



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:09 PM UTC

PDB ID : 4CAE / pdb_00004cae
Title : Plasmodium vivax N-myristoyltransferase in complex with a benzothiophene inhibitor (compound 20b)
Authors : Rackham, M.D.; Brannigan, J.A.; Rangachari, K.; Wilkinson, A.J.; Holder, A.A.; Tate, E.W.; Leatherbarrow, R.J.
Deposited on : 2013-10-08
Resolution : 1.46 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)
Xtrriage (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

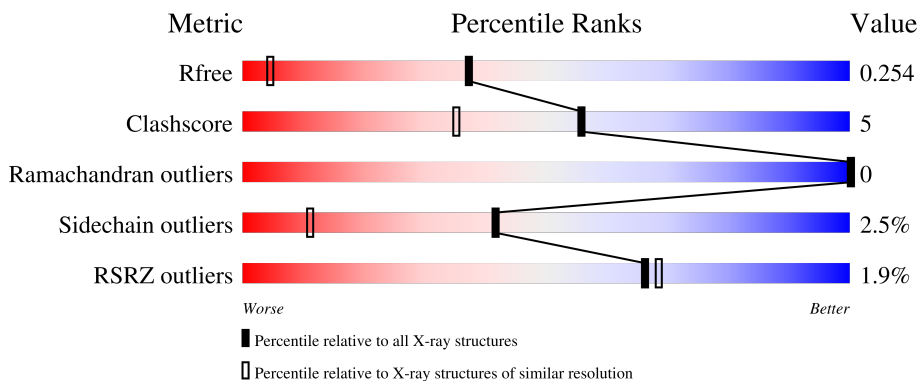
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



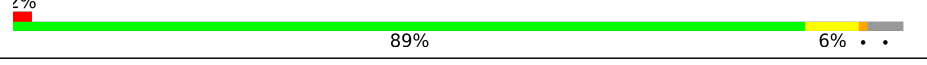
The reported resolution of this entry is 1.46 Å.

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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	384	 2% 81% 17% .
1	B	384	 2% 89% 10% .
1	C	384	 2% 89% 6% . .

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
5	DMS	B	1415	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11329 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
			Total	C	N	O	S			
1	A	384	3321	2162	540	607	12	0	25	0
1	B	384	3278	2139	531	596	12	3	18	0
1	C	367	3133	2045	499	579	10	1	17	0

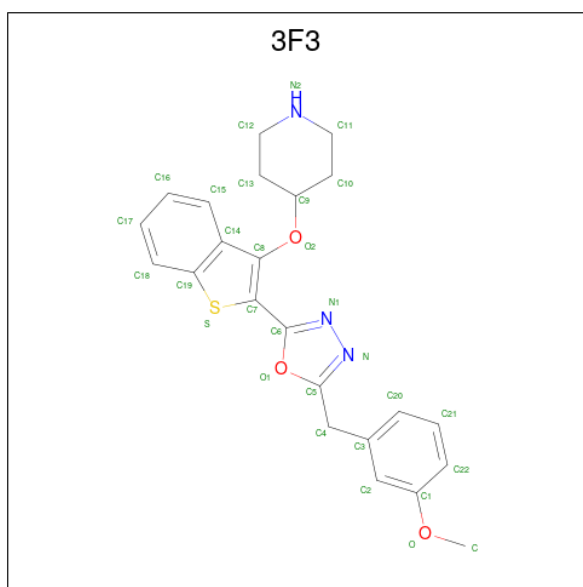
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

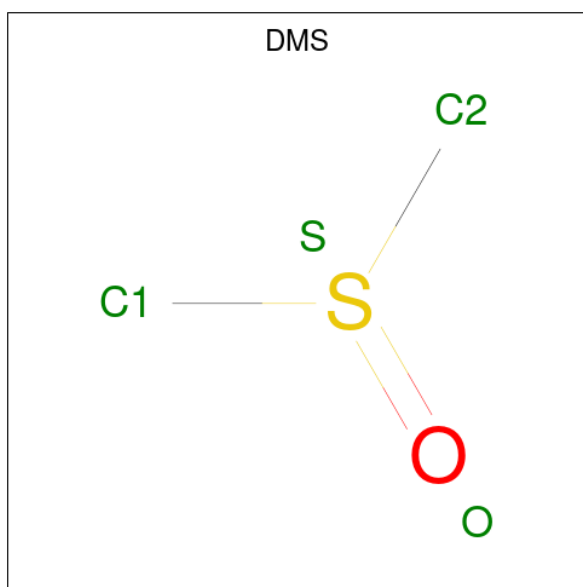
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Cl 2	0	0
3	B	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0

- Molecule 4 is 4-[(2-{5-[(3-METHOXYPHENYL)METHYL]-1,3,4-OXADIAZOL-2-YL}-1-BENZOTHIOPHEN-3-YL)OXY]PIPERIDINE (CCD ID: 3F3) (formula: C₂₃H₂₃N₃O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			30	23	3	3	1		
4	B	1	Total	C	N	O	S	0	0
			30	23	3	3	1		
4	C	1	Total	C	N	O	S	0	0
			30	23	3	3	1		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



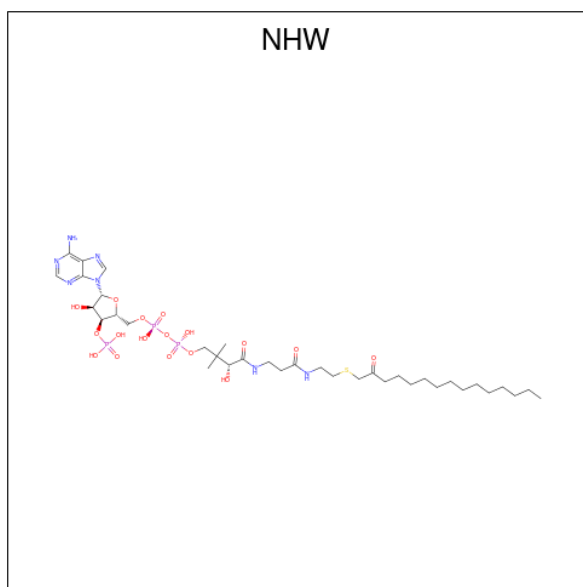
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

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

- Molecule 6 is 2-oxopentadecyl-CoA (CCD ID: NHW) (formula: $C_{36}H_{64}N_7O_{17}P_3S$).



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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

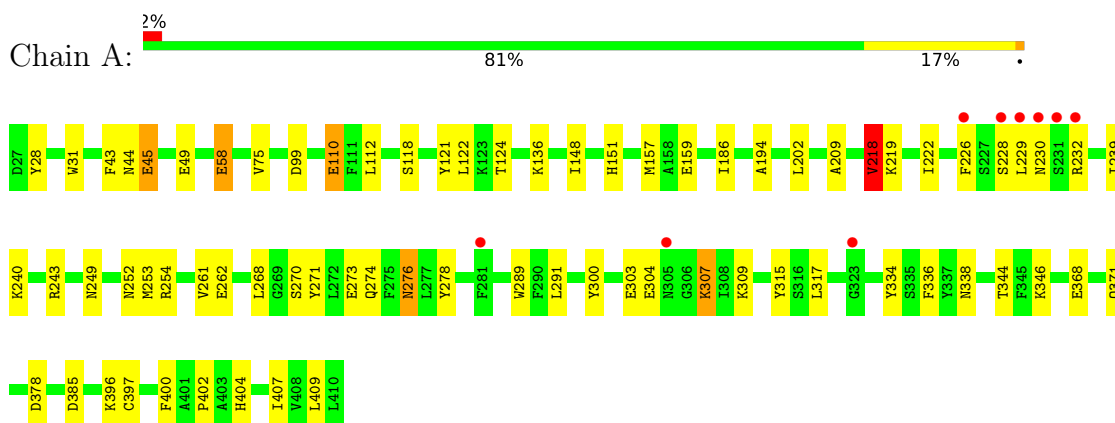
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	437	Total	O	0	0
			437	437		
8	B	453	Total	O	0	0
			453	453		
8	C	401	Total	O	0	0
			401	401		

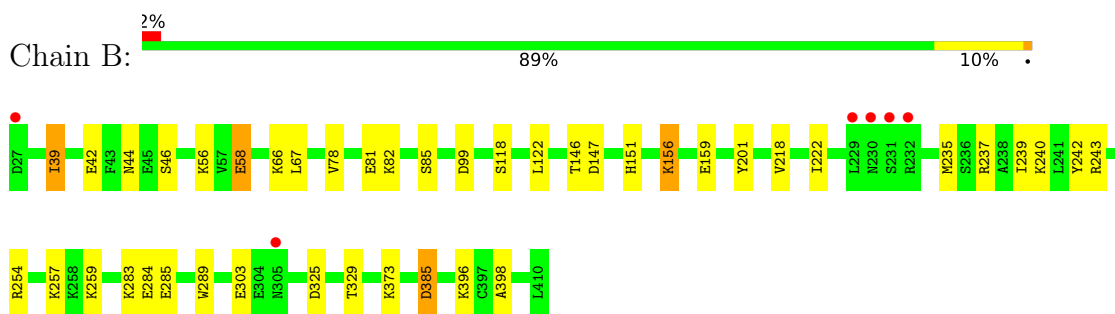
3 Residue-property plots [i](#)

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.

