



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:15 PM UTC

PDB ID : 1T57 / pdb_00001t57
Title : Crystal Structure of the Conserved Protein MTH1675 from Methanobacterium thermoautotrophicum
Authors : Kim, Y.; Joachimiak, A.; Saridakis, V.; Xu, X.; Arrowsmith, C.H.; Christendat, D.; Edwards, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2004-05-03
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

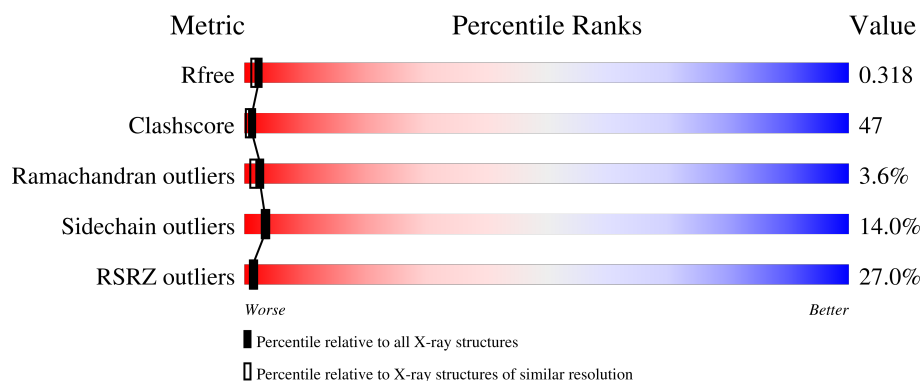
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	206	
1	B	206	
1	C	206	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4441 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 Conserved Protein MTH1675.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	Se	0	0	0
			1406	879	247	271	2	7			
1	B	186	Total	C	N	O	S	Se	0	0	0
			1406	879	247	271	2	7			
1	C	186	Total	C	N	O	S	Se	0	0	0
			1406	879	247	271	2	7			

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	cloning artifact	UNP O27711
A	-18	GLY	-	cloning artifact	UNP O27711
A	-17	SER	-	cloning artifact	UNP O27711
A	-16	SER	-	cloning artifact	UNP O27711
A	-15	HIS	-	cloning artifact	UNP O27711
A	-14	HIS	-	cloning artifact	UNP O27711
A	-13	HIS	-	cloning artifact	UNP O27711
A	-12	HIS	-	cloning artifact	UNP O27711
A	-11	HIS	-	cloning artifact	UNP O27711
A	-10	HIS	-	cloning artifact	UNP O27711
A	-9	SER	-	cloning artifact	UNP O27711
A	-8	SER	-	cloning artifact	UNP O27711
A	-7	GLY	-	cloning artifact	UNP O27711
A	-6	LEU	-	cloning artifact	UNP O27711
A	-5	VAL	-	cloning artifact	UNP O27711
A	-4	PRO	-	cloning artifact	UNP O27711
A	-3	ARG	-	cloning artifact	UNP O27711
A	-2	GLY	-	cloning artifact	UNP O27711
A	-1	SER	-	cloning artifact	UNP O27711
A	0	HIS	-	cloning artifact	UNP O27711
A	1	MSE	MET	modified residue	UNP O27711
A	51	MSE	MET	modified residue	UNP O27711
A	115	MSE	MET	modified residue	UNP O27711

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Chain	Residue	Modelled	Actual	Comment	Reference
A	121	MSE	MET	modified residue	UNP O27711
A	135	MSE	MET	modified residue	UNP O27711
A	169	MSE	MET	modified residue	UNP O27711
A	183	MSE	MET	modified residue	UNP O27711
B	-19	MSE	-	cloning artifact	UNP O27711
B	-18	GLY	-	cloning artifact	UNP O27711
B	-17	SER	-	cloning artifact	UNP O27711
B	-16	SER	-	cloning artifact	UNP O27711
B	-15	HIS	-	cloning artifact	UNP O27711
B	-14	HIS	-	cloning artifact	UNP O27711
B	-13	HIS	-	cloning artifact	UNP O27711
B	-12	HIS	-	cloning artifact	UNP O27711
B	-11	HIS	-	cloning artifact	UNP O27711
B	-10	HIS	-	cloning artifact	UNP O27711
B	-9	SER	-	cloning artifact	UNP O27711
B	-8	SER	-	cloning artifact	UNP O27711
B	-7	GLY	-	cloning artifact	UNP O27711
B	-6	LEU	-	cloning artifact	UNP O27711
B	-5	VAL	-	cloning artifact	UNP O27711
B	-4	PRO	-	cloning artifact	UNP O27711
B	-3	ARG	-	cloning artifact	UNP O27711
B	-2	GLY	-	cloning artifact	UNP O27711
B	-1	SER	-	cloning artifact	UNP O27711
B	0	HIS	-	cloning artifact	UNP O27711
B	1	MSE	MET	modified residue	UNP O27711
B	51	MSE	MET	modified residue	UNP O27711
B	115	MSE	MET	modified residue	UNP O27711
B	121	MSE	MET	modified residue	UNP O27711
B	135	MSE	MET	modified residue	UNP O27711
B	169	MSE	MET	modified residue	UNP O27711
B	183	MSE	MET	modified residue	UNP O27711
C	-19	MSE	-	cloning artifact	UNP O27711
C	-18	GLY	-	cloning artifact	UNP O27711
C	-17	SER	-	cloning artifact	UNP O27711
C	-16	SER	-	cloning artifact	UNP O27711
C	-15	HIS	-	cloning artifact	UNP O27711
C	-14	HIS	-	cloning artifact	UNP O27711
C	-13	HIS	-	cloning artifact	UNP O27711
C	-12	HIS	-	cloning artifact	UNP O27711
C	-11	HIS	-	cloning artifact	UNP O27711
C	-10	HIS	-	cloning artifact	UNP O27711
C	-9	SER	-	cloning artifact	UNP O27711

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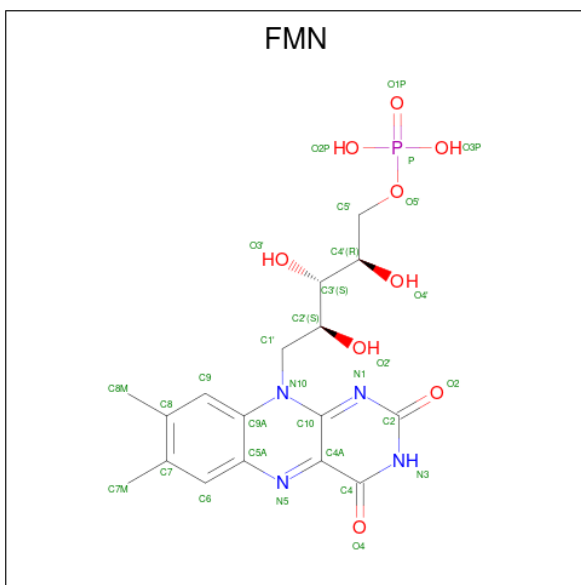
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	cloning artifact	UNP O27711
C	-7	GLY	-	cloning artifact	UNP O27711
C	-6	LEU	-	cloning artifact	UNP O27711
C	-5	VAL	-	cloning artifact	UNP O27711
C	-4	PRO	-	cloning artifact	UNP O27711
C	-3	ARG	-	cloning artifact	UNP O27711
C	-2	GLY	-	cloning artifact	UNP O27711
C	-1	SER	-	cloning artifact	UNP O27711
C	0	HIS	-	cloning artifact	UNP O27711
C	1	MSE	MET	modified residue	UNP O27711
C	51	MSE	MET	modified residue	UNP O27711
C	115	MSE	MET	modified residue	UNP O27711
C	121	MSE	MET	modified residue	UNP O27711
C	135	MSE	MET	modified residue	UNP O27711
C	169	MSE	MET	modified residue	UNP O27711
C	183	MSE	MET	modified residue	UNP O27711

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total 1 Mg 1	0	0
2	B	2	Total 2 Mg 2	0	0
2	C	1	Total 1 Mg 1	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



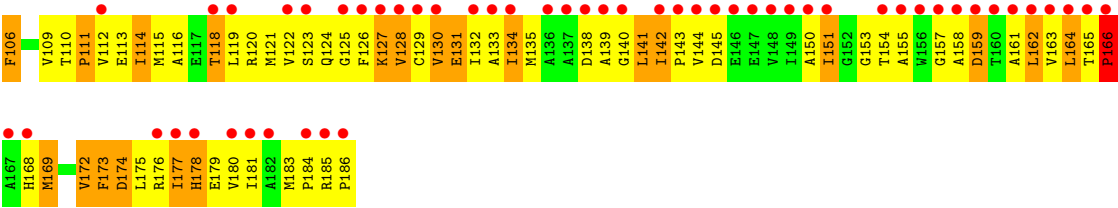
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	B	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	C	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	64	Total O 64 64	0	0
4	B	46	Total O 46 46	0	0
4	C	16	Total O 16 16	0	0

