



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:23 pm GMT

PDB ID : 4A95
Title : Plasmodium vivax N-myristoyltransferase with quinoline inhibitor
Authors : Goncalves, V.; Brannigan, J.A.; Whalley, D.; Ansell, K.H.; Saxty, B.; Holder, A.A.; Wilkinson, A.J.; Tate, E.W.; Leatherbarrow, R.J.
Deposited on : 2011-11-24
Resolution : 1.55 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

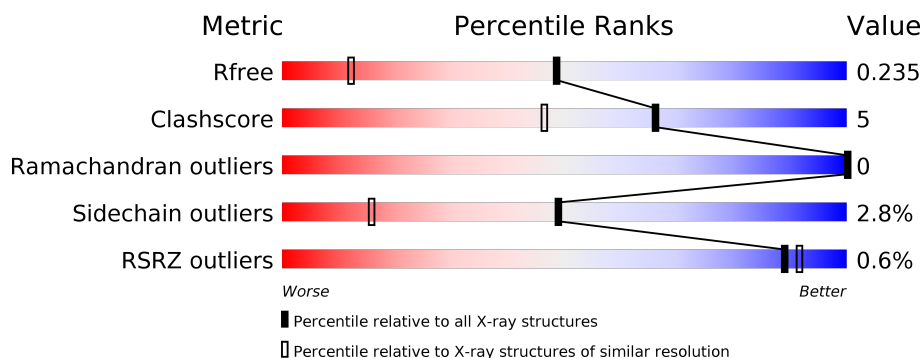
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	100719	1088 (1.56-1.56)
Clashscore	112137	1132 (1.56-1.56)
Ramachandran outliers	110173	1110 (1.56-1.56)
Sidechain outliers	110143	1108 (1.56-1.56)
RSRZ outliers	101464	1089 (1.56-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	384	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 87%; height: 10px; background-color: red;"></div> <div style="width: 11%; height: 10px; background-color: orange;"></div> <div style="width: 2%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: green;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> </div> </div>
1	B	384	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 89%; height: 10px; background-color: red;"></div> <div style="width: 11%; height: 10px; background-color: orange;"></div> <div style="width: 0%; height: 10px; background-color: yellow;"></div> <div style="width: 0%; height: 10px; background-color: green;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> </div> </div>
1	C	384	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 83%; height: 10px; background-color: red;"></div> <div style="width: 11%; height: 10px; background-color: orange;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: green;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> </div> </div>

2 Entry composition [i](#)

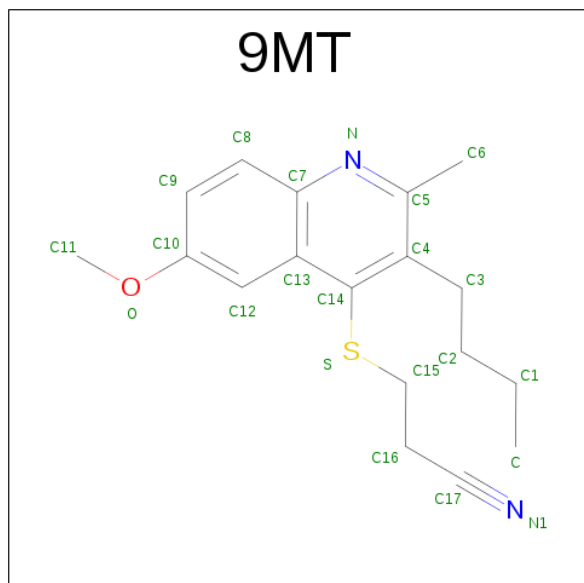
There are 7 unique types of molecules in this entry. The entry contains 11498 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	17	0
			3279	2132	535	600	12			
1	B	384	Total	C	N	O	S	0	18	0
			3282	2139	532	599	12			
1	C	366	Total	C	N	O	S	0	14	0
			3126	2039	501	575	11			

- Molecule 2 is 3-(3-BUTYL-6-METHOXY-2-METHYL-QUINOLIN-4-YL)SULFANYLPROPANENITRILE (three-letter code: 9MT) (formula: C₁₈H₂₂N₂OS).



