



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:36 PM GMT

PDB ID : 2ISJ  
Title : BluB bound to oxidized FMN  
Authors : Larsen, N.A.; Taga, M.E.; Howard-Jones, A.R.; Walsh, C.T.; Walker, G.C.  
Deposited on : 2006-10-17  
Resolution : 2.30 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

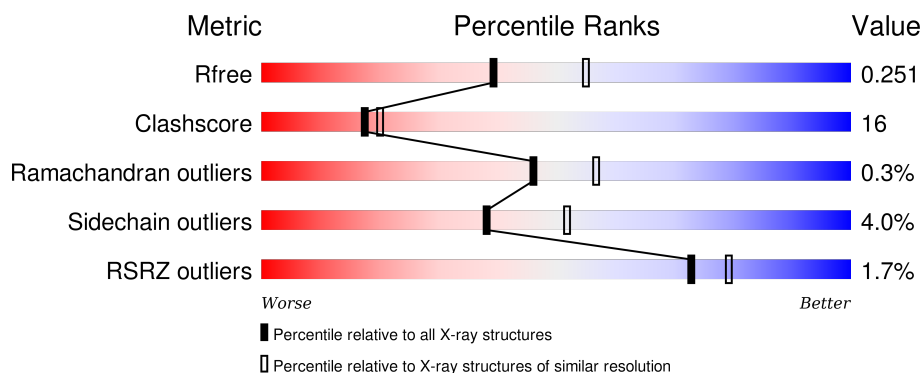
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	230	<div> <div>67%</div> <div>26%</div> <div>• 5%</div> </div>
1	B	230	<div> <div>68%</div> <div>26%</div> <div>• 5%</div> </div>
1	C	230	<div> <div>71%</div> <div>21%</div> <div>• 5%</div> </div>
1	D	230	<div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div>
1	E	230	<div> <div>69%</div> <div>24%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	230	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>69%</div><div>25%</div><div>• 5%</div></div></div>
1	G	230	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>65%</div><div>28%</div><div>• 5%</div></div></div>
1	H	230	<div><div><div></div><div></div><div></div></div><div><div>6%</div><div>56%</div><div>39%</div><div>5%</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14695 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 BluB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	B	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	C	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	D	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	E	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	F	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	G	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			
1	H	219	Total	C	N	O	S	0	0	0
			1741	1103	314	317	7			

There are 24 discrepancies between the modelled and reference sequences:

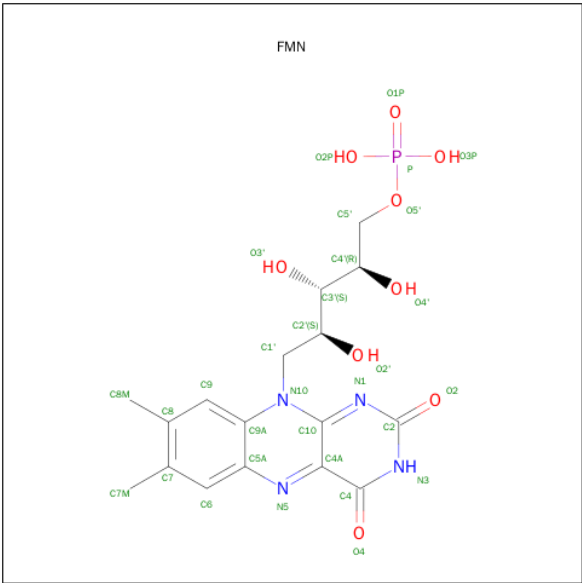
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
A	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
A	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
B	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
B	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
B	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
C	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
C	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
C	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
D	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
D	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
D	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
E	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
E	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
F	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
F	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
F	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
G	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
G	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
G	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8
H	-2	GLY	-	CLONING ARTIFACT	UNP Q92PC8
H	-1	SER	-	CLONING ARTIFACT	UNP Q92PC8
H	0	HIS	-	CLONING ARTIFACT	UNP Q92PC8

- 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	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	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	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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

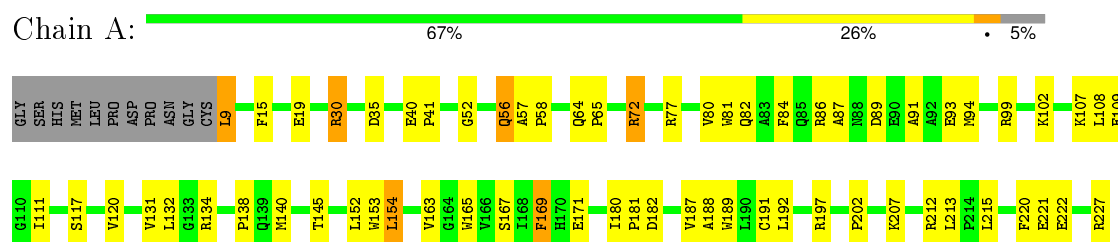
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total	O	0	0
			88	88		
3	B	86	Total	O	0	0
			86	86		
3	C	69	Total	O	0	0
			69	69		
3	D	87	Total	O	0	0
			87	87		
3	E	59	Total	O	0	0
			59	59		
3	F	55	Total	O	0	0
			55	55		
3	G	36	Total	O	0	0
			36	36		
3	H	39	Total	O	0	0
			39	39		

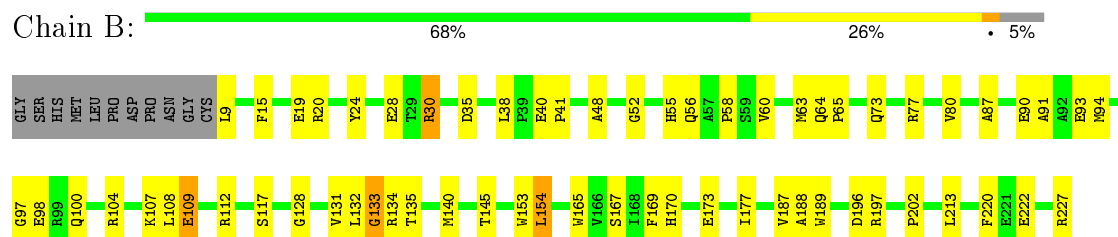
### 3 Residue-property plots [i](#)

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.

