



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:59 pm BST

PDB ID : 4B14  
Title : Plasmodium vivax N-myristoyltransferase with a bound benzofuran inhibitor (compound 26)  
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 : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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 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

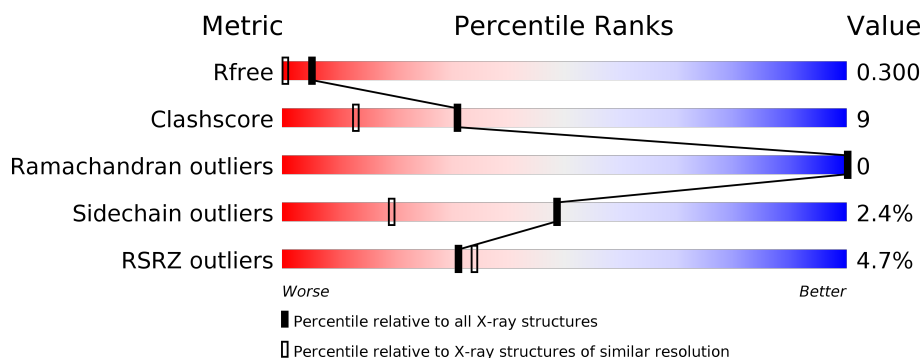
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>5%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div></div> </div> </div>
1	B	385	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div></div> </div> </div>
1	C	385	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>5%</div> </div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11054 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.

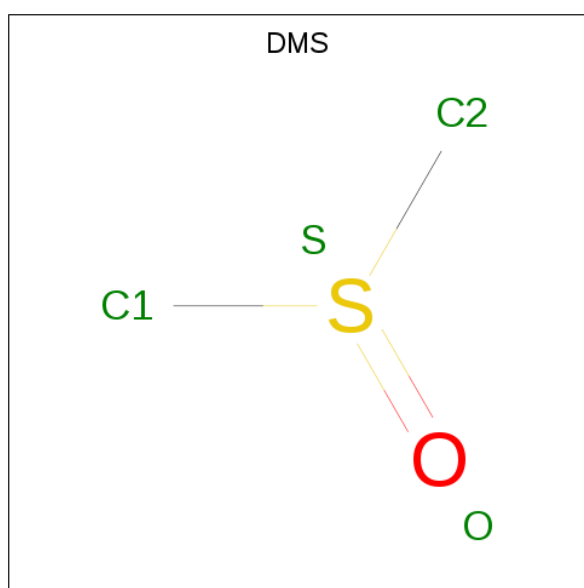
- Molecule 1 is a protein called GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	15	0
			3266	2126	527	600	13			
1	B	385	Total	C	N	O	S	0	10	0
			3233	2101	527	592	13			
1	C	367	Total	C	N	O	S	0	13	0
			3116	2031	499	576	10			

There are 3 discrepancies between the modelled and reference sequences:

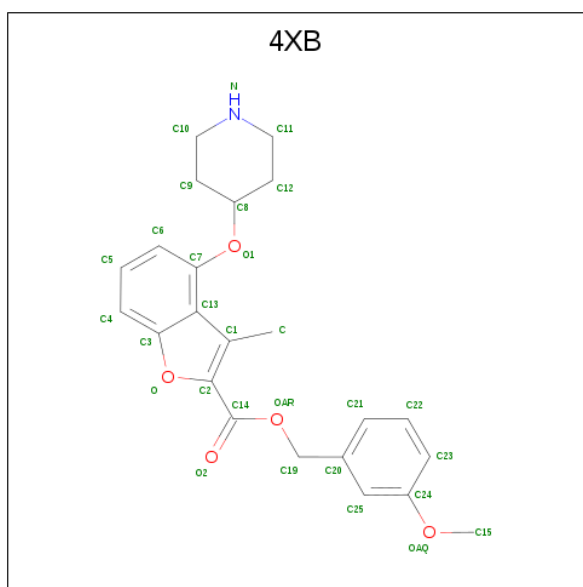
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	expression tag	UNP A5K1A2
B	26	MET	-	expression tag	UNP A5K1A2
C	26	MET	-	expression tag	UNP A5K1A2

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



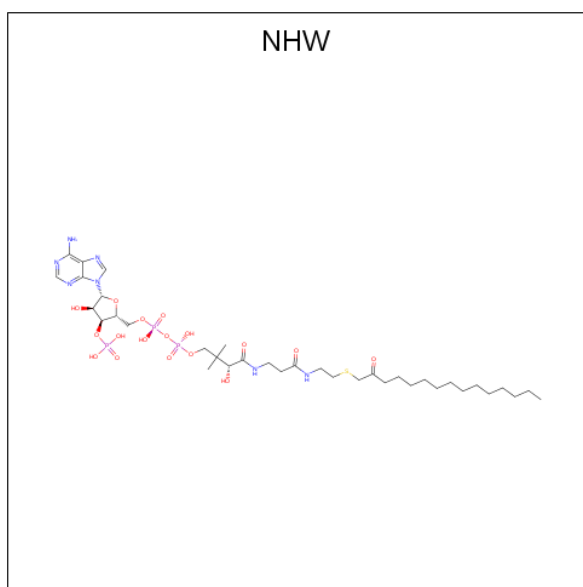
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is 3-methoxybenzyl 3-methyl-4-(piperidin-4-yloxy)-1-benzofuran-2-carboxylate (three-letter code: 4XB) (formula: C<sub>23</sub>H<sub>25</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	23	1	5		
3	B	1	Total	C	N	O	0	0
			29	23	1	5		
3	C	1	Total	C	N	O	0	0
			29	23	1	5		

- Molecule 4 is 2-oxopentadecyl-CoA (three-letter code: NHW) (formula: C<sub>36</sub>H<sub>64</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



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

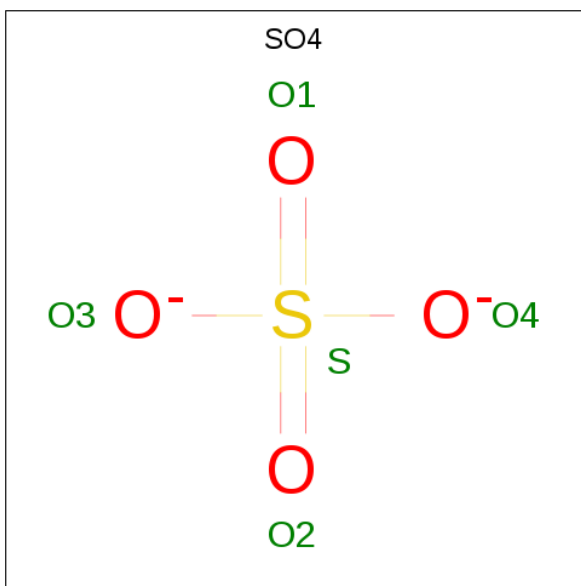
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

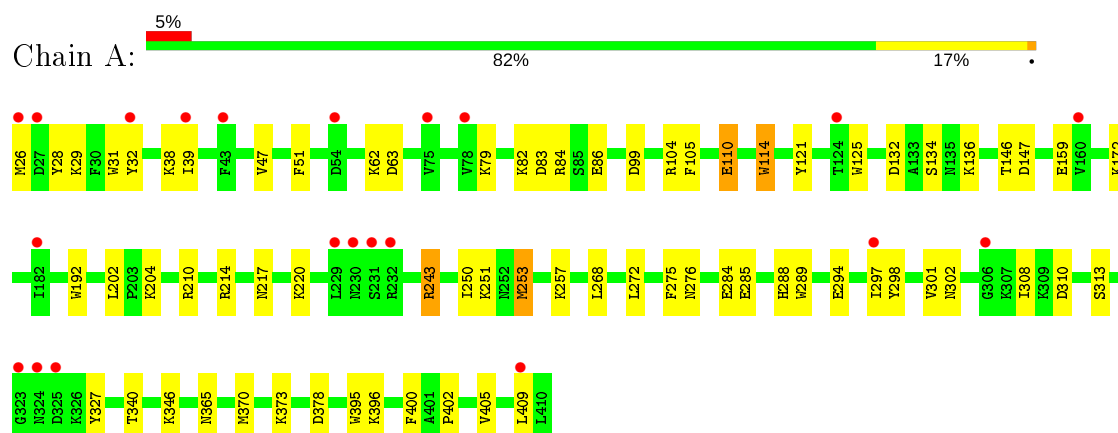
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	411	Total	O	0	4
			415	415		
8	B	382	Total	O	0	1
			383	383		
8	C	339	Total	O	0	0
			339	339		

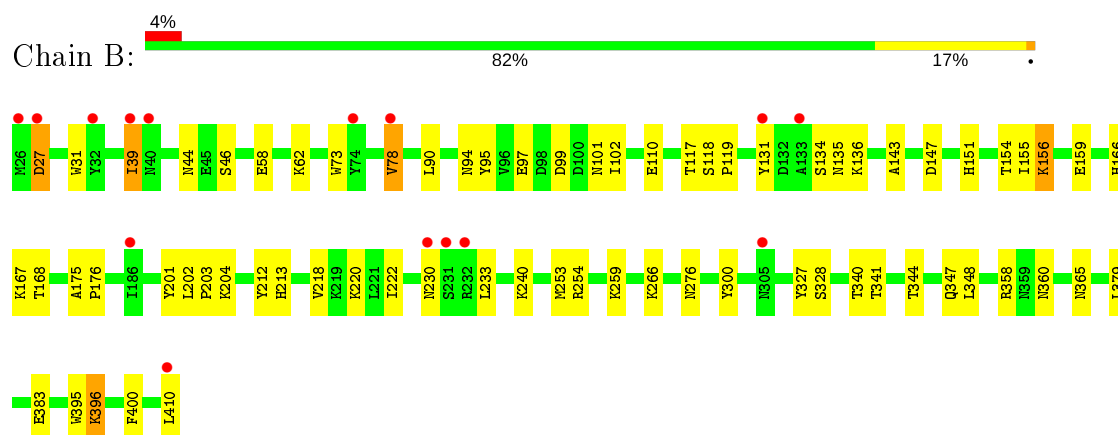
### 3 Residue-property plots [i](#)

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.