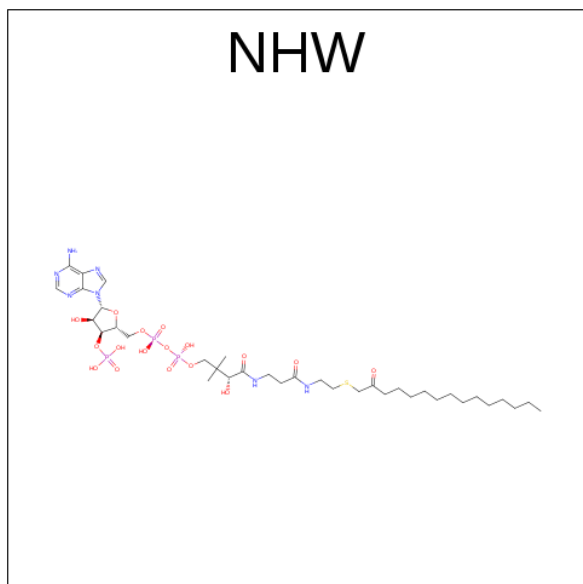
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			22	18	2	1	1		
2	B	1	Total	C	N	O	S	0	0
			22	18	2	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			22	18	2	1	1		

- Molecule 3 is 2-OXOPENTADECYL-COA (three-letter code: NHW) (formula: $C_{36}H_{64}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

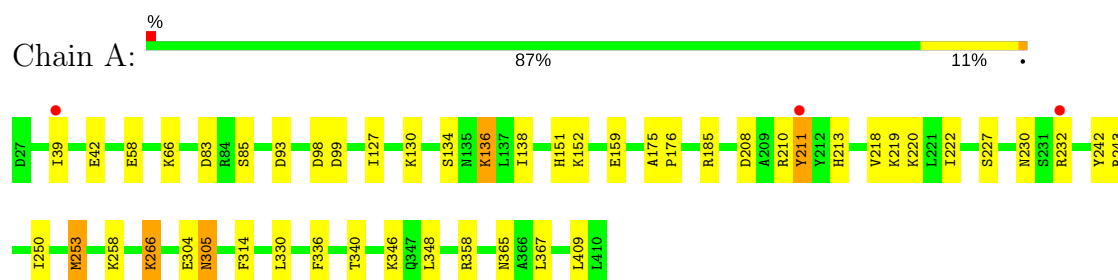
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	574	Total	O	0	0
			574	574		
7	B	522	Total	O	0	0
			522	522		
7	C	446	Total	O	0	0
			446	446		