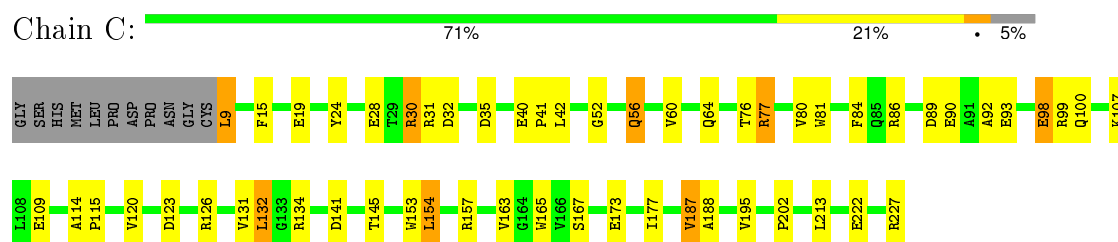
#### • Molecule 1: BluB



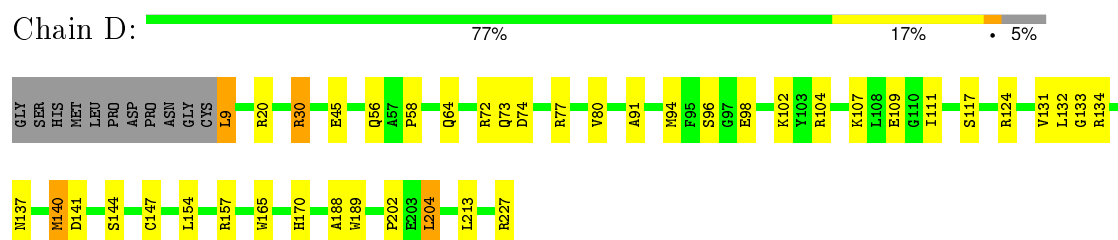
#### • Molecule 1: BluB



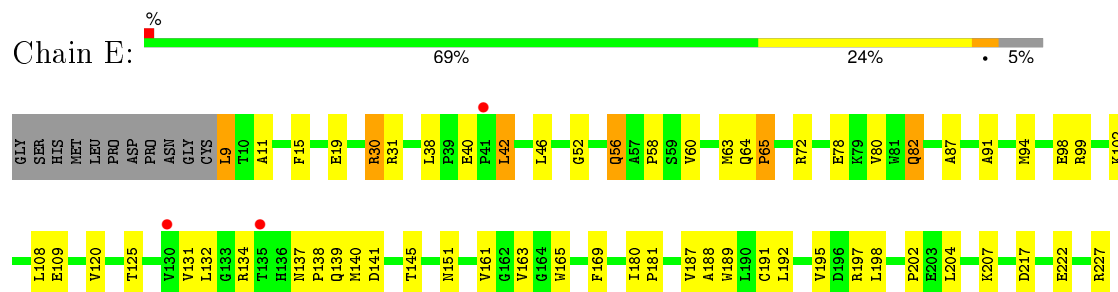
#### • Molecule 1: BluB



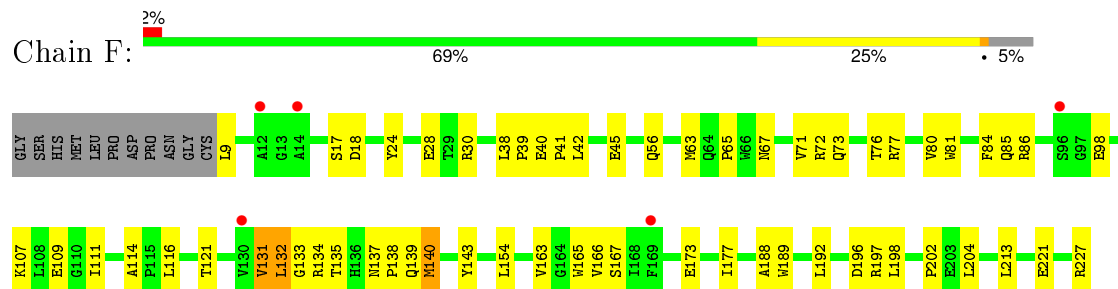
#### • Molecule 1: BluB



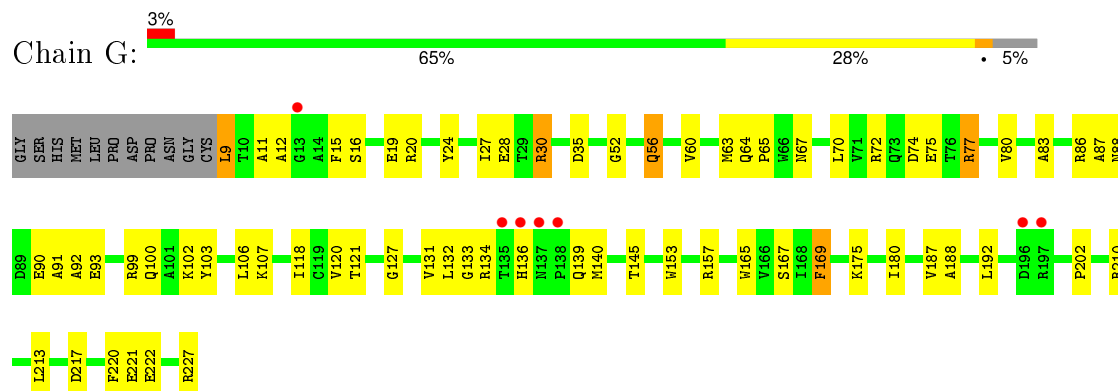
- Molecule 1: BluB



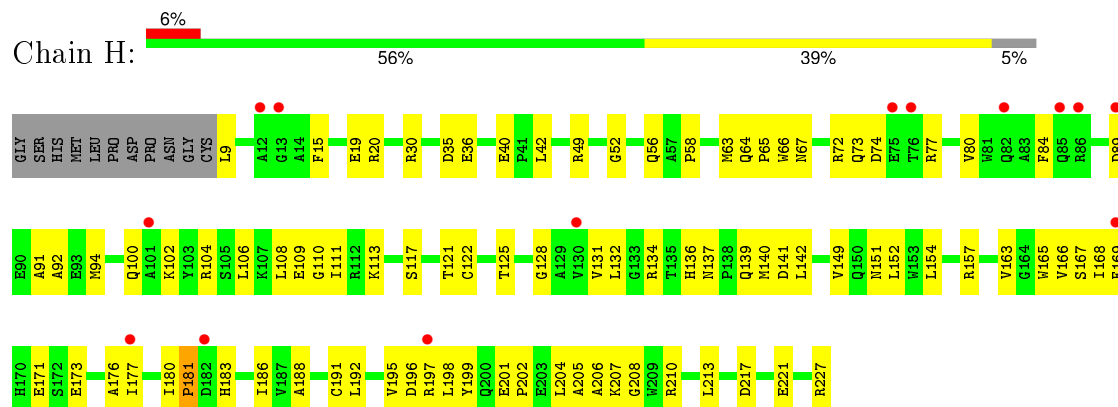
- Molecule 1: BluB



- Molecule 1: BluB



- Molecule 1: BluB





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.15Å 172.72Å 92.06Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 48.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	80.0 (50.00-2.30) 88.6 (48.81-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.207 , 0.252 0.207 , 0.251	Depositor DCC
$R_{free}$ test set	3618 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.2	EDS
Estimated twinning fraction	0.238 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 79967 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	14695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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	0.38	0/1780	0.65	0/2412
1	B	0.38	0/1780	0.65	1/2412 (0.0%)
1	C	0.39	0/1780	0.64	0/2412
1	D	0.38	0/1780	0.65	1/2412 (0.0%)
1	E	0.33	0/1780	0.59	0/2412
1	F	0.34	0/1780	0.59	0/2412
1	G	0.34	0/1780	0.58	0/2412
1	H	0.32	0/1780	0.58	0/2412
All	All	0.36	0/14240	0.62	2/19296 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	D	170	HIS	N-CA-C	-5.17	97.05	111.00

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	1741	0	1716	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1741	0	1716	75	0
1	C	1741	0	1716	60	0
1	D	1741	0	1716	49	0
1	E	1741	0	1716	73	0
1	F	1741	0	1716	66	0
1	G	1741	0	1716	65	0
1	H	1741	0	1716	86	0
2	A	31	0	19	2	0
2	B	31	0	19	6	0
2	C	31	0	19	4	0
2	D	31	0	19	2	0
2	E	31	0	19	7	0
2	F	31	0	19	2	0
2	G	31	0	19	3	0
2	H	31	0	19	3	0
3	A	88	0	0	7	0
3	B	86	0	0	8	0
3	C	69	0	0	8	0
3	D	87	0	0	4	0
3	E	59	0	0	2	0
3	F	55	0	0	2	0
3	G	36	0	0	1	0
3	H	39	0	0	6	0
All	All	14695	0	13880	450	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 16.

