



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:20 AM GMT

PDB ID : 3AE1
Title : Crystal structure of porcine heart mitochondrial complex II bound with N-P
henyl-2-(trifluoromethyl)-benzamide
Authors : Harada, S.; Sasaki, T.; Shindo, M.; Kido, Y.; Inaoka, D.K.; Omori, J.; Osanai,
A.; Sakamoto, K.; Mao, J.; Matsuoka, S.; Inoue, M.; Honma, T.; Tanaka, A.;
Kita, K.
Deposited on : 2010-02-04
Resolution : 3.14 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

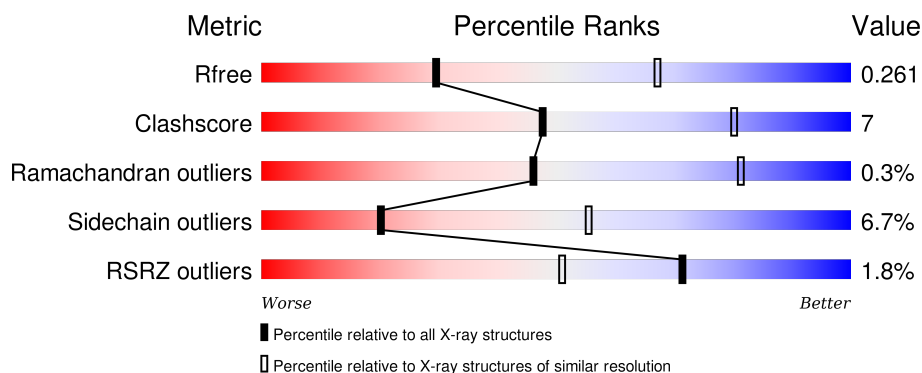
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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	1095 (3.18-3.10)
Clashscore	102246	1202 (3.18-3.10)
Ramachandran outliers	100387	1162 (3.18-3.10)
Sidechain outliers	100360	1162 (3.18-3.10)
RSRZ outliers	91569	1097 (3.18-3.10)

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>2%</div> <div>77%</div> <div>19%</div> <div>• •</div> </div>
2	B	252	<div> <div>3%</div> <div>75%</div> <div>17%</div> <div>• 5%</div> </div>
3	C	140	<div> <div>2%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
4	D	103	<div> <div>2%</div> <div>92%</div> <div>7%</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
10	HEM	C	1305	-	-	-	X
11	EPH	D	1306	X	-	-	X
12	TFZ	C	1201	-	-	-	X
9	MLI	A	701	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 8665 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

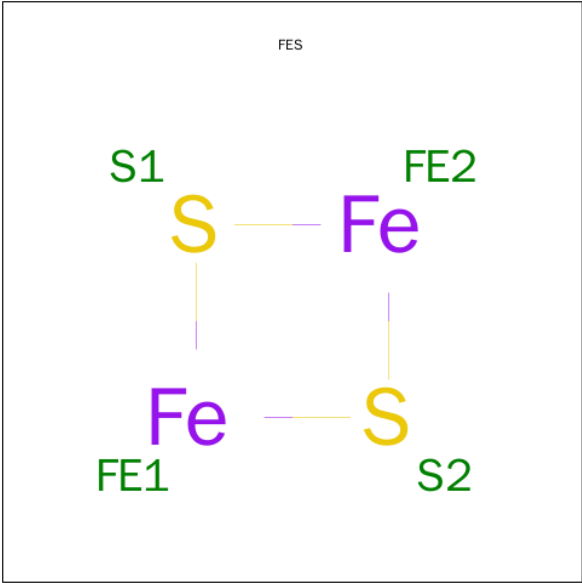
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			765	499	128	133	5			

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



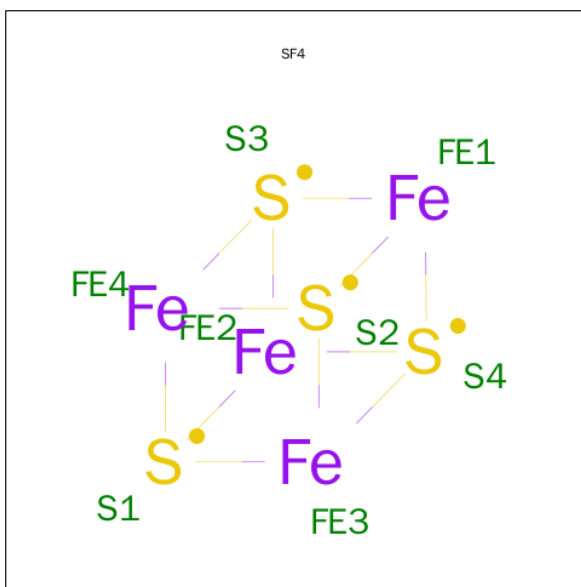
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



