



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:06 PM GMT

PDB ID : 1GAQ
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN FERREDOXIN
AND FERREDOXIN-NADP+ REDUCTASE
Authors : Kurisu, G.; Kusunoki, M.; Hase, T.
Deposited on : 2000-05-08
Resolution : 2.59 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

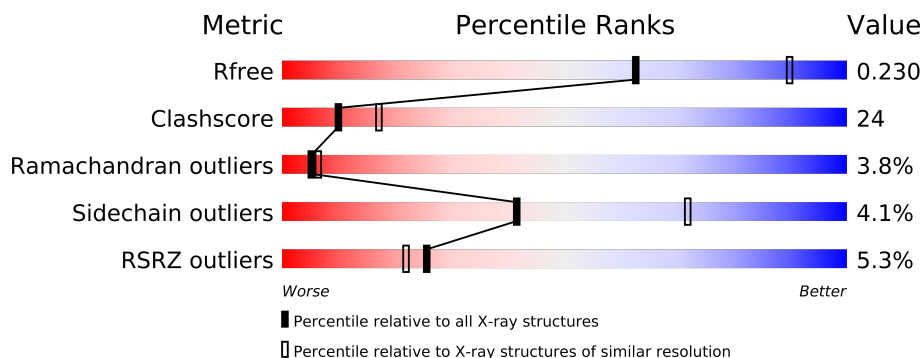
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.59 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	314	
1	C	314	
2	B	98	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5685 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

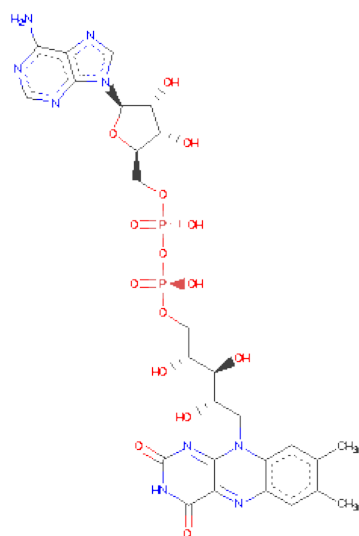
- Molecule 1 is a protein called FERREDOXIN-NADP+ REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2355	1502	390	447	16			
1	C	296	Total	C	N	O	S	0	0	0
			2355	1502	390	447	16			

- Molecule 2 is a protein called FERREDOXIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			732	450	115	163	4			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



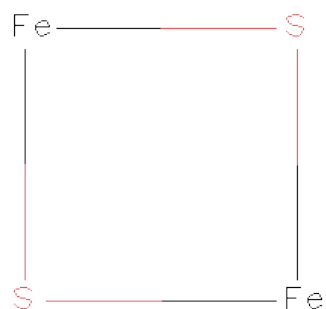
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total	O	0	0
			40	40		
5	B	13	Total	O	0	0
			13	13		
5	C	80	Total	O	0	0
			80	80		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.07Å 93.41Å 135.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.56 – 2.59 35.44 – 2.68	Depositor EDS
% Data completeness (in resolution range)	97.8 (39.56-2.59) 88.3 (35.44-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.45 (at 2.68Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.232 , 0.297 0.236 , 0.230	Depositor DCC
R_{free} test set	950 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 18578 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5685	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, 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	0.35	0/2407	0.58	0/3241
1	C	0.42	0/2407	0.66	1/3241 (0.0%)
2	B	0.29	0/744	0.55	0/1015
All	All	0.37	0/5558	0.61	1/7497 (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	C	55	GLY	N-CA-C	6.43	129.18	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2355	0	2328	117	0
1	C	2355	0	2328	85	0
2	B	732	0	675	63	0
3	A	53	0	31	0	0
3	C	53	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	0	0	0
5	A	40	0	0	4	0
5	B	13	0	0	3	0
5	C	80	0	0	4	0
