



## Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:26 AM UTC

PDB ID : 2YNC / pdb\_00002ync  
Title : Plasmodium vivax N-myristoyltransferase in complex with YnC12-CoA thioester.  
Authors : Wright, M.H.; Clough, B.; Rackham, M.D.; Brannigan, J.A.; Grainger, M.; Bottrill, A.R.; Heal, W.P.; Broncel, M.; Serwa, R.A.; Mann, D.; Leatherbarrow, R.J.; Wilkinson, A.J.; Holder, A.A.; Tate, E.W.  
Deposited on : 2012-10-13  
Resolution : 1.75 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

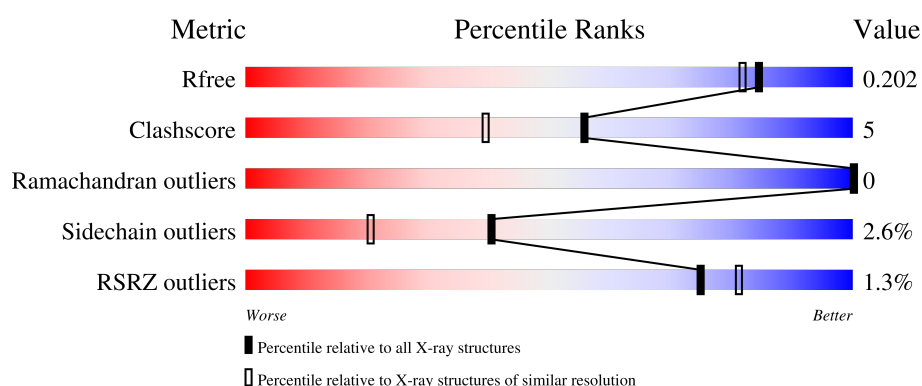
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	384	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	B	384	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	C	384	<div> <div>84%</div> <div>11%</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
3	DMS	A	999	-	-	X	-
3	DMS	B	999	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11267 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	17	0
			3290	2145	532	601	12			
1	B	384	Total	C	N	O	S	0	18	0
			3278	2137	529	600	12			

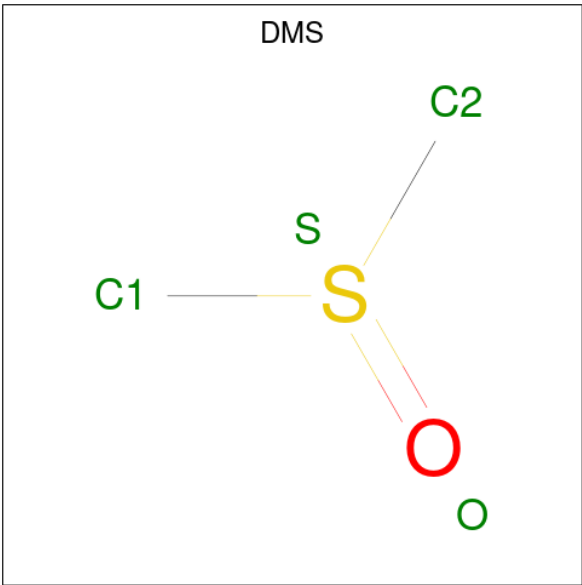
- Molecule 2 is a protein called GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	370	Total	C	N	O	S	0	25	0
			3222	2111	513	587	11			

There is a discrepancy between the modelled and reference sequences:

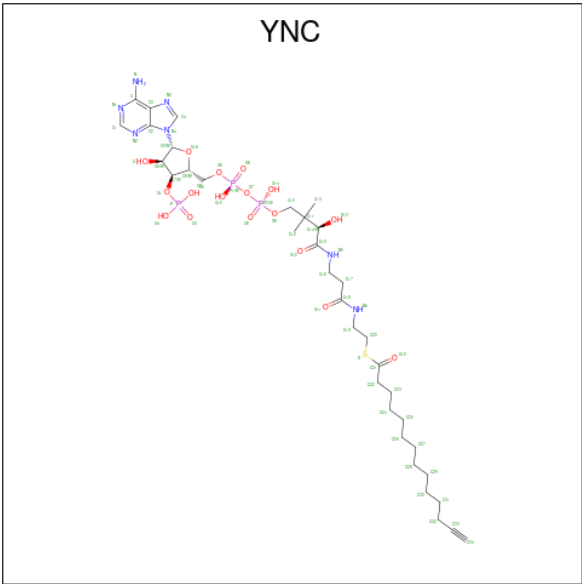
Chain	Residue	Modelled	Actual	Comment	Reference
C	243	LYS	ARG	conflict	UNP A5K1A2

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



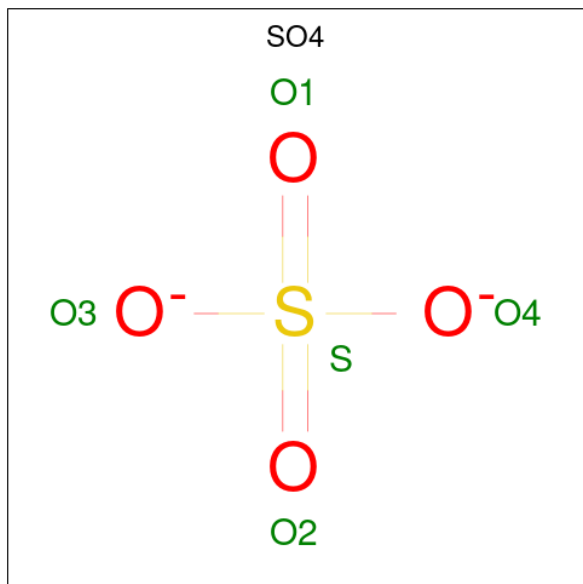
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is TETRADEC-13-YNOIC ACID - COA THIOESTER (CCD ID: YNC) (formula:  $C_{35}H_{58}N_7O_{17}P_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	
			63	35	7	17	3	1	
4	B	1	Total	C	N	O	P	S	
			63	35	7	17	3	1	
4	C	1	Total	C	N	O	P	S	
			63	35	7	17	3	1	

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 8 is water.

