W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 06:22 PM GMT

PDB ID	:	2HFO
Title	:	Crystal Structures of the Synechocystis Photoreceptor Slr1694 Reveal Distinct Structural States Related to Signaling
Authors	:	Yuan, H.; Anderson, S.; Masuda, S.; Dragnea, V.; Moffat, K.; Bauer, C.E.
Deposited on	:	2006-06-24
Resolution	:	2.10 Å(reported)

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

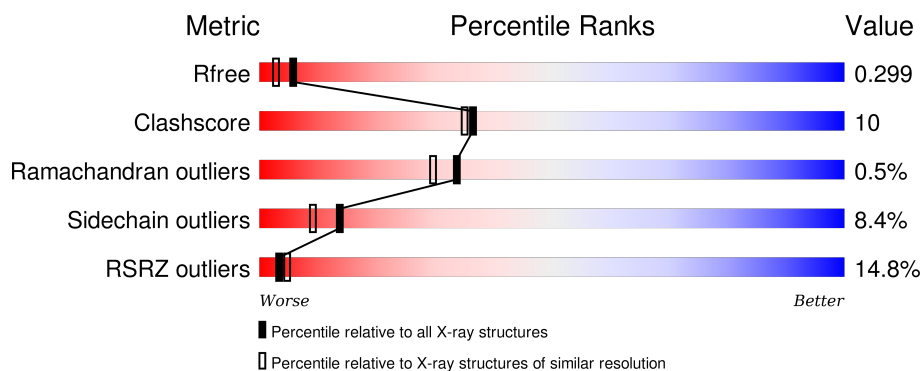|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.10 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		0.299
Clashscore		10
Ramachandran outliers		0.5%
Sidechain outliers		8.4%
RSRZ outliers		14.8%

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	153	11% / 80% · 15% · ·
1	B	153	19% / 71% · 18% · · 8%
1	C	153	18% / 66% · 19% · 11%
1	D	153	17% / 69% · 21% · 5% · ·
1	E	153	10% / 76% · 14% · 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	153	9% 75% 16% · 8%
1	G	153	13% 75% 15% · 9%
1	H	153	12% 74% 16% · 8%
1	I	153	13% 74% 16% · 7%
1	J	153	14% 72% 16% ·· 9%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 11646 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 Activator of photopigment and puc expression.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total 1205	C 762	N 205	O 230	S 8	0	0	0
1	B	140	Total 1109	C 702	N 193	O 206	S 8	0	0	0
1	C	136	Total 1067	C 675	N 186	O 198	S 8	0	0	0
1	D	147	Total 1167	C 737	N 201	O 221	S 8	0	0	0
1	E	141	Total 1107	C 700	N 190	O 209	S 8	0	0	0
1	F	140	Total 1115	C 704	N 194	O 209	S 8	0	0	0
1	G	139	Total 1099	C 693	N 192	O 206	S 8	0	0	0
1	H	141	Total 1121	C 708	N 195	O 210	S 8	0	0	0
1	I	142	Total 1117	C 707	N 193	O 209	S 8	0	0	0
1	J	139	Total 1100	C 692	N 190	O 210	S 8	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	CLONING ARTIFACT	UNP P74295
A	2	GLY	-	CLONING ARTIFACT	UNP P74295
A	3	HIS	-	CLONING ARTIFACT	UNP P74295
B	1	ALA	-	CLONING ARTIFACT	UNP P74295
B	2	GLY	-	CLONING ARTIFACT	UNP P74295
B	3	HIS	-	CLONING ARTIFACT	UNP P74295
C	1	ALA	-	CLONING ARTIFACT	UNP P74295
C	2	GLY	-	CLONING ARTIFACT	UNP P74295
C	3	HIS	-	CLONING ARTIFACT	UNP P74295