All	All	5685	0	5393	261	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (261) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:102:ILE:HG22	1:C:106:GLY:HA2	1.41	0.99
1:A:71:ARG:H	1:A:74:GLN:HE21	0.97	0.96
1:C:180:PHE:HB3	1:C:184:MET:HE2	1.49	0.94
1:C:255:LYS:HG2	1:C:288:LEU:HD21	1.52	0.91
1:C:33:LYS:HG2	1:C:34:PRO:HD2	1.54	0.89
1:A:71:ARG:N	1:A:74:GLN:HE21	1.72	0.86
2:B:16:LEU:HD23	2:B:17:GLN:H	1.39	0.85
2:B:16:LEU:CD2	2:B:17:GLN:H	1.90	0.84
2:B:95:LEU:HG	2:B:96:THR:H	1.44	0.82
1:A:259:TRP:HB2	1:A:288:LEU:HD21	1.59	0.82
1:C:76:ILE:HD12	1:C:147:ILE:HD12	1.65	0.78
1:A:75:SER:HA	1:A:97:ILE:HG13	1.65	0.78
2:B:2:THR:HA	2:B:19:PRO:HA	1.64	0.77
2:B:2:THR:HG22	2:B:17:GLN:HE21	1.50	0.77
2:B:61:GLN:HA	2:B:64:LEU:HD12	1.68	0.76
2:B:19:PRO:HG2	2:B:22:VAL:HB	1.68	0.75
1:A:119:ILE:HG12	1:A:129:LYS:HG2	1.68	0.75
1:A:160:ASP:OD2	1:A:163:ALA:HB2	1.88	0.73
1:A:37:PRO:HG3	1:A:146:GLN:HE21	1.54	0.73
1:A:170:THR:OG1	1:A:277:MET:HG2	1.89	0.72
1:A:107:ASP:OD1	1:A:109:LYS:HB3	1.91	0.71
1:A:76:ILE:HG23	1:A:97:ILE:HD11	1.74	0.70
1:C:102:ILE:CG2	1:C:106:GLY:HA2	2.22	0.68
1:C:93:ARG:HD3	3:C:321:FAD:O1P	1.92	0.68
2:B:26:ASP:O	2:B:30:GLU:HG2	1.93	0.68
1:A:102:ILE:HD12	1:A:187:GLU:OE2	1.94	0.67
1:A:236:GLU:O	1:A:237:GLN:HG3	1.95	0.67
2:B:51:VAL:HG22	2:B:52:VAL:H	1.59	0.66
1:A:28:VAL:HG11	1:A:31:LEU:HD21	1.77	0.66
2:B:6:LYS:HB2	2:B:86:VAL:HG22	1.76	0.66
1:C:180:PHE:HB3	1:C:184:MET:CE	2.25	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:93:ARG:HD2	1:C:132:CYS:HB2	1.77	0.66
1:A:282:ASP:O	1:A:286:VAL:HG23	1.96	0.65
1:C:33:LYS:CG	1:C:34:PRO:HD2	2.27	0.64
1:C:85:LYS:C	1:C:87:GLY:H	2.01	0.64
2:B:7:LEU:N	2:B:7:LEU:HD12	2.13	0.63
1:A:302:GLN:O	1:A:305:ARG:HB2	1.98	0.63
1:C:107:ASP:O	1:C:109:LYS:HD3	1.99	0.63
2:B:2:THR:HG22	2:B:17:GLN:NE2	2.12	0.62
2:B:20:ASP:O	2:B:80:TYR:HB3	2.00	0.62
1:C:239:ASN:ND2	1:C:243:GLU:H	1.98	0.62
1:C:181:LEU:HD23	1:C:184:MET:HE3	1.82	0.62
1:C:34:PRO:HA	1:C:79:ILE:HD11	1.81	0.62
2:B:61:GLN:HA	2:B:64:LEU:CD1	2.29	0.62
1:A:162:ASN:ND2	1:A:195:ASN:HB3	2.15	0.61
2:B:83:SER:O	2:B:85:VAL:HG23	2.00	0.61
1:A:285:MET:CE	1:A:288:LEU:HD23	2.29	0.61
1:A:145:VAL:HB	5:A:326:HOH:O	2.00	0.61
1:C:75:SER:HB3	1:C:96:SER:HA	1.82	0.61
1:A:36:GLU:HG3	1:C:25:GLU:HB2	1.82	0.61
1:C:94:LEU:HD12	3:C:321:FAD:HM82	1.81	0.61
1:A:158:PRO:HD3	1:A:270:TYR:OH	2.01	0.61
1:C:181:LEU:HA	1:C:184:MET:HE3	1.83	0.61
2:B:7:LEU:HD13	2:B:14:VAL:HB	1.83	0.60
