



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:26 PM UTC

PDB ID : 7VVV / pdb_00007vvv
Title : Crystal structure of MmtN
Authors : Peng, M.; Li, C.Y.
Deposited on : 2021-11-09
Resolution : 2.45 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
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

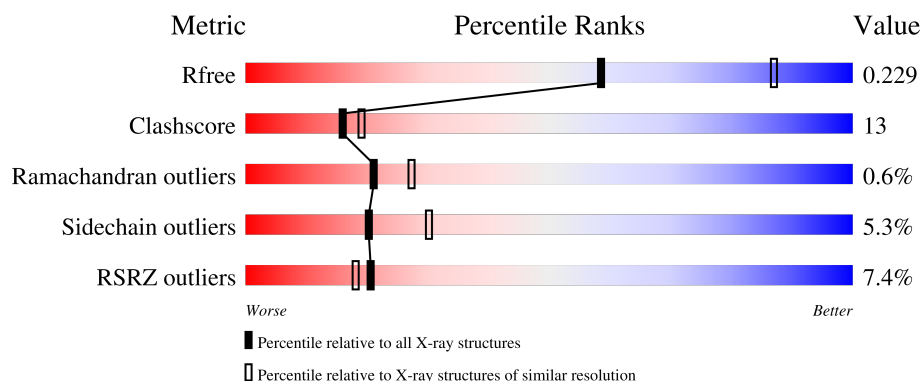
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	305	6% 64% 24% • 8%
1	B	305	7% 57% 22% 5% • 15%
1	C	305	7% 70% 15% • • 10%

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	PO4	A	401	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6304 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.

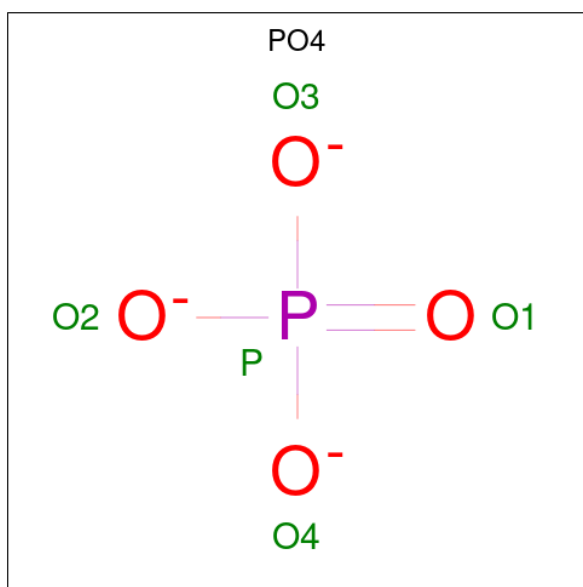
- Molecule 1 is a protein called SAM-dependent methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2132	1338	378	411	5			
1	B	258	Total	C	N	O	S	0	0	0
			1965	1240	341	379	5			
1	C	273	Total	C	N	O	S	0	0	0
			2075	1309	364	397	5			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
A	143	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
A	146	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
B	141	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
B	143	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
B	146	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
C	141	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
C	143	ALA	LYS	engineered mutation	UNP A0A0T5PCK9
C	146	ALA	LYS	engineered mutation	UNP A0A0T5PCK9

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		
3	B	45	Total	O	0	0
			45	45		
3	C	44	Total	O	0	0
			44	44		

- Molecule 1: SAM-dependent methyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.73Å 131.28Å 134.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.36 – 2.45 47.36 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.36-2.45) 98.7 (47.36-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.195 , 0.240 0.206 , 0.229	Depositor DCC
R_{free} test set	2257 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.938	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6304	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: PO4

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	1.54	29/2176 (1.3%)	1.01	19/2963 (0.6%)
1	B	1.61	30/2008 (1.5%)	1.06	7/2735 (0.3%)
1	C	1.15	14/2118 (0.7%)	0.84	13/2883 (0.5%)
All	All	1.45	73/6302 (1.2%)	0.97	39/8581 (0.5%)

