



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:57 PM GMT

PDB ID : 4B11  
Title : Plasmodium vivax N-myristoyltransferase with a bound benzofuran inhibitor (compound 13)  
Authors : Yu, Z.; Brannigan, J.A.; Moss, D.K.; Brzozowski, A.M.; Wilkinson, A.J.; Holder, A.A.; Tate, E.W.; Leatherbarrow, R.J.  
Deposited on : 2012-07-06  
Resolution : 1.59 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

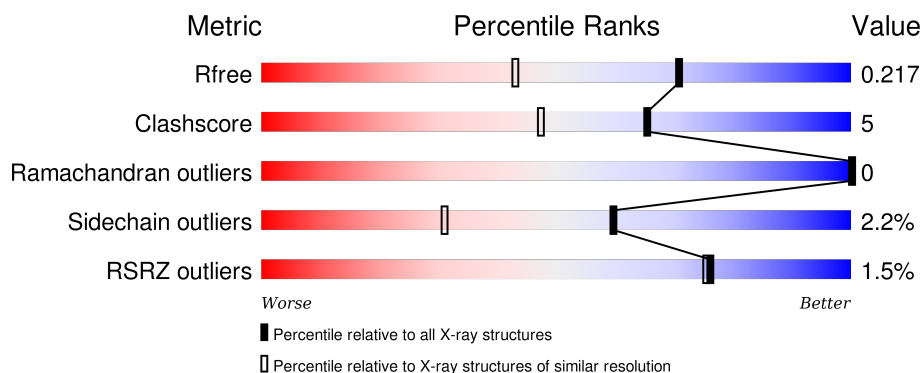
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.59 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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  $\geq 3$ , 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>83%</div> <div>15%</div> <div>.</div> </div>
1	B	385	<div> <div>90%</div> <div>10%</div> <div>.</div> </div>
1	C	385	<div> <div>3%</div> <div>83%</div> <div>12%</div> <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
2	7I1	B	999	-	-	-	X
2	7I1	C	999	-	-	-	X
4	DMS	A	1001	-	-	-	X
4	DMS	B	1001	-	-	-	X
4	DMS	C	1001	-	-	-	X
5	SO4	A	1411	-	-	-	X
6	CL	C	1414	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11552 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.

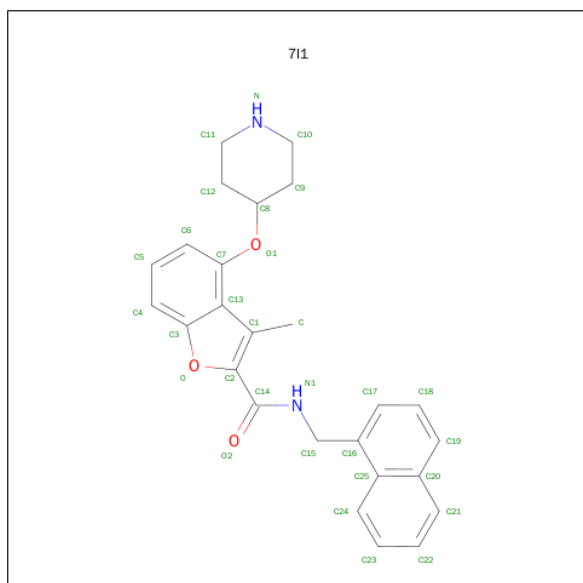
- Molecule 1 is a protein called GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	23	0
			3316	2161	533	609	13			
1	B	385	Total	C	N	O	S	0	13	0
			3254	2118	529	594	13			
1	C	374	Total	C	N	O	S	0	25	0
			3253	2128	519	594	12			

There are 3 discrepancies between the modelled and reference sequences:

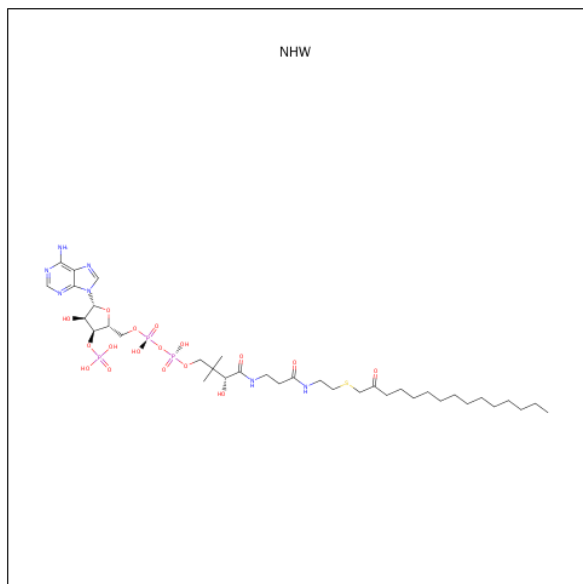
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	EXPRESSION TAG	UNP A5K1A2
B	26	MET	-	EXPRESSION TAG	UNP A5K1A2
C	26	MET	-	EXPRESSION TAG	UNP A5K1A2

- Molecule 2 is 3-METHYL-N-(NAPHTHALEN-1-YLMETHYL)-4-PIPERIDIN-4-YLOXY-1-BENZOFURAN-2-CARBOXAMIDE (three-letter code: 7I1) (formula: C<sub>26</sub>H<sub>26</sub>N<sub>2</sub>O<sub>3</sub>).



