Full wwPDB X-ray Structure Validation Report (i)

May 1, 2024 – 02:45 am BST

PDB ID	:	4CAE
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 (i) 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 (i)) were used in the production of this report:

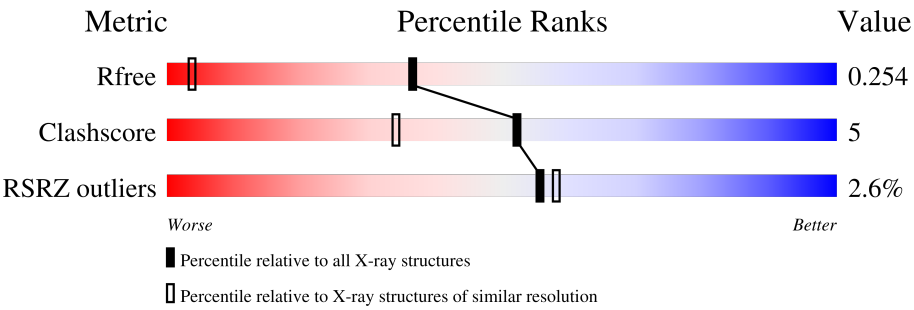
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
RSRZ outliers	127900	1139 (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 <=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% 85% 15%
1	B	384	3% 89% 11% •
1	C	384	3% 90% 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

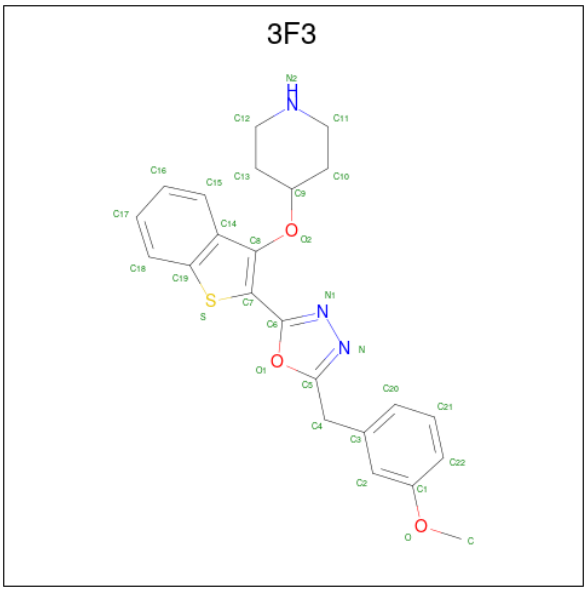
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

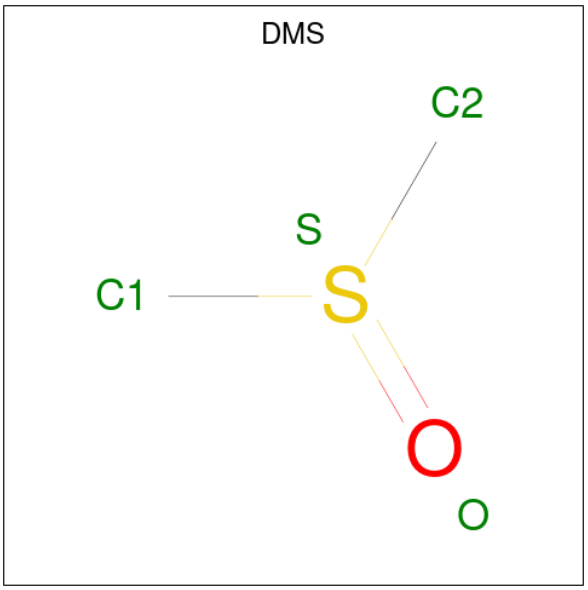
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	2	2	2	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0

- Molecule 4 is 4-[(2-{5-[(3-METHOXYPHENYL)METHYL]-1,3,4-OXADIAZOL-2-YL}-1-BENZOTHIOPHEN-3-YL)OXY]PIPERIDINE (three-letter code: 3F3) (formula: $C_{23}H_{23}N_3O_3S$).



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

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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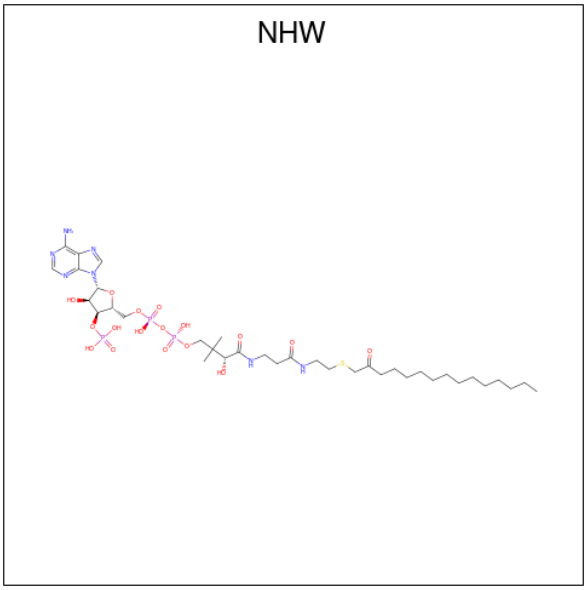
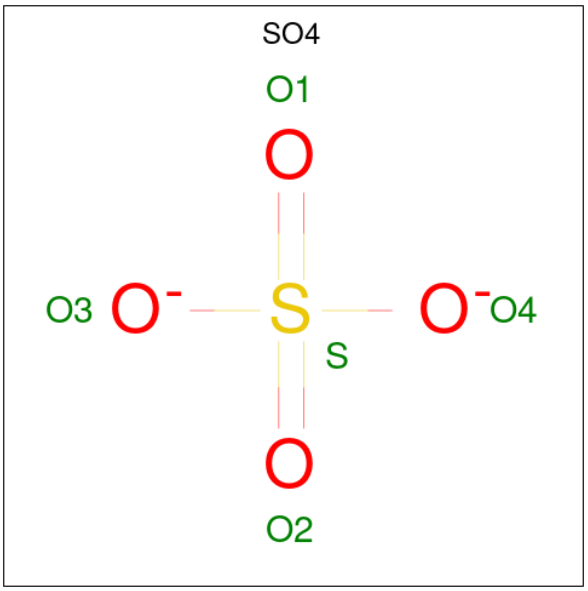
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
5	B	1	4	2	1	1	0	0
			Total	C	O	S		
5	C	1	4	2	1	1	0	0

- Molecule 6 is 2-oxopentadecyl-CoA (three-letter code: 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
			Total	C	N	O	P	S		
6	B	1	64	36	7	17	3	1	0	0
			Total	C	N	O	P	S		
6	C	1	64	36	7	17	3	1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 8 is water.

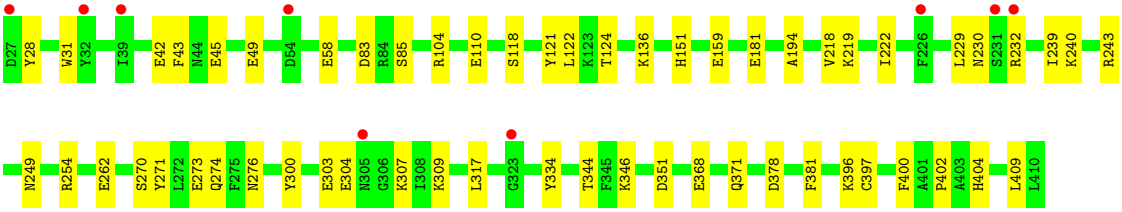
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	437	437	437	0	0
			Total	O		
8	B	453	453	453	0	0
			Total	O		
8	C	401	401	401	0	0

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.