All (450) 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:C:90:GLU:HA	3:C:568:HOH:O	1.47	1.14
1:D:131:VAL:HG13	1:D:134:ARG:HB3	1.39	1.02
1:C:145:THR:HG21	1:C:187:VAL:HG11	1.45	0.99
1:C:64:GLN:HE22	1:D:213:LEU:H	1.11	0.98
1:A:89:ASP:HB2	3:A:889:HOH:O	1.74	0.86
1:A:120:VAL:O	1:A:187:VAL:HG12	1.77	0.85
1:D:20:ARG:NH1	1:D:20:ARG:HB2	1.92	0.84
1:D:20:ARG:HH11	1:D:20:ARG:HB2	1.46	0.80
1:B:131:VAL:HG13	1:B:134:ARG:HB3	1.64	0.79
1:E:11:ALA:HA	1:F:197:ARG:HD2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:VAL:HG13	1:C:134:ARG:HB3	1.63	0.78
1:G:222:GLU:HG3	1:H:73:GLN:NE2	1.98	0.78
2:G:508:FMN:H6	1:H:140:MET:HE2	1.64	0.78
1:A:213:LEU:H	1:B:64:GLN:HE22	1.28	0.78
1:D:77:ARG:HD3	3:D:671:HOH:O	1.84	0.78
1:B:187:VAL:HB	3:B:868:HOH:O	1.84	0.77
3:C:1088:HOH:O	1:D:132:LEU:HD22	1.86	0.75
1:H:131:VAL:HG13	1:H:134:ARG:HB3	1.69	0.75
1:E:222:GLU:HG3	1:F:73:GLN:NE2	2.02	0.75
1:A:140:MET:HE2	2:B:501:FMN:H6	1.70	0.74
1:C:92:ALA:O	1:C:100:GLN:HG3	1.87	0.74
1:H:132:LEU:HD22	3:H:1090:HOH:O	1.88	0.73
1:B:24:TYR:O	1:B:28:GLU:HG3	1.88	0.73
1:B:145:THR:HG21	3:B:868:HOH:O	1.89	0.73
2:C:504:FMN:H6	1:D:140:MET:HE2	1.70	0.73
1:H:227:ARG:HG2	1:H:227:ARG:HH11	1.54	0.73
1:B:100:GLN:NE2	1:B:104:ARG:HH21	1.87	0.72
1:E:145:THR:HG21	1:E:187:VAL:HG11	1.71	0.72
1:G:64:GLN:HE22	1:H:213:LEU:H	1.35	0.72
1:A:107:LYS:HE2	1:A:109:GLU:O	1.91	0.71
1:A:182:ASP:HB2	3:A:792:HOH:O	1.90	0.71
1:E:131:VAL:HG13	1:E:134:ARG:HB3	1.71	0.71
1:F:134:ARG:HG2	1:F:138:PRO:HA	1.74	0.70
1:C:222:GLU:HG3	1:D:73:GLN:NE2	2.07	0.70
1:E:137:ASN:HB2	3:E:934:HOH:O	1.92	0.70
1:C:24:TYR:O	1:C:28:GLU:HG3	1.91	0.70
1:C:64:GLN:NE2	1:D:213:LEU:H	1.87	0.70
1:A:15:PHE:HB3	1:A:19:GLU:HB2	1.75	0.69
1:G:87:ALA:CB	1:G:169:PHE:HA	2.22	0.68
1:B:132:LEU:HD23	1:B:133:GLY:H	1.58	0.68
1:A:154:LEU:HD23	1:B:154:LEU:HD23	1.74	0.68
1:A:213:LEU:H	1:B:64:GLN:NE2	1.92	0.68
1:A:140:MET:CE	1:B:167:SER:HB3	2.24	0.68
1:A:87:ALA:CB	1:A:169:PHE:HA	2.24	0.67
3:C:743:HOH:O	1:D:137:ASN:HB2	1.94	0.67
1:A:9:LEU:N	1:A:9:LEU:HD23	2.08	0.67
1:H:196:ASP:O	1:H:197:ARG:HD2	1.94	0.67
1:G:120:VAL:O	1:G:187:VAL:HG12	1.95	0.67
1:B:132:LEU:HD23	1:B:133:GLY:N	2.08	0.67
2:E:506:FMN:HM73	1:F:140:MET:HG3	1.78	0.67
1:C:213:LEU:H	1:D:64:GLN:HE22	1.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:ARG:HD3	3:F:565:HOH:O	1.94	0.66
1:G:139:GLN:HE21	1:H:139:GLN:HE21	1.43	0.66
1:H:204:LEU:HD13	3:H:764:HOH:O	1.95	0.66
1:H:191:CYS:C	1:H:192:LEU:HD12	2.17	0.65
1:D:131:VAL:CG1	1:D:134:ARG:HB3	2.21	0.65
1:D:202:PRO:HB3	2:D:503:FMN:H5'2	1.77	0.65
1:E:120:VAL:O	1:E:187:VAL:HG12	1.97	0.65
1:A:145:THR:CG2	1:A:187:VAL:HG11	2.28	0.65
1:E:145:THR:CG2	1:E:187:VAL:HG11	2.26	0.65
1:G:30:ARG:HA	1:G:157:ARG:HD3	1.79	0.65
1:C:145:THR:CG2	1:C:187:VAL:HG11	2.24	0.64
1:E:131:VAL:CG1	1:E:134:ARG:HB3	2.27	0.64
1:A:64:GLN:HE22	1:B:213:LEU:H	1.44	0.64
1:E:94:MET:HE3	1:F:135:THR:HB	1.80	0.64
1:A:72:ARG:C	1:A:77:ARG:HH12	2.01	0.64
1:D:107:LYS:HE2	1:D:109:GLU:O	1.98	0.64
1:B:128:GLY:HA3	3:B:1067:HOH:O	1.97	0.63
1:E:102:LYS:HE2	1:E:207:LYS:O	1.99	0.63
1:E:132:LEU:HD22	3:E:572:HOH:O	1.97	0.63
1:F:132:LEU:HD23	1:F:133:GLY:N	2.14	0.63
1:D:80:VAL:HG21	1:D:189:TRP:CH2	2.34	0.63
1:C:77:ARG:HD3	3:C:815:HOH:O	1.99	0.62
1:G:9:LEU:N	1:G:9:LEU:HD23	2.14	0.62
1:B:30:ARG:NH1	2:B:501:FMN:O2P	2.32	0.62
1:H:125:THR:HG23	1:H:183:HIS:HB2	1.83	0.61
1:F:165:TRP:CZ2	1:F:188:ALA:HB2	2.36	0.61
1:E:140:MET:HE3	2:F:505:FMN:H6	1.83	0.61
1:E:91:ALA:HA	1:E:94:MET:HE3	1.82	0.61
1:E:94:MET:CE	1:F:135:THR:HB	2.31	0.61
1:A:167:SER:HB3	1:B:140:MET:HE2	1.81	0.60
2:A:502:FMN:H6	1:B:140:MET:HE2	1.83	0.60
1:A:77:ARG:HD3	3:A:811:HOH:O	1.99	0.60
1:F:24:TYR:O	1:F:28:GLU:HG3	2.01	0.60
1:G:132:LEU:HD22	3:G:1089:HOH:O	2.00	0.60
1:E:165:TRP:CZ2	1:E:188:ALA:HB2	2.37	0.60
1:C:131:VAL:CG1	1:C:134:ARG:HB3	2.30	0.60
1:B:91:ALA:HA	1:B:94:MET:HE3	1.83	0.60
1:C:89:ASP:O	3:C:568:HOH:O	2.15	0.60
1:H:52:GLY:O	1:H:56:GLN:HG2	2.01	0.60
1:G:213:LEU:H	1:H:64:GLN:HE22	1.47	0.59
1:A:140:MET:HE1	1:B:167:SER:HB3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:GLU:HG2	1:D:56:GLN:OE1	2.01	0.59
1:A:222:GLU:HG3	1:B:73:GLN:NE2	2.16	0.59
1:E:30:ARG:NH2	2:E:506:FMN:O2P	2.35	0.59
1:F:67:ASN:HB2	1:F:121:THR:OG1	2.02	0.59
1:G:15:PHE:HB3	1:G:19:GLU:HB2	1.84	0.59
1:G:132:LEU:HD21	1:H:108:LEU:HD22	1.84	0.59
1:C:154:LEU:HD23	1:D:154:LEU:HD12	1.84	0.59
1:A:227:ARG:HG2	1:A:227:ARG:HH11	1.68	0.59
1:E:139:GLN:HE21	1:F:139:GLN:HE21	1.51	0.58
1:F:42:LEU:HD22	1:F:116:LEU:HD23	1.84	0.58
1:D:102:LYS:HE2	3:D:1077:HOH:O	2.04	0.58
1:H:163:VAL:HG22	1:H:192:LEU:HG	1.86	0.58
1:F:76:THR:O	1:F:80:VAL:HG23	2.03	0.57
1:C:120:VAL:O	1:C:187:VAL:HG13	2.04	0.57
1:E:217:ASP:HA	1:E:227:ARG:HH21	1.70	0.57
1:E:15:PHE:HB3	1:E:19:GLU:HB2	1.86	0.57
1:E:140:MET:HE2	1:F:167:SER:CB	2.34	0.57
1:F:173:GLU:O	1:F:177:ILE:HG13	2.04	0.57
1:G:127:GLY:HA2	1:H:210:ARG:NH1	2.19	0.57
1:C:154:LEU:HD23	1:D:154:LEU:CD1	2.34	0.57
1:D:74:ASP:HA	1:D:77:ARG:NH1	2.20	0.57
1:E:87:ALA:CB	1:E:169:PHE:HA	2.35	0.57
1:A:134:ARG:HG2	1:A:138:PRO:HA	1.87	0.57
1:E:80:VAL:HG21	1:E:189:TRP:CH2	2.39	0.57
1:A:145:THR:HG22	1:A:187:VAL:HG11	1.87	0.57
1:A:82:GLN:NE2	3:A:551:HOH:O	2.37	0.57
1:B:227:ARG:HG2	1:B:227:ARG:HH11	1.70	0.56
1:B:131:VAL:HG11	1:B:134:ARG:NE	2.20	0.56
1:G:64:GLN:NE2	1:H:213:LEU:H	2.01	0.56
1:A:87:ALA:HB2	1:A:169:PHE:HA	1.87	0.56
1:F:227:ARG:HG2	1:F:227:ARG:HH11	1.70	0.56
1:G:52:GLY:O	1:G:56:GLN:HG2	2.05	0.56
1:F:63:MET:CE	1:F:65:PRO:HB3	2.36	0.56
1:G:74:ASP:HA	1:G:77:ARG:NH1	2.20	0.56
1:D:227:ARG:HG2	1:D:227:ARG:HH11	1.70	0.56
1:E:60:VAL:HG22	1:E:132:LEU:O	2.05	0.55
1:B:52:GLY:O	1:B:56:GLN:HG2	2.06	0.55
1:A:64:GLN:NE2	1:B:213:LEU:H	2.04	0.55
1:G:35:ASP:HB2	1:G:107:LYS:HD2	1.89	0.55
1:C:35:ASP:HB2	1:C:107:LYS:HD2	1.88	0.55
1:A:102:LYS:HE2	1:A:207:LYS:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:MET:HE3	1:H:167:SER:HB3	1.89	0.55
1:G:27:ILE:HG23	1:H:151:ASN:ND2	2.22	0.55
1:F:86:ARG:NH2	1:F:173:GLU:OE1	2.40	0.55
1:F:134:ARG:CG	1:F:138:PRO:HA	2.36	0.55
1:E:91:ALA:HA	1:E:94:MET:CE	2.36	0.55
1:A:197:ARG:HD2	1:B:9:LEU:HD21	1.88	0.55
1:A:52:GLY:O	1:A:56:GLN:HG3	2.07	0.55
1:C:165:TRP:CE2	1:D:140:MET:HE3	2.41	0.54
1:E:204:LEU:HD12	2:E:506:FMN:O4'	2.06	0.54
1:B:220:PHE:HE1	1:B:227:ARG:HH12	1.55	0.54
1:A:140:MET:HE2	1:B:167:SER:HB3	1.89	0.54
1:F:39:PRO:HG2	1:F:40:GLU:OE2	2.06	0.54
1:G:16:SER:OG	1:G:19:GLU:HG3	2.07	0.54
1:E:195:VAL:HG21	1:E:198:LEU:HD21	1.88	0.54
1:D:131:VAL:HG11	1:D:134:ARG:NE	2.23	0.54
1:H:227:ARG:HG2	1:H:227:ARG:NH1	2.22	0.54
1:G:60:VAL:HG22	1:G:132:LEU:O	2.07	0.54
1:H:132:LEU:CD2	3:H:1090:HOH:O	2.53	0.54
1:A:163:VAL:HG22	1:A:192:LEU:HG	1.89	0.54