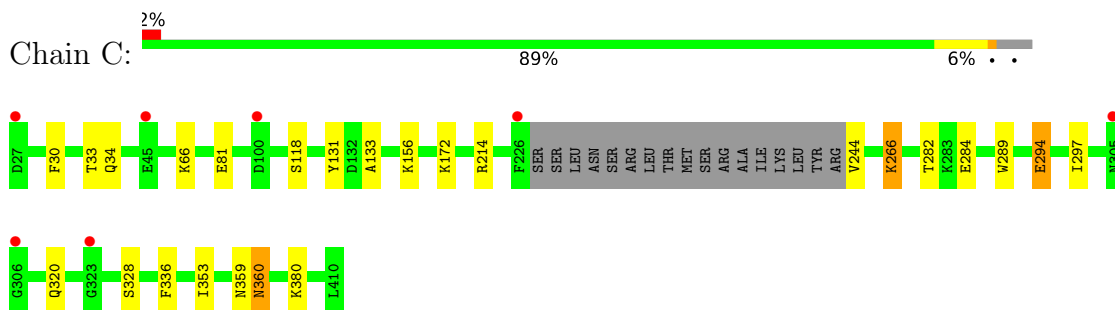
- Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.50Å 121.05Å 178.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.22 – 1.46 100.22 – 1.46	Depositor EDS
% Data completeness (in resolution range)	99.4 (100.22-1.46) 99.4 (100.22-1.46)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.46Å)	Xtrriage
Refinement program	REFMAC 5.8.0029	Depositor
R, R_{free}	0.215 , 0.254 0.214 , 0.254	Depositor DCC
R_{free} test set	10864 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtrriage
Anisotropy	0.265	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11329	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: CL, DMS, SO4, MG, NHW, 3F3

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	1.23	8/3468 (0.2%)	1.19	13/4694 (0.3%)
1	B	1.21	4/3411 (0.1%)	1.12	2/4617 (0.0%)
1	C	1.17	2/3257 (0.1%)	1.13	1/4412 (0.0%)
All	All	1.20	14/10136 (0.1%)	1.15	16/13723 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	336	PHE	CA-C	7.28	1.56	1.52
1	A	336	PHE	CA-C	6.38	1.56	1.52
1	B	303	GLU	C-O	-6.35	1.16	1.24
1	A	278	TYR	C-O	-6.12	1.16	1.23
1	A	276[A]	ASN	C-O	5.78	1.31	1.24
1	A	276[B]	ASN	C-O	5.78	1.31	1.24
1	C	297	ILE	C-O	5.77	1.29	1.24
1	A	112	LEU	C-O	-5.71	1.17	1.24
1	B	259	LYS	N-CA	5.64	1.53	1.46
1	B	373	LYS	CA-C	5.45	1.60	1.52
1	A	315	TYR	N-CA	5.38	1.52	1.45
1	A	407	ILE	C-O	5.22	1.29	1.23
1	A	338	ASN	N-CA	-5.19	1.39	1.46
1	B	67	LEU	C-O	-5.07	1.20	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	VAL	N-CA-C	6.79	117.49	110.36
1	A	202	LEU	CA-C-N	-6.22	112.58	120.23
1	A	202	LEU	C-N-CA	-6.22	112.58	120.23
1	A	252	ASN	N-CA-C	6.18	120.44	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	ASP	N-CA-C	6.06	120.75	113.23
1	A	268	LEU	N-CA-C	5.67	117.54	111.36
1	A	291	LEU	CA-C-N	-5.63	113.96	119.76
1	A	291	LEU	C-N-CA	-5.63	113.96	119.76
1	A	209	ALA	N-CA-C	5.55	117.46	108.41
1	B	385	ASP	CB-CA-C	-5.45	100.17	109.65
1	A	218[A]	VAL	N-CA-C	5.32	115.95	110.36
1	A	218[B]	VAL	N-CA-C	5.32	115.95	110.36
1	B	396	LYS	N-CA-CB	-5.29	101.81	110.43
1	C	282	THR	CB-CA-C	-5.21	100.66	110.51
1	A	186	ILE	N-CA-C	-5.15	105.38	111.00
1	A	226	PHE	N-CA-C	-5.09	105.82	112.23

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	3321	0	3353	46	0
1	B	3278	0	3310	36	0
1	C	3133	0	3128	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	30	0	23	1	0
4	B	30	0	23	0	0
4	C	30	0	23	0	0
5	A	4	0	6	1	0
5	B	4	0	6	5	0
5	C	4	0	6	1	0
6	A	64	0	60	1	0
6	B	64	0	60	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	64	0	60	0	0
7	B	5	0	0	0	0
8	A	437	0	0	7	0
8	B	453	0	0	8	0
8	C	401	0	0	5	0
All	All	11329	0	10058	95	0

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

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:PHE:O	1:C:33[A]:THR:HG22	1.42	1.19
1:B:289:TRP:CE2	5:B:1415:DMS:H21	1.99	0.97
1:A:344:THR:HG21	1:B:42[B]:GLU:HG2	1.53	0.87
1:A:344:THR:HG21	1:B:42[B]:GLU:CG	2.07	0.84
1:B:240:LYS:HG3	1:B:243[A]:ARG:NH2	1.93	0.84
1:B:289:TRP:CZ2	5:B:1415:DMS:H21	2.13	0.82
1:A:262[B]:GLU:HG3	8:A:2318:HOH:O	1.81	0.81
1:A:122:LEU:HB3	1:A:124:THR:HG22	1.65	0.78
1:A:159:GLU:CD	1:A:409:LEU:HD22	2.14	0.71
1:A:148:ILE:HB	1:A:157:MET:HE3	1.74	0.69
1:B:159:GLU:OE2	5:B:1415:DMS:H13	1.96	0.65
1:C:266:LYS:HG2	8:C:2285:HOH:O	1.96	0.64
1:A:218[B]:VAL:CG2	1:A:239:ILE:HG12	2.28	0.63
1:B:240:LYS:CG	1:B:243[A]:ARG:NH2	2.62	0.62
1:A:218[B]:VAL:HG21	1:A:239:ILE:HA	1.80	0.61
1:A:218[B]:VAL:HG21	1:A:239:ILE:HG12	1.82	0.61
1:B:257[B]:LYS:HD2	8:B:2322:HOH:O	1.99	0.61
1:B:289:TRP:NE1	5:B:1415:DMS:H21	2.17	0.59
1:A:194:ALA:HB2	6:A:1422:NHW:HDM	1.86	0.57
1:B:218:VAL:CG1	1:B:239[B]:ILE:HD13	2.35	0.56
1:B:218:VAL:HB	1:B:239[B]:ILE:CD1	2.36	0.56
1:A:371:GLN:HG2	8:A:2337:HOH:O	2.05	0.56
1:A:317:LEU:HB3	1:A:334:TYR:CE1	2.43	0.53
1:C:156[B]:LYS:NZ	1:C:156[B]:LYS:HB3	2.24	0.53
1:B:235:MET:O	1:B:239[B]:ILE:HG12	2.07	0.53
1:A:151[B]:HIS:CD2	8:A:2021:HOH:O	2.62	0.53
1:A:346:LYS:HE2	1:A:378:ASP:HB3	1.91	0.52
4:A:1414:3F3:C15	4:A:1414:3F3:H9	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222[A]:ILE:HD12	1:A:229:LEU:HG	1.93	0.51
1:A:118:SER:O	1:A:121[A]:TYR:HB3	2.10	0.50
1:B:329:THR:HG23	8:B:2161:HOH:O	2.10	0.50
1:B:156[A]:LYS:HE2	1:B:156[A]:LYS:HA	1.95	0.49
1:A:230[B]:ASN:HD22	1:A:232:ARG:HD2	1.78	0.49
1:A:368:GLU:O	1:A:402:PRO:HB2	2.13	0.49
1:C:294:GLU:HG3	8:C:2157:HOH:O	2.12	0.49
1:B:283:LYS:HD2	8:B:2333:HOH:O	2.12	0.48
1:A:110[A]:GLU:HG3	8:A:2159:HOH:O	2.11	0.48
1:B:78:VAL:HG12	8:B:2094:HOH:O	2.12	0.48
1:B:254:ARG:NH1	1:B:257[B]:LYS:HD3	2.29	0.48
1:B:147:ASP:OD2	1:B:156[B]:LYS:HE2	2.14	0.48
1:A:404:HIS:HE1	8:A:2427:HOH:O	1.97	0.47
1:B:243[A]:ARG:CZ	8:B:2291:HOH:O	2.62	0.47
1:B:218:VAL:HG21	1:B:242:TYR:HB2	1.95	0.47
1:A:121[A]:TYR:CD1	1:A:121[A]:TYR:C	2.92	0.47
1:C:118:SER:HB3	1:C:289:TRP:CZ2	2.49	0.47
1:C:328:SER:HA	8:C:2329:HOH:O	2.14	0.47
1:B:284[A]:GLU:HG3	1:B:285:GLU:N	2.30	0.47
1:C:214:ARG:HG2	1:C:353:ILE:HD13	1.96	0.47
1:A:218[B]:VAL:HG23	1:A:219:LYS:N	2.30	0.47
1:C:284[A]:GLU:H	1:C:284[A]:GLU:CD	2.23	0.47
1:B:237:ARG:NH2	8:B:2285:HOH:O	2.48	0.46
1:A:249:ASN:ND2	8:A:2303:HOH:O	2.48	0.46
1:A:289:TRP:CE2	5:A:1415:DMS:H11	2.50	0.46
1:A:303:GLU:HA	1:A:307:LYS:O	2.15	0.46
1:C:131:TYR:CE2	1:C:133:ALA:HB3	2.51	0.46
1:A:58:GLU:O	1:A:58:GLU:HG3	2.16	0.46
1:A:43:PHE:CZ	1:A:396:LYS:HG3	2.51	0.45
1:B:218:VAL:HB	1:B:239[B]:ILE:HD13	1.98	0.45
1:A:45:GLU:O	1:A:151[A]:HIS:CE1	2.70	0.45
1:A:151[B]:HIS:CD2	1:A:397:CYS:HB2	2.53	0.44
1:A:218[B]:VAL:HG23	1:A:219:LYS:H	1.82	0.44
1:B:39:ILE:HD11	1:B:201:TYR:HE2	1.82	0.44
1:B:56:LYS:HB3	1:B:58:GLU:HG2	1.98	0.44
1:B:218:VAL:O	1:B:222[A]:ILE:HG12	2.18	0.44
1:B:325:ASP:OD1	1:B:325:ASP:N	2.50	0.43
1:C:266:LYS:HB2	1:C:266:LYS:HE2	1.65	0.43
1:B:118:SER:HB3	1:B:289:TRP:CZ2	2.53	0.43
1:A:304:GLU:O	1:A:307:LYS:HB2	2.18	0.43
1:B:66:LYS:HE3	8:B:2082:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146[B]:THR:HG21	5:B:1415:DMS:H22	2.01	0.43
1:B:243[A]:ARG:HE	1:B:243[A]:ARG:HB3	1.34	0.43
1:B:44[B]:ASN:HD22	1:B:46:SER:H	1.67	0.43
1:C:33[A]:THR:HG23	1:C:34:GLN:OE1	2.18	0.43
1:C:359:ASN:O	1:C:360[A]:ASN:HB2	2.19	0.43
1:A:271:TYR:HE1	1:A:371:GLN:NE2	2.17	0.42
5:C:1414:DMS:H13	8:C:2345:HOH:O	2.19	0.42
1:A:274:GLN:HB3	8:A:2328:HOH:O	2.20	0.42
1:A:270[A]:SER:OG	1:A:273[A]:GLU:OE2	2.33	0.42
1:A:136:LYS:HA	1:A:136:LYS:HD2	1.70	0.42
1:A:276[A]:ASN:ND2	1:A:400:PHE:CE1	2.85	0.42
1:B:151[B]:HIS:HE1	1:B:398:ALA:O	2.03	0.42
1:A:49:GLU:OE2	1:A:396:LYS:NZ	2.53	0.41
1:A:304:GLU:HB2	1:A:309:LYS:HG3	2.02	0.41
1:B:85:SER:HB2	8:B:2111:HOH:O	2.20	0.41
1:C:172:LYS:HE3	8:C:2203:HOH:O	2.19	0.41
1:A:240[A]:LYS:HG3	1:A:243[A]:ARG:NH2	2.35	0.41
1:A:28:TYR:HB3	1:A:31:TRP:HB2	2.02	0.41
1:B:39:ILE:HD11	1:B:201:TYR:CE2	2.56	0.41
1:A:254[B]:ARG:NH2	1:A:303:GLU:OE1	2.49	0.40
1:A:396:LYS:HB2	1:A:396:LYS:HE3	1.67	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	407/384 (106%)	395 (97%)	12 (3%)	0	100	100
1	B	400/384 (104%)	392 (98%)	8 (2%)	0	100	100
1	C	380/384 (99%)	367 (97%)	13 (3%)	0	100	100
All	All	1187/1152 (103%)	1154 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	375/350 (107%)	361 (96%)	14 (4%)	30 4
1	B	368/350 (105%)	359 (98%)	9 (2%)	43 12
1	C	351/350 (100%)	341 (97%)	10 (3%)	38 8
All	All	1094/1050 (104%)	1061 (97%)	33 (3%)	42 7