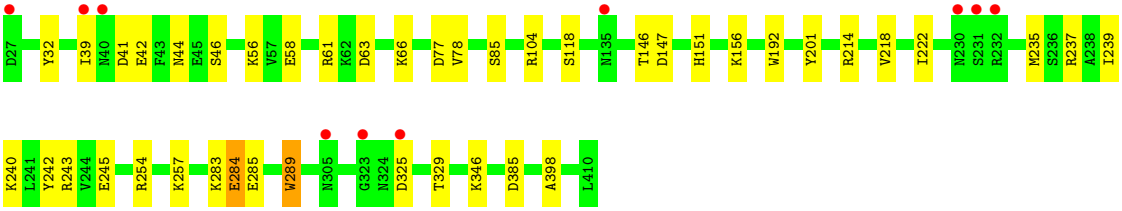
• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE

Chain A:



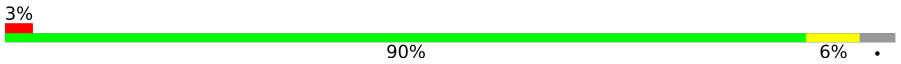
• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE

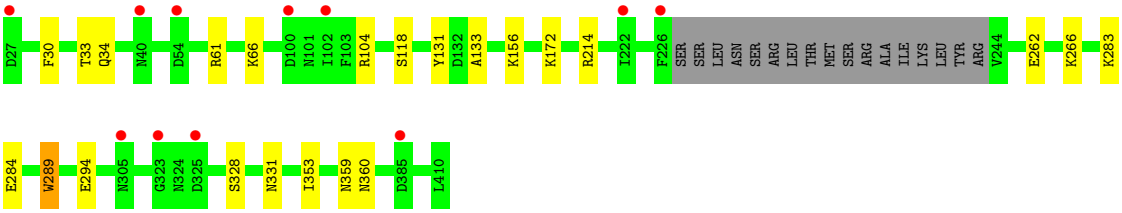
Chain B:



• Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE

Chain C:





4 Data and refinement statistics (i)

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 24.43 – 1.46	Depositor EDS
% Data completeness (in resolution range)	99.4 (100.22-1.46) 99.5 (24.43-1.46)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.8.0029	Depositor
R, R_{free}	0.215 , 0.254 0.214 , 0.254	Depositor DCC
R_{free} test set	10801 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11329	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 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NHW, CL, DMS, MG, 3F3, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.98	2/3453 (0.1%)	1.03	4/4674 (0.1%)
1	B	0.99	3/3411 (0.1%)	1.04	10/4617 (0.2%)
1	C	1.08	5/3257 (0.2%)	1.00	3/4412 (0.1%)
All	All	1.02	10/10121 (0.1%)	1.02	17/13703 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66[A]	LYS	CE-NZ	-17.38	1.05	1.49
1	C	66[B]	LYS	CE-NZ	-17.38	1.05	1.49
1	C	66[A]	LYS	CD-CE	9.20	1.74	1.51
1	C	66[B]	LYS	CD-CE	9.20	1.74	1.51
1	A	181	GLU	CD-OE1	-7.25	1.17	1.25
1	B	192	TRP	CE3-CZ3	6.71	1.49	1.38
1	A	381	PHE	CG-CD1	5.27	1.46	1.38
1	B	289	TRP	CZ3-CH2	5.26	1.48	1.40
1	C	289	TRP	CE3-CZ3	5.24	1.47	1.38
1	B	245	GLU	CD-OE2	5.10	1.31	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	284[A]	GLU	CB-CG-CD	11.19	144.41	114.20
1	B	284[B]	GLU	CB-CG-CD	11.19	144.41	114.20
1	B	104	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	A	104	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	B	61	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	C	61	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	104	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	C	104	ARG	NE-CZ-NH2	-6.92	116.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	214	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	77	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	63	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	104	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	351	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	385	ASP	CB-CA-C	-5.12	100.17	110.40
1	A	83	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	41	ASP	CB-CG-OD1	-5.08	113.73	118.30

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	52	0
1	B	3278	0	3310	43	0
1	C	3133	0	3128	18	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	0	0
5	B	4	0	6	4	0
5	C	4	0	6	0	0
6	A	64	0	60	1	0
6	B	64	0	60	0	0
6	C	64	0	60	0	0
7	B	5	0	0	0	0
8	A	437	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	453	0	0	13	0
8	C	401	0	0	6	0
All	All	11329	0	10058	110	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 (110) 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:32[A]:TYR:CD1	8:B:2007:HOH:O	1.83	1.25
1:C:30:PHE:O	1:C:33[A]:THR:HG22	1.42	1.19
1:A:218[B]:VAL:HG22	8:A:2269:HOH:O	1.43	1.13
1:C:331[A]:ASN:OD1	8:C:2338:HOH:O	1.80	0.97
1:B:289:TRP:CE2	5:B:1415:DMS:H23	2.05	0.92
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:NE1	5:B:1415:DMS:H23	1.95	0.82
1:A:262[B]:GLU:HG3	8:A:2318:HOH:O	1.81	0.81
1:A:121[A]:TYR:OH	8:A:2180:HOH:O	2.01	0.79
1:A:122:LEU:HB3	1:A:124:THR:HG22	1.65	0.78
1:B:32[A]:TYR:HD1	8:B:2007:HOH:O	1.36	0.76
1:B:151[B]:HIS:NE2	8:B:2028:HOH:O	1.73	0.72
1:A:276[B]:ASN:OD1	8:A:2336:HOH:O	2.08	0.70
1:B:257[B]:LYS:NZ	8:B:2321:HOH:O	2.26	0.69
1:B:32[A]:TYR:CE1	8:B:2007:HOH:O	2.23	0.68
1:A:159:GLU:CD	1:A:409:LEU:HD22	2.14	0.67
1:C:266:LYS:HG2	8:C:2285:HOH:O	1.96	0.64
1:C:262[B]:GLU:HG3	1:C:283:LYS:HE2	1.78	0.64
1:A:218[B]:VAL:CG2	1:A:239:ILE:HG12	2.28	0.63
1:A:42[A]:GLU:OE2	1:B:346:LYS:NZ	2.23	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:A:85[A]:SER:OG	8:A:2110:HOH:O	2.16	0.58
1:A:194:ALA:HB2	6:A:1422:NHW:HDM	1.86	0.57
1:C:262[B]:GLU:HG3	1:C:283:LYS:CE	2.35	0.56
1:B:218:VAL:CG1	1:B:239[B]:ILE:HD13	2.35	0.56
1:A:42[A]:GLU:OE1	1:B:346:LYS:HE3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:156[B]:LYS:HB3	1:C:156[B]:LYS:HZ2	1.73	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
1:B:146[B]:THR:HG21	5:B:1415:DMS:H22	1.92	0.51
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:A:270[B]:SER:OG	8:A:2326:HOH:O	2.20	0.49
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:C:284[B]:GLU:HG2	8:C:2305:HOH:O	2.12	0.48
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
8:A:2390:HOH:O	1:B:44[A]:ASN:OD1	2.20	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: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:B:289:TRP:CZ2	5:B:1415:DMS:H23	2.50	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: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:151[A]:HIS:CE1	8:A:2206:HOH:O	2.69	0.46
1:A:43:PHE:CZ	1:A:396:LYS:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:325:ASP:OD1	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
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
1:A:121[A]:TYR:CD1	1:A:121[A]:TYR:C	2.92	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:C:284[A]:GLU:H	1:C:284[A]:GLU:CD	2.23	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)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	3F3	B	1414	-	24,34,34	1.96	4 (16%)	23,47,47	1.43	5 (21%)
5	DMS	C	1414	-	3,3,3	0.35	0	3,3,3	1.32	1 (33%)
6	NHW	B	1422	2	58,66,66	1.30	6 (10%)	70,92,92	1.25	8 (11%)
6	NHW	A	1422	2	58,66,66	1.24	5 (8%)	70,92,92	1.43	11 (15%)
7	SO4	B	1411	-	4,4,4	0.28	0	6,6,6	0.73	0
4	3F3	C	1413	-	24,34,34	1.95	2 (8%)	23,47,47	1.30	2 (8%)
6	NHW	C	1422	2	58,66,66	1.25	7 (12%)	70,92,92	1.31	7 (10%)
5	DMS	B	1415	-	3,3,3	0.28	0	3,3,3	2.21	1 (33%)
5	DMS	A	1415	-	3,3,3	0.33	0	3,3,3	1.12	0
4	3F3	A	1414	-	24,34,34	1.41	2 (8%)	23,47,47	1.82	8 (34%)