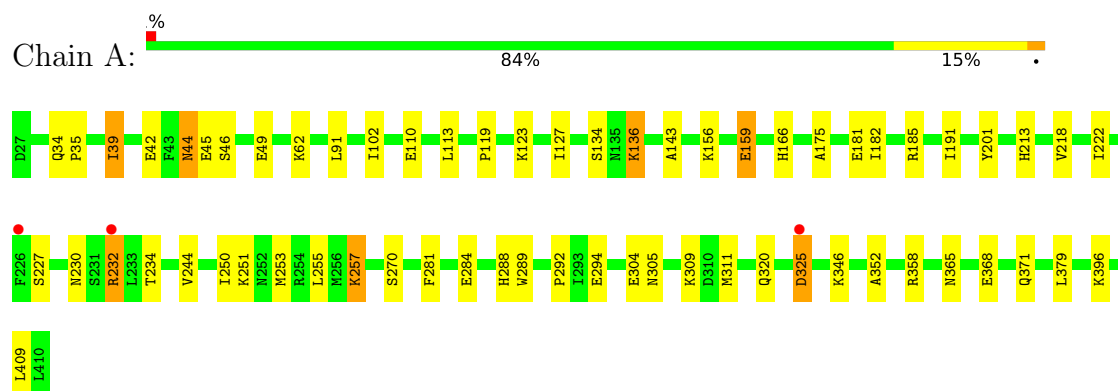
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	466	Total 466	O 466	0	0
8	B	412	Total 412	O 412	0	0
8	C	385	Total 385	O 385	0	0



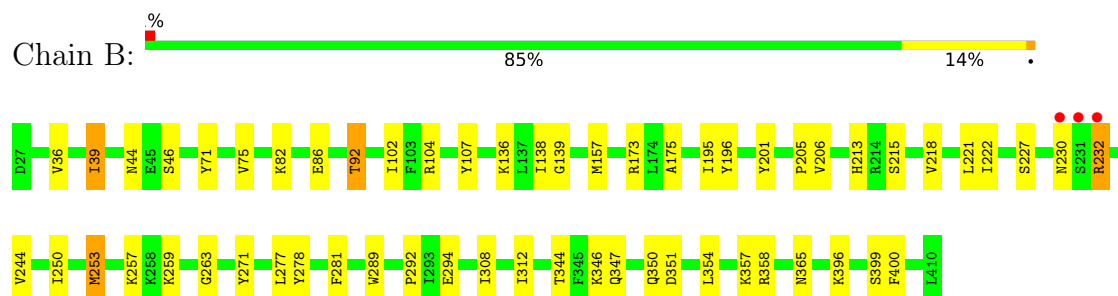
### 3 Residue-property plots [i](#)

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

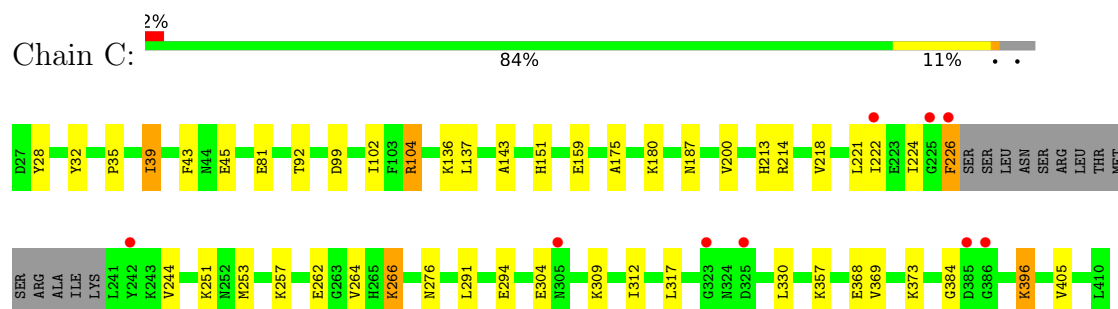
#### • Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



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



#### • Molecule 2: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.45Å 119.05Å 176.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.74 – 1.75 98.74 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.7 (98.74-1.75) 98.0 (98.74-1.75)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.159 , 0.203 0.158 , 0.202	Depositor DCC
$R_{free}$ test set	6018 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.9	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11267	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 4.06% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.52	23/3408 (0.7%)	1.22	2/4611 (0.0%)
1	B	1.53	21/3404 (0.6%)	1.26	6/4608 (0.1%)
2	C	1.41	10/3368 (0.3%)	1.21	4/4560 (0.1%)
All	All	1.49	54/10180 (0.5%)	1.23	12/13779 (0.1%)