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

Mol	Chain	Res	Type
1	A	44[A]	ASN
1	A	44[B]	ASN
1	A	45	GLU
1	A	58	GLU
1	A	75	VAL
1	A	99	ASP
1	A	110[A]	GLU
1	A	110[B]	GLU
1	A	218[A]	VAL
1	A	218[B]	VAL
1	A	228	SER
1	A	253[A]	MET
1	A	253[B]	MET
1	A	307	LYS
1	B	39	ILE
1	B	58	GLU
1	B	81	GLU
1	B	82	LYS
1	B	99	ASP
1	B	122	LEU
1	B	156[A]	LYS
1	B	156[B]	LYS
1	B	385	ASP

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Mol	Chain	Res	Type
1	C	66[A]	LYS
1	C	66[B]	LYS
1	C	81	GLU
1	C	244	VAL
1	C	266	LYS
1	C	294	GLU
1	C	320	GLN
1	C	360[A]	ASN
1	C	360[B]	ASN
1	C	380	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	249	ASN
1	A	252	ASN
1	A	350	GLN
1	A	359	ASN
1	A	372	ASN
1	B	34	GLN
1	B	106	ASN
1	B	187	ASN
1	B	249	ASN
1	B	359	ASN
1	B	360	ASN
1	B	372	ASN
1	C	302	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 7 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
7	SO4	B	1411	-	4,4,4	0.38	0	6,6,6	0.72	0
5	DMS	A	1415	-	3,3,3	0.36	0	3,3,3	1.14	0
4	3F3	B	1414	-	34,34,34	2.03	9 (26%)	41,47,47	2.65	13 (31%)
6	NHW	C	1422	2	64,66,66	1.52	10 (15%)	87,92,92	1.78	18 (20%)
4	3F3	C	1413	-	34,34,34	2.09	8 (23%)	41,47,47	2.46	13 (31%)
5	DMS	B	1415	-	3,3,3	0.30	0	3,3,3	2.24	2 (66%)
4	3F3	A	1414	-	34,34,34	2.26	8 (23%)	41,47,47	3.31	20 (48%)
5	DMS	C	1414	-	3,3,3	0.37	0	3,3,3	1.35	1 (33%)
6	NHW	A	1422	2	64,66,66	1.34	9 (14%)	87,92,92	1.52	18 (20%)
6	NHW	B	1422	2	64,66,66	1.44	11 (17%)	87,92,92	1.46	16 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3F3	B	1414	-	-	3/14/22/22	0/5/5/5
6	NHW	C	1422	2	-	1/65/81/81	0/3/3/3
4	3F3	C	1413	-	-	3/14/22/22	0/5/5/5
4	3F3	A	1414	-	-	1/14/22/22	0/5/5/5
6	NHW	B	1422	2	-	3/65/81/81	0/3/3/3
6	NHW	A	1422	2	-	4/65/81/81	0/3/3/3

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1414	3F3	C14-C19	7.50	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1414	3F3	C8-C7	6.77	1.47	1.37
4	B	1414	3F3	C8-C7	6.00	1.46	1.37
4	C	1413	3F3	C14-C19	5.23	1.48	1.41
4	C	1413	3F3	C5-N	5.14	1.35	1.28
4	B	1414	3F3	C5-N	5.06	1.35	1.28
6	C	1422	NHW	P1A-O3A	4.83	1.64	1.59
4	A	1414	3F3	C5-N	4.81	1.34	1.28
4	C	1413	3F3	C8-C7	4.79	1.44	1.37
6	B	1422	NHW	C6-C5	4.33	1.60	1.51
4	B	1414	3F3	C14-C19	4.19	1.47	1.41
6	C	1422	NHW	O10-C10	4.05	1.49	1.42
6	C	1422	NHW	O4X-C4X	4.00	1.53	1.45
6	C	1422	NHW	C12-C11	3.90	1.59	1.52
4	C	1413	3F3	C6-N1	3.86	1.32	1.29
6	B	1422	NHW	P3X-O3X	3.61	1.65	1.59
4	B	1414	3F3	C19-S	-3.45	1.67	1.74
6	A	1422	NHW	P3X-O3X	3.44	1.65	1.59
6	B	1422	NHW	CP-S1	3.30	1.89	1.81
6	C	1422	NHW	C5A-N7A	-3.30	1.33	1.39
6	B	1422	NHW	P2A-O3A	3.24	1.63	1.59
6	A	1422	NHW	P1A-O3A	-3.09	1.56	1.59
6	B	1422	NHW	P3X-O8A	3.06	1.66	1.54
4	C	1413	3F3	O1-C5	3.00	1.41	1.36
6	A	1422	NHW	P3X-O7A	-2.82	1.44	1.54
4	B	1414	3F3	O1-C5	2.79	1.41	1.36
4	B	1414	3F3	C16-C17	2.76	1.44	1.38
4	C	1413	3F3	C19-S	-2.75	1.68	1.74
6	B	1422	NHW	C5A-C4A	2.63	1.43	1.39
4	A	1414	3F3	C4-C5	2.63	1.53	1.50
6	B	1422	NHW	C8A-N7A	2.56	1.36	1.31
6	C	1422	NHW	P3X-O7A	-2.56	1.45	1.54
6	B	1422	NHW	P1A-O2A	-2.50	1.43	1.55
6	C	1422	NHW	C7-N8	2.49	1.51	1.46
4	B	1414	3F3	C14-C8	2.47	1.51	1.45
6	A	1422	NHW	C8A-N7A	2.39	1.36	1.31
4	A	1414	3F3	C2-C3	2.39	1.43	1.39
6	B	1422	NHW	P2A-O4A	-2.38	1.44	1.55
4	A	1414	3F3	C19-S	-2.37	1.69	1.74
4	A	1414	3F3	C18-C19	-2.35	1.36	1.39
6	A	1422	NHW	C5A-N7A	-2.34	1.34	1.39
4	B	1414	3F3	C6-N1	2.33	1.31	1.29
4	C	1413	3F3	C14-C8	2.32	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1422	NHW	C4A-N9A	-2.32	1.32	1.37
6	A	1422	NHW	C7-C6	2.31	1.59	1.51
4	B	1414	3F3	O2-C9	-2.29	1.41	1.46
6	A	1422	NHW	P2A-O3A	-2.19	1.57	1.59
6	A	1422	NHW	C4A-N3A	2.19	1.38	1.34
4	C	1413	3F3	C18-C19	-2.11	1.36	1.39
4	A	1414	3F3	C7-S	-2.09	1.70	1.74
6	C	1422	NHW	P2A-O3A	-2.08	1.57	1.59
6	C	1422	NHW	P2A-O4A	-2.04	1.45	1.55
6	C	1422	NHW	C8A-N7A	2.03	1.35	1.31
6	B	1422	NHW	P3X-O7A	-2.02	1.47	1.54
6	A	1422	NHW	O6A-C12	2.02	1.50	1.43

