



# Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2020 – 12:00 am BST

PDB ID : 4B10  
Title : Plasmodium vivax N-myristoyltransferase with a non-hydrolysable co- factor  
Authors : Yu, Z.; Brannigan, J.A.; Moss, D.K.; Brzozowski, A.M.; Wilkinson, A.J.;  
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Deposited on : 2012-07-06  
Resolution : 1.56 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

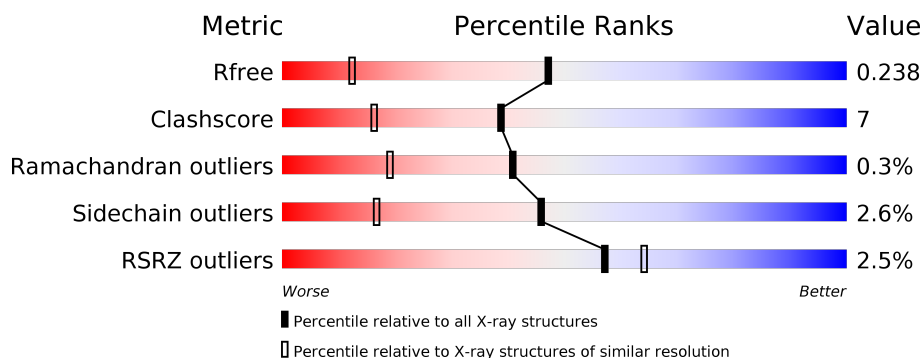
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.56 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))
$R_{free}$	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	385	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div>
1	B	385	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div> </div>
1	C	385	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>..</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11496 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.

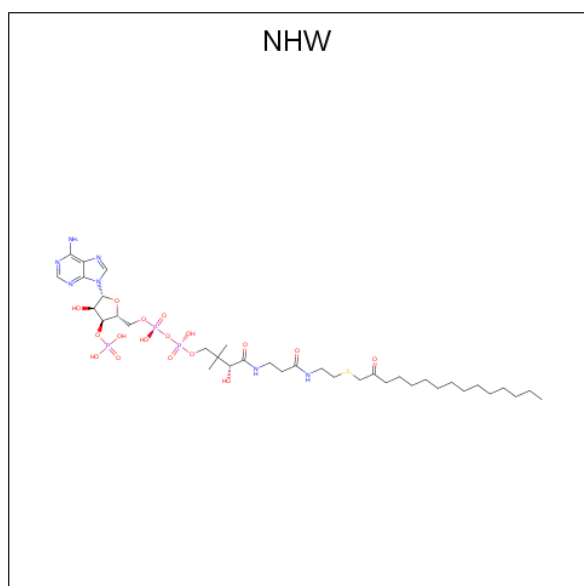
- Molecule 1 is a protein called GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	5	25	0
			3336	2175	539	609	13			
1	B	385	Total	C	N	O	S	0	23	0
			3338	2179	540	606	13			
1	C	374	Total	C	N	O	S	0	21	0
			3223	2108	517	586	12			

There are 3 discrepancies between the modelled and reference sequences:

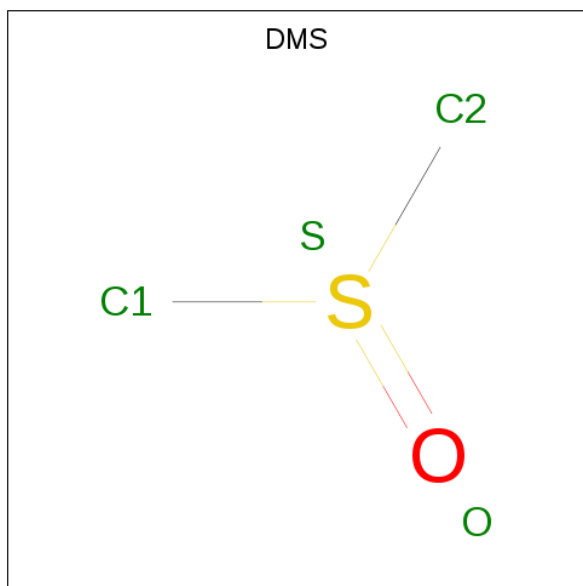
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	expression tag	UNP A5K1A2
B	26	MET	-	expression tag	UNP A5K1A2
C	26	MET	-	expression tag	UNP A5K1A2

- Molecule 2 is 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	0	0
			64	36	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	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: O<sub>4</sub>S).



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

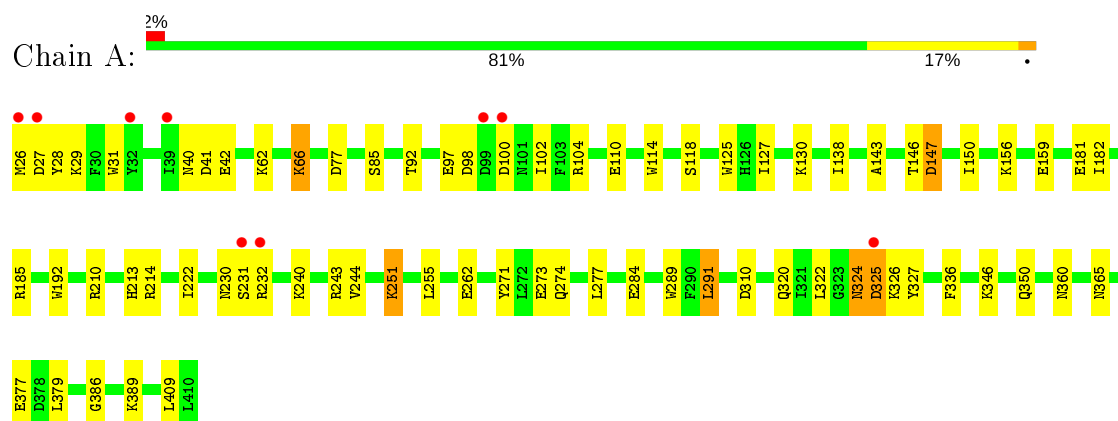
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	530	Total	O	0	0
			530	530		
7	B	445	Total	O	0	0
			445	445		
7	C	409	Total	O	0	0
			409	409		

