Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 11:09 AM EDT

PDB ID	:	2I7H
Title	:	Crystal Structure of the Nitroreductase-like Family Protein from Bacillus cereus
Authors	:	Kim, Y.; Li, H.; Moy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2006-08-30
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

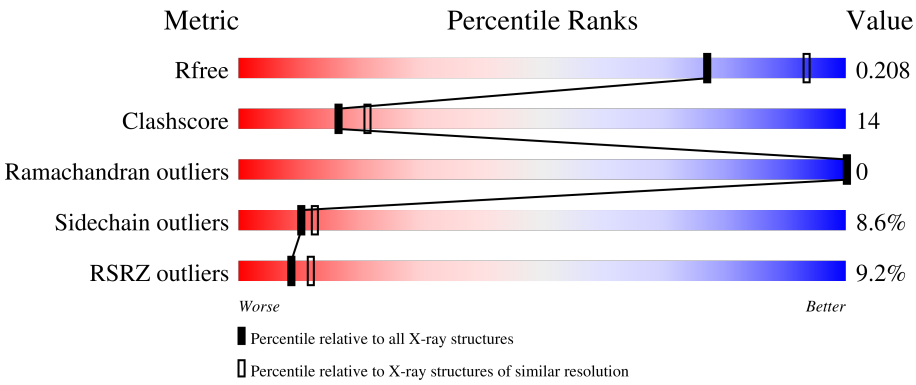
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	189	10%; 70%; 25%; • •
1	B	189	10%; 72%; 22%; 5% •
1	C	189	5%; 75%; 21%; • •
1	D	189	6%; 72%; 23%; • ••

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Mol	Chain	Length	Quality of chain
1	E	189	8% 77% 18%
1	F	189	15% 67% 27% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	C	1003[A]	-	-	X	-
2	FMN	C	1003[B]	-	-	X	-
2	FMN	D	1004	-	-	X	-
3	SO4	C	1207	-	-	X	-
3	SO4	E	1205	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10972 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 Nitroreductase-like family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	187	1672	1051	292	321	4	4	0	21	0
1	B	187	1647	1035	291	313	4	4	0	17	0
1	C	187	1660	1048	290	313	4	5	0	19	0
1	D	187	1645	1034	293	310	4	4	0	16	0
1	E	185	1624	1021	293	301	5	4	0	16	0
1	F	187	1636	1032	291	305	4	4	0	15	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	CLONING ARTIFACT	UNP Q81HL8
A	-1	ASN	-	CLONING ARTIFACT	UNP Q81HL8
A	0	ALA	-	CLONING ARTIFACT	UNP Q81HL8
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
A	97	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
A	117	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
A	181	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
B	-2	SER	-	CLONING ARTIFACT	UNP Q81HL8
B	-1	ASN	-	CLONING ARTIFACT	UNP Q81HL8
B	0	ALA	-	CLONING ARTIFACT	UNP Q81HL8
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
B	97	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
B	117	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
B	181	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
C	-2	SER	-	CLONING ARTIFACT	UNP Q81HL8
C	-1	ASN	-	CLONING ARTIFACT	UNP Q81HL8
C	0	ALA	-	CLONING ARTIFACT	UNP Q81HL8

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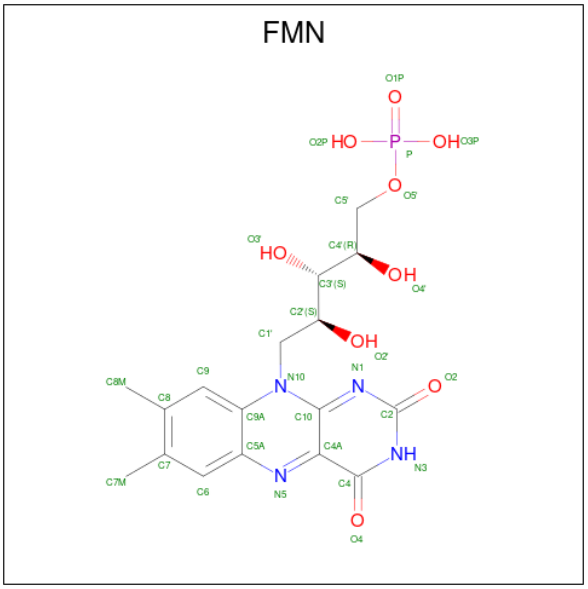
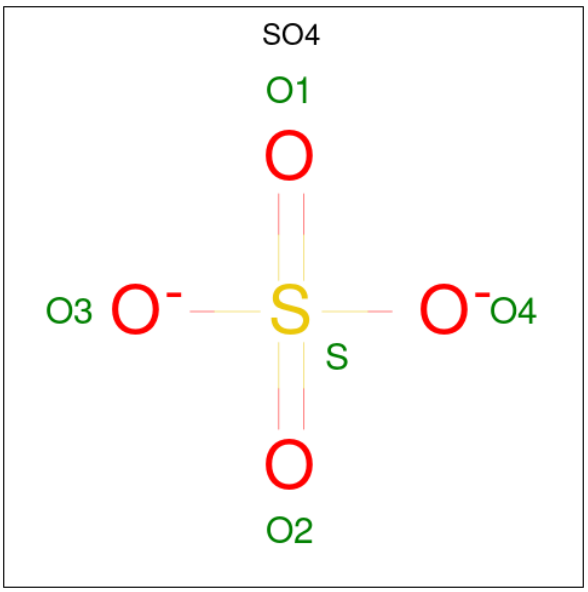
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
C	97	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
C	117	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
C	181	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
D	-2	SER	-	CLONING ARTIFACT	UNP Q81HL8
D	-1	ASN	-	CLONING ARTIFACT	UNP Q81HL8
D	0	ALA	-	CLONING ARTIFACT	UNP Q81HL8
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
D	97	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
D	117	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
D	181	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
E	-2	SER	-	CLONING ARTIFACT	UNP Q81HL8
E	-1	ASN	-	CLONING ARTIFACT	UNP Q81HL8
E	0	ALA	-	CLONING ARTIFACT	UNP Q81HL8
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
E	97	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
E	117	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
E	181	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
F	-2	SER	-	CLONING ARTIFACT	UNP Q81HL8
F	-1	ASN	-	CLONING ARTIFACT	UNP Q81HL8
F	0	ALA	-	CLONING ARTIFACT	UNP Q81HL8
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
F	97	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
F	117	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8
F	181	MSE	MET	MODIFIED RESIDUE	UNP Q81HL8

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	17	4	9	1	0	0
			Total	C	N	O	P		
2	B	1	31	17	4	9	1	0	0
			Total	C	N	O	P		
2	C	1	62	34	8	18	2	0	1
			Total	C	N	O	P		
2	D	1	31	17	4	9	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	C	1	5	4	1	0	0
			Total	O	S		
3	C	1	5	4	1	0	0
			Total	O	S		
3	D	1	5	4	1	0	0
			Total	O	S		
3	E	1	5	4	1	0	0
			Total	O	S		
3	F	1	5	4	1	0	0

- Molecule 4 is water.

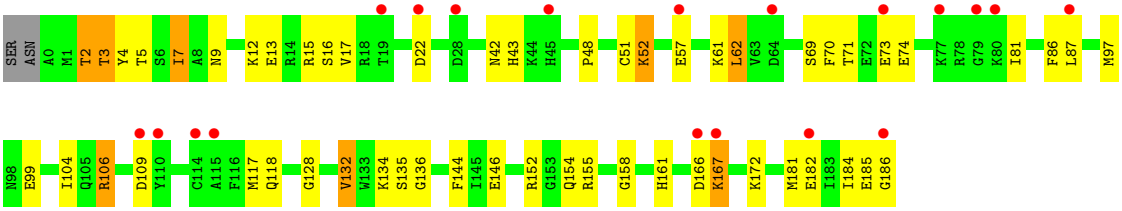
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	154	154	154	0	0
			Total	O		
4	B	178	178	178	0	0
			Total	O		
4	C	150	150	150	0	0
			Total	O		
4	D	163	163	163	0	0
			Total	O		
4	E	142	142	142	0	0
			Total	O		
4	F	111	111	111	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

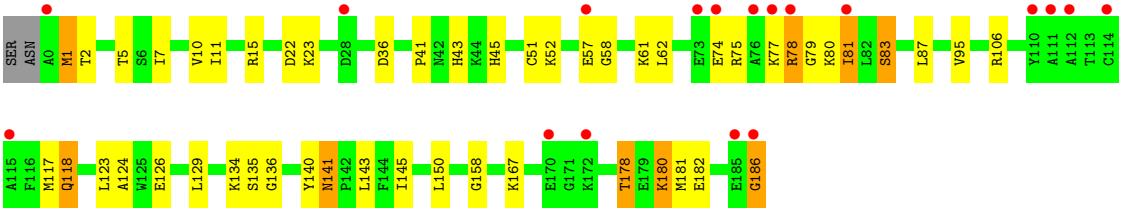
• Molecule 1: Nitroreductase-like family protein

Chain A:



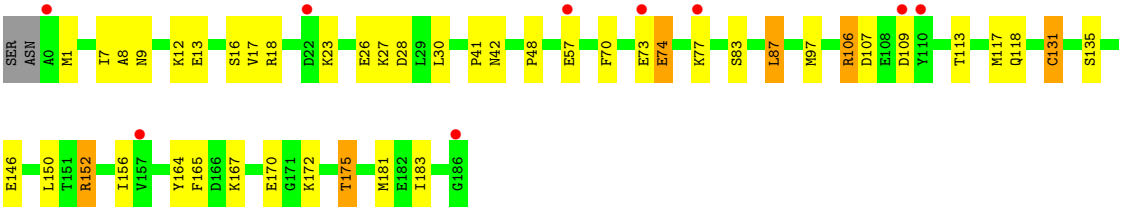
• Molecule 1: Nitroreductase-like family protein

Chain B:



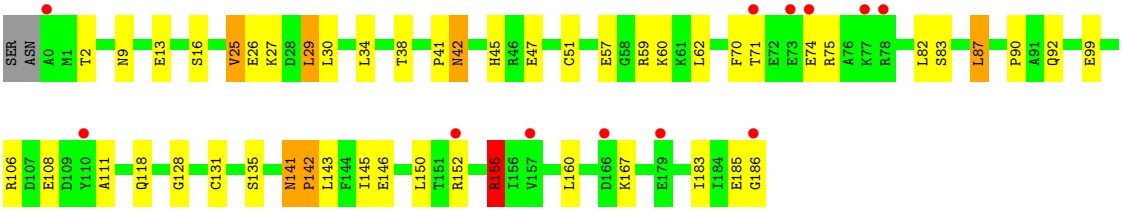
• Molecule 1: Nitroreductase-like family protein

Chain C:



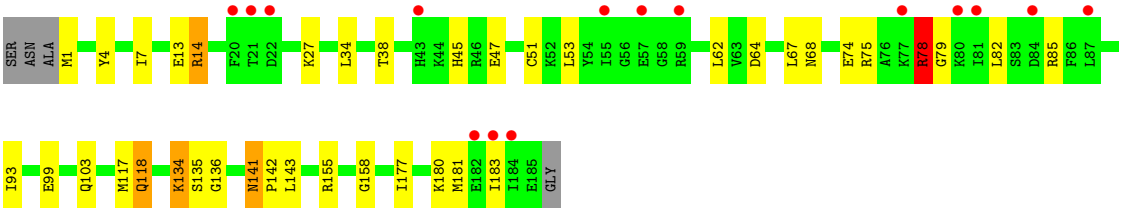
• Molecule 1: Nitroreductase-like family protein

Chain D:



