



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2016 – 06:55 PM EDT

PDB ID : 4UFW
Title : Plasmodium vivax N-myristoyltransferase in complex with a pyridyl inhibitor (compound 23)
Authors : Yu, Z.; Brannigan, J.A.; Rangachari, K.; Heal, W.P.; Wilkinson, A.J.; Holder, A.A.; Tate, E.W.; Leatherbarrow, R.J.
Deposited on : 2015-03-19
Resolution : 1.50 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20027107

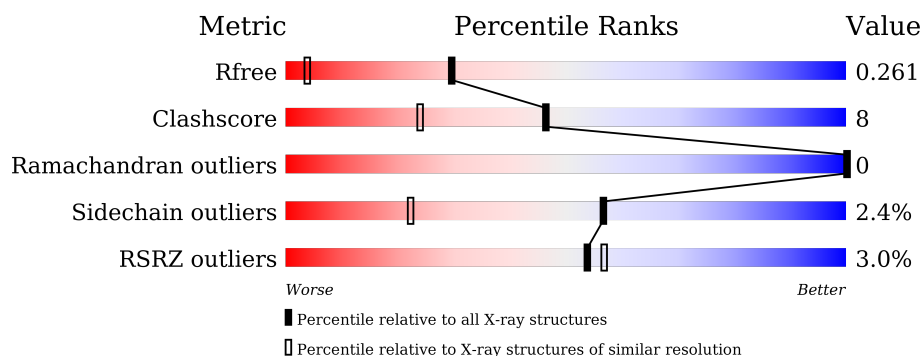
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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	385	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>.</div> </div> </div>
1	B	385	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>
1	C	385	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>.</div> <div>5%</div> </div> </div>

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
4	SO4	A	1412	-	-	-	X
7	DMS	C	1414	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11389 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.

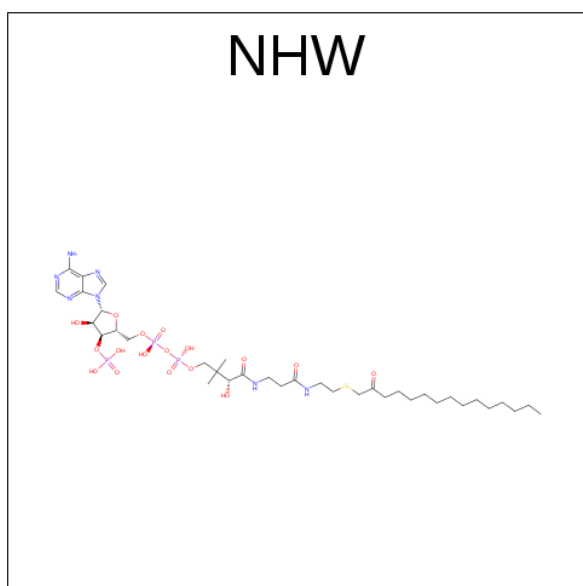
- Molecule 1 is a protein called GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	29	0
			3357	2184	546	614	13			
1	B	385	Total	C	N	O	S	0	16	0
			3269	2127	530	599	13			
1	C	367	Total	C	N	O	S	0	32	0
			3224	2112	515	587	10			

There are 3 discrepancies between the modelled and reference sequences:

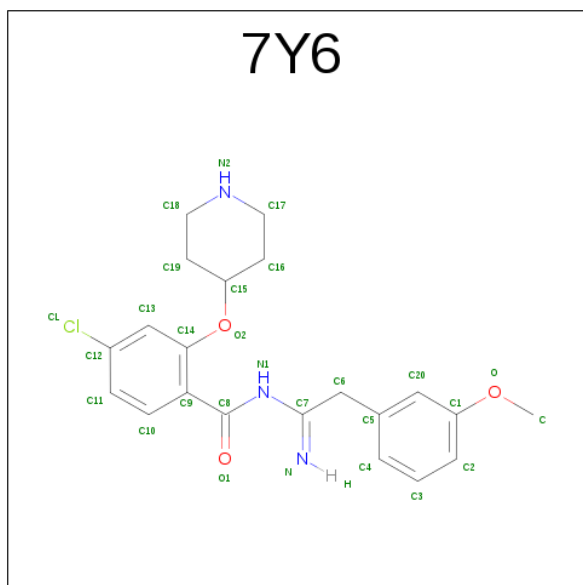
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	EXPRESSION TAG	UNP A5K1A2
B	26	MET	-	EXPRESSION TAG	UNP A5K1A2
C	26	MET	-	EXPRESSION TAG	UNP A5K1A2

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



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

- Molecule 3 is 4-CHLORANYL-N-[2-(3-METHOXYPHENYL)ETHANIMIDOYL]-2-PIPERIDIN-4-YLOXY-BENZAMIDE (three-letter code: 7Y6) (formula: $C_{21}H_{24}ClN_3O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O		
			28	21	1	3	3	0	0
3	B	1	Total	C	Cl	N	O		
			28	21	1	3	3	0	0
3	C	1	Total	C	Cl	N	O		
			28	21	1	3	3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