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	42	VAL	C-O	-7.94	1.16	1.24
1	B	81	ASN	C-O	-7.29	1.15	1.24
1	A	42	VAL	C-O	-7.20	1.16	1.24
1	A	197	ASN	C-O	-7.04	1.15	1.24
1	C	291	ILE	C-O	-6.98	1.17	1.24
1	B	210	LEU	C-O	-6.87	1.16	1.24
1	A	294	ARG	CA-C	-6.80	1.47	1.52
1	B	65	VAL	C-O	-6.72	1.17	1.24
1	B	225	ILE	C-O	-6.67	1.16	1.24
1	B	219	GLU	C-O	-6.56	1.16	1.23
1	C	187	ALA	C-O	-6.50	1.15	1.24
1	A	98	GLY	C-O	-6.49	1.16	1.23
1	B	19	ASP	CA-C	-6.49	1.46	1.53
1	A	176	GLY	C-O	-6.42	1.16	1.23
1	B	93	PHE	C-O	-6.42	1.16	1.24
1	B	223	SER	C-O	-6.42	1.15	1.23
1	C	98	GLY	C-O	-6.40	1.17	1.24
1	B	188	THR	C-O	-6.29	1.15	1.24
1	A	292	ARG	C-O	-6.22	1.16	1.24
1	A	162	TRP	C-O	-6.11	1.17	1.24
1	B	227	LEU	CA-C	-5.99	1.45	1.52
1	A	211	PHE	C-O	-5.99	1.17	1.24
1	A	178	ASN	C-O	-5.99	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	GLN	C-O	-5.96	1.17	1.24
1	B	178	ASN	C-O	-5.93	1.17	1.24
1	C	171	ASN	C-O	-5.92	1.16	1.24
1	C	292	ARG	C-O	-5.85	1.17	1.24
1	B	41	ARG	C-O	-5.85	1.17	1.23
1	C	255	CYS	C-O	-5.83	1.16	1.23
1	B	202	VAL	C-O	-5.83	1.17	1.24
1	C	41	ARG	C-O	-5.82	1.17	1.24
1	B	92	ARG	C-O	-5.79	1.16	1.24
1	A	226	VAL	C-O	-5.73	1.17	1.23
1	B	115	SER	C-O	-5.70	1.16	1.23
1	C	62	ALA	C-O	-5.68	1.16	1.23
1	A	201	ARG	C-O	-5.66	1.17	1.24
1	B	208	PHE	N-CA	-5.62	1.39	1.46
1	A	200	ALA	C-O	-5.61	1.16	1.24
1	B	80	ARG	CA-C	-5.59	1.46	1.52
1	B	64	LEU	C-O	-5.56	1.16	1.23
1	C	258	TYR	C-O	-5.55	1.17	1.23
1	A	184	ARG	C-O	-5.54	1.17	1.24
1	C	256	GLU	C-O	-5.50	1.17	1.24
1	C	294	ARG	C-O	-5.48	1.18	1.24
1	A	95	PRO	C-O	-5.45	1.16	1.24
1	A	180	ALA	C-O	-5.43	1.17	1.24
1	A	181	LEU	C-O	-5.42	1.17	1.24
1	A	198	PHE	C-O	-5.36	1.17	1.23
1	A	202	VAL	C-O	-5.33	1.17	1.24
1	A	110	ALA	C-O	-5.33	1.18	1.24
1	A	22	ASP	N-CA	-5.31	1.41	1.46
1	B	218	PRO	C-O	-5.31	1.17	1.23
1	A	27	THR	C-O	-5.26	1.18	1.24
1	A	28	PHE	C-O	-5.26	1.18	1.24
1	B	226	VAL	C-O	-5.25	1.18	1.23
1	A	163	ALA	C-O	-5.25	1.17	1.24
1	A	108	ALA	C-O	-5.21	1.18	1.24
1	B	114	ARG	C-O	-5.21	1.16	1.23
1	B	224	GLN	C-O	-5.20	1.17	1.23
1	B	284	ILE	C-O	-5.20	1.18	1.24
1	C	162	TRP	N-CA	-5.19	1.40	1.46
1	B	190	PRO	C-O	-5.17	1.16	1.24
1	B	108	ALA	C-O	-5.12	1.18	1.24
1	C	40	LYS	C-O	-5.12	1.17	1.23