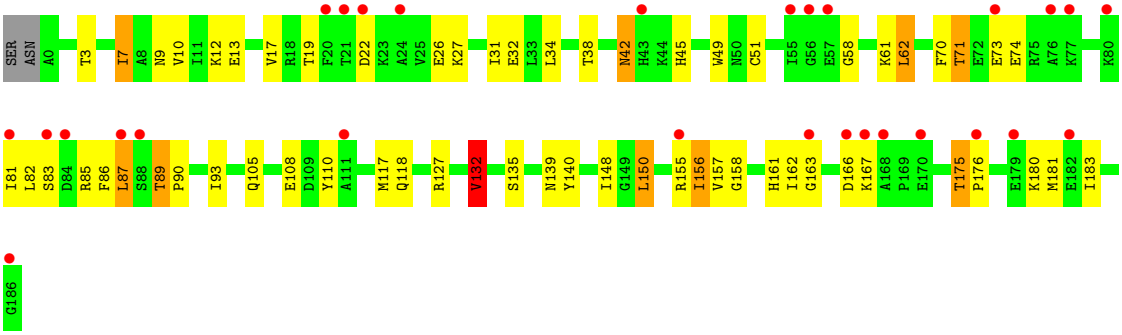
• Molecule 1: Nitroreductase-like family protein

Chain E:



• Molecule 1: Nitroreductase-like family protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	242.72Å 87.22Å 81.19Å 90.00° 103.03° 90.00°	Depositor
Resolution (Å)	40.91 – 2.30 40.91 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.91-2.30) 99.6 (40.91-2.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.213 0.170 , 0.208	Depositor DCC
R_{free} test set	7501 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10972	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, SO4

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	0.67	0/1698	0.71	1/2284 (0.0%)
1	B	0.81	2/1674 (0.1%)	0.81	2/2249 (0.1%)
1	C	0.81	1/1686 (0.1%)	0.80	3/2263 (0.1%)
1	D	0.73	1/1671 (0.1%)	0.78	3/2244 (0.1%)
1	E	0.63	0/1652	0.75	2/2219 (0.1%)
1	F	0.61	0/1663	0.74	1/2235 (0.0%)
All	All	0.72	4/10044 (0.0%)	0.76	12/13494 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	186	GLY	C-O	12.85	1.44	1.23
1	C	131	CYS	CB-SG	-12.76	1.60	1.82
1	D	131	CYS	CB-SG	-8.40	1.68	1.82
1	B	186	GLY	CA-C	6.52	1.62	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	155	ARG	NE-CZ-NH1	-9.29	115.65	120.30
1	B	186	GLY	CA-C-O	-8.94	104.52	120.60
1	B	106	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	D	155	ARG	NE-CZ-NH2	6.23	123.41	120.30
1	C	106	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	C	152	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	E	78	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	E	14	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	F	132	VAL	CB-CA-C	-5.22	101.48	111.40
1	C	131	CYS	CB-CA-C	-5.18	100.05	110.40
1	D	131	CYS	CB-CA-C	-5.08	100.24	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	106	ARG	NE-CZ-NH1	-5.04	117.78	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	1672	0	1642	55	0
1	B	1647	0	1616	69	0
1	C	1660	0	1647	60	0
1	D	1645	0	1625	52	0
1	E	1624	0	1614	45	0
1	F	1636	0	1622	50	0
2	A	31	0	19	4	0
2	B	31	0	19	6	0
2	C	62	0	38	28	0
2	D	31	0	19	9	0
3	B	10	0	0	1	0
3	C	10	0	0	2	0
3	D	5	0	0	1	0
3	E	5	0	0	2	0
3	F	5	0	0	0	0
4	A	154	0	0	12	1
4	B	178	0	0	10	0
4	C	150	0	0	3	0
4	D	163	0	0	5	1
4	E	142	0	0	11	0
4	F	111	0	0	3	0
All	All	10972	0	9861	287	1

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 14.

