



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:05 PM EDT

PDB ID : 4B14 / pdb_00004b14
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

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 ⓘ](#)) 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

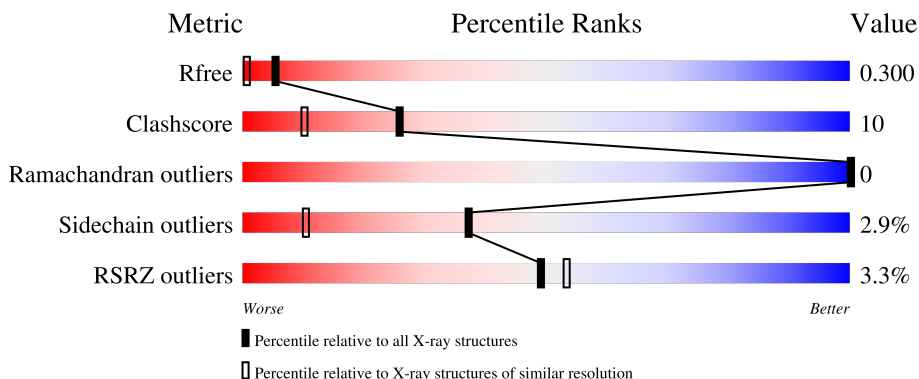
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

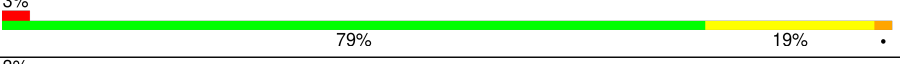
The reported resolution of this entry is 1.50 Å.

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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	B	385	
1	C	385	

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.

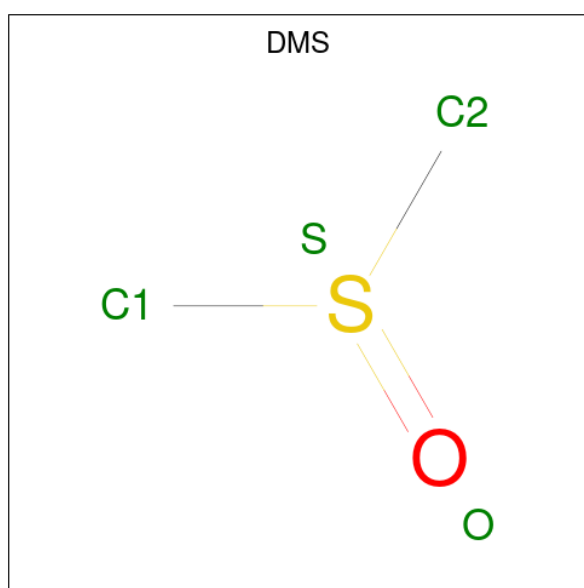
- Molecule 1 is a protein called GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

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:

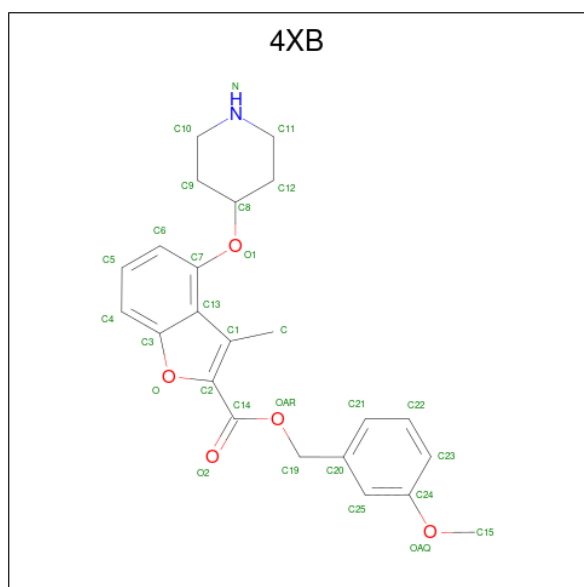
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	expression tag	UNP A5K1A2
B	26	MET	-	expression tag	UNP A5K1A2
C	26	MET	-	expression tag	UNP A5K1A2

- Molecule 2 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



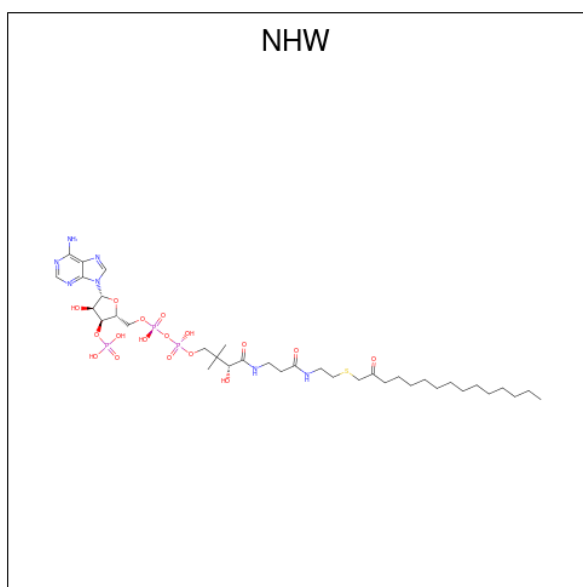
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is 3-methoxybenzyl 3-methyl-4-(piperidin-4-yloxy)-1-benzofuran-2-carboxylate (CCD ID: 4XB) (formula: $C_{23}H_{25}NO_5$).



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 (CCD ID: NHW) (formula: $C_{36}H_{64}N_7O_{17}P_3S$).



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

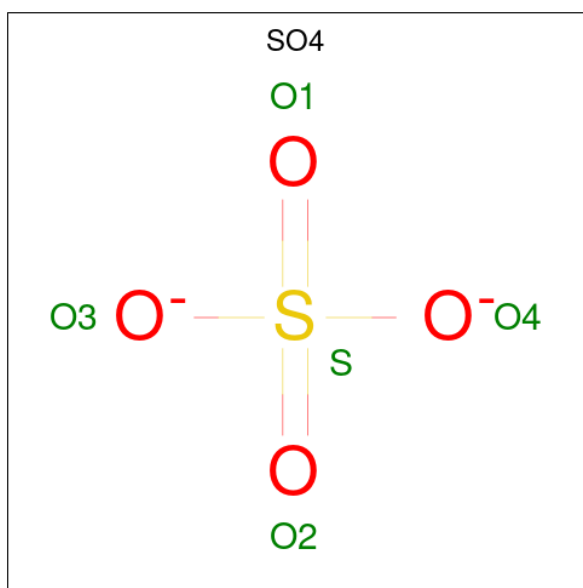
- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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

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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

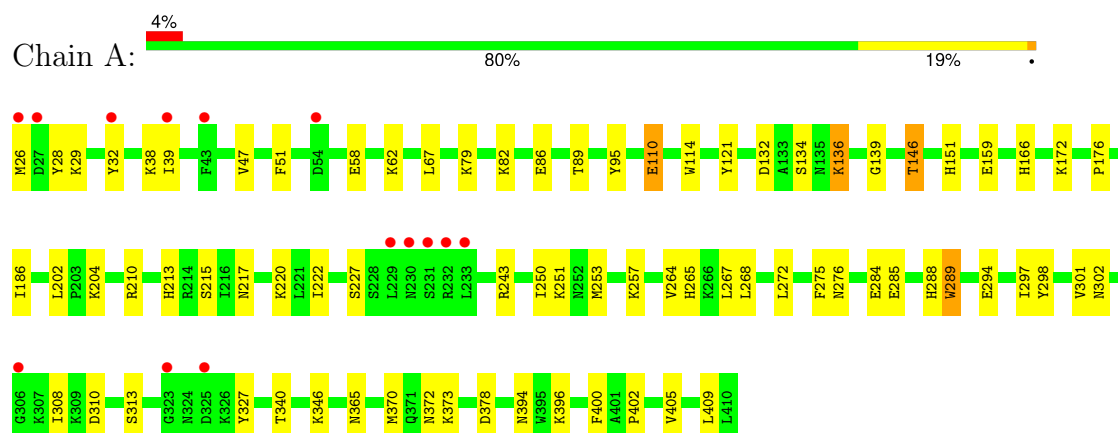
- Molecule 8 is water.

