



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:20 AM UTC

PDB ID : 4UFX / pdb_00004ufx
Title : Plasmodium vivax N-myristoyltransferase in complex with a pyridyl inhibitor (compound 19)
Authors : Yu, Z.; Brannigan, J.A.; Rangachari, K.; Heal, W.P.; Wilkinson, A.J.; Holder, A.A.; Tate, E.W.; Leatherbarrow, R.J.
Deposited on : 2015-03-19
Resolution : 1.49 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

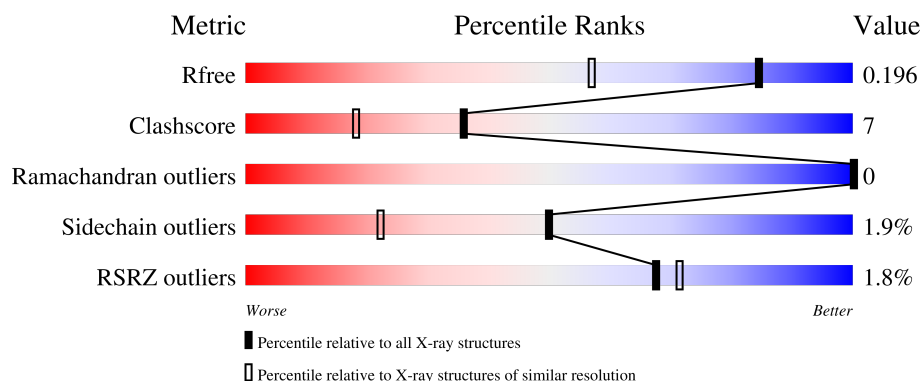
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.49 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	85% 14% .
1	B	385	87% 11% .
1	C	385	81% 13% ..

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
6	CL	A	1415	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11935 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.

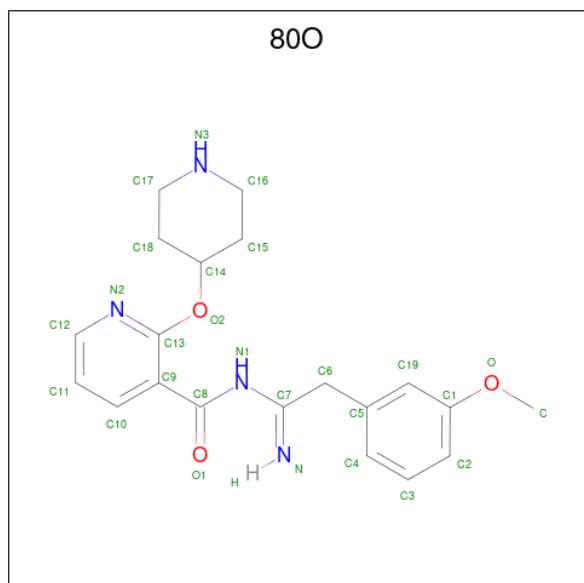
- Molecule 1 is a protein called GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	29	0
			3335	2185	536	601	13			
1	B	385	Total	C	N	O	S	0	42	0
			3413	2241	543	616	13			
1	C	372	Total	C	N	O	S	0	41	0
			3308	2187	518	591	12			

There are 3 discrepancies between the modelled and reference sequences:

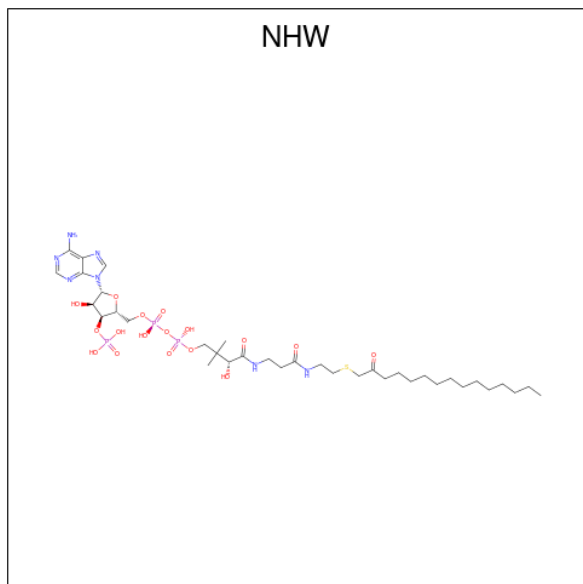
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	expression tag	UNP A5K1A2
B	26	MET	-	expression tag	UNP A5K1A2
C	26	MET	-	expression tag	UNP A5K1A2

- Molecule 2 is N-[2-(3-methoxyphenyl)ethanimidoyl]-2-piperidin-4-yloxy-pyridine-3-carboxamide (CCD ID: 800) (formula: C₂₀H₂₄N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	20	4	3		
2	B	1	Total	C	N	O	0	0
			27	20	4	3		
2	C	1	Total	C	N	O	0	0
			27	20	4	3		

- Molecule 3 is 2-oxopentadecyl-CoA (CCD ID: NHW) (formula: $C_{36}H_{64}N_7O_{17}P_3S$).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Cl	0	0
			3	3		
6	B	2	Total	Cl	0	0
			2	2		
6	C	1	Total	Cl	0	0
			1	1		

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

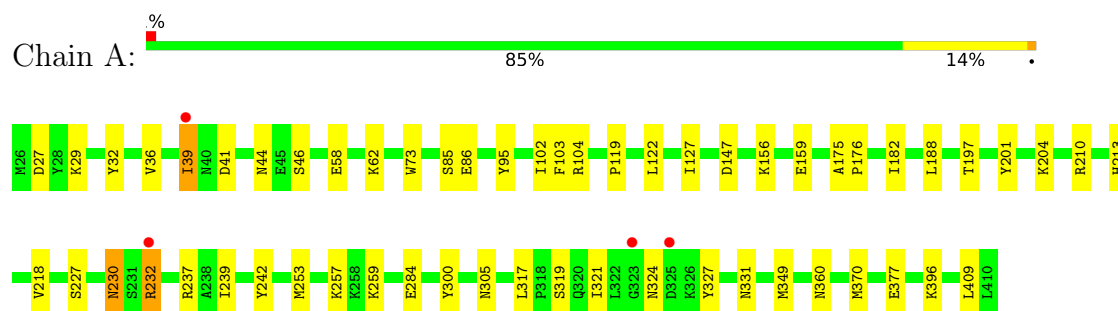
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	583	Total	O	0	0
			583	583		
8	B	466	Total	O	0	0
			466	466		
8	C	518	Total	O	0	0
			518	518		

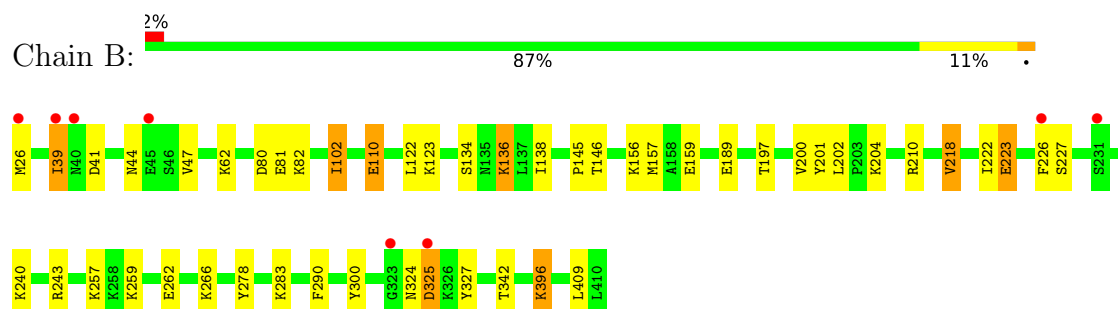
3 Residue-property plots [i](#)

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.

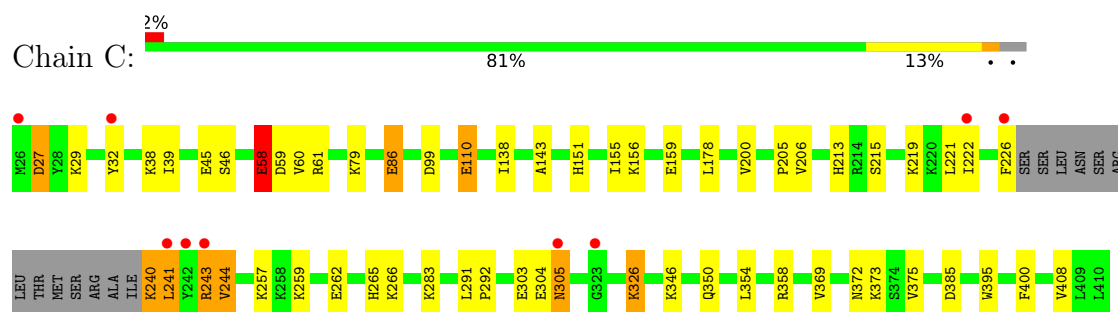
• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



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• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.33Å 118.89Å 174.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.32 – 1.49 98.32 – 1.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (98.32-1.49) 99.8 (98.32-1.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.49Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.158 , 0.197 0.158 , 0.196	Depositor DCC
R_{free} test set	9861 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	10.3	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11935	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 80O, DMS, CL, NHW, MG