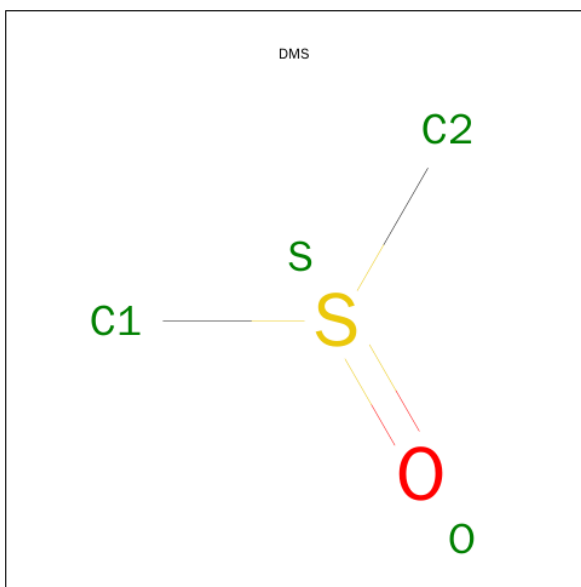
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	26	2	3		
2	B	1	Total	C	N	O	0	0
			31	26	2	3		
2	C	1	Total	C	N	O	0	0
			31	26	2	3		

- 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 DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



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

- Molecule 5 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

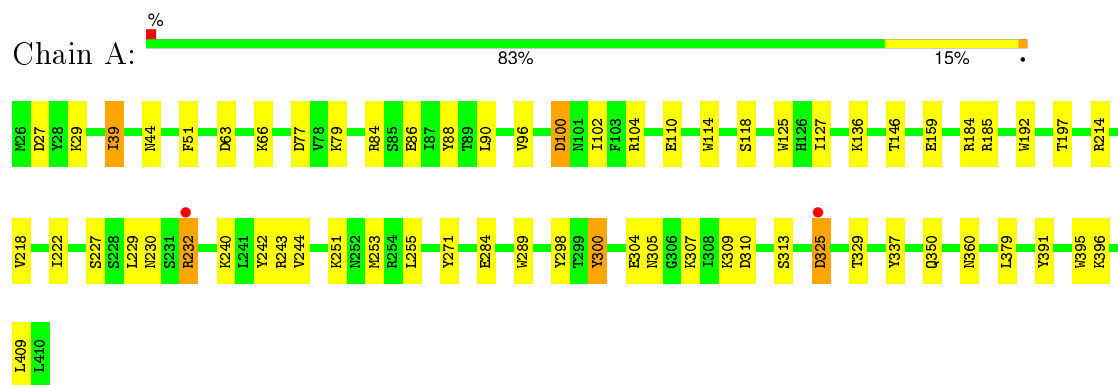
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	530	Total 533	O 533	0	3
8	B	449	Total 449	O 449	0	0
8	C	438	Total 438	O 438	0	0

