



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:40 PM GMT

PDB ID : 2IFA
Title : Crystal Structure of the PUTATIVE NITROREDUCTASE (SMU.260) IN COMPLEX WITH FMN FROM STREPTOCOCCUS MUTANS, NORTH-EAST STRUCTURAL GENOMICS TARGET SMR5.
Authors : Forouhar, F.; Chen, Y.; Xiao, R.; Ma, L.C.; Byler, T.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2006-09-20
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

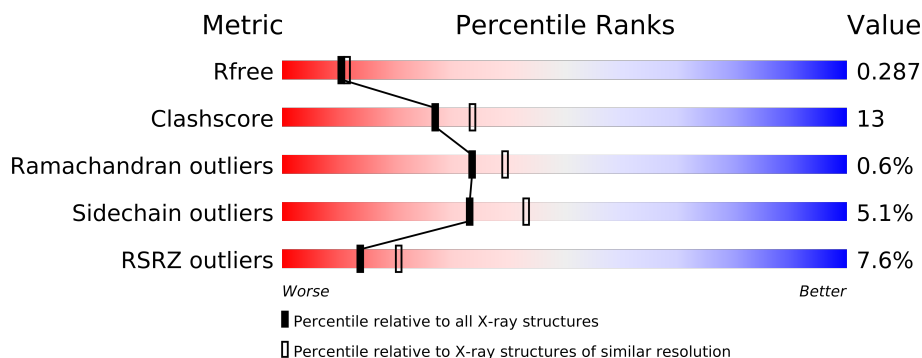
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	208	
1	B	208	
1	C	208	
1	D	208	
1	E	208	
1	F	208	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10188 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Hypothetical protein SMU.260.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	Se	0	0	0
			1582	1017	263	299	3			
1	B	201	Total	C	N	O	Se	0	0	0
			1591	1022	264	302	3			
1	C	201	Total	C	N	O	Se	0	0	0
			1591	1022	264	302	3			
1	D	200	Total	C	N	O	Se	0	0	0
			1582	1017	263	299	3			
1	E	201	Total	C	N	O	Se	0	0	0
			1591	1022	264	302	3			
1	F	199	Total	C	N	O	Se	0	0	0
			1574	1011	262	298	3			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
A	145	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
A	170	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
A	189	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
A	201	LEU	-	EXPRESSION TAG	UNP Q8DW21
A	202	GLU	-	EXPRESSION TAG	UNP Q8DW21
A	203	HIS	-	EXPRESSION TAG	UNP Q8DW21
A	204	HIS	-	EXPRESSION TAG	UNP Q8DW21
A	205	HIS	-	EXPRESSION TAG	UNP Q8DW21
A	206	HIS	-	EXPRESSION TAG	UNP Q8DW21
A	207	HIS	-	EXPRESSION TAG	UNP Q8DW21
A	208	HIS	-	EXPRESSION TAG	UNP Q8DW21
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
B	145	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
B	170	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
B	189	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
B	201	LEU	-	EXPRESSION TAG	UNP Q8DW21

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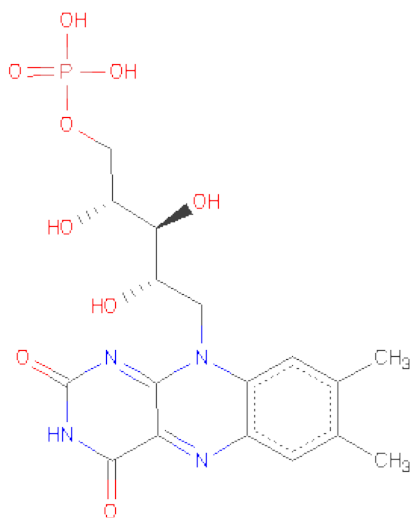
Chain	Residue	Modelled	Actual	Comment	Reference
B	202	GLU	-	EXPRESSION TAG	UNP Q8DW21
B	203	HIS	-	EXPRESSION TAG	UNP Q8DW21
B	204	HIS	-	EXPRESSION TAG	UNP Q8DW21
B	205	HIS	-	EXPRESSION TAG	UNP Q8DW21
B	206	HIS	-	EXPRESSION TAG	UNP Q8DW21
B	207	HIS	-	EXPRESSION TAG	UNP Q8DW21
B	208	HIS	-	EXPRESSION TAG	UNP Q8DW21
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
C	145	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
C	170	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
C	189	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
C	201	LEU	-	EXPRESSION TAG	UNP Q8DW21
C	202	GLU	-	EXPRESSION TAG	UNP Q8DW21
C	203	HIS	-	EXPRESSION TAG	UNP Q8DW21
C	204	HIS	-	EXPRESSION TAG	UNP Q8DW21
C	205	HIS	-	EXPRESSION TAG	UNP Q8DW21
C	206	HIS	-	EXPRESSION TAG	UNP Q8DW21
C	207	HIS	-	EXPRESSION TAG	UNP Q8DW21
C	208	HIS	-	EXPRESSION TAG	UNP Q8DW21
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
D	145	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
D	170	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
D	189	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
D	201	LEU	-	EXPRESSION TAG	UNP Q8DW21
D	202	GLU	-	EXPRESSION TAG	UNP Q8DW21
D	203	HIS	-	EXPRESSION TAG	UNP Q8DW21
D	204	HIS	-	EXPRESSION TAG	UNP Q8DW21
D	205	HIS	-	EXPRESSION TAG	UNP Q8DW21
D	206	HIS	-	EXPRESSION TAG	UNP Q8DW21
D	207	HIS	-	EXPRESSION TAG	UNP Q8DW21
D	208	HIS	-	EXPRESSION TAG	UNP Q8DW21
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
E	145	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
E	170	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
E	189	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
E	201	LEU	-	EXPRESSION TAG	UNP Q8DW21
E	202	GLU	-	EXPRESSION TAG	UNP Q8DW21
E	203	HIS	-	EXPRESSION TAG	UNP Q8DW21
E	204	HIS	-	EXPRESSION TAG	UNP Q8DW21
E	205	HIS	-	EXPRESSION TAG	UNP Q8DW21
E	206	HIS	-	EXPRESSION TAG	UNP Q8DW21
E	207	HIS	-	EXPRESSION TAG	UNP Q8DW21

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Chain	Residue	Modelled	Actual	Comment	Reference
E	208	HIS	-	EXPRESSION TAG	UNP Q8DW21
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
F	145	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
F	170	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
F	189	MSE	MET	MODIFIED RESIDUE	UNP Q8DW21
F	201	LEU	-	EXPRESSION TAG	UNP Q8DW21
F	202	GLU	-	EXPRESSION TAG	UNP Q8DW21
F	203	HIS	-	EXPRESSION TAG	UNP Q8DW21
F	204	HIS	-	EXPRESSION TAG	UNP Q8DW21
F	205	HIS	-	EXPRESSION TAG	UNP Q8DW21
F	206	HIS	-	EXPRESSION TAG	UNP Q8DW21
F	207	HIS	-	EXPRESSION TAG	UNP Q8DW21
F	208	HIS	-	EXPRESSION TAG	UNP Q8DW21

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



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

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

- Molecule 3 is water.