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	-	-	2/7/22/22	0/5/5/5
6	NHW	B	1422	2	-	3/61/81/81	0/3/3/3
6	NHW	A	1422	2	-	6/61/81/81	0/3/3/3
4	3F3	C	1413	-	-	2/7/22/22	0/5/5/5
6	NHW	C	1422	2	-	1/61/81/81	0/3/3/3
4	3F3	A	1414	-	-	1/7/22/22	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1414	3F3	C8-C14	7.96	1.51	1.40
4	C	1413	3F3	C8-C14	7.70	1.50	1.40
6	B	1422	NHW	C6-C5	4.55	1.60	1.51
6	C	1422	NHW	O4X-C4X	3.98	1.53	1.45
6	C	1422	NHW	O10-C10	3.90	1.49	1.42
4	A	1414	3F3	C8-C14	3.70	1.45	1.40
6	B	1422	NHW	P3X-O3X	3.47	1.65	1.59
6	A	1422	NHW	P3X-O3X	3.31	1.65	1.59
6	B	1422	NHW	CP-S1	3.18	1.89	1.81
4	B	1414	3F3	N-N1	3.10	1.43	1.37
6	B	1422	NHW	P3X-O8A	2.94	1.66	1.54
6	A	1422	NHW	P3X-O7A	-2.73	1.44	1.54
6	A	1422	NHW	O4X-C1X	2.64	1.44	1.41
6	C	1422	NHW	P3X-O7A	-2.48	1.45	1.54
4	B	1414	3F3	C17-C18	2.47	1.42	1.36
6	B	1422	NHW	P1A-O2A	-2.46	1.43	1.55
6	C	1422	NHW	C7-N8	2.45	1.51	1.46
6	A	1422	NHW	C7-C6	2.41	1.59	1.51
4	B	1414	3F3	C16-C17	2.38	1.44	1.38
4	A	1414	3F3	C2-C3	2.37	1.43	1.39
6	B	1422	NHW	P2A-O4A	-2.35	1.44	1.55
4	C	1413	3F3	C16-C15	2.27	1.41	1.36
6	A	1422	NHW	C4A-N3A	2.07	1.38	1.35
6	C	1422	NHW	O4X-C1X	-2.03	1.38	1.41
6	C	1422	NHW	C2A-N3A	2.02	1.35	1.32
6	C	1422	NHW	P2A-O4A	-2.00	1.45	1.55

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1422	NHW	N3A-C2A-N1A	-4.95	120.94	128.68
4	A	1414	3F3	C16-C15-C14	-4.66	114.43	120.89
6	B	1422	NHW	N3A-C2A-N1A	-4.07	122.32	128.68
6	C	1422	NHW	O1M-C1M-CP	-3.88	116.64	122.17
6	A	1422	NHW	C13-C11-C10	3.85	115.50	108.82
6	A	1422	NHW	O1M-C1M-CP	-3.79	116.76	122.17
6	C	1422	NHW	O6A-C12-C11	-3.67	104.65	110.55
6	A	1422	NHW	CP-C1M-C2M	3.53	123.08	115.52
6	A	1422	NHW	C13-C11-C12	-3.41	102.67	108.23
6	C	1422	NHW	C1X-N9A-C4A	-3.25	120.93	126.64
6	B	1422	NHW	O1M-C1M-CP	-3.20	117.61	122.17
6	B	1422	NHW	C6-C7-N8	-3.16	105.52	111.90
6	A	1422	NHW	C2A-N1A-C6A	3.14	124.12	118.75
6	A	1422	NHW	N3A-C2A-N1A	-3.10	123.83	128.68
6	B	1422	NHW	C2A-N1A-C6A	3.03	123.94	118.75
6	B	1422	NHW	C13-C11-C10	3.02	114.06	108.82
4	A	1414	3F3	C-O-C1	2.87	123.75	117.51
6	C	1422	NHW	C14-C11-C10	2.86	113.78	108.82
6	A	1422	NHW	C5X-C4X-C3X	-2.81	105.10	114.40
5	B	1415	DMS	C2-S-C1	2.76	112.62	98.44
4	A	1414	3F3	C17-C16-C15	2.74	124.28	120.44
4	B	1414	3F3	C16-C17-C18	-2.72	116.63	120.44
4	C	1413	3F3	C11-N2-C12	2.71	118.14	110.34
4	B	1414	3F3	C1-C2-C3	-2.66	116.79	119.73
6	A	1422	NHW	C2-C3-N4	-2.58	107.00	112.42
6	A	1422	NHW	C5A-C6A-N1A	-2.58	114.51	120.35
4	A	1414	3F3	C21-C22-C1	2.34	122.72	118.96
4	A	1414	3F3	C10-C11-N2	2.29	115.29	110.64
4	A	1414	3F3	C21-C20-C3	-2.26	117.16	120.63
4	C	1413	3F3	C17-C16-C15	-2.20	117.36	120.44
5	C	1414	DMS	O-S-C2	2.14	117.48	106.54
4	B	1414	3F3	C20-C3-C2	2.12	121.50	118.54
6	C	1422	NHW	C6-C7-N8	-2.11	107.65	111.90
4	A	1414	3F3	C20-C3-C2	2.10	121.48	118.54
6	B	1422	NHW	O4A-P2A-O5A	2.06	122.41	112.24
6	C	1422	NHW	C10-C9-N8	-2.06	112.48	116.58
4	B	1414	3F3	C4-C3-C20	-2.05	115.33	120.92
6	A	1422	NHW	N6A-C6A-N1A	2.04	122.81	118.57
6	B	1422	NHW	P2A-O3A-P1A	-2.03	125.87	132.83
6	A	1422	NHW	C2-S1-CP	-2.02	98.33	101.71
6	B	1422	NHW	O6A-C12-C11	-2.01	107.31	110.55
4	B	1414	3F3	C20-C21-C22	-2.01	117.39	120.25
4	A	1414	3F3	C8-O2-C9	-2.00	112.09	117.16

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1422	NHW	C12-O6A-P2A-O5A
6	C	1422	NHW	C6-C7-N8-C9
6	B	1422	NHW	C6-C7-N8-C9
4	B	1414	3F3	C13-C9-O2-C8
4	B	1414	3F3	C10-C9-O2-C8
4	C	1413	3F3	C13-C9-O2-C8
4	C	1413	3F3	C10-C9-O2-C8
4	A	1414	3F3	C13-C9-O2-C8
6	A	1422	NHW	C12-O6A-P2A-O3A
6	B	1422	NHW	P2A-O3A-P1A-O1A
6	A	1422	NHW	C11-C12-O6A-P2A
6	A	1422	NHW	C5X-O5X-P1A-O1A
6	A	1422	NHW	C12-O6A-P2A-O4A
6	B	1422	NHW	C4M-C5M-C6M-C7M
6	A	1422	NHW	C7M-C8M-C9M-CAM