- Molecule 1: Conserved Protein MTH1675





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.98Å 69.40Å 90.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.92 – 2.30 32.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	83.9 (32.92-2.30) 83.9 (32.92-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.66 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.252 , 0.318 0.253 , 0.318	Depositor DCC
R_{free} test set	2475 reflections (8.51%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4441	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.70	0/1420	1.13	4/1908 (0.2%)
1	B	0.64	0/1420	1.17	16/1908 (0.8%)
1	C	0.64	0/1420	1.37	25/1908 (1.3%)
All	All	0.66	0/4260	1.23	45/5724 (0.8%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	GLY	N-CA-C	15.28	131.05	110.43
1	C	144	VAL	N-CA-C	-13.39	100.35	113.20
1	A	144	VAL	N-CA-C	-10.62	102.66	112.43
1	C	142	ILE	CA-C-N	8.89	129.44	119.92
1	C	142	ILE	C-N-CA	8.89	129.44	119.92
1	C	86	VAL	N-CA-C	8.31	120.16	107.78
1	B	12	GLY	N-CA-C	7.86	121.82	111.52
1	C	10	GLU	CA-C-N	7.66	127.59	119.85
1	C	10	GLU	C-N-CA	7.66	127.59	119.85
1	B	65	PHE	N-CA-C	-7.62	103.83	113.43
1	C	37	VAL	N-CA-C	7.47	118.91	108.23
1	C	114	ILE	N-CA-C	-7.24	103.47	110.42
1	A	94	ALA	N-CA-C	7.22	120.02	111.71
1	C	2	GLU	N-CA-C	7.18	119.05	108.14
1	C	46	LEU	N-CA-C	-7.09	103.16	111.03
1	C	106	PHE	N-CA-C	7.01	121.96	113.41
1	C	178	HIS	N-CA-C	6.81	122.26	113.88
1	B	16	THR	N-CA-C	6.59	119.30	111.33
1	C	71	LEU	N-CA-C	-6.41	102.07	110.53
1	B	70	GLN	N-CA-C	6.38	120.22	109.76
1	B	109	VAL	CB-CA-C	-6.32	102.07	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ALA	N-CA-C	-6.29	105.74	113.41
1	C	38	ALA	N-CA-C	6.10	119.29	107.71
1	C	7	TYR	N-CA-C	6.07	118.30	107.80
1	B	110	THR	CA-C-N	6.03	125.51	119.24
1	B	110	THR	C-N-CA	6.03	125.51	119.24
1	C	11	PRO	N-CA-C	5.97	120.87	111.38
1	B	89	TYR	N-CA-C	5.90	118.73	108.76
1	B	174	ASP	N-CA-C	-5.83	106.33	113.50
1	C	159	ASP	N-CA-C	5.76	120.38	113.23
1	C	4	LYS	N-CA-C	5.53	117.80	109.23
1	C	12	GLY	CA-C-N	5.48	127.88	120.65
1	C	12	GLY	C-N-CA	5.48	127.88	120.65
1	C	87	ASN	N-CA-C	5.43	122.36	110.80
1	C	174	ASP	N-CA-C	-5.43	106.69	113.15
1	B	15	ASN	N-CA-C	5.39	119.71	113.18
1	B	110	THR	N-CA-C	-5.37	103.86	110.31
1	A	158	ALA	N-CA-C	5.33	117.49	109.23
1	B	78	ARG	N-CA-C	-5.30	106.50	112.87
1	B	142	ILE	CA-C-N	5.30	125.28	120.03
1	B	142	ILE	C-N-CA	5.30	125.28	120.03
1	A	37	VAL	N-CA-C	5.21	115.63	108.12
1	C	134	ILE	N-CA-C	5.21	115.94	110.62
1	C	6	CYS	N-CA-C	5.07	116.90	109.24
1	B	163	VAL	N-CA-C	-5.06	99.97	107.51