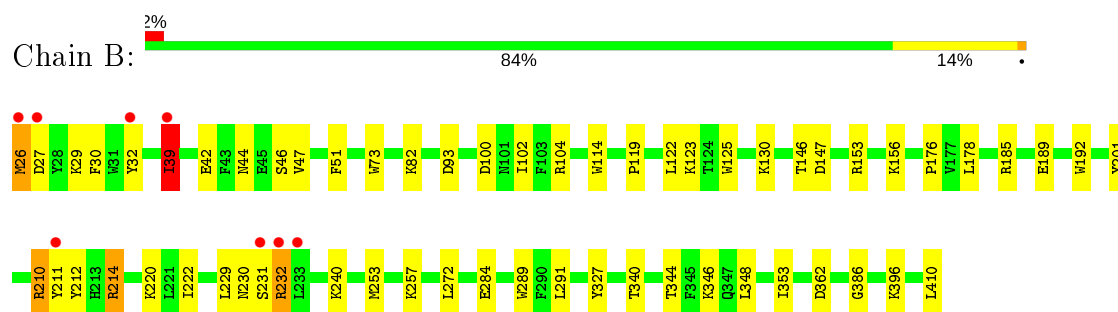
### 3 Residue-property plots [i](#)

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

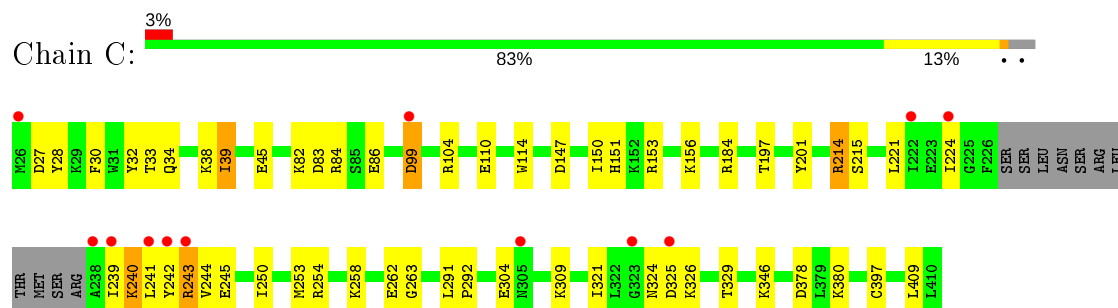
#### • Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.37Å 119.06Å 176.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.83 – 1.56 41.83 – 1.56	Depositor EDS
% Data completeness (in resolution range)	97.8 (41.83-1.56) 97.8 (41.83-1.56)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.7.0025	Depositor
R, $R_{free}$	0.188 , 0.238 0.188 , 0.238	Depositor DCC
$R_{free}$ test set	8406 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.7	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11496	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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, 0.333 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: SO4, MG, DMS, NHW, 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	1.07	5/3479 (0.1%)	1.10	9/4708 (0.2%)
1	B	1.03	3/3481 (0.1%)	1.08	9/4706 (0.2%)
1	C	1.05	2/3361 (0.1%)	1.05	6/4550 (0.1%)
All	All	1.05	10/10321 (0.1%)	1.07	24/13964 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	GLU	CD-OE2	6.84	1.33	1.25
1	A	125	TRP	CD2-CE2	6.75	1.49	1.41
1	B	192	TRP	CD2-CE2	6.40	1.49	1.41
1	B	289	TRP	CD2-CE2	5.97	1.48	1.41
1	B	114	TRP	CD2-CE2	5.88	1.48	1.41
1	C	245	GLU	CD-OE2	5.57	1.31	1.25
1	A	114	TRP	CD2-CE2	5.33	1.47	1.41
1	A	192	TRP	CD2-CE2	5.26	1.47	1.41
1	A	181	GLU	CD-OE2	5.15	1.31	1.25
1	C	114	TRP	CD2-CE2	5.11	1.47	1.41

All (24) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	B	210	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B	272	LEU	CB-CG-CD1	-7.66	97.98	111.00
1	B	104	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	185	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	C	104	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	336	PHE	CB-CG-CD2	-6.27	116.41	120.80
1	C	104	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	B	185	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	B	410	LEU	CB-CG-CD1	-5.83	101.09	111.00
1	C	153	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	362	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	77	ASP	CB-CG-OD1	5.62	123.35	118.30
1	A	255	LEU	CB-CG-CD1	-5.59	101.50	111.00
1	B	93	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	251[A]	LYS	CD-CE-NZ	5.50	124.34	111.70
1	A	251[B]	LYS	CD-CE-NZ	5.50	124.34	111.70
1	A	147[A]	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	147[B]	ASP	CB-CG-OD2	5.37	123.14	118.30
1	C	254	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	291	LEU	CB-CG-CD1	-5.35	101.90	111.00
1	C	184	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	310	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	84	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	386	GLY	Peptide
1	B	386	GLY	Peptide

## 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	3336	0	3357	61	0
1	B	3338	0	3375	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3223	0	3246	48	0
2	A	64	0	60	0	0
2	B	64	0	60	0	0
2	C	64	0	60	0	0
3	A	4	0	6	1	0
3	B	4	0	6	0	0
3	C	4	0	6	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
6	B	5	0	0	1	0
7	A	530	0	0	13	0
7	B	445	0	0	8	0
7	C	409	0	0	10	0
All	All	11496	0	10176	152	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 7.