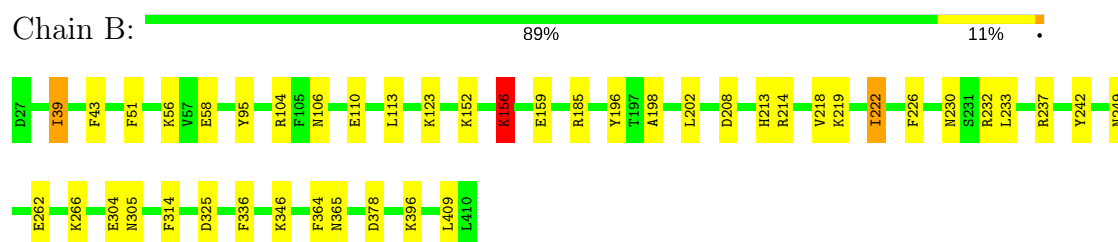
3 Residue-property plots

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

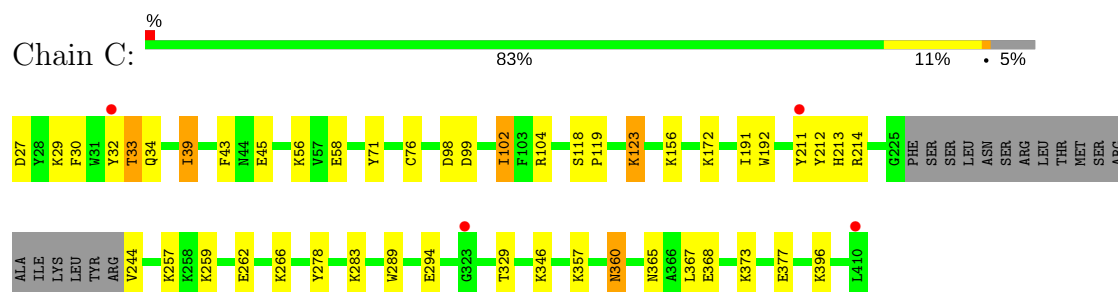
• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.49Å 121.56Å 179.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.08 – 1.55 60.78 – 1.55	Depositor EDS
% Data completeness (in resolution range)	85.3 (72.08-1.55) 85.3 (60.78-1.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.186 , 0.236 0.186 , 0.235	Depositor DCC
R_{free} test set	7732 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11498	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: NHW, SO4, MG, 9MT, CL

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	1.20	3/3389 (0.1%)	1.06	7/4586 (0.2%)
1	B	1.19	6/3404 (0.2%)	1.08	9/4603 (0.2%)
1	C	1.17	5/3235 (0.2%)	1.01	2/4381 (0.0%)
All	All	1.18	14/10028 (0.1%)	1.05	18/13570 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	ALA	CA-CB	5.81	1.64	1.52
1	C	377	GLU	CG-CD	-5.79	1.43	1.51
1	C	368	GLU	CD-OE1	-5.77	1.19	1.25
1	A	314	PHE	CE1-CZ	5.60	1.48	1.37
1	A	211[A]	TYR	CD1-CE1	5.40	1.47	1.39
1	A	211[B]	TYR	CD1-CE1	5.40	1.47	1.39
1	B	95	TYR	CD2-CE2	5.38	1.47	1.39
1	C	368	GLU	CD-OE2	-5.36	1.19	1.25
1	B	364	PHE	CE2-CZ	5.27	1.47	1.37
1	C	192	TRP	CE3-CZ3	5.19	1.47	1.38
1	B	314	PHE	CE2-CZ	5.17	1.47	1.37
1	C	71	TYR	CE1-CZ	5.14	1.45	1.38
1	B	51	PHE	CE2-CZ	5.12	1.47	1.37
1	B	196	TYR	CG-CD2	5.05	1.45	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156[A]	LYS	CD-CE-NZ	6.66	127.02	111.70
1	B	156[B]	LYS	CD-CE-NZ	6.66	127.02	111.70
1	A	208	ASP	CB-CG-OD1	6.22	123.89	118.30
1	A	130	LYS	CD-CE-NZ	-5.86	98.21	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	PHE	CB-CG-CD2	-5.84	116.71	120.80
1	A	336	PHE	CB-CG-CD2	-5.68	116.83	120.80
1	B	219	LYS	CD-CE-NZ	-5.53	98.99	111.70
1	B	208	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	104	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	358	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	202	LEU	CB-CG-CD1	-5.37	101.86	111.00
1	C	278	TYR	CZ-CE2-CD2	-5.29	115.03	119.80
1	A	93	ASP	CB-CG-OD1	5.23	123.01	118.30
1	C	104	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	83	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	336	PHE	CB-CG-CD1	5.10	124.37	120.80
1	B	185	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	113	LEU	CB-CG-CD2	-5.02	102.47	111.00

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	3279	0	3295	33	0
1	B	3282	0	3316	31	0
1	C	3126	0	3117	24	0
2	A	22	0	22	8	0
2	B	22	0	22	2	0
2	C	22	0	22	2	0
3	A	64	0	60	0	0
3	B	64	0	60	0	0
3	C	64	0	60	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	5	0	0	1	0
7	A	574	0	0	7	0
7	B	522	0	0	7	0
7	C	446	0	0	7	0
All	All	11498	0	9974	92	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 5.