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	1406	0	1408	76	0
1	B	1406	0	1408	118	0
1	C	1406	0	1408	234	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
3	A	31	0	19	5	0
3	B	31	0	19	2	0
3	C	31	0	19	6	0
4	A	64	0	0	4	0
4	B	46	0	0	6	0
4	C	16	0	0	3	0
All	All	4441	0	4281	405	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (405) 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:48:LEU:HD22	1:C:56:ILE:HD11	1.21	1.20
1:C:120:ARG:HG2	1:C:127:LYS:HG2	1.31	1.10
1:C:26:ARG:HH12	1:C:30:LEU:HD23	1.09	1.07
1:A:131:GLU:HG2	1:A:135:MSE:HE2	1.09	1.04
1:B:131:GLU:HG2	1:B:135:MSE:HE2	1.32	1.03
1:A:132:ILE:HA	1:A:135:MSE:HE3	1.42	1.02
1:B:180:VAL:HG11	1:B:183:MSE:HE3	1.42	1.01
1:C:34:ASN:C	1:C:35:PHE:HD1	1.69	1.00
1:A:180:VAL:HG11	1:A:183:MSE:HE2	1.48	0.95
1:C:26:ARG:NH1	1:C:30:LEU:HD23	1.81	0.95
1:C:55:ASN:C	1:C:55:ASN:HD22	1.76	0.94
1:C:130:VAL:O	1:C:134:ILE:HG13	1.66	0.94
1:C:131:GLU:HG2	1:C:135:MSE:HE2	1.48	0.93
1:B:180:VAL:HG11	1:B:183:MSE:CE	1.99	0.93
1:B:78:ARG:O	1:B:82:LEU:HD23	1.70	0.92
1:B:110:THR:HG22	1:B:113:GLU:OE1	1.70	0.91
1:C:56:ILE:CB	1:C:86:VAL:HG11	2.01	0.91
1:C:63:ALA:HB2	1:C:71:LEU:HG	1.52	0.91
1:A:73:LEU:HD11	1:A:78:ARG:HB2	1.54	0.90
1:C:15:ASN:O	1:C:19:VAL:HG23	1.70	0.90
1:C:26:ARG:HH12	1:C:30:LEU:CD2	1.86	0.89
1:C:19:VAL:HG12	1:C:23:VAL:HG11	1.56	0.87
1:C:19:VAL:HG21	1:C:159:ASP:HA	1.57	0.87
1:C:48:LEU:HD22	1:C:56:ILE:CD1	2.03	0.86
1:C:8:PHE:CE2	1:C:15:ASN:HB3	2.11	0.85
1:C:37:VAL:HG22	1:C:38:ALA:H	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:VAL:HG11	1:C:158:ALA:O	1.77	0.84
1:B:104:ASN:HA	4:B:304:HOH:O	1.78	0.83
1:C:164:LEU:HB3	1:C:177:ILE:HA	1.59	0.83
1:C:56:ILE:HB	1:C:86:VAL:HG11	1.59	0.83
1:B:135:MSE:HE1	3:B:201:FMN:HM73	1.59	0.83
1:C:5:ILE:HG12	1:C:6:CYS:N	1.91	0.83
1:C:19:VAL:O	1:C:23:VAL:HG13	1.78	0.82
1:A:132:ILE:CA	1:A:135:MSE:HE3	2.10	0.82
1:C:120:ARG:CG	1:C:127:LYS:HG2	2.10	0.82
1:A:131:GLU:HG2	1:A:135:MSE:CE	2.02	0.81
1:B:37:VAL:HG13	1:B:151:ILE:HB	1.61	0.81
1:C:20:LEU:HA	1:C:23:VAL:HG22	1.61	0.80
1:C:2:GLU:O	1:C:3:LYS:HD2	1.80	0.80
1:C:34:ASN:C	1:C:35:PHE:CD1	2.59	0.80
1:C:48:LEU:CD2	1:C:56:ILE:HD11	2.09	0.80
1:C:83:GLU:C	1:C:85:GLY:H	1.89	0.80
1:C:57:VAL:HG11	4:C:305:HOH:O	1.81	0.79
1:C:6:CYS:SG	1:C:22:LEU:HD11	2.22	0.79
1:B:131:GLU:CG	1:B:135:MSE:HE2	2.14	0.78
1:C:39:SER:OG	1:C:44:THR:HB	1.83	0.78
1:C:115:MSE:O	1:C:118:THR:HG22	1.83	0.78
1:C:164:LEU:HD13	1:C:166:PRO:HG3	1.66	0.77
1:A:17:GLU:O	1:A:21:GLU:HG3	1.84	0.77
1:C:56:ILE:CG2	1:C:86:VAL:HG11	2.15	0.77
1:C:58:SER:HB3	1:C:81:LEU:HD21	1.66	0.77
1:A:73:LEU:CD1	1:A:78:ARG:HB2	2.16	0.75
1:C:115:MSE:HA	1:C:118:THR:HG22	1.69	0.75
1:A:112:VAL:HG11	4:A:352:HOH:O	1.87	0.74
1:C:83:GLU:O	1:C:85:GLY:N	2.19	0.74
1:C:19:VAL:HG12	1:C:23:VAL:CG1	2.16	0.74
1:A:121:MSE:CE	1:B:119:LEU:HD21	2.17	0.74
1:C:37:VAL:HG23	1:C:151:ILE:HG13	1.69	0.73
1:C:172:VAL:HG13	1:C:173:PHE:H	1.54	0.73
1:C:118:THR:HG23	1:C:119:LEU:H	1.53	0.73
1:C:129:CYS:O	1:C:133:ALA:HB2	1.87	0.73
1:C:44:THR:HG21	1:C:158:ALA:HB2	1.71	0.73
1:B:1:MSE:HE3	1:B:3:LYS:NZ	2.05	0.72
1:C:35:PHE:HD1	1:C:35:PHE:N	1.87	0.72
1:C:8:PHE:CZ	1:C:19:VAL:HG22	2.25	0.72
1:C:43:GLU:O	1:C:46:LEU:N	2.21	0.72
1:C:37:VAL:HG22	1:C:38:ALA:N	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:HG23	3:A:200:FMN:H5'2	1.72	0.71
1:A:121:MSE:HE1	1:B:119:LEU:HD21	1.73	0.71
1:C:38:ALA:HB2	1:C:132:ILE:HD13	1.72	0.71
1:C:109:VAL:HG23	1:C:113:GLU:HB2	1.72	0.71
1:C:20:LEU:O	1:C:23:VAL:HG22	1.91	0.70
1:B:74:GLU:C	1:B:76:GLU:H	1.96	0.70
1:C:81:LEU:HD23	1:C:88:VAL:HG22	1.74	0.70
1:C:35:PHE:CD1	1:C:35:PHE:N	2.60	0.70
1:C:19:VAL:C	1:C:23:VAL:HG13	2.17	0.70
1:C:56:ILE:HG22	1:C:86:VAL:HG11	1.72	0.70
1:B:110:THR:HG22	1:B:113:GLU:HG3	1.74	0.69
4:A:362:HOH:O	1:B:183:MSE:SE	2.61	0.69
1:C:20:LEU:CA	1:C:23:VAL:HG22	2.22	0.69
1:B:1:MSE:HE3	1:B:3:LYS:HZ1	1.57	0.69
1:C:162:LEU:HD23	1:C:177:ILE:HD12	1.73	0.69
1:B:78:ARG:HG3	1:B:88:VAL:HG11	1.75	0.68
1:A:37:VAL:HG21	1:A:48:LEU:HD22	1.75	0.68
1:C:115:MSE:O	1:C:118:THR:CG2	2.40	0.68
1:B:20:LEU:HB3	1:B:51:MSE:HE1	1.74	0.68
1:C:5:ILE:HG12	1:C:6:CYS:H	1.56	0.68
1:C:56:ILE:O	1:C:86:VAL:CG1	2.42	0.67
1:A:128:VAL:O	1:A:132:ILE:HG12	1.93	0.67
1:C:26:ARG:HG2	1:C:181:ILE:HG12	1.76	0.67
1:B:103:SER:O	4:B:304:HOH:O	2.12	0.67
1:A:19:VAL:O	1:A:23:VAL:HG13	1.95	0.67
1:B:130:VAL:O	1:B:134:ILE:HG13	1.95	0.66
1:C:20:LEU:HA	1:C:23:VAL:CG2	2.25	0.66
1:B:122:VAL:HG21	1:B:126:PHE:CD1	2.31	0.66
1:C:120:ARG:HG2	1:C:127:LYS:CG	2.18	0.65
1:C:141:LEU:HB3	4:C:305:HOH:O	1.96	0.65
1:C:175:LEU:C	1:C:175:LEU:HD23	2.22	0.65
1:B:74:GLU:C	1:B:76:GLU:N	2.55	0.65
1:C:164:LEU:HD13	1:C:166:PRO:CG	2.27	0.64
1:C:79:ASP:OD1	1:C:80:ALA:N	2.30	0.64
1:B:101:GLY:HA3	1:C:172:VAL:HG12	1.78	0.64
1:B:19:VAL:O	1:B:23:VAL:HG23	1.97	0.64
1:B:110:THR:OG1	1:B:111:PRO:HD2	1.98	0.64
1:C:153:GLY:HA3	1:C:158:ALA:HA	1.79	0.63
1:C:8:PHE:HE2	1:C:15:ASN:HB3	1.60	0.63
1:C:49:SER:HA	1:C:56:ILE:HD12	1.79	0.63
1:C:17:GLU:HG3	1:C:47:ARG:HH12	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:HIS:HB3	1:C:131:GLU:OE2	1.98	0.63
1:B:93:HIS:HB3	1:B:131:GLU:OE1	1.99	0.63
1:B:132:ILE:HA	1:B:135:MSE:HE3	1.80	0.63
1:C:172:VAL:HG13	1:C:173:PHE:N	2.13	0.63
1:B:71:LEU:HD23	1:B:72:GLU:N	2.15	0.62
1:C:18:ARG:HD3	1:C:18:ARG:O	2.00	0.62
1:C:83:GLU:C	1:C:85:GLY:N	2.51	0.62
1:C:37:VAL:HG23	1:C:151:ILE:CG1	2.29	0.62
1:C:164:LEU:O	1:C:166:PRO:HD3	2.00	0.61
1:C:110:THR:HG23	1:C:113:GLU:OE2	2.00	0.61
1:C:20:LEU:C	1:C:23:VAL:HG22	2.25	0.61
1:C:115:MSE:O	1:C:116:ALA:C	2.41	0.61
1:B:151:ILE:HD12	1:B:151:ILE:N	2.16	0.61
1:C:6:CYS:SG	1:C:22:LEU:CD1	2.89	0.61
1:B:110:THR:HG22	1:B:113:GLU:CG	2.31	0.60
1:C:56:ILE:HG22	1:C:86:VAL:CG1	2.30	0.60
1:C:2:GLU:HG3	1:C:3:LYS:N	2.14	0.60
1:C:16:THR:O	1:C:20:LEU:N	2.33	0.60
1:C:64:GLY:HA2	1:C:67:GLU:O	2.02	0.60
1:B:139:ALA:CB	1:B:141:LEU:HD23	2.31	0.60
1:A:164:LEU:C	1:A:164:LEU:HD12	2.27	0.60
1:B:139:ALA:O	1:B:141:LEU:HD22	2.01	0.59
1:C:55:ASN:HD21	1:C:57:VAL:HG12	1.67	0.59
1:C:43:GLU:HG3	1:C:44:THR:N	2.16	0.59
1:A:48:LEU:O	1:A:52:VAL:HG22	2.03	0.59
1:B:139:ALA:HB3	1:B:141:LEU:HD23	1.84	0.59
1:A:36:VAL:HA	1:A:57:VAL:HG13	1.83	0.59
1:B:146:GLU:HA	4:B:315:HOH:O	2.03	0.59
1:B:110:THR:HG22	1:B:113:GLU:CD	2.28	0.59
1:C:32:ILE:HG22	1:C:33:ARG:N	2.18	0.59
1:C:74:GLU:O	1:C:78:ARG:N	2.34	0.58
1:B:9:GLU:HG3	1:B:10:GLU:HG2	1.84	0.58
1:C:17:GLU:HG3	1:C:47:ARG:NH1	2.18	0.58
1:C:56:ILE:O	1:C:86:VAL:HG13	2.02	0.58
1:C:168:HIS:O	1:C:172:VAL:HA	2.03	0.58
1:A:93:HIS:CD2	3:A:200:FMN:HM72	2.39	0.58
1:C:5:ILE:CG1	1:C:6:CYS:N	2.63	0.58
1:C:81:LEU:HD23	1:C:88:VAL:CG2	2.34	0.58
1:C:132:ILE:N	1:C:135:MSE:HE3	2.19	0.58
1:B:132:ILE:CA	1:B:135:MSE:HE3	2.34	0.57
1:C:122:VAL:HB	1:C:126:PHE:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:CG1	1:C:6:CYS:H	2.16	0.57
1:B:62:HIS:CD2	1:B:65:PHE:HD1	2.23	0.57
1:C:121:MSE:SE	4:C:319:HOH:O	2.71	0.57
1:B:76:GLU:HB2	4:B:337:HOH:O	2.04	0.57
1:C:15:ASN:C	1:C:19:VAL:HG23	2.30	0.57
1:A:37:VAL:HG21	1:A:48:LEU:CD2	2.35	0.57
1:B:43:GLU:O	1:B:47:ARG:HG3	2.05	0.57
1:C:118:THR:O	1:C:121:MSE:HG3	2.04	0.57
1:A:165:THR:OG1	1:A:178:HIS:HE1	1.89	0.56
1:B:110:THR:CG2	1:B:113:GLU:HG3	2.36	0.56
1:C:115:MSE:HA	1:C:118:THR:CG2	2.35	0.56
1:B:26:ARG:HG3	1:B:30:LEU:HD12	1.86	0.56
1:A:34:ASN:O	1:A:148:VAL:HG13	2.06	0.56
1:C:98:VAL:O	1:C:101:GLY:N	2.38	0.56
1:C:123:SER:OG	1:C:126:PHE:HB2	2.06	0.56
1:B:148:VAL:HG12	1:B:149:ILE:N	2.20	0.56
1:C:21:GLU:O	1:C:25:GLU:HG3	2.05	0.56
1:C:180:VAL:HG21	1:C:183:MSE:CE	2.37	0.55
1:B:93:HIS:H	1:B:93:HIS:CD2	2.24	0.55
1:A:135:MSE:HE1	3:A:200:FMN:HM73	1.88	0.55
1:C:115:MSE:CA	1:C:118:THR:HG22	2.37	0.55
1:A:179:GLU:HG2	1:B:7:TYR:CE1	2.42	0.55
1:B:154:THR:O	1:B:155:ALA:HB3	2.06	0.55
1:C:18:ARG:HD3	1:C:18:ARG:C	2.30	0.55
1:B:49:SER:HA	1:B:56:ILE:CD1	2.37	0.55
1:C:26:ARG:CZ	1:C:30:LEU:HD23	2.36	0.55
1:C:93:HIS:CE1	3:C:202:FMN:HM72	2.42	0.55
1:C:56:ILE:C	1:C:86:VAL:CG1	2.80	0.54
1:C:164:LEU:C	1:C:166:PRO:HD3	2.32	0.54
1:A:115:MSE:HG2	1:B:118:THR:OG1	2.08	0.54
1:A:80:ALA:O	1:A:84:ARG:HG2	2.08	0.54
1:B:77:ALA:C	1:B:79:ASP:N	2.65	0.54
1:B:37:VAL:CG1	1:B:151:ILE:HB	2.36	0.53
1:C:124:GLN:O	1:C:127:LYS:HG3	2.09	0.53
1:C:132:ILE:CA	1:C:135:MSE:HE3	2.38	0.53
1:B:180:VAL:HG11	1:B:183:MSE:HE2	1.89	0.53
1:A:131:GLU:O	1:A:135:MSE:HG3	2.09	0.53
1:B:132:ILE:N	1:B:135:MSE:HE3	2.24	0.53
1:C:16:THR:O	1:C:20:LEU:HB2	2.08	0.53
1:C:180:VAL:HG21	1:C:183:MSE:HE3	1.91	0.53
1:B:98:VAL:O	1:B:101:GLY:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:HIS:CD2	1:C:64:GLY:HA3	2.42	0.53
1:C:5:ILE:HD12	1:C:180:VAL:CG1	2.39	0.53
1:C:131:GLU:HG2	1:C:135:MSE:CE	2.31	0.53
1:C:23:VAL:O	1:C:27:ALA:HB2	2.09	0.52
1:C:46:LEU:O	1:C:49:SER:OG	2.27	0.52
1:C:111:PRO:O	1:C:114:ILE:N	2.37	0.52
1:C:154:THR:HG23	1:C:159:ASP:OD1	2.09	0.52
1:B:74:GLU:O	1:B:76:GLU:N	2.42	0.52
1:C:75:ASP:HA	1:C:78:ARG:HB3	1.90	0.52
1:B:62:HIS:NE2	1:B:65:PHE:HD1	2.07	0.52
1:C:163:VAL:HB	1:C:179:GLU:HB2	1.92	0.52