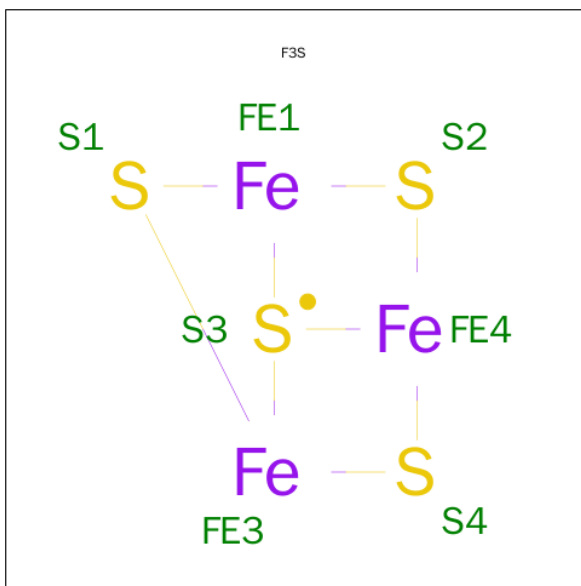
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		

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



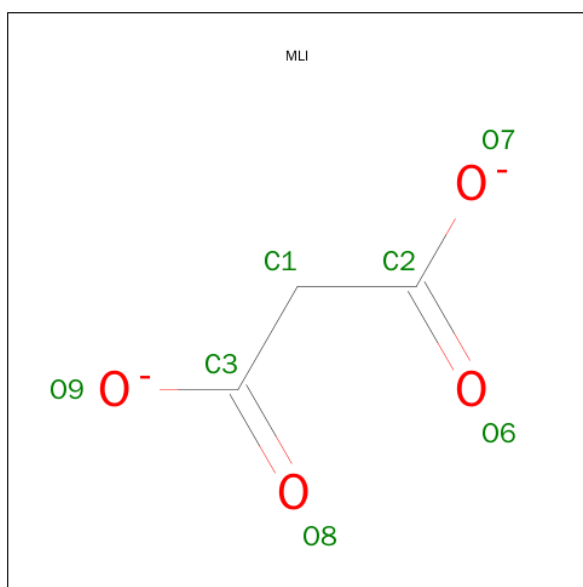
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		

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



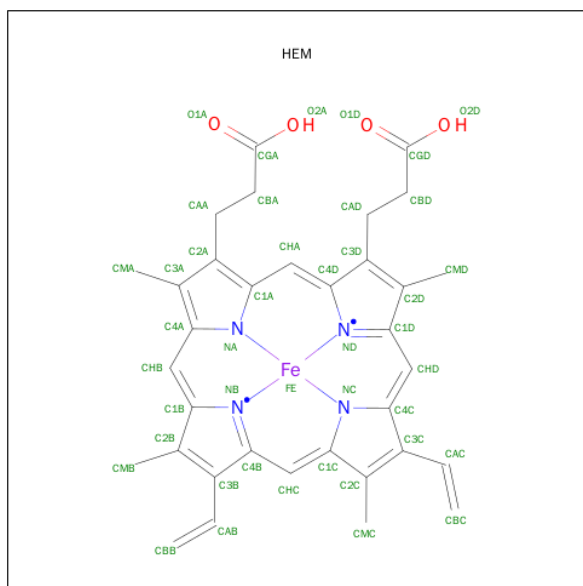
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

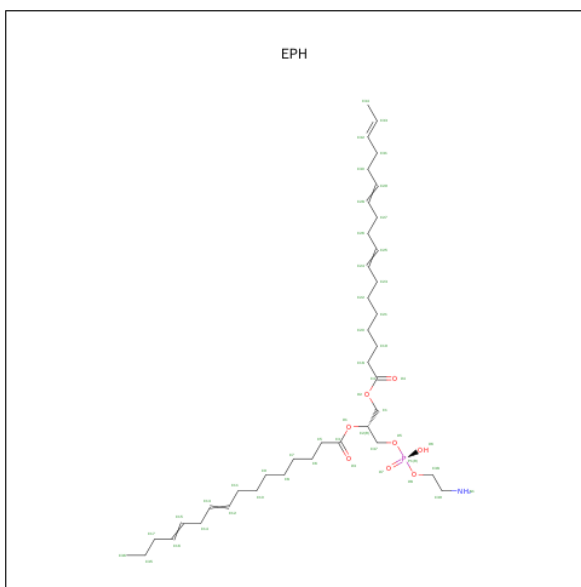
- Molecule 9 is MALONATE ION (three-letter code: MLI) (formula: $\text{C}_3\text{H}_2\text{O}_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	O		0	0
			7	3	4			