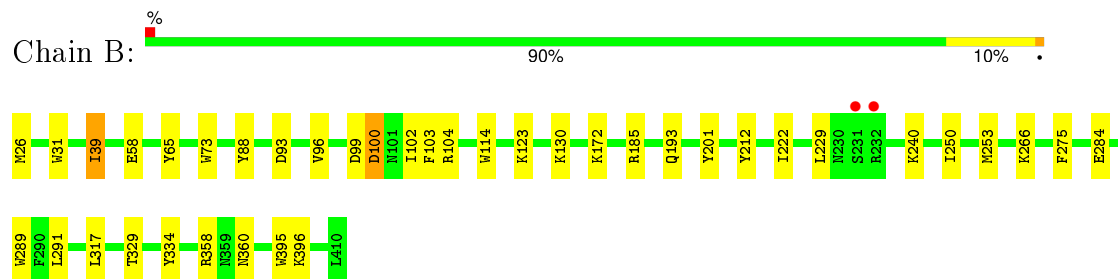
### 3 Residue-property plots

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

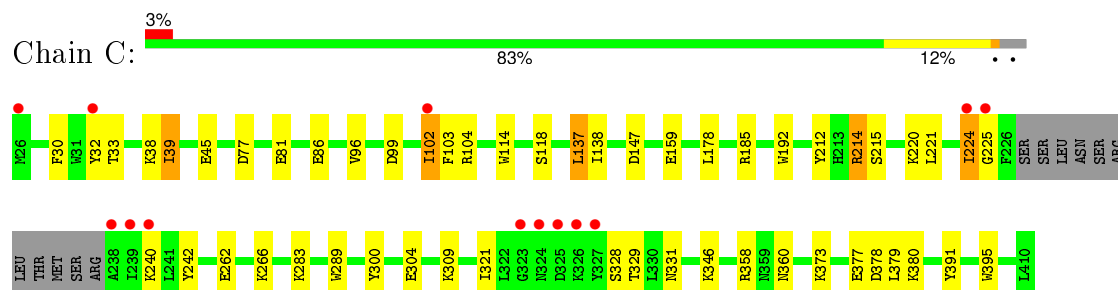
#### • Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



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#### • 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, $\alpha$ , $\beta$ , $\gamma$	57.34Å 119.03Å 175.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.72 – 1.59 70.62 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.7 (70.72-1.59) 99.7 (70.62-1.59)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.7.0025	Depositor
R, $R_{free}$	0.171 , 0.219 0.170 , 0.217	Depositor DCC
$R_{free}$ test set	8110 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.4	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 161160 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NHW, DMS, SO4, 7I1

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	1.24	8/3450 (0.2%)	1.18	13/4669 (0.3%)
1	B	1.22	9/3367 (0.3%)	1.16	7/4554 (0.2%)
1	C	1.20	7/3389 (0.2%)	1.20	11/4583 (0.2%)
All	All	1.22	24/10206 (0.2%)	1.18	31/13806 (0.2%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	TYR	CE1-CZ	6.82	1.47	1.38
1	B	73	TRP	CD2-CE2	6.56	1.49	1.41
1	C	391	TYR	CE2-CZ	6.34	1.46	1.38
1	C	192	TRP	CG-CD1	6.31	1.45	1.36
1	C	114	TRP	CD2-CE2	6.28	1.48	1.41
1	B	114	TRP	CD2-CE2	6.14	1.48	1.41
1	A	271	TYR	CG-CD2	6.04	1.47	1.39
1	B	65	TYR	CE2-CZ	-6.03	1.30	1.38
1	B	395	TRP	CD2-CE2	6.02	1.48	1.41
1	B	193	GLN	C-O	5.94	1.34	1.23
1	A	395	TRP	CD2-CE2	5.93	1.48	1.41
1	B	31	TRP	CD2-CE2	5.85	1.48	1.41
1	A	192	TRP	CD2-CE2	5.82	1.48	1.41
1	C	395	TRP	CD2-CE2	5.79	1.48	1.41
1	C	395	TRP	NE1-CE2	-5.76	1.30	1.37
1	A	90	LEU	C-O	5.74	1.34	1.23
1	B	275	PHE	CE2-CZ	5.54	1.47	1.37
1	C	86	GLU	CD-OE1	5.49	1.31	1.25
1	C	300	TYR	CG-CD1	5.32	1.46	1.39
1	A	88	TYR	CG-CD1	5.26	1.46	1.39
1	B	289	TRP	CD2-CE2	5.23	1.47	1.41
1	A	337	TYR	CE1-CZ	5.14	1.45	1.38
1	A	114	TRP	CD2-CE2	5.07	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	TRP	CD2-CE2	5.01	1.47	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ARG	NE-CZ-NH1	12.21	126.41	120.30
1	C	104	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	C	104	ARG	NE-CZ-NH1	11.79	126.20	120.30
1	A	104	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	C	185	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	C	137	LEU	CB-CG-CD1	7.01	122.91	111.00
1	C	358	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	172	LYS	CD-CE-NZ	-6.52	96.70	111.70
1	A	84	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	77	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	396	LYS	CD-CE-NZ	-6.07	97.74	111.70
1	C	300	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	A	391	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	C	147	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	185	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	358	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	C	214[A]	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	214[B]	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	84	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	184	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	79	LYS	CD-CE-NZ	-5.36	99.36	111.70
1	B	93	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	212	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	C	309	LYS	CD-CE-NZ	-5.29	99.54	111.70
1	C	77	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	229	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	A	255	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	A	310	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	284	GLU	CG-CD-OE1	5.08	128.46	118.30
1	A	63	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	300	TYR	CB-CG-CD1	-5.00	118.00	121.00

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	3316	0	3346	39	1
1	B	3254	0	3277	24	0
1	C	3253	0	3288	36	1
2	A	31	0	26	2	0
2	B	31	0	26	2	0
2	C	31	0	26	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	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	1	0
5	A	5	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	533	0	0	11	1
8	B	449	0	0	8	1
8	C	438	0	0	8	0
All	All	11552	0	10187	102	2

