



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:16 AM UTC

PDB ID : 4UFW / pdb_00004ufw
Title : Plasmodium vivax N-myristoyltransferase in complex with a pyridyl inhibitor (compound 22)
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 : 1.50 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

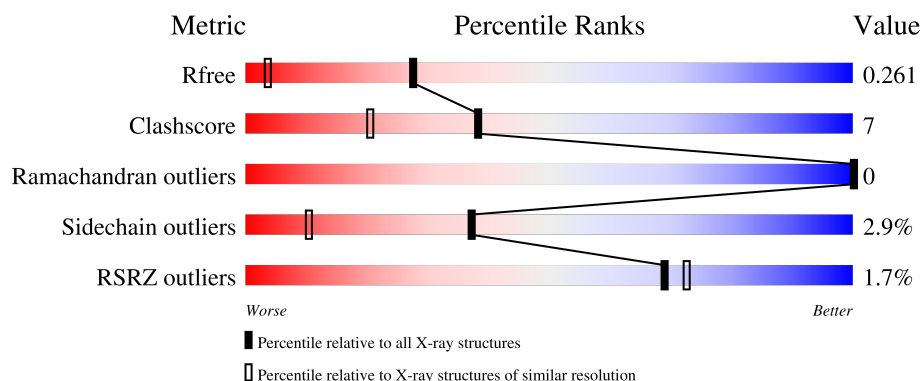
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

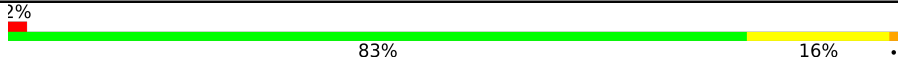
The reported resolution of this entry is 1.50 Å.

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 11389 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.

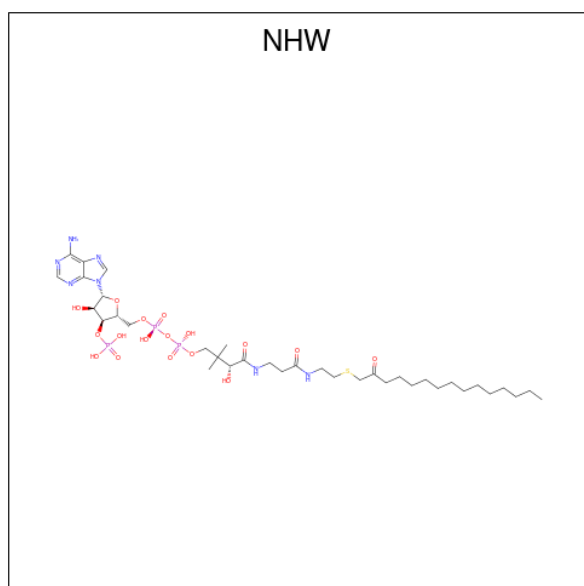
- Molecule 1 is a protein called GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	29	0
			3357	2184	546	614	13			
1	B	385	Total	C	N	O	S	0	16	0
			3269	2127	530	599	13			
1	C	367	Total	C	N	O	S	0	32	0
			3224	2112	515	587	10			

There are 3 discrepancies between the modelled and reference sequences:

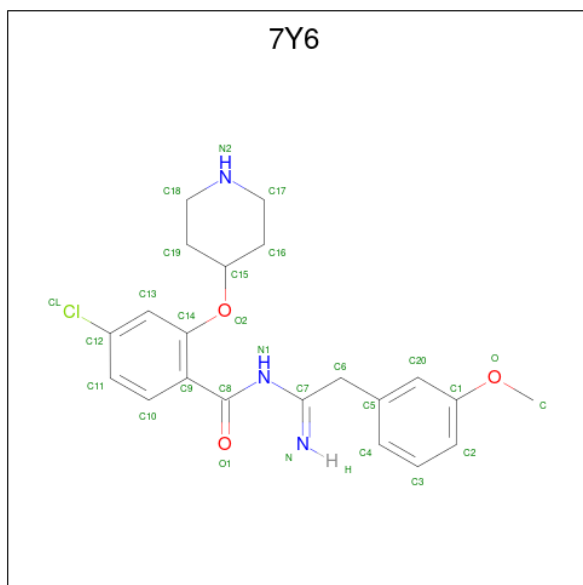
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	expression tag	UNP A5K1A2
B	26	MET	-	expression tag	UNP A5K1A2
C	26	MET	-	expression tag	UNP A5K1A2

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



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

- Molecule 3 is 4-chloranyl-N-[2-(3-methoxyphenyl)ethanimidoyl]-2-piperidin-4-yloxy-benzamide (CCD ID: 7Y6) (formula: $C_{21}H_{24}ClN_3O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O		
			28	21	1	3	3	0	0
3	B	1	Total	C	Cl	N	O		
			28	21	1	3	3	0	0
3	C	1	Total	C	Cl	N	O		
			28	21	1	3	3	0	0

- 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		

- 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	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		
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	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		

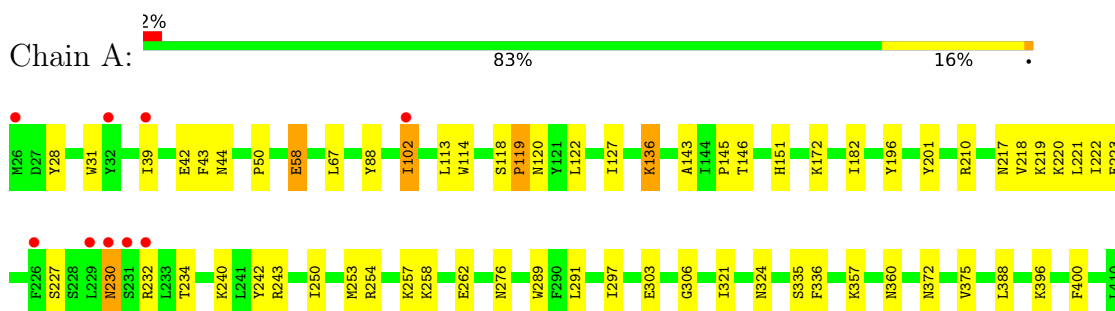
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	474	Total	O	0	0
			474	474		
8	B	404	Total	O	0	0
			404	404		
8	C	362	Total	O	0	0
			362	362		

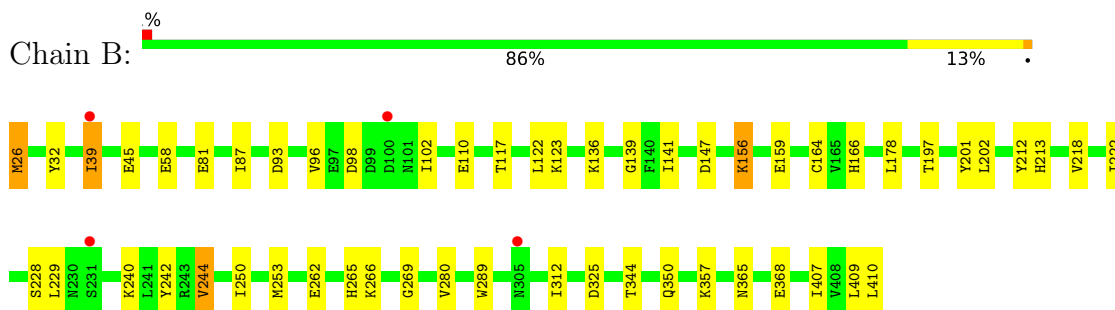
3 Residue-property plots

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.

