



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:04 PM GMT

PDB ID : 3SFE
Title : crystal structure of porcine mitochondrial respiratory complex II bound with oxaloacetate and thiabendazole
Authors : Zhou, Q.J.; Zhai, Y.J.; Liu, M.; Sun, F.
Deposited on : 2011-06-13
Resolution : 2.81 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

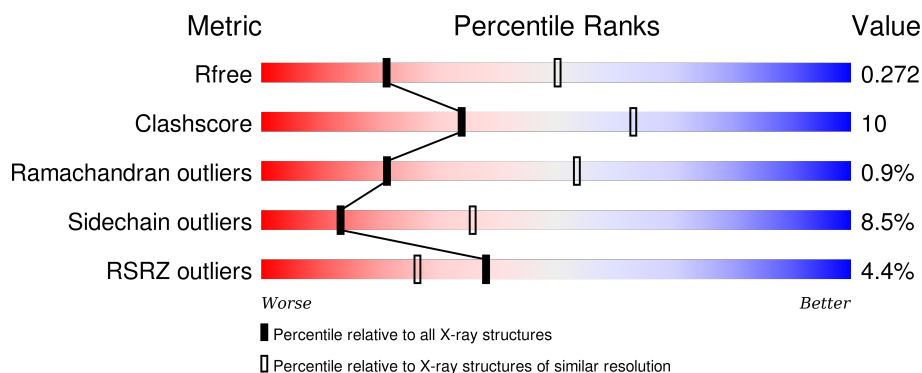
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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. 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>5%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
2	B	252	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>• 5%</div> </div> </div>
3	C	140	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
4	D	103	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>20%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	OAA	A	701	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 8687 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	1	0
			4737	2959	851	895	32			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	0	0	0
			1927	1217	327	361	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	139	Total	C	N	O	S	0	0	0
			1068	697	180	184	7			

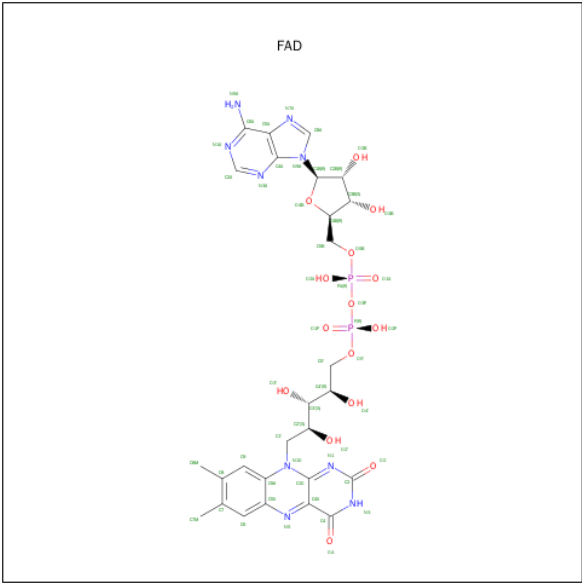
- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

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:

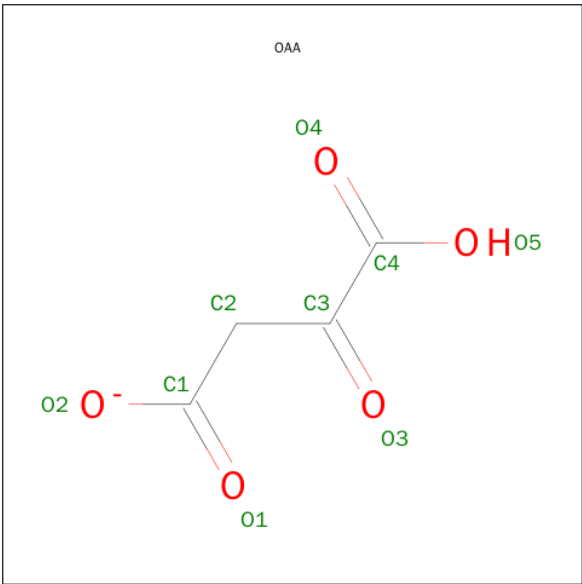
Chain	Residue	Modelled	Actual	Comment	Reference
D	100	ALA	VAL	SEE REMARK 999	UNP A5GZW8

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



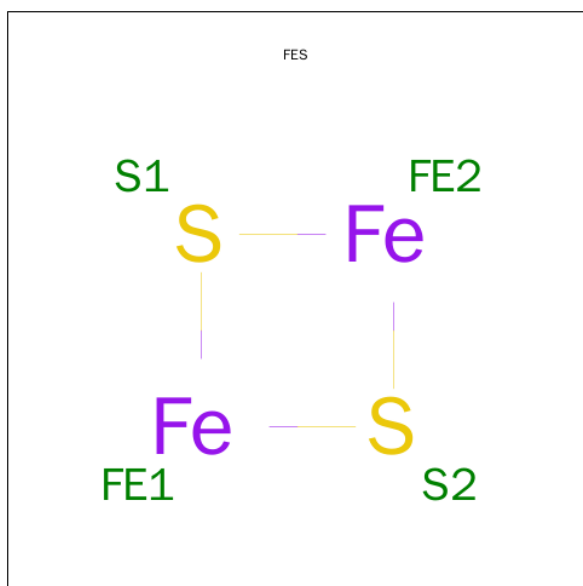
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	53	27	9	15	2	0	0

- Molecule 6 is OXALOACETATE ION (three-letter code: OAA) (formula: C₄H₃O₅).