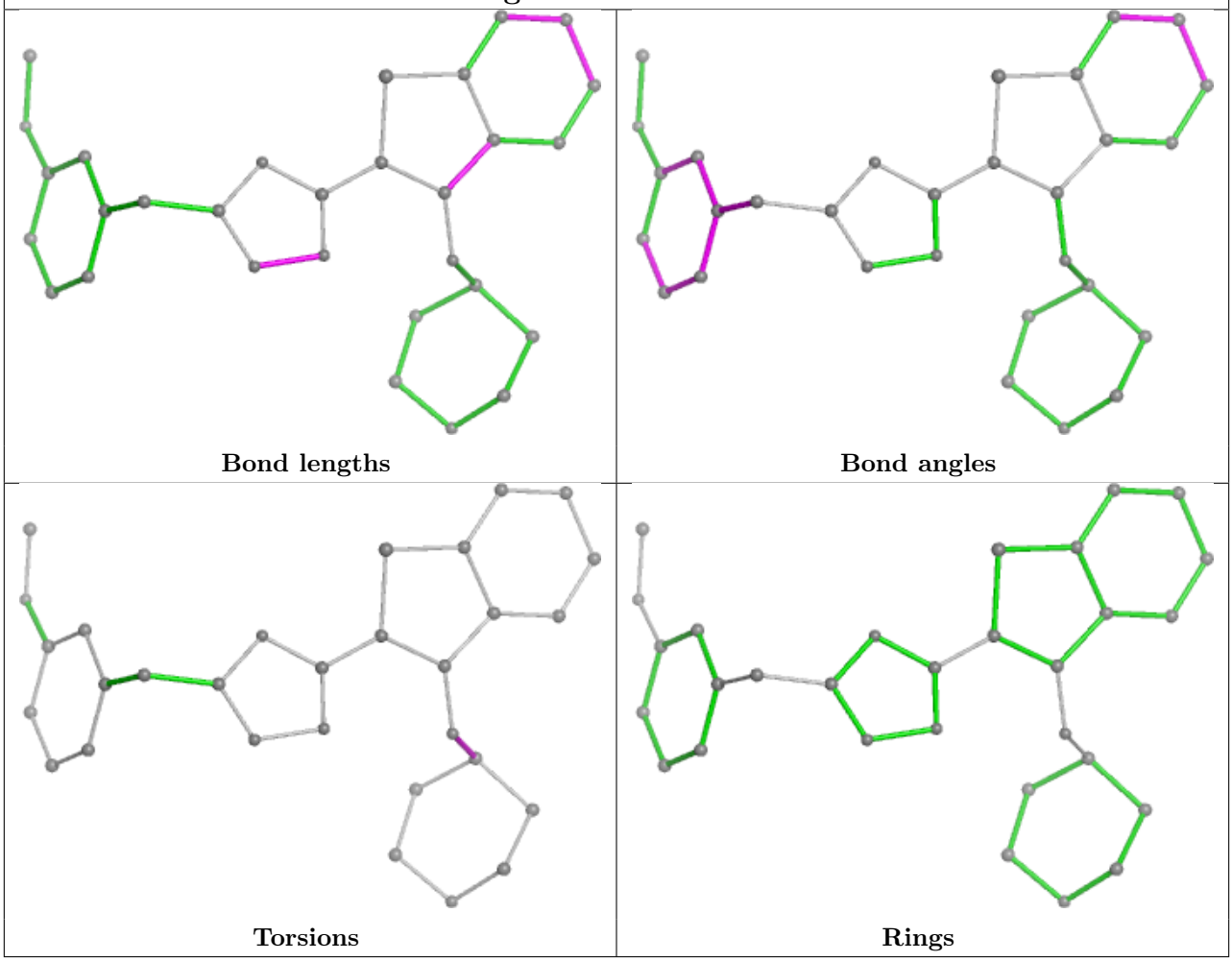
There are no ring outliers.

3 monomers are involved in 6 short contacts:

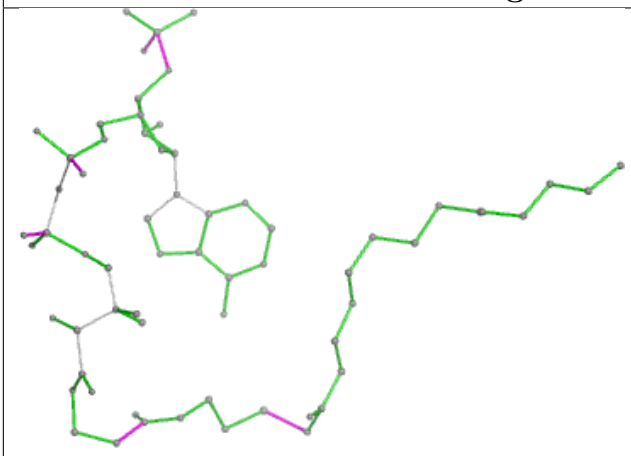
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1422	NHW	1	0
5	B	1415	DMS	4	0
4	A	1414	3F3	1	0

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 then 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.