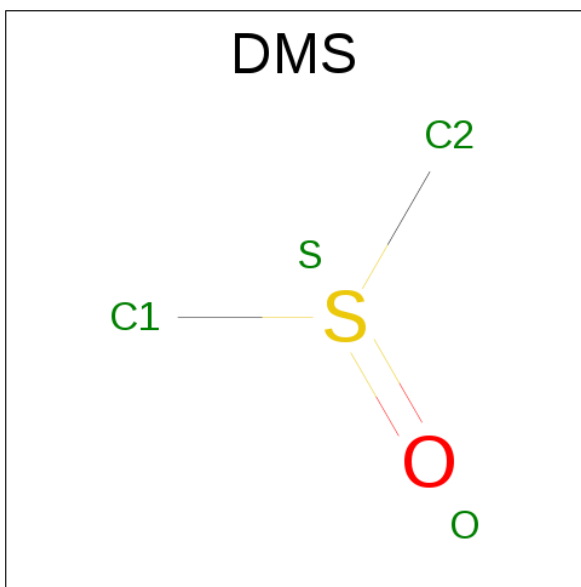
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	B	1	Total	C	O	S	0	0
			4	2	1	1		
7	C	1	Total	C	O	S	0	0
			4	2	1	1		

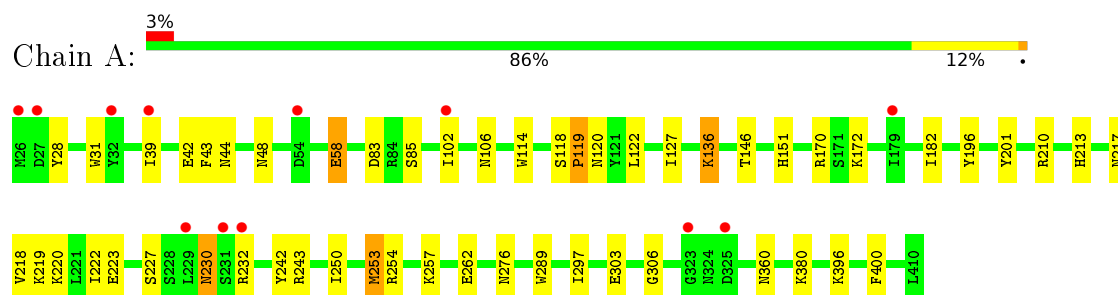
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	474	Total	O	0	0
			474	474		
8	B	404	Total	O	0	0
			404	404		
8	C	362	Total	O	0	0
			362	362		

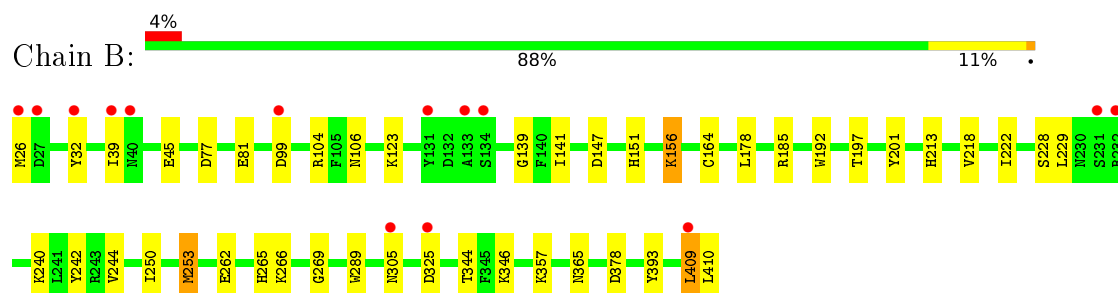
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

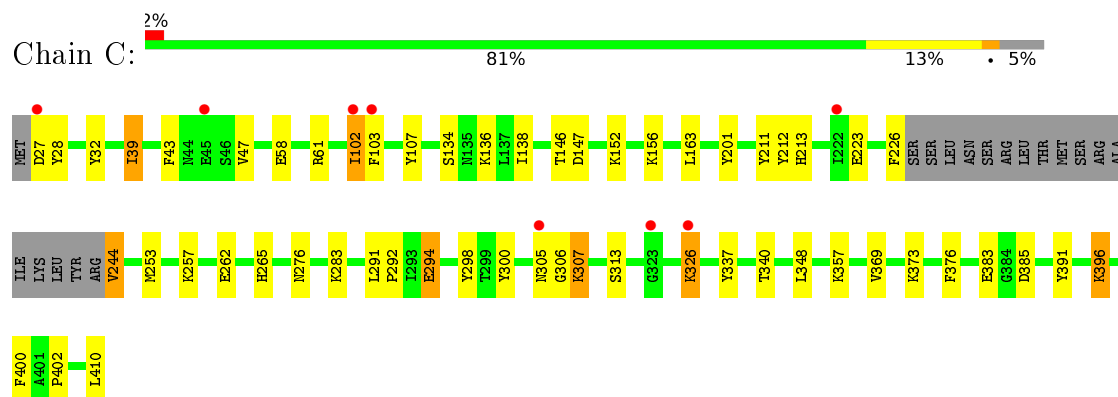
• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