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	ALA	-	CLONING ARTIFACT	UNP P74295
D	2	GLY	-	CLONING ARTIFACT	UNP P74295
D	3	HIS	-	CLONING ARTIFACT	UNP P74295
E	1	ALA	-	CLONING ARTIFACT	UNP P74295
E	2	GLY	-	CLONING ARTIFACT	UNP P74295
E	3	HIS	-	CLONING ARTIFACT	UNP P74295
F	1	ALA	-	CLONING ARTIFACT	UNP P74295
F	2	GLY	-	CLONING ARTIFACT	UNP P74295
F	3	HIS	-	CLONING ARTIFACT	UNP P74295
G	1	ALA	-	CLONING ARTIFACT	UNP P74295
G	2	GLY	-	CLONING ARTIFACT	UNP P74295
G	3	HIS	-	CLONING ARTIFACT	UNP P74295
H	1	ALA	-	CLONING ARTIFACT	UNP P74295
H	2	GLY	-	CLONING ARTIFACT	UNP P74295
H	3	HIS	-	CLONING ARTIFACT	UNP P74295
I	1	ALA	-	CLONING ARTIFACT	UNP P74295
I	2	GLY	-	CLONING ARTIFACT	UNP P74295
I	3	HIS	-	CLONING ARTIFACT	UNP P74295
J	1	ALA	-	CLONING ARTIFACT	UNP P74295
J	2	GLY	-	CLONING ARTIFACT	UNP P74295
J	3	HIS	-	CLONING ARTIFACT	UNP P74295

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).
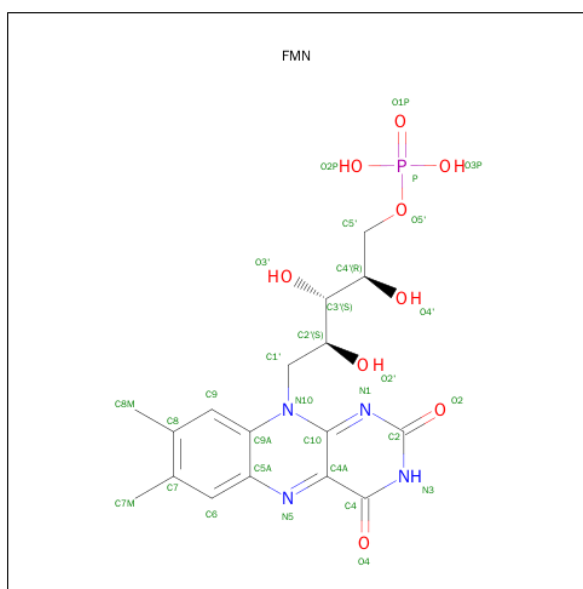
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	17	4	9	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total 31	C 17	N 4	O 9	P 1		0	0
2	C	1	Total 31	C 17	N 4	O 9	P 1		0	0
2	D	1	Total 31	C 17	N 4	O 9	P 1		0	0
2	E	1	Total 31	C 17	N 4	O 9	P 1		0	0
2	F	1	Total 31	C 17	N 4	O 9	P 1		0	0
2	G	1	Total 31	C 17	N 4	O 9	P 1		0	0
2	H	1	Total 31	C 17	N 4	O 9	P 1		0	0
2	I	1	Total 31	C 17	N 4	O 9	P 1		0	0
2	J	1	Total 31	C 17	N 4	O 9	P 1		0	0

- Molecule 3 is water.

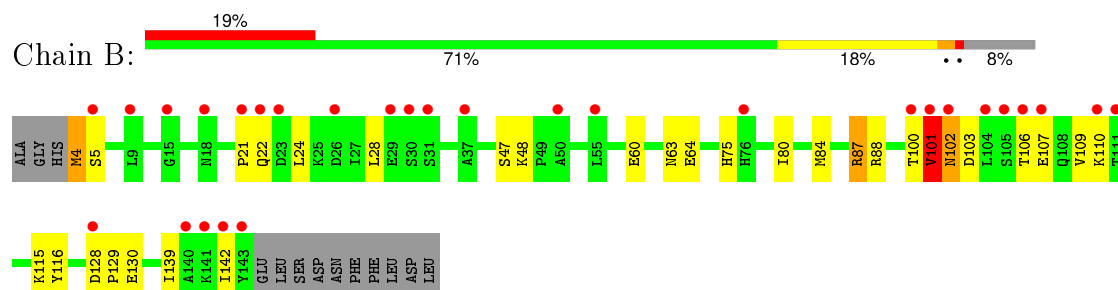| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total 22	O 22	0	0
3	B	6	Total 6	O 6	0	0
3	C	12	Total 12	O 12	0	0
3	D	29	Total 29	O 29	0	0
3	E	12	Total 12	O 12	0	0
3	F	8	Total 8	O 8	0	0
3	G	13	Total 13	O 13	0	0
3	H	10	Total 10	O 10	0	0
3	I	9	Total 9	O 9	0	0
3	J	8	Total 8	O 8	0	0