1:A:109:VAL:HG13	1:C:106:PHE:CG	2.45	0.52
1:A:93:HIS:NE2	3:A:200:FMN:HM72	2.24	0.52
1:C:135:MSE:HE1	3:C:202:FMN:HM73	1.92	0.52
1:C:165:THR:O	1:C:166:PRO:O	2.27	0.52
1:C:125:GLY:H	1:C:154:THR:HG22	1.73	0.52
1:B:71:LEU:HD22	1:B:73:LEU:H	1.75	0.51
1:B:77:ALA:C	1:B:79:ASP:H	2.17	0.51
1:C:128:VAL:O	1:C:132:ILE:HG12	2.10	0.51
1:B:100:ARG:O	1:B:104:ASN:ND2	2.43	0.51
1:B:118:THR:O	1:B:121:MSE:HB2	2.09	0.51
1:C:26:ARG:HH22	1:C:30:LEU:HD23	1.76	0.51
1:C:50:GLU:HG3	1:C:51:MSE:HE3	1.93	0.51
1:A:153:GLY:HA2	1:A:159:ASP:OD2	2.11	0.51
1:B:144:VAL:HG12	1:B:144:VAL:O	2.10	0.51
1:C:19:VAL:O	1:C:23:VAL:N	2.29	0.51
1:A:109:VAL:CG1	1:C:106:PHE:CG	2.94	0.51
1:C:115:MSE:C	1:C:118:THR:HG22	2.36	0.51
1:C:43:GLU:O	1:C:46:LEU:HB3	2.11	0.51
1:C:56:ILE:CG2	1:C:57:VAL:N	2.74	0.51
1:C:73:LEU:HD23	1:C:78:ARG:HB2	1.93	0.51
1:B:125:GLY:HA2	1:B:128:VAL:CG1	2.41	0.50
1:C:132:ILE:HA	1:C:135:MSE:HE3	1.92	0.50
1:C:175:LEU:HD23	1:C:176:ARG:N	2.26	0.50
1:A:177:ILE:HB	1:B:122:VAL:HA	1.94	0.50
1:C:55:ASN:C	1:C:55:ASN:ND2	2.49	0.50
1:A:169:MSE:HG3	1:A:170:ASN:N	2.27	0.50
1:C:132:ILE:HA	1:C:135:MSE:HG3	1.94	0.50
1:B:19:VAL:HG21	1:B:159:ASP:HA	1.94	0.49
1:B:109:VAL:HG12	1:B:113:GLU:HB2	1.92	0.49
1:B:34:ASN:O	1:B:148:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HB3	1:B:186:PRO:HD3	1.95	0.49
1:C:72:GLU:O	1:C:74:GLU:N	2.45	0.49
1:B:164:LEU:HD12	1:B:164:LEU:C	2.37	0.49
1:C:40:VAL:HG12	3:C:202:FMN:C5'	2.42	0.49
1:B:105:ARG:HG3	1:B:105:ARG:HH11	1.76	0.49
1:C:118:THR:HG23	1:C:119:LEU:N	2.25	0.49
1:C:32:ILE:HG22	1:C:34:ASN:H	1.77	0.49
1:C:75:ASP:O	1:C:79:ASP:HB3	2.12	0.49
1:C:6:CYS:C	1:C:7:TYR:CD1	2.91	0.49
1:C:26:ARG:NH1	1:C:26:ARG:HG3	2.28	0.49
1:A:12:GLY:HA3	4:A:350:HOH:O	2.12	0.49
1:C:40:VAL:HG22	1:C:40:VAL:O	2.13	0.49
1:B:95:LEU:HB2	1:B:131:GLU:HG3	1.94	0.48
1:C:20:LEU:CD1	1:C:47:ARG:HD2	2.43	0.48
1:C:26:ARG:NH2	1:C:30:LEU:HD23	2.28	0.48
1:C:138:ASP:OD1	1:C:169:MSE:HG2	2.12	0.48
1:C:157:GLY:O	3:C:202:FMN:O4'	2.21	0.48
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.69	0.48
1:A:128:VAL:HG22	1:A:152:GLY:HA3	1.94	0.48
1:A:60:THR:OG1	1:A:61:HIS:N	2.47	0.48
1:B:40:VAL:HA	1:B:60:THR:OG1	2.14	0.48
1:B:20:LEU:CB	1:B:51:MSE:HE1	2.44	0.48
1:A:75:ASP:O	1:A:79:ASP:OD1	2.32	0.47
1:B:79:ASP:HA	1:B:82:LEU:HB2	1.94	0.47
1:B:140:GLY:HA3	1:C:71:LEU:CD1	2.44	0.47
1:A:171:SER:O	1:A:174:ASP:HB2	2.14	0.47
1:C:19:VAL:CG1	1:C:158:ALA:O	2.57	0.47
1:C:26:ARG:HG3	1:C:26:ARG:HH11	1.79	0.47
1:C:8:PHE:HZ	1:C:19:VAL:HG22	1.74	0.47
1:C:37:VAL:CG2	1:C:151:ILE:HG13	2.42	0.47
1:B:10:GLU:OE2	1:B:10:GLU:HA	2.14	0.47
1:C:8:PHE:HB2	1:C:184:PRO:HA	1.97	0.47
1:A:46:LEU:HD21	1:A:81:LEU:HD12	1.96	0.47
1:A:172:VAL:C	1:A:174:ASP:H	2.22	0.47
1:B:75:ASP:HB3	4:B:333:HOH:O	2.14	0.47
1:B:98:VAL:O	1:B:99:GLY:C	2.58	0.47
1:B:126:PHE:O	1:B:130:VAL:HG23	2.15	0.47
1:C:16:THR:O	1:C:20:LEU:CB	2.63	0.47
1:C:111:PRO:O	1:C:114:ILE:HB	2.14	0.47
1:C:163:VAL:HG12	1:C:178:HIS:HB2	1.96	0.47
1:B:20:LEU:HB3	1:B:51:MSE:CE	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:VAL:HG23	1:A:173:PHE:N	2.29	0.47
1:B:93:HIS:CD2	1:B:93:HIS:N	2.80	0.47
1:C:105:ARG:HD3	1:C:105:ARG:C	2.40	0.47
1:C:19:VAL:CG1	1:C:23:VAL:CG1	2.91	0.47
1:C:32:ILE:CG2	1:C:33:ARG:N	2.78	0.47
1:B:149:ILE:HA	1:B:162:LEU:O	2.15	0.46
1:C:105:ARG:HD3	1:C:105:ARG:O	2.15	0.46
1:A:142:ILE:HB	1:A:143:PRO:HD2	1.96	0.46
1:B:138:ASP:OD1	1:B:169:MSE:HB3	2.14	0.46
1:C:123:SER:O	1:C:126:PHE:N	2.42	0.46
1:B:137:ALA:O	1:B:168:HIS:HE1	1.98	0.46
1:B:62:HIS:HE2	1:B:65:PHE:HD1	1.62	0.46
1:B:131:GLU:O	1:B:135:MSE:HG3	2.14	0.46
1:A:185:ARG:HG2	4:A:311:HOH:O	2.16	0.46
1:A:62:HIS:HD2	1:A:63:ALA:O	1.98	0.46
1:B:169:MSE:SE	1:C:92:SER:HB3	2.66	0.46
1:C:75:ASP:OD2	1:C:78:ARG:HD3	2.15	0.46
1:C:142:ILE:HA	1:C:143:PRO:HD3	1.73	0.46
1:C:161:ALA:O	1:C:162:LEU:HD12	2.15	0.46
1:B:92:SER:HB3	1:C:138:ASP:OD1	2.16	0.46
1:B:63:ALA:HB2	1:C:140:GLY:N	2.31	0.46
1:C:89:TYR:CE1	1:C:139:ALA:HB2	2.51	0.46
1:A:43:GLU:O	1:A:46:LEU:HB2	2.16	0.46
1:C:24:GLY:O	1:C:25:GLU:C	2.59	0.46
1:C:89:TYR:CD2	1:C:90:ALA:N	2.84	0.46
1:C:150:ALA:O	1:C:162:LEU:N	2.49	0.46
1:C:40:VAL:HA	1:C:60:THR:OG1	2.16	0.45
1:B:172:VAL:HG21	1:C:98:VAL:HG13	1.98	0.45
1:A:131:GLU:CG	1:A:135:MSE:HE2	2.05	0.45
1:C:55:ASN:HD21	1:C:57:VAL:CG1	2.30	0.45
1:B:160:THR:HA	1:B:182:ALA:O	2.16	0.45
1:B:36:VAL:HG21	1:B:142:ILE:HD13	1.98	0.45
1:C:56:ILE:O	1:C:57:VAL:HG12	2.17	0.45
1:C:62:HIS:HB3	1:C:91:GLY:O	2.17	0.45
1:A:109:VAL:HG11	1:C:106:PHE:CD1	2.51	0.45
1:C:19:VAL:HG21	1:C:158:ALA:O	2.17	0.45
1:C:8:PHE:CD1	1:C:8:PHE:N	2.85	0.45
1:C:55:ASN:ND2	1:C:57:VAL:HG12	2.31	0.44
1:A:179:GLU:HG2	1:B:7:TYR:CZ	2.52	0.44
1:C:185:ARG:O	1:C:186:PRO:O	2.35	0.44
1:A:25:GLU:O	1:A:29:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:LEU:C	1:C:175:LEU:CD2	2.90	0.44
1:A:5:ILE:HD11	1:A:183:MSE:HE3	1.99	0.44
1:A:75:ASP:OD1	1:A:75:ASP:N	2.45	0.44
1:C:47:ARG:O	1:C:51:MSE:HE3	2.17	0.44
1:C:151:ILE:HD11	1:C:158:ALA:HB1	1.99	0.44
1:A:164:LEU:C	1:A:164:LEU:CD1	2.91	0.44
1:C:5:ILE:HD12	1:C:180:VAL:HG13	2.00	0.44
1:B:140:GLY:HA3	1:C:71:LEU:HD11	2.00	0.44
1:B:98:VAL:C	1:B:100:ARG:N	2.74	0.44
1:C:157:GLY:N	3:C:202:FMN:O4'	2.51	0.44
1:A:94:ALA:HB2	1:A:135:MSE:HG2	2.00	0.44
1:C:17:GLU:CD	1:C:17:GLU:H	2.24	0.44
1:C:50:GLU:CD	1:C:84:ARG:HH22	2.26	0.44
1:C:74:GLU:OE2	1:C:74:GLU:HA	2.18	0.44
1:C:40:VAL:HG12	3:C:202:FMN:H5'2	1.99	0.43
1:C:162:LEU:CD2	1:C:177:ILE:HD12	2.47	0.43
1:B:148:VAL:CG1	1:B:149:ILE:N	2.80	0.43
1:B:39:SER:HA	3:B:201:FMN:H5'1	2.01	0.43
1:B:67:GLU:O	1:B:68:LYS:C	2.62	0.43
1:C:37:VAL:CG2	1:C:38:ALA:H	2.21	0.43
1:C:56:ILE:C	1:C:57:VAL:CG1	2.91	0.43
1:C:122:VAL:CB	1:C:126:PHE:CD2	3.02	0.43
1:A:46:LEU:CD2	1:A:81:LEU:HD12	2.48	0.43
1:C:37:VAL:CG2	1:C:38:ALA:N	2.77	0.43
1:C:55:ASN:ND2	1:C:55:ASN:O	2.51	0.43
1:C:127:LYS:HE2	1:C:127:LYS:HB2	1.85	0.43
1:C:36:VAL:HA	1:C:57:VAL:HG22	2.00	0.43
1:C:78:ARG:CZ	1:C:82:LEU:HD11	2.48	0.43
1:B:63:ALA:HB2	1:C:140:GLY:CA	2.48	0.43
1:A:149:ILE:HD13	1:A:181:ILE:HD11	2.01	0.43
1:C:19:VAL:CG2	1:C:159:ASP:HA	2.38	0.43
1:A:164:LEU:HD12	1:A:164:LEU:O	2.19	0.43
1:C:98:VAL:O	1:C:99:GLY:C	2.61	0.43
1:C:172:VAL:O	1:C:174:ASP:N	2.52	0.43
1:B:13:LYS:O	1:B:14:GLU:C	2.61	0.42
1:A:52:VAL:HG23	1:A:56:ILE:HD11	2.02	0.42
1:B:63:ALA:HB2	1:C:140:GLY:HA2	2.00	0.42
1:B:110:THR:OG1	1:B:111:PRO:CD	2.66	0.42
1:B:172:VAL:HG13	1:B:173:PHE:N	2.33	0.42
1:C:48:LEU:O	1:C:48:LEU:HD23	2.19	0.42
1:B:127:LYS:HD3	1:B:127:LYS:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ILE:HD12	1:B:166:PRO:HG2	2.01	0.42
1:A:60:THR:C	3:A:200:FMN:HM82	2.45	0.42
1:C:33:ARG:HE	1:C:33:ARG:HB3	1.64	0.42
1:C:185:ARG:HB3	1:C:186:PRO:HD3	2.01	0.42
1:B:17:GLU:HB2	4:B:334:HOH:O	2.19	0.42
1:B:17:GLU:CD	1:B:47:ARG:NH2	2.78	0.42
1:C:23:VAL:O	1:C:27:ALA:CB	2.67	0.42
1:A:42:GLY:O	1:A:43:GLU:C	2.63	0.42
1:A:16:THR:HG22	1:A:20:LEU:HD12	2.01	0.41
1:A:20:LEU:O	1:A:23:VAL:HG22	2.21	0.41
1:A:47:ARG:HA	1:A:47:ARG:HD3	1.70	0.41
1:B:101:GLY:O	1:B:104:ASN:HB2	2.19	0.41
1:C:43:GLU:O	1:C:46:LEU:CB	2.68	0.41
1:A:16:THR:HG22	1:A:20:LEU:CD1	2.50	0.41
1:A:175:LEU:C	1:A:175:LEU:HD23	2.45	0.41
1:B:75:ASP:HA	1:B:78:ARG:HB3	2.02	0.41
1:C:14:GLU:H	1:C:14:GLU:CD	2.28	0.41
1:C:58:SER:CB	1:C:81:LEU:HD21	2.44	0.41
1:C:62:HIS:CD2	1:C:63:ALA:O	2.73	0.41
1:A:23:VAL:CG2	1:A:24:GLY:N	2.83	0.41
1:B:10:GLU:HA	1:B:11:PRO:HD3	1.92	0.41
1:B:172:VAL:HG11	1:C:98:VAL:HG13	2.02	0.41
1:B:102:ILE:C	1:B:104:ASN:N	2.76	0.41
1:A:125:GLY:HA2	1:A:128:VAL:HG13	2.02	0.41
1:C:8:PHE:CD2	1:C:15:ASN:HB3	2.53	0.41
1:A:36:VAL:O	1:A:36:VAL:HG13	2.21	0.41
1:B:17:GLU:HG2	1:B:47:ARG:HH22	1.85	0.41
1:C:120:ARG:O	1:C:121:MSE:C	2.63	0.41
1:A:2:GLU:CD	1:B:4:LYS:HD2	2.46	0.41
1:A:56:ILE:HB	1:A:86:VAL:HG22	2.03	0.41
1:C:19:VAL:CG1	1:C:23:VAL:HG11	2.39	0.41
1:C:37:VAL:CG2	1:C:151:ILE:CG1	2.98	0.41
1:A:117:GLU:HB3	1:B:173:PHE:CE1	2.56	0.41
1:B:126:PHE:N	1:B:160:THR:HG21	2.36	0.41
1:C:120:ARG:HE	1:C:127:LYS:HE3	1.85	0.41
1:B:79:ASP:C	1:B:81:LEU:N	2.79	0.40
1:C:16:THR:HA	1:C:19:VAL:HB	2.03	0.40
1:C:172:VAL:C	1:C:174:ASP:H	2.28	0.40
1:A:179:GLU:HA	1:B:7:TYR:CE2	2.56	0.40
1:C:35:PHE:HE2	1:C:52:VAL:CG1	2.34	0.40
1:C:48:LEU:O	1:C:49:SER:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LEU:O	1:C:82:LEU:C	2.64	0.40
1:A:5:ILE:HG13	1:A:180:VAL:O	2.22	0.40
1:A:18:ARG:HD2	1:A:18:ARG:HA	1.89	0.40
1:B:75:ASP:HA	1:B:78:ARG:CB	2.51	0.40
1:C:49:SER:HB2	1:C:84:ARG:HG2	2.04	0.40
1:C:142:ILE:O	1:C:142:ILE:HG13	2.19	0.40
1:C:164:LEU:HD12	1:C:164:LEU:H	1.87	0.40
1:A:23:VAL:HG23	1:A:24:GLY:N	2.36	0.40
1:A:172:VAL:HG23	1:A:173:PHE:H	1.86	0.40
1:C:36:VAL:O	1:C:151:ILE:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/206 (89%)	173 (94%)	10 (5%)	1 (0%)	24	31
1	B	184/206 (89%)	162 (88%)	19 (10%)	3 (2%)	7	7
1	C	184/206 (89%)	138 (75%)	30 (16%)	16 (9%)	0	0
All	All	552/618 (89%)	473 (86%)	59 (11%)	20 (4%)	2	1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	14	GLU
1	C	84	ARG
1	C	166	PRO
1	A	108	GLY
1	B	64	GLY
1	C	73	LEU
1	C	87	ASN

