



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:18 PM GMT

PDB ID : 1X0P
Title : Structure of a cyanobacterial BLUF protein, Tll0078
Authors : Kita, A.; Okajima, K.; Morimoto, Y.; Ikeuchi, M.; Miki, K.
Deposited on : 2005-03-27
Resolution : 2.00 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

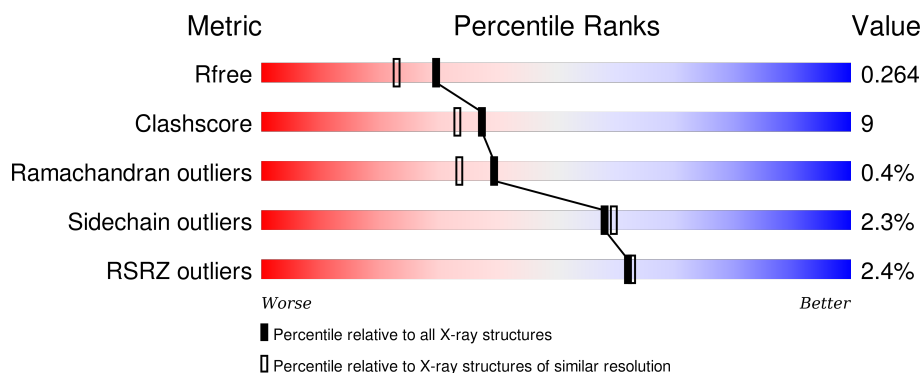
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	143	<div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	B	143	<div> <div>84%</div> <div>13%</div> <div>.</div> </div>
1	C	143	<div> <div>80%</div> <div>17%</div> <div>.</div> </div>
1	D	143	<div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	E	143	<div> <div>78%</div> <div>20%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	143	
1	G	143	
1	H	143	
1	I	143	
1	J	143	

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
2	FAD	B	9151	-	-	-	X
2	FAD	D	9153	-	-	-	X
2	FAD	E	9154	-	-	-	X
2	FAD	G	9156	-	-	-	X
2	FAD	H	9157	-	-	-	X
2	FAD	I	9158	-	-	-	X
2	FAD	J	9159	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11816 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 hypothetical protein Tll0078.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1144	716	204	214	10			
1	B	139	Total	C	N	O	S	0	0	0
			1128	708	200	210	10			
1	C	139	Total	C	N	O	S	0	0	0
			1124	706	200	208	10			
1	D	139	Total	C	N	O	S	0	0	0
			1128	708	200	210	10			
1	E	141	Total	C	N	O	S	0	0	0
			1135	712	200	213	10			
1	F	142	Total	C	N	O	S	0	0	0
			1148	718	204	216	10			
1	G	139	Total	C	N	O	S	0	0	0
			1116	701	199	206	10			
1	H	138	Total	C	N	O	S	0	0	0
			1118	703	199	206	10			
1	I	141	Total	C	N	O	S	0	0	0
			1101	691	194	207	9			
1	J	139	Total	C	N	O	S	0	0	0
			1128	708	200	210	10			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	17	4	6		
2	B	1	Total	C	N	O	0	0
			27	17	4	6		
2	C	1	Total	C	N	O	0	0
			27	17	4	6		
2	D	1	Total	C	N	O	0	0
			27	17	4	6		
2	E	1	Total	C	N	O	0	0
			27	17	4	6		
2	F	1	Total	C	N	O	0	0
			27	17	4	6		
2	G	1	Total	C	N	O	0	0
			27	17	4	6		
2	H	1	Total	C	N	O	0	0
			27	17	4	6		
2	I	1	Total	C	N	O	0	0
			27	17	4	6		
2	J	1	Total	C	N	O	0	0
			27	17	4	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	32	Total	O	0	0
			32	32		

Continued on next page...

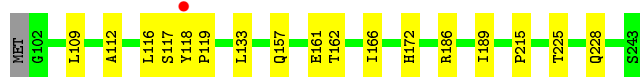
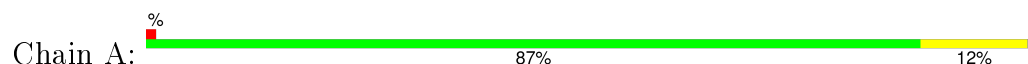
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	30	Total	O	0	0
			30	30		
3	D	25	Total	O	0	0
			25	25		
3	E	22	Total	O	0	0
			22	22		
3	F	35	Total	O	0	0
			35	35		
3	G	29	Total	O	0	0
			29	29		
3	H	22	Total	O	0	0
			22	22		
3	I	20	Total	O	0	0
			20	20		
3	J	22	Total	O	0	0
			22	22		

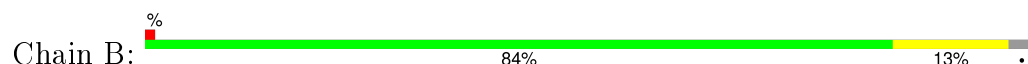
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

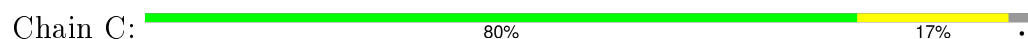
- Molecule 1: hypothetical protein Tll0078



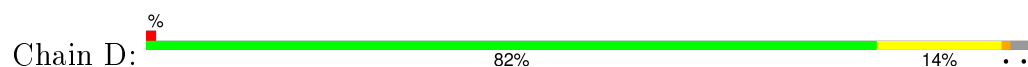
- Molecule 1: hypothetical protein Tll0078



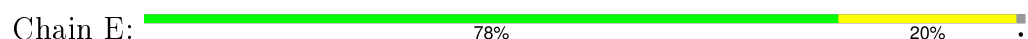
- Molecule 1: hypothetical protein Tll0078



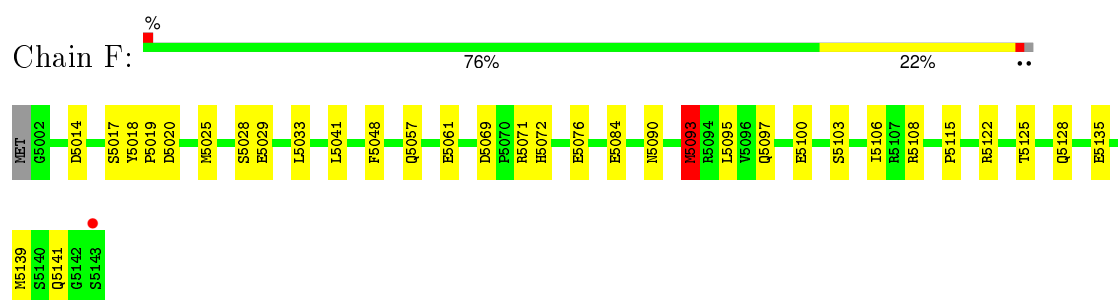
- Molecule 1: hypothetical protein Tll0078