All (287) 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:135[B]:SER:CB	2:C:1003[B]:FMN:H6	1.61	1.31
1:A:181:MSE:HE3	1:B:51[B]:CYS:SG	1.94	1.07
1:B:95[B]:VAL:HG21	1:B:117:MSE:SE	2.07	1.04
1:A:186:GLY:HA3	1:B:61[A]:LYS:NZ	1.73	1.04
1:C:135[B]:SER:OG	2:C:1003[B]:FMN:H6	1.56	1.03
1:C:135[B]:SER:HB3	2:C:1003[B]:FMN:H6	1.38	1.01
1:D:9[B]:ASN:ND2	1:D:13[B]:GLU:OE2	1.94	1.00
1:E:181:MSE:HE1	1:F:31:ILE:HG12	1.46	0.96
1:B:45[A]:HIS:ND1	4:B:1367:HOH:O	1.98	0.96
2:C:1003[B]:FMN:H9	2:C:1003[B]:FMN:O2'	1.66	0.94
1:B:135[B]:SER:O	4:B:1352:HOH:O	1.86	0.91
1:A:52:LYS:HE2	1:B:182[B]:GLU:HG3	1.50	0.89
3:B:1201:SO4:O4	4:B:1371:HOH:O	1.89	0.89
1:C:135[B]:SER:CB	2:C:1003[B]:FMN:C6	2.51	0.88
1:C:150:LEU:HD12	1:C:156[A]:ILE:HD11	1.56	0.88
1:F:110:TYR:CE1	1:F:155[B]:ARG:NH2	2.41	0.87
1:F:140:TYR:OH	1:F:155[B]:ARG:NH1	2.08	0.87
1:A:51[B]:CYS:SG	1:B:181:MSE:HE3	2.14	0.87
1:C:175:THR:HG23	1:D:47:GLU:OE1	1.75	0.87
1:C:135[B]:SER:OG	2:C:1003[B]:FMN:C6	2.23	0.86
1:F:71:THR:HG22	1:F:73:GLU:H	1.41	0.86
1:A:186:GLY:HA3	1:B:61[A]:LYS:HZ2	1.37	0.85
3:C:1207:SO4:O3	4:C:1357:HOH:O	1.95	0.85
1:F:110:TYR:HE1	1:F:155[B]:ARG:HH21	1.19	0.84
1:C:150:LEU:CD1	1:C:156[A]:ILE:HD11	2.07	0.84
1:C:26[B]:GLU:HG2	1:C:28[B]:ASP:OD1	1.77	0.84
1:B:23:LYS:NZ	1:C:1[B]:MSE:HG2	1.92	0.84
1:A:97:MSE:CE	1:A:109[B]:ASP:OD2	2.24	0.84
1:C:135[B]:SER:HB3	2:C:1003[B]:FMN:C6	2.07	0.82
1:E:51[B]:CYS:SG	1:E:93:ILE:HG23	2.19	0.82
4:E:1292:HOH:O	1:F:155[A]:ARG:HD2	1.80	0.80
1:A:135[A]:SER:OG	1:A:136:GLY:N	2.15	0.79
1:D:26[B]:GLU:HG2	1:D:29:LEU:HB2	1.65	0.79
1:A:97:MSE:HE1	1:A:109[B]:ASP:OD2	1.83	0.79
1:A:52:LYS:CE	1:B:182[B]:GLU:HG3	2.12	0.78
1:A:186:GLY:HA3	1:B:61[A]:LYS:HZ1	1.46	0.78
1:F:110:TYR:OH	1:F:155[B]:ARG:NH2	2.17	0.78
1:B:135[B]:SER:OG	1:B:136:GLY:N	2.10	0.77
1:F:110:TYR:HE1	1:F:155[B]:ARG:NH2	1.80	0.77
1:E:118:GLN:HE21	1:E:118:GLN:HA	1.50	0.76
1:F:9:ASN:O	1:F:13[A]:GLU:HB2	1.85	0.76
1:E:134:LYS:NZ	4:E:1343:HOH:O	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:THR:OG1	1:A:74[A]:GLU:HG3	1.87	0.75
1:A:135[B]:SER:OG	2:A:1001:FMN:H6	1.87	0.75
1:C:26[B]:GLU:HG3	4:C:1243:HOH:O	1.85	0.75
2:C:1003[B]:FMN:H4'	1:D:42:ASN:H	1.52	0.73
2:C:1003[B]:FMN:H5'2	1:D:41:PRO:HA	1.68	0.73
3:E:1205:SO4:O2	4:E:1309:HOH:O	2.06	0.73
1:A:7[B]:ILE:HD12	1:B:7:ILE:HB	1.71	0.73
1:A:152:ARG:HB2	4:A:1113:HOH:O	1.89	0.72
1:B:95[B]:VAL:CG2	1:B:117:MSE:SE	2.88	0.72
1:B:15:ARG:HD3	4:B:1376:HOH:O	1.89	0.71
1:D:16:SER:OG	2:D:1004:FMN:C5'	2.39	0.71
4:A:1125:HOH:O	1:B:7:ILE:HG23	1.91	0.71
1:B:23:LYS:HZ2	1:C:1[B]:MSE:HG2	1.56	0.70
1:D:9[B]:ASN:C	1:D:9[B]:ASN:HD22	1.95	0.70
1:E:155[B]:ARG:HD2	4:E:1240:HOH:O	1.92	0.69
1:C:135[B]:SER:OG	2:C:1003[B]:FMN:N5	2.25	0.69
1:B:74[B]:GLU:OE2	1:B:78[B]:ARG:NE	2.26	0.69
1:E:45:HIS:ND1	4:E:1308:HOH:O	2.24	0.69
2:B:1002:FMN:H4'	2:B:1002:FMN:O1P	1.92	0.68
1:A:97:MSE:SE	1:A:109[B]:ASP:OD2	2.61	0.68
1:B:117:MSE:HE1	1:B:158:GLY:HA3	1.75	0.67
1:C:175:THR:CG2	1:D:47:GLU:OE1	2.42	0.67
2:A:1001:FMN:H2'	1:B:43:HIS:HA	1.75	0.67
1:F:110:TYR:CZ	1:F:155[B]:ARG:NH2	2.63	0.66
1:E:155[B]:ARG:CD	4:E:1240:HOH:O	2.43	0.66
1:E:13:GLU:OE1	4:E:1294:HOH:O	2.12	0.66
1:E:135[B]:SER:OG	1:E:136:GLY:N	2.28	0.66
2:B:1002:FMN:O2'	2:B:1002:FMN:H9	1.95	0.66
1:C:135[A]:SER:HB2	2:C:1003[A]:FMN:H6	1.78	0.66
2:C:1003[B]:FMN:O2'	2:C:1003[B]:FMN:C9	2.43	0.65
1:D:16:SER:OG	2:D:1004:FMN:H5'1	1.96	0.65
1:A:117:MSE:HE1	1:A:158:GLY:HA3	1.77	0.65
1:C:26[B]:GLU:OE2	1:C:28[B]:ASP:OD1	2.15	0.65
1:F:89:THR:HG21	4:F:1215:HOH:O	1.97	0.65
1:B:74[B]:GLU:HG2	1:B:78[B]:ARG:HG2	1.78	0.65
1:D:70:PHE:HB3	1:D:74[B]:GLU:HB3	1.77	0.64
1:C:26[B]:GLU:CG	1:C:28[B]:ASP:OD1	2.45	0.64
1:B:135[A]:SER:OG	2:B:1002:FMN:H6	1.97	0.64
1:B:118:GLN:HA	1:B:118:GLN:HE21	1.62	0.64
1:F:51[B]:CYS:SG	1:F:93:ILE:HG23	2.37	0.64
1:B:2:THR:HG23	4:B:1318:HOH:O	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LYS:HZ1	1:C:1[B]:MSE:HG2	1.61	0.63
1:E:14:ARG:NH2	4:E:1307:HOH:O	2.24	0.62
1:E:27:LYS:HE2	1:F:183:ILE:HD13	1.82	0.62
1:B:23:LYS:NZ	1:C:1[B]:MSE:HE2	2.14	0.62
1:F:85:ARG:O	1:F:89:THR:HG23	2.00	0.62
1:C:135[A]:SER:CB	2:C:1003[A]:FMN:H6	2.30	0.61
1:D:57[B]:GLU:OE1	1:D:60[B]:LYS:CE	2.49	0.60
1:B:23:LYS:HZ3	1:C:1[B]:MSE:HE2	1.65	0.60
1:E:141:ASN:C	1:E:141:ASN:HD22	2.03	0.60
1:F:32:GLU:OE1	1:F:127:ARG:NH2	2.32	0.60
1:F:70:PHE:HB3	1:F:74[A]:GLU:HG3	1.84	0.60
1:A:182[B]:GLU:HG2	1:B:52:LYS:HG2	1.82	0.60
1:F:155[B]:ARG:NH2	1:F:157:VAL:HA	2.17	0.60
1:D:141:ASN:C	1:D:141:ASN:HD22	2.05	0.60
1:A:2:THR:HG21	4:A:1124:HOH:O	2.00	0.59
1:C:181:MSE:HG3	1:D:51[B]:CYS:SG	2.42	0.59
1:B:74[B]:GLU:CD	1:B:78[B]:ARG:HE	2.06	0.59
1:D:9[B]:ASN:O	1:D:13[B]:GLU:HG3	2.02	0.59
1:E:7:ILE:HB	1:F:7:ILE:HG12	1.85	0.58
1:C:107:ASP:OD2	1:D:155:ARG:NH1	2.36	0.58
1:F:71:THR:HB	1:F:74[A]:GLU:HG2	1.86	0.58
1:D:135:SER:OG	2:D:1004:FMN:H6	2.04	0.58
1:D:141:ASN:ND2	1:D:143:LEU:H	2.02	0.58
1:A:17:VAL:O	1:A:132:VAL:HG22	2.04	0.57
1:A:118:GLN:HE21	1:A:118:GLN:HA	1.67	0.57
1:E:141:ASN:ND2	1:E:143:LEU:H	2.02	0.57
1:A:69[B]:SER:OG	1:A:144:PHE:HB2	2.03	0.57
1:D:9[B]:ASN:CG	1:D:13[B]:GLU:OE2	2.43	0.57
1:C:18:ARG:NH2	2:C:1003[A]:FMN:O3'	2.36	0.57
1:C:172:LYS:HG2	1:D:45:HIS:CE1	2.39	0.57
2:C:1003[A]:FMN:HM71	1:D:111:ALA:HB3	1.85	0.57
1:A:7[A]:ILE:HG21	1:B:10:VAL:HG21	1.85	0.57
1:E:181:MSE:CE	1:F:31:ILE:HG12	2.28	0.57
1:F:71:THR:HG22	1:F:73:GLU:N	2.14	0.56
1:A:7[A]:ILE:HD11	1:B:123:LEU:HA	1.87	0.56
1:E:181:MSE:HE1	1:F:31:ILE:CG1	2.30	0.56
1:A:73[B]:GLU:HG2	4:A:1080:HOH:O	2.05	0.56
1:A:181:MSE:HE3	1:B:51[A]:CYS:HB2	1.86	0.56
1:D:9[B]:ASN:ND2	1:D:9[B]:ASN:C	2.59	0.56
1:D:16:SER:OG	2:D:1004:FMN:H5'2	2.06	0.56
1:B:23:LYS:HB2	1:C:1[A]:MSE:HE3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLU:O	1:B:57[A]:GLU:HG3	2.05	0.56
1:F:26[B]:GLU:HG2	4:F:1270:HOH:O	2.07	0.56
2:C:1003[B]:FMN:HM81	1:D:41:PRO:HB2	1.89	0.55
1:D:141:ASN:HD22	1:D:143:LEU:H	1.54	0.55
1:D:99:GLU:OE2	1:D:155:ARG:HD2	2.07	0.54
2:C:1003[B]:FMN:C5'	1:D:41:PRO:HA	2.37	0.54
1:E:51[B]:CYS:SG	1:F:181:MSE:HE3	2.47	0.54
1:C:48:PRO:HG3	1:C:109[B]:ASP:HB2	1.90	0.54
1:E:74[B]:GLU:CD	1:E:78:ARG:HE	2.11	0.54
2:C:1003[A]:FMN:H5'1	1:D:41:PRO:HA	1.89	0.53
1:D:26[B]:GLU:CG	1:D:29:LEU:HB2	2.36	0.53
1:C:16:SER:HG	2:C:1003[A]:FMN:HO4'	1.56	0.53
1:C:83:SER:O	1:C:87:LEU:HB2	2.09	0.53
1:E:180:LYS:HE3	1:F:49:TRP:O	2.08	0.53
1:B:45[B]:HIS:HD2	4:B:1261:HOH:O	1.91	0.53
1:A:12:LYS:O	1:A:15:ARG:NH2	2.39	0.52
1:B:45[A]:HIS:CE1	4:B:1367:HOH:O	2.52	0.52
1:D:25:VAL:HG13	1:D:90:PRO:HB3	1.91	0.52
1:A:166:ASP:HB3	1:A:167[A]:LYS:HD3	1.92	0.52
1:B:141:ASN:HD22	1:B:143:LEU:H	1.57	0.52
4:A:1102:HOH:O	1:B:180:LYS:NZ	2.41	0.52
1:B:57[A]:GLU:HG2	4:B:1297:HOH:O	2.10	0.52
1:A:4:TYR:CE2	1:B:5:THR:HG22	2.45	0.52
1:B:79:GLY:O	1:B:83[A]:SER:OG	2.28	0.52
1:E:99:GLU:OE2	1:E:155[A]:ARG:NE	2.36	0.52
1:C:113:THR:O	1:C:117:MSE:HG3	2.10	0.51
1:C:135[B]:SER:OG	2:C:1003[B]:FMN:C5A	2.57	0.51
1:D:118:GLN:HE21	1:D:118:GLN:HA	1.74	0.51
1:F:81:ILE:HG13	1:F:82[B]:LEU:N	2.25	0.51
1:F:81:ILE:HG13	1:F:82[A]:LEU:N	2.25	0.51
1:F:117:MSE:HE1	1:F:158:GLY:HA3	1.93	0.51
2:D:1004:FMN:O3'	4:D:1363:HOH:O	2.19	0.51
1:A:3[A]:THR:HG22	4:A:1013:HOH:O	2.10	0.51
1:E:53:LEU:HB2	1:F:181:MSE:HE2	1.92	0.50
2:A:1001:FMN:O4'	2:A:1001:FMN:H1'2	2.12	0.50
1:D:57[B]:GLU:OE1	1:D:60[B]:LYS:HE3	2.12	0.50
2:A:1001:FMN:HM81	1:B:41:PRO:HB2	1.93	0.50
1:C:97:MSE:SE	1:C:109[B]:ASP:OD2	2.79	0.50
1:E:155[B]:ARG:HD3	4:E:1240:HOH:O	2.11	0.50
1:D:92:GLN:HA	1:D:160:LEU:O	2.12	0.50
1:E:141:ASN:HD22	1:E:142:PRO:N	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99[B]:GLU:HG2	1:A:155:ARG:HB2	1.93	0.49
1:E:141:ASN:HD22	1:E:143:LEU:H	1.59	0.49
1:A:61:LYS:NZ	1:B:186:GLY:O	2.44	0.49
1:A:132:VAL:HG23	1:A:161:HIS:HB2	1.95	0.49
1:A:70:PHE:HB3	1:A:74[A]:GLU:HB2	1.95	0.49
1:E:85:ARG:NH2	3:E:1205:SO4:O3	2.45	0.49
1:C:150:LEU:CD1	1:C:156[A]:ILE:CD1	2.84	0.48
1:E:118:GLN:HA	1:E:118:GLN:NE2	2.23	0.48
1:D:145:ILE:HG23	1:D:150:LEU:HB2	1.94	0.48
1:E:183:ILE:HD13	1:F:27:LYS:HD3	1.94	0.48
1:B:7:ILE:HD12	1:B:11:ILE:HD12	1.94	0.48
1:A:9[B]:ASN:O	1:A:13[B]:GLU:HB2	2.14	0.48
1:C:97:MSE:CE	1:C:109[B]:ASP:OD2	2.61	0.48
1:B:78[A]:ARG:HH11	1:B:81:ILE:HG13	1.79	0.48
1:B:141:ASN:HD22	1:B:141:ASN:C	2.17	0.48
1:E:51[B]:CYS:SG	1:E:93:ILE:CG2	2.98	0.48
1:C:175:THR:HG23	1:D:47:GLU:CD	2.33	0.48
1:F:118:GLN:HE21	1:F:118:GLN:HA	1.77	0.48
1:D:9[A]:ASN:O	1:D:13[A]:GLU:HB2	2.13	0.47
2:C:1003[B]:FMN:H9	2:C:1003[B]:FMN:C2'	2.43	0.47
1:E:34:LEU:CD1	1:F:181:MSE:HE1	2.44	0.47
2:C:1003[B]:FMN:O2P	4:C:1333:HOH:O	2.20	0.47
2:C:1003[A]:FMN:HM81	1:D:41:PRO:HB2	1.96	0.47
1:B:1:MSE:HE2	1:C:23[B]:LYS:HG3	1.96	0.47
1:C:41:PRO:HB2	2:D:1004:FMN:HM81	1.97	0.47
1:F:155[B]:ARG:CZ	1:F:156[B]:ILE:O	2.64	0.46
1:B:141:ASN:ND2	1:B:143:LEU:H	2.13	0.46
1:D:128:GLY:HA2	4:D:1342:HOH:O	2.15	0.46
1:C:70:PHE:HB3	1:C:74[B]:GLU:HB2	1.97	0.46
1:D:82[A]:LEU:HD22	3:D:1204:SO4:O4	2.16	0.46
1:D:71:THR:OG1	1:D:74[B]:GLU:HB2	2.15	0.46
1:E:177:ILE:O	1:E:181:MSE:HG2	2.15	0.46
1:D:34:LEU:O	1:D:38:THR:HG23	2.15	0.46
1:C:9:ASN:O	1:C:13:GLU:HB2	2.15	0.46
1:A:154:GLN:O	4:A:1115:HOH:O	2.21	0.46
1:C:118:GLN:HA	1:C:118:GLN:HE21	1.79	0.46
4:A:1022:HOH:O	1:B:178:THR:HB	2.16	0.46
1:B:135[A]:SER:CB	2:B:1002:FMN:H6	2.46	0.46
1:E:67:LEU:CD2	1:E:79:GLY:HA2	2.46	0.46
1:C:23[A]:LYS:HD3	1:C:164:TYR:CD1	2.51	0.45
1:A:7[A]:ILE:CG2	1:B:10:VAL:HG21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:ILE:HG21	1:F:10:VAL:HG21	1.99	0.45
1:B:45[B]:HIS:CD2	4:B:1261:HOH:O	2.68	0.45
1:B:145:ILE:HG23	1:B:150:LEU:HB2	1.98	0.45
1:B:23:LYS:NZ	1:C:1[B]:MSE:CG	2.74	0.45
1:C:183:ILE:HD13	1:D:27:LYS:HD3	1.98	0.45
1:E:135[A]:SER:OG	1:F:108:GLU:OE1	2.31	0.45
2:D:1004:FMN:C3'	4:D:1363:HOH:O	2.64	0.45
1:E:78:ARG:HG2	1:E:78:ARG:HH21	1.81	0.45
1:E:181:MSE:HB3	1:F:51[A]:CYS:HB2	1.99	0.45
1:F:148:ILE:HD11	1:F:150:LEU:HD22	1.99	0.45
1:A:16:SER:HB3	1:A:132:VAL:HG13	1.99	0.44
1:F:156[A]:ILE:O	1:F:156[A]:ILE:HG13	2.17	0.44
1:C:106:ARG:HD2	3:C:1207:SO4:O2	2.17	0.44
1:B:36:ASP:HB2	1:B:123:LEU:HD13	1.99	0.44
2:B:1002:FMN:O1P	2:B:1002:FMN:C4'	2.62	0.44
1:E:4:TYR:OH	4:E:1294:HOH:O	2.21	0.44
1:E:68[A]:ASN:OD1	1:E:75:ARG:NH2	2.51	0.44
1:A:81:ILE:HG12	4:A:1061:HOH:O	2.18	0.44
1:C:27:LYS:HD3	1:D:183:ILE:HD13	2.00	0.44
1:F:135:SER:HA	1:F:139:ASN:ND2	2.33	0.44
1:A:73[A]:GLU:HG3	1:A:74[A]:GLU:N	2.33	0.44
1:A:73[A]:GLU:HG3	1:A:74[A]:GLU:H	1.82	0.44
1:C:97:MSE:SE	1:C:109[B]:ASP:OD1	2.85	0.44
1:F:17:VAL:O	1:F:132:VAL:HG22	2.17	0.44
1:B:23:LYS:HD2	1:C:1[A]:MSE:CG	2.48	0.44
1:E:51[B]:CYS:O	1:F:181:MSE:HA	2.18	0.44
1:B:124:ALA:HB1	1:B:129:LEU:HB3	2.00	0.43
1:A:48:PRO:HB3	1:A:109[B]:ASP:HB2	1.99	0.43
1:E:34:LEU:O	1:E:38:THR:HG23	2.18	0.43
1:A:181:MSE:CE	1:B:51[B]:CYS:SG	2.86	0.43
1:C:48:PRO:HB2	1:C:109[B]:ASP:OD1	2.18	0.43
1:A:118:GLN:HA	1:A:118:GLN:NE2	2.33	0.43
1:A:51[B]:CYS:O	1:B:181:MSE:HA	2.19	0.43
1:A:182[B]:GLU:CG	1:B:52:LYS:HG2	2.49	0.43
1:C:23[A]:LYS:HD3	1:C:164:TYR:CG	2.54	0.43
1:C:8:ALA:O	1:C:12[A]:LYS:HG3	2.19	0.43
2:C:1003[A]:FMN:HM73	1:D:108:GLU:HA	1.99	0.43
1:C:97:MSE:SE	1:C:109[B]:ASP:CG	3.07	0.42
1:E:117:MSE:HE1	1:E:158:GLY:HA3	2.01	0.42
1:A:106:ARG:HG3	1:A:106:ARG:HH11	1.84	0.42
1:C:73:GLU:O	1:C:77[B]:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:LEU:O	1:F:38:THR:HG23	2.18	0.42
1:C:135[A]:SER:HB2	2:C:1003[A]:FMN:N5	2.34	0.42
1:F:58:GLY:O	1:F:61:LYS:HB2	2.20	0.42
1:F:62:LEU:HD13	1:F:86:PHE:CE2	2.55	0.42
1:A:5:THR:HA	4:A:1133:HOH:O	2.20	0.42
1:F:42:ASN:OD1	1:F:45:HIS:HA	2.19	0.42
1:A:7[B]:ILE:CD1	1:B:7:ILE:HB	2.46	0.41
1:A:184:ILE:O	1:B:58:GLY:HA3	2.19	0.41
1:A:43:HIS:CD2	2:B:1002:FMN:C4A	3.02	0.41
4:A:1125:HOH:O	1:B:7:ILE:CG2	2.58	0.41
1:D:106:ARG:NH1	4:D:1352:HOH:O	2.53	0.41
1:D:87:LEU:HA	1:D:87:LEU:HD12	1.79	0.41
1:E:1:MSE:HG2	4:F:1253:HOH:O	2.20	0.41
1:B:126:GLU:HG3	4:B:1359:HOH:O	2.19	0.41
1:B:23:LYS:HZ2	1:C:1[B]:MSE:CG	2.27	0.41
1:D:25:VAL:HG13	1:D:90:PRO:CB	2.50	0.41
1:A:7[A]:ILE:HG22	1:B:7:ILE:HG22	2.03	0.41
1:C:57[A]:GLU:HG3	1:D:186:GLY:HA3	2.01	0.41
1:B:1:MSE:HB2	1:B:2:THR:H	1.78	0.41
1:E:103:GLN:NE2	4:E:1207:HOH:O	2.42	0.41
2:C:1003[A]:FMN:HM71	1:D:111:ALA:CB	2.49	0.41
1:D:141:ASN:HD22	1:D:142:PRO:N	2.19	0.41
1:F:83:SER:O	1:F:87:LEU:HB2	2.21	0.41
1:A:62:LEU:HD13	1:A:86:PHE:HE2	1.85	0.41
1:C:16:SER:OG	2:C:1003[A]:FMN:O4'	2.35	0.41
1:F:90:PRO:HG2	1:F:163:GLY:HA3	2.03	0.41
1:C:18:ARG:NE	2:C:1003[A]:FMN:O2	2.41	0.41
1:D:83:SER:O	1:D:87:LEU:HB2	2.21	0.41
1:A:128:GLY:HA2	4:A:1108:HOH:O	2.20	0.40
1:E:47:GLU:OE1	1:F:175:THR:CG2	2.69	0.40
1:E:67:LEU:HD21	1:E:79:GLY:HA2	2.02	0.40
1:A:104:ILE:HG12	1:B:140:TYR:CE1	2.56	0.40
1:D:26[B]:GLU:HG3	1:D:29:LEU:H	1.86	0.40
2:D:1004:FMN:H3'	4:D:1363:HOH:O	2.21	0.40
1:F:175:THR:HA	1:F:176:PRO:HD3	1.91	0.40
1:D:16:SER:CB	2:D:1004:FMN:H5'1	2.52	0.40
1:F:161:HIS:C	1:F:162:ILE:HG13	2.42	0.40
1:C:17:VAL:HG11	1:C:165:PHE:HB3	2.03	0.40
1:B:1:MSE:CE	1:C:23[B]:LYS:CG	3.00	0.40
1:E:177:ILE:HD12	1:E:177:ILE:HA	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1096:HOH:O	4:D:1226:HOH:O[1_556]	2.03	0.17

