Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:31 pm BST

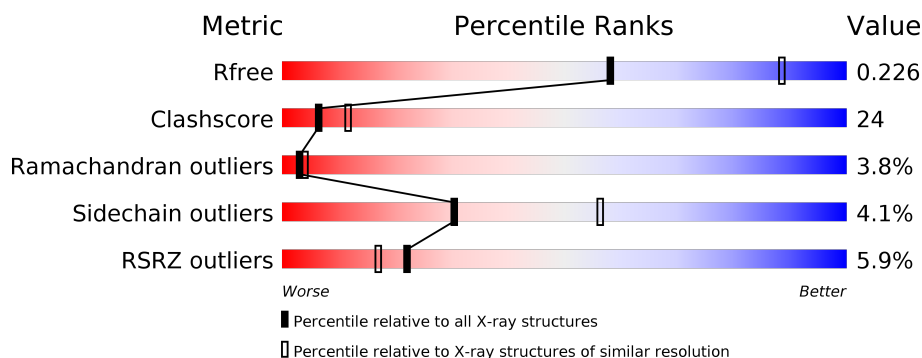|		
PDB ID	:	1GAQ
Title	:	CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN FERREDOXIN AND FERREDOXIN-NADP+ REDUCTASE
Authors	:	Kurisu, G.; Kusunoki, M.; Hase, T.
Deposited on	:	2000-05-08
Resolution	:	2.59 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	Percentile Ranks	Value
Rfree		0.226
Clashscore		24
Ramachandran outliers		3.8%
Sidechain outliers		4.1%
RSRZ outliers		5.9%

Worse   Better

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	314	3% 50% 40% • 6%
1	C	314	62% 30% • 6%
2	B	98	33% 41% 48% 10% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5685 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 FERREDOXIN-NADP+ REDUCTASE.

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

- Molecule 2 is a protein called FERREDOXIN I.

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

- 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 53	C 27	N 9	O 15	P 2	0	0

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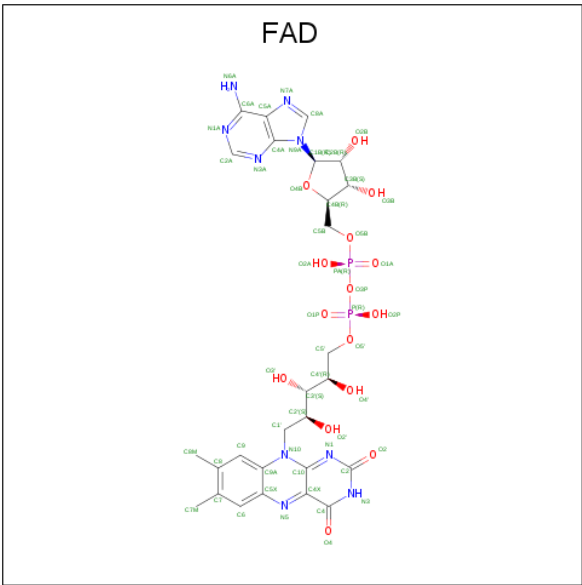
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).
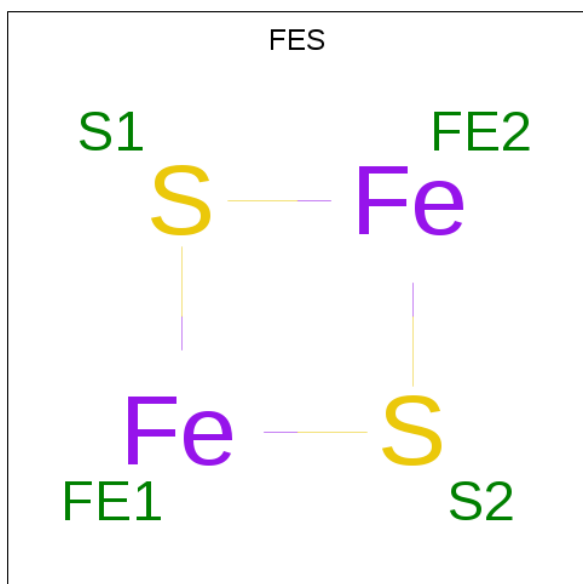
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 4	Fe 2	S 2	0	0

- Molecule 5 is water.