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Mol	Chain	Res	Type
1	C	173	PHE
1	B	68	LYS
1	C	31	GLY
1	C	44	THR
1	C	131	GLU
1	C	81	LEU
1	B	75	ASP
1	C	43	GLU
1	C	111	PRO
1	C	155	ALA
1	C	141	LEU
1	C	172	VAL
1	C	112	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	148/157 (94%)	133 (90%)	15 (10%)	7	9
1	B	148/157 (94%)	130 (88%)	18 (12%)	5	5
1	C	148/157 (94%)	119 (80%)	29 (20%)	1	1
All	All	444/471 (94%)	382 (86%)	62 (14%)	3	3

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	17	GLU
1	A	19	VAL
1	A	57	VAL
1	A	59	VAL
1	A	60	THR
1	A	66	ARG
1	A	109	VAL
1	A	112	VAL

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Mol	Chain	Res	Type
1	A	114	ILE
1	A	127	LYS
1	A	128	VAL
1	A	130	VAL
1	A	149	ILE
1	A	183	MSE
1	B	1	MSE
1	B	3	LYS
1	B	9	GLU
1	B	14	GLU
1	B	18	ARG
1	B	33	ARG
1	B	37	VAL
1	B	53	GLU
1	B	83	GLU
1	B	95	LEU
1	B	109	VAL
1	B	111	PRO
1	B	112	VAL
1	B	122	VAL
1	B	123	SER
1	B	128	VAL
1	B	169	MSE
1	B	171	SER
1	C	1	MSE
1	C	2	GLU
1	C	4	LYS
1	C	5	ILE
1	C	18	ARG
1	C	22	LEU
1	C	30	LEU
1	C	33	ARG
1	C	35	PHE
1	C	36	VAL
1	C	39	SER
1	C	43	GLU
1	C	55	ASN
1	C	56	ILE
1	C	57	VAL
1	C	79	ASP
1	C	82	LEU
1	C	84	ARG

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Mol	Chain	Res	Type
1	C	118	THR
1	C	127	LYS
1	C	128	VAL
1	C	130	VAL
1	C	145	ASP
1	C	151	ILE
1	C	162	LEU
1	C	164	LEU
1	C	166	PRO
1	C	169	MSE
1	C	177	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	34	ASN
1	A	55	ASN
1	A	62	HIS
1	A	104	ASN
1	A	168	HIS
1	A	178	HIS
1	B	34	ASN
1	B	62	HIS
1	B	70	GLN
1	B	104	ASN
1	C	55	ASN
1	C	61	HIS
1	C	124	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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
3	FMN	C	202	-	33,33,33	2.09	8 (24%)	48,50,50	2.58	20 (41%)
3	FMN	A	200	-	33,33,33	1.04	1 (3%)	48,50,50	1.99	12 (25%)
3	FMN	B	201	2	33,33,33	2.11	9 (27%)	48,50,50	2.45	18 (37%)