1:C:210:LEU:HD13	1:C:213:LYS:HD2	1.82	0.60
1:A:83:VAL:HG12	1:A:89:PRO:HA	1.82	0.60
1:A:71:ARG:H	1:A:74:GLN:NE2	1.82	0.60
2:B:61:GLN:HB3	2:B:64:LEU:HB2	1.84	0.60
2:B:46:SER:HA	5:B:101:HOH:O	2.00	0.60
2:B:95:LEU:HG	2:B:96:THR:N	2.16	0.60
2:B:51:VAL:HG22	2:B:52:VAL:N	2.17	0.60
1:A:55:GLY:HA3	1:A:116:LYS:HE3	1.83	0.60
1:A:289:ALA:C	1:A:291:LYS:H	2.05	0.60
1:A:181:LEU:HB3	1:A:219:MET:SD	2.42	0.59
2:B:2:THR:CG2	2:B:17:GLN:HE21	2.15	0.58
1:A:247:ILE:O	1:A:251:MET:HE2	2.03	0.58
2:B:9:THR:C	2:B:11:GLU:H	2.06	0.58
2:B:9:THR:HG22	2:B:89:THR:HG21	1.84	0.58
1:A:107:ASP:CG	1:A:109:LYS:HB3	2.24	0.58
1:C:33:LYS:HG2	1:C:34:PRO:CD	2.31	0.57
1:A:102:ILE:HG22	1:A:106:GLY:C	2.24	0.57
1:A:165:ILE:HG23	1:A:198:GLY:HA2	1.87	0.57
1:C:26:GLY:HA3	1:C:71:ARG:HH12	1.70	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:239:ASN:HD21	1:C:243:GLU:H	1.50	0.56
2:B:60:ASP:HB3	2:B:78:HIS:ND1	2.20	0.56
1:C:180:PHE:O	1:C:184:MET:HG3	2.05	0.56
1:C:26:GLY:HA3	1:C:71:ARG:NH1	2.21	0.56
1:A:90:HIS:CD2	1:A:131:VAL:HG11	2.41	0.56
2:B:54:GLY:HA3	2:B:84:ASP:O	2.06	0.56
1:C:88:LYS:HB2	1:C:89:PRO:CD	2.36	0.56
1:C:133:SER:HB3	3:C:321:FAD:H5'1	1.87	0.56
1:C:301:LYS:NZ	1:C:301:LYS:HB2	2.21	0.56
2:B:93:GLU:HB3	5:B:107:HOH:O	2.05	0.55
1:A:155:MET:HE2	1:A:272:CYS:HB2	1.89	0.55
1:A:93:ARG:HG3	1:A:132:CYS:CB	2.37	0.55
1:C:239:ASN:C	1:C:239:ASN:HD22	2.09	0.55
1:A:239:ASN:OD1	1:A:243:GLU:HB2	2.07	0.55
1:A:35:LYS:O	1:C:25:GLU:HG2	2.08	0.54
1:A:234:SER:HA	1:A:245:MET:O	2.07	0.54
2:B:6:LYS:HD2	2:B:86:VAL:HG22	1.90	0.54
1:A:40:GLY:O	1:A:41:ARG:HG2	2.08	0.54
1:A:286:VAL:HA	1:A:296:TRP:HB2	1.88	0.54
1:A:93:ARG:HG3	1:A:132:CYS:HB2	1.89	0.54
1:C:75:SER:O	1:C:151:VAL:HG12	2.07	0.54
2:B:60:ASP:HA	1:C:190:ASP:OD1	2.07	0.54
1:A:171:GLY:C	1:A:173:GLY:H	2.11	0.54
2:B:66:ASP:HA	5:B:103:HOH:O	2.08	0.54
2:B:16:LEU:HD23	2:B:17:GLN:N	2.18	0.54
1:A:56:GLU:O	1:A:116:LYS:HD2	2.09	0.53
1:A:246:TYR:H	1:A:249:THR:HB	1.73	0.53
2:B:7:LEU:HB2	2:B:14:VAL:HB	1.91	0.53
2:B:14:VAL:HG12	2:B:15:GLU:N	2.24	0.53
1:A:22:LYS:HA	1:A:158:PRO:HA	1.90	0.52
1:C:155:MET:HG2	1:C:312:GLU:HG3	1.91	0.52
1:A:264:LYS:HA	5:A:322:HOH:O	2.09	0.52
2:B:8:ILE:HG22	2:B:8:ILE:O	2.09	0.52
1:A:294:ILE:N	1:A:294:ILE:HD13	2.25	0.52
1:A:22:LYS:CD	1:A:307:ASP:HB3	2.40	0.52
1:A:186:PHE:CZ	1:A:219:MET:HG3	2.45	0.52
1:C:83:VAL:HG12	1:C:88:LYS:O	2.10	0.51
1:A:294:ILE:HD11	1:A:299:TYR:HB2	1.93	0.51