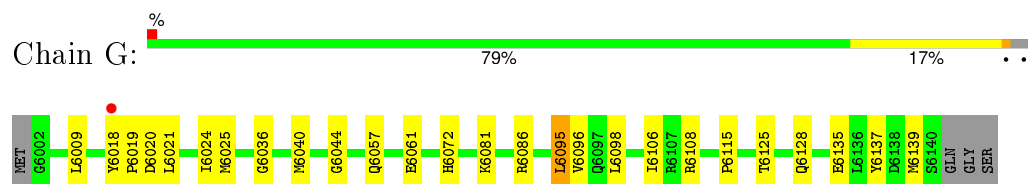
- Molecule 1: hypothetical protein Tll0078



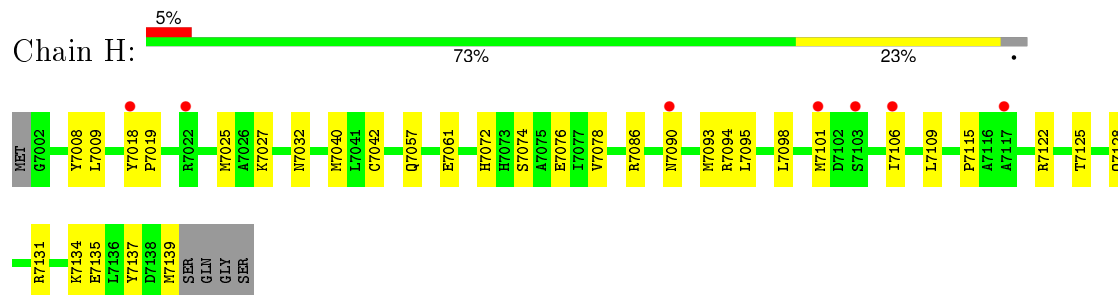
- Molecule 1: hypothetical protein Tll0078



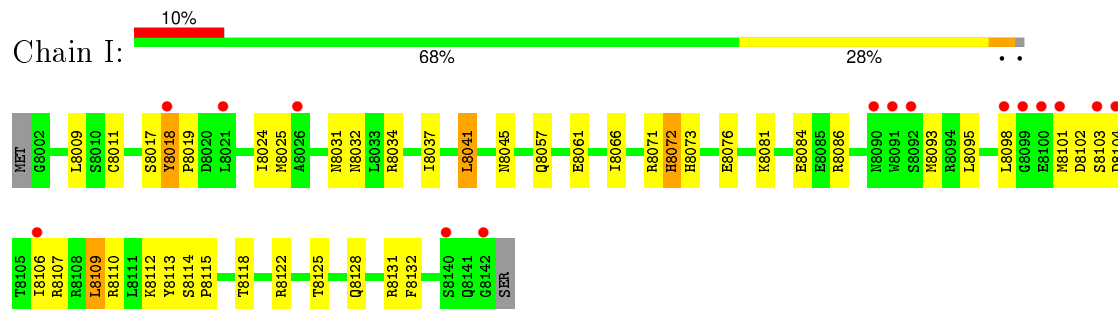
- Molecule 1: hypothetical protein Tll0078



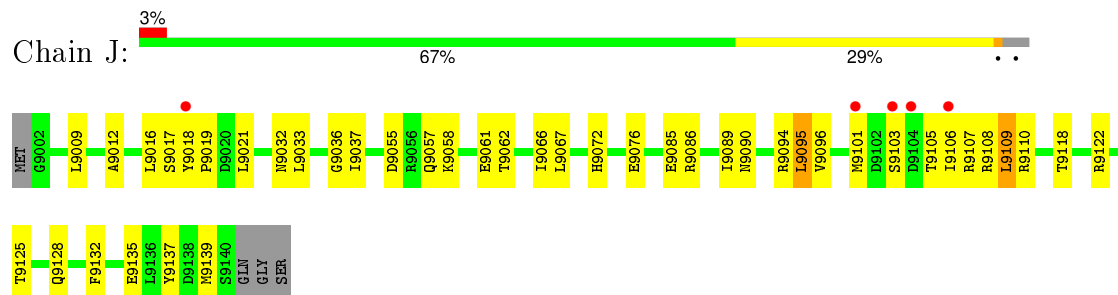
- Molecule 1: hypothetical protein Tll0078



- Molecule 1: hypothetical protein Tll0078



- Molecule 1: hypothetical protein Tll0078



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.51Å 109.85Å 169.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 84.94 – 1.91	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.00) 84.5 (84.94-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 1.91Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.231 , 0.268 0.227 , 0.264	Depositor DCC
R_{free} test set	5177 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 114000 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11816	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.43	0/1164	0.60	0/1562
1	B	0.38	0/1148	0.58	0/1542
1	C	0.39	0/1144	0.58	0/1537
1	D	0.38	0/1148	0.57	0/1542
1	E	0.37	0/1155	0.56	0/1552
1	F	0.37	0/1168	0.58	0/1567
1	G	0.37	0/1136	0.54	0/1528
1	H	0.38	0/1138	0.55	0/1529
1	I	0.36	0/1119	0.52	0/1507
1	J	0.35	0/1148	0.54	0/1542
All	All	0.38	0/11468	0.56	0/15408

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

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	1144	0	1133	11	0
1	B	1128	0	1121	13	0
1	C	1124	0	1117	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1128	0	1121	22	0
1	E	1135	0	1121	21	0
1	F	1148	0	1137	20	0
1	G	1116	0	1102	23	0
1	H	1118	0	1112	32	0
1	I	1101	0	1069	36	0
1	J	1128	0	1121	30	0
2	A	27	0	19	1	0
2	B	27	0	19	0	0
2	C	27	0	19	1	0
2	D	27	0	19	0	0
2	E	27	0	19	0	0
2	F	27	0	19	0	0
2	G	27	0	19	0	0
2	H	27	0	19	1	0
2	I	27	0	19	2	0
2	J	27	0	19	0	0
3	A	39	0	0	0	0
3	B	32	0	0	1	0
3	C	30	0	0	1	0
3	D	25	0	0	0	0
3	E	22	0	0	0	0
3	F	35	0	0	0	0
3	G	29	0	0	2	0
3	H	22	0	0	0	0
3	I	20	0	0	2	0
3	J	22	0	0	1	0
All	All	11816	0	11344	212	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 9.