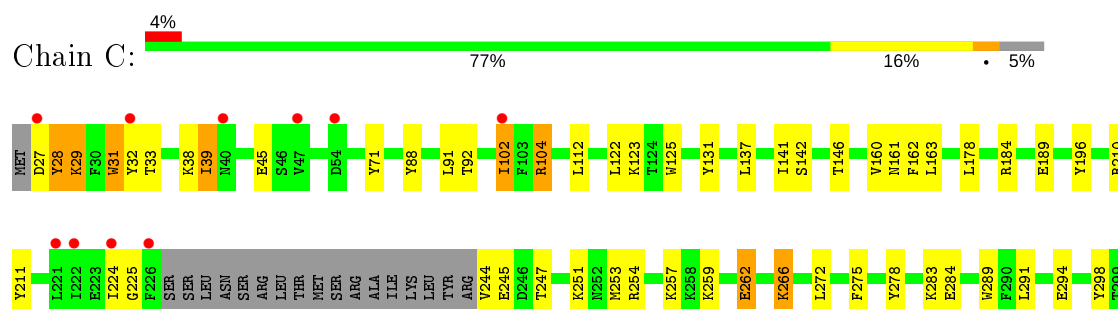
#### • Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



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



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







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.38Å 118.96Å 179.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.64 – 1.50 32.62 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (32.64-1.50) 99.5 (32.62-1.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.73 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.7.0025	Depositor
R, $R_{free}$	0.252 , 0.302 0.250 , 0.300	Depositor DCC
$R_{free}$ test set	9804 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.1	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 32.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11054	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 3.95% 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: MG, CL, 4XB, NHW, DMS, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.05	5/3381 (0.1%)	1.13	11/4577 (0.2%)
1	B	1.05	4/3336 (0.1%)	1.12	6/4513 (0.1%)
1	C	1.03	5/3224 (0.2%)	1.14	10/4368 (0.2%)
All	All	1.04	14/9941 (0.1%)	1.13	27/13458 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	289	TRP	CD2-CE2	6.39	1.49	1.41
1	C	31	TRP	CD2-CE2	5.96	1.48	1.41
1	B	73	TRP	CD2-CE2	5.80	1.48	1.41
1	A	192	TRP	CD2-CE2	5.70	1.48	1.41
1	C	393	TYR	CE2-CZ	5.57	1.45	1.38
1	A	114	TRP	CD2-CE2	5.48	1.48	1.41
1	B	31	TRP	CD2-CE2	5.48	1.48	1.41
1	A	31	TRP	CD2-CE2	5.42	1.47	1.41
1	B	395	TRP	CD2-CE2	5.40	1.47	1.41
1	C	189	GLU	CD-OE1	5.39	1.31	1.25
1	A	395	TRP	CD2-CE2	5.38	1.47	1.41
1	C	278	TYR	CG-CD2	5.28	1.46	1.39
1	A	125	TRP	CD2-CE2	5.23	1.47	1.41
1	B	95	TYR	CG-CD2	-5.09	1.32	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	ARG	NE-CZ-NH1	11.91	126.26	120.30
1	C	104	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	99	ASP	CB-CG-OD1	8.50	125.95	118.30
1	B	358	ARG	NE-CZ-NH2	-8.27	116.17	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	409	LEU	CA-CB-CG	7.29	132.06	115.30
1	C	184	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	84	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	83	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	C	137	LEU	CB-CG-CD1	6.24	121.60	111.00
1	B	90	LEU	CB-CG-CD2	-6.22	100.42	111.00
1	A	253[A]	MET	CG-SD-CE	6.15	110.04	100.20
1	A	253[B]	MET	CG-SD-CE	6.15	110.04	100.20
1	A	104	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	C	39	ILE	CG1-CB-CG2	-6.02	98.16	111.40
1	B	62	LYS	CD-CE-NZ	5.97	125.44	111.70
1	A	214	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	202	LEU	CB-CG-CD1	-5.85	101.05	111.00
1	A	84	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	243	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	210	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	B	240	LYS	CD-CE-NZ	-5.67	98.66	111.70
1	C	225	GLY	N-CA-C	5.52	126.91	113.10
1	A	83	ASP	CB-CG-OD1	5.46	123.22	118.30
1	C	310	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	B	110	GLU	OE1-CD-OE2	-5.29	116.96	123.30
1	C	122	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	63	ASP	CB-CG-OD1	5.03	122.83	118.30

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	3266	0	3283	67	0
1	B	3233	0	3248	50	0
1	C	3116	0	3104	61	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	29	0	25	2	0
3	B	29	0	25	3	0
3	C	29	0	25	3	0
4	A	64	0	60	1	0
4	B	64	0	60	0	0
4	C	64	0	60	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	B	5	0	0	1	0
8	A	415	0	0	17	0
8	B	383	0	0	9	0
8	C	339	0	0	19	0
All	All	11054	0	9908	180	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 9.