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 (102) 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:30:PHE:O	1:C:33[A]:THR:HG22	1.61	0.99
1:C:32[B]:TYR:HE2	8:C:2010:HOH:O	1.50	0.93
1:A:230:ASN:OD1	1:A:232:ARG:HG3	1.72	0.90
1:A:243:ARG:HD3	8:A:2360:HOH:O	1.81	0.79
1:C:224[B]:ILE:HG22	1:C:225:GLY:H	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44[A]:ASN:OD1	8:A:2028:HOH:O	2.04	0.75
1:C:377[B]:GLU:HG2	8:C:2407:HOH:O	1.91	0.70
1:A:159:GLU:CD	1:A:409[A]:LEU:HD22	2.13	0.69
1:A:100:ASP:HB3	1:A:102:ILE:HG12	1.74	0.69
1:B:100:ASP:HB3	1:B:102[A]:ILE:HD13	1.76	0.67
1:A:251[B]:LYS:HG3	8:A:2377:HOH:O	1.96	0.66
1:A:325:ASP:OD1	1:A:325:ASP:N	2.25	0.65
1:A:304[B]:GLU:OE2	1:A:309:LYS:NZ	2.22	0.64
1:B:100:ASP:HB3	1:B:102[A]:ILE:CD1	2.31	0.61
1:C:224[B]:ILE:HG22	1:C:225:GLY:N	2.15	0.60
1:A:304[B]:GLU:HG2	1:A:305:ASN:HD22	1.66	0.60
1:A:127:ILE:HD11	1:A:185:ARG:HD2	1.85	0.58
1:C:32[B]:TYR:CE2	8:C:2010:HOH:O	2.36	0.57
1:C:304[B]:GLU:HG2	8:C:2309:HOH:O	2.04	0.57
1:A:197:THR:HG23	1:A:409[A]:LEU:HD12	1.87	0.57
1:C:346:LYS:CE	1:C:378:ASP:HB3	2.35	0.56
1:A:86[B]:GLU:HG3	8:A:2147:HOH:O	2.06	0.56
1:A:350[B]:GLN:NE2	8:A:2472:HOH:O	2.38	0.55
1:B:102[A]:ILE:HG23	8:B:2149:HOH:O	2.07	0.55
1:C:224[A]:ILE:HG21	1:C:321:ILE:HG21	1.89	0.55
1:C:215:SER:HB3	1:C:221:LEU:HD12	1.90	0.54
1:B:284[A]:GLU:CG	8:B:2346:HOH:O	2.57	0.53
1:B:123:LYS:HB3	8:B:2099:HOH:O	2.08	0.52
1:B:317:LEU:HB3	1:B:334:TYR:CE1	2.45	0.52
1:A:222[A]:ILE:HD13	1:A:227:SER:HB2	1.92	0.52
1:A:251[B]:LYS:HB2	1:A:251[B]:LYS:HZ2	1.75	0.52
1:C:262[B]:GLU:HG3	1:C:283:LYS:HE3	1.91	0.52
1:B:100:ASP:CB	1:B:102[A]:ILE:HD13	2.40	0.52
1:A:253[A]:MET:HG3	1:A:300:TYR:HB3	1.92	0.52
1:C:96:VAL:HG12	2:C:999:7I1:H23	1.91	0.51
1:C:102:ILE:O	1:C:102:ILE:HG13	2.10	0.51
1:C:102:ILE:HG12	1:C:103:PHE:CE2	2.46	0.51
1:C:346:LYS:HE2	1:C:378:ASP:HB3	1.92	0.50
1:A:118:SER:HB3	1:A:289:TRP:CZ2	2.47	0.50
1:C:331[B]:ASN:OD1	8:C:2372:HOH:O	2.18	0.50
1:C:360[A]:ASN:ND2	8:C:2401:HOH:O	2.44	0.50
1:B:284[A]:GLU:HG3	8:B:2346:HOH:O	2.11	0.50
1:A:218[B]:VAL:HG21	1:A:242:TYR:HD2	1.77	0.49
1:B:102[A]:ILE:HG22	1:B:103:PHE:CE1	2.47	0.49
1:B:250:ILE:O	1:B:253[B]:MET:HG2	2.13	0.49
1:A:329:THR:HG23	8:A:2202:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218[B]:VAL:HG21	1:A:242:TYR:CD2	2.47	0.48
1:B:130:LYS:NZ	8:B:2091:HOH:O	2.44	0.48
1:A:27:ASP:HB3	1:A:29:LYS:HE2	1.95	0.48
1:A:350[B]:GLN:OE1	1:A:379:LEU:HD22	2.14	0.47
