



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:43 PM GMT

PDB ID : 2HFN  
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 : 1.80 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-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

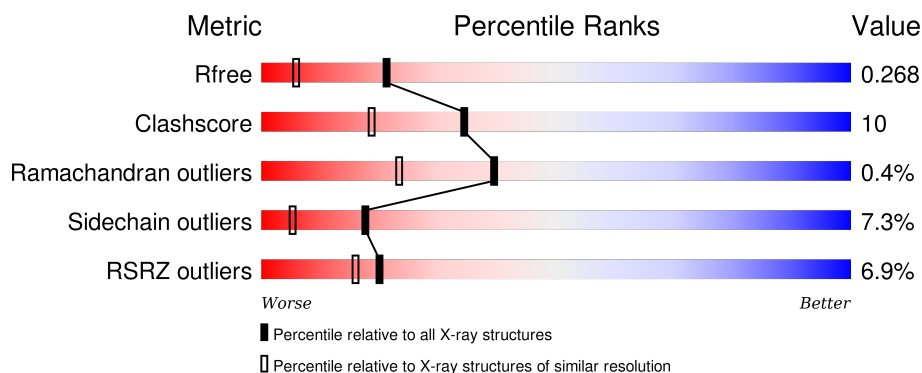
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	153	<div> <div>8%</div> <div>71% 23% . . .</div> </div>
1	B	153	<div> <div>4%</div> <div>75% 16% . 8%</div> </div>
1	C	153	<div> <div>6%</div> <div>75% 15% . 8%</div> </div>
1	D	153	<div> <div>3%</div> <div>74% 18% . . 5%</div> </div>
1	E	153	<div> <div>3%</div> <div>78% 10% . 9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	153	<div><div></div><div>7%</div><div>78%</div><div>10%</div><div>•</div><div>9%</div></div>
1	G	153	<div><div></div><div>7%</div><div>75%</div><div>15%</div><div>•</div><div>9%</div></div>
1	H	153	<div><div></div><div>19%</div><div>78%</div><div>11%</div><div>•</div><div>9%</div></div>
1	I	153	<div><div></div><div>3%</div><div>71%</div><div>16%</div><div>• •</div><div>9%</div></div>
1	J	153	<div><div></div><div>4%</div><div>69%</div><div>20%</div><div>• •</div><div>7%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11655 atoms, of which 2 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 Synechocystis Photoreceptor (Slr1694).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	149	Total	C	H	N	O	S	0	0	0
			1198	757	1	204	229	7			
1	B	140	Total	C	N	O	S		0	0	0
			1094	690	191	205	8				
1	C	140	Total	C	N	O	S		0	0	0
			1104	695	193	208	8				
1	D	146	Total	C	N	O	S		0	0	0
			1177	741	201	227	8				
1	E	139	Total	C	H	N	O	S	0	0	0
			1092	687	1	192	205	7			
1	F	139	Total	C	N	O	S		0	0	0
			1101	693	193	208	7				
1	G	139	Total	C	N	O	S		0	0	0
			1092	688	189	208	7				
1	H	139	Total	C	N	O	S		0	0	0
			1099	691	192	209	7				
1	I	139	Total	C	N	O	S		0	0	0
			1109	700	194	208	7				
1	J	142	Total	C	N	O	S		0	0	0
			1131	714	197	213	7				

There are 30 discrepancies between the modelled and reference sequences:

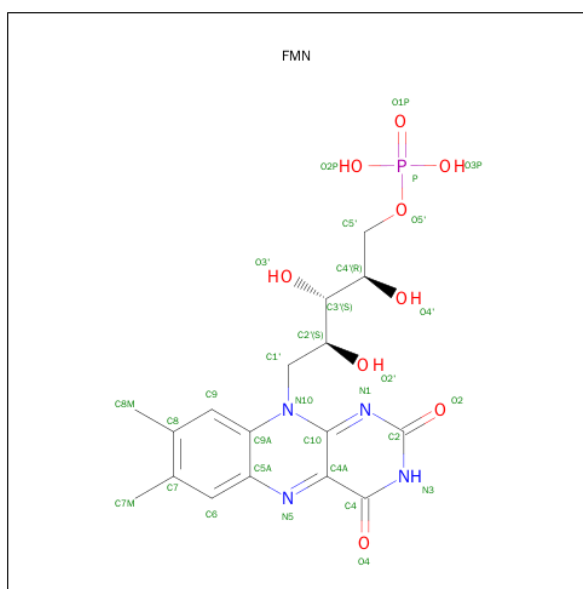
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	CLONING ARTIFACT	UNP P74295
A	2	GLY	-	CLONING ARTIFACT	UNP P74295
A	3	HIS	-	CLONING ARTIFACT	UNP P74295
B	1	ALA	-	CLONING ARTIFACT	UNP P74295
B	2	GLY	-	CLONING ARTIFACT	UNP P74295
B	3	HIS	-	CLONING ARTIFACT	UNP P74295
C	1	ALA	-	CLONING ARTIFACT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

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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<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		

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

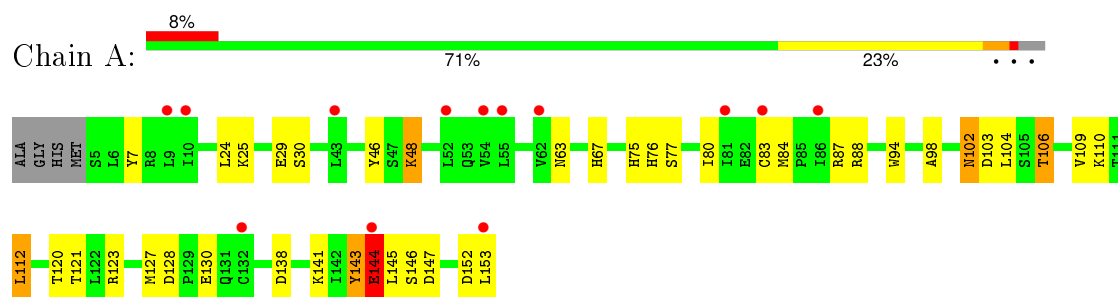
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	14	Total	O	0	0
			14	14		
3	C	15	Total	O	0	0
			15	15		
3	D	33	Total	O	0	0
			33	33		
3	E	4	Total	O	0	0
			4	4		
3	F	11	Total	O	0	0
			11	11		
3	G	2	Total	O	0	0
			2	2		
3	I	15	Total	O	0	0
			15	15		
3	J	12	Total	O	0	0
			12	12		