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	1.40	8/3500 (0.2%)	1.25	3/4734 (0.1%)
1	B	1.37	9/3620 (0.2%)	1.17	8/4888 (0.2%)
1	C	1.37	10/3513 (0.3%)	1.23	10/4746 (0.2%)
All	All	1.38	27/10633 (0.3%)	1.22	21/14368 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	LEU	N-CA	9.86	1.52	1.46
1	B	396[A]	LYS	CA-C	8.27	1.62	1.52
1	B	396[B]	LYS	CA-C	8.27	1.62	1.52
1	C	408	VAL	C-O	6.18	1.31	1.24
1	C	60	VAL	CA-CB	5.92	1.60	1.54
1	A	95	TYR	C-O	5.70	1.29	1.23
1	A	370	MET	C-O	5.66	1.29	1.24
1	B	200	VAL	N-CA	5.62	1.52	1.46
1	B	342	THR	N-CA	5.51	1.53	1.46
1	C	155	ILE	C-O	5.45	1.29	1.24
1	A	36	VAL	C-O	5.43	1.28	1.24
1	C	46	SER	CA-C	5.38	1.60	1.52
1	B	189	GLU	N-CA	5.34	1.52	1.46
1	C	61	ARG	C-O	5.34	1.30	1.23
1	A	349	MET	N-CA	5.29	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	ARG	N-CA	5.28	1.52	1.46
1	A	122	LEU	N-CA	5.24	1.52	1.46
1	A	73	TRP	C-O	5.24	1.30	1.23
1	B	300	TYR	CA-C	-5.19	1.46	1.52
1	B	278	TYR	N-CA	5.14	1.52	1.46
1	B	122	LEU	N-CA	5.13	1.52	1.46
1	A	319	SER	N-CA	5.11	1.52	1.46
1	C	79	LYS	N-CA	5.11	1.52	1.46
1	C	292	PRO	C-O	5.10	1.29	1.23
1	C	205	PRO	N-CA	5.05	1.53	1.47
1	C	303	GLU	C-O	5.04	1.30	1.24
1	C	395	TRP	N-CA	5.01	1.52	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	ASN	CB-CA-C	-7.66	101.02	111.89
1	C	241	LEU	N-CA-C	-6.85	104.40	112.89
1	B	102	ILE	CB-CA-C	-6.56	100.53	111.29
1	C	58	GLU	CB-CG-CD	6.53	123.71	112.60
1	B	325	ASP	N-CA-C	6.16	118.07	111.36
1	B	226	PHE	N-CA-C	-6.09	104.76	111.82
1	C	372	ASN	N-CA-C	5.75	118.32	111.71
1	C	305	ASN	N-CA-C	5.74	119.31	111.39
1	C	27	ASP	N-CA-C	-5.57	101.50	110.14
1	A	305	ASN	CB-CA-C	-5.56	102.93	111.66
1	B	102	ILE	CA-CB-CG1	5.49	119.74	110.40
1	C	86	GLU	CA-CB-CG	-5.28	103.54	114.10
1	B	324	ASN	N-CA-C	-5.26	100.60	109.07
1	C	244	VAL	CG1-CB-CG2	5.26	122.37	110.80
1	B	218	VAL	N-CA-CB	-5.24	103.87	110.57
1	A	317	LEU	O-C-N	5.21	125.44	121.27
1	A	230	ASN	N-CA-C	5.19	114.98	108.45
1	C	350	GLN	N-CA-C	-5.17	105.72	111.36
1	B	290	PHE	CA-C-N	-5.06	113.89	120.67
1	B	290	PHE	C-N-CA	-5.06	113.89	120.67
1	C	369	VAL	O-C-N	5.01	127.35	122.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	240	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3335	0	3419	45	0
1	B	3413	0	3539	55	0
1	C	3308	0	3428	49	2
2	A	27	0	23	1	0
2	B	27	0	23	1	0
2	C	27	0	23	1	0
3	A	64	0	60	0	0
3	B	64	0	60	0	0
3	C	64	0	59	0	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	3	0	0	2	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
7	A	8	0	12	2	0
7	B	8	0	12	0	0
7	C	4	0	6	1	0
8	A	583	0	0	9	1
8	B	466	0	0	15	0
8	C	518	0	0	10	1
All	All	11935	0	10664	153	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (153) 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:257[A]:LYS:HD2	1:B:259[A]:LYS:NZ	1.59	1.17
1:B:257[B]:LYS:HD2	8:B:2340:HOH:O	1.42	1.17
1:B:243[B]:ARG:NH2	8:B:2308:HOH:O	1.76	1.17
1:C:151[B]:HIS:HE1	8:C:2043:HOH:O	1.38	1.06
1:A:232:ARG:O	1:A:237[B]:ARG:NH1	1.92	1.03
1:B:39:ILE:HD11	1:B:201:TYR:HE1	1.20	1.02
1:C:200[A]:VAL:CG2	8:C:2311:HOH:O	2.13	0.97
1:B:159[A]:GLU:CD	1:B:409[A]:LEU:HD22	1.92	0.95
1:B:62[B]:LYS:HG3	8:B:2067:HOH:O	1.67	0.94
1:B:39:ILE:HD11	1:B:201:TYR:CE1	2.03	0.92
1:B:156[A]:LYS:NZ	1:B:157:MET:O	2.04	0.89
1:B:257[A]:LYS:HD2	1:B:259[A]:LYS:HZ3	1.28	0.89
1:C:262[B]:GLU:HG3	1:C:283[B]:LYS:HE3	1.55	0.88
1:B:257[A]:LYS:HE3	8:B:2338:HOH:O	1.75	0.87
1:B:257[A]:LYS:CD	1:B:259[A]:LYS:NZ	2.39	0.85
1:A:44:ASN:HD22	1:A:46:SER:H	1.25	0.84
1:B:44[B]:ASN:ND2	1:B:44[B]:ASN:H	1.75	0.83
1:A:257:LYS:HE2	1:A:259[A]:LYS:NZ	1.93	0.83
1:C:346[B]:LYS:HG2	1:C:375:VAL:HG12	1.68	0.76
1:A:39:ILE:HD11	1:A:201:TYR:HE1	1.52	0.74
1:B:159[A]:GLU:CD	1:B:409[A]:LEU:CD2	2.60	0.74
1:C:151[B]:HIS:CE1	8:C:2043:HOH:O	2.23	0.74
2:C:1000:80O:N	2:C:1000:80O:O1	2.16	0.73
1:B:82[B]:LYS:HE3	8:B:2117:HOH:O	1.90	0.71
1:B:145:PRO:HB2	1:B:156[A]:LYS:HE2	1.74	0.70
1:A:159:GLU:CD	1:A:409[A]:LEU:HD22	2.17	0.70
1:B:257[A]:LYS:HD2	1:B:259[A]:LYS:HZ1	1.53	0.70
1:A:39:ILE:HD11	1:A:201:TYR:CE1	2.26	0.70
1:A:147[A]:ASP:OD2	8:A:2281:HOH:O	2.10	0.69
1:B:39:ILE:CD1	1:B:201:TYR:HE1	2.01	0.69
1:A:85[A]:SER:OG	8:A:2163:HOH:O	2.12	0.67
1:C:257:LYS:HE3	1:C:259[B]:LYS:NZ	2.11	0.66
1:B:44[B]:ASN:H	1:B:44[B]:ASN:HD22	1.43	0.65
1:A:44:ASN:ND2	1:A:46:SER:H	1.94	0.65
1:C:326[B]:LYS:CE	8:C:2447:HOH:O	2.44	0.65
2:A:1000:80O:O1	2:A:1000:80O:N	2.23	0.64
1:A:230:ASN:OD1	1:A:232:ARG:HB2	1.98	0.64
1:B:243[B]:ARG:HD3	8:B:2314:HOH:O	1.97	0.63
1:A:119:PRO:CG	1:A:284[B]:GLU:HG2	2.29	0.63
1:B:123[C]:LYS:HB3	8:B:2105:HOH:O	1.99	0.63
1:B:41:ASP:O	1:B:204[B]:LYS:HE3	1.99	0.63
1:A:259[B]:LYS:HB2	1:A:259[B]:LYS:HZ3	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASP:HB3	1:A:29:LYS:HE3	1.82	0.62
1:B:159[A]:GLU:OE1	1:B:409[A]:LEU:CD2	2.48	0.61
