



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:20 AM GMT

PDB ID : 3AE4  
Title : Crystal structure of porcine heart mitochondrial complex II bound with 2-Iodo-N-methyl-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 : 2.91 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

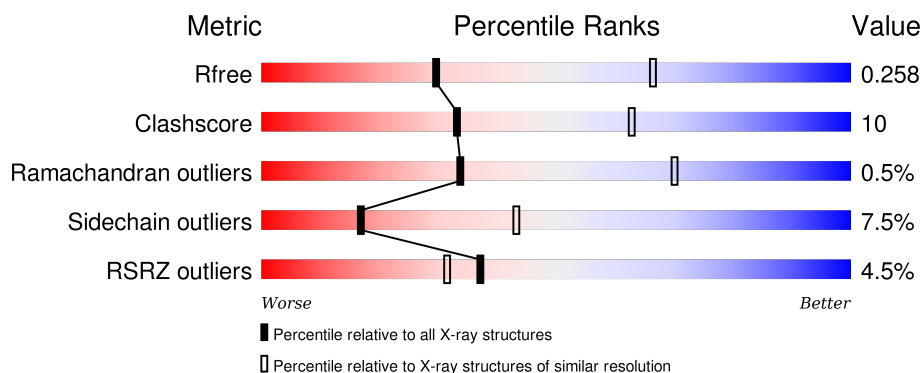
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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))
$R_{free}$	91344	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>74%</div> <div>21%</div> <div>• •</div> </div>
2	B	252	<div> <div>5%</div> <div>69%</div> <div>23%</div> <div>• 5%</div> </div>
3	C	140	<div> <div>9%</div> <div>81%</div> <div>15%</div> <div>• •</div> </div>
4	D	103	<div> <div>5%</div> <div>87%</div> <div>12%</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 criteria:

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

## 2 Entry composition

There are 12 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			

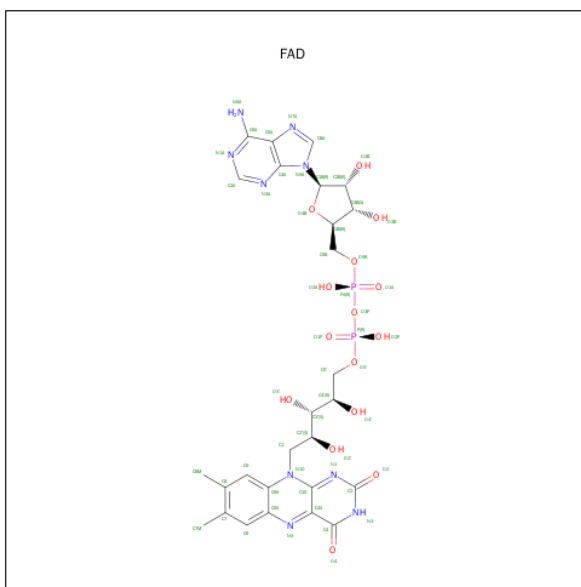
- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b560 subunit, mitochondrial.

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.

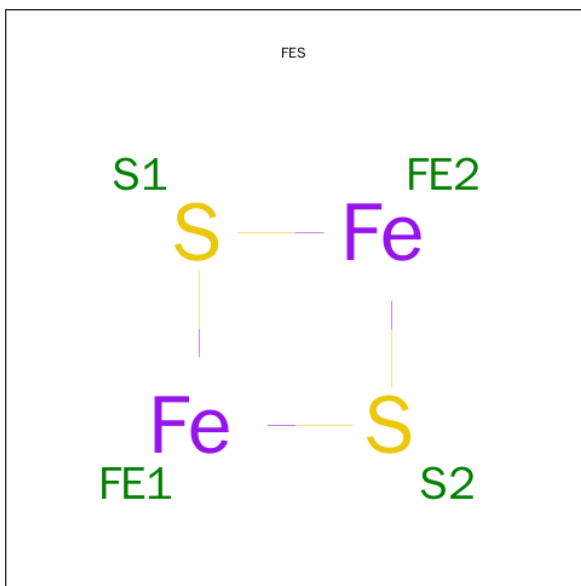
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			765	499	128	133	5			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



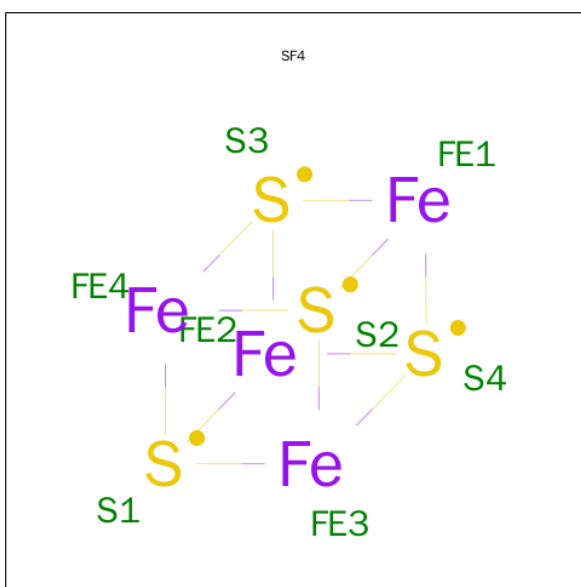
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



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:  $\text{Fe}_4\text{S}_4$ ).