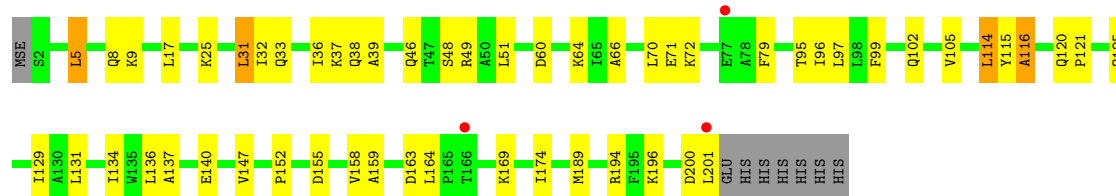
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total	O	0	0
			129	129		
3	B	105	Total	O	0	0
			105	105		
3	C	78	Total	O	0	0
			78	78		
3	D	70	Total	O	0	0
			70	70		
3	E	62	Total	O	0	0
			62	62		
3	F	47	Total	O	0	0
			47	47		

3 Residue-property plots

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.

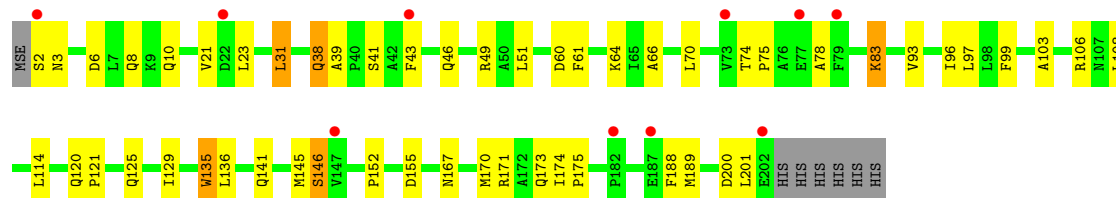
• Molecule 1: Hypothetical protein SMU.260

Chain A: 



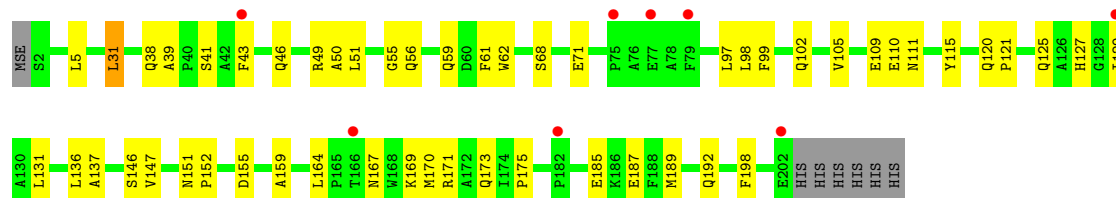
• Molecule 1: Hypothetical protein SMU.260

Chain B: 



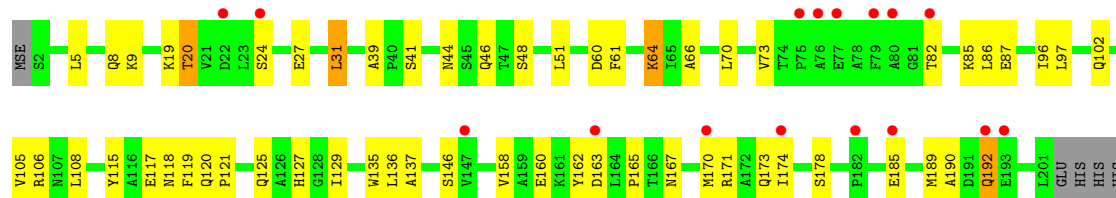
• Molecule 1: Hypothetical protein SMU.260

Chain C: 



• Molecule 1: Hypothetical protein SMU.260

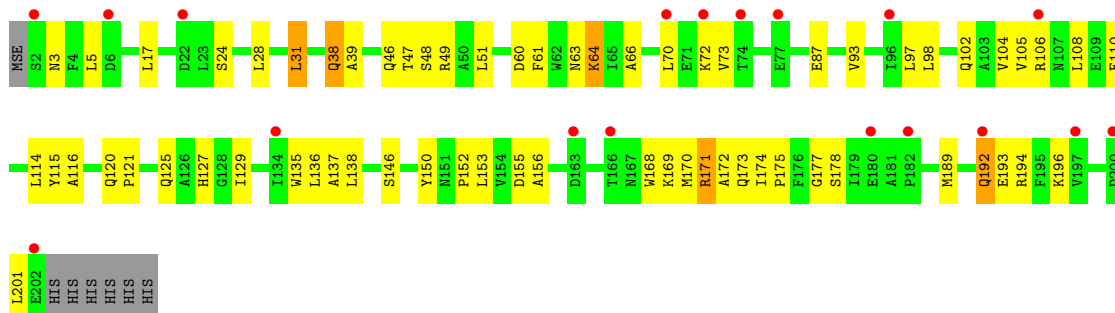
Chain D: 



HIS
HIS
HIS

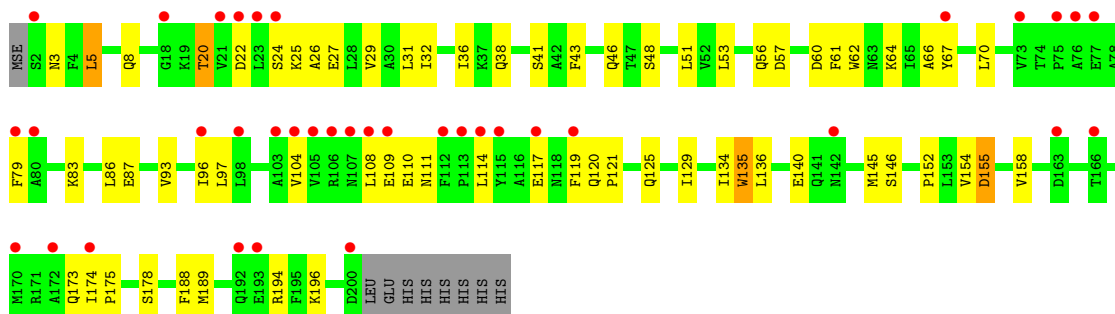
• Molecule 1: Hypothetical protein SMU.260

Chain E: 



• Molecule 1: Hypothetical protein SMU.260

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.44Å 60.87Å 109.16Å 90.00° 117.83° 90.00°	Depositor
Resolution (Å)	29.03 – 2.30 29.03 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.3 (29.03-2.30) 96.3 (29.03-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.51 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1, XTALVIEW	Depositor
R, R_{free}	0.218 , 0.273 0.233 , 0.287	Depositor DCC
R_{free} test set	5330 reflections (9.73%)	DCC
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 26.1	EDS
Estimated twinning fraction	0.006 for l,k,-h-l 0.006 for -h-l,k,h 0.019 for -h-l,-k,l 0.017 for h,-k,-h-l 0.018 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 106929 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10188	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.40	0/1615	0.54	0/2184
1	B	0.40	0/1624	0.55	0/2196
1	C	0.39	0/1624	0.53	0/2196
1	D	0.38	0/1615	0.53	0/2184
1	E	0.35	0/1624	0.47	0/2196
1	F	0.34	0/1607	0.47	0/2173
All	All	0.38	0/9709	0.52	0/13129

