



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:19 PM GMT

PDB ID : 1YRH  
Title : Crystal Structure Of Trp Repressor Binding Protein Wrba in complex with FMN  
Authors : Gorman, J.; Shapiro, L.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2005-02-03  
Resolution : 3.11 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

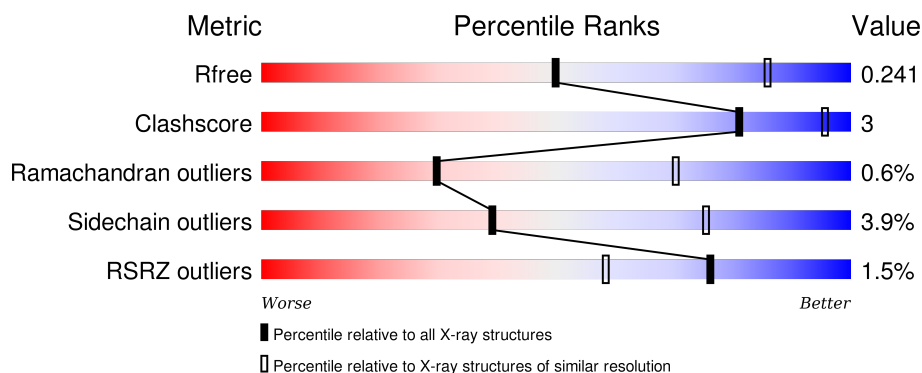
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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	211	<div> <div>89%</div> <div>6% 5%</div> </div>
1	B	211	<div> <div>86%</div> <div>8% 5%</div> </div>
1	C	211	<div> <div>%</div> <div>84%</div> <div>10% 5%</div> </div>
1	D	211	<div> <div>%</div> <div>86%</div> <div>9% 5%</div> </div>
1	E	211	<div> <div>%</div> <div>83%</div> <div>9% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	211	<div><div></div><div>3%</div><div>86%</div><div>9%</div><div></div></div>
1	G	211	<div><div></div><div>4%</div><div>82%</div><div>13%</div><div>5%</div></div>
1	H	211	<div><div></div><div>%</div><div>83%</div><div>11%</div><div>5%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12386 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 trp repressor binding protein WrbA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	Se	0	0	0
			1495	935	260	294	6			
1	B	200	Total	C	N	O	Se	0	0	0
			1495	935	260	294	6			
1	C	201	Total	C	N	O	Se	0	0	0
			1500	938	261	295	6			
1	D	201	Total	C	N	O	Se	0	0	0
			1500	938	261	295	6			
1	E	198	Total	C	N	O	Se	0	0	0
			1485	930	258	291	6			
1	F	202	Total	C	N	O	Se	0	0	0
			1507	942	262	297	6			
1	G	200	Total	C	N	O	Se	0	0	0
			1495	935	260	294	6			
1	H	201	Total	C	N	O	Se	0	0	0
			1500	938	261	295	6			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	UNP Q9RYU4
A	0	SER	-	cloning artifact	UNP Q9RYU4
A	1	LEU	-	cloning artifact	UNP Q9RYU4
A	21	MSE	MET	modified residue	UNP Q9RYU4
A	63	MSE	MET	modified residue	UNP Q9RYU4
A	95	MSE	MET	modified residue	UNP Q9RYU4
A	119	MSE	MET	modified residue	UNP Q9RYU4
A	138	MSE	MET	modified residue	UNP Q9RYU4
A	141	MSE	MET	modified residue	UNP Q9RYU4
A	200	GLU	-	cloning artifact	UNP Q9RYU4
A	202	GLY	-	cloning artifact	UNP Q9RYU4
A	203	SER	-	cloning artifact	UNP Q9RYU4
A	204	HIS	-	cloning artifact	UNP Q9RYU4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	205	HIS	-	cloning artifact	UNP Q9RYU4
A	206	HIS	-	cloning artifact	UNP Q9RYU4
A	207	HIS	-	cloning artifact	UNP Q9RYU4
A	208	HIS	-	cloning artifact	UNP Q9RYU4
A	209	HIS	-	cloning artifact	UNP Q9RYU4
B	-1	MET	-	cloning artifact	UNP Q9RYU4
B	0	SER	-	cloning artifact	UNP Q9RYU4
B	1	LEU	-	cloning artifact	UNP Q9RYU4
B	21	MSE	MET	modified residue	UNP Q9RYU4
B	63	MSE	MET	modified residue	UNP Q9RYU4
B	95	MSE	MET	modified residue	UNP Q9RYU4
B	119	MSE	MET	modified residue	UNP Q9RYU4
B	138	MSE	MET	modified residue	UNP Q9RYU4
B	141	MSE	MET	modified residue	UNP Q9RYU4