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	195	ILE	C-O	7.67	1.31	1.24
1	B	292	PRO	C-O	6.92	1.31	1.23
1	A	311	MET	C-O	6.85	1.32	1.23
1	A	35	PRO	CA-C	6.72	1.59	1.52
1	B	278	TYR	N-CA	6.72	1.54	1.46
1	A	102	ILE	CA-C	6.59	1.61	1.52
1	B	358	ARG	N-CA	6.55	1.54	1.46
1	B	277	LEU	N-CA	6.54	1.54	1.46
1	B	351	ASP	N-CA	6.50	1.54	1.46
2	C	291	LEU	CA-C	6.45	1.59	1.53
1	B	107	TYR	C-O	6.43	1.31	1.23
1	A	368	GLU	CA-CB	6.20	1.60	1.52
1	A	113	LEU	CA-C	6.18	1.60	1.52
1	B	399	SER	N-CA	6.14	1.53	1.45
2	C	180	LYS	C-O	6.06	1.31	1.24
1	B	205	PRO	C-O	6.05	1.30	1.23
1	A	34	GLN	C-O	5.99	1.30	1.23
1	B	396	LYS	CA-CB	5.87	1.61	1.53
1	A	123	LYS	C-O	5.85	1.31	1.24
2	C	330	LEU	CA-C	5.83	1.59	1.52
2	C	264	VAL	C-O	5.82	1.30	1.24
2	C	175	ALA	N-CA	5.80	1.52	1.46
1	B	92	THR	N-CA	5.78	1.53	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	HIS	CA-C	5.72	1.60	1.52
1	A	91	LEU	N-CA	5.65	1.53	1.46
2	C	28	TYR	N-CA	5.63	1.54	1.46
1	A	91	LEU	C-O	5.52	1.30	1.24
1	A	292	PRO	C-O	5.52	1.29	1.23
2	C	317	LEU	N-CA	5.49	1.52	1.46
2	C	405	VAL	N-CA	5.46	1.52	1.46
1	A	255	LEU	N-CA	5.37	1.52	1.46
1	B	354	LEU	C-O	5.32	1.30	1.24
1	B	263	GLY	CA-C	5.29	1.58	1.52
1	B	157	MET	N-CA	5.25	1.52	1.45
1	B	71	TYR	N-CA	5.24	1.52	1.45
1	B	350	GLN	C-O	5.23	1.30	1.24
1	A	234	THR	CB-CG2	5.20	1.69	1.52
1	A	371	GLN	N-CA	5.20	1.52	1.46
1	A	166	HIS	CA-C	5.17	1.59	1.52
1	A	270	SER	C-O	5.17	1.30	1.24
1	B	271	TYR	N-CA	-5.16	1.40	1.46
1	B	308	ILE	N-CA	5.16	1.52	1.46
1	A	175	ALA	N-CA	5.15	1.51	1.46
1	A	320	GLN	N-CA	-5.13	1.39	1.46
1	A	257	LYS	N-CA	5.12	1.52	1.45
1	B	139	GLY	N-CA	5.10	1.50	1.45
2	C	35	PRO	CA-C	5.10	1.57	1.52
2	C	369	VAL	N-CA	5.04	1.52	1.45
1	B	173	ARG	CA-CB	5.03	1.61	1.53
1	A	181	GLU	N-CA	5.03	1.52	1.46
1	B	196	TYR	C-O	5.02	1.29	1.23
1	A	175	ALA	C-N	5.01	1.40	1.33
1	A	159	GLU	C-O	5.01	1.30	1.24
1	A	352	ALA	N-CA	5.01	1.52	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	104	ARG	NE-CZ-NH1	6.72	128.22	121.50
1	B	36	VAL	N-CA-C	-6.24	101.96	109.01
1	B	396	LYS	N-CA-CB	-5.73	101.56	110.55
2	C	104	ARG	NE-CZ-NH2	-5.70	114.07	119.20
1	A	305	ASN	N-CA-C	5.35	118.81	111.54
2	C	187	ASN	N-CA-C	5.30	117.80	111.71
1	B	175	ALA	CA-C-N	-5.26	114.25	119.56

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ALA	C-N-CA	-5.26	114.25	119.56
2	C	200	VAL	N-CA-C	5.25	116.79	109.55
1	B	102	ILE	CB-CA-C	-5.09	102.94	111.29
1	B	75	VAL	CB-CA-C	-5.09	106.41	111.80
1	A	358	ARG	N-CA-C	-5.06	106.37	112.54