2:B:999:7I1:O2	2:B:999:7I1:H24	2.14	0.47
1:A:96:VAL:HG12	2:A:999:7I1:H23	1.96	0.47
2:C:999:7I1:H102	8:C:2259:HOH:O	2.13	0.47
1:A:350[B]:GLN:CD	8:A:2472:HOH:O	2.53	0.47
1:A:350[B]:GLN:OE1	1:A:350[B]:GLN:HA	2.14	0.47
1:C:212:TYR:OH	1:C:373[B]:LYS:HE2	2.14	0.47
1:C:32[A]:TYR:CE1	1:C:38:LYS:HE3	2.50	0.47
1:A:251[B]:LYS:NZ	1:A:251[B]:LYS:CB	2.79	0.46
1:A:51:PHE:CE1	1:A:396:LYS:HG3	2.50	0.46
1:C:102:ILE:HD11	1:C:224[B]:ILE:HG22	1.97	0.46
2:A:999:7I1:O2	2:A:999:7I1:H24	2.15	0.46
1:C:346:LYS:HE3	1:C:378:ASP:HB3	1.97	0.46
1:B:100:ASP:O	1:B:102[A]:ILE:HD12	2.15	0.46
1:A:240:LYS:HD3	8:A:2357:HOH:O	2.16	0.45
1:A:298:TYR:O	1:A:313:SER:HA	2.17	0.45
1:A:253[A]:MET:HB2	1:A:253[A]:MET:HE3	1.76	0.44
1:B:329:THR:HG23	8:B:2156:HOH:O	2.17	0.44
1:B:39:ILE:HA	1:B:39:ILE:HD13	1.66	0.44
1:B:360:ASN:ND2	8:B:2264:HOH:O	2.51	0.44
1:C:159[B]:GLU:OE2	4:C:1001:DMS:O	2.36	0.44
1:A:39:ILE:HA	1:A:39:ILE:HD13	1.70	0.44
1:A:240:LYS:CD	8:A:2357:HOH:O	2.66	0.43
1:A:110[A]:GLU:H	1:A:110[A]:GLU:CD	2.22	0.43
1:B:100:ASP:O	1:B:102[A]:ILE:CD1	2.67	0.43
1:C:240:LYS:HG2	1:C:380:LYS:HZ3	1.82	0.43
8:A:2404:HOH:O	1:C:45[A]:GLU:HG2	2.18	0.43
1:C:138:ILE:C	1:C:138:ILE:HD12	2.39	0.43
1:B:266[B]:LYS:HE3	1:B:266[B]:LYS:HB3	1.55	0.43
1:C:266[B]:LYS:HG2	8:C:2323:HOH:O	2.19	0.42
1:C:39[A]:ILE:HD13	1:C:39[A]:ILE:HA	1.71	0.42
1:A:100:ASP:CB	1:A:102:ILE:HG12	2.45	0.42
1:C:103:PHE:CE1	1:C:224[B]:ILE:HG21	2.55	0.42
1:C:214[B]:ARG:NH1	1:C:379:LEU:O	2.52	0.42
1:C:178[B]:LEU:N	1:C:178[B]:LEU:HD12	2.33	0.42
1:B:39:ILE:HD11	1:B:201:TYR:HE1	1.85	0.42
1:A:251[B]:LYS:HG3	1:A:251[B]:LYS:H	1.46	0.41
1:C:220:LYS:O	1:C:224[B]:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LEU:HD23	1:B:291:LEU:HA	1.93	0.41
1:B:96:VAL:HG12	2:B:999:7I1:H23	2.03	0.41
1:B:222:ILE:HD12	1:B:229:LEU:HG	2.03	0.41
1:C:102:ILE:HD11	1:C:225:GLY:H	1.85	0.41
1:C:102:ILE:HD13	1:C:225:GLY:HA3	2.03	0.41
1:A:304[A]:GLU:HG2	8:A:2387:HOH:O	2.20	0.41
1:C:266[A]:LYS:HB3	1:C:266[A]:LYS:HE3	1.78	0.41
1:B:102[A]:ILE:HG22	1:B:103:PHE:CD1	2.55	0.41
1:B:317:LEU:HB3	1:B:334:TYR:CD1	2.56	0.41
1:A:218[B]:VAL:HG21	1:A:242:TYR:HB2	2.04	0.40
1:C:118:SER:HB3	1:C:289:TRP:CZ2	2.57	0.40
1:C:30:PHE:O	1:C:33[A]:THR:CG2	2.51	0.40
1:A:251[B]:LYS:HB2	1:A:251[B]:LYS:NZ	2.36	0.40
1:B:240:LYS:HD3	8:B:2282:HOH:O	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:NZ	8:A:2476:HOH:O[1_655]	2.16	0.04
1:C:242:TYR:OH	8:B:2193:HOH:O[2_455]	2.18	0.02