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
3	FMN	C	202	-	-	7/18/18/18	0/3/3/3
3	FMN	A	200	-	-	3/18/18/18	0/3/3/3
3	FMN	B	201	2	-	4/18/18/18	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	FMN	C9-C9A	6.09	1.49	1.39
3	C	202	FMN	C9-C9A	5.82	1.49	1.39
3	C	202	FMN	C9A-C5A	4.65	1.48	1.41
3	C	202	FMN	C6-C7	4.15	1.45	1.39
3	B	201	FMN	C2-N3	4.03	1.47	1.39
3	B	201	FMN	C6-C7	3.96	1.45	1.39
3	B	201	FMN	C9A-C5A	3.94	1.47	1.41
3	C	202	FMN	C2-N3	3.76	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	202	FMN	C4A-C10	3.40	1.54	1.44
3	A	200	FMN	C4A-N5	3.40	1.38	1.30
3	B	201	FMN	C4A-C10	2.81	1.52	1.44
3	C	202	FMN	C5'-C4'	2.53	1.55	1.51
3	B	201	FMN	C8-C7	2.39	1.46	1.40
3	B	201	FMN	C5'-C4'	2.35	1.55	1.51
3	B	201	FMN	C4-N3	2.34	1.43	1.38
3	C	202	FMN	C4-N3	2.33	1.43	1.38
3	C	202	FMN	C8M-C8	-2.30	1.46	1.51
3	B	201	FMN	C8M-C8	-2.09	1.47	1.51

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	200	FMN	C5'-C4'-C3'	7.02	125.46	112.22
3	C	202	FMN	C5A-C9A-N10	6.73	124.05	117.97
3	B	201	FMN	C7M-C7-C6	-6.27	108.53	119.57
3	C	202	FMN	C7M-C7-C6	-6.15	108.74	119.57
3	B	201	FMN	C5A-C9A-N10	5.84	123.24	117.97
3	B	201	FMN	C9A-C5A-N5	-5.46	116.66	122.45
3	A	200	FMN	O4'-C4'-C5'	-5.36	98.17	109.99
3	B	201	FMN	C7M-C7-C8	5.20	131.38	120.76
3	C	202	FMN	C7M-C7-C8	4.93	130.84	120.76
3	C	202	FMN	C9A-C5A-N5	-4.84	117.31	122.45
3	C	202	FMN	C1'-N10-C9A	4.64	129.64	120.63
3	A	200	FMN	C4'-C3'-C2'	4.35	120.81	113.57
3	C	202	FMN	C9A-N10-C10	-4.21	114.33	120.75
3	C	202	FMN	O2-C2-N1	3.98	128.41	121.80
3	B	201	FMN	C4'-C3'-C2'	3.85	119.98	113.57
3	B	201	FMN	C1'-N10-C9A	3.77	127.95	120.63
3	B	201	FMN	O2-C2-N1	3.76	128.05	121.80
3	C	202	FMN	C4A-C10-N10	3.71	121.79	116.48
3	B	201	FMN	C9A-N10-C10	-3.69	115.12	120.75
3	C	202	FMN	C5'-C4'-C3'	3.65	119.11	112.22
3	B	201	FMN	C10-N1-C2	3.56	124.55	116.85
3	C	202	FMN	C10-N1-C2	3.34	124.08	116.85
3	A	200	FMN	C4-N3-C2	-3.26	119.86	125.64
3	B	201	FMN	C4A-C10-N10	3.22	121.09	116.48
3	A	200	FMN	C4A-C10-N10	3.02	120.81	116.48
3	C	202	FMN	C4'-C3'-C2'	2.98	118.53	113.57
3	B	201	FMN	C6-C5A-N5	2.97	123.38	118.44
3	B	201	FMN	C4A-C10-N1	-2.96	117.32	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	202	FMN	C4A-C10-N1	-2.89	117.51	124.59
3	A	200	FMN	O5'-C5'-C4'	-2.82	101.83	109.36
3	C	202	FMN	O4-C4-N3	-2.69	115.05	120.11
3	C	202	FMN	O3'-C3'-C4'	-2.63	102.95	108.93
3	C	202	FMN	C4-N3-C2	-2.61	121.01	125.64
3	C	202	FMN	C6-C5A-N5	2.60	122.76	118.44
3	A	200	FMN	C10-C4A-N5	-2.58	119.54	124.81
3	A	200	FMN	O2P-P-O5'	2.48	113.13	106.67
3	A	200	FMN	O4'-C4'-C3'	-2.44	103.54	109.25
3	C	202	FMN	O2-C2-N3	-2.41	113.96	118.58
3	B	201	FMN	O4-C4-N3	-2.41	115.58	120.11
3	B	201	FMN	O3'-C3'-C4'	-2.38	103.51	108.93
3	B	201	FMN	C4-C4A-C10	2.35	120.97	116.93
3	B	201	FMN	C4-N3-C2	-2.30	121.56	125.64
3	A	200	FMN	C4-C4A-C10	2.24	120.78	116.93
3	C	202	FMN	C4-C4A-C10	2.22	120.73	116.93
3	B	201	FMN	O2-C2-N3	-2.20	114.37	118.58
3	C	202	FMN	C9-C9A-C5A	-2.08	116.36	120.03
3	A	200	FMN	O3'-C3'-C4'	2.07	113.64	108.93
3	C	202	FMN	O5'-C5'-C4'	-2.02	103.98	109.36
3	B	201	FMN	C10-C4A-N5	-2.02	120.69	124.81
3	A	200	FMN	O4-C4-C4A	-2.00	121.24	126.53

There are no chirality outliers.

All (14) torsion outliers are listed below:

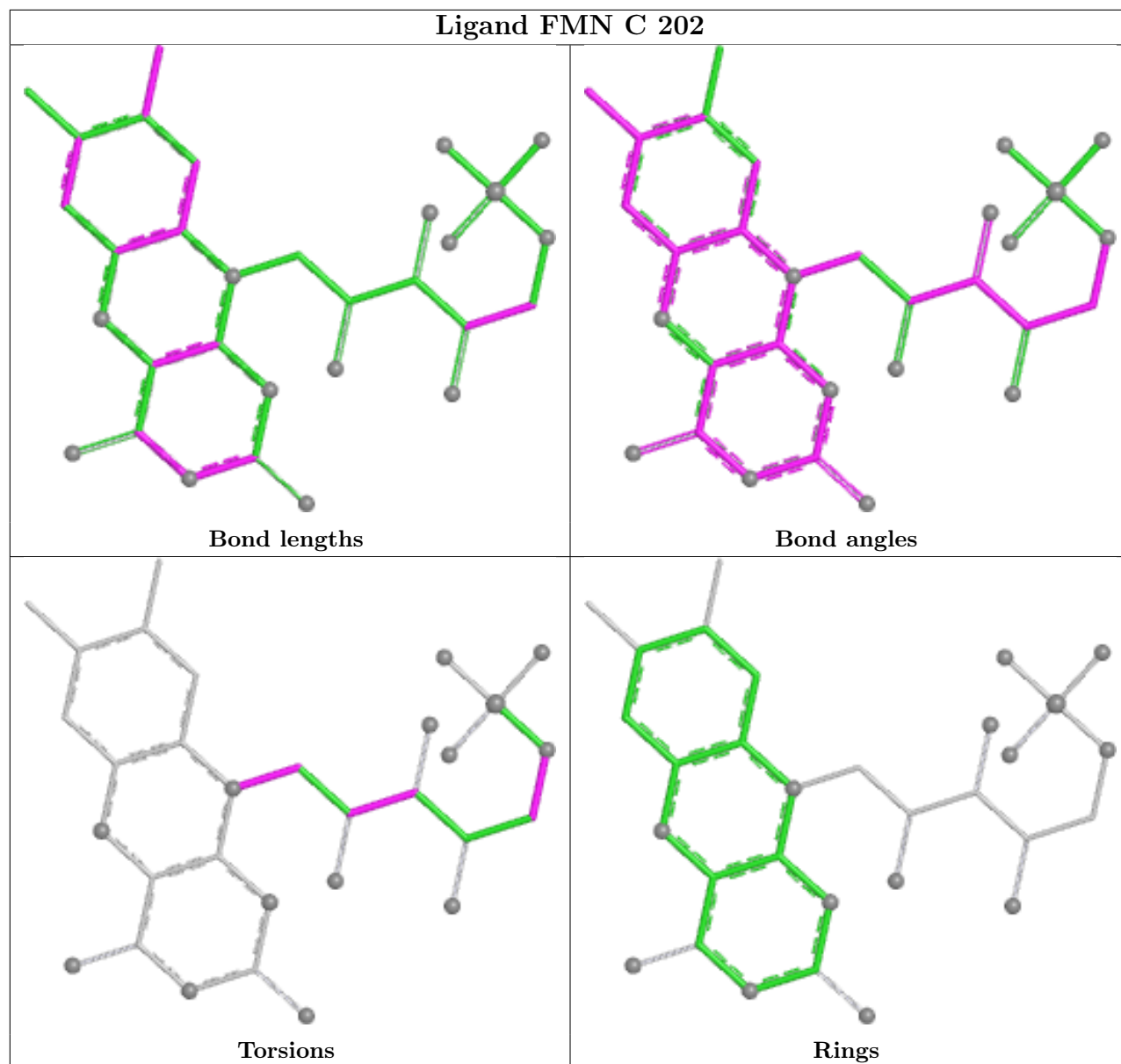
Mol	Chain	Res	Type	Atoms
3	C	202	FMN	C2'-C1'-N10-C10
3	C	202	FMN	C1'-C2'-C3'-O3'
3	C	202	FMN	C1'-C2'-C3'-C4'
3	C	202	FMN	O2'-C2'-C3'-O3'
3	C	202	FMN	O2'-C2'-C3'-C4'
3	B	201	FMN	C2'-C3'-C4'-O4'
3	C	202	FMN	C2'-C1'-N10-C9A
3	B	201	FMN	O3'-C3'-C4'-O4'
3	A	200	FMN	C2'-C3'-C4'-C5'
3	B	201	FMN	C2'-C3'-C4'-C5'
3	C	202	FMN	C4'-C5'-O5'-P
3	B	201	FMN	O3'-C3'-C4'-C5'
3	A	200	FMN	O2'-C2'-C3'-C4'
3	A	200	FMN	C1'-C2'-C3'-C4'