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	3290	0	3304	35	0
1	B	3278	0	3301	33	0
2	C	3222	0	3238	28	0
3	A	4	0	6	5	0
3	B	4	0	6	5	0
3	C	4	0	6	1	0
4	A	63	0	54	0	0
4	B	63	0	54	0	0
4	C	63	0	54	0	0
5	A	5	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	2	0	0	0	0
7	B	1	0	0	0	0
7	C	2	0	0	0	0
8	A	466	0	0	2	0
8	B	412	0	0	0	0
8	C	385	0	0	6	0
All	All	11267	0	10023	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (95) 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)
3:C:999:DMS:H21	8:C:2343:HOH:O	1.07	1.22
1:A:213[A]:HIS:HD2	1:A:365:ASN:OD1	1.46	0.97
1:B:213[A]:HIS:HD2	1:B:365:ASN:OD1	1.56	0.89
2:C:251[B]:LYS:HZ2	2:C:251[B]:LYS:HB2	1.42	0.85
1:A:213[A]:HIS:CD2	1:A:365:ASN:OD1	2.30	0.85
1:A:230:ASN:OD1	1:A:232:ARG:HG3	1.86	0.76
2:C:251[B]:LYS:CB	2:C:251[B]:LYS:NZ	2.50	0.74
1:A:44:ASN:HD22	1:A:46:SER:H	1.37	0.72
1:A:156[B]:LYS:HE2	1:A:191:ILE:HD11	1.69	0.72
1:A:42:GLU:HG3	1:B:344:THR:HG21	1.74	0.70
1:B:232:ARG:HH11	1:B:232:ARG:HG2	1.55	0.70
1:A:284[B]:GLU:H	1:A:284[B]:GLU:CD	2.00	0.69
1:B:232:ARG:HH11	1:B:232:ARG:CG	2.10	0.65
2:C:251[B]:LYS:HB2	2:C:251[B]:LYS:NZ	2.02	0.65
2:C:262[B]:GLU:HG3	8:C:2285:HOH:O	1.97	0.65
1:B:232:ARG:HG2	1:B:232:ARG:NH1	2.09	0.64
1:B:215[B]:SER:HB2	1:B:221:LEU:CD1	2.27	0.64
1:A:325:ASP:OD1	1:A:325:ASP:N	2.31	0.63
1:A:289:TRP:CE2	3:A:999:DMS:H11	2.34	0.63
1:A:127:ILE:HD11	1:A:182[B]:ILE:HD12	1.79	0.63
2:C:32[B]:TYR:OH	2:C:39[B]:ILE:HG22	2.00	0.62
1:A:127:ILE:CD1	1:A:182[B]:ILE:HD12	2.30	0.61
1:A:289:TRP:NE1	3:A:999:DMS:H11	2.15	0.61
1:B:215[B]:SER:HB2	1:B:221:LEU:HD12	1.81	0.61
1:A:222[A]:ILE:HD13	1:A:227:SER:HB2	1.82	0.60
1:A:42:GLU:CG	1:B:344:THR:HG21	2.31	0.60
2:C:32[B]:TYR:HE2	8:C:2015:HOH:O	1.85	0.59
1:A:346[A]:LYS:HD3	1:A:379:LEU:HD21	1.88	0.56
1:B:213[A]:HIS:CD2	1:B:365:ASN:OD1	2.47	0.56
1:B:230[A]:ASN:OD1	1:B:232:ARG:HB2	2.07	0.55
2:C:304[B]:GLU:HG2	8:C:2277:HOH:O	2.05	0.55
2:C:304[A]:GLU:OE2	2:C:309:LYS:NZ	2.37	0.54
1:A:45:GLU:HG3	8:A:2023:HOH:O	2.06	0.54
1:A:289:TRP:CD1	3:A:999:DMS:H11	2.43	0.54
1:B:244:VAL:CG2	1:B:357[B]:LYS:HD3	2.37	0.54
1:B:346[B]:LYS:HG3	1:B:347:GLN:N	2.22	0.53
2:C:213[A]:HIS:CE1	2:C:384:GLY:HA3	2.44	0.53
2:C:92:THR:O	2:C:104:ARG:HD2	2.09	0.52
2:C:357:LYS:HE2	8:C:2254:HOH:O	2.10	0.52
1:A:304:GLU:OE2	1:A:309:LYS:NZ	2.31	0.51
1:A:44:ASN:ND2	1:A:46:SER:H	2.06	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:HD11	1:A:185:ARG:HD2	1.92	0.51
1:B:244:VAL:HG21	1:B:357[B]:LYS:HD3	1.91	0.51
1:B:44[A]:ASN:HB3	1:B:46:SER:H	1.76	0.51
1:B:289:TRP:NE1	3:B:999:DMS:H21	2.25	0.50
1:A:281:PHE:HE1	3:A:999:DMS:C1	2.24	0.50
2:C:373[B]:LYS:HB2	8:C:2360:HOH:O	2.11	0.49
1:A:159:GLU:CD	1:A:409:LEU:HD22	2.38	0.49
1:A:44:ASN:HD22	1:A:44:ASN:C	2.21	0.48
1:A:218:VAL:O	1:A:222[A]:ILE:HG12	2.13	0.48
2:C:151[A]:HIS:HA	2:C:276[A]:ASN:OD1	2.14	0.47
2:C:266:LYS:HB2	2:C:266:LYS:NZ	2.29	0.47
1:B:218:VAL:O	1:B:222[A]:ILE:HG12	2.14	0.47
1:B:253[B]:MET:HE2	1:B:312:ILE:HD12	1.96	0.47
1:B:138:ILE:C	1:B:138:ILE:HD12	2.41	0.46
1:A:49:GLU:OE2	1:A:396:LYS:HE3	2.16	0.46
1:A:39:ILE:HD12	1:A:201:TYR:HE2	1.81	0.45
2:C:32[B]:TYR:HH	2:C:39[B]:ILE:HG22	1.80	0.45
1:B:39:ILE:HD11	1:B:201:TYR:CE1	2.51	0.45
1:B:92:THR:O	1:B:104:ARG:HD2	2.17	0.44
2:C:218:VAL:O	2:C:222:ILE:HG12	2.17	0.44
1:B:222[A]:ILE:HD13	1:B:227:SER:HB2	1.99	0.44
1:B:289:TRP:CD1	3:B:999:DMS:H21	2.53	0.44
2:C:43:PHE:CE1	2:C:396:LYS:HG3	2.53	0.44
2:C:45:GLU:OE2	2:C:151[A]:HIS:HE1	2.00	0.44
1:A:143:ALA:HA	1:A:159:GLU:O	2.18	0.44
1:B:289:TRP:CE2	3:B:999:DMS:H21	2.52	0.43
1:A:251[A]:LYS:NZ	1:A:251[A]:LYS:HB3	2.34	0.43
1:B:281:PHE:CE1	3:B:999:DMS:H22	2.54	0.43
1:A:134:SER:OG	1:A:136:LYS:HB2	2.19	0.43
1:B:39:ILE:HD11	1:B:201:TYR:HE1	1.83	0.43
2:C:214[B]:ARG:HA	2:C:214[B]:ARG:HD2	1.89	0.43
1:A:284[B]:GLU:CD	1:A:284[B]:GLU:N	2.73	0.43
1:A:281:PHE:HE1	3:A:999:DMS:H12	1.84	0.42
2:C:253[B]:MET:HE2	2:C:312:ILE:HD12	2.01	0.42
1:A:251[A]:LYS:NZ	1:A:251[A]:LYS:CB	2.82	0.42
1:A:250:ILE:O	1:A:253[B]:MET:HG2	2.20	0.42
1:B:257:LYS:HD2	1:B:259:LYS:HE2	2.00	0.42
1:B:39:ILE:HA	1:B:39:ILE:HD12	1.79	0.42
1:B:206[B]:VAL:HG12	1:B:400:PHE:CE2	2.54	0.42
2:C:251[B]:LYS:CB	2:C:251[B]:LYS:HZ3	2.32	0.42
1:A:62[B]:LYS:HE3	8:A:2058:HOH:O	2.19	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:PHE:HE1	3:B:999:DMS:H22	1.85	0.41
2:C:32[B]:TYR:OH	2:C:39[B]:ILE:CG2	2.67	0.41
2:C:368:GLU:HB2	2:C:373[B]:LYS:HG2	2.00	0.41
1:B:244:VAL:CG2	1:B:357[A]:LYS:HD2	2.50	0.41
1:A:127:ILE:CD1	1:A:182[B]:ILE:CD1	2.98	0.41
2:C:39[A]:ILE:HD13	2:C:39[A]:ILE:HA	1.72	0.41
2:C:143:ALA:HA	2:C:159:GLU:O	2.21	0.41
1:B:250:ILE:O	1:B:253[B]:MET:HG2	2.21	0.41
2:C:213[A]:HIS:HE1	2:C:384:GLY:HA3	1.85	0.41
2:C:221:LEU:O	2:C:226:PHE:HB3	2.21	0.41
1:B:82:LYS:O	1:B:86[B]:GLU:HG2	2.21	0.40
1:B:244:VAL:HG21	1:B:357[A]:LYS:HD2	2.02	0.40
2:C:224:ILE:HG13	2:C:226:PHE:HB2	2.04	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	399/384 (104%)	390 (98%)	9 (2%)	0	100	100
1	B	400/384 (104%)	391 (98%)	9 (2%)	0	100	100
2	C	391/384 (102%)	383 (98%)	8 (2%)	0	100	100
All	All	1190/1152 (103%)	1164 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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