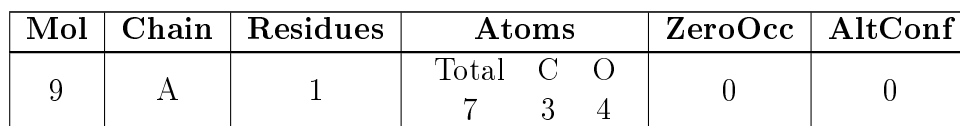
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



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

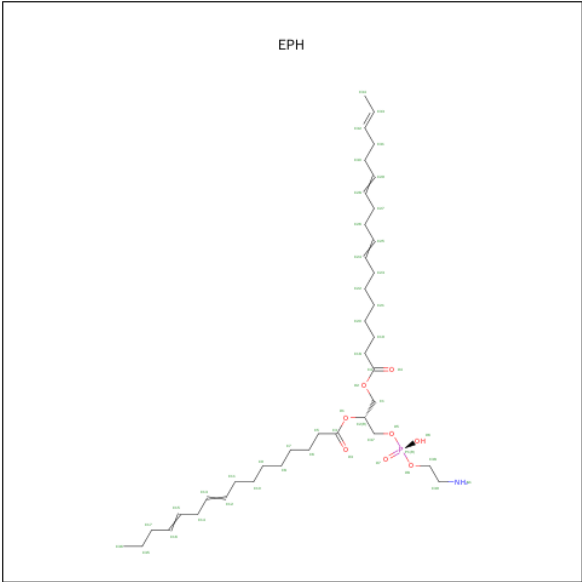
- Molecule 9 is MALONATE ION (three-letter code: MLI) (formula:  $\text{C}_3\text{H}_2\text{O}_4$ ).



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- Chemical structure of HEM (heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme group.

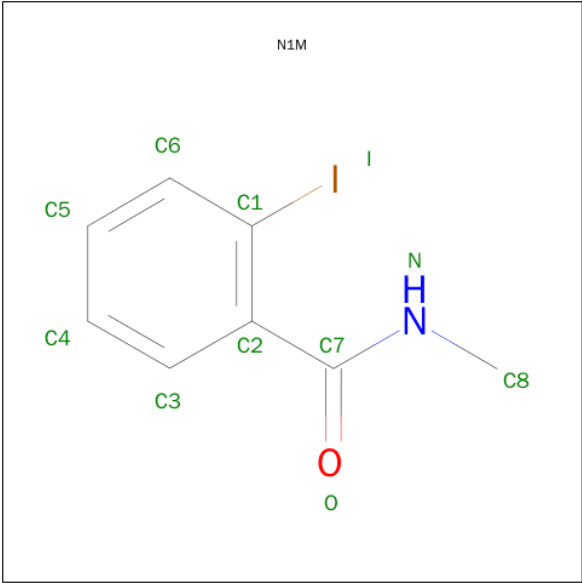
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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		

- Molecule 12 is 2-iodo-N-methylbenzamide (three-letter code: N1M) (formula: C<sub>8</sub>H<sub>8</sub>INO).



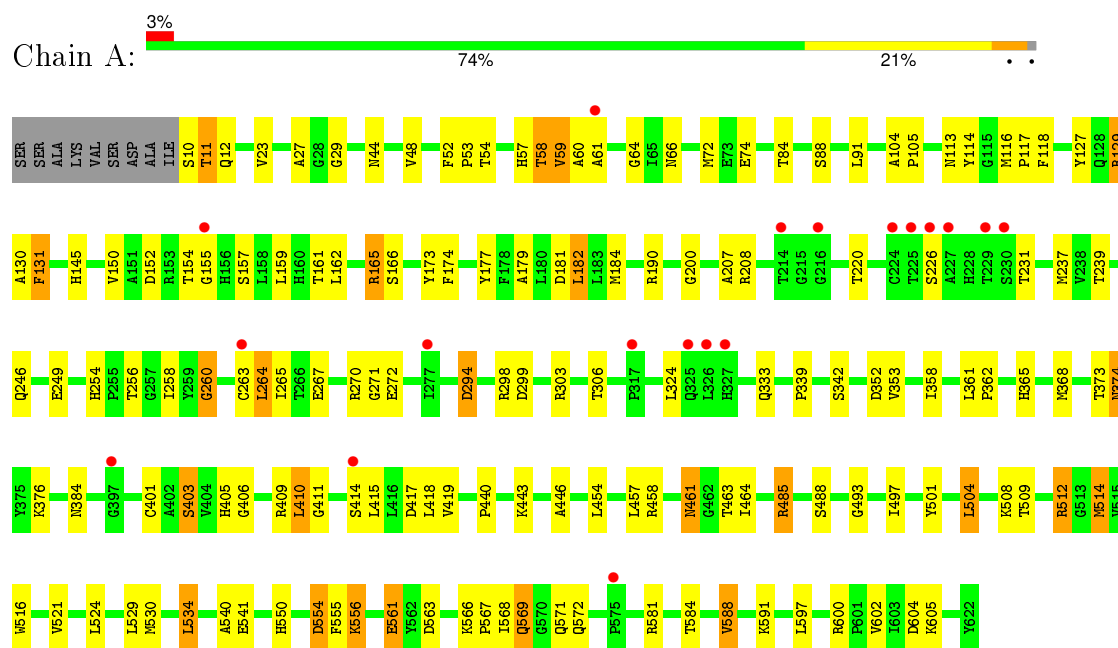
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	I	N	O	0	0
			11	8	1	1	1		