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 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.
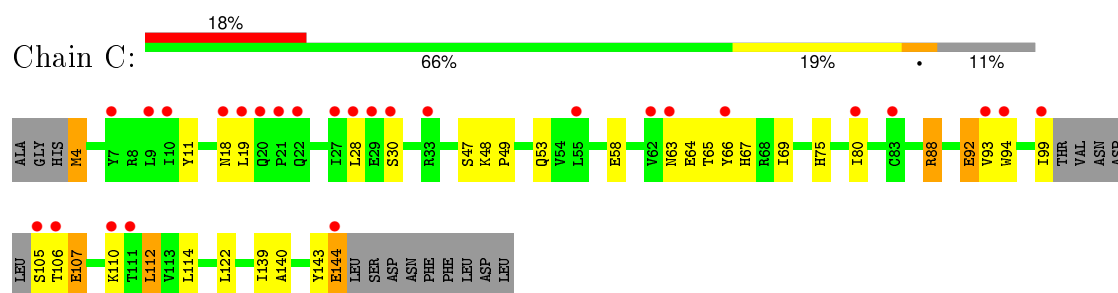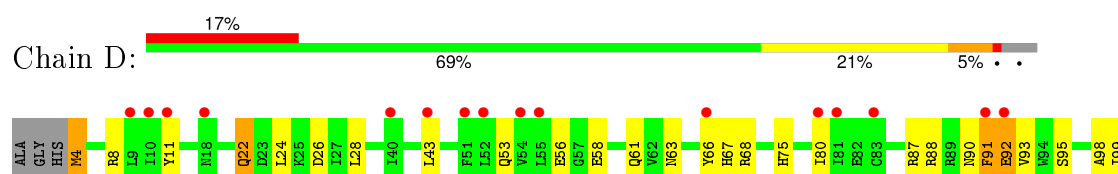
- Molecule 1: Activator of photopigment and puc expression

- Molecule 1: Activator of photopigment and puc expression

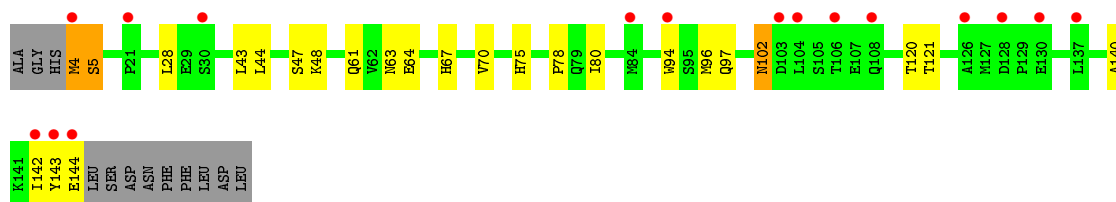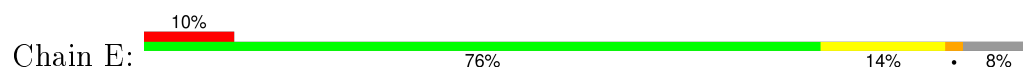- Molecule 1: Activator of photopigment and puc expression

- Molecule 1: Activator of photopigment and puc expression

T100 V101 M102 D103 L104 S105 T106 E107 Q108 K115 T120 T121 L122 E130 F135 L136 K141 I142 Y143 E144 L145 S146 D147 N148 F149 F150 LEU ASP LEU

● Molecule 1: Activator of photopigment and puc expression

Chain E:

10%

76%　　　　　14%　　8%

ALA GLY HIS M4 S5 P21 L28 E29 S30 L43 L44 S47 K48 Q61 V62 N63 E64 H67 V70 H75 P78 Q79 I80 M84 W94 S95 M96 Q97 M102 D103 L104 S105 T106 E107 Q108 T120 T121 A126 M127 D128 P129 E130 L137 A140

K141 I142 Y143 E144 LEU SER ASP ASN PHE LEU ASP LEU

● Molecule 1: Activator of photopigment and puc expression

Chain F:

9%

75%　　　　　16%　　8%

ALA GLY HIS M4 S5 I16 Q20 D23 D26 I27 L28 E29 S30 S31 N34 L43 L44 K48 P49 Q53 N63 E64 H67 H75 I80 V93 M96 Q97 A98 I99 N102 D103 L104 S105 T106 E107 K115 Y116 D128 L136 I139

