



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2016 – 02:02 PM EDT

PDB ID : 5J3W  
Title : Crystal structures reveal signaling states of a short blue light photoreceptor protein PpSB1-LOV (dark state)  
Authors : Granzin, J.; Batra-Safferling, R.  
Deposited on : 2016-03-31  
Resolution : 2.55 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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-20027939  
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-20027939

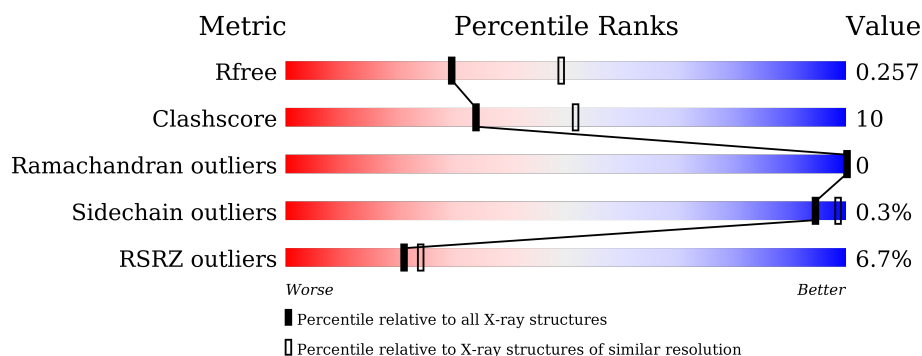
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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  $\geq 3$ , 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	162	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>18%</div> <div>•</div> <div>18%</div> </div> </div>
1	B	162	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>13%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	162	<div> <div>12%</div> <div> <div></div> <div>63%</div> <div>19%</div> <div>•</div> <div>17%</div> </div> </div>
1	D	162	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>15%</div> <div>•</div> <div>17%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	C	500	-	-	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4194 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 Sensory box protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1011	635	174	197	5			
1	B	134	Total	C	N	O	S	0	0	0
			1041	650	187	200	4			
1	C	134	Total	C	N	O	S	0	0	0
			972	613	163	192	4			
1	D	134	Total	C	N	O	S	0	0	0
			1046	652	184	206	4			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q88E39
A	-18	GLY	-	expression tag	UNP Q88E39
A	-17	SER	-	expression tag	UNP Q88E39
A	-16	SER	-	expression tag	UNP Q88E39
A	-15	HIS	-	expression tag	UNP Q88E39
A	-14	HIS	-	expression tag	UNP Q88E39
A	-13	HIS	-	expression tag	UNP Q88E39
A	-12	HIS	-	expression tag	UNP Q88E39
A	-11	HIS	-	expression tag	UNP Q88E39
A	-10	HIS	-	expression tag	UNP Q88E39
A	-9	SER	-	expression tag	UNP Q88E39
A	-8	SER	-	expression tag	UNP Q88E39
A	-7	GLY	-	expression tag	UNP Q88E39
A	-6	LEU	-	expression tag	UNP Q88E39
A	-5	VAL	-	expression tag	UNP Q88E39
A	-4	PRO	-	expression tag	UNP Q88E39
A	-3	ARG	-	expression tag	UNP Q88E39
A	-2	GLY	-	expression tag	UNP Q88E39
A	-1	SER	-	expression tag	UNP Q88E39
A	0	HIS	-	expression tag	UNP Q88E39
B	-19	MET	-	initiating methionine	UNP Q88E39