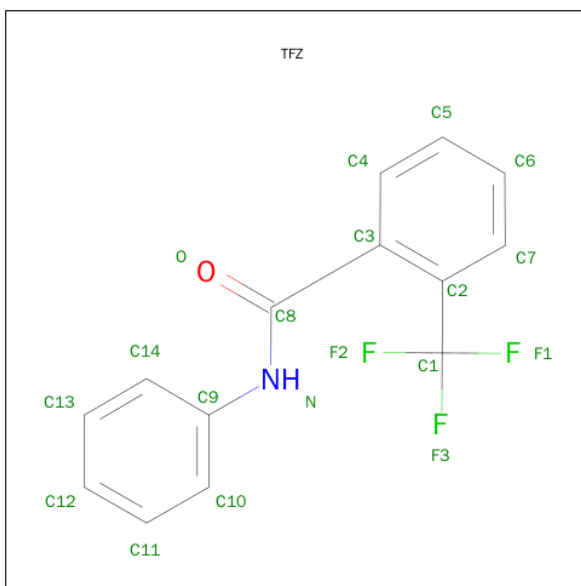
- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





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

- Molecule 12 is N-PHENYL-2-(TRIFLUOROMETHYL)BENZAMIDE (three-letter code: TFZ) (formula: $C_{14}H_{10}F_3NO$).