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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/350 (105%)	355 (97%)	12 (3%)	33	13
1	B	368/350 (105%)	362 (98%)	6 (2%)	55	38
2	C	362/350 (103%)	347 (96%)	15 (4%)	27	8
All	All	1097/1050 (104%)	1064 (97%)	33 (3%)	40	16

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

Mol	Chain	Res	Type
1	A	39	ILE
1	A	44	ASN
1	A	110[A]	GLU
1	A	110[B]	GLU
1	A	119	PRO
1	A	136	LYS
1	A	232	ARG
1	A	244	VAL
1	A	257	LYS
1	A	294[A]	GLU
1	A	294[B]	GLU
1	A	325	ASP
1	B	39	ILE
1	B	136	LYS
1	B	232	ARG
1	B	253[A]	MET
1	B	253[B]	MET
1	B	294	GLU
2	C	39[A]	ILE
2	C	39[B]	ILE
2	C	81	GLU
2	C	99	ASP
2	C	102	ILE
2	C	136	LYS
2	C	137	LEU
2	C	226	PHE
2	C	244	VAL
2	C	257[A]	LYS
2	C	257[B]	LYS
2	C	266	LYS
2	C	294[A]	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	294[B]	GLU
2	C	396	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	249	ASN
1	A	295	ASN
1	A	350	GLN
1	A	359	ASN
1	A	372	ASN
1	B	249	ASN
1	B	295	ASN
1	B	320	GLN
1	B	359	ASN
1	B	360	ASN
1	B	372	ASN
2	C	101	ASN
2	C	120	ASN
2	C	359	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 oligosaccharides in this entry.

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

Of 15 ligands modelled in this entry, 8 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$
5	SO4	A	1411	-	4,4,4	0.46	0	6,6,6	0.96	0
4	YNC	B	1000	6	63,65,65	1.72	9 (14%)	85,91,91	1.97	14 (16%)
3	DMS	A	999	-	3,3,3	0.38	0	3,3,3	0.76	0
3	DMS	B	999	-	3,3,3	0.46	0	3,3,3	1.33	0
3	DMS	C	999	-	3,3,3	0.97	0	3,3,3	1.59	1 (33%)
4	YNC	A	1000	6	63,65,65	1.54	9 (14%)	85,91,91	2.08	22 (25%)
4	YNC	C	1000	6	63,65,65	1.64	12 (19%)	85,91,91	2.03	19 (22%)

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
4	YNC	B	1000	6	-	2/63/80/80	0/3/3/3
4	YNC	A	1000	6	-	0/63/80/80	0/3/3/3
4	YNC	C	1000	6	-	3/63/80/80	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1000	YNC	C22-C21	5.64	1.56	1.50
4	B	1000	YNC	O10-C21	5.46	1.29	1.21
4	B	1000	YNC	C3-C2	5.12	1.48	1.39
4	C	1000	YNC	P1-O7	4.86	1.64	1.59
4	A	1000	YNC	O13-C14	4.32	1.50	1.42
4	C	1000	YNC	C3-C2	4.29	1.46	1.39
4	A	1000	YNC	P-O1	4.16	1.66	1.59
4	C	1000	YNC	P-O1	4.01	1.66	1.59
4	A	1000	YNC	C3-C2	3.82	1.45	1.39
4	A	1000	YNC	C4-N3	3.49	1.38	1.31
4	C	1000	YNC	C4-N3	3.48	1.38	1.31
4	B	1000	YNC	C4-N3	3.20	1.37	1.31

