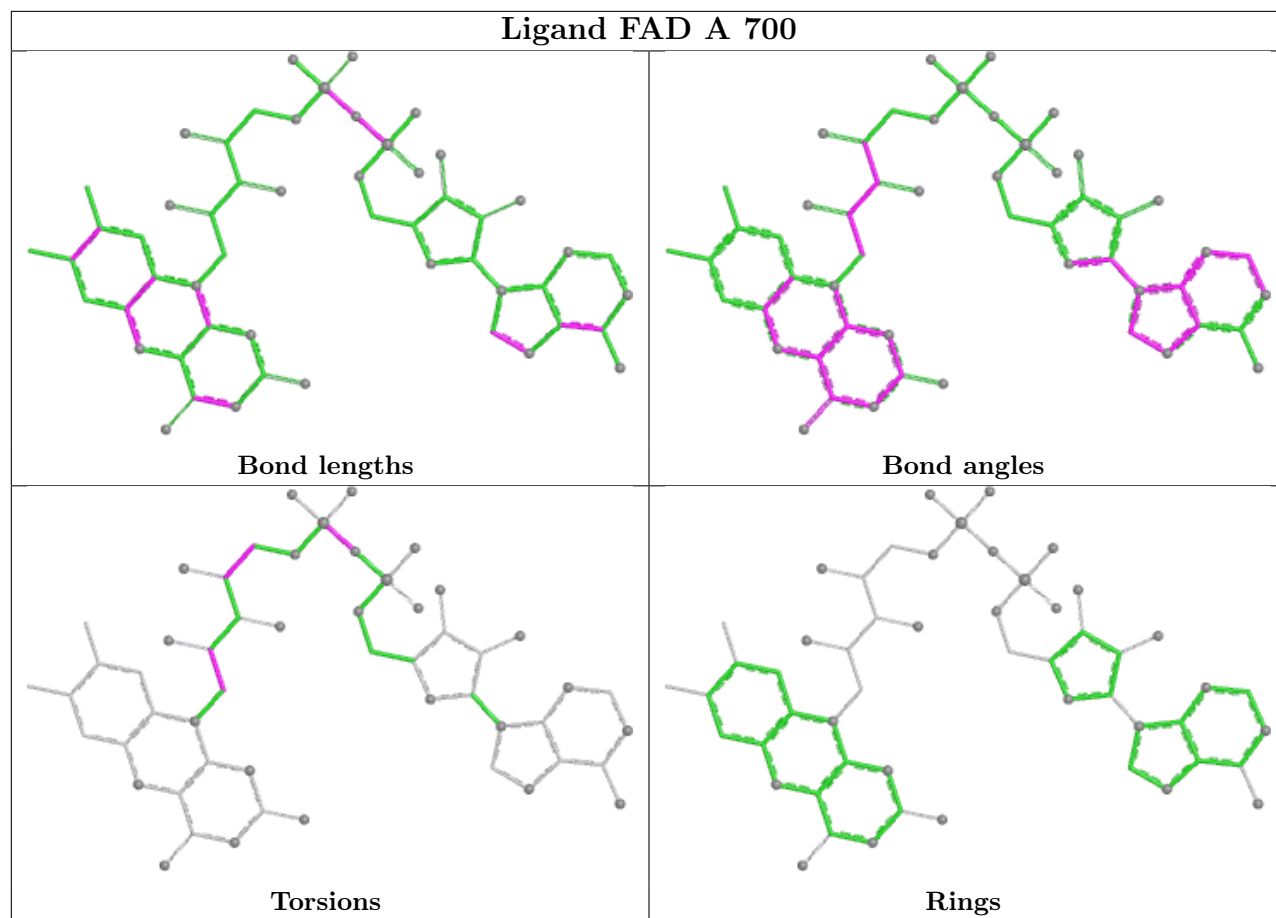
Mol	Chain	Res	Type	Atoms
10	C	1305	HEM	C3D-CAD-CBD-CGD
5	A	700	FAD	PA-O3P-P-O5'
6	A	701	OAA	O3-C3-C4-O4
10	C	1305	HEM	C2B-C3B-CAB-CBB
10	C	1305	HEM	C4B-C3B-CAB-CBB
5	A	700	FAD	C3'-C4'-C5'-O5'
10	C	1305	HEM	CAA-CBA-CGA-O1A
10	C	1305	HEM	CAA-CBA-CGA-O2A
6	A	701	OAA	O1-C1-C2-C3
5	A	700	FAD	PA-O3P-P-O1P
5	A	700	FAD	PA-O3P-P-O2P