All (212) 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:G:6098:LEU:HB3	1:G:6106:ILE:HD12	1.53	0.88
1:J:9125:THR:H	1:J:9128:GLN:HE21	1.27	0.81
1:D:3042:CYS:SG	1:D:3098:LEU:HD21	2.21	0.80
1:J:9125:THR:H	1:J:9128:GLN:NE2	1.78	0.80
1:H:7125:THR:H	1:H:7128:GLN:HE21	1.31	0.76
1:H:7125:THR:H	1:H:7128:GLN:NE2	1.87	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3040:MET:HE1	1:D:3094:ARG:HH11	1.54	0.72
1:E:4125:THR:H	1:E:4128:GLN:HE21	1.38	0.71
1:G:6098:LEU:HB3	1:G:6106:ILE:CD1	2.21	0.70
1:D:3125:THR:H	1:D:3128:GLN:NE2	1.89	0.69
1:F:5125:THR:H	1:F:5128:GLN:NE2	1.93	0.66
1:I:8125:THR:H	1:I:8128:GLN:HE21	1.44	0.66
1:H:7074:SER:HB3	1:H:7122:ARG:HH22	1.63	0.63
1:J:9018:TYR:N	1:J:9019:PRO:HD2	2.13	0.63
1:A:225:THR:H	1:A:228:GLN:NE2	1.96	0.63
1:I:8122:ARG:HH11	1:I:8122:ARG:HG2	1.64	0.63
1:F:5103:SER:HA	1:F:5106:ILE:HD12	1.80	0.62
1:A:225:THR:H	1:A:228:GLN:HE21	1.47	0.62
1:C:2125:THR:H	1:C:2128:GLN:HE21	1.46	0.62
1:G:6040:MET:HE1	1:G:6137:TYR:HA	1.82	0.62
1:I:8112:LYS:HE2	1:J:9085:GLU:OE1	2.00	0.62
1:I:8018:TYR:N	1:I:8019:PRO:HD2	2.15	0.61
1:I:8125:THR:H	1:I:8128:GLN:NE2	1.98	0.61
1:F:5057:GLN:O	1:F:5061:GLU:HG3	2.02	0.60
1:H:7040:MET:HE3	1:H:7137:TYR:HD1	1.67	0.60
1:D:3098:LEU:H	1:D:3098:LEU:HD22	1.67	0.59
1:H:7018:TYR:N	1:H:7019:PRO:HD2	2.17	0.59
1:C:2125:THR:H	1:C:2128:GLN:NE2	1.99	0.59
1:I:8107:ARG:HG2	1:I:8110:ARG:NH2	2.18	0.59
1:I:8107:ARG:HG2	1:I:8110:ARG:HH21	1.67	0.59
1:G:6108:ARG:HH21	1:H:7090:ASN:ND2	1.99	0.59
1:I:8041:LEU:HD11	2:I:9158:FAD:HM73	1.85	0.59
1:G:6125:THR:H	1:G:6128:GLN:HE21	1.49	0.58
1:F:5125:THR:H	1:F:5128:GLN:HE21	1.51	0.58
1:B:1131:ARG:NH2	1:F:5084:GLU:HG3	2.18	0.58
1:I:8045:ASN:ND2	1:I:8118:THR:HB	2.18	0.58
1:J:9101:MET:SD	1:J:9106:ILE:HD11	2.43	0.58
1:D:3091:TRP:CG	1:D:3094:ARG:HB2	2.38	0.58
1:I:8031:ASN:HA	1:I:8034:ARG:NH1	2.18	0.58
1:E:4057:GLN:O	1:E:4061:GLU:HG3	2.04	0.58
1:H:7101:MET:HE3	1:H:7106:ILE:HB	1.85	0.58
1:D:3106:ILE:HD13	1:D:3106:ILE:O	2.04	0.58
1:D:3125:THR:H	1:D:3128:GLN:HE21	1.50	0.57
1:H:7040:MET:CE	1:H:7094:ARG:HD3	2.34	0.57
1:E:4136:LEU:HA	1:E:4139:MET:HE3	1.87	0.56
1:J:9012:ALA:HB1	1:J:9016:LEU:HD22	1.88	0.56
1:F:5041:LEU:HD21	1:F:5048:PHE:CD2	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6125:THR:H	1:G:6128:GLN:NE2	2.03	0.56
1:I:8098:LEU:HB3	1:I:8106:ILE:HG21	1.88	0.55
1:B:1018:TYR:N	1:B:1019:PRO:HD2	2.21	0.55
1:F:5025:MET:O	1:F:5029:GLU:HG3	2.07	0.55
1:C:2086:ARG:NH2	1:D:3115:PRO:HA	2.21	0.55
1:E:4125:THR:H	1:E:4128:GLN:NE2	2.05	0.54
1:C:2136:LEU:HA	1:C:2139:MET:HE3	1.89	0.54
1:D:3018:TYR:N	1:D:3019:PRO:HD2	2.23	0.53
1:J:9055:ASP:HB3	1:J:9058:LYS:HB2	1.91	0.53
1:G:6057:GLN:O	1:G:6061:GLU:HG3	2.07	0.53
1:B:1081:LYS:HA	3:G:9405:HOH:O	2.09	0.53
1:H:7040:MET:HE1	1:H:7094:ARG:HD3	1.91	0.53
1:J:9105:THR:HA	1:J:9108:ARG:NH2	2.23	0.52
1:H:7135:GLU:O	1:H:7139:MET:HG3	2.08	0.52
1:F:5097:GLN:HB2	1:F:5100:GLU:OE1	2.08	0.52
1:C:2017:SER:OG	1:C:2019:PRO:HD2	2.10	0.52
1:G:6018:TYR:N	1:G:6019:PRO:HD2	2.25	0.52
1:F:5076:GLU:OE2	1:F:5122:ARG:HD2	2.09	0.52
1:A:157:GLN:O	1:A:161:GLU:HG3	2.09	0.51
1:D:3086:ARG:NH2	1:E:4115:PRO:HA	2.26	0.51
1:C:2063:TYR:CE2	1:C:2067:LEU:HD11	2.46	0.51
1:J:9057:GLN:O	1:J:9061:GLU:HG3	2.11	0.51
1:J:9109:LEU:HD22	1:J:9132:PHE:CD1	2.46	0.51
1:G:6036:GLY:HA2	3:G:9273:HOH:O	2.10	0.51
1:E:4003:LEU:HG	1:E:4083:ILE:HG13	1.92	0.50
1:H:7057:GLN:O	1:H:7061:GLU:HG3	2.10	0.50
1:F:5108:ARG:HH11	1:F:5108:ARG:HG2	1.76	0.50
1:I:8102:ASP:C	1:I:8104:ASP:H	2.13	0.50