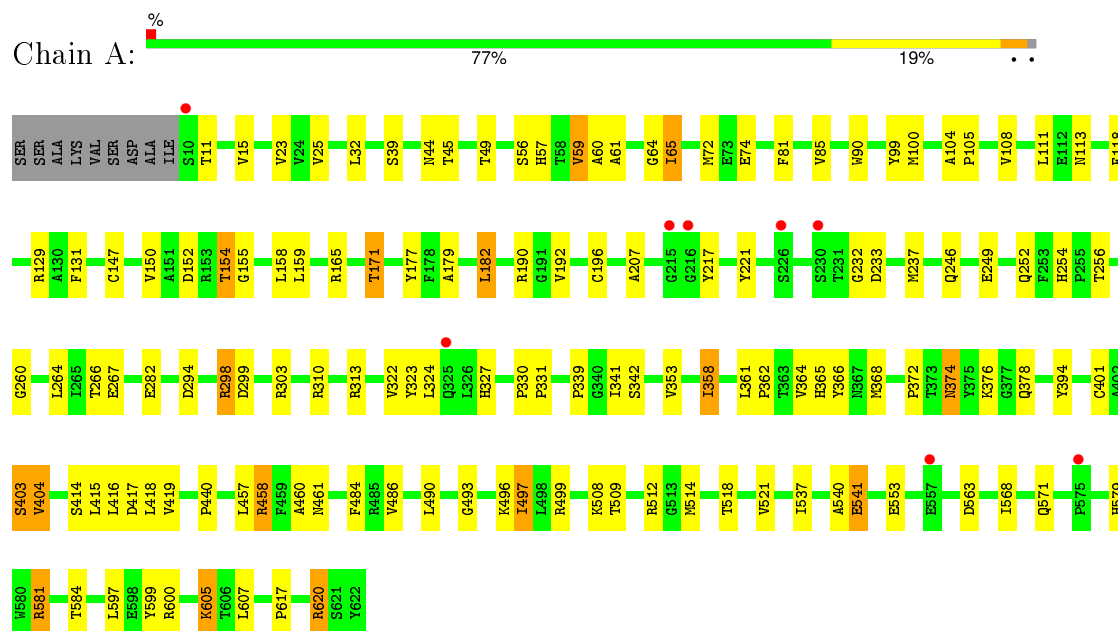


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	F	N	O	0	0
			19	14	3	1	1		

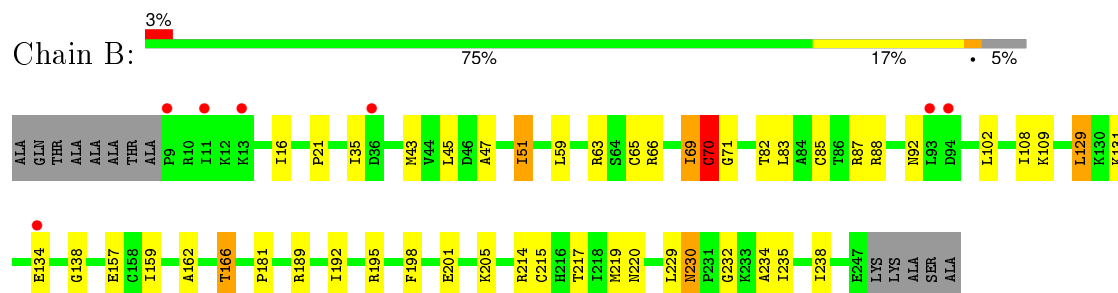
3 Residue-property plots

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

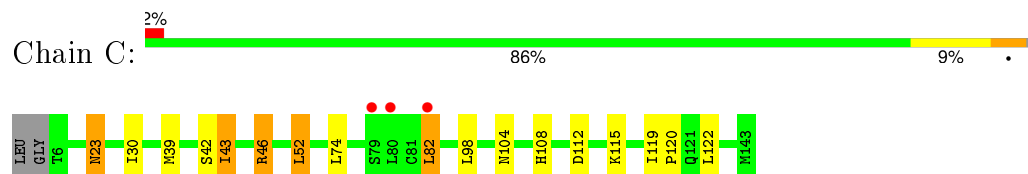
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial



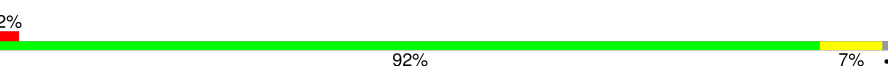
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



- Molecule 3: Succinate dehydrogenase cytochrome b560 subunit, mitochondrial



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

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.47Å 84.06Å 294.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.62 – 3.14 47.62 – 3.14	Depositor EDS
% Data completeness (in resolution range)	95.3 (47.62-3.14) 95.3 (47.62-3.14)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.220 , 0.268 0.220 , 0.261	Depositor DCC
R_{free} test set	1536 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30472 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8665	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: SF4, MLI, F3S, FES, EPH, TFZ, HEM, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/4828	0.52	0/6531
2	B	0.32	0/1964	0.48	0/2648
3	C	0.33	0/1091	0.48	0/1483
4	D	0.31	0/784	0.46	0/1066
All	All	0.32	0/8667	0.50	0/11728

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4729	0	4618	84	0
2	B	1922	0	1901	30	0
3	C	1064	0	1104	12	0
4	D	765	0	773	4	0
5	A	53	0	31	9	0
6	B	4	0	0	1	0
7	B	8	0	0	0	0
8	B	7	0	0	1	0
9	A	7	0	2	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	43	0	30	1	0
11	D	44	0	53	0	0
12	C	19	0	10	3	0
All	All	8665	0	8522	125	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 7.