All (152) 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:262[B]:GLU:HG3	7:C:2288:HOH:O	1.37	1.24
1:C:30:PHE:O	1:C:33[A]:THR:HG22	1.50	1.10
1:A:147[B]:ASP:OD1	1:A:156:LYS:HD3	1.54	1.08
1:A:62:LYS:HE3	7:A:2092:HOH:O	1.51	1.07
1:C:32[B]:TYR:HE2	7:C:2011:HOH:O	1.38	1.05
1:C:33[A]:THR:HG23	1:C:34:GLN:HE21	1.34	0.92
1:C:243:ARG:HG2	1:C:243:ARG:HH11	1.39	0.86
1:B:147:ASP:OD1	1:B:156[A]:LYS:HD3	1.75	0.85
1:A:324:ASN:ND2	1:A:327:TYR:H	1.74	0.85
1:A:346[B]:LYS:HZ3	1:A:379:LEU:HD21	1.42	0.84
1:B:122[A]:LEU:HD21	1:B:189:GLU:HG3	1.60	0.83
1:C:32[B]:TYR:OH	1:C:39[B]:ILE:HG22	1.81	0.80
1:A:251[B]:LYS:NZ	1:A:251[B]:LYS:CB	2.45	0.79
1:A:251[B]:LYS:HZ1	1:A:251[B]:LYS:HB2	1.46	0.79
1:C:214[B]:ARG:HH11	1:C:214[B]:ARG:HG2	1.49	0.77
1:C:45[A]:GLU:OE2	1:C:151[A]:HIS:HE1	1.70	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262[B]:GLU:CG	7:C:2288:HOH:O	2.09	0.74
1:C:110:GLU:OE2	7:C:2158:HOH:O	2.04	0.73
1:B:47:VAL:HG11	1:B:396[B]:LYS:HG2	1.69	0.73
1:A:159:GLU:CD	1:A:409:LEU:HD22	2.09	0.73
1:B:210:ARG:C	1:B:211[C]:TYR:CA	2.58	0.71
1:B:47:VAL:CG1	1:B:396[B]:LYS:HG2	2.19	0.71
1:C:325:ASP:HB3	7:C:2342:HOH:O	1.91	0.71
1:A:42[B]:GLU:HG3	1:B:344:THR:HG21	1.72	0.71
1:B:82[B]:LYS:HG3	7:B:2099:HOH:O	1.90	0.70
1:C:214[B]:ARG:HD2	1:C:215:SER:N	2.07	0.70
1:B:123:LYS:HB3	7:B:2093:HOH:O	1.91	0.70
1:B:122[A]:LEU:HD22	1:B:125:TRP:CE2	2.27	0.69
1:A:110:GLU:HG2	7:A:2221:HOH:O	1.93	0.69
1:A:251[B]:LYS:NZ	1:A:251[B]:LYS:HB2	2.03	0.69
1:B:122[A]:LEU:CD2	1:B:189:GLU:HG3	2.22	0.69
1:C:147:ASP:OD1	1:C:156:LYS:NZ	2.25	0.69
1:B:222:ILE:HD12	1:B:229:LEU:HG	1.74	0.68
1:C:147:ASP:OD1	1:C:156:LYS:CE	2.41	0.68
1:C:32[B]:TYR:HH	1:C:39[B]:ILE:HG22	1.58	0.68
1:C:239:ILE:HA	1:C:242:TYR:HB2	1.75	0.68
1:A:147[B]:ASP:OD1	1:A:156:LYS:CD	2.38	0.67
1:B:211[C]:TYR:CA	1:B:212:TYR:N	2.58	0.67
1:A:213[A]:HIS:ND1	1:A:365:ASN:OD1	2.19	0.67
1:A:346[B]:LYS:HZ3	1:A:379:LEU:CD2	2.08	0.66
1:A:346[B]:LYS:NZ	1:A:379:LEU:HD21	2.10	0.66
1:C:214[B]:ARG:HD2	1:C:214[B]:ARG:C	2.14	0.66
1:B:26:MET:HA	7:B:2001:HOH:O	1.95	0.66
1:C:45[A]:GLU:OE2	1:C:151[A]:HIS:CE1	2.50	0.65
1:C:215:SER:HB3	1:C:221:LEU:HD12	1.79	0.64
1:C:243:ARG:HH11	1:C:243:ARG:CG	2.08	0.64
1:C:147:ASP:OD1	1:C:156:LYS:HE2	1.99	0.61
1:A:240:LYS:HG3	1:A:243:ARG:HH12	1.64	0.61
1:C:214[B]:ARG:NH1	1:C:214[B]:ARG:HG2	2.16	0.60
1:C:82:LYS:O	1:C:86[A]:GLU:HG3	2.01	0.59
1:A:324:ASN:HD22	1:A:327:TYR:H	1.48	0.59
1:C:262[B]:GLU:HG3	1:C:263:GLY:H	1.67	0.58
1:B:122[A]:LEU:HD22	1:B:125:TRP:NE1	2.19	0.58
1:B:214:ARG:HG2	1:B:353:ILE:HD13	1.86	0.58
1:A:147[A]:ASP:CG	1:A:156:LYS:HZ3	2.07	0.58
1:A:147[A]:ASP:OD2	1:A:156:LYS:NZ	2.37	0.57
1:B:47:VAL:HG11	1:B:396[B]:LYS:CG	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:TYR:CE2	1:C:39[A]:ILE:HG13	2.40	0.57
1:A:66[B]:LYS:HE2	7:A:2034:HOH:O	2.05	0.56
1:C:32[A]:TYR:CE2	1:C:38:LYS:HE3	2.40	0.56
1:A:324:ASN:ND2	1:A:326:LYS:H	2.03	0.56
1:A:42[B]:GLU:CG	1:B:344:THR:HG21	2.37	0.55
1:A:85[A]:SER:OG	7:A:2149:HOH:O	2.18	0.55
1:C:262[B]:GLU:HG2	7:C:2285:HOH:O	2.05	0.55
1:A:251[B]:LYS:CB	1:A:251[B]:LYS:HZ1	2.10	0.55
1:A:118:SER:HB3	1:A:289:TRP:CZ2	2.42	0.55
1:A:147[A]:ASP:OD2	1:A:156:LYS:CE	2.55	0.55
1:A:284[A]:GLU:H	1:A:284[A]:GLU:CD	2.11	0.53
1:C:250:ILE:O	1:C:253[A]:MET:HG2	2.09	0.53
1:A:62:LYS:HE2	7:A:2073:HOH:O	2.09	0.52
1:A:102:ILE:HG23	7:A:2200:HOH:O	2.09	0.52
1:A:360[A]:ASN:ND2	7:A:2340:HOH:O	2.43	0.52
1:A:130:LYS:NZ	7:A:2242:HOH:O	2.31	0.51
1:B:39:ILE:HD11	1:B:201:TYR:HE2	1.75	0.51
1:A:350[B]:GLN:OE1	1:A:350[B]:GLN:HA	2.11	0.51
1:C:262[B]:GLU:HG3	1:C:263:GLY:N	2.25	0.51