• 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	57.52Å 121.91Å 178.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.73 – 1.50 30.37 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (100.73-1.50) 99.1 (30.37-1.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.214 , 0.261 0.214 , 0.261	Depositor DCC
R_{free} test set	10013 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 199396 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11389	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 3.26% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 7Y6, MG, CL, NHW, DMS, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.06	0/3501	1.06	5/4738 (0.1%)
1	B	1.07	2/3395 (0.1%)	1.07	9/4594 (0.2%)
1	C	1.02	2/3388 (0.1%)	1.03	4/4582 (0.1%)
All	All	1.05	4/10284 (0.0%)	1.05	18/13914 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	337	TYR	CG-CD1	5.68	1.46	1.39
1	B	192	TRP	CB-CG	5.59	1.60	1.50
1	C	337	TYR	CE1-CZ	5.25	1.45	1.38
1	B	393	TYR	CG-CD1	5.00	1.45	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	409	LEU	CB-CG-CD2	-6.42	100.09	111.00
1	A	380	LYS	CD-CE-NZ	-6.17	97.51	111.70
1	A	170	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	253[A]	MET	CG-SD-CE	5.93	109.69	100.20
1	A	253[B]	MET	CG-SD-CE	5.93	109.69	100.20
1	B	77	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	C	410	LEU	CB-CG-CD1	-5.61	101.45	111.00
1	B	185	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	391	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	A	83	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	378	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	B	77	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	163	LEU	CB-CG-CD1	5.28	119.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	104	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	253[A]	MET	CG-SD-CE	5.00	108.20	100.20
1	B	253[B]	MET	CG-SD-CE	5.00	108.20	100.20

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	3357	0	3387	57	0
1	B	3269	0	3285	37	0
1	C	3224	0	3273	59	0
2	A	64	0	60	0	0
2	B	64	0	60	0	0
2	C	64	0	60	0	0
3	A	28	0	23	4	0
3	B	28	0	23	1	0
3	C	28	0	23	3	0
4	A	5	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	4	0	6	0	0
7	B	4	0	6	0	0
7	C	4	0	6	0	0
8	A	474	0	0	15	0
8	B	404	0	0	15	0
8	C	362	0	0	9	0
All	All	11389	0	10212	155	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 8.