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		

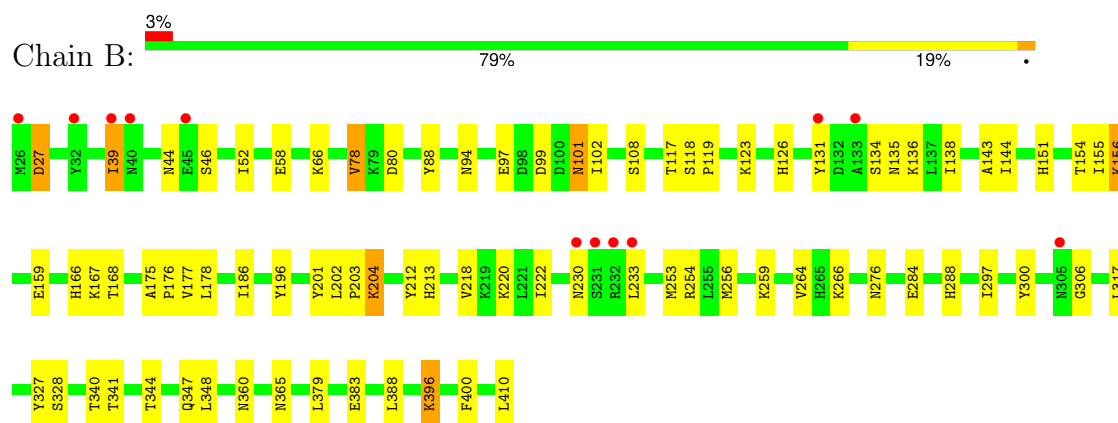
3 Residue-property plots

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.

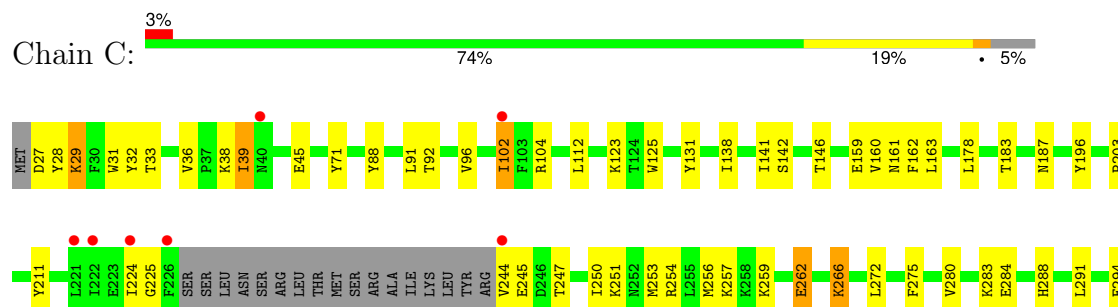
• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE

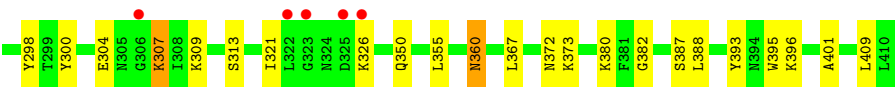


• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.38Å 118.96Å 179.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.64 – 1.50 32.64 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (32.64-1.50) 99.4 (32.64-1.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	12.1	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11054	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, MG, SO4, DMS, NHW, 4XB

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	1.33	12/3381 (0.4%)	1.32	6/4577 (0.1%)
1	B	1.32	10/3336 (0.3%)	1.32	12/4513 (0.3%)
1	C	1.28	7/3224 (0.2%)	1.33	10/4368 (0.2%)
All	All	1.31	29/9941 (0.3%)	1.32	28/13458 (0.2%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	HIS	C-O	7.10	1.32	1.24
1	A	176	PRO	C-O	6.67	1.31	1.24
1	B	178	LEU	C-O	-6.58	1.16	1.24
1	B	126	HIS	CG-CD2	6.53	1.43	1.35
1	A	267	LEU	C-O	6.51	1.31	1.24
1	A	166	HIS	ND1-CE1	6.35	1.39	1.32
1	B	108	SER	N-CA	6.11	1.53	1.45
1	C	395	TRP	CA-C	-6.05	1.45	1.52
1	A	215	SER	N-CA	5.83	1.53	1.46
1	A	95	TYR	C-O	5.77	1.29	1.23
1	C	187	ASN	N-CA	5.74	1.53	1.46
1	C	138	ILE	CA-CB	5.72	1.60	1.54
1	B	186	ILE	C-O	5.63	1.30	1.24
1	A	146	THR	N-CA	5.46	1.52	1.46
1	C	387	SER	C-O	5.44	1.30	1.23
1	A	265	HIS	ND1-CE1	5.35	1.38	1.32
1	A	89	THR	N-CA	5.32	1.52	1.46
1	B	52	ILE	CA-C	5.27	1.59	1.52
1	A	394	ASN	N-CA	5.22	1.54	1.46
1	B	88	TYR	CA-C	5.21	1.59	1.52
1	A	139	GLY	C-O	5.19	1.29	1.24
1	C	280	VAL	CA-C	5.17	1.57	1.53
1	C	183	THR	C-O	-5.13	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	388	LEU	C-O	-5.12	1.18	1.24
1	B	196	TYR	C-O	-5.11	1.17	1.23
1	A	213	HIS	ND1-CE1	5.11	1.37	1.32
1	B	177	VAL	C-O	-5.11	1.18	1.24
1	C	350	GLN	N-CA	-5.11	1.40	1.46
1	A	151	HIS	CG-CD2	5.08	1.41	1.35

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	LEU	CA-C-N	-9.01	111.10	120.38
1	A	67	LEU	C-N-CA	-9.01	111.10	120.38
1	C	36	VAL	CA-C-N	-8.88	111.23	120.03
1	C	36	VAL	C-N-CA	-8.88	111.23	120.03
1	A	289	TRP	N-CA-C	7.59	121.64	112.38
1	C	401	ALA	CA-C-N	-7.31	112.15	120.04
1	C	401	ALA	C-N-CA	-7.31	112.15	120.04
1	B	204	LYS	CA-C-N	-7.22	112.56	119.85
1	B	204	LYS	C-N-CA	-7.22	112.56	119.85
1	B	202	LEU	CA-C-N	-7.08	112.47	119.90
1	B	202	LEU	C-N-CA	-7.08	112.47	119.90
1	C	225	GLY	N-CA-C	6.88	126.91	114.46
1	A	186	ILE	N-CA-C	-6.77	103.88	110.72
1	B	138	ILE	CA-C-O	6.72	125.03	118.98
1	C	372	ASN	N-CA-C	6.54	118.41	111.28
1	B	288	HIS	N-CA-C	6.26	117.77	111.07
1	A	264	VAL	N-CA-C	-5.97	104.69	110.72
1	B	306	GLY	N-CA-C	5.92	122.13	115.08
1	A	372	ASN	N-CA-C	5.85	117.66	111.28
1	B	144	ILE	O-C-N	5.54	125.18	121.69
1	C	250	ILE	N-CA-CB	-5.44	105.14	111.83
1	C	288	HIS	N-CA-C	5.33	116.77	111.07
1	C	96	VAL	N-CA-C	5.27	116.48	109.37
1	C	203	PRO	N-CA-C	5.22	118.77	110.21
1	B	80	ASP	N-CA-C	5.12	117.09	109.25
1	B	101	ASN	N-CA-C	5.12	118.67	111.90
1	B	52	ILE	CB-CG1-CD1	5.09	124.48	113.80
1	B	66	LYS	N-CA-C	5.08	117.80	110.28

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	68	0
1	B	3233	0	3248	55	0
1	C	3116	0	3104	64	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
2	C	4	0	6	2	0
3	A	29	0	25	1	0
3	B	29	0	25	3	0
3	C	29	0	25	2	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	20	0
All	All	11054	0	9908	189	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 10.