1:A:58[B]:GLU:HG3	8:A:2079:HOH:O	1.99	0.61
1:B:145:PRO:HB2	1:B:156[A]:LYS:CE	2.31	0.61
1:C:354[B]:LEU:HD21	1:C:358:ARG:NE	2.16	0.61
1:C:206[B]:VAL:HG22	1:C:400:PHE:CE1	2.36	0.60
2:B:1000:80O:N	2:B:1000:80O:O1	2.26	0.60
1:A:127:ILE:CD1	1:A:182[B]:ILE:HD13	2.32	0.60
1:B:110[B]:GLU:HG3	8:B:2176:HOH:O	2.02	0.59
1:A:218[A]:VAL:HG21	1:A:239:ILE:HA	1.83	0.59
1:A:86:GLU:OE2	8:A:2173:HOH:O	2.17	0.59
1:B:240[A]:LYS:HG3	1:B:243[A]:ARG:NH2	2.18	0.59
1:B:134:SER:OG	1:B:136[B]:LYS:HB3	2.03	0.58
1:C:156[B]:LYS:HE2	8:C:2168:HOH:O	2.03	0.58
1:B:262[A]:GLU:HG3	1:B:283[A]:LYS:HZ1	1.69	0.57
1:B:240[A]:LYS:HG3	1:B:243[A]:ARG:HH21	1.70	0.56
1:C:32[A]:TYR:OH	1:C:39:ILE:HG22	2.05	0.56
1:A:58[A]:GLU:HG2	8:A:2041:HOH:O	2.05	0.56
1:A:284[B]:GLU:HG3	8:A:2465:HOH:O	2.05	0.56
1:C:262[B]:GLU:CG	1:C:283[B]:LYS:HE3	2.31	0.55
1:C:326[B]:LYS:HE2	1:C:326[B]:LYS:CA	2.37	0.55
1:C:222:ILE:HB	8:C:2333:HOH:O	2.07	0.54
1:B:82[B]:LYS:CD	8:B:2117:HOH:O	2.54	0.54
1:B:257[A]:LYS:CD	1:B:259[A]:LYS:HZ1	2.17	0.54
1:B:82[B]:LYS:HD2	8:B:2117:HOH:O	2.09	0.53
1:B:80:ASP:OD2	1:B:82[B]:LYS:HD2	2.07	0.53
1:B:197:THR:HG23	1:B:409[B]:LEU:HD22	1.91	0.53
1:B:262[B]:GLU:HG3	8:B:2343:HOH:O	2.10	0.52
1:C:110[A]:GLU:HG3	8:C:2211:HOH:O	2.09	0.52
1:B:146:THR:H	1:B:156[A]:LYS:HZ3	1.58	0.52
1:C:346[B]:LYS:CG	1:C:375:VAL:HG12	2.38	0.51
1:A:257:LYS:HE2	1:A:259[A]:LYS:HZ3	1.72	0.51
1:C:326[B]:LYS:HE2	1:C:326[B]:LYS:HA	1.93	0.51
1:A:218[A]:VAL:HG11	1:A:242:TYR:HD2	1.76	0.50
1:B:257[B]:LYS:CD	8:B:2340:HOH:O	2.24	0.50
1:A:218[A]:VAL:HG22	8:A:2371:HOH:O	2.11	0.50
1:B:223[A]:GLU:HG2	1:B:327:TYR:HE2	1.76	0.50
1:B:262[A]:GLU:HG2	1:B:266[A]:LYS:HE3	1.93	0.50
1:B:39:ILE:O	1:B:204[A]:LYS:NZ	2.43	0.49
1:A:360[A]:ASN:ND2	8:A:2377:HOH:O	2.45	0.49
1:A:218[A]:VAL:CG2	1:A:239:ILE:HG12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:GLU:OE2	1:C:151[A]:HIS:HE1	1.96	0.49
1:A:227:SER:O	6:A:1415:CL:CL	2.68	0.49
1:C:32[A]:TYR:CE2	1:C:38:LYS:HD2	2.48	0.48
1:B:82[B]:LYS:CE	8:B:2117:HOH:O	2.54	0.48
1:B:145:PRO:CA	1:B:156[A]:LYS:HZ1	2.26	0.48
1:A:331[A]:ASN:HB3	7:A:1417:DMS:H13	1.95	0.48
1:A:213:HIS:HD2	8:A:2191:HOH:O	1.96	0.47
1:B:159[A]:GLU:OE1	1:B:409[A]:LEU:HD21	2.15	0.47
1:C:110[B]:GLU:H	1:C:110[B]:GLU:CD	2.23	0.47
1:C:304:GLU:O	1:C:305:ASN:HB2	2.13	0.47
1:A:32:TYR:OH	1:A:39:ILE:HB	2.15	0.47
1:B:47:VAL:HG11	1:B:396[A]:LYS:HD2	1.97	0.47
1:A:257:LYS:HE2	1:A:259[B]:LYS:HD3	1.96	0.46
1:C:200[A]:VAL:HG23	8:C:2311:HOH:O	1.99	0.46
1:A:127:ILE:HD11	1:A:182[B]:ILE:CD1	2.45	0.46
1:A:218[A]:VAL:HG23	1:A:239:ILE:HG12	1.98	0.46
1:B:145:PRO:HA	1:B:156[A]:LYS:HZ1	1.79	0.46
1:B:222[A]:ILE:HD13	1:B:227:SER:HB2	1.97	0.46
1:B:218:VAL:O	1:B:222[A]:ILE:HG12	2.15	0.46
1:C:265:HIS:CE1	1:C:283[A]:LYS:HG2	2.50	0.46
1:A:331[B]:ASN:HB3	7:A:1417:DMS:H13	1.98	0.46
1:A:62[B]:LYS:HE3	1:A:188:LEU:CD2	2.46	0.46
1:A:218[A]:VAL:HG11	1:A:242:TYR:CD2	2.51	0.46
1:C:45:GLU:OE2	1:C:151[A]:HIS:CE1	2.69	0.45
1:B:102:ILE:HG22	8:B:2161:HOH:O	2.17	0.45
1:B:146:THR:HG22	1:B:159[B]:GLU:HG3	1.97	0.45
1:A:41:ASP:O	1:A:204[B]:LYS:HE3	2.17	0.45
1:A:197:THR:HG23	1:A:409[A]:LEU:HD12	1.99	0.45
1:A:324:ASN:HB3	1:A:327:TYR:O	2.17	0.45
1:B:102:ILE:HD13	1:B:102:ILE:HG21	1.78	0.45
1:C:159[B]:GLU:OE2	7:C:1413:DMS:O	2.35	0.44
1:B:110[A]:GLU:HG3	8:B:2175:HOH:O	2.17	0.44
1:A:253[A]:MET:HG3	1:A:300:TYR:HB3	2.00	0.44
1:C:138:ILE:HD12	1:C:138:ILE:C	2.42	0.44
1:A:159:GLU:OE2	1:A:409[A]:LEU:HD22	2.17	0.44
1:C:86:GLU:OE1	8:C:2171:HOH:O	2.21	0.43
1:A:127:ILE:HD11	1:A:182[B]:ILE:HD13	2.00	0.43
1:C:240:LYS:CB	1:C:243:ARG:HB2	2.48	0.43
1:B:197:THR:HG23	1:B:409[A]:LEU:HD12	2.00	0.43
1:C:257:LYS:HE3	1:C:259[B]:LYS:CE	2.49	0.43
1:C:291:LEU:HD23	1:C:291:LEU:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:HD3	4:A:1411:SO4:O1	2.18	0.43
1:C:265:HIS:ND1	1:C:283[A]:LYS:HG2	2.34	0.43
1:B:262[A]:GLU:HG3	1:B:283[A]:LYS:NZ	2.34	0.43
1:C:262[A]:GLU:HA	1:C:283[A]:LYS:HZ2	1.83	0.43
1:C:58:GLU:HG2	1:C:59:ASP:N	2.31	0.43
1:C:326[B]:LYS:HE3	8:C:2447:HOH:O	2.13	0.43
1:C:213:HIS:CG	1:C:226:PHE:HE1	2.37	0.42
1:C:27:ASP:HB3	1:C:29:LYS:HE2	2.01	0.42
1:C:215:SER:HB3	1:C:221:LEU:HD12	2.01	0.42
1:B:146:THR:CG2	1:B:159[B]:GLU:HG3	2.50	0.42
1:C:257:LYS:HE3	1:C:259[B]:LYS:HZ1	1.81	0.42
1:C:262[A]:GLU:HG2	1:C:266[A]:LYS:HE2	2.02	0.42
1:A:159:GLU:CD	1:A:409[A]:LEU:CD2	2.89	0.41
1:A:175:ALA:HB3	1:A:176:PRO:HD3	2.02	0.41
1:A:321:ILE:HG22	1:A:324:ASN:HB2	2.02	0.41
1:A:102[B]:ILE:HG13	1:A:103:PHE:CE2	2.55	0.41
1:B:210:ARG:HD3	4:B:1411:SO4:O3	2.21	0.41
1:C:346[B]:LYS:HG2	1:C:375:VAL:CG1	2.46	0.41
1:B:138:ILE:HD12	1:B:138:ILE:C	2.46	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373[A]:LYS:NZ	8:A:2159:HOH:O[4_456]	1.64	0.56
1:C:110[B]:GLU:OE1	8:C:2240:HOH:O[4_446]	2.02	0.18