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	206/189 (109%)	200 (97%)	6 (3%)	0	100	100
1	B	202/189 (107%)	196 (97%)	6 (3%)	0	100	100
1	C	204/189 (108%)	199 (98%)	5 (2%)	0	100	100
1	D	201/189 (106%)	196 (98%)	5 (2%)	0	100	100
1	E	199/189 (105%)	195 (98%)	4 (2%)	0	100	100
1	F	200/189 (106%)	197 (98%)	3 (2%)	0	100	100
All	All	1212/1134 (107%)	1183 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	180/157 (115%)	162 (90%)	18 (10%)	7	9
1	B	176/157 (112%)	157 (89%)	19 (11%)	6	7
1	C	178/157 (113%)	164 (92%)	14 (8%)	12	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	175/157 (112%)	157 (90%)	18 (10%)	7 8
1	E	175/157 (112%)	168 (96%)	7 (4%)	31 44
1	F	174/157 (111%)	153 (88%)	21 (12%)	5 5
All	All	1058/942 (112%)	961 (91%)	97 (9%)	10 11

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3[A]	THR
1	A	3[B]	THR
1	A	7[A]	ILE
1	A	7[B]	ILE
1	A	22[A]	ASP
1	A	22[B]	ASP
1	A	42	ASN
1	A	52	LYS
1	A	57	GLU
1	A	62	LEU
1	A	87	LEU
1	A	132	VAL
1	A	134	LYS
1	A	146	GLU
1	A	167[A]	LYS
1	A	167[B]	LYS
1	A	172	LYS
1	B	1	MSE
1	B	22[A]	ASP
1	B	22[B]	ASP
1	B	62	LEU
1	B	75	ARG
1	B	77	LYS
1	B	78[A]	ARG
1	B	78[B]	ARG
1	B	80	LYS
1	B	81	ILE
1	B	83[A]	SER
1	B	83[B]	SER
1	B	87	LEU
1	B	118	GLN
1	B	134	LYS

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Mol	Chain	Res	Type
1	B	141	ASN
1	B	167	LYS
1	B	178	THR
1	B	180	LYS
1	C	7	ILE
1	C	30	LEU
1	C	42	ASN
1	C	74[A]	GLU
1	C	74[B]	GLU
1	C	87	LEU
1	C	131	CYS
1	C	146[A]	GLU
1	C	146[B]	GLU
1	C	152	ARG
1	C	167[A]	LYS
1	C	167[B]	LYS
1	C	170	GLU
1	C	175	THR
1	D	2	THR
1	D	25	VAL
1	D	29	LEU
1	D	30	LEU
1	D	42	ASN
1	D	59	ARG
1	D	62	LEU
1	D	75	ARG
1	D	87	LEU
1	D	141	ASN
1	D	142	PRO
1	D	146[A]	GLU
1	D	146[B]	GLU
1	D	152[A]	ARG
1	D	152[B]	ARG
1	D	155	ARG
1	D	167	LYS
1	D	185	GLU
1	E	62	LEU
1	E	64	ASP
1	E	78	ARG
1	E	82	LEU
1	E	118	GLN
1	E	134	LYS

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Mol	Chain	Res	Type
1	E	141	ASN
1	F	3	THR
1	F	7	ILE
1	F	12[A]	LYS
1	F	12[B]	LYS
1	F	19	THR
1	F	22[A]	ASP
1	F	22[B]	ASP
1	F	42	ASN
1	F	62	LEU
1	F	71	THR
1	F	87	LEU
1	F	89	THR
1	F	105	GLN
1	F	132	VAL
1	F	150	LEU
1	F	156[A]	ILE
1	F	156[B]	ILE
1	F	166	ASP
1	F	167	LYS
1	F	175	THR
1	F	180	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	118	GLN
1	B	118	GLN
1	B	121	GLN
1	B	141	ASN
1	C	45	HIS
1	C	118	GLN
1	C	119	ASN
1	C	121	GLN
1	D	103	GLN
1	D	118	GLN
1	D	119	ASN
1	D	121	GLN
1	D	141	ASN
1	E	118	GLN
1	E	121	GLN

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Mol	Chain	Res	Type
1	E	141	ASN
1	F	103	GLN
1	F	118	GLN
1	F	121	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	B	1002	-	33,33,33	1.22	2 (6%)	48,50,50	1.65	10 (20%)
3	SO4	B	1201	-	4,4,4	0.26	0	6,6,6	0.18	0
3	SO4	C	1207	-	4,4,4	0.30	0	6,6,6	0.18	0
3	SO4	D	1204	-	4,4,4	0.45	0	6,6,6	0.58	0
3	SO4	E	1205	-	4,4,4	0.26	0	6,6,6	0.61	0
2	FMN	A	1001	-	33,33,33	1.26	2 (6%)	48,50,50	1.73	13 (27%)
2	FMN	C	1003[A]	-	33,33,33	1.22	3 (9%)	48,50,50	1.46	10 (20%)
2	FMN	D	1004	-	33,33,33	1.30	3 (9%)	48,50,50	1.79	16 (33%)
3	SO4	C	1203	-	4,4,4	0.34	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	F	1206	-	4,4,4	0.30	0	6,6,6	0.37	0
3	SO4	B	1202	-	4,4,4	0.23	0	6,6,6	0.17	0
2	FMN	C	1003[B]	-	33,33,33	1.25	3 (9%)	48,50,50	1.67	13 (27%)