1:D:3040:MET:HE2	1:D:3094:ARG:HD3	1.92	0.50
1:I:8009:LEU:HD12	1:I:8009:LEU:C	2.31	0.50
1:C:2110:ARG:HD2	1:C:2118:THR:C	2.32	0.49
1:J:9021:LEU:HD22	1:J:9095:LEU:HD11	1.94	0.49
1:A:117:SER:HB2	1:A:119:PRO:HD2	1.94	0.49
1:I:8057:GLN:O	1:I:8061:GLU:HG3	2.12	0.49
1:G:6025:MET:SD	1:G:6095:LEU:HB2	2.52	0.48
1:C:2025:MET:SD	1:C:2095:LEU:HB2	2.53	0.48
1:J:9009:LEU:C	1:J:9009:LEU:HD12	2.33	0.48
1:I:8103:SER:O	1:I:8107:ARG:HB2	2.14	0.48
1:C:2086:ARG:HH21	1:D:3115:PRO:HA	1.78	0.48
1:C:2022:ARG:HG2	1:C:2022:ARG:HH11	1.79	0.48
1:D:3098:LEU:N	1:D:3098:LEU:HD22	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8113:TYR:CE2	1:I:8131:ARG:HD3	2.48	0.48
1:J:9110:ARG:HD2	1:J:9118:THR:C	2.33	0.48
1:J:9095:LEU:HD23	1:J:9096:VAL:N	2.28	0.48
1:D:3040:MET:CE	1:D:3094:ARG:HH11	2.25	0.48
1:E:4017:SER:HB2	1:E:4019:PRO:HD2	1.94	0.48
1:F:5041:LEU:HD23	1:F:5041:LEU:C	2.34	0.47
1:F:5017:SER:O	1:F:5020:ASP:HB2	2.14	0.47
1:I:8017:SER:HB2	1:I:8019:PRO:HD2	1.96	0.47
1:D:3086:ARG:HH21	1:E:4115:PRO:HA	1.79	0.47
1:E:4018:TYR:O	1:E:4022:ARG:HG3	2.15	0.47
1:C:2040:MET:HE1	1:C:2136:LEU:HB2	1.96	0.47
1:I:8110:ARG:O	1:I:8114:SER:HB3	2.15	0.47
1:I:8109:LEU:HD22	1:I:8132:PHE:CD1	2.50	0.47
1:D:3040:MET:HE3	1:D:3137:TYR:HD1	1.80	0.47
1:B:1086:ARG:HH21	1:C:2115:PRO:HA	1.78	0.47
1:G:6025:MET:CG	1:G:6095:LEU:HD12	2.45	0.47
1:D:3055:ASP:OD2	1:D:3057:GLN:HB3	2.14	0.47
1:B:1057:GLN:HG2	1:B:1061:GLU:OE2	2.15	0.46
1:G:6044:GLY:HA3	1:G:6098:LEU:HD12	1.96	0.46
1:G:6021:LEU:HB3	1:G:6095:LEU:HD11	1.97	0.46
1:I:8076:GLU:OE2	1:I:8122:ARG:NH1	2.49	0.46
1:A:112:ALA:HB1	1:A:116:LEU:HD22	1.96	0.46
1:H:7009:LEU:HD11	1:H:7076:GLU:HB2	1.98	0.46
1:C:2136:LEU:HD23	1:C:2139:MET:CE	2.46	0.46
1:E:4109:LEU:HD22	1:E:4139:MET:HE1	1.97	0.46
1:C:2057:GLN:HA	1:H:7076:GLU:HG2	1.98	0.46
1:G:6115:PRO:HA	1:H:7086:ARG:NH2	2.30	0.46
1:A:186:ARG:HB2	1:A:189:ILE:HG12	1.98	0.46
1:E:4032:ASN:HD22	1:E:4093:MET:HB2	1.81	0.46
1:H:7115:PRO:HA	1:I:8086:ARG:NH2	2.31	0.45
1:B:1086:ARG:NH2	1:C:2115:PRO:HA	2.31	0.45
1:F:5028:SER:HB3	1:F:5093:MET:HG3	1.98	0.45
1:G:6135:GLU:O	1:G:6139:MET:HG2	2.16	0.45
1:B:1025:MET:SD	1:B:1095:LEU:HB2	2.55	0.45
1:B:1098:LEU:HD22	1:B:1106:ILE:CD1	2.47	0.45
1:B:1135:GLU:O	1:B:1139:MET:HG3	2.17	0.45
1:J:9125:THR:N	1:J:9128:GLN:HE21	2.06	0.45
1:J:9018:TYR:N	1:J:9019:PRO:CD	2.80	0.45
1:I:8031:ASN:HA	1:I:8034:ARG:HH12	1.81	0.45
1:H:7025:MET:SD	1:H:7095:LEU:HB2	2.57	0.45
1:I:8025:MET:SD	1:I:8095:LEU:HB2	2.57	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7131:ARG:NH2	1:I:8084:GLU:OE2	2.49	0.45
1:H:7042:CYS:SG	1:H:7098:LEU:HD21	2.57	0.45
1:G:6025:MET:HG2	1:G:6095:LEU:HD12	1.98	0.45
1:C:2136:LEU:HD23	1:C:2139:MET:HE1	1.97	0.44
1:I:8102:ASP:C	1:I:8104:ASP:N	2.70	0.44
1:H:7134:LYS:O	1:H:7137:TYR:HB3	2.17	0.44
1:J:9017:SER:OG	1:J:9019:PRO:HG2	2.18	0.44
1:J:9135:GLU:O	1:J:9139:MET:HG3	2.17	0.44
1:E:4086:ARG:NH2	1:F:5115:PRO:HA	2.32	0.44
1:H:7040:MET:HE2	1:H:7094:ARG:HD3	1.99	0.44
1:J:9036:GLY:HA2	3:J:9249:HOH:O	2.15	0.44
1:G:6108:ARG:HH21	1:H:7090:ASN:HD21	1.65	0.44
1:G:6009:LEU:HD12	1:G:6009:LEU:C	2.38	0.44
1:E:4106:ILE:N	1:E:4106:ILE:HD12	2.33	0.44
1:I:8122:ARG:HB2	3:I:9393:HOH:O	2.17	0.44
1:E:4017:SER:CB	1:E:4019:PRO:HD2	2.48	0.44
1:J:9017:SER:HB2	1:J:9019:PRO:HD2	2.00	0.44
1:J:9086:ARG:HB2	1:J:9089:ILE:HG12	2.00	0.44
1:I:8017:SER:OG	1:I:8019:PRO:HG2	2.18	0.43
1:D:3025:MET:SD	1:D:3095:LEU:HB2	2.58	0.43
1:J:9033:LEU:O	1:J:9033:LEU:HD13	2.19	0.43
1:D:3066:ILE:HG22	1:D:3072:HIS:CE1	2.53	0.43