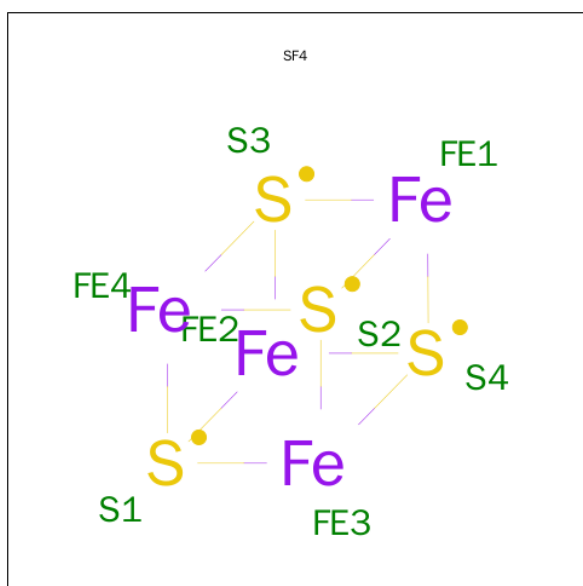
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	4	5		

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



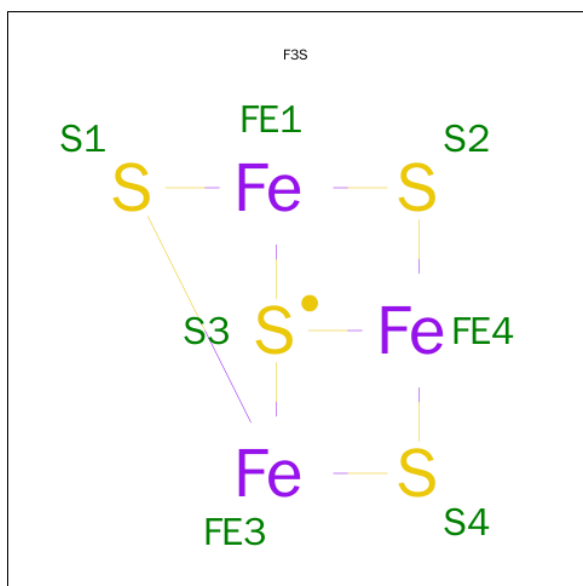
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		

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



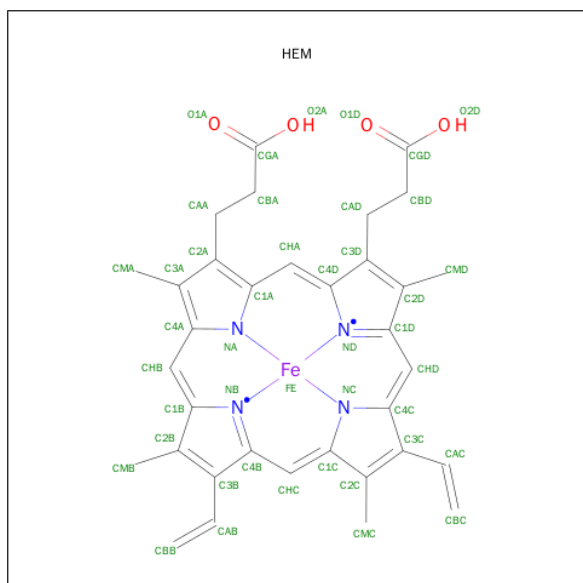
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		

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



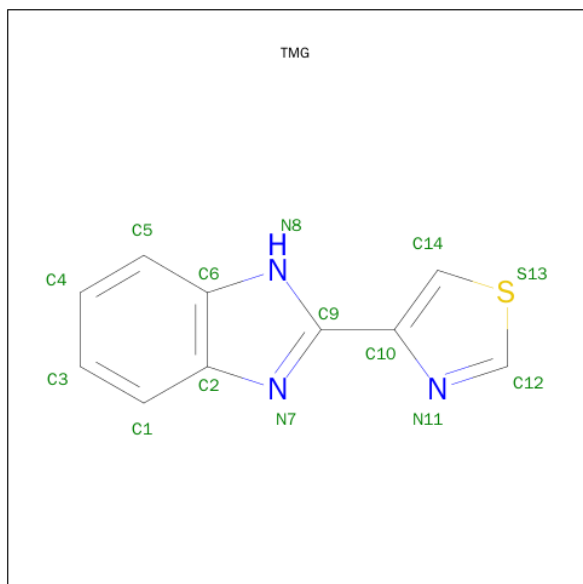
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		

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



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

- Molecule 11 is 2-(1,3-THIAZOL-4-YL)-1H-BENZIMIDAZOLE (three-letter code: TMG) (formula: C₁₀H₇N₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	N	S		
			14	10	3	1		
							0	0