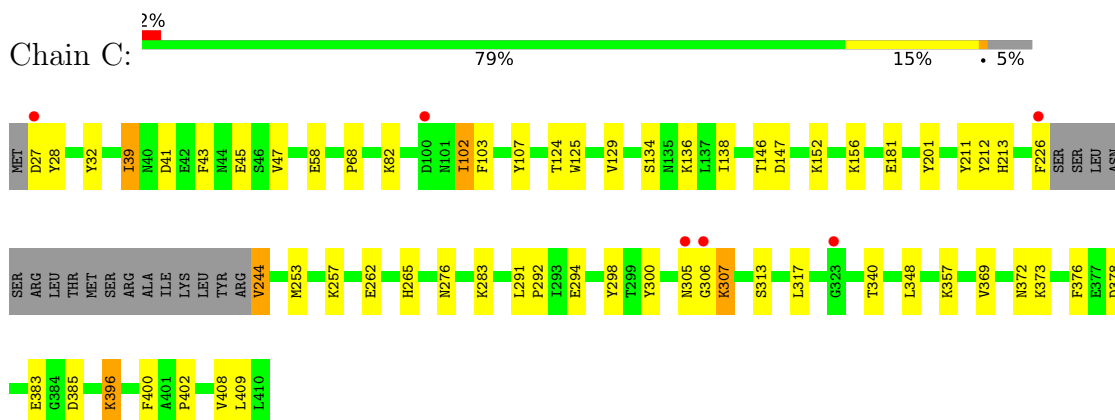
• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



• 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	57.52Å 121.91Å 178.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.73 – 1.50 100.72 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (100.73-1.50) 99.1 (100.72-1.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.214 , 0.261 0.214 , 0.261	Depositor DCC
R_{free} test set	10015 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11389	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: MG, SO4, NHW, 7Y6, DMS, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.33	9/3501 (0.3%)	1.20	11/4738 (0.2%)
1	B	1.34	12/3395 (0.4%)	1.20	4/4594 (0.1%)
1	C	1.26	6/3388 (0.2%)	1.18	3/4582 (0.1%)
All	All	1.31	27/10284 (0.3%)	1.19	18/13914 (0.1%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	336	PHE	CA-C	9.90	1.57	1.52
1	B	166	HIS	CA-C	6.07	1.60	1.52
1	C	68	PRO	CA-C	5.85	1.57	1.52
1	B	87	ILE	N-CA	5.79	1.53	1.46
1	B	244[A]	VAL	C-O	-5.72	1.17	1.24
1	B	244[B]	VAL	C-O	-5.72	1.17	1.24
1	B	407	ILE	N-CA	5.70	1.52	1.46
1	A	221	LEU	CA-C	5.60	1.60	1.52
1	B	110	GLU	C-O	-5.57	1.17	1.24
1	A	335	SER	C-O	5.54	1.30	1.23
1	C	181	GLU	CA-C	5.51	1.59	1.52
1	A	388	LEU	C-O	5.50	1.30	1.24
1	B	202	LEU	C-O	-5.49	1.19	1.24
1	C	317	LEU	C-O	5.48	1.29	1.24
1	C	408	VAL	C-O	5.46	1.30	1.24
1	C	129	VAL	C-O	5.41	1.29	1.24
1	A	113	LEU	C-O	-5.32	1.18	1.24
1	A	357	LYS	C-O	5.27	1.30	1.24
1	A	50	PRO	C-O	5.25	1.29	1.23
1	B	280	VAL	N-CA	-5.23	1.40	1.46
1	B	212	TYR	C-O	5.21	1.30	1.23
1	B	117	THR	N-CA	5.18	1.52	1.46
1	A	234	THR	C-O	5.18	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	368	GLU	N-CA	5.11	1.52	1.46
1	B	122	LEU	N-CA	5.06	1.52	1.46
1	A	143	ALA	CA-CB	-5.05	1.44	1.54
1	C	82	LYS	CA-C	5.03	1.59	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	PRO	CB-CA-C	-7.55	102.27	111.11
1	B	98	ASP	N-CA-C	-6.79	102.06	110.41
1	B	93	ASP	N-CA-C	6.58	121.05	112.89
1	A	291	LEU	CA-C-N	-6.36	113.21	119.76
1	A	291	LEU	C-N-CA	-6.36	113.21	119.76
1	C	372	ASN	N-CA-C	5.98	117.80	111.28
1	A	88	TYR	N-CA-C	-5.93	104.73	111.07
1	B	96	VAL	N-CA-C	5.85	116.96	109.30
1	A	113	LEU	N-CA-C	-5.67	104.79	110.97
1	A	324	ASN	N-CA-C	-5.47	100.26	109.07
1	C	41	ASP	N-CA-C	5.37	118.02	110.23
1	C	378	ASP	N-CA-C	5.24	117.74	111.71
1	A	321	ILE	N-CA-C	-5.22	100.36	107.99
1	A	67	LEU	CA-C-N	-5.20	115.03	120.38
1	A	67	LEU	C-N-CA	-5.20	115.03	120.38
1	A	102	ILE	CB-CA-C	-5.16	102.83	111.29
1	A	372	ASN	N-CA-C	5.10	116.84	111.28
1	B	350	GLN	N-CA-C	-5.05	105.85	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3357	0	3387	52	0
1	B	3269	0	3285	33	0
1	C	3224	0	3273	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	64	0	60	0	0
2	B	64	0	60	0	0
2	C	64	0	60	0	0
3	A	28	0	23	4	0
3	B	28	0	23	1	0
3	C	28	0	23	3	0
4	A	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	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	4	0	6	0	0
7	B	4	0	6	1	0
7	C	4	0	6	0	0
8	A	474	0	0	11	0
8	B	404	0	0	10	0
8	C	362	0	0	2	0
All	All	11389	0	10212	140	0