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	412/385 (107%)	402 (98%)	10 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	425/385 (110%)	416 (98%)	9 (2%)	0	100	100
1	C	409/385 (106%)	400 (98%)	9 (2%)	0	100	100
All	All	1246/1155 (108%)	1218 (98%)	28 (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	379/351 (108%)	373 (98%)	6 (2%)	55	28
1	B	393/351 (112%)	383 (98%)	10 (2%)	42	14
1	C	379/351 (108%)	368 (97%)	11 (3%)	37	10
All	All	1151/1053 (109%)	1124 (98%)	27 (2%)	50	16

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

Mol	Chain	Res	Type
1	A	39	ILE
1	A	156[A]	LYS
1	A	156[B]	LYS
1	A	232	ARG
1	A	377	GLU
1	A	396	LYS
1	B	26	MET
1	B	39	ILE
1	B	81	GLU
1	B	110[A]	GLU
1	B	110[B]	GLU
1	B	136[A]	LYS
1	B	136[B]	LYS
1	B	223[A]	GLU
1	B	223[B]	GLU
1	B	325	ASP

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Mol	Chain	Res	Type
1	C	58	GLU
1	C	99	ASP
1	C	110[A]	GLU
1	C	110[B]	GLU
1	C	219[A]	LYS
1	C	219[B]	LYS
1	C	241	LEU
1	C	243	ARG
1	C	244	VAL
1	C	326[A]	LYS
1	C	326[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	44	ASN
1	A	101	ASN
1	A	187	ASN
1	A	213	HIS
1	A	249	ASN
1	A	302	ASN
1	A	305	ASN
1	A	350	GLN
1	A	359	ASN
1	A	372	ASN
1	B	34	GLN
1	B	187	ASN
1	B	249	ASN
1	B	331	ASN
1	B	350	GLN
1	B	359	ASN
1	B	360	ASN
1	B	371	GLN
1	C	34	GLN
1	C	55	ASN
1	C	249	ASN
1	C	302	ASN
1	C	350	GLN
1	C	359	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 9 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NHW	B	1001	5	64,66,66	1.56	9 (14%)	87,92,92	1.44	12 (13%)
2	80O	A	1000	-	29,29,29	1.33	3 (10%)	29,38,38	1.28	5 (17%)
7	DMS	A	1416	-	3,3,3	0.91	0	3,3,3	2.15	2 (66%)
7	DMS	B	1416	-	3,3,3	0.84	0	3,3,3	1.87	1 (33%)
3	NHW	C	1001	5	64,66,66	1.70	11 (17%)	87,92,92	1.64	18 (20%)
4	SO4	B	1411	-	4,4,4	0.23	0	6,6,6	1.14	0
7	DMS	A	1417	-	3,3,3	0.74	0	3,3,3	1.87	2 (66%)
3	NHW	A	1001	5	64,66,66	1.35	11 (17%)	87,92,92	1.72	16 (18%)
4	SO4	A	1411	-	4,4,4	0.53	0	6,6,6	0.90	0
7	DMS	C	1413	-	3,3,3	0.58	0	3,3,3	0.92	0
2	80O	C	1000	-	29,29,29	2.23	7 (24%)	29,38,38	1.45	3 (10%)
2	80O	B	1000	-	29,29,29	1.60	6 (20%)	29,38,38	1.27	4 (13%)
7	DMS	B	1415	-	3,3,3	0.57	0	3,3,3	1.26	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
3	NHW	B	1001	5	-	1/65/81/81	0/3/3/3
2	80O	A	1000	-	-	3/16/26/26	0/3/3/3
3	NHW	C	1001	5	-	1/65/81/81	0/3/3/3
3	NHW	A	1001	5	-	1/65/81/81	0/3/3/3
2	80O	C	1000	-	-	2/16/26/26	0/3/3/3
2	80O	B	1000	-	-	2/16/26/26	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	NHW	P1A-O3A	9.07	1.69	1.59
2	C	1000	80O	C6-C7	9.07	1.57	1.51
3	B	1001	NHW	C13-C11	4.22	1.62	1.53
3	A	1001	NHW	O4X-C1X	4.00	1.51	1.42
3	B	1001	NHW	P3X-O3X	3.52	1.65	1.59
3	B	1001	NHW	C8A-N7A	3.39	1.38	1.31
2	B	1000	80O	C6-C7	3.39	1.53	1.51
3	B	1001	NHW	C4A-N9A	-3.36	1.30	1.37
2	C	1000	80O	C6-C5	3.34	1.57	1.51
2	A	1000	80O	C2-C1	3.28	1.44	1.38
2	B	1000	80O	C9-C13	-3.18	1.35	1.40
2	A	1000	80O	C6-C7	3.13	1.53	1.51
3	C	1001	NHW	O10-C10	-3.12	1.36	1.42
3	A	1001	NHW	P1A-O3A	3.11	1.62	1.59
2	B	1000	80O	C8-N1	-3.09	1.32	1.37
2	C	1000	80O	C8-N1	-2.94	1.32	1.37
3	B	1001	NHW	P2A-O3A	2.91	1.62	1.59
3	A	1001	NHW	P3X-O3X	2.91	1.64	1.59
3	B	1001	NHW	O4X-C4X	2.89	1.51	1.45
3	C	1001	NHW	P3X-O3X	2.81	1.64	1.59
3	A	1001	NHW	C4A-N9A	-2.78	1.31	1.37
2	B	1000	80O	C6-C5	2.75	1.56	1.51
3	C	1001	NHW	C8A-N7A	2.72	1.36	1.31
2	B	1000	80O	C7-N	2.62	1.33	1.27
2	C	1000	80O	C3-C4	2.61	1.43	1.38
3	A	1001	NHW	P2A-O4A	-2.60	1.43	1.55
3	B	1001	NHW	C6-C5	2.58	1.56	1.51
2	B	1000	80O	C17-N3	2.51	1.56	1.47
2	C	1000	80O	C19-C1	2.48	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	NHW	O4X-C1X	2.44	1.47	1.42
3	A	1001	NHW	C6-C5	2.34	1.56	1.51
3	A	1001	NHW	C12-C11	2.33	1.56	1.52
3	B	1001	NHW	C7-C6	2.33	1.59	1.51
2	A	1000	80O	O-C1	2.33	1.42	1.37
3	A	1001	NHW	P2A-O3A	2.32	1.62	1.59
3	B	1001	NHW	C5A-C4A	2.20	1.43	1.39
3	A	1001	NHW	C13-C11	2.20	1.58	1.53
2	C	1000	80O	C2-C1	2.18	1.42	1.38
3	C	1001	NHW	O1M-C1M	2.16	1.25	1.21
3	A	1001	NHW	CP-S1	2.15	1.87	1.81
3	C	1001	NHW	P2A-O3A	-2.12	1.57	1.59
3	C	1001	NHW	O5X-C5X	2.10	1.52	1.44
3	C	1001	NHW	C7-C6	2.08	1.58	1.51
2	C	1000	80O	C7-N	2.07	1.31	1.27
3	C	1001	NHW	O6A-C12	2.03	1.50	1.43
3	C	1001	NHW	CAM-C9M	2.03	1.61	1.51
3	A	1001	NHW	P1A-O2A	-2.02	1.46	1.55