A140 K141 I142 Y143 GLU LEU SER ASP ASN PHE LEU ASP LEU

● Molecule 1: Activator of photopigment and puc expression

Chain G:

13%

75%　　　　　15%　　9%

ALA GLY HIS M4 L9 I10 N18 P21 Q22 D23 L24 K25 D26 I27 L28 E29 S30 S31 Q32 L43 L52 L55 E56 G57 N63 E64 T65 Y66 H67 R68 H75 I80 C83 R87 N90 Q97 A98 I99 N102 D103 L104 S105 T106 E107 Q108 L112 T120 A126 M127 D128 L137 D138 I139 A140 K141 I142 TYR GLU LEU SER ASP ASN PHE PHE LEU ASP LEU

● Molecule 1: Activator of photopigment and puc expression

Chain H:

12%

74%　　　　　16%　　8%

ALA GLY HIS M4 S5 L9 N18 L19 Q20 P21 Q22 L28 E29 S30 S47 K48 P49 L55 E58 Q61 V62 N63 E64 T65 Y66 H67 H75 I80 C83 R87 I99 N102 D103 L104 S105 T106 E107 Q108 T111 L112 T120 T121 E130
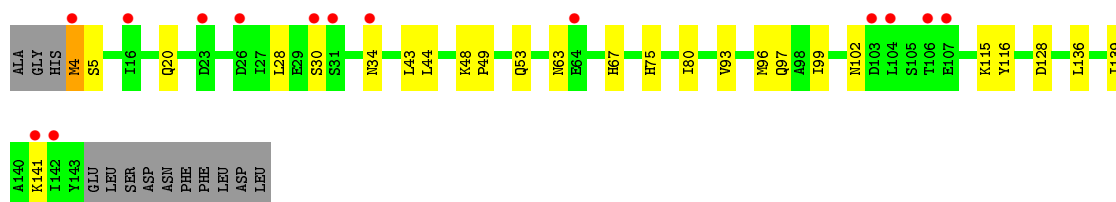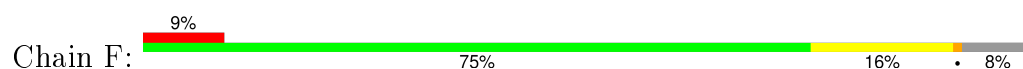
L137 K141 I142 Y143 E144 LEU SER ASP ASN PHE PHE LEU ASP LEU

● Molecule 1: Activator of photopigment and puc expression

Chain I:

13%

74%　　　　　16%　　7%

• Molecule 1: Activator of photopigment and puc expression

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	119.42Å 147.68Å 96.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.10 47.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.8 (48.00-2.10) 90.8 (47.96-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.237 , 0.286 0.265 , 0.299	Depositor DCC
R_{free} test set	4477 reflections (4.96%)	DCC
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 65.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	0 of 90451 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11646	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN

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	0.70	0/1229	0.74	0/1667
1	B	0.73	1/1131 (0.1%)	0.72	0/1536
1	C	0.68	0/1088	0.73	0/1478
1	D	0.70	0/1190	0.90	5/1616 (0.3%)
1	E	0.55	0/1129	0.70	0/1536
1	F	0.80	1/1137 (0.1%)	0.71	1/1544 (0.1%)
1	G	0.55	0/1120	0.73	0/1521
1	H	0.58	0/1143	0.66	0/1552
1	I	0.55	0/1139	0.69	1/1549 (0.1%)
1	J	0.60	0/1119	0.73	1/1518 (0.1%)
All	All	0.65	2/11425 (0.0%)	0.74	8/15517 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	D	0	2
1	H	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	20	GLN	CD-OE1	17.50	1.62	1.24
1	B	22	GLN	CD-NE2	10.33	1.58	1.32

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	148	ASN	N-CA-C	-6.91	92.34	111.00
1	F	20	GLN	CG-CD-OE1	-6.27	109.06	121.60
1	D	91	PHE	C-N-CA	6.17	137.12	121.70
1	D	144	GLU	N-CA-C	-6.05	94.68	111.00
1	I	114	LEU	CA-CB-CG	5.97	129.03	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	101	VAL	Peptide
1	B	102	ASN	Peptide
1	D	143	TYR	Peptide
1	D	147	ASP	Peptide
1	H	142	ILE	Peptide

