wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2023 – 07:43 PM JST

PDB ID	:	5H2U
Title	:	Crystal structure of PTK6 Kinase Domain complexed with Dasatinib
Authors	:	Thakur, M.K.; Birudukota, S.; Swaminathan, S.; Tyagi, R.; Gosu, R.
Deposited on	:	2016-10-18
Resolution	:	2.24 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

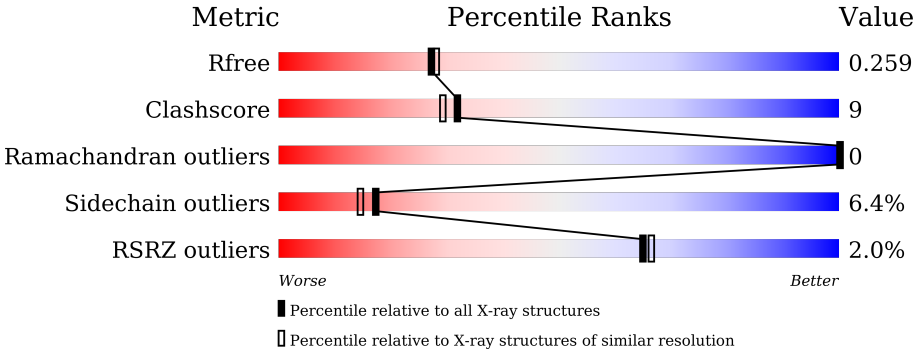
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	267	% 78% 17% •
1	B	267	80% 17% ••
1	C	267	3% 77% 21% ••
1	D	267	3% 79% 18% ••

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9541 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 Protein-tyrosine kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	2211	1413	390	390	18	0	10	0
1	B	264	2202	1406	389	390	17	0	12	0
1	C	265	2201	1406	387	389	19	0	12	0
1	D	264	2190	1399	382	391	18	0	11	0

There are 24 discrepancies between the modelled and reference sequences:

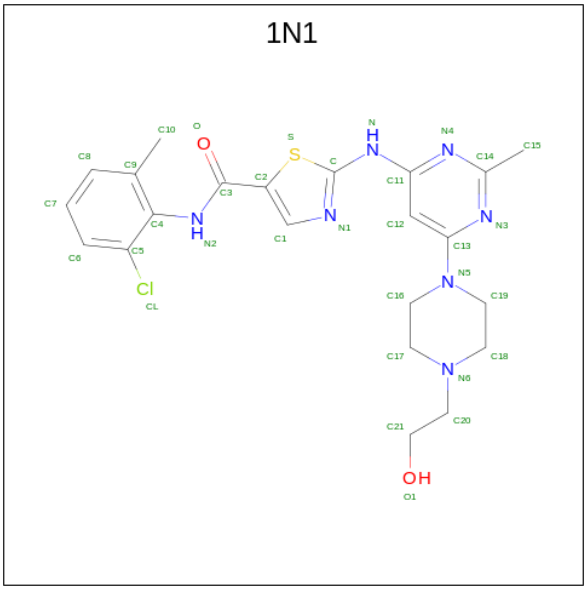
Chain	Residue	Modelled	Actual	Comment	Reference
A	184	CXM	-	expression tag	UNP Q13882
A	433	THR	CYS	engineered mutation	UNP Q13882
A	447	HIS	-	expression tag	UNP Q13882
A	448	HIS	-	expression tag	UNP Q13882
A	449	HIS	-	expression tag	UNP Q13882
A	450	HIS	-	expression tag	UNP Q13882
B	184	CXM	-	expression tag	UNP Q13882
B	433	THR	CYS	engineered mutation	UNP Q13882
B	447	HIS	-	expression tag	UNP Q13882
B	448	HIS	-	expression tag	UNP Q13882
B	449	HIS	-	expression tag	UNP Q13882
B	450	HIS	-	expression tag	UNP Q13882
C	184	CXM	-	expression tag	UNP Q13882
C	433	THR	CYS	engineered mutation	UNP Q13882
C	447	HIS	-	expression tag	UNP Q13882
C	448	HIS	-	expression tag	UNP Q13882
C	449	HIS	-	expression tag	UNP Q13882
C	450	HIS	-	expression tag	UNP Q13882
D	184	CXM	-	expression tag	UNP Q13882
D	433	THR	CYS	engineered mutation	UNP Q13882
D	447	HIS	-	expression tag	UNP Q13882

Continued on next page...

Continued from previous page...

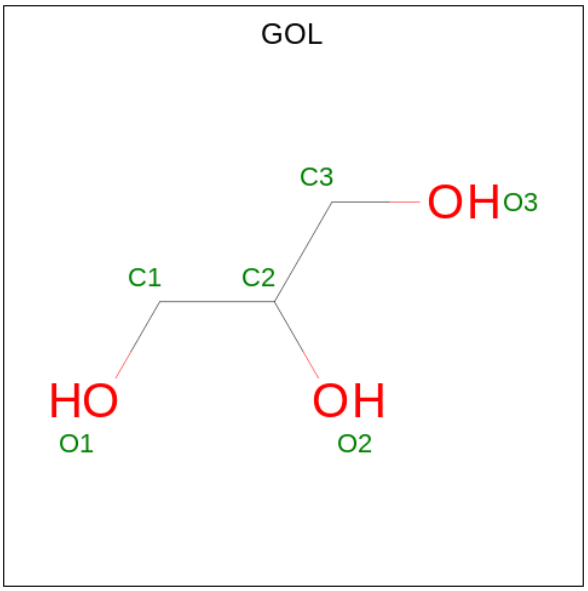
Chain	Residue	Modelled	Actual	Comment	Reference
D	448	HIS	-	expression tag	UNP Q13882
D	449	HIS	-	expression tag	UNP Q13882
D	450	HIS	-	expression tag	UNP Q13882

- Molecule 2 is N-(2-CHLORO-6-METHYLPHENYL)-2-({6-[4-(2-HYDROXYETHYL)PIPERAZIN-1-YL]-2-METHYLPYRIMIDIN-4-YL}AMINO)-1,3-THIAZOLE-5-CARBOXAMIDE (three-letter code: 1N1) (formula: $C_{22}H_{26}ClN_7O_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
2	A	1	41	29	2	7	2	1	0	1
2	B	1	41	29	2	7	2	1	0	1
2	C	1	41	29	2	7	2	1	0	1
2	D	1	41	29	2	7	2	1	0	1

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	C	1	6	3	3	0	0
			Total	C	O		
3	C	1	6	3	3	0	0
			Total	C	O		
3	C	1	6	3	3	0	0
			Total	C	O		
3	D	1	6	3	3	0	0
			Total	C	O		
3	D	1	6	3	3	0	0
			Total	C	O		
3	D	1	6	3	3	0	0

- Molecule 4 is water.

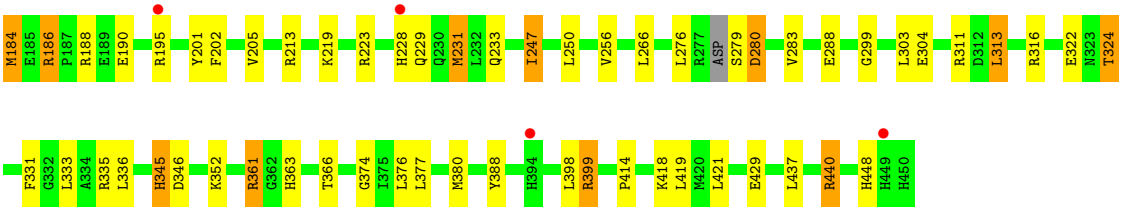
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	138	138	138	0	0
			Total	O		
4	B	120	120	120	0	0
			Total	O		
4	C	112	112	112	0	0
			Total	O		
4	D	131	131	131	0	0

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.