All (92) 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:56:LYS:HB3	1:C:58:GLU:OE1	1.46	1.15
1:B:262:GLU:OE2	1:B:266[B]:LYS:NZ	1.89	1.03
1:B:159:GLU:CD	1:B:409[A]:LEU:HD22	1.88	0.93
1:C:30:PHE:O	1:C:33[A]:THR:HG22	1.70	0.92
1:C:257[B]:LYS:HD3	1:C:259:LYS:HE2	1.53	0.91
1:B:346[B]:LYS:HD2	7:B:2484:HOH:O	1.74	0.85
2:A:1000:9MT:H21C	2:A:1000:9MT:H61C	1.56	0.84
1:C:58:GLU:H	1:C:58:GLU:CD	1.84	0.81
1:A:66:LYS:HE2	7:A:2113:HOH:O	1.81	0.81
1:C:76:CYS:O	1:C:123[A]:LYS:HE3	1.81	0.80
1:B:110:GLU:HG3	7:B:2196:HOH:O	1.88	0.71
1:C:346:LYS:HD3	7:C:2415:HOH:O	1.93	0.69
1:C:262[B]:GLU:HG3	1:C:283:LYS:HE3	1.75	0.68
1:C:360[B]:ASN:ND2	7:C:2407:HOH:O	2.28	0.67
1:B:123[B]:LYS:HG3	7:B:2224:HOH:O	1.94	0.66
1:B:159:GLU:OE2	1:B:409[A]:LEU:HD22	1.93	0.66
1:A:85[A]:SER:OG	7:A:2157:HOH:O	2.12	0.66
1:A:346[A]:LYS:HE2	7:A:2525:HOH:O	1.96	0.64
1:A:213:HIS:HE1	7:A:2350:HOH:O	1.81	0.63
1:B:159:GLU:CD	1:B:409[A]:LEU:CD2	2.66	0.62
1:C:27:ASP:OD2	1:C:29:LYS:HE3	2.00	0.62
1:B:346[B]:LYS:HE3	1:B:378:ASP:CB	2.30	0.62
1:A:211[A]:TYR:CD1	2:A:1000:9MT:C17	2.85	0.59
1:A:266[A]:LYS:HE3	7:C:2028:HOH:O	2.02	0.59
1:A:42:GLU:OE1	1:B:346[A]:LYS:HE3	2.01	0.59
1:A:218:VAL:O	1:A:222[A]:ILE:HG12	2.03	0.58
1:A:346[B]:LYS:NZ	7:A:2515:HOH:O	2.39	0.55
1:C:262[A]:GLU:HG2	7:C:2314:HOH:O	2.04	0.55
1:A:213:HIS:HD2	1:A:365:ASN:OD1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLU:OE2	1:A:409[B]:LEU:HD12	2.07	0.54
1:A:211[A]:TYR:CE1	2:A:1000:9MT:H161	2.45	0.52
1:C:213:HIS:HD2	1:C:365:ASN:OD1	1.91	0.52
1:B:346[B]:LYS:HE3	1:B:378:ASP:HB3	1.91	0.52
1:C:33[A]:THR:HG23	1:C:34:GLN:OE1	2.10	0.52
1:A:134:SER:OG	1:A:136:LYS:HB2	2.09	0.52
1:A:151:HIS:O	1:A:152:LYS:HB2	2.09	0.52
1:B:213:HIS:HD2	1:B:365:ASN:OD1	1.95	0.50
1:C:98:ASP:OD2	1:C:102:ILE:HG23	2.12	0.50
1:A:210:ARG:NH1	6:B:1411:SO4:O4	2.32	0.50
1:B:152:LYS:NZ	7:B:2248:HOH:O	2.30	0.49
1:B:230[B]:ASN:CB	1:B:233:LEU:H	2.25	0.49
1:A:222[A]:ILE:HD13	1:A:227:SER:HB2	1.95	0.49
1:A:218:VAL:HG21	1:A:242:TYR:HB2	1.93	0.49
1:C:212:TYR:OH	1:C:373:LYS:HE2	2.13	0.48
1:A:230:ASN:OD1	1:A:232:ARG:HG3	2.15	0.47
1:B:123[A]:LYS:HB3	7:B:2120:HOH:O	2.14	0.47
1:A:218:VAL:CG2	1:A:242:TYR:HB2	2.45	0.46
1:A:175:ALA:HB3	1:A:176:PRO:HD3	1.98	0.46
1:A:66:LYS:HE3	7:A:2112:HOH:O	2.17	0.45