1:E:4009:LEU:C	1:E:4009:LEU:HD12	2.38	0.43
1:A:215:PRO:HA	1:G:6086:ARG:NH2	2.32	0.43
1:I:8122:ARG:NH1	1:I:8122:ARG:HG2	2.30	0.43
1:A:118:TYR:N	1:A:119:PRO:CD	2.82	0.43
1:E:4018:TYR:N	1:E:4019:PRO:CD	2.81	0.43
1:E:4140:SER:C	1:E:4142:GLY:H	2.20	0.43
1:I:8081:LYS:HA	3:I:9451:HOH:O	2.17	0.43
1:H:7098:LEU:HA	1:H:7101:MET:HE2	2.01	0.43
1:H:7027:LYS:HG2	2:H:9157:FAD:H4'	2.00	0.43
1:H:7009:LEU:CD1	1:H:7076:GLU:HB2	2.49	0.43
1:I:8024:ILE:HD11	1:I:8071:ARG:HD2	2.00	0.43
1:F:5069:ASP:OD1	1:F:5071:ARG:HB2	2.18	0.43
1:G:6108:ARG:HH21	1:H:7090:ASN:CG	2.22	0.43
1:C:2109:LEU:HG	1:C:2132:PHE:CD1	2.54	0.43
1:E:4003:LEU:HG	1:E:4083:ILE:CG1	2.49	0.42
1:J:9090:ASN:ND2	1:J:9137:TYR:OH	2.52	0.42
1:H:7040:MET:HE3	1:H:7137:TYR:CD1	2.51	0.42
1:B:1017:SER:HB2	1:B:1019:PRO:HD2	2.00	0.42
1:B:1125:THR:H	1:B:1128:GLN:HE21	1.65	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4024:ILE:HG13	1:E:4071:ARG:NH1	2.35	0.42
1:D:3016:LEU:HD23	1:D:3043:TYR:CZ	2.54	0.42
1:B:1009:LEU:C	1:B:1009:LEU:HD12	2.40	0.42
1:H:7009:LEU:C	1:H:7009:LEU:HD12	2.40	0.42
1:H:7115:PRO:HA	1:I:8086:ARG:HH21	1.85	0.42
1:C:2036:GLY:HA2	3:C:9243:HOH:O	2.20	0.42
1:J:9062:THR:O	1:J:9066:ILE:HG13	2.20	0.42
1:C:2033:LEU:O	1:C:2033:LEU:HD13	2.19	0.41
1:F:5041:LEU:HD21	1:F:5048:PHE:CE2	2.55	0.41
1:J:9107:ARG:HA	1:J:9110:ARG:NH1	2.36	0.41
1:D:3009:LEU:C	1:D:3009:LEU:HD12	2.41	0.41
1:E:4057:GLN:NE2	1:J:9122:ARG:HH21	2.18	0.41
1:H:7008:TYR:HA	1:H:7078:VAL:HG23	2.02	0.41
1:G:6020:ASP:O	1:G:6024:ILE:HG13	2.20	0.41
1:E:4102:ASP:O	1:E:4106:ILE:HD13	2.21	0.41
1:A:109:LEU:HD12	1:A:109:LEU:C	2.40	0.41
1:J:9095:LEU:HD23	1:J:9096:VAL:H	1.84	0.41
1:I:8011:CYS:HB2	1:I:8073:HIS:CE1	2.56	0.41
1:J:9009:LEU:HG	1:J:9076:GLU:HB2	2.03	0.41
1:C:2020:ASP:O	1:C:2024:ILE:HG13	2.21	0.41
1:H:7032:ASN:HD22	1:H:7093:MET:HB2	1.86	0.41
1:F:5090:ASN:HD22	1:F:5141:GLN:NE2	2.19	0.41
1:C:2033:LEU:C	1:C:2033:LEU:HD13	2.42	0.41
1:I:8032:ASN:HB3	1:I:8037:ILE:O	2.20	0.41
1:A:162:THR:O	1:A:166:ILE:HG13	2.21	0.41
2:A:9150:FAD:H1'1	2:A:9150:FAD:H9	1.86	0.41
2:I:9158:FAD:H1'1	2:I:9158:FAD:H9	1.88	0.41
1:I:8109:LEU:HD22	1:I:8132:PHE:HD1	1.86	0.41
1:I:8115:PRO:HA	1:J:9086:ARG:NH2	2.36	0.41
3:B:9453:HOH:O	1:G:6081:LYS:HA	2.21	0.41
1:D:3106:ILE:HD13	1:D:3106:ILE:C	2.42	0.40
1:I:8066:ILE:HG22	1:I:8072:HIS:CE1	2.56	0.40
1:G:6095:LEU:HD23	1:G:6096:VAL:N	2.37	0.40
2:C:9152:FAD:H9	2:C:9152:FAD:H1'1	1.87	0.40
1:H:7098:LEU:CD2	1:H:7101:MET:HE1	2.52	0.40
1:F:5018:TYR:N	1:F:5019:PRO:HD2	2.36	0.40
1:F:5135:GLU:O	1:F:5139:MET:HG2	2.20	0.40
1:B:1125:THR:H	1:B:1128:GLN:NE2	2.19	0.40
1:J:9032:ASN:HB3	1:J:9037:ILE:O	2.21	0.40
1:H:7098:LEU:HD22	1:H:7101:MET:HE1	2.04	0.40
1:F:5041:LEU:HD22	1:F:5095:LEU:HD13	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:TYR:HB2	1:A:119:PRO:HD3	2.04	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	140/143 (98%)	140 (100%)	0	0	100	100
1	B	137/143 (96%)	135 (98%)	2 (2%)	0	100	100
1	C	137/143 (96%)	134 (98%)	3 (2%)	0	100	100
1	D	137/143 (96%)	135 (98%)	2 (2%)	0	100	100
1	E	139/143 (97%)	136 (98%)	2 (1%)	1 (1%)	26	19
1	F	140/143 (98%)	138 (99%)	1 (1%)	1 (1%)	26	19
1	G	137/143 (96%)	135 (98%)	2 (2%)	0	100	100
1	H	136/143 (95%)	131 (96%)	5 (4%)	0	100	100
1	I	139/143 (97%)	130 (94%)	7 (5%)	2 (1%)	14	6
1	J	137/143 (96%)	133 (97%)	3 (2%)	1 (1%)	26	19
All	All	1379/1430 (96%)	1347 (98%)	27 (2%)	5 (0%)	39	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	5093	MET
1	I	8093	MET
1	J	9103	SER
1	I	8101	MET
1	E	4141	GLN