1:A:37:PRO:HG3	1:A:146:GLN:NE2	2.24	0.51
1:A:61:VAL:HG22	1:A:112:SER:OG	2.11	0.51
1:C:90:HIS:CE1	1:C:131:VAL:HG11	2.46	0.51
1:C:271:MET:SD	1:C:278:GLU:HB3	2.51	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:181:LEU:HD23	1:C:184:MET:CE	2.41	0.51
1:A:248:GLN:HA	1:A:251:MET:CE	2.40	0.51
1:C:32:TYR:CE2	1:C:38:TYR:HB2	2.46	0.51
1:C:301:LYS:HZ2	1:C:301:LYS:HB2	1.76	0.51
1:A:174:ILE:HD11	1:A:200:LEU:HD21	1.92	0.51
1:A:222:ARG:HH11	1:A:222:ARG:HG3	1.76	0.50
1:A:294:ILE:HD13	1:A:294:ILE:H	1.76	0.50
1:C:169:ALA:HB2	1:C:177:PHE:HE2	1.76	0.50
1:A:76:ILE:HD12	1:A:147:ILE:HG23	1.94	0.50
2:B:93:GLU:C	2:B:94:GLU:HG3	2.31	0.50
1:A:42:CYS:O	1:A:141:PRO:HA	2.12	0.50
1:A:257:GLU:O	1:A:261:LEU:HG	2.11	0.50
1:A:300:LYS:HD3	1:A:304:LYS:HE3	1.94	0.50
1:A:130:GLY:O	1:A:134:ASN:HB2	2.12	0.50
2:B:92:GLU:HA	2:B:92:GLU:OE1	2.12	0.50
2:B:9:THR:HG22	2:B:89:THR:CG2	2.41	0.49
1:A:221:GLU:O	1:A:224:PRO:HD3	2.12	0.49
1:C:55:GLY:O	1:C:56:GLU:HB2	2.12	0.49
1:C:169:ALA:HB2	1:C:177:PHE:CE2	2.47	0.49
2:B:8:ILE:N	2:B:8:ILE:HD12	2.28	0.49
1:A:50:GLY:C	1:A:52:ASP:H	2.16	0.49
1:A:28:VAL:O	1:A:150:PRO:HG2	2.12	0.49
1:A:83:VAL:HG12	1:A:89:PRO:CA	2.42	0.49
2:B:19:PRO:HG2	2:B:22:VAL:CB	2.41	0.48
1:A:248:GLN:HA	1:A:251:MET:HE3	1.94	0.48
1:C:146:GLN:HG3	5:C:355:HOH:O	2.13	0.48
1:A:285:MET:HG2	1:A:296:TRP:CE2	2.47	0.48
1:A:285:MET:HE3	1:A:288:LEU:HD23	1.95	0.48
1:A:285:MET:HG2	1:A:296:TRP:CZ2	2.48	0.48
2:B:85:VAL:HG12	2:B:87:ILE:HG13	1.96	0.48
2:B:45:SER:HB3	2:B:63:TYR:CE2	2.49	0.48
1:C:93:ARG:HD2	1:C:132:CYS:CB	2.41	0.48
1:C:130:GLY:O	1:C:134:ASN:HB2	2.13	0.48
1:C:286:VAL:O	1:C:290:GLU:HG3	2.13	0.47
1:A:22:LYS:HD2	1:A:307:ASP:HB3	1.96	0.47
1:C:275:LYS:HG3	1:C:314:TYR:C	2.34	0.47
1:C:118:LEU:HD22	1:C:120:TYR:HD1	1.80	0.47
1:A:213:LYS:HG3	1:A:214:GLU:N	2.29	0.47
1:A:186:PHE:HA	1:A:222:ARG:HH12	1.79	0.47
2:B:67:GLY:O	2:B:71:ASP:HB2	2.15	0.47
1:A:163:ALA:HB1	1:A:266:ASN:O	2.15	0.46
1:A:157:MET:HG2	1:A:180:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:286:VAL:HG22	1:A:296:TRP:HB3	1.97	0.46
1:C:84:ASP:CG	1:C:85:LYS:H	2.19	0.46
1:A:165:ILE:HD11	1:A:180:PHE:CE2	2.51	0.46
1:C:27:VAL:HG22	1:C:71:ARG:HG3	1.97	0.46
1:A:239:ASN:CG	1:A:240:ALA:N	2.69	0.46
1:A:251:MET:HE3	1:A:281:ILE:HG12	1.98	0.46
1:C:47:LYS:NZ	1:C:51:ASP:OD1	2.48	0.46
1:A:71:ARG:N	1:A:74:GLN:NE2	2.53	0.46
1:A:171:GLY:C	1:A:173:GLY:N	2.69	0.46
1:A:86:ASN:HB2	2:B:97:GLY:O	2.16	0.46