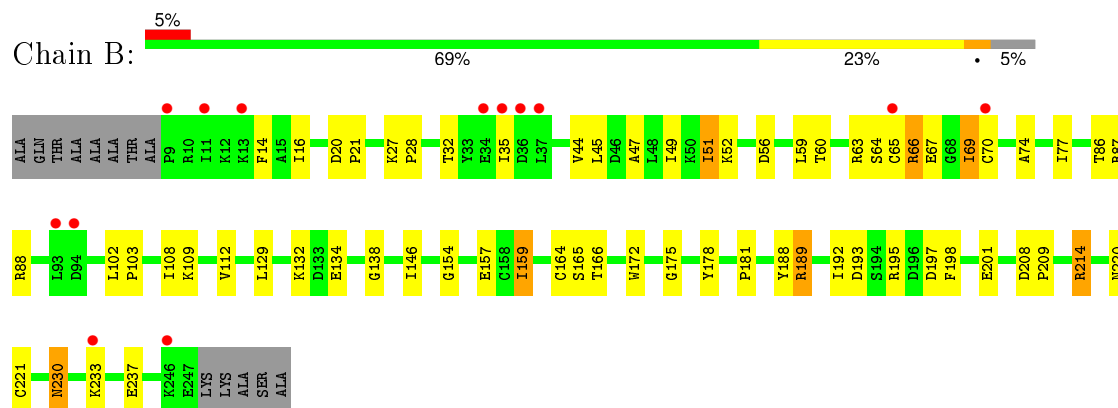
### 3 Residue-property plots

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

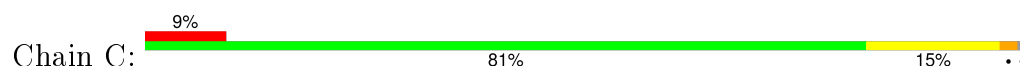
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial



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

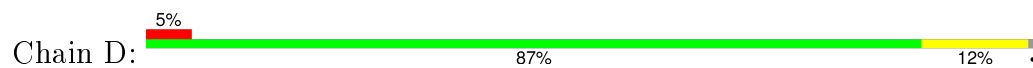


- Molecule 3: Succinate dehydrogenase cytochrome b560 subunit, mitochondrial





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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.56 Å 84.22 Å 294.22 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.24 – 2.91 48.24 – 2.91	Depositor EDS
% Data completeness (in resolution range)	85.0 (48.24-2.91) 84.9 (48.24-2.91)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 2.91 Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.222 , 0.257 0.220 , 0.258	Depositor DCC
$R_{free}$ test set	1682 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.2	Xtriage
Anisotropy	0.857	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 33975 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8657	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, MLI, F3S, FES, EPH, HEM, FAD, N1M

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	0.36	0/4828	0.55	1/6531 (0.0%)
2	B	0.37	0/1964	0.54	0/2648
3	C	0.36	0/1091	0.49	0/1483
4	D	0.35	0/784	0.50	0/1066
All	All	0.36	0/8667	0.54	1/11728 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	LEU	CA-CB-CG	5.32	127.54	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4729	0	4618	113	0
2	B	1922	0	1900	44	0
3	C	1064	0	1104	15	0
4	D	765	0	773	7	0
5	A	53	0	31	16	0
6	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	8	0	0	0	0
8	B	7	0	0	0	0
9	A	7	0	2	1	0
10	C	43	0	30	3	0
11	D	44	0	53	2	0
12	D	11	0	8	0	0
All	All	8657	0	8519	175	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 10.