2:A:1000:9MT:H12	2:A:1000:9MT:H152	1.99	0.45
1:A:340:THR:HB	1:A:348:LEU:HD22	1.98	0.45
1:A:211[B]:TYR:CE2	1:A:367:LEU:HD21	2.51	0.45
1:B:237:ARG:NH2	7:B:2341:HOH:O	2.50	0.45
1:A:220:LYS:HE2	1:A:330:LEU:HD12	1.99	0.44
1:A:138:ILE:HD12	1:A:138:ILE:C	2.38	0.44
1:C:211[C]:TYR:CE2	1:C:367:LEU:HD21	2.53	0.44
1:A:98:ASP:HA	2:A:1000:9MT:H112	1.99	0.44
1:B:304[A]:GLU:O	1:B:305:ASN:C	2.56	0.44
1:C:123[A]:LYS:HD2	1:C:123[A]:LYS:HA	1.48	0.44
1:B:346[B]:LYS:HE3	1:B:378:ASP:HB2	2.00	0.43
1:B:156[A]:LYS:HE2	1:B:156[A]:LYS:HA	1.99	0.43
1:A:127:ILE:HD11	1:A:185:ARG:HD2	2.01	0.43
1:C:211[C]:TYR:CD1	2:C:1000:9MT:N1	2.86	0.43
1:B:226:PHE:CZ	2:B:1000:9MT:H12C	2.54	0.43
1:B:159:GLU:OE1	1:B:409[A]:LEU:CD2	2.68	0.42
1:A:243[A]:ARG:HG2	7:A:2394:HOH:O	2.19	0.42
2:B:1000:9MT:H61C	2:B:1000:9MT:H31C	1.84	0.42
1:C:156:LYS:HG3	1:C:191:ILE:HG12	2.00	0.42
1:B:43:PHE:CZ	1:B:396:LYS:HG3	2.55	0.42
1:A:250:ILE:O	1:A:253[B]:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LYS:HE3	7:C:2228:HOH:O	2.19	0.42
1:B:218:VAL:HG21	1:B:242:TYR:HB2	2.02	0.41
1:A:211[A]:TYR:CD1	2:A:1000:9MT:H151	2.55	0.41
2:C:1000:9MT:H31C	2:C:1000:9MT:H61C	1.78	0.41
1:B:230[B]:ASN:HB3	1:B:233:LEU:H	1.84	0.41
1:C:213:HIS:HE1	7:C:2263:HOH:O	2.02	0.41
1:A:211[A]:TYR:HD1	2:A:1000:9MT:C17	2.33	0.41
2:A:1000:9MT:H21C	2:A:1000:9MT:C6	2.37	0.41
1:C:32[B]:TYR:OH	1:C:39:ILE:HB	2.20	0.41
1:B:230[B]:ASN:HB2	1:B:233:LEU:H	1.86	0.41
1:B:56:LYS:HB3	1:B:58:GLU:HG2	2.03	0.41
1:C:118:SER:HB3	1:C:289:TRP:CZ2	2.56	0.41
1:C:43:PHE:CE1	1:C:396:LYS:HG3	2.56	0.41
1:A:213:HIS:CD2	1:A:365:ASN:OD1	2.71	0.41
1:A:304:GLU:O	1:A:305[A]:ASN:ND2	2.53	0.40
1:B:249:ASN:ND2	7:B:2365:HOH:O	2.37	0.40
1:C:357:LYS:HE2	7:C:2275:HOH:O	2.20	0.40
1:B:218:VAL:O	1:B:222[A]:ILE:HG23	2.21	0.40
1:B:39:ILE:HD12	1:B:39:ILE:HA	1.70	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	399/384 (104%)	385 (96%)	14 (4%)	0	100	100
1	B	399/384 (104%)	387 (97%)	12 (3%)	0	100	100
1	C	377/384 (98%)	362 (96%)	15 (4%)	0	100	100
All	All	1175/1152 (102%)	1134 (96%)	41 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	367/350 (105%)	355 (97%)	12 (3%)	43	12
1	B	368/350 (105%)	359 (98%)	9 (2%)	54	22
1	C	348/350 (99%)	330 (95%)	18 (5%)	27	3
All	All	1083/1050 (103%)	1044 (96%)	39 (4%)	49	9