1:C:259:TRP:CZ2	1:C:294:ILE:HD11	2.50	0.46
1:A:252:ALA:O	1:A:255:LYS:HG2	2.15	0.46
2:B:89:THR:O	2:B:90:HIS:HB2	2.17	0.45
1:A:239:ASN:CG	1:A:240:ALA:H	2.18	0.45
1:C:88:LYS:CB	1:C:89:PRO:CD	2.95	0.45
2:B:45:SER:HB3	2:B:63:TYR:HE2	1.82	0.45
1:A:157:MET:HG2	1:A:180:PHE:CE1	2.51	0.45
1:C:248:GLN:H	1:C:248:GLN:NE2	2.15	0.45
1:C:91:LYS:HB3	1:C:91:LYS:NZ	2.31	0.45
1:A:197:LEU:HD12	1:A:226:ASN:O	2.16	0.45
1:A:294:ILE:CD1	1:A:294:ILE:H	2.30	0.45
1:A:188:LYS:NZ	1:A:188:LYS:HB2	2.32	0.45
2:B:6:LYS:HD2	2:B:86:VAL:CG2	2.47	0.45
2:B:25:LEU:CB	2:B:77:CYS:HA	2.47	0.45
1:A:311:VAL:HG12	1:A:312:GLU:N	2.30	0.45
1:A:117:ARG:NH2	1:A:138:ASP:OD2	2.48	0.45
1:A:235:ARG:NH2	5:A:355:HOH:O	2.49	0.45
2:B:37:TYR:HD2	2:B:40:ARG:HD2	1.82	0.45
1:A:274:LEU:O	1:A:277:MET:HG3	2.16	0.44
2:B:56:VAL:CG1	2:B:85:VAL:HG21	2.47	0.44
1:C:304:LYS:HG2	1:C:309:TRP:O	2.16	0.44
1:C:181:LEU:HB3	1:C:219:MET:SD	2.56	0.44
2:B:61:GLN:CA	2:B:64:LEU:HD12	2.44	0.44
2:B:64:LEU:HD23	2:B:68:GLN:NE2	2.32	0.44
1:A:169:ALA:HB2	1:A:177:PHE:CD2	2.52	0.44
2:B:23:TYR:HB2	2:B:26:ASP:OD2	2.17	0.44
1:C:107:ASP:OD1	1:C:109:LYS:HB2	2.16	0.44
1:A:109:LYS:HD3	1:A:110:THR:CG2	2.47	0.44
1:A:289:ALA:C	1:A:291:LYS:N	2.70	0.44
2:B:9:THR:C	2:B:11:GLU:N	2.71	0.44
1:C:191:ASP:HB2	5:C:345:HOH:O	2.18	0.44
1:C:77:GLY:HA3	1:C:148:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:167:MET:O	1:A:200:LEU:HD12	2.18	0.44
1:C:157:MET:CE	1:C:183:LYS:HD3	2.48	0.44
1:A:63:SER:HB2	1:A:109:LYS:CE	2.47	0.44
2:B:5:VAL:HG21	2:B:18:VAL:HG23	2.00	0.44
1:C:83:VAL:HG23	1:C:83:VAL:O	2.18	0.44
1:A:205:PRO:HA	1:A:234:SER:OG	2.18	0.44
1:C:158:PRO:HD3	1:C:270:TYR:OH	2.18	0.44
1:A:50:GLY:O	1:A:52:ASP:N	2.51	0.43
1:C:134:ASN:O	1:C:138:ASP:HB2	2.18	0.43
2:B:56:VAL:HG12	2:B:81:PRO:HA	1.99	0.43
2:B:7:LEU:N	2:B:7:LEU:CD1	2.82	0.43
2:B:68:GLN:HG2	2:B:73:TRP:HB2	1.99	0.43
1:A:186:PHE:CE1	1:A:219:MET:HG3	2.54	0.43
1:C:157:MET:HE1	1:C:183:LYS:HD3	2.00	0.43
1:C:248:GLN:H	1:C:248:GLN:HE21	1.65	0.43
1:C:161:PRO:O	1:C:194:PHE:HA	2.19	0.43
2:B:95:LEU:CG	2:B:96:THR:H	2.14	0.43
2:B:3:TYR:CD2	2:B:83:SER:HA	2.53	0.43
2:B:57:ASP:O	2:B:79:ALA:HA	2.18	0.43
1:C:151:VAL:HG22	1:C:152:GLY:N	2.34	0.43
1:A:24:GLU:HA	1:A:27:VAL:HG21	2.01	0.43
1:C:235:ARG:HA	1:C:244:ARG:HH11	1.83	0.43
1:A:169:ALA:HB2	1:A:177:PHE:CE2	2.54	0.43
2:B:61:GLN:HG2	2:B:64:LEU:HD12	2.01	0.42
1:A:171:GLY:O	1:A:173:GLY:N	2.51	0.42