All (189) 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:HB3	1.35	1.03
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:253[B]:MET:CE	1:B:300:TYR:CB	2.44	0.95
1:A:289:TRP:O	1:A:297[B]:ILE:CD1	2.14	0.95
1:C:284[B]:GLU:HA	1:C:284[B]:GLU:OE1	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:NZ	1:A:251[B]:LYS:HB2	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:B:253[B]:MET:HE1	1:B:300:TYR:CB	2.05	0.87
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
1:A:114:TRP:HZ2	1:A:297[B]:ILE:HD12	1.40	0.83
1:C:304[A]:GLU:HG2	1:C:309:LYS:HZ3	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:B:156[A]:LYS:HE2	1:B:156[A]:LYS:CA	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:251[B]:LYS:HB2	1:A:251[B]:LYS:HZ2	1.44	0.79
1:B:253[B]:MET:HE3	1:B:300:TYR:CB	2.08	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: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:A:159:GLU:CD	1:A:409:LEU:HD22	2.16	0.71
1:B:344:THR:HG1	1:B:347:GLN:HG3	1.55	0.71
1:C:45:GLU:HB3	8:C:2016:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ILE:HB	8:C:2007:HOH:O	1.91	0.69
1:B:253[B]:MET:HE1	1:B:300:TYR:HB2	1.68	0.69
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
1:A:62:LYS:NZ	8:A:2073:HOH:O	2.30	0.59
1:B:410:LEU:O	3:B:1001:4XB:H10	2.02	0.59
1:B:253[B]:MET:HE1	1:B:300:TYR:C	2.27	0.59
2:C:999:DMS:H13	8:C:2291:HOH:O	2.02	0.59
1:C:382:GLY:HA3	8:C:2194:HOH:O	2.02	0.59
1:A:51:PHE:CE1	1:A:396:LYS:HE2	2.38	0.59
1:A:79:LYS:HE3	1:A:121:TYR:OH	2.02	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: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:159:GLU:OE2	2:C:999:DMS:H23	2.04	0.57
1:C:141:ILE:HG22	1:C:178:LEU:HD22	1.87	0.56
1:A:251[B]:LYS:CB	1:A:251[B]:LYS:HZ3	2.19	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:410:LEU:C	3:B:1001:4XB:H11A	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284[B]:GLU:OE1	1:C:284[B]:GLU:CA	2.50	0.53
1:A:159:GLU:OE2	1:A:409:LEU:HD22	2.09	0.52
1:A:253[B]:MET:SD	1:A:302:ASN:HB2	2.50	0.52
4:A:1411:NHW:H8A	8:A:2412:HOH:O	2.09	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: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:210:ARG:NH1	7:B:1412:SO4:O1	2.30	0.51
1:A:220:LYS:HE3	1:A:327:TYR:CD1	2.45	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
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
1:A:268[B]:LEU:HD21	1:A:272:LEU:CD1	2.25	0.48
1:B:256:MET:HE3	1:B:264:VAL:HG21	1.95	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:29:LYS:HA	1:C:29:LYS:HD3	1.65	0.47
1:C:71:TYR:CE1	1:C:131:TYR:CD1	3.03	0.47
1:C:123:LYS:HB3	8:C:2064:HOH:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ASP:N	1:B:27:ASP:OD1	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:28:TYR:HB3	1:C:31:TRP:HB2	1.97	0.45
1:C:254:ARG:O	1:C:300:TYR:HA	2.16	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:HD23	1:C:355:LEU:HA	1.86	0.45
1:C:272:LEU:HD23	1:C:272:LEU:HA	1.80	0.45
1:A:38[A]:LYS:HE2	8:A:2005:HOH:O	2.17	0.44
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:47:VAL:HG11	1:A:396:LYS:HG2	2.00	0.43
1:A:294:GLU:HG3	8:A:2335:HOH:O	2.18	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:C:256:MET:HE2	1:C:291:LEU:CD2	2.49	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:C:256:MET:HE2	1:C:291:LEU:HD21	2.01	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:HD23	1:B:379:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:222:ILE:HD13	1:A:227:SER:C	2.46	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:HB3	1:A:172:LYS:HE3	1.93	0.41
1:B:203:PRO:HA	1:B:204:LYS:HA	1.93	0.41
1:B:284:GLU:H	1:B:284:GLU:CD	2.28	0.41
1:A:210:ARG:NH2	1:A:373:LYS:HE3	2.36	0.41
1:A:365:ASN:HB3	3:A:1001:4XB:H4	2.02	0.41
1:B:344:THR:HG1	1:B:347:GLN:CG	2.30	0.40
1:C:298:TYR:O	1:C:313:SER:HA	2.22	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 [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	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%)	362 (99%)	4 (1%)	65	41
1	B	361/351 (103%)	348 (96%)	13 (4%)	31	6
1	C	347/351 (99%)	330 (95%)	17 (5%)	22	3
All	All	1074/1053 (102%)	1040 (97%)	34 (3%)	37	8

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	110	GLU
1	A	136	LYS
1	A	146	THR
1	B	27	ASP
1	B	39	ILE
1	B	58	GLU
1	B	78	VAL
1	B	99	ASP
1	B	123	LYS
1	B	136	LYS
1	B	156[A]	LYS
1	B	156[B]	LYS
1	B	297	ILE
1	B	317	LEU
1	B	328	SER
1	B	396	LYS
1	C	29	LYS
1	C	33[A]	THR
1	C	33[B]	THR
1	C	39	ILE
1	C	102	ILE
1	C	146[A]	THR
1	C	146[B]	THR
1	C	244	VAL
1	C	262	GLU

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Mol	Chain	Res	Type
1	C	266	LYS
1	C	294[A]	GLU
1	C	294[B]	GLU
1	C	307	LYS
1	C	326	LYS
1	C	360	ASN
1	C	396	LYS
1	C	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	151	HIS
1	A	187	ASN
1	A	193	GLN
1	A	249	ASN
1	A	350	GLN
1	A	371	GLN
1	A	372	ASN
1	B	34	GLN
1	B	106	ASN
1	B	151	HIS
1	B	213	HIS
1	B	249	ASN
1	B	320	GLN
1	B	359	ASN
1	B	360	ASN
1	C	40	ASN
1	C	55	ASN
1	C	187	ASN
1	C	372	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DMS	C	999	-	3,3,3	0.45	0	3,3,3	1.24	1 (33%)
3	4XB	B	1001	-	32,32,32	1.68	7 (21%)	40,44,44	2.47	16 (40%)
2	DMS	A	999	-	3,3,3	0.51	0	3,3,3	0.85	0
3	4XB	A	1001	-	32,32,32	1.73	6 (18%)	40,44,44	2.09	9 (22%)
7	SO4	B	1412	-	4,4,4	0.49	0	6,6,6	0.56	0
4	NHW	A	1411	6	64,66,66	1.44	5 (7%)	87,92,92	1.68	19 (21%)
2	DMS	B	999	-	3,3,3	0.39	0	3,3,3	0.79	0
3	4XB	C	1001	-	32,32,32	1.75	6 (18%)	40,44,44	1.72	6 (15%)
4	NHW	C	1411	6	64,66,66	1.39	6 (9%)	87,92,92	1.53	16 (18%)
4	NHW	B	1411	6	64,66,66	1.40	5 (7%)	87,92,92	1.81	19 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	4XB	B	1001	-	-	4/15/23/23	0/4/4/4
3	4XB	A	1001	-	-	1/15/23/23	0/4/4/4
4	NHW	A	1411	6	-	2/65/81/81	0/3/3/3
3	4XB	C	1001	-	-	0/15/23/23	0/4/4/4
4	NHW	C	1411	6	-	4/65/81/81	0/3/3/3
4	NHW	B	1411	6	-	2/65/81/81	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1411	NHW	P2A-O3A	7.19	1.67	1.59
3	C	1001	4XB	C2-C1	5.97	1.50	1.36
3	A	1001	4XB	OAR-C14	5.59	1.44	1.33
4	C	1411	NHW	P3X-O3X	5.16	1.68	1.59
4	B	1411	NHW	P3X-O3X	5.03	1.68	1.59
4	A	1411	NHW	P1A-O3A	-4.74	1.54	1.59
3	B	1001	4XB	C2-C1	4.64	1.46	1.36
3	B	1001	4XB	OAR-C14	4.61	1.42	1.33
4	C	1411	NHW	C12-C11	4.17	1.59	1.52
3	C	1001	4XB	OAR-C14	4.14	1.41	1.33
4	B	1411	NHW	P2A-O3A	3.94	1.63	1.59
3	A	1001	4XB	C2-C1	3.89	1.45	1.36
4	B	1411	NHW	P3X-O7A	3.63	1.68	1.54
4	B	1411	NHW	C5A-N7A	-3.36	1.33	1.39
3	B	1001	4XB	O-C3	-3.16	1.33	1.38
4	B	1411	NHW	C4A-N9A	-3.07	1.31	1.37
3	A	1001	4XB	O-C2	-3.02	1.33	1.39
3	A	1001	4XB	C4-C3	2.89	1.45	1.39
4	C	1411	NHW	P2A-O6A	-2.78	1.48	1.59
3	C	1001	4XB	C13-C1	-2.73	1.39	1.45
4	C	1411	NHW	C5A-N7A	-2.70	1.34	1.39
3	C	1001	4XB	C25-C24	2.58	1.43	1.39
4	A	1411	NHW	C1X-N9A	2.49	1.53	1.46
3	B	1001	4XB	O-C2	-2.45	1.34	1.39
3	C	1001	4XB	C-C1	2.44	1.54	1.50
3	A	1001	4XB	OAR-C19	-2.39	1.40	1.45
4	A	1411	NHW	O10-C10	2.34	1.46	1.42
3	B	1001	4XB	C13-C1	-2.33	1.40	1.45
4	A	1411	NHW	O4X-C1X	-2.28	1.36	1.42
3	B	1001	4XB	C5-C4	-2.23	1.35	1.38
3	A	1001	4XB	O-C3	-2.21	1.35	1.38
4	C	1411	NHW	P2A-O3A	2.19	1.61	1.59
3	C	1001	4XB	OAR-C19	-2.18	1.41	1.45
3	B	1001	4XB	C25-C20	2.09	1.42	1.39
4	C	1411	NHW	O10-C10	2.01	1.45	1.42