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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: FERREDOXIN-NADP+ REDUCTASE
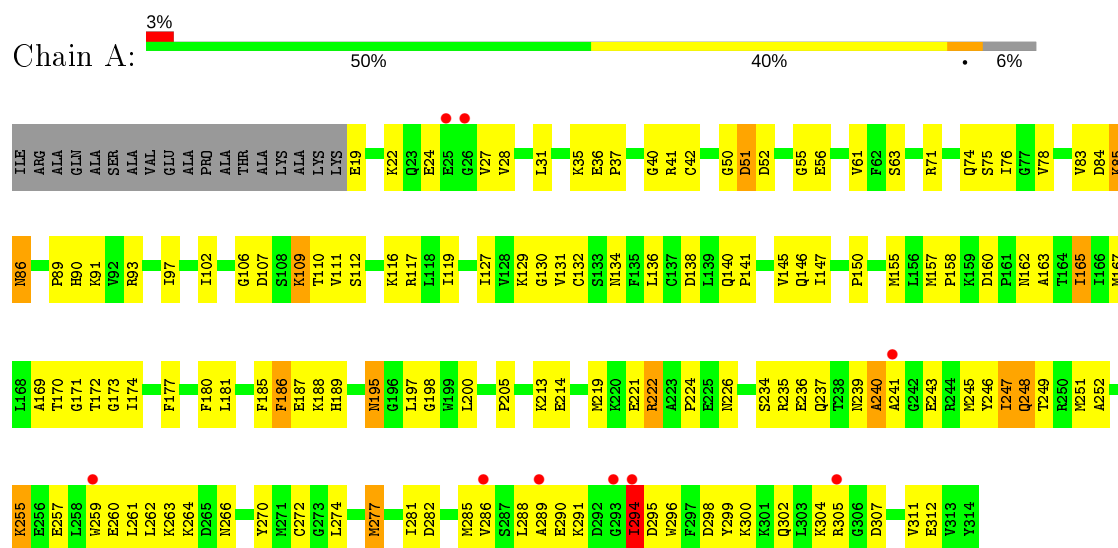
- Molecule 1: FERREDOXIN-NADP+ REDUCTASE

- Molecule 2: FERREDOXIN I

G72 W73 V74 L75 T76 C77 H78 A79 Y80 P81 T82 S83 D84 V85 V86 I87 E88 T89 H90 K91 E92 E93 E94 L95 T96 G97 A98
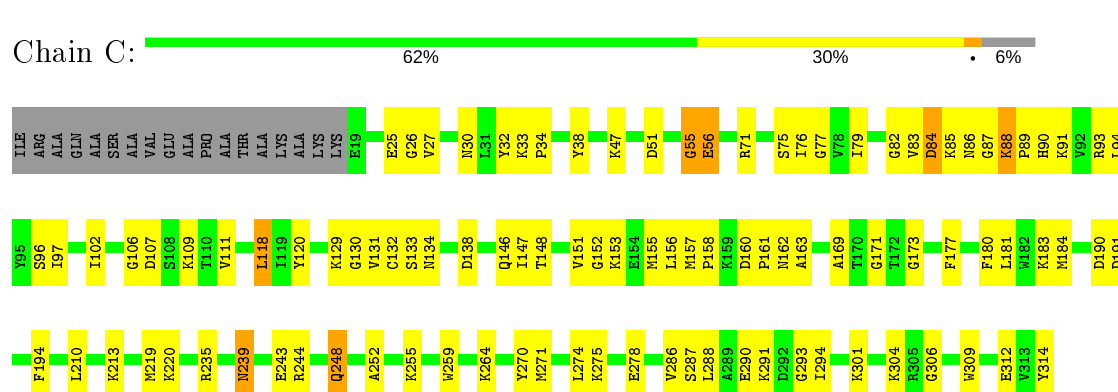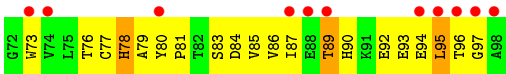
4 Data and refinement statistics (i)

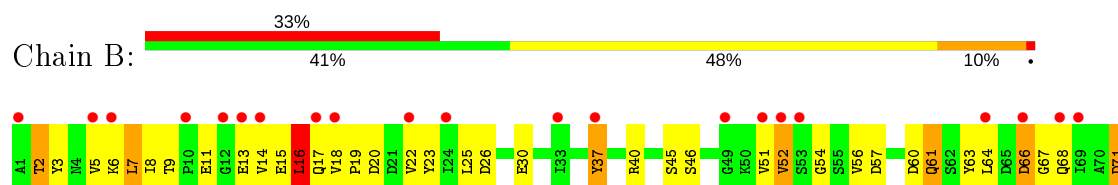| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.07Å 93.41Å 135.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.56 – 2.59 35.44 – 2.68	Depositor EDS
% Data completeness (in resolution range)	97.8 (39.56-2.59) 88.3 (35.44-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.45 (at 2.68Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.232 , 0.297 0.228 , 0.226	Depositor DCC
R_{free} test set	950 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 53.3	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, 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(^{o})	Ideal(^{o})
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 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	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
4	B	4	0	0	0	0
5	A	40	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	13	0	0	3	0
5	C	80	0	0	4	0
All	All	5685	0	5393	261	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 24.