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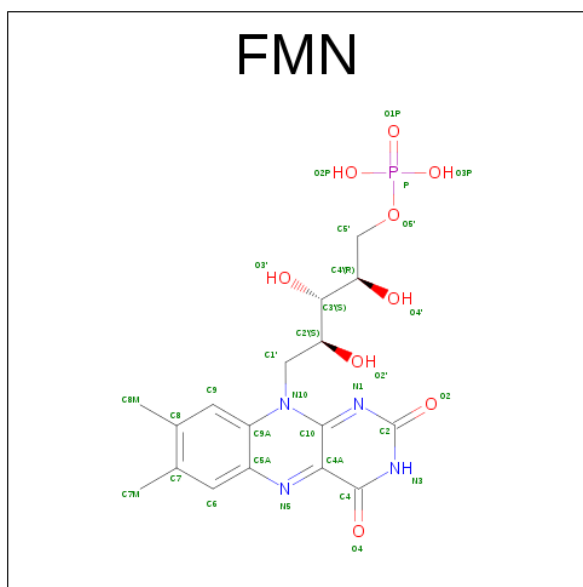
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q88E39
B	-17	SER	-	expression tag	UNP Q88E39
B	-16	SER	-	expression tag	UNP Q88E39
B	-15	HIS	-	expression tag	UNP Q88E39
B	-14	HIS	-	expression tag	UNP Q88E39
B	-13	HIS	-	expression tag	UNP Q88E39
B	-12	HIS	-	expression tag	UNP Q88E39
B	-11	HIS	-	expression tag	UNP Q88E39
B	-10	HIS	-	expression tag	UNP Q88E39
B	-9	SER	-	expression tag	UNP Q88E39
B	-8	SER	-	expression tag	UNP Q88E39
B	-7	GLY	-	expression tag	UNP Q88E39
B	-6	LEU	-	expression tag	UNP Q88E39
B	-5	VAL	-	expression tag	UNP Q88E39
B	-4	PRO	-	expression tag	UNP Q88E39
B	-3	ARG	-	expression tag	UNP Q88E39
B	-2	GLY	-	expression tag	UNP Q88E39
B	-1	SER	-	expression tag	UNP Q88E39
B	0	HIS	-	expression tag	UNP Q88E39
C	-19	MET	-	initiating methionine	UNP Q88E39
C	-18	GLY	-	expression tag	UNP Q88E39
C	-17	SER	-	expression tag	UNP Q88E39
C	-16	SER	-	expression tag	UNP Q88E39
C	-15	HIS	-	expression tag	UNP Q88E39
C	-14	HIS	-	expression tag	UNP Q88E39
C	-13	HIS	-	expression tag	UNP Q88E39
C	-12	HIS	-	expression tag	UNP Q88E39
C	-11	HIS	-	expression tag	UNP Q88E39
C	-10	HIS	-	expression tag	UNP Q88E39
C	-9	SER	-	expression tag	UNP Q88E39
C	-8	SER	-	expression tag	UNP Q88E39
C	-7	GLY	-	expression tag	UNP Q88E39
C	-6	LEU	-	expression tag	UNP Q88E39
C	-5	VAL	-	expression tag	UNP Q88E39
C	-4	PRO	-	expression tag	UNP Q88E39
C	-3	ARG	-	expression tag	UNP Q88E39
C	-2	GLY	-	expression tag	UNP Q88E39
C	-1	SER	-	expression tag	UNP Q88E39
C	0	HIS	-	expression tag	UNP Q88E39
D	-19	MET	-	initiating methionine	UNP Q88E39
D	-18	GLY	-	expression tag	UNP Q88E39
D	-17	SER	-	expression tag	UNP Q88E39

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q88E39
D	-15	HIS	-	expression tag	UNP Q88E39
D	-14	HIS	-	expression tag	UNP Q88E39
D	-13	HIS	-	expression tag	UNP Q88E39
D	-12	HIS	-	expression tag	UNP Q88E39
D	-11	HIS	-	expression tag	UNP Q88E39
D	-10	HIS	-	expression tag	UNP Q88E39
D	-9	SER	-	expression tag	UNP Q88E39
D	-8	SER	-	expression tag	UNP Q88E39
D	-7	GLY	-	expression tag	UNP Q88E39
D	-6	LEU	-	expression tag	UNP Q88E39
D	-5	VAL	-	expression tag	UNP Q88E39
D	-4	PRO	-	expression tag	UNP Q88E39
D	-3	ARG	-	expression tag	UNP Q88E39
D	-2	GLY	-	expression tag	UNP Q88E39
D	-1	SER	-	expression tag	UNP Q88E39
D	0	HIS	-	expression tag	UNP Q88E39

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		



- Molecule 1: Sensory box protein





Q116	
V123	
E124	
L125	
E126	
R127	
E128	
L129	
A134	
ARG	
PRO	
LYS	
PRO	
ASP	
GLU	
ARG	
ALA	

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.38Å 71.09Å 91.26Å 90.00° 91.08° 90.00°	Depositor
Resolution (Å)	45.00 – 2.55 45.62 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.3 (45.00-2.55) 97.5 (45.62-2.55)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.192 , 0.255 0.193 , 0.257	Depositor DCC
$R_{free}$ test set	1070 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.6	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 74.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.53	0/1025	0.75	1/1386 (0.1%)
1	B	0.54	0/1055	0.77	1/1424 (0.1%)
1	C	0.50	0/985	0.72	0/1340
1	D	0.56	0/1059	0.80	2/1429 (0.1%)
All	All	0.53	0/4124	0.76	4/5579 (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	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	LEU	CB-CG-CD1	-7.30	98.59	111.00
1	D	129	LEU	CB-CG-CD2	-5.80	101.14	111.00
1	D	123	VAL	C-N-CA	-5.44	108.10	121.70
1	A	60	ASP	N-CA-C	-5.29	96.73	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	63	GLN	Peptide

## 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	1011	0	946	22	0
1	B	1041	0	998	21	0
1	C	972	0	872	24	0
1	D	1046	0	1002	19	0
2	A	31	0	19	0	0
2	B	31	0	19	2	0
2	C	31	0	19	3	0
2	D	31	0	19	1	0
All	All	4194	0	3894	82	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.