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1411	NHW	N3A-C2A-N1A	-6.94	118.08	128.58
3	A	1001	4XB	OAR-C14-C2	6.43	120.82	111.52
3	B	1001	4XB	OAR-C14-C2	6.40	120.78	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	4XB	C-C1-C13	-5.28	117.47	126.26
4	C	1411	NHW	N3A-C2A-N1A	-4.93	121.12	128.58
3	A	1001	4XB	O1-C8-C9	4.89	119.73	108.31
4	A	1411	NHW	N3A-C2A-N1A	-4.79	121.33	128.58
3	A	1001	4XB	C15-OAQ-C24	4.77	127.74	117.50
3	B	1001	4XB	C12-C8-C9	4.74	121.34	111.67
3	C	1001	4XB	O-C3-C13	4.73	115.43	110.69
3	B	1001	4XB	C19-OAR-C14	4.71	122.73	116.16
4	B	1411	NHW	C2A-N1A-C6A	4.44	126.02	118.73
4	A	1411	NHW	C7-C6-C5	4.20	119.38	112.39
3	B	1001	4XB	O1-C8-C12	-4.09	98.77	108.31
3	C	1001	4XB	OAR-C14-C2	4.08	117.42	111.52
3	C	1001	4XB	C-C1-C2	4.07	136.24	128.21
3	C	1001	4XB	C-C1-C13	-4.04	119.53	126.26
4	A	1411	NHW	C5A-C4A-N3A	-3.94	121.29	126.72
4	C	1411	NHW	N3A-C4A-N9A	3.72	133.49	127.17
4	C	1411	NHW	O4A-P2A-O3A	3.71	117.30	107.27
4	C	1411	NHW	C5A-C4A-N3A	-3.66	121.67	126.72
4	A	1411	NHW	C5X-C4X-C3X	-3.66	102.19	114.38
3	B	1001	4XB	C-C1-C2	3.65	135.41	128.21
4	B	1411	NHW	C6-C5-N4	-3.63	109.73	116.34
4	B	1411	NHW	C3-N4-C5	3.58	129.49	122.82
3	A	1001	4XB	C11-N-C10	3.57	120.47	110.40
4	B	1411	NHW	N9A-C8A-N7A	-3.54	108.91	113.94
4	A	1411	NHW	N9A-C8A-N7A	-3.54	108.92	113.94
4	A	1411	NHW	O1M-C1M-CP	-3.50	117.18	122.17
3	A	1001	4XB	C9-C10-N	3.35	117.12	110.81
4	A	1411	NHW	O6A-C12-C11	-3.23	105.35	110.55
4	B	1411	NHW	O1M-C1M-CP	-3.19	117.62	122.17
4	B	1411	NHW	C4A-C5A-N7A	-3.14	106.99	110.58
4	C	1411	NHW	O4X-C4X-C5X	-3.14	99.28	109.33
4	B	1411	NHW	C5A-C4A-N3A	-3.08	122.47	126.72
4	A	1411	NHW	C6-C7-N8	3.07	118.53	112.00
3	A	1001	4XB	O-C3-C13	3.06	113.75	110.69
4	A	1411	NHW	C2A-N3A-C4A	3.04	119.25	111.83
4	A	1411	NHW	O4X-C1X-C2X	-3.02	100.15	106.62
4	B	1411	NHW	C5A-N7A-C8A	2.99	108.15	103.45
4	B	1411	NHW	C5X-C4X-C3X	-2.95	104.54	114.38
4	A	1411	NHW	C5A-N7A-C8A	2.90	108.01	103.45
4	C	1411	NHW	N6A-C6A-N1A	2.90	124.83	118.38
3	B	1001	4XB	O-C3-C4	-2.88	120.43	126.49
4	A	1411	NHW	P3X-O3X-C3X	-2.87	115.76	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1411	NHW	CP-C1M-C2M	2.86	121.60	115.55
4	B	1411	NHW	C13-C11-C10	2.85	113.62	108.77
3	A	1001	4XB	C4-C3-C13	-2.83	119.44	124.01
4	B	1411	NHW	C10-C9-N8	-2.81	111.15	116.48
4	B	1411	NHW	C2A-N3A-C4A	2.81	118.69	111.83
3	A	1001	4XB	C3-C13-C1	-2.73	102.77	106.69
4	B	1411	NHW	C4A-N9A-C8A	2.60	108.46	105.74
3	B	1001	4XB	C23-C24-C25	-2.58	117.03	120.50
4	A	1411	NHW	C3-N4-C5	-2.56	118.06	122.82
3	B	1001	4XB	C3-O-C2	2.55	107.93	105.26
3	B	1001	4XB	O1-C7-C13	2.53	123.01	117.51
4	B	1411	NHW	O4X-C1X-C2X	-2.52	101.21	106.62
3	C	1001	4XB	C19-OAR-C14	2.50	119.65	116.16
3	B	1001	4XB	C5-C6-C7	2.48	124.10	119.60
4	A	1411	NHW	C2X-C3X-C4X	-2.44	98.97	103.24
4	A	1411	NHW	C2-S1-CP	2.43	105.73	101.72
3	B	1001	4XB	C6-C7-C13	-2.42	115.23	120.14
4	C	1411	NHW	C14-C11-C13	-2.42	104.39	109.20
4	C	1411	NHW	C2A-N1A-C6A	2.39	122.66	118.73
3	B	1001	4XB	O-C3-C13	2.39	113.08	110.69
4	C	1411	NHW	C2A-N3A-C4A	2.38	117.64	111.83
4	C	1411	NHW	C13-C11-C10	2.36	112.79	108.77
4	C	1411	NHW	O4X-C1X-C2X	-2.33	101.64	106.62
4	C	1411	NHW	C5A-C6A-N6A	-2.32	117.54	123.29
4	C	1411	NHW	C6-C5-N4	-2.32	112.12	116.34
4	A	1411	NHW	N3A-C4A-N9A	2.29	131.06	127.17
4	A	1411	NHW	C13-C11-C12	-2.25	104.51	108.22
4	B	1411	NHW	C4M-C3M-C2M	-2.25	104.86	113.13
4	B	1411	NHW	O4X-C4X-C5X	-2.24	102.17	109.33
4	A	1411	NHW	C4A-C5A-N7A	-2.23	108.04	110.58
4	C	1411	NHW	C2-C3-N4	-2.21	107.79	112.41
3	A	1001	4XB	OAR-C14-O2	-2.20	119.42	123.37
3	B	1001	4XB	C3-C13-C1	-2.20	103.53	106.69
3	C	1001	4XB	C22-C23-C24	-2.17	115.70	118.98
3	B	1001	4XB	C5-C4-C3	-2.15	115.69	119.60
2	C	999	DMS	O-S-C2	2.14	117.22	106.49
3	B	1001	4XB	C7-C13-C1	2.12	138.81	134.09
4	C	1411	NHW	O5-C5-N4	2.07	127.09	123.03
4	A	1411	NHW	O3A-P2A-O5A	-2.04	104.56	110.70
4	C	1411	NHW	C7-N8-C9	-2.04	118.88	122.55
4	B	1411	NHW	O6A-C12-C11	-2.03	107.28	110.55

There are no chirality outliers.