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	B	1002	-	-	7/18/18/18	0/2/3/3
2	FMN	A	1001	-	-	8/18/18/18	0/3/3/3
2	FMN	C	1003[A]	-	-	10/18/18/18	0/3/3/3
2	FMN	D	1004	-	-	9/18/18/18	0/3/3/3
2	FMN	C	1003[B]	-	-	11/18/18/18	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1004	FMN	C4A-N5	4.19	1.39	1.30
2	A	1001	FMN	C4A-N5	3.78	1.38	1.30
2	C	1003[A]	FMN	C4A-N5	3.72	1.38	1.30
2	B	1002	FMN	C4A-N5	3.61	1.38	1.30
2	C	1003[B]	FMN	C4A-N5	3.50	1.38	1.30
2	B	1002	FMN	C10-N1	3.38	1.40	1.33
2	C	1003[B]	FMN	C10-N1	3.15	1.39	1.33
2	C	1003[A]	FMN	C10-N1	2.95	1.39	1.33
2	D	1004	FMN	C10-N1	2.60	1.38	1.33
2	A	1001	FMN	C10-N1	2.49	1.38	1.33
2	D	1004	FMN	C9-C8	2.18	1.42	1.39
2	C	1003[A]	FMN	C10-N10	2.04	1.41	1.37
2	C	1003[B]	FMN	C1'-N10	2.02	1.52	1.47

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1002	FMN	C7M-C7-C6	-4.66	111.35	119.57
2	A	1001	FMN	C4-N3-C2	-3.98	118.57	125.64
2	D	1004	FMN	O2P-P-O5'	3.62	116.11	106.67
2	C	1003[B]	FMN	C4-N3-C2	-3.57	119.31	125.64
2	C	1003[B]	FMN	C4A-C10-N10	3.54	121.55	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	FMN	O4-C4-C4A	-3.51	117.27	126.53
2	C	1003[A]	FMN	C7M-C7-C6	-3.46	113.47	119.57
2	C	1003[A]	FMN	C4-N3-C2	-3.46	119.49	125.64
2	A	1001	FMN	C1'-C2'-C3'	3.42	118.93	109.66
2	B	1002	FMN	C1'-N10-C9A	-3.41	114.00	120.63
2	D	1004	FMN	C4A-C10-N10	3.39	121.33	116.48
2	B	1002	FMN	C4-N3-C2	-3.32	119.74	125.64
2	A	1001	FMN	C4A-C10-N10	3.14	120.97	116.48
2	D	1004	FMN	C10-C4A-N5	-3.04	118.61	124.81
2	A	1001	FMN	C4A-C4-N3	3.02	120.94	113.25
2	D	1004	FMN	O5'-C5'-C4'	3.01	117.40	109.36
2	B	1002	FMN	C4A-C10-N10	2.99	120.76	116.48
2	D	1004	FMN	C4'-C3'-C2'	2.94	118.46	113.57
2	C	1003[B]	FMN	C1'-C2'-C3'	2.93	117.59	109.66
2	D	1004	FMN	C1'-C2'-C3'	2.90	117.53	109.66
2	C	1003[B]	FMN	C4A-C4-N3	2.83	120.47	113.25
2	B	1002	FMN	C4A-C10-N1	-2.83	117.65	124.59
2	A	1001	FMN	C4A-C10-N1	-2.83	117.66	124.59
2	C	1003[A]	FMN	C4A-C10-N1	-2.82	117.67	124.59
2	C	1003[A]	FMN	C4A-C10-N10	2.81	120.50	116.48
2	C	1003[B]	FMN	C4A-C10-N1	-2.77	117.80	124.59
2	B	1002	FMN	C4A-C4-N3	2.76	120.27	113.25
2	C	1003[A]	FMN	C4A-C4-N3	2.75	120.25	113.25
2	C	1003[A]	FMN	C10-C4A-N5	-2.73	119.23	124.81
2	D	1004	FMN	O4-C4-C4A	-2.70	119.40	126.53
2	A	1001	FMN	O3'-C3'-C2'	2.69	115.05	108.93
2	D	1004	FMN	C10-N1-C2	2.68	122.65	116.85
2	A	1001	FMN	O3P-P-O5'	2.68	113.66	106.67
2	C	1003[B]	FMN	O2P-P-O5'	2.59	113.42	106.67
2	C	1003[B]	FMN	C10-C4A-N5	-2.58	119.55	124.81
2	B	1002	FMN	C10-C4A-N5	-2.56	119.59	124.81
2	B	1002	FMN	O4-C4-C4A	-2.55	119.80	126.53
2	C	1003[B]	FMN	O4-C4-C4A	-2.48	119.98	126.53
2	C	1003[B]	FMN	C2'-C1'-N10	2.47	121.89	110.20
2	D	1004	FMN	O4'-C4'-C3'	-2.47	103.47	109.25
2	A	1001	FMN	C10-N1-C2	2.38	122.00	116.85
2	D	1004	FMN	C4-N3-C2	-2.38	121.42	125.64
2	C	1003[A]	FMN	C4'-C3'-C2'	2.34	117.47	113.57
2	D	1004	FMN	O2-C2-N3	2.28	122.97	118.58
2	B	1002	FMN	C4-C4A-C10	2.27	120.83	116.93
2	A	1001	FMN	C9-C9A-N10	2.27	124.91	121.85
2	D	1004	FMN	C4A-C10-N1	-2.26	119.05	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1004	FMN	C9-C9A-N10	2.26	124.89	121.85
2	A	1001	FMN	C10-C4A-N5	-2.26	120.20	124.81
2	A	1001	FMN	C4-C4A-C10	2.25	120.79	116.93
2	D	1004	FMN	C4-C4A-C10	2.22	120.73	116.93
2	C	1003[B]	FMN	O5'-C5'-C4'	2.19	115.22	109.36
2	C	1003[A]	FMN	C4-C4A-C10	2.19	120.69	116.93
2	A	1001	FMN	C5'-C4'-C3'	-2.19	108.09	112.22
2	C	1003[B]	FMN	C4-C4A-C10	2.18	120.67	116.93
2	C	1003[B]	FMN	C10-N1-C2	2.15	121.50	116.85
2	C	1003[A]	FMN	C10-N1-C2	2.12	121.44	116.85
2	C	1003[A]	FMN	C1'-C2'-C3'	2.11	115.37	109.66
2	B	1002	FMN	C10-N1-C2	2.07	121.34	116.85
2	C	1003[B]	FMN	C9A-N10-C10	-2.05	117.62	120.75
2	D	1004	FMN	O3'-C3'-C4'	2.03	113.54	108.93
2	D	1004	FMN	C7M-C7-C6	-2.00	116.05	119.57

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	FMN	C1'-C2'-C3'-O3'
2	A	1001	FMN	C1'-C2'-C3'-C4'
2	A	1001	FMN	O2'-C2'-C3'-O3'
2	A	1001	FMN	C3'-C4'-C5'-O5'
2	A	1001	FMN	O4'-C4'-C5'-O5'
2	A	1001	FMN	C4'-C5'-O5'-P
2	B	1002	FMN	C2'-C1'-N10-C10
2	B	1002	FMN	C2'-C3'-C4'-O4'
2	B	1002	FMN	C2'-C3'-C4'-C5'
2	B	1002	FMN	O3'-C3'-C4'-O4'
2	B	1002	FMN	O3'-C3'-C4'-C5'
2	B	1002	FMN	C4'-C5'-O5'-P
2	B	1002	FMN	C5'-O5'-P-O2P
2	C	1003[A]	FMN	N10-C1'-C2'-O2'
2	C	1003[A]	FMN	C1'-C2'-C3'-C4'
2	C	1003[A]	FMN	C3'-C4'-C5'-O5'
2	C	1003[A]	FMN	O4'-C4'-C5'-O5'
2	C	1003[A]	FMN	C5'-O5'-P-O2P
2	C	1003[A]	FMN	C5'-O5'-P-O3P
2	C	1003[B]	FMN	C2'-C1'-N10-C10
2	C	1003[B]	FMN	C2'-C3'-C4'-C5'
2	C	1003[B]	FMN	O3'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
2	C	1003[B]	FMN	C5'-O5'-P-O1P
2	D	1004	FMN	C1'-C2'-C3'-O3'
2	D	1004	FMN	C3'-C4'-C5'-O5'
2	D	1004	FMN	O4'-C4'-C5'-O5'
2	D	1004	FMN	C5'-O5'-P-O1P
2	D	1004	FMN	C5'-O5'-P-O2P
2	D	1004	FMN	C5'-O5'-P-O3P
2	C	1003[B]	FMN	O3'-C3'-C4'-C5'
2	D	1004	FMN	C4'-C5'-O5'-P
2	A	1001	FMN	O2'-C2'-C3'-C4'
2	C	1003[B]	FMN	C2'-C3'-C4'-O4'
2	D	1004	FMN	C2'-C3'-C4'-C5'
2	D	1004	FMN	C2'-C3'-C4'-O4'
2	C	1003[B]	FMN	C2'-C1'-N10-C9A
2	C	1003[A]	FMN	C5'-O5'-P-O1P
2	C	1003[B]	FMN	C4'-C5'-O5'-P
2	C	1003[A]	FMN	O2'-C2'-C3'-C4'
2	C	1003[B]	FMN	C3'-C4'-C5'-O5'
2	C	1003[A]	FMN	C4'-C5'-O5'-P
2	C	1003[A]	FMN	O2'-C2'-C3'-O3'
2	A	1001	FMN	C5'-O5'-P-O3P
2	C	1003[B]	FMN	C5'-O5'-P-O2P
2	C	1003[B]	FMN	C5'-O5'-P-O3P

There are no ring outliers.

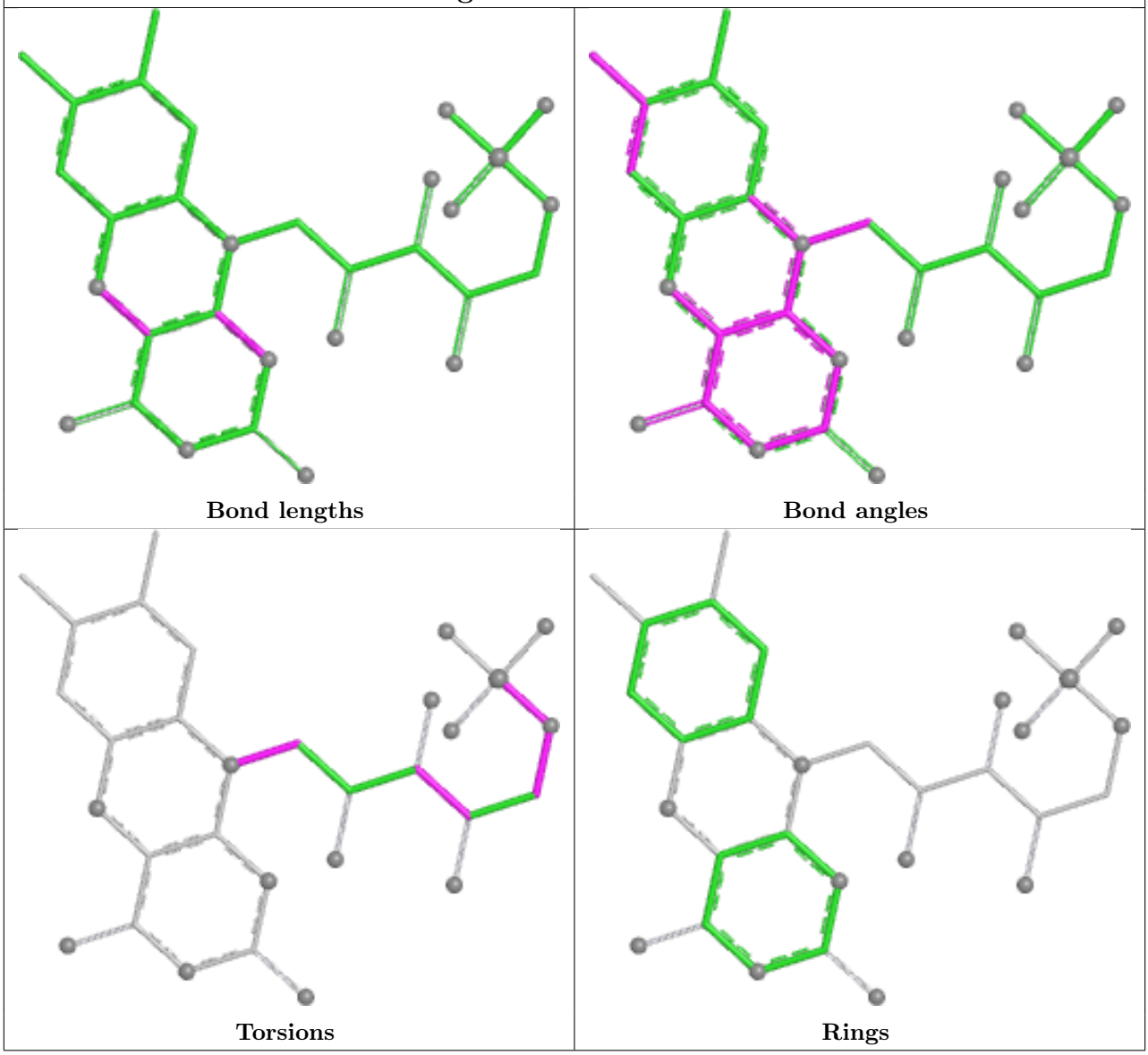
9 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	FMN	6	0
3	B	1201	SO4	1	0
3	C	1207	SO4	2	0
3	D	1204	SO4	1	0
3	E	1205	SO4	2	0
2	A	1001	FMN	4	0
2	C	1003[A]	FMN	12	0
2	D	1004	FMN	9	0
2	C	1003[B]	FMN	16	0