All (175) 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	1.38	1.34
2:B:102:LEU:HB3	2:B:166:THR:HG21	1.34	1.08
1:A:57:HIS:CE1	5:A:700:FAD:HM82	1.91	1.06
1:A:509:THR:HG23	1:A:512:ARG:HH12	1.30	0.97
1:A:61:ALA:HB3	1:A:155:GLY:HA3	1.49	0.93
1:A:57:HIS:NE2	5:A:700:FAD:HM81	1.86	0.91
1:A:150:VAL:H	1:A:154:THR:HG22	1.35	0.90
1:A:59:VAL:HG23	1:A:159:LEU:HD23	1.61	0.82
3:C:52:LEU:HB3	10:C:1305:HEM:HAC	1.62	0.80
1:A:60:ALA:HB1	5:A:700:FAD:HM72	1.63	0.79
1:A:179:ALA:N	5:A:700:FAD:N1A	2.31	0.77
1:A:254:HIS:HD2	1:A:256:THR:H	1.33	0.76
1:A:415:LEU:HG	5:A:700:FAD:C2	2.15	0.75
1:A:353:VAL:HG12	1:A:358:ILE:HD11	1.70	0.73
1:A:29:GLY:H	1:A:58:THR:HG21	1.52	0.71
1:A:373:THR:HG22	1:A:374:ASN:O	1.89	0.71
2:B:27:LYS:HB3	2:B:28:PRO:CD	2.21	0.70
4:D:72:LEU:O	4:D:76:LEU:HB2	1.91	0.69
1:A:361:LEU:HD12	1:A:362:PRO:HD2	1.73	0.69
1:A:418:LEU:HD11	5:A:700:FAD:H4'	1.75	0.68
1:A:254:HIS:CD2	1:A:256:THR:H	2.12	0.68
1:A:561:GLU:OE2	1:A:581:ARG:HD3	1.94	0.67
2:B:129:LEU:HD11	2:B:195:ARG:HB2	1.75	0.67
1:A:246:GLN:NE2	1:A:600:ARG:HE	1.93	0.67
1:A:54:THR:O	1:A:59:VAL:HG21	1.94	0.67
1:A:504:LEU:HD21	1:A:530:MET:HG3	1.76	0.66
3:C:29:HIS:HD2	3:C:30:ILE:HG13	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:HIS:ND1	1:A:409:ARG:HG3	2.10	0.66
2:B:35:ILE:HD11	2:B:51:ILE:HG22	1.78	0.65
3:C:46:ARG:HE	10:C:1305:HEM:CGD	2.10	0.65
1:A:258:ILE:HD11	1:A:265:ILE:HG13	1.80	0.63
1:A:265:ILE:HD12	1:A:358:ILE:HG21	1.81	0.63
1:A:246:GLN:HA	1:A:584:THR:O	1.98	0.62
2:B:166:THR:O	2:B:166:THR:HG22	1.99	0.62
1:A:61:ALA:HA	5:A:700:FAD:N5	2.15	0.61
1:A:239:THR:HG23	1:A:588:VAL:HG13	1.82	0.61
1:A:150:VAL:N	1:A:154:THR:HG22	2.12	0.61
1:A:563:ASP:H	1:A:571:GLN:NE2	1.99	0.61
1:A:264:LEU:HD13	1:A:365:HIS:CE1	2.36	0.60
1:A:258:ILE:HG22	1:A:260:GLY:H	1.67	0.60
1:A:116:MET:HA	1:A:161:THR:HG21	1.84	0.59
1:A:181:ASP:HA	1:A:237:MET:HG2	1.83	0.59
1:A:166:SER:HB2	1:A:173:TYR:OH	2.03	0.58
1:A:563:ASP:H	1:A:571:GLN:HE22	1.52	0.58
2:B:102:LEU:CB	2:B:166:THR:HG21	2.22	0.57
1:A:84:THR:HA	1:A:410:LEU:HD22	1.86	0.57
1:A:118:PHE:HA	1:A:150:VAL:HG22	1.86	0.57
1:A:265:ILE:CD1	1:A:358:ILE:HG21	2.35	0.57
1:A:485:ARG:HH21	1:A:550:HIS:HD2	1.53	0.56
3:C:29:HIS:CD2	3:C:30:ILE:HG13	2.40	0.56
1:A:190:ARG:HD2	1:A:440:PRO:HB2	1.87	0.56
1:A:409:ARG:NH2	9:A:701:MLI:O9	2.37	0.56
1:A:129:ARG:NH1	1:A:130:ALA:H	2.04	0.56
2:B:69:ILE:O	2:B:159:ILE:HD11	2.05	0.55
1:A:246:GLN:HE22	1:A:600:ARG:HE	1.51	0.55
2:B:21:PRO:HG3	2:B:108:ILE:O	2.06	0.55
3:C:52:LEU:HD21	3:C:98:LEU:HA	1.89	0.54
1:A:91:LEU:HA	1:A:602:VAL:HG11	1.89	0.54
1:A:566:LYS:HB2	1:A:567:PRO:HD2	1.89	0.53
1:A:414:SER:O	1:A:418:LEU:HD13	2.09	0.53
1:A:516:TRP:HB3	2:B:60:THR:HG21	1.90	0.53