All (180) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253[B]:MET:HE3	1:B:300:TYR:CB	1.81	1.11
1:B:253[B]:MET:HE3	1:B:300:TYR:HB3	1.07	1.07
1:C:259:LYS:HE2	8:C:2236:HOH:O	1.61	0.99
1:C:373[A]:LYS:NZ	8:C:2319:HOH:O	1.97	0.98
1:A:114:TRP:CZ2	1:A:297[B]:ILE:HD12	1.98	0.98
1:A:132[A]:ASP:HB2	8:A:2087:HOH:O	1.64	0.96
1:B:253[B]:MET:CE	1:B:300:TYR:HB3	1.95	0.96
1:A:32:TYR:HB3	8:A:2006:HOH:O	1.65	0.96
1:A:289:TRP:O	1:A:297[B]:ILE:CD1	2.14	0.95
1:B:253[B]:MET:CE	1:B:300:TYR:CB	2.44	0.94
1:C:284[B]:GLU:OE1	1:C:284[B]:GLU:HA	1.67	0.93
1:B:156[A]:LYS:HE2	1:B:156[A]:LYS:HA	1.52	0.92
1:A:251[B]:LYS:HB2	1:A:251[B]:LYS:NZ	1.85	0.92
1:A:289:TRP:O	1:A:297[B]:ILE:HD11	1.70	0.91
1:A:268[B]:LEU:HD21	1:A:272:LEU:HD11	1.53	0.88
1:A:134:SER:HB2	1:A:136:LYS:HD3	1.56	0.87
1:C:160[B]:VAL:HG13	1:C:196:TYR:HB3	1.57	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:TRP:HZ2	1:A:297[B]:ILE:HD12	1.40	0.83
1:A:284:GLU:N	1:A:284:GLU:OE1	2.11	0.82
1:A:28:TYR:CE2	1:A:39:ILE:HD11	2.15	0.82
1:C:304[A]:GLU:HG2	1:C:309:LYS:HZ3	1.43	0.81
1:B:156[A]:LYS:CA	1:B:156[A]:LYS:HE2	2.10	0.80
1:A:268[B]:LEU:CD2	1:A:272:LEU:CD1	2.59	0.80
1:A:268[B]:LEU:CD2	1:A:272:LEU:HD11	2.11	0.79
1:A:110:GLU:HG3	8:A:2068:HOH:O	1.84	0.78
1:B:253[B]:MET:CE	1:B:300:TYR:HB2	2.12	0.78
1:A:251[B]:LYS:HB2	1:A:251[B]:LYS:HZ2	1.45	0.77
1:C:88:TYR:HA	8:C:2079:HOH:O	1.84	0.77
1:B:213:HIS:HD2	1:B:365:ASN:OD1	1.67	0.77
1:A:346:LYS:HE3	1:A:378:ASP:HB3	1.67	0.76
1:C:245:GLU:OE2	1:C:247[B]:THR:HG23	1.85	0.76
1:C:32[A]:TYR:CE1	1:C:38:LYS:HE3	2.21	0.75
1:B:396:LYS:HA	8:B:2368:HOH:O	1.86	0.74
1:B:102:ILE:HG23	8:B:2127:HOH:O	1.87	0.73
1:A:62:LYS:CE	8:A:2073:HOH:O	2.36	0.73
1:B:360:ASN:HB2	8:B:2345:HOH:O	1.89	0.72
1:A:251[B]:LYS:NZ	1:A:251[B]:LYS:CB	2.53	0.71
1:B:410:LEU:OXT	3:B:1001:4XB:H11A	1.89	0.71
1:A:62:LYS:HD3	8:A:2055:HOH:O	1.89	0.71
1:C:304[A]:GLU:HG2	1:C:309:LYS:NZ	2.04	0.71
1:A:268[B]:LEU:HD23	1:A:272:LEU:HG	1.72	0.71
1:C:388:LEU:HD21	3:C:1001:4XB:H9	1.73	0.71
1:C:45:GLU:HB3	8:C:2016:HOH:O	1.91	0.70
1:C:39:ILE:HB	8:C:2007:HOH:O	1.91	0.69
1:A:159:GLU:CD	1:A:409:LEU:HD22	2.16	0.66
1:A:268[B]:LEU:CD2	1:A:272:LEU:HG	2.25	0.66
1:C:28:TYR:CE2	1:C:39:ILE:HG13	2.31	0.66
1:A:51:PHE:CD1	1:A:396:LYS:HE2	2.31	0.65
1:C:32[A]:TYR:CD1	1:C:38:LYS:HE3	2.30	0.65
8:A:2306:HOH:O	1:C:45:GLU:HG2	1.96	0.64
1:A:346:LYS:HE3	1:A:378:ASP:CB	2.27	0.64
1:A:243:ARG:HD3	8:A:2272:HOH:O	1.97	0.64
1:C:112:LEU:HD11	8:C:2079:HOH:O	1.98	0.64
1:A:268[B]:LEU:HD22	1:A:272:LEU:CD1	2.28	0.63
1:A:402:PRO:HA	1:A:405:VAL:HG23	1.80	0.62
1:C:45:GLU:CB	8:C:2016:HOH:O	2.47	0.61
1:B:344:THR:OG1	1:B:347:GLN:HG3	1.99	0.61
1:C:27:ASP:OD1	1:C:29:LYS:HE3	2.00	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253[B]:MET:HE1	1:B:300:TYR:HB2	1.82	0.60
1:B:410:LEU:O	3:B:1001:4XB:H10	2.02	0.59
1:C:382:GLY:HA3	8:C:2194:HOH:O	2.02	0.59
1:A:79:LYS:HE3	1:A:121:TYR:OH	2.02	0.59
1:A:51:PHE:CE1	1:A:396:LYS:HE2	2.38	0.59
1:C:253:MET:HG3	1:C:300:TYR:HB3	1.83	0.58
1:A:268[B]:LEU:CD2	1:A:272:LEU:CG	2.81	0.58
1:A:310[B]:ASP:HB3	1:A:340:THR:HA	1.86	0.58
1:B:78:VAL:HG11	1:B:117:THR:HG23	1.85	0.58
1:A:39:ILE:O	1:A:204:LYS:NZ	2.27	0.58
1:A:251[B]:LYS:HZ3	1:A:251[B]:LYS:CB	2.17	0.58
1:A:29:LYS:HE2	8:A:2004:HOH:O	2.02	0.58
1:C:141:ILE:HD12	1:C:163:LEU:HD13	1.85	0.57
1:C:141:ILE:HG22	1:C:178:LEU:HD22	1.87	0.56
1:C:28:TYR:HA	4:C:1411:NHW:P3X	2.45	0.56
1:B:97:GLU:OE1	1:B:101:ASN:ND2	2.38	0.56
1:B:253[A]:MET:HG3	1:B:300:TYR:HB3	1.88	0.55
1:B:44[B]:ASN:ND2	1:B:46:SER:OG	2.40	0.55
1:A:82:LYS:O	1:A:86[B]:GLU:HG3	2.07	0.54
1:A:110:GLU:HA	1:A:110:GLU:OE1	2.07	0.54
1:A:257:LYS:HE2	8:A:2293:HOH:O	2.08	0.54
1:C:360:ASN:HA	8:C:2198:HOH:O	2.08	0.53
1:C:284[B]:GLU:OE1	1:C:284[B]:GLU:CA	2.50	0.53
1:B:253[B]:MET:HE1	1:B:300:TYR:CB	2.35	0.53
1:A:159:GLU:OE2	1:A:409:LEU:HD22	2.09	0.52
4:A:1411:NHW:H8A	8:A:2412:HOH:O	2.09	0.52
1:A:253[B]:MET:SD	1:A:302:ASN:HB2	2.50	0.52
1:B:213:HIS:CD2	1:B:365:ASN:OD1	2.56	0.52
1:B:220:LYS:HE3	1:B:327:TYR:CD1	2.45	0.52
1:B:341:THR:HG21	8:B:2311:HOH:O	2.08	0.52
1:A:285:GLU:HG3	8:A:2324:HOH:O	2.08	0.52
1:A:250:ILE:HD13	1:A:310[B]:ASP:OD2	2.10	0.51
1:C:32[B]:TYR:CE2	1:C:38:LYS:HD2	2.45	0.51
1:A:62:LYS:NZ	8:A:2073:HOH:O	2.30	0.51
1:C:307:LYS:HE2	8:C:2277:HOH:O	2.11	0.51
1:C:224:ILE:HG21	1:C:321:ILE:HD13	1.91	0.51
1:A:220:LYS:HE3	1:A:327:TYR:CD1	2.45	0.51
1:A:210:ARG:NH1	7:B:1412:SO4:O1	2.30	0.51
1:B:410:LEU:C	3:B:1001:4XB:H11A	2.30	0.51
1:B:78:VAL:HG11	1:B:117:THR:CG2	2.41	0.51
1:C:71:TYR:CZ	1:C:131:TYR:CD1	2.99	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LYS:CE	8:C:2231:HOH:O	2.59	0.50
1:A:28:TYR:HE2	1:A:39:ILE:HD11	1.74	0.50
1:C:245:GLU:OE2	1:C:247[B]:THR:CG2	2.57	0.50
1:A:202:LEU:O	1:A:204:LYS:HA	2.11	0.49
1:C:161:ASN:HB3	1:C:162:PHE:CD2	2.47	0.49
1:B:230[B]:ASN:HB2	1:B:233:LEU:H	1.78	0.49
1:C:304[B]:GLU:HG2	8:C:2229:HOH:O	2.13	0.49
1:C:388:LEU:CD2	3:C:1001:4XB:H9	2.40	0.49
1:B:276:ASN:ND2	1:B:400:PHE:CD1	2.81	0.49
1:B:154:THR:O	1:B:155:ILE:HD13	2.13	0.48
1:B:254:ARG:NH2	1:B:259:LYS:HE3	2.28	0.48
3:C:1001:4XB:O1	3:C:1001:4XB:H	2.13	0.48
1:A:268[B]:LEU:HD21	1:A:272:LEU:CD1	2.25	0.48
1:B:131:TYR:HB3	8:B:2155:HOH:O	2.13	0.47
1:C:251:LYS:HG2	8:C:2218:HOH:O	2.12	0.47
1:B:175:ALA:HB3	1:B:176:PRO:HD3	1.96	0.47
1:C:300:TYR:CD2	1:C:355:LEU:HD13	2.50	0.47
1:A:26:MET:HG3	8:A:2002:HOH:O	2.14	0.47
1:C:123:LYS:HB3	8:C:2064:HOH:O	2.15	0.47
1:C:71:TYR:CE1	1:C:131:TYR:CD1	3.03	0.47
1:C:29:LYS:HA	1:C:29:LYS:HD3	1.65	0.47
1:C:91:LEU:HB2	8:C:2079:HOH:O	2.14	0.47
1:B:39:ILE:HD11	1:B:201:TYR:HE2	1.80	0.47
1:C:262:GLU:HG3	1:C:283:LYS:HE3	1.96	0.47
1:A:268[B]:LEU:HD22	1:A:272:LEU:HD12	1.97	0.46
1:B:27:ASP:OD1	1:B:27:ASP:N	2.48	0.46
1:C:257:LYS:HD3	1:C:259:LYS:CE	2.44	0.46
1:A:217[A]:ASN:ND2	8:A:2253:HOH:O	2.47	0.46
1:C:380:LYS:HD3	8:C:2323:HOH:O	2.14	0.46
1:A:276:ASN:ND2	1:A:400:PHE:CE1	2.84	0.46
1:C:102:ILE:O	1:C:102:ILE:HG13	2.16	0.46
1:C:266:LYS:HE3	1:C:266:LYS:HB2	1.58	0.46
1:C:254:ARG:O	1:C:300:TYR:HA	2.16	0.45
1:C:28:TYR:HB3	1:C:31:TRP:HB2	1.97	0.45
1:B:151:HIS:HD2	8:B:2031:HOH:O	1.98	0.45
1:C:39:ILE:HD12	1:C:39:ILE:HG23	1.67	0.45
1:B:266:LYS:CE	8:B:2270:HOH:O	2.63	0.45
1:C:259:LYS:NZ	8:C:2231:HOH:O	2.29	0.45
1:C:355:LEU:HA	1:C:355:LEU:HD23	1.86	0.45
1:C:272:LEU:HA	1:C:272:LEU:HD23	1.80	0.45
1:A:38[A]:LYS:HE2	8:A:2005:HOH:O	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LYS:HB2	1:A:62:LYS:HE3	1.82	0.44
1:B:118:SER:HB2	1:B:119:PRO:CD	2.46	0.44
1:C:211:TYR:HB3	1:C:367:LEU:HD23	1.99	0.44
1:A:288:HIS:CE1	8:A:2329:HOH:O	2.70	0.44
1:B:166:HIS:CE1	1:B:168:THR:HG23	2.53	0.44
1:C:259:LYS:HD2	8:C:2231:HOH:O	2.16	0.44
1:B:266:LYS:HE2	8:B:2270:HOH:O	2.18	0.44
1:C:291:LEU:HA	1:C:291:LEU:HD23	1.76	0.44
1:A:250:ILE:O	1:A:253[B]:MET:HG2	2.16	0.44
1:C:92:THR:O	1:C:104:ARG:HD2	2.18	0.44
1:A:346:LYS:CE	1:A:378:ASP:HB3	2.43	0.43
1:C:125:TRP:O	1:C:142:SER:HA	2.18	0.43
1:C:393:TYR:CD2	4:C:1411:NHW:H9M	2.54	0.43
1:A:276:ASN:ND2	1:A:400:PHE:CD1	2.87	0.43
1:A:294:GLU:HG3	8:A:2335:HOH:O	2.18	0.43
1:A:47:VAL:HG11	1:A:396:LYS:HG2	2.00	0.43
1:B:78:VAL:CG1	1:B:117:THR:CG2	2.97	0.42
1:B:212:TYR:CE2	1:B:383:GLU:HB2	2.54	0.42
1:A:298:TYR:O	1:A:313:SER:HA	2.20	0.42
1:B:94:ASN:OD1	1:B:167:LYS:HG3	2.19	0.42
1:B:151:HIS:CD2	8:B:2031:HOH:O	2.72	0.42
1:C:275:PHE:HA	8:C:2256:HOH:O	2.20	0.42
1:B:379:LEU:HA	1:B:379:LEU:HD23	1.80	0.41
1:A:275:PHE:CZ	1:A:370:MET:HG2	2.55	0.41
1:B:143:ALA:HA	1:B:159:GLU:O	2.20	0.41
1:B:340:THR:HB	1:B:348:LEU:HD22	2.01	0.41
1:C:257:LYS:HD3	1:C:259:LYS:HE3	2.02	0.41
1:B:134:SER:O	1:B:135:ASN:HB3	2.21	0.41
1:B:218:VAL:O	1:B:222:ILE:HG12	2.20	0.41
1:A:172:LYS:HE3	1:A:172:LYS:HB3	1.93	0.41
1:B:203:PRO:HA	1:B:204:LYS:HA	1.93	0.41
1:A:365:ASN:HB3	3:A:1001:4XB:H4	2.02	0.41
1:A:210:ARG:NH2	1:A:373:LYS:HE3	2.36	0.41
1:C:298:TYR:O	1:C:313:SER:HA	2.22	0.40
1:A:105:PHE:CZ	3:A:1001:4XB:HA	2.57	0.40
1:A:301:VAL:HB	1:A:308:ILE:HD12	2.04	0.40
1:C:102:ILE:HD11	1:C:224:ILE:O	2.21	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	398/385 (103%)	384 (96%)	14 (4%)	0	100	100
1	B	393/385 (102%)	380 (97%)	13 (3%)	0	100	100
1	C	376/385 (98%)	366 (97%)	10 (3%)	0	100	100
All	All	1167/1155 (101%)	1130 (97%)	37 (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	366/351 (104%)	363 (99%)	3 (1%)	81	66
1	B	361/351 (103%)	350 (97%)	11 (3%)	41	12
1	C	347/351 (99%)	332 (96%)	15 (4%)	29	5
All	All	1074/1053 (102%)	1045 (97%)	29 (3%)	49	15