All (155) 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:B:213[B]:HIS:CE1	8:B:2234:HOH:O	1.77	1.28
1:C:213[A]:HIS:CE1	8:C:2206:HOH:O	1.80	1.25
1:A:213[B]:HIS:CE1	8:A:2281:HOH:O	1.88	1.23
1:B:151[B]:HIS:HE1	8:B:2026:HOH:O	0.88	1.20
1:C:136[A]:LYS:HE2	8:C:2149:HOH:O	1.45	1.16
1:A:243[B]:ARG:HG3	1:A:243[B]:ARG:HH11	1.11	1.12
1:A:48[B]:ASN:ND2	8:A:2038:HOH:O	1.60	1.10
1:A:254:ARG:HD2	1:A:257:LYS:HZ1	1.15	1.07
1:C:373[B]:LYS:HE3	8:C:2335:HOH:O	0.88	1.04
3:A:1411:7Y6:H191	8:A:2467:HOH:O	1.53	1.04
1:A:114:TRP:CZ2	1:A:297[A]:ILE:HD12	1.96	1.00
1:B:147[B]:ASP:OD1	1:B:156[B]:LYS:HE3	1.61	1.00
1:A:289:TRP:O	1:A:297[A]:ILE:HD11	1.65	0.96
1:B:39:ILE:HD11	1:B:201:TYR:HE1	1.30	0.95
1:B:156[A]:LYS:HE3	8:B:2178:HOH:O	1.68	0.94
1:C:147:ASP:OD1	1:C:156[A]:LYS:HE3	1.67	0.93
1:C:294[B]:GLU:OE1	8:C:2279:HOH:O	1.90	0.89
1:A:85[A]:SER:OG	8:A:2122:HOH:O	1.90	0.89
1:C:265:HIS:ND1	1:C:283[B]:LYS:HD2	1.89	0.87
1:A:243[B]:ARG:NH1	1:A:243[B]:ARG:HG3	1.88	0.87
1:A:114:TRP:HZ2	1:A:297[A]:ILE:HD12	1.38	0.87
1:A:254:ARG:HD2	1:A:257:LYS:NZ	1.90	0.87
1:B:156[A]:LYS:HE2	1:B:156[A]:LYS:HA	1.57	0.85
1:A:289:TRP:O	1:A:297[A]:ILE:CD1	2.25	0.83
1:C:305:ASN:OD1	1:C:307:LYS:HD2	1.79	0.82
1:C:102[A]:ILE:HD11	1:C:103:PHE:CZ	2.15	0.81
1:C:213[B]:HIS:CD2	1:C:226:PHE:HE1	2.00	0.79
1:C:305:ASN:HD21	1:C:307:LYS:HD3	1.48	0.78
1:A:254:ARG:CD	1:A:257:LYS:HZ1	1.95	0.76
1:C:305:ASN:OD1	1:C:306:GLY:N	2.17	0.75
1:A:42[B]:GLU:HG3	1:B:344:THR:HG21	1.69	0.74
1:B:151[B]:HIS:CE1	8:B:2026:HOH:O	1.78	0.73
1:B:156[A]:LYS:CA	1:B:156[A]:LYS:HE2	2.14	0.73
1:C:244[B]:VAL:HG11	1:C:357:LYS:HD2	1.72	0.72
1:C:136[A]:LYS:HG3	8:C:2149:HOH:O	1.90	0.72
1:B:39:ILE:HD11	1:B:201:TYR:CE1	2.19	0.71
1:A:303:GLU:OE2	1:A:306:GLY:HA2	1.90	0.71
1:C:223:GLU:OE1	1:C:326[B]:LYS:HE2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ILE:HD12	1:A:201:TYR:HE1	1.56	0.70
1:C:136[A]:LYS:CE	8:C:2149:HOH:O	2.16	0.70
1:C:134:SER:OG	1:C:136[A]:LYS:HG2	1.92	0.69
1:C:102[A]:ILE:HD11	1:C:103:PHE:CE2	2.28	0.69
1:A:230[A]:ASN:HD22	1:A:230[A]:ASN:H	1.36	0.69
1:A:230[B]:ASN:OD1	1:A:232:ARG:HB2	1.93	0.69
1:B:240:LYS:HG2	8:B:2264:HOH:O	1.92	0.69
3:A:1411:7Y6:H11	8:A:2281:HOH:O	1.92	0.67
1:A:254:ARG:HH11	1:A:257:LYS:HZ3	1.42	0.67
1:B:99[B]:ASP:OD1	8:B:2131:HOH:O	2.11	0.67
1:C:27[A]:ASP:OD1	1:C:27[A]:ASP:N	2.26	0.66
1:A:254:ARG:NH1	1:A:257:LYS:HZ3	1.92	0.66
1:A:213[B]:HIS:ND1	8:A:2281:HOH:O	2.13	0.64
1:C:213[A]:HIS:ND1	8:C:2206:HOH:O	2.02	0.62
1:A:42[B]:GLU:CG	1:B:344:THR:HG21	2.29	0.62
8:A:2417:HOH:O	1:B:45[B]:GLU:HG3	2.01	0.61
1:C:265:HIS:ND1	1:C:283[B]:LYS:CD	2.64	0.61
1:C:213[B]:HIS:CD2	1:C:226:PHE:CE1	2.87	0.60
1:A:119:PRO:O	1:A:120[B]:ASN:CB	2.48	0.60
1:A:172:LYS:HE3	8:A:2244:HOH:O	2.00	0.60
1:A:262:GLU:HG3	8:A:2351:HOH:O	2.01	0.59
1:A:243[B]:ARG:CG	1:A:243[B]:ARG:HH11	2.00	0.59
1:A:254:ARG:NH1	1:A:257:LYS:NZ	2.50	0.58
1:C:276[A]:ASN:ND2	1:C:400:PHE:CE2	2.72	0.57
1:C:211:TYR:HB2	3:C:1411:7Y6:H11	1.88	0.56
1:A:151[B]:HIS:HE1	8:A:2217:HOH:O	1.88	0.56
1:C:305:ASN:HD21	1:C:307:LYS:CD	2.16	0.56
1:C:47:VAL:CG1	1:C:396:LYS:HG2	2.34	0.56
1:B:266:LYS:HE2	8:B:2303:HOH:O	2.05	0.55
1:B:266:LYS:HG3	8:B:2303:HOH:O	2.07	0.55
1:C:28:TYR:CE2	1:C:39[A]:ILE:HG13	2.42	0.55
1:C:244[B]:VAL:HG11	1:C:357:LYS:CD	2.36	0.54
1:C:152[B]:LYS:CB	1:C:152[B]:LYS:NZ	2.71	0.54
1:B:213[B]:HIS:ND1	8:B:2234:HOH:O	2.15	0.54
1:A:114:TRP:CZ2	1:A:297[A]:ILE:CD1	2.82	0.54
1:A:222[A]:ILE:HD13	1:A:227:SER:HB2	1.89	0.54
3:A:1411:7Y6:C19	8:A:2467:HOH:O	2.32	0.54
1:C:262[B]:GLU:HG2	1:C:283[B]:LYS:HE2	1.90	0.53
1:B:32:TYR:OH	1:B:39:ILE:HB	2.08	0.53
1:C:305:ASN:CG	1:C:306:GLY:H	2.09	0.52