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1000	YNC	C1-N1	3.06	1.39	1.33
4	B	1000	YNC	C33-C34	3.02	1.27	1.18
4	A	1000	YNC	O12-C15	2.90	1.29	1.23
4	C	1000	YNC	P-O3	2.85	1.59	1.50
4	A	1000	YNC	O10-C21	2.81	1.25	1.21
4	C	1000	YNC	C33-C34	2.77	1.26	1.18
4	B	1000	YNC	P-O1	2.70	1.64	1.59
4	B	1000	YNC	O13-C14	2.64	1.47	1.42
4	C	1000	YNC	C22-C21	2.62	1.53	1.50
4	C	1000	YNC	O13-C14	2.58	1.46	1.42
4	C	1000	YNC	C2-N4	-2.49	1.32	1.37
4	A	1000	YNC	C10-C11	2.44	1.56	1.52
4	B	1000	YNC	C17-C18	2.39	1.56	1.51
4	C	1000	YNC	P1-O15	-2.35	1.44	1.55
4	A	1000	YNC	P2-O7	-2.34	1.57	1.59
4	C	1000	YNC	P2-O7	2.28	1.62	1.59
4	B	1000	YNC	C3-N3	-2.13	1.35	1.39
4	C	1000	YNC	C3-C	2.11	1.46	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1000	YNC	O10-C21-C22	-9.05	113.54	123.98
4	B	1000	YNC	C22-C21-S	8.57	123.62	113.40
4	A	1000	YNC	C22-C21-S	7.92	122.84	113.40
4	C	1000	YNC	C22-C21-S	6.75	121.45	113.40
4	C	1000	YNC	O10-C21-C22	-6.61	116.35	123.98
4	C	1000	YNC	N2-C1-N1	-6.20	119.20	128.58
4	A	1000	YNC	C23-C22-C21	-5.42	100.31	112.27
4	A	1000	YNC	O10-C21-C22	-5.11	118.09	123.98
4	A	1000	YNC	N2-C1-N1	-5.06	120.92	128.58
4	A	1000	YNC	C3-C2-N2	-4.84	120.05	126.72
4	C	1000	YNC	C3-C2-N2	-4.71	120.23	126.72
4	B	1000	YNC	C23-C22-C21	-4.19	103.02	112.27
4	A	1000	YNC	C16-N5-C15	-4.17	115.05	122.55
4	C	1000	YNC	C1-N2-C2	4.13	121.93	111.83
4	C	1000	YNC	C23-C22-C21	-4.04	103.34	112.27
4	C	1000	YNC	N2-C2-N4	3.95	133.89	127.17
4	A	1000	YNC	C2-C3-N3	-3.94	106.08	110.58
4	A	1000	YNC	P-O1-C7	-3.91	113.00	123.43
4	B	1000	YNC	C3-C2-N2	-3.88	121.38	126.72
4	C	1000	YNC	C1-N1-C	3.71	124.82	118.73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1000	YNC	C1-N2-C2	3.68	120.81	111.83
4	C	1000	YNC	O9-C10-C11	-3.45	105.00	110.55
4	B	1000	YNC	N2-C2-N4	3.34	132.84	127.17
4	B	1000	YNC	C1-N1-C	3.24	124.06	118.73
4	B	1000	YNC	C13-C11-C14	-3.22	103.28	108.77
4	A	1000	YNC	N2-C2-N4	3.15	132.53	127.17
4	C	1000	YNC	O15-P1-O6	3.09	126.83	112.44
4	A	1000	YNC	C12-C11-C14	3.05	113.97	108.77
4	A	1000	YNC	C2-N4-C4	2.97	108.86	105.74
4	A	1000	YNC	C2-N4-C5	-2.92	119.80	126.63
4	A	1000	YNC	O10-C21-S	-2.89	119.01	122.68
4	B	1000	YNC	N2-C1-N1	-2.81	124.32	128.58
4	C	1000	YNC	C2-N4-C4	2.79	108.67	105.74
4	A	1000	YNC	O9-C10-C11	-2.67	106.25	110.55
4	C	1000	YNC	O11-C18-N6	2.64	128.21	123.03
4	C	1000	YNC	C12-C11-C10	-2.64	103.87	108.22
4	C	1000	YNC	O11-C18-C17	-2.59	117.32	122.02
4	A	1000	YNC	O15-P1-O7	2.57	114.23	107.27
4	C	1000	YNC	O1-C7-C8	-2.57	100.98	110.03
4	B	1000	YNC	C9-C8-C7	-2.53	105.94	114.38
4	B	1000	YNC	C3-N3-C4	2.50	107.39	103.45
4	A	1000	YNC	O14-P2-O7	-2.49	100.55	107.27
4	A	1000	YNC	N4-C4-N3	-2.41	110.52	113.94
4	A	1000	YNC	C3-N3-C4	2.39	107.20	103.45
4	B	1000	YNC	O9-C10-C11	-2.33	106.80	110.55
4	B	1000	YNC	C2-C3-N3	-2.29	107.96	110.58
4	A	1000	YNC	C6-C5-N4	-2.27	107.67	113.30
4	B	1000	YNC	O15-P1-O7	2.23	113.30	107.27
4	A	1000	YNC	O-C6-C5	2.21	117.73	110.10
4	C	1000	YNC	O2-P-O3	2.20	119.41	110.83
4	C	1000	YNC	C6-C5-N4	-2.17	107.91	113.30
4	B	1000	YNC	C1-N2-C2	2.09	116.93	111.83
4	C	1000	YNC	O14-P2-O9	2.07	116.93	107.57
4	A	1000	YNC	C-C3-N3	2.04	136.03	132.09
3	C	999	DMS	C2-S-C1	2.04	108.89	98.42
4	C	1000	YNC	C12-C11-C14	2.01	112.19	108.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1000	YNC	C17-C16-N5-C15

*Continued on next page...*

*Continued from previous page...*

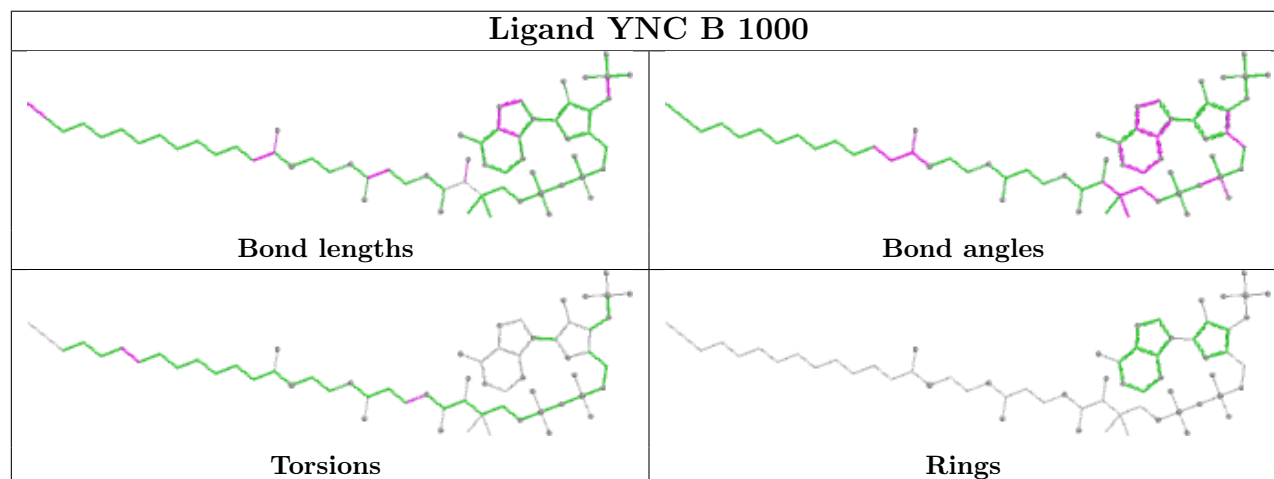
Mol	Chain	Res	Type	Atoms
4	B	1000	YNC	C27-C28-C29-C30
4	C	1000	YNC	C24-C25-C26-C27
4	B	1000	YNC	C17-C16-N5-C15
4	C	1000	YNC	P2-O7-P1-O6