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	GLU
1	A	146	THR
1	A	147	ASP
1	B	27	ASP
1	B	39	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	58	GLU
1	B	78	VAL
1	B	99	ASP
1	B	136	LYS
1	B	147	ASP
1	B	156[A]	LYS
1	B	156[B]	LYS
1	B	328	SER
1	B	396	LYS
1	C	28	TYR
1	C	29	LYS
1	C	33[A]	THR
1	C	33[B]	THR
1	C	102	ILE
1	C	146[A]	THR
1	C	146[B]	THR
1	C	244	VAL
1	C	262	GLU
1	C	266	LYS
1	C	294[A]	GLU
1	C	294[B]	GLU
1	C	307	LYS
1	C	360	ASN
1	C	396	LYS

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

Mol	Chain	Res	Type
1	A	34	GLN
1	A	55	ASN
1	A	106	ASN
1	A	249	ASN
1	A	350	GLN
1	A	371	GLN
1	B	34	GLN
1	B	106	ASN
1	B	151	HIS
1	B	213	HIS
1	B	249	ASN
1	B	295	ASN
1	B	360	ASN
1	C	331	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	360	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 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NHW	C	1411	6	58,66,66	1.23	3 (5%)	70,92,92	1.48	13 (18%)
3	4XB	C	1001	-	27,32,32	1.23	3 (11%)	30,44,44	1.44	6 (20%)
3	4XB	A	1001	-	27,32,32	1.28	2 (7%)	30,44,44	2.14	7 (23%)
3	4XB	B	1001	-	27,32,32	1.10	2 (7%)	30,44,44	2.43	9 (30%)
2	DMS	C	999	-	3,3,3	0.42	0	3,3,3	1.22	1 (33%)
2	DMS	A	999	-	3,3,3	0.48	0	3,3,3	0.84	0
7	SO4	B	1412	-	4,4,4	0.41	0	6,6,6	0.61	0
4	NHW	B	1411	6	58,66,66	1.19	2 (3%)	70,92,92	1.81	16 (22%)
4	NHW	A	1411	6	58,66,66	0.98	3 (5%)	70,92,92	1.61	11 (15%)
2	DMS	B	999	-	3,3,3	0.37	0	3,3,3	0.77	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
4	NHW	C	1411	6	-	4/61/81/81	0/3/3/3
3	4XB	C	1001	-	-	0/13/23/23	0/4/4/4
3	4XB	A	1001	-	-	0/13/23/23	0/4/4/4
3	4XB	B	1001	-	-	2/13/23/23	0/4/4/4
4	NHW	B	1411	6	-	2/61/81/81	0/3/3/3
4	NHW	A	1411	6	-	2/61/81/81	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1411	NHW	P3X-O3X	4.91	1.68	1.59
4	B	1411	NHW	P3X-O3X	4.78	1.68	1.59
3	A	1001	4XB	OAR-C14	4.21	1.44	1.33
4	B	1411	NHW	P3X-O7A	3.49	1.68	1.54
3	B	1001	4XB	OAR-C14	3.49	1.42	1.33
3	C	1001	4XB	OAR-C14	3.14	1.41	1.33
4	A	1411	NHW	O4X-C1X	-3.11	1.36	1.41
4	C	1411	NHW	P2A-O6A	-2.66	1.48	1.59
3	A	1001	4XB	OAR-C19	-2.46	1.40	1.45
3	C	1001	4XB	C25-C24	2.45	1.43	1.38
4	A	1411	NHW	C2A-N3A	2.44	1.36	1.32
4	C	1411	NHW	O4X-C1X	-2.33	1.37	1.41
4	A	1411	NHW	O10-C10	2.26	1.46	1.42
3	C	1001	4XB	OAR-C19	-2.25	1.41	1.45
3	B	1001	4XB	C25-C20	2.08	1.42	1.39

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1411	NHW	N3A-C2A-N1A	-6.78	118.08	128.68
3	A	1001	4XB	O1-C8-C9	5.17	119.73	108.31
3	B	1001	4XB	C4-C3-C13	5.12	126.35	117.84
3	B	1001	4XB	C12-C8-C9	4.97	121.34	111.74
4	C	1411	NHW	N3A-C2A-N1A	-4.84	121.12	128.68
3	A	1001	4XB	C15-OAQ-C24	4.71	127.74	117.51
4	A	1411	NHW	N3A-C2A-N1A	-4.70	121.33	128.68
4	A	1411	NHW	O4X-C1X-C2X	-4.64	100.15	106.93
3	A	1001	4XB	C1-C13-C3	-4.51	102.77	110.65