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1414	3F3	O1-C5-C4	11.10	128.79	117.73
4	C	1413	3F3	O1-C5-C4	10.15	127.84	117.73
4	A	1414	3F3	C5-N-N1	8.80	111.03	106.25
4	A	1414	3F3	O1-C5-N	-8.38	106.03	112.75
4	B	1414	3F3	O1-C5-C4	7.38	125.08	117.73
4	B	1414	3F3	C5-N-N1	6.59	109.83	106.25
4	B	1414	3F3	C6-N1-N	-5.98	101.34	106.03
4	C	1413	3F3	O1-C5-N	-5.52	108.32	112.75
4	B	1414	3F3	O1-C6-N1	5.35	118.01	113.00
4	B	1414	3F3	O1-C5-N	-5.27	108.53	112.75
4	A	1414	3F3	C6-N1-N	-5.25	101.91	106.03
6	C	1422	NHW	C5A-C4A-N3A	-5.16	119.61	126.72
6	C	1422	NHW	N9A-C8A-N7A	-5.12	106.68	113.94
6	C	1422	NHW	N3A-C2A-N1A	-5.05	120.94	128.58
4	C	1413	3F3	C5-N-N1	4.72	108.81	106.25
6	C	1422	NHW	N3A-C4A-N9A	4.20	134.32	127.17
6	B	1422	NHW	N3A-C2A-N1A	-4.14	122.32	128.58
6	C	1422	NHW	C4A-N9A-C8A	4.03	109.97	105.74
6	A	1422	NHW	C13-C11-C10	3.95	115.50	108.77
6	C	1422	NHW	C2A-N3A-C4A	3.89	121.33	111.83
6	C	1422	NHW	O1M-C1M-CP	-3.88	116.64	122.17
6	B	1422	NHW	C5A-C4A-N3A	-3.88	121.38	126.72
6	C	1422	NHW	C5A-N7A-C8A	3.83	109.47	103.45
6	A	1422	NHW	O1M-C1M-CP	-3.79	116.76	122.17
6	A	1422	NHW	C5A-C4A-N3A	-3.78	121.50	126.72
4	B	1414	3F3	C4-C3-C20	-3.78	115.33	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1414	3F3	C8-C7-S	3.73	114.21	111.49
6	C	1422	NHW	O6A-C12-C11	-3.67	104.65	110.55
6	A	1422	NHW	CP-C1M-C2M	3.56	123.08	115.55
4	A	1414	3F3	C14-C19-S	3.51	116.36	112.24
4	B	1414	3F3	C19-S-C7	3.44	94.68	91.02
4	A	1414	3F3	C5-O1-C6	3.37	105.86	102.67
6	A	1422	NHW	C13-C11-C12	-3.36	102.67	108.22
6	A	1422	NHW	C2A-N1A-C6A	3.28	124.12	118.73
4	A	1414	3F3	C17-C16-C15	3.27	124.28	120.24
4	A	1414	3F3	C19-C14-C8	-3.26	105.73	110.45
6	B	1422	NHW	P3X-O3X-C3X	-3.23	114.81	123.43
6	B	1422	NHW	O1M-C1M-CP	-3.20	117.61	122.17
6	B	1422	NHW	C2A-N1A-C6A	3.17	123.94	118.73
4	A	1414	3F3	C4-C3-C20	-3.17	116.23	120.89
4	B	1414	3F3	C18-C19-C14	-3.16	118.16	121.47
4	C	1413	3F3	C18-C19-C14	-3.15	118.17	121.47
6	A	1422	NHW	N3A-C2A-N1A	-3.14	123.83	128.58
6	B	1422	NHW	C13-C11-C10	3.10	114.06	108.77
6	B	1422	NHW	C6-C7-N8	-3.04	105.52	112.00
6	B	1422	NHW	O3A-P2A-O5A	-3.04	101.56	110.70
4	A	1414	3F3	C16-C15-C14	-2.97	114.43	119.80
6	C	1422	NHW	C2X-C1X-N9A	-2.97	105.94	113.30
6	C	1422	NHW	C14-C11-C10	2.94	113.78	108.77
4	B	1414	3F3	C16-C17-C18	-2.92	116.63	120.24
4	A	1414	3F3	C-O-C1	2.91	123.75	117.50
4	C	1413	3F3	C19-C14-C8	-2.86	106.31	110.45
6	A	1422	NHW	C5X-C4X-C3X	-2.79	105.10	114.38
5	B	1415	DMS	C2-S-C1	2.77	112.62	98.42
4	C	1413	3F3	C19-S-C7	2.75	93.95	91.02
4	C	1413	3F3	C11-N2-C12	2.74	118.14	110.40
6	A	1422	NHW	C4A-C5A-N7A	-2.73	107.46	110.58
4	B	1414	3F3	C1-C2-C3	-2.71	116.79	119.76
6	B	1422	NHW	C2A-N3A-C4A	2.69	118.40	111.83
4	A	1414	3F3	C15-C14-C19	2.64	121.78	118.77
6	B	1422	NHW	C4A-C5A-N7A	-2.64	107.57	110.58
6	C	1422	NHW	O3A-P2A-O5A	-2.62	102.83	110.70
6	A	1422	NHW	C2-C3-N4	-2.59	107.00	112.41
6	B	1422	NHW	O3A-P1A-O1A	-2.54	103.08	110.70
6	A	1422	NHW	C4X-O4X-C1X	-2.54	103.87	109.47
4	A	1414	3F3	C21-C22-C1	2.47	122.72	118.98
6	C	1422	NHW	C4A-C5A-N7A	-2.47	107.76	110.58
6	A	1422	NHW	C2X-C1X-N9A	-2.47	107.18	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1414	3F3	C21-C20-C3	-2.45	117.16	120.61
6	C	1422	NHW	C4A-N9A-C1X	-2.44	120.93	126.63
4	C	1413	3F3	C14-C19-S	2.39	115.04	112.24
6	B	1422	NHW	O2A-P1A-O3A	2.39	113.72	107.27
4	A	1414	3F3	C10-C11-N2	2.38	115.29	110.81
6	A	1422	NHW	N9A-C8A-N7A	-2.34	110.62	113.94
4	C	1413	3F3	C17-C16-C15	-2.33	117.36	120.24
6	B	1422	NHW	N3A-C4A-N9A	2.33	131.13	127.17
6	A	1422	NHW	C5A-N7A-C8A	2.30	107.06	103.45
6	C	1422	NHW	C4X-O4X-C1X	-2.29	104.42	109.47
6	A	1422	NHW	O4A-P2A-O3A	2.28	113.42	107.27
4	B	1414	3F3	C20-C21-C22	-2.22	117.39	120.24
6	B	1422	NHW	C4A-N9A-C8A	2.21	108.06	105.74
4	A	1414	3F3	O1-C6-N1	2.20	115.06	113.00
5	C	1414	DMS	O-S-C2	2.19	117.48	106.49
4	C	1413	3F3	C13-C12-N2	-2.18	106.70	110.81
4	A	1414	3F3	C9-O2-C8	-2.16	112.09	122.72
4	C	1413	3F3	C6-N1-N	-2.14	104.35	106.03
6	B	1422	NHW	O4A-P2A-O5A	2.14	122.41	112.44
4	B	1414	3F3	C20-C3-C2	2.14	121.50	118.55
4	A	1414	3F3	C18-C19-C14	-2.14	119.22	121.47
4	A	1414	3F3	C20-C3-C2	2.13	121.48	118.55
6	C	1422	NHW	C10-C9-N8	-2.11	112.48	116.48
4	C	1413	3F3	C21-C22-C1	2.06	122.09	118.98
4	B	1414	3F3	C17-C18-C19	2.06	123.02	119.57
6	A	1422	NHW	C2-S1-CP	-2.06	98.33	101.72
6	A	1422	NHW	N3A-C4A-N9A	2.05	130.66	127.17
6	C	1422	NHW	C6-C7-N8	-2.05	107.65	112.00
5	B	1415	DMS	O-S-C1	2.03	116.66	106.49
6	B	1422	NHW	O6A-C12-C11	-2.01	107.31	110.55
6	A	1422	NHW	C6A-C5A-C4A	2.01	119.92	117.18
6	C	1422	NHW	O2A-P1A-O3A	2.01	112.71	107.27
4	C	1413	3F3	C16-C17-C18	2.01	122.72	120.24