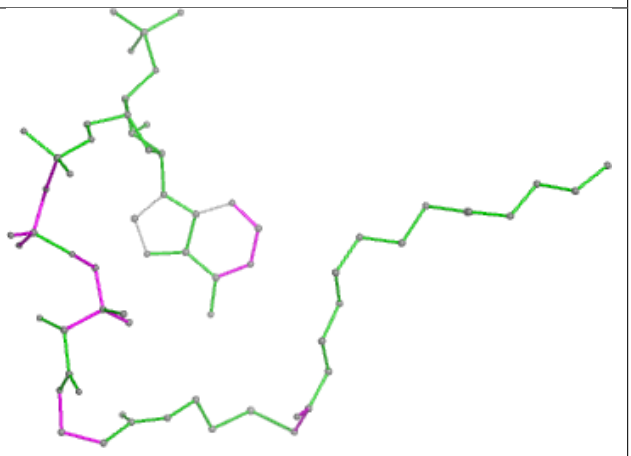
Ligand 3F3 B 1414



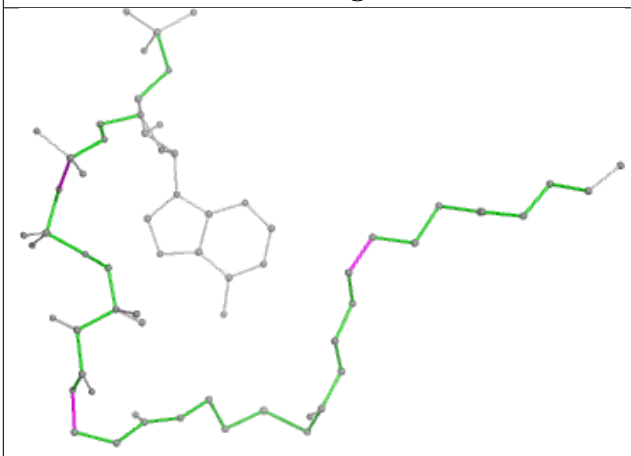
Ligand NHW B 1422



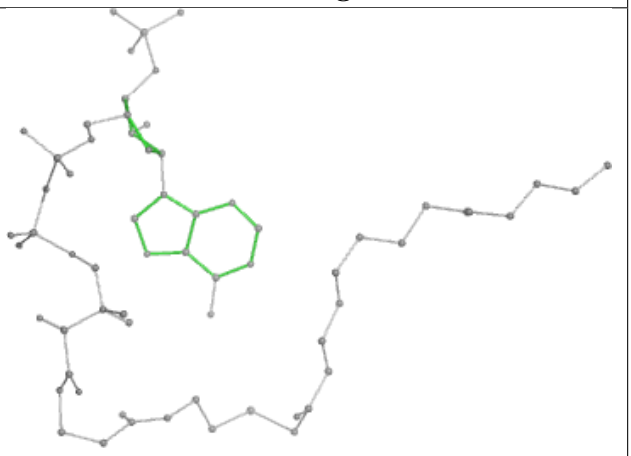
Bond lengths



Bond angles

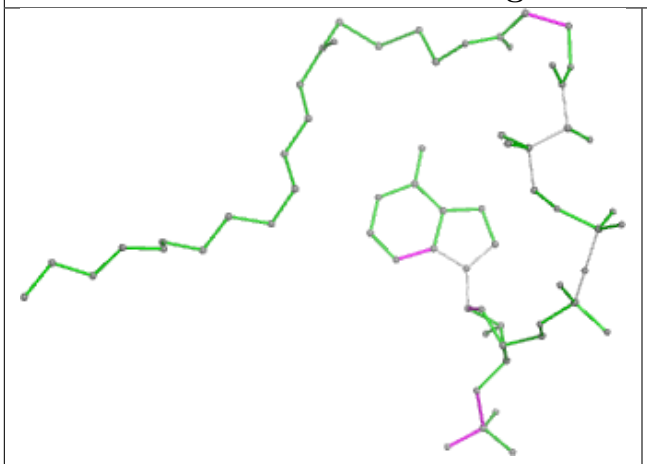


Torsions



Rings

Ligand NHW A 1422



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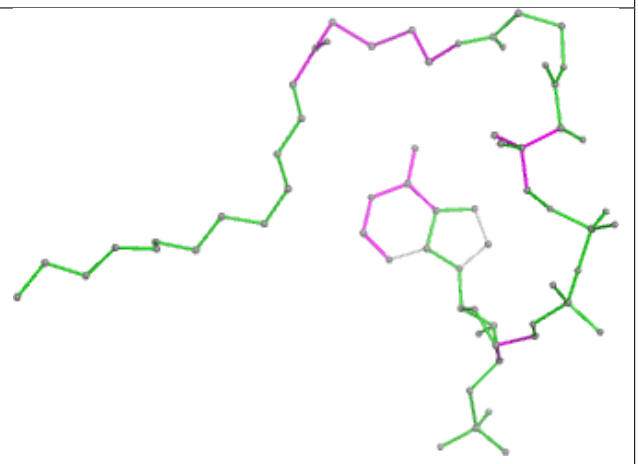
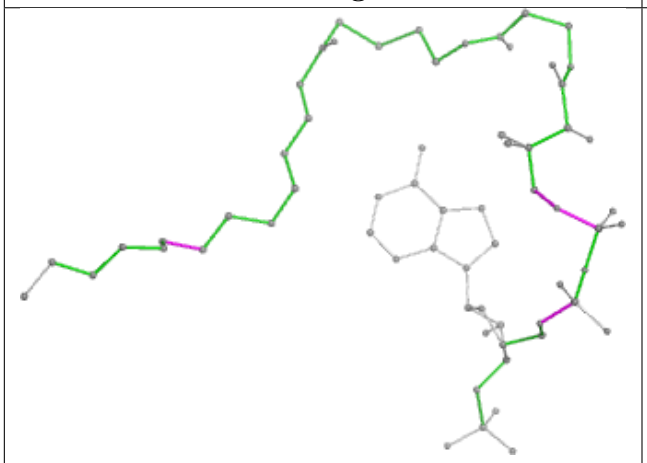
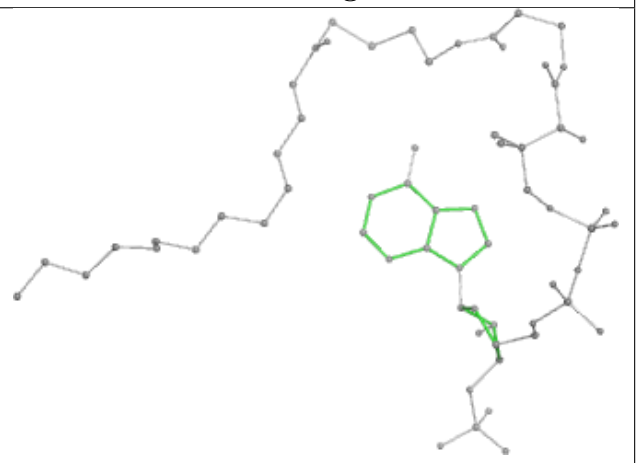