All (82) 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:B:60:ASP:OD2	1:B:84:ARG:NH2	2.00	0.94
1:B:60:ASP:CG	1:B:84:ARG:HH21	1.69	0.94
1:D:124:GLU:HG3	1:D:127:ARG:HB3	1.57	0.86
1:C:21:ALA:HB1	1:C:28:THR:HG22	1.64	0.79
1:A:116:GLN:OE1	1:A:116:GLN:N	2.22	0.73
1:C:124:GLU:CD	1:C:127:ARG:HH12	1.91	0.72
1:B:129:LEU:CD1	1:D:129:LEU:HB2	2.21	0.71
1:A:33:VAL:HG21	1:A:48:ILE:HD11	1.80	0.64
1:A:61:ARG:O	1:A:66:ARG:NH1	2.32	0.62
1:D:57:GLN:OE1	1:D:61:ARG:NH1	2.33	0.61
1:B:80:ARG:CZ	1:B:98:SER:OG	2.49	0.61
1:C:19:VAL:HG12	1:C:33:VAL:HG12	1.82	0.61
1:C:44:SER:OG	1:C:47:GLU:HG3	2.01	0.61
1:D:38:GLU:OE2	1:D:45:ARG:NH2	2.34	0.61
1:C:59:ASP:O	1:C:61:ARG:HD3	2.01	0.60
1:C:44:SER:H	1:C:47:GLU:CD	2.05	0.60
1:D:116:GLN:N	1:D:116:GLN:OE1	2.35	0.60
1:A:30:LEU:HD21	1:A:53:CYS:SG	2.42	0.59
1:D:80:ARG:NH1	1:D:96:GLU:OE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:VAL:HB	1:C:111:TYR:HB2	1.84	0.58
1:A:103:LYS:NZ	1:A:108:GLN:C	2.58	0.57
1:C:124:GLU:CD	1:C:127:ARG:NH1	2.58	0.56
1:D:19:VAL:HG12	1:D:33:VAL:HG22	1.88	0.56
1:C:124:GLU:OE1	1:C:127:ARG:NH1	2.41	0.54
1:B:68:ARG:HD3	1:B:81:GLU:OE1	2.08	0.53
1:C:73:MET:SD	2:C:500:FMN:HM81	2.48	0.53
1:B:126:GLU:HG3	1:D:125:LEU:HD13	1.91	0.53
1:A:3:ASN:ND2	1:A:5:GLN:OE1	2.41	0.53
1:C:121:ARG:HD3	1:D:62:ASP:O	2.10	0.52
1:B:57:GLN:OE1	1:B:61:ARG:NH1	2.43	0.52
1:B:129:LEU:HD13	1:D:129:LEU:HB2	1.92	0.51
1:D:61:ARG:O	1:D:66:ARG:NH1	2.41	0.51
1:B:37:PHE:HE2	1:B:48:ILE:HD12	1.76	0.51
1:B:60:ASP:CG	1:B:84:ARG:NH2	2.51	0.50
1:A:89:ASP:OD1	1:A:91:SER:OG	2.26	0.50
1:B:19:VAL:HG12	1:B:33:VAL:HG12	1.94	0.50
1:D:47:GLU:OE2	1:D:88:LYS:NZ	2.44	0.49
1:A:122:GLN:O	1:A:126:GLU:HG2	2.11	0.49
1:C:7:LEU:HD23	1:C:10:MET:HE3	1.95	0.48
1:D:129:LEU:HD12	1:D:129:LEU:O	2.14	0.48
1:C:19:VAL:HB	1:C:30:LEU:HD22	1.94	0.48
1:A:103:LYS:HZ2	1:A:108:GLN:C	2.17	0.48
1:A:33:VAL:HG23	1:A:45:ARG:HG2	1.95	0.48
1:D:33:VAL:HG13	1:D:37:PHE:HB3	1.95	0.48
1:A:103:LYS:NZ	1:A:108:GLN:O	2.47	0.47
1:B:44:SER:O	1:B:48:ILE:HG12	2.15	0.47
1:B:43:TYR:HB3	1:B:48:ILE:CG2	2.45	0.46