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	4XB	O1-C8-C12	-4.31	98.77	108.31
4	B	1411	NHW	C2A-N1A-C6A	4.25	126.02	118.75
4	A	1411	NHW	C7-C6-C5	4.22	119.38	112.36
3	A	1001	4XB	OAR-C14-C2	4.17	120.82	111.92
3	B	1001	4XB	OAR-C14-C2	4.15	120.78	111.92
3	B	1001	4XB	C1-C13-C3	-4.07	103.53	110.65
4	B	1411	NHW	C6-C5-N4	-3.98	109.73	116.42
4	B	1411	NHW	O4X-C1X-C2X	-3.91	101.21	106.93
3	B	1001	4XB	C19-OAR-C14	3.86	122.73	115.91
4	A	1411	NHW	C5X-C4X-C3X	-3.68	102.19	114.40
4	C	1411	NHW	O4X-C1X-C2X	-3.62	101.64	106.93
4	B	1411	NHW	C3-N4-C5	3.58	129.49	122.84
3	A	1001	4XB	C11-N-C10	3.53	120.47	110.34
4	A	1411	NHW	O1M-C1M-CP	-3.50	117.18	122.17
4	A	1411	NHW	C6-C7-N8	3.29	118.53	111.90
4	A	1411	NHW	O6A-C12-C11	-3.23	105.35	110.55
3	A	1001	4XB	C9-C10-N	3.20	117.12	110.64
4	B	1411	NHW	O1M-C1M-CP	-3.19	117.62	122.17
4	C	1411	NHW	O4X-C4X-C5X	-3.07	99.28	109.37
3	C	1001	4XB	C1-C13-C3	-3.04	105.34	110.65
4	C	1411	NHW	N6A-C6A-N1A	3.02	124.83	118.57
4	B	1411	NHW	C5X-C4X-C3X	-2.97	104.54	114.40
3	B	1001	4XB	C6-C7-C13	-2.89	115.23	120.61
4	B	1411	NHW	CP-C1M-C2M	2.83	121.60	115.52
4	B	1411	NHW	C13-C11-C10	2.77	113.62	108.82
3	B	1001	4XB	C5-C6-C7	2.74	124.10	119.89
4	B	1411	NHW	C10-C9-N8	-2.73	111.15	116.58
4	B	1411	NHW	C5A-C6A-N6A	2.68	124.42	120.35
3	C	1001	4XB	C1-C2-C14	2.66	132.62	126.14
3	C	1001	4XB	OAR-C14-C2	2.58	117.42	111.92
4	A	1411	NHW	C3-N4-C5	-2.57	118.06	122.84
4	C	1411	NHW	C6-C5-N4	-2.55	112.12	116.42
3	B	1001	4XB	C23-C24-C25	-2.55	117.03	120.53
3	C	1001	4XB	C4-C3-C13	2.51	122.01	117.84
4	C	1411	NHW	C4A-C5A-N7A	2.46	111.96	109.40
4	A	1411	NHW	C2-S1-CP	2.41	105.73	101.71
4	A	1411	NHW	C2X-C3X-C4X	-2.40	98.97	103.22
4	C	1411	NHW	C14-C11-C13	-2.35	104.39	109.17
4	B	1411	NHW	C4M-C3M-C2M	-2.32	104.86	113.19
4	B	1411	NHW	C4A-C5A-N7A	-2.31	106.99	109.40
4	B	1411	NHW	C5A-C6A-N1A	-2.29	115.16	120.35
4	C	1411	NHW	C13-C11-C10	2.29	112.79	108.82

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	1411	NHW	C13-C11-C12	-2.28	104.51	108.23
4	C	1411	NHW	C2A-N1A-C6A	2.28	122.66	118.75
4	C	1411	NHW	C2-C3-N4	-2.20	107.79	112.42
4	B	1411	NHW	O4X-C4X-C5X	-2.19	102.17	109.37
4	C	1411	NHW	O5-C5-N4	2.16	127.09	123.01
3	C	1001	4XB	C19-OAR-C14	2.11	119.65	115.91
3	A	1001	4XB	OAR-C14-O2	-2.10	119.42	123.67
2	C	999	DMS	O-S-C2	2.09	117.22	106.54
4	C	1411	NHW	C7-N8-C9	-2.08	118.88	122.59
4	B	1411	NHW	O6A-C12-C11	-2.03	107.28	110.55
3	C	1001	4XB	C22-C23-C24	-2.03	115.70	118.96
4	C	1411	NHW	C7-C6-C5	2.01	115.70	112.36

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1411	NHW	C5X-O5X-P1A-O1A
4	B	1411	NHW	C4M-C5M-C6M-C7M
4	A	1411	NHW	C7M-C8M-C9M-CAM
3	B	1001	4XB	C2-C14-OAR-C19
4	C	1411	NHW	C5X-O5X-P1A-O3A
4	A	1411	NHW	C4M-C5M-C6M-C7M
4	B	1411	NHW	C6-C7-N8-C9
3	B	1001	4XB	C20-C19-OAR-C14
4	C	1411	NHW	O4X-C4X-C5X-O5X
4	C	1411	NHW	C12-O6A-P2A-O5A

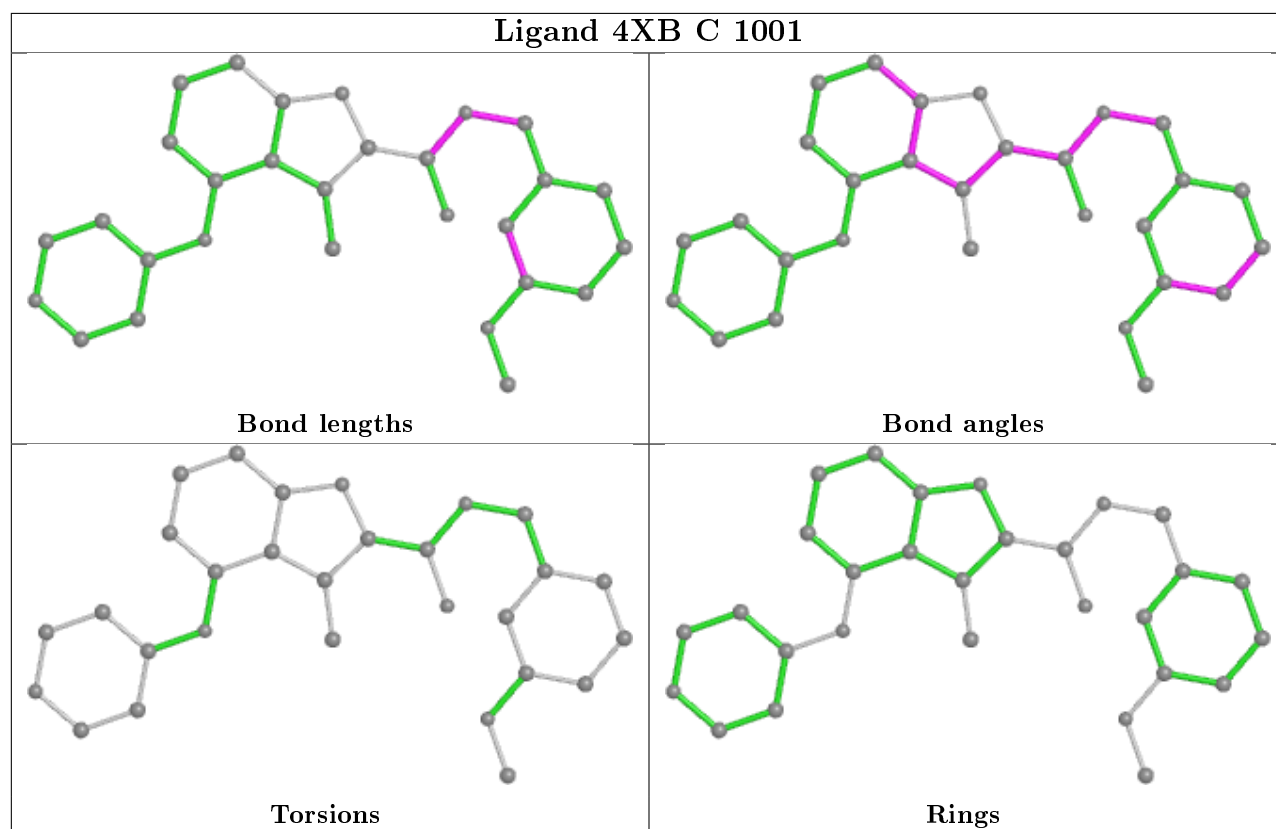
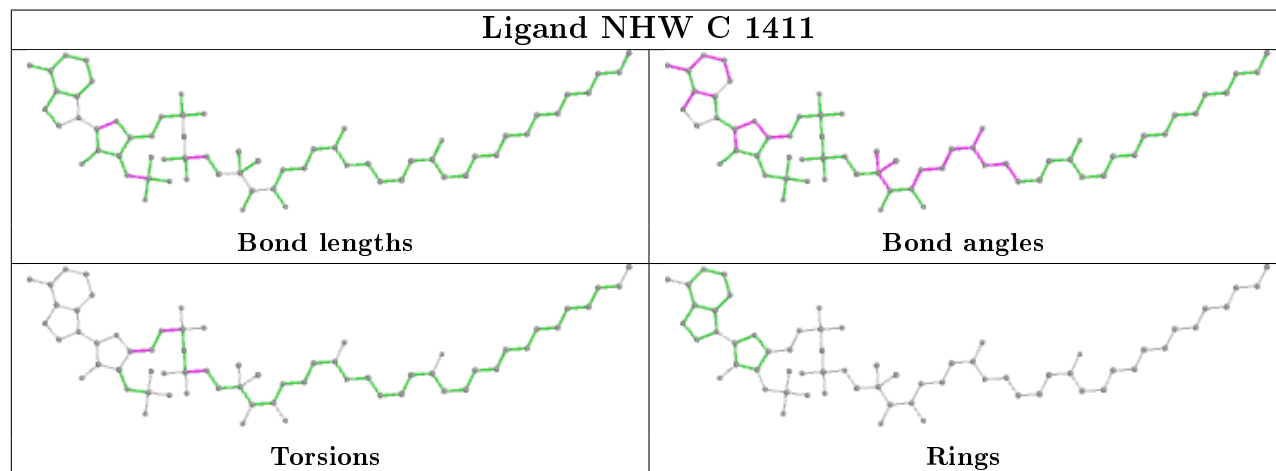
There are no ring outliers.