1	A	213	ALA	C-O	-5.11	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	LYS	C-O	-5.10	1.17	1.23
1	B	228	GLN	CA-C	-5.09	1.46	1.52
1	B	266	ARG	C-O	-5.07	1.17	1.23
1	A	103	ILE	C-O	-5.06	1.18	1.24
1	B	163	ALA	C-O	-5.05	1.17	1.24
1	C	165	PHE	C-O	-5.05	1.17	1.24
1	A	19	ASP	CA-C	-5.00	1.46	1.52
1	A	41	ARG	C-O	-5.00	1.18	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	TRP	N-CA-C	9.24	130.48	110.80
1	B	277	ASP	N-CA-C	-8.81	102.31	113.23
1	C	244	LEU	N-CA-C	8.59	122.07	112.97
1	B	97	GLU	N-CA-C	-7.98	98.06	110.42
1	B	244	LEU	N-CA-C	-7.94	100.64	110.41
1	B	17	ALA	N-CA-C	7.92	119.99	111.36
1	A	200	ALA	N-CA-C	7.49	121.31	112.93
1	C	230	ALA	N-CA-C	7.44	119.39	111.28
1	C	161	PRO	CA-C-N	-7.14	111.28	122.49
1	C	161	PRO	C-N-CA	-7.14	111.28	122.49
1	C	42	VAL	N-CA-C	6.99	119.52	108.89
1	B	190	PRO	N-CA-C	6.86	122.83	113.98
1	C	160	TYR	N-CA-C	-6.80	99.36	109.42
1	A	150	THR	N-CA-C	6.48	119.76	109.65
1	C	277	ASP	N-CA-C	-6.32	104.27	112.23
1	A	198	PHE	N-CA-C	6.28	118.96	109.23
1	A	159	TYR	CA-C-N	6.25	132.94	121.70
1	A	159	TYR	C-N-CA	6.25	132.94	121.70
1	A	59	ILE	CB-CA-C	-6.15	104.19	111.94
1	C	252	GLU	N-CA-C	-6.06	99.84	109.59
1	A	160	TYR	CA-C-N	-5.96	114.61	120.98
1	A	160	TYR	C-N-CA	-5.96	114.61	120.98
1	A	97	GLU	N-CA-C	5.95	118.59	110.55
1	A	18	PHE	N-CA-C	5.93	118.42	110.35
1	A	42	VAL	N-CA-C	5.80	116.83	108.48
1	B	278	THR	N-CA-C	-5.80	104.33	111.40
1	A	294	ARG	CA-C-N	-5.78	114.64	120.31
1	A	294	ARG	C-N-CA	-5.78	114.64	120.31
1	A	277	ASP	N-CA-C	-5.77	106.58	113.97
1	C	97	GLU	N-CA-C	5.64	118.86	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ASP	N-CA-C	5.61	122.75	110.80
1	A	19	ASP	N-CA-C	-5.61	102.71	109.72
1	C	160	TYR	CA-C-N	-5.54	114.89	120.21
1	C	160	TYR	C-N-CA	-5.54	114.89	120.21
1	C	171	ASN	N-CA-C	-5.39	106.21	112.89
1	A	163	ALA	N-CA-C	5.32	117.83	111.71
1	A	246	GLN	N-CA-C	-5.18	105.75	111.71
1	C	255	CYS	N-CA-C	-5.16	103.88	110.53
1	A	86	ALA	O-C-N	5.07	125.07	121.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	2132	0	2062	62	0
1	B	1965	0	1898	67	0
1	C	2075	0	2015	45	0
2	A	5	0	0	2	0
3	A	38	0	0	0	0
3	B	45	0	0	1	0
3	C	44	0	0	0	0
All	All	6304	0	5975	160	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 13.