1:A:80:VAL:HG21	1:A:189:TRP:CH2	2.43	0.54
1:C:165:TRP:CZ2	1:D:140:MET:HE3	2.44	0.53
1:C:90:GLU:CA	3:C:568:HOH:O	2.25	0.53
1:B:131:VAL:CG1	1:B:134:ARG:NE	2.71	0.53
1:E:140:MET:CE	1:F:167:SER:HB3	2.38	0.53
1:H:205:ALA:HA	1:H:210:ARG:O	2.08	0.53
1:E:227:ARG:HH11	1:E:227:ARG:HG2	1.74	0.53
1:H:15:PHE:HB3	1:H:19:GLU:HB2	1.90	0.53
1:A:165:TRP:CE2	1:B:140:MET:HE3	2.43	0.53
1:A:58:PRO:HG3	1:B:153:TRP:CZ3	2.43	0.53
1:G:165:TRP:CZ2	1:G:188:ALA:HB2	2.44	0.53
1:E:58:PRO:HD3	1:F:30:ARG:HH21	1.73	0.53
1:H:74:ASP:OD1	1:H:77:ARG:NH2	2.42	0.53
1:E:9:LEU:N	1:E:9:LEU:HD23	2.24	0.53
1:A:167:SER:HB3	1:B:140:MET:CE	2.38	0.52
1:H:152:LEU:HD23	1:H:152:LEU:O	2.09	0.52
1:A:165:TRP:CZ2	1:A:188:ALA:HB2	2.45	0.52
1:C:202:PRO:HA	2:C:504:FMN:O3P	2.10	0.52
1:E:9:LEU:HB2	1:F:198:LEU:O	2.09	0.52
1:A:30:ARG:HG3	1:A:30:ARG:O	2.10	0.52
1:E:64:GLN:HE22	1:F:213:LEU:H	1.57	0.52
1:G:70:LEU:HD23	1:G:118:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:TRP:CZ2	1:B:188:ALA:HB2	2.44	0.52
1:B:87:ALA:O	1:B:90:GLU:HG2	2.10	0.52
1:B:100:GLN:HE21	1:B:104:ARG:HH21	1.56	0.52
1:H:35:ASP:OD1	1:H:113:LYS:HE3	2.10	0.52
1:A:165:TRP:CZ2	1:B:140:MET:HE3	2.44	0.52
1:A:15:PHE:HB3	1:A:19:GLU:CB	2.40	0.52
1:H:108:LEU:HD13	1:H:168:ILE:CD1	2.40	0.52
1:F:84:PHE:CE2	1:F:109:GLU:HG2	2.44	0.52
1:B:15:PHE:HB3	1:B:19:GLU:HB2	1.92	0.52
1:H:42:LEU:HD12	1:H:42:LEU:N	2.25	0.52
1:A:35:ASP:HB2	1:A:107:LYS:CD	2.40	0.52
1:H:201:GLU:HB2	3:H:950:HOH:O	2.10	0.52
1:C:131:VAL:HG11	1:C:134:ARG:NE	2.25	0.51
1:B:38:LEU:HD11	1:B:196:ASP:OD2	2.11	0.51
1:G:221:GLU:OE1	1:H:72:ARG:NH2	2.42	0.51
1:D:9:LEU:N	3:D:622:HOH:O	2.42	0.51
1:B:80:VAL:HG21	1:B:189:TRP:CH2	2.45	0.51
1:B:90:GLU:OE1	1:B:170:HIS:NE2	2.44	0.51
1:H:171:GLU:HG3	1:H:186:ILE:HD12	1.93	0.51
1:G:139:GLN:NE2	1:H:139:GLN:HE21	2.08	0.51
1:F:38:LEU:HB3	1:F:40:GLU:OE1	2.11	0.51
1:E:42:LEU:HD23	1:E:42:LEU:N	2.26	0.51
1:D:20:ARG:NH1	1:D:20:ARG:CB	2.69	0.51
1:E:197:ARG:HB2	1:F:9:LEU:HD22	1.93	0.51
1:C:173:GLU:O	1:C:177:ILE:HG13	2.10	0.51
1:C:227:ARG:HG2	1:C:227:ARG:HH11	1.76	0.51
1:C:52:GLY:O	1:C:56:GLN:HG2	2.11	0.51
1:C:153:TRP:CD1	1:C:163:VAL:HB	2.46	0.51
1:G:63:MET:CE	1:G:65:PRO:HB3	2.40	0.51
1:B:48:ALA:HB3	3:B:607:HOH:O	2.11	0.51
1:H:166:VAL:HG12	1:H:169:PHE:CE1	2.46	0.51
1:H:84:PHE:CE2	1:H:109:GLU:HG2	2.46	0.50
1:A:108:LEU:HD22	1:B:132:LEU:HD21	1.92	0.50
1:E:58:PRO:CD	1:F:30:ARG:HH21	2.24	0.50
1:G:217:ASP:HA	1:G:227:ARG:HH21	1.74	0.50
1:A:91:ALA:HA	1:A:94:MET:HE3	1.93	0.50
1:D:202:PRO:HA	2:D:503:FMN:O1P	2.12	0.50
1:C:60:VAL:HG22	1:C:132:LEU:O	2.11	0.50
1:B:134:ARG:HG3	1:B:140:MET:HB2	1.94	0.50
1:E:140:MET:HE1	1:F:165:TRP:HE1	1.76	0.50
1:E:139:GLN:NE2	1:F:139:GLN:HE21	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:LEU:N	1:G:192:LEU:HD12	2.27	0.50
1:B:108:LEU:O	1:B:109:GLU:HB3	2.12	0.50
1:A:35:ASP:HB2	1:A:107:LYS:HD3	1.94	0.50
1:C:98:GLU:HG3	1:C:99:ARG:N	2.27	0.50
1:E:163:VAL:HG22	1:E:192:LEU:HG	1.92	0.50
1:A:140:MET:HE3	1:B:165:TRP:CE2	2.47	0.50
1:C:213:LEU:H	1:D:64:GLN:NE2	2.07	0.50
1:H:77:ARG:CB	1:H:77:ARG:HH11	2.25	0.50
1:E:46:LEU:HD21	1:E:161:VAL:HG21	1.93	0.50
1:H:49:ARG:HH11	1:H:49:ARG:HG3	1.76	0.50
1:C:134:ARG:NH1	1:C:141:ASP:OD2	2.45	0.49
1:E:132:LEU:HD13	1:F:204:LEU:HD21	1.94	0.49
1:G:131:VAL:HG13	1:G:134:ARG:HB3	1.94	0.49
1:C:132:LEU:HD12	1:D:204:LEU:HD21	1.93	0.49
1:C:123:ASP:OD2	1:C:126:ARG:HB2	2.12	0.49
1:G:145:THR:HG22	1:G:187:VAL:HG11	1.93	0.49
1:E:72:ARG:NH2	1:F:221:GLU:OE1	2.46	0.49
1:B:35:ASP:HB2	1:B:107:LYS:HD2	1.94	0.49
1:G:87:ALA:HB2	1:G:169:PHE:HA	1.92	0.49
1:E:222:GLU:OE2	1:F:72:ARG:N	2.41	0.49
1:E:139:GLN:HE21	1:F:139:GLN:NE2	2.11	0.49
1:H:132:LEU:C	1:H:132:LEU:HD23	2.33	0.49
1:A:145:THR:HG21	1:A:187:VAL:HG11	1.94	0.49
1:E:58:PRO:HD3	1:F:30:ARG:NH2	2.28	0.48
1:C:165:TRP:NE1	1:D:140:MET:CE	2.76	0.48
1:B:227:ARG:NH2	3:B:718:HOH:O	2.45	0.48
1:G:93:GLU:OE1	1:G:93:GLU:HA	2.14	0.48
1:F:17:SER:HB3	1:G:86:ARG:HD2	1.95	0.48
1:E:42:LEU:HB3	1:E:46:LEU:HD23	1.95	0.48
1:B:112:ARG:NH2	3:B:597:HOH:O	2.34	0.48
1:H:131:VAL:HG23	3:H:814:HOH:O	2.14	0.48
1:C:165:TRP:CZ2	1:C:188:ALA:HB2	2.48	0.48
1:D:77:ARG:NH1	3:D:857:HOH:O	2.47	0.48
1:G:167:SER:O	1:H:137:ASN:ND2	2.46	0.48
1:E:140:MET:HE2	1:F:167:SER:HB3	1.95	0.48
1:A:9:LEU:CD2	1:A:9:LEU:N	2.77	0.48
1:H:77:ARG:HB3	1:H:77:ARG:HH11	1.79	0.48
1:C:9:LEU:HD23	1:C:9:LEU:N	2.29	0.48
1:A:140:MET:CE	1:B:167:SER:CB	2.92	0.48
1:H:122:CYS:SG	1:H:142:LEU:HD23	2.54	0.48
1:F:132:LEU:HD23	1:F:133:GLY:H	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:THR:O	1:C:80:VAL:HG23	2.14	0.47
1:E:58:PRO:N	1:F:30:ARG:HH21	2.12	0.47
1:F:81:TRP:CH2	1:F:85:GLN:HG3	2.49	0.47
1:C:30:ARG:HA	1:C:157:ARG:HD3	1.96	0.47
1:A:167:SER:CB	1:B:140:MET:HE2	2.43	0.47
1:H:202:PRO:HD2	3:H:950:HOH:O	2.14	0.47
1:G:72:ARG:NH2	1:H:221:GLU:OE2	2.46	0.47
1:G:165:TRP:CZ2	2:G:508:FMN:HM72	2.50	0.47
1:C:167:SER:HB3	1:D:140:MET:CE	2.45	0.47
1:F:202:PRO:HB3	2:F:505:FMN:H5'2	1.96	0.47
1:A:221:GLU:O	1:A:222:GLU:HB2	2.13	0.47
1:H:9:LEU:HD23	1:H:9:LEU:C	2.34	0.47
1:H:66:TRP:HA	1:H:121:THR:O	2.15	0.47
1:H:100:GLN:O	1:H:104:ARG:HB2	2.15	0.47
1:D:132:LEU:HD23	1:D:133:GLY:N	2.30	0.47
1:A:180:ILE:HA	1:A:181:PRO:HD3	1.76	0.47
1:D:91:ALA:HA	1:D:94:MET:HE3	1.97	0.47
1:H:80:VAL:HG12	1:H:111:ILE:HD13	1.97	0.47
1:C:107:LYS:HE2	1:C:109:GLU:O	2.15	0.46
1:A:30:ARG:NH1	1:A:30:ARG:O	2.48	0.46
1:G:80:VAL:O	1:G:83:ALA:HB3	2.15	0.46
1:G:165:TRP:CZ2	1:H:140:MET:HE3	2.50	0.46
1:E:222:GLU:OE2	1:F:71:VAL:HA	2.15	0.46
1:B:100:GLN:NE2	3:B:697:HOH:O	2.47	0.46
1:E:31:ARG:HH21	2:E:506:FMN:P	2.39	0.46
1:C:64:GLN:HE22	1:D:213:LEU:N	1.94	0.46
1:B:202:PRO:HB3	2:B:501:FMN:H5'2	1.97	0.46
1:C:167:SER:HB3	1:D:140:MET:HE2	1.98	0.46
1:E:202:PRO:HA	2:E:506:FMN:O3P	2.14	0.46
1:A:227:ARG:HG3	1:E:125:THR:O	2.16	0.46
1:G:127:GLY:HA2	1:H:210:ARG:HH12	1.80	0.46
1:H:141:ASP:OD1	1:H:142:LEU:N	2.48	0.46
1:F:140:MET:HE3	1:F:143:TYR:HD2	1.80	0.46
1:F:137:ASN:OD1	1:F:139:GLN:HB2	2.15	0.46
1:E:15:PHE:HB3	1:E:19:GLU:CB	2.45	0.46
1:C:165:TRP:NE1	1:D:140:MET:HE3	2.31	0.46
1:E:140:MET:HE2	1:F:167:SER:HB2	1.96	0.46
1:G:12:ALA:O	1:H:196:ASP:HA	2.15	0.46
1:B:202:PRO:HB3	2:B:501:FMN:C5'	2.46	0.45
1:F:227:ARG:HG2	1:F:227:ARG:NH1	2.30	0.45
1:E:222:GLU:HG3	1:F:73:GLN:HE21	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:VAL:CG2	1:G:133:GLY:HA3	2.46	0.45
1:B:227:ARG:NH1	1:B:227:ARG:HG2	2.31	0.45
1:A:94:MET:HE3	1:B:135:THR:HB	1.98	0.45
1:E:151:ASN:OD1	1:F:154:LEU:HD11	2.16	0.45
1:H:217:ASP:O	1:H:227:ARG:NH2	2.50	0.45
1:A:72:ARG:N	1:B:222:GLU:OE2	2.36	0.45
1:C:15:PHE:HB3	1:C:19:GLU:HB2	1.99	0.45
1:E:52:GLY:O	1:E:56:GLN:HG2	2.16	0.45
1:G:145:THR:CG2	1:G:187:VAL:HG11	2.46	0.45
1:C:86:ARG:NH2	1:C:173:GLU:OE1	2.35	0.45