All (261) 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: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
1:A:119:ILE:HG12	1:A:129:LYS:HG2	1.68	0.75
2:B:19:PRO:HG2	2:B:22:VAL:HB	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:93:ARG:HD2	1:C:132:CYS:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:PHE:HB3	1:C:184:MET:CE	2.25	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
2:B:61:GLN:HA	2:B:64:LEU:CD1	2.29	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
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:145:VAL:HB	5:A:326:HOH:O	2.00	0.61
1:A:285:MET:CE	1:A:288:LEU:HD23	2.29	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
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
2:B:51:VAL:HG22	2:B:52:VAL:N	2.17	0.60
2:B:95:LEU:HG	2:B:96:THR:N	2.16	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:A:102:ILE:HG22	1:A:106:GLY:C	2.24	0.57
1:C:33:LYS:HG2	1:C:34:PRO:CD	2.31	0.57
1:A:165:ILE:HG23	1:A:198:GLY:HA2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:GLY:HA3	1:C:71:ARG:HH12	1.70	0.57
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
1:A:155:MET:HE2	1:A:272:CYS:HB2	1.89	0.55
2:B:93:GLU:HB3	5:B:107:HOH:O	2.05	0.55
1:A:93:ARG:HG3	1:A:132:CYS:CB	2.37	0.55
1:A:239:ASN:OD1	1:A:243:GLU:HB2	2.07	0.55
1:C:239:ASN:C	1:C:239:ASN:HD22	2.09	0.55
1:A:234:SER:HA	1:A:245:MET:O	2.07	0.54
1:A:35:LYS:O	1:C:25:GLU:HG2	2.08	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
1:A:171:GLY:C	1:A:173:GLY:H	2.11	0.54
2:B:60:ASP:HA	1:C:190:ASP:OD1	2.07	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:A:264:LYS:HA	5:A:322:HOH:O	2.09	0.52
1:C:155:MET:HG2	1:C:312:GLU:HG3	1.91	0.52
1:A:294:ILE:N	1:A:294:ILE:HD13	2.25	0.52
2:B:8:ILE:HG22	2:B:8:ILE:O	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:174:ILE:HD11	1:A:200:LEU:HD21	1.92	0.51
1:C:301:LYS:HZ2	1:C:301:LYS:HB2	1.76	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:257:GLU:O	1:A:261:LEU:HG	2.11	0.50
1:A:42:CYS:O	1:A:141:PRO:HA	2.12	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: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
1:A:50:GLY:C	1:A:52:ASP:H	2.16	0.49
2:B:8:ILE:N	2:B:8:ILE:HD12	2.28	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:45:SER:HB3	2:B:63:TYR:CE2	2.49	0.48
2:B:85:VAL:HG12	2:B:87:ILE:HG13	1.96	0.48
1:C:130:GLY:O	1:C:134:ASN:HB2	2.13	0.48
1:C:93:ARG:HD2	1:C:132:CYS:CB	2.41	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:A:213:LYS:HG3	1:A:214:GLU:N	2.29	0.47
1:C:118:LEU:HD22	1:C:120:TYR:HD1	1.80	0.47
1:A:186:PHE:HA	1:A:222:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:165:ILE:HD11	1:A:180:PHE:CE2	2.51	0.46
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:239:ASN:CG	1:A:240:ALA:N	2.69	0.46
1:C:27:VAL:HG22	1:C:71:ARG:HG3	1.97	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:171:GLY:C	1:A:173:GLY:N	2.69	0.46