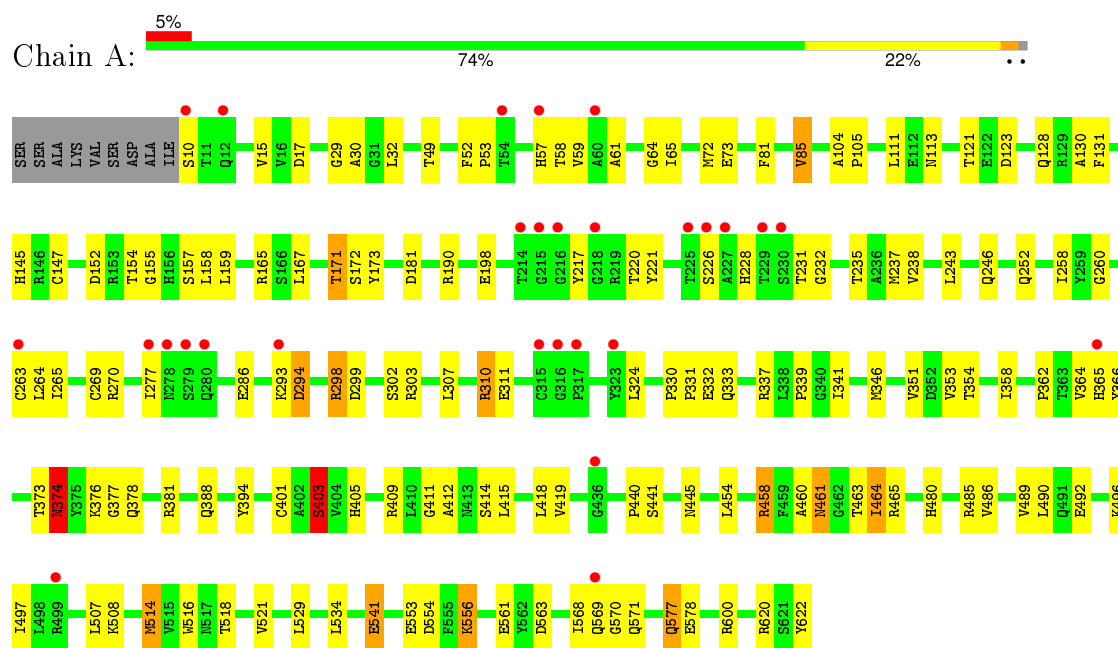
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	22	Total	O		
			22	22	0	0
12	B	12	Total	O		
			12	12	0	0
12	C	10	Total	O		
			10	10	0	0
12	D	8	Total	O		
			8	8	0	0

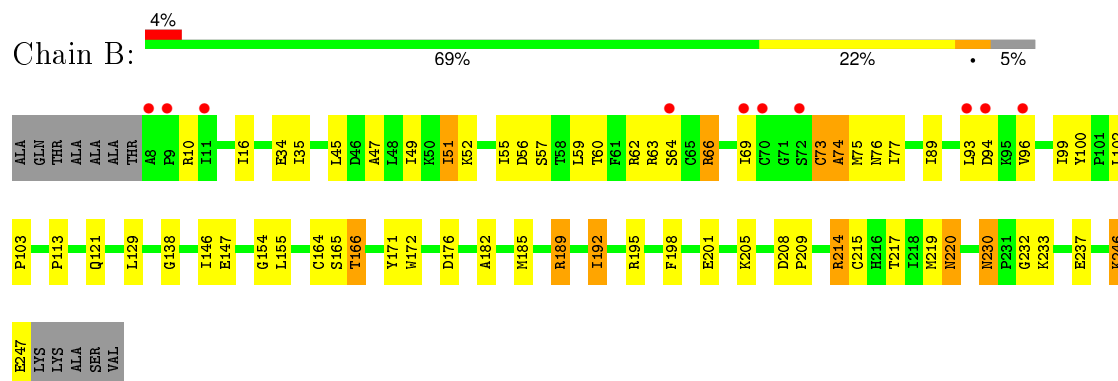
3 Residue-property plots

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.

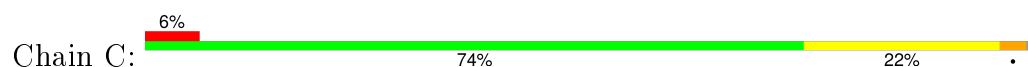
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

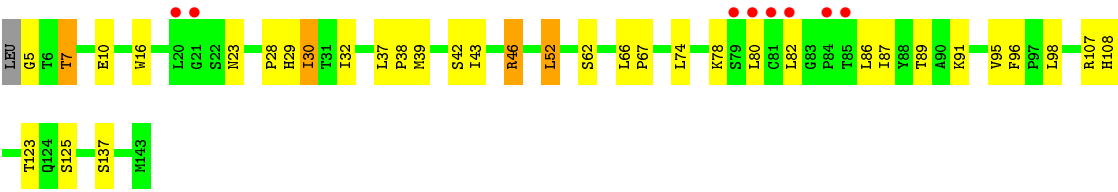


- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

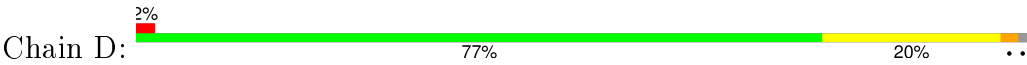


- Molecule 3: Succinate dehydrogenase cytochrome b560 subunit, mitochondrial





• 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, α , β , γ	70.71Å 83.42Å 294.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.81 45.21 – 2.81	Depositor EDS
% Data completeness (in resolution range)	78.1 (50.00-2.81) 78.2 (45.21-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.31 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.214 , 0.270 0.215 , 0.272	Depositor DCC
R_{free} test set	1717 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 34068 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8687	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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, 0.375 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: OAA, SF4, F3S, FES, TMG, 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	0.38	0/4839	0.56	0/6545
2	B	0.39	0/1969	0.53	0/2656
3	C	0.38	0/1095	0.52	0/1488
4	D	0.35	0/784	0.49	0/1066
All	All	0.38	0/8687	0.54	0/11755