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	124/126 (98%)	122 (98%)	2 (2%)	70	73
1	B	123/126 (98%)	121 (98%)	2 (2%)	70	73
1	C	122/126 (97%)	121 (99%)	1 (1%)	86	89
1	D	123/126 (98%)	121 (98%)	2 (2%)	70	73
1	E	123/126 (98%)	119 (97%)	4 (3%)	45	43
1	F	125/126 (99%)	121 (97%)	4 (3%)	46	44
1	G	120/126 (95%)	118 (98%)	2 (2%)	68	71
1	H	121/126 (96%)	119 (98%)	2 (2%)	68	71
1	I	115/126 (91%)	111 (96%)	4 (4%)	43	40
1	J	123/126 (98%)	118 (96%)	5 (4%)	37	32
All	All	1219/1260 (97%)	1191 (98%)	28 (2%)	58	60

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	LEU
1	A	172	HIS
1	B	1041	LEU
1	B	1072	HIS
1	C	2072	HIS
1	D	3072	HIS
1	D	3106	ILE
1	E	4014	ASP
1	E	4041	LEU
1	E	4072	HIS
1	E	4107	ARG
1	F	5014	ASP
1	F	5033	LEU
1	F	5072	HIS
1	F	5093	MET
1	G	6072	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	6095	LEU
1	H	7072	HIS
1	H	7109	LEU
1	I	8018	TYR
1	I	8041	LEU
1	I	8072	HIS
1	I	8109	LEU
1	J	9067	LEU
1	J	9072	HIS
1	J	9094	ARG
1	J	9095	LEU
1	J	9109	LEU

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	157	GLN
1	A	228	GLN
1	B	1057	GLN
1	B	1128	GLN
1	C	2120	GLN
1	C	2128	GLN
1	D	3120	GLN
1	D	3128	GLN
1	E	4057	GLN
1	E	4120	GLN
1	E	4128	GLN
1	F	5057	GLN
1	F	5120	GLN
1	F	5128	GLN
1	F	5141	GLN
1	G	6128	GLN
1	H	7128	GLN
1	I	8045	ASN
1	I	8057	GLN
1	I	8120	GLN
1	I	8128	GLN
1	J	9057	GLN
1	J	9090	ASN
1	J	9128	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 ⓘ