1:B:44[B]:ASN:ND2	1:B:46:SER:OG	2.40	0.50
1:A:92:THR:O	1:A:104:ARG:HD2	2.11	0.50
1:A:262:GLU:HG3	7:A:2394:HOH:O	2.10	0.50
1:C:39[B]:ILE:HD11	1:C:201:TYR:CE2	2.47	0.50
1:A:40[B]:ASN:ND2	7:A:2019:HOH:O	2.45	0.49
1:B:51:PHE:CD1	1:B:396[A]:LYS:HE2	2.48	0.49
1:C:33[A]:THR:CG2	1:C:34:GLN:HE21	2.18	0.49
1:B:130:LYS:NZ	7:B:2087:HOH:O	2.45	0.49
1:B:32:TYR:OH	1:B:39:ILE:HB	2.13	0.48
1:B:257:LYS:HE3	7:B:2304:HOH:O	2.13	0.48
1:B:123:LYS:HG3	7:B:2171:HOH:O	2.13	0.48
1:B:230[A]:ASN:OD1	1:B:232:ARG:HG3	2.13	0.48
1:B:73:TRP:HZ3	1:B:178:LEU:HD23	1.77	0.48
1:A:251[B]:LYS:HB3	1:A:251[B]:LYS:NZ	2.26	0.48
1:A:389:LYS:HD2	1:A:389:LYS:N	2.29	0.48
1:C:151[A]:HIS:CD2	7:C:2036:HOH:O	2.67	0.47
1:C:324:ASN:OD1	1:C:326:LYS:HB3	2.14	0.47
1:A:147[B]:ASP:OD1	1:A:156:LYS:NZ	2.43	0.47
1:A:97:GLU:HG2	1:A:104:ARG:HB2	1.97	0.47
1:B:119:PRO:HG3	1:B:284[C]:GLU:HG3	1.96	0.47
1:A:325:ASP:OD1	1:A:325:ASP:N	2.48	0.47
1:C:28:TYR:HE2	1:C:39[A]:ILE:HG13	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:NH1	6:B:1411:SO4:O1	2.32	0.46
1:A:127:ILE:HD11	1:A:182[B]:ILE:HD12	1.96	0.46
1:C:243:ARG:HG2	1:C:243:ARG:NH1	2.17	0.46
1:C:321:ILE:HG22	1:C:324:ASN:HB2	1.98	0.45
1:A:150:ILE:HD13	1:A:277:LEU:HD13	1.99	0.45
1:B:47:VAL:HG11	1:B:396[B]:LYS:CD	2.47	0.45
7:A:2481:HOH:O	1:B:44[A]:ASN:OD1	2.20	0.45
1:A:251[B]:LYS:HB3	1:A:251[B]:LYS:HZ2	1.82	0.44
1:B:27:ASP:HB3	1:B:29:LYS:HE3	1.99	0.44
1:C:304:GLU:HB3	1:C:309[A]:LYS:HE3	1.97	0.44
1:A:27:ASP:HB3	1:A:29:LYS:HE3	1.98	0.44
1:C:32[B]:TYR:CE2	7:C:2011:HOH:O	2.29	0.44
1:A:138:ILE:C	1:A:138:ILE:HD12	2.38	0.44
1:A:377[A]:GLU:HG2	7:A:2503:HOH:O	2.18	0.44
1:B:340:THR:HB	1:B:348:LEU:HD22	1.98	0.44
1:C:346:LYS:HD2	1:C:378:ASP:HB3	1.98	0.44
1:A:320:GLN:HG2	1:A:322:LEU:HD23	2.00	0.43
1:A:41:ASP:O	1:A:42[A]:GLU:HG3	2.18	0.43
1:A:271:TYR:O	1:A:274:GLN:HG2	2.18	0.43
1:B:240:LYS:HD3	7:B:2139:HOH:O	2.17	0.43
1:A:251[B]:LYS:HZ2	1:A:251[B]:LYS:CB	2.29	0.43
1:C:83:ASP:HA	1:C:86[A]:GLU:HG3	1.99	0.43
1:A:346[B]:LYS:NZ	1:A:379:LEU:CD2	2.77	0.43
1:C:214[B]:ARG:CG	1:C:214[B]:ARG:NH1	2.82	0.43
1:C:240:LYS:HG2	1:C:380:LYS:HE2	1.99	0.43
1:B:220:LYS:HE3	1:B:327:TYR:CD1	2.54	0.43
1:C:291:LEU:HA	1:C:292:PRO:HD3	1.91	0.43
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.88	0.43
1:A:230:ASN:OD1	1:A:232:ARG:HG2	2.18	0.42
1:A:28:TYR:HB3	1:A:31:TRP:HB2	2.00	0.42
1:B:147:ASP:OD1	1:B:156[A]:LYS:CD	2.58	0.42
1:B:102:ILE:HA	1:B:102:ILE:HD13	1.85	0.42
1:B:51:PHE:HA	1:B:396[A]:LYS:HE3	2.01	0.42
1:A:98:ASP:OD1	1:A:102:ILE:N	2.47	0.42
3:A:1001:DMS:H22	7:A:2470:HOH:O	2.19	0.42
1:B:122[A]:LEU:HD13	1:B:125:TRP:CE3	2.55	0.42
1:A:147[B]:ASP:CG	1:A:156:LYS:HZ3	2.12	0.42
1:B:30:PHE:CD1	1:B:176:PRO:HB3	2.54	0.42
1:C:346:LYS:HD3	7:C:2384:HOH:O	2.20	0.42
1:C:86[B]:GLU:HB3	7:C:2118:HOH:O	2.20	0.42
1:C:151[B]:HIS:HD2	1:C:397:CYS:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:HD11	1:A:185:ARG:HD2	2.02	0.41
1:B:291:LEU:HD23	1:B:291:LEU:HA	1.95	0.41
1:A:66[B]:LYS:HD3	1:A:66[B]:LYS:HA	1.68	0.41
1:B:346[A]:LYS:HB3	1:B:346[A]:LYS:HE3	1.78	0.41
1:A:143:ALA:HA	1:A:159:GLU:O	2.21	0.41
1:B:42:GLU:HG2	7:B:2023:HOH:O	2.21	0.41
1:B:44[B]:ASN:HD22	1:B:46:SER:H	1.67	0.41
1:C:215:SER:HB2	1:C:241:LEU:HD13	2.03	0.41
1:C:197:THR:HG23	1:C:409[B]:LEU:HD13	2.03	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	408/385 (106%)	399 (98%)	9 (2%)	0	100	100
1	B	408/385 (106%)	399 (98%)	8 (2%)	1 (0%)	47	23
1	C	391/385 (102%)	372 (95%)	17 (4%)	2 (0%)	29	9
All	All	1207/1155 (104%)	1170 (97%)	34 (3%)	3 (0%)	41	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	224	ILE
1	C	99	ASP
1	B	39	ILE