All (160) 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:244:LEU:HD12	1:C:249:LEU:O	1.44	1.18
1:A:162:TRP:CH2	1:B:251:ARG:HB2	1.85	1.11
1:A:279:ASP:OD1	1:A:280:SER:N	1.93	1.00
1:A:157:ALA:HB1	1:A:159:TYR:CE2	1.98	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ARG:HH21	1:A:88:ARG:HG3	1.27	0.96
1:A:162:TRP:HH2	1:B:251:ARG:CB	1.80	0.94
1:A:162:TRP:HH2	1:B:251:ARG:HB2	1.23	0.93
1:A:162:TRP:CH2	1:B:251:ARG:HA	2.05	0.92
1:B:227:LEU:HD12	1:B:285:TYR:CE1	2.06	0.89
1:C:143:ALA:C	1:C:144:LEU:HD23	1.97	0.89
1:A:261:PRO:HD3	1:A:285:TYR:CZ	2.07	0.88
1:C:247:THR:HB	1:C:249:LEU:HD21	1.56	0.88
1:C:249:LEU:H	1:C:249:LEU:HD23	1.40	0.87
1:A:19:ASP:OD1	1:A:21:THR:HG23	1.76	0.85
1:C:143:ALA:O	1:C:144:LEU:HD23	1.76	0.85
1:B:128:PRO:O	1:B:131:VAL:HG13	1.77	0.84
1:A:156:ILE:HG22	1:A:157:ALA:H	1.43	0.83
1:A:261:PRO:HD3	1:A:285:TYR:CE1	2.14	0.83
1:A:70:LEU:HD23	1:A:159:TYR:HB3	1.60	0.81
1:A:162:TRP:CH2	1:B:251:ARG:CB	2.57	0.80
1:C:144:LEU:HA	1:C:145:ALA:C	2.06	0.80
1:C:249:LEU:HD23	1:C:249:LEU:N	1.96	0.79
1:A:157:ALA:HB1	1:A:159:TYR:CD2	2.17	0.79
1:B:247:THR:OG1	1:B:248:GLY:HA2	1.82	0.78
1:B:273:GLN:O	1:B:273:GLN:NE2	2.12	0.78
1:B:160:TYR:HB3	1:B:161:PRO:CD	2.14	0.77
1:C:244:LEU:HD12	1:C:249:LEU:C	2.10	0.77
1:B:130:ASP:OD1	1:B:131:VAL:N	2.18	0.77
1:C:252:GLU:OE2	1:C:253:PHE:N	2.17	0.77
1:C:73:ARG:HH21	1:C:139:ALA:HB1	1.52	0.74
1:C:244:LEU:CD1	1:C:249:LEU:O	2.33	0.73
1:A:183:ARG:NH2	2:A:401:PO4:O4	2.20	0.73
1:A:162:TRP:CZ3	1:B:251:ARG:HB2	2.23	0.73
1:B:251:ARG:O	1:B:251:ARG:HG3	1.88	0.72
1:C:279:ASP:O	1:C:280:SER:HB2	1.88	0.72
1:A:156:ILE:HG22	1:A:157:ALA:N	2.02	0.72
1:B:250:GLU:O	1:B:251:ARG:HB3	1.88	0.71
1:A:162:TRP:CH2	1:B:251:ARG:CA	2.74	0.71
1:B:243:ALA:O	1:B:251:ARG:HG2	1.90	0.70
1:B:273:GLN:HE21	1:B:273:GLN:C	1.99	0.70
1:B:228:GLN:OE1	1:B:232:THR:HB	1.92	0.70
1:C:247:THR:CB	1:C:249:LEU:HD21	2.23	0.69
1:C:244:LEU:O	1:C:245:ALA:HB3	1.91	0.69
1:B:71:ASP:OD1	1:B:73:ARG:HD3	1.93	0.69
1:B:286:HIS:NE2	3:B:402:HOH:O	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ARG:O	1:B:92:ARG:HG3	1.93	0.68
1:B:102:LEU:H	1:B:160:TYR:HE2	1.41	0.68
1:C:126:GLY:O	1:C:201:ARG:NH2	2.27	0.67
1:B:252:GLU:N	1:B:252:GLU:OE2	2.27	0.67
1:C:193:ASP:OD1	1:C:294:ARG:HD3	1.95	0.66
1:C:250:GLU:HG3	1:C:251:ARG:N	2.11	0.66
1:A:88:ARG:HG3	1:A:88:ARG:NH2	2.02	0.66
1:B:252:GLU:O	1:B:252:GLU:HG2	1.98	0.63
1:A:30:ARG:HG2	1:A:30:ARG:HH11	1.62	0.62