Bond angles

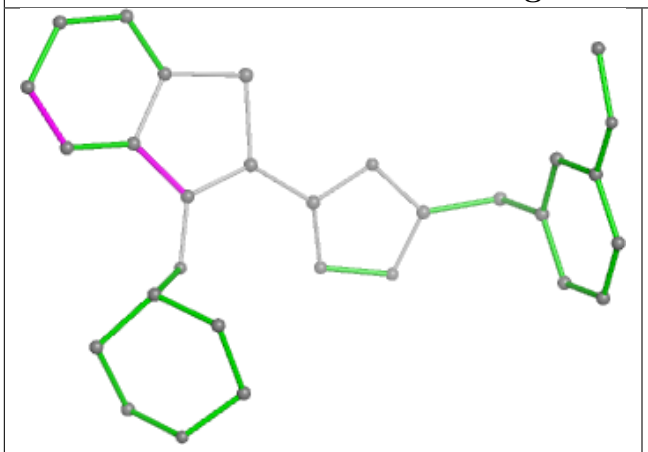


Torsions

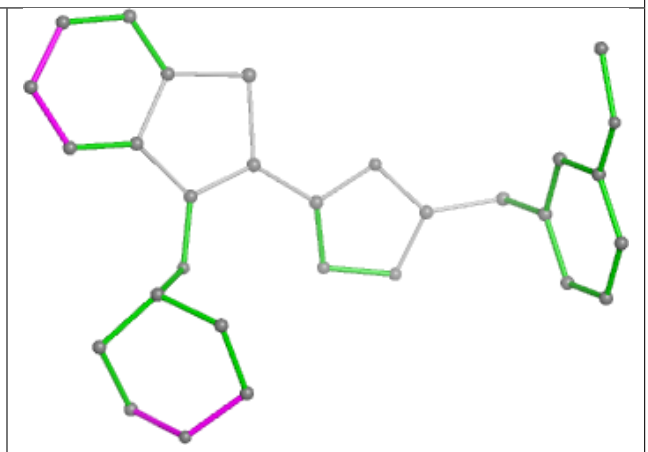


Rings

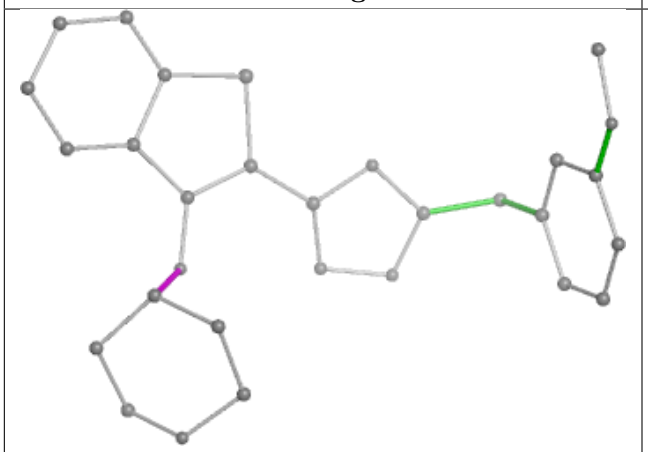
Ligand 3F3 C 1413



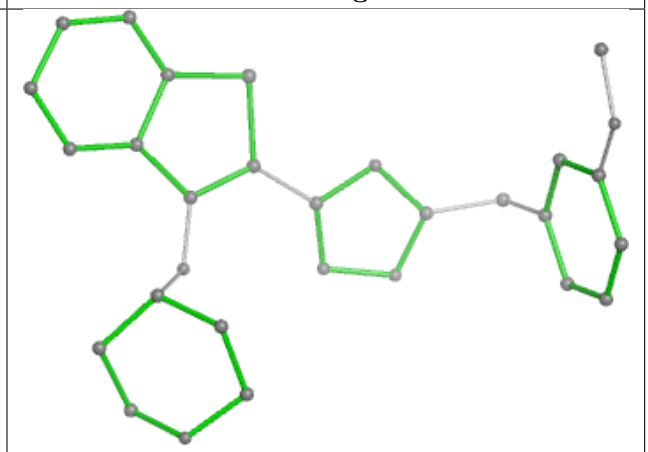
Bond lengths



Bond angles

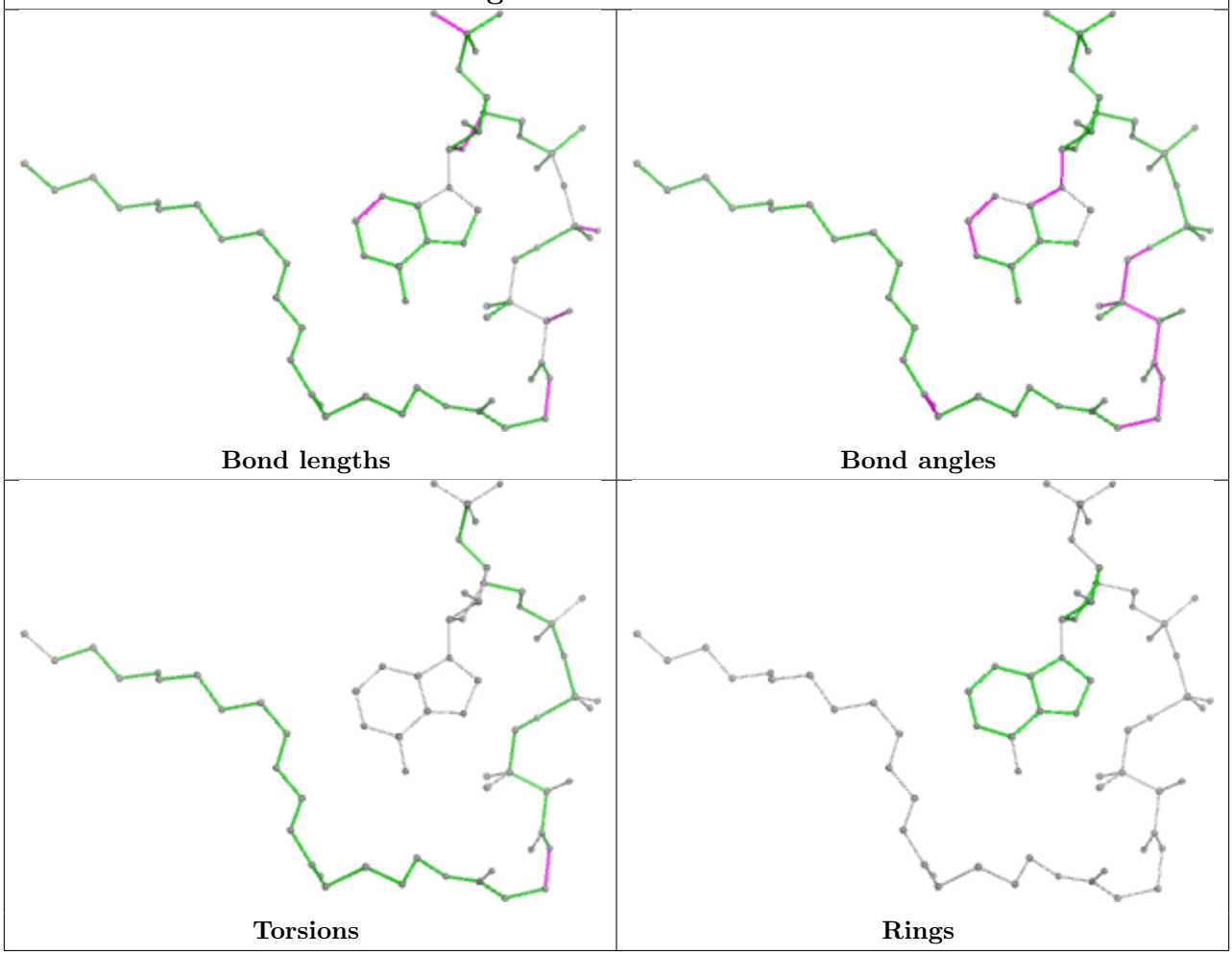


Torsions

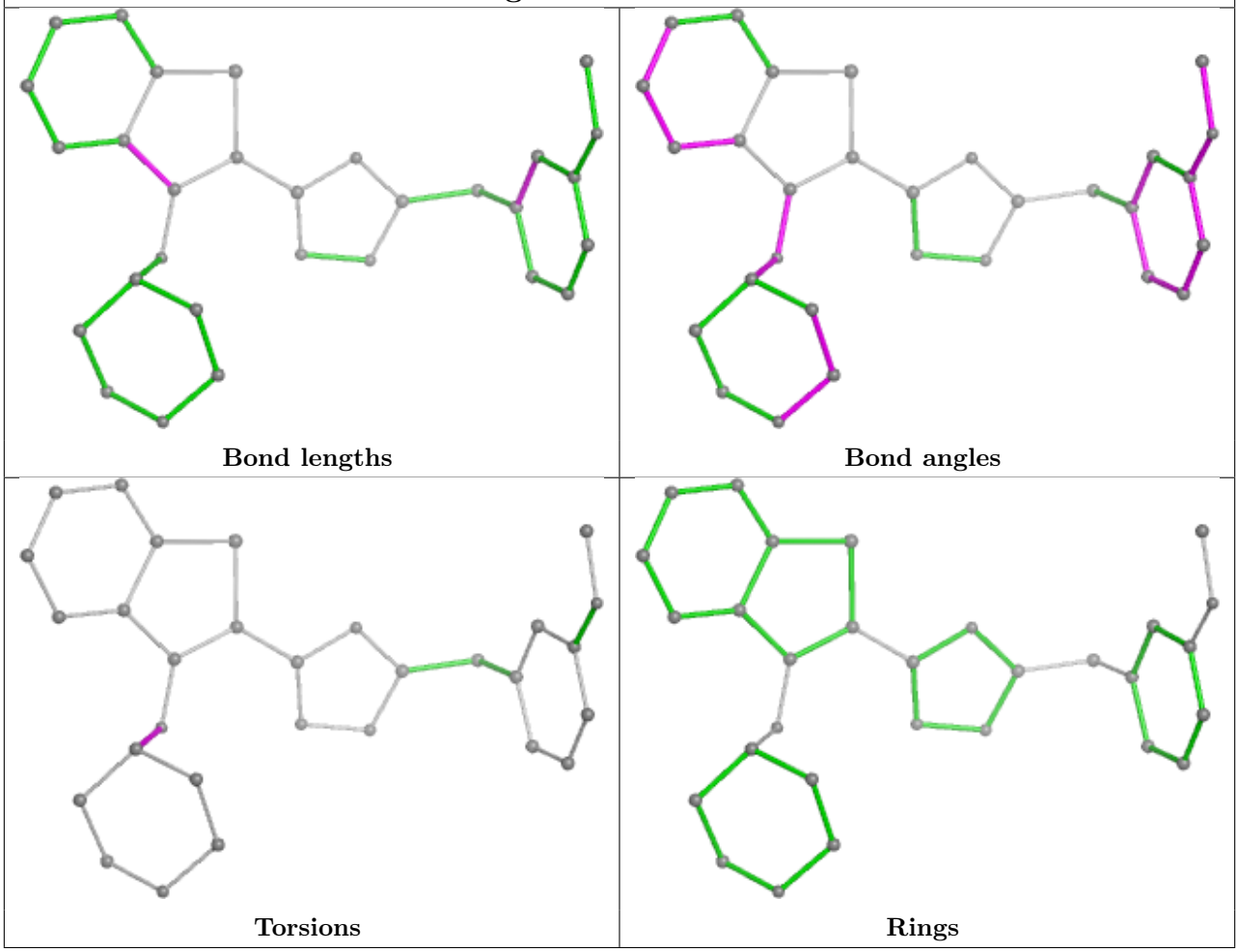


Rings

Ligand NHW C 1422



Ligand 3F3 A 1414



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	60	63	10, 16, 30, 60	5 (1%)
1	B	384/384 (100%)	-0.05	10 (2%)	56	58	7, 12, 26, 53	10 (2%)
1	C	367/384 (95%)	0.02	11 (2%)	50	53	7, 14, 27, 45	10 (2%)
All	All	1135/1152 (98%)	0.04	30 (2%)	56	58	7, 14, 28, 60	25 (2%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	ARG	5.9
1	A	232	ARG	5.8
1	A	231	SER	4.6
1	B	231	SER	4.4
1	C	27	ASP	4.3
1	C	305	ASN	4.1
1	A	54	ASP	3.9
1	B	323	GLY	3.2
1	B	305	ASN	3.2
1	B	325	ASP	2.9
1	A	323	GLY	2.8
1	C	222	ILE	2.8
1	A	226	PHE	2.7
1	C	100	ASP	2.5
1	B	135	ASN	2.5
1	A	305	ASN	2.4
1	C	323	GLY	2.4
1	A	27	ASP	2.4
1	C	385	ASP	2.3
1	C	102	ILE	2.2
1	B	27	ASP	2.2
1	C	54	ASP	2.2
1	A	32	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	226	PHE	2.1
1	B	40	ASN	2.1
1	C	40	ASN	2.1
1	C	325	ASP	2.1
1	B	230	ASN	2.1
1	B	39	ILE	2.0