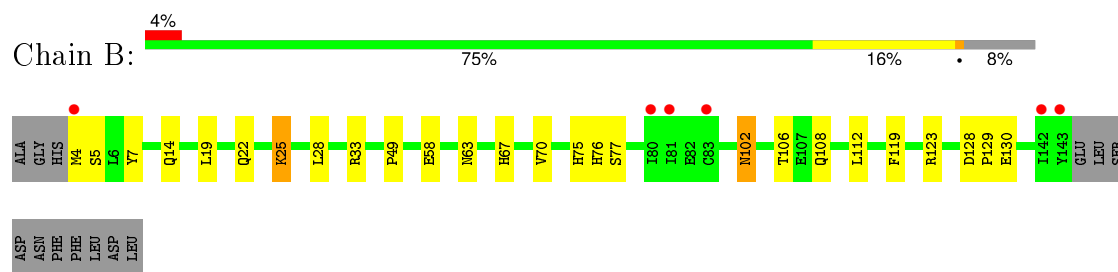
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

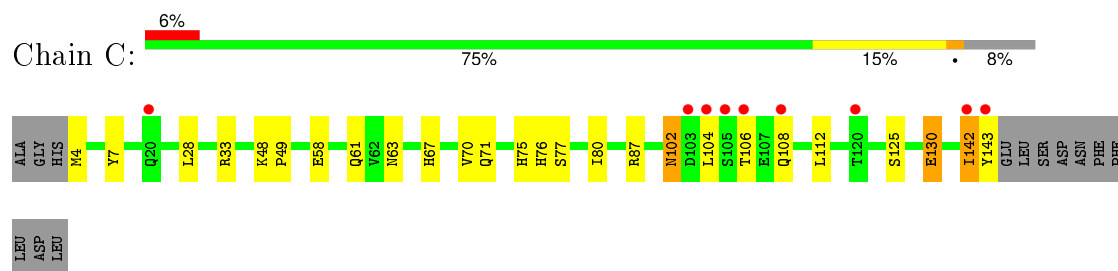
- Molecule 1: Synechocystis Photoreceptor (Slr1694)



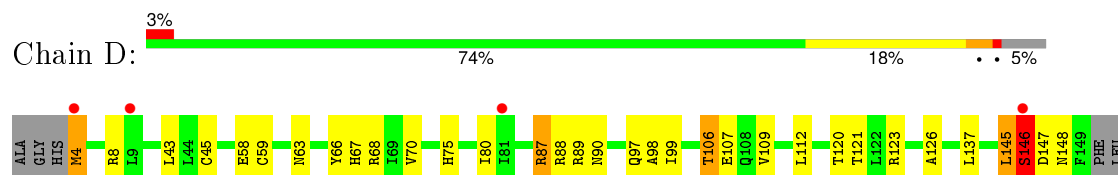
- Molecule 1: Synechocystis Photoreceptor (Slr1694)



- Molecule 1: Synechocystis Photoreceptor (Slr1694)




- Molecule 1: Synechocystis Photoreceptor (Slr1694)




ASP  
LEU

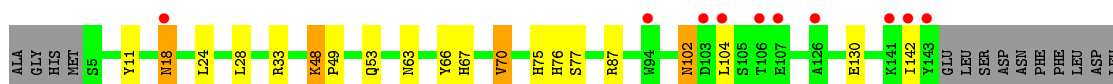
- Molecule 1: Synechocystis Photoreceptor (Slr1694)

Chain E: 




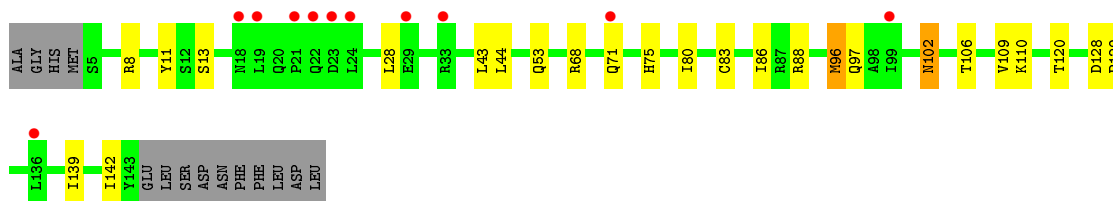
- Molecule 1: Synechocystis Photoreceptor (Slr1694)

Chain F: 




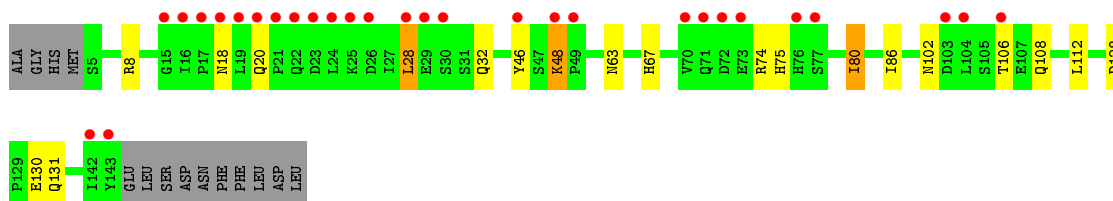
- Molecule 1: Synechocystis Photoreceptor (Slr1694)

Chain G: 



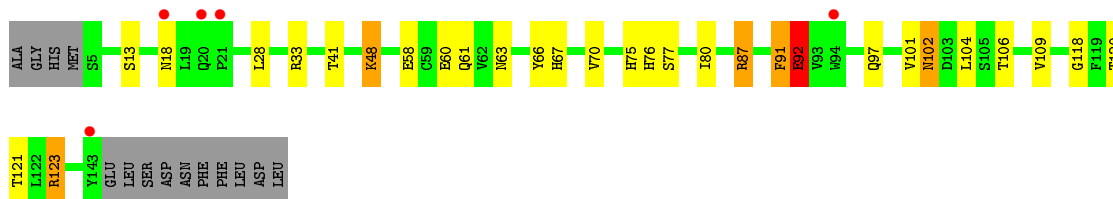
- Molecule 1: Synechocystis Photoreceptor (Slr1694)

Chain H: 



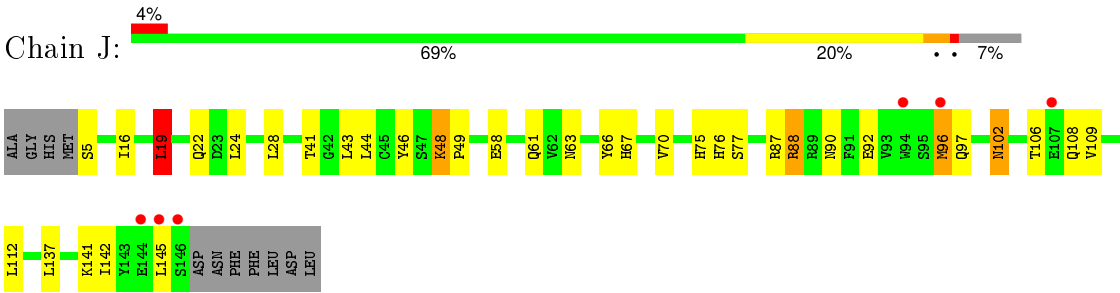
- Molecule 1: Synechocystis Photoreceptor (Slr1694)

Chain I: 