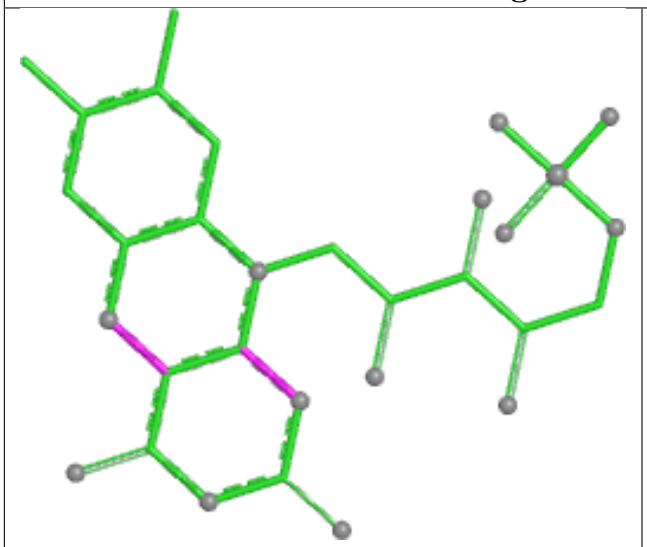
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

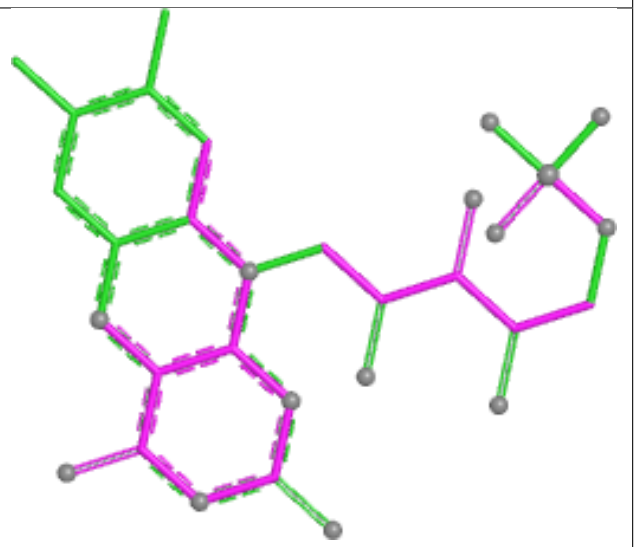
Ligand FMN B 1002



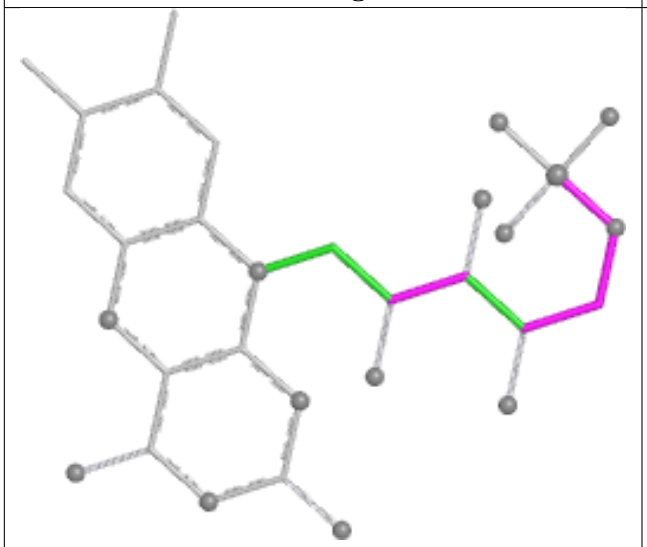
Ligand FMN A 1001



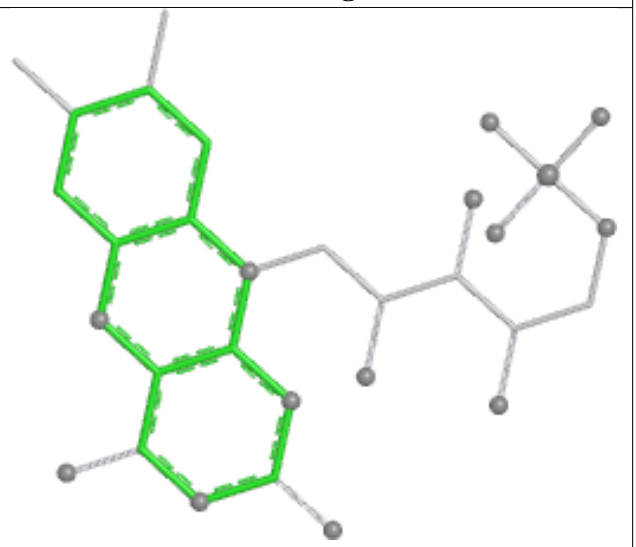
Bond lengths



Bond angles

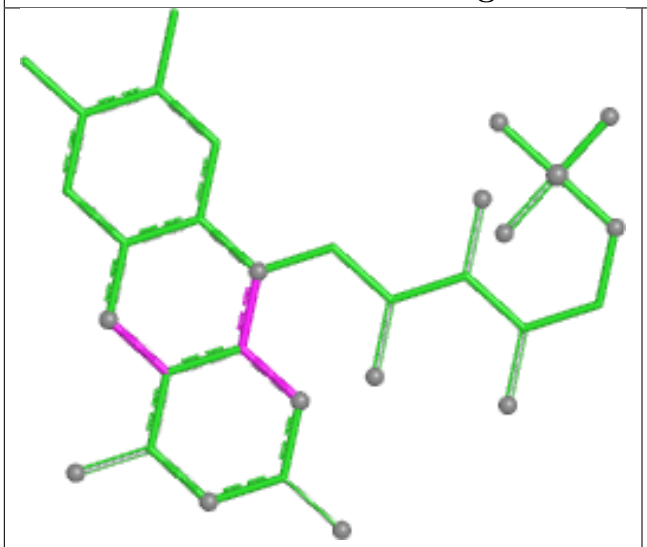


Torsions

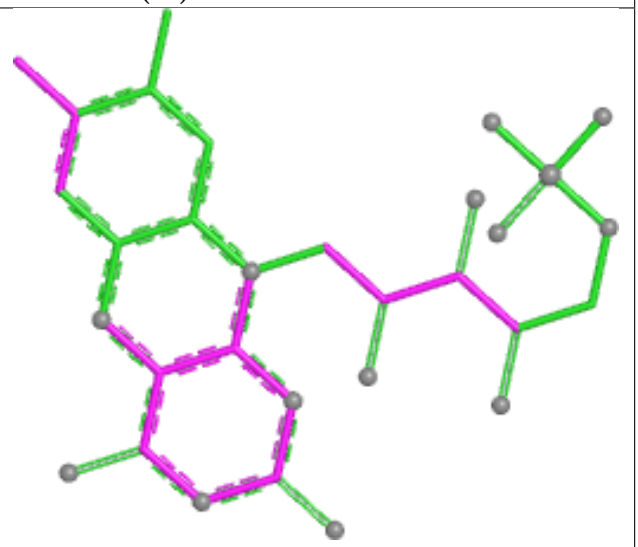


Rings

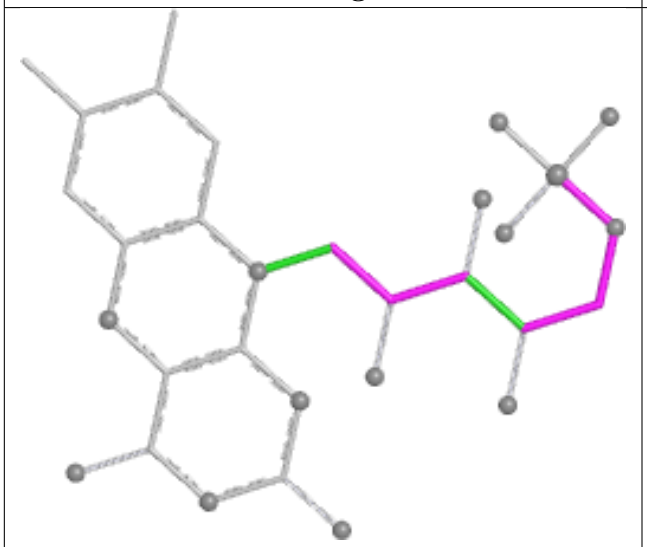
Ligand FMN C 1003 (A)