1:A:254:ARG:HH11	1:A:257:LYS:NZ	2.05	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230[A]:ASN:H	1:A:230[A]:ASN:ND2	2.03	0.51
3:A:1411:7Y6:O1	3:A:1411:7Y6:N	2.42	0.50
1:C:152[B]:LYS:HB2	1:C:152[B]:LYS:NZ	2.26	0.50
1:A:127:ILE:CD1	1:A:182[B]:ILE:HD12	2.42	0.49
1:B:213[B]:HIS:ND1	1:B:365:ASN:OD1	2.34	0.49
1:B:244[A]:VAL:CG2	1:B:357:LYS:HD2	2.42	0.49
1:A:127:ILE:HD11	1:A:182[B]:ILE:HD12	1.93	0.49
8:A:2423:HOH:O	1:B:45[B]:GLU:HG2	2.13	0.49
1:B:222:ILE:HD12	1:B:229:LEU:HG	1.95	0.48
1:C:262[B]:GLU:HG2	1:C:283[B]:LYS:CE	2.43	0.48
1:A:217[A]:ASN:ND2	1:A:220:LYS:HB2	2.29	0.48
1:A:218[A]:VAL:HG21	1:A:242:TYR:HB2	1.95	0.48
1:C:340:THR:HB	1:C:348:LEU:HD22	1.96	0.48
1:A:119:PRO:O	1:A:120[B]:ASN:HB2	2.13	0.47
1:C:253:MET:HG3	1:C:300:TYR:HB3	1.96	0.47
1:C:276[A]:ASN:ND2	1:C:400:PHE:CD2	2.82	0.47
1:C:47:VAL:HG11	1:C:396:LYS:HG2	1.96	0.47
1:C:262[A]:GLU:HG3	8:C:2250:HOH:O	2.14	0.47
1:A:58:GLU:HB3	8:A:2061:HOH:O	2.14	0.47
1:C:223:GLU:OE1	1:C:326[B]:LYS:CE	2.61	0.47
1:B:123[B]:LYS:NZ	8:B:2168:HOH:O	2.48	0.47
1:C:102[A]:ILE:CD1	1:C:103:PHE:CZ	2.93	0.47
1:A:243[B]:ARG:NH1	1:A:243[B]:ARG:CG	2.65	0.47
1:A:196:TYR:CD1	1:A:196:TYR:N	2.82	0.46
1:B:289:TRP:CZ3	1:B:410:LEU:HD11	2.49	0.46
1:B:123[B]:LYS:HB3	8:B:2088:HOH:O	2.15	0.46
1:C:369:VAL:HA	1:C:402:PRO:O	2.16	0.46
1:C:400:PHE:HB3	8:C:2023:HOH:O	2.16	0.46
1:A:42[A]:GLU:OE2	1:B:346:LYS:NZ	2.47	0.46
1:C:298:TYR:O	1:C:313:SER:HA	2.17	0.45
1:C:39[B]:ILE:HD11	1:C:201:TYR:CE2	2.52	0.45
1:A:219:LYS:O	1:A:223:GLU:HG3	2.17	0.45
3:B:1411:7Y6:H15	3:B:1411:7Y6:H13	1.79	0.45
1:C:373[A]:LYS:HA	1:C:376:PHE:CD2	2.52	0.44
1:B:123[A]:LYS:HB3	8:B:2088:HOH:O	2.16	0.44
1:A:114:TRP:HZ2	1:A:297[A]:ILE:CD1	2.18	0.44
1:A:151[B]:HIS:CE1	8:A:2217:HOH:O	2.68	0.44
1:A:43:PHE:CZ	1:A:396:LYS:HG3	2.52	0.44
1:C:212:TYR:CD2	1:C:383:GLU:HA	2.53	0.44
1:A:360[A]:ASN:ND2	8:A:2291:HOH:O	2.51	0.43
1:A:210:ARG:NH1	4:A:1412:SO4:O1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ILE:HD12	1:B:39:ILE:HA	1.91	0.43
1:C:107:TYR:OH	3:C:1411:7Y6:H172	2.19	0.43
1:C:152[B]:LYS:HB2	1:C:152[B]:LYS:HZ2	1.82	0.43
1:B:141:ILE:HG22	1:B:178:LEU:HD22	1.99	0.43
1:C:43:PHE:CE1	1:C:396:LYS:HG3	2.54	0.43
1:B:197:THR:HG23	1:B:409:LEU:HD13	2.01	0.43
1:C:152[B]:LYS:CB	1:C:152[B]:LYS:HZ3	2.32	0.43
1:C:138:ILE:C	1:C:138:ILE:HD12	2.39	0.43
1:C:265:HIS:CG	1:C:283[B]:LYS:HD2	2.53	0.42
1:A:276[A]:ASN:ND2	1:A:400:PHE:CE1	2.84	0.42
1:C:32[B]:TYR:OH	1:C:39[B]:ILE:HG22	2.19	0.42
1:A:250:ILE:HB	1:A:253[B]:MET:HG2	2.01	0.42
1:B:250:ILE:O	1:B:253[B]:MET:HG2	2.20	0.42
1:B:262:GLU:HG2	1:B:266:LYS:HE3	2.02	0.42
1:B:218:VAL:CG2	1:B:242:TYR:HB2	2.50	0.42
1:C:291:LEU:HA	1:C:292:PRO:HD3	1.92	0.42
1:B:269:GLY:HA3	8:B:2305:HOH:O	2.20	0.41
1:C:373[B]:LYS:HA	1:C:376:PHE:CD2	2.55	0.41
1:A:118:SER:HB3	1:A:289:TRP:CZ2	2.55	0.41
1:A:39:ILE:CD1	1:A:201:TYR:HE1	2.30	0.41
1:C:39[A]:ILE:HA	1:C:39[A]:ILE:HD13	1.99	0.41
1:C:211:TYR:CB	3:C:1411:7Y6:C11	2.99	0.41
1:B:139:GLY:HA2	1:B:164:CYS:O	2.21	0.41
1:A:28:TYR:HB3	1:A:31:TRP:HB2	2.03	0.41
1:B:265:HIS:CE1	8:B:2306:HOH:O	2.74	0.40
1:B:357:LYS:HE2	8:B:2270:HOH:O	2.22	0.40
1:A:122[B]:LEU:HA	1:A:122[B]:LEU:HD23	1.91	0.40
1:A:136:LYS:HD2	1:A:136:LYS:HA	1.71	0.40
1:C:47:VAL:HG12	1:C:396:LYS:HG2	2.02	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	412/385 (107%)	400 (97%)	12 (3%)	0	100	100
1	B	399/385 (104%)	389 (98%)	10 (2%)	0	100	100
1	C	393/385 (102%)	381 (97%)	12 (3%)	0	100	100
All	All	1204/1155 (104%)	1170 (97%)	34 (3%)	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	380/351 (108%)	371 (98%)	9 (2%)	57	22
1	B	367/351 (105%)	359 (98%)	8 (2%)	60	25
1	C	366/351 (104%)	347 (95%)	19 (5%)	29	4
All	All	1113/1053 (106%)	1077 (97%)	36 (3%)	57	13