- Molecule 1: Synechocystis Photoreceptor (Slr1694)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.93Å 118.11Å 97.10Å 90.00° 110.79° 90.00°	Depositor
Resolution (Å)	48.51 – 1.80 48.50 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.51-1.80) 97.3 (48.50-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.240 , 0.266 0.240 , 0.268	Depositor DCC
$R_{free}$ test set	8644 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 62.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 172322 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, 0.375 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: 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	0.73	0/1221	0.86	5/1656 (0.3%)
1	B	0.59	0/1116	0.67	0/1516
1	C	0.61	0/1126	0.65	0/1527
1	D	0.74	1/1200 (0.1%)	0.94	1/1628 (0.1%)
1	E	0.50	0/1113	0.67	0/1512
1	F	0.54	0/1122	0.63	0/1522
1	G	0.49	0/1114	0.62	0/1511
1	H	0.78	5/1121 (0.4%)	0.70	2/1522 (0.1%)
1	I	0.60	0/1131	0.73	1/1535 (0.1%)
1	J	0.58	0/1153	0.68	1/1565 (0.1%)
All	All	0.63	6/11417 (0.1%)	0.72	10/15494 (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	A	0	1
1	D	1	3
All	All	1	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	74	ARG	CZ-NH1	15.80	1.53	1.33
1	H	74	ARG	CZ-NH2	8.77	1.44	1.33
1	H	74	ARG	CD-NE	6.47	1.57	1.46
1	D	45	CYS	CB-SG	-5.93	1.72	1.81
1	H	20	GLN	CD-NE2	5.92	1.47	1.32
1	H	20	GLN	CD-OE1	5.59	1.36	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	74	ARG	NE-CZ-NH2	-13.65	113.48	120.30
1	D	146	SER	N-CA-C	11.64	142.44	111.00
1	I	91	PHE	CB-CA-C	6.48	123.37	110.40
1	A	144	GLU	CB-CA-C	-6.44	97.52	110.40
1	A	127	MET	CG-SD-CE	-6.42	89.93	100.20
1	A	144	GLU	CA-C-N	-6.16	103.64	117.20
1	A	123	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	H	74	ARG	NH1-CZ-NH2	5.59	125.54	119.40
1	J	19	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	144	GLU	CA-C-O	5.16	130.94	120.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	146	SER	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	TYR	Peptide
1	D	145	LEU	Peptide
1	D	146	SER	Peptide
1	D	97	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	1197	1	1174	29	0
1	B	1094	0	1065	23	0
1	C	1104	0	1079	24	0
1	D	1177	0	1155	31	0
1	E	1091	1	1063	19	0
1	F	1101	0	1087	24	0
1	G	1092	0	1065	19	0
1	H	1099	0	1068	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1109	0	1097	36	0
1	J	1131	0	1116	45	0
2	A	31	0	19	1	0
2	B	31	0	19	1	0
2	C	31	0	19	2	0
2	D	31	0	19	1	0
2	E	31	0	19	1	0
2	F	31	0	19	1	0
2	G	31	0	19	0	0
2	H	31	0	19	0	0
2	I	31	0	19	0	0
2	J	31	0	19	0	0
3	A	42	0	0	2	0
3	B	14	0	0	1	0
3	C	15	0	0	1	0
3	D	33	0	0	1	0
3	E	4	0	0	0	0
3	F	11	0	0	0	0
3	G	2	0	0	0	0
3	I	15	0	0	1	0
3	J	12	0	0	2	0
All	All	11653	2	11159	226	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 (226) 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:E:48:LYS:N	1:E:48:LYS:HD2	1.62	1.11
1:J:48:LYS:HD3	1:J:48:LYS:H	0.93	1.07
1:E:48:LYS:H	1:E:48:LYS:CD	1.66	1.05
1:I:48:LYS:H	1:I:48:LYS:CD	1.64	1.05
1:I:48:LYS:H	1:I:48:LYS:HD3	1.21	1.00
1:J:48:LYS:HD3	1:J:48:LYS:N	1.74	1.00
1:J:48:LYS:CD	1:J:48:LYS:H	1.67	0.96
1:A:46:TYR:CE2	1:A:48:LYS:HD3	2.01	0.95
1:E:48:LYS:H	1:E:48:LYS:HD2	0.77	0.93
1:I:87:ARG:HA	1:I:87:ARG:HE	1.37	0.90
1:J:5:SER:HA	3:J:1113:HOH:O	1.71	0.90
1:J:96:MET:CE	1:J:97:GLN:H	1.88	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:TYR:CA	1:A:144:GLU:HB2	2.05	0.86
1:G:44:LEU:N	1:G:96:MET:HE1	1.92	0.84
1:E:102:ASN:HD22	1:E:104:LEU:H	1.22	0.83
1:F:87:ARG:HE	1:F:87:ARG:HA	1.43	0.83
1:A:143:TYR:HA	1:A:144:GLU:HB2	1.61	0.82
1:D:43:LEU:HD11	1:D:99:ILE:HG12	1.60	0.82
1:J:96:MET:HE2	1:J:97:GLN:N	1.95	0.82
1:F:33:ARG:NH1	2:F:201:FMN:O3P	2.13	0.81
1:B:128:ASP:OD1	1:J:87:ARG:NH2	2.13	0.81
1:J:44:LEU:N	1:J:96:MET:HE1	1.97	0.80
1:J:43:LEU:HA	1:J:96:MET:CE	2.11	0.80
1:J:43:LEU:HA	1:J:96:MET:HE1	1.64	0.80
1:G:128:ASP:OD1	1:I:87:ARG:NH2	2.16	0.79
1:F:48:LYS:H	1:F:48:LYS:HD2	1.48	0.78
1:J:96:MET:HE2	1:J:97:GLN:H	1.49	0.76
1:J:88:ARG:HG2	1:J:88:ARG:HH11	1.52	0.75
1:G:96:MET:HE3	1:G:97:GLN:H	1.53	0.74
1:J:43:LEU:CA	1:J:96:MET:HE1	2.17	0.74
1:G:68:ARG:O	1:G:71:GLN:HG2	1.88	0.74
1:D:8:ARG:HD3	3:D:1036:HOH:O	1.89	0.72
1:J:58:GLU:OE2	1:J:61:GLN:HG2	1.89	0.72
1:J:46:TYR:CE2	1:J:48:LYS:HD2	2.24	0.72
1:F:87:ARG:HH12	1:H:130:GLU:HB3	1.54	0.72
1:F:48:LYS:H	1:F:48:LYS:CD	2.00	0.72