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	NHW	N3A-C2A-N1A	-6.16	119.26	128.58
3	A	1001	NHW	C4A-C5A-N7A	-6.06	103.65	110.58
3	A	1001	NHW	C5A-C4A-N3A	-4.93	119.93	126.72
3	A	1001	NHW	C6A-C5A-C4A	4.79	123.71	117.18
3	C	1001	NHW	C4A-N9A-C8A	4.74	110.72	105.74
3	A	1001	NHW	C5A-C4A-N9A	4.61	110.84	105.81
3	C	1001	NHW	C5A-C4A-N3A	-3.91	121.33	126.72
3	C	1001	NHW	N3A-C4A-N9A	3.60	133.29	127.17
3	C	1001	NHW	N3A-C2A-N1A	-3.59	123.15	128.58
3	C	1001	NHW	C6-C5-N4	-3.56	109.86	116.34
3	A	1001	NHW	C5A-N7A-C8A	3.55	109.02	103.45
3	B	1001	NHW	C2A-N1A-C6A	3.43	124.36	118.73
3	B	1001	NHW	O6A-C12-C11	-3.36	105.15	110.55
3	B	1001	NHW	P3X-O3X-C3X	-3.29	114.65	123.43
3	A	1001	NHW	N9A-C8A-N7A	-3.27	109.30	113.94
3	A	1001	NHW	C6-C5-N4	-3.25	110.42	116.34
3	C	1001	NHW	N9A-C8A-N7A	-3.18	109.42	113.94
3	C	1001	NHW	P3X-O3X-C3X	-3.16	114.99	123.43
2	C	1000	80O	C9-C8-N1	3.06	121.15	115.39
3	C	1001	NHW	O5-C5-C6	3.05	127.55	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1001	NHW	C2-C3-N4	-3.03	106.08	112.41
2	B	1000	80O	C11-C12-N2	-3.02	118.63	123.42
2	C	1000	80O	C6-C5-C4	-2.99	116.49	120.89
3	A	1001	NHW	C5X-C4X-C3X	-2.98	104.46	114.38
3	C	1001	NHW	O1M-C1M-CP	-2.95	117.96	122.17
3	A	1001	NHW	O3A-P2A-O5A	-2.91	101.95	110.70
3	B	1001	NHW	C5A-C4A-N3A	-2.90	122.72	126.72
3	C	1001	NHW	O4X-C1X-C2X	-2.88	100.45	106.62
7	A	1416	DMS	C2-S-C1	2.87	113.13	98.42
3	B	1001	NHW	C7-C6-C5	2.82	117.09	112.39
3	C	1001	NHW	O3A-P2A-O5A	-2.76	102.39	110.70
3	C	1001	NHW	C2A-N3A-C4A	2.72	118.48	111.83
3	A	1001	NHW	P3X-O3X-C3X	-2.63	116.39	123.43
3	A	1001	NHW	C2-C3-N4	-2.62	106.94	112.41
3	B	1001	NHW	C7-N8-C9	-2.61	117.86	122.55
3	A	1001	NHW	O4X-C1X-C2X	-2.58	101.09	106.62
3	B	1001	NHW	C2A-N3A-C4A	2.56	118.07	111.83
3	B	1001	NHW	N9A-C8A-N7A	-2.55	110.31	113.94
2	B	1000	80O	C1-C19-C5	-2.53	117.00	119.76
2	A	1000	80O	C16-N3-C17	2.49	117.44	110.40
3	B	1001	NHW	O2A-P1A-O3A	2.48	113.98	107.27
7	B	1416	DMS	O-S-C1	2.48	118.90	106.49
3	B	1001	NHW	C4A-N9A-C8A	2.46	108.32	105.74
7	A	1417	DMS	C2-S-C1	2.44	110.91	98.42
3	A	1001	NHW	O1M-C1M-CP	-2.41	118.73	122.17
2	C	1000	80O	C12-N2-C13	2.40	123.56	116.28
7	A	1416	DMS	O-S-C1	-2.28	95.06	106.49
3	A	1001	NHW	C13-C11-C10	2.25	112.60	108.77
3	C	1001	NHW	O6A-C12-C11	-2.23	106.96	110.55
2	A	1000	80O	C2-C3-C4	-2.22	117.40	120.24
3	C	1001	NHW	C5X-C4X-C3X	-2.21	107.01	114.38
3	C	1001	NHW	C3X-C2X-C1X	2.21	104.74	99.89
2	B	1000	80O	C5-C6-C7	-2.20	109.07	113.62
3	A	1001	NHW	C3M-C2M-C1M	-2.19	109.05	114.59
7	A	1417	DMS	O-S-C2	2.09	116.97	106.49
2	A	1000	80O	C12-N2-C13	2.09	122.62	116.28
2	A	1000	80O	C3-C4-C5	2.07	123.53	120.61
3	C	1001	NHW	CP-C1M-C2M	2.05	119.88	115.55
2	B	1000	80O	C12-N2-C13	2.04	122.49	116.28
3	A	1001	NHW	O4A-P2A-O5A	2.03	121.88	112.44
2	A	1000	80O	C11-C12-N2	-2.02	120.23	123.42
3	C	1001	NHW	O4X-C4X-C5X	-2.01	102.90	109.33

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	NHW	O3A-P2A-O5A	-2.00	104.67	110.70

There are no chirality outliers.

All (10) torsion outliers are listed below:

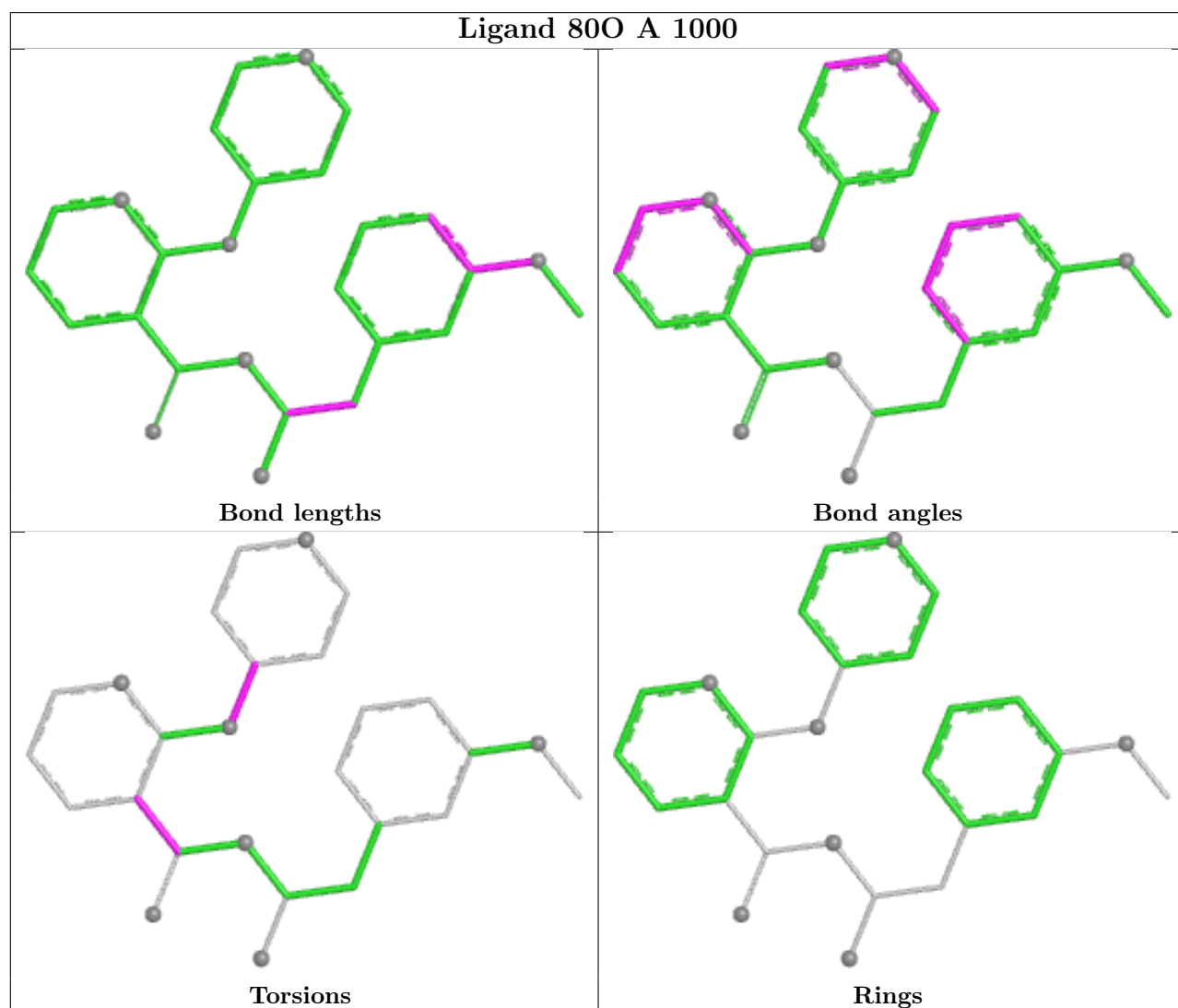
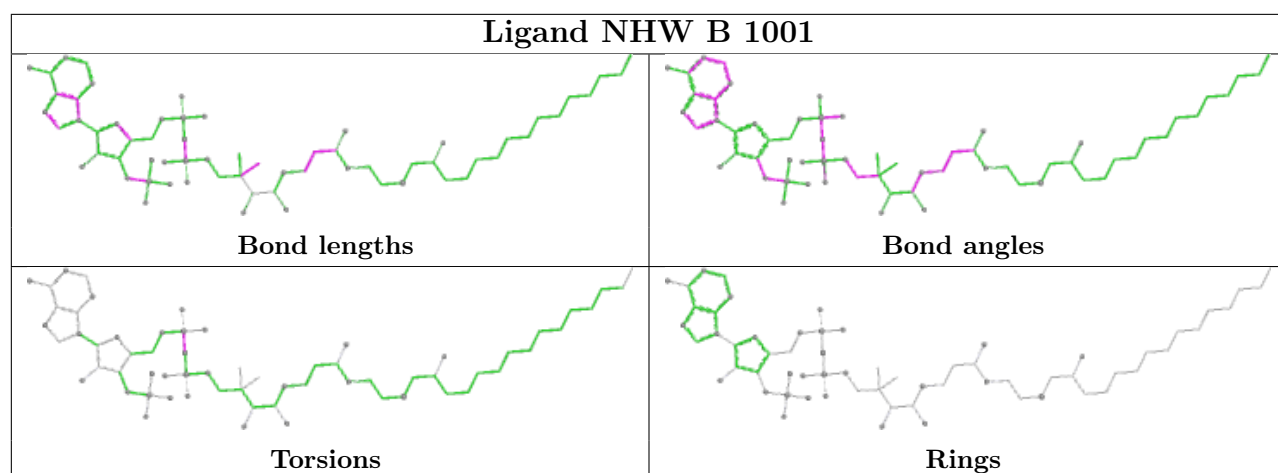
Mol	Chain	Res	Type	Atoms
2	B	1000	80O	C18-C14-O2-C13
2	A	1000	80O	O1-C8-C9-C13
2	A	1000	80O	C18-C14-O2-C13
2	A	1000	80O	C15-C14-O2-C13
2	B	1000	80O	C15-C14-O2-C13
2	C	1000	80O	C18-C14-O2-C13
2	C	1000	80O	C15-C14-O2-C13
3	B	1001	NHW	P2A-O3A-P1A-O1A
3	C	1001	NHW	P2A-O3A-P1A-O1A
3	A	1001	NHW	P2A-O3A-P1A-O1A

There are no ring outliers.