1:G:86:ARG:O	1:G:90:GLU:HG3	2.17	0.45
1:H:36:GLU:N	1:H:36:GLU:CD	2.70	0.45
1:G:67:ASN:HB2	1:G:121:THR:OG1	2.17	0.45
1:F:77:ARG:HD2	1:F:111:ILE:O	2.16	0.45
1:G:30:ARG:NH2	1:H:58:PRO:HD3	2.31	0.45
1:A:220:PHE:HE1	1:A:227:ARG:NH1	2.15	0.45
1:D:227:ARG:CG	1:D:227:ARG:HH11	2.29	0.45
1:F:114:ALA:HB1	1:F:192:LEU:O	2.16	0.45
1:F:45:GLU:N	1:F:45:GLU:CD	2.70	0.45
1:A:165:TRP:NE1	1:B:140:MET:HE3	2.32	0.45
1:E:202:PRO:HG3	2:E:506:FMN:O3P	2.17	0.44
1:C:145:THR:HG21	1:C:187:VAL:CG1	2.31	0.44
1:E:78:GLU:OE1	1:E:82:GLN:NE2	2.50	0.44
1:H:177:ILE:HG22	1:H:177:ILE:O	2.16	0.44
1:A:140:MET:HE3	2:B:501:FMN:HM72	1.98	0.44
1:F:131:VAL:HG13	1:F:134:ARG:HB3	2.00	0.44
1:F:30:ARG:O	1:F:30:ARG:HG3	2.18	0.44
1:C:9:LEU:N	3:C:642:HOH:O	2.50	0.44
1:G:60:VAL:O	1:G:60:VAL:HG13	2.18	0.44
1:A:30:ARG:HH21	1:B:58:PRO:N	2.16	0.44
1:H:15:PHE:HB2	1:H:20:ARG:HG3	1.99	0.44
1:E:191:CYS:C	1:E:192:LEU:HD12	2.38	0.44
1:H:92:ALA:C	1:H:94:MET:H	2.19	0.44
1:B:60:VAL:O	1:B:63:MET:HB2	2.18	0.44
1:H:192:LEU:HD12	1:H:192:LEU:N	2.32	0.44
1:A:191:CYS:C	1:A:192:LEU:HD12	2.38	0.44
1:C:42:LEU:HD12	1:C:42:LEU:N	2.33	0.44
1:E:38:LEU:HB3	1:E:40:GLU:OE2	2.18	0.44
1:H:67:ASN:HB2	1:H:121:THR:OG1	2.18	0.44
1:E:134:ARG:NH1	1:E:141:ASP:OD2	2.51	0.43
1:C:153:TRP:CZ3	1:D:58:PRO:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:204:LEU:HD22	2:H:507:FMN:O4'	2.18	0.43
1:A:57:ALA:HB1	1:A:58:PRO:HD2	1.99	0.43
1:C:40:GLU:HA	1:C:41:PRO:HD3	1.92	0.43
1:B:77:ARG:HD3	3:B:902:HOH:O	2.17	0.43
1:E:134:ARG:HD2	1:E:138:PRO:O	2.19	0.43
1:H:108:LEU:HD13	1:H:168:ILE:HD11	2.00	0.43
1:C:40:GLU:OE2	1:C:40:GLU:N	2.45	0.43
1:E:180:ILE:HA	1:E:181:PRO:HD3	1.84	0.43
1:H:165:TRP:CZ2	1:H:188:ALA:HB2	2.54	0.43
1:A:82:GLN:O	1:A:86:ARG:HG3	2.18	0.43
1:A:64:GLN:N	1:A:65:PRO:CD	2.81	0.43
1:A:153:TRP:CD1	1:A:163:VAL:HB	2.54	0.43
1:B:35:ASP:HB2	1:B:107:LYS:CD	2.49	0.43
1:B:131:VAL:CG1	1:B:134:ARG:HE	2.31	0.43
1:A:108:LEU:CD2	1:B:132:LEU:HD21	2.49	0.43
1:C:132:LEU:CD1	1:D:204:LEU:HD21	2.49	0.43
1:H:206:ALA:C	1:H:208:GLY:H	2.22	0.43
1:G:88:ASN:O	1:G:91:ALA:HB3	2.18	0.43
1:A:35:ASP:HA	1:A:107:LYS:NZ	2.34	0.43
1:E:131:VAL:CG1	1:E:134:ARG:HE	2.31	0.43
1:E:140:MET:HE1	1:F:165:TRP:NE1	2.34	0.43
1:F:40:GLU:HA	1:F:41:PRO:HD3	1.91	0.43
1:B:63:MET:CE	1:B:65:PRO:HB3	2.49	0.43
1:C:31:ARG:HH21	2:C:504:FMN:P	2.42	0.43
1:B:15:PHE:HB2	1:B:20:ARG:HG3	2.00	0.43
1:E:40:GLU:H	1:E:40:GLU:CD	2.21	0.43
1:A:81:TRP:O	1:A:84:PHE:HB3	2.19	0.43
1:A:140:MET:CE	1:B:165:TRP:NE1	2.82	0.42
1:A:40:GLU:HA	1:A:41:PRO:HD3	1.95	0.42
1:G:35:ASP:HB2	1:G:107:LYS:CD	2.49	0.42
1:H:109:GLU:OE2	1:H:110:GLY:N	2.52	0.42
1:G:136:HIS:HE1	1:H:91:ALA:HB2	1.83	0.42
1:H:217:ASP:HA	1:H:227:ARG:HH21	1.84	0.42
1:H:149:VAL:HG11	1:H:165:TRP:CZ3	2.54	0.42
1:E:102:LYS:HD2	1:E:102:LYS:HA	1.84	0.42
1:B:173:GLU:O	1:B:177:ILE:HG13	2.19	0.42
1:H:195:VAL:HG21	1:H:198:LEU:HD21	2.01	0.42
1:G:11:ALA:HB2	1:H:197:ARG:CZ	2.49	0.42
1:F:227:ARG:HA	1:F:227:ARG:HD3	1.86	0.42
1:E:63:MET:CE	1:E:65:PRO:HB3	2.49	0.42
1:A:215:LEU:HD13	1:B:55:HIS:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ARG:CZ	1:D:20:ARG:CB	2.98	0.42
1:H:180:ILE:HA	1:H:181:PRO:HD3	1.86	0.42
1:A:152:LEU:C	1:A:152:LEU:HD23	2.39	0.42
1:A:9:LEU:N	3:A:538:HOH:O	2.53	0.42
1:A:91:ALA:HA	1:A:94:MET:CE	2.50	0.42
1:D:144:SER:O	1:D:147:CYS:HB2	2.19	0.42
1:B:40:GLU:HA	1:B:41:PRO:HD3	1.84	0.42
1:C:195:VAL:HG23	1:C:195:VAL:O	2.19	0.42
1:D:30:ARG:HA	1:D:157:ARG:HD3	2.01	0.42
1:G:167:SER:HB3	1:H:140:MET:CE	2.49	0.42
1:C:227:ARG:HE	1:H:128:GLY:HA2	1.85	0.42
1:G:175:LYS:HE3	1:G:180:ILE:HG22	2.02	0.42
1:C:222:GLU:OE2	1:D:72:ARG:N	2.46	0.42
1:E:204:LEU:HD23	1:E:204:LEU:HA	1.90	0.42
1:F:165:TRP:HD1	1:F:166:VAL:N	2.18	0.42
1:G:15:PHE:HE1	1:H:157:ARG:CZ	2.33	0.42
1:F:77:ARG:NE	3:F:618:HOH:O	2.51	0.42
1:B:220:PHE:CE1	1:B:227:ARG:NH1	2.88	0.42
1:G:220:PHE:HE1	1:G:227:ARG:NH1	2.18	0.42
1:A:77:ARG:HD2	1:A:111:ILE:O	2.20	0.41
1:A:30:ARG:HH21	1:B:58:PRO:HD3	1.85	0.41
1:C:81:TRP:O	1:C:84:PHE:HB3	2.20	0.41
1:G:153:TRP:CZ3	1:H:58:PRO:HG3	2.56	0.41
1:C:93:GLU:HB2	3:C:568:HOH:O	2.20	0.41
1:A:213:LEU:N	1:B:64:GLN:HE22	2.06	0.41
1:G:102:LYS:O	1:G:106:LEU:HG	2.20	0.41
1:E:99:ARG:HA	1:E:99:ARG:HD2	1.88	0.41
1:A:202:PRO:HA	2:A:502:FMN:O3P	2.21	0.41
1:G:202:PRO:HA	2:G:508:FMN:O3P	2.21	0.41
1:B:30:ARG:HH22	2:B:501:FMN:P	2.43	0.41
1:F:165:TRP:CE2	1:F:188:ALA:HB2	2.55	0.41
1:D:131:VAL:CG1	1:D:134:ARG:NE	2.83	0.41
1:F:196:ASP:O	1:F:197:ARG:HD2	2.20	0.41
1:B:64:GLN:N	1:B:65:PRO:CD	2.83	0.41
1:G:87:ALA:HB1	1:H:136:HIS:CD2	2.55	0.41
1:A:153:TRP:CZ3	1:B:58:PRO:HG3	2.55	0.41
1:F:81:TRP:O	1:F:84:PHE:HB3	2.20	0.41
1:G:99:ARG:O	1:G:103:TYR:N	2.46	0.41
1:D:80:VAL:HG12	1:D:111:ILE:HD13	2.02	0.41
1:H:173:GLU:O	1:H:176:ALA:HB3	2.21	0.41
1:D:124:ARG:NE	1:D:141:ASP:OD2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:165:TRP:HD1	1:H:166:VAL:N	2.18	0.41
1:E:192:LEU:N	1:E:192:LEU:HD12	2.36	0.41
1:E:11:ALA:HB2	1:F:197:ARG:NH1	2.35	0.41
1:A:9:LEU:HA	3:A:538:HOH:O	2.19	0.41
1:H:49:ARG:NH1	1:H:49:ARG:HG3	2.35	0.41
1:H:89:ASP:C	1:H:91:ALA:H	2.23	0.41
1:G:75:GLU:H	1:G:75:GLU:CD	2.24	0.41
1:H:102:LYS:O	1:H:106:LEU:HG	2.21	0.41
1:D:165:TRP:CZ2	1:D:188:ALA:HB2	2.56	0.41
1:A:212:ARG:HA	1:B:64:GLN:HE22	1.87	0.41
1:E:108:LEU:O	1:E:109:GLU:HB3	2.20	0.41
1:G:213:LEU:H	1:H:64:GLN:NE2	2.17	0.40
1:G:102:LYS:HA	1:G:102:LYS:HD2	1.88	0.40
1:A:171:GLU:CD	3:A:1050:HOH:O	2.59	0.40
2:E:506:FMN:C7M	1:F:140:MET:HG3	2.49	0.40
1:F:80:VAL:HG21	1:F:189:TRP:CH2	2.56	0.40
1:H:202:PRO:HB3	2:H:507:FMN:H5'2	2.03	0.40
1:H:165:TRP:CZ2	2:H:507:FMN:HM72	2.56	0.40
1:G:20:ARG:O	1:G:24:TYR:HD1	2.05	0.40
1:A:187:VAL:HG13	1:A:188:ALA:N	2.36	0.40
1:A:140:MET:HE2	1:B:167:SER:CB	2.52	0.40
1:C:32:ASP:N	2:C:504:FMN:O1P	2.54	0.40
1:H:196:ASP:C	1:H:197:ARG:HD2	2.41	0.40
1:G:9:LEU:HD22	1:H:199:TYR:CE1	2.56	0.40
1:F:163:VAL:HG22	1:F:192:LEU:HG	2.03	0.40
1:G:24:TYR:O	1:G:28:GLU:HG3	2.21	0.40
1:H:63:MET:CE	1:H:65:PRO:HB3	2.52	0.40
1:G:92:ALA:O	1:G:100:GLN:HG3	2.22	0.40
1:D:45:GLU:H	1:D:45:GLU:CD	2.25	0.40
1:C:114:ALA:HA	1:C:115:PRO:HD2	1.92	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	217/230 (94%)	214 (99%)	3 (1%)	0	100	100
1	B	217/230 (94%)	208 (96%)	6 (3%)	3 (1%)	14	13
1	C	217/230 (94%)	211 (97%)	6 (3%)	0	100	100
1	D	217/230 (94%)	211 (97%)	6 (3%)	0	100	100
1	E	217/230 (94%)	207 (95%)	10 (5%)	0	100	100
1	F	217/230 (94%)	206 (95%)	11 (5%)	0	100	100
1	G	217/230 (94%)	212 (98%)	5 (2%)	0	100	100
1	H	217/230 (94%)	202 (93%)	13 (6%)	2 (1%)	21	24
All	All	1736/1840 (94%)	1671 (96%)	60 (4%)	5 (0%)	46	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	207	LYS
1	B	97	GLY
1	B	109	GLU
1	B	133	GLY
1	H	181	PRO