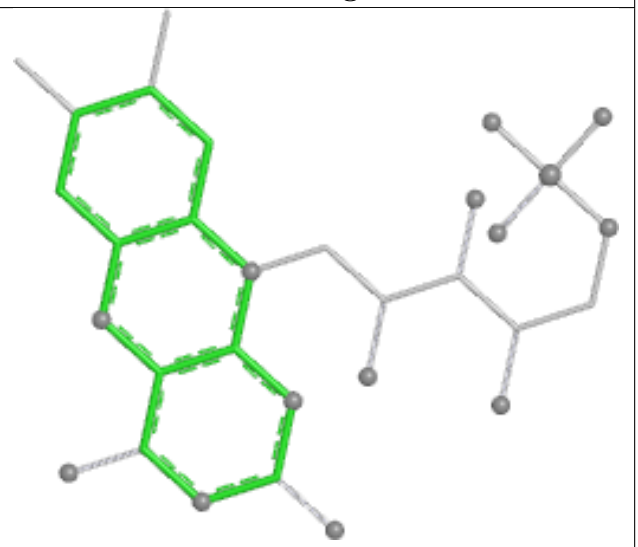
Bond lengths



Bond angles

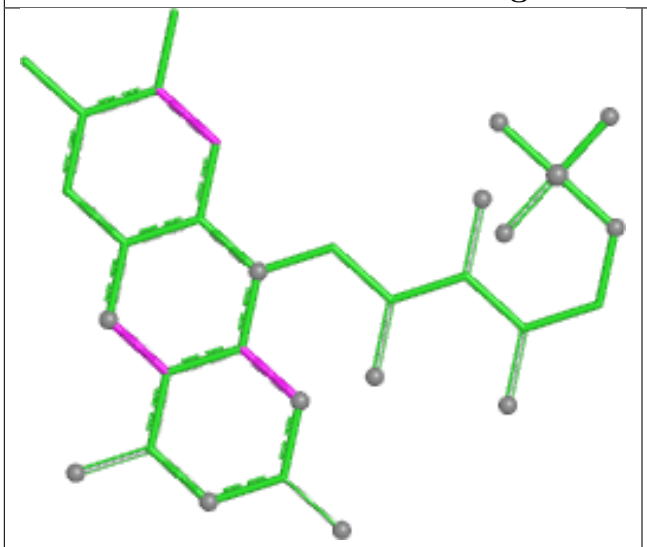


Torsions

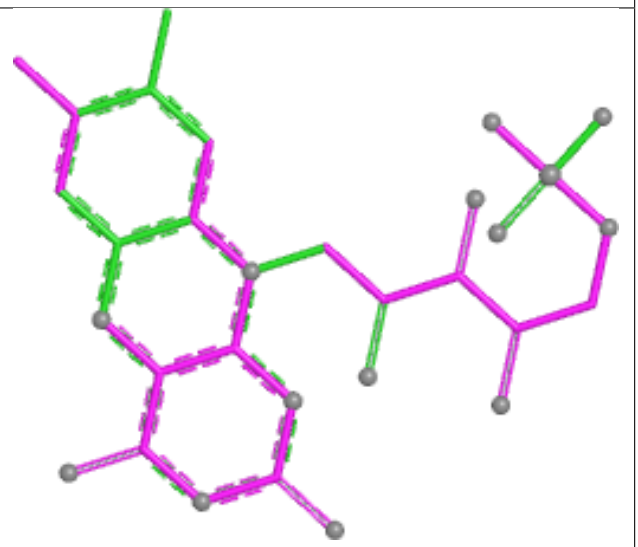


Rings

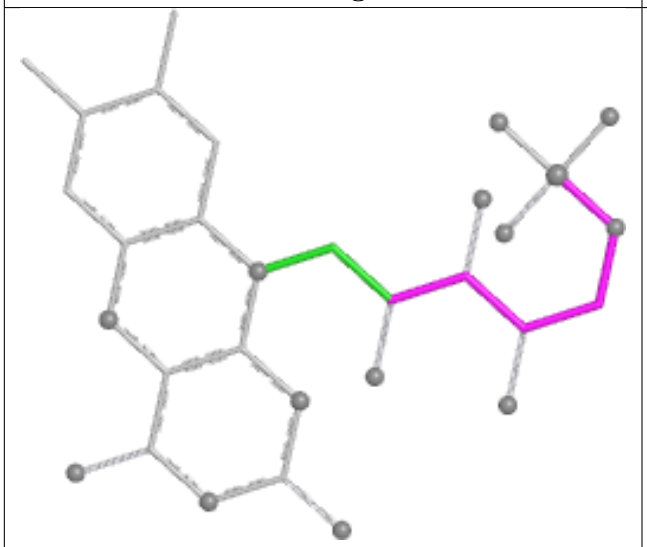
Ligand FMN D 1004



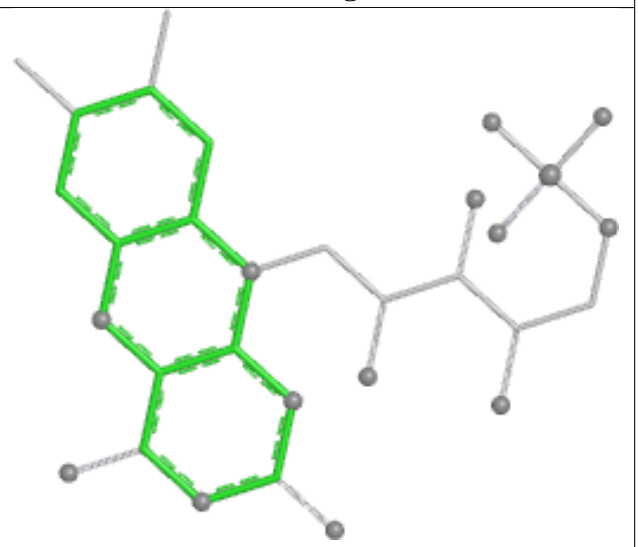
Bond lengths



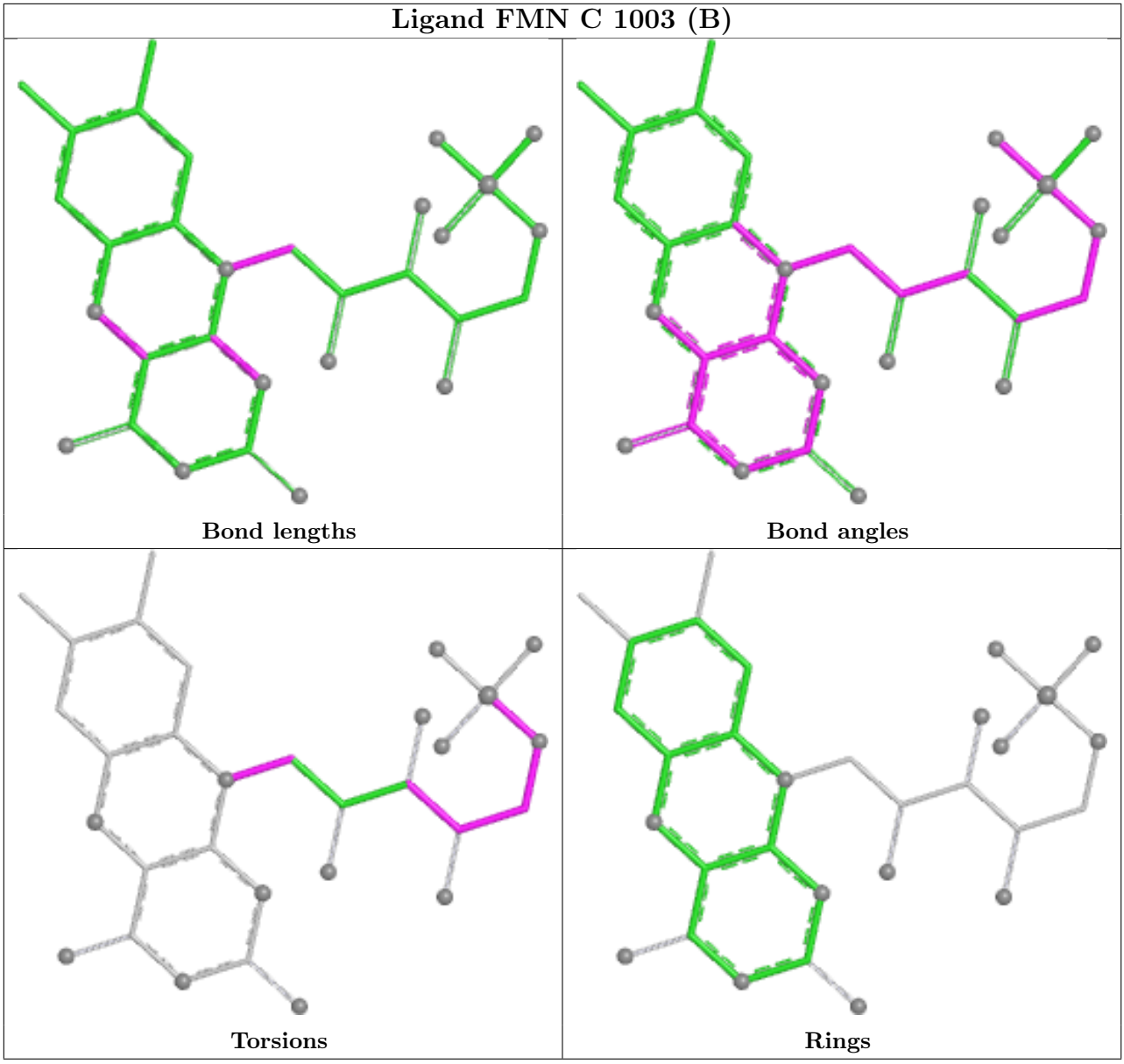
Bond angles



Torsions



Rings



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	183/189 (96%)	0.72	19 (10%)	6	9	32, 43, 53, 57	0
1	B	183/189 (96%)	0.71	18 (9%)	7	10	32, 41, 57, 65	0
1	C	183/189 (96%)	0.63	9 (4%)	29	36	29, 39, 53, 66	0
1	D	183/189 (96%)	0.60	12 (6%)	18	23	31, 40, 51, 59	0
1	E	181/189 (95%)	0.72	15 (8%)	11	15	39, 48, 59, 68	0
1	F	183/189 (96%)	0.96	28 (15%)	2	3	39, 49, 62, 73	0
All	All	1096/1134 (96%)	0.72	101 (9%)	9	12	29, 43, 58, 73	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	186	GLY	6.0
1	C	186	GLY	5.7
1	B	76	ALA	5.6
1	A	186	GLY	5.3
1	D	186	GLY	4.8
1	C	22	ASP	4.6
1	D	0	ALA	4.5
1	E	57	GLU	4.5
1	B	0	ALA	4.2
1	F	167	LYS	4.2
1	A	73[A]	GLU	4.2
1	F	168	ALA	4.1
1	C	0	ALA	4.0
1	F	20	PHE	3.8
1	F	166	ASP	3.8
1	C	77[A]	LYS	3.7
1	B	170	GLU	3.7
1	B	77	LYS	3.6
1	E	84	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	73	GLU	3.5
1	E	43[A]	HIS	3.4
1	B	57[A]	GLU	3.4
1	F	80	LYS	3.4
1	F	22[A]	ASP	3.3
1	F	55	ILE	3.3
1	E	80	LYS	3.2
1	E	22	ASP	3.2
1	B	186	GLY	3.2
1	D	157	VAL	3.1
1	F	84	ASP	3.1
1	A	22[A]	ASP	3.1
1	E	183	ILE	3.1
1	D	77[A]	LYS	3.0
1	E	87	LEU	3.0
1	A	87	LEU	3.0
1	E	81	ILE	3.0
1	C	110	TYR	2.9
1	E	21	THR	2.9
1	F	182[A]	GLU	2.9
1	D	166	ASP	2.9
1	B	81	ILE	2.8
1	A	77	LYS	2.8
1	A	166	ASP	2.8
1	A	19[A]	THR	2.8
1	F	56	GLY	2.8
1	F	21	THR	2.8
1	B	115	ALA	2.7
1	B	114	CYS	2.7
1	B	111	ALA	2.6
1	A	80	LYS	2.6
1	F	170	GLU	2.6
1	D	110	TYR	2.6
1	B	78[A]	ARG	2.6
1	F	24	ALA	2.6
1	A	167[A]	LYS	2.6
1	F	81	ILE	2.6
1	A	45	HIS	2.5
1	F	155[A]	ARG	2.5
1	D	78[A]	ARG	2.5
1	B	110	TYR	2.5
1	A	64[A]	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	57[A]	GLU	2.4
1	A	109[A]	ASP	2.4
1	F	43[A]	HIS	2.4
1	A	57	GLU	2.3
1	C	157	VAL	2.3
1	E	20	PHE	2.3
1	B	112	ALA	2.3
1	B	28[A]	ASP	2.3
1	F	77	LYS	2.3
1	A	79	GLY	2.3
1	B	74[A]	GLU	2.3
1	D	73[A]	GLU	2.3
1	B	172[A]	LYS	2.3
1	A	115	ALA	2.3
1	A	114	CYS	2.3
1	A	110	TYR	2.2
1	A	28	ASP	2.2
1	C	73	GLU	2.2
1	E	55	ILE	2.2
1	F	163	GLY	2.2
1	F	88	SER	2.2
1	C	109[A]	ASP	2.2
1	E	184	ILE	2.2
1	F	57[A]	GLU	2.2
1	F	73	GLU	2.2
1	E	77	LYS	2.2
1	F	87	LEU	2.2
1	F	111	ALA	2.1
1	D	179	GLU	2.1
1	E	59	ARG	2.1
1	B	185	GLU	2.1
1	D	71	THR	2.1
1	A	182[A]	GLU	2.1
1	E	182	GLU	2.1
1	D	74[A]	GLU	2.1
1	F	176	PRO	2.1
1	F	76	ALA	2.0
1	F	179	GLU	2.0
1	F	83	SER	2.0
1	D	152[A]	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