All (13) torsion outliers are listed below:

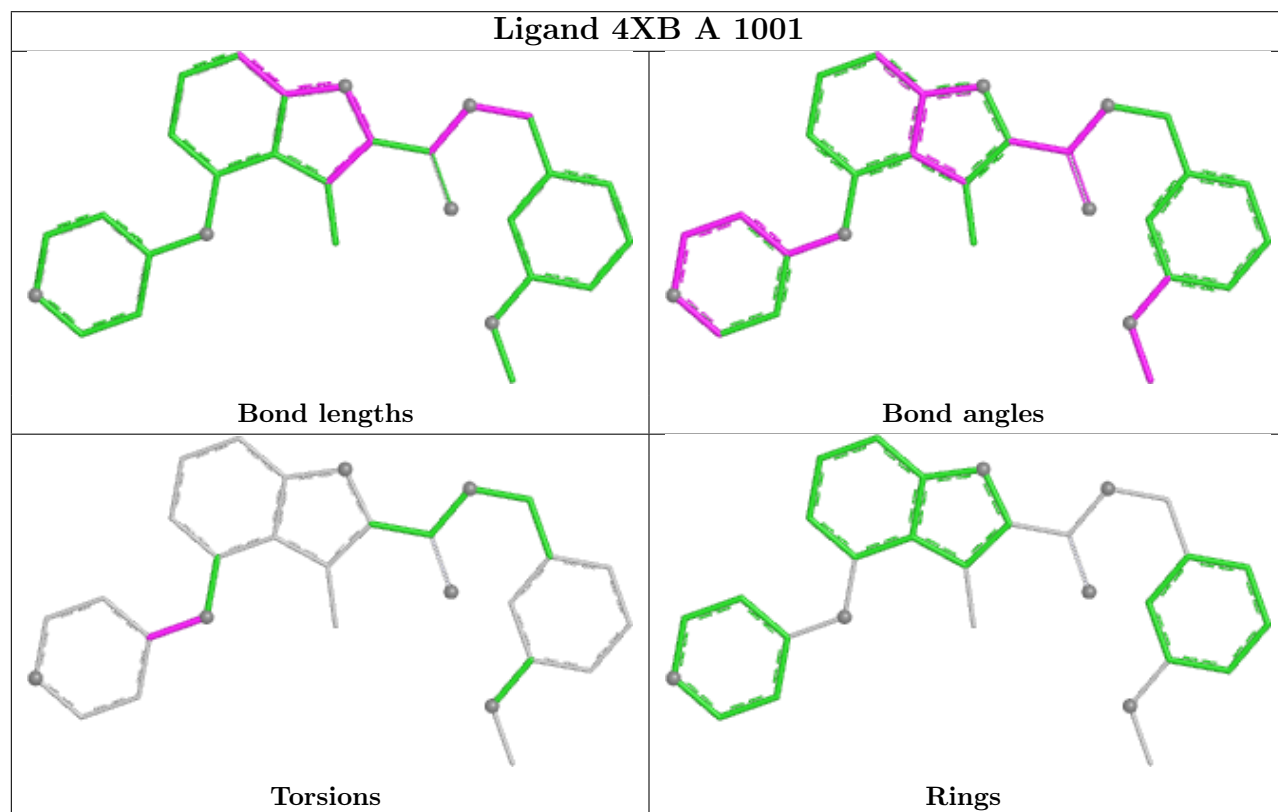
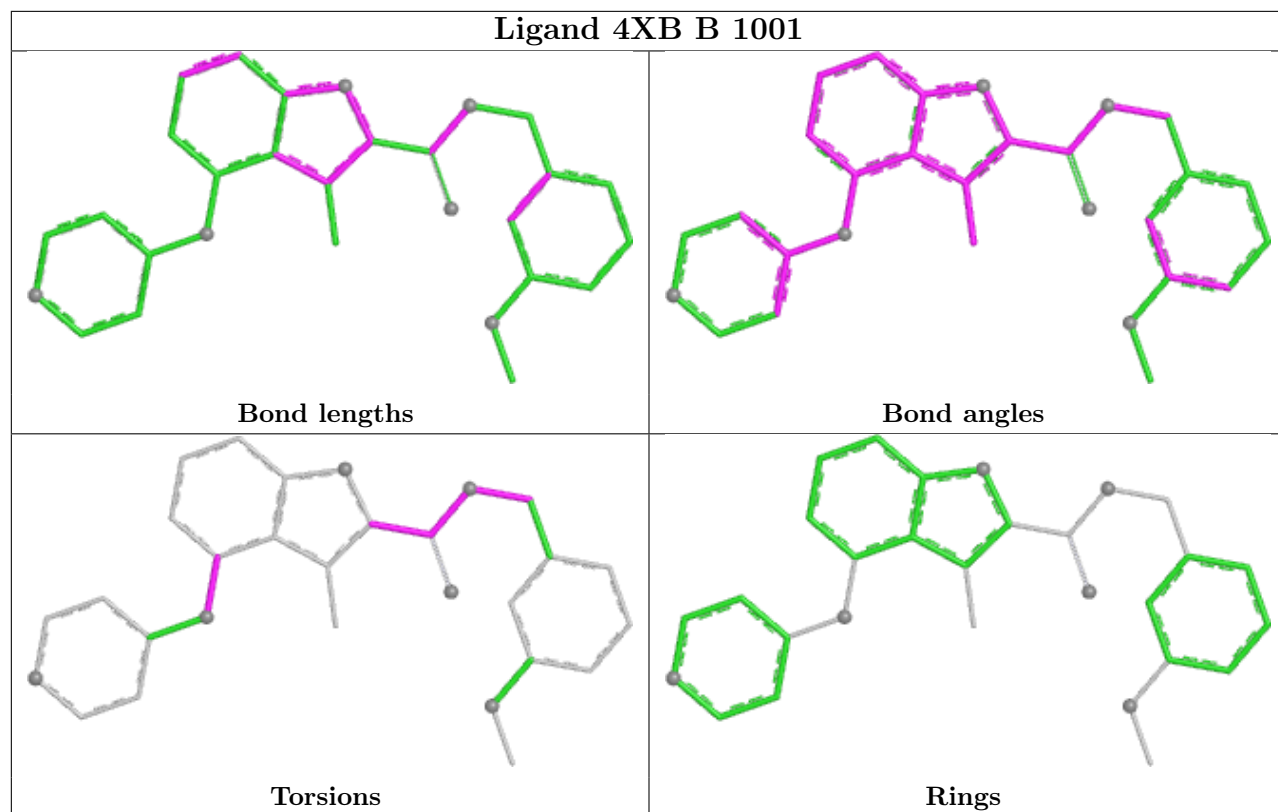
Mol	Chain	Res	Type	Atoms
4	C	1411	NHW	C5X-O5X-P1A-O1A
4	B	1411	NHW	C4M-C5M-C6M-C7M
3	B	1001	4XB	C2-C14-OAR-C19
4	A	1411	NHW	C7M-C8M-C9M-CAM
4	C	1411	NHW	C5X-O5X-P1A-O3A
4	C	1411	NHW	C12-O6A-P2A-O5A
4	A	1411	NHW	C4M-C5M-C6M-C7M
4	B	1411	NHW	C6-C7-N8-C9
3	B	1001	4XB	C20-C19-OAR-C14
3	B	1001	4XB	O2-C14-C2-C1
4	C	1411	NHW	O4X-C4X-C5X-O5X
3	B	1001	4XB	C6-C7-O1-C8
3	A	1001	4XB	C12-C8-O1-C7

There are no ring outliers.