2:B:27:LYS:HE2	2:B:28:PRO:HD3	1.91	0.53
1:A:239:THR:CG2	1:A:588:VAL:HG13	2.39	0.53
1:A:157:SER:O	1:A:161:THR:HG23	2.08	0.53
1:A:401:CYS:C	1:A:403:SER:H	2.12	0.52
3:C:69:ASN:ND2	3:C:71:GLU:HB2	2.24	0.52
1:A:497:ILE:HG22	1:A:534:LEU:HD13	1.91	0.52
1:A:254:HIS:HD2	1:A:256:THR:N	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:ASN:HD21	3:C:71:GLU:HB2	1.75	0.52
1:A:246:GLN:HE22	1:A:600:ARG:HH21	1.59	0.51
1:A:127:TYR:OH	1:A:129:ARG:HD3	2.10	0.51
2:B:65:CYS:O	2:B:66:ARG:HG3	2.10	0.51
2:B:21:PRO:HD3	2:B:109:LYS:HG3	1.92	0.51
1:A:61:ALA:HA	5:A:700:FAD:C5X	2.41	0.51
2:B:178:TYR:CD1	2:B:214:ARG:HB2	2.46	0.51
2:B:208:ASP:HB2	2:B:209:PRO:CD	2.41	0.51
2:B:27:LYS:HB3	2:B:28:PRO:HD3	1.93	0.51
2:B:52:LYS:HA	2:B:56:ASP:O	2.10	0.51
2:B:74:ALA:O	2:B:102:LEU:HG	2.11	0.51
2:B:189:ARG:NH2	2:B:193:ASP:OD1	2.44	0.51
1:A:374:ASN:HB3	1:A:376:LYS:H	1.76	0.50
1:A:104:ALA:HB3	1:A:105:PRO:HD3	1.93	0.50
1:A:27:ALA:H	5:A:700:FAD:H4B	1.75	0.49
1:A:581:ARG:HH22	1:A:604:ASP:CG	2.15	0.49
1:A:66:ASN:ND2	1:A:411:GLY:O	2.41	0.49
3:C:57:SER:O	3:C:61:LEU:HB2	2.13	0.49
2:B:230:ASN:HD22	2:B:230:ASN:C	2.15	0.49
1:A:60:ALA:CB	5:A:700:FAD:HM72	2.41	0.49
3:C:104:ASN:HD22	3:C:107:ARG:HE	1.61	0.49
1:A:48:VAL:HG12	5:A:700:FAD:H2A	1.95	0.49
1:A:568:ILE:HG13	1:A:569:GLN:N	2.27	0.49
1:A:61:ALA:HA	5:A:700:FAD:C6	2.43	0.48
1:A:113:ASN:HD22	2:B:138:GLY:H	1.60	0.48
4:D:61:TYR:HA	11:D:1306:EPH:H52	1.95	0.48
1:A:130:ALA:HB2	1:A:145:HIS:CD2	2.48	0.48
1:A:29:GLY:N	1:A:58:THR:HG21	2.24	0.48
2:B:14:PHE:O	2:B:32:THR:HA	2.13	0.48
1:A:258:ILE:HD12	1:A:263:CYS:O	2.13	0.48
2:B:166:THR:O	2:B:166:THR:CG2	2.62	0.47
1:A:64:GLY:HA2	1:A:154:THR:HG21	1.95	0.47
1:A:298:ARG:HH22	1:A:409:ARG:NH2	2.13	0.47
1:A:342:SER:OG	1:A:353:VAL:HG21	2.14	0.47
2:B:129:LEU:HD11	2:B:195:ARG:CB	2.43	0.47
3:C:109:LEU:HD13	4:D:51:VAL:HG12	1.97	0.47
1:A:117:PRO:O	1:A:150:VAL:HG13	2.14	0.47
1:A:249:GLU:HB2	1:A:540:ALA:HB2	1.97	0.46
1:A:113:ASN:ND2	2:B:138:GLY:H	2.13	0.46
4:D:124:VAL:HG13	4:D:128:LYS:HB3	1.97	0.46
1:A:414:SER:O	1:A:417:ASP:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:HIS:CG	1:A:409:ARG:HG3	2.50	0.46
1:A:182:LEU:HD23	1:A:184:MET:HE1	1.97	0.46
1:A:114:TYR:CD2	1:A:165:ARG:HD2	2.50	0.46
1:A:415:LEU:HG	5:A:700:FAD:N3	2.28	0.46
1:A:554:ASP:HB2	1:A:555:PHE:CD2	2.51	0.46
2:B:69:ILE:O	2:B:159:ILE:CD1	2.64	0.45
1:A:353:VAL:CG1	1:A:358:ILE:HD11	2.44	0.45
3:C:62:SER:HB2	3:C:66:LEU:HD12	1.98	0.45
1:A:267:GLU:OE1	1:A:298:ARG:HD3	2.17	0.45
1:A:10:SER:C	1:A:12:GLN:H	2.19	0.45
2:B:64:SER:HB3	2:B:70:CYS:SG	2.56	0.45
2:B:188:TYR:OH	2:B:237:GLU:HG2	2.17	0.45
1:A:57:HIS:O	1:A:59:VAL:N	2.51	0.44
2:B:230:ASN:ND2	2:B:233:LYS:H	2.15	0.44