1:B:14:GLN:HE22	1:B:49:PRO:HG2	1.53	0.72
1:B:119:PHE:HD2	1:B:123:ARG:HH12	1.36	0.72
1:I:80:ILE:H	1:J:63:ASN:HD21	1.37	0.71
1:A:80:ILE:H	1:B:63:ASN:HD21	1.38	0.71
1:I:91:PHE:O	1:I:92:GLU:OE1	2.08	0.71
1:I:58:GLU:OE2	1:I:61:GLN:HG2	1.92	0.70
1:J:96:MET:HE2	1:J:97:GLN:O	1.92	0.70
1:I:41:THR:HG21	1:I:92:GLU:HA	1.73	0.69
1:C:58:GLU:HB3	1:C:61:GLN:HE21	1.58	0.68
1:I:91:PHE:O	1:I:92:GLU:CB	2.35	0.68
1:G:139:ILE:O	1:G:142:ILE:HG12	1.94	0.68
1:I:80:ILE:H	1:J:63:ASN:ND2	1.92	0.68
1:E:63:ASN:O	1:E:67:HIS:HD2	1.76	0.68
1:J:96:MET:HE3	1:J:97:GLN:H	1.58	0.68
1:A:80:ILE:H	1:B:63:ASN:ND2	1.91	0.68
1:D:106:THR:HG22	1:D:109:VAL:H	1.58	0.68
1:F:48:LYS:N	1:F:48:LYS:HD2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:LYS:N	1:I:48:LYS:CD	2.46	0.67
1:B:119:PHE:HD2	1:B:123:ARG:NH1	1.93	0.67
1:A:130:GLU:OE1	1:C:87:ARG:HD3	1.95	0.66
1:G:80:ILE:H	1:H:63:ASN:HD21	1.44	0.66
1:J:48:LYS:HE3	1:J:102:ASN:HB3	1.77	0.65
1:I:48:LYS:N	1:I:48:LYS:HD3	2.04	0.65
1:E:102:ASN:ND2	1:E:104:LEU:H	1.91	0.65
1:D:87:ARG:HH22	1:F:130:GLU:CD	2.00	0.65
1:G:80:ILE:H	1:H:63:ASN:ND2	1.95	0.65
1:A:110:LYS:HB3	1:A:120:THR:OG1	1.97	0.64
1:A:144:GLU:HG3	1:A:145:LEU:HG	1.79	0.64
1:J:96:MET:CE	1:J:97:GLN:O	2.46	0.64
1:J:43:LEU:C	1:J:96:MET:HE1	2.18	0.64
1:B:67:HIS:O	1:B:70:VAL:HG22	1.98	0.64
1:C:106:THR:HG22	1:C:108:GLN:H	1.63	0.63
1:F:87:ARG:NE	1:F:87:ARG:HA	2.14	0.62
1:I:91:PHE:O	1:I:92:GLU:HB3	1.99	0.62
1:B:76:HIS:HD2	1:B:77:SER:OG	1.81	0.62
1:H:106:THR:HG22	1:H:108:GLN:H	1.63	0.62
1:B:106:THR:HG22	1:B:108:GLN:H	1.66	0.61
1:E:102:ASN:HD22	1:E:104:LEU:N	1.95	0.61
1:A:46:TYR:HE2	1:A:48:LYS:HD3	1.58	0.61
1:I:87:ARG:CA	1:I:87:ARG:HE	2.10	0.60
1:J:96:MET:CE	1:J:97:GLN:N	2.58	0.60
1:D:4:MET:N	1:D:58:GLU:OE2	2.34	0.60
1:G:128:ASP:CG	1:I:87:ARG:HH22	2.06	0.59
1:F:87:ARG:NH1	1:H:130:GLU:HB3	2.17	0.59
1:C:80:ILE:H	1:D:63:ASN:HD21	1.51	0.59
1:J:5:SER:CA	3:J:1113:HOH:O	2.42	0.58
1:A:106:THR:HG22	1:A:109:VAL:H	1.68	0.58
1:D:87:ARG:NH2	1:F:130:GLU:CD	2.57	0.58
1:C:63:ASN:ND2	1:D:80:ILE:H	2.01	0.58
1:J:88:ARG:CG	1:J:88:ARG:HH11	2.16	0.57
1:C:87:ARG:CZ	1:C:87:ARG:HA	2.34	0.57
1:I:123:ARG:CZ	1:I:123:ARG:HB2	2.35	0.57
1:C:63:ASN:HD21	1:D:80:ILE:H	1.53	0.57
1:J:43:LEU:CA	1:J:96:MET:CE	2.79	0.56
1:D:4:MET:HE2	1:D:59:CYS:HB3	1.88	0.56
1:J:43:LEU:HA	1:J:96:MET:HE3	1.86	0.56
1:C:48:LYS:HD2	1:C:49:PRO:CA	2.36	0.56
1:C:48:LYS:HD2	1:C:49:PRO:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:MET:N	3:B:1063:HOH:O	2.39	0.55
1:I:48:LYS:HE3	1:I:102:ASN:HB3	1.88	0.55
1:J:106:THR:HG22	1:J:108:GLN:H	1.71	0.55
1:A:48:LYS:HG2	3:A:1003:HOH:O	2.07	0.55
1:C:63:ASN:O	1:C:67:HIS:HD2	1.90	0.55
1:B:119:PHE:CD2	1:B:123:ARG:NH1	2.75	0.55
1:I:63:ASN:O	1:I:67:HIS:HD2	1.90	0.55
1:B:14:GLN:HE22	1:B:49:PRO:CG	2.18	0.54
1:I:106:THR:HG22	1:I:109:VAL:H	1.72	0.54
1:I:102:ASN:ND2	1:I:104:LEU:H	2.06	0.54
1:J:63:ASN:O	1:J:67:HIS:HD2	1.90	0.54
1:C:80:ILE:H	1:D:63:ASN:ND2	2.06	0.54
1:C:33:ARG:NH1	2:C:201:FMN:O3P	2.41	0.54
1:F:87:ARG:NH1	1:H:128:ASP:OD2	2.42	0.53
1:J:41:THR:HG21	1:J:92:GLU:HA	1.89	0.53
1:J:67:HIS:O	1:J:70:VAL:HG22	2.09	0.53
1:C:102:ASN:HD22	1:C:104:LEU:H	1.55	0.53
1:B:102:ASN:C	1:B:102:ASN:HD22	2.12	0.53
1:E:63:ASN:O	1:E:67:HIS:CD2	2.60	0.53
1:I:76:HIS:HD2	1:I:77:SER:OG	1.91	0.53
1:G:106:THR:HG23	1:G:109:VAL:H	1.74	0.53
1:I:66:TYR:OH	1:J:67:HIS:HE1	1.93	0.52
1:I:91:PHE:O	1:I:92:GLU:CD	2.47	0.52
1:A:112:LEU:HD21	1:A:138:ASP:CB	2.39	0.52
1:A:76:HIS:HD2	1:A:77:SER:OG	1.92	0.52
1:G:110:LYS:HB3	1:G:120:THR:OG1	2.10	0.52
1:B:4:MET:O	1:B:58:GLU:HG3	2.11	0.51
1:C:76:HIS:HD2	1:C:77:SER:OG	1.93	0.51
1:A:102:ASN:HD22	1:A:102:ASN:C	2.14	0.51
1:C:102:ASN:ND2	1:C:104:LEU:H	2.09	0.51
1:C:130:GLU:HB3	1:E:87:ARG:HH11	1.76	0.51
1:F:76:HIS:HD2	1:F:77:SER:OG	1.94	0.51
1:G:96:MET:CE	1:G:97:GLN:O	2.59	0.51
1:J:48:LYS:CD	1:J:48:LYS:N	2.46	0.50
1:E:80:ILE:H	1:F:63:ASN:ND2	2.08	0.50
1:J:102:ASN:HD22	1:J:102:ASN:C	2.14	0.50
1:I:102:ASN:C	1:I:102:ASN:HD22	2.15	0.50
1:I:101:VAL:HG12	3:I:1124:HOH:O	2.11	0.50
1:I:102:ASN:HD22	1:I:104:LEU:H	1.58	0.50
1:G:102:ASN:HD22	1:G:102:ASN:C	2.15	0.49
1:A:87:ARG:HG2	1:A:87:ARG:HH21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ASP:CG	1:A:153:LEU:H	2.16	0.49
1:H:46:TYR:CE2	1:H:48:LYS:HG3	2.48	0.49
1:A:25:LYS:O	1:A:29:GLU:HG3	2.13	0.48
1:C:70:VAL:CG2	3:C:1111:HOH:O	2.60	0.48