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	102	ILE
1	A	106	ASN
1	A	119	PRO
1	A	136	LYS
1	A	146[A]	THR
1	A	146[B]	THR
1	A	230[A]	ASN
1	A	230[B]	ASN
1	B	26	MET
1	B	81	GLU
1	B	106	ASN
1	B	156[A]	LYS
1	B	156[B]	LYS
1	B	228	SER

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Mol	Chain	Res	Type
1	B	305	ASN
1	B	325	ASP
1	C	39[A]	ILE
1	C	39[B]	ILE
1	C	58[A]	GLU
1	C	58[B]	GLU
1	C	102[A]	ILE
1	C	102[B]	ILE
1	C	146[A]	THR
1	C	146[B]	THR
1	C	244[A]	VAL
1	C	244[B]	VAL
1	C	257[A]	LYS
1	C	257[B]	LYS
1	C	294[A]	GLU
1	C	294[B]	GLU
1	C	307	LYS
1	C	326[A]	LYS
1	C	326[B]	LYS
1	C	385	ASP
1	C	396	LYS

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

Mol	Chain	Res	Type
1	A	34	GLN
1	A	106	ASN
1	A	371	GLN
1	B	34	GLN
1	B	106	ASN
1	B	249	ASN
1	B	265	HIS
1	C	34	GLN
1	C	44	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	NHW	A	1000	5	57,66,66	1.28	5 (8%)	67,92,92	1.63	10 (14%)
3	7Y6	A	1411	-	29,30,30	1.50	2 (6%)	36,40,40	2.37	12 (33%)
4	SO4	A	1412	-	4,4,4	0.36	0	6,6,6	0.56	0
7	DMS	A	1415	-	3,3,3	0.33	0	3,3,3	1.28	0
2	NHW	B	1000	5	57,66,66	1.43	4 (7%)	67,92,92	1.73	10 (14%)
3	7Y6	B	1411	-	29,30,30	1.82	4 (13%)	36,40,40	2.88	15 (41%)
7	DMS	B	1414	-	3,3,3	0.41	0	3,3,3	1.47	1 (33%)
2	NHW	C	1000	5	57,66,66	1.30	5 (8%)	67,92,92	1.96	7 (10%)
3	7Y6	C	1411	-	29,30,30	1.66	5 (17%)	36,40,40	2.20	13 (36%)
7	DMS	C	1414	-	3,3,3	0.51	0	3,3,3	1.17	0

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	NHW	A	1000	5	-	0/61/81/81	0/3/3/3
3	7Y6	A	1411	-	-	0/16/26/26	0/3/3/3
4	SO4	A	1412	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DMS	A	1415	-	-	0/0/0/0	0/0/0/0
2	NHW	B	1000	5	-	0/61/81/81	0/3/3/3
3	7Y6	B	1411	-	-	0/16/26/26	0/3/3/3
7	DMS	B	1414	-	-	0/0/0/0	0/0/0/0
2	NHW	C	1000	5	-	0/61/81/81	0/3/3/3
3	7Y6	C	1411	-	-	0/16/26/26	0/3/3/3
7	DMS	C	1414	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1411	7Y6	C8-N1	-6.29	1.26	1.37
3	C	1411	7Y6	C8-N1	-5.72	1.27	1.37
3	A	1411	7Y6	C8-N1	-5.70	1.27	1.37
2	C	1000	NHW	O4X-C1X	-4.19	1.35	1.41
2	C	1000	NHW	P3X-O7A	-2.78	1.45	1.54
3	B	1411	7Y6	C9-C8	-2.30	1.45	1.50
2	A	1000	NHW	C14-C11	-2.21	1.48	1.53
2	C	1000	NHW	P1A-O1A	-2.11	1.43	1.51
3	C	1411	7Y6	C2-C1	2.04	1.42	1.38
2	B	1000	NHW	O4X-C4X	2.13	1.49	1.45
2	A	1000	NHW	P1A-O5X	2.14	1.68	1.59
2	A	1000	NHW	O4X-C4X	2.19	1.50	1.45
2	C	1000	NHW	CP-C1M	2.21	1.55	1.51
3	C	1411	7Y6	C6-C7	2.32	1.52	1.49
3	C	1411	7Y6	C6-C5	2.45	1.55	1.51
2	A	1000	NHW	O1M-C1M	2.72	1.26	1.21
3	B	1411	7Y6	O2-C14	3.01	1.43	1.37
2	B	1000	NHW	C6-C5	3.15	1.57	1.51
2	C	1000	NHW	O4X-C4X	3.77	1.53	1.45
3	A	1411	7Y6	O1-C8	3.81	1.31	1.23
3	C	1411	7Y6	O1-C8	3.95	1.31	1.23
3	B	1411	7Y6	O1-C8	4.14	1.31	1.23
2	B	1000	NHW	O10-C10	4.22	1.50	1.42
2	A	1000	NHW	O4X-C1X	4.57	1.47	1.41
2	B	1000	NHW	CP-S1	6.54	1.96	1.81