B	200	GLU	-	cloning artifact	UNP Q9RYU4
B	202	GLY	-	cloning artifact	UNP Q9RYU4
B	203	SER	-	cloning artifact	UNP Q9RYU4
B	204	HIS	-	cloning artifact	UNP Q9RYU4
B	205	HIS	-	cloning artifact	UNP Q9RYU4
B	206	HIS	-	cloning artifact	UNP Q9RYU4
B	207	HIS	-	cloning artifact	UNP Q9RYU4
B	208	HIS	-	cloning artifact	UNP Q9RYU4
B	209	HIS	-	cloning artifact	UNP Q9RYU4
C	-1	MET	-	cloning artifact	UNP Q9RYU4
C	0	SER	-	cloning artifact	UNP Q9RYU4
C	1	LEU	-	cloning artifact	UNP Q9RYU4
C	21	MSE	MET	modified residue	UNP Q9RYU4
C	63	MSE	MET	modified residue	UNP Q9RYU4
C	95	MSE	MET	modified residue	UNP Q9RYU4
C	119	MSE	MET	modified residue	UNP Q9RYU4
C	138	MSE	MET	modified residue	UNP Q9RYU4
C	141	MSE	MET	modified residue	UNP Q9RYU4
C	200	GLU	-	cloning artifact	UNP Q9RYU4
C	202	GLY	-	cloning artifact	UNP Q9RYU4
C	203	SER	-	cloning artifact	UNP Q9RYU4
C	204	HIS	-	cloning artifact	UNP Q9RYU4
C	205	HIS	-	cloning artifact	UNP Q9RYU4
C	206	HIS	-	cloning artifact	UNP Q9RYU4
C	207	HIS	-	cloning artifact	UNP Q9RYU4
C	208	HIS	-	cloning artifact	UNP Q9RYU4
C	209	HIS	-	cloning artifact	UNP Q9RYU4
D	-1	MET	-	cloning artifact	UNP Q9RYU4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	cloning artifact	UNP Q9RYU4
D	1	LEU	-	cloning artifact	UNP Q9RYU4
D	21	MSE	MET	modified residue	UNP Q9RYU4
D	63	MSE	MET	modified residue	UNP Q9RYU4
D	95	MSE	MET	modified residue	UNP Q9RYU4
D	119	MSE	MET	modified residue	UNP Q9RYU4
D	138	MSE	MET	modified residue	UNP Q9RYU4
D	141	MSE	MET	modified residue	UNP Q9RYU4
D	200	GLU	-	cloning artifact	UNP Q9RYU4
D	202	GLY	-	cloning artifact	UNP Q9RYU4
D	203	SER	-	cloning artifact	UNP Q9RYU4
D	204	HIS	-	cloning artifact	UNP Q9RYU4
D	205	HIS	-	cloning artifact	UNP Q9RYU4
D	206	HIS	-	cloning artifact	UNP Q9RYU4
D	207	HIS	-	cloning artifact	UNP Q9RYU4
D	208	HIS	-	cloning artifact	UNP Q9RYU4
D	209	HIS	-	cloning artifact	UNP Q9RYU4
E	-1	MET	-	cloning artifact	UNP Q9RYU4
E	0	SER	-	cloning artifact	UNP Q9RYU4
E	1	LEU	-	cloning artifact	UNP Q9RYU4
E	21	MSE	MET	modified residue	UNP Q9RYU4
E	63	MSE	MET	modified residue	UNP Q9RYU4
E	95	MSE	MET	modified residue	UNP Q9RYU4
E	119	MSE	MET	modified residue	UNP Q9RYU4
E	138	MSE	MET	modified residue	UNP Q9RYU4
E	141	MSE	MET	modified residue	UNP Q9RYU4
E	200	GLU	-	cloning artifact	UNP Q9RYU4
E	202	GLY	-	cloning artifact	UNP Q9RYU4
E	203	SER	-	cloning artifact	UNP Q9RYU4
E	204	HIS	-	cloning artifact	UNP Q9RYU4
E	205	HIS	-	cloning artifact	UNP Q9RYU4
E	206	HIS	-	cloning artifact	UNP Q9RYU4
E	207	HIS	-	cloning artifact	UNP Q9RYU4
E	208	HIS	-	cloning artifact	UNP Q9RYU4
E	209	HIS	-	cloning artifact	UNP Q9RYU4
F	-1	MET	-	cloning artifact	UNP Q9RYU4
F	0	SER	-	cloning artifact	UNP Q9RYU4
F	1	LEU	-	cloning artifact	UNP Q9RYU4
F	21	MSE	MET	modified residue	UNP Q9RYU4
F	63	MSE	MET	modified residue	UNP Q9RYU4
F	95	MSE	MET	modified residue	UNP Q9RYU4
F	119	MSE	MET	modified residue	UNP Q9RYU4