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1582	0	1549	43	0
1	B	1591	0	1555	47	0
1	C	1591	0	1555	46	0
1	D	1582	0	1549	43	0
1	E	1591	0	1555	56	0
1	F	1574	0	1538	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	0	19	4	0
2	B	31	0	19	2	0
2	C	31	0	19	5	0
2	D	31	0	19	3	0
2	E	31	0	19	5	0
2	F	31	0	19	3	0
3	A	129	0	0	4	0
3	B	105	0	0	4	0
3	C	78	0	0	3	0
3	D	70	0	0	3	0
3	E	62	0	0	4	0
3	F	47	0	0	5	0
All	All	10188	0	9415	249	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (249) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:39:ALA:HB1	1:D:129:ILE:HG22	1.57	0.86
1:A:120:GLN:HB3	1:A:121:PRO:HD3	1.60	0.83
1:E:170:MSE:HE2	1:E:173:GLN:HE21	1.45	0.82
1:B:6:ASP:O	1:B:10:GLN:HG3	1.79	0.82
1:C:46:GLN:HE22	1:D:189:MSE:H	1.29	0.81
1:C:102:GLN:HE22	1:C:120:GLN:HE22	1.27	0.81
1:C:105:VAL:O	1:C:109:GLU:HG3	1.83	0.79
2:A:501:FMN:HM72	1:B:125:GLN:HE21	1.48	0.79
1:C:125:GLN:HE21	2:D:504:FMN:HM72	1.49	0.77
1:E:125:GLN:NE2	2:F:506:FMN:HM72	1.99	0.76
2:A:501:FMN:HM72	1:B:125:GLN:NE2	2.02	0.74
1:E:46:GLN:HE22	1:F:189:MSE:H	1.36	0.73
2:E:505:FMN:HM72	1:F:125:GLN:HE21	1.55	0.72
1:B:120:GLN:HB3	1:B:121:PRO:HD3	1.71	0.71
2:C:503:FMN:HM72	1:D:125:GLN:HE21	1.55	0.71
2:C:503:FMN:HM72	1:D:125:GLN:NE2	2.05	0.71
1:E:171:ARG:HA	1:E:171:ARG:HE	1.56	0.71
1:A:36:ILE:HD11	1:A:134:ILE:HD11	1.73	0.70
1:E:98:LEU:HD13	1:E:174:ILE:HD13	1.72	0.70
1:A:125:GLN:HE21	2:B:502:FMN:HM72	1.56	0.69
1:D:120:GLN:HB3	1:D:121:PRO:HD3	1.72	0.69
1:A:196:LYS:HB2	1:B:51:LEU:HD12	1.74	0.69
1:C:189:MSE:H	1:D:46:GLN:HE22	1.41	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:51:LEU:HD23	1:C:97:LEU:HD22	1.75	0.69
1:B:39:ALA:HB1	1:B:129:ILE:HG22	1.75	0.68
1:D:106:ARG:HH12	1:D:167:ASN:HD21	1.42	0.68
1:F:24:SER:HB3	1:F:27:GLU:HG3	1.76	0.68
1:E:189:MSE:H	1:F:46:GLN:HE22	1.40	0.67
1:E:170:MSE:HE3	1:E:171:ARG:H	1.59	0.67
1:F:104:VAL:HB	3:F:519:HOH:O	1.95	0.66
1:E:120:GLN:HB3	1:E:121:PRO:HD3	1.78	0.66
1:E:60:ASP:HA	1:E:64:LYS:HD3	1.78	0.65
1:C:167:ASN:HA	3:C:513:HOH:O	1.96	0.65
1:B:43:PHE:HZ	1:B:108:LEU:HD13	1.61	0.64
1:E:48:SER:HB3	3:E:514:HOH:O	1.97	0.64
1:F:120:GLN:HB3	1:F:121:PRO:HD3	1.80	0.64
1:A:46:GLN:HE22	1:B:189:MSE:H	1.45	0.63
1:D:5:LEU:HD11	1:D:9:LYS:HE3	1.81	0.63
1:E:189:MSE:HE2	1:E:194:ARG:HB2	1.78	0.63
1:A:125:GLN:NE2	2:B:502:FMN:HM72	2.14	0.63
1:D:185:GLU:HB3	3:F:521:HOH:O	1.99	0.63
1:B:114:LEU:HB2	3:B:529:HOH:O	1.99	0.63
1:D:61:PHE:CZ	1:D:173:GLN:HG2	2.35	0.61
1:E:51:LEU:HD23	1:E:97:LEU:HD12	1.81	0.61
1:E:60:ASP:O	1:E:64:LYS:HB2	2.00	0.61
1:F:96:ILE:HB	1:F:174:ILE:HB	1.81	0.61
1:F:60:ASP:O	1:F:64:LYS:HB2	2.01	0.61
1:C:125:GLN:NE2	2:D:504:FMN:HM72	2.15	0.60
1:B:31:LEU:HD11	1:B:141:GLN:HG3	1.84	0.60
1:D:192:GLN:CD	1:D:192:GLN:H	2.03	0.60
1:D:158:VAL:HG21	1:D:170:MSE:HE1	1.83	0.59
1:F:32:ILE:HD13	1:F:96:ILE:HD11	1.85	0.59
1:F:66:ALA:O	1:F:70:LEU:HD23	2.02	0.59
1:C:115:TYR:OH	1:F:114:LEU:HB2	2.02	0.59
1:B:152:PRO:HA	1:B:155:ASP:OD1	2.03	0.58
1:E:174:ILE:HD12	1:E:174:ILE:N	2.19	0.58
1:C:51:LEU:HB3	1:C:97:LEU:HB2	1.86	0.57
1:A:66:ALA:O	1:A:70:LEU:HD23	2.04	0.57
1:A:25:LYS:HB2	1:B:201:LEU:HD13	1.86	0.57
1:E:125:GLN:HE21	2:F:506:FMN:HM72	1.70	0.57
1:C:120:GLN:HB2	1:C:121:PRO:HD3	1.87	0.57
1:F:24:SER:HB3	1:F:27:GLU:CG	2.34	0.57
1:C:31:LEU:HD21	1:C:137:ALA:HB1	1.87	0.56
1:D:60:ASP:O	1:D:64:LYS:HB3	2.05	0.56
1:C:31:LEU:CD2	1:C:137:ALA:HB1	2.36	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:66:ALA:O	1:B:70:LEU:HD23	2.05	0.56
1:E:46:GLN:NE2	1:F:189:MSE:H	2.02	0.55
1:F:20:THR:HG23	1:F:178:SER:OG	2.07	0.55
1:A:49:ARG:HB2	1:A:99:PHE:HB2	1.88	0.55
1:A:115:TYR:OH	1:E:114:LEU:HB2	2.07	0.54
1:B:61:PHE:CZ	1:B:173:GLN:HG2	2.42	0.54
1:D:20:THR:O	1:D:178:SER:HB3	2.08	0.54
1:C:111:ASN:ND2	1:F:43:PHE:H	2.06	0.54
2:E:505:FMN:HM72	1:F:125:GLN:NE2	2.22	0.53
1:F:20:THR:O	1:F:178:SER:HB3	2.08	0.53
1:C:61:PHE:CZ	1:C:173:GLN:HG2	2.43	0.53