### 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	178/187 (95%)	167 (94%)	11 (6%)	23	30
1	B	178/187 (95%)	172 (97%)	6 (3%)	44	59
1	C	178/187 (95%)	170 (96%)	8 (4%)	34	46
1	D	178/187 (95%)	170 (96%)	8 (4%)	34	46
1	E	178/187 (95%)	171 (96%)	7 (4%)	39	53
1	F	178/187 (95%)	171 (96%)	7 (4%)	39	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	178/187 (95%)	172 (97%)	6 (3%)	44	59
1	H	178/187 (95%)	174 (98%)	4 (2%)	60	77
All	All	1424/1496 (95%)	1367 (96%)	57 (4%)	38	52

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	30	ARG
1	A	56	GLN
1	A	72	ARG
1	A	93	GLU
1	A	99	ARG
1	A	117	SER
1	A	131	VAL
1	A	132	LEU
1	A	154	LEU
1	A	169	PHE
1	B	30	ARG
1	B	93	GLU
1	B	98	GLU
1	B	117	SER
1	B	154	LEU
1	B	169	PHE
1	C	9	LEU
1	C	30	ARG
1	C	56	GLN
1	C	77	ARG
1	C	98	GLU
1	C	132	LEU
1	C	154	LEU
1	C	187	VAL
1	D	9	LEU
1	D	30	ARG
1	D	96	SER
1	D	98	GLU
1	D	104	ARG
1	D	117	SER
1	D	140	MET
1	D	204	LEU
1	E	9	LEU