All (125) 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	1.01	1.33
1:A:61:ALA:HB3	1:A:155:GLY:HA3	1.39	1.04
1:A:57:HIS:CE1	5:A:700:FAD:HM82	1.99	0.95
2:B:102:LEU:HB3	2:B:166:THR:HG21	1.50	0.94
1:A:11:THR:O	1:A:11:THR:HG22	1.79	0.80
1:A:486:VAL:HG12	1:A:553:GLU:HB2	1.70	0.73
1:A:59:VAL:HG13	1:A:159:LEU:HD23	1.71	0.72
4:D:72:LEU:O	4:D:76:LEU:HB2	1.91	0.70
3:C:52:LEU:HB3	10:C:1305:HEM:HAC	1.73	0.69
1:A:104:ALA:HB3	1:A:105:PRO:HD3	1.76	0.68
1:A:415:LEU:HG	5:A:700:FAD:C2	2.24	0.67
1:A:310:ARG:HG2	1:A:310:ARG:HH11	1.59	0.66
1:A:64:GLY:HA2	1:A:154:THR:HG21	1.76	0.66
1:A:150:VAL:H	1:A:154:THR:HB	1.62	0.65
1:A:374:ASN:HB3	1:A:376:LYS:H	1.61	0.64
3:C:23:ASN:HD22	3:C:23:ASN:H	1.44	0.64
1:A:56:SER:O	1:A:59:VAL:HG22	1.97	0.64
1:A:457:LEU:O	1:A:509:THR:HG21	2.02	0.60
2:B:65:CYS:HG	6:B:302:FES:FE1	1.18	0.59
1:A:190:ARG:HD2	1:A:440:PRO:HB2	1.84	0.59
2:B:215:CYS:HA	8:B:304:F3S:S4	2.45	0.57
1:A:246:GLN:HB2	1:A:372:PRO:HG3	1.87	0.57
1:A:620:ARG:HG3	1:A:620:ARG:O	2.06	0.56
1:A:458:ARG:NH2	1:A:514:MET:HG2	2.21	0.56
1:A:518:THR:HA	1:A:521:VAL:HG22	1.87	0.56
1:A:605:LYS:HE3	1:A:605:LYS:O	2.06	0.55
1:A:254:HIS:HD2	1:A:256:THR:H	1.54	0.55
2:B:219:MET:HE2	2:B:232:GLY:HA3	1.89	0.54
1:A:61:ALA:HA	5:A:700:FAD:N5	2.23	0.54
2:B:35:ILE:HD11	2:B:51:ILE:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:HD11	2:B:59:LEU:HD22	1.89	0.54
3:C:46:ARG:HD3	4:D:87:VAL:HG22	1.89	0.54
2:B:198:PHE:CD2	2:B:201:GLU:HG3	2.43	0.54
3:C:42:SER:O	12:C:1201:TFZ:H10	2.09	0.53
1:A:57:HIS:CD2	5:A:700:FAD:C8M	2.84	0.53
2:B:129:LEU:HD21	2:B:195:ARG:HB2	1.91	0.52
1:A:579:HIS:HD2	1:A:581:ARG:H	1.54	0.52
1:A:150:VAL:HB	1:A:154:THR:HA	1.92	0.52
1:A:158:LEU:HD23	1:A:415:LEU:HD22	1.92	0.52
2:B:219:MET:CE	2:B:232:GLY:HA3	2.39	0.52
1:A:150:VAL:O	1:A:150:VAL:HG12	2.10	0.51
1:A:57:HIS:NE2	5:A:700:FAD:C8	2.68	0.50
1:A:217:TYR:HB3	1:A:232:GLY:HA3	1.92	0.50
3:C:52:LEU:HD21	3:C:98:LEU:HA	1.94	0.50
1:A:64:GLY:HA3	1:A:147:CYS:SG	2.52	0.49
1:A:353:VAL:HG12	1:A:358:ILE:HD11	1.93	0.49
3:C:39:MET:HG2	12:C:1201:TFZ:H6	1.94	0.49
2:B:65:CYS:O	2:B:66:ARG:HG3	2.13	0.49
1:A:111:LEU:HD11	1:A:419:VAL:HG21	1.94	0.48
1:A:267:GLU:OE1	1:A:298:ARG:HD3	2.13	0.48
1:A:310:ARG:CG	1:A:310:ARG:HH11	2.26	0.48
1:A:461:ASN:HD22	1:A:508:LYS:HE3	1.78	0.48
1:A:11:THR:O	1:A:11:THR:CG2	2.51	0.48
1:A:266:THR:HA	9:A:701:MLI:O8	2.14	0.48
2:B:235:ILE:HA	2:B:238:ILE:HD12	1.96	0.48
2:B:69:ILE:O	2:B:70:CYS:C	2.52	0.47
2:B:21:PRO:HD3	2:B:109:LYS:HG3	1.95	0.47
1:A:509:THR:HG23	1:A:512:ARG:HH12	1.80	0.47
1:A:60:ALA:HB1	5:A:700:FAD:HM72	1.96	0.47
1:A:65:ILE:HD12	1:A:108:VAL:HG22	1.96	0.47
2:B:230:ASN:HD22	2:B:230:ASN:C	2.17	0.47
3:C:112:ASP:OD1	4:D:47:ARG:HD2	2.15	0.47
1:A:179:ALA:N	5:A:700:FAD:N1A	2.46	0.46
1:A:496:LYS:HG3	1:A:499:ARG:HH22	1.80	0.46
2:B:131:LYS:HB2	2:B:134:GLU:HG3	1.97	0.46
1:A:414:SER:HA	1:A:417:ASP:HB3	1.97	0.46
1:A:81:PHE:O	1:A:85:VAL:HG12	2.15	0.46