1:C:55:GLY:O	1:C:59:GLN:HG2	2.08	0.53
1:D:61:PHE:HZ	1:D:173:GLN:HG2	1.72	0.53
1:A:201:LEU:HD23	1:B:93:VAL:O	2.08	0.53
1:D:165:PRO:HB3	3:D:565:HOH:O	2.06	0.53
1:C:152:PRO:HA	1:C:155:ASP:OD1	2.08	0.53
1:A:102:GLN:HA	1:A:105:VAL:HG22	1.90	0.53
1:A:31:LEU:CD2	1:A:137:ALA:HB1	2.39	0.53
1:C:49:ARG:HB2	1:C:99:PHE:HB2	1.91	0.53
1:C:198:PHE:HD2	1:D:51:LEU:HD11	1.73	0.53
1:C:43:PHE:CE2	1:F:111:ASN:HB3	2.43	0.53
1:E:127:HIS:HE1	3:E:522:HOH:O	1.92	0.53
1:A:48:SER:HB2	3:A:566:HOH:O	2.09	0.53
1:A:169:LYS:HE2	3:A:508:HOH:O	2.08	0.53
1:C:97:LEU:HG	1:C:170:MSE:HE1	1.91	0.52
1:F:189:MSE:HE2	1:F:194:ARG:HB2	1.91	0.52
1:F:36:ILE:HD11	1:F:134:ILE:HD11	1.90	0.52
1:F:31:LEU:O	1:F:31:LEU:HD13	2.10	0.52
1:C:169:LYS:HE3	3:C:521:HOH:O	2.10	0.52
1:A:152:PRO:HA	1:A:155:ASP:OD1	2.09	0.52
1:B:146:SER:O	1:B:175:PRO:HD2	2.10	0.52
1:A:5:LEU:HD22	1:A:9:LYS:HE3	1.91	0.52
1:C:111:ASN:HD21	1:F:43:PHE:H	1.57	0.51
1:D:31:LEU:CD1	1:D:137:ALA:HB1	2.41	0.51
1:D:24:SER:OG	1:D:27:GLU:HG3	2.10	0.51
1:E:61:PHE:CZ	1:E:173:GLN:HG2	2.46	0.51
1:D:48:SER:HB2	3:D:528:HOH:O	2.11	0.51
1:A:95:THR:HA	1:A:174:ILE:O	2.10	0.51
1:C:68:SER:O	1:C:71:GLU:HG2	2.11	0.51
1:B:2:SER:HA	1:B:6:ASP:OD2	2.11	0.51
2:E:505:FMN:HM83	1:F:41:SER:HA	1.94	0.50
1:C:131:LEU:HD11	1:C:147:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:3:ASN:ND2	1:F:5:LEU:HB2	2.26	0.50
1:F:62:TRP:O	1:F:86:LEU:HD13	2.12	0.50
1:B:135:TRP:CG	1:B:145:MSE:HE2	2.47	0.50
1:C:56:GLN:HA	1:C:59:GLN:CG	2.42	0.50
1:A:189:MSE:H	1:B:46:GLN:HE22	1.60	0.50
1:E:46:GLN:HE22	1:F:188:PHE:HA	1.77	0.50
1:E:46:GLN:HE22	1:F:189:MSE:N	2.06	0.49
1:E:102:GLN:HA	1:E:105:VAL:HG22	1.94	0.49
1:B:120:GLN:HG3	3:B:506:HOH:O	2.10	0.49
1:A:46:GLN:HE22	1:B:188:PHE:HA	1.76	0.49
1:E:121:PRO:O	1:E:125:GLN:HG3	2.11	0.49
1:D:127:HIS:HE1	3:D:552:HOH:O	1.95	0.49
1:A:114:LEU:HB2	1:E:115:TYR:OH	2.13	0.49
1:E:66:ALA:O	1:E:70:LEU:HD13	2.13	0.49
1:E:63:ASN:C	1:E:64:LYS:HD2	2.33	0.49
1:E:31:LEU:HD12	1:E:138:LEU:HD12	1.95	0.49
1:D:5:LEU:HD11	1:D:9:LYS:CE	2.43	0.48
2:A:501:FMN:HM83	1:B:41:SER:HA	1.93	0.48
1:A:158:VAL:HG12	1:A:164:LEU:HD12	1.95	0.48
1:E:146:SER:O	1:E:175:PRO:HD2	2.12	0.48
1:E:24:SER:O	1:E:28:LEU:HG	2.14	0.48
1:D:102:GLN:HA	1:D:105:VAL:HG22	1.96	0.48
1:F:3:ASN:HD22	1:F:5:LEU:HB2	1.79	0.48
1:A:46:GLN:NE2	1:B:189:MSE:H	2.11	0.48
1:A:200:ASP:O	1:A:201:LEU:HB2	2.13	0.48
1:E:93:VAL:HG23	1:E:177:GLY:HA2	1.94	0.48
1:E:70:LEU:HD21	1:E:150:TYR:CE1	2.49	0.47
1:A:194:ARG:NH1	1:B:46:GLN:HE21	2.13	0.47
1:E:127:HIS:HD2	3:E:518:HOH:O	1.96	0.47
1:A:33:GLN:O	1:A:37:LYS:HG3	2.15	0.47
1:C:120:GLN:CB	1:C:121:PRO:HD3	2.44	0.47
1:E:169:LYS:O	1:E:171:ARG:HG2	2.14	0.47
1:A:51:LEU:HB3	1:A:97:LEU:HB2	1.96	0.47
1:A:131:LEU:HD11	1:A:147:VAL:HG22	1.96	0.47
1:B:103:ALA:HB2	1:B:167:ASN:CG	2.34	0.47
1:E:38:GLN:CG	1:F:8:GLN:HB3	2.44	0.47
1:D:70:LEU:HA	1:D:73:VAL:HG22	1.97	0.47
1:E:150:TYR:O	1:E:153:LEU:HB2	2.14	0.47
1:E:201:LEU:HD23	3:F:545:HOH:O	2.15	0.47
1:D:51:LEU:HB3	1:D:97:LEU:HB2	1.97	0.47
1:A:159:ALA:HA	1:A:164:LEU:HB2	1.96	0.47
1:D:190:ALA:HB1	1:D:192:GLN:HE21	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:127:HIS:HE1	3:C:522:HOH:O	1.96	0.46
1:A:194:ARG:HH12	1:B:46:GLN:HE21	1.63	0.46
1:A:71:GLU:HB3	1:A:79:PHE:CZ	2.50	0.46
1:C:97:LEU:CD2	1:C:170:MSE:HE1	2.45	0.46
1:F:146:SER:O	1:F:175:PRO:HD2	2.16	0.46
1:F:152:PRO:HA	1:F:155:ASP:OD1	2.15	0.46
1:E:49:ARG:HD2	1:E:168:TRP:CZ2	2.51	0.46
2:C:503:FMN:O4'	1:D:44:ASN:HB2	2.16	0.46
1:C:189:MSE:H	1:D:46:GLN:NE2	2.10	0.46
1:E:38:GLN:HG2	1:F:8:GLN:HB3	1.98	0.46
2:A:501:FMN:C7M	1:B:125:GLN:HE21	2.24	0.46
1:E:106:ARG:O	1:E:110:GLU:HG3	2.14	0.46
1:C:151:ASN:HB3	1:C:170:MSE:CG	2.46	0.45
1:A:8:GLN:HB3	1:B:38:GLN:HB3	1.98	0.45
1:B:96:ILE:HB	1:B:174:ILE:HB	1.98	0.45
1:B:170:MSE:O	1:B:171:ARG:HD2	2.16	0.45
1:B:121:PRO:O	1:B:125:GLN:HG3	2.16	0.45
1:D:96:ILE:HB	1:D:174:ILE:HB	1.99	0.45