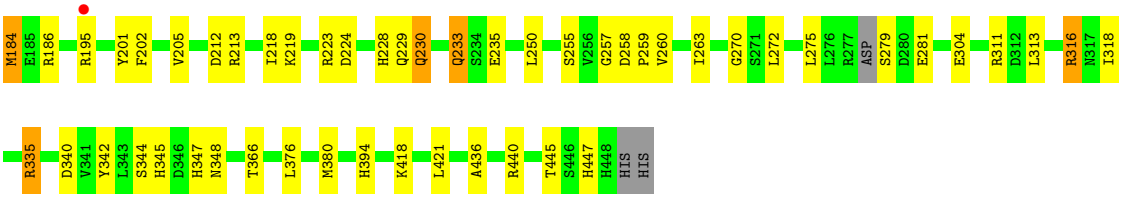
• Molecule 1: Protein-tyrosine kinase 6

Chain A:



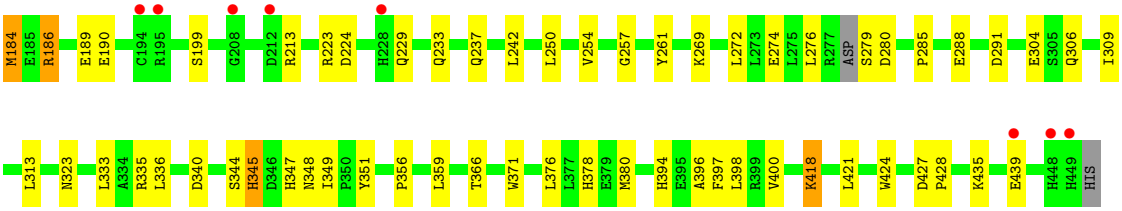
• Molecule 1: Protein-tyrosine kinase 6

Chain B:



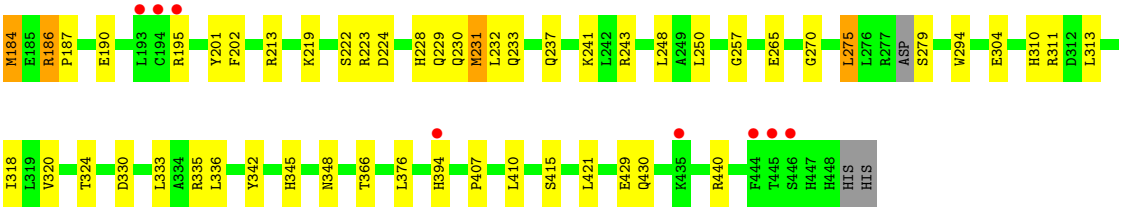
• Molecule 1: Protein-tyrosine kinase 6

Chain C:



• Molecule 1: Protein-tyrosine kinase 6

Chain D:


M184
E185
R186
P187
E190
L193
C194
R195
Y201
F202
R213
K219
S222
R223
D224
H228
Q229
Q230
M231
L232
Q233
Q237
K241
L242
R243
L248
A249
L250
G257
E265
G270
L275
L276
R277
ASP
S279
W294
E304
H310
R311
D312
L313
I318
L319
V320
T324
D330
L333
A334
R335
L336
Y342
H345
N348
T366
L376
H394
P407
L410
S415
L421
E429
Q430
K435
R440
F444
T445
S446
H447
H448
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.88Å 77.02Å 87.41Å 81.36° 75.76° 74.92°	Depositor
Resolution (Å)	84.52 – 2.24 42.18 – 2.24	Depositor EDS
% Data completeness (in resolution range)	94.5 (84.52-2.24) 94.5 (42.18-2.24)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.205 , 0.260 0.204 , 0.259	Depositor DCC
R_{free} test set	2789 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9541	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.20% 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: CXM, GOL, 1N1

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	0.47	0/2285	0.64	0/3087
1	B	0.47	0/2282	0.63	0/3085
1	C	0.45	0/2280	0.61	0/3081
1	D	0.45	0/2266	0.63	1/3063 (0.0%)
All	All	0.46	0/9113	0.63	1/12316 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	275	LEU	CA-CB-CG	5.90	128.87	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	184	CXM	Mainchain

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	2211	0	2219	41	0
1	B	2202	0	2202	37	0
1	C	2201	0	2200	45	0
1	D	2190	0	2188	36	0
2	A	41	0	14	0	0
2	B	41	0	14	0	0
2	C	41	0	14	0	0
2	D	41	0	14	0	0
3	A	18	0	24	1	0
3	B	18	0	24	5	0
3	C	18	0	24	1	0
3	D	18	0	24	0	0
4	A	138	0	0	4	0
4	B	120	0	0	2	0
4	C	112	0	0	6	0
4	D	131	0	0	3	0
All	All	9541	0	8961	155	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 9.

The worst 5 of 155 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:276:LEU:O	1:C:279:SER:HB3	1.55	1.05
1:A:399:ARG:HG2	1:A:399:ARG:HH11	1.18	1.04
1:C:223:ARG:NH2	1:C:229:GLN:OE1	1.94	1.00
1:B:223:ARG:NH2	1:B:229:GLN:OE1	1.96	0.99
1:D:223:ARG:HH22	1:D:229:GLN:HE22	1.14	0.96

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	272/267 (102%)	265 (97%)	7 (3%)	0	100	100
1	B	272/267 (102%)	264 (97%)	8 (3%)	0	100	100
1	C	273/267 (102%)	266 (97%)	7 (3%)	0	100	100
1	D	271/267 (102%)	265 (98%)	6 (2%)	0	100	100
All	All	1088/1068 (102%)	1060 (97%)	28 (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	244/236 (103%)	220 (90%)	24 (10%)	8	4
1	B	243/236 (103%)	230 (95%)	13 (5%)	22	21
1	C	242/236 (102%)	230 (95%)	12 (5%)	24	24
1	D	242/236 (102%)	228 (94%)	14 (6%)	20	18
All	All	971/944 (103%)	908 (94%)	63 (6%)	17	14

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	233	GLN
1	D	250	LEU
1	B	418	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	243	ARG
1	D	330	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	385	GLN
1	D	448	HIS
1	C	317	ASN
1	C	348	ASN
1	C	378	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	CXM	A	184	1	8,10,11	0.87	0	7,11,13	1.49	2 (28%)
1	CXM	D	184	1	8,10,11	1.02	1 (12%)	7,11,13	1.67	1 (14%)
1	CXM	B	184	1	8,10,11	0.92	1 (12%)	7,11,13	1.54	2 (28%)
1	CXM	C	184	1	8,10,11	0.79	0	7,11,13	1.82	2 (28%)

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
1	CXM	A	184	1	-	3/9/10/12	-
1	CXM	D	184	1	-	5/9/10/12	-
1	CXM	B	184	1	-	2/9/10/12	-
1	CXM	C	184	1	-	4/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	184	CXM	ON1-CN	2.21	1.25	1.21
1	B	184	CXM	ON1-CN	2.10	1.25	1.21

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	184	CXM	ON1-CN-N	-3.50	119.10	124.85
1	C	184	CXM	ON1-CN-N	-3.35	119.35	124.85
1	A	184	CXM	ON1-CN-N	-2.81	120.24	124.85
1	B	184	CXM	ON1-CN-N	-2.68	120.45	124.85
1	C	184	CXM	C-CA-N	2.49	114.23	109.73

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	184	CXM	C-CA-CB-CG
1	C	184	CXM	C-CA-CB-CG
1	D	184	CXM	O-C-CA-CB
1	A	184	CXM	N-CA-CB-CG
1	B	184	CXM	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	184	CXM	1	0
1	D	184	CXM	1	0
1	C	184	CXM	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

20 ligands are modelled in this entry.

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	1N1	C	501[A]	-	32,36,36	0.79	0	40,50,50	1.83	11 (27%)
2	1N1	C	501[B]	-	32,36,36	0.81	0	40,50,50	1.78	9 (22%)
3	GOL	B	503	-	5,5,5	0.31	0	5,5,5	0.49	0
3	GOL	A	503	-	5,5,5	0.33	0	5,5,5	0.30	0
2	1N1	A	501[A]	-	32,36,36	0.76	0	40,50,50	1.51	7 (17%)
3	GOL	B	502	-	5,5,5	0.35	0	5,5,5	0.42	0
2	1N1	A	501[B]	-	32,36,36	0.78	0	40,50,50	1.55	7 (17%)
3	GOL	D	503	-	5,5,5	0.23	0	5,5,5	0.80	0
3	GOL	A	502	-	5,5,5	0.40	0	5,5,5	0.43	0
3	GOL	A	504	-	5,5,5	0.28	0	5,5,5	0.63	0
2	1N1	D	504[A]	-	32,36,36	0.79	1 (3%)	40,50,50	1.40	7 (17%)
2	1N1	D	504[B]	-	32,36,36	0.82	1 (3%)	40,50,50	1.47	8 (20%)
3	GOL	C	503	-	5,5,5	0.36	0	5,5,5	0.32	0
3	GOL	C	504	-	5,5,5	0.39	0	5,5,5	0.41	0
2	1N1	B	501[A]	-	32,36,36	0.74	0	40,50,50	1.45	8 (20%)
2	1N1	B	501[B]	-	32,36,36	0.76	0	40,50,50	1.48	8 (20%)
3	GOL	C	502	-	5,5,5	0.34	0	5,5,5	0.46	0
3	GOL	B	504	-	5,5,5	0.30	0	5,5,5	0.54	0
3	GOL	D	501	-	5,5,5	0.28	0	5,5,5	0.62	0
3	GOL	D	502	-	5,5,5	0.31	0	5,5,5	0.43	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	1N1	C	501[A]	-	-	3/13/29/29	0/4/4/4
2	1N1	C	501[B]	-	-	3/13/29/29	0/4/4/4
3	GOL	B	503	-	-	4/4/4/4	-
3	GOL	A	503	-	-	4/4/4/4	-
2	1N1	A	501[A]	-	-	3/13/29/29	0/4/4/4
3	GOL	B	502	-	-	0/4/4/4	-
2	1N1	A	501[B]	-	-	3/13/29/29	0/4/4/4
3	GOL	D	503	-	-	4/4/4/4	-
3	GOL	A	502	-	-	0/4/4/4	-
3	GOL	A	504	-	-	2/4/4/4	-
2	1N1	D	504[A]	-	-	3/13/29/29	0/4/4/4
2	1N1	D	504[B]	-	-	3/13/29/29	0/4/4/4
3	GOL	C	503	-	-	4/4/4/4	-
3	GOL	C	504	-	-	2/4/4/4	-
2	1N1	B	501[A]	-	-	2/13/29/29	0/4/4/4
2	1N1	B	501[B]	-	-	2/13/29/29	0/4/4/4
3	GOL	C	502	-	-	0/4/4/4	-
3	GOL	B	504	-	-	4/4/4/4	-
3	GOL	D	501	-	-	2/4/4/4	-
3	GOL	D	502	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	504[A]	1N1	C13-N5	2.05	1.41	1.37
2	D	504[B]	1N1	C13-N5	2.05	1.41	1.37

