Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 01:26 pm GMT

PDB ID	:	4BZ7
Title	:	Crystal structure of Schistosoma mansoni HDAC8 complexed with M344
Authors	:	Marek, M.; Romier, C.
Deposited on	:	2013-07-24
Resolution	:	1.65 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:

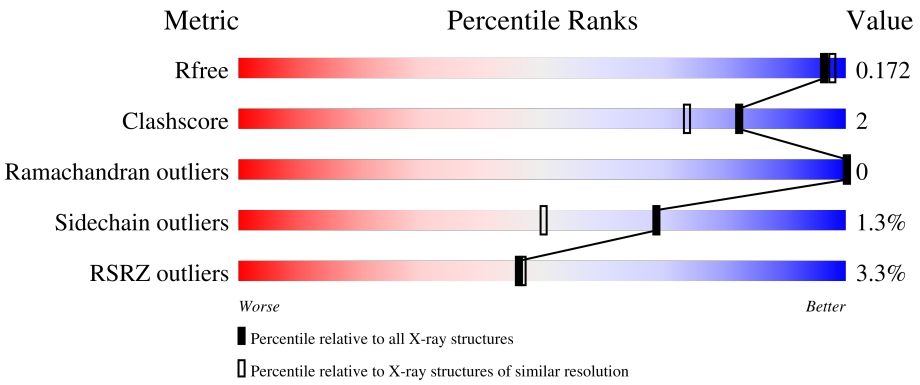
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	446	5% 85% • 11%
1	B	446	2% 90% • 7%
1	C	446	% 90% • 7%
1	D	446	4% 85% 5% 11%

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	GOL	D	800	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14549 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 HISTONE DEACETYLASE 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	399	3226	2086	532	593	15	0	9	0
1	B	413	3310	2136	551	607	16	0	5	0
1	C	416	3352	2164	557	613	18	0	8	0
1	D	399	3218	2079	532	592	15	0	7	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	GLY	-	expression tag	UNP A5H660
A	442	SER	-	expression tag	UNP A5H660
A	443	LEU	-	expression tag	UNP A5H660
A	444	VAL	-	expression tag	UNP A5H660
A	445	PRO	-	expression tag	UNP A5H660
A	446	ARG	-	expression tag	UNP A5H660
B	441	GLY	-	expression tag	UNP A5H660
B	442	SER	-	expression tag	UNP A5H660
B	443	LEU	-	expression tag	UNP A5H660
B	444	VAL	-	expression tag	UNP A5H660
B	445	PRO	-	expression tag	UNP A5H660
B	446	ARG	-	expression tag	UNP A5H660
C	441	GLY	-	expression tag	UNP A5H660
C	442	SER	-	expression tag	UNP A5H660
C	443	LEU	-	expression tag	UNP A5H660
C	444	VAL	-	expression tag	UNP A5H660
C	445	PRO	-	expression tag	UNP A5H660
C	446	ARG	-	expression tag	UNP A5H660
D	441	GLY	-	expression tag	UNP A5H660
D	442	SER	-	expression tag	UNP A5H660
D	443	LEU	-	expression tag	UNP A5H660

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Chain	Residue	Modelled	Actual	Comment	Reference
D	444	VAL	-	expression tag	UNP A5H660
D	445	PRO	-	expression tag	UNP A5H660
D	446	ARG	-	expression tag	UNP A5H660

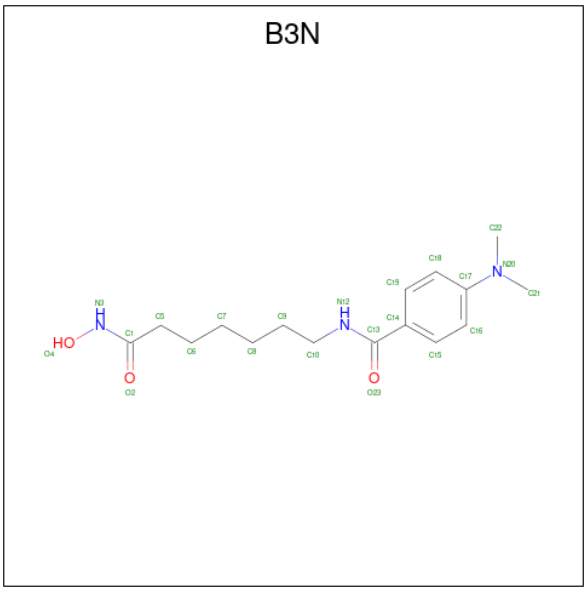
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

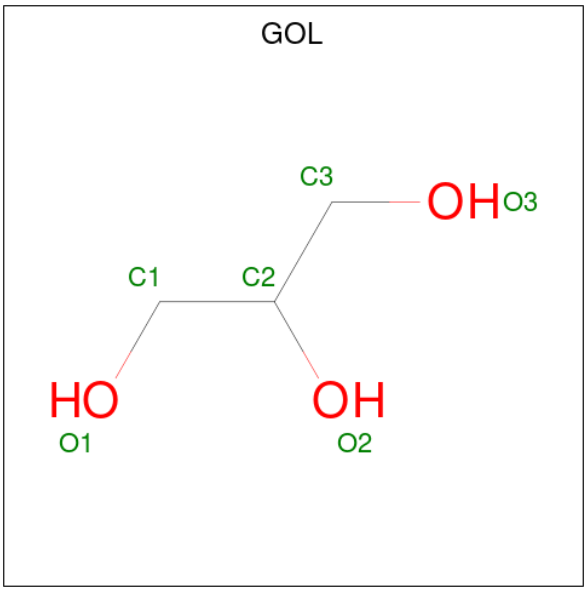
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
3	A	2	2	2	0	0
3	B	2	2	2	0	0
3	C	2	2	2	0	0
3	D	2	2	2	0	0