2:B:69:ILE:O	2:B:71:GLY:N	2.48	0.46
1:A:104:ALA:HA	1:A:416:LEU:HD11	1.96	0.46
1:A:497:ILE:HG21	1:A:537:ILE:HG21	1.98	0.46
1:A:361:LEU:HD12	1:A:362:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:SER:O	1:A:418:LEU:HD13	2.15	0.46
3:C:119:ILE:N	3:C:120:PRO:HD2	2.31	0.46
1:A:299:ASP:O	1:A:303:ARG:HB2	2.16	0.46
2:B:43:MET:HA	2:B:88:ARG:HA	1.97	0.45
1:A:25:VAL:HG21	1:A:192:VAL:HG11	1.98	0.45
3:C:74:LEU:HD22	4:D:136:LEU:HD13	1.99	0.45
1:A:39:SER:OG	1:A:171:THR:HG23	2.16	0.45
1:A:45:THR:HB	1:A:171:THR:HG22	1.99	0.45
3:C:43:ILE:HG13	3:C:43:ILE:H	1.52	0.44
1:A:254:HIS:O	1:A:362:PRO:HA	2.17	0.44
1:A:90:TRP:HZ3	1:A:620:ARG:HB3	1.83	0.44
1:A:246:GLN:HE22	1:A:600:ARG:HE	1.64	0.44
1:A:99:TYR:HB2	1:A:607:LEU:HD11	1.98	0.44
1:A:584:THR:HA	1:A:599:TYR:CD2	2.53	0.43
1:A:378:GLN:HG2	1:A:394:TYR:CE2	2.54	0.43
1:A:113:ASN:HD22	2:B:138:GLY:H	1.65	0.43
3:C:82:LEU:HD23	3:C:82:LEU:H	1.83	0.43
1:A:493:GLY:O	1:A:497:ILE:HB	2.18	0.43
1:A:113:ASN:ND2	2:B:138:GLY:H	2.17	0.43
1:A:182:LEU:HD13	1:A:237:MET:HB3	1.99	0.43
1:A:100:MET:SD	1:A:404:VAL:HG11	2.58	0.43
3:C:42:SER:C	12:C:1201:TFZ:H10	2.39	0.43
1:A:563:ASP:H	1:A:571:GLN:NE2	2.17	0.43
1:A:254:HIS:HB2	1:A:365:HIS:HB2	2.01	0.42
2:B:181:PRO:HA	2:B:235:ILE:HD11	2.00	0.42
1:A:221:TYR:CG	1:A:364:VAL:HG21	2.54	0.42
2:B:16:ILE:HG21	2:B:59:LEU:HD11	2.01	0.42
1:A:249:GLU:HB2	1:A:540:ALA:HB2	2.01	0.42
1:A:401:CYS:C	1:A:403:SER:H	2.21	0.42
2:B:162:ALA:O	2:B:166:THR:OG1	2.25	0.42
1:A:490:LEU:HD13	1:A:541:GLU:HA	2.02	0.42
1:A:264:LEU:HD21	9:A:701:MLI:O8	2.20	0.42
2:B:21:PRO:HG3	2:B:108:ILE:O	2.19	0.42
1:A:152:ASP:HB2	1:A:339:PRO:HD2	2.01	0.42
1:A:90:TRP:CE2	1:A:617:PRO:HA	2.55	0.42
1:A:233:ASP:O	1:A:237:MET:HG3	2.20	0.42
1:A:118:PHE:HA	1:A:150:VAL:HG22	2.02	0.41
2:B:47:ALA:O	2:B:51:ILE:HG23	2.21	0.41
2:B:45:LEU:HD22	2:B:85:CYS:HB3	2.02	0.41
1:A:563:ASP:HB3	1:A:571:GLN:HE22	1.85	0.41
2:B:157:GLU:HB2	2:B:229:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:THR:HB	2:B:83:LEU:H	1.73	0.41
1:A:23:VAL:HG23	1:A:207:ALA:HB3	2.02	0.41
1:A:49:THR:OG1	5:A:700:FAD:O2B	2.34	0.41
2:B:70:CYS:SG	2:B:71:GLY:N	2.94	0.41
1:A:303:ARG:HG3	1:A:484:PHE:CZ	2.55	0.41
1:A:341:ILE:HG13	1:A:342:SER:N	2.35	0.41
2:B:198:PHE:HD2	2:B:201:GLU:HG3	1.86	0.40
1:A:366:TYR:HE1	1:A:414:SER:HG	1.66	0.40
1:A:330:PRO:HA	1:A:331:PRO:HD3	1.92	0.40
1:A:322:VAL:CG1	1:A:323:TYR:N	2.84	0.40
2:B:234:ALA:O	2:B:238:ILE:HG13	2.22	0.40
1:A:177:TYR:CE2	1:A:196:CYS:HB2	2.56	0.40
1:A:298:ARG:HH22	9:A:701:MLI:C2	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	611/622 (98%)	580 (95%)	29 (5%)	2 (0%)	46	81
2	B	237/252 (94%)	221 (93%)	15 (6%)	1 (0%)	39	77
3	C	136/140 (97%)	133 (98%)	3 (2%)	0	100	100
4	D	100/103 (97%)	97 (97%)	3 (3%)	0	100	100
All	All	1084/1117 (97%)	1031 (95%)	50 (5%)	3 (0%)	46	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	70	CYS
1	A	460	ALA