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501[A]	1N1	N3-C13-N5	4.50	121.59	116.55
2	C	501[B]	1N1	N3-C13-N5	4.50	121.59	116.55
2	C	501[A]	1N1	C12-C13-N5	-4.39	117.08	122.29
2	C	501[B]	1N1	C12-C13-N5	-4.39	117.08	122.29
2	A	501[A]	1N1	C19-N5-C16	3.91	120.14	111.52

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	GOL	O1-C1-C2-C3
3	B	504	GOL	O1-C1-C2-C3
3	D	501	GOL	C1-C2-C3-O3
3	B	504	GOL	O1-C1-C2-O2
3	D	503	GOL	O2-C2-C3-O3

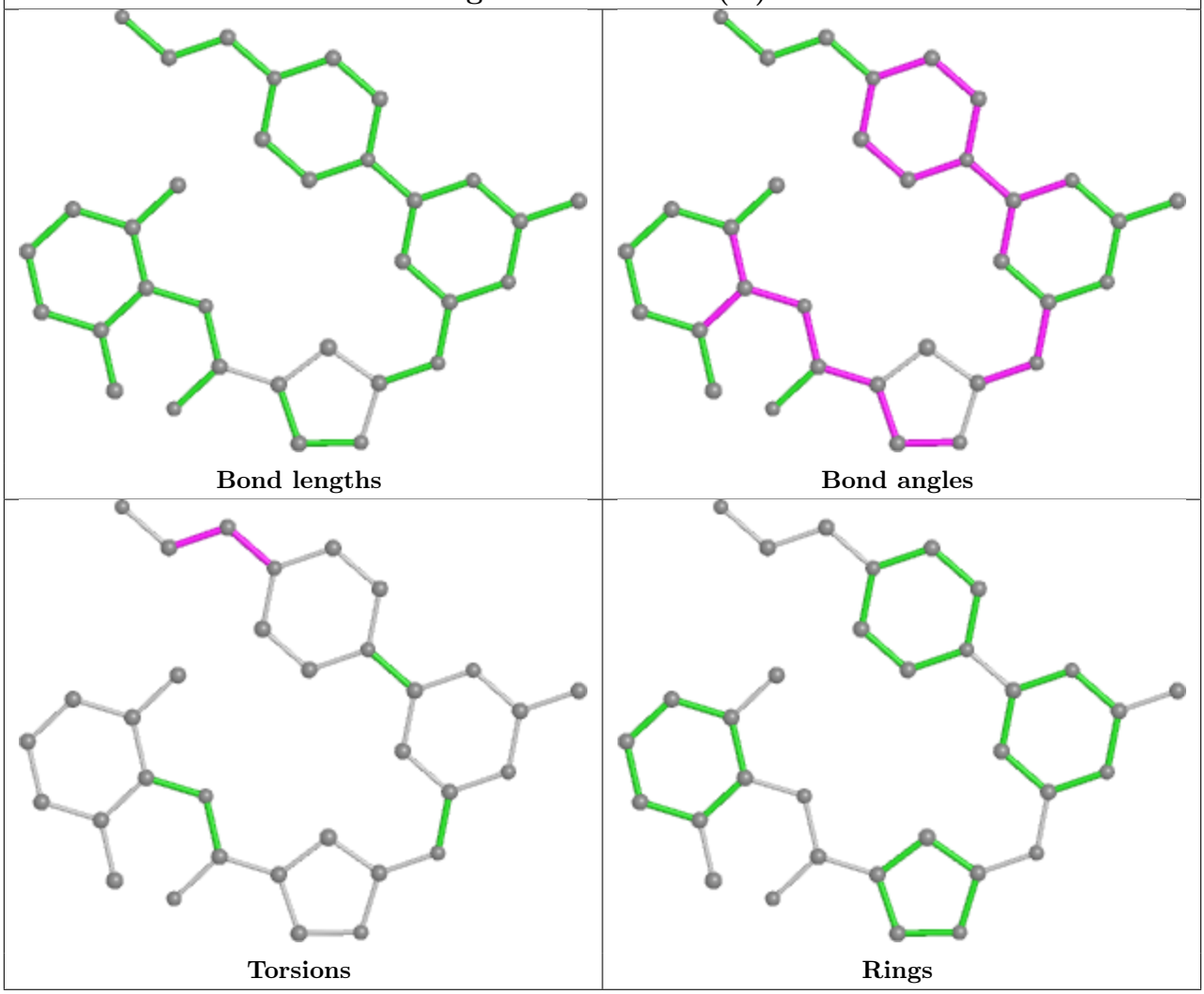
There are no ring outliers.

5 monomers are involved in 7 short contacts:

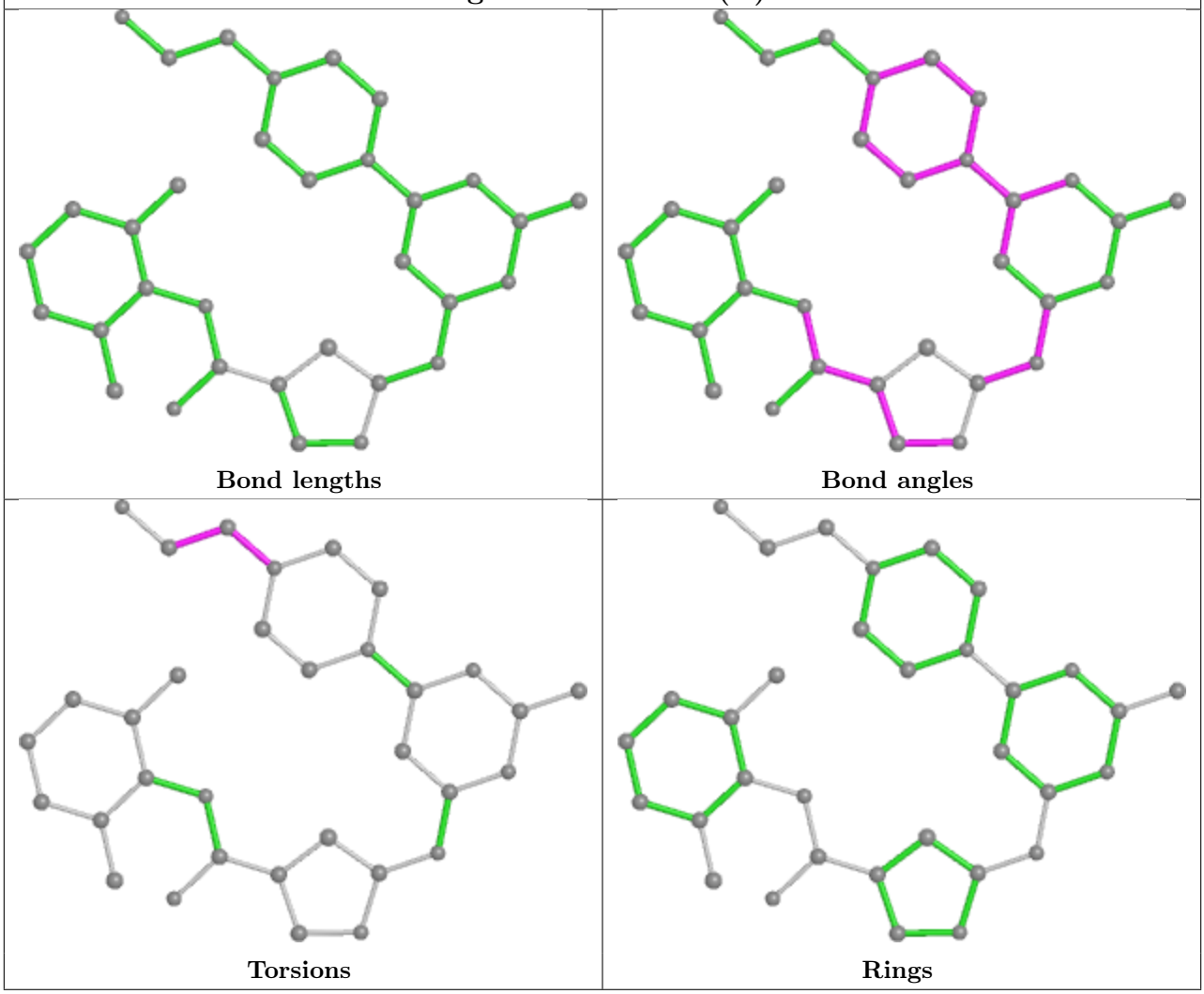
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	GOL	3	0
3	B	502	GOL	1	0
3	A	504	GOL	1	0
3	C	504	GOL	1	0
3	B	504	GOL	1	0

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.