1:A:71:ARG:N	1:A:74:GLN:NE2	2.53	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
1:A:239:ASN:CG	1:A:240:ALA:H	2.18	0.45
2:B:89:THR:O	2:B:90:HIS:HB2	2.17	0.45
2:B:45:SER:HB3	2:B:63:TYR:HE2	1.82	0.45
1:C:88:LYS:CB	1:C:89:PRO:CD	2.95	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:A:197:LEU:HD12	1:A:226:ASN:O	2.16	0.45
1:C:91:LYS:HB3	1:C:91:LYS:NZ	2.31	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:25:LEU:CB	2:B:77:CYS:HA	2.47	0.45
2:B:6:LYS:HD2	2:B:86:VAL:CG2	2.47	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
1:A:311:VAL:HG12	1:A:312:GLU:N	2.30	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:A:169:ALA:HB2	1:A:177:PHE:CD2	2.52	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:C:181:LEU:HB3	1:C:219:MET:SD	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:83:VAL:HG23	1:C:83:VAL:O	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:161:PRO:O	1:C:194:PHE:HA	2.19	0.43
1:C:248:GLN:H	1:C:248:GLN:HE21	1.65	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
2:B:95:LEU:CG	2:B:96:THR:H	2.14	0.43
1:A:24:GLU:HA	1:A:27:VAL:HG21	2.01	0.43
1:C:151:VAL:HG22	1:C:152:GLY:N	2.34	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: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:C:85:LYS:C	1:C:87:GLY:N	2.69	0.42
1:A:260:GLU:HA	1:A:260:GLU:OE2	2.20	0.42
1:A:289:ALA:O	1:A:291:LYS:N	2.52	0.42
1:A:102:ILE:HD11	1:A:189:HIS:CE1	2.55	0.42
1:A:109:LYS:HD3	1:A:110:THR:HG23	2.02	0.42
2:B:64:LEU:HD23	2:B:68:GLN:HE22	1.85	0.42
1:C:111:VAL:HG13	1:C:111:VAL:O	2.20	0.42
1:C:171:GLY:C	1:C:173:GLY:N	2.73	0.42
2:B:25:LEU:HB3	2:B:77:CYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:222:ARG:HG3	1:A:222:ARG:NH1	2.34	0.41
1:A:295:ASP:O	1:A:296:TRP:C	2.58	0.41
1:A:84:ASP:OD1	1:A:86:ASN:HB3	2.21	0.41
1:A:22:LYS:HD3	1:A:307:ASP:HB3	2.03	0.41
1:A:78:VAL:HG11	1:A:136:LEU:HD21	2.03	0.41
1:C:252:ALA:O	1:C:255:LYS:HB2	2.21	0.41
1:C:82:GLY:O	1:C:83:VAL:HG13	2.20	0.41
1:C:129:LYS:HB3	1:C:134:ASN:ND2	2.36	0.41
1:C:146:GLN:N	5:C:355:HOH:O	2.40	0.41
1:C:75:SER:HA	1:C:97:ILE:HG13	2.02	0.41
1:A:305:ARG:HH11	1:A:305:ARG:HG3	1.86	0.41
1:A:85:LYS:O	1:A:85:LYS:HG2	2.21	0.41
1:C:26:GLY:CA	1:C:71:ARG:HH12	2.33	0.40
1:C:85:LYS:O	1:C:86:ASN:HB3	2.21	0.40
2:B:14:VAL:HG12	2:B:15:GLU:H	1.85	0.40
1:A:140:GLN:O	1:A:141:PRO:C	2.59	0.40
1:A:246:TYR:N	1:A:249:THR:HB	2.36	0.40
1:C:153:LYS:HA	1:C:156:LEU:HG	2.03	0.40
1:A:165:ILE:HG23	1:A:165:ILE:O	2.22	0.40
1:A:185:PHE:C	1:A:187:GLU:H	2.25	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 (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	294/314 (94%)	241 (82%)	41 (14%)	12 (4%)	3	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	294/314 (94%)	271 (92%)	17 (6%)	6 (2%)	7	14
2	B	96/98 (98%)	64 (67%)	24 (25%)	8 (8%)	1	1
All	All	684/726 (94%)	576 (84%)	82 (12%)	26 (4%)	3	4