1:B:4:MET:HA	1:B:58:GLU:CG	2.43	0.48
1:C:4:MET:O	1:C:58:GLU:HG3	2.12	0.48
1:I:67:HIS:HE1	1:J:66:TYR:OH	1.96	0.48
1:J:88:ARG:CG	1:J:88:ARG:NH1	2.76	0.47
1:H:8:ARG:HB2	1:H:86:ILE:HD13	1.97	0.47
1:D:87:ARG:HH21	1:D:87:ARG:CG	2.28	0.47
1:B:4:MET:HA	1:B:58:GLU:HG2	1.96	0.47
1:G:8:ARG:HB2	1:G:86:ILE:HD13	1.97	0.47
1:D:87:ARG:NH2	1:F:130:GLU:OE1	2.48	0.47
1:J:44:LEU:H	1:J:96:MET:HE1	1.75	0.46
1:E:67:HIS:O	1:E:70:VAL:HG22	2.15	0.46
1:E:106:THR:HG22	1:E:109:VAL:HG23	1.96	0.46
1:D:87:ARG:HB3	1:D:87:ARG:NH2	2.31	0.46
1:J:109:VAL:HG22	1:J:142:ILE:HD11	1.96	0.46
1:G:83:CYS:SG	1:H:80:ILE:HG12	2.54	0.46
1:I:48:LYS:H	1:I:48:LYS:HD2	1.67	0.46
1:C:67:HIS:HE1	1:D:66:TYR:OH	1.99	0.46
1:D:68:ARG:NH1	2:D:201:FMN:O4'	2.48	0.46
1:F:102:ASN:HD22	1:F:104:LEU:H	1.63	0.46
1:B:4:MET:HB3	1:D:126:ALA:CB	2.46	0.46
1:I:67:HIS:CE1	1:J:66:TYR:OH	2.69	0.46
1:G:44:LEU:CB	1:G:96:MET:HE1	2.46	0.45
1:E:48:LYS:HD3	1:E:102:ASN:HB3	1.98	0.45
1:I:66:TYR:OH	1:J:67:HIS:CE1	2.69	0.45
1:D:146:SER:OG	1:D:147:ASP:HA	2.16	0.45
1:E:46:TYR:CD2	1:E:48:LYS:HE2	2.52	0.45
1:F:87:ARG:HH11	1:H:131:GLN:HG3	1.80	0.45
1:E:18:ASN:N	1:E:18:ASN:OD1	2.49	0.45
1:G:43:LEU:HA	1:G:96:MET:HE3	1.97	0.45
1:D:4:MET:CE	1:D:59:CYS:HB3	2.47	0.45
1:G:96:MET:CE	1:G:97:GLN:H	2.26	0.44
1:D:87:ARG:HH12	1:F:130:GLU:HB3	1.81	0.44
1:A:83:CYS:O	1:A:84:MET:HG3	2.17	0.44
1:B:63:ASN:HD22	1:B:67:HIS:HE1	1.64	0.44
1:B:128:ASP:HB2	1:B:129:PRO:CD	2.48	0.44
1:F:48:LYS:HA	1:F:49:PRO:HA	1.79	0.44
1:B:22:GLN:HE22	1:B:25:LYS:NZ	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:LYS:N	1:E:48:LYS:CD	2.46	0.44
1:I:118:GLY:H	1:I:123:ARG:HH12	1.66	0.44
1:B:4:MET:HB3	1:D:126:ALA:HB1	1.99	0.44
1:A:128:ASP:OD1	1:C:87:ARG:NH2	2.50	0.44
1:D:67:HIS:HA	1:D:70:VAL:HG22	2.00	0.44
1:A:48:LYS:H	1:A:48:LYS:HG2	1.55	0.43
1:D:4:MET:N	1:D:58:GLU:CG	2.81	0.43
1:E:11:TYR:CE1	1:E:53:GLN:HB3	2.53	0.43
1:A:48:LYS:HE2	3:A:1003:HOH:O	2.18	0.43
1:D:88:ARG:NH1	1:D:89:ARG:O	2.52	0.43
1:A:102:ASN:ND2	1:A:104:LEU:H	2.16	0.43
1:I:58:GLU:OE2	1:I:60:GLU:HB3	2.19	0.43
1:A:112:LEU:HD21	1:A:138:ASP:HB3	2.00	0.43
1:D:90:ASN:HB3	1:D:137:LEU:HD21	2.00	0.42
1:E:67:HIS:HE1	1:F:66:TYR:OH	2.02	0.42
1:B:33:ARG:NH1	2:B:201:FMN:O3P	2.52	0.42
1:E:80:ILE:H	1:F:63:ASN:HD21	1.66	0.42
1:C:63:ASN:O	1:C:67:HIS:CD2	2.71	0.42
1:A:98:ALA:O	1:A:147:ASP:HA	2.19	0.42
1:A:143:TYR:CB	1:A:144:GLU:HB2	2.49	0.42
1:H:63:ASN:O	1:H:67:HIS:HD2	2.03	0.42
1:I:87:ARG:NE	1:I:87:ARG:HA	2.17	0.42
1:A:30:SER:HB3	2:A:201:FMN:H4'	2.01	0.42
1:H:28:LEU:O	1:H:32:GLN:HG3	2.20	0.42
1:J:48:LYS:HA	1:J:49:PRO:HA	1.89	0.41
1:I:91:PHE:O	1:I:92:GLU:CG	2.68	0.41
1:I:63:ASN:O	1:I:67:HIS:CD2	2.71	0.41
1:D:88:ARG:NH2	1:D:148:ASN:OD1	2.52	0.41
2:E:201:FMN:H9	2:E:201:FMN:H1'1	1.84	0.41
1:A:63:ASN:O	1:A:67:HIS:HD2	2.03	0.41
1:F:11:TYR:CE1	1:F:53:GLN:HB3	2.56	0.41
1:F:18:ASN:N	1:F:18:ASN:OD1	2.52	0.41
1:C:67:HIS:CE1	1:D:66:TYR:OH	2.73	0.41
1:G:11:TYR:CE1	1:G:53:GLN:HB3	2.55	0.41
1:J:16:ILE:O	1:J:19:LEU:HB2	2.21	0.41
1:D:99:ILE:HD11	1:D:145:LEU:HD11	2.03	0.41
1:B:130:GLU:OE1	1:J:87:ARG:NH1	2.49	0.41
1:F:67:HIS:HA	1:F:70:VAL:HG12	2.03	0.41
1:G:128:ASP:HB2	1:G:129:PRO:CD	2.50	0.41
1:F:87:ARG:CZ	1:H:130:GLU:OE1	2.69	0.41
1:D:146:SER:HB3	1:D:147:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ARG:HA	1:D:87:ARG:NE	2.36	0.41
1:C:33:ARG:HH12	2:C:201:FMN:P	2.44	0.41
1:C:142:ILE:HG13	1:C:143:TYR:N	2.36	0.41
1:A:141:LYS:HB2	1:A:141:LYS:HE2	1.67	0.40
1:D:87:ARG:HH21	1:D:87:ARG:HG3	1.85	0.40
1:J:90:ASN:HB3	1:J:137:LEU:HD21	2.04	0.40
1:J:76:HIS:HD2	1:J:77:SER:OG	2.05	0.40
1:I:87:ARG:CA	1:I:87:ARG:NE	2.81	0.40
1:A:94:TRP:CZ3	1:A:146:SER:HB3	2.57	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	147/153 (96%)	145 (99%)	1 (1%)	1 (1%)	26	11
1	B	138/153 (90%)	138 (100%)	0	0	100	100
1	C	138/153 (90%)	134 (97%)	4 (3%)	0	100	100
1	D	144/153 (94%)	142 (99%)	0	2 (1%)	14	3
1	E	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	F	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	G	137/153 (90%)	133 (97%)	4 (3%)	0	100	100
1	H	137/153 (90%)	136 (99%)	1 (1%)	0	100	100
1	I	137/153 (90%)	132 (96%)	4 (3%)	1 (1%)	26	11
1	J	140/153 (92%)	134 (96%)	5 (4%)	1 (1%)	26	11
All	All	1392/1530 (91%)	1364 (98%)	23 (2%)	5 (0%)	39	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	GLU
1	D	98	ALA
1	I	92	GLU
1	J	145	LEU
1	D	146	SER