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Mol	Chain	Res	Type
1	E	30	ARG
1	E	42	LEU
1	E	56	GLN
1	E	65	PRO
1	E	82	GLN
1	E	98	GLU
1	F	18	ASP
1	F	56	GLN
1	F	98	GLU
1	F	107	LYS
1	F	131	VAL
1	F	132	LEU
1	F	140	MET
1	G	9	LEU
1	G	30	ARG
1	G	56	GLN
1	G	77	ARG
1	G	169	PHE
1	G	210	ARG
1	H	30	ARG
1	H	40	GLU
1	H	117	SER
1	H	154	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	64	GLN
1	A	82	GLN
1	A	85	GLN
1	A	211	GLN
1	B	56	GLN
1	B	64	GLN
1	B	73	GLN
1	B	82	GLN
1	B	100	GLN
1	B	139	GLN
1	B	211	GLN
1	C	56	GLN
1	C	64	GLN
1	D	64	GLN

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Mol	Chain	Res	Type
1	D	73	GLN
1	D	139	GLN
1	E	56	GLN
1	E	64	GLN
1	E	82	GLN
1	E	200	GLN
1	E	211	GLN
1	F	56	GLN
1	F	73	GLN
1	F	82	GLN
1	F	139	GLN
1	F	211	GLN
1	G	56	GLN
1	G	64	GLN
1	G	139	GLN
1	G	211	GLN
1	H	56	GLN
1	H	64	GLN
1	H	73	GLN
1	H	137	ASN
1	H	150	GLN
1	H	211	GLN

### 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](#)

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	502	-	32,33,33	2.83	12 (37%)	34,50,50	2.27	10 (29%)
2	FMN	B	501	-	32,33,33	2.68	12 (37%)	34,50,50	2.06	9 (26%)
2	FMN	C	504	-	32,33,33	2.56	9 (28%)	34,50,50	2.20	9 (26%)
2	FMN	D	503	-	32,33,33	2.78	12 (37%)	34,50,50	2.07	9 (26%)
2	FMN	E	506	-	32,33,33	2.68	13 (40%)	34,50,50	2.25	9 (26%)
2	FMN	F	505	-	32,33,33	2.78	9 (28%)	34,50,50	1.98	7 (20%)
2	FMN	G	508	-	32,33,33	2.60	9 (28%)	34,50,50	2.23	9 (26%)
2	FMN	H	507	-	32,33,33	2.72	9 (28%)	34,50,50	1.99	8 (23%)

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	502	-	-	0/18/18/18	0/3/3/3
2	FMN	B	501	-	-	0/18/18/18	0/3/3/3
2	FMN	C	504	-	-	0/18/18/18	0/3/3/3
2	FMN	D	503	-	-	0/18/18/18	0/3/3/3
2	FMN	E	506	-	-	0/18/18/18	0/3/3/3
2	FMN	F	505	-	-	0/18/18/18	0/3/3/3
2	FMN	G	508	-	-	0/18/18/18	0/3/3/3
2	FMN	H	507	-	-	0/18/18/18	0/3/3/3

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	FMN	C2'-C3'	-2.95	1.47	1.53
2	D	503	FMN	P-O2P	-2.91	1.44	1.54
2	E	506	FMN	P-O2P	-2.70	1.45	1.54
2	H	507	FMN	P-O2P	-2.67	1.45	1.54
2	B	501	FMN	P-O2P	-2.63	1.45	1.54
2	D	503	FMN	C2'-C3'	-2.59	1.48	1.53
2	F	505	FMN	P-O2P	-2.52	1.46	1.54
2	G	508	FMN	P-O2P	-2.47	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	FMN	P-O2P	-2.39	1.46	1.54
2	C	504	FMN	C2'-C3'	-2.37	1.48	1.53
2	C	504	FMN	P-O2P	-2.10	1.47	1.54
2	A	502	FMN	P-O5'	-2.06	1.54	1.59
2	E	506	FMN	C2'-C3'	-2.03	1.49	1.53
2	E	506	FMN	P-O3P	-2.02	1.47	1.54
2	E	506	FMN	C8M-C8	2.01	1.55	1.51
2	E	506	FMN	C10-N1	2.03	1.39	1.35
2	E	506	FMN	C9-C9A	2.04	1.45	1.40
2	G	508	FMN	C9-C9A	2.06	1.45	1.40
2	F	505	FMN	C9-C9A	2.07	1.45	1.40
2	D	503	FMN	C4'-C3'	2.09	1.57	1.53
2	D	503	FMN	C10-N1	2.14	1.39	1.35
2	A	502	FMN	C10-N1	2.15	1.39	1.35
2	B	501	FMN	C10-N1	2.15	1.39	1.35
2	B	501	FMN	C9-C9A	2.18	1.45	1.40
2	H	507	FMN	C5'-C4'	2.21	1.55	1.51
2	C	504	FMN	C6-C7	2.25	1.44	1.37
2	H	507	FMN	C6-C7	2.28	1.44	1.37
2	B	501	FMN	C6-C7	2.29	1.44	1.37
2	A	502	FMN	P-O1P	2.34	1.58	1.50
2	F	505	FMN	C6-C7	2.37	1.44	1.37
2	D	503	FMN	C5'-C4'	2.40	1.55	1.51
2	D	503	FMN	P-O1P	2.44	1.58	1.50
2	D	503	FMN	C6-C7	2.45	1.44	1.37
2	G	508	FMN	C6-C7	2.45	1.44	1.37
2	C	504	FMN	P-O1P	2.46	1.58	1.50
2	A	502	FMN	C9-C9A	2.48	1.46	1.40
2	E	506	FMN	C6-C7	2.48	1.44	1.37
2	F	505	FMN	P-O1P	2.52	1.58	1.50
2	G	508	FMN	P-O1P	2.57	1.58	1.50
2	E	506	FMN	P-O1P	2.62	1.59	1.50
2	B	501	FMN	P-O1P	2.74	1.59	1.50
2	H	507	FMN	P-O1P	2.77	1.59	1.50
2	A	502	FMN	C6-C7	2.79	1.45	1.37
2	B	501	FMN	C4'-C3'	2.87	1.59	1.53
2	B	501	FMN	C5'-C4'	3.05	1.56	1.51
2	C	504	FMN	C10-N10	3.22	1.42	1.39
2	A	502	FMN	C10-N10	3.39	1.43	1.39
2	E	506	FMN	C10-N10	4.20	1.44	1.39
2	D	503	FMN	C10-N10	4.24	1.44	1.39
2	F	505	FMN	C10-N10	4.40	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	508	FMN	C10-N10	4.65	1.44	1.39
2	B	501	FMN	C10-N10	4.73	1.44	1.39
2	H	507	FMN	C10-N10	4.89	1.44	1.39
2	G	508	FMN	C9A-N10	4.89	1.45	1.38
2	B	501	FMN	C5A-N5	4.95	1.43	1.35
2	C	504	FMN	C9A-N10	4.96	1.45	1.38
2	G	508	FMN	C4-N3	5.11	1.42	1.33
2	E	506	FMN	C5A-N5	5.25	1.43	1.35
2	C	504	FMN	C5A-N5	5.26	1.43	1.35
2	D	503	FMN	C4-N3	5.28	1.42	1.33
2	G	508	FMN	C5A-N5	5.37	1.43	1.35
2	A	502	FMN	C9A-N10	5.39	1.46	1.38
2	E	506	FMN	C4-N3	5.43	1.42	1.33
2	A	502	FMN	C5A-N5	5.47	1.43	1.35
2	C	504	FMN	C4-N3	5.47	1.42	1.33
2	B	501	FMN	C4-N3	5.49	1.42	1.33
2	D	503	FMN	C5A-N5	5.53	1.44	1.35
2	H	507	FMN	C5A-N5	5.61	1.44	1.35
2	B	501	FMN	C9A-N10	5.69	1.46	1.38
2	H	507	FMN	C4-N3	5.70	1.43	1.33
2	F	505	FMN	C5A-N5	5.79	1.44	1.35
2	A	502	FMN	C4-N3	5.93	1.43	1.33
2	F	505	FMN	C4-N3	5.95	1.43	1.33
2	E	506	FMN	C9A-N10	6.08	1.47	1.38
2	H	507	FMN	C9A-N10	6.15	1.47	1.38
2	D	503	FMN	C9A-N10	6.20	1.47	1.38
2	F	505	FMN	C9A-N10	6.33	1.47	1.38
2	B	501	FMN	C4A-N5	6.85	1.43	1.33
2	H	507	FMN	C4A-N5	7.07	1.44	1.33
2	C	504	FMN	C4A-N5	7.31	1.44	1.33
2	F	505	FMN	C4A-N5	7.36	1.44	1.33
2	E	506	FMN	C4A-N5	7.45	1.44	1.33
2	G	508	FMN	C4A-N5	7.53	1.44	1.33
2	D	503	FMN	C4A-N5	7.81	1.45	1.33
2	A	502	FMN	C4A-N5	8.68	1.46	1.33