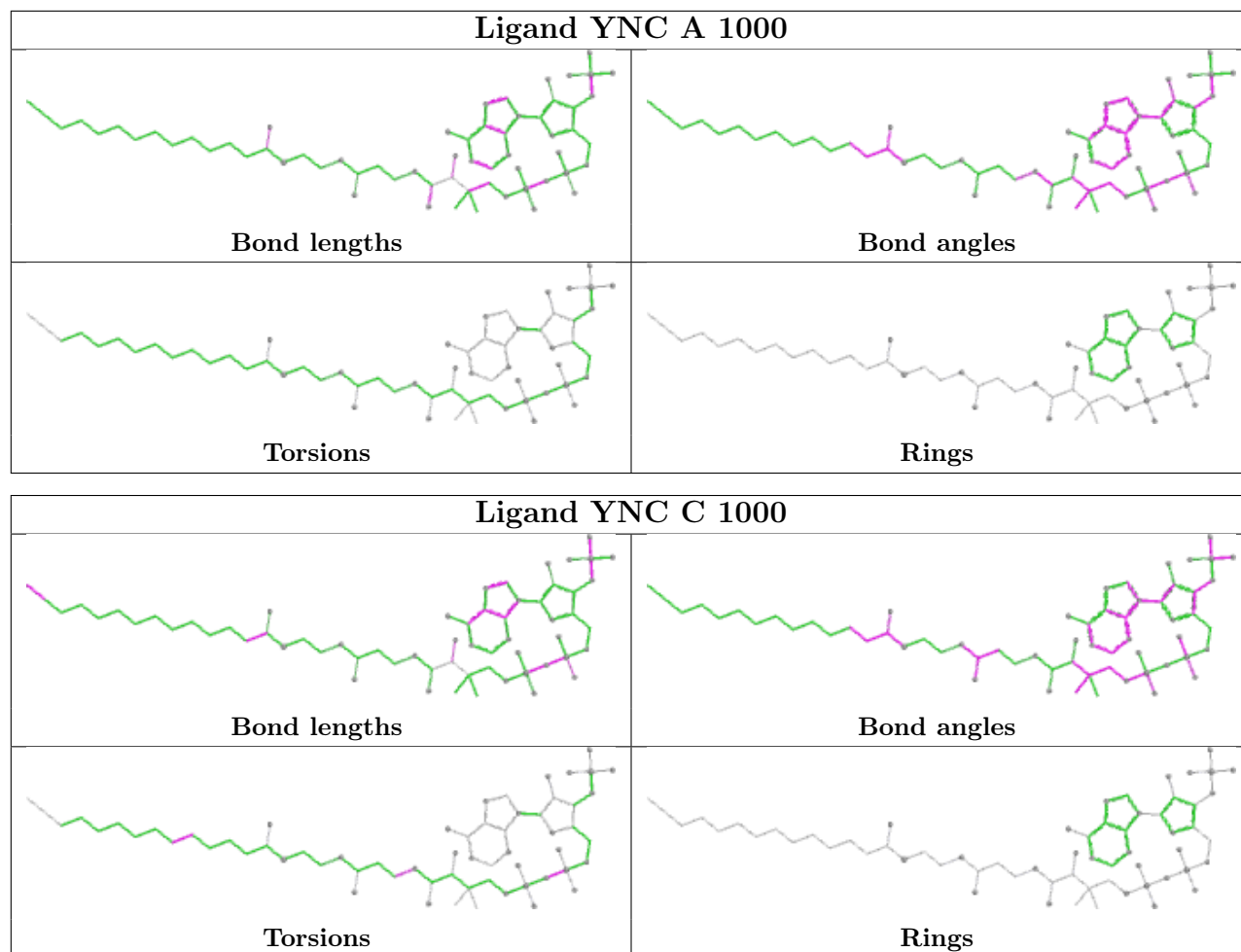
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	DMS	5	0
3	B	999	DMS	5	0
3	C	999	DMS	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 [i](#)

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	384/384 (100%)	-0.59	3 (0%) 82 86	3, 9, 26, 55	27 (7%)
1	B	384/384 (100%)	-0.55	3 (0%) 82 86	4, 10, 25, 66	29 (7%)
2	C	370/384 (96%)	-0.48	9 (2%) 59 66	4, 10, 29, 52	35 (9%)
All	All	1138/1152 (98%)	-0.54	15 (1%) 75 81	3, 10, 27, 66	91 (7%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	226	PHE	6.1
1	A	325	ASP	3.5
2	C	225	GLY	3.4
2	C	222	ILE	3.4
2	C	323	GLY	3.2
2	C	386	GLY	2.9
1	A	232	ARG	2.7
2	C	325	ASP	2.4
1	B	230[A]	ASN	2.3
2	C	305	ASN	2.3
1	B	232	ARG	2.3
1	A	226	PHE	2.3
1	B	231	SER	2.2
2	C	242	TYR	2.1
2	C	385	ASP	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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