## 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	406/385 (106%)	395 (97%)	11 (3%)	0	100	100
1	B	396/385 (103%)	384 (97%)	12 (3%)	0	100	100
1	C	395/385 (103%)	378 (96%)	17 (4%)	0	100	100
All	All	1197/1155 (104%)	1157 (97%)	40 (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	374/351 (107%)	362 (97%)	12 (3%)	46	18
1	B	364/351 (104%)	359 (99%)	5 (1%)	74	53
1	C	365/351 (104%)	355 (97%)	10 (3%)	52	23
All	All	1103/1053 (105%)	1076 (98%)	27 (2%)	60	27

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ILE
1	A	100	ASP
1	A	136	LYS
1	A	146[A]	THR
1	A	146[B]	THR
1	A	214	ARG
1	A	232	ARG
1	A	244	VAL
1	A	307	LYS
1	A	325	ASP
1	A	360[A]	ASN
1	A	360[B]	ASN
1	B	26	MET
1	B	39	ILE
1	B	58	GLU
1	B	99	ASP
1	B	100	ASP
1	C	39[A]	ILE
1	C	39[B]	ILE
1	C	81	GLU
1	C	99	ASP
1	C	102	ILE
1	C	137	LEU

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Mol	Chain	Res	Type
1	C	224[A]	ILE
1	C	224[B]	ILE
1	C	328	SER
1	C	329	THR

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	34	GLN
1	A	106	ASN
1	A	249	ASN
1	A	305	ASN
1	A	371	GLN
1	B	34	GLN
1	B	249	ASN
1	B	295	ASN
1	B	360	ASN
1	C	34	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 7 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	$\# Z  > 2$
3	NHW	A	1000	7	56,66,66	1.40	8 (14%)	68,92,92	1.62	11 (16%)
4	DMS	A	1001	-	3,3,3	0.30	0	3,3,3	3.79	1 (33%)
5	SO4	A	1411	-	4,4,4	0.65	0	6,6,6	1.18	1 (16%)
2	7I1	A	999	-	31,35,35	1.29	3 (9%)	35,49,49	1.74	9 (25%)
3	NHW	B	1000	7	56,66,66	1.80	14 (25%)	68,92,92	1.70	11 (16%)
4	DMS	B	1001	-	3,3,3	0.26	0	3,3,3	1.29	0
2	7I1	B	999	-	31,35,35	1.17	4 (12%)	35,49,49	2.23	11 (31%)
3	NHW	C	1000	7	56,66,66	1.30	6 (10%)	68,92,92	1.68	16 (23%)
4	DMS	C	1001	-	3,3,3	0.24	0	3,3,3	0.95	0
2	7I1	C	999	-	31,35,35	1.33	4 (12%)	35,49,49	1.95	10 (28%)

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	NHW	A	1000	7	-	0/61/81/81	0/3/3/3
4	DMS	A	1001	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1411	-	-	0/0/0/0	0/0/0/0
2	7I1	A	999	-	-	0/9/21/21	0/4/5/5
3	NHW	B	1000	7	-	0/61/81/81	0/3/3/3
4	DMS	B	1001	-	-	0/0/0/0	0/0/0/0
2	7I1	B	999	-	-	0/9/21/21	0/4/5/5
3	NHW	C	1000	7	-	0/61/81/81	0/3/3/3
4	DMS	C	1001	-	-	0/0/0/0	0/0/0/0
2	7I1	C	999	-	-	0/9/21/21	0/4/5/5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1000	NHW	P2A-O4A	-2.69	1.43	1.54
3	B	1000	NHW	C2A-N3A	-2.31	1.28	1.32
3	A	1000	NHW	O2X-C2X	2.02	1.47	1.43
3	B	1000	NHW	O1M-C1M	2.02	1.25	1.21
2	C	999	7I1	C18-C19	2.04	1.41	1.36
3	B	1000	NHW	C3M-C2M	2.05	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	7I1	C2-C14	2.14	1.53	1.49
3	B	1000	NHW	C2-C3	2.14	1.59	1.51
2	B	999	7I1	C18-C19	2.17	1.41	1.36
2	C	999	7I1	C22-C21	2.22	1.41	1.36
3	A	1000	NHW	CP-C1M	2.25	1.55	1.51
3	C	1000	NHW	O4X-C1X	2.25	1.44	1.41
2	B	999	7I1	C1-C13	2.27	1.43	1.40
3	B	1000	NHW	C2X-C3X	2.31	1.58	1.53
2	B	999	7I1	C5-C4	2.32	1.42	1.36
3	C	1000	NHW	CP-C1M	2.32	1.55	1.51
2	B	999	7I1	C9-C8	2.33	1.57	1.51
3	C	1000	NHW	C6-C5	2.35	1.55	1.51
2	A	999	7I1	C18-C19	2.42	1.42	1.36
2	A	999	7I1	C17-C16	2.48	1.42	1.37
3	C	1000	NHW	O10-C10	2.56	1.47	1.42
3	B	1000	NHW	CP-C1M	2.60	1.55	1.51
3	B	1000	NHW	C7-N8	2.66	1.52	1.46
3	A	1000	NHW	C7-N8	2.75	1.52	1.46
3	C	1000	NHW	O5-C5	2.85	1.29	1.23
3	A	1000	NHW	O10-C10	2.85	1.48	1.42
3	A	1000	NHW	O5-C5	2.89	1.29	1.23
3	B	1000	NHW	C8A-N7A	2.91	1.40	1.34
3	A	1000	NHW	C3-N4	3.11	1.53	1.46
3	C	1000	NHW	P3X-O3X	3.14	1.69	1.60
2	C	999	7I1	C1-C13	3.20	1.44	1.40
3	B	1000	NHW	O10-C10	3.34	1.49	1.42
2	C	999	7I1	C5-C4	3.40	1.44	1.36
3	A	1000	NHW	CP-S1	3.57	1.89	1.81
3	B	1000	NHW	O4X-C1X	3.70	1.45	1.41
3	A	1000	NHW	C6-C5	3.78	1.58	1.51
3	B	1000	NHW	O4X-C4X	3.99	1.54	1.45
3	B	1000	NHW	CP-S1	4.16	1.90	1.81
3	B	1000	NHW	C6-C5	5.21	1.61	1.51