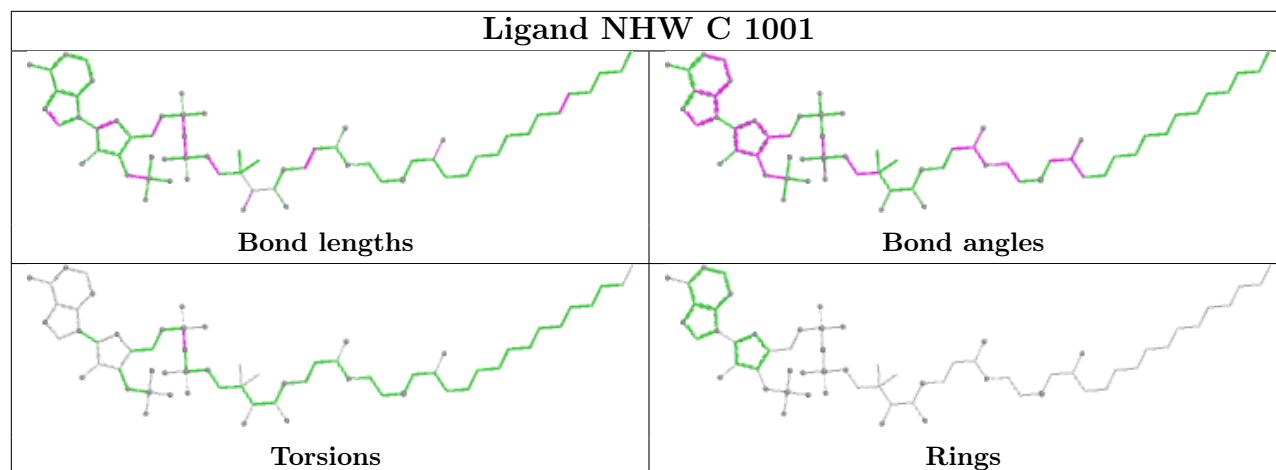
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	80O	1	0
4	B	1411	SO4	1	0
7	A	1417	DMS	2	0
4	A	1411	SO4	1	0
7	C	1413	DMS	1	0
2	C	1000	80O	1	0
2	B	1000	80O	1	0

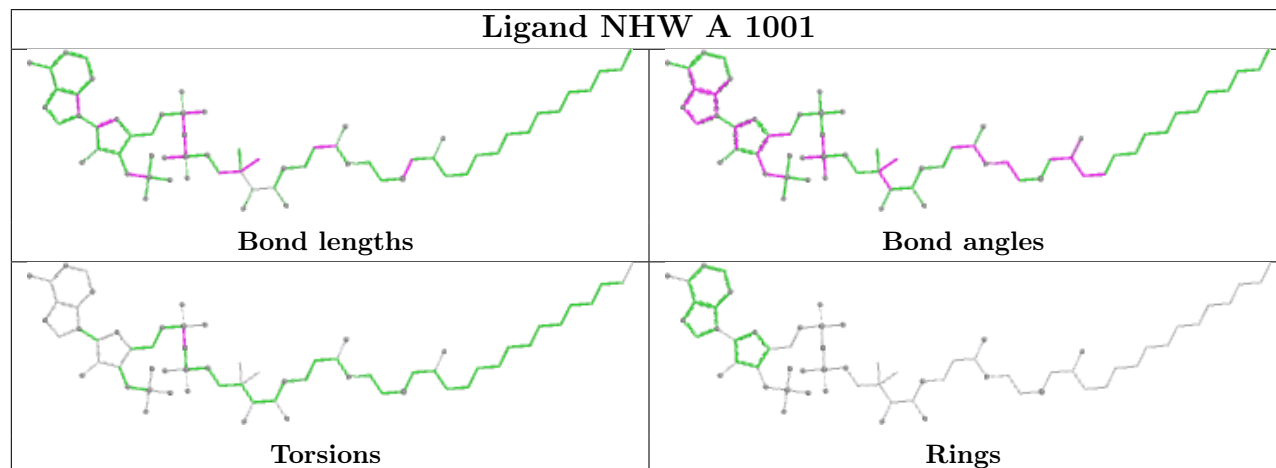
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