1:C:244:LEU:CD1	1:C:250:GLU:HA	2.30	0.61
1:B:72:PRO:HG3	1:B:99:ALA:HB2	1.83	0.61
1:A:44:GLU:HG3	1:A:119:VAL:HG23	1.83	0.60
1:C:254:THR:CG2	1:C:268:SER:HB3	2.31	0.60
1:B:249:LEU:O	1:B:250:GLU:HG3	2.01	0.60
1:B:247:THR:CB	1:B:248:GLY:HA2	2.29	0.60
1:B:102:LEU:HD21	1:B:177:LEU:HD11	1.82	0.60
1:B:247:THR:N	1:B:248:GLY:HA2	2.15	0.59
1:B:245:ALA:O	1:B:246:GLN:HG3	2.02	0.59
1:B:131:VAL:HG23	1:B:131:VAL:O	2.01	0.59
1:C:247:THR:HB	1:C:249:LEU:CD2	2.29	0.59
1:A:19:ASP:OD1	1:A:21:THR:N	2.34	0.57
1:A:162:TRP:CZ2	1:B:251:ARG:HA	2.39	0.57
1:C:254:THR:HG22	1:C:268:SER:HB3	1.86	0.57
1:B:227:LEU:CD1	1:B:285:TYR:CE1	2.85	0.56
1:A:73:ARG:NH2	1:A:156:ILE:O	2.34	0.56
1:A:193:ASP:OD1	1:A:294:ARG:HD3	2.05	0.56
1:C:30:ARG:HD2	1:C:224:GLN:NE2	2.20	0.56
1:A:158:HIS:C	1:A:159:TYR:CD1	2.84	0.56
1:A:88:ARG:HH21	1:A:88:ARG:CG	2.09	0.55
1:B:245:ALA:O	1:B:246:GLN:CG	2.54	0.55
1:B:276:VAL:O	1:B:276:VAL:HG12	2.05	0.55
1:A:122:LEU:HD11	1:A:181:LEU:HD22	1.88	0.55
1:A:156:ILE:CG2	1:A:157:ALA:H	2.18	0.54
1:A:157:ALA:CB	1:A:159:TYR:CE2	2.82	0.54
1:A:162:TRP:N	1:A:162:TRP:CD1	2.75	0.54
1:A:236:PHE:HE1	1:B:247:THR:HB	1.71	0.54
1:C:276:VAL:O	1:C:276:VAL:HG12	2.08	0.54
1:B:227:LEU:HD12	1:B:285:TYR:CZ	2.42	0.53
1:B:275:LEU:HD12	1:B:275:LEU:N	2.23	0.53
1:A:156:ILE:CG2	1:A:157:ALA:N	2.72	0.53
1:A:80:ARG:O	1:A:83:ARG:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:PO4:O2	1:C:183:ARG:NH2	2.38	0.53
1:A:162:TRP:CH2	1:B:251:ARG:HD3	2.44	0.52
1:A:164:GLU:O	1:B:209:GLU:HG2	2.10	0.52
1:A:119:VAL:HG12	1:A:195:VAL:HB	1.92	0.51
1:C:247:THR:CB	1:C:249:LEU:CD2	2.87	0.51
1:B:273:GLN:NE2	1:B:273:GLN:CA	2.73	0.51
1:B:160:TYR:HB3	1:B:161:PRO:HD3	1.93	0.50
1:B:128:PRO:O	1:B:131:VAL:CG1	2.55	0.50
1:B:119:VAL:HG12	1:B:195:VAL:HB	1.94	0.50
1:A:41:ARG:HD3	1:A:114:ARG:O	2.12	0.50
1:B:249:LEU:O	1:B:250:GLU:CG	2.60	0.50
1:A:272:ALA:HB1	1:A:284:ILE:HD13	1.93	0.49
1:B:261:PRO:HD3	1:B:285:TYR:CZ	2.47	0.49
1:C:14:PRO:HB2	1:C:16:PHE:CD2	2.47	0.49
1:C:142:ALA:C	1:C:144:LEU:H	2.21	0.49
1:A:30:ARG:HG2	1:A:30:ARG:NH1	2.28	0.48
1:A:70:LEU:CD2	1:A:159:TYR:HB3	2.37	0.48
1:B:89:ARG:HH11	1:B:92:ARG:NH1	2.11	0.48
1:B:124:GLN:O	1:B:127:GLU:HG2	2.13	0.48
1:B:271:GLU:O	1:B:274:ALA:HB3	2.13	0.48
1:A:260:ASP:CG	1:A:264:ALA:H	2.21	0.48
1:C:247:THR:O	1:C:249:LEU:HD23	2.14	0.48
1:A:53:VAL:HG11	1:A:93:PHE:CD1	2.48	0.47
1:A:250:GLU:OE1	1:A:250:GLU:HA	2.13	0.47
1:A:260:ASP:OD1	1:A:265:THR:HG22	2.15	0.47