1:A:23:VAL:HG23	1:A:207:ALA:HB3	1.99	0.44
1:A:57:HIS:CE1	1:A:226:SER:HA	2.52	0.44
5:A:700:FAD:H9	5:A:700:FAD:H1'1	1.84	0.44
1:A:58:THR:HG22	5:A:700:FAD:O4'	2.17	0.44
1:A:457:LEU:O	1:A:509:THR:HG21	2.17	0.44
4:D:128:LYS:O	4:D:132:MET:HG3	2.17	0.44
1:A:270:ARG:HD2	1:A:294:ASP:O	2.18	0.44
1:A:556:LYS:HB3	1:A:556:LYS:HE2	1.85	0.44
4:D:58:PRO:HB3	11:D:1306:EPH:H28	2.00	0.44
2:B:103:PRO:O	2:B:166:THR:HG23	2.17	0.44
1:A:299:ASP:O	1:A:303:ARG:HB2	2.17	0.44
4:D:89:THR:HG23	4:D:102:LYS:NZ	2.33	0.43
2:B:44:VAL:HG11	2:B:77:ILE:HD12	2.00	0.43
1:A:174:PHE:HB3	1:A:177:TYR:CD1	2.53	0.43
1:A:461:ASN:ND2	1:A:508:LYS:HE3	2.34	0.43
1:A:464:ILE:O	1:A:508:LYS:N	2.51	0.43
2:B:172:TRP:HZ3	3:C:30:ILE:HG23	1.83	0.43
2:B:164:CYS:HB2	2:B:221:CYS:HB2	2.01	0.43
1:A:131:PHE:CD1	1:A:411:GLY:HA3	2.54	0.43
1:A:272:GLU:HB3	1:A:333:GLN:HE21	1.84	0.43
1:A:129:ARG:HA	1:A:129:ARG:HD2	1.54	0.42
1:A:200:GLY:HA3	1:A:514:MET:HB3	2.01	0.42
2:B:208:ASP:HB2	2:B:209:PRO:HD3	2.01	0.42
2:B:132:LYS:HG2	2:B:197:ASP:HB3	2.01	0.42
2:B:27:LYS:HB3	2:B:28:PRO:HD2	2.00	0.42
2:B:67:GLU:HB3	2:B:69:ILE:HD11	2.00	0.42
2:B:45:LEU:O	2:B:49:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:TYR:HA	1:A:504:LEU:HD23	2.01	0.42
2:B:165:SER:HA	2:B:181:PRO:HD2	2.02	0.42
1:A:374:ASN:HA	1:A:374:ASN:HD22	1.67	0.41
1:A:88:SER:HB2	1:A:406:GLY:HA3	2.02	0.41
1:A:52:PHE:CD1	1:A:53:PRO:HD2	2.56	0.41
2:B:198:PHE:HD2	2:B:201:GLU:HG3	1.86	0.41
3:C:46:ARG:HG2	10:C:1305:HEM:O2D	2.21	0.41
1:A:130:ALA:O	1:A:271:GLY:HA3	2.21	0.41
1:A:57:HIS:C	1:A:59:VAL:N	2.73	0.41
2:B:47:ALA:O	2:B:51:ILE:HG23	2.21	0.41
1:A:493:GLY:O	1:A:497:ILE:HG12	2.20	0.41
1:A:231:THR:HA	1:A:529:LEU:HD21	2.03	0.41
1:A:162:LEU:HA	1:A:162:LEU:HD23	1.96	0.41
1:A:29:GLY:HA3	1:A:418:LEU:HD23	2.03	0.41
2:B:20:ASP:HA	2:B:21:PRO:HD3	1.88	0.41
1:A:152:ASP:HB2	1:A:339:PRO:HD2	2.03	0.41
1:A:521:VAL:HA	1:A:524:LEU:HD12	2.02	0.41
3:C:104:ASN:ND2	3:C:107:ARG:HE	2.19	0.41
1:A:114:TYR:CE2	1:A:165:ARG:HD2	2.56	0.41
1:A:556:LYS:HD2	1:A:556:LYS:H	1.86	0.41
2:B:154:GLY:N	2:B:157:GLU:OE1	2.54	0.41
1:A:443:LYS:HB2	1:A:446:ALA:HB2	2.02	0.40
2:B:108:ILE:HD12	2:B:112:VAL:HG12	2.02	0.40
3:C:78:LYS:HA	3:C:82:LEU:HD21	2.03	0.40
2:B:16:ILE:HG21	2:B:59:LEU:HD11	2.04	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%)	573 (94%)	36 (6%)	2 (0%)	46	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	237/252 (94%)	225 (95%)	11 (5%)	1 (0%)	39	74
3	C	136/140 (97%)	129 (95%)	5 (4%)	2 (2%)	13	41
4	D	100/103 (97%)	95 (95%)	5 (5%)	0	100	100
All	All	1084/1117 (97%)	1022 (94%)	57 (5%)	5 (0%)	34	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	84	PRO
1	A	260	GLY
1	A	11	THR
2	B	175	GLY
3	C	81	CYS