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

All (140) 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:A:243[B]:ARG:HG3	1:A:243[B]:ARG:HH11	1.11	1.12
1:A:254:ARG:HD2	1:A:257:LYS:HZ1	1.15	1.07
3:A:1411:7Y6:H191	8:A:2467:HOH:O	1.53	1.04
1:A:114:TRP:CZ2	1:A:297[A]:ILE:HD12	1.96	1.00
1:B:147[B]:ASP:OD1	1:B:156[B]:LYS:HE3	1.61	1.00
1:A:289:TRP:O	1:A:297[A]:ILE:HD11	1.65	0.96
1:B:39:ILE:HD11	1:B:201:TYR:HE1	1.30	0.95
1:C:147:ASP:OD1	1:C:156[A]:LYS:HE3	1.67	0.93
1:C:265:HIS:ND1	1:C:283[B]:LYS:HD2	1.89	0.87
1:A:243[B]:ARG:HG3	1:A:243[B]:ARG:NH1	1.88	0.87
1:A:114:TRP:HZ2	1:A:297[A]:ILE:HD12	1.38	0.87
1:A:254:ARG:HD2	1:A:257:LYS:NZ	1.90	0.87
1:B:156[A]:LYS:HE2	1:B:156[A]:LYS:HA	1.57	0.85
1:A:289:TRP:O	1:A:297[A]:ILE:CD1	2.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ASN:OD1	1:C:307:LYS:HD2	1.79	0.82
1:C:102[A]:ILE:HD11	1:C:103:PHE:CZ	2.15	0.81
1:C:213[B]:HIS:CD2	1:C:226:PHE:HE1	2.00	0.79
1:C:305:ASN:HD21	1:C:307:LYS:HD3	1.48	0.78
1:A:254:ARG:CD	1:A:257:LYS:HZ1	1.95	0.76
1:C:305:ASN:OD1	1:C:306:GLY:N	2.17	0.75
1:A:42[B]:GLU:HG3	1:B:344:THR:HG21	1.69	0.74
1:B:156[A]:LYS:HE2	1:B:156[A]:LYS:CA	2.14	0.73
1:C:244[B]:VAL:HG11	1:C:357:LYS:HD2	1.72	0.72
1:B:39:ILE:HD11	1:B:201:TYR:CE1	2.19	0.71
1:A:303:GLU:OE2	1:A:306:GLY:HA2	1.90	0.71
1:A:39:ILE:HD12	1:A:201:TYR:HE1	1.56	0.70
1:B:26:MET:HE3	8:B:2003:HOH:O	1.90	0.70
1:C:134:SER:OG	1:C:136[A]:LYS:HG2	1.92	0.69
1:A:230[A]:ASN:HD22	1:A:230[A]:ASN:H	1.36	0.69
1:A:230[B]:ASN:OD1	1:A:232:ARG:HB2	1.93	0.69
1:C:102[A]:ILE:HD11	1:C:103:PHE:CE2	2.28	0.69
1:B:240:LYS:HG2	8:B:2264:HOH:O	1.92	0.69
3:A:1411:7Y6:H11	8:A:2281:HOH:O	1.92	0.67
1:A:254:ARG:HH11	1:A:257:LYS:HZ3	1.42	0.67
1:C:27[A]:ASP:N	1:C:27[A]:ASP:OD1	2.26	0.66
1:A:254:ARG:NH1	1:A:257:LYS:HZ3	1.92	0.66
1:B:159:GLU:OE2	7:B:1414:DMS:H13	1.96	0.65
1:A:42[B]:GLU:CG	1:B:344:THR:HG21	2.29	0.62
8:A:2417:HOH:O	1:B:45[B]:GLU:HG3	2.01	0.61
1:C:265:HIS:ND1	1:C:283[B]:LYS:CD	2.64	0.61
1:C:213[B]:HIS:CD2	1:C:226:PHE:CE1	2.87	0.60
1:A:119:PRO:O	1:A:120[B]:ASN:CB	2.48	0.60
1:A:172:LYS:HE3	8:A:2244:HOH:O	2.00	0.60
1:A:262:GLU:HG3	8:A:2351:HOH:O	2.01	0.59
1:A:243[B]:ARG:HH11	1:A:243[B]:ARG:CG	2.00	0.59
1:A:254:ARG:NH1	1:A:257:LYS:NZ	2.50	0.58
1:B:253[B]:MET:HE2	1:B:312:ILE:HD12	1.86	0.57
1:C:276[A]:ASN:ND2	1:C:400:PHE:CE2	2.72	0.57
1:C:305:ASN:CG	1:C:306:GLY:H	2.09	0.57
1:C:152[B]:LYS:HB2	1:C:152[B]:LYS:HZ2	1.69	0.56
1:C:211:TYR:HB2	3:C:1411:7Y6:H11	1.88	0.56
1:A:151[B]:HIS:HE1	8:A:2217:HOH:O	1.88	0.56
1:C:305:ASN:HD21	1:C:307:LYS:CD	2.16	0.56
1:C:47:VAL:CG1	1:C:396:LYS:HG2	2.34	0.56
1:B:266:LYS:HE2	8:B:2303:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LYS:HG3	8:B:2303:HOH:O	2.07	0.55
1:C:28:TYR:CE2	1:C:39[A]:ILE:HG13	2.42	0.55
1:C:244[B]:VAL:HG11	1:C:357:LYS:CD	2.36	0.54
1:C:152[B]:LYS:CB	1:C:152[B]:LYS:NZ	2.71	0.54
1:A:114:TRP:CZ2	1:A:297[A]:ILE:CD1	2.82	0.54
1:A:222[A]:ILE:HD13	1:A:227:SER:HB2	1.89	0.54
3:A:1411:7Y6:C19	8:A:2467:HOH:O	2.32	0.54
1:C:262[B]:GLU:HG2	1:C:283[B]:LYS:HE2	1.90	0.53
1:B:32:TYR:OH	1:B:39:ILE:HB	2.08	0.53
1:A:254:ARG:HH11	1:A:257:LYS:NZ	2.05	0.51
1:A:230[A]:ASN:ND2	1:A:230[A]:ASN:H	2.03	0.51
3:A:1411:7Y6:O1	3:A:1411:7Y6:N	2.42	0.50
1:C:152[B]:LYS:HB2	1:C:152[B]:LYS:NZ	2.26	0.50
1:A:127:ILE:CD1	1:A:182[B]:ILE:HD12	2.42	0.49
1:B:213[B]:HIS:ND1	1:B:365:ASN:OD1	2.34	0.49
1:B:244[A]:VAL:CG2	1:B:357:LYS:HD2	2.42	0.49
1:A:127:ILE:HD11	1:A:182[B]:ILE:HD12	1.93	0.49
8:A:2423:HOH:O	1:B:45[B]:GLU:HG2	2.13	0.49
1:B:222:ILE:HD12	1:B:229:LEU:HG	1.95	0.48
1:C:262[B]:GLU:HG2	1:C:283[B]:LYS:CE	2.43	0.48
1:A:217[A]:ASN:ND2	1:A:220:LYS:HB2	2.29	0.48
1:A:218[A]:VAL:HG21	1:A:242:TYR:HB2	1.95	0.48
1:C:340:THR:HB	1:C:348:LEU:HD22	1.96	0.48
1:C:253:MET:HG3	1:C:300:TYR:HB3	1.96	0.47
1:C:276[A]:ASN:ND2	1:C:400:PHE:CD2	2.82	0.47
1:C:47:VAL:HG11	1:C:396:LYS:HG2	1.96	0.47
1:C:138:ILE:HD12	1:C:138:ILE:C	2.39	0.47
1:C:262[A]:GLU:HG3	8:C:2250:HOH:O	2.14	0.47
1:A:58:GLU:HB3	8:A:2061:HOH:O	2.14	0.47
1:B:123[B]:LYS:NZ	8:B:2168:HOH:O	2.48	0.47
1:C:102[A]:ILE:CD1	1:C:103:PHE:CZ	2.93	0.47
1:A:243[B]:ARG:NH1	1:A:243[B]:ARG:CG	2.65	0.47
1:A:196:TYR:N	1:A:196:TYR:CD1	2.82	0.46
1:B:289:TRP:CZ3	1:B:410:LEU:HD11	2.49	0.46
1:B:123[B]:LYS:HB3	8:B:2088:HOH:O	2.15	0.46
1:C:369:VAL:HA	1:C:402:PRO:O	2.16	0.46
1:C:400:PHE:HB3	8:C:2023:HOH:O	2.16	0.46
1:A:119:PRO:O	1:A:120[B]:ASN:HB2	2.13	0.45
1:C:298:TYR:O	1:C:313:SER:HA	2.17	0.45
1:C:39[B]:ILE:HD11	1:C:201:TYR:CE2	2.52	0.45
1:A:219:LYS:O	1:A:223:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1411:7Y6:H13	3:B:1411:7Y6:H15	1.79	0.45
1:C:373[A]:LYS:HA	1:C:376:PHE:CD2	2.52	0.44
1:B:123[A]:LYS:HB3	8:B:2088:HOH:O	2.16	0.44
1:A:114:TRP:HZ2	1:A:297[A]:ILE:CD1	2.18	0.44
1:A:151[B]:HIS:CE1	8:A:2217:HOH:O	2.68	0.44
1:A:43:PHE:CZ	1:A:396:LYS:HG3	2.52	0.44
1:C:212:TYR:CD2	1:C:383:GLU:HA	2.53	0.44
1:A:360[A]:ASN:ND2	8:A:2291:HOH:O	2.51	0.43
1:A:210:ARG:NH1	4:A:1412:SO4:O1	2.34	0.43
1:B:39:ILE:HD12	1:B:39:ILE:HA	1.91	0.43
1:C:107:TYR:OH	3:C:1411:7Y6:H172	2.19	0.43
1:B:141:ILE:HG22	1:B:178:LEU:HD22	1.99	0.43
1:C:43:PHE:CE1	1:C:396:LYS:HG3	2.54	0.43
1:B:197:THR:HG23	1:B:409:LEU:HD13	2.01	0.43
1:C:265:HIS:CG	1:C:283[B]:LYS:HD2	2.53	0.42
1:A:276[A]:ASN:ND2	1:A:400:PHE:CE1	2.84	0.42
1:C:32[B]:TYR:OH	1:C:39[B]:ILE:HG22	2.19	0.42
1:A:250:ILE:HB	1:A:253[B]:MET:HG2	2.01	0.42
1:B:250:ILE:O	1:B:253[B]:MET:HG2	2.20	0.42
1:B:262:GLU:HG2	1:B:266:LYS:HE3	2.02	0.42
1:B:218:VAL:CG2	1:B:242:TYR:HB2	2.50	0.42
1:C:291:LEU:HA	1:C:292:PRO:HD3	1.92	0.42
1:B:269:GLY:HA3	8:B:2305:HOH:O	2.20	0.41
1:C:373[B]:LYS:HA	1:C:376:PHE:CD2	2.55	0.41
1:C:305:ASN:CG	1:C:307:LYS:HD2	2.45	0.41
1:A:118:SER:HB3	1:A:289:TRP:CZ2	2.55	0.41
1:A:39:ILE:CD1	1:A:201:TYR:HE1	2.30	0.41
1:C:39[A]:ILE:HD13	1:C:39[A]:ILE:HA	1.99	0.41
1:C:211:TYR:CB	3:C:1411:7Y6:C11	2.99	0.41
1:A:28:TYR:HB3	1:A:31:TRP:HB2	2.03	0.41
1:B:139:GLY:HA2	1:B:164:CYS:O	2.21	0.41
1:B:265:HIS:CE1	8:B:2306:HOH:O	2.74	0.40
1:B:357:LYS:HE2	8:B:2270:HOH:O	2.22	0.40
1:C:124:THR:HG1	1:C:125:TRP:CD1	2.40	0.40
1:A:122[B]:LEU:HD23	1:A:122[B]:LEU:HA	1.91	0.40
1:A:136:LYS:HD2	1:A:136:LYS:HA	1.71	0.40
1:C:47:VAL:HG12	1:C:396:LYS:HG2	2.02	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	412/385 (107%)	400 (97%)	12 (3%)	0	100	100
1	B	399/385 (104%)	389 (98%)	10 (2%)	0	100	100
1	C	393/385 (102%)	381 (97%)	12 (3%)	0	100	100
All	All	1204/1155 (104%)	1170 (97%)	34 (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	380/351 (108%)	369 (97%)	11 (3%)	37	10
1	B	367/351 (105%)	357 (97%)	10 (3%)	39	12
1	C	366/351 (104%)	347 (95%)	19 (5%)	21	3
All	All	1113/1053 (106%)	1073 (96%)	40 (4%)	37	6