1:B:21:VAL:HG12	1:B:23:LEU:H	1.81	0.45
1:A:38:GLN:HG2	1:B:8:GLN:HB3	1.98	0.45
1:D:108:LEU:HB3	1:D:119:PHE:CE1	2.51	0.45
1:C:110:GLU:HB3	2:E:505:FMN:O2	2.17	0.45
1:D:19:LYS:NZ	1:D:19:LYS:HB2	2.32	0.45
1:F:61:PHE:HZ	1:F:173:GLN:HG2	1.80	0.45
1:D:171:ARG:NE	1:D:171:ARG:HA	2.32	0.45
1:D:118:ASN:O	1:D:121:PRO:HD2	2.17	0.45
1:E:98:LEU:O	1:E:170:MSE:HE3	2.17	0.44
1:A:60:ASP:O	1:A:64:LYS:HB2	2.16	0.44
1:B:83:LYS:C	1:B:83:LYS:HD3	2.38	0.44
1:F:154:VAL:O	1:F:158:VAL:HG23	2.17	0.44
1:C:62:TRP:CZ2	1:C:175:PRO:HB3	2.52	0.44
1:E:196:LYS:HB2	1:F:51:LEU:HD12	1.99	0.44
1:E:51:LEU:HD12	1:F:196:LYS:O	2.17	0.44
1:C:125:GLN:O	1:C:129:ILE:HG13	2.17	0.44
1:A:131:LEU:HD11	1:A:147:VAL:CG2	2.48	0.44
1:F:135:TRP:CG	1:F:145:MSE:HE2	2.52	0.44
1:E:5:LEU:HD23	1:E:5:LEU:O	2.17	0.44
1:F:26:ALA:HB2	3:F:553:HOH:O	2.18	0.44
1:E:105:VAL:HA	1:E:108:LEU:HD12	2.00	0.44
1:B:120:GLN:HB2	3:B:593:HOH:O	2.18	0.44
1:C:146:SER:O	1:C:175:PRO:HD2	2.17	0.44
2:C:503:FMN:HM83	1:D:41:SER:HA	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:505:FMN:HM82	1:F:129:ILE:HD12	2.00	0.43
1:F:25:LYS:O	1:F:29:VAL:HG23	2.19	0.43
1:E:192:GLN:HG2	1:E:193:GLU:HG2	2.00	0.43
1:A:31:LEU:HD21	1:A:137:ALA:HB1	1.99	0.43
1:E:152:PRO:HA	1:E:155:ASP:OD1	2.18	0.43
1:A:115:TYR:O	1:A:116:ALA:C	2.57	0.43
1:E:31:LEU:HD11	1:E:137:ALA:HB1	2.01	0.43
1:A:17:LEU:HD12	3:A:576:HOH:O	2.18	0.43
1:F:48:SER:HB3	3:F:540:HOH:O	2.19	0.43
1:F:53:LEU:HD22	1:F:57:ASP:HB3	2.00	0.43
1:F:51:LEU:HB3	1:F:97:LEU:HB2	2.01	0.43
2:C:503:FMN:HM82	1:D:129:ILE:HD12	2.01	0.43
1:C:39:ALA:HB1	1:C:129:ILE:HG22	2.01	0.43
1:E:39:ALA:HB1	1:E:129:ILE:HG22	2.00	0.43
1:B:61:PHE:HZ	1:B:173:GLN:HG2	1.84	0.43
1:B:21:VAL:CG2	1:B:93:VAL:HG21	2.48	0.43
1:C:159:ALA:HA	1:C:164:LEU:HB2	2.01	0.43
1:A:72:LYS:HD2	3:A:628:HOH:O	2.18	0.43
1:F:20:THR:HG23	1:F:178:SER:CB	2.48	0.43
1:E:201:LEU:HD21	1:F:93:VAL:HG13	2.00	0.43
1:E:170:MSE:CE	1:E:172:ALA:H	2.32	0.42
1:C:43:PHE:HD2	1:F:108:LEU:HG	1.84	0.42
1:D:115:TYR:HB2	1:D:119:PHE:CE2	2.53	0.42
1:A:39:ALA:HB1	1:A:129:ILE:HG22	2.01	0.42
1:C:41:SER:HA	2:D:504:FMN:HM83	2.01	0.42
1:E:17:LEU:HA	1:E:178:SER:O	2.19	0.42
1:B:106:ARG:HH21	1:B:106:ARG:HG3	1.84	0.42
1:A:32:ILE:HD13	1:A:96:ILE:HD11	2.01	0.42
1:E:3:ASN:HB2	1:F:140:GLU:OE1	2.19	0.42
1:E:129:ILE:HD12	2:F:506:FMN:HM82	2.01	0.42
1:C:61:PHE:HZ	1:C:173:GLN:HG2	1.84	0.42
1:D:31:LEU:HD11	1:D:137:ALA:HB1	2.01	0.42
1:F:61:PHE:CZ	1:F:173:GLN:HG2	2.54	0.42
1:C:97:LEU:CG	1:C:170:MSE:HE1	2.49	0.41
1:D:162:TYR:O	1:D:163:ASP:C	2.58	0.41
1:D:66:ALA:O	1:D:70:LEU:HD23	2.19	0.41
1:B:49:ARG:HB2	1:B:99:PHE:HB2	2.02	0.41
1:D:82:THR:O	1:D:86:LEU:HG	2.20	0.41
1:B:146:SER:HB2	3:B:562:HOH:O	2.19	0.41
1:B:74:THR:HA	1:B:75:PRO:HD3	1.96	0.41
1:A:140:GLU:OE2	1:B:3:ASN:HA	2.20	0.41
1:D:146:SER:O	1:D:174:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:50:ALA:HA	1:C:97:LEU:O	2.20	0.41
1:E:47:THR:HG22	1:E:104:VAL:HB	2.03	0.41
1:D:118:ASN:C	1:D:121:PRO:HD2	2.41	0.41
1:A:196:LYS:HB2	1:B:51:LEU:CD1	2.47	0.41
1:B:38:GLN:HE21	1:B:38:GLN:N	2.19	0.41
1:B:60:ASP:O	1:B:64:LYS:HB2	2.20	0.41
1:E:31:LEU:CD1	1:E:137:ALA:HB1	2.51	0.41
1:F:67:TYR:CZ	1:F:83:LYS:HB2	2.56	0.40
1:C:38:GLN:HG3	1:D:8:GLN:HB3	2.02	0.40
1:F:31:LEU:C	1:F:31:LEU:HD13	2.42	0.40
1:E:156:ALA:HB2	3:E:547:HOH:O	2.20	0.40
1:B:106:ARG:NH2	1:B:106:ARG:HG3	2.36	0.40
1:C:38:GLN:HA	1:C:38:GLN:OE1	2.20	0.40
1:B:125:GLN:O	1:B:129:ILE:HG13	2.21	0.40
1:C:170:MSE:O	1:C:171:ARG:HD2	2.21	0.40
1:C:111:ASN:ND2	1:F:43:PHE:N	2.69	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	198/208 (95%)	191 (96%)	6 (3%)	1 (0%)	38	45
1	B	199/208 (96%)	184 (92%)	14 (7%)	1 (0%)	38	45
1	C	199/208 (96%)	191 (96%)	8 (4%)	0	100	100
1	D	198/208 (95%)	189 (96%)	9 (4%)	0	100	100
1	E	199/208 (96%)	185 (93%)	12 (6%)	2 (1%)	22	23
1	F	197/208 (95%)	181 (92%)	13 (7%)	3 (2%)	15	13
All	All	1190/1248 (95%)	1121 (94%)	62 (5%)	7 (1%)	33	39