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1000	NHW	N3A-C2A-N1A	-12.18	119.31	128.87
2	B	1000	NHW	N3A-C2A-N1A	-7.85	122.71	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	NHW	N3A-C2A-N1A	-7.35	123.10	128.87
3	B	1411	7Y6	O1-C8-C9	-6.82	107.57	120.94
3	B	1411	7Y6	C16-C15-C19	-6.33	101.11	111.56
3	C	1411	7Y6	O1-C8-C9	-5.26	110.63	120.94
3	A	1411	7Y6	C16-C15-C19	-4.89	103.48	111.56
2	B	1000	NHW	C1X-N9A-C4A	-3.91	122.44	126.81
2	A	1000	NHW	C2-S1-CP	-3.88	95.37	101.86
3	A	1411	7Y6	O2-C14-C13	-3.44	115.35	123.39
3	A	1411	7Y6	C10-C9-C8	-3.40	109.12	118.28
3	B	1411	7Y6	C10-C9-C8	-3.40	109.12	118.28
2	B	1000	NHW	P3X-O3X-C3X	-3.37	112.94	121.56
3	C	1411	7Y6	C10-C9-C8	-3.37	109.21	118.28
3	B	1411	7Y6	O2-C14-C13	-3.29	115.70	123.39
3	C	1411	7Y6	C10-C11-C12	-3.28	115.66	119.22
2	A	1000	NHW	C4X-O4X-C1X	-3.23	106.21	109.64
3	C	1411	7Y6	C13-C14-C9	-3.20	115.37	121.34
3	B	1411	7Y6	C13-C14-C9	-3.10	115.55	121.34
3	C	1411	7Y6	C16-C15-C19	-3.10	106.44	111.56
2	C	1000	NHW	C1X-N9A-C4A	-3.05	123.40	126.81
2	B	1000	NHW	C10-C9-N8	-3.05	109.11	116.31
2	B	1000	NHW	C7-N8-C9	-3.05	116.51	122.62
2	A	1000	NHW	C13-C11-C12	-3.00	104.61	108.50
2	C	1000	NHW	C2-C3-N4	-2.97	106.47	112.43
3	A	1411	7Y6	O1-C8-C9	-2.96	115.13	120.94
2	A	1000	NHW	C2-C3-N4	-2.93	106.54	112.43
3	B	1411	7Y6	C17-C16-C15	-2.92	107.17	110.28
2	A	1000	NHW	O1M-C1M-CP	-2.66	118.41	122.14
3	A	1411	7Y6	C10-C11-C12	-2.61	116.40	119.22
2	C	1000	NHW	P3X-O3X-C3X	-2.51	115.13	121.56
2	C	1000	NHW	C6-C5-N4	-2.44	112.21	116.46
3	B	1411	7Y6	C10-C11-C12	-2.41	116.61	119.22
3	A	1411	7Y6	C13-C14-C9	-2.28	117.08	121.34
3	C	1411	7Y6	O2-C14-C13	-2.22	118.19	123.39
2	A	1000	NHW	C3-N4-C5	-2.18	118.46	122.79
3	C	1411	7Y6	C18-C19-C15	-2.18	107.95	110.28
3	B	1411	7Y6	C2-C1-C20	-2.13	117.61	120.56
2	A	1000	NHW	O4X-C4X-C5X	-2.01	102.10	109.29
2	A	1000	NHW	C13-C11-C10	2.01	112.84	109.17
3	C	1411	7Y6	C16-C17-N2	2.02	114.10	110.62
2	B	1000	NHW	O8A-P3X-O7A	2.07	115.03	107.44
3	B	1411	7Y6	C11-C12-C13	2.13	124.45	121.53
2	C	1000	NHW	O2X-C2X-C3X	2.16	117.36	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1414	DMS	C2-S-C1	2.16	109.92	98.50
2	B	1000	NHW	O4A-P2A-O5A	2.22	124.13	112.56
3	C	1411	7Y6	O2-C15-C16	2.26	113.90	108.31
3	A	1411	7Y6	C17-C16-C15	2.31	112.75	110.28
2	C	1000	NHW	O2A-P1A-O3A	2.37	115.42	105.27
3	C	1411	7Y6	O1-C8-N1	2.39	126.07	122.32
2	B	1000	NHW	O8A-P3X-O3X	2.50	114.11	106.62
2	B	1000	NHW	C2A-N1A-C6A	2.77	123.72	118.77
2	A	1000	NHW	O3X-P3X-O9A	2.78	114.11	107.48
3	A	1411	7Y6	C11-C12-C13	3.11	125.78	121.53
3	B	1411	7Y6	C9-C8-N1	3.39	121.43	115.37
3	B	1411	7Y6	C18-C19-C15	3.68	114.21	110.28
3	C	1411	7Y6	C9-C8-N1	3.69	121.98	115.37
3	A	1411	7Y6	C10-C9-C14	3.70	122.95	118.24
3	B	1411	7Y6	O2-C15-C16	3.72	117.54	108.31
3	A	1411	7Y6	O2-C15-C16	4.39	119.19	108.31
2	B	1000	NHW	C2-S1-CP	4.39	109.19	101.86
3	A	1411	7Y6	C9-C8-N1	4.48	123.39	115.37
3	C	1411	7Y6	C10-C9-C14	4.57	124.06	118.24
3	B	1411	7Y6	O1-C8-N1	5.09	130.31	122.32
3	B	1411	7Y6	C10-C9-C14	5.10	124.74	118.24
3	C	1411	7Y6	O2-C14-C9	5.16	126.36	116.56
3	A	1411	7Y6	O2-C14-C9	5.66	127.31	116.56
3	B	1411	7Y6	O2-C14-C9	6.25	128.43	116.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1411	7Y6	4	0
4	A	1412	SO4	1	0
3	B	1411	7Y6	1	0
3	C	1411	7Y6	3	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 ⓘ