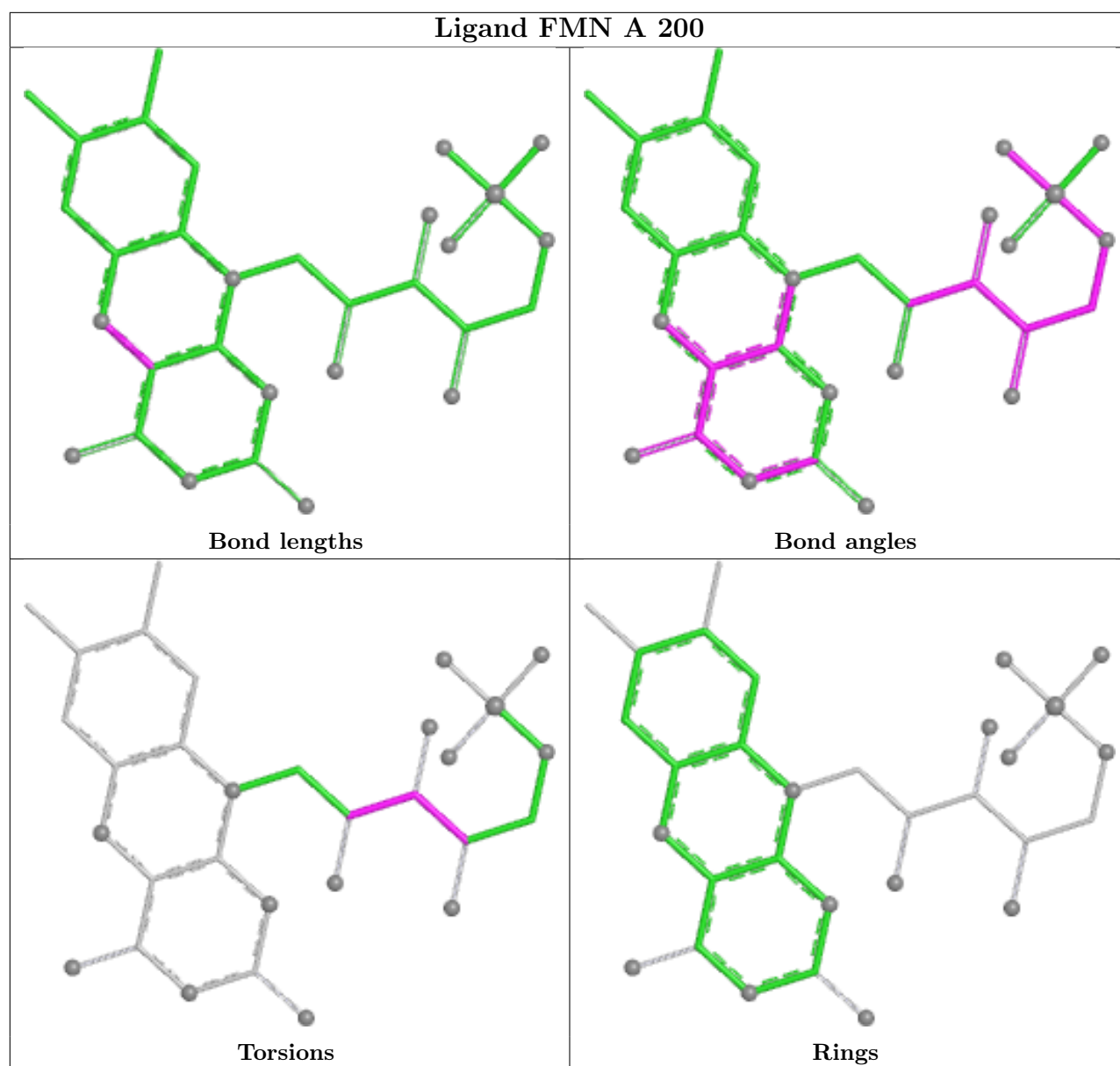
There are no ring outliers.

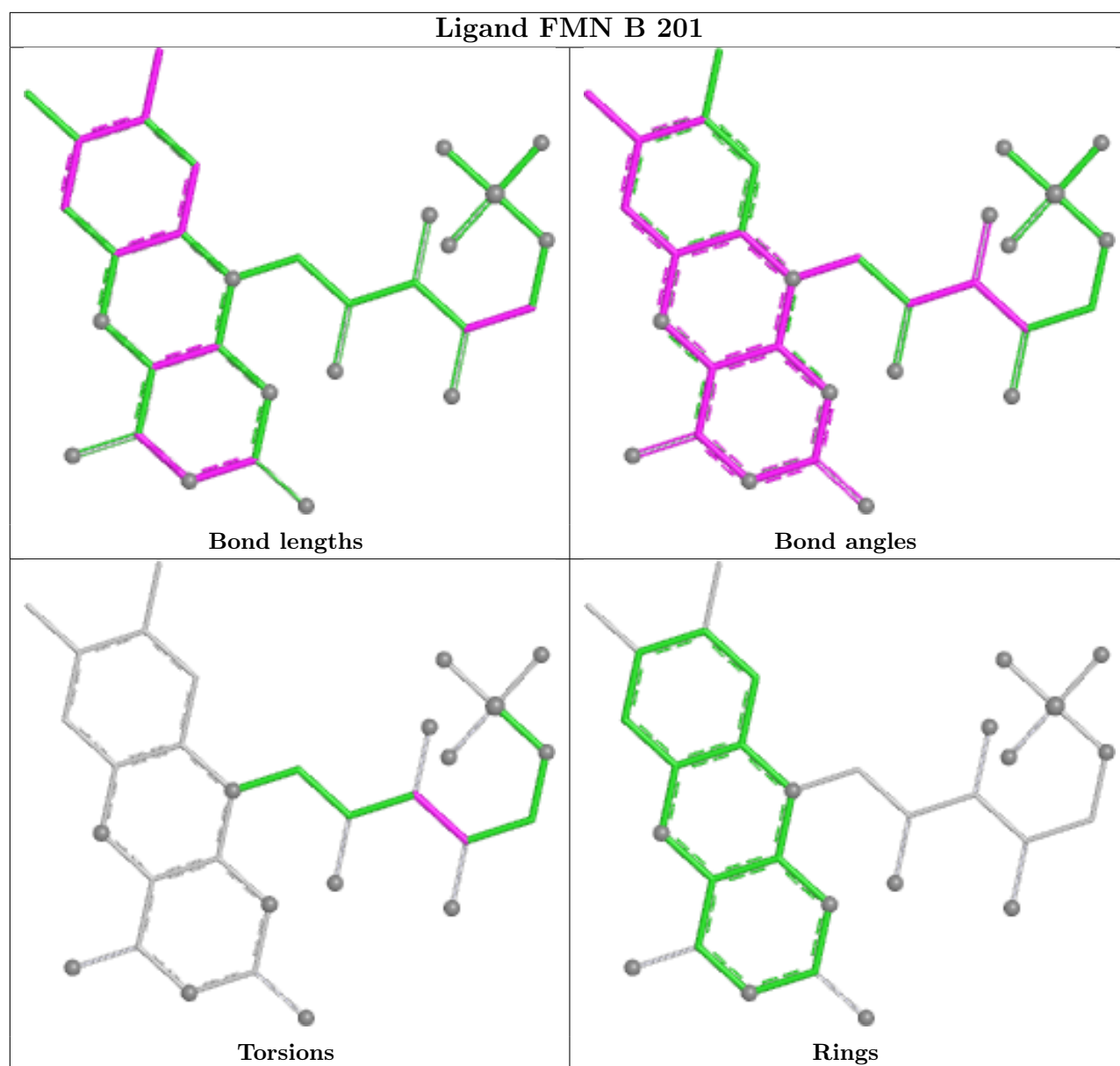
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	202	FMN	6	0
3	A	200	FMN	5	0
3	B	201	FMN	2	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 than 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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	179/206 (86%)	0.38	5 (2%) 55 57	18, 38, 78, 106	0
1	B	179/206 (86%)	0.89	27 (15%) 5 6	26, 46, 92, 117	0
1	C	179/206 (86%)	2.49	113 (63%) 0 0	33, 83, 122, 146	0
All	All	537/618 (86%)	1.26	145 (27%) 1 1	18, 54, 109, 146	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	181	ILE	7.2
1	C	144	VAL	6.7
1	C	81	LEU	6.6
1	C	182	ALA	5.7
1	C	82	LEU	5.7
1	C	163	VAL	5.3
1	C	143	PRO	5.3
1	C	73	LEU	5.3
1	C	52	VAL	5.3
1	C	12	GLY	5.1
1	C	142	ILE	4.9
1	C	16	THR	4.9
1	C	168	HIS	4.7
1	C	58	SER	4.6
1	C	178	HIS	4.3
1	C	162	LEU	4.2
1	C	184	PRO	4.2
1	B	69	GLY	4.1
1	C	20	LEU	4.0
1	C	15	ASN	4.0
1	C	34	ASN	4.0
1	C	69	GLY	3.9
1	C	150	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	158	ALA	3.8
1	C	7	TYR	3.8
1	C	167	ALA	3.7
1	C	5	ILE	3.7
1	C	160	THR	3.7
1	C	137	ALA	3.6
1	C	155	ALA	3.6
1	C	164	LEU	3.6
1	C	71	LEU	3.5
1	C	161	ALA	3.5
1	C	126	PHE	3.5
1	C	156	TRP	3.5
1	C	61	HIS	3.4
1	C	39	SER	3.4
1	C	77	ALA	3.4
1	C	40	VAL	3.4
1	C	91	GLY	3.3
1	C	8	PHE	3.3
1	C	35	PHE	3.3
1	C	148	VAL	3.3
1	B	71	LEU	3.2
1	C	22	LEU	3.2
1	C	165	THR	3.2
1	B	62	HIS	3.2
1	C	11	PRO	3.2
1	C	30	LEU	3.1
1	C	176	ARG	3.1
1	C	27	ALA	3.1
1	C	186	PRO	3.1
1	C	177	ILE	3.0
1	B	153	GLY	3.0
1	C	38	ALA	3.0
1	C	54	GLY	3.0
1	C	157	GLY	3.0
1	C	122	VAL	3.0
1	C	13	LYS	3.0
1	C	145	ASP	2.9
1	C	80	ALA	2.9
1	C	36	VAL	2.9
1	C	37	VAL	2.9
1	C	60	THR	2.9
1	B	74	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	77	ALA	2.9
1	C	65	PHE	2.9
1	C	18	ARG	2.9
1	C	72	GLU	2.9
1	C	56	ILE	2.8
1	A	54	GLY	2.8
1	C	123	SER	2.8
1	C	147	GLU	2.8
1	C	128	VAL	2.8
1	C	42	GLY	2.7
1	C	53	GLU	2.7
1	C	119	LEU	2.7
1	B	92	SER	2.7
1	C	129	CYS	2.7
1	C	149	ILE	2.7
1	B	110	THR	2.7
1	C	140	GLY	2.7
1	C	136	ALA	2.6
1	C	118	THR	2.6
1	B	43	GLU	2.6
1	B	139	ALA	2.6
1	C	159	ASP	2.6
1	C	31	GLY	2.6
1	C	139	ALA	2.6
1	C	24	GLY	2.6
1	A	82	LEU	2.5
1	C	185	ARG	2.5
1	C	79	ASP	2.5
1	A	107	GLY	2.5
1	C	86	VAL	2.5
1	C	130	VAL	2.5
1	C	68	LYS	2.5
1	B	156	TRP	2.5
1	C	180	VAL	2.5
1	C	127	LYS	2.5
1	B	80	ALA	2.4
1	B	101	GLY	2.4
1	B	78	ARG	2.4
1	C	89	TYR	2.4
1	C	49	SER	2.4
1	C	151	ILE	2.4
1	B	79	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	41	SER	2.3
1	C	138	ASP	2.3
1	B	70	GLN	2.3
1	C	25	GLU	2.3
1	C	55	ASN	2.3
1	C	84	ARG	2.3
1	C	134	ILE	2.3
1	C	154	THR	2.3
1	C	132	ILE	2.3
1	B	170	ASN	2.2
1	B	63	ALA	2.2
1	B	81	LEU	2.2
1	B	82	LEU	2.2
1	C	23	VAL	2.2
1	B	105	ARG	2.2
1	B	140	GLY	2.2
1	C	45	ALA	2.2
1	B	102	ILE	2.2
1	B	40	VAL	2.2
1	B	77	ALA	2.2
1	C	133	ALA	2.2
1	C	88	VAL	2.2
1	C	83	GLU	2.2
1	A	25	GLU	2.1
1	B	68	LYS	2.1
1	B	91	GLY	2.1
1	B	47	ARG	2.1
1	C	33	ARG	2.1
1	C	3	LYS	2.1
1	C	32	ILE	2.1
1	C	46	LEU	2.1
1	C	57	VAL	2.1
1	C	112	VAL	2.1
1	C	28	ASP	2.1
1	C	166	PRO	2.1
1	C	26	ARG	2.0
1	C	125	GLY	2.0
1	C	146	GLU	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 oligosaccharides in this entry.