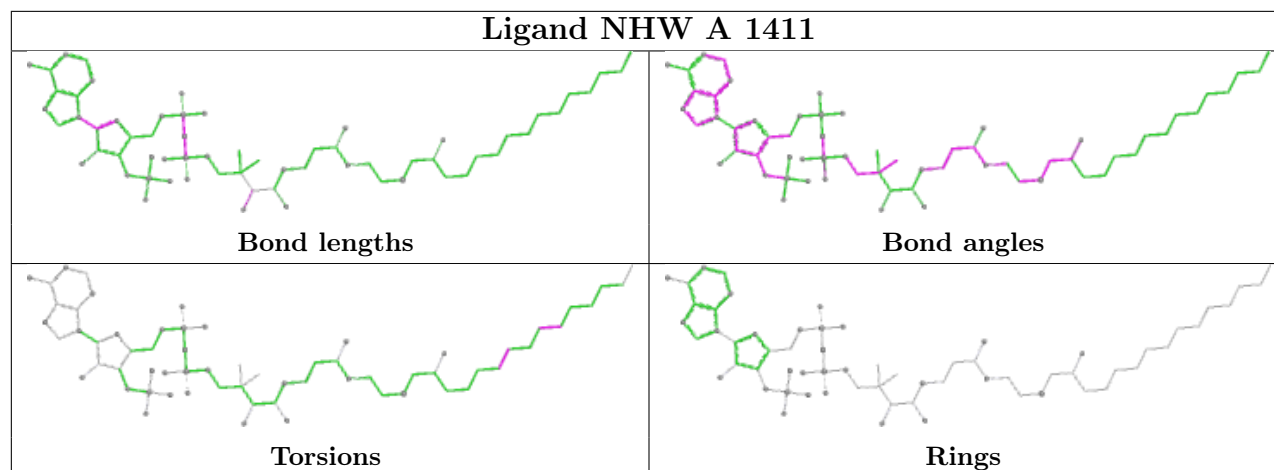
7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	999	DMS	2	0
3	B	1001	4XB	3	0
3	A	1001	4XB	1	0
7	B	1412	SO4	1	0
4	A	1411	NHW	1	0
3	C	1001	4XB	2	0
4	C	1411	NHW	2	0

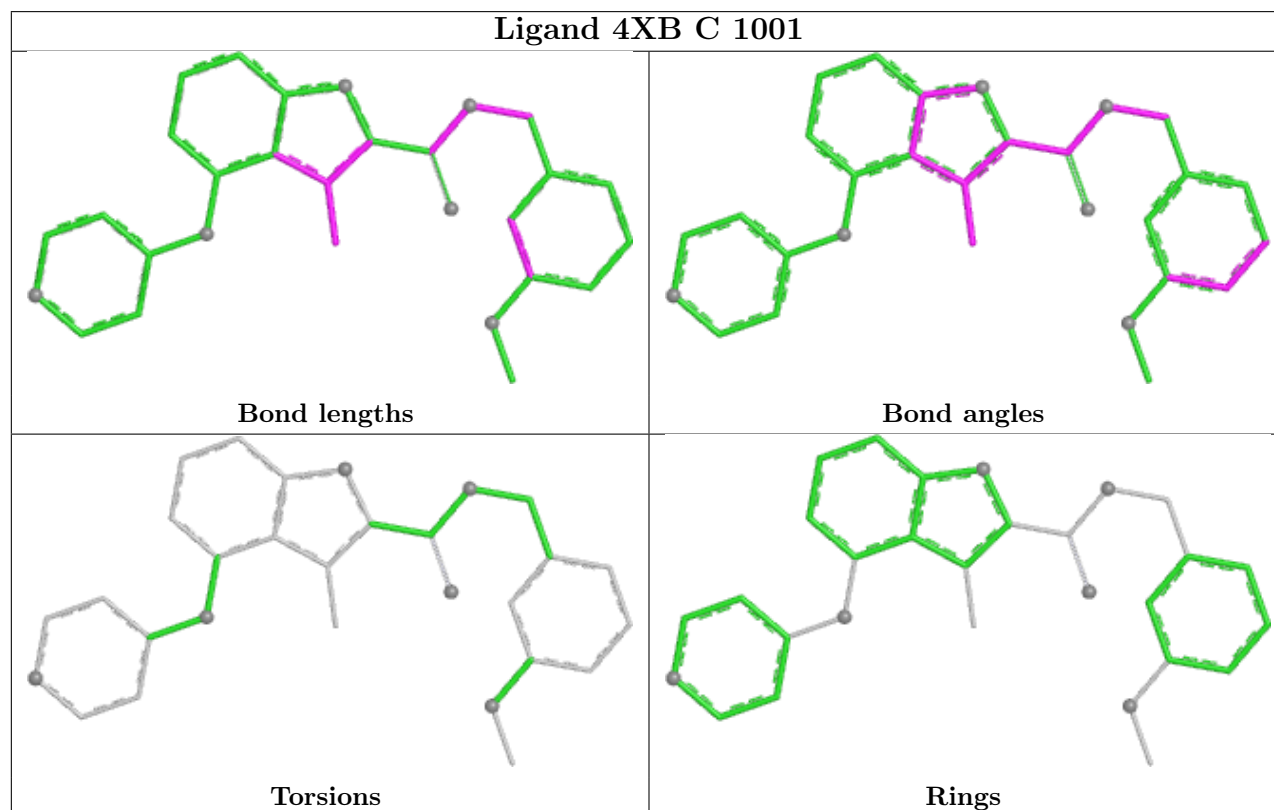
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