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	ALA
1	B	78	ALA
1	F	109	GLU
1	F	79	PHE
1	F	119	PHE
1	E	116	ALA
1	E	73	VAL

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	163/167 (98%)	158 (97%)	5 (3%)	52	68
1	B	164/167 (98%)	156 (95%)	8 (5%)	35	45
1	C	164/167 (98%)	157 (96%)	7 (4%)	40	52
1	D	163/167 (98%)	153 (94%)	10 (6%)	26	34
1	E	164/167 (98%)	155 (94%)	9 (6%)	30	39
1	F	162/167 (97%)	151 (93%)	11 (7%)	22	28
All	All	980/1002 (98%)	930 (95%)	50 (5%)	33	43

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	31	LEU
1	A	114	LEU
1	A	136	LEU
1	A	163	ASP
1	B	31	LEU
1	B	38	GLN
1	B	83	LYS
1	B	97	LEU
1	B	135	TRP
1	B	136	LEU
1	B	146	SER
1	B	200	ASP

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Mol	Chain	Res	Type
1	C	5	LEU
1	C	31	LEU
1	C	98	LEU
1	C	136	LEU
1	C	185	GLU
1	C	187	GLU
1	C	192	GLN
1	D	20	THR
1	D	31	LEU
1	D	64	LYS
1	D	85	LYS
1	D	87	GLU
1	D	117	GLU
1	D	135	TRP
1	D	136	LEU
1	D	160	GLU
1	D	192	GLN
1	E	31	LEU
1	E	38	GLN
1	E	64	LYS
1	E	72	LYS
1	E	87	GLU
1	E	135	TRP
1	E	136	LEU
1	E	171	ARG
1	E	192	GLN
1	F	5	LEU
1	F	20	THR
1	F	22	ASP
1	F	38	GLN
1	F	56	GLN
1	F	87	GLU
1	F	110	GLU
1	F	117	GLU
1	F	135	TRP
1	F	136	LEU
1	F	155	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN

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Mol	Chain	Res	Type
1	A	46	GLN
1	A	125	GLN
1	B	33	GLN
1	B	38	GLN
1	B	46	GLN
1	B	125	GLN
1	B	141	GLN
1	C	33	GLN
1	C	46	GLN
1	C	59	GLN
1	C	102	GLN
1	C	111	ASN
1	C	118	ASN
1	C	125	GLN
1	C	127	HIS
1	C	141	GLN
1	C	148	GLN
1	D	10	GLN
1	D	33	GLN
1	D	46	GLN
1	D	63	ASN
1	D	102	GLN
1	D	125	GLN
1	D	127	HIS
1	D	167	ASN
1	D	192	GLN
1	E	10	GLN
1	E	33	GLN
1	E	46	GLN
1	E	102	GLN
1	E	118	ASN
1	E	125	GLN
1	E	127	HIS
1	E	141	GLN
1	E	157	GLN
1	E	192	GLN
1	F	33	GLN
1	F	46	GLN
1	F	59	GLN
1	F	125	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 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	501	-	33,33,33	3.27	19 (57%)	46,50,50	3.66	18 (39%)
2	FMN	B	502	-	33,33,33	3.07	18 (54%)	46,50,50	3.60	18 (39%)
2	FMN	C	503	-	33,33,33	3.20	16 (48%)	46,50,50	3.73	15 (32%)
2	FMN	D	504	-	33,33,33	2.92	16 (48%)	46,50,50	3.61	17 (36%)
2	FMN	E	505	-	33,33,33	2.90	16 (48%)	46,50,50	3.57	16 (34%)
2	FMN	F	506	-	33,33,33	2.99	16 (48%)	46,50,50	3.64	16 (34%)

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	501	-	-	0/18/18/18	0/0/3/3
2	FMN	B	502	-	-	0/18/18/18	0/0/3/3
2	FMN	C	503	-	-	0/18/18/18	0/0/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	D	504	-	-	0/18/18/18	0/0/3/3
2	FMN	E	505	-	-	0/18/18/18	0/0/3/3
2	FMN	F	506	-	-	0/18/18/18	0/0/3/3

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	503	FMN	C6-C5A	7.65	1.50	1.41
2	F	506	FMN	C6-C5A	7.44	1.50	1.41
2	A	501	FMN	C6-C5A	6.90	1.50	1.41
2	D	504	FMN	C6-C5A	6.77	1.49	1.41
2	B	502	FMN	C6-C5A	6.74	1.49	1.41
2	A	501	FMN	C9A-N10	6.65	1.48	1.38
2	B	502	FMN	C9A-N10	6.57	1.48	1.38
2	A	501	FMN	C1'-N10	6.50	1.55	1.48
2	C	503	FMN	C9A-N10	6.42	1.48	1.38
2	E	505	FMN	C6-C5A	6.30	1.49	1.41
2	C	503	FMN	C1'-N10	6.15	1.55	1.48
2	A	501	FMN	C1'-C2'	6.11	1.57	1.51
2	F	506	FMN	C9A-N10	5.92	1.47	1.38
2	E	505	FMN	C9A-N10	5.91	1.47	1.38
2	B	502	FMN	C1'-C2'	5.89	1.57	1.51
2	D	504	FMN	C9A-N10	5.77	1.47	1.38
2	C	503	FMN	C1'-C2'	5.60	1.56	1.51
2	B	502	FMN	C1'-N10	5.28	1.54	1.48
2	D	504	FMN	C1'-C2'	5.25	1.56	1.51
2	C	503	FMN	C4-N3	5.22	1.45	1.37
2	E	505	FMN	C1'-N10	5.06	1.53	1.48
2	E	505	FMN	C1'-C2'	5.00	1.56	1.51
2	A	501	FMN	C4A-C10	4.92	1.49	1.40
2	F	506	FMN	C1'-N10	4.69	1.53	1.48
2	F	506	FMN	C1'-C2'	4.68	1.56	1.51
2	D	504	FMN	C1'-N10	4.65	1.53	1.48
2	F	506	FMN	C4-N3	4.47	1.44	1.37
2	C	503	FMN	C6-C7	4.40	1.50	1.37
2	D	504	FMN	C6-C7	4.35	1.49	1.37
2	F	506	FMN	C6-C7	4.34	1.49	1.37
2	E	505	FMN	C4A-C10	4.34	1.48	1.40
2	D	504	FMN	C4-N3	4.34	1.44	1.37
2	B	502	FMN	C4A-C10	4.33	1.48	1.40
2	B	502	FMN	C8-C7	4.28	1.53	1.40
2	C	503	FMN	C4A-C10	4.23	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FMN	C4-N3	4.18	1.44	1.37
2	B	502	FMN	C4-N3	4.15	1.44	1.37
2	F	506	FMN	C4A-C10	4.10	1.48	1.40
2	E	505	FMN	C6-C7	4.05	1.49	1.37
2	B	502	FMN	C6-C7	4.03	1.48	1.37
2	A	501	FMN	C6-C7	3.99	1.48	1.37
2	C	503	FMN	C2-N3	3.95	1.45	1.37
2	D	504	FMN	C4A-C10	3.93	1.47	1.40
2	A	501	FMN	C8-C7	3.89	1.52	1.40
2	D	504	FMN	C8-C7	3.85	1.52	1.40
2	E	505	FMN	C4-N3	3.81	1.43	1.37
2	E	505	FMN	C8-C7	3.80	1.51	1.40
2	F	506	FMN	C8-C7	3.79	1.51	1.40
2	A	501	FMN	C2-N3	3.72	1.44	1.37
2	A	501	FMN	P-O3P	-3.67	1.41	1.54
2	C	503	FMN	C8-C7	3.64	1.51	1.40
2	F	506	FMN	P-O3P	-3.54	1.41	1.54
2	D	504	FMN	C9-C9A	3.53	1.47	1.40
2	F	506	FMN	C2-N3	3.47	1.44	1.37
2	D	504	FMN	P-O3P	-3.45	1.42	1.54
2	A	501	FMN	C9-C8	3.42	1.47	1.37
2	A	501	FMN	C9-C9A	3.41	1.47	1.40
2	B	502	FMN	P-O3P	-3.41	1.42	1.54
2	C	503	FMN	C9-C9A	3.40	1.47	1.40
2	F	506	FMN	C9-C9A	3.35	1.47	1.40
2	E	505	FMN	P-O3P	-3.31	1.42	1.54
2	A	501	FMN	C10-N10	3.21	1.45	1.38
2	C	503	FMN	P-O3P	-3.18	1.43	1.54
2	E	505	FMN	C9-C9A	3.15	1.47	1.40
2	F	506	FMN	C5A-N5	3.14	1.40	1.35
2	B	502	FMN	C9-C9A	3.10	1.46	1.40
2	C	503	FMN	C9-C8	3.08	1.46	1.37
2	B	502	FMN	C9-C8	3.05	1.46	1.37
2	D	504	FMN	C2-N3	3.03	1.43	1.37
2	B	502	FMN	C2-N3	3.01	1.43	1.37
2	D	504	FMN	C9-C8	2.95	1.45	1.37
2	E	505	FMN	C2-N3	2.95	1.43	1.37
2	F	506	FMN	C9-C8	2.88	1.45	1.37
2	E	505	FMN	C5A-N5	2.74	1.39	1.35
2	E	505	FMN	C9-C8	2.73	1.45	1.37
2	E	505	FMN	C10-N10	2.72	1.44	1.38
2	A	501	FMN	C8M-C8	2.61	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	503	FMN	C10-N10	2.56	1.44	1.38
2	C	503	FMN	C8M-C8	2.45	1.56	1.51
2	A	501	FMN	C5A-N5	2.42	1.39	1.35
2	C	503	FMN	C5A-N5	2.36	1.38	1.35
2	B	502	FMN	C10-N10	2.35	1.43	1.38
2	D	504	FMN	C8M-C8	2.34	1.56	1.51
2	F	506	FMN	C8M-C8	2.32	1.56	1.51
2	E	505	FMN	C8M-C8	2.32	1.56	1.51
2	C	503	FMN	C10-N1	2.29	1.39	1.35
2	D	504	FMN	C5A-N5	2.28	1.38	1.35
2	A	501	FMN	C10-N1	2.24	1.39	1.35
2	F	506	FMN	C10-N10	2.22	1.43	1.38
2	B	502	FMN	C8M-C8	2.16	1.55	1.51
2	B	502	FMN	C10-N1	2.15	1.39	1.35
2	D	504	FMN	C10-N10	2.14	1.43	1.38
2	A	501	FMN	C4'-C3'	2.13	1.57	1.53
2	A	501	FMN	P-O1P	-2.11	1.44	1.51
2	E	505	FMN	P-O2P	-2.11	1.47	1.54
2	A	501	FMN	O5'-C5'	-2.09	1.36	1.44
2	B	502	FMN	O5'-C5'	-2.08	1.36	1.44
2	F	506	FMN	P-O2P	-2.08	1.47	1.54
2	D	504	FMN	P-O2P	-2.05	1.47	1.54
2	B	502	FMN	C5A-N5	2.05	1.38	1.35
2	B	502	FMN	P-O2P	-2.03	1.47	1.54