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	102	ILE
1	A	119	PRO
1	A	136	LYS
1	A	146[A]	THR

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Mol	Chain	Res	Type
1	A	146[B]	THR
1	A	230[A]	ASN
1	A	230[B]	ASN
1	A	240	LYS
1	A	258	LYS
1	A	375	VAL
1	B	26	MET
1	B	39	ILE
1	B	58	GLU
1	B	81	GLU
1	B	102	ILE
1	B	136	LYS
1	B	156[A]	LYS
1	B	156[B]	LYS
1	B	228	SER
1	B	325	ASP
1	C	39[A]	ILE
1	C	39[B]	ILE
1	C	45	GLU
1	C	58[A]	GLU
1	C	58[B]	GLU
1	C	102[A]	ILE
1	C	102[B]	ILE
1	C	146[A]	THR
1	C	146[B]	THR
1	C	244[A]	VAL
1	C	244[B]	VAL
1	C	257[A]	LYS
1	C	257[B]	LYS
1	C	294[A]	GLU
1	C	294[B]	GLU
1	C	307	LYS
1	C	385	ASP
1	C	396	LYS
1	C	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	135	ASN
1	A	249	ASN

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Mol	Chain	Res	Type
1	A	350	GLN
1	A	371	GLN
1	A	372	ASN
1	B	34	GLN
1	B	106	ASN
1	B	187	ASN
1	B	249	ASN
1	B	265	HIS
1	B	331	ASN
1	B	359	ASN
1	B	360	ASN
1	B	372	ASN
1	C	34	GLN
1	C	101	ASN
1	C	187	ASN
1	C	295	ASN
1	C	359	ASN
1	C	371	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	NHW	A	1000	5	64,66,66	1.42	8 (12%)	87,92,92	1.53	18 (20%)
7	DMS	B	1414	-	3,3,3	0.46	0	3,3,3	1.55	1 (33%)
7	DMS	A	1415	-	3,3,3	0.38	0	3,3,3	1.38	0
3	7Y6	C	1411	-	30,30,30	1.74	6 (20%)	34,40,40	2.38	13 (38%)
3	7Y6	A	1411	-	30,30,30	1.61	3 (10%)	34,40,40	2.48	12 (35%)
2	NHW	B	1000	5	64,66,66	1.83	9 (14%)	87,92,92	1.61	16 (18%)
4	SO4	A	1412	-	4,4,4	0.31	0	6,6,6	0.54	0
2	NHW	C	1000	5	64,66,66	1.88	10 (15%)	87,92,92	1.77	15 (17%)
3	7Y6	B	1411	-	30,30,30	1.88	6 (20%)	34,40,40	3.01	17 (50%)
7	DMS	C	1414	-	3,3,3	0.55	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
2	NHW	A	1000	5	-	0/65/81/81	0/3/3/3
3	7Y6	C	1411	-	-	4/16/26/26	0/3/3/3
3	7Y6	A	1411	-	-	5/16/26/26	0/3/3/3
2	NHW	B	1000	5	-	5/65/81/81	0/3/3/3
2	NHW	C	1000	5	-	1/65/81/81	0/3/3/3
3	7Y6	B	1411	-	-	4/16/26/26	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	NHW	P1A-O3A	9.33	1.69	1.59
2	B	1000	NHW	P2A-O3A	-7.13	1.51	1.59
3	B	1411	7Y6	C8-N1	-6.56	1.26	1.37
3	C	1411	7Y6	C8-N1	-5.96	1.27	1.37
3	A	1411	7Y6	C8-N1	-5.93	1.27	1.37
2	B	1000	NHW	CP-S1	5.76	1.96	1.81
2	C	1000	NHW	P3X-O3X	5.22	1.68	1.59
2	B	1000	NHW	P3X-O3X	5.17	1.68	1.59
2	B	1000	NHW	O10-C10	4.77	1.50	1.42
2	A	1000	NHW	P2A-O3A	-4.65	1.54	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	NHW	O4X-C4X	3.90	1.53	1.45
3	B	1411	7Y6	O1-C8	3.60	1.31	1.23
3	C	1411	7Y6	O1-C8	3.43	1.31	1.23
2	C	1000	NHW	C5A-N7A	-3.43	1.32	1.39
3	A	1411	7Y6	C7-N	3.38	1.34	1.27
3	A	1411	7Y6	O1-C8	3.31	1.31	1.23
3	B	1411	7Y6	O2-C14	3.21	1.43	1.37
2	B	1000	NHW	P1A-O3A	3.21	1.63	1.59
2	A	1000	NHW	P1A-O3A	3.08	1.62	1.59
2	B	1000	NHW	C6-C5	3.07	1.57	1.51
2	C	1000	NHW	C8A-N9A	-2.93	1.32	1.37
2	C	1000	NHW	O4X-C1X	-2.91	1.35	1.42
3	C	1411	7Y6	C7-N	2.83	1.33	1.27
3	B	1411	7Y6	C7-N	2.80	1.33	1.27
2	A	1000	NHW	O1M-C1M	2.77	1.26	1.21
3	C	1411	7Y6	C6-C5	2.60	1.55	1.51
2	C	1000	NHW	P3X-O7A	-2.60	1.45	1.54
2	A	1000	NHW	O4X-C1X	2.49	1.47	1.42
3	B	1411	7Y6	C9-C8	-2.48	1.45	1.50
2	A	1000	NHW	C8A-N9A	-2.46	1.33	1.37
2	C	1000	NHW	C8A-N7A	2.45	1.36	1.31
2	A	1000	NHW	C14-C11	-2.37	1.48	1.53
3	C	1411	7Y6	C6-C7	2.29	1.52	1.51
2	A	1000	NHW	O4X-C4X	2.27	1.50	1.45
2	A	1000	NHW	P1A-O5X	2.27	1.68	1.59
2	B	1000	NHW	O4X-C4X	2.22	1.49	1.45
2	C	1000	NHW	CP-C1M	2.21	1.55	1.51
3	C	1411	7Y6	C2-C1	2.17	1.42	1.38
2	B	1000	NHW	C14-C11	2.10	1.58	1.53
2	C	1000	NHW	P1A-O1A	-2.09	1.43	1.50
2	B	1000	NHW	C8A-N7A	2.03	1.35	1.31
3	B	1411	7Y6	C3-C2	2.02	1.42	1.38