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 (i)

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%)	26	50
1	C	254/265 (96%)	248 (98%)	6 (2%)	49	74
2	B	82/83 (99%)	76 (93%)	6 (7%)	14	28
All	All	590/613 (96%)	566 (96%)	24 (4%)	30	56

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

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Mol	Chain	Res	Type
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
1	C	248	GLN

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 ⓘ

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	-	51,58,58	2.68	23 (45%)	60,89,89	1.70	10 (16%)
3	FAD	C	321	-	51,58,58	2.63	20 (39%)	60,89,89	1.71	11 (18%)
4	FES	B	99	2	0,4,4	0.00	-	-		

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	-	-	1/30/50/50	0/6/6/6
3	FAD	C	321	-	-	9/30/50/50	0/6/6/6
4	FES	B	99	2	-	-	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	320	FAD	C4X-C10	9.93	1.48	1.38
3	C	321	FAD	C4X-C10	9.83	1.48	1.38
3	A	320	FAD	C9A-N10	7.67	1.48	1.38
3	C	321	FAD	C9A-N10	6.95	1.47	1.38
3	A	320	FAD	O4B-C1B	5.09	1.48	1.41
3	C	321	FAD	O4B-C1B	4.66	1.47	1.41
3	C	321	FAD	C5'-C4'	-4.44	1.45	1.51
3	A	320	FAD	PA-O2A	-3.85	1.37	1.55
3	C	321	FAD	PA-O2A	-3.83	1.37	1.55
3	A	320	FAD	C4-N3	3.76	1.39	1.33
3	C	321	FAD	C10-N1	3.48	1.37	1.33
3	C	321	FAD	P-O2P	-3.46	1.39	1.55
3	A	320	FAD	P-O2P	-3.43	1.39	1.55
3	A	320	FAD	C4-C4X	3.41	1.47	1.41
3	C	321	FAD	C4-N3	3.38	1.38	1.33
3	A	320	FAD	C4X-N5	3.24	1.38	1.33
3	C	321	FAD	C8-C7	3.21	1.48	1.40
3	C	321	FAD	C2A-N3A	3.19	1.37	1.32
3	A	320	FAD	C8-C7	3.09	1.48	1.40
3	A	320	FAD	O5'-C5'	2.96	1.56	1.44
3	C	321	FAD	C4-C4X	2.95	1.46	1.41
3	A	320	FAD	C10-N1	2.86	1.36	1.33
3	A	320	FAD	C2A-N1A	2.81	1.39	1.33
3	C	321	FAD	C4X-N5	2.80	1.37	1.33
3	A	320	FAD	C4A-N3A	2.76	1.39	1.35
3	A	320	FAD	C2A-N3A	2.74	1.36	1.32
3	C	321	FAD	C2-N3	2.69	1.43	1.38
3	A	320	FAD	C2-N3	2.67	1.43	1.38
3	C	321	FAD	C2A-N1A	2.62	1.38	1.33
3	A	320	FAD	O4B-C4B	2.60	1.50	1.45
3	C	321	FAD	C9-C8	2.47	1.44	1.37
3	C	321	FAD	C4A-N3A	2.42	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	321	FAD	O5'-C5'	2.36	1.53	1.44
3	C	321	FAD	O4B-C4B	2.35	1.50	1.45
3	C	321	FAD	P-O5'	-2.24	1.50	1.59
3	A	320	FAD	C5B-C4B	2.20	1.58	1.51
3	A	320	FAD	C9-C8	2.17	1.43	1.37
3	A	320	FAD	C9A-C5X	2.14	1.46	1.42
3	A	320	FAD	C2-N1	-2.13	1.33	1.38
3	A	320	FAD	C5X-N5	2.12	1.38	1.35
3	C	321	FAD	PA-O5B	-2.05	1.51	1.59
3	A	320	FAD	C1'-N10	2.04	1.50	1.48
3	A	320	FAD	P-O5'	-2.03	1.51	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	320	FAD	C4-N3-C2	7.77	121.70	115.14
3	C	321	FAD	C4-N3-C2	7.73	121.67	115.14
3	A	320	FAD	C4X-C4-N3	-4.56	117.19	123.43
3	C	321	FAD	C4X-C4-N3	-4.29	117.56	123.43
3	A	320	FAD	C4-C4X-C10	-3.47	117.65	119.95
3	A	320	FAD	C5X-C9A-N10	-3.04	115.51	117.72
3	C	321	FAD	C4-C4X-C10	-2.97	117.99	119.95
3	C	321	FAD	C5X-C9A-N10	-2.92	115.60	117.72
3	C	321	FAD	O5B-PA-O1A	-2.73	98.39	109.07
3	A	320	FAD	C5'-C4'-C3'	-2.65	107.08	112.20
3	C	321	FAD	C3B-C2B-C1B	2.60	104.89	100.98
3	A	320	FAD	C5A-C6A-N1A	-2.32	115.08	120.35
3	C	321	FAD	C5A-C6A-N1A	-2.29	115.16	120.35
3	A	320	FAD	O5B-PA-O1A	-2.29	100.13	109.07
3	A	320	FAD	C2A-N1A-C6A	2.28	122.66	118.75
3	A	320	FAD	C4A-C5A-N7A	2.24	111.73	109.40
3	C	321	FAD	C2A-N1A-C6A	2.23	122.56	118.75
3	C	321	FAD	C5'-C4'-C3'	-2.22	107.91	112.20
3	A	320	FAD	C3B-C2B-C1B	2.19	104.27	100.98
3	C	321	FAD	C5A-C6A-N6A	2.06	123.49	120.35
3	C	321	FAD	C1'-N10-C10	2.03	120.23	118.41

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	321	FAD	C2'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
3	C	321	FAD	O3'-C3'-C4'-O4'
3	C	321	FAD	O3'-C3'-C4'-C5'
3	C	321	FAD	C5'-O5'-P-O1P
3	C	321	FAD	C2'-C3'-C4'-C5'
3	C	321	FAD	C3B-C4B-C5B-O5B
3	C	321	FAD	O4B-C4B-C5B-O5B
3	C	321	FAD	O2'-C2'-C3'-C4'
3	C	321	FAD	C5'-O5'-P-O3P
3	A	320	FAD	P-O3P-PA-O1A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	321	FAD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FAD A 320