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ILE
1	A	58	GLU
1	A	99	ASP
1	A	136	LYS
1	A	219	LYS
1	A	253[A]	MET
1	A	253[B]	MET
1	A	258	LYS
1	A	266[A]	LYS
1	A	266[B]	LYS
1	A	305[A]	ASN
1	A	305[B]	ASN
1	B	39	ILE
1	B	106	ASN
1	B	156[A]	LYS
1	B	156[B]	LYS
1	B	214	ARG
1	B	222[A]	ILE
1	B	222[B]	ILE
1	B	232	ARG
1	B	325	ASP
1	C	33[A]	THR
1	C	33[B]	THR
1	C	39	ILE
1	C	45	GLU
1	C	99	ASP

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Mol	Chain	Res	Type
1	C	102	ILE
1	C	119	PRO
1	C	123[A]	LYS
1	C	123[B]	LYS
1	C	214[A]	ARG
1	C	214[B]	ARG
1	C	244	VAL
1	C	266	LYS
1	C	294[A]	GLU
1	C	294[B]	GLU
1	C	329	THR
1	C	360[A]	ASN
1	C	360[B]	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	A	249	ASN
1	A	350	GLN
1	B	34	GLN
1	B	106	ASN
1	B	213	HIS
1	B	331	ASN
1	B	371	GLN
1	C	106	ASN
1	C	213	HIS

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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
2	9MT	A	1000	-	23,23,23	1.39	5 (21%)	27,30,30	2.37	12 (44%)
3	NHW	A	1001	5	59,66,66	1.16	5 (8%)	66,92,92	1.46	10 (15%)
2	9MT	B	1000	-	23,23,23	1.10	2 (8%)	27,30,30	2.12	8 (29%)
3	NHW	B	1001	5	59,66,66	1.26	3 (5%)	66,92,92	1.65	9 (13%)
6	SO4	B	1411	-	4,4,4	0.31	0	6,6,6	0.93	0
2	9MT	C	1000	-	23,23,23	0.93	0	27,30,30	1.72	8 (29%)
3	NHW	C	1001	5	59,66,66	1.35	4 (6%)	66,92,92	1.79	6 (9%)