There are no ring outliers.

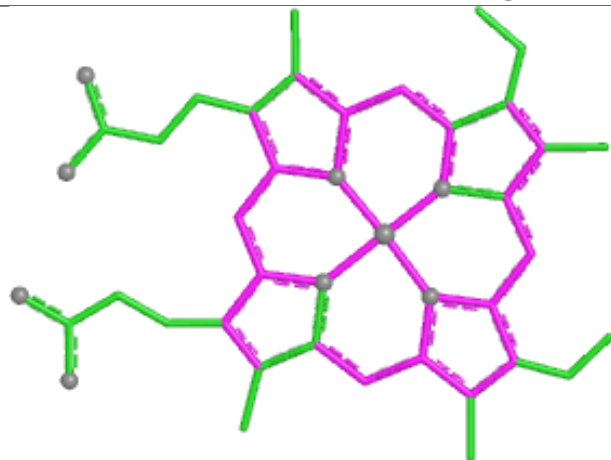
7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	302	FES	1	0
5	A	700	FAD	13	0
10	C	1305	HEM	1	0
6	A	701	OAA	5	0
9	B	304	F3S	2	0
8	B	303	SF4	1	0
11	D	1	PCI	1	0

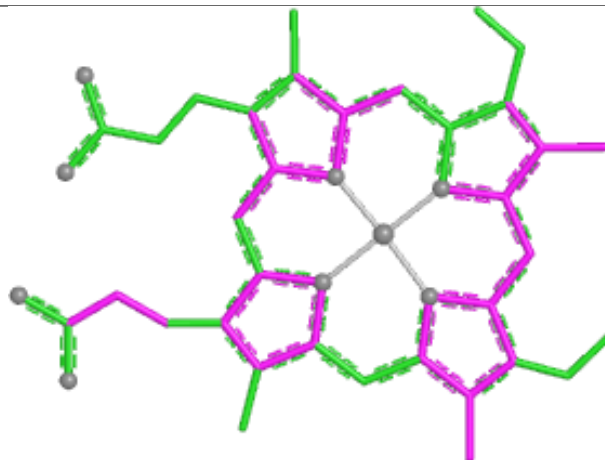
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