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	4737	0	4631	103	0
2	B	1927	0	1904	46	0
3	C	1068	0	1107	23	0
4	D	765	0	773	12	0
5	A	53	0	31	12	0
6	A	9	0	0	4	0
7	B	4	0	0	0	0
8	B	8	0	0	0	0
9	B	7	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	43	0	30	0	0
11	C	14	0	7	2	0
12	A	22	0	0	0	0
12	B	12	0	0	0	0
12	C	10	0	0	0	0
12	D	8	0	0	0	0
All	All	8687	0	8483	172	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 (172) 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	1.67	1.07
1:A:310:ARG:HG3	1:A:310:ARG:HH11	1.29	0.92
1:A:374:ASN:HB3	1:A:376:LYS:H	1.36	0.88
1:A:57:HIS:CE1	5:A:700:FAD:HM82	2.11	0.85
1:A:577:GLN:HE21	1:A:577:GLN:H	1.23	0.84
1:A:29:GLY:H	1:A:58:THR:HG21	1.47	0.77
1:A:152:ASP:HB2	1:A:339:PRO:HD2	1.71	0.72
1:A:298:ARG:HH22	6:A:701:OAA:C1	2.02	0.71
1:A:373:THR:HG22	1:A:374:ASN:O	1.90	0.71
4:D:53:LEU:HD11	4:D:76:LEU:HD12	1.73	0.70
1:A:57:HIS:NE2	5:A:700:FAD:HM81	2.05	0.69
1:A:264:LEU:CB	5:A:700:FAD:HM73	2.22	0.69
2:B:129:LEU:HD11	2:B:195:ARG:HB2	1.75	0.69
1:A:181:ASP:HA	1:A:237:MET:HG2	1.74	0.68
4:D:72:LEU:O	4:D:76:LEU:HB2	1.93	0.68
2:B:246:LYS:O	2:B:247:GLU:HB2	1.92	0.68
1:A:298:ARG:NH2	6:A:701:OAA:C1	2.57	0.67
1:A:264:LEU:HB3	5:A:700:FAD:HM73	1.77	0.67
4:D:60:ALA:HA	4:D:68:MET:HG2	1.78	0.66
1:A:190:ARG:HD2	1:A:440:PRO:HB2	1.77	0.65
1:A:563:ASP:H	1:A:571:GLN:HE22	1.46	0.64
2:B:52:LYS:HD2	2:B:57:SER:HA	1.78	0.64
3:C:46:ARG:HE	4:D:87:VAL:HG22	1.62	0.63
1:A:58:THR:HG23	5:A:700:FAD:O1A	1.97	0.63
2:B:215:CYS:HA	9:B:304:F3S:S1	2.38	0.63
2:B:164:CYS:SG	2:B:182:ALA:HB2	2.39	0.62
1:A:486:VAL:HG22	1:A:553:GLU:HG3	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASP:O	1:A:303:ARG:HB2	2.00	0.62
1:A:264:LEU:HD22	5:A:700:FAD:H6	1.81	0.61
1:A:61:ALA:HB3	1:A:155:GLY:HA3	1.81	0.61
3:C:46:ARG:NE	4:D:87:VAL:HG22	2.16	0.61
1:A:569:GLN:C	1:A:571:GLN:H	2.03	0.61
2:B:51:ILE:HD11	2:B:59:LEU:HD22	1.83	0.60
2:B:230:ASN:ND2	2:B:233:LYS:H	1.99	0.60
1:A:58:THR:HG22	5:A:700:FAD:O4'	2.01	0.60
1:A:310:ARG:CG	1:A:310:ARG:HH11	2.12	0.60
1:A:264:LEU:HD22	5:A:700:FAD:C6	2.33	0.59
1:A:190:ARG:CD	1:A:440:PRO:HB2	2.33	0.58
2:B:103:PRO:HD2	2:B:166:THR:HG23	1.83	0.58
2:B:164:CYS:SG	2:B:165:SER:N	2.77	0.58
1:A:310:ARG:HG3	1:A:310:ARG:NH1	2.07	0.57
2:B:219:MET:CE	2:B:232:GLY:HA3	2.34	0.57
1:A:171:THR:HB	1:A:173:TYR:CE1	2.39	0.57
3:C:52:LEU:HD21	3:C:98:LEU:HA	1.85	0.57
2:B:198:PHE:CD2	2:B:201:GLU:HG3	2.40	0.57
1:A:458:ARG:NH2	1:A:514:MET:HG2	2.20	0.57
2:B:155:LEU:HD12	2:B:192:ILE:HD11	1.86	0.56
1:A:81:PHE:O	1:A:85:VAL:HG12	2.06	0.56
1:A:246:GLN:NE2	1:A:600:ARG:HE	2.04	0.56
1:A:405:HIS:ND1	1:A:409:ARG:HG3	2.21	0.55
1:A:59:VAL:HB	1:A:159:LEU:HD23	1.89	0.55
4:D:49:VAL:HG11	4:D:78:LEU:HD13	1.88	0.54
1:A:104:ALA:HB3	1:A:105:PRO:HD3	1.90	0.54
3:C:37:LEU:HB3	3:C:38:PRO:HD3	1.89	0.54
2:B:214:ARG:NH2	4:D:86:GLN:OE1	2.41	0.54
1:A:258:ILE:HG13	1:A:265:ILE:HD11	1.89	0.53
2:B:75:MET:HG3	2:B:77:ILE:HD11	1.89	0.53
1:A:72:MET:HG2	1:A:128:GLN:HB2	1.89	0.53
1:A:409:ARG:HH22	6:A:701:OAA:C1	2.22	0.53
2:B:208:ASP:HB2	2:B:209:PRO:HD2	1.91	0.53
3:C:28:PRO:HB2	3:C:32:ILE:HG12	1.89	0.52
1:A:49:THR:HG1	5:A:700:FAD:HO2A	1.58	0.52
2:B:198:PHE:HD2	2:B:201:GLU:HG3	1.74	0.52
1:A:246:GLN:HE22	1:A:600:ARG:HE	1.56	0.52
1:A:353:VAL:HG12	1:A:358:ILE:HD11	1.92	0.52
1:A:113:ASN:ND2	2:B:138:GLY:H	2.07	0.52
1:A:518:THR:HA	1:A:521:VAL:HG22	1.91	0.52
1:A:217:TYR:HB3	1:A:232:GLY:HA3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:GLU:O	1:A:496:LYS:HB2	2.10	0.51
1:A:111:LEU:HD11	1:A:419:VAL:HG21	1.92	0.51
1:A:415:LEU:HG	5:A:700:FAD:C2	2.40	0.51
3:C:78:LYS:HA	3:C:82:LEU:HD11	1.93	0.51
1:A:158:LEU:HD23	1:A:415:LEU:HD22	1.91	0.51
1:A:172:SER:HG	3:C:5:GLY:N	2.07	0.51
2:B:219:MET:HE2	2:B:232:GLY:HA3	1.92	0.51
1:A:220:THR:HG23	1:A:529:LEU:HD22	1.92	0.51
4:D:43:TRP:O	4:D:47:ARG:HG2	2.11	0.50
1:A:401:CYS:C	1:A:403:SER:H	2.12	0.50
1:A:57:HIS:CE1	1:A:226:SER:HA	2.47	0.50
2:B:52:LYS:HA	2:B:56:ASP:O	2.11	0.49
1:A:480:HIS:HD2	1:A:489:VAL:O	1.95	0.49
3:C:46:ARG:NH2	11:C:1:TMG:H14	2.28	0.49
2:B:230:ASN:HD22	2:B:230:ASN:C	2.16	0.49
1:A:569:GLN:C	1:A:571:GLN:N	2.66	0.49
1:A:231:THR:HA	1:A:529:LEU:HD21	1.94	0.48
1:A:228:HIS:NE2	2:B:66:ARG:HG2	2.28	0.48
1:A:298:ARG:NH2	1:A:411:GLY:HA2	2.28	0.48
1:A:190:ARG:NH1	1:A:441:SER:O	2.47	0.48
1:A:374:ASN:HB2	1:A:378:GLN:H	1.79	0.48
2:B:102:LEU:HD22	2:B:166:THR:HG21	1.96	0.48