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	9MT	A	1000	-	-	0/11/11/11	0/2/2/2
3	NHW	A	1001	5	-	0/61/81/81	0/3/3/3
2	9MT	B	1000	-	-	0/11/11/11	0/2/2/2
3	NHW	B	1001	5	-	0/61/81/81	0/3/3/3
6	SO4	B	1411	-	-	0/0/0/0	0/0/0/0
2	9MT	C	1000	-	-	0/11/11/11	0/2/2/2
3	NHW	C	1001	5	-	0/61/81/81	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	9MT	C14-C13	-2.52	1.39	1.43
2	A	1000	9MT	C14-S	-2.27	1.74	1.77
3	A	1001	NHW	C12-C11	-2.23	1.49	1.52
2	A	1000	9MT	C13-C7	-2.19	1.39	1.42
2	B	1000	9MT	C8-C9	2.10	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	NHW	C12-C11	2.20	1.55	1.52
2	A	1000	9MT	C4-C5	2.33	1.42	1.39
3	C	1001	NHW	O4X-C4X	2.44	1.50	1.45
3	B	1001	NHW	C13-C11	2.48	1.59	1.53
3	C	1001	NHW	CP-S1	2.57	1.87	1.81
2	B	1000	9MT	C12-C10	2.59	1.41	1.37
3	B	1001	NHW	CP-S1	2.79	1.87	1.81
3	A	1001	NHW	C7-C6	2.79	1.60	1.51
3	A	1001	NHW	CP-C1M	2.87	1.56	1.51
2	A	1000	9MT	C5-N	2.92	1.35	1.32
3	A	1001	NHW	O4X-C1X	3.07	1.45	1.41
3	A	1001	NHW	P3X-O3X	4.30	1.67	1.59
3	B	1001	NHW	P3X-O3X	5.01	1.68	1.59
3	C	1001	NHW	P3X-O3X	6.92	1.71	1.59