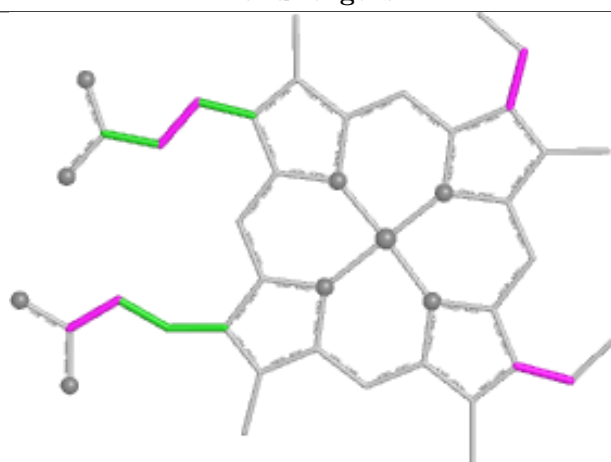
Ligand HEM C 1305



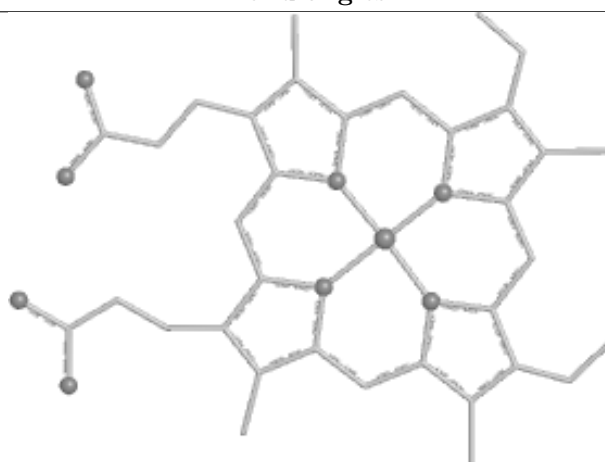
Bond lengths



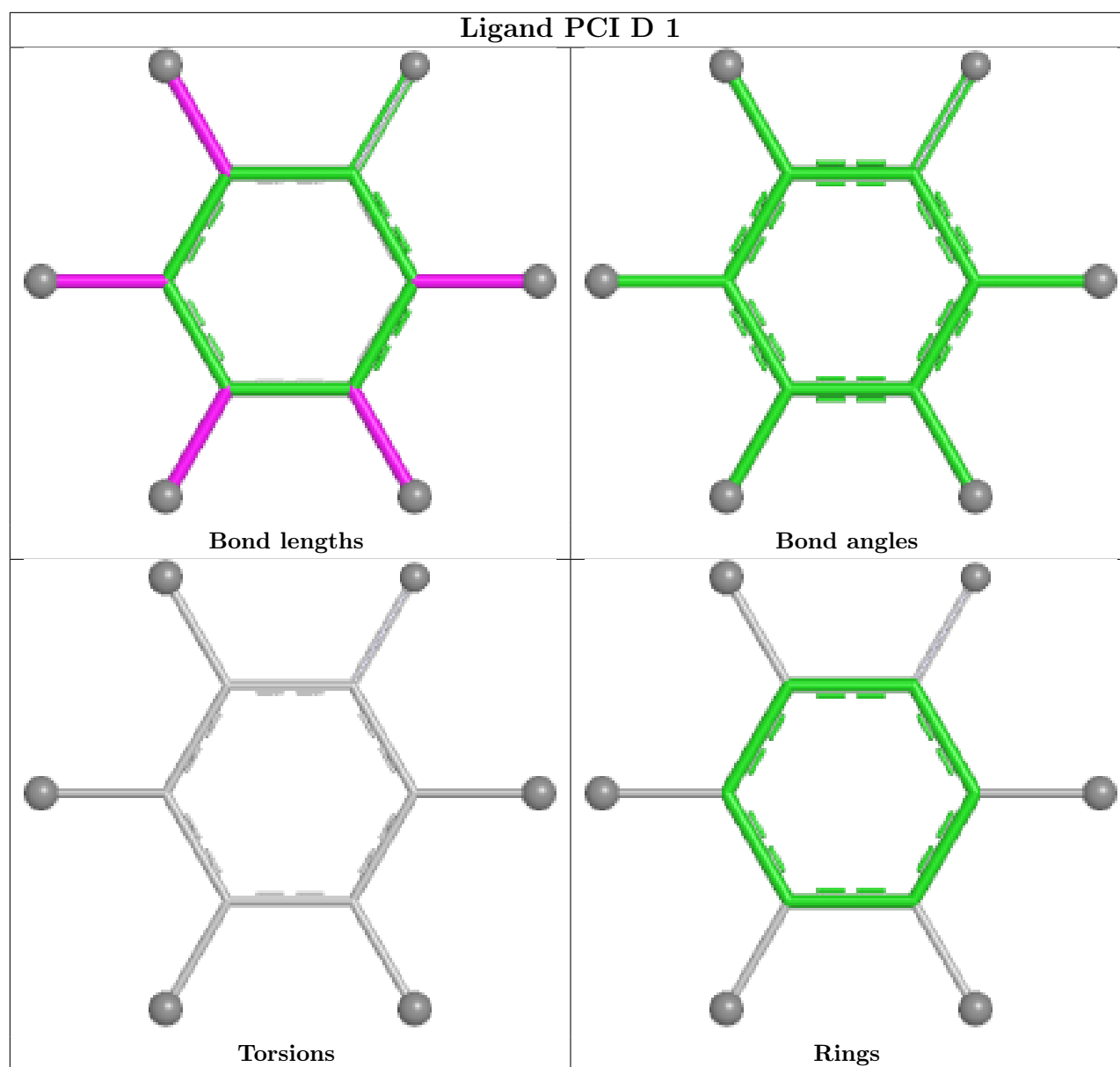
Bond angles



Torsions



Rings



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%)	0.78	53 (8%) 16 13	33, 56, 98, 108	0
2	B	239/252 (94%)	0.82	21 (8%) 15 12	37, 52, 72, 76	0
3	C	138/140 (98%)	1.31	23 (16%) 4 3	50, 64, 89, 92	0
4	D	102/103 (99%)	0.96	8 (7%) 19 15	48, 65, 74, 77	0
All	All	1092/1117 (97%)	0.87	105 (9%) 13 10	33, 58, 92, 108	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	LYS	3.8
2	B	9	PRO	3.7
4	D	35	SER	3.6
1	A	326	LEU	3.6
1	A	10	SER	3.6
2	B	212	LEU	3.6
1	A	11	THR	3.5
3	C	123	THR	3.4
3	C	80	LEU	3.4
1	A	297	SER	3.3
1	A	298	ARG	3.3
3	C	142	ALA	3.3
3	C	82	LEU	3.2
3	C	94	ILE	3.2
2	B	25	GLY	3.2
2	B	32	THR	3.1
2	B	236	ALA	3.1
1	A	324	LEU	3.0
1	A	317	PRO	3.0
3	C	6	THR	3.0
1	A	410	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	457	LEU	2.9
1	A	307	LEU	2.9
4	D	130	VAL	2.9
1	A	461	ASN	2.9
3	C	141	ALA	2.9
1	A	132	GLY	2.8
1	A	316	GLY	2.8
1	A	296	ALA	2.8
1	A	511	ASP	2.8
1	A	291	VAL	2.8
2	B	100	TYR	2.8
3	C	127	VAL	2.7
1	A	277	ILE	2.7
3	C	42	SER	2.7
1	A	356	GLU	2.7