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD C 321

Bond lengths

Bond angles

Torsions

Rings
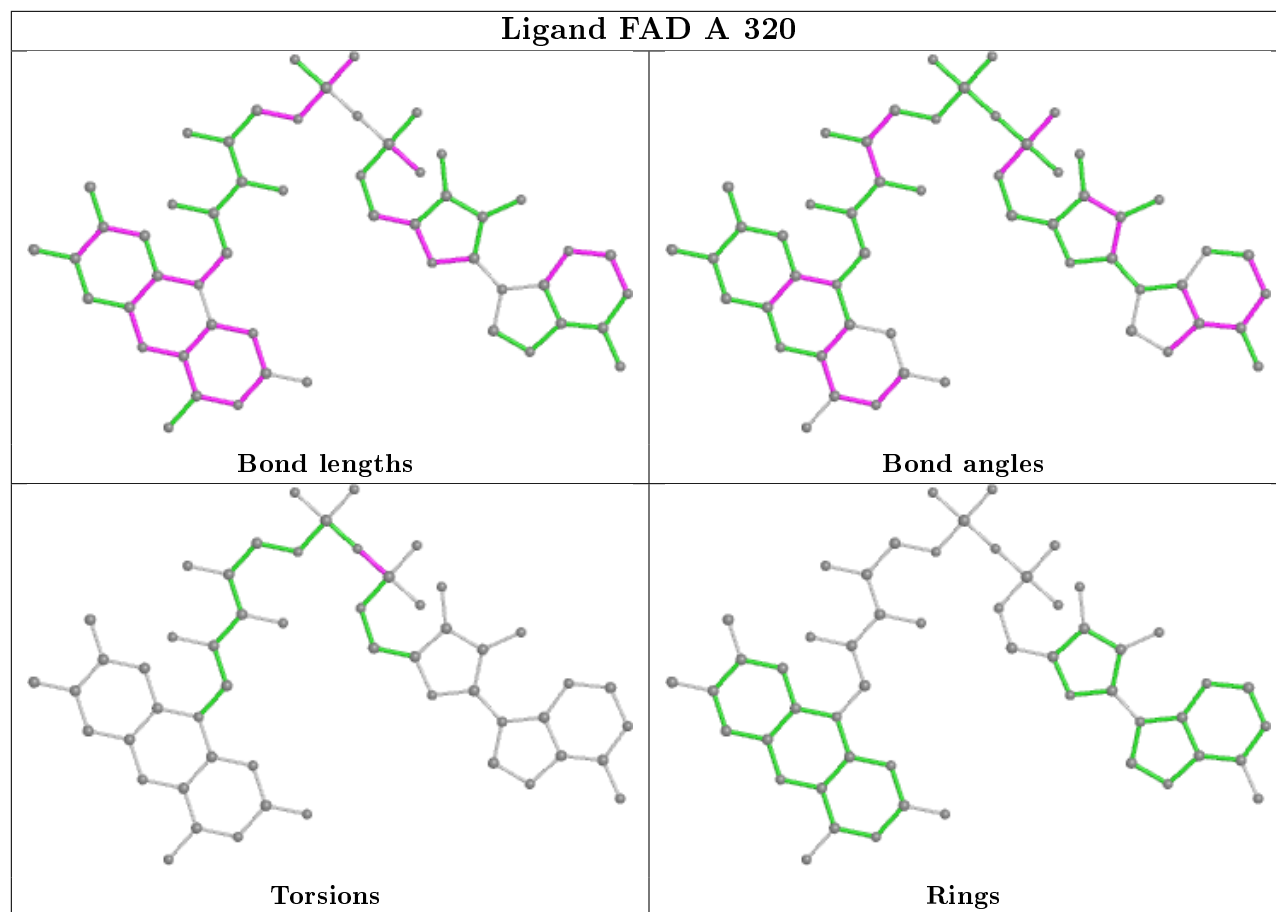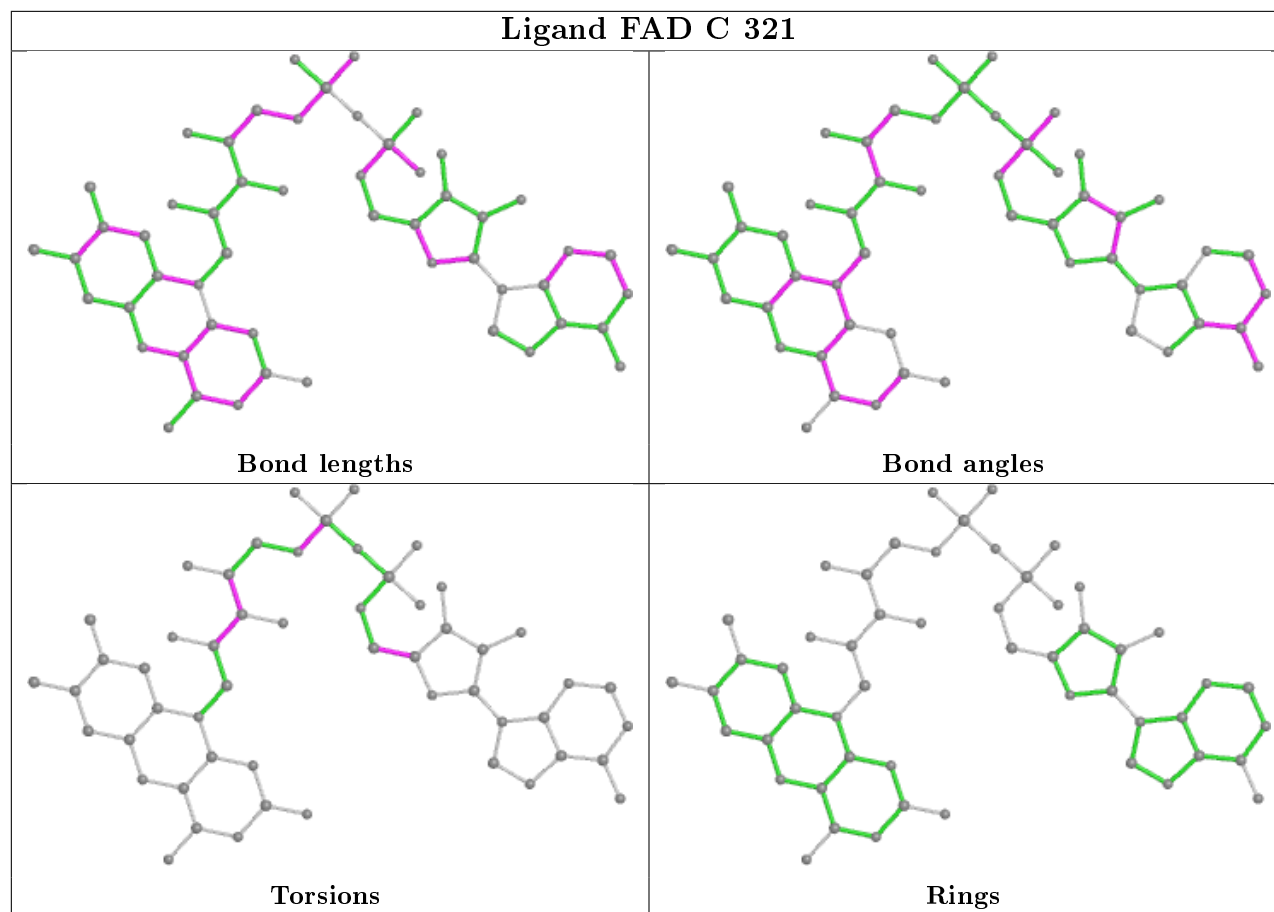
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.38	9 (3%)	50	43	25, 49, 79, 89	0
1	C	296/314 (94%)	-0.14	0	100	100	9, 32, 59, 77	0
2	B	98/98 (100%)	1.52	32 (32%)	0	0	55, 77, 98, 116	0
All	All	690/726 (95%)	0.32	41 (5%)	22	17	9, 44, 84, 116	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	VAL	5.4
2	B	22	VAL	5.3
2	B	49	GLY	4.8
1	A	293	GLY	4.6
2	B	98	ALA	4.5
2	B	69	ILE	4.4
2	B	97	GLY	4.3
1	A	294	ILE	4.2
2	B	14	VAL	3.6
2	B	89	THR	3.4
2	B	24	ILE	3.4
2	B	64	LEU	3.4
2	B	18	VAL	3.2
2	B	96	THR	3.2
2	B	52	VAL	3.1
2	B	80	TYR	3.1
2	B	74	VAL	3.1
2	B	53	SER	3.1
1	A	241	ALA	3.1
2	B	88	GLU	3.0
1	A	259	TRP	2.9
1	A	26	GLY	2.8
2	B	1	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	94	GLU	2.7
2	B	87	ILE	2.7
2	B	10	PRO	2.7
2	B	13	GLU	2.6
1	A	25	GLU	2.5
2	B	12	GLY	2.5
1	A	305	ARG	2.5
2	B	73	TRP	2.5
2	B	95	LEU	2.4
2	B	66	ASP	2.4
2	B	6	LYS	2.3
2	B	68	GLN	2.3
2	B	37	TYR	2.3
2	B	51	VAL	2.2
1	A	289	ALA	2.1
2	B	17	GLN	2.1
2	B	33	ILE	2.1
2	B	5	VAL	2.0