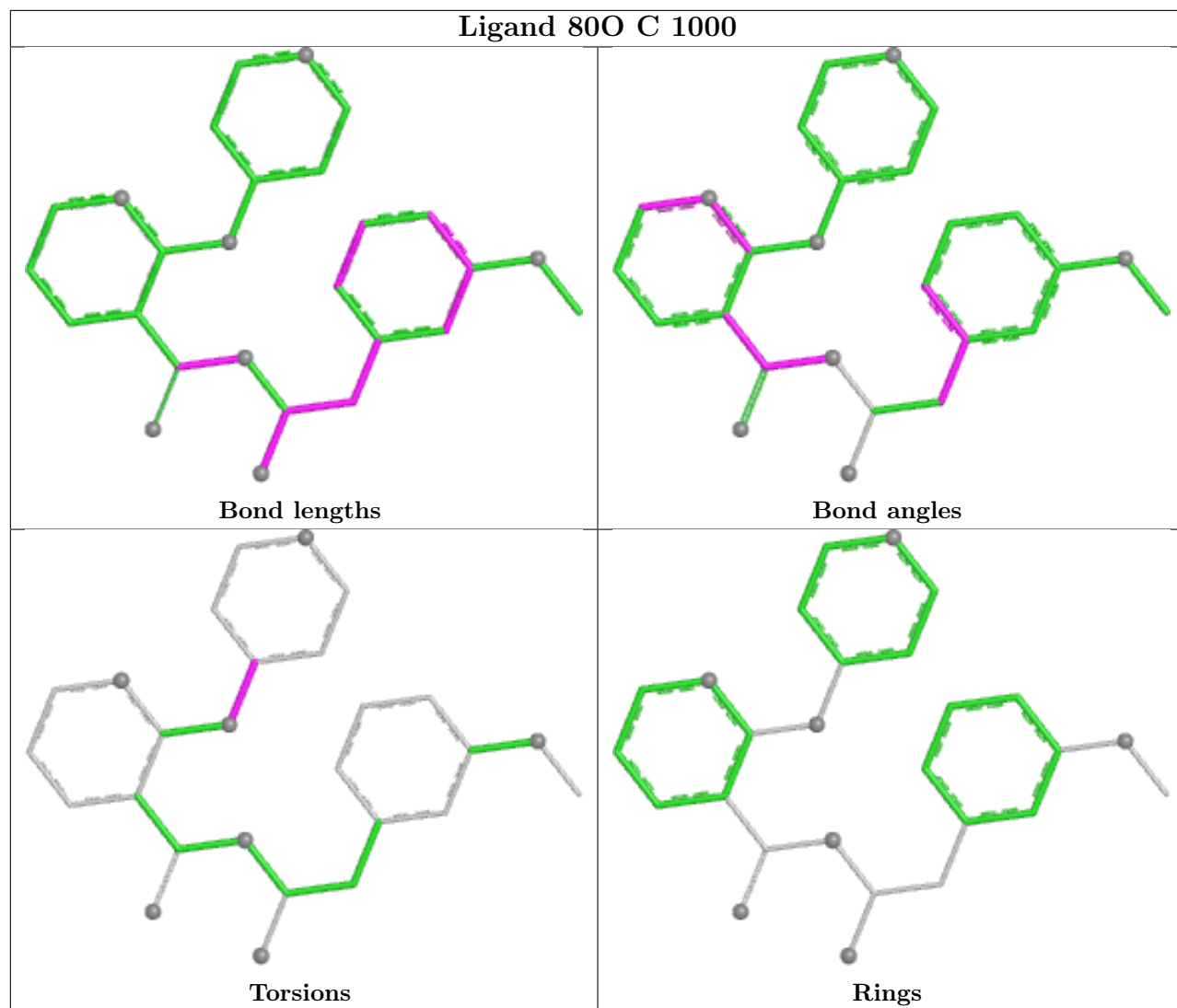


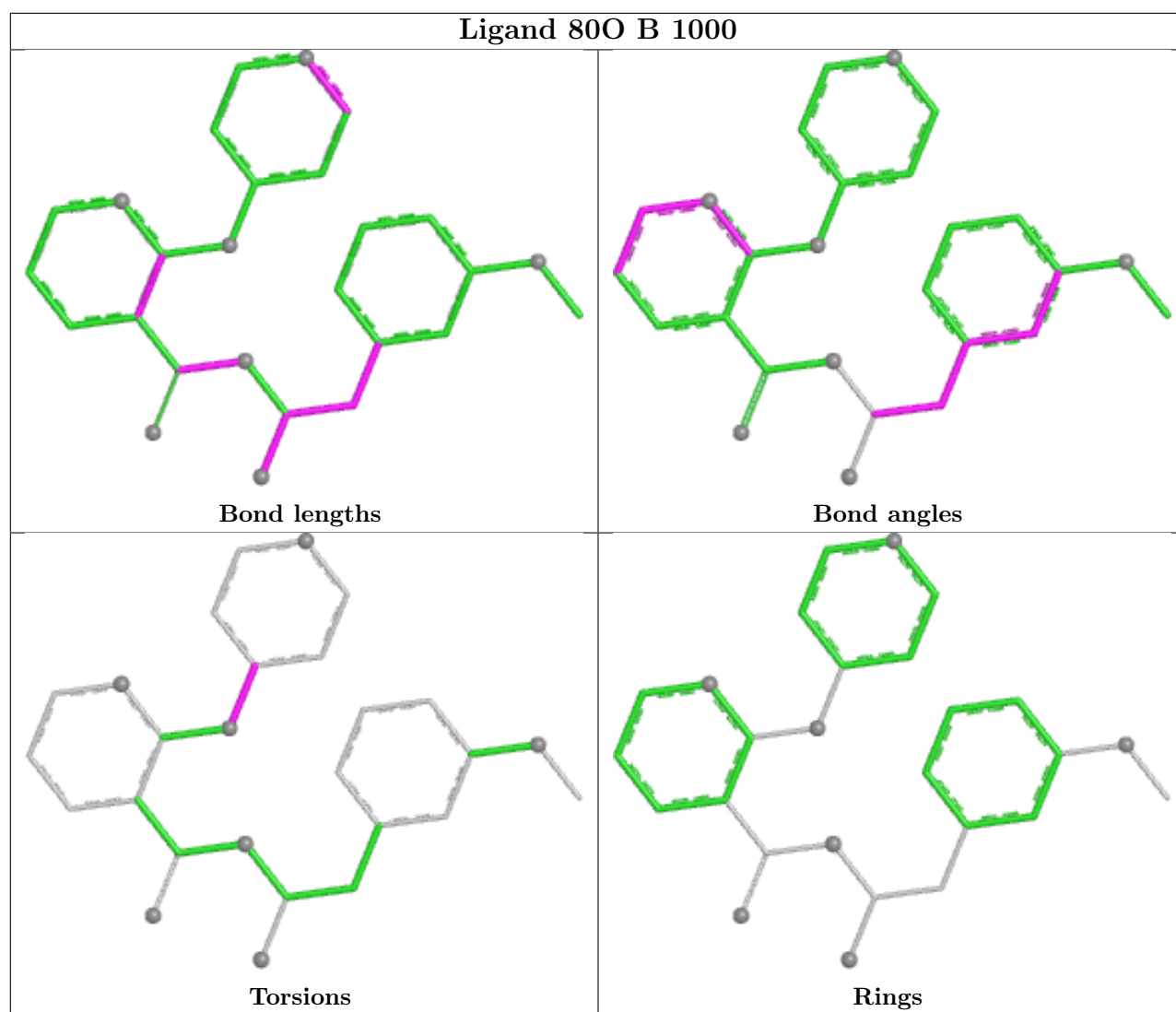
Ligand NHW C 1001



Ligand NHW A 1001







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%)	-0.57	4 (1%) 79 82	4, 10, 24, 40	37 (9%)
1	B	385/385 (100%)	-0.48	8 (2%) 63 67	4, 10, 25, 53	45 (11%)
1	C	372/385 (96%)	-0.52	9 (2%) 59 63	4, 10, 26, 59	44 (11%)
All	All	1142/1155 (98%)	-0.52	21 (1%) 67 71	4, 10, 25, 59	126 (11%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	PHE	3.7
1	A	39	ILE	3.7
1	C	26	MET	3.5
1	B	231	SER	3.0
1	C	242	TYR	3.0
1	B	26	MET	3.0
1	C	32[A]	TYR	3.0
1	B	39	ILE	2.9
1	A	325	ASP	2.8
1	B	45[A]	GLU	2.7
1	A	323[A]	GLY	2.6
1	C	222	ILE	2.5
1	B	226	PHE	2.5
1	C	323	GLY	2.5
1	A	232	ARG	2.4
1	B	323	GLY	2.4
1	C	243	ARG	2.3
1	C	305	ASN	2.2
1	B	325	ASP	2.2
1	B	40[A]	ASN	2.2
1	C	241	LEU	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](#)

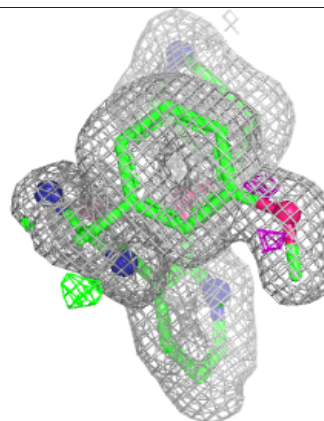
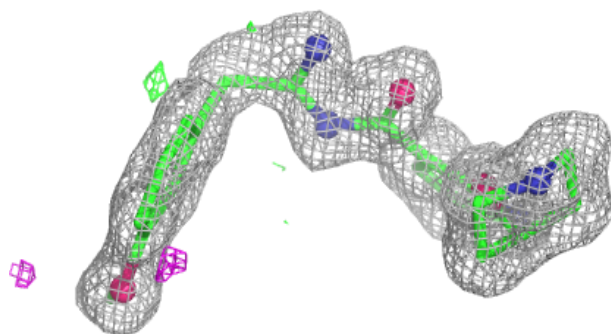
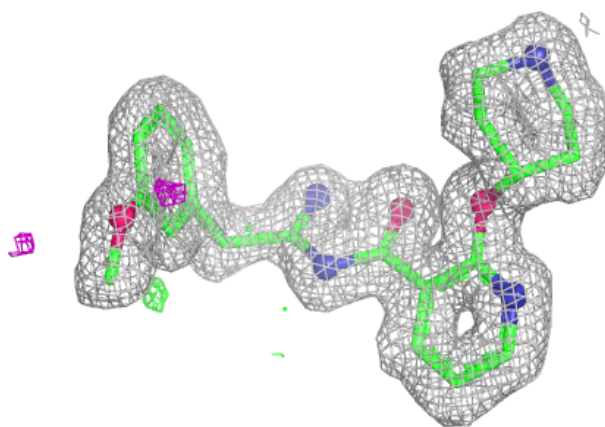
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	DMS	B	1416	4/4	0.82	0.16	35,38,39,46	0
7	DMS	A	1417	4/4	0.83	0.17	45,45,53,59	0
4	SO4	B	1411	5/5	0.89	0.14	22,23,26,28	5
6	CL	A	1415	1/1	0.94	0.28	39,39,39,39	0
4	SO4	A	1411	5/5	0.95	0.08	14,17,18,20	5
7	DMS	A	1416	4/4	0.97	0.10	16,19,21,21	0
2	80O	C	1000	27/27	0.97	0.06	8,11,19,22	0
7	DMS	B	1415	4/4	0.97	0.09	16,19,19,19	0
2	80O	B	1000	27/27	0.97	0.05	9,12,18,25	0
7	DMS	C	1413	4/4	0.97	0.10	15,19,20,20	0
2	80O	A	1000	27/27	0.98	0.04	9,11,15,25	0
3	NHW	A	1001	64/64	0.99	0.04	6,9,12,14	0
3	NHW	B	1001	64/64	0.99	0.04	6,9,12,14	0
5	MG	A	1412	1/1	0.99	0.06	18,18,18,18	0
5	MG	B	1412	1/1	0.99	0.06	17,17,17,17	0
3	NHW	C	1001	64/64	0.99	0.03	5,8,11,14	0
6	CL	C	1412	1/1	1.00	0.02	9,9,9,9	0
6	CL	A	1413	1/1	1.00	0.01	9,9,9,9	0
6	CL	A	1414	1/1	1.00	0.02	13,13,13,13	0
5	MG	C	1411	1/1	1.00	0.07	16,16,16,16	0
6	CL	B	1413	1/1	1.00	0.01	10,10,10,10	0
6	CL	B	1414	1/1	1.00	0.03	13,13,13,13	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.