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	FMN	C4A-C10-N10	-14.68	113.18	120.51
2	A	501	FMN	C4A-C10-N10	-14.35	113.35	120.51
2	F	506	FMN	C4A-C10-N10	-14.04	113.50	120.51
2	C	503	FMN	C4A-N5-C5A	14.02	132.44	116.69
2	D	504	FMN	C4A-C10-N10	-13.94	113.55	120.51
2	A	501	FMN	C4A-N5-C5A	13.89	132.29	116.69
2	B	502	FMN	C4A-C10-N10	-13.88	113.59	120.51
2	E	505	FMN	C4A-C10-N10	-13.69	113.68	120.51
2	D	504	FMN	C4A-N5-C5A	13.46	131.81	116.69
2	B	502	FMN	C4A-N5-C5A	13.45	131.80	116.69
2	E	505	FMN	C4A-N5-C5A	13.40	131.75	116.69
2	F	506	FMN	C4A-N5-C5A	13.33	131.66	116.69
2	F	506	FMN	C9A-N10-C10	7.25	128.88	121.77
2	D	504	FMN	C9A-N10-C10	6.79	128.43	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	505	FMN	C9A-N10-C10	6.60	128.24	121.77
2	C	503	FMN	C9A-N10-C10	6.58	128.22	121.77
2	B	502	FMN	C9A-N10-C10	6.51	128.16	121.77
2	A	501	FMN	C9A-N10-C10	6.31	127.96	121.77
2	C	503	FMN	C2-N1-C10	6.26	121.29	114.98
2	E	505	FMN	C2-N1-C10	6.21	121.23	114.98
2	B	502	FMN	C2-N1-C10	6.09	121.12	114.98
2	D	504	FMN	C2-N1-C10	6.04	121.06	114.98
2	A	501	FMN	C2-N1-C10	6.01	121.04	114.98
2	F	506	FMN	C2-N1-C10	6.00	121.02	114.98
2	C	503	FMN	C9A-C5A-N5	-4.97	114.75	122.37
2	F	506	FMN	C9A-C5A-N5	-4.81	115.00	122.37
2	D	504	FMN	C9A-C5A-N5	-4.67	115.21	122.37
2	E	505	FMN	C9A-C5A-N5	-4.55	115.40	122.37
2	B	502	FMN	C9A-C5A-N5	-4.52	115.44	122.37
2	A	501	FMN	C9A-C5A-N5	-4.40	115.62	122.37
2	A	501	FMN	C10-C4A-N5	-3.64	116.03	120.45
2	F	506	FMN	C10-C4A-N5	-3.63	116.05	120.45
2	E	505	FMN	C10-C4A-N5	-3.60	116.08	120.45
2	C	503	FMN	C1'-N10-C9A	-3.59	115.38	118.87
2	C	503	FMN	C10-C4A-N5	-3.52	116.18	120.45
2	D	504	FMN	C10-C4A-N5	-3.49	116.22	120.45
2	B	502	FMN	C10-C4A-N5	-3.39	116.34	120.45
2	D	504	FMN	C1'-N10-C9A	-3.29	115.67	118.87
2	A	501	FMN	C1'-N10-C9A	-3.22	115.74	118.87
2	C	503	FMN	C6-C5A-N5	3.10	122.59	118.97
2	F	506	FMN	C6-C5A-N5	3.09	122.57	118.97
2	A	501	FMN	N1-C10-N10	3.08	124.08	115.97
2	C	503	FMN	N3-C2-N1	-3.08	114.65	121.19
2	A	501	FMN	C9-C9A-N10	3.01	128.07	121.59
2	B	502	FMN	N1-C10-N10	3.00	123.87	115.97
2	E	505	FMN	N1-C10-N10	2.98	123.81	115.97
2	B	502	FMN	C9-C9A-N10	2.96	127.97	121.59
2	F	506	FMN	C1'-N10-C10	-2.95	114.98	119.17
2	A	501	FMN	C6-C5A-C9A	2.90	123.03	119.02
2	C	503	FMN	N1-C10-N10	2.88	123.54	115.97
2	D	504	FMN	N3-C2-N1	-2.86	115.12	121.19
2	A	501	FMN	N3-C2-N1	-2.82	115.19	121.19
2	F	506	FMN	C1'-N10-C9A	-2.82	116.13	118.87
2	F	506	FMN	N3-C2-N1	-2.81	115.21	121.19
2	D	504	FMN	C9-C9A-N10	2.81	127.63	121.59
2	D	504	FMN	N1-C10-N10	2.80	123.33	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	FMN	C6-C5A-C9A	2.79	122.89	119.02
2	E	505	FMN	C1'-N10-C9A	-2.79	116.16	118.87
2	E	505	FMN	N3-C2-N1	-2.77	115.30	121.19
2	E	505	FMN	C9-C9A-N10	2.77	127.55	121.59
2	B	502	FMN	C8M-C8-C7	2.74	127.07	120.74
2	F	506	FMN	N1-C10-N10	2.72	123.12	115.97
2	B	502	FMN	N3-C2-N1	-2.71	115.43	121.19
2	C	503	FMN	C9-C9A-N10	2.70	127.42	121.59
2	F	506	FMN	C9-C9A-N10	2.69	127.38	121.59
2	D	504	FMN	C6-C5A-N5	2.67	122.08	118.97
2	D	504	FMN	C6-C5A-C9A	2.66	122.71	119.02
2	C	503	FMN	C6-C5A-C9A	2.63	122.66	119.02
2	A	501	FMN	O4'-C4'-C5'	-2.62	104.75	110.12
2	E	505	FMN	C6-C5A-N5	2.60	122.00	118.97
2	B	502	FMN	C1'-N10-C9A	-2.59	116.35	118.87
2	B	502	FMN	C1'-N10-C10	-2.59	115.48	119.17
2	E	505	FMN	C6-C5A-C9A	2.59	122.60	119.02
2	B	502	FMN	C8M-C8-C9	-2.54	114.25	120.38
2	E	505	FMN	C1'-N10-C10	-2.51	115.60	119.17
2	F	506	FMN	C6-C5A-C9A	2.46	122.43	119.02