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Mol	Chain	Res	Type
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%)	466 (93%)	33 (7%)	21	56
2	B	214/220 (97%)	198 (92%)	16 (8%)	17	51
3	C	117/118 (99%)	107 (92%)	10 (8%)	13	45
4	D	76/76 (100%)	74 (97%)	2 (3%)	54	84
All	All	906/920 (98%)	845 (93%)	61 (7%)	20	55

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	32	LEU
1	A	44	ASN
1	A	59	VAL
1	A	65	ILE
1	A	72	MET
1	A	74	GLU
1	A	129	ARG
1	A	131	PHE
1	A	154	THR
1	A	165	ARG
1	A	171	THR
1	A	182	LEU
1	A	252	GLN
1	A	282	GLU
1	A	294	ASP
1	A	298	ARG
1	A	313	ARG
1	A	324	LEU
1	A	327	HIS

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Mol	Chain	Res	Type
1	A	358	ILE
1	A	368	MET
1	A	374	ASN
1	A	403	SER
1	A	404	VAL
1	A	458	ARG
1	A	497	ILE
1	A	541	GLU
1	A	568	ILE
1	A	581	ARG
1	A	597	LEU
1	A	605	LYS
1	A	620	ARG
2	B	51	ILE
2	B	63	ARG
2	B	69	ILE
2	B	70	CYS
2	B	87	ARG
2	B	92	ASN
2	B	129	LEU
2	B	159	ILE
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
3	C	23	ASN
3	C	30	ILE
3	C	43	ILE
3	C	46	ARG
3	C	52	LEU
3	C	82	LEU
3	C	104	ASN
3	C	108	HIS
3	C	115	LYS
3	C	122	LEU
4	D	78	LEU
4	D	124	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	113	ASN
1	A	128	GLN
1	A	246	GLN
1	A	254	HIS
1	A	382	HIS
1	A	384	ASN
1	A	408	ASN
1	A	445	ASN
1	A	461	ASN
1	A	474	GLN
1	A	550	HIS
1	A	569	GLN
1	A	571	GLN
1	A	579	HIS
2	B	92	ASN
2	B	121	GLN
2	B	220	ASN
2	B	230	ASN
3	C	17	ASN
3	C	23	ASN
3	C	104	ASN
3	C	121	GLN
4	D	42	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	1.23	6 (12%)	54,89,89	2.18	7 (12%)
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	-
12	TFZ	C	1201	-	20,20,20	1.63	2 (10%)	27,28,28	0.93	2 (7%)
10	HEM	C	1305	3,4	30,50,50	2.18	9 (30%)	24,82,82	2.35	10 (41%)
11	EPH	D	1306	-	42,43,48	1.56	7 (16%)	43,48,53	1.42	9 (20%)