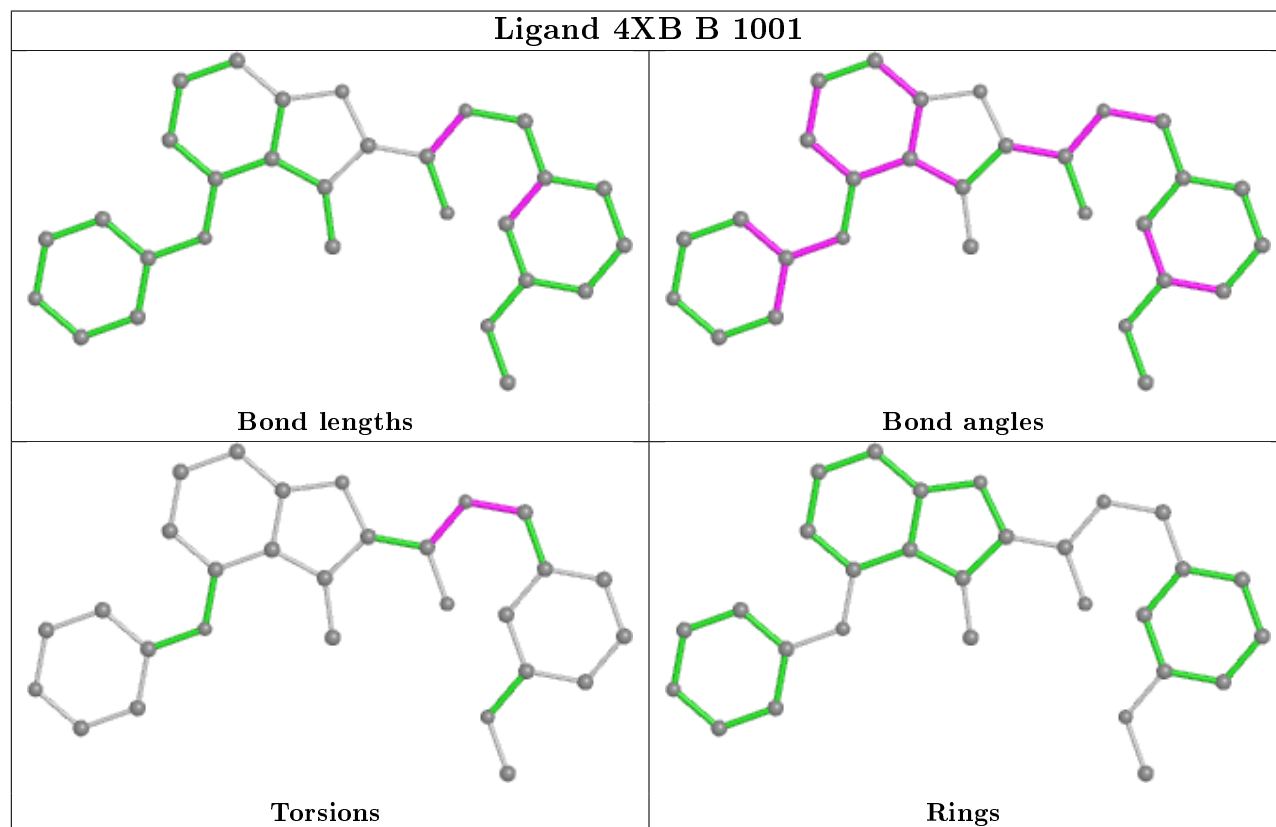
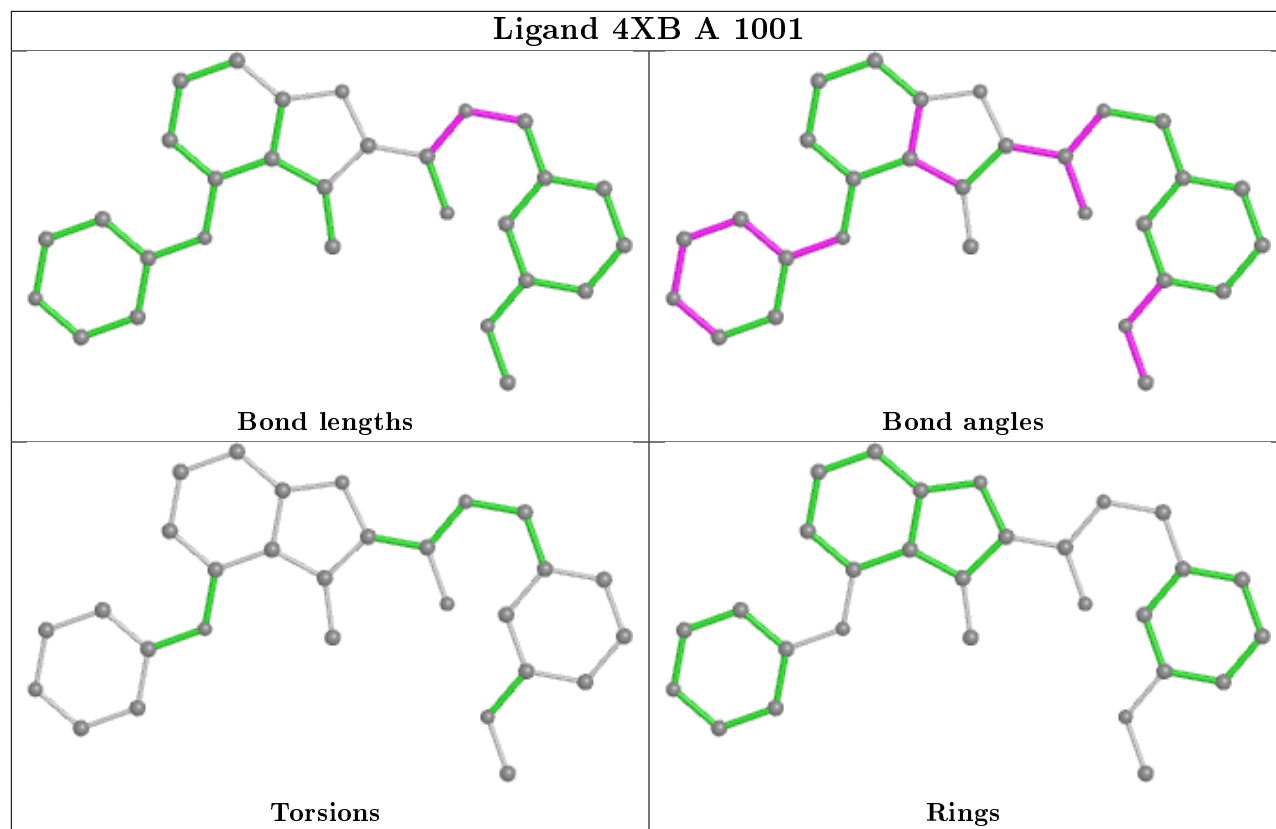
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1411	NHW	2	0
3	C	1001	4XB	3	0
3	A	1001	4XB	2	0
3	B	1001	4XB	3	0
7	B	1412	SO4	1	0
4	A	1411	NHW	1	0

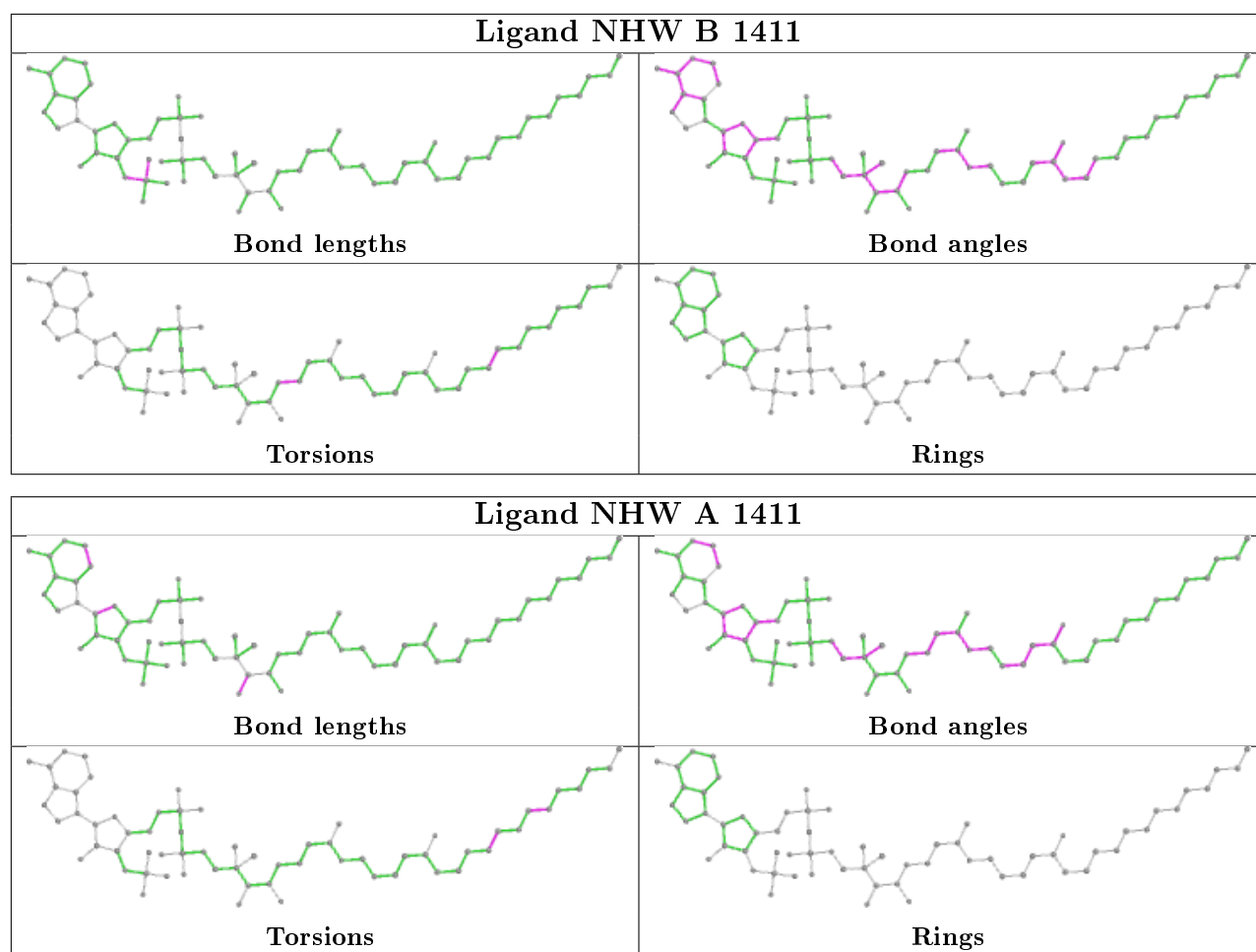
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 ⓘ