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1414	3F3	O1-C6-C7-S
4	B	1414	3F3	N1-C6-C7-S
6	A	1422	NHW	C12-O6A-P2A-O5A
6	C	1422	NHW	C6-C7-N8-C9

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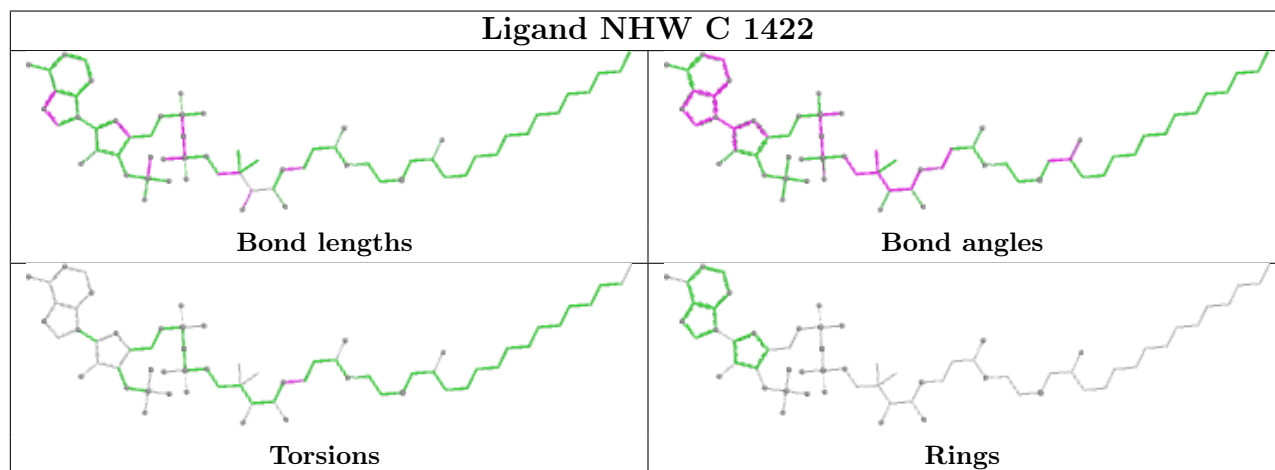
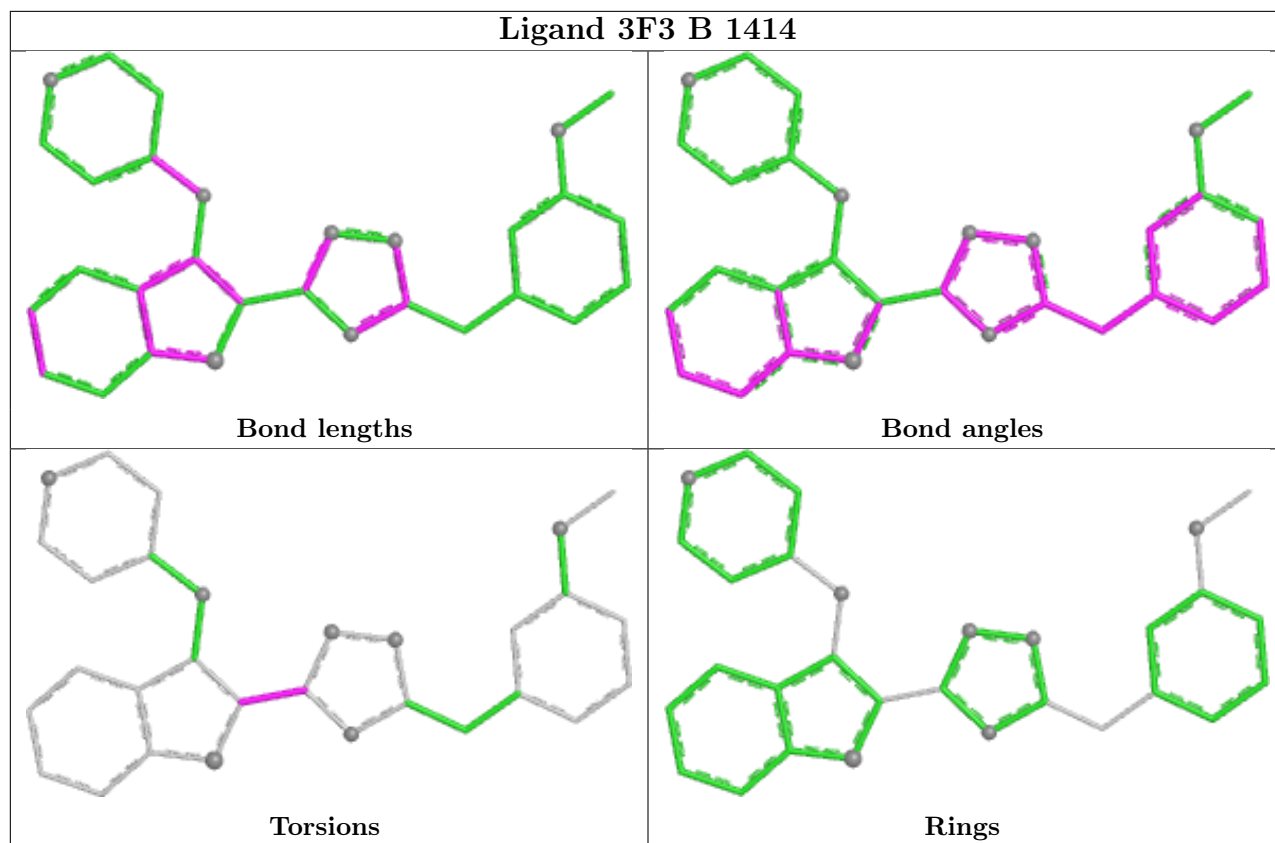
Mol	Chain	Res	Type	Atoms
4	A	1414	3F3	O1-C6-C7-C8
4	B	1414	3F3	O1-C6-C7-C8
4	C	1413	3F3	O1-C6-C7-C8
6	A	1422	NHW	C5X-O5X-P1A-O1A
6	B	1422	NHW	C6-C7-N8-C9
4	C	1413	3F3	N1-C6-C7-C8
6	B	1422	NHW	P2A-O3A-P1A-O1A
6	A	1422	NHW	C11-C12-O6A-P2A
6	B	1422	NHW	C4M-C5M-C6M-C7M
6	A	1422	NHW	C7M-C8M-C9M-CAM
4	C	1413	3F3	N1-C6-C7-S