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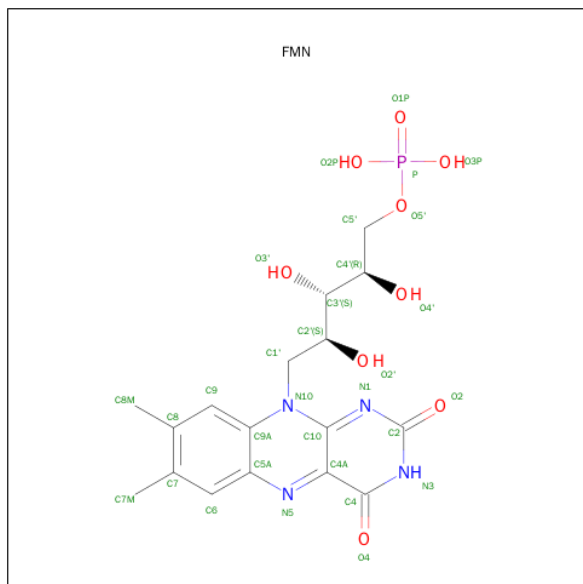
Chain	Residue	Modelled	Actual	Comment	Reference
F	138	MSE	MET	modified residue	UNP Q9RYU4
F	141	MSE	MET	modified residue	UNP Q9RYU4
F	200	GLU	-	cloning artifact	UNP Q9RYU4
F	202	GLY	-	cloning artifact	UNP Q9RYU4
F	203	SER	-	cloning artifact	UNP Q9RYU4
F	204	HIS	-	cloning artifact	UNP Q9RYU4
F	205	HIS	-	cloning artifact	UNP Q9RYU4
F	206	HIS	-	cloning artifact	UNP Q9RYU4
F	207	HIS	-	cloning artifact	UNP Q9RYU4
F	208	HIS	-	cloning artifact	UNP Q9RYU4
F	209	HIS	-	cloning artifact	UNP Q9RYU4
G	-1	MET	-	cloning artifact	UNP Q9RYU4
G	0	SER	-	cloning artifact	UNP Q9RYU4
G	1	LEU	-	cloning artifact	UNP Q9RYU4
G	21	MSE	MET	modified residue	UNP Q9RYU4
G	63	MSE	MET	modified residue	UNP Q9RYU4
G	95	MSE	MET	modified residue	UNP Q9RYU4
G	119	MSE	MET	modified residue	UNP Q9RYU4
G	138	MSE	MET	modified residue	UNP Q9RYU4
G	141	MSE	MET	modified residue	UNP Q9RYU4
G	200	GLU	-	cloning artifact	UNP Q9RYU4
G	202	GLY	-	cloning artifact	UNP Q9RYU4
G	203	SER	-	cloning artifact	UNP Q9RYU4
G	204	HIS	-	cloning artifact	UNP Q9RYU4
G	205	HIS	-	cloning artifact	UNP Q9RYU4
G	206	HIS	-	cloning artifact	UNP Q9RYU4
G	207	HIS	-	cloning artifact	UNP Q9RYU4
G	208	HIS	-	cloning artifact	UNP Q9RYU4
G	209	HIS	-	cloning artifact	UNP Q9RYU4
H	-1	MET	-	cloning artifact	UNP Q9RYU4
H	0	SER	-	cloning artifact	UNP Q9RYU4
H	1	LEU	-	cloning artifact	UNP Q9RYU4
H	21	MSE	MET	modified residue	UNP Q9RYU4
H	63	MSE	MET	modified residue	UNP Q9RYU4
H	95	MSE	MET	modified residue	UNP Q9RYU4
H	119	MSE	MET	modified residue	UNP Q9RYU4
H	138	MSE	MET	modified residue	UNP Q9RYU4
H	141	MSE	MET	modified residue	UNP Q9RYU4
H	200	GLU	-	cloning artifact	UNP Q9RYU4
H	202	GLY	-	cloning artifact	UNP Q9RYU4
H	203	SER	-	cloning artifact	UNP Q9RYU4
H	204	HIS	-	cloning artifact	UNP Q9RYU4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	205	HIS	-	cloning artifact	UNP Q9RYU4
H	206	HIS	-	cloning artifact	UNP Q9RYU4
H	207	HIS	-	cloning artifact	UNP Q9RYU4
H	208	HIS	-	cloning artifact	UNP Q9RYU4
H	209	HIS	-	cloning artifact	UNP Q9RYU4