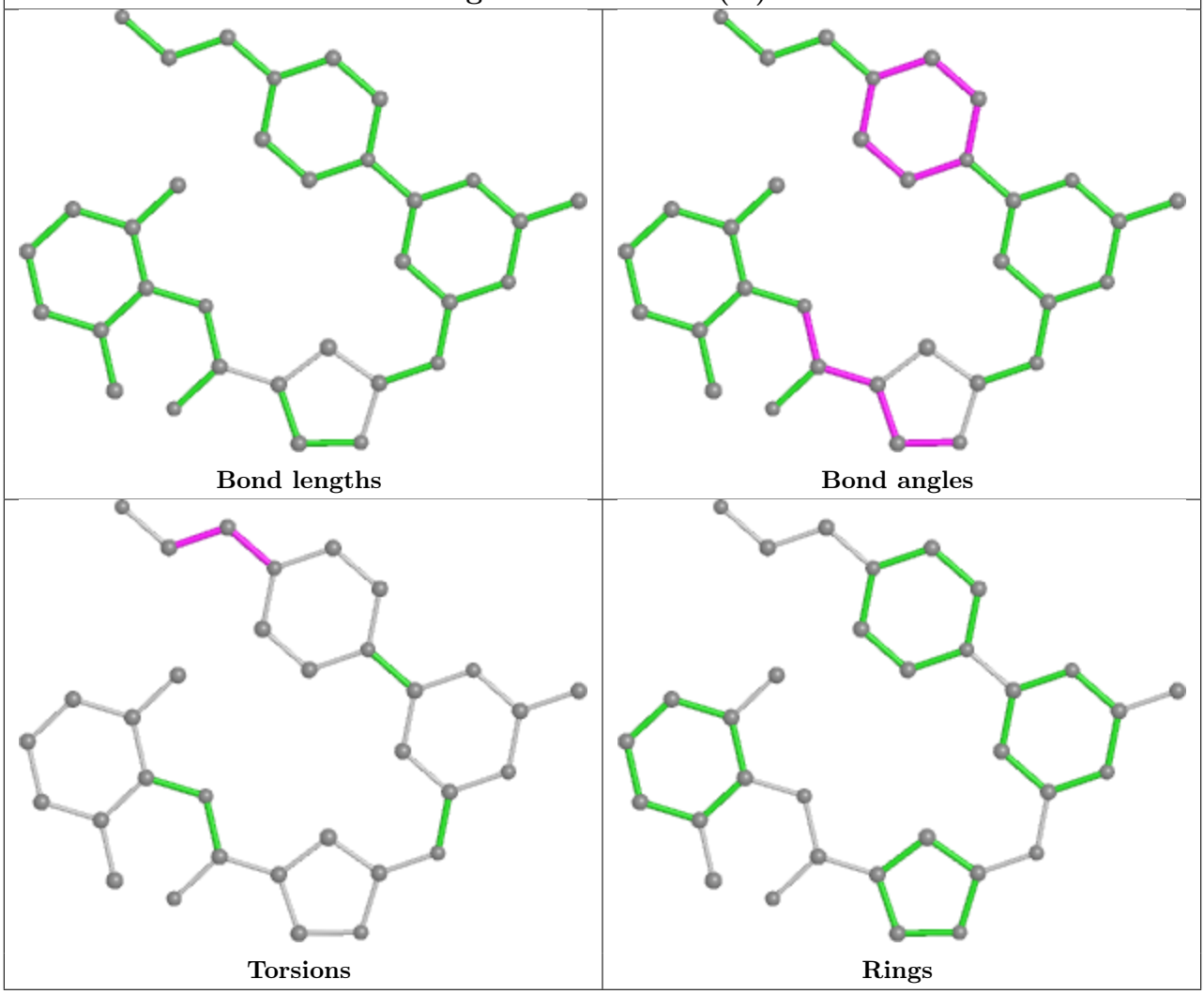
Ligand 1N1 C 501 (A)



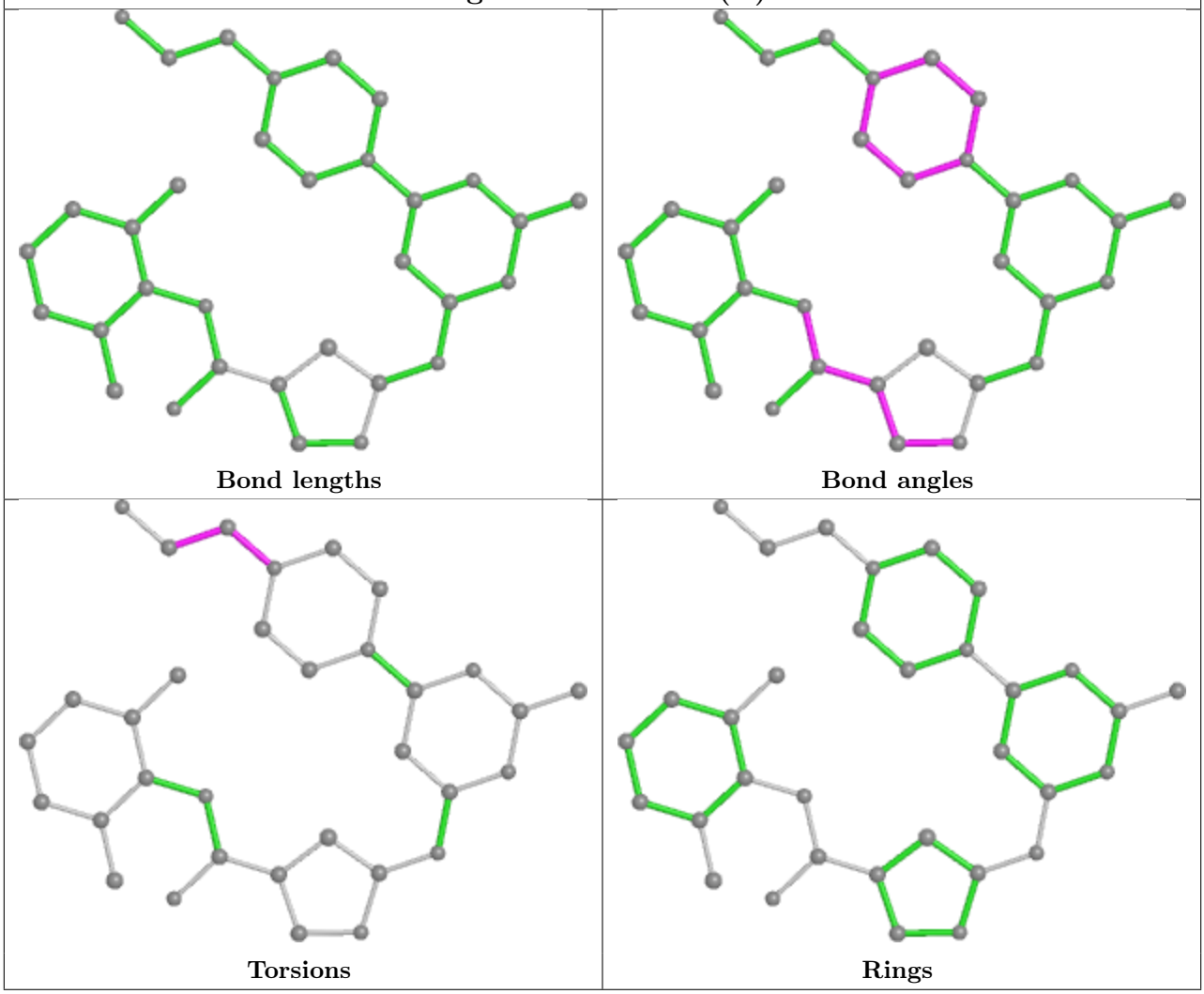
Ligand 1N1 C 501 (B)