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	508	FMN	O5'-P-O1P	-4.35	96.16	107.08
2	E	506	FMN	O5'-P-O1P	-4.23	96.44	107.08
2	A	502	FMN	N3-C2-N1	-4.19	120.64	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	506	FMN	C4A-C4-N3	-4.15	118.09	123.52
2	H	507	FMN	C4A-C4-N3	-4.10	118.16	123.52
2	F	505	FMN	C4A-C4-N3	-4.00	118.30	123.52
2	C	504	FMN	N3-C2-N1	-3.98	120.98	127.69
2	D	503	FMN	N3-C2-N1	-3.96	121.02	127.69
2	A	502	FMN	O5'-P-O1P	-3.91	97.25	107.08
2	F	505	FMN	N3-C2-N1	-3.88	121.16	127.69
2	A	502	FMN	C4-C4A-C10	-3.87	117.46	119.94
2	H	507	FMN	N3-C2-N1	-3.85	121.20	127.69
2	B	501	FMN	N3-C2-N1	-3.85	121.20	127.69
2	E	506	FMN	N3-C2-N1	-3.83	121.24	127.69
2	G	508	FMN	N3-C2-N1	-3.82	121.26	127.69
2	B	501	FMN	C4A-C4-N3	-3.82	118.53	123.52
2	G	508	FMN	C4A-C4-N3	-3.82	118.53	123.52
2	C	504	FMN	C4A-C4-N3	-3.73	118.64	123.52
2	A	502	FMN	C4A-C4-N3	-3.63	118.78	123.52
2	D	503	FMN	C4A-C4-N3	-3.60	118.81	123.52
2	C	504	FMN	O5'-P-O1P	-3.60	98.03	107.08
2	D	503	FMN	C4-C4A-C10	-3.46	117.73	119.94
2	C	504	FMN	C4-C4A-C10	-3.37	117.78	119.94
2	E	506	FMN	C4-C4A-C10	-3.22	117.88	119.94
2	G	508	FMN	C4-C4A-C10	-3.15	117.92	119.94
2	D	503	FMN	O5'-P-O1P	-3.13	99.22	107.08
2	F	505	FMN	O5'-P-O1P	-3.10	99.29	107.08
2	F	505	FMN	C4-C4A-C10	-3.08	117.97	119.94
2	H	507	FMN	C4-C4A-C10	-2.87	118.10	119.94
2	C	504	FMN	C1'-C2'-C3'	-2.75	101.96	109.82
2	B	501	FMN	C4-C4A-C10	-2.73	118.19	119.94
2	A	502	FMN	C1'-C2'-C3'	-2.67	102.17	109.82
2	H	507	FMN	O5'-P-O1P	-2.67	100.36	107.08
2	G	508	FMN	C1'-C2'-C3'	-2.48	102.72	109.82
2	A	502	FMN	C4A-C10-N10	-2.26	118.88	120.52
2	B	501	FMN	O5'-P-O1P	-2.25	101.42	107.08
2	B	501	FMN	C4A-C10-N10	-2.20	118.92	120.52
2	E	506	FMN	C1'-C2'-C3'	-2.16	103.65	109.82
2	E	506	FMN	C4A-C10-N10	-2.06	119.02	120.52
2	D	503	FMN	C4A-C10-N10	-2.02	119.05	120.52
2	D	503	FMN	C4-C4A-N5	2.02	121.15	118.70
2	C	504	FMN	C4-C4A-N5	2.02	121.16	118.70
2	B	501	FMN	C6-C5A-C9A	2.08	121.40	119.11
2	G	508	FMN	C4-C4A-N5	2.18	121.34	118.70
2	H	507	FMN	C6-C5A-C9A	2.22	121.56	119.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	FMN	C4-C4A-N5	2.39	121.61	118.70
2	A	502	FMN	C4A-N5-C5A	2.62	119.81	116.72
2	C	504	FMN	C4A-N5-C5A	2.69	119.89	116.72
2	F	505	FMN	C4A-N5-C5A	2.71	119.91	116.72
2	H	507	FMN	C4A-N5-C5A	2.79	120.01	116.72
2	G	508	FMN	C4A-N5-C5A	2.98	120.24	116.72
2	D	503	FMN	C4A-N5-C5A	2.98	120.24	116.72
2	E	506	FMN	C4A-N5-C5A	3.07	120.34	116.72
2	B	501	FMN	C4A-N5-C5A	3.13	120.41	116.72
2	H	507	FMN	O3P-P-O2P	3.20	119.18	107.44
2	D	503	FMN	O3P-P-O2P	3.33	119.67	107.44
2	B	501	FMN	O3P-P-O2P	3.46	120.14	107.44
2	F	505	FMN	O3P-P-O2P	3.55	120.47	107.44
2	E	506	FMN	O3P-P-O2P	3.65	120.84	107.44
2	G	508	FMN	O3P-P-O2P	3.98	122.07	107.44
2	A	502	FMN	O3P-P-O2P	3.99	122.08	107.44
2	C	504	FMN	O3P-P-O2P	4.01	122.15	107.44
2	F	505	FMN	C4-N3-C2	6.04	120.20	115.16
2	C	504	FMN	C4-N3-C2	6.06	120.21	115.16
2	H	507	FMN	C4-N3-C2	6.17	120.31	115.16
2	G	508	FMN	C4-N3-C2	6.18	120.31	115.16
2	B	501	FMN	C4-N3-C2	6.22	120.35	115.16
2	D	503	FMN	C4-N3-C2	6.27	120.39	115.16
2	A	502	FMN	C4-N3-C2	6.34	120.44	115.16
2	E	506	FMN	C4-N3-C2	6.65	120.71	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	FMN	2	0
2	B	501	FMN	6	0
2	C	504	FMN	4	0
2	D	503	FMN	2	0
2	E	506	FMN	7	0
2	F	505	FMN	2	0
2	G	508	FMN	3	0
2	H	507	FMN	3	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	219/230 (95%)	-0.30	0 100 100	2, 12, 27, 45	0
1	B	219/230 (95%)	-0.24	0 100 100	3, 14, 34, 48	0
1	C	219/230 (95%)	-0.20	0 100 100	4, 15, 35, 43	0
1	D	219/230 (95%)	-0.24	0 100 100	2, 14, 31, 45	0
1	E	219/230 (95%)	0.01	3 (1%) 78 83	9, 23, 41, 50	0
1	F	219/230 (95%)	0.06	5 (2%) 64 72	8, 24, 40, 51	0
1	G	219/230 (95%)	0.22	7 (3%) 51 60	12, 26, 44, 51	0
1	H	219/230 (95%)	0.45	14 (6%) 23 31	9, 32, 50, 55	0
All	All	1752/1840 (95%)	-0.03	29 (1%) 73 79	2, 19, 42, 55	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	196	ASP	3.7
1	F	169	PHE	3.6
1	E	130	VAL	3.5
1	H	76	THR	3.4
1	H	169	PHE	3.3
1	E	41	PRO	3.2
1	F	14	ALA	2.9
1	H	85	GLN	2.9
1	G	137	ASN	2.8
1	G	13	GLY	2.8
1	H	12	ALA	2.7
1	H	13	GLY	2.7
1	G	138	PRO	2.5
1	F	96	SER	2.5
1	G	135	THR	2.5
1	H	86	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	130	VAL	2.5
1	H	177	ILE	2.5
1	H	182	ASP	2.5
1	H	130	VAL	2.3
1	G	197	ARG	2.3
1	F	12	ALA	2.3
1	H	82	GLN	2.3
1	H	197	ARG	2.2
1	G	136	HIS	2.1
1	H	75	GLU	2.1
1	H	101	ALA	2.1
1	E	135	THR	2.0
1	H	89	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	504	31/31	0.93	0.16	0.93	2,5,22,30	0
2	FMN	G	508	31/31	0.89	0.18	0.91	17,22,27,30	0
2	FMN	F	505	31/31	0.93	0.14	0.56	17,21,32,34	0
2	FMN	E	506	31/31	0.91	0.15	0.52	9,15,30,34	0
2	FMN	B	501	31/31	0.95	0.13	0.50	1,6,13,17	0
2	FMN	D	503	31/31	0.94	0.15	0.50	1,3,15,22	0
2	FMN	A	502	31/31	0.94	0.14	0.10	2,6,25,32	0
2	FMN	H	507	31/31	0.90	0.16	0.05	18,26,27,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.