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	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	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	A	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	G	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	E	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	29	Total 29	O 29	0	0
3	B	21	Total 21	O 21	0	0
3	C	23	Total 23	O 23	0	0
3	D	24	Total 24	O 24	0	0
3	E	12	Total 12	O 12	0	0
3	F	21	Total 21	O 21	0	0
3	G	12	Total 12	O 12	0	0
3	H	19	Total 19	O 19	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.

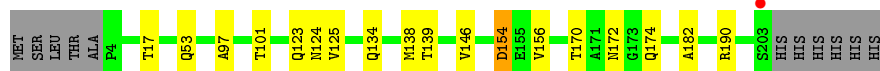
- Molecule 1: trp repressor binding protein WrbA

Chain A: 




- Molecule 1: trp repressor binding protein WrbA

Chain B: 




- Molecule 1: trp repressor binding protein WrbA

Chain C: 




- Molecule 1: trp repressor binding protein WrbA

Chain D: 

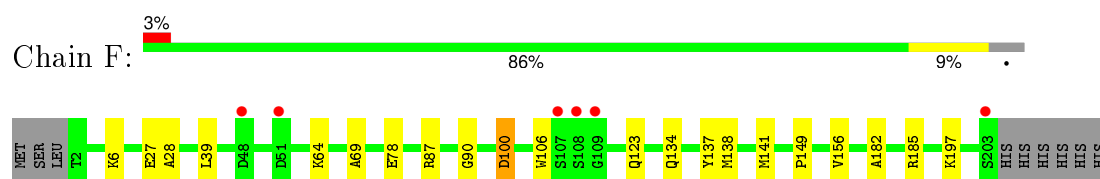


- Molecule 1: trp repressor binding protein WrbA

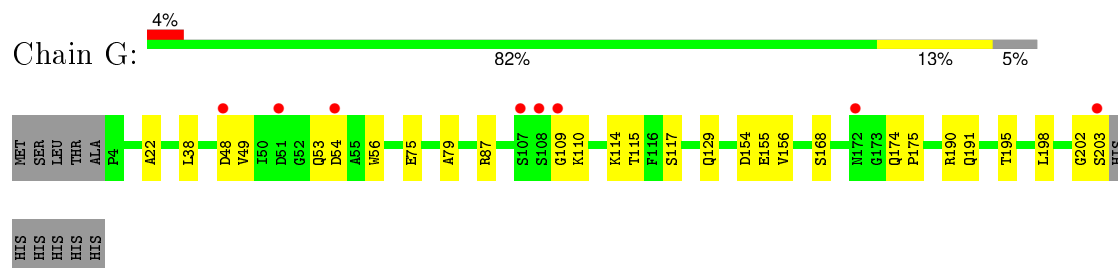
Chain E: 



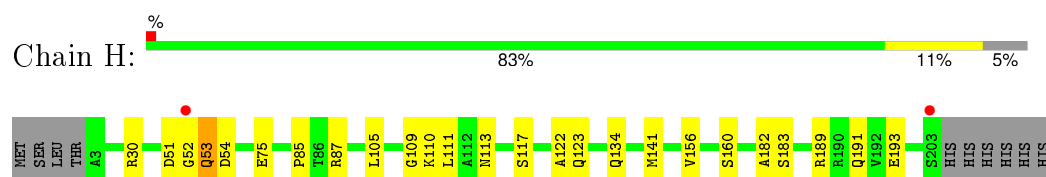
- Molecule 1: trp repressor binding protein WrbA



- Molecule 1: trp repressor binding protein WrbA



- Molecule 1: trp repressor binding protein WrbA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.33Å 122.33Å 208.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.11 20.02 – 3.11	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-3.11) 97.1 (20.02-3.11)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.65 (at 3.09Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.198 , 0.233 0.204 , 0.241	Depositor DCC
$R_{free}$ test set	1632 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 26.2	EDS
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 32058 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	12386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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 [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	0.56	0/1518	0.60	0/2051
1	B	0.55	0/1518	0.61	0/2051
1	C	0.55	0/1523	0.57	0/2059
1	D	0.55	0/1523	0.59	0/2059
1	E	0.53	0/1508	0.59	0/2038
1	F	0.51	0/1530	0.55	0/2069
1	G	0.53	0/1518	0.56	0/2051
1	H	0.52	0/1523	0.62	1/2059 (0.0%)
All	All	0.54	0/12161	0.59	1/16437 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	H	30	ARG	NE-CZ-NH1	5.35	122.97	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1495	0	1466	6	0
1	B	1495	0	1466	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1500	0	1470	11	0
1	D	1500	0	1470	14	0
1	E	1485	0	1458	15	0
1	F	1507	0	1477	14	0
1	G	1495	0	1466	11	0
1	H	1500	0	1470	14	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
2	F	31	0	19	1	0
2	G	31	0	19	0	0
2	H	31	0	19	2	0
3	A	29	0	0	0	0
3	B	21	0	0	0	0
3	C	23	0	0	1	0
3	D	24	0	0	1	0
3	E	12	0	0	2	0
3	F	21	0	0	1	0
3	G	12	0	0	1	0
3	H	19	0	0	1	0
All	All	12386	0	11895	80	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 3.