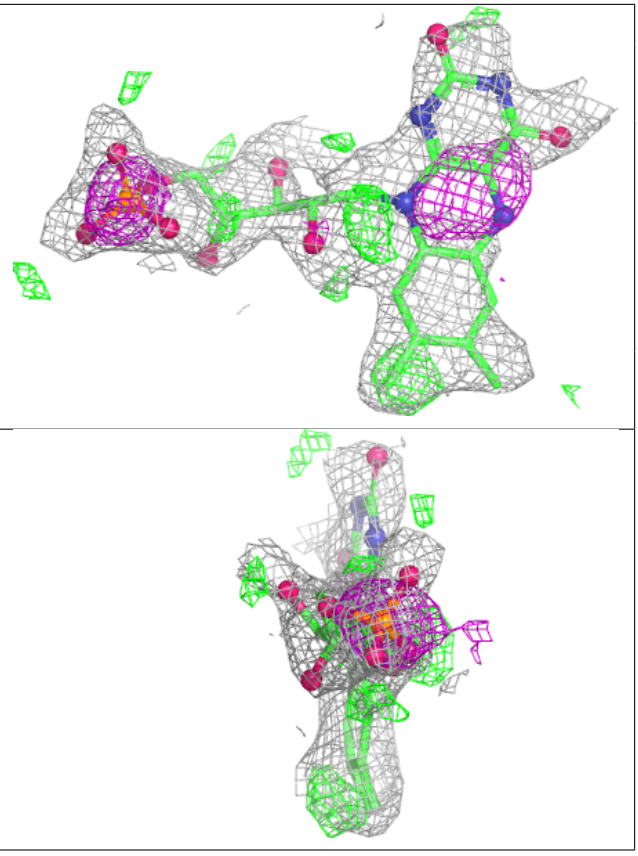
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FMN	B	1002	31/31	0.67	0.36	49,54,57,59	31
2	FMN	C	1003[A]	31/31	0.71	0.37	38,45,49,49	31
2	FMN	C	1003[B]	31/31	0.71	0.37	27,46,47,47	31
3	SO4	F	1206	5/5	0.73	0.33	93,93,93,95	0
3	SO4	D	1204	5/5	0.78	0.29	49,52,54,58	5
3	SO4	E	1205	5/5	0.80	0.33	53,55,56,59	5
3	SO4	C	1203	5/5	0.82	0.27	71,72,74,75	5
3	SO4	B	1202	5/5	0.83	0.27	82,84,84,85	5
3	SO4	C	1207	5/5	0.86	0.46	67,68,69,70	5
2	FMN	A	1001	31/31	0.86	0.23	34,39,42,44	31
2	FMN	D	1004	31/31	0.88	0.18	38,42,44,48	31
3	SO4	B	1201	5/5	0.90	0.23	82,82,84,84	5

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

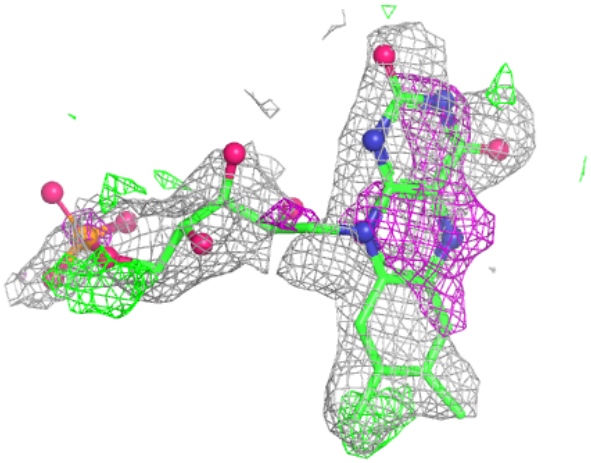
Electron density around FMN B 1002:

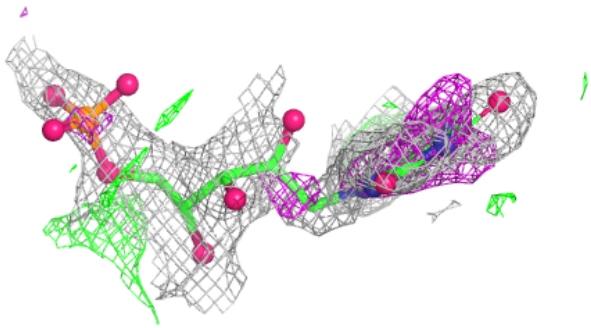
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

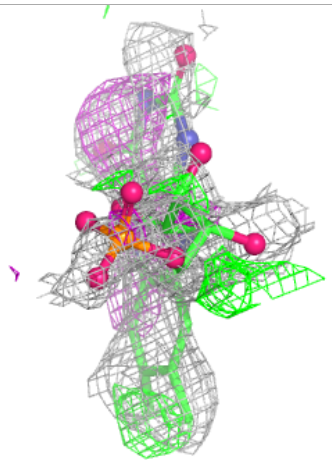


Electron density around FMN C 1003 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

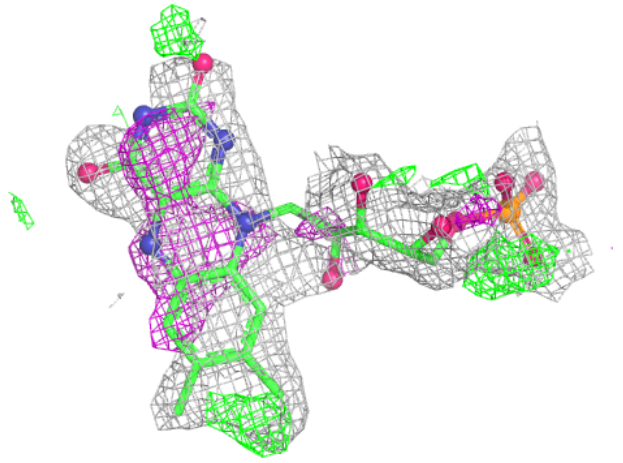


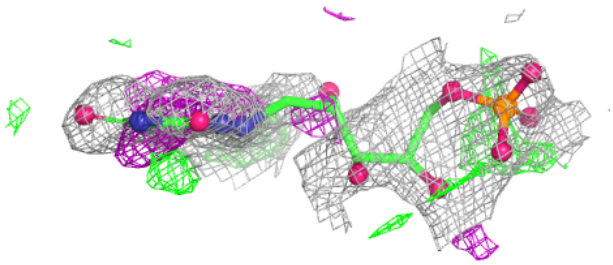


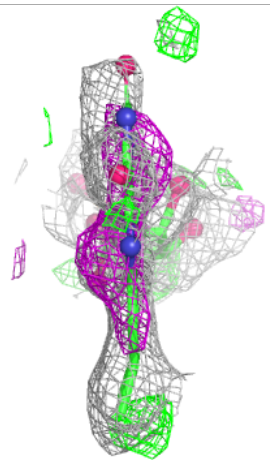


Electron density around FMN C 1003 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

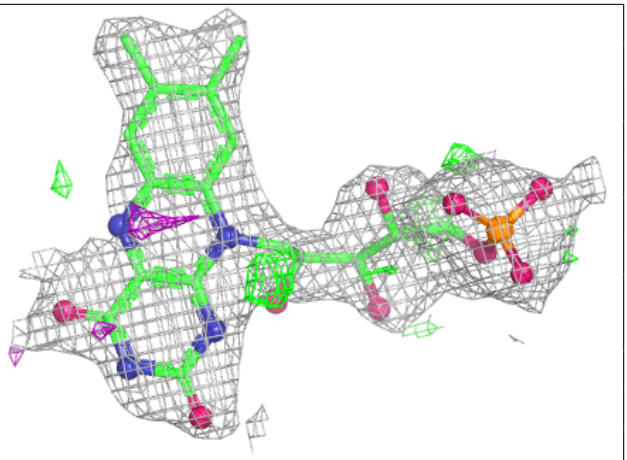


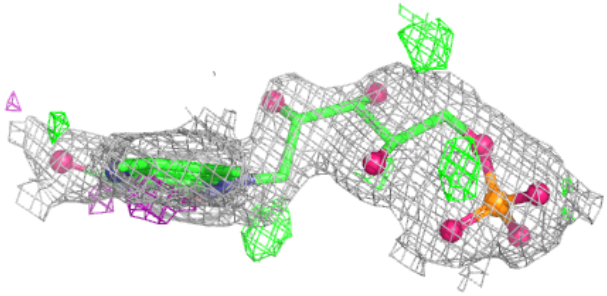


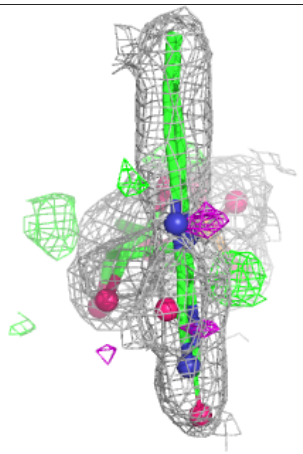


Electron density around FMN A 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

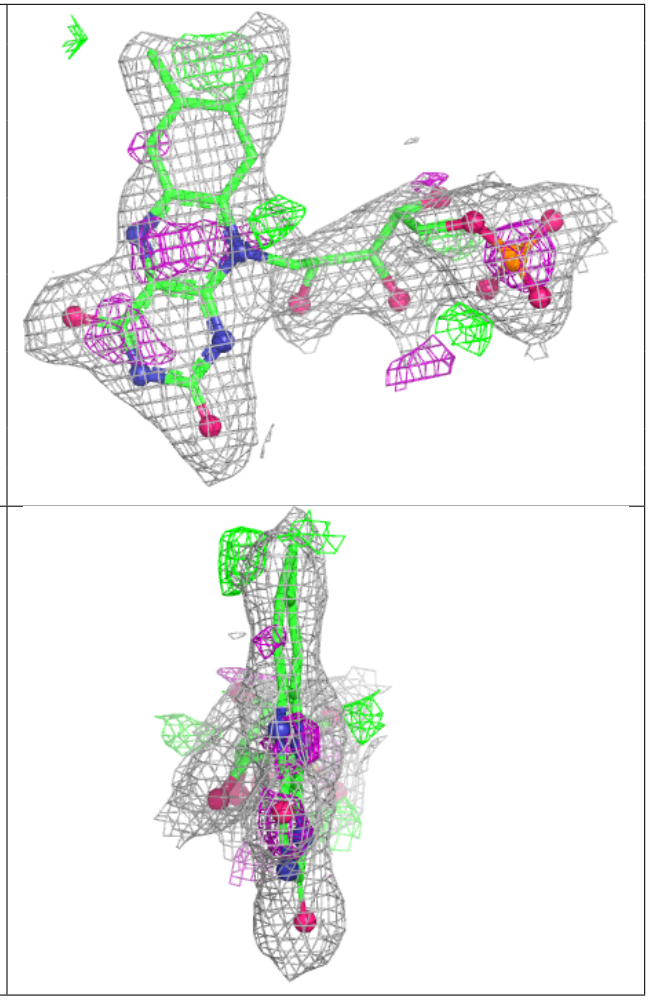






Electron density around FMN D 1004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.