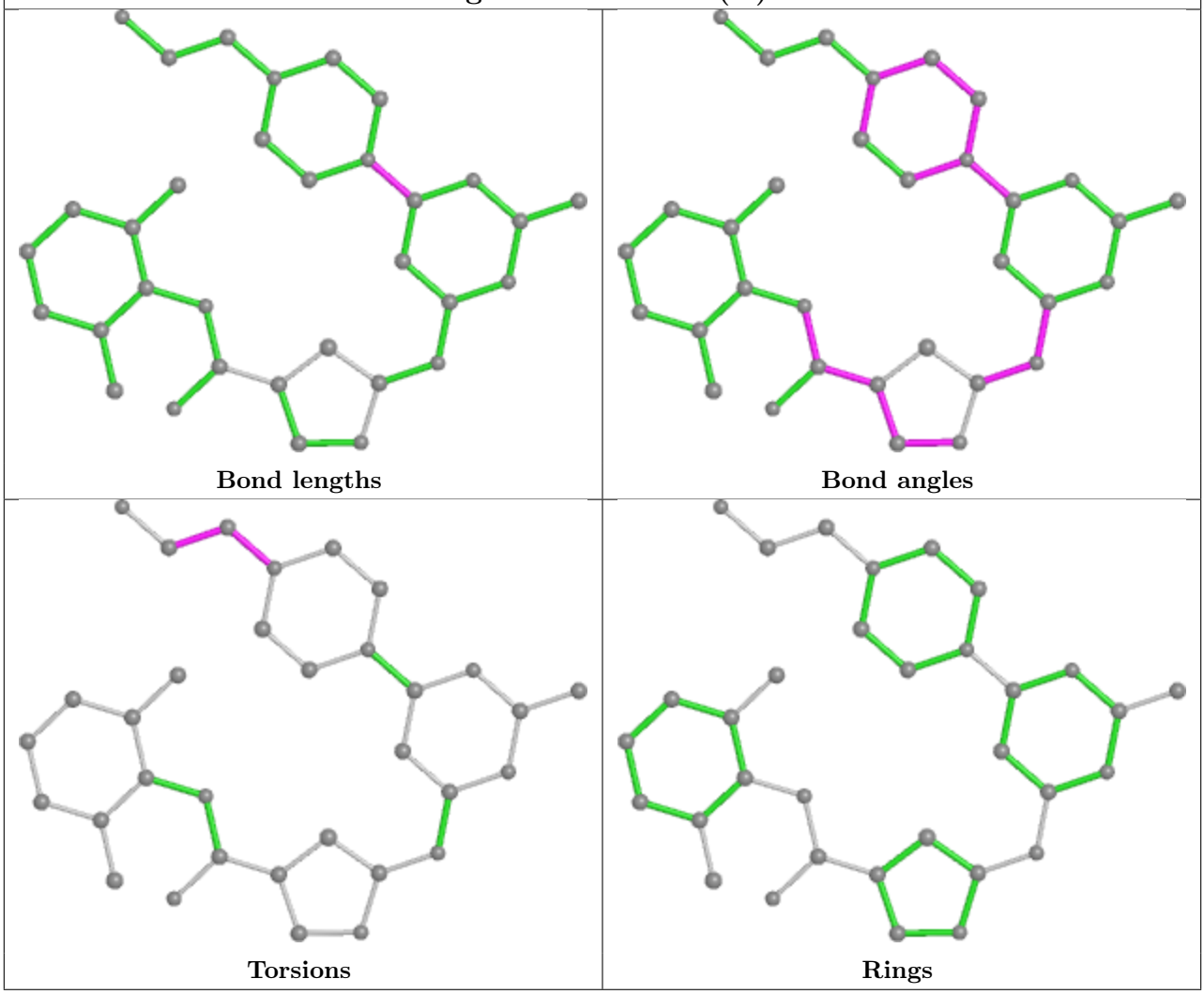
Ligand 1N1 A 501 (A)



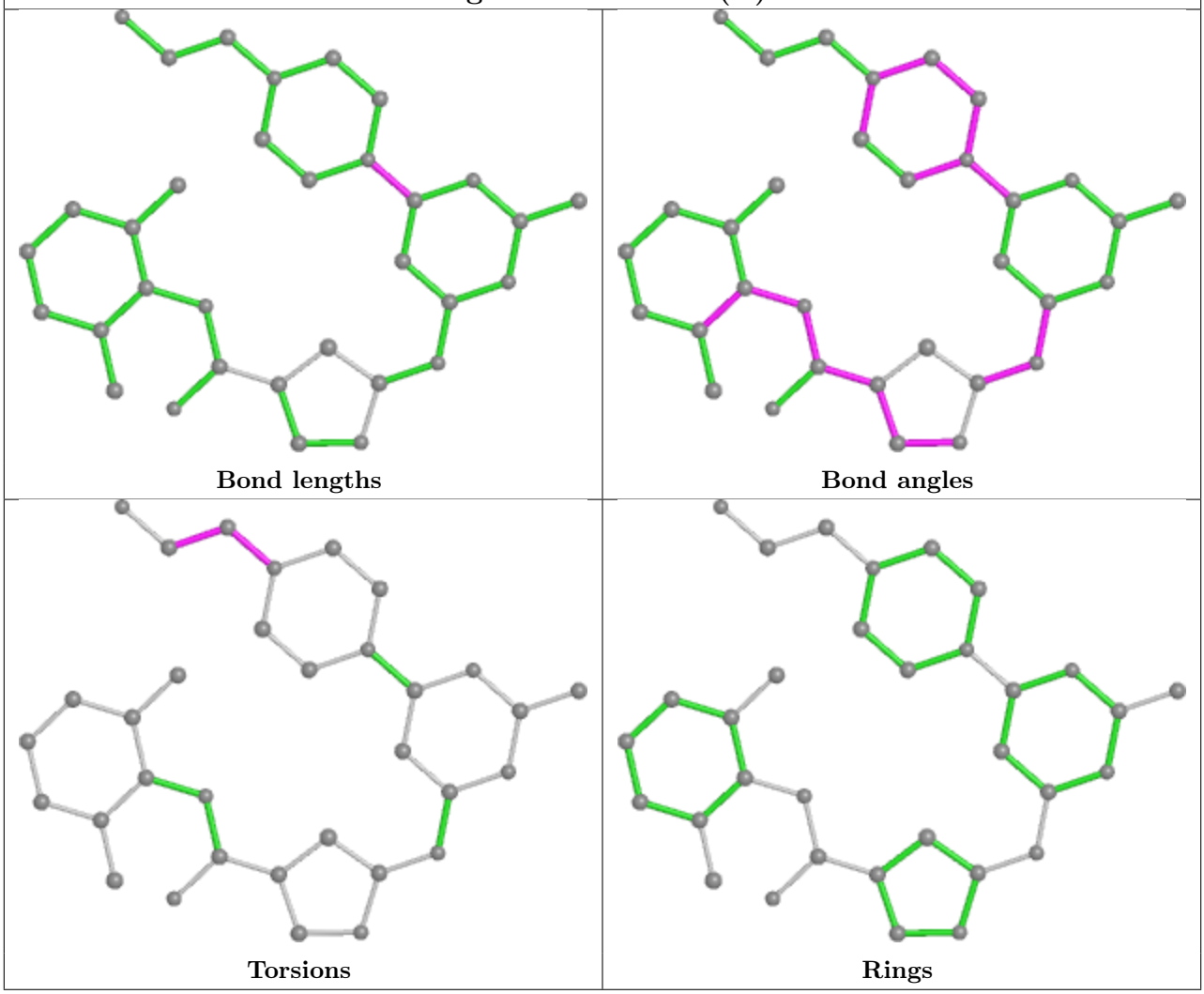
Ligand 1N1 A 501 (B)