All (80) 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:134:GLN:HE22	1:D:134:GLN:HE22	1.26	0.81
1:F:134:GLN:HE22	1:H:134:GLN:HE22	1.34	0.75
1:F:134:GLN:O	1:F:138:MSE:HG2	1.88	0.73
1:E:134:GLN:HE21	1:F:134:GLN:NE2	1.87	0.71
1:G:115:THR:HG21	1:G:195:THR:OG1	1.93	0.69
1:B:134:GLN:HE22	1:D:134:GLN:NE2	1.93	0.67
1:E:4:PRO:N	3:E:416:HOH:O	2.28	0.66
1:D:3:ALA:N	3:D:421:HOH:O	2.28	0.65
1:C:117:SER:OG	1:C:191:GLN:NE2	2.31	0.64
1:B:134:GLN:NE2	1:D:134:GLN:HE22	1.94	0.64
1:F:134:GLN:NE2	1:H:134:GLN:HE22	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:418:HOH:O	1:H:141:MSE:HE1	2.00	0.62
1:C:117:SER:HB3	1:C:187:GLN:HE21	1.68	0.59
1:E:19:TYR:CZ	1:E:23:GLN:NE2	2.70	0.59
1:B:97:ALA:O	1:B:101:THR:HG23	2.03	0.58
1:H:117:SER:OG	1:H:191:GLN:NE2	2.37	0.58
1:H:105:LEU:HD23	1:H:111:LEU:HD21	1.85	0.57
1:B:156:VAL:HG21	1:B:182:ALA:HB1	1.85	0.57
1:H:189:ARG:O	1:H:193:GLU:HG3	2.05	0.56
1:F:106:TRP:HB2	3:F:428:HOH:O	2.06	0.56
1:C:28:ALA:HB2	1:C:185:ARG:HG2	1.87	0.55
1:D:81:VAL:HG22	1:D:191:GLN:HE22	1.71	0.54
1:C:138:MSE:SE	1:D:134:GLN:HG3	2.58	0.54
1:A:87:ARG:HG2	1:D:100:ASP:OD1	2.08	0.53
1:E:134:GLN:HE21	1:F:134:GLN:HE21	1.55	0.52
1:A:174:GLN:HB3	1:A:175:PRO:CD	2.38	0.52
1:G:117:SER:HB3	1:G:191:GLN:HE22	1.74	0.52
1:A:117:SER:OG	1:A:191:GLN:NE2	2.43	0.52
1:E:179:ASN:HA	3:E:417:HOH:O	2.10	0.51
1:F:156:VAL:HG21	1:F:182:ALA:HB1	1.93	0.51
1:E:141:MSE:HG2	1:F:149:PRO:HG3	1.95	0.49
1:C:72:ALA:HB1	1:E:54:ASP:HA	1.93	0.49
1:C:138:MSE:HE3	1:D:138:MSE:HE1	1.95	0.49
1:B:154:ASP:HB3	1:B:156:VAL:HG12	1.95	0.48
1:B:53:GLN:HA	1:H:75:GLU:OE1	2.14	0.48
1:E:86:THR:HG22	1:E:132:THR:OG1	2.14	0.48
1:H:51:ASP:C	3:H:424:HOH:O	2.51	0.48
1:H:53:GLN:HE21	1:H:53:GLN:N	2.12	0.47
1:A:134:GLN:O	1:A:138:MSE:HG2	2.14	0.47
1:F:123:GLN:HB2	2:F:407:FMN:H1'	1.97	0.47
1:H:85:PRO:HB2	2:H:405:FMN:H4'	1.95	0.47
1:C:159:LYS:HA	3:C:407:HOH:O	2.15	0.47
1:C:128:GLY:O	1:C:132:THR:HG22	2.15	0.46
1:F:6:LYS:HB2	1:F:78:GLU:HG3	1.97	0.46
1:D:156:VAL:HG21	1:D:182:ALA:HB1	1.96	0.46
1:D:117:SER:OG	1:D:191:GLN:NE2	2.49	0.46
1:G:129:GLN:HE21	1:G:168:SER:CB	2.29	0.46
1:H:160:SER:HB2	1:H:183:SER:OG	2.15	0.45
1:G:190:ARG:NH2	1:H:113:ASN:OD1	2.50	0.45
1:A:174:GLN:HB3	1:A:175:PRO:HD2	1.98	0.45
1:D:83:SER:HB2	1:D:119:MSE:HE3	1.99	0.45
1:E:27:GLU:HG2	1:E:28:ALA:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:SER:CB	1:G:191:GLN:HE22	2.30	0.45
1:C:50:ILE:HG22	1:C:57:LYS:HG2	1.99	0.44
1:D:17:THR:HG1	1:D:17:THR:H	1.62	0.44
1:C:154:ASP:OD2	1:C:155:GLU:N	2.51	0.44
1:G:53:GLN:CG	1:G:56:TRP:HB2	2.48	0.43
1:G:129:GLN:HE21	1:G:168:SER:HB2	1.84	0.43
1:H:156:VAL:HG21	1:H:182:ALA:HB1	2.00	0.43
1:H:122:ALA:HB1	2:H:405:FMN:O2	2.19	0.43
1:B:156:VAL:CG2	1:B:182:ALA:HB1	2.49	0.43
1:C:3:ALA:HB1	1:C:4:PRO:HD2	2.01	0.43
1:G:154:ASP:OD2	1:G:155:GLU:N	2.52	0.42
1:B:172:ASN:OD1	1:B:174:GLN:N	2.49	0.42
1:F:28:ALA:HB2	1:F:185:ARG:HG2	2.02	0.42
1:E:156:VAL:HG21	1:E:182:ALA:HB1	2.00	0.42
1:F:137:TYR:O	1:F:141:MSE:HG3	2.19	0.42
1:E:86:THR:HG22	1:E:132:THR:CB	2.49	0.42
1:A:134:GLN:HG3	1:B:138:MSE:SE	2.70	0.42
1:E:93:SER:O	1:E:97:ALA:N	2.53	0.41
1:D:152:TYR:CD2	1:D:158:PHE:CE1	3.08	0.41
1:G:79:ALA:HA	1:G:115:THR:HG22	2.02	0.41
1:F:87:ARG:N	1:F:90:GLY:O	2.52	0.41
1:G:22:ALA:HB1	1:G:38:LEU:HD11	2.02	0.41
1:G:75:GLU:HA	1:G:114:LYS:HZ1	1.86	0.41
1:F:39:LEU:HB3	1:F:69:ALA:HB2	2.02	0.41
1:E:110:LYS:O	1:E:111:LEU:HB2	2.21	0.40
1:D:94:GLN:O	1:D:95:MSE:C	2.59	0.40
1:E:134:GLN:O	1:E:138:MSE:HG2	2.22	0.40
1:E:19:TYR:CE2	1:E:23:GLN:NE2	2.89	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	198/211 (94%)	191 (96%)	7 (4%)	0	100	100
1	B	198/211 (94%)	192 (97%)	6 (3%)	0	100	100
1	C	199/211 (94%)	189 (95%)	8 (4%)	2 (1%)	19	59
1	D	199/211 (94%)	192 (96%)	7 (4%)	0	100	100
1	E	196/211 (93%)	181 (92%)	12 (6%)	3 (2%)	13	47
1	F	200/211 (95%)	178 (89%)	21 (10%)	1 (0%)	34	73
1	G	198/211 (94%)	183 (92%)	13 (7%)	2 (1%)	19	59
1	H	199/211 (94%)	192 (96%)	5 (2%)	2 (1%)	19	59
All	All	1587/1688 (94%)	1498 (94%)	79 (5%)	10 (1%)	30	70