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1000	NHW	N3A-C2A-N1A	-9.27	121.79	128.89
3	C	1000	NHW	N3A-C2A-N1A	-5.20	124.91	128.89
3	A	1000	NHW	C1X-N9A-C4A	-4.50	120.15	126.94
3	A	1000	NHW	N3A-C2A-N1A	-4.47	125.47	128.89
3	A	1000	NHW	C4A-C5A-N7A	-4.39	105.44	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	7I1	C1-C13-C3	-4.15	102.70	110.03
2	B	999	7I1	C1-C13-C3	-3.75	103.40	110.03
3	A	1000	NHW	C2X-C1X-N9A	-3.72	108.61	114.29
3	B	1000	NHW	C4X-O4X-C1X	-3.64	105.72	109.72
2	C	999	7I1	O2-C14-C2	-3.59	116.15	121.01
3	C	1000	NHW	C2X-C1X-N9A	-3.55	108.87	114.29
2	B	999	7I1	C24-C25-C16	-3.47	116.90	122.64
3	C	1000	NHW	C5X-C4X-C3X	-3.41	102.05	114.31
3	A	1000	NHW	O4X-C1X-N9A	-3.29	101.20	108.10
2	C	999	7I1	C1-C13-C3	-3.25	104.28	110.03
3	A	1000	NHW	O1M-C1M-CP	-3.10	117.70	122.14
2	B	999	7I1	C11-C12-C8	-3.04	106.98	110.19
2	B	999	7I1	C16-C15-N1	-3.04	105.55	113.13
2	B	999	7I1	C23-C24-C25	-3.03	116.60	120.88
3	C	1000	NHW	O3X-C3X-C4X	-3.02	98.15	109.99
2	C	999	7I1	C24-C25-C16	-2.99	117.69	122.64
3	A	1000	NHW	P3X-O3X-C3X	-2.96	114.46	121.56
2	A	999	7I1	C24-C25-C16	-2.83	117.96	122.64
3	C	1000	NHW	O6A-C12-C11	-2.70	106.21	110.55
3	C	1000	NHW	C2X-C3X-C4X	-2.67	98.28	103.29
2	A	999	7I1	C18-C19-C20	-2.56	116.33	120.44
3	C	1000	NHW	C6-C5-N4	-2.44	112.21	116.46
3	C	1000	NHW	CAM-C9M-C8M	-2.42	102.02	114.53
3	A	1000	NHW	C2-C3-N4	-2.40	107.56	112.36
3	B	1000	NHW	C2-C3-N4	-2.35	107.66	112.36
3	B	1000	NHW	C6-C5-N4	-2.35	112.38	116.46
3	B	1000	NHW	C3-C2-S1	-2.30	105.72	114.25
3	B	1000	NHW	C2X-C1X-N9A	-2.29	110.79	114.29
3	B	1000	NHW	P3X-O3X-C3X	-2.26	116.14	121.56
3	C	1000	NHW	C6-C7-N8	-2.25	106.94	111.88
3	A	1000	NHW	C2-S1-CP	-2.22	98.20	101.89
3	C	1000	NHW	O3X-P3X-O9A	-2.21	101.60	107.11
3	B	1000	NHW	C3M-C2M-C1M	-2.20	109.76	115.12
3	B	1000	NHW	C7-N8-C9	-2.13	118.31	122.53
3	C	1000	NHW	C3-N4-C5	-2.12	118.62	122.79
3	C	1000	NHW	O10-C10-C9	-2.12	105.51	110.38
3	C	1000	NHW	C3-C2-S1	-2.06	106.60	114.25
2	C	999	7I1	C16-C15-N1	-2.06	107.98	113.13
3	B	1000	NHW	C4M-C3M-C2M	-2.05	105.76	113.29
5	A	1411	SO4	O4-S-O3	-2.03	100.73	108.98
2	A	999	7I1	C16-C15-N1	-2.03	108.07	113.13
2	B	999	7I1	C16-C25-C20	2.03	121.63	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	999	7I1	C19-C20-C25	2.17	122.04	119.10
2	A	999	7I1	C12-C11-N	2.33	114.41	110.46
3	C	1000	NHW	O8A-P3X-O7A	2.39	116.48	107.38
3	A	1000	NHW	O2X-C2X-C3X	2.41	118.13	111.16
3	C	1000	NHW	C3X-C2X-C1X	2.44	105.84	99.98
2	C	999	7I1	C-C1-C2	2.48	133.20	127.84
2	C	999	7I1	C15-N1-C14	2.50	128.36	121.84
2	A	999	7I1	C9-C8-C12	2.58	115.81	111.61
2	B	999	7I1	C-C1-C2	2.66	133.59	127.84
2	A	999	7I1	C16-C25-C20	2.68	122.48	118.97
2	C	999	7I1	C24-C25-C20	2.72	121.47	117.91
2	B	999	7I1	C24-C25-C20	2.72	121.47	117.91
2	B	999	7I1	C9-C8-C12	2.91	116.34	111.61
3	A	1000	NHW	C13-C11-C10	2.91	114.66	109.34
2	A	999	7I1	C10-N-C11	2.93	120.04	110.33
3	B	1000	NHW	C2A-N1A-C6A	3.09	124.28	118.77
2	A	999	7I1	C10-C9-C8	3.98	114.39	110.19
2	B	999	7I1	C10-N-C11	4.02	123.68	110.33
2	C	999	7I1	C10-C9-C8	4.18	114.60	110.19
3	C	1000	NHW	C13-C11-C10	4.49	117.55	109.34
2	C	999	7I1	C10-N-C11	4.77	126.16	110.33
4	A	1001	DMS	C2-S-C1	6.23	130.63	98.46
2	B	999	7I1	C10-C9-C8	7.11	117.68	110.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	7I1	2	0
2	B	999	7I1	2	0
4	C	1001	DMS	1	0
2	C	999	7I1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	385/385 (100%)	-0.44	2 (0%) 91 91	7, 12, 26, 70	12 (3%)
1	B	385/385 (100%)	-0.44	2 (0%) 91 91	8, 14, 28, 62	13 (3%)
1	C	374/385 (97%)	-0.34	13 (3%) 48 44	8, 13, 32, 60	11 (2%)
All	All	1144/1155 (99%)	-0.40	17 (1%) 76 75	7, 13, 30, 70	36 (3%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	323	GLY	4.5
1	C	224[A]	ILE	4.4
1	A	232	ARG	4.4
1	C	225	GLY	3.5
1	C	325	ASP	3.4
1	B	231	SER	3.2
1	C	32[A]	TYR	3.2
1	C	239	ILE	3.0
1	A	325	ASP	2.9
1	C	26	MET	2.7
1	B	232	ARG	2.6
1	C	324	ASN	2.5
1	C	240	LYS	2.3
1	C	326	LYS	2.2
1	C	238	ALA	2.1
1	C	327	TYR	2.1
1	C	102	ILE	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 ⓘ