1:A:497:ILE:HG22	1:A:534:LEU:HD13	1.96	0.48
1:A:374:ASN:HB3	1:A:376:LYS:N	2.17	0.47
2:B:230:ASN:ND2	2:B:233:LYS:HB3	2.29	0.47
1:A:310:ARG:NH1	1:A:310:ARG:CG	2.75	0.47
1:A:414:SER:O	1:A:418:LEU:HD13	2.15	0.47
4:D:123:ASP:OD1	4:D:124:VAL:HG23	2.14	0.47
1:A:264:LEU:HD13	1:A:365:HIS:CE1	2.49	0.47
3:C:74:LEU:HD12	4:D:132:MET:HE2	1.95	0.47
1:A:464:ILE:O	1:A:508:LYS:N	2.48	0.47
1:A:490:LEU:HD13	1:A:541:GLU:HA	1.96	0.47
2:B:209:PRO:O	2:B:214:ARG:NH1	2.47	0.46
2:B:76:ASN:HB3	2:B:100:TYR:HB2	1.97	0.46
1:A:64:GLY:HA2	1:A:154:THR:HG21	1.97	0.46
1:A:415:LEU:HA	1:A:418:LEU:HD22	1.97	0.46
2:B:198:PHE:O	2:B:201:GLU:HG2	2.15	0.46
1:A:458:ARG:HH22	1:A:514:MET:HG2	1.80	0.46
2:B:121:GLN:NE2	2:B:171:TYR:OH	2.47	0.46
1:A:113:ASN:HD22	2:B:138:GLY:H	1.63	0.46
2:B:47:ALA:O	2:B:51:ILE:HG23	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:ARG:HA	2:B:214:ARG:NE	2.30	0.45
1:A:461:ASN:HD22	1:A:508:LYS:HE3	1.81	0.45
4:D:92:VAL:CG1	4:D:97:LEU:HB3	2.47	0.45
1:A:72:MET:HE2	1:A:121:THR:HG21	1.99	0.45
2:B:155:LEU:CD1	2:B:192:ILE:HD11	2.47	0.45
3:C:7:THR:HB	3:C:10:GLU:H	1.82	0.44
1:A:514:MET:HA	1:A:514:MET:HE3	1.98	0.44
1:A:516:TRP:HB3	2:B:60:THR:HG21	1.99	0.44
1:A:252:GLN:HB3	1:A:366:TYR:HB3	1.99	0.44
1:A:307:LEU:O	1:A:311:GLU:HG2	2.18	0.44
2:B:129:LEU:HD11	2:B:195:ARG:CB	2.45	0.43
1:A:221:TYR:CG	1:A:364:VAL:HG21	2.53	0.43
1:A:30:ALA:H	1:A:418:LEU:HG	1.83	0.43
1:A:130:ALA:HB2	1:A:145:HIS:CD2	2.53	0.43
3:C:29:HIS:HD2	3:C:30:ILE:HD12	1.84	0.43
3:C:96:PHE:HA	3:C:137:SER:OG	2.18	0.43
2:B:45:LEU:O	2:B:49:ILE:HG12	2.18	0.43
3:C:91:LYS:O	3:C:95:VAL:HG23	2.19	0.43
2:B:51:ILE:HA	2:B:55:ILE:HG12	2.00	0.43
1:A:72:MET:CE	1:A:121:THR:HG21	2.49	0.43
1:A:553:GLU:O	1:A:556:LYS:HE3	2.18	0.43
3:C:82:LEU:HB3	3:C:87:ILE:HD13	2.00	0.42
1:A:238:VAL:HG13	1:A:243:LEU:HB2	2.02	0.42
2:B:62:ARG:NH1	2:B:113:PRO:HD2	2.35	0.42
3:C:107:ARG:HD2	3:C:125:SER:HB2	2.00	0.42
3:C:62:SER:HB2	3:C:66:LEU:HD12	2.00	0.42
2:B:155:LEU:HD13	2:B:189:ARG:HA	2.01	0.42
1:A:330:PRO:HA	1:A:331:PRO:HD3	1.85	0.42
2:B:10:ARG:HG2	2:B:93:LEU:HD21	2.02	0.42
4:D:57:LEU:HB2	4:D:58:PRO:CD	2.50	0.42
2:B:154:GLY:O	2:B:185:MET:HE1	2.20	0.42
2:B:16:ILE:HG12	2:B:99:ILE:HB	2.03	0.41
1:A:269:CYS:SG	1:A:341:ILE:HD13	2.60	0.41
1:A:286:GLU:HG3	1:A:293:LYS:HE2	2.02	0.41
1:A:460:ALA:HB1	1:A:507:LEU:O	2.19	0.41
1:A:373:THR:HG23	1:A:377:GLY:HA2	2.02	0.41
1:A:563:ASP:H	1:A:571:GLN:NE2	2.15	0.41
1:A:171:THR:HB	1:A:173:TYR:HE1	1.82	0.41
1:A:258:ILE:HD13	1:A:263:CYS:HB2	2.01	0.41
1:A:346:MET:HA	1:A:351:VAL:H	1.85	0.41
1:A:52:PHE:CD1	1:A:53:PRO:HD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:SER:HB2	1:A:362:PRO:HB3	2.03	0.41
1:A:411:GLY:O	1:A:412:ALA:HB3	2.20	0.41
3:C:42:SER:HB2	11:C:1:TMG:N11	2.35	0.41
2:B:220:ASN:HD21	3:C:39:MET:HE2	1.86	0.41
2:B:102:LEU:HB3	2:B:166:THR:HG21	2.02	0.41
1:A:217:TYR:HB3	1:A:232:GLY:CA	2.51	0.41
3:C:87:ILE:O	3:C:91:LYS:HB3	2.20	0.41
1:A:270:ARG:HD2	1:A:294:ASP:O	2.21	0.41
1:A:264:LEU:HB2	5:A:700:FAD:HM73	1.98	0.41
1:A:374:ASN:HA	1:A:374:ASN:HD22	1.65	0.41
1:A:128:GLN:HA	1:A:147:CYS:O	2.20	0.41
2:B:73:CYS:HB2	2:B:74:ALA:H	1.73	0.41
2:B:176:ASP:HB3	3:C:16:TRP:CZ2	2.56	0.41
2:B:35:ILE:HD11	2:B:51:ILE:HG22	2.03	0.41
1:A:333:GLN:HG2	1:A:337:ARG:HG3	2.02	0.41
1:A:264:LEU:HD11	6:A:701:OAA:O3	2.21	0.40
1:A:577:GLN:NE2	1:A:577:GLN:H	2.04	0.40
1:A:620:ARG:HE	1:A:622:TYR:HE1	1.68	0.40
1:A:378:GLN:HG2	1:A:394:TYR:CE2	2.57	0.40
3:C:28:PRO:HB2	3:C:32:ILE:CG1	2.52	0.40
3:C:66:LEU:HA	3:C:67:PRO:HD3	1.90	0.40
2:B:172:TRP:HZ3	3:C:30:ILE:HG22	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	612/622 (98%)	565 (92%)	42 (7%)	5 (1%)	24 56
2	B	238/252 (94%)	217 (91%)	18 (8%)	3 (1%)	15 42
3	C	137/140 (98%)	128 (93%)	8 (6%)	1 (1%)	26 60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	100/103 (97%)	92 (92%)	7 (7%)	1 (1%)	19	51
All	All	1087/1117 (97%)	1002 (92%)	75 (7%)	10 (1%)	21	53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	86	LEU
1	A	374	ASN
2	B	73	CYS
1	A	403	SER
2	B	74	ALA
4	D	37	LYS
1	A	260	GLY
1	A	568	ILE
2	B	64	SER
1	A	570	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	500/506 (99%)	459 (92%)	41 (8%)	14	38
2	B	214/221 (97%)	194 (91%)	20 (9%)	11	31
3	C	117/118 (99%)	107 (92%)	10 (8%)	13	36
4	D	76/76 (100%)	70 (92%)	6 (8%)	15	39
All	All	907/921 (98%)	830 (92%)	77 (8%)	13	36