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1411	7Y6	O2-C14-C9	7.36	128.43	116.57
3	B	1411	7Y6	O1-C8-C9	-7.34	107.57	121.03
3	A	1411	7Y6	O2-C14-C9	6.66	127.31	116.57
2	C	1000	NHW	N3A-C2A-N1A	-6.13	119.31	128.58
3	C	1411	7Y6	O2-C14-C9	6.07	126.36	116.57
3	C	1411	7Y6	O1-C8-C9	-5.67	110.63	121.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1000	NHW	C5A-C4A-N3A	-5.56	119.06	126.72
3	B	1411	7Y6	O1-C8-N1	5.50	130.31	122.27
3	B	1411	7Y6	C16-C15-C19	-5.17	101.11	111.67
3	B	1411	7Y6	C10-C9-C14	4.97	124.74	118.21
3	A	1411	7Y6	O2-C15-C16	4.66	119.19	108.31
2	B	1000	NHW	C2-S1-CP	4.53	109.19	101.72
3	C	1411	7Y6	C10-C9-C14	4.45	124.06	118.21
2	C	1000	NHW	C2A-N3A-C4A	4.37	122.50	111.83
2	B	1000	NHW	C5A-C4A-N3A	-4.29	120.81	126.72
3	A	1411	7Y6	C9-C8-N1	4.25	123.39	115.39
3	A	1411	7Y6	C16-C15-C19	-4.01	103.48	111.67
3	B	1411	7Y6	O2-C15-C16	3.96	117.54	108.31
2	B	1000	NHW	P3X-O3X-C3X	-3.93	112.94	123.43
2	A	1000	NHW	C5A-C4A-N3A	-3.93	121.31	126.72
2	C	1000	NHW	N3A-C4A-N9A	3.92	133.83	127.17
2	B	1000	NHW	C10-C9-N8	-3.89	109.11	116.48
2	B	1000	NHW	N3A-C2A-N1A	-3.88	122.71	128.58
2	A	1000	NHW	C2-S1-CP	-3.85	95.37	101.72
3	A	1411	7Y6	O2-C14-C13	-3.80	115.35	123.87
3	B	1411	7Y6	O2-C14-C13	-3.64	115.70	123.87
2	A	1000	NHW	N3A-C2A-N1A	-3.62	123.10	128.58
3	A	1411	7Y6	C10-C9-C14	3.61	122.95	118.21
3	C	1411	7Y6	C10-C11-C12	-3.56	115.66	119.24
3	A	1411	7Y6	C10-C9-C8	-3.53	109.12	118.53
3	B	1411	7Y6	C10-C9-C8	-3.53	109.12	118.53
3	C	1411	7Y6	C9-C8-N1	3.49	121.98	115.39
3	C	1411	7Y6	C10-C9-C8	-3.49	109.21	118.53
2	A	1000	NHW	N3A-C4A-N9A	3.42	132.98	127.17
2	C	1000	NHW	O3A-P2A-O5A	-3.41	100.44	110.70
2	B	1000	NHW	C7-N8-C9	-3.36	116.51	122.55
2	C	1000	NHW	N9A-C8A-N7A	-3.35	109.18	113.94
3	B	1411	7Y6	C5-C6-C7	-3.25	106.90	113.62
3	A	1411	7Y6	C11-C12-C13	3.25	125.78	121.53
2	C	1000	NHW	C5A-N7A-C8A	3.24	108.54	103.45
2	A	1000	NHW	C4A-N9A-C8A	3.23	109.13	105.74
3	A	1411	7Y6	O1-C8-C9	-3.22	115.13	121.03
3	B	1411	7Y6	C9-C8-N1	3.21	121.43	115.39
3	C	1411	7Y6	C13-C14-C9	-3.21	115.37	121.39
3	B	1411	7Y6	C13-C14-C9	-3.11	115.55	121.39
2	C	1000	NHW	P3X-O3X-C3X	-3.11	115.13	123.43
2	B	1000	NHW	C2A-N1A-C6A	3.04	123.72	118.73
2	C	1000	NHW	O2A-P1A-O3A	3.01	115.42	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1411	7Y6	C5-C6-C7	-2.93	107.55	113.62
2	B	1000	NHW	N3A-C4A-N9A	2.92	132.13	127.17
2	C	1000	NHW	C2-C3-N4	-2.85	106.47	112.41
3	A	1411	7Y6	C10-C11-C12	-2.83	116.40	119.24
2	A	1000	NHW	C2-C3-N4	-2.81	106.54	112.41
2	B	1000	NHW	O4X-C1X-C2X	-2.67	100.89	106.62
2	C	1000	NHW	C4A-C5A-N7A	-2.67	107.53	110.58
2	A	1000	NHW	C2A-N3A-C4A	2.66	118.33	111.83
2	A	1000	NHW	O3A-P1A-O1A	-2.64	102.77	110.70
2	A	1000	NHW	O1M-C1M-CP	-2.64	118.41	122.17
3	B	1411	7Y6	C10-C11-C12	-2.62	116.61	119.24
3	C	1411	7Y6	O1-C8-N1	2.60	126.07	122.27
2	B	1000	NHW	C4A-N9A-C8A	2.60	108.47	105.74
3	C	1411	7Y6	C16-C15-C19	-2.56	106.44	111.67
2	B	1000	NHW	N9A-C8A-N7A	-2.54	110.33	113.94
3	C	1411	7Y6	O2-C14-C13	-2.54	118.19	123.87
2	B	1000	NHW	O4A-P2A-O5A	2.51	124.13	112.44
2	A	1000	NHW	O4X-C1X-C2X	-2.49	101.28	106.62
3	C	1411	7Y6	O2-C15-C16	2.40	113.90	108.31
2	A	1000	NHW	C13-C11-C10	2.39	112.84	108.77
2	A	1000	NHW	O4A-P2A-O3A	2.39	113.73	107.27
2	A	1000	NHW	C3-N4-C5	-2.34	118.46	122.82
2	C	1000	NHW	O4A-P2A-O3A	2.33	113.56	107.27
2	B	1000	NHW	C2A-N3A-C4A	2.30	117.44	111.83
3	A	1411	7Y6	C13-C14-C9	-2.30	117.08	121.39
2	A	1000	NHW	O3A-P2A-O5A	-2.27	103.86	110.70
2	A	1000	NHW	C7-N8-C9	2.27	126.62	122.55
2	C	1000	NHW	C6-C5-N4	-2.27	112.21	116.34
3	B	1411	7Y6	C17-N2-C18	2.26	116.78	110.40
2	A	1000	NHW	O4X-C4X-C5X	-2.26	102.10	109.33
2	B	1000	NHW	O4A-P2A-O3A	-2.25	101.19	107.27
3	C	1411	7Y6	C11-C12-CL	-2.25	116.04	119.36
7	B	1414	DMS	C2-S-C1	2.24	109.92	98.42
3	B	1411	7Y6	C11-C12-C13	2.23	124.45	121.53
2	C	1000	NHW	O2X-C2X-C3X	2.21	117.36	111.19
2	A	1000	NHW	C13-C11-C12	-2.19	104.61	108.22
3	B	1411	7Y6	C2-C1-C20	-2.15	117.61	120.50
3	B	1411	7Y6	C-O-C1	2.15	122.11	117.50
2	C	1000	NHW	O4X-C1X-C2X	-2.14	102.03	106.62
2	B	1000	NHW	O8A-P3X-O3X	2.12	114.11	105.85
3	A	1411	7Y6	C5-C6-C7	-2.10	109.28	113.62
3	B	1411	7Y6	C13-C12-CL	-2.08	116.56	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	NHW	C4A-C5A-N7A	-2.04	108.24	110.58
2	A	1000	NHW	O2X-C2X-C3X	2.02	116.83	111.19

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1000	NHW	C12-O6A-P2A-O4A
3	C	1411	7Y6	O1-C8-C9-C14
2	C	1000	NHW	C7M-C8M-C9M-CAM
3	B	1411	7Y6	C19-C15-O2-C14
3	B	1411	7Y6	C16-C15-O2-C14
3	C	1411	7Y6	C19-C15-O2-C14
3	C	1411	7Y6	C16-C15-O2-C14
3	B	1411	7Y6	O1-C8-C9-C14
3	C	1411	7Y6	N1-C8-C9-C14
3	A	1411	7Y6	C16-C15-O2-C14
3	A	1411	7Y6	O1-C8-C9-C14
2	B	1000	NHW	C4M-C5M-C6M-C7M
3	B	1411	7Y6	N1-C8-C9-C14
3	A	1411	7Y6	C19-C15-O2-C14
3	A	1411	7Y6	C9-C14-O2-C15
2	B	1000	NHW	C7M-C8M-C9M-CAM
3	A	1411	7Y6	C13-C14-O2-C15
2	B	1000	NHW	P2A-O3A-P1A-O1A
2	B	1000	NHW	P2A-O3A-P1A-O2A