### 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%)	457 (92%)	42 (8%)	14	37
2	B	214/220 (97%)	199 (93%)	15 (7%)	19	47
3	C	117/118 (99%)	108 (92%)	9 (8%)	16	41
4	D	76/76 (100%)	74 (97%)	2 (3%)	54	84
All	All	906/920 (98%)	838 (92%)	68 (8%)	17	43

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	44	ASN
1	A	58	THR
1	A	59	VAL
1	A	72	MET
1	A	74	GLU

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Mol	Chain	Res	Type
1	A	129	ARG
1	A	131	PHE
1	A	165	ARG
1	A	182	LEU
1	A	208	ARG
1	A	220	THR
1	A	264	LEU
1	A	294	ASP
1	A	306	THR
1	A	324	LEU
1	A	352	ASP
1	A	368	MET
1	A	374	ASN
1	A	384	ASN
1	A	403	SER
1	A	410	LEU
1	A	419	VAL
1	A	458	ARG
1	A	461	ASN
1	A	463	THR
1	A	485	ARG
1	A	488	SER
1	A	504	LEU
1	A	512	ARG
1	A	514	MET
1	A	534	LEU
1	A	541	GLU
1	A	554	ASP
1	A	556	LYS
1	A	561	GLU
1	A	569	GLN
1	A	572	GLN
1	A	588	VAL
1	A	591	LYS
1	A	597	LEU
1	A	605	LYS
2	B	51	ILE
2	B	63	ARG
2	B	66	ARG
2	B	69	ILE
2	B	86	THR
2	B	87	ARG

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Mol	Chain	Res	Type
2	B	88	ARG
2	B	134	GLU
2	B	146	ILE
2	B	159	ILE
2	B	189	ARG
2	B	192	ILE
2	B	214	ARG
2	B	220	ASN
2	B	230	ASN
3	C	13	GLU
3	C	23	ASN
3	C	26	LEU
3	C	30	ILE
3	C	31	THR
3	C	46	ARG
3	C	98	LEU
3	C	115	LYS
3	C	123	THR
4	D	78	LEU
4	D	134	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	113	ASN
1	A	145	HIS
1	A	246	GLN
1	A	254	HIS
1	A	374	ASN
1	A	384	ASN
1	A	408	ASN
1	A	461	ASN
1	A	474	GLN
1	A	550	HIS
1	A	571	GLN
1	A	572	GLN
1	A	579	HIS
2	B	38	ASN
2	B	121	GLN
2	B	174	ASN
2	B	186	GLN