### 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	376/351 (107%)	367 (98%)	9 (2%)	49	20
1	B	376/351 (107%)	366 (97%)	10 (3%)	44	15
1	C	361/351 (103%)	349 (97%)	12 (3%)	38	10
All	All	1113/1053 (106%)	1082 (97%)	31 (3%)	46	14

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	MET
1	A	66[A]	LYS
1	A	66[B]	LYS
1	A	146	THR
1	A	214	ARG
1	A	231	SER
1	A	244	VAL
1	A	324	ASN
1	A	325	ASP
1	B	26	MET
1	B	39	ILE
1	B	100	ASP
1	B	146	THR
1	B	153	ARG
1	B	214	ARG
1	B	231	SER
1	B	232	ARG
1	B	253[A]	MET
1	B	253[B]	MET
1	C	27	ASP
1	C	39[A]	ILE
1	C	39[B]	ILE
1	C	99	ASP
1	C	150	ILE
1	C	214[A]	ARG
1	C	214[B]	ARG

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Mol	Chain	Res	Type
1	C	240	LYS
1	C	243	ARG
1	C	244	VAL
1	C	258	LYS
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	249	ASN
1	A	320	GLN
1	A	324	ASN
1	B	34	GLN
1	B	249	ASN
1	B	295	ASN
1	B	305	ASN
1	B	320	GLN
1	C	40	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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
3	DMS	B	1001	-	3,3,3	0.53	0	3,3,3	1.51	1 (33%)
2	NHW	B	1000	5	58,66,66	1.48	8 (13%)	70,92,92	1.31	7 (10%)
3	DMS	A	1001	-	3,3,3	0.47	0	3,3,3	1.13	0
2	NHW	C	1000	5	58,66,66	1.47	7 (12%)	70,92,92	1.41	11 (15%)
3	DMS	C	1001	-	3,3,3	0.36	0	3,3,3	1.28	1 (33%)
2	NHW	A	1000	5	58,66,66	2.09	7 (12%)	70,92,92	1.73	13 (18%)
6	SO4	B	1411	-	4,4,4	0.23	0	6,6,6	0.63	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	-	1/61/81/81	0/3/3/3
2	NHW	C	1000	5	-	4/61/81/81	0/3/3/3
2	NHW	B	1000	5	-	2/61/81/81	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	NHW	P3X-O3X	9.87	1.78	1.59
2	A	1000	NHW	O4X-C1X	7.91	1.52	1.41
2	C	1000	NHW	P3X-O3X	6.09	1.70	1.59
2	B	1000	NHW	C6-C5	4.66	1.60	1.51
2	B	1000	NHW	O4X-C1X	4.22	1.47	1.41
2	A	1000	NHW	C7-N8	4.01	1.55	1.46
2	A	1000	NHW	O10-C10	3.79	1.49	1.42
2	B	1000	NHW	P3X-O8A	3.23	1.67	1.54
2	A	1000	NHW	C2A-N3A	3.16	1.37	1.32
2	B	1000	NHW	CP-C1M	3.14	1.56	1.51
2	C	1000	NHW	C2X-C1X	-3.12	1.49	1.53
2	C	1000	NHW	CP-C1M	2.82	1.56	1.51
2	B	1000	NHW	P1A-O2A	-2.68	1.42	1.55
2	B	1000	NHW	O6A-C12	2.54	1.52	1.43
2	B	1000	NHW	C13-C11	2.48	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	NHW	C7-N8	2.39	1.51	1.46
2	C	1000	NHW	O4X-C1X	2.31	1.44	1.41
2	C	1000	NHW	O10-C10	2.24	1.46	1.42
2	C	1000	NHW	P3X-O7A	-2.15	1.46	1.54
2	A	1000	NHW	C2M-C1M	2.14	1.56	1.50
2	C	1000	NHW	O1M-C1M	2.13	1.25	1.21
2	A	1000	NHW	C6-C5	2.04	1.55	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	NHW	N3A-C2A-N1A	-5.71	119.75	128.68
2	A	1000	NHW	N3A-C2A-N1A	-5.37	120.28	128.68
2	C	1000	NHW	O4X-C1X-C2X	-5.00	99.62	106.93
2	A	1000	NHW	O6A-C12-C11	-4.90	102.67	110.55
2	A	1000	NHW	O1M-C1M-CP	-4.90	115.18	122.17
2	A	1000	NHW	O4X-C1X-C2X	-3.93	101.18	106.93
2	C	1000	NHW	O7A-P3X-O9A	3.54	124.56	110.68
2	C	1000	NHW	C5X-C4X-C3X	-3.51	102.75	114.40
2	A	1000	NHW	CP-C1M-C2M	3.46	122.94	115.52
2	A	1000	NHW	C4A-C5A-N7A	-3.45	105.80	109.40
2	A	1000	NHW	C2-S1-CP	-3.38	96.05	101.71
2	C	1000	NHW	N3A-C2A-N1A	-3.36	123.43	128.68
2	A	1000	NHW	C5X-C4X-C3X	-3.30	103.47	114.40
2	B	1000	NHW	O6A-C12-C11	-3.24	105.34	110.55
2	C	1000	NHW	O4X-C4X-C5X	-2.53	101.05	109.37
2	B	1000	NHW	C5X-C4X-C3X	-2.53	106.02	114.40
2	B	1000	NHW	C2A-N1A-C6A	2.50	123.04	118.75
2	C	1000	NHW	C3-N4-C5	-2.47	118.26	122.84
2	C	1000	NHW	C13-C11-C12	-2.40	104.31	108.23
2	A	1000	NHW	C2-C3-N4	-2.33	107.53	112.42
2	C	1000	NHW	C13-C11-C10	2.27	112.76	108.82
2	C	1000	NHW	C6-C5-N4	-2.23	112.67	116.42
3	C	1001	DMS	O-S-C1	2.22	117.86	106.54
2	C	1000	NHW	O2A-P1A-O1A	2.20	123.11	112.24
2	C	1000	NHW	C14-C11-C13	2.19	113.62	109.17
2	B	1000	NHW	O4A-P2A-O5A	2.16	122.93	112.24
2	A	1000	NHW	O2X-C2X-C3X	2.12	117.18	111.17
3	B	1001	DMS	O-S-C2	2.11	117.33	106.54
2	A	1000	NHW	O7A-P3X-O9A	2.10	118.91	110.68
2	B	1000	NHW	C7-C6-C5	2.10	115.85	112.36
2	B	1000	NHW	C2-S1-CP	-2.09	98.22	101.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	NHW	C2X-C3X-C4X	2.03	106.81	103.22
2	A	1000	NHW	O4A-P2A-O5A	2.01	122.18	112.24

There are no chirality outliers.

All (7) torsion outliers are listed below:

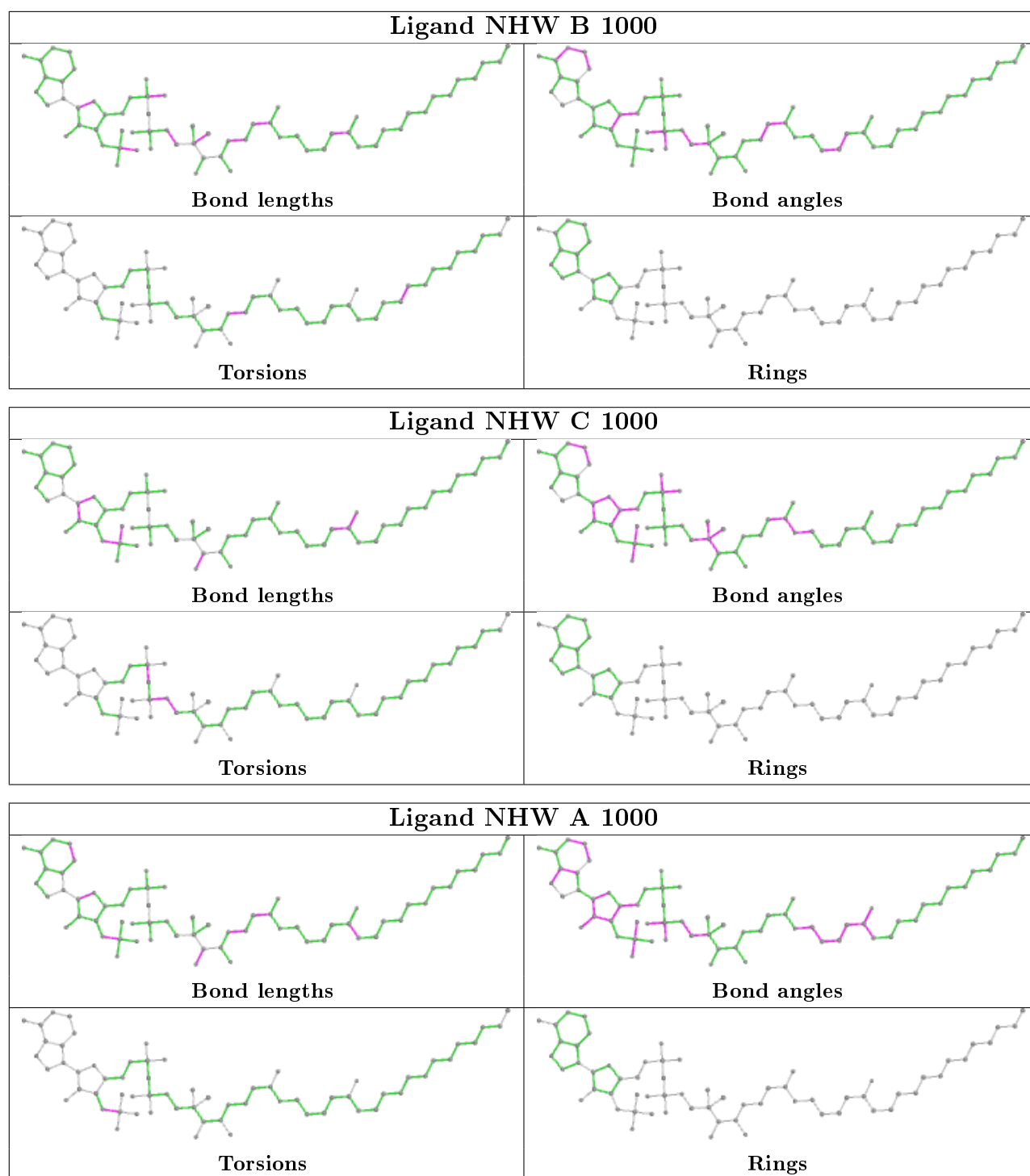
Mol	Chain	Res	Type	Atoms
2	C	1000	NHW	C12-O6A-P2A-O5A
2	A	1000	NHW	C3X-O3X-P3X-O7A
2	B	1000	NHW	C6-C7-N8-C9
2	B	1000	NHW	C4M-C5M-C6M-C7M
2	C	1000	NHW	C12-O6A-P2A-O3A
2	C	1000	NHW	P2A-O3A-P1A-O1A
2	C	1000	NHW	C11-C12-O6A-P2A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	DMS	1	0
6	B	1411	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 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%)	-0.18	9 (2%) 60 66	4, 9, 26, 65	13 (3%)
1	B	385/385 (100%)	-0.20	8 (2%) 63 69	5, 11, 26, 59	10 (2%)
1	C	374/385 (97%)	-0.12	12 (3%) 47 55	6, 11, 31, 53	13 (3%)
All	All	1144/1155 (99%)	-0.17	29 (2%) 57 64	4, 10, 27, 65	36 (3%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	239	ILE	7.0
1	A	231	SER	5.3
1	B	231	SER	5.0
1	A	232	ARG	5.0
1	C	26	MET	4.8
1	C	241	LEU	4.5
1	B	232	ARG	4.3
1	A	325	ASP	4.1
1	B	26	MET	3.7
1	C	242	TYR	3.6
1	C	243	ARG	3.0
1	B	39	ILE	2.9
1	B	211[A]	TYR	2.9
1	C	325	ASP	2.9
1	A	32	TYR	2.8
1	C	224	ILE	2.7
1	C	238	ALA	2.6
1	A	26	MET	2.6