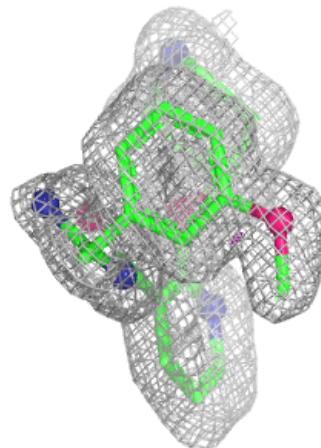
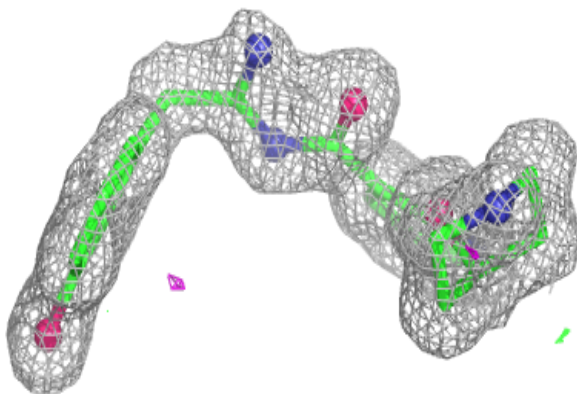
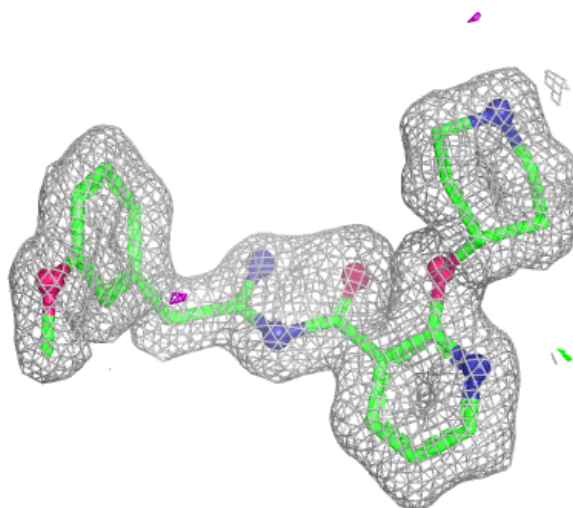
Electron density around 80O C 1000:

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



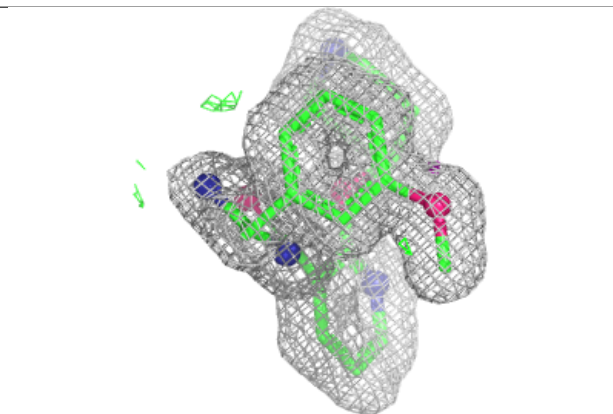
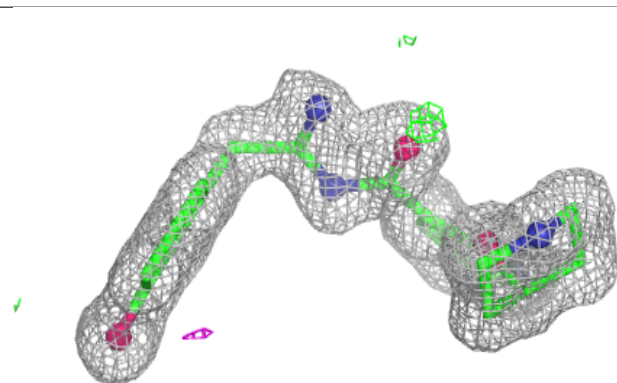
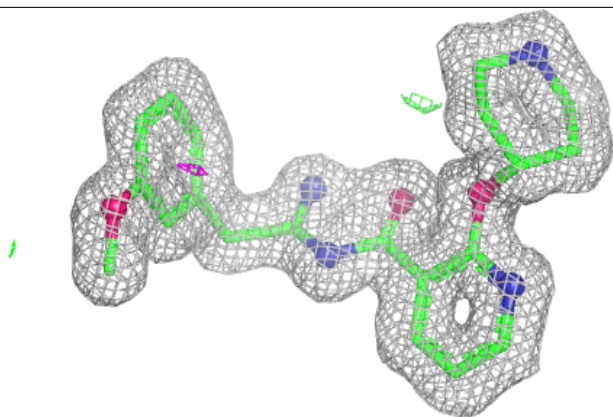
Electron density around 80O B 1000:

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

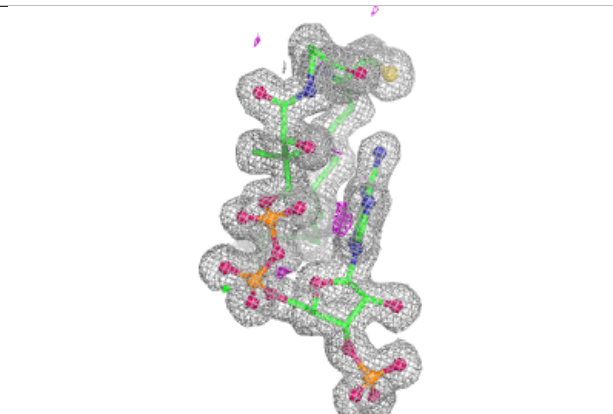
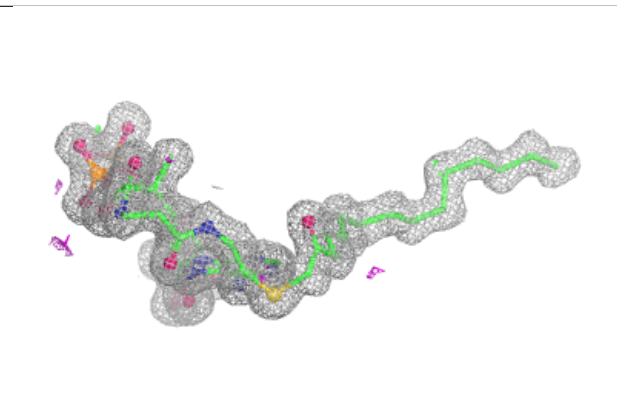
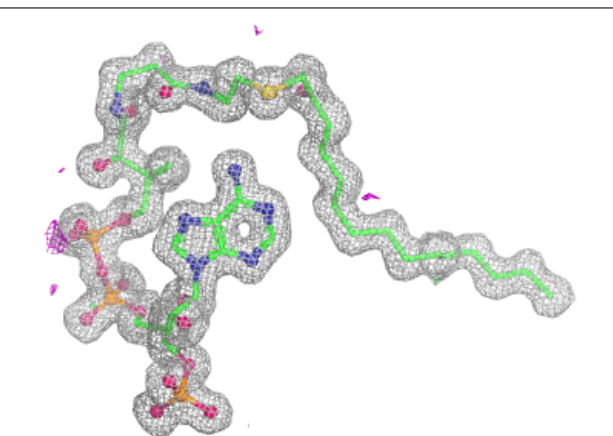


Electron density around 80O A 1000:

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

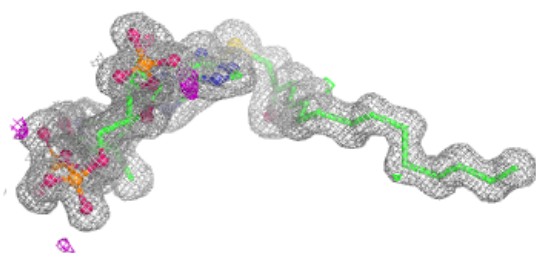
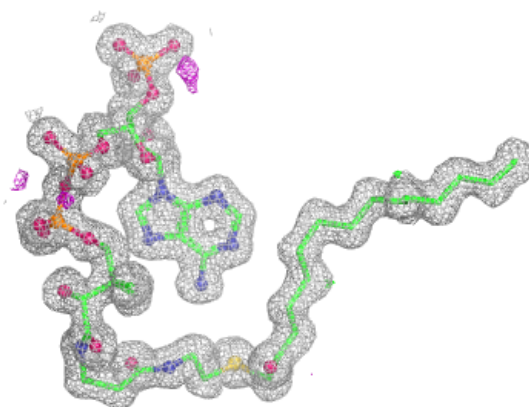
**Electron density around NHW A 1001:**

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

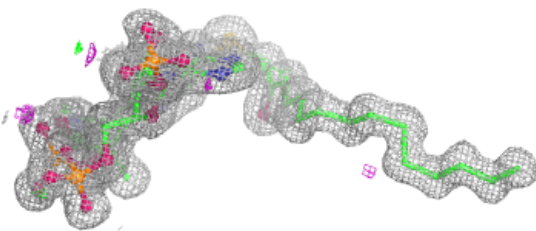
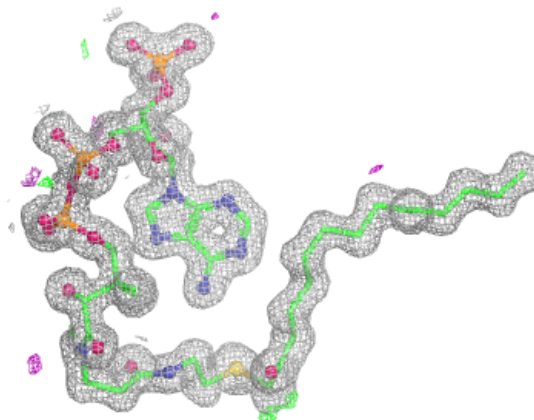


Electron density around NHW B 1001:

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

**Electron density around NHW C 1001:**

$2mF_o-DF_c$ (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.