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1001	NHW	N3A-C2A-N1A	-11.75	118.62	128.86
3	B	1001	NHW	N3A-C2A-N1A	-8.29	121.64	128.86
3	A	1001	NHW	C6-C5-N4	-4.79	108.23	116.49
2	A	1000	9MT	C3-C4-C14	-4.76	112.77	119.44
2	A	1000	9MT	C9-C8-C7	-4.56	115.25	120.84
2	A	1000	9MT	C12-C13-C14	-4.32	119.50	123.34
3	B	1001	NHW	C6-C5-N4	-4.29	109.09	116.49
3	A	1001	NHW	N3A-C2A-N1A	-4.27	125.14	128.86
2	A	1000	9MT	C4-C5-N	-4.04	117.59	122.16
2	C	1000	9MT	C15-C16-C17	-3.44	102.46	111.92
3	B	1001	NHW	C4X-O4X-C1X	-3.30	106.25	109.77
3	B	1001	NHW	O1M-C1M-CP	-3.16	117.67	122.17
2	B	1000	9MT	C13-C7-N	-3.02	119.72	122.84
2	C	1000	9MT	C9-C8-C7	-2.85	117.34	120.84
2	B	1000	9MT	C15-C16-C17	-2.79	104.27	111.92
3	A	1001	NHW	C6-C7-N8	-2.78	106.11	111.87
2	B	1000	9MT	C1-C2-C3	-2.45	101.99	114.06
3	A	1001	NHW	C3M-C2M-C1M	-2.37	108.82	114.78
2	B	1000	9MT	C16-C15-S	-2.37	106.79	113.33
3	A	1001	NHW	C4A-C5A-N7A	-2.33	107.16	109.41
2	A	1000	9MT	C10-C12-C13	-2.33	116.75	120.05
3	B	1001	NHW	C7-C6-C5	-2.30	108.52	112.22
3	A	1001	NHW	C2-C3-N4	-2.27	107.48	112.49
2	C	1000	9MT	C13-C7-N	-2.22	120.55	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	9MT	O-C10-C12	-2.19	118.74	124.49
3	C	1001	NHW	C2-C3-N4	-2.15	107.74	112.49
3	A	1001	NHW	C1X-N9A-C4A	-2.07	123.06	126.64
3	A	1001	NHW	O4A-P2A-O5A	2.21	123.71	112.28
2	C	1000	9MT	C4-C14-S	2.29	122.77	119.91
3	B	1001	NHW	O5-C5-C6	2.29	126.32	122.01
3	C	1001	NHW	C2A-N1A-C6A	2.30	122.79	118.77
2	A	1000	9MT	C8-C7-C13	2.30	121.81	119.11
3	B	1001	NHW	C3-N4-C5	2.30	127.27	122.84
2	A	1000	9MT	C12-C13-C7	2.31	121.76	118.92
3	B	1001	NHW	C13-C11-C10	2.34	112.87	108.82
2	C	1000	9MT	C3-C4-C14	2.38	122.78	119.44
2	B	1000	9MT	C15-S-C14	2.39	109.80	102.11
3	C	1001	NHW	O6A-C12-C11	2.47	114.52	110.55
3	B	1001	NHW	C2A-N1A-C6A	2.51	123.16	118.77
3	C	1001	NHW	C13-C11-C10	2.52	113.19	108.82
3	C	1001	NHW	O5-C5-N4	2.55	127.84	122.97
2	C	1000	9MT	C14-C13-C7	2.55	120.45	117.57
3	A	1001	NHW	C14-C11-C13	2.71	114.94	109.19
2	C	1000	9MT	C5-N-C7	2.81	120.51	118.35
2	A	1000	9MT	C8-C9-C10	2.85	123.97	120.15
2	A	1000	9MT	C6-C5-C4	2.93	127.04	122.42
2	B	1000	9MT	C8-C7-C13	2.94	122.56	119.11
2	A	1000	9MT	C2-C3-C4	2.97	121.94	113.88
2	B	1000	9MT	C3-C4-C14	3.41	124.23	119.44
2	C	1000	9MT	C8-C7-C13	3.42	123.13	119.11
3	A	1001	NHW	O5-C5-C6	3.66	128.88	122.01
2	A	1000	9MT	C5-N-C7	4.01	121.43	118.35
2	B	1000	9MT	C5-N-C7	6.83	123.60	118.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	9MT	8	0
2	B	1000	9MT	2	0
6	B	1411	SO4	1	0
2	C	1000	9MT	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	384/384 (100%)	-0.41	3 (0%) 86 89	8, 13, 23, 50	20 (5%)
1	B	384/384 (100%)	-0.41	0 100 100	7, 13, 27, 38	19 (4%)
1	C	366/384 (95%)	-0.35	4 (1%) 80 84	9, 14, 28, 50	20 (5%)
All	All	1134/1152 (98%)	-0.39	7 (0%) 89 91	7, 14, 27, 50	59 (5%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211[A]	TYR	3.3
1	C	211[A]	TYR	3.3
1	A	39	ILE	2.2
1	C	323	GLY	2.1
1	A	232	ARG	2.1
1	C	410	LEU	2.0
1	C	32[A]	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	9MT	B	1000	22/22	0.92	0.11	1.95	16,20,26,28	0
6	SO4	B	1411	5/5	0.93	0.10	1.79	41,45,49,49	0
5	MG	C	1412	1/1	0.99	0.09	1.37	21,21,21,21	0
4	CL	B	1412	1/1	1.00	0.07	1.05	12,12,12,12	0
2	9MT	C	1000	22/22	0.94	0.10	0.35	15,18,23,26	0
2	9MT	A	1000	22/22	0.94	0.09	0.17	12,17,23,24	0
3	NHW	A	1001	64/64	0.98	0.07	-0.06	9,11,15,17	0
3	NHW	B	1001	64/64	0.98	0.06	-0.51	7,12,15,17	0
3	NHW	C	1001	64/64	0.98	0.06	-0.57	8,12,16,22	0
5	MG	B	1413	1/1	0.99	0.05	-1.15	20,20,20,20	0
5	MG	A	1412	1/1	0.98	0.04	-2.54	20,20,20,20	0
4	CL	A	1411	1/1	0.99	0.04	-5.42	12,12,12,12	0
4	CL	C	1411	1/1	0.99	0.03	-6.85	13,13,13,13	0

6.5 Other polymers

There are no such residues in this entry.