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	15	VAL
1	A	17	ASP
1	A	32	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	65	ILE
1	A	73	GLU
1	A	85	VAL
1	A	123	ASP
1	A	131	PHE
1	A	157	SER
1	A	165	ARG
1	A	167	LEU
1	A	171	THR
1	A	198	GLU
1	A	235	THR
1	A	277	ILE
1	A	294	ASP
1	A	298	ARG
1	A	310	ARG
1	A	324	LEU
1	A	332	GLU
1	A	354	THR
1	A	374	ASN
1	A	381	ARG
1	A	388	GLN
1	A	403	SER
1	A	445	ASN
1	A	454	LEU
1	A	458	ARG
1	A	461	ASN
1	A	463	THR
1	A	464	ILE
1	A	465	ARG
1	A	485	ARG
1	A	514	MET
1	A	541	GLU
1	A	554	ASP
1	A	556	LYS
1	A	561	GLU
1	A	577	GLN
1	A	578	GLU
2	B	34	GLU
2	B	51	ILE
2	B	63	ARG
2	B	66	ARG
2	B	69	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	89	ILE
2	B	94	ASP
2	B	96	VAL
2	B	146	ILE
2	B	147	GLU
2	B	166	THR
2	B	189	ARG
2	B	192	ILE
2	B	205	LYS
2	B	214	ARG
2	B	217	THR
2	B	220	ASN
2	B	230	ASN
2	B	237	GLU
2	B	246	LYS
3	C	7	THR
3	C	23	ASN
3	C	30	ILE
3	C	43	ILE
3	C	46	ARG
3	C	52	LEU
3	C	80	LEU
3	C	89	THR
3	C	108	HIS
3	C	123	THR
4	D	47	ARG
4	D	52	LEU
4	D	78	LEU
4	D	98	GLN
4	D	134	TRP
4	D	136	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	384	ASN
1	A	461	ASN
1	A	474	GLN
1	A	480	HIS
1	A	506	HIS
1	A	550	HIS
1	A	571	GLN
1	A	577	GLN
1	A	579	HIS
2	B	31	GLN
2	B	39	ASN
2	B	92	ASN
2	B	121	GLN
2	B	220	ASN
2	B	230	ASN
3	C	17	ASN
3	C	29	HIS
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 carbohydrates 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$
5	FAD	A	700	1	48,58,58	1.11	4 (8%)	54,89,89	2.08	11 (20%)
6	OAA	A	701	-	2,8,8	20.06	2 (100%)	2,10,10	22.63	1 (50%)
7	FES	B	302	2	0,4,4	0.00	-	0,4,4	0.00	-
8	SF4	B	303	2	0,12,12	0.00	-	0,24,24	0.00	-
9	F3S	B	304	2	0,9,9	0.00	-	0,15,15	0.00	-
11	TMG	C	1	-	13,16,16	1.06	1 (7%)	8,22,22	3.19	2 (25%)
10	HEM	C	1305	3,4	30,50,50	4.15	15 (50%)	24,82,82	2.59	9 (37%)