1:D:70:ARG:NH1	2:D:500:FMN:O3P	2.48	0.46
1:A:80:ARG:HA	1:A:97:LEU:O	2.16	0.46
1:C:97:LEU:HD21	1:C:99:ILE:HD11	1.98	0.45
1:B:129:LEU:HD12	1:B:129:LEU:HA	1.67	0.45
1:C:114:GLY:N	2:C:500:FMN:HM73	2.32	0.45
1:D:60:ASP:OD2	1:D:84:ARG:NE	2.38	0.45
1:A:6:LEU:HA	1:A:6:LEU:HD12	1.82	0.44
1:C:63:GLN:O	1:C:66:ARG:N	2.50	0.44
1:C:117:LYS:HG2	1:C:119:VAL:HG13	2.00	0.43
1:B:7:LEU:HB3	1:D:7:LEU:HB3	2.01	0.43
1:A:44:SER:O	1:A:48:ILE:HG12	2.18	0.43
1:B:37:PHE:HE2	1:B:48:ILE:CD1	2.31	0.43
1:C:125:LEU:HA	1:C:125:LEU:HD23	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HD23	1:C:20:VAL:HG11	2.01	0.42
1:C:70:ARG:HA	1:C:73:MET:HE2	2.01	0.42
1:D:49:LEU:HD12	1:D:49:LEU:HA	1.84	0.42
1:C:21:ALA:CB	1:C:28:THR:HG22	2.44	0.42
1:C:80:ARG:HA	1:C:97:LEU:O	2.19	0.42
1:D:19:VAL:HB	1:D:30:LEU:HD22	2.01	0.42
1:B:43:TYR:CZ	1:B:88:LYS:HA	2.55	0.42
1:A:94:TRP:CG	1:A:123:VAL:HG21	2.55	0.41
1:A:71:LYS:O	1:A:75:GLU:HG3	2.20	0.41
1:B:73:MET:SD	2:B:500:FMN:HM81	2.60	0.41
1:A:60:ASP:O	1:A:61:ARG:HD2	2.21	0.41
1:A:69:ILE:O	1:A:73:MET:HG2	2.21	0.41
1:C:45:ARG:HG2	1:C:46:ASP:OD1	2.20	0.41
1:A:19:VAL:HG12	1:A:33:VAL:HG12	2.03	0.41
1:B:80:ARG:NH1	1:B:98:SER:OG	2.54	0.41
1:A:37:PHE:CD1	1:A:116:GLN:NE2	2.89	0.41
1:B:30:LEU:HD21	1:B:53:CYS:SG	2.61	0.40
2:C:500:FMN:H4'	2:C:500:FMN:H1'2	1.83	0.40
1:B:80:ARG:HA	1:B:97:LEU:O	2.22	0.40
2:B:500:FMN:H9	2:B:500:FMN:H1'1	1.83	0.40
1:C:24:GLU:O	1:C:25:GLY:C	2.59	0.40
1:A:52:ASP:O	1:A:55:PHE:HD2	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	131/162 (81%)	129 (98%)	2 (2%)	0	100	100
1	B	132/162 (82%)	130 (98%)	2 (2%)	0	100	100
1	C	132/162 (82%)	130 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	132/162 (82%)	130 (98%)	2 (2%)	0	100	100
All	All	527/648 (81%)	519 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	98/139 (70%)	97 (99%)	1 (1%)	82	94
1	B	104/139 (75%)	104 (100%)	0	100	100
1	C	87/139 (63%)	87 (100%)	0	100	100
1	D	106/139 (76%)	106 (100%)	0	100	100
All	All	395/556 (71%)	394 (100%)	1 (0%)	94	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