### 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	136/141 (96%)	125 (92%)	11 (8%)	15	4
1	B	121/141 (86%)	113 (93%)	8 (7%)	21	7
1	C	123/141 (87%)	114 (93%)	9 (7%)	17	5
1	D	135/141 (96%)	125 (93%)	10 (7%)	17	5
1	E	121/141 (86%)	113 (93%)	8 (7%)	21	7
1	F	124/141 (88%)	116 (94%)	8 (6%)	21	7
1	G	122/141 (86%)	116 (95%)	6 (5%)	31	13
1	H	123/141 (87%)	116 (94%)	7 (6%)	25	10
1	I	125/141 (89%)	111 (89%)	14 (11%)	7	1
1	J	127/141 (90%)	116 (91%)	11 (9%)	13	3
All	All	1257/1410 (89%)	1165 (93%)	92 (7%)	17	5

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	TYR
1	A	24	LEU
1	A	48	LYS
1	A	75	HIS
1	A	88	ARG
1	A	102	ASN
1	A	103	ASP
1	A	106	THR
1	A	112	LEU

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Mol	Chain	Res	Type
1	A	121	THR
1	A	144	GLU
1	B	5	SER
1	B	7	TYR
1	B	19	LEU
1	B	25	LYS
1	B	28	LEU
1	B	75	HIS
1	B	102	ASN
1	B	112	LEU
1	C	7	TYR
1	C	28	LEU
1	C	71	GLN
1	C	75	HIS
1	C	102	ASN
1	C	112	LEU
1	C	125	SER
1	C	130	GLU
1	C	142	ILE
1	D	4	MET
1	D	75	HIS
1	D	87	ARG
1	D	106	THR
1	D	107	GLU
1	D	112	LEU
1	D	120	THR
1	D	121	THR
1	D	123	ARG
1	D	146	SER
1	E	18	ASN
1	E	22	GLN
1	E	28	LEU
1	E	48	LYS
1	E	75	HIS
1	E	102	ASN
1	E	112	LEU
1	E	120	THR
1	F	18	ASN
1	F	24	LEU
1	F	28	LEU
1	F	48	LYS
1	F	70	VAL

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Mol	Chain	Res	Type
1	F	75	HIS
1	F	102	ASN
1	F	142	ILE
1	G	13	SER
1	G	28	LEU
1	G	75	HIS
1	G	88	ARG
1	G	96	MET
1	G	102	ASN
1	H	18	ASN
1	H	28	LEU
1	H	48	LYS
1	H	75	HIS
1	H	80	ILE
1	H	102	ASN
1	H	112	LEU
1	I	13	SER
1	I	18	ASN
1	I	28	LEU
1	I	33	ARG
1	I	48	LYS
1	I	70	VAL
1	I	75	HIS
1	I	87	ARG
1	I	92	GLU
1	I	97	GLN
1	I	102	ASN
1	I	120	THR
1	I	121	THR
1	I	123	ARG
1	J	19	LEU
1	J	22	GLN
1	J	24	LEU
1	J	28	LEU
1	J	48	LYS
1	J	75	HIS
1	J	88	ARG
1	J	96	MET
1	J	102	ASN
1	J	112	LEU
1	J	141	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	32	GLN
1	A	67	HIS
1	A	76	HIS
1	A	97	GLN
1	A	102	ASN
1	B	14	GLN
1	B	22	GLN
1	B	32	GLN
1	B	63	ASN
1	B	76	HIS
1	B	102	ASN
1	C	32	GLN
1	C	61	GLN
1	C	63	ASN
1	C	67	HIS
1	C	76	HIS
1	C	102	ASN
1	D	18	ASN
1	D	53	GLN
1	D	63	ASN
1	D	90	ASN
1	E	32	GLN
1	E	67	HIS
1	E	76	HIS
1	E	102	ASN
1	F	32	GLN
1	F	63	ASN
1	F	67	HIS
1	F	76	HIS
1	G	32	GLN
1	G	61	GLN
1	G	67	HIS
1	G	102	ASN
1	G	108	GLN
1	H	32	GLN
1	H	61	GLN
1	H	63	ASN
1	H	67	HIS
1	H	90	ASN
1	H	102	ASN
1	I	32	GLN