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
6	OAA	A	701	-	-	0/2/8/8	0/0/0/0
7	FES	B	302	2	-	0/0/4/4	0/1/1/1
8	SF4	B	303	2	-	0/0/48/48	0/6/5/5
9	F3S	B	304	2	-	0/0/24/24	0/0/3/3
11	TMG	C	1	-	-	0/0/4/4	0/3/3/3
10	HEM	C	1305	3,4	-	0/10/54/54	0/0/8/8

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	OAA	C2-C3	-27.74	1.25	1.51
10	C	1305	HEM	C3B-C4B	-15.02	1.38	1.51
10	C	1305	HEM	C3D-C4D	-9.74	1.39	1.51
10	C	1305	HEM	C2D-C3D	-4.98	1.39	1.54
10	C	1305	HEM	C2D-C1D	-3.75	1.39	1.51
10	C	1305	HEM	C2B-C1B	-3.73	1.39	1.51
11	C	1	TMG	C14-S13	2.01	1.73	1.70
10	C	1305	HEM	FE-ND	2.17	2.09	1.97
10	C	1305	HEM	FE-NB	2.22	2.09	1.97
5	A	700	FAD	C9A-N10	2.41	1.42	1.38
10	C	1305	HEM	C1A-CHA	2.90	1.47	1.39
5	A	700	FAD	C10-N10	3.06	1.42	1.39
10	C	1305	HEM	C4A-CHB	3.10	1.48	1.39
5	A	700	FAD	C8-C7	3.24	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1305	HEM	CHD-C1D	3.44	1.48	1.38
10	C	1305	HEM	FE-NC	3.50	2.09	1.95
10	C	1305	HEM	CHC-C4B	3.50	1.48	1.38
5	A	700	FAD	C9A-C5X	3.65	1.50	1.42
10	C	1305	HEM	C2A-C3A	3.71	1.48	1.37
10	C	1305	HEM	CHD-C4C	5.33	1.48	1.36
10	C	1305	HEM	CHC-C1C	5.33	1.48	1.36
6	A	701	OAA	O3-C3	5.93	1.32	1.22