### 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%)	0.55	21 (5%)	25 27	6, 11, 22, 55	15 (3%)
1	B	385/385 (100%)	0.54	15 (3%)	39 44	5, 11, 24, 40	15 (3%)
1	C	367/385 (95%)	0.54	17 (4%)	32 35	6, 11, 21, 32	13 (3%)
All	All	1137/1155 (98%)	0.54	53 (4%)	31 34	5, 11, 22, 55	43 (3%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	ARG	6.2
1	A	32	TYR	5.2
1	B	133	ALA	4.8
1	A	26	MET	4.2
1	B	39	ILE	4.1
1	C	40	ASN	4.1
1	B	231[A]	SER	4.0
1	B	232	ARG	4.0
1	B	305	ASN	3.7
1	B	26	MET	3.6
1	B	32	TYR	3.6
1	B	131	TYR	3.5
1	B	27	ASP	3.4
1	A	39	ILE	3.3
1	A	230	ASN	3.3
1	A	323	GLY	3.2
1	C	222	ILE	3.1
1	C	323	GLY	2.9
1	A	27	ASP	2.8
1	A	229	LEU	2.8
1	A	409	LEU	2.8
1	B	230[A]	ASN	2.8
1	A	306	GLY	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	27	ASP	2.7
1	A	324	ASN	2.7
1	C	367	LEU	2.6
1	A	54	ASP	2.6
1	A	297[A]	ILE	2.5
1	C	409	LEU	2.5
1	A	78[A]	VAL	2.5
1	C	54	ASP	2.4
1	C	325	ASP	2.4
1	C	326	LYS	2.4
1	C	305	ASN	2.4
1	C	224	ILE	2.4
1	C	102	ILE	2.4
1	B	410	LEU	2.4
1	C	32[A]	TYR	2.4
1	A	43	PHE	2.3
1	A	231	SER	2.3
1	C	322	LEU	2.3
1	A	160	VAL	2.2
1	A	325	ASP	2.2
1	B	40	ASN	2.2
1	A	75	VAL	2.2
1	B	78	VAL	2.2
1	C	226	PHE	2.2
1	A	182	ILE	2.2
1	C	221	LEU	2.1
1	B	186	ILE	2.1
1	B	74	TYR	2.0
1	C	47	VAL	2.0
1	A	124	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

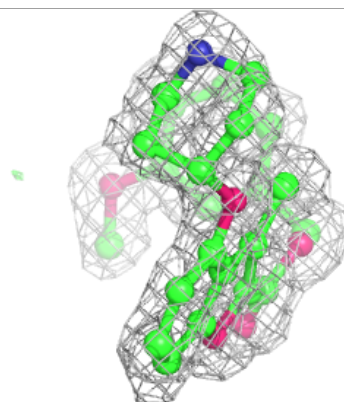
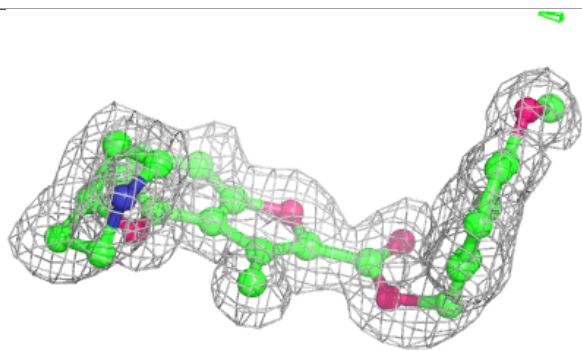
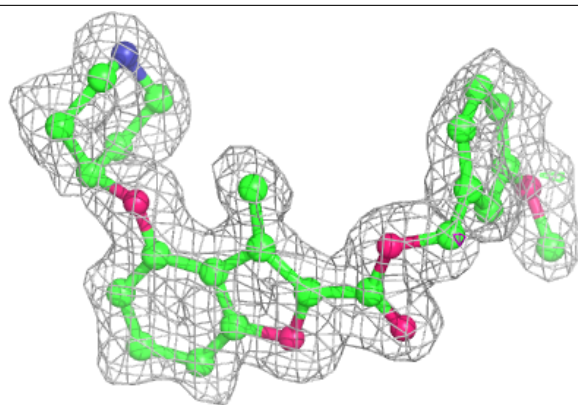
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	DMS	C	999	4/4	0.75	0.35	15,16,16,17	4
2	DMS	A	999	4/4	0.85	0.27	11,11,12,12	4
7	SO4	B	1412	5/5	0.86	0.17	38,41,43,43	0
3	4XB	C	1001	29/29	0.90	0.12	10,13,18,19	0
3	4XB	B	1001	29/29	0.92	0.11	9,12,14,14	0
4	NHW	C	1411	64/64	0.94	0.10	6,9,13,15	0
3	4XB	A	1001	29/29	0.94	0.10	10,11,13,14	0
4	NHW	B	1411	64/64	0.94	0.10	5,9,13,14	0
4	NHW	A	1411	64/64	0.94	0.10	6,9,12,17	0
2	DMS	B	999	4/4	0.94	0.15	22,23,26,26	0
6	MG	C	1413	1/1	0.97	0.07	18,18,18,18	0
6	MG	A	1413	1/1	0.98	0.05	23,23,23,23	0
6	MG	B	1414	1/1	0.98	0.04	21,21,21,21	0
5	CL	B	1413	1/1	0.99	0.07	9,9,9,9	0
5	CL	C	1412	1/1	0.99	0.08	9,9,9,9	0
5	CL	A	1412	1/1	1.00	0.04	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.

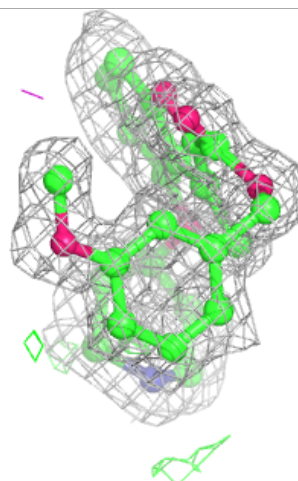
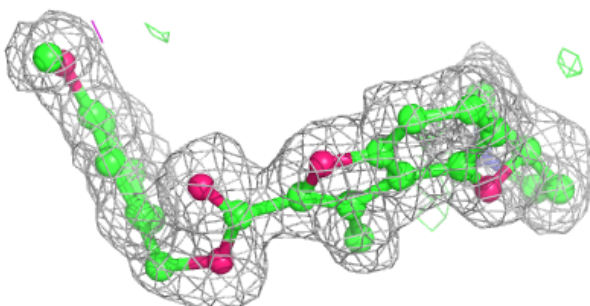
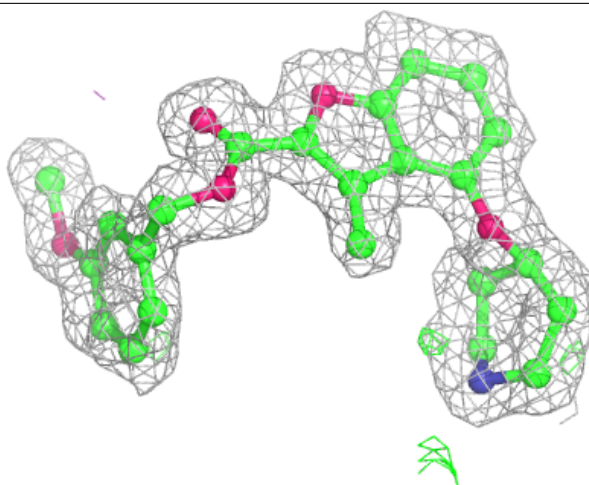
**Electron density around 4XB C 1001:**