1	A	39	ILE	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 monosaccharides 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(Å^2)	Q<0.9
5	DMS	B	1415	4/4	0.92	0.17	25,26,27,36	0
5	DMS	A	1415	4/4	0.93	0.13	27,28,30,31	0
5	DMS	C	1414	4/4	0.93	0.15	22,25,27,28	0
4	3F3	C	1413	30/30	0.94	0.09	14,17,21,21	0
4	3F3	A	1414	30/30	0.95	0.09	12,16,18,21	0
7	SO4	B	1411	5/5	0.95	0.15	36,38,41,44	0
6	NHW	A	1422	64/64	0.96	0.08	10,13,16,18	0
6	NHW	C	1422	64/64	0.96	0.08	8,11,15,17	0
4	3F3	B	1414	30/30	0.96	0.09	10,12,14,19	0
6	NHW	B	1422	64/64	0.97	0.07	7,10,13,14	0
2	MG	C	1411	1/1	0.98	0.07	20,20,20,20	0
3	CL	A	1412	1/1	0.98	0.07	34,34,34,34	0
2	MG	B	1412	1/1	0.98	0.07	21,21,21,21	0
3	CL	B	1413	1/1	0.99	0.06	13,13,13,13	0
3	CL	C	1412	1/1	0.99	0.03	12,12,12,12	0
2	MG	A	1411	1/1	0.99	0.06	22,22,22,22	0

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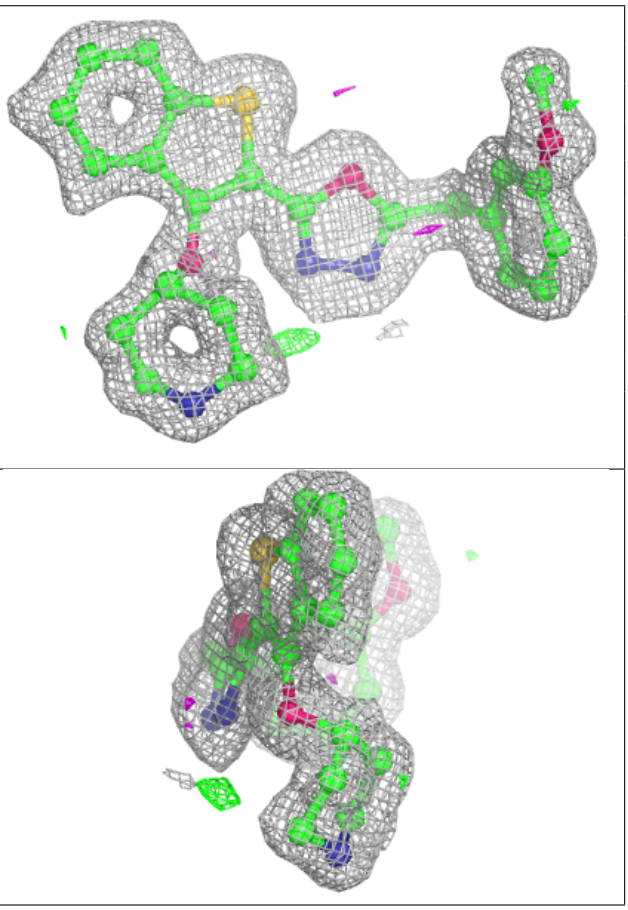
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	A	1413	1/1	0.99	0.05	15,15,15,15	0

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.

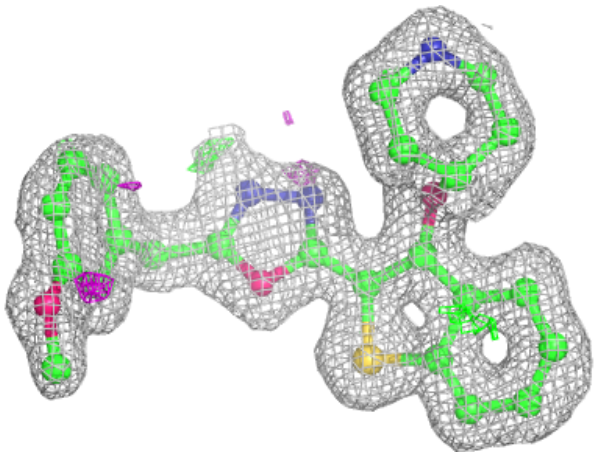
Electron density around 3F3 C 1413:

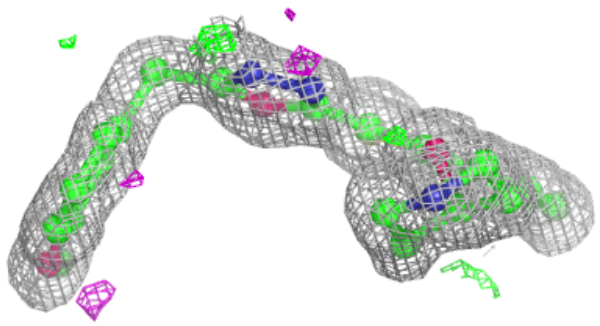
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