2	F	506	FMN	C8M-C8-C7	2.38	126.24	120.74
2	D	504	FMN	C8M-C8-C7	2.38	126.23	120.74
2	B	502	FMN	C6-C5A-N5	2.31	121.67	118.97
2	D	504	FMN	C1'-N10-C10	-2.31	115.89	119.17
2	E	505	FMN	C8M-C8-C7	2.30	126.04	120.74
2	E	505	FMN	O4'-C4'-C5'	-2.28	105.44	110.12
2	F	506	FMN	C8M-C8-C9	-2.27	114.91	120.38
2	F	506	FMN	O3P-P-O5'	-2.26	100.40	106.65
2	D	504	FMN	O3P-P-O5'	-2.26	100.42	106.65
2	A	501	FMN	C8M-C8-C7	2.24	125.91	120.74
2	D	504	FMN	C8M-C8-C9	-2.23	115.01	120.38
2	B	502	FMN	O3P-P-O5'	-2.23	100.50	106.65
2	A	501	FMN	O3P-P-O5'	-2.22	100.52	106.65
2	E	505	FMN	C8M-C8-C9	-2.20	115.08	120.38
2	C	503	FMN	C8M-C8-C7	2.19	125.81	120.74
2	B	502	FMN	C5A-C9A-N10	-2.19	114.65	116.80
2	A	501	FMN	C5A-C9A-N10	-2.12	114.72	116.80
2	C	503	FMN	C8M-C8-C9	-2.10	115.31	120.38
2	D	504	FMN	C5A-C9A-N10	-2.07	114.76	116.80
2	A	501	FMN	C8M-C8-C9	-2.05	115.44	120.38
2	A	501	FMN	C6-C5A-N5	2.03	121.34	118.97
2	B	502	FMN	O4'-C4'-C5'	-2.03	105.95	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FMN	C1'-N10-C10	-2.02	116.29	119.17
2	C	503	FMN	O4'-C4'-C3'	2.02	114.07	109.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	200/208 (96%)	0.05	3 (1%) 70 78	8, 19, 37, 46	0
1	B	201/208 (96%)	0.23	10 (4%) 28 38	7, 21, 46, 54	0
1	C	201/208 (96%)	0.21	8 (3%) 36 47	9, 22, 41, 58	0
1	D	200/208 (96%)	0.40	16 (8%) 12 19	7, 26, 54, 64	0
1	E	201/208 (96%)	0.71	18 (8%) 10 16	15, 37, 52, 59	0
1	F	199/208 (95%)	1.13	37 (18%) 2 3	15, 40, 64, 72	0
All	All	1202/1248 (96%)	0.45	92 (7%) 14 20	7, 26, 53, 72	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	79	PHE	7.1
1	F	107	ASN	7.1
1	F	103	ALA	6.3
1	F	119	PHE	6.1
1	F	80	ALA	6.0
1	F	163	ASP	5.4
1	F	104	VAL	4.9
1	F	113	PRO	4.8
1	F	106	ARG	4.7
1	F	105	VAL	4.6
1	F	166	THR	4.4
1	F	112	PHE	4.4
1	F	114	LEU	4.4
1	A	201	LEU	4.4
1	B	182	PRO	4.3
1	F	109	GLU	4.3
1	C	43	PHE	4.3
1	C	202	GLU	4.0
1	D	80	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	202	GLU	3.9
1	D	77	GLU	3.9
1	E	163	ASP	3.8
1	D	185	GLU	3.7
1	D	22	ASP	3.7
1	B	2	SER	3.7
1	B	77	GLU	3.6
1	A	166	THR	3.6
1	C	79	PHE	3.5
1	F	108	LEU	3.5
1	E	166	THR	3.4
1	F	23	LEU	3.4
1	E	77	GLU	3.4
1	F	115	TYR	3.3
1	A	77	GLU	3.3
1	F	21	VAL	3.2
1	F	67	TYR	3.2
1	D	163	ASP	3.2
1	B	43	PHE	3.2
1	F	192	GLN	3.2
1	C	166	THR	3.1
1	F	77	GLU	3.1
1	F	22	ASP	3.0
1	F	76	ALA	3.0
1	D	182	PRO	3.0
1	E	22	ASP	2.8
1	C	75	PRO	2.8
1	E	106	ARG	2.8
1	E	6	ASP	2.7
1	D	192	GLN	2.7
1	F	193	GLU	2.7
1	F	98	LEU	2.6
1	B	202	GLU	2.6
1	E	192	GLN	2.6
1	C	182	PRO	2.6
1	F	174	ILE	2.6
1	E	72	LYS	2.6
1	F	2	SER	2.6
1	F	170	MSE	2.5
1	F	73	VAL	2.5
1	C	77	GLU	2.5
1	D	76	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	200	ASP	2.4
1	D	174	ILE	2.4
1	D	75	PRO	2.4
1	E	197	VAL	2.4
1	F	18	GLY	2.4
1	B	187	GLU	2.4
1	E	96	ILE	2.4
1	F	142	ASN	2.4
1	E	180	GLU	2.4
1	F	117	GLU	2.3
1	B	73	VAL	2.3
1	E	200	ASP	2.3
1	E	134	ILE	2.3
1	E	2	SER	2.2
1	D	82	THR	2.2
1	B	147	VAL	2.2
1	B	79	PHE	2.2
1	F	75	PRO	2.1
1	F	172	ALA	2.1
1	D	147	VAL	2.1
1	D	193	GLU	2.1
1	F	96	ILE	2.1
1	D	170	MSE	2.1
1	E	74	THR	2.1
1	B	22	ASP	2.1
1	C	129	ILE	2.1
1	D	79	PHE	2.1
1	E	182	PRO	2.0
1	F	24	SER	2.0
1	E	70	LEU	2.0
1	D	24	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FMN	C	503	31/31	0.16	0.77	9,17,22,27	0
2	FMN	E	505	31/31	0.18	0.47	16,19,27,28	0
2	FMN	A	501	31/31	0.16	0.41	9,17,21,24	0
2	FMN	B	502	31/31	0.16	0.25	11,15,21,22	0
2	FMN	F	506	31/31	0.14	-0.13	16,18,22,24	0
2	FMN	D	504	31/31	0.17	-0.30	19,23,27,31	0

6.5 Other polymers

There are no such residues in this entry.