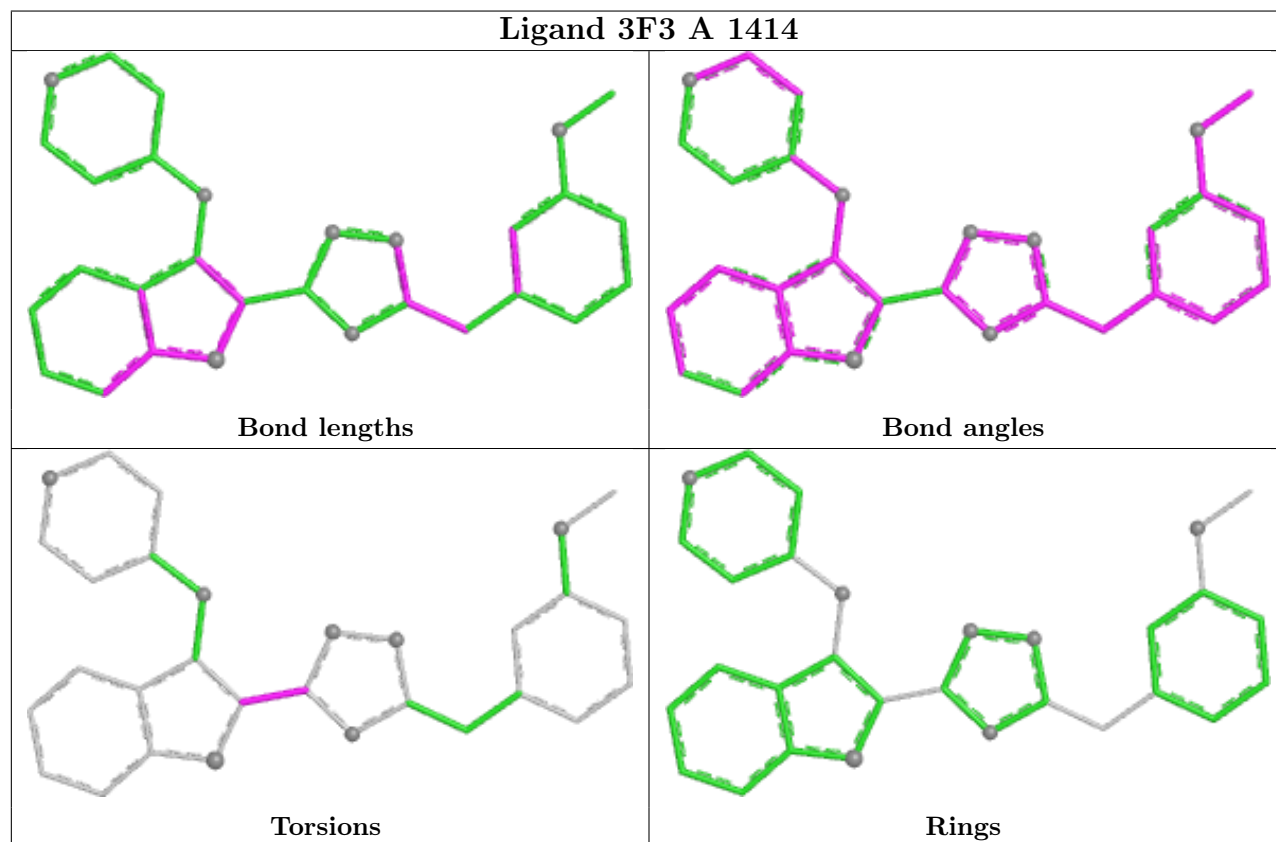
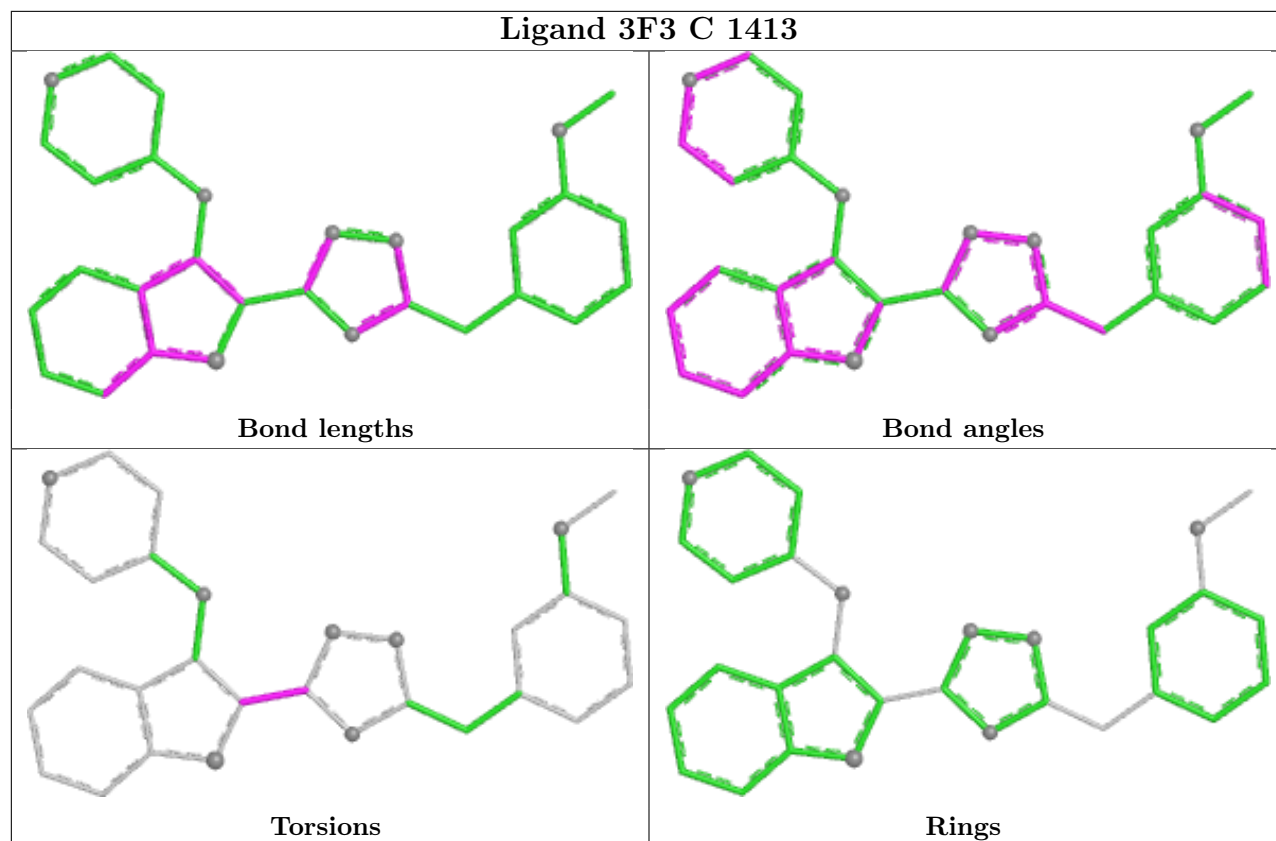
There are no ring outliers.

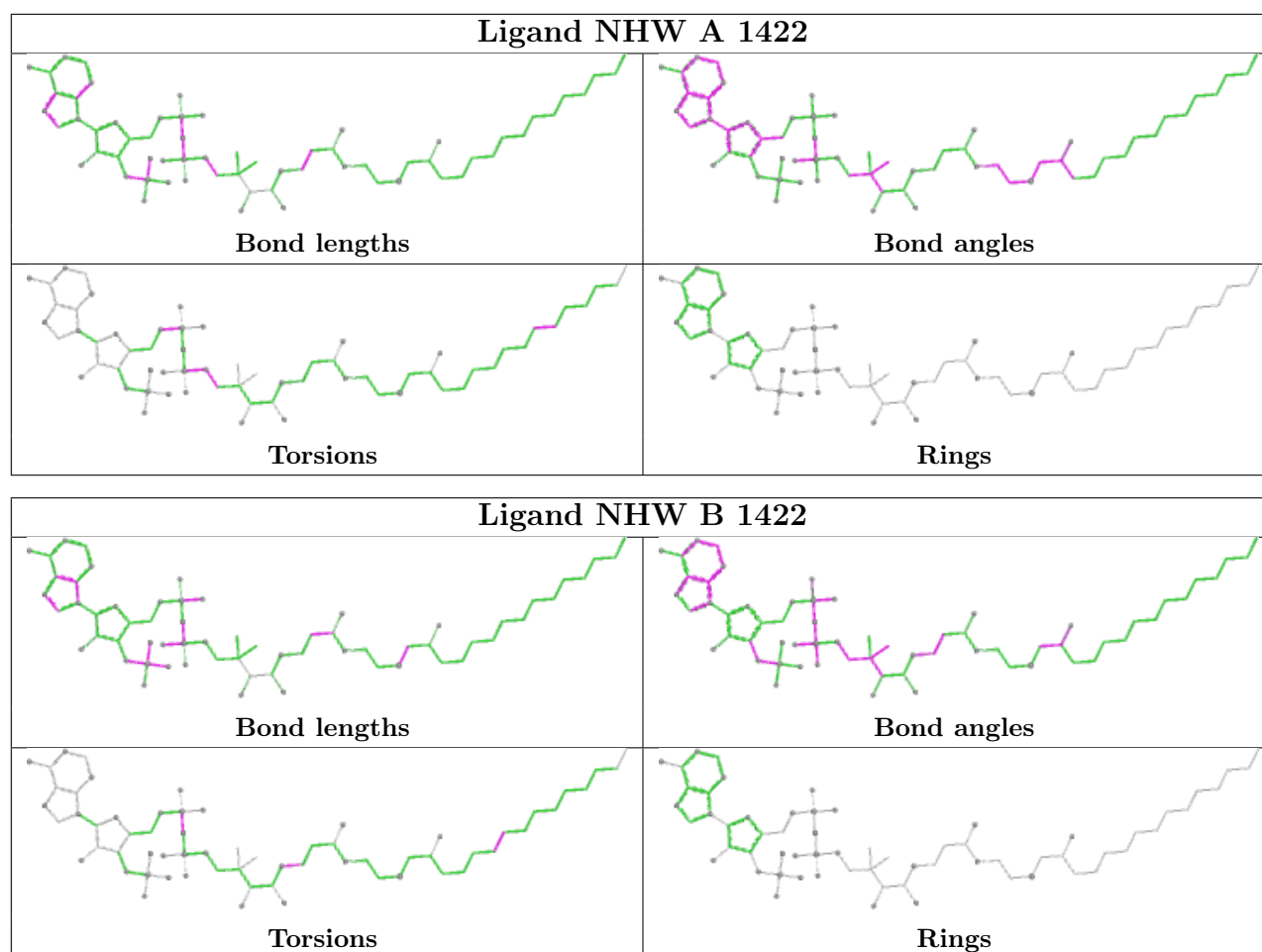
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1415	DMS	1	0
5	B	1415	DMS	5	0
4	A	1414	3F3	1	0
5	C	1414	DMS	1	0
6	A	1422	NHW	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	384/384 (100%)	0.16	9 (2%) 61 63	6, 15, 29, 60	30 (7%)
1	B	384/384 (100%)	-0.27	6 (1%) 70 73	6, 12, 25, 53	27 (7%)
1	C	367/384 (95%)	-0.15	7 (1%) 66 68	6, 13, 26, 45	27 (7%)
All	All	1135/1152 (98%)	-0.08	22 (1%) 66 68	6, 14, 28, 60	84 (7%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	PHE	3.8
1	A	231	SER	3.6
1	B	232	ARG	3.0
1	C	323	GLY	2.9
1	B	231	SER	2.7
1	A	232	ARG	2.7
1	C	27	ASP	2.6
1	A	230[A]	ASN	2.6
1	C	45	GLU	2.5
1	A	281	PHE	2.5
1	B	230	ASN	2.4
1	C	226	PHE	2.4
1	A	305	ASN	2.4
1	C	306	GLY	2.4
1	A	229	LEU	2.3
1	C	100	ASP	2.3
1	C	305	ASN	2.3
1	B	229	LEU	2.2
1	A	323	GLY	2.1
1	A	228	SER	2.1
1	B	27	ASP	2.0
1	B	305	ASN	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](#)