1	A	358	ILE	2.6
2	B	235	ILE	2.6
1	A	343	GLU	2.6
1	A	15	VAL	2.6
3	C	67	PRO	2.6
3	C	139	GLY	2.6
2	B	11	ILE	2.6
1	A	295	LEU	2.6
2	B	74	ALA	2.6
3	C	83	GLY	2.6
1	A	353	VAL	2.6
1	A	334	LEU	2.5
2	B	192	ILE	2.5
3	C	77	VAL	2.5
1	A	261	ALA	2.5
3	C	90	ALA	2.5
1	A	88	SER	2.5
4	D	126	ILE	2.5
1	A	222	PHE	2.5
2	B	60	THR	2.4
3	C	36	SER	2.4
1	A	13	TYR	2.4
3	C	40	ALA	2.4
2	B	91	THR	2.4
2	B	173	TRP	2.4
4	D	131	ALA	2.4
3	C	128	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	122	HIS	2.3
1	A	313	ARG	2.3
3	C	93	GLY	2.3
1	A	131	PHE	2.3
1	A	354	THR	2.3
2	B	53	ASN	2.3
1	A	12	GLN	2.3
1	A	542	ALA	2.2
2	B	105	MET	2.2
3	C	88	TYR	2.2
1	A	265	ILE	2.2
2	B	213	TYR	2.2
4	D	36	SER	2.2
2	B	69	ILE	2.2
1	A	129	ARG	2.2
1	A	259	TYR	2.2
1	A	288	TYR	2.2
1	A	507	LEU	2.2
2	B	143	LEU	2.2
3	C	66	LEU	2.2
1	A	442	ILE	2.2
1	A	564	TYR	2.1
1	A	309	ILE	2.1
2	B	77	ILE	2.1
1	A	287	ARG	2.1
1	A	622	TYR	2.1
4	D	52	LEU	2.1
3	C	92	PHE	2.1
3	C	89	THR	2.1
1	A	572	GLN	2.1
1	A	292	ALA	2.1
2	B	134	GLU	2.1
1	A	14	PRO	2.1
4	D	106	LEU	2.1
1	A	323	TYR	2.1
1	A	568	ILE	2.1
1	A	16	VAL	2.0
1	A	322	VAL	2.0
3	C	70	PHE	2.0
1	A	359	PRO	2.0
2	B	58	THR	2.0
1	A	351	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