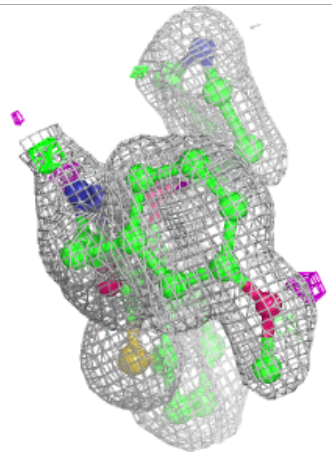


Electron density around 3F3 A 1414:

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

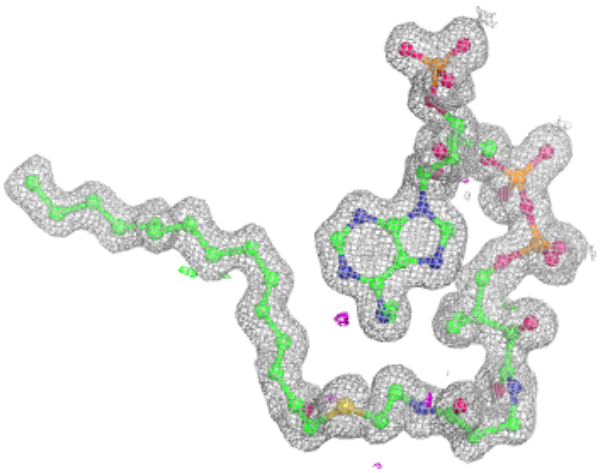


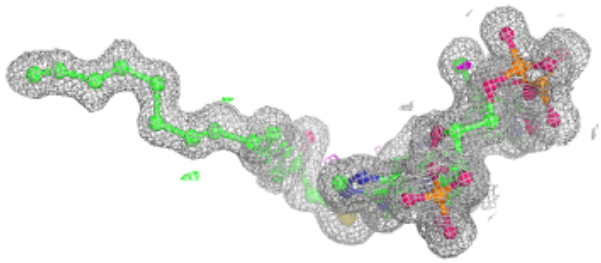




Electron density around NHW A 1422:

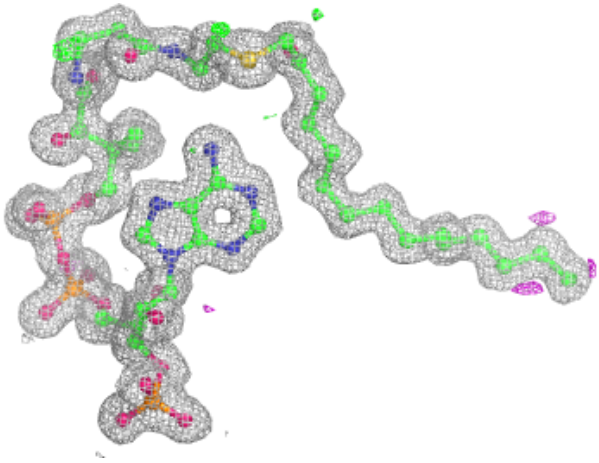
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

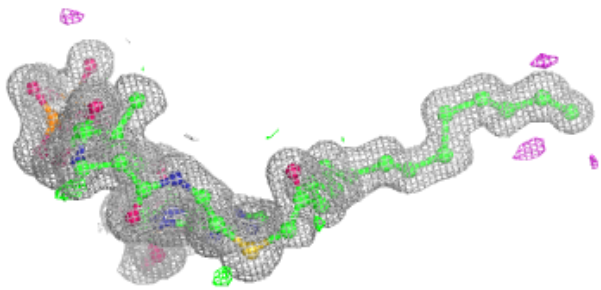


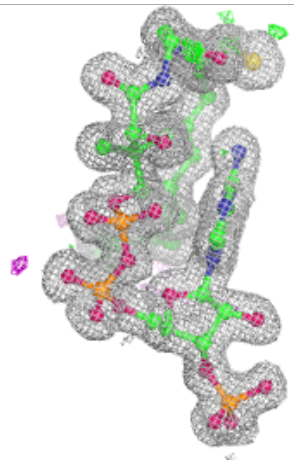


Electron density around NHW C 1422:

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

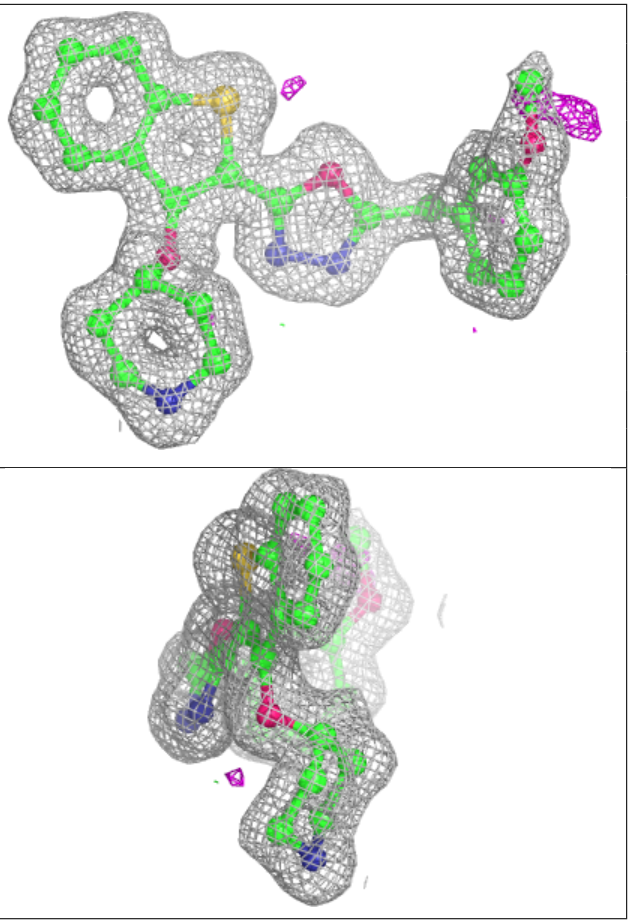


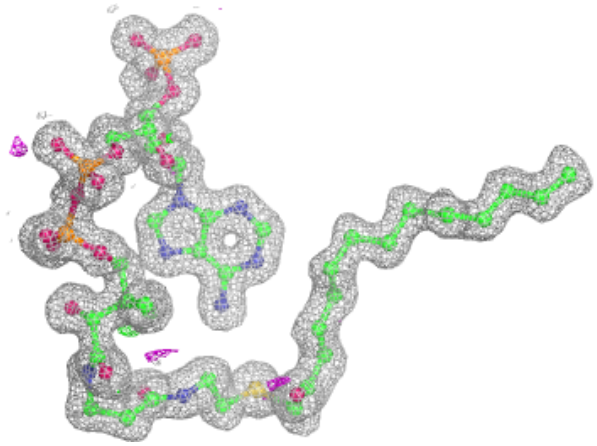
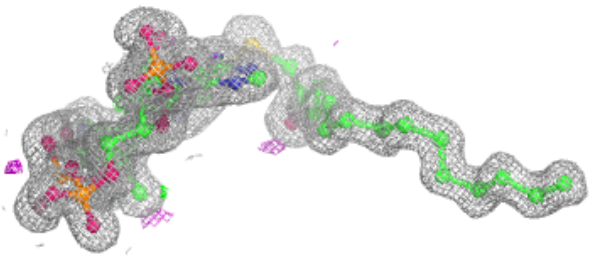




Electron density around 3F3 B 1414:

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



Electron density around NHW B 1422: 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.