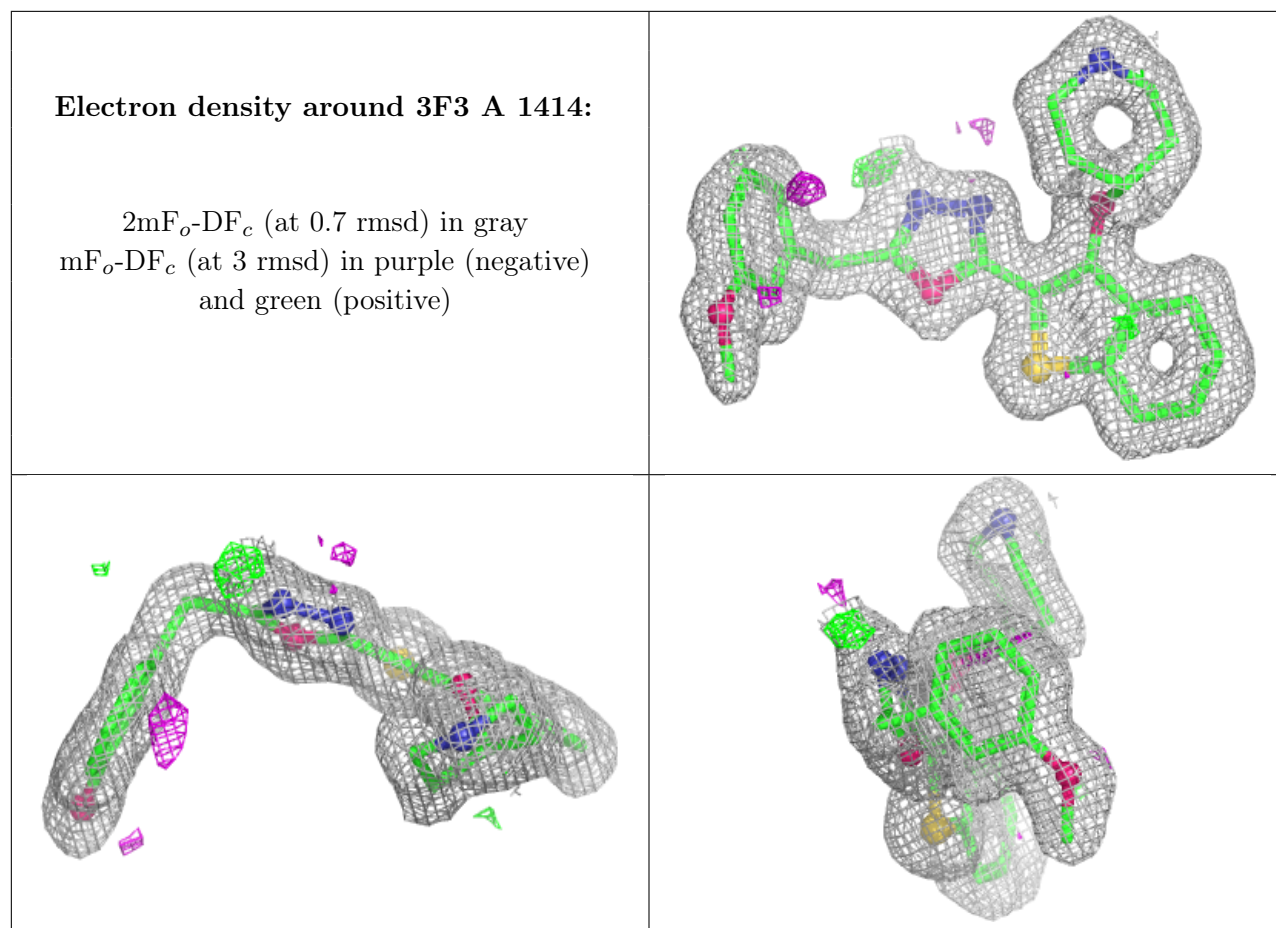
There are no oligosaccharides in this entry.

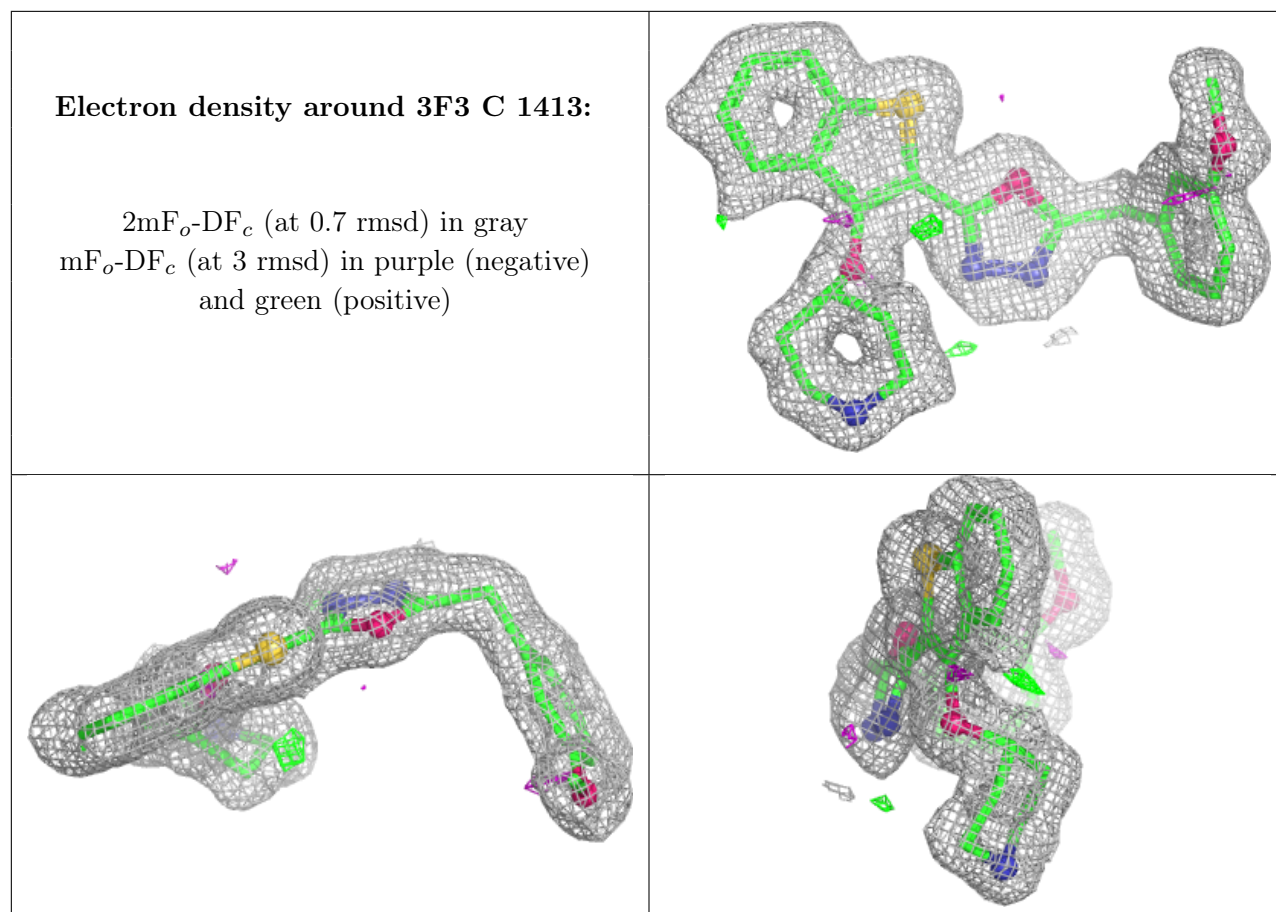
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
5	DMS	C	1414	4/4	0.91	0.17	22,25,27,28	0
7	SO4	B	1411	5/5	0.91	0.10	36,38,41,44	0
5	DMS	A	1415	4/4	0.92	0.14	27,28,30,31	0
5	DMS	B	1415	4/4	0.93	0.16	25,26,27,36	0
4	3F3	A	1414	30/30	0.96	0.07	12,16,18,21	0
4	3F3	C	1413	30/30	0.96	0.07	14,17,21,21	0
4	3F3	B	1414	30/30	0.97	0.06	10,12,14,19	0
2	MG	B	1412	1/1	0.97	0.04	21,21,21,21	0
3	CL	A	1412	1/1	0.98	0.05	34,34,34,34	0
6	NHW	A	1422	64/64	0.98	0.05	10,13,16,18	0
6	NHW	B	1422	64/64	0.98	0.04	7,10,13,14	0
6	NHW	C	1422	64/64	0.98	0.05	8,11,15,17	0
2	MG	C	1411	1/1	0.98	0.09	20,20,20,20	0
3	CL	A	1413	1/1	0.99	0.03	15,15,15,15	0
3	CL	B	1413	1/1	0.99	0.02	13,13,13,13	0
2	MG	A	1411	1/1	0.99	0.02	22,22,22,22	0
3	CL	C	1412	1/1	1.00	0.06	12,12,12,12	0