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	385/385 (100%)	0.17	12 (3%) 52 55	9, 14, 27, 64	11 (2%)
1	B	385/385 (100%)	0.17	14 (3%) 46 49	8, 14, 28, 61	13 (3%)
1	C	367/385 (95%)	0.17	8 (2%) 65 68	8, 15, 28, 45	8 (2%)
All	All	1137/1155 (98%)	0.17	34 (2%) 54 57	8, 14, 28, 64	32 (2%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	MET	6.0
1	B	232	ARG	5.8
1	A	26	MET	5.3
1	A	232	ARG	5.0
1	B	39	ILE	4.1
1	A	231	SER	4.0
1	B	305	ASN	4.0
1	A	229	LEU	3.4
1	B	231	SER	3.2
1	C	222	ILE	3.2
1	C	323	GLY	3.1
1	B	131	TYR	3.0
1	A	39	ILE	2.7
1	B	133	ALA	2.6
1	A	54	ASP	2.6
1	C	326[A]	LYS	2.5
1	C	305	ASN	2.4
1	B	99[A]	ASP	2.4
1	B	32	TYR	2.4
1	C	103	PHE	2.4
1	B	40	ASN	2.3
1	C	102[A]	ILE	2.3
1	C	27[A]	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	102	ILE	2.2
1	B	325	ASP	2.2
1	A	323	GLY	2.2
1	A	32	TYR	2.2
1	A	325	ASP	2.2
1	B	409	LEU	2.1
1	B	27[A]	ASP	2.0
1	C	45	GLU	2.0
1	A	27	ASP	2.0
1	A	179	ILE	2.0
1	B	134	SER	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(Å ²)	Q<0.9
4	SO4	A	1412	5/5	0.95	0.15	5.18	42,43,46,46	0
7	DMS	C	1414	4/4	0.88	0.17	2.83	26,30,30,34	0
3	7Y6	B	1411	28/28	0.88	0.14	1.76	19,24,28,30	0
3	7Y6	A	1411	28/28	0.90	0.12	0.68	18,26,29,30	0
3	7Y6	C	1411	28/28	0.87	0.12	0.55	19,26,31,36	0
7	DMS	B	1414	4/4	0.97	0.11	0.47	20,21,22,25	0
7	DMS	A	1415	4/4	0.95	0.11	0.13	25,26,26,26	0
2	NHW	A	1000	64/64	0.95	0.09	-0.15	9,11,15,17	0
6	CL	B	1413	1/1	1.00	0.08	-0.31	13,13,13,13	0
2	NHW	B	1000	64/64	0.96	0.09	-0.39	8,11,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NHW	C	1000	64/64	0.97	0.08	-0.55	8,12,15,18	0
5	MG	C	1412	1/1	0.97	0.07	-1.00	22,22,22,22	0
6	CL	A	1414	1/1	0.99	0.06	-1.67	13,13,13,13	0
5	MG	A	1413	1/1	0.98	0.06	-1.87	22,22,22,22	0
5	MG	B	1412	1/1	0.98	0.06	-1.97	27,27,27,27	0
6	CL	C	1413	1/1	1.00	0.05	-2.72	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.