10 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	$\# Z > 2$
2	FAD	A	9150	-	26,29,58	2.58	10 (38%)	29,43,89	3.64	10 (34%)
2	FAD	B	9151	-	26,29,58	2.67	13 (50%)	29,43,89	3.63	9 (31%)
2	FAD	C	9152	-	26,29,58	2.50	11 (42%)	29,43,89	3.63	8 (27%)
2	FAD	D	9153	-	26,29,58	2.76	13 (50%)	29,43,89	3.59	8 (27%)
2	FAD	E	9154	-	26,29,58	2.77	12 (46%)	29,43,89	3.60	9 (31%)
2	FAD	F	9155	-	26,29,58	2.54	11 (42%)	29,43,89	3.70	8 (27%)
2	FAD	G	9156	-	26,29,58	2.50	13 (50%)	29,43,89	3.69	8 (27%)
2	FAD	H	9157	-	26,29,58	2.59	11 (42%)	29,43,89	3.64	8 (27%)
2	FAD	I	9158	-	26,29,58	2.60	10 (38%)	29,43,89	3.70	9 (31%)
2	FAD	J	9159	-	26,29,58	2.70	12 (46%)	29,43,89	3.76	9 (31%)

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
2	FAD	A	9150	-	-	0/14/14/50	0/3/3/6
2	FAD	B	9151	-	-	0/14/14/50	0/3/3/6
2	FAD	C	9152	-	-	0/14/14/50	0/3/3/6
2	FAD	D	9153	-	-	0/14/14/50	0/3/3/6
2	FAD	E	9154	-	-	0/14/14/50	0/3/3/6
2	FAD	F	9155	-	-	0/14/14/50	0/3/3/6
2	FAD	G	9156	-	-	0/14/14/50	0/3/3/6
2	FAD	H	9157	-	-	0/14/14/50	0/3/3/6
2	FAD	I	9158	-	-	0/14/14/50	0/3/3/6
2	FAD	J	9159	-	-	0/14/14/50	0/3/3/6

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9150	FAD	C1'-N10	-5.28	1.42	1.48
2	D	9153	FAD	C1'-N10	-4.30	1.43	1.48
2	G	9156	FAD	C1'-N10	-3.74	1.44	1.48
2	F	9155	FAD	C1'-N10	-3.74	1.44	1.48
2	J	9159	FAD	C1'-N10	-3.47	1.44	1.48
2	B	9151	FAD	C1'-N10	-3.43	1.44	1.48
2	E	9154	FAD	C1'-N10	-2.75	1.45	1.48
2	I	9158	FAD	C1'-N10	-2.36	1.45	1.48
2	B	9151	FAD	C2'-C3'	-2.36	1.48	1.53
2	C	9152	FAD	C1'-N10	-2.26	1.46	1.48
2	E	9154	FAD	C2'-C3'	-2.25	1.48	1.53
2	H	9157	FAD	C1'-N10	-2.16	1.46	1.48
2	G	9156	FAD	C2'-C3'	-2.11	1.49	1.53
2	D	9153	FAD	C2'-C3'	-2.10	1.49	1.53
2	E	9154	FAD	C8-C7	2.02	1.46	1.41
2	F	9155	FAD	C8-C7	2.03	1.46	1.41
2	J	9159	FAD	O2'-C2'	2.07	1.48	1.43
2	G	9156	FAD	C4X-C10	2.07	1.44	1.41
2	G	9156	FAD	C8-C7	2.09	1.46	1.41
2	G	9156	FAD	C5'-C4'	2.10	1.58	1.52
2	J	9159	FAD	C10-N10	2.10	1.41	1.39
2	B	9151	FAD	O2'-C2'	2.16	1.48	1.43
2	B	9151	FAD	O4'-C4'	2.16	1.48	1.43
2	I	9158	FAD	C4X-C10	2.16	1.45	1.41
2	D	9153	FAD	O2'-C2'	2.17	1.48	1.43
2	H	9157	FAD	O4'-C4'	2.17	1.48	1.43
2	H	9157	FAD	C4X-C10	2.18	1.45	1.41
2	A	9150	FAD	C8-C7	2.18	1.46	1.41
2	I	9158	FAD	C4-C4X	2.22	1.45	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	9152	FAD	C8-C7	2.24	1.47	1.41
2	G	9156	FAD	C10-N1	2.26	1.39	1.35
2	D	9153	FAD	C4X-C10	2.27	1.45	1.41
2	D	9153	FAD	C10-N10	2.28	1.41	1.39
2	G	9156	FAD	O4'-C4'	2.35	1.48	1.43
2	F	9155	FAD	C4-C4X	2.37	1.46	1.41
2	F	9155	FAD	O4'-C4'	2.38	1.48	1.43
2	D	9153	FAD	O4'-C4'	2.41	1.48	1.43
2	B	9151	FAD	C10-N10	2.44	1.42	1.39
2	I	9158	FAD	O4'-C4'	2.45	1.48	1.43
2	H	9157	FAD	C10-N1	2.45	1.39	1.35
2	A	9150	FAD	C10-N1	2.51	1.39	1.35
2	A	9150	FAD	O4'-C4'	2.56	1.49	1.43
2	C	9152	FAD	C10-N1	2.56	1.39	1.35
2	J	9159	FAD	C4X-C10	2.57	1.45	1.41
2	F	9155	FAD	C5X-N5	2.61	1.39	1.35
2	B	9151	FAD	C4X-C10	2.64	1.46	1.41
2	E	9154	FAD	C4X-C10	2.69	1.46	1.41
2	F	9155	FAD	C4X-C10	2.73	1.46	1.41
2	E	9154	FAD	O4'-C4'	2.76	1.49	1.43
2	C	9152	FAD	O4'-C4'	2.79	1.49	1.43
2	H	9157	FAD	C10-N10	2.81	1.42	1.39
2	F	9155	FAD	C10-N1	2.90	1.40	1.35
2	A	9150	FAD	C4X-C10	2.91	1.46	1.41
2	G	9156	FAD	C4-C4X	2.92	1.47	1.41
2	C	9152	FAD	C4-C4X	2.93	1.47	1.41
2	I	9158	FAD	C5X-N5	2.98	1.40	1.35
2	J	9159	FAD	O4'-C4'	3.01	1.50	1.43
2	C	9152	FAD	C4X-C10	3.02	1.46	1.41
2	B	9151	FAD	C9A-N10	3.07	1.43	1.38
2	C	9152	FAD	C4'-C3'	3.07	1.59	1.53
2	A	9150	FAD	C9A-N10	3.12	1.43	1.38
2	C	9152	FAD	C9A-N10	3.15	1.43	1.38
2	G	9156	FAD	C5X-N5	3.23	1.40	1.35
2	D	9153	FAD	C4-C4X	3.25	1.47	1.41
2	A	9150	FAD	C5X-N5	3.34	1.40	1.35
2	D	9153	FAD	C4'-C3'	3.35	1.60	1.53
2	J	9159	FAD	C10-N1	3.45	1.41	1.35
2	E	9154	FAD	C10-N1	3.47	1.41	1.35
2	I	9158	FAD	C10-N1	3.47	1.41	1.35
2	H	9157	FAD	C4-C4X	3.49	1.48	1.41
2	B	9151	FAD	C10-N1	3.50	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	9153	FAD	C10-N1	3.50	1.41	1.35
2	E	9154	FAD	C4-C4X	3.53	1.48	1.41
2	C	9152	FAD	C5X-N5	3.56	1.41	1.35
2	B	9151	FAD	C4'-C3'	3.59	1.60	1.53
2	H	9157	FAD	C5X-N5	3.59	1.41	1.35
2	J	9159	FAD	C4-C4X	3.63	1.48	1.41
2	B	9151	FAD	C4-C4X	3.65	1.48	1.41
2	J	9159	FAD	C5X-N5	3.84	1.41	1.35
2	E	9154	FAD	C5X-N5	3.86	1.41	1.35
2	E	9154	FAD	C4'-C3'	3.86	1.61	1.53
2	G	9156	FAD	C4'-C3'	3.87	1.61	1.53
2	F	9155	FAD	C4'-C3'	3.91	1.61	1.53
2	G	9156	FAD	C9A-N10	3.96	1.44	1.38
2	D	9153	FAD	C5X-N5	4.03	1.41	1.35
2	J	9159	FAD	C9A-N10	4.04	1.44	1.38
2	I	9158	FAD	C4'-C3'	4.06	1.61	1.53
2	H	9157	FAD	C4'-C3'	4.10	1.61	1.53
2	F	9155	FAD	C9A-N10	4.19	1.44	1.38
2	B	9151	FAD	C5X-N5	4.19	1.42	1.35
2	F	9155	FAD	C4X-N5	4.23	1.40	1.33
2	A	9150	FAD	C4'-C3'	4.24	1.62	1.53
2	E	9154	FAD	C9A-N10	4.29	1.44	1.38
2	J	9159	FAD	C4'-C3'	4.34	1.62	1.53
2	D	9153	FAD	C9A-N10	4.42	1.44	1.38
2	H	9157	FAD	C9A-N10	4.49	1.45	1.38
2	G	9156	FAD	C4X-N5	4.87	1.41	1.33
2	A	9150	FAD	C4X-N5	5.10	1.41	1.33
2	J	9159	FAD	C4X-N5	5.10	1.41	1.33
2	J	9159	FAD	C4-N3	5.19	1.42	1.33
2	G	9156	FAD	C4-N3	5.20	1.42	1.33
2	H	9157	FAD	C4X-N5	5.31	1.41	1.33
2	A	9150	FAD	C4-N3	5.32	1.43	1.33
2	H	9157	FAD	C4-N3	5.33	1.43	1.33
2	I	9158	FAD	C4X-N5	5.38	1.41	1.33
2	I	9158	FAD	C9A-N10	5.39	1.46	1.38
2	I	9158	FAD	C4-N3	5.41	1.43	1.33
2	B	9151	FAD	C4X-N5	5.48	1.41	1.33
2	B	9151	FAD	C4-N3	5.49	1.43	1.33
2	D	9153	FAD	C4-N3	5.56	1.43	1.33
2	C	9152	FAD	C4-N3	5.60	1.43	1.33
2	C	9152	FAD	C4X-N5	5.61	1.42	1.33
2	D	9153	FAD	C4X-N5	5.84	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	9154	FAD	C4-N3	5.88	1.44	1.33
2	E	9154	FAD	C4X-N5	5.93	1.42	1.33
2	F	9155	FAD	C4-N3	5.98	1.44	1.33