1:C:171:GLY:C	1:C:173:GLY:H	2.22	0.42
1:C:85:LYS:C	1:C:87:GLY:N	2.69	0.42
1:A:261:LEU:C	1:A:263:LYS:H	2.23	0.42
1:C:264:LYS:HG2	5:C:387:HOH:O	2.18	0.42
1:A:289:ALA:O	1:A:291:LYS:N	2.52	0.42
1:A:260:GLU:HA	1:A:260:GLU:OE2	2.20	0.42
1:A:109:LYS:HD3	1:A:110:THR:HG23	2.02	0.42
1:A:102:ILE:HD11	1:A:189:HIS:CE1	2.55	0.42
2:B:64:LEU:HD23	2:B:68:GLN:HE22	1.85	0.42
1:C:171:GLY:C	1:C:173:GLY:N	2.73	0.42
1:C:111:VAL:HG13	1:C:111:VAL:O	2.20	0.42
2:B:25:LEU:HB3	2:B:77:CYS:HA	2.02	0.41
1:C:118:LEU:HD22	1:C:120:TYR:CD1	2.55	0.41
1:C:160:ASP:HB3	1:C:163:ALA:HB2	2.02	0.41
1:A:111:VAL:O	1:A:111:VAL:HG13	2.19	0.41
1:A:295:ASP:O	1:A:296:TRP:C	2.58	0.41
1:A:222:ARG:HG3	1:A:222:ARG:NH1	2.34	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:84:ASP:OD1	1:A:86:ASN:HB3	2.21	0.41
1:C:252:ALA:O	1:C:255:LYS:HB2	2.21	0.41
1:A:22:LYS:HD3	1:A:307:ASP:HB3	2.03	0.41
1:C:82:GLY:O	1:C:83:VAL:HG13	2.20	0.41
1:A:78:VAL:HG11	1:A:136:LEU:HD21	2.03	0.41
1:A:305:ARG:HH11	1:A:305:ARG:HG3	1.86	0.41
1:C:75:SER:HA	1:C:97:ILE:HG13	2.02	0.41
1:C:146:GLN:N	5:C:355:HOH:O	2.40	0.41
1:C:129:LYS:HB3	1:C:134:ASN:ND2	2.36	0.41
1:A:85:LYS:O	1:A:85:LYS:HG2	2.21	0.41
1:C:85:LYS:O	1:C:86:ASN:HB3	2.21	0.40
1:C:26:GLY:CA	1:C:71:ARG:HH12	2.33	0.40
2:B:14:VAL:HG12	2:B:15:GLU:H	1.85	0.40
1:A:246:TYR:N	1:A:249:THR:HB	2.36	0.40
1:A:140:GLN:O	1:A:141:PRO:C	2.59	0.40
1:C:153:LYS:HA	1:C:156:LEU:HG	2.03	0.40
1:A:185:PHE:C	1:A:187:GLU:H	2.25	0.40
1:A:165:ILE:HG23	1:A:165:ILE:O	2.22	0.40
1:A:28:VAL:N	5:A:331:HOH:O	2.50	0.40
1:C:287:SER:O	1:C:291:LYS:HG2	2.21	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	294/314 (94%)	241 (82%)	41 (14%)	12 (4%)	4	5
1	C	294/314 (94%)	271 (92%)	17 (6%)	6 (2%)	11	21
2	B	96/98 (98%)	64 (67%)	24 (25%)	8 (8%)	1	1
All	All	684/726 (94%)	576 (84%)	82 (12%)	26 (4%)	5	6

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	ALA
2	B	16	LEU
2	B	61	GLN
1	C	84	ASP
1	C	88	LYS
1	A	290	GLU
2	B	2	THR
2	B	52	VAL
2	B	66	ASP
2	B	76	THR
2	B	95	LEU
1	A	51	ASP
1	A	262	LEU
1	A	294	ILE
1	A	85	LYS
1	C	293	GLY
1	C	306	GLY
1	A	86	ASN
1	A	172	THR
1	A	186	PHE
1	A	241	ALA
1	C	30	ASN
1	C	56	GLU
1	A	255	LYS
2	B	13	GLU
1	A	165	ILE

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	254/265 (96%)	242 (95%)	12 (5%)	36	65
1	C	254/265 (96%)	248 (98%)	6 (2%)	61	87
2	B	82/83 (99%)	76 (93%)	6 (7%)	20	38
All	All	590/613 (96%)	566 (96%)	24 (4%)	41	72