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Mol	Chain	Res	Type
1	I	67	HIS
1	I	76	HIS
1	I	97	GLN
1	I	102	ASN
1	J	32	GLN
1	J	63	ASN
1	J	67	HIS
1	J	76	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	201	-	32,33,33	1.43	4 (12%)	34,50,50	1.95	6 (17%)
2	FMN	B	201	-	32,33,33	1.27	4 (12%)	34,50,50	1.81	5 (14%)
2	FMN	C	201	-	32,33,33	1.28	4 (12%)	34,50,50	2.12	7 (20%)
2	FMN	D	201	-	32,33,33	1.41	5 (15%)	34,50,50	1.96	4 (11%)
2	FMN	E	201	-	32,33,33	1.31	4 (12%)	34,50,50	1.73	6 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FMN	F	201	-	32,33,33	1.31	4 (12%)	34,50,50	1.81	6 (17%)
2	FMN	G	201	-	32,33,33	1.26	5 (15%)	34,50,50	1.86	6 (17%)
2	FMN	H	201	-	32,33,33	1.19	4 (12%)	34,50,50	1.75	5 (14%)
2	FMN	I	201	-	32,33,33	1.41	5 (15%)	34,50,50	1.82	4 (11%)
2	FMN	J	201	-	32,33,33	1.26	4 (12%)	34,50,50	2.12	6 (17%)

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

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	FMN	C10-N1	2.05	1.39	1.35
2	H	201	FMN	C5A-N5	2.10	1.38	1.35
2	D	201	FMN	C5A-N5	2.11	1.38	1.35
2	J	201	FMN	C4A-N5	2.13	1.36	1.33
2	G	201	FMN	C10-N1	2.20	1.39	1.35
2	I	201	FMN	C5A-N5	2.26	1.38	1.35
2	C	201	FMN	C4A-N5	2.27	1.36	1.33
2	I	201	FMN	C10-N1	2.28	1.39	1.35
2	G	201	FMN	C5A-N5	2.37	1.39	1.35
2	J	201	FMN	C5A-N5	2.56	1.39	1.35
2	F	201	FMN	C5A-N5	2.56	1.39	1.35
2	H	201	FMN	C1'-N10	2.64	1.51	1.48
2	G	201	FMN	C1'-N10	2.68	1.51	1.48
2	C	201	FMN	C4-N3	2.69	1.37	1.33
2	B	201	FMN	C4-N3	2.71	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	FMN	C4A-N5	2.75	1.37	1.33
2	F	201	FMN	C1'-N10	2.93	1.51	1.48
2	E	201	FMN	C5A-N5	2.95	1.40	1.35
2	B	201	FMN	C5A-N5	2.96	1.40	1.35
2	E	201	FMN	C1'-N10	2.98	1.51	1.48
2	H	201	FMN	C4-N3	3.01	1.38	1.33
2	D	201	FMN	C4-N3	3.09	1.38	1.33
2	C	201	FMN	C5A-N5	3.11	1.40	1.35
2	A	201	FMN	C5A-N5	3.23	1.40	1.35
2	I	201	FMN	C4A-N5	3.25	1.38	1.33
2	E	201	FMN	C4-N3	3.26	1.38	1.33
2	J	201	FMN	C4-N3	3.26	1.38	1.33
2	G	201	FMN	C4A-N5	3.29	1.38	1.33
2	A	201	FMN	C4-N3	3.30	1.39	1.33
2	H	201	FMN	C4A-N5	3.38	1.38	1.33
2	F	201	FMN	C4A-N5	3.39	1.38	1.33
2	A	201	FMN	C1'-N10	3.41	1.52	1.48
2	B	201	FMN	C1'-N10	3.41	1.52	1.48
2	D	201	FMN	C4A-N5	3.53	1.38	1.33
2	F	201	FMN	C4-N3	3.53	1.39	1.33
2	C	201	FMN	C1'-N10	3.53	1.52	1.48
2	G	201	FMN	C4-N3	3.55	1.39	1.33
2	I	201	FMN	C4-N3	3.67	1.39	1.33
2	I	201	FMN	C1'-N10	3.70	1.52	1.48
2	J	201	FMN	C1'-N10	3.70	1.52	1.48
2	E	201	FMN	C4A-N5	3.77	1.39	1.33
2	A	201	FMN	C4A-N5	3.77	1.39	1.33
2	D	201	FMN	C1'-N10	4.36	1.53	1.48

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	FMN	N3-C2-N1	-5.25	118.84	127.69
2	I	201	FMN	N3-C2-N1	-5.12	119.07	127.69
2	D	201	FMN	N3-C2-N1	-4.89	119.46	127.69
2	J	201	FMN	N3-C2-N1	-4.76	119.68	127.69
2	G	201	FMN	N3-C2-N1	-4.69	119.80	127.69
2	J	201	FMN	C4A-C4-N3	-4.62	117.48	123.52
2	H	201	FMN	N3-C2-N1	-4.53	120.07	127.69
2	A	201	FMN	N3-C2-N1	-4.49	120.14	127.69
2	E	201	FMN	N3-C2-N1	-4.39	120.31	127.69
2	B	201	FMN	N3-C2-N1	-4.32	120.42	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	FMN	N3-C2-N1	-4.09	120.80	127.69
2	A	201	FMN	C4A-C4-N3	-4.05	118.23	123.52
2	B	201	FMN	C4A-C4-N3	-3.72	118.66	123.52
2	D	201	FMN	C4A-C4-N3	-3.72	118.67	123.52
2	F	201	FMN	C4A-C4-N3	-3.48	118.97	123.52
2	C	201	FMN	C4A-C4-N3	-3.37	119.11	123.52
2	G	201	FMN	C4A-C4-N3	-3.27	119.24	123.52
2	H	201	FMN	C4A-C4-N3	-3.25	119.27	123.52
2	E	201	FMN	C4A-C4-N3	-2.85	119.80	123.52
2	C	201	FMN	C9A-C5A-N5	-2.25	118.52	122.18
2	A	201	FMN	C5A-C9A-N10	2.01	119.08	117.58
2	J	201	FMN	O3'-C3'-C4'	2.04	114.01	108.73
2	G	201	FMN	C4-C4A-N5	2.10	121.26	118.70
2	F	201	FMN	C5A-C9A-N10	2.13	119.17	117.58
2	F	201	FMN	C4-C4A-N5	2.26	121.45	118.70
2	A	201	FMN	C4-C4A-N5	2.37	121.58	118.70
2	E	201	FMN	C4-C4A-N5	2.39	121.61	118.70
2	B	201	FMN	C5A-C9A-N10	2.47	119.43	117.58
2	G	201	FMN	C5A-C9A-N10	2.54	119.48	117.58
2	H	201	FMN	C5A-C9A-N10	2.62	119.54	117.58
2	C	201	FMN	C1'-N10-C9A	2.64	121.89	118.83
2	E	201	FMN	C5A-C9A-N10	2.93	119.78	117.58
2	J	201	FMN	C5A-C9A-N10	2.97	119.80	117.58
2	D	201	FMN	C4A-N5-C5A	3.14	120.42	116.72
2	C	201	FMN	C5A-C9A-N10	3.14	119.93	117.58
2	J	201	FMN	C4A-N5-C5A	3.17	120.46	116.72
2	H	201	FMN	C4A-N5-C5A	3.18	120.47	116.72
2	A	201	FMN	C4A-N5-C5A	3.23	120.53	116.72
2	I	201	FMN	C4-C4A-N5	3.25	122.65	118.70
2	E	201	FMN	C4A-N5-C5A	3.66	121.03	116.72
2	B	201	FMN	C4A-N5-C5A	3.80	121.20	116.72
2	G	201	FMN	C4A-N5-C5A	3.84	121.25	116.72
2	C	201	FMN	C4A-N5-C5A	4.28	121.76	116.72
2	F	201	FMN	C4A-N5-C5A	4.44	121.95	116.72
2	I	201	FMN	C4A-N5-C5A	4.47	121.99	116.72
2	I	201	FMN	C4-N3-C2	5.48	119.73	115.16
2	E	201	FMN	C4-N3-C2	5.77	119.97	115.16
2	F	201	FMN	C4-N3-C2	6.00	120.17	115.16
2	B	201	FMN	C4-N3-C2	6.45	120.54	115.16
2	H	201	FMN	C4-N3-C2	6.58	120.64	115.16
2	G	201	FMN	C4-N3-C2	6.75	120.79	115.16
2	C	201	FMN	C4-N3-C2	7.17	121.14	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	FMN	C4-N3-C2	7.49	121.41	115.16
2	D	201	FMN	C4-N3-C2	7.89	121.74	115.16
2	J	201	FMN	C4-N3-C2	8.03	121.85	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	FMN	1	0
2	B	201	FMN	1	0
2	C	201	FMN	2	0
2	D	201	FMN	1	0
2	E	201	FMN	1	0
2	F	201	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 ⓘ