4 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	500	-	32,33,33	1.20	4 (12%)	34,50,50	1.93	6 (17%)
2	FMN	B	500	-	32,33,33	1.24	3 (9%)	34,50,50	1.77	5 (14%)
2	FMN	C	500	-	32,33,33	1.10	2 (6%)	34,50,50	1.55	5 (14%)
2	FMN	D	500	-	32,33,33	1.25	3 (9%)	34,50,50	1.72	5 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	A	500	-	-	0/18/18/18	0/3/3/3
2	FMN	B	500	-	-	0/18/18/18	0/3/3/3
2	FMN	C	500	-	-	0/18/18/18	0/3/3/3
2	FMN	D	500	-	-	0/18/18/18	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FMN	C10-N1	2.05	1.39	1.35
2	A	500	FMN	C1'-N10	2.28	1.50	1.48
2	D	500	FMN	C1'-N10	2.43	1.51	1.48
2	B	500	FMN	C1'-N10	2.65	1.51	1.48
2	C	500	FMN	C4-N3	2.84	1.38	1.33
2	B	500	FMN	C4-N3	2.84	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	FMN	C4-N3	2.85	1.38	1.33
2	A	500	FMN	C4-N3	2.99	1.38	1.33
2	C	500	FMN	C4A-N5	3.02	1.38	1.33
2	D	500	FMN	C4A-N5	3.42	1.38	1.33
2	A	500	FMN	C4A-N5	3.48	1.38	1.33
2	B	500	FMN	C4A-N5	3.52	1.38	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	FMN	N3-C2-N1	-4.70	119.78	127.69
2	A	500	FMN	N3-C2-N1	-4.58	119.99	127.69
2	D	500	FMN	N3-C2-N1	-4.54	120.04	127.69
2	C	500	FMN	N3-C2-N1	-3.95	121.05	127.69
2	A	500	FMN	C4A-C4-N3	-3.48	118.97	123.52
2	C	500	FMN	C4A-C4-N3	-3.22	119.32	123.52
2	D	500	FMN	C4A-C4-N3	-2.79	119.87	123.52
2	B	500	FMN	C4A-C4-N3	-2.01	120.89	123.52
2	A	500	FMN	O3'-C3'-C2'	2.09	114.14	108.73
2	C	500	FMN	C5A-C9A-N10	2.34	119.33	117.58
2	C	500	FMN	C4A-N5-C5A	2.85	120.08	116.72
2	D	500	FMN	C4A-N5-C5A	3.16	120.44	116.72
2	A	500	FMN	C4A-N5-C5A	3.16	120.45	116.72
2	B	500	FMN	C4A-N5-C5A	3.39	120.72	116.72
2	D	500	FMN	C5A-C9A-N10	3.58	120.26	117.58
2	A	500	FMN	C5A-C9A-N10	3.59	120.27	117.58
2	B	500	FMN	C5A-C9A-N10	3.91	120.51	117.58
2	B	500	FMN	C4-N3-C2	5.37	119.64	115.16
2	C	500	FMN	C4-N3-C2	5.51	119.75	115.16
2	D	500	FMN	C4-N3-C2	6.01	120.17	115.16
2	A	500	FMN	C4-N3-C2	7.21	121.17	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	FMN	2	0
2	C	500	FMN	3	0
2	D	500	FMN	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	133/162 (82%)	0.26	8 (6%) 25 29	62, 104, 152, 210	0
1	B	134/162 (82%)	0.32	7 (5%) 31 36	62, 94, 164, 191	0
1	C	134/162 (82%)	0.70	19 (14%) 4 4	72, 125, 200, 230	0
1	D	134/162 (82%)	0.03	2 (1%) 76 80	58, 84, 144, 177	0
All	All	535/648 (82%)	0.33	36 (6%) 21 24	58, 100, 171, 230	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	57	GLN	8.2
1	C	56	LEU	7.2
1	C	55	PHE	5.6
1	A	48	ILE	4.5
1	C	61	ARG	4.5
1	B	132	LEU	4.3
1	C	58	GLY	4.3
1	C	62	ASP	4.3
1	C	60	ASP	4.3
1	C	59	ASP	4.2
1	C	130	ALA	4.2
1	C	86	TYR	3.6
1	C	65	GLY	3.6
1	A	30	LEU	3.4
1	C	134	ALA	3.3
1	B	129	LEU	3.3
1	A	49	LEU	3.2
1	A	129	LEU	3.2
1	A	56	LEU	3.2
1	C	28	THR	3.1
1	B	134	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	45	ARG	3.0
1	C	30	LEU	2.9
1	D	2	ILE	2.9
1	B	116	GLN	2.5
1	C	69	ILE	2.3
1	A	125	LEU	2.3
1	C	83	LEU	2.3
1	C	2	ILE	2.3
1	C	26	ASP	2.2
1	A	44	SER	2.2
1	B	30	LEU	2.1
1	A	47	GLU	2.1
1	C	54	ARG	2.1
1	D	82	VAL	2.0
1	B	133	ARG	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	FMN	C	500	31/31	0.87	0.50	1.55	104,116,132,138	31
2	FMN	B	500	31/31	0.94	0.25	1.07	110,117,135,141	0
2	FMN	A	500	31/31	0.95	0.18	-0.14	93,111,125,145	0
2	FMN	D	500	31/31	0.97	0.14	-0.66	66,85,97,101	0

## 6.5 Other polymers

There are no such residues in this entry.