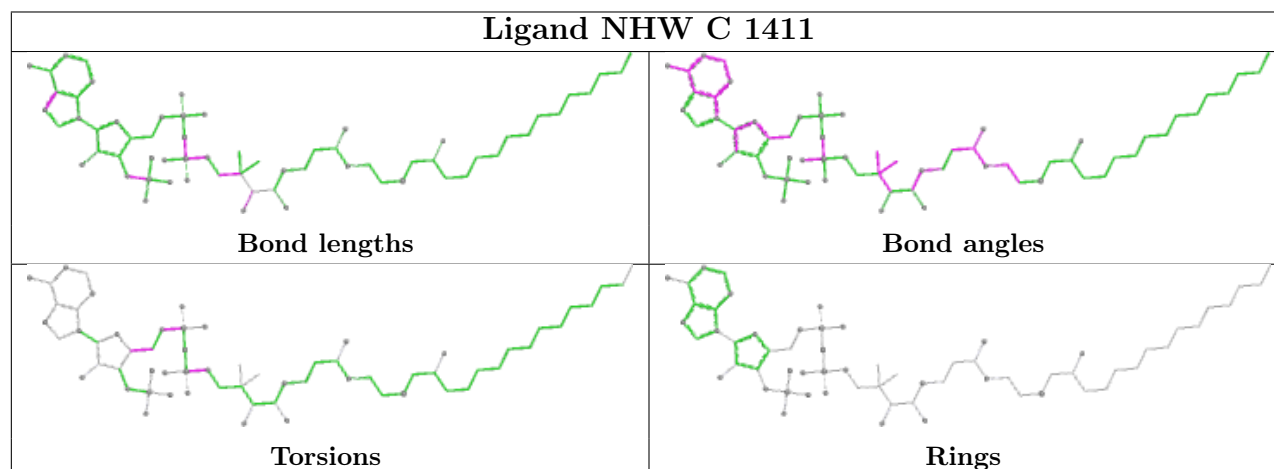
Ligand NHW A 1411

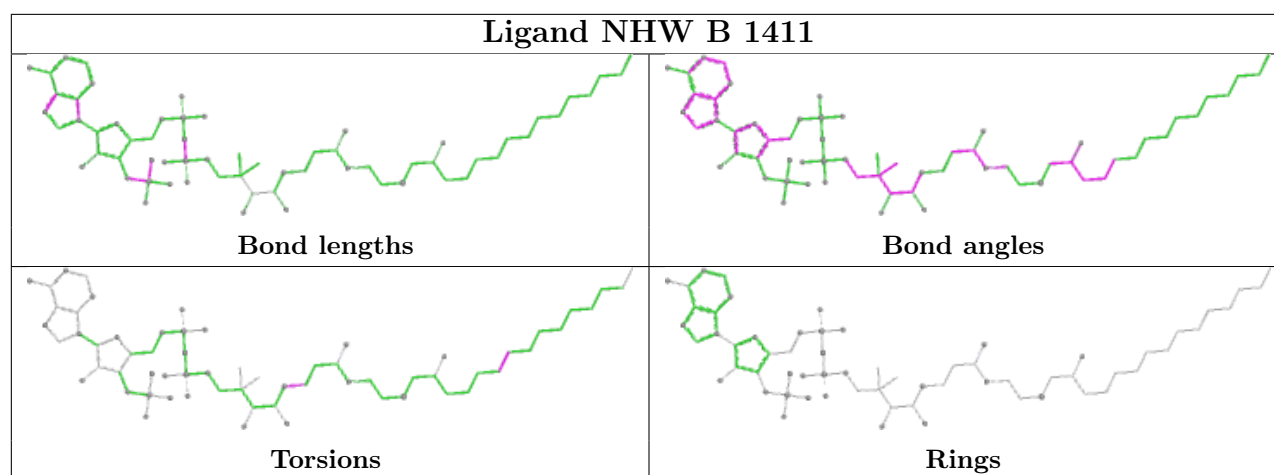


Ligand 4XB C 1001



Ligand NHW C 1411





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	385/385 (100%)	0.26	14 (3%)	46 50	4, 10, 22, 55	30 (7%)
1	B	385/385 (100%)	0.29	12 (3%)	51 55	5, 11, 23, 40	25 (6%)
1	C	367/385 (95%)	0.27	12 (3%)	49 53	4, 11, 21, 32	26 (7%)
All	All	1137/1155 (98%)	0.27	38 (3%)	49 53	4, 11, 22, 55	81 (7%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	LEU	3.9
1	A	26	MET	3.8
1	C	323	GLY	3.8
1	A	32	TYR	3.7
1	B	32	TYR	3.5
1	B	231[A]	SER	3.3
1	A	232	ARG	3.3
1	A	231	SER	3.3
1	B	133	ALA	3.3
1	A	323	GLY	3.2
1	B	131	TYR	3.1
1	C	306	GLY	3.0
1	A	39	ILE	2.9
1	C	325	ASP	2.7
1	C	102	ILE	2.7
1	B	233	LEU	2.6
1	A	27	ASP	2.6
1	A	230	ASN	2.6
1	B	40	ASN	2.6
1	C	224	ILE	2.5
1	B	230[A]	ASN	2.5
1	B	26	MET	2.5
1	A	325	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	306	GLY	2.4
1	C	326	LYS	2.4
1	C	40	ASN	2.4
1	C	322	LEU	2.4
1	B	232	ARG	2.3
1	B	39	ILE	2.3
1	B	45	GLU	2.3
1	C	222	ILE	2.2
1	A	54	ASP	2.2
1	C	226	PHE	2.2
1	C	221	LEU	2.1
1	A	43	PHE	2.1
1	A	233	LEU	2.0
1	B	305	ASN	2.0
1	C	244	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

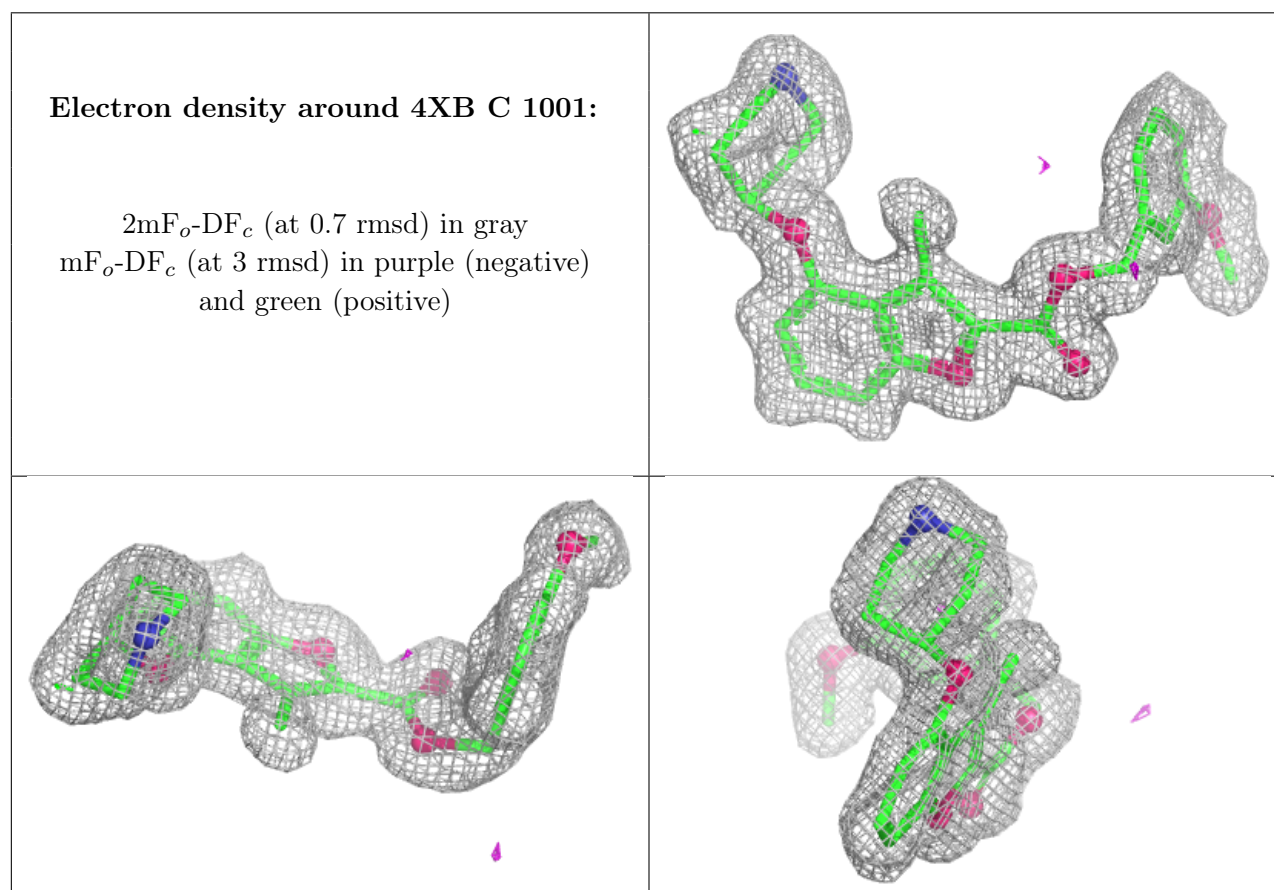
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	C	999	4/4	0.77	0.23	15,16,16,17	4
7	SO4	B	1412	5/5	0.80	0.14	38,41,43,43	0
2	DMS	A	999	4/4	0.89	0.14	11,11,12,12	4
3	4XB	C	1001	29/29	0.93	0.08	10,13,18,19	0
2	DMS	B	999	4/4	0.94	0.15	22,23,26,26	0
3	4XB	B	1001	29/29	0.94	0.07	9,12,14,14	0
3	4XB	A	1001	29/29	0.95	0.06	10,11,13,14	0
4	NHW	C	1411	64/64	0.96	0.06	6,9,13,15	0

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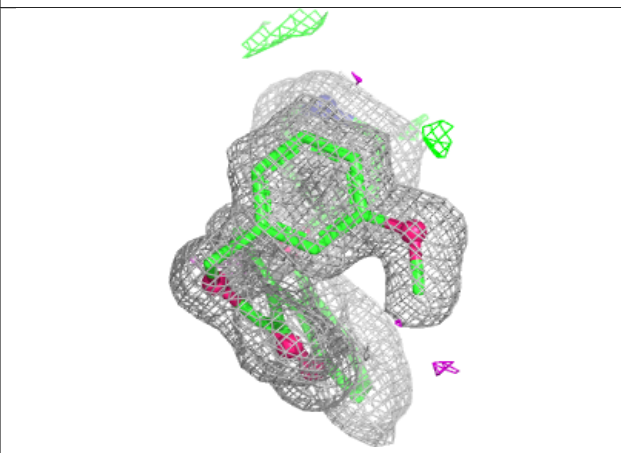
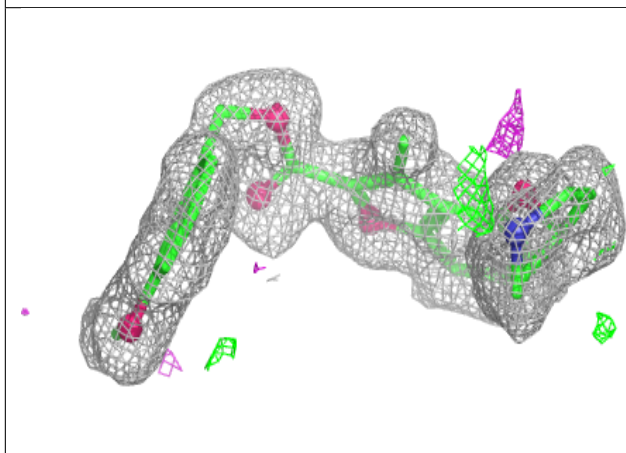
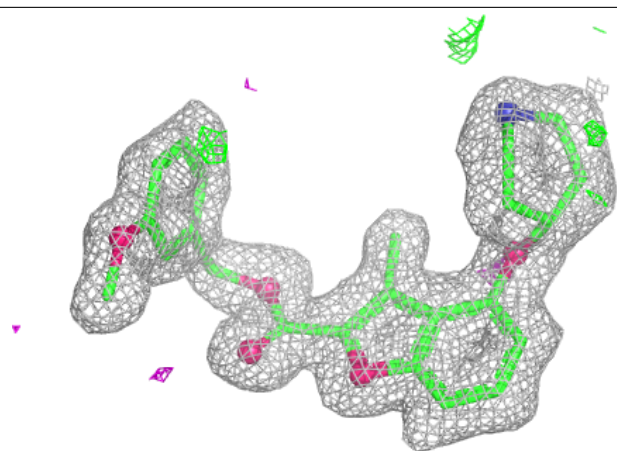
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NHW	A	1411	64/64	0.96	0.06	6,9,12,17	0
6	MG	B	1414	1/1	0.97	0.06	21,21,21,21	0
4	NHW	B	1411	64/64	0.97	0.06	5,9,13,14	0
6	MG	C	1413	1/1	0.98	0.07	18,18,18,18	0
6	MG	A	1413	1/1	0.98	0.09	23,23,23,23	0
5	CL	B	1413	1/1	0.99	0.03	9,9,9,9	0
5	CL	C	1412	1/1	0.99	0.02	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.