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	51	ASP
1	A	91	LYS
1	A	109	LYS
1	A	127	ILE
1	A	195	ASN
1	A	222	ARG
1	A	247	ILE
1	A	248	GLN
1	A	277	MET
1	A	294	ILE
1	A	298	ASP
2	B	7	LEU
2	B	16	LEU
2	B	37	TYR
2	B	71	ASP
2	B	78	HIS
2	B	89	THR
1	C	118	LEU
1	C	162	ASN
1	C	220	LYS
1	C	239	ASN
1	C	248	GLN
1	C	274	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	90	HIS
1	A	140	GLN
1	A	144	ASN
1	A	146	GLN
1	A	195	ASN
1	A	248	GLN
1	A	310	ASN
2	B	17	GLN
2	B	27	GLN
2	B	58	GLN
2	B	61	GLN
1	C	195	ASN
1	C	226	ASN
1	C	239	ASN

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Mol	Chain	Res	Type
1	C	248	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

3 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	$\# Z > 2$
3	FAD	A	320	-	58,58,58	2.41	19 (32%)	85,89,89	1.38	12 (14%)
4	FES	B	99	2	0,4,4	0.00	-	0,4,4	0.00	-
3	FAD	C	321	-	58,58,58	2.39	18 (31%)	85,89,89	1.47	12 (14%)

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
3	FAD	A	320	-	-	0/34/50/50	0/1/6/6
4	FES	B	99	2	-	0/0/4/4	0/0/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	C	321	-	-	0/34/50/50	0/1/6/6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	321	FAD	P-O3P	-7.87	1.45	1.59
3	A	320	FAD	P-O3P	-7.81	1.45	1.59
3	A	320	FAD	C9A-N10	6.79	1.48	1.38
3	C	321	FAD	C1'-C2'	6.34	1.57	1.51
3	C	321	FAD	C9A-N10	6.13	1.47	1.38
3	A	320	FAD	C1'-C2'	5.73	1.57	1.51
3	A	320	FAD	C4X-C10	4.51	1.48	1.40
3	A	320	FAD	O4B-C1B	4.45	1.48	1.41
3	C	321	FAD	C4X-C10	4.45	1.48	1.40
3	C	321	FAD	O4B-C1B	4.05	1.47	1.41
3	A	320	FAD	PA-O2A	-3.98	1.37	1.55
3	C	321	FAD	PA-O2A	-3.97	1.37	1.55
3	C	321	FAD	C5'-C4'	-3.88	1.45	1.51
3	A	320	FAD	C4-C4X	3.68	1.47	1.41
3	C	321	FAD	P-O2P	-3.57	1.39	1.55
3	A	320	FAD	P-O2P	-3.54	1.39	1.55
3	C	321	FAD	C4-C4X	3.19	1.46	1.41
3	C	321	FAD	C2-N3	3.18	1.43	1.37
3	A	320	FAD	C2-N3	3.15	1.43	1.37
3	C	321	FAD	C8-C7	2.78	1.48	1.40
3	A	320	FAD	O5'-C5'	2.73	1.56	1.44
3	A	320	FAD	C8-C7	2.68	1.48	1.40
3	A	320	FAD	C2A-N1A	2.65	1.39	1.33
3	C	321	FAD	C2A-N3A	2.56	1.37	1.32
3	A	320	FAD	C4A-N3A	2.52	1.39	1.35
3	C	321	FAD	C2A-N1A	2.47	1.38	1.33
3	A	320	FAD	O4B-C4B	2.47	1.50	1.45
3	C	321	FAD	C8A-N9A	2.38	1.40	1.36
3	A	320	FAD	C5X-N5	2.32	1.38	1.35
3	C	321	FAD	C9-C8	2.25	1.44	1.37
3	C	321	FAD	O4B-C4B	2.22	1.50	1.45
3	C	321	FAD	C4A-N3A	2.22	1.39	1.35
3	A	320	FAD	C8A-N9A	2.20	1.39	1.36
3	A	320	FAD	C2A-N3A	2.19	1.36	1.32