### 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	149/153 (97%)	0.66	13 (8%) 13 10	17, 31, 38, 43	0
1	B	140/153 (91%)	0.60	6 (4%) 39 32	25, 36, 49, 56	0
1	C	140/153 (91%)	0.74	9 (6%) 23 18	23, 33, 50, 58	0
1	D	146/153 (95%)	0.59	4 (2%) 58 53	23, 28, 39, 43	0
1	E	139/153 (90%)	0.56	5 (3%) 46 40	20, 41, 49, 56	0
1	F	139/153 (90%)	0.51	10 (7%) 18 14	34, 39, 52, 57	0
1	G	139/153 (90%)	0.73	11 (7%) 15 12	42, 50, 60, 64	0
1	H	139/153 (90%)	1.11	29 (20%) 1 1	45, 51, 60, 64	0
1	I	139/153 (90%)	0.31	5 (3%) 46 40	32, 36, 47, 55	0
1	J	142/153 (92%)	0.53	6 (4%) 40 34	30, 36, 52, 64	0
All	All	1412/1530 (92%)	0.63	98 (6%) 20 16	17, 38, 54, 64	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	18	ASN	7.1
1	J	144	GLU	6.3
1	H	19	LEU	6.3
1	C	104	LEU	6.1
1	C	142	ILE	5.8
1	H	21	PRO	5.6
1	J	145	LEU	5.4
1	H	20	GLN	5.3
1	C	106	THR	4.9
1	F	18	ASN	4.4
1	H	22	GLN	4.4
1	H	142	ILE	4.3
1	F	126	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	142	ILE	3.9
1	F	106	THR	3.9
1	C	105	SER	3.8
1	H	71	GLN	3.7
1	I	143	TYR	3.7
1	A	153	LEU	3.6
1	H	104	LEU	3.5
1	J	94	TRP	3.5
1	C	103	ASP	3.5
1	F	103	ASP	3.5
1	B	142	ILE	3.5
1	H	16	ILE	3.5
1	D	4	MET	3.4
1	F	142	ILE	3.4
1	H	48	LYS	3.3
1	H	17	PRO	3.3
1	H	26	ASP	3.1
1	H	24	LEU	3.1
1	H	103	ASP	3.0
1	H	143	TYR	3.0
1	C	143	TYR	3.0
1	H	106	THR	2.9
1	B	83	CYS	2.9
1	G	21	PRO	2.9
1	C	120	THR	2.9
1	J	146	SER	2.8
1	H	23	ASP	2.8
1	H	72	ASP	2.8
1	D	146	SER	2.8
1	F	141	LYS	2.7
1	H	46	TYR	2.7
1	A	83	CYS	2.7
1	B	81	ILE	2.6
1	J	96	MET	2.6
1	A	132	CYS	2.6
1	H	15	GLY	2.6
1	B	4	MET	2.6
1	A	9	LEU	2.6
1	F	94	TRP	2.5
1	F	143	TYR	2.5
1	H	49	PRO	2.5
1	G	29	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	103	ASP	2.4
1	I	18	ASN	2.4
1	G	18	ASN	2.4
1	B	80	ILE	2.4
1	A	43	LEU	2.4
1	I	21	PRO	2.4
1	H	25	LYS	2.4
1	A	10	ILE	2.4
1	H	77	SER	2.3
1	A	55	LEU	2.3
1	C	20	GLN	2.3
1	A	86	ILE	2.3
1	H	29	GLU	2.3
1	A	52	LEU	2.3
1	H	30	SER	2.3
1	G	22	GLN	2.3
1	I	20	GLN	2.3
1	H	28	LEU	2.3
1	E	143	TYR	2.2
1	G	33	ARG	2.3
1	H	70	VAL	2.2
1	A	81	ILE	2.2
1	B	143	TYR	2.2
1	D	81	ILE	2.2
1	F	107	GLU	2.2
1	J	107	GLU	2.2
1	G	23	ASP	2.2
1	G	99	ILE	2.1
1	H	73	GLU	2.1
1	A	62	VAL	2.1
1	G	71	GLN	2.1
1	F	104	LEU	2.1
1	G	24	LEU	2.1
1	G	136	LEU	2.1
1	E	18	ASN	2.1
1	A	144	GLU	2.1
1	A	54	VAL	2.1
1	I	94	TRP	2.1
1	D	9	LEU	2.1
1	G	19	LEU	2.1
1	E	106	THR	2.0
1	C	108	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	76	HIS	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	H	201	31/31	0.86	0.25	1.53	51,52,57,58	5
2	FMN	G	201	31/31	0.77	0.22	1.47	42,44,47,49	5
2	FMN	I	201	31/31	0.92	0.14	0.68	28,31,38,41	5
2	FMN	B	201	31/31	0.90	0.11	-0.78	29,32,40,45	5
2	FMN	J	201	31/31	0.91	0.11	-0.85	26,29,40,44	5
2	FMN	F	201	31/31	0.88	0.11	-0.91	29,34,38,45	5
2	FMN	A	201	31/31	0.92	0.09	-1.64	26,28,36,41	5
2	FMN	D	201	31/31	0.94	0.08	-2.83	20,24,29,33	5
2	FMN	C	201	31/31	0.93	0.08	-3.13	28,30,37,41	5
2	FMN	E	201	31/31	0.92	0.09	-3.71	32,34,42,45	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.