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	FAD	N3A-C2A-N1A	-9.20	121.85	128.89
11	C	1	TMG	C10-C14-S13	-8.57	101.36	111.83
10	C	1305	HEM	CAA-CBA-CGA	-3.93	105.53	112.75
10	C	1305	HEM	C3B-CAB-CBB	-3.60	118.94	124.46
5	A	700	FAD	C2B-C1B-N9A	-2.99	109.72	114.29
5	A	700	FAD	C4A-C5A-N7A	-2.69	107.00	109.48
5	A	700	FAD	C4-C4X-C10	-2.43	118.39	119.94
5	A	700	FAD	C4X-C4-N3	-2.37	120.34	123.59
10	C	1305	HEM	C3C-CAC-CBC	-2.18	121.11	124.46
5	A	700	FAD	P-O3P-PA	-2.04	126.99	132.73
5	A	700	FAD	C1'-C2'-C3'	2.18	116.04	109.82
5	A	700	FAD	C4B-O4B-C1B	2.35	112.31	109.72
5	A	700	FAD	O4B-C1B-N9A	2.57	113.48	108.10
10	C	1305	HEM	C2C-C1C-NC	2.73	114.82	110.21
11	C	1	TMG	C14-S13-C12	2.79	98.05	92.37
10	C	1305	HEM	CMD-C2D-C3D	2.97	127.50	114.35
10	C	1305	HEM	CAD-C3D-C4D	4.32	127.72	112.47
5	A	700	FAD	C4X-N5-C5X	4.78	122.27	116.76
10	C	1305	HEM	CMC-C2C-C3C	4.86	128.66	116.53
10	C	1305	HEM	CMB-C2B-C3B	4.98	128.95	116.53
10	C	1305	HEM	CAD-C3D-C2D	5.15	128.03	113.22
5	A	700	FAD	C4-N3-C2	6.64	120.99	115.25
6	A	701	OAA	C1-C2-C3	31.98	173.74	115.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	700	FAD	12	0
6	A	701	OAA	4	0
9	B	304	F3S	1	0
11	C	1	TMG	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, 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%)	0.20	28 (4%) 36 25	32, 52, 84, 92	0
2	B	240/252 (95%)	0.11	10 (4%) 40 28	38, 48, 69, 76	0
3	C	139/140 (99%)	0.20	8 (5%) 26 17	51, 60, 83, 85	0
4	D	102/103 (99%)	0.06	2 (1%) 68 58	50, 64, 73, 78	0
All	All	1094/1117 (97%)	0.17	48 (4%) 38 26	32, 55, 81, 92	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	35	SER	4.0
1	A	317	PRO	3.9
3	C	81	CYS	3.9
1	A	323	TYR	3.5
3	C	21	GLY	3.4
2	B	64	SER	3.4
2	B	94	ASP	3.3
1	A	226	SER	3.2
1	A	315	CYS	3.2
1	A	436	GLY	3.2
2	B	8	ALA	3.2
1	A	279	SER	3.1
1	A	10	SER	3.1
1	A	365	HIS	3.0
3	C	84	PRO	3.0
1	A	280	GLN	3.0
2	B	70	CYS	2.9
2	B	11	ILE	2.8
3	C	80	LEU	2.8
2	B	9	PRO	2.7
1	A	277	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	215	GLY	2.7
3	C	79	SER	2.6
1	A	218	GLY	2.6
1	A	230	SER	2.5
1	A	57	HIS	2.5
1	A	225	THR	2.5
1	A	229	THR	2.5
1	A	12	GLN	2.4
1	A	227	ALA	2.4
1	A	60	ALA	2.3
1	A	278	ASN	2.3
1	A	316	GLY	2.3
2	B	93	LEU	2.3
1	A	499[A]	ARG	2.3
1	A	216	GLY	2.2
3	C	20	LEU	2.2
2	B	72	SER	2.1
2	B	69	ILE	2.1
1	A	214	THR	2.1
2	B	96	VAL	2.1
4	D	135	LYS	2.1
1	A	54	THR	2.1
3	C	82	LEU	2.1
1	A	263	CYS	2.1
1	A	293	LYS	2.0
3	C	85	THR	2.0
1	A	569	GLN	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
10	HEM	C	1305	43/43	0.97	0.21	1.28	64,66,67,68	0
5	FAD	A	700	53/53	0.96	0.31	0.60	37,40,44,45	0
6	OAA	A	701	9/9	0.96	0.27	0.49	75,75,76,76	0
11	TMG	C	1	14/14	0.97	0.17	-0.38	44,45,48,49	0
8	SF4	B	303	8/8	0.99	0.17	-0.40	37,38,39,40	0
7	FES	B	302	4/4	0.99	0.22	-1.01	49,49,51,51	0
9	F3S	B	304	7/7	0.99	0.13	-1.54	45,45,47,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.