1:B:275:LEU:N	1:B:275:LEU:CD1	2.77	0.47
1:A:200:ALA:HB3	1:A:287:GLU:HB3	1.97	0.47
1:B:260:ASP:OD1	1:B:265:THR:N	2.39	0.47
1:C:249:LEU:N	1:C:249:LEU:CD2	2.72	0.47
1:B:64:LEU:HD23	1:B:65:VAL:N	2.30	0.46
1:B:161:PRO:O	1:B:162:TRP:CB	2.62	0.46
1:A:247:THR:HB	1:A:249:LEU:HG	1.98	0.46
1:A:261:PRO:CD	1:A:285:TYR:CZ	2.92	0.46
1:C:144:LEU:HA	1:C:146:ALA:N	2.30	0.45
1:B:66:SER:OG	1:B:111:GLN:HG2	2.16	0.45
1:B:273:GLN:NE2	1:B:273:GLN:HA	2.31	0.45
1:B:274:ALA:C	1:B:276:VAL:N	2.73	0.45
1:C:30:ARG:HD2	1:C:224:GLN:HE21	1.82	0.45
1:A:162:TRP:HH2	1:B:251:ARG:HD3	1.81	0.45
1:A:247:THR:HG22	1:C:236:PHE:CE2	2.52	0.44
1:C:142:ALA:C	1:C:144:LEU:N	2.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ASP:HB2	1:B:20:PRO:HD2	1.98	0.44
1:B:260:ASP:CG	1:B:264:ALA:H	2.25	0.44
1:B:247:THR:CB	1:B:248:GLY:CA	2.96	0.44
1:A:58:GLN:OE1	1:A:86:ALA:HB2	2.17	0.44
1:C:247:THR:C	1:C:249:LEU:HD23	2.42	0.44
1:A:158:HIS:O	1:A:159:TYR:CD1	2.70	0.44
1:C:111:GLN:NE2	1:C:114:ARG:NH1	2.66	0.44
1:C:244:LEU:HA	1:C:244:LEU:HD13	1.80	0.44
1:C:252:GLU:O	1:C:253:PHE:HB2	2.17	0.43
1:A:88:ARG:HD3	1:A:88:ARG:HA	1.88	0.43
1:B:270:THR:O	1:B:271:GLU:C	2.58	0.43
1:A:156:ILE:O	1:A:157:ALA:HB2	2.18	0.43
1:B:261:PRO:HD3	1:B:285:TYR:CE2	2.54	0.43
1:A:79:GLU:HG3	1:A:95:PRO:HG3	2.01	0.42
1:A:153:GLU:CD	1:A:153:GLU:H	2.27	0.42
1:C:14:PRO:HG2	1:C:16:PHE:CE2	2.55	0.42
1:A:162:TRP:CD1	1:A:162:TRP:H	2.38	0.41
1:B:274:ALA:O	1:B:276:VAL:N	2.52	0.41
1:A:105:THR:O	1:A:106:PRO:C	2.61	0.41
1:C:244:LEU:HD11	1:C:250:GLU:HA	2.02	0.41
1:A:236:PHE:CE1	1:B:247:THR:HB	2.53	0.41
1:C:166:ASP:HA	1:C:171:ASN:ND2	2.35	0.41
1:B:274:ALA:C	1:B:276:VAL:H	2.29	0.41
1:C:201:ARG:HD3	1:C:257:PHE:CE2	2.55	0.41
1:C:52:ASN:O	1:C:56:MET:HG3	2.20	0.41
1:A:109:ARG:HH11	1:A:109:ARG:HD2	1.74	0.41
1:B:260:ASP:CG	1:B:264:ALA:HB3	2.46	0.41
1:A:19:ASP:OD1	1:A:20:PRO:HD2	2.21	0.41
1:B:102:LEU:HD21	1:B:177:LEU:CD1	2.47	0.40
1:C:142:ALA:O	1:C:144:LEU:N	2.54	0.40
1:C:161:PRO:HG2	1:C:164:GLU:OE2	2.22	0.40
1:A:88:ARG:NH2	1:A:88:ARG:CG	2.72	0.40
1:C:71:ASP:HB2	1:C:159:TYR:HE2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/305 (91%)	264 (95%)	14 (5%)	0	100	100
1	B	254/305 (83%)	237 (93%)	13 (5%)	4 (2%)	7	7
1	C	269/305 (88%)	255 (95%)	13 (5%)	1 (0%)	30	37
All	All	801/915 (88%)	756 (94%)	40 (5%)	5 (1%)	21	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	245	ALA
1	B	251	ARG
1	C	280	SER
1	B	162	TRP
1	B	246	GLN