There are no carbohydrates 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. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	SO4	A	1411	5/5	0.83	0.17	8.51	43,46,61,62	0
6	CL	C	1414	1/1	0.96	0.08	8.14	37,37,37,37	0
4	DMS	C	1001	4/4	0.94	0.17	5.78	13,14,15,15	4
4	DMS	B	1001	4/4	0.93	0.12	3.62	25,26,28,28	0
2	7I1	B	999	31/31	0.91	0.13	3.08	20,23,29,31	0
4	DMS	A	1001	4/4	0.93	0.14	2.92	25,28,28,40	0
2	7I1	C	999	31/31	0.88	0.11	2.24	19,25,32,39	0
2	7I1	A	999	31/31	0.92	0.11	1.47	17,21,28,31	0
3	NHW	A	1000	64/64	0.98	0.06	-0.26	7,10,13,16	0
3	NHW	C	1000	64/64	0.98	0.06	-0.44	6,11,14,16	0
3	NHW	B	1000	64/64	0.98	0.05	-0.66	7,11,15,16	0
7	MG	C	1412	1/1	0.98	0.06	-0.92	19,19,19,19	0
7	MG	B	1412	1/1	0.98	0.05	-0.96	21,21,21,21	0
6	CL	B	1411	1/1	1.00	0.05	-1.41	14,14,14,14	0
7	MG	A	1413	1/1	0.99	0.05	-3.86	18,18,18,18	0
6	CL	A	1412	1/1	1.00	0.04	-7.29	11,11,11,11	0
6	CL	C	1411	1/1	1.00	0.04	-10.47	11,11,11,11	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.