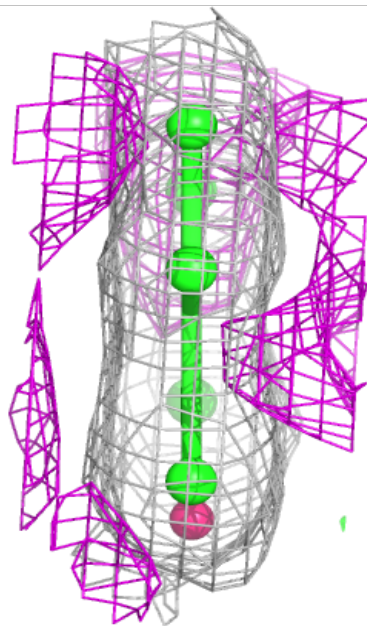
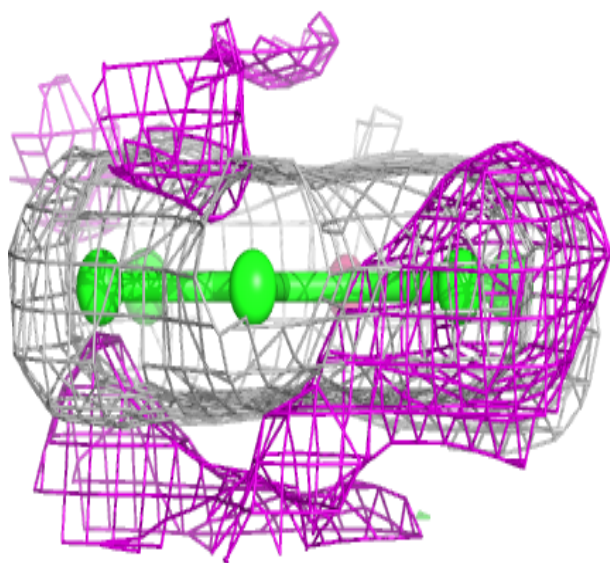
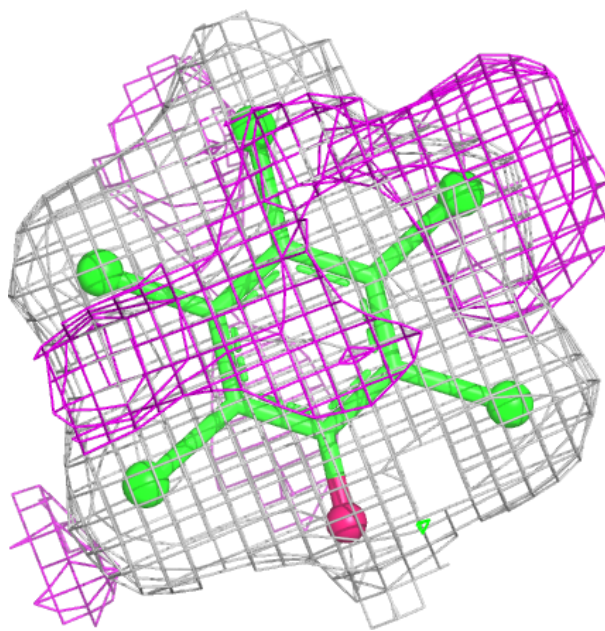
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	OAA	A	701	9/9	0.91	0.11	77,77,78,78	0
11	PCI	D	1	12/12	0.92	0.13	34,35,38,38	0
10	HEM	C	1305	43/43	0.93	0.16	69,73,74,75	0
5	FAD	A	700	53/53	0.94	0.08	34,38,41,42	0
9	F3S	B	304	7/7	0.98	0.05	35,40,41,43	0
8	SF4	B	303	8/8	0.99	0.03	34,35,36,36	0
7	FES	B	302	4/4	0.99	0.03	38,39,41,42	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.