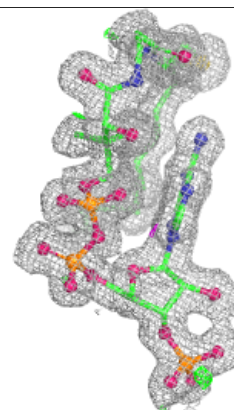
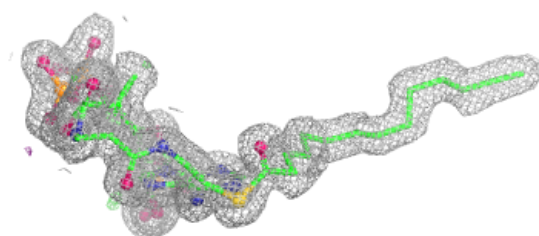
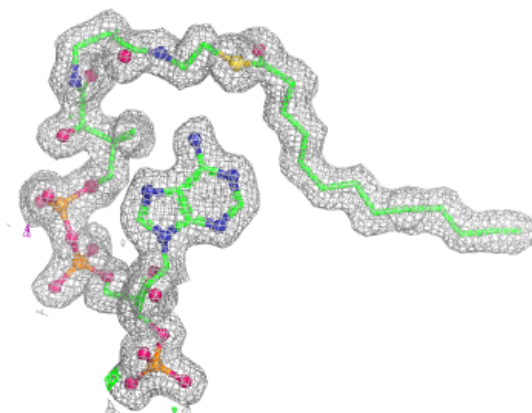
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	999	4/4	0.81	0.17	27,27,30,38	0
3	DMS	A	999	4/4	0.86	0.18	23,28,30,37	0
3	DMS	B	999	4/4	0.91	0.13	25,29,29,32	0
7	CL	C	1500	1/1	0.94	0.08	34,34,34,34	0
5	SO4	A	1411	5/5	0.95	0.10	27,28,36,37	0
7	CL	A	1500	1/1	0.96	0.09	31,31,31,31	0
4	YNC	A	1000	63/63	0.98	0.04	6,9,11,14	0
4	YNC	B	1000	63/63	0.98	0.04	6,10,13,15	0
4	YNC	C	1000	63/63	0.98	0.04	6,10,13,17	0
6	MG	C	1411	1/1	0.99	0.02	19,19,19,19	0
6	MG	A	1412	1/1	0.99	0.08	19,19,19,19	0
6	MG	B	1411	1/1	0.99	0.07	20,20,20,20	0
7	CL	B	1412	1/1	1.00	0.02	9,9,9,9	0
7	CL	C	1412	1/1	1.00	0.01	10,10,10,10	0
7	CL	A	1413	1/1	1.00	0.01	9,9,9,9	0

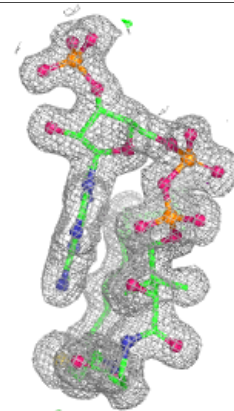
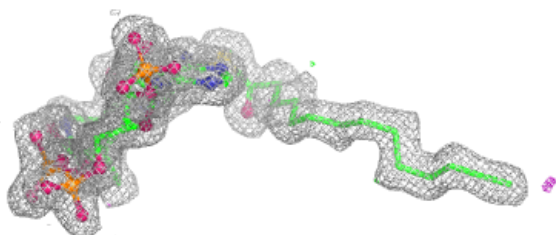
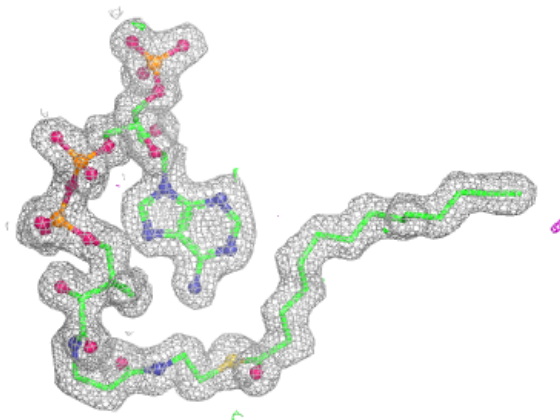
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around YNC 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)

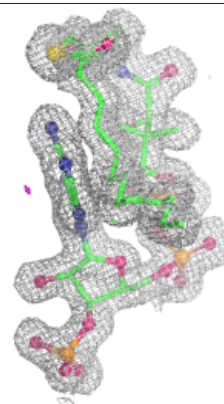
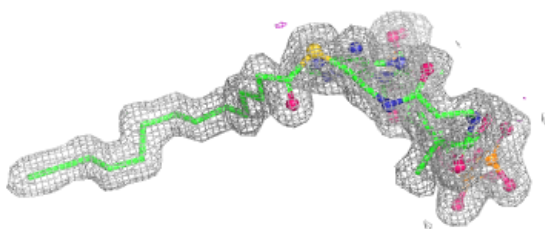
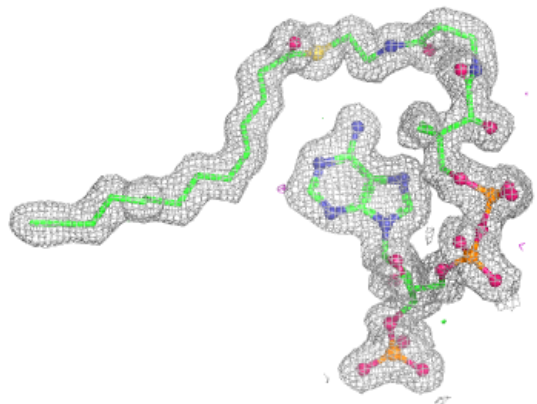
**Electron density around YNC B 1000:**

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



**Electron density around YNC C 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 ⓘ

There are no such residues in this entry.