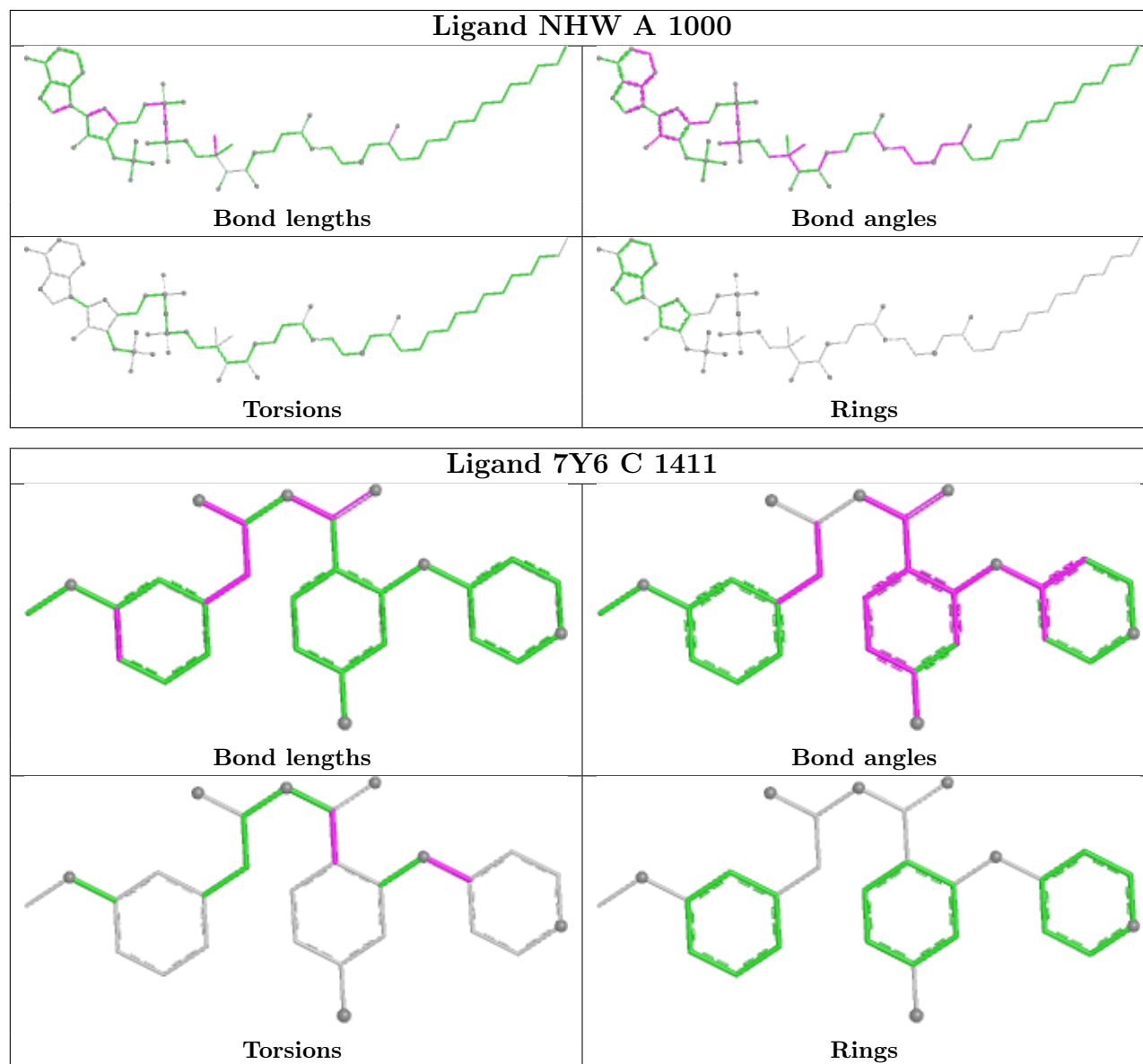
There are no ring outliers.

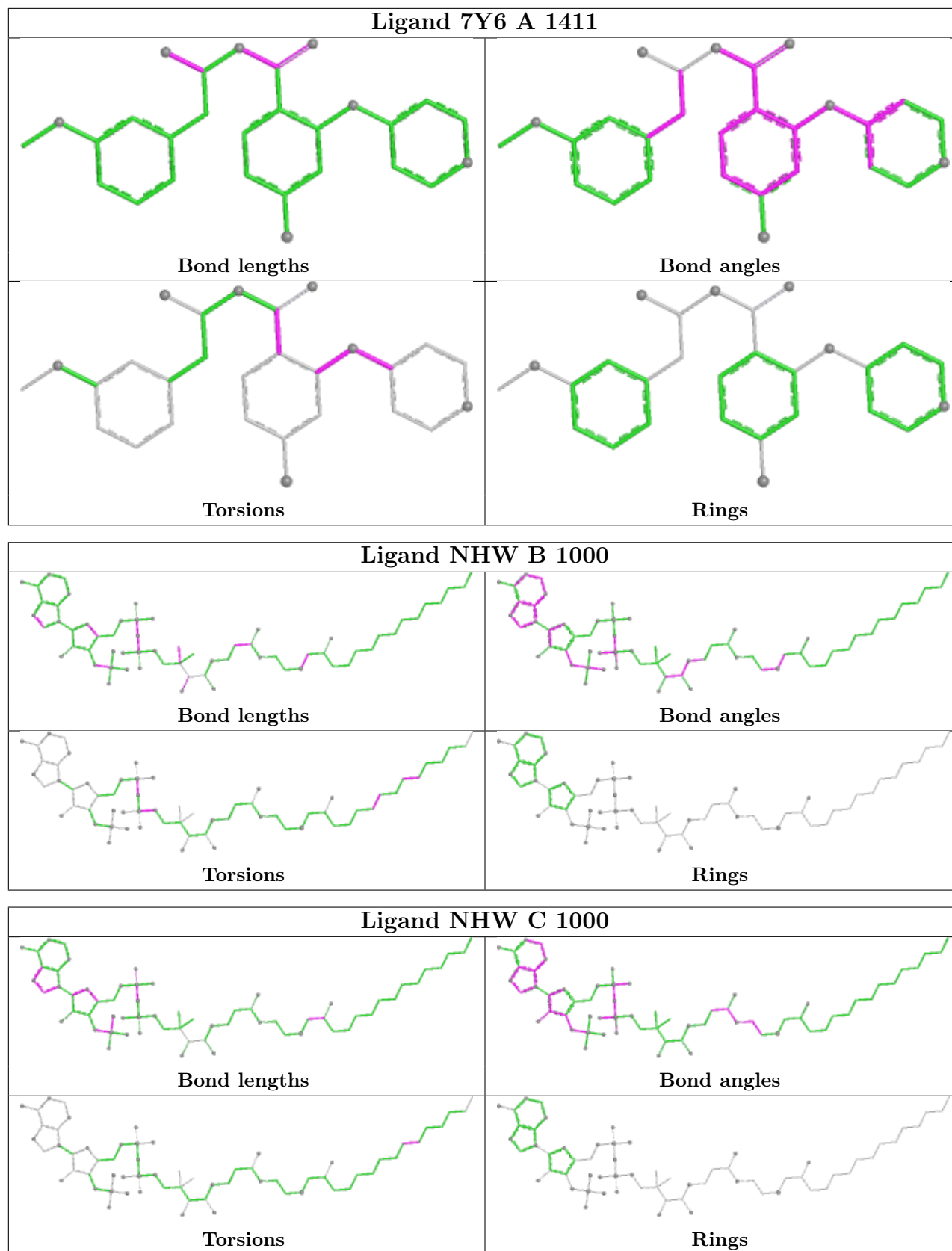
5 monomers are involved in 10 short contacts:

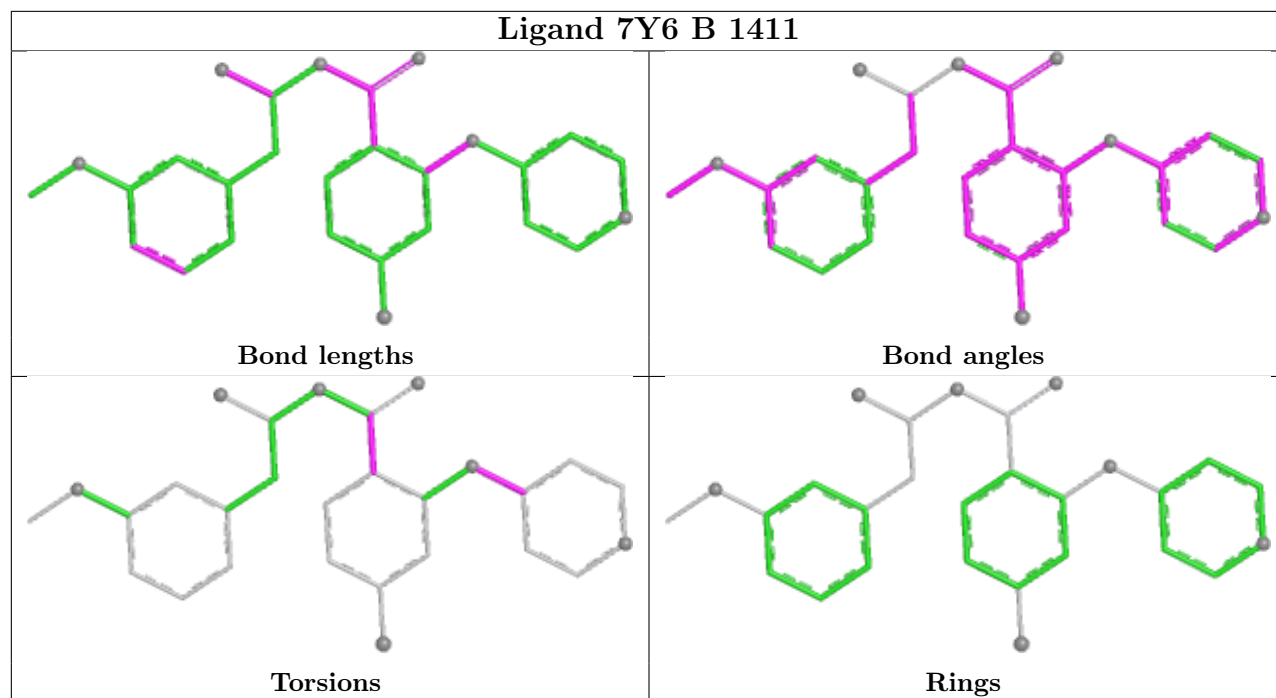
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1414	DMS	1	0
3	C	1411	7Y6	3	0
3	A	1411	7Y6	4	0
4	A	1412	SO4	1	0
3	B	1411	7Y6	1	0