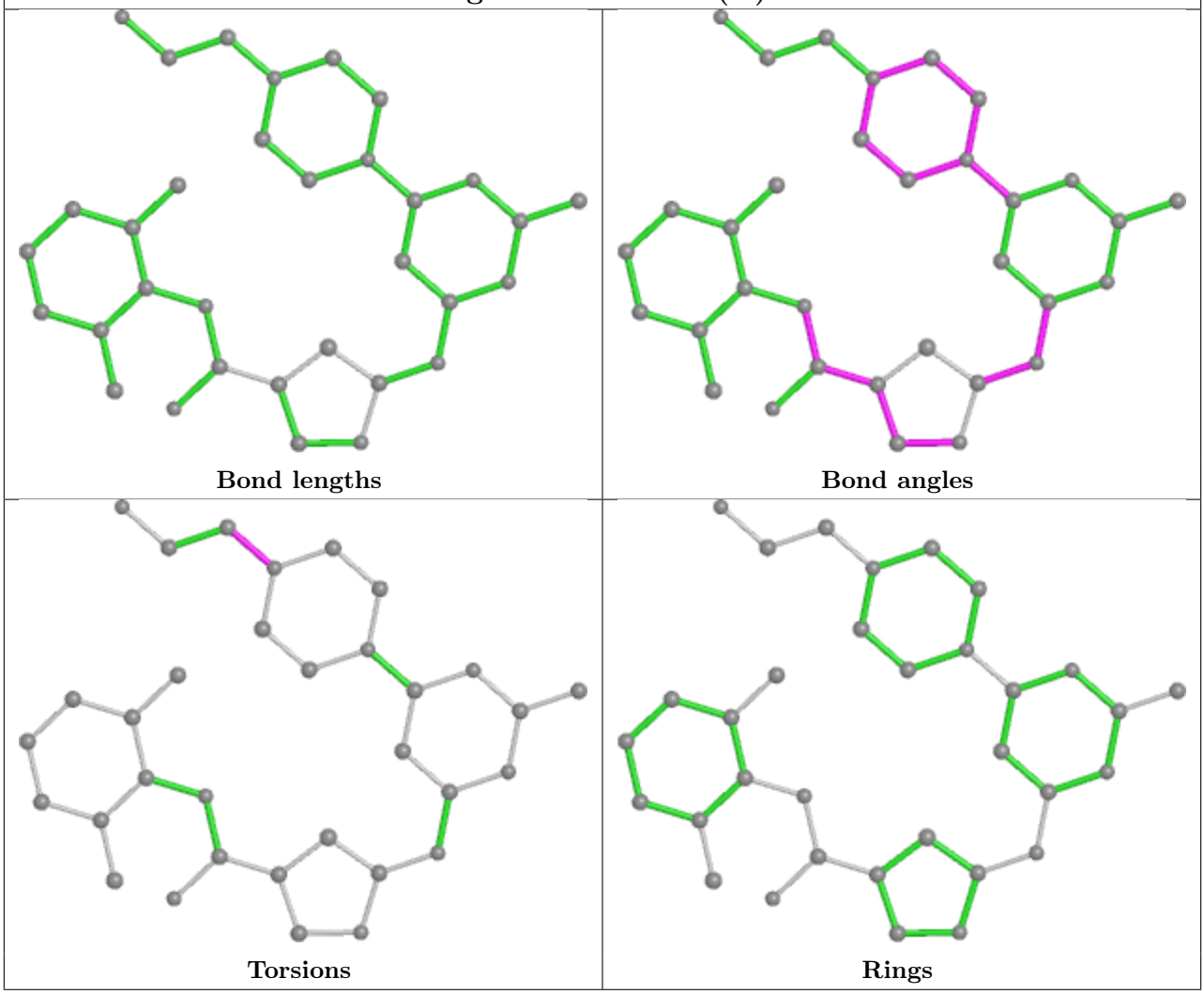
Ligand 1N1 D 504 (A)



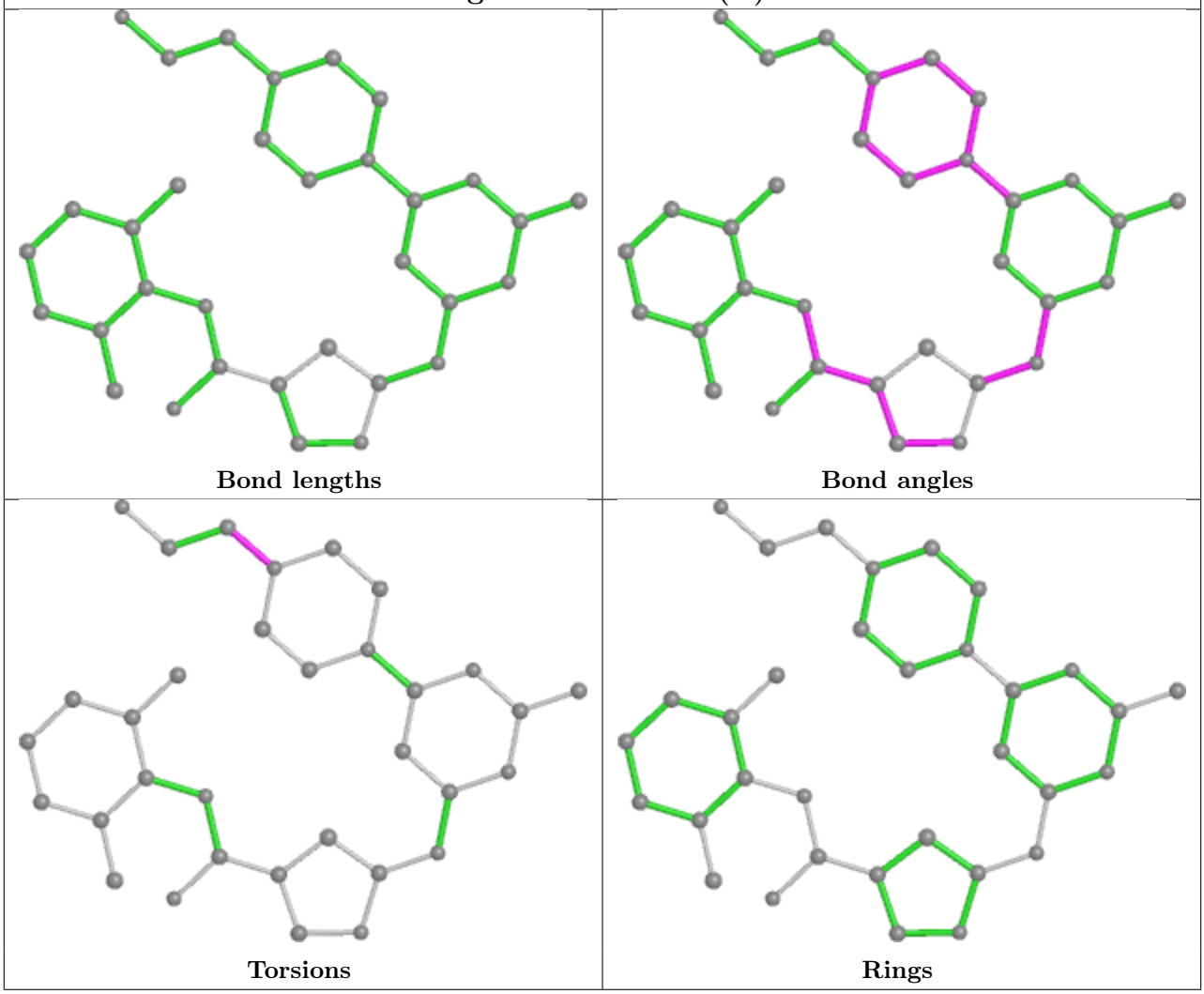
Ligand 1N1 D 504 (B)



Ligand 1N1 B 501 (A)



Ligand 1N1 B 501 (B)



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	265/267 (99%)	0.05	4 (1%)	73	74	23, 31, 42, 55	0
1	B	263/267 (98%)	-0.03	1 (0%)	92	93	24, 31, 41, 50	0
1	C	264/267 (98%)	0.23	8 (3%)	50	50	26, 33, 44, 54	0
1	D	263/267 (98%)	0.27	8 (3%)	50	50	26, 34, 44, 52	0
All	All	1055/1068 (98%)	0.13	21 (1%)	65	66	23, 32, 44, 55	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	444	PHE	4.4
1	D	195	ARG	4.4
1	C	195[A]	ARG	3.9
1	A	449	HIS	3.4
1	C	448	HIS	3.3

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CXM	C	184	11/12	0.88	0.19	42,43,44,46	0
1	CXM	D	184	11/12	0.92	0.15	41,42,46,46	0
1	CXM	A	184	11/12	0.95	0.13	38,39,40,41	0
1	CXM	B	184	11/12	0.96	0.11	36,37,43,43	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

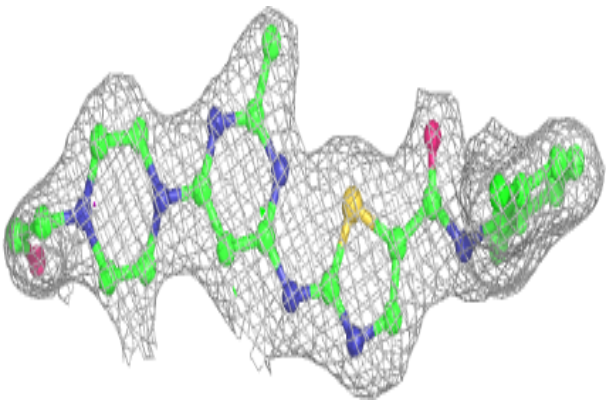
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