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

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

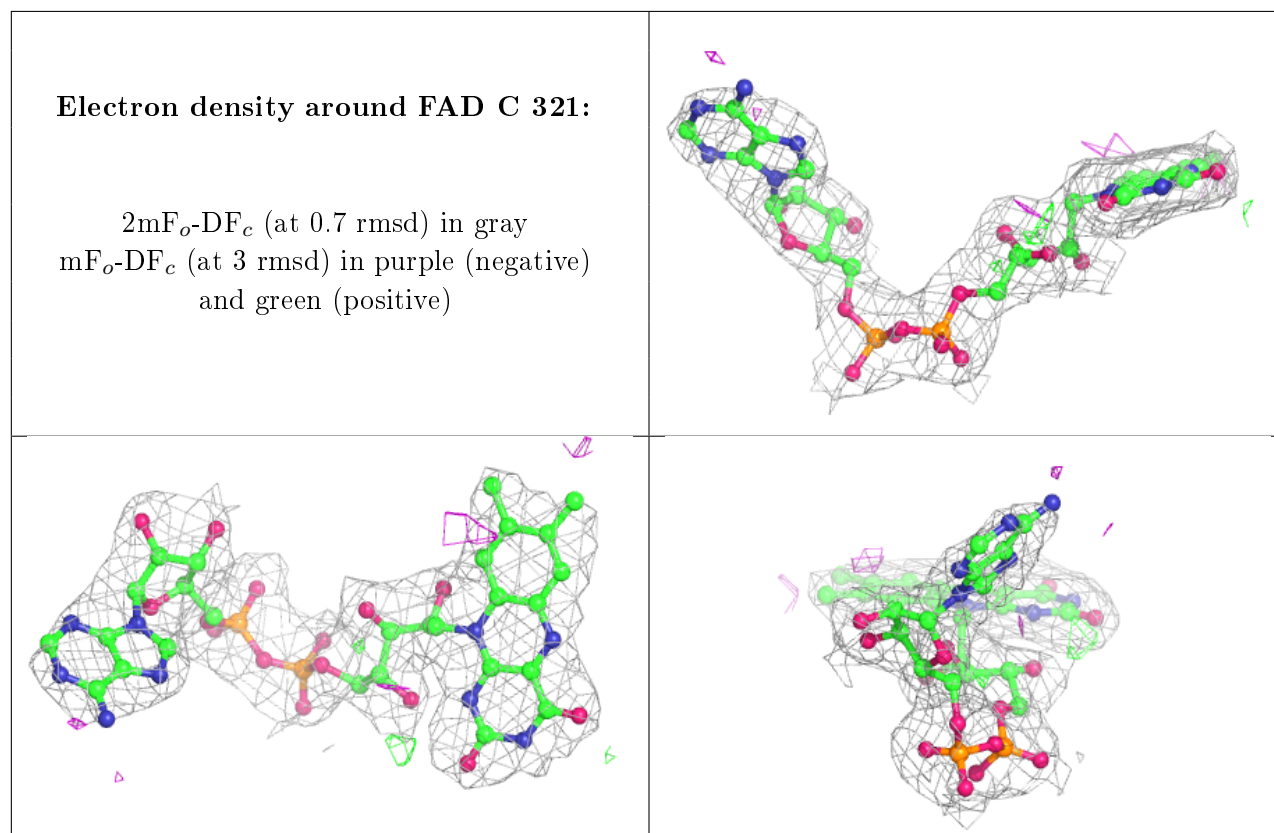## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.
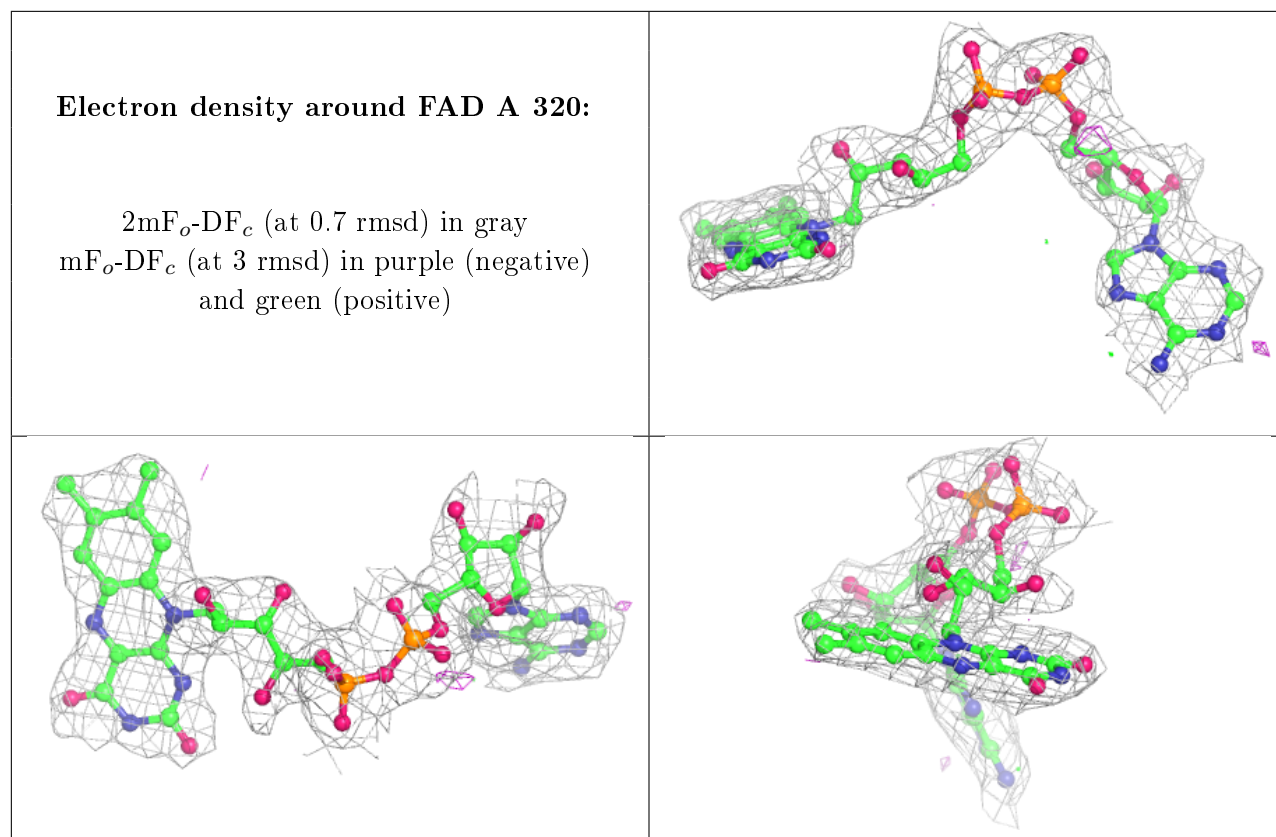
6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FAD	C	321	53/53	0.95	0.14	12,34,53,56	0
3	FAD	A	320	53/53	0.96	0.15	20,34,50,51	0
4	FES	B	99	4/4	0.98	0.09	56,58,59,60	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD C 321:

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

Electron density around FAD A 320:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.