3	C	321	FAD	O5'-C5'	2.17	1.53	1.44
3	A	320	FAD	C5B-C4B	2.09	1.58	1.51
3	A	320	FAD	C9A-C5X	2.09	1.46	1.42

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	320	FAD	C2-N1-C10	6.21	121.23	114.98
3	C	321	FAD	C2-N1-C10	5.62	120.64	114.98
3	C	321	FAD	O4B-C1B-N9A	-5.44	103.38	108.44
3	A	320	FAD	O4B-C1B-N9A	-4.05	104.67	108.44
3	C	321	FAD	C4X-C10-N10	-3.66	118.68	120.51
3	C	321	FAD	N3A-C2A-N1A	-3.14	126.08	128.71
3	A	320	FAD	N3A-C2A-N1A	-2.96	126.23	128.71
3	A	320	FAD	C4X-C10-N10	-2.92	119.05	120.51
3	C	321	FAD	O5B-PA-O1A	-2.80	98.39	109.37
3	A	320	FAD	C5'-C4'-C3'	-2.64	107.08	112.06
3	A	320	FAD	C4A-C5A-N7A	2.58	111.73	109.52
3	C	321	FAD	C3B-C2B-C1B	2.55	104.89	100.91
3	A	320	FAD	C5A-C4A-N9A	-2.38	103.73	107.16
3	A	320	FAD	N3A-C4A-N9A	2.37	129.72	125.43
3	A	320	FAD	O5B-PA-O1A	-2.36	100.13	109.37
3	C	321	FAD	C4X-C10-N1	-2.28	120.45	122.73
3	C	321	FAD	C4A-C5A-N7A	2.27	111.46	109.52
3	C	321	FAD	C5'-C4'-C3'	-2.20	107.91	112.06
3	C	321	FAD	N3A-C4A-N9A	2.17	129.36	125.43
3	A	320	FAD	C2A-N1A-C6A	2.15	122.66	118.77
3	A	320	FAD	C3B-C2B-C1B	2.15	104.27	100.91
3	A	320	FAD	C4X-C10-N1	-2.14	120.59	122.73
3	C	321	FAD	C5A-C4A-N9A	-2.11	104.11	107.16
3	C	321	FAD	C2A-N1A-C6A	2.10	122.56	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	296/314 (94%)	0.39	6 (2%) 62 60	25, 49, 79, 89	0
1	C	296/314 (94%)	-0.12	2 (0%) 84 86	9, 32, 59, 77	0
2	B	98/98 (100%)	1.45	29 (29%) 1 1	55, 77, 98, 116	0
All	All	690/726 (95%)	0.32	37 (5%) 25 21	9, 44, 84, 116	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	98	ALA	5.0
2	B	69	ILE	4.8
2	B	49	GLY	4.6
2	B	14	VAL	4.5
1	A	293	GLY	4.4
1	A	286	VAL	4.2
1	A	294	ILE	4.2
2	B	97	GLY	4.0
2	B	24	ILE	3.8
2	B	22	VAL	3.8
1	A	259	TRP	3.5
2	B	87	ILE	3.3
2	B	89	THR	3.2
2	B	53	SER	3.2
2	B	95	LEU	3.0
2	B	18	VAL	2.9
2	B	64	LEU	2.9
2	B	88	GLU	2.9
2	B	80	TYR	2.9
2	B	33	ILE	2.8
2	B	74	VAL	2.8
2	B	96	THR	2.8
2	B	6	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	13	GLU	2.6
2	B	52	VAL	2.6
1	C	147	ILE	2.4
2	B	12	GLY	2.4
2	B	94	GLU	2.2
2	B	37	TYR	2.2
1	C	88	LYS	2.2
2	B	73	TRP	2.1
1	A	305	ARG	2.1
2	B	1	ALA	2.0
2	B	65	ASP	2.0
2	B	79	ALA	2.0
2	B	16	LEU	2.0
1	A	26	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	FAD	C	321	53/53	0.14	-0.27	12,34,53,56	0
3	FAD	A	320	53/53	0.14	-0.44	20,34,50,51	0
4	FES	B	99	4/4	0.08	-2.24	56,58,59,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.