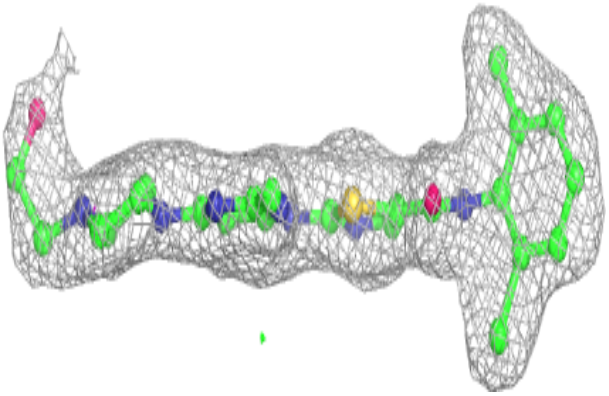
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	503	6/6	0.88	0.13	44,46,46,46	0
3	GOL	C	503	6/6	0.88	0.17	49,50,51,52	0
3	GOL	A	503	6/6	0.89	0.16	51,52,53,53	0
3	GOL	A	504	6/6	0.90	0.15	35,38,38,40	0
2	1N1	D	504[B]	33/33	0.90	0.17	32,37,47,48	8
2	1N1	D	504[A]	33/33	0.90	0.17	32,37,47,48	8
3	GOL	C	504	6/6	0.90	0.16	42,43,44,46	0
3	GOL	D	503	6/6	0.91	0.18	32,34,38,39	0
2	1N1	C	501[A]	33/33	0.92	0.15	31,36,46,48	8
2	1N1	C	501[B]	33/33	0.92	0.15	30,36,46,48	8
3	GOL	C	502	6/6	0.93	0.18	36,38,38,40	0
3	GOL	D	502	6/6	0.93	0.14	47,48,49,49	0
3	GOL	B	504	6/6	0.93	0.20	35,37,39,41	0
2	1N1	B	501[B]	33/33	0.94	0.14	30,33,41,44	8
2	1N1	B	501[A]	33/33	0.94	0.14	29,33,41,44	8
2	1N1	A	501[A]	33/33	0.95	0.14	27,30,39,42	8
2	1N1	A	501[B]	33/33	0.95	0.14	27,30,39,42	8
3	GOL	A	502	6/6	0.95	0.17	36,38,39,40	0
3	GOL	D	501	6/6	0.96	0.21	39,40,40,40	0
3	GOL	B	502	6/6	0.97	0.12	28,30,32,32	0

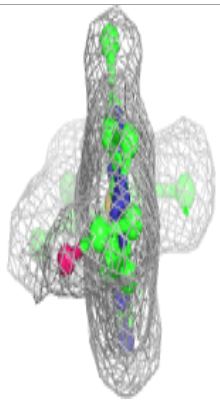
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1N1 D 504 (B):

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

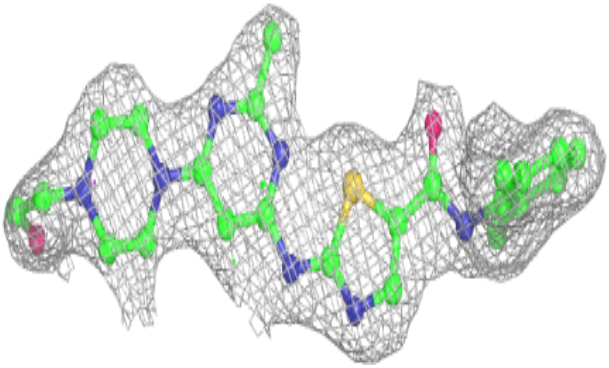


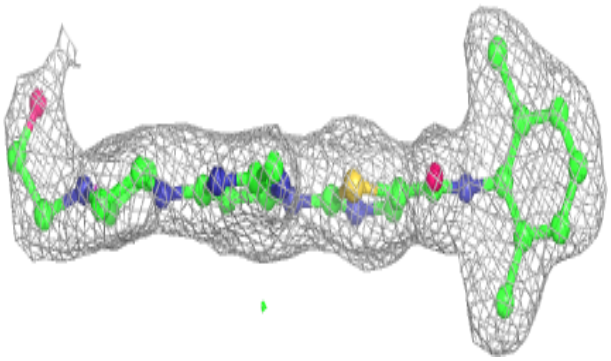


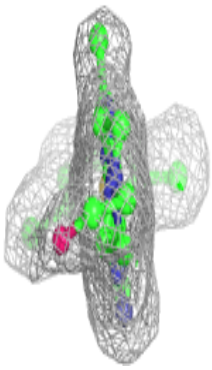


Electron density around 1N1 D 504 (A):