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, 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%)	-0.05	9 (2%) 61 65	6, 13, 26, 64	40 (10%)
1	B	385/385 (100%)	-0.12	4 (1%) 79 82	7, 13, 27, 61	29 (7%)
1	C	367/385 (95%)	-0.03	6 (1%) 70 74	6, 14, 28, 45	40 (10%)
All	All	1137/1155 (98%)	-0.07	19 (1%) 69 72	6, 14, 27, 64	109 (9%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	323	GLY	3.5
1	A	231	SER	3.3
1	A	229	LEU	3.1
1	C	305	ASN	2.9
1	A	39	ILE	2.9
1	A	26	MET	2.9
1	B	305	ASN	2.6
1	C	27[A]	ASP	2.6
1	B	100	ASP	2.6
1	A	232	ARG	2.6
1	B	39	ILE	2.3
1	B	231	SER	2.3
1	A	230[A]	ASN	2.2
1	A	102	ILE	2.1
1	A	226	PHE	2.1
1	C	306	GLY	2.1
1	C	100	ASP	2.1
1	C	226	PHE	2.0
1	A	32	TYR	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](#)

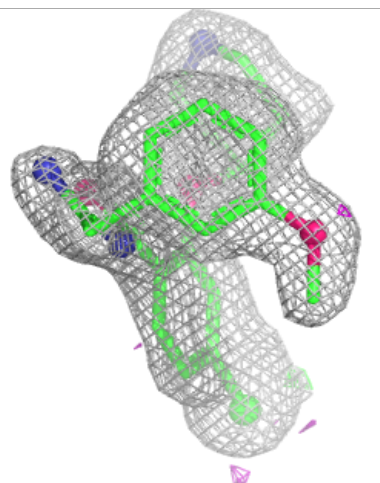
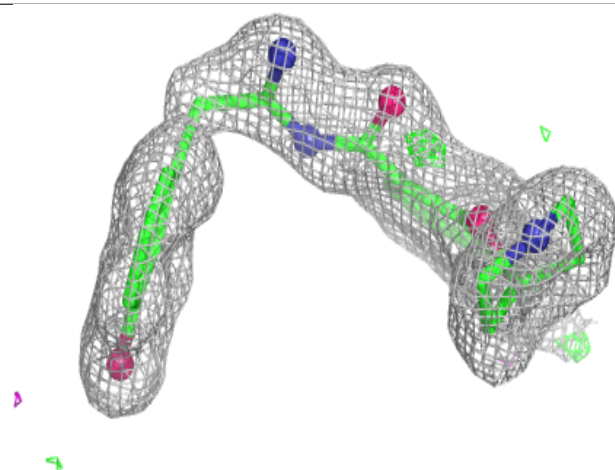
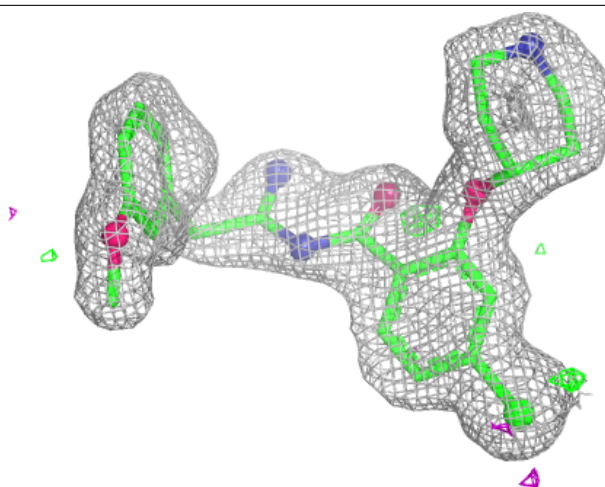
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	1414	4/4	0.89	0.16	26,30,30,34	0
4	SO4	A	1412	5/5	0.90	0.10	42,43,46,46	0
3	7Y6	C	1411	28/28	0.92	0.10	19,26,31,36	0
3	7Y6	B	1411	28/28	0.93	0.10	19,24,28,30	0
3	7Y6	A	1411	28/28	0.93	0.10	18,26,29,30	0
7	DMS	A	1415	4/4	0.95	0.14	25,26,26,26	0
7	DMS	B	1414	4/4	0.96	0.09	20,21,22,25	0
5	MG	C	1412	1/1	0.97	0.07	22,22,22,22	0
5	MG	B	1412	1/1	0.97	0.05	27,27,27,27	0
2	NHW	A	1000	64/64	0.98	0.05	9,11,15,17	0
2	NHW	B	1000	64/64	0.98	0.04	8,11,14,14	0
2	NHW	C	1000	64/64	0.98	0.04	8,12,15,18	0
5	MG	A	1413	1/1	0.99	0.03	22,22,22,22	0
6	CL	A	1414	1/1	0.99	0.03	13,13,13,13	0
6	CL	B	1413	1/1	0.99	0.02	13,13,13,13	0
6	CL	C	1413	1/1	1.00	0.04	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.

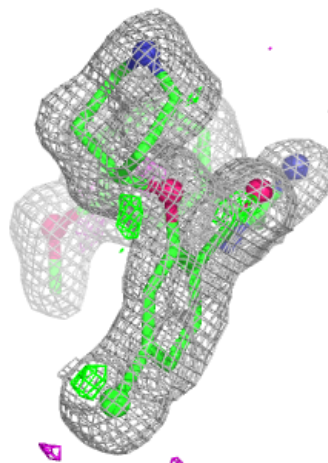
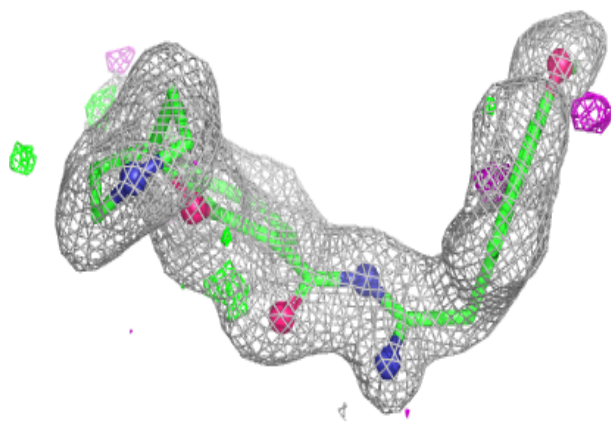
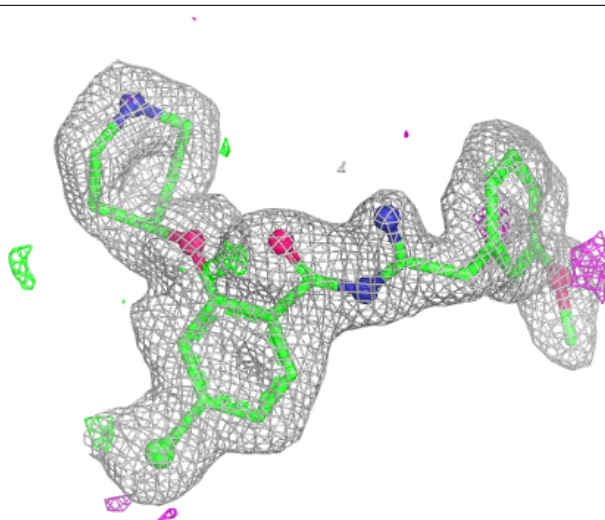
Electron density around 7Y6 C 1411:

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



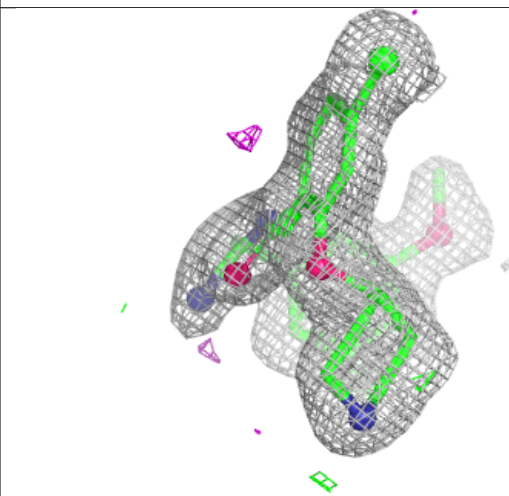
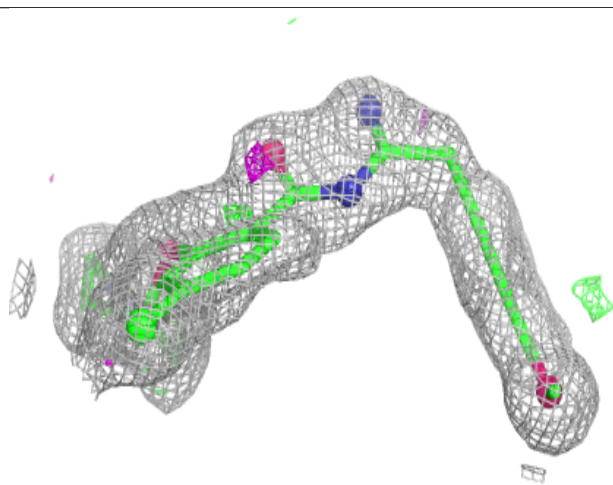
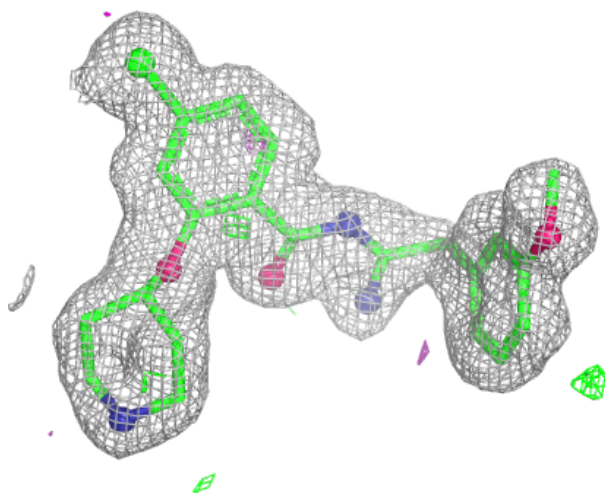
Electron density around 7Y6 B 1411:

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



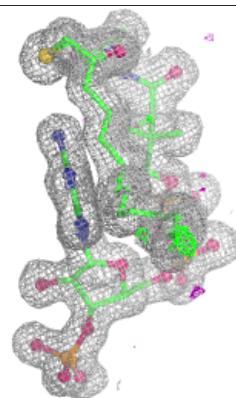
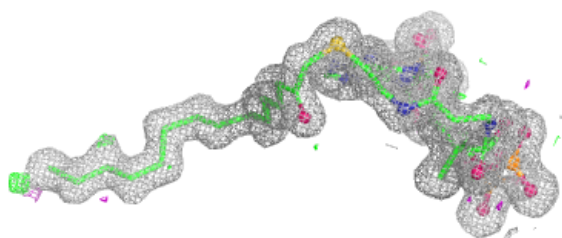
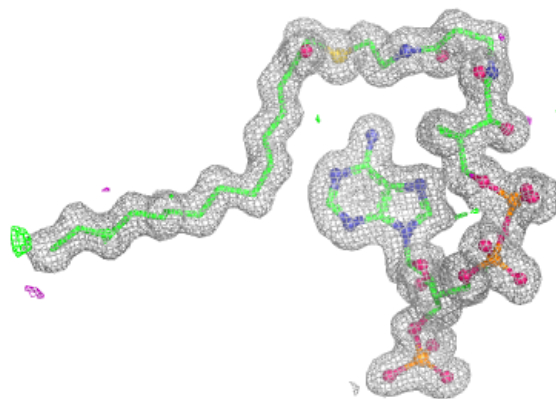
Electron density around 7Y6 A 1411:

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

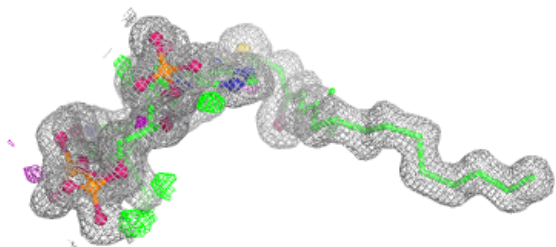
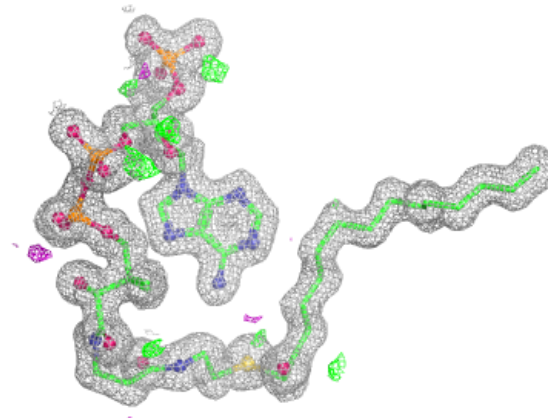


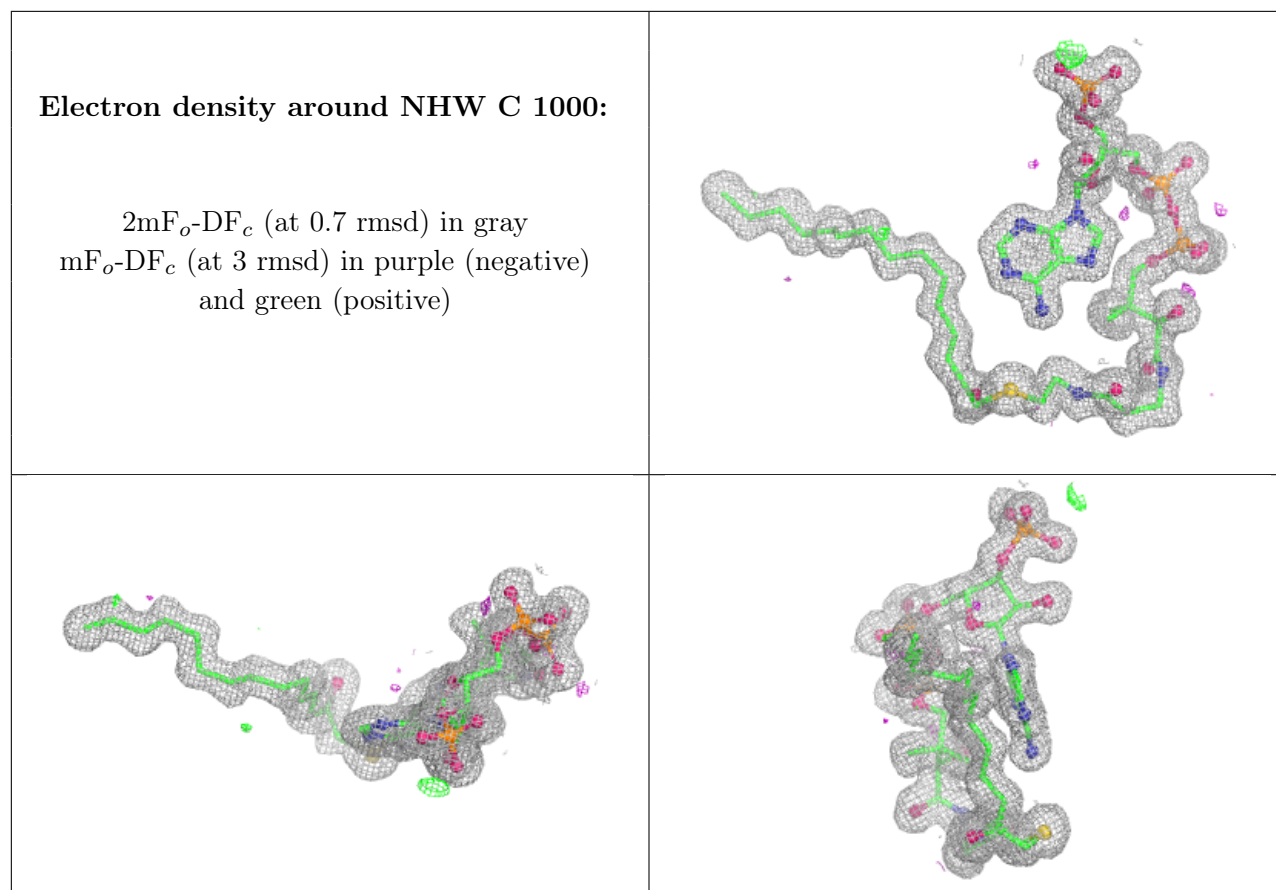
Electron density around NHW A 1000:

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

**Electron density around NHW 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.