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	215/238 (90%)	205 (95%)	10 (5%)	23	35
1	B	202/238 (85%)	188 (93%)	14 (7%)	14	19
1	C	209/238 (88%)	200 (96%)	9 (4%)	26	38
All	All	626/714 (88%)	593 (95%)	33 (5%)	20	30

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	41	ARG
1	A	80	ARG
1	A	81	ASN
1	A	84	ASP
1	A	88	ARG
1	A	107	GLU
1	A	250	GLU
1	A	266	ARG
1	A	280	SER
1	B	21	THR
1	B	41	ARG
1	B	92	ARG
1	B	97	GLU
1	B	107	GLU
1	B	129	ASP
1	B	235	SER
1	B	238	VAL
1	B	244	LEU
1	B	247	THR
1	B	250	GLU
1	B	251	ARG
1	B	266	ARG
1	B	278	THR
1	C	144	LEU
1	C	159	TYR
1	C	244	LEU
1	C	249	LEU
1	C	250	GLU
1	C	251	ARG
1	C	252	GLU
1	C	254	THR
1	C	280	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	155	HIS
1	A	171	ASN
1	A	178	ASN
1	A	224	GLN
1	B	58	GLN

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Mol	Chain	Res	Type
1	B	224	GLN
1	C	178	ASN
1	C	224	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	PO4	A	401	-	4,4,4	0.98	0	6,6,6	0.46	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	280/305 (91%)	0.47	17 (6%) 27 24	30, 58, 86, 95	0
1	B	258/305 (84%)	0.48	21 (8%) 18 16	37, 51, 92, 109	0
1	C	273/305 (89%)	0.33	22 (8%) 18 16	35, 50, 85, 106	0
All	All	811/915 (88%)	0.43	60 (7%) 20 18	30, 54, 88, 109	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	THR	6.1
1	B	244	LEU	5.9
1	C	147	GLY	5.8
1	B	11	PRO	5.6
1	B	162	TRP	4.9
1	A	159	TYR	4.7
1	C	248	GLY	4.6
1	A	158	HIS	4.6
1	B	249	LEU	4.6
1	B	245	ALA	4.3
1	A	160	TYR	4.3
1	C	162	TRP	4.0
1	C	144	LEU	4.0
1	C	245	ALA	3.9
1	B	284	ILE	3.7
1	A	246	GLN	3.6
1	A	161	PRO	3.6
1	C	246	GLN	3.4
1	A	245	ALA	3.3
1	B	131	VAL	3.3
1	C	249	LEU	3.1
1	B	246	GLN	3.0
1	A	17	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	244	LEU	2.9
1	C	142	ALA	2.9
1	C	145	ALA	2.8
1	C	159	TYR	2.8
1	C	97	GLU	2.7
1	B	231	GLY	2.7
1	B	296	ALA	2.7
1	A	278	THR	2.7
1	C	143	ALA	2.7
1	B	243	ALA	2.6
1	C	252	GLU	2.6
1	A	162	TRP	2.6
1	C	296	ALA	2.5
1	A	87	PRO	2.5
1	B	248	GLY	2.5
1	C	247	THR	2.4
1	C	141	ALA	2.3
1	A	157	ALA	2.3
1	A	244	LEU	2.3
1	A	251	ARG	2.3
1	B	278	THR	2.2
1	B	250	GLU	2.2
1	A	18	PHE	2.2
1	C	253	PHE	2.2
1	C	275	LEU	2.2
1	A	91	ASP	2.2
1	B	283	GLU	2.2
1	C	160	TYR	2.1
1	A	63	ALA	2.1
1	B	160	TYR	2.1
1	B	275	LEU	2.1
1	C	250	GLU	2.1
1	B	251	ARG	2.0
1	C	251	ARG	2.0
1	A	296	ALA	2.0
1	B	91	ASP	2.0
1	B	229	HIS	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 [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	PO4	A	401	5/5	0.94	0.31	41,43,45,54	5

6.5 Other polymers [i](#)

There are no such residues in this entry.