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

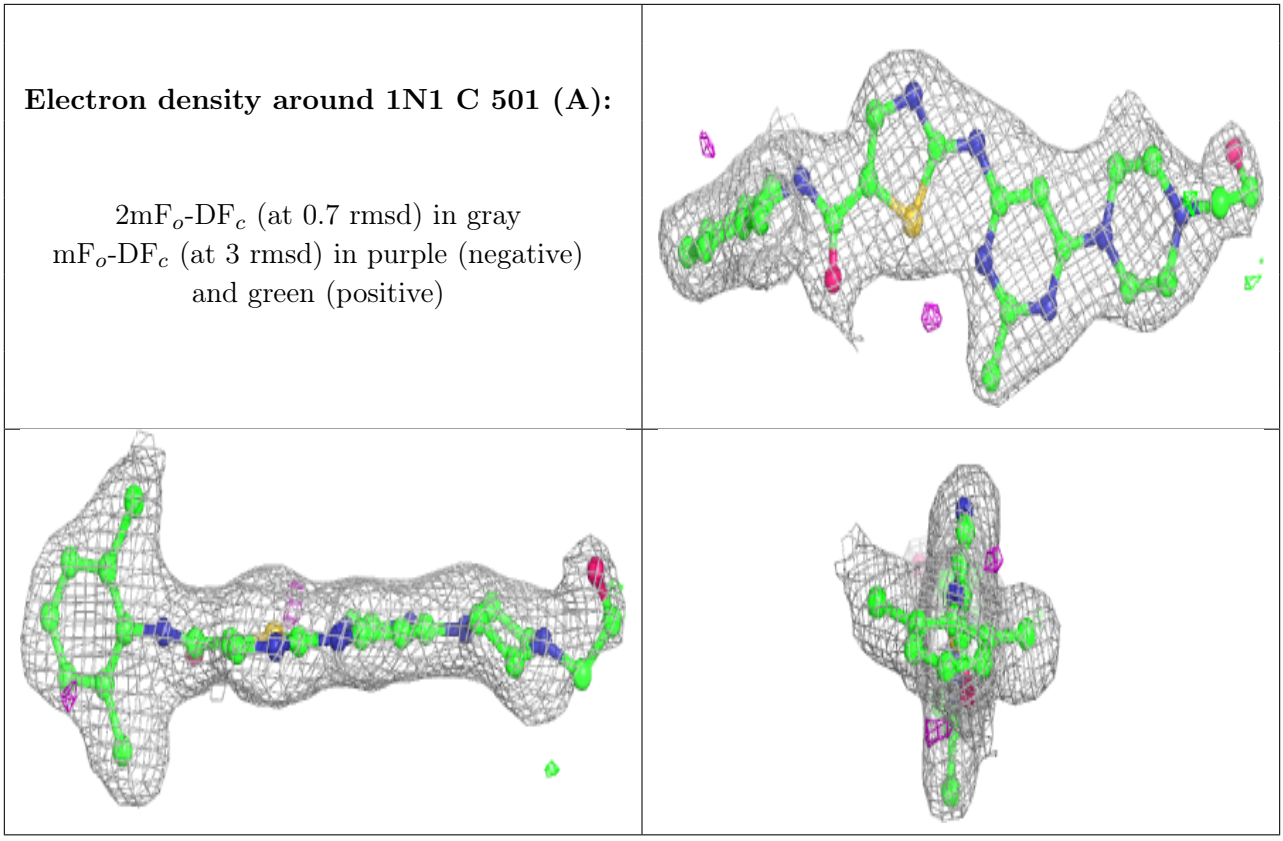






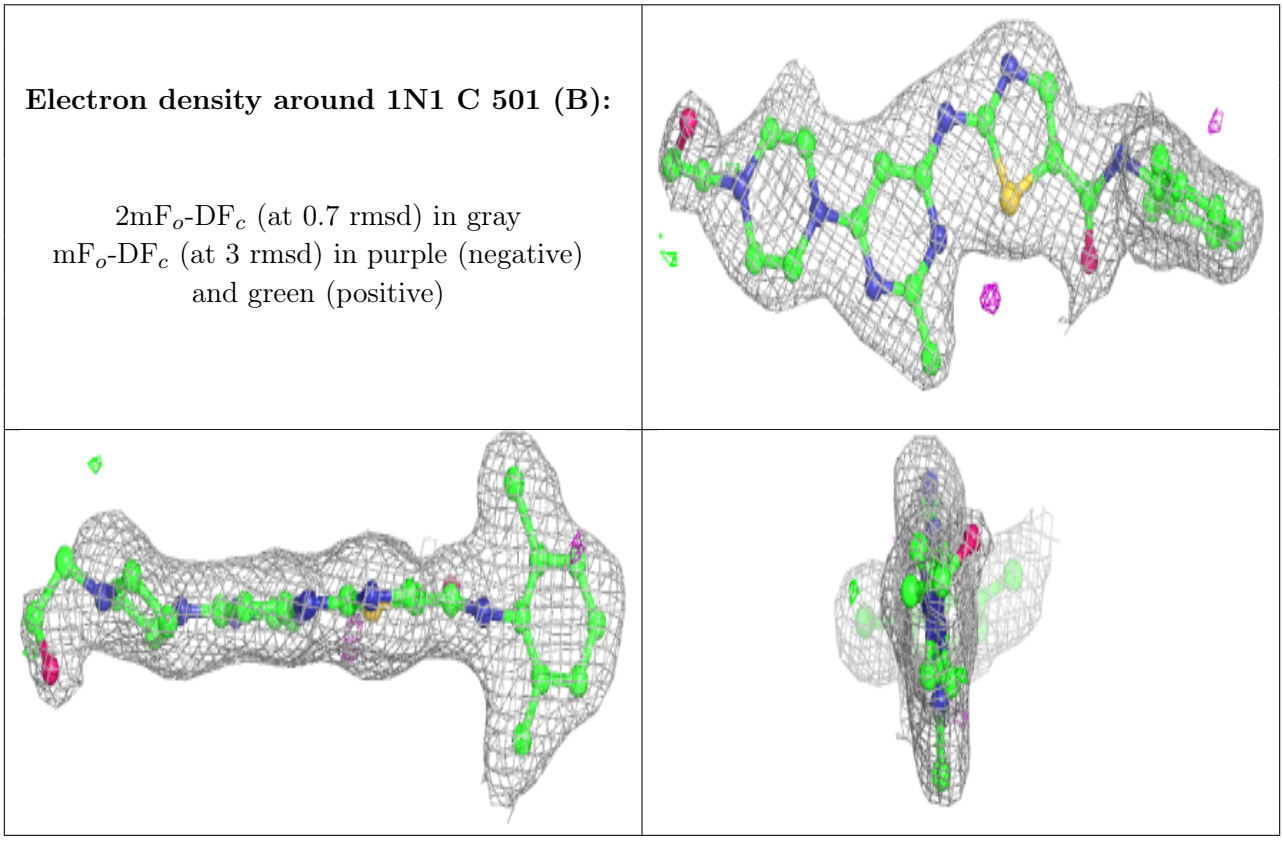
Electron density around 1N1 C 501 (A):

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



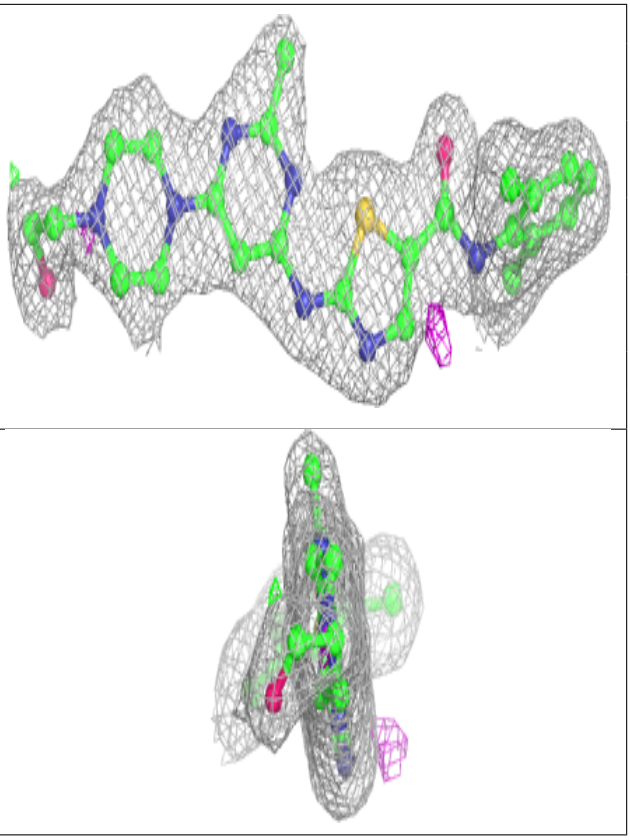
Electron density around 1N1 C 501 (B):

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



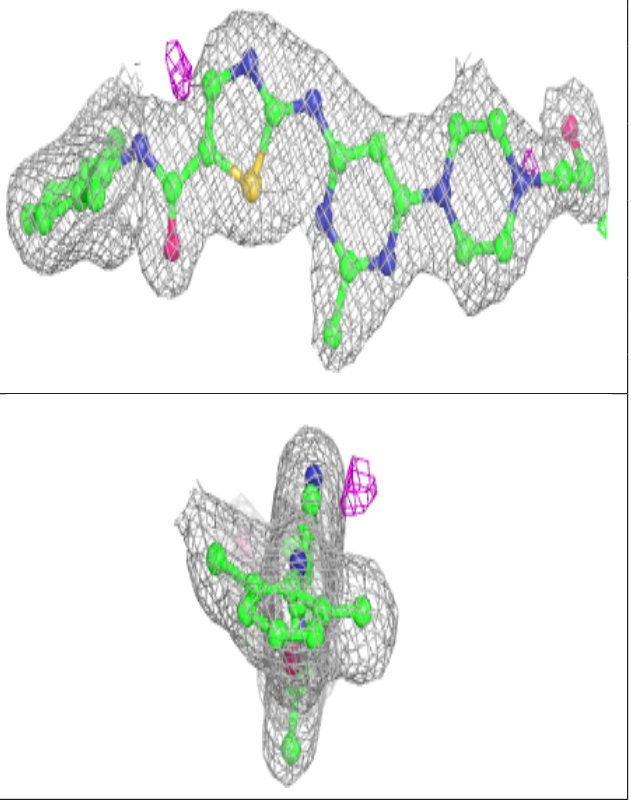
Electron density around 1N1 B 501 (B):

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



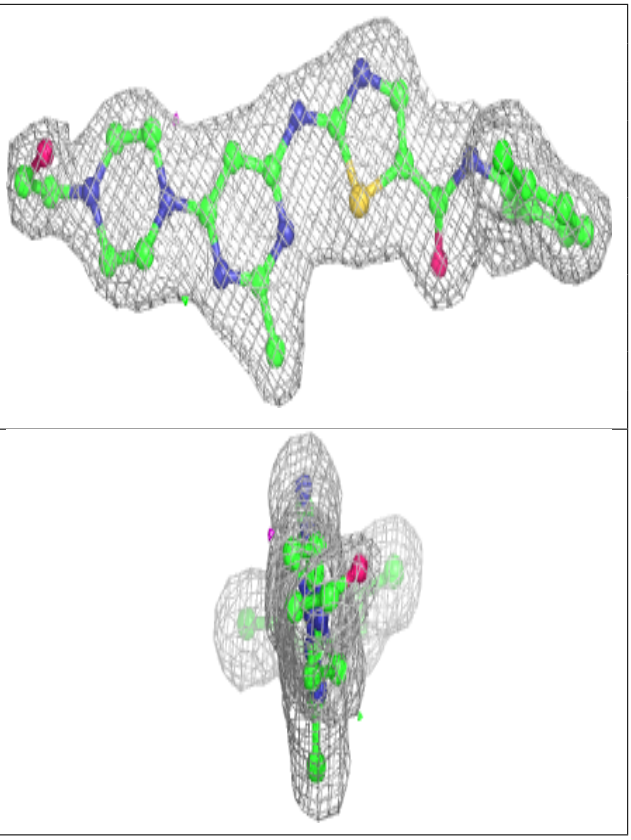
Electron density around 1N1 B 501 (A):

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



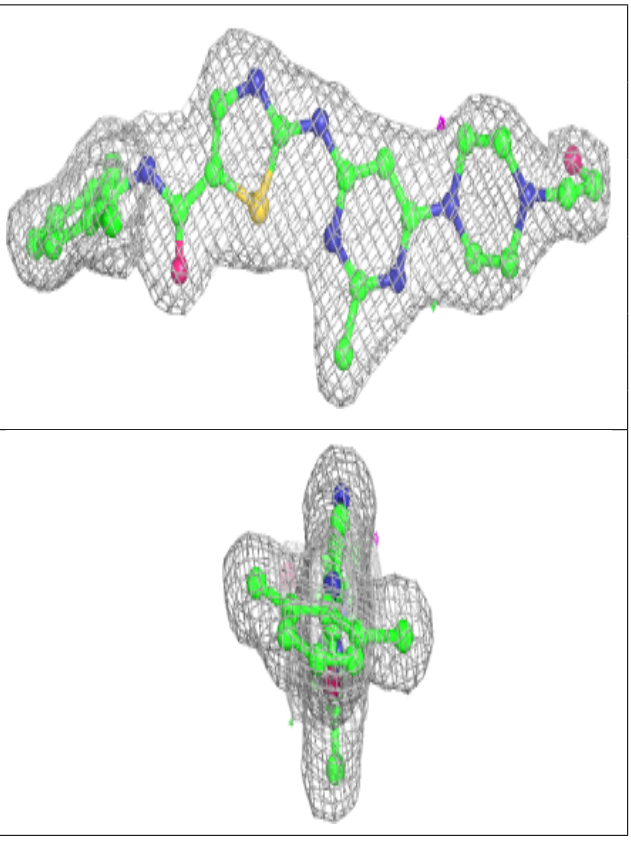
Electron density around 1N1 A 501 (A):

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



Electron density around 1N1 A 501 (B):

$2mF_o$-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.