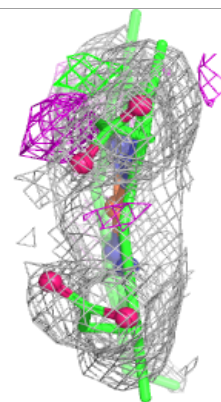
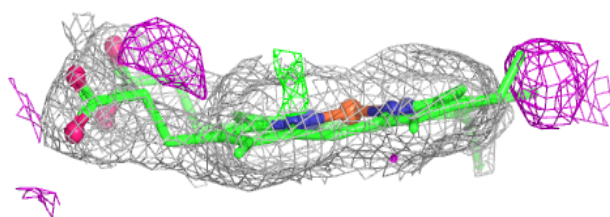
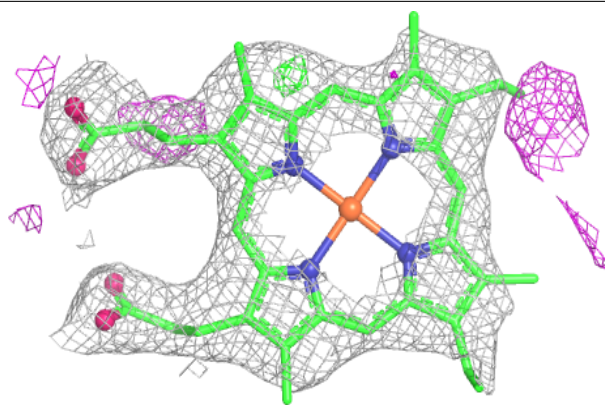
Electron density around PCI D 1:

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

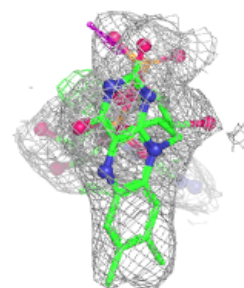
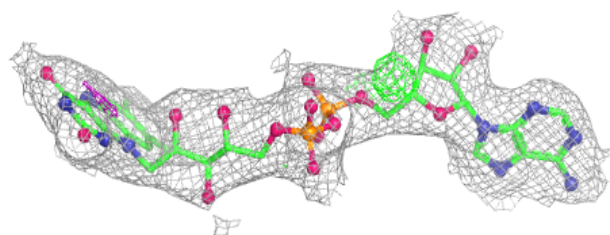
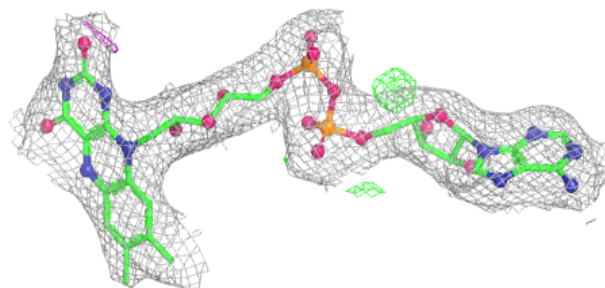


Electron density around HEM C 1305:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.