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	9152	FAD	C4X-C4-N3	-7.70	113.07	123.59
2	H	9157	FAD	C4X-C4-N3	-7.53	113.29	123.59
2	J	9159	FAD	C4X-C4-N3	-7.42	113.45	123.59
2	G	9156	FAD	C4X-C4-N3	-7.35	113.54	123.59
2	B	9151	FAD	C4X-C4-N3	-7.19	113.76	123.59
2	A	9150	FAD	C4X-C4-N3	-7.16	113.80	123.59
2	F	9155	FAD	C4X-C4-N3	-7.16	113.80	123.59
2	I	9158	FAD	C4X-C4-N3	-7.12	113.86	123.59
2	E	9154	FAD	C4X-C4-N3	-7.08	113.90	123.59
2	D	9153	FAD	C4X-C4-N3	-7.01	114.01	123.59
2	F	9155	FAD	C4-C4X-N5	-3.70	114.22	118.72
2	I	9158	FAD	C4-C4X-N5	-3.63	114.32	118.72
2	A	9150	FAD	C4-C4X-N5	-3.08	114.98	118.72
2	G	9156	FAD	C4-C4X-N5	-2.99	115.09	118.72
2	D	9153	FAD	C4-C4X-N5	-2.88	115.23	118.72
2	H	9157	FAD	C4-C4X-N5	-2.82	115.30	118.72
2	J	9159	FAD	C4-C4X-N5	-2.77	115.36	118.72
2	C	9152	FAD	C4-C4X-N5	-2.62	115.54	118.72
2	B	9151	FAD	C4-C4X-N5	-2.54	115.64	118.72
2	E	9154	FAD	C4-C4X-N5	-2.31	115.91	118.72
2	A	9150	FAD	O4'-C4'-C5'	-2.27	103.92	109.22
2	I	9158	FAD	O2'-C2'-C1'	-2.03	104.96	109.94
2	J	9159	FAD	O3'-C3'-C4'	2.14	114.14	108.75
2	B	9151	FAD	O3'-C3'-C4'	2.19	114.27	108.75
2	E	9154	FAD	O3'-C3'-C4'	2.39	114.78	108.75
2	A	9150	FAD	O3'-C3'-C4'	2.43	114.86	108.75
2	B	9151	FAD	C1'-N10-C9A	2.96	122.19	118.86
2	E	9154	FAD	C1'-N10-C9A	2.99	122.22	118.86
2	H	9157	FAD	C5X-C9A-N10	3.05	119.94	117.62
2	G	9156	FAD	C5X-C9A-N10	3.06	119.95	117.62
2	F	9155	FAD	C5X-C9A-N10	3.08	119.96	117.62
2	C	9152	FAD	C5X-C9A-N10	3.19	120.04	117.62
2	D	9153	FAD	C1'-N10-C9A	3.30	122.56	118.86
2	C	9152	FAD	C1'-N10-C9A	3.30	122.57	118.86
2	A	9150	FAD	C5X-C9A-N10	3.30	120.13	117.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	9157	FAD	C1'-N10-C9A	3.37	122.64	118.86
2	A	9150	FAD	C1'-N10-C9A	3.42	122.70	118.86
2	J	9159	FAD	C5X-C9A-N10	3.43	120.22	117.62
2	I	9158	FAD	C5X-C9A-N10	3.43	120.23	117.62
2	I	9158	FAD	C1'-N10-C9A	3.44	122.73	118.86
2	D	9153	FAD	C5X-C9A-N10	3.49	120.27	117.62
2	E	9154	FAD	C5X-C9A-N10	3.53	120.30	117.62
2	F	9155	FAD	C1'-N10-C9A	3.59	122.89	118.86
2	B	9151	FAD	O2'-C2'-C3'	3.66	118.22	109.02
2	E	9154	FAD	O2'-C2'-C3'	3.74	118.42	109.02
2	G	9156	FAD	C1'-N10-C9A	3.82	123.15	118.86
2	B	9151	FAD	C5X-C9A-N10	3.87	120.56	117.62
2	G	9156	FAD	O2'-C2'-C3'	3.90	118.83	109.02
2	I	9158	FAD	O2'-C2'-C3'	3.91	118.86	109.02
2	D	9153	FAD	O2'-C2'-C3'	3.94	118.91	109.02
2	H	9157	FAD	O2'-C2'-C3'	3.98	119.01	109.02
2	J	9159	FAD	C1'-N10-C9A	4.05	123.40	118.86
2	F	9155	FAD	O2'-C2'-C3'	4.10	119.32	109.02
2	J	9159	FAD	O2'-C2'-C3'	4.11	119.34	109.02
2	A	9150	FAD	O2'-C2'-C3'	4.22	119.64	109.02
2	C	9152	FAD	O2'-C2'-C3'	4.27	119.76	109.02
2	E	9154	FAD	C4-C4X-C10	4.81	123.02	119.94
2	C	9152	FAD	C4-C4X-C10	5.13	123.22	119.94
2	A	9150	FAD	C4-C4X-C10	5.21	123.27	119.94
2	B	9151	FAD	C4-C4X-C10	5.25	123.30	119.94
2	J	9159	FAD	C4-C4X-C10	5.39	123.39	119.94
2	D	9153	FAD	C4-C4X-C10	5.59	123.52	119.94
2	G	9156	FAD	C4-C4X-C10	5.79	123.65	119.94
2	H	9157	FAD	C4-C4X-C10	5.97	123.76	119.94
2	I	9158	FAD	C4-C4X-C10	6.07	123.82	119.94
2	F	9155	FAD	C4-C4X-C10	6.35	124.00	119.94
2	C	9152	FAD	O5'-C5'-C4'	7.97	128.42	111.10
2	D	9153	FAD	O5'-C5'-C4'	8.06	128.61	111.10
2	A	9150	FAD	O5'-C5'-C4'	8.10	128.72	111.10
2	H	9157	FAD	O5'-C5'-C4'	8.10	128.72	111.10
2	I	9158	FAD	O5'-C5'-C4'	8.32	129.19	111.10
2	E	9154	FAD	O5'-C5'-C4'	8.65	129.91	111.10
2	B	9151	FAD	O5'-C5'-C4'	8.85	130.35	111.10
2	J	9159	FAD	O5'-C5'-C4'	8.87	130.38	111.10
2	G	9156	FAD	O5'-C5'-C4'	8.93	130.52	111.10
2	F	9155	FAD	O5'-C5'-C4'	8.97	130.59	111.10
2	F	9155	FAD	C4-N3-C2	12.14	125.74	115.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	9156	FAD	C4-N3-C2	12.53	126.08	115.25
2	H	9157	FAD	C4-N3-C2	12.61	126.15	115.25
2	D	9153	FAD	C4-N3-C2	12.72	126.24	115.25
2	B	9151	FAD	C4-N3-C2	12.73	126.25	115.25
2	E	9154	FAD	C4-N3-C2	12.90	126.40	115.25
2	I	9158	FAD	C4-N3-C2	12.92	126.41	115.25
2	A	9150	FAD	C4-N3-C2	12.95	126.44	115.25
2	C	9152	FAD	C4-N3-C2	13.15	126.61	115.25
2	J	9159	FAD	C4-N3-C2	13.31	126.75	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9150	FAD	1	0
2	C	9152	FAD	1	0
2	H	9157	FAD	1	0
2	I	9158	FAD	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	142/143 (99%)	-0.10	1 (0%) 89 89	16, 24, 33, 39	0
1	B	139/143 (97%)	-0.09	1 (0%) 89 89	16, 26, 36, 42	0
1	C	139/143 (97%)	-0.11	0 100 100	20, 27, 36, 43	0
1	D	139/143 (97%)	-0.02	2 (1%) 78 78	20, 29, 36, 43	0
1	E	141/143 (98%)	-0.00	0 100 100	21, 30, 39, 46	0
1	F	142/143 (99%)	-0.06	1 (0%) 89 89	17, 27, 38, 47	0
1	G	139/143 (97%)	-0.02	1 (0%) 89 89	19, 29, 42, 48	0
1	H	138/143 (96%)	0.16	7 (5%) 32 33	22, 31, 41, 46	0
1	I	141/143 (98%)	0.57	15 (10%) 8 9	22, 35, 45, 49	0
1	J	139/143 (97%)	0.19	5 (3%) 46 48	22, 32, 42, 46	0
All	All	1399/1430 (97%)	0.05	33 (2%) 62 63	16, 29, 41, 49	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	8101	MET	8.3
1	I	8099	GLY	6.1
1	I	8100	GLU	5.8
1	G	6018	TYR	5.1
1	I	8142	GLY	5.1
1	I	8106	ILE	4.4
1	I	8018	TYR	4.2
1	I	8098	LEU	3.7
1	I	8103	SER	3.2
1	H	7106	ILE	3.1
1	I	8140	SER	3.0
1	J	9018	TYR	3.0
1	I	8090	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	3018	TYR	2.9
1	I	8104	ASP	2.8
1	J	9101	MET	2.8
1	B	1018	TYR	2.6
1	I	8026	ALA	2.6
1	I	8021	LEU	2.5
1	F	5143	SER	2.5
1	A	118	TYR	2.5
1	H	7018	TYR	2.5
1	H	7090	ASN	2.5
1	I	8092	SER	2.4
1	H	7101	MET	2.3
1	I	8091	TRP	2.2
1	J	9106	ILE	2.2
1	H	7022	ARG	2.2
1	H	7117	ALA	2.2
1	H	7103	SER	2.1
1	D	3099	GLY	2.0
1	J	9103	SER	2.0
1	J	9104	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(Å ²)	Q<0.9
2	FAD	E	9154	27/53	0.79	0.25	5.87	29,36,43,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FAD	B	9151	27/53	0.82	0.21	5.33	29,35,38,41	0
2	FAD	G	9156	27/53	0.84	0.16	4.77	31,37,43,48	0
2	FAD	I	9158	27/53	0.83	0.26	4.54	35,42,47,48	0
2	FAD	D	9153	27/53	0.81	0.20	3.87	31,34,41,46	0
2	FAD	H	9157	27/53	0.86	0.18	3.85	31,35,42,43	0
2	FAD	J	9159	27/53	0.85	0.19	3.67	35,38,43,47	0
2	FAD	F	9155	27/53	0.86	0.18	1.92	30,33,38,39	0
2	FAD	A	9150	27/53	0.90	0.16	1.46	25,29,34,38	0
2	FAD	C	9152	27/53	0.91	0.15	1.36	23,29,35,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.