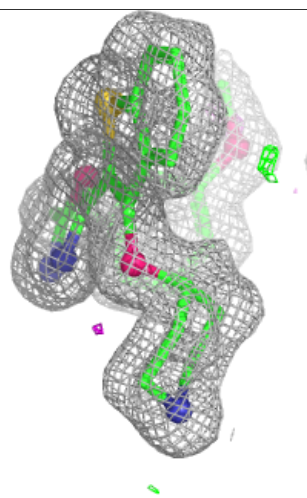
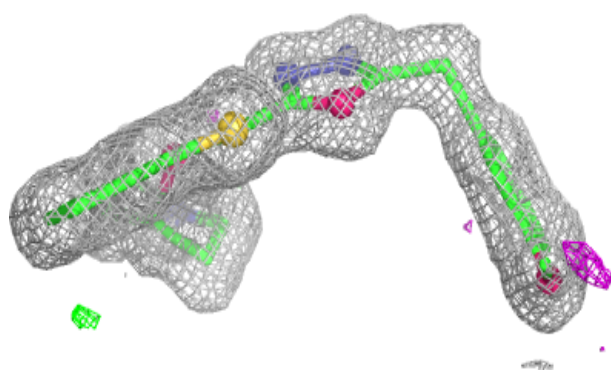
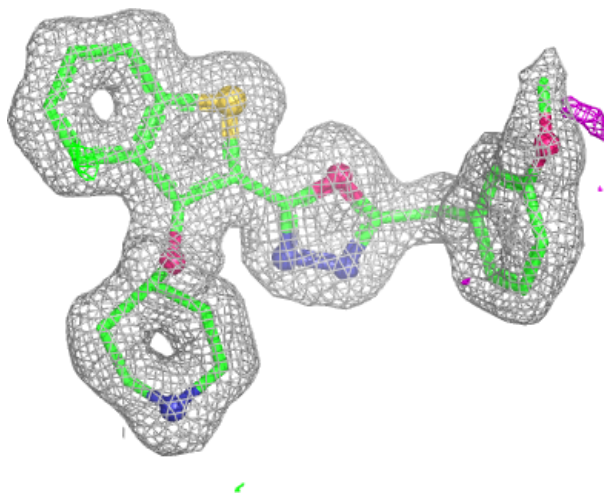
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

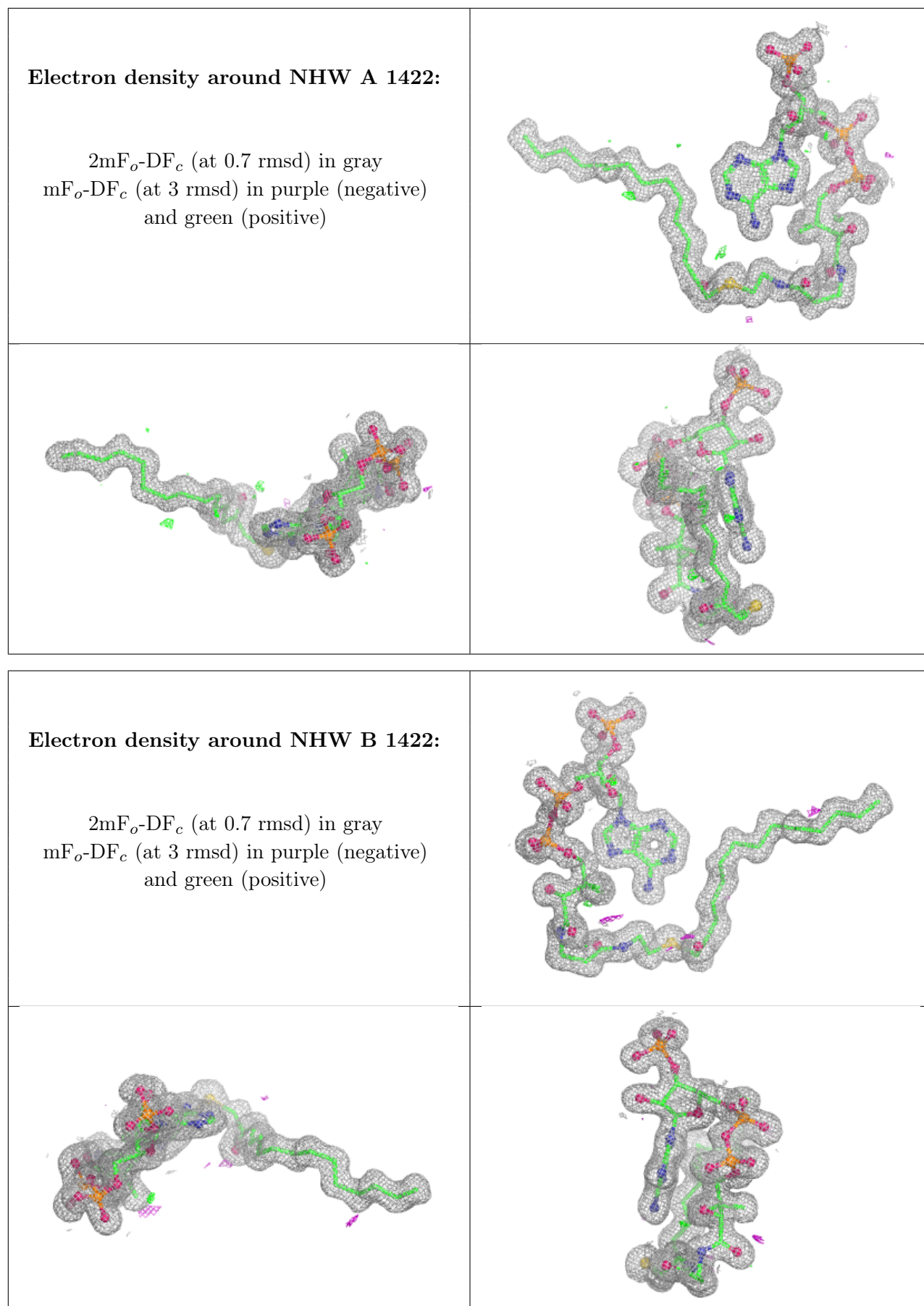


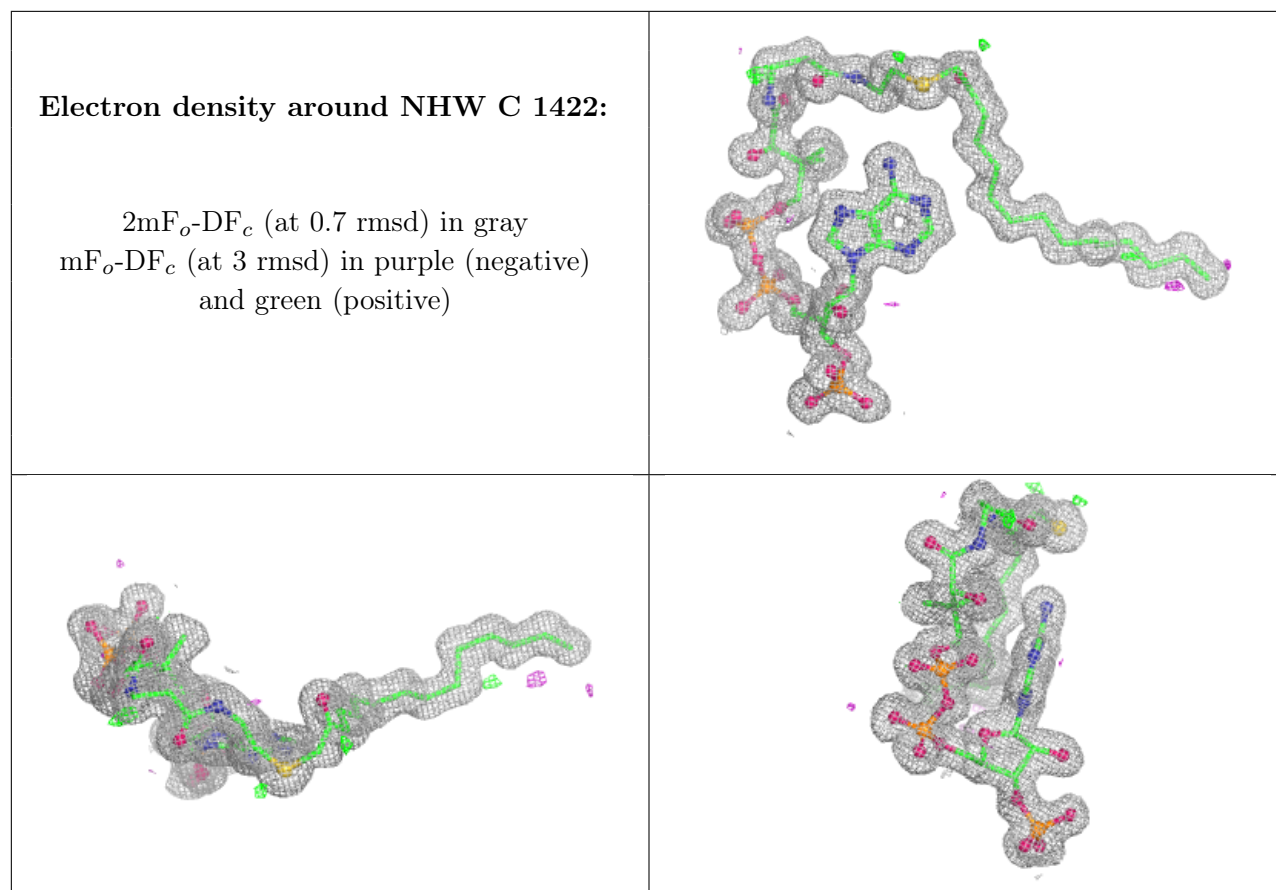


Electron density around 3F3 B 1414:

$2mF_o-DF_c$ (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.