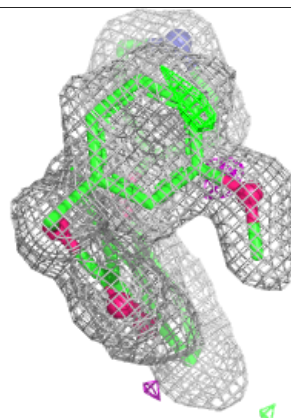
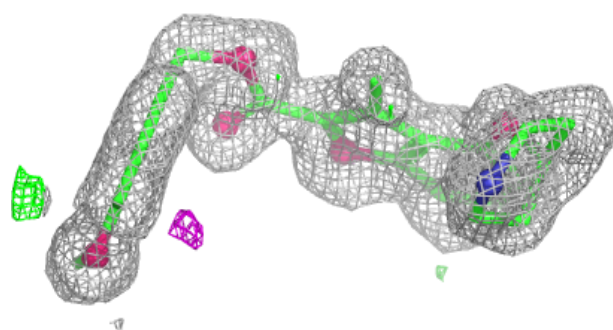
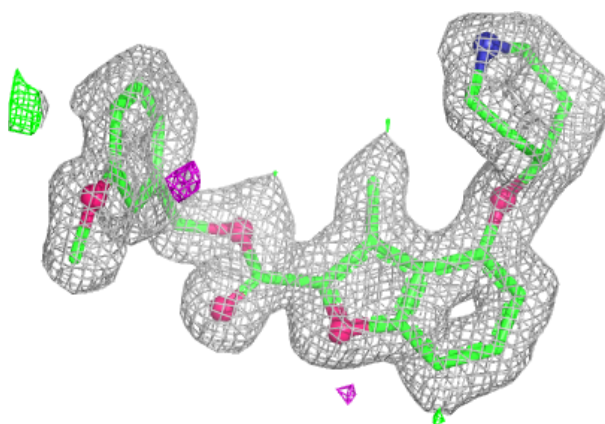
Electron density around 4XB B 1001:

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



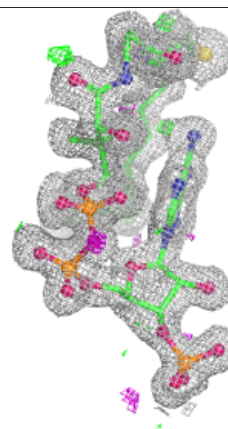
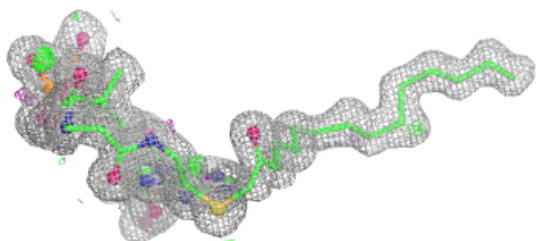
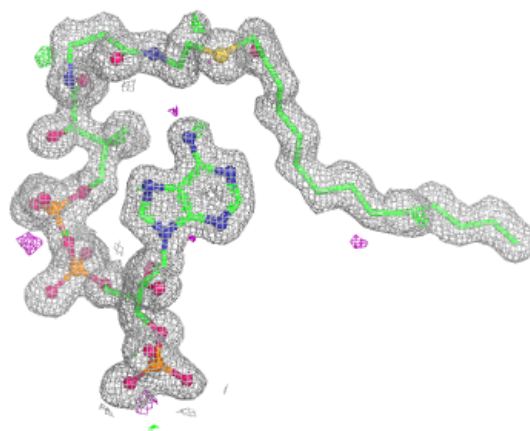
Electron density around 4XB A 1001:

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



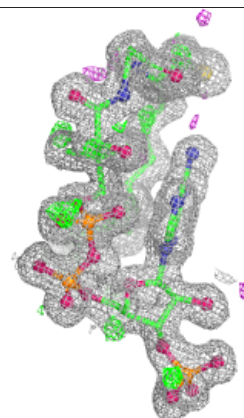
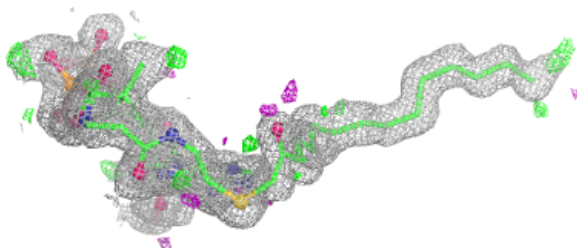
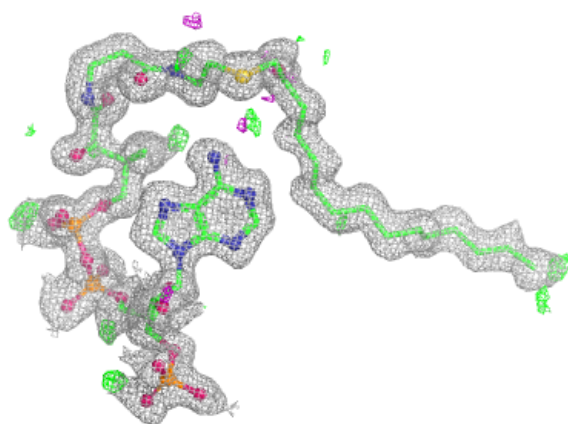
Electron density around NHW C 1411:

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

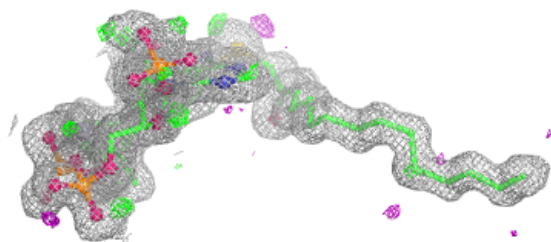
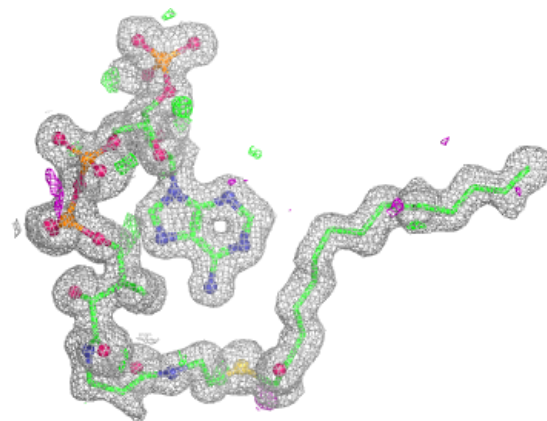


Electron density around NHW A 1411:

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

**Electron density around 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 [i](#)

There are no such residues in this entry.