1	C	222	ILE	2.5
1	C	323	GLY	2.4
1	B	27	ASP	2.4
1	C	99	ASP	2.3
1	A	100[A]	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	305	ASN	2.2
1	B	32	TYR	2.2
1	A	99	ASP	2.2
1	A	27	ASP	2.1
1	B	233	LEU	2.1
1	A	39	ILE	2.1

## 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](#)

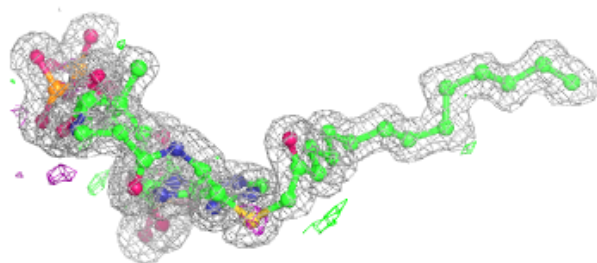
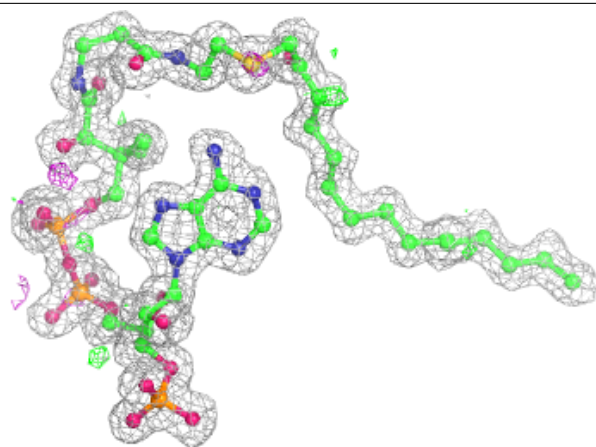
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DMS	C	1001	4/4	0.92	0.14	16,16,17,17	4
6	SO4	B	1411	5/5	0.94	0.09	33,39,39,40	0
3	DMS	B	1001	4/4	0.95	0.17	12,13,13,15	4
3	DMS	A	1001	4/4	0.95	0.23	15,15,16,16	4
2	NHW	B	1000	64/64	0.97	0.06	6,10,13,15	0
2	NHW	A	1000	64/64	0.97	0.07	5,8,10,13	0
2	NHW	C	1000	64/64	0.97	0.07	4,9,11,12	0
5	MG	A	1412	1/1	0.99	0.03	16,16,16,16	0
5	MG	B	1413	1/1	0.99	0.09	19,19,19,19	0
5	MG	C	1412	1/1	0.99	0.05	19,19,19,19	0
4	CL	C	1411	1/1	1.00	0.04	8,8,8,8	0
4	CL	A	1411	1/1	1.00	0.04	9,9,9,9	0
4	CL	B	1412	1/1	1.00	0.05	8,8,8,8	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around NHW B 1000:**