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	109	GLY
1	E	88	PHE
1	F	100	ASP
1	H	109	GLY
1	C	155	GLU
1	E	110	LYS
1	G	109	GLY
1	E	89	GLY
1	H	52	GLY
1	G	202	GLY

### 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	152/156 (97%)	147 (97%)	5 (3%)	45	79
1	B	152/156 (97%)	143 (94%)	9 (6%)	24	60
1	C	152/156 (97%)	146 (96%)	6 (4%)	39	75
1	D	152/156 (97%)	146 (96%)	6 (4%)	39	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	151/156 (97%)	148 (98%)	3 (2%)	63	87
1	F	153/156 (98%)	149 (97%)	4 (3%)	54	83
1	G	152/156 (97%)	142 (93%)	10 (7%)	21	57
1	H	152/156 (97%)	147 (97%)	5 (3%)	45	79
All	All	1216/1248 (97%)	1168 (96%)	48 (4%)	39	75

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	SER
1	A	110	LYS
1	A	155	GLU
1	A	198	LEU
1	A	200	GLU
1	B	17	THR
1	B	123	GLN
1	B	124	ASN
1	B	125	VAL
1	B	139	THR
1	B	146	VAL
1	B	154	ASP
1	B	170	THR
1	B	190	ARG
1	C	35	GLU
1	C	48	ASP
1	C	64	LYS
1	C	110	LYS
1	C	115	THR
1	C	189	ARG
1	D	17	THR
1	D	64	LYS
1	D	87	ARG
1	D	123	GLN
1	D	155	GLU
1	D	156	VAL
1	E	17	THR
1	E	27	GLU
1	E	155	GLU
1	F	27	GLU
1	F	64	LYS
1	F	100	ASP

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Mol	Chain	Res	Type
1	F	197	LYS
1	G	48	ASP
1	G	49	VAL
1	G	54	ASP
1	G	87	ARG
1	G	110	LYS
1	G	156	VAL
1	G	174	GLN
1	G	175	PRO
1	G	198	LEU
1	G	203	SER
1	H	53	GLN
1	H	54	ASP
1	H	87	ARG
1	H	110	LYS
1	H	123	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	191	GLN
1	B	124	ASN
1	B	129	GLN
1	B	191	GLN
1	C	126	ASN
1	C	129	GLN
1	C	191	GLN
1	D	134	GLN
1	D	191	GLN
1	E	129	GLN
1	E	191	GLN
1	F	134	GLN
1	G	47	GLN
1	G	129	GLN
1	G	134	GLN
1	G	191	GLN
1	H	53	GLN
1	H	123	GLN
1	H	129	GLN
1	H	191	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 ⓘ