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Mol	Chain	Res	Type
2	B	220	ASN
2	B	230	ASN
3	C	23	ASN
3	C	29	HIS
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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	FAD	A	700	1	48,58,58	1.26	6 (12%)	54,89,89	2.23	6 (11%)
9	MLI	A	701	-	0,6,6	0.00	-	0,7,7	0.00	-
6	FES	B	302	2	0,4,4	0.00	-	0,4,4	0.00	-
7	SF4	B	303	2	0,12,12	0.00	-	0,24,24	0.00	-
8	F3S	B	304	2	0,9,9	0.00	-	0,15,15	0.00	-
10	HEM	C	1305	3,4	30,50,50	2.09	9 (30%)	24,82,82	2.40	10 (41%)
12	N1M	D	1201	-	11,11,11	0.72	0	14,14,14	0.86	0
11	EPH	D	1306	-	42,43,48	1.79	8 (19%)	43,48,53	1.39	6 (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
5	FAD	A	700	1	-	0/30/50/50	0/6/6/6
9	MLI	A	701	-	-	0/0/4/4	0/0/0/0
6	FES	B	302	2	-	0/0/4/4	0/1/1/1
7	SF4	B	303	2	-	0/0/48/48	0/6/5/5
8	F3S	B	304	2	-	0/0/24/24	0/0/3/3
10	HEM	C	1305	3,4	-	0/10/54/54	0/0/8/8
12	N1M	D	1201	-	-	0/6/6/6	0/1/1/1
11	EPH	D	1306	-	-	0/47/47/52	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1305	HEM	C3B-C4B	-7.03	1.45	1.51
10	C	1305	HEM	C3D-C4D	-4.98	1.45	1.51
10	C	1305	HEM	C2C-C1C	-3.34	1.46	1.52
10	C	1305	HEM	C2D-C1D	-2.05	1.45	1.51
10	C	1305	HEM	C2B-C1B	-2.05	1.45	1.51
5	A	700	FAD	C5X-N5	2.07	1.38	1.35
10	C	1305	HEM	C3C-CAC	2.09	1.55	1.51
10	C	1305	HEM	FE-NB	2.18	2.09	1.97
10	C	1305	HEM	C1C-NC	2.21	1.38	1.36
10	C	1305	HEM	CAA-C2A	2.24	1.55	1.52
11	D	1306	EPH	P1-O7	2.37	1.59	1.51
5	A	700	FAD	C1'-N10	2.42	1.51	1.48
5	A	700	FAD	C2A-N1A	2.52	1.38	1.33
5	A	700	FAD	C4-N3	3.00	1.38	1.33
11	D	1306	EPH	C15-C16	3.16	1.53	1.29
5	A	700	FAD	C4X-N5	3.55	1.38	1.33
5	A	700	FAD	C2A-N3A	3.58	1.38	1.32
11	D	1306	EPH	C13-C12	3.70	1.53	1.31
11	D	1306	EPH	C25-C24	3.72	1.53	1.31
11	D	1306	EPH	C29-C28	3.76	1.53	1.31
11	D	1306	EPH	O1-C3	4.19	1.46	1.34
11	D	1306	EPH	O2-C4	4.24	1.46	1.33
11	D	1306	EPH	P1-O6	5.74	1.79	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	FAD	N3A-C2A-N1A	-12.60	119.24	128.89
5	A	700	FAD	P-O3P-PA	-4.58	119.86	132.73
10	C	1305	HEM	C3B-CAB-CBB	-4.03	118.27	124.46
11	D	1306	EPH	C30-C29-C28	-3.32	111.86	127.06
10	C	1305	HEM	C3C-CAC-CBC	-3.26	119.45	124.46
5	A	700	FAD	C4X-C4-N3	-2.40	120.30	123.59
10	C	1305	HEM	CMA-C3A-C4A	-2.24	124.66	128.36
11	D	1306	EPH	C14-C13-C12	-2.09	112.09	125.00
11	D	1306	EPH	C14-C15-C16	-2.08	112.14	125.00
11	D	1306	EPH	C11-C12-C13	-2.02	111.27	125.34
10	C	1305	HEM	C2D-C3D-C4D	2.01	104.90	101.50
5	A	700	FAD	C5X-C9A-N10	2.18	119.27	117.62
10	C	1305	HEM	C3B-C4B-CHC	2.65	126.89	123.16
11	D	1306	EPH	O2-C4-C18	2.76	120.32	111.90
10	C	1305	HEM	CMD-C2D-C3D	2.86	126.99	114.35
5	A	700	FAD	C4X-N5-C5X	3.68	121.00	116.76
10	C	1305	HEM	CMC-C2C-C3C	3.77	125.95	116.53
10	C	1305	HEM	CMB-C2B-C3B	3.99	126.48	116.53
11	D	1306	EPH	O1-C3-C5	4.37	121.03	111.53
10	C	1305	HEM	CAD-C3D-C4D	4.40	128.00	112.47
10	C	1305	HEM	CAD-C3D-C2D	4.83	127.10	113.22
5	A	700	FAD	C4-N3-C2	5.43	119.94	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	700	FAD	16	0
9	A	701	MLI	1	0
10	C	1305	HEM	3	0
11	D	1306	EPH	2	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	613/622 (98%)	0.11	19 (3%)	52 46	56, 75, 106, 131	0
2	B	239/252 (94%)	0.18	13 (5%)	29 24	56, 70, 105, 126	0
3	C	138/140 (98%)	0.07	12 (8%)	13 8	56, 79, 126, 138	0
4	D	102/103 (99%)	0.10	5 (4%)	33 28	61, 79, 99, 115	0
All	All	1092/1117 (97%)	0.12	49 (4%)	37 31	56, 75, 107, 138	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	35	SER	8.5
2	B	11	ILE	4.6
1	A	224	CYS	3.6
3	C	86	LEU	3.3
1	A	230	SER	3.2
3	C	87	ILE	3.1
2	B	37	LEU	3.1
1	A	225	THR	3.0
2	B	93	LEU	3.0
1	A	317	PRO	2.9
3	C	88	TYR	2.9
1	A	326	LEU	2.9
2	B	94	ASP	2.8
3	C	84	PRO	2.8
1	A	575	PRO	2.7
1	A	214	THR	2.7
3	C	85	THR	2.7
1	A	277	ILE	2.6
1	A	227	ALA	2.6
1	A	226	SER	2.6
3	C	81	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	36	ASP	2.6
2	B	246	LYS	2.5
1	A	216	GLY	2.5
2	B	65	CYS	2.4
1	A	325	GLN	2.4
1	A	414	SER	2.4
2	B	35	ILE	2.4
3	C	82	LEU	2.3
3	C	143	MET	2.3
2	B	34	GLU	2.3
1	A	61	ALA	2.3
2	B	70	CYS	2.3
2	B	233	LYS	2.2
4	D	128	LYS	2.2
3	C	63	ALA	2.2
4	D	62	LEU	2.2
1	A	327	HIS	2.1
3	C	80	LEU	2.1
2	B	9	PRO	2.1
1	A	229	THR	2.1
1	A	155	GLY	2.1
3	C	140	LEU	2.1
4	D	124	VAL	2.1
4	D	36	SER	2.1
1	A	263	CYS	2.0
2	B	13	LYS	2.0
3	C	142	ALA	2.0
1	A	397	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 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	EPH	D	1306	44/49	0.77	0.61	4.68	106,118,123,123	0
9	MLI	A	701	7/7	0.94	0.32	1.83	79,81,82,82	0
10	HEM	C	1305	43/43	0.96	0.21	1.36	62,64,70,72	0
5	FAD	A	700	53/53	0.91	0.33	0.82	47,60,75,75	0
7	SF4	B	303	8/8	0.99	0.17	-0.28	59,59,60,60	0
8	F3S	B	304	7/7	0.99	0.16	-0.38	66,67,70,70	0
6	FES	B	302	4/4	0.98	0.21	-0.96	61,62,64,64	0
12	N1M	D	1201	11/11	0.99	0.15	-1.41	80,80,81,84	0

## 6.5 Other polymers

There are no such residues in this entry.