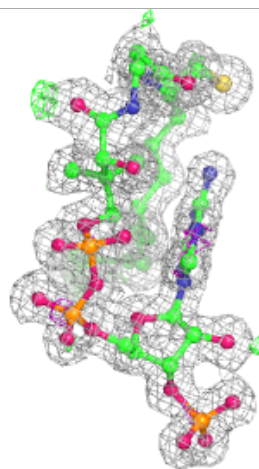
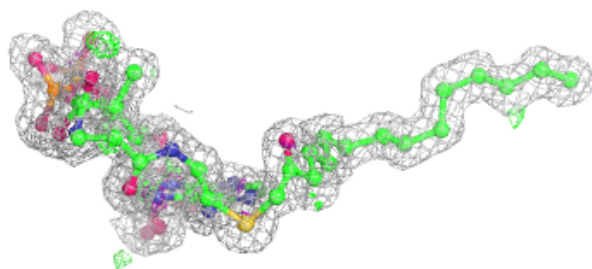
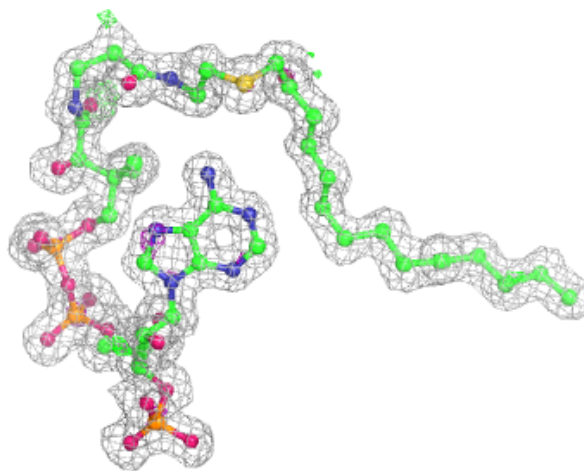
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

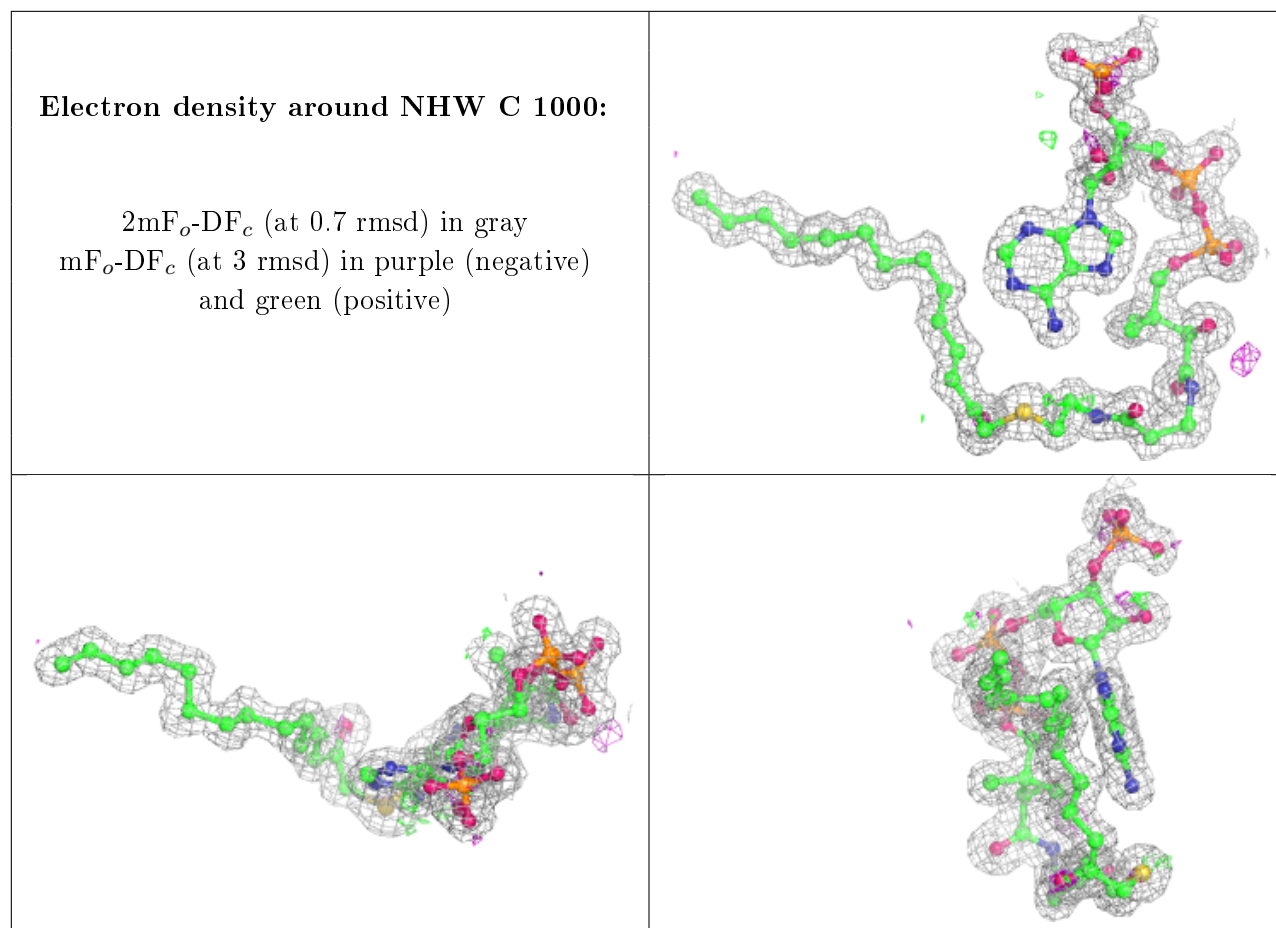




**Electron density around NHW A 1000:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.