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



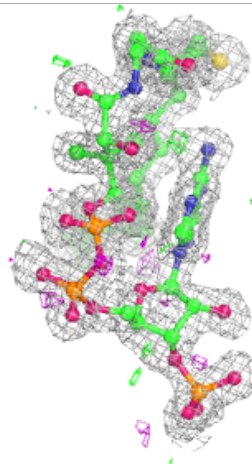
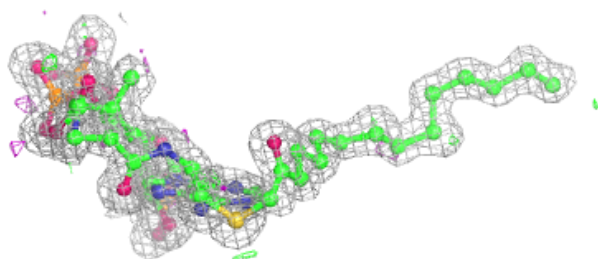
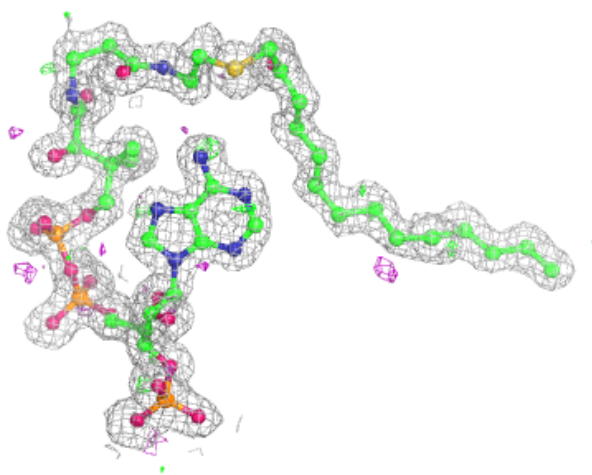
**Electron density around 4XB B 1001:**

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



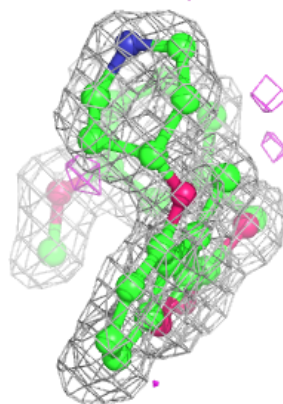
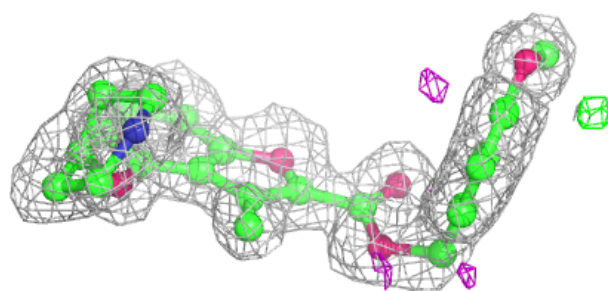
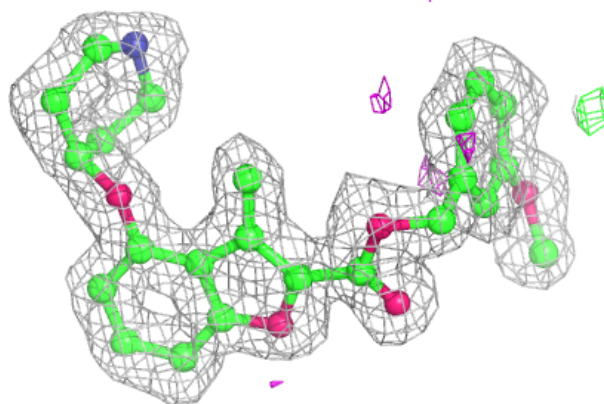
**Electron density around NHW C 1411:**

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



**Electron density around 4XB A 1001:**

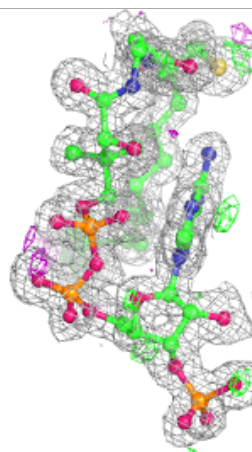
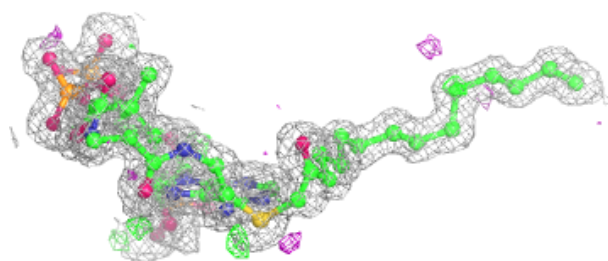
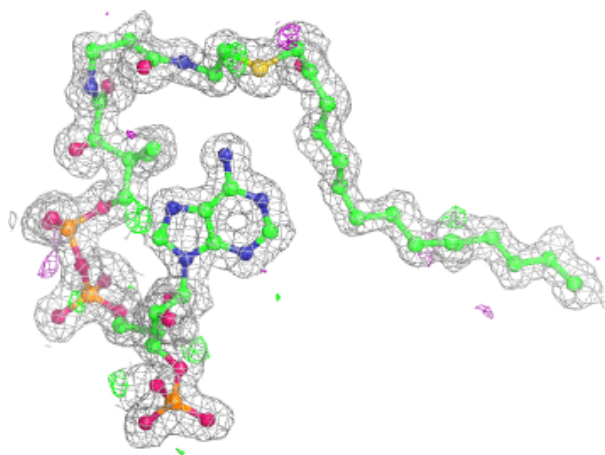
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

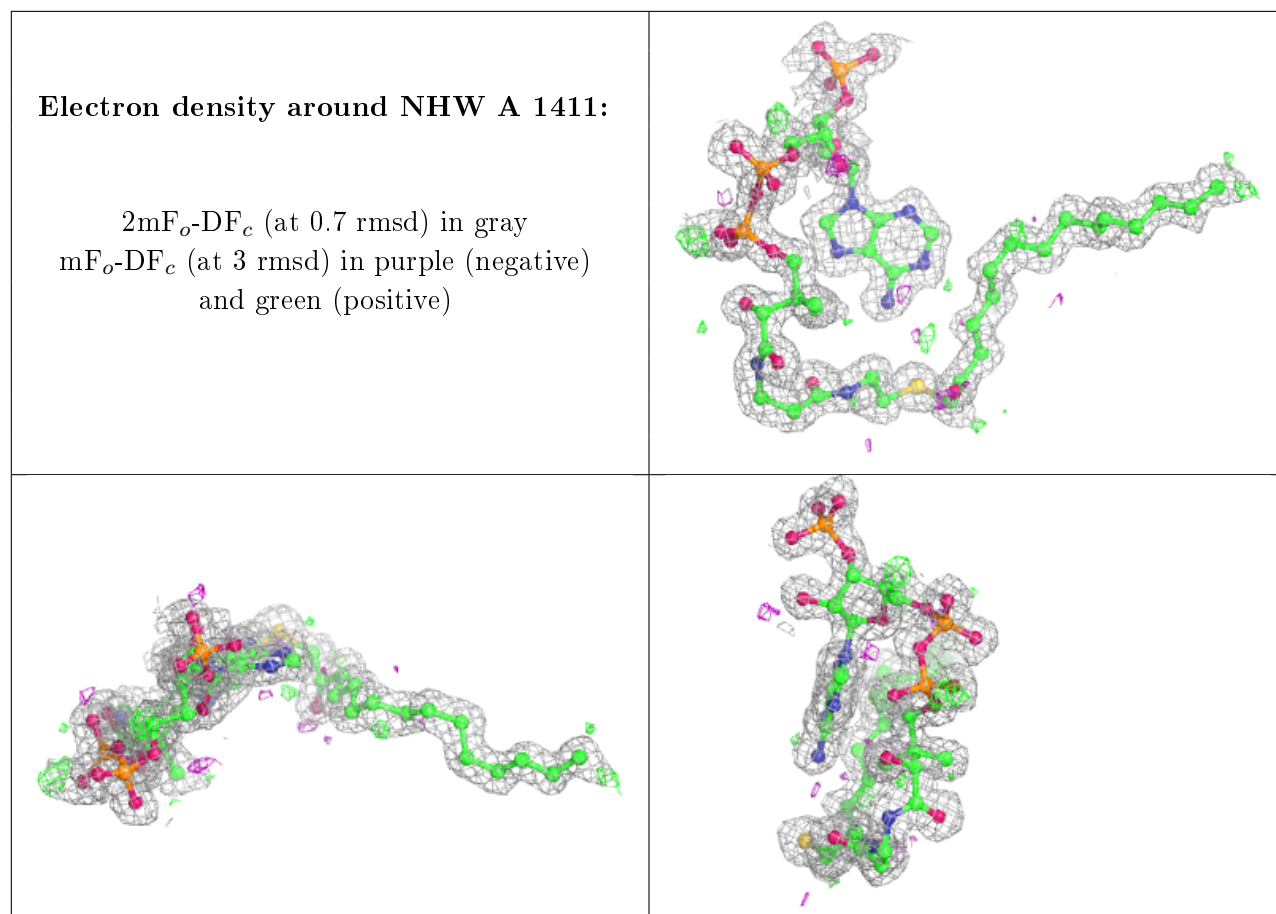




**Electron density around NHW B 1411:**

$2mF_o-DF_c$  (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.