8 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	404	-	32,33,33	1.33	4 (12%)	34,50,50	1.51	4 (11%)
2	FMN	B	403	-	32,33,33	1.21	3 (9%)	34,50,50	1.90	7 (20%)
2	FMN	C	402	-	32,33,33	1.20	3 (9%)	34,50,50	1.76	5 (14%)
2	FMN	D	401	-	32,33,33	1.22	3 (9%)	34,50,50	1.91	8 (23%)
2	FMN	E	408	-	32,33,33	1.36	4 (12%)	34,50,50	1.97	7 (20%)
2	FMN	F	407	-	32,33,33	1.25	4 (12%)	34,50,50	1.64	5 (14%)
2	FMN	G	406	-	32,33,33	1.22	4 (12%)	34,50,50	1.71	6 (17%)
2	FMN	H	405	-	32,33,33	1.33	5 (15%)	34,50,50	1.82	4 (11%)

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	404	-	-	0/18/18/18	0/3/3/3
2	FMN	B	403	-	-	0/18/18/18	0/3/3/3
2	FMN	C	402	-	-	0/18/18/18	0/3/3/3
2	FMN	D	401	-	-	0/18/18/18	0/3/3/3
2	FMN	E	408	-	-	0/18/18/18	0/3/3/3
2	FMN	F	407	-	-	0/18/18/18	0/3/3/3
2	FMN	G	406	-	-	0/18/18/18	0/3/3/3
2	FMN	H	405	-	-	0/18/18/18	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	FMN	C6-C5A	-2.05	1.38	1.41
2	G	406	FMN	C10-N1	2.01	1.39	1.35
2	H	405	FMN	C5A-N5	2.06	1.38	1.35
2	E	408	FMN	C5A-N5	2.13	1.38	1.35
2	H	405	FMN	C10-N1	2.22	1.39	1.35
2	F	407	FMN	C5A-N5	2.26	1.38	1.35
2	A	404	FMN	C5A-N5	2.49	1.39	1.35
2	C	402	FMN	C4-N3	2.50	1.37	1.33
2	D	401	FMN	C1'-N10	2.54	1.51	1.48
2	H	405	FMN	C1'-N10	2.58	1.51	1.48
2	A	404	FMN	C4-N3	2.65	1.37	1.33
2	C	402	FMN	C4A-N5	2.65	1.37	1.33
2	G	406	FMN	C1'-N10	2.72	1.51	1.48
2	A	404	FMN	C4A-N5	2.82	1.37	1.33
2	F	407	FMN	C1'-N10	2.89	1.51	1.48
2	D	401	FMN	C4-N3	2.90	1.38	1.33
2	F	407	FMN	C4-N3	2.91	1.38	1.33
2	B	403	FMN	C4A-N5	2.94	1.37	1.33
2	G	406	FMN	C4A-N5	2.97	1.37	1.33
2	C	402	FMN	C1'-N10	2.98	1.51	1.48
2	H	405	FMN	C4-N3	2.98	1.38	1.33
2	D	401	FMN	C4A-N5	3.27	1.38	1.33
2	E	408	FMN	C4-N3	3.29	1.39	1.33
2	B	403	FMN	C4-N3	3.37	1.39	1.33
2	A	404	FMN	C1'-N10	3.52	1.52	1.48
2	E	408	FMN	C1'-N10	3.54	1.52	1.48
2	F	407	FMN	C4A-N5	3.55	1.38	1.33
2	G	406	FMN	C4-N3	3.55	1.39	1.33
2	E	408	FMN	C4A-N5	3.69	1.39	1.33
2	H	405	FMN	C4A-N5	3.83	1.39	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	FMN	N3-C2-N1	-5.09	119.11	127.69
2	H	405	FMN	N3-C2-N1	-5.02	119.23	127.69
2	G	406	FMN	N3-C2-N1	-4.61	119.92	127.69
2	E	408	FMN	N3-C2-N1	-4.52	120.08	127.69
2	D	401	FMN	N3-C2-N1	-4.36	120.36	127.69
2	F	407	FMN	N3-C2-N1	-4.13	120.74	127.69
2	A	404	FMN	N3-C2-N1	-3.89	121.14	127.69
2	C	402	FMN	N3-C2-N1	-3.77	121.35	127.69
2	E	408	FMN	C4A-C4-N3	-3.51	118.93	123.52
2	C	402	FMN	C4A-C4-N3	-3.12	119.45	123.52
2	B	403	FMN	C4A-C4-N3	-3.10	119.46	123.52
2	D	401	FMN	C4A-C4-N3	-2.97	119.64	123.52
2	G	406	FMN	C4A-C4-N3	-2.86	119.78	123.52
2	H	405	FMN	C4A-C4-N3	-2.51	120.25	123.52
2	F	407	FMN	C4A-C4-N3	-2.43	120.35	123.52
2	G	406	FMN	O4'-C4'-C5'	-2.14	105.43	110.09
2	E	408	FMN	C8M-C8-C7	-2.04	116.34	120.73
2	D	401	FMN	C4A-C10-N10	-2.02	119.05	120.52
2	D	401	FMN	C1'-N10-C9A	2.08	121.24	118.83
2	A	404	FMN	C1'-N10-C9A	2.12	121.29	118.83