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	1205	0	1182	20	0
1	B	1109	0	1096	18	0
1	C	1067	0	1036	34	0
1	D	1167	0	1141	44	0
1	E	1107	0	1078	26	0
1	F	1115	0	1102	22	0
1	G	1099	0	1087	19	0
1	H	1121	0	1106	21	0
1	I	1117	0	1094	30	0
1	J	1100	0	1079	20	0
2	A	31	0	19	0	0
2	B	31	0	19	1	0
2	C	31	0	19	1	0
2	D	31	0	19	1	0
2	E	31	0	19	0	0
2	F	31	0	19	2	0
2	G	31	0	19	1	0
2	H	31	0	19	0	0

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	31	0	19	0	0
2	J	31	0	19	0	0
3	A	22	0	0	3	0
3	B	6	0	0	0	0
3	C	12	0	0	0	0
3	D	29	0	0	5	0
3	E	12	0	0	1	0
3	F	8	0	0	1	0
3	G	13	0	0	1	0
3	H	10	0	0	1	0
3	I	9	0	0	2	0
3	J	8	0	0	1	0
All	All	11646	0	11191	216	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 216 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:I:59:CYS:HB3	3:I:160:HOH:O	1.26	1.27
1:D:93:VAL:HB	3:D:176:HOH:O	1.43	1.18
1:F:44:LEU:HB2	1:F:96:MET:CE	1.91	1.01
1:E:43:LEU:C	1:E:96:MET:HE1	1.81	1.00
1:A:84:MET:HB3	3:A:173:HOH:O	1.64	0.97

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	148/153 (97%)	145 (98%)	3 (2%)	0	100	100
1	B	138/153 (90%)	131 (95%)	5 (4%)	2 (1%)	14	7
1	C	132/153 (86%)	128 (97%)	3 (2%)	1 (1%)	24	17
1	D	145/153 (95%)	140 (97%)	3 (2%)	2 (1%)	14	7
1	E	139/153 (91%)	137 (99%)	2 (1%)	0	100	100
1	F	138/153 (90%)	134 (97%)	4 (3%)	0	100	100
1	G	137/153 (90%)	132 (96%)	5 (4%)	0	100	100
1	H	139/153 (91%)	135 (97%)	3 (2%)	1 (1%)	26	21
1	I	140/153 (92%)	139 (99%)	1 (1%)	0	100	100
1	J	135/153 (88%)	129 (96%)	5 (4%)	1 (1%)	26	21
All	All	1391/1530 (91%)	1350 (97%)	34 (2%)	7 (0%)	34	30

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	VAL
1	C	107	GLU
1	D	92	GLU
1	H	143	TYR
1	J	92	GLU

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	137/141 (97%)	124 (90%)	13 (10%)	11	7
1	B	124/141 (88%)	115 (93%)	9 (7%)	17	13
1	C	117/141 (83%)	104 (89%)	13 (11%)	8	4
1	D	131/141 (93%)	121 (92%)	10 (8%)	16	12
1	E	123/141 (87%)	114 (93%)	9 (7%)	17	13
1	F	126/141 (89%)	118 (94%)	8 (6%)	22	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	124/141 (88%)	113 (91%)	11 (9%)	12	8
1	H	126/141 (89%)	115 (91%)	11 (9%)	13	8
1	I	124/141 (88%)	112 (90%)	12 (10%)	10	6
1	J	124/141 (88%)	114 (92%)	10 (8%)	15	10
All	All	1256/1410 (89%)	1150 (92%)	106 (8%)	14	9

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	28	LEU
1	F	102	ASN
1	J	19	LEU
1	E	75	HIS
1	E	142	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	148	ASN
1	F	61	GLN
1	J	61	GLN
1	E	32	GLN
1	E	67	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	FMN	A	154	-	32,33,33	1.34	4 (12%)	34,50,50	1.49	6 (17%)
2	FMN	B	154	-	32,33,33	1.39	4 (12%)	34,50,50	1.75	4 (11%)
2	FMN	C	154	-	32,33,33	1.20	4 (12%)	34,50,50	1.63	6 (17%)
2	FMN	D	154	-	32,33,33	1.51	6 (18%)	34,50,50	1.71	5 (14%)
2	FMN	E	154	-	32,33,33	1.36	4 (12%)	34,50,50	2.19	8 (23%)
2	FMN	F	154	-	32,33,33	1.29	4 (12%)	34,50,50	1.69	5 (14%)
2	FMN	G	154	-	32,33,33	1.23	4 (12%)	34,50,50	1.63	5 (14%)
2	FMN	H	154	-	32,33,33	1.30	5 (15%)	34,50,50	1.83	7 (20%)
2	FMN	I	154	-	32,33,33	1.28	4 (12%)	34,50,50	1.79	6 (17%)
2	FMN	J	201	-	32,33,33	1.47	4 (12%)	34,50,50	1.82	9 (26%)