6.4 Ligands

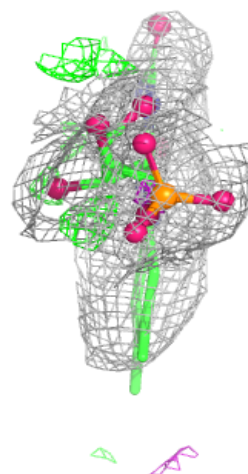
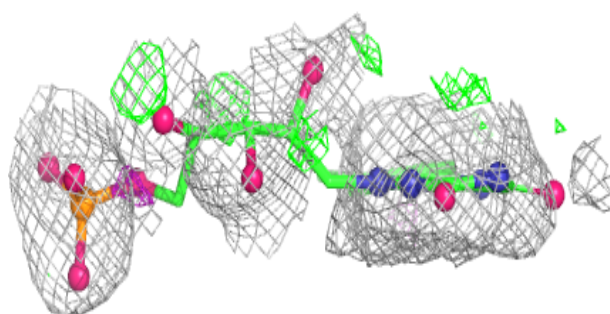
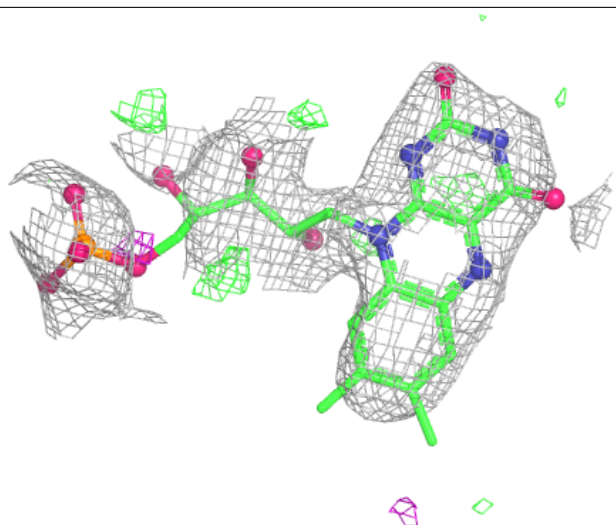
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	C	304	1/1	0.58	0.14	75,75,75,75	0
3	FMN	C	202	31/31	0.82	0.21	84,102,105,108	0
2	MG	B	303	1/1	0.85	0.21	71,71,71,71	0
3	FMN	A	200	31/31	0.91	0.10	29,39,54,58	0
3	FMN	B	201	31/31	0.92	0.12	23,48,71,76	0
2	MG	B	301	1/1	0.92	0.14	52,52,52,52	0
2	MG	A	302	1/1	0.95	0.06	46,46,46,46	0

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.

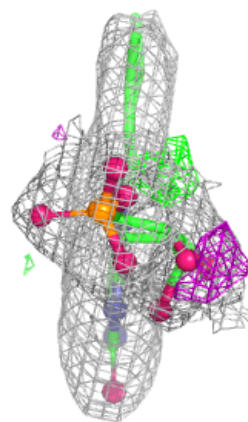
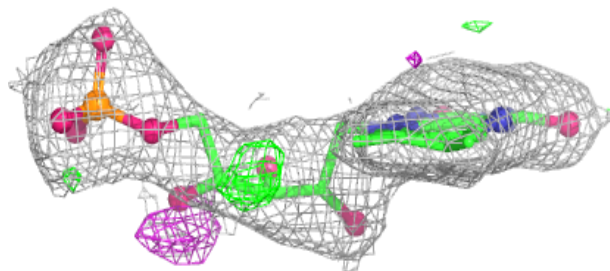
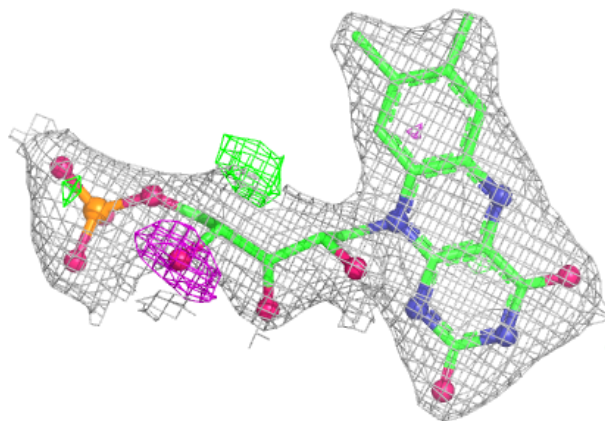
Electron density around FMN C 202:

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



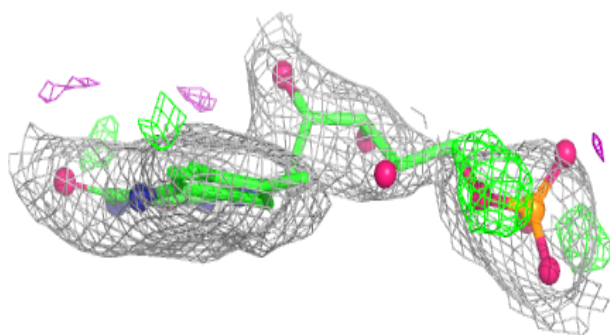
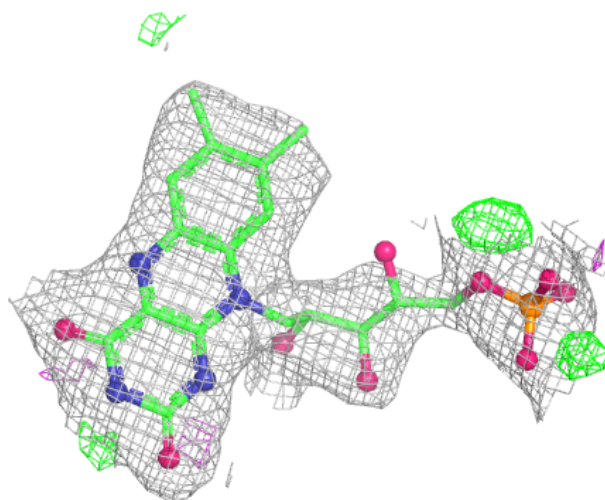
Electron density around FMN A 200:

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



Electron density around FMN B 201:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.