2	B	403	FMN	C6-C5A-C9A	2.14	121.47	119.11
2	B	403	FMN	C5A-C9A-N10	2.19	119.22	117.58
2	G	406	FMN	C1'-N10-C9A	2.41	121.62	118.83
2	E	408	FMN	C5A-C9A-N10	2.43	119.40	117.58
2	D	401	FMN	C6-C5A-C9A	2.67	122.06	119.11
2	F	407	FMN	C4A-N5-C5A	2.79	120.01	116.72
2	C	402	FMN	C4A-N5-C5A	2.80	120.02	116.72
2	G	406	FMN	C4A-N5-C5A	2.87	120.11	116.72
2	B	403	FMN	C1'-N10-C9A	3.04	122.35	118.83
2	E	408	FMN	C1'-N10-C9A	3.13	122.46	118.83
2	D	401	FMN	C5A-C9A-N10	3.13	119.93	117.58
2	C	402	FMN	C5A-C9A-N10	3.17	119.95	117.58
2	F	407	FMN	C5A-C9A-N10	3.21	119.98	117.58
2	B	403	FMN	C4A-N5-C5A	3.34	120.65	116.72
2	D	401	FMN	C4A-N5-C5A	3.48	120.82	116.72
2	H	405	FMN	C4A-N5-C5A	3.74	121.13	116.72
2	A	404	FMN	C4A-N5-C5A	3.88	121.29	116.72
2	E	408	FMN	C4A-N5-C5A	3.90	121.32	116.72
2	A	404	FMN	C4-N3-C2	4.11	118.59	115.16
2	F	407	FMN	C4-N3-C2	5.19	119.48	115.16
2	C	402	FMN	C4-N3-C2	5.42	119.68	115.16
2	G	406	FMN	C4-N3-C2	5.78	119.98	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	405	FMN	C4-N3-C2	6.30	120.41	115.16
2	D	401	FMN	C4-N3-C2	6.37	120.47	115.16
2	E	408	FMN	C4-N3-C2	6.45	120.54	115.16
2	B	403	FMN	C4-N3-C2	6.49	120.57	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	407	FMN	1	0
2	H	405	FMN	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, 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	194/211 (91%)	-0.42	1 (0%) 91 84	25, 26, 32, 36	0
1	B	194/211 (91%)	-0.37	1 (0%) 91 84	25, 28, 39, 51	0
1	C	195/211 (92%)	-0.36	2 (1%) 84 70	25, 28, 37, 44	0
1	D	195/211 (92%)	-0.40	2 (1%) 84 70	25, 27, 34, 42	0
1	E	192/211 (90%)	-0.26	2 (1%) 84 70	29, 37, 46, 49	0
1	F	196/211 (92%)	-0.05	6 (3%) 52 28	35, 44, 58, 61	0
1	G	194/211 (91%)	0.00	8 (4%) 41 19	33, 44, 61, 64	0
1	H	195/211 (92%)	-0.38	2 (1%) 84 70	26, 29, 38, 42	0
All	All	1555/1688 (92%)	-0.28	24 (1%) 76 58	25, 30, 50, 64	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	108	SER	5.4
1	C	203	SER	4.1
1	F	107	SER	3.7
1	G	54	ASP	3.6
1	G	51	ASP	3.4
1	F	48	ASP	3.3
1	A	203	SER	3.2
1	G	172	ASN	2.9
1	H	203	SER	2.9
1	E	174	GLN	2.8
1	E	108	SER	2.8
1	G	203	SER	2.7
1	D	203	SER	2.5
1	F	51	ASP	2.5
1	F	203	SER	2.4
1	G	109	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	108	SER	2.2
1	D	173	GLY	2.2
1	C	65	ASP	2.2
1	H	52	GLY	2.1
1	G	107	SER	2.1
1	F	109	GLY	2.1
1	B	203	SER	2.1
1	G	48	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, 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( $\text{\AA}^2$ )	Q<0.9
2	FMN	C	402	31/31	0.95	0.18	0.38	25,25,27,28	0
2	FMN	A	404	31/31	0.96	0.17	0.12	25,25,26,27	0
2	FMN	H	405	31/31	0.97	0.15	-0.08	27,29,30,33	0
2	FMN	E	408	31/31	0.95	0.15	-0.55	30,31,33,34	0
2	FMN	B	403	31/31	0.97	0.15	-0.60	25,26,27,27	0
2	FMN	G	406	31/31	0.95	0.15	-0.73	33,34,45,46	0
2	FMN	F	407	31/31	0.95	0.15	-0.75	35,37,38,39	0
2	FMN	D	401	31/31	0.97	0.13	-1.36	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.