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	FMN	A	154	-	-	0/18/18/18	0/3/3/3
2	FMN	B	154	-	-	0/18/18/18	0/3/3/3
2	FMN	C	154	-	-	0/18/18/18	0/3/3/3
2	FMN	D	154	-	-	0/18/18/18	0/3/3/3
2	FMN	E	154	-	-	0/18/18/18	0/3/3/3
2	FMN	F	154	-	-	0/18/18/18	0/3/3/3
2	FMN	G	154	-	-	0/18/18/18	0/3/3/3
2	FMN	H	154	-	-	0/18/18/18	0/3/3/3
2	FMN	I	154	-	-	0/18/18/18	0/3/3/3
2	FMN	J	201	-	-	0/18/18/18	0/3/3/3

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	154	FMN	C4A-C10	-2.24	1.36	1.40
2	D	154	FMN	C4-C4A	-2.13	1.36	1.41
2	H	154	FMN	C9A-C5A	-2.10	1.38	1.42
2	I	154	FMN	C5A-N5	2.02	1.38	1.35
2	C	154	FMN	C5A-N5	2.10	1.38	1.35

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	154	FMN	N3-C2-N1	-5.86	117.81	127.69
2	D	154	FMN	N3-C2-N1	-4.71	119.76	127.69
2	I	154	FMN	N3-C2-N1	-4.37	120.33	127.69
2	C	154	FMN	N3-C2-N1	-4.11	120.77	127.69
2	F	154	FMN	N3-C2-N1	-4.08	120.82	127.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	154	FMN	1	0
2	C	154	FMN	1	0
2	D	154	FMN	1	0
2	F	154	FMN	2	0
2	G	154	FMN	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	150/153 (98%)	0.85	17 (11%)	7	9	32, 41, 47, 57	0
1	B	140/153 (91%)	1.29	29 (20%)	1	1	36, 42, 51, 64	0
1	C	136/153 (88%)	1.20	27 (19%)	1	2	35, 42, 50, 63	0
1	D	147/153 (96%)	1.26	26 (17%)	2	3	36, 42, 48, 55	0
1	E	141/153 (92%)	0.81	16 (11%)	7	9	35, 42, 48, 65	0
1	F	140/153 (91%)	1.03	14 (10%)	9	13	35, 41, 47, 68	0
1	G	139/153 (90%)	0.99	20 (14%)	3	5	37, 42, 47, 64	0
1	H	141/153 (92%)	1.06	19 (13%)	4	6	36, 42, 48, 64	0
1	I	142/153 (92%)	1.11	20 (14%)	4	5	36, 42, 50, 70	0
1	J	139/153 (90%)	1.16	22 (15%)	3	4	36, 42, 50, 66	0
All	All	1415/1530 (92%)	1.07	210 (14%)	3	5	32, 42, 49, 70	0

The worst 5 of 210 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106	THR	9.6
1	F	104	LEU	7.4
1	F	103	ASP	7.1
1	B	101	VAL	7.0
1	H	21	PRO	5.8

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	FMN	B	154	31/31	0.85	0.20	0.56	33,35,48,51	5
2	FMN	G	154	31/31	0.85	0.18	-0.26	34,36,48,48	5
2	FMN	E	154	31/31	0.85	0.17	-0.30	30,37,51,52	5
2	FMN	I	154	31/31	0.81	0.17	-0.36	41,45,54,57	5
2	FMN	H	154	31/31	0.91	0.16	-0.42	35,36,43,50	5
2	FMN	F	154	31/31	0.85	0.14	-0.57	39,41,51,52	5
2	FMN	A	154	31/31	0.85	0.15	-0.68	26,29,39,44	5
2	FMN	J	201	31/31	0.91	0.18	-0.69	31,35,37,41	5
2	FMN	C	154	31/31	0.90	0.15	-0.79	26,29,43,45	5
2	FMN	D	154	31/31	0.91	0.15	-1.10	17,23,36,40	5

6.5 Other polymers (i)

There are no such residues in this entry.