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
12	TFZ	C	1201	-	-	0/14/14/14	0/2/2/2
10	HEM	C	1305	3,4	-	0/10/54/54	0/0/8/8
11	EPH	D	1306	-	1/1/4/14	0/47/47/52	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1305	HEM	C3B-C4B	-7.17	1.45	1.51
10	C	1305	HEM	C3D-C4D	-4.92	1.45	1.51
10	C	1305	HEM	C2C-C1C	-3.49	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	1201	TFZ	C9-N	-2.77	1.36	1.41
10	C	1305	HEM	C2D-C1D	-2.12	1.44	1.51
10	C	1305	HEM	CAA-C2A	2.03	1.55	1.52
10	C	1305	HEM	C4C-NC	2.05	1.38	1.36
10	C	1305	HEM	FE-ND	2.12	2.08	1.97
5	A	700	FAD	C5X-N5	2.12	1.38	1.35
5	A	700	FAD	C1'-N10	2.32	1.50	1.48
11	D	1306	EPH	P1-O7	2.35	1.59	1.51
10	C	1305	HEM	C1C-NC	2.45	1.39	1.36
5	A	700	FAD	C2A-N1A	2.59	1.38	1.33
10	C	1305	HEM	FE-NC	2.72	2.06	1.95
5	A	700	FAD	C4-N3	2.99	1.38	1.33
11	D	1306	EPH	C15-C16	3.15	1.52	1.29
5	A	700	FAD	C2A-N3A	3.44	1.38	1.32
5	A	700	FAD	C4X-N5	3.64	1.39	1.33
11	D	1306	EPH	C13-C12	3.66	1.52	1.31
11	D	1306	EPH	C29-C28	3.66	1.52	1.31
11	D	1306	EPH	C25-C24	3.68	1.52	1.31
11	D	1306	EPH	O2-C4	4.20	1.46	1.33
11	D	1306	EPH	O1-C3	4.26	1.47	1.34
12	C	1201	TFZ	C3-C2	6.47	1.51	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	FAD	N3A-C2A-N1A	-12.12	119.61	128.89
11	D	1306	EPH	C30-C29-C28	-3.47	111.17	127.06
10	C	1305	HEM	C3B-CAB-CBB	-3.30	119.40	124.46
10	C	1305	HEM	C3C-CAC-CBC	-3.07	119.75	124.46
5	A	700	FAD	P-O3P-PA	-3.01	124.27	132.73
5	A	700	FAD	C4X-C4-N3	-2.28	120.47	123.59
11	D	1306	EPH	C14-C15-C16	-2.16	111.63	125.00
11	D	1306	EPH	C14-C13-C12	-2.14	111.77	125.00
10	C	1305	HEM	CMA-C3A-C4A	-2.13	124.84	128.36
12	C	1201	TFZ	F3-C1-C2	-2.09	109.00	112.68
11	D	1306	EPH	C23-C24-C25	-2.06	111.03	125.34
11	D	1306	EPH	C11-C12-C13	-2.05	111.03	125.34
11	D	1306	EPH	C27-C28-C29	-2.04	111.11	125.34
11	D	1306	EPH	C26-C25-C24	-2.04	111.15	125.34
12	C	1201	TFZ	C1-C2-C3	2.12	125.15	122.11
10	C	1305	HEM	C3B-C4B-CHC	2.12	126.15	123.16
5	A	700	FAD	C4-C4X-N5	2.28	121.49	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1305	HEM	C2D-C3D-C4D	2.38	105.54	101.50
11	D	1306	EPH	O2-C4-C18	2.76	120.31	111.90
10	C	1305	HEM	CMD-C2D-C3D	2.79	126.68	114.35
5	A	700	FAD	C5X-C9A-N10	2.94	119.85	117.62
5	A	700	FAD	C4X-N5-C5X	3.59	120.89	116.76
10	C	1305	HEM	CMB-C2B-C3B	3.80	126.02	116.53
10	C	1305	HEM	CMC-C2C-C3C	3.81	126.05	116.53
10	C	1305	HEM	CAD-C3D-C2D	4.23	125.37	113.22
11	D	1306	EPH	O1-C3-C5	4.33	120.95	111.53
10	C	1305	HEM	CAD-C3D-C4D	4.71	129.08	112.47
5	A	700	FAD	C4-N3-C2	5.49	119.99	115.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	D	1306	EPH	C2

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	700	FAD	9	0
9	A	701	MLI	3	0
6	B	302	FES	1	0
8	B	304	F3S	1	0
12	C	1201	TFZ	3	0
10	C	1305	HEM	1	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%)	-0.02	8 (1%)	79 63	57, 78, 109, 132	0
2	B	239/252 (94%)	-0.03	7 (2%)	55 32	58, 73, 109, 131	0
3	C	138/140 (98%)	-0.11	3 (2%)	65 44	66, 85, 128, 138	0
4	D	102/103 (99%)	-0.13	2 (1%)	68 48	67, 83, 105, 118	0
All	All	1092/1117 (97%)	-0.05	20 (1%)	71 51	57, 79, 112, 138	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	35	SER	7.1
3	C	80	LEU	3.1
2	B	11	ILE	3.0
3	C	82	LEU	2.9
1	A	230	SER	2.7
1	A	10	SER	2.7
1	A	216	GLY	2.6
2	B	134	GLU	2.6
3	C	79	SER	2.6
2	B	9	PRO	2.5
1	A	575	PRO	2.5
1	A	325	GLN	2.4
1	A	215	GLY	2.3
1	A	557	GLU	2.3
1	A	226	SER	2.3
2	B	13	LYS	2.2
4	D	36	SER	2.2
2	B	94	ASP	2.2
2	B	93	LEU	2.1
2	B	36	ASP	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
12	TFZ	C	1201	19/19	0.81	0.37	5.32	108,108,109,109	0
11	EPH	D	1306	44/49	0.83	0.55	4.52	115,121,127,127	0
10	HEM	C	1305	43/43	0.96	0.25	2.00	76,77,79,79	0
9	MLI	A	701	7/7	0.85	0.37	1.93	87,87,88,88	0
5	FAD	A	700	53/53	0.92	0.35	0.62	62,63,68,69	0
7	SF4	B	303	8/8	0.99	0.19	-0.54	53,54,55,55	0
6	FES	B	302	4/4	0.99	0.20	-0.70	58,58,59,60	0
8	F3S	B	304	7/7	0.99	0.17	-0.71	68,68,68,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.