- Molecule 4 is 4-(dimethylamino)-N-[7-(hydroxyamino)-7-oxoheptyl]benzamide (three-letter code: B3N) (formula: $C_{16}H_{25}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	22	16	3	3	0	0
			Total	C	N	O		
4	A	1	22	16	3	3	0	0
			Total	C	N	O		
4	B	1	22	16	3	3	0	0
			Total	C	N	O		
4	B	1	22	16	3	3	0	0
			Total	C	N	O		
4	C	1	22	16	3	3	0	0
			Total	C	N	O		
4	C	1	22	16	3	3	0	0
			Total	C	N	O		
4	D	1	22	16	3	3	0	0
			Total	C	N	O		
4	D	1	22	16	3	3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

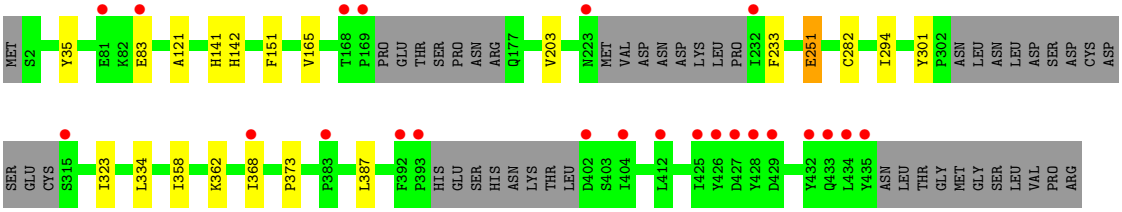
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	330	330	330	0	0
			Total	O		
6	B	293	293	293	0	0
			Total	O		
6	C	303	303	303	0	0
			Total	O		
6	D	245	245	245	0	0

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.

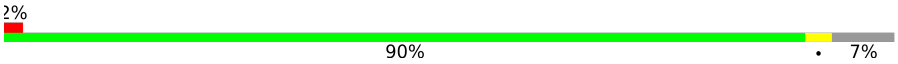
- Molecule 1: HISTONE DEACETYLASE 8

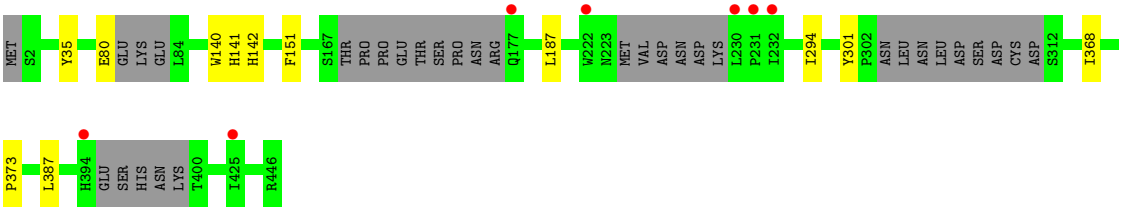
Chain A:



- Molecule 1: HISTONE DEACETYLASE 8

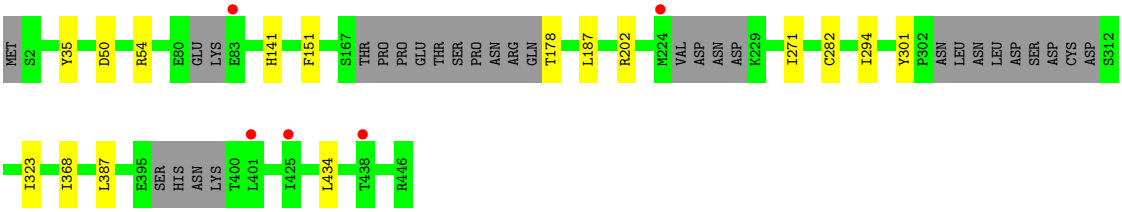
Chain B:





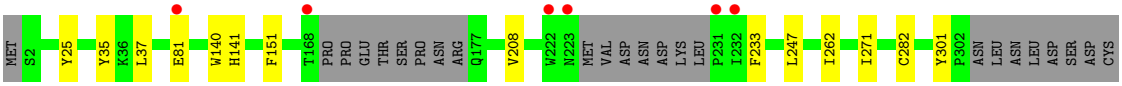
- Molecule 1: HISTONE DEACETYLASE 8

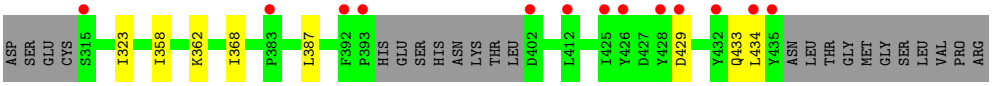
Chain C:



- Molecule 1: HISTONE DEACETYLASE 8

Chain D:




ASP
SER
GLU
CYS
S315
I323
I358
K362
I368
P383
L387
F392
P393
HIS
GLU
SER
HIS
ASN
LYS
THR
LEU
D402
L412
I425
Y426
D427
Y428
D429
Y432
Q433
L434
Y435
ASN
LEU
THR
GLY
MET
GLY
SER
LEU
VAL
PRO
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.56Å 70.58Å 98.51Å 78.05° 75.41° 85.49°	Depositor
Resolution (Å)	24.16 – 1.65 49.71 – 1.65	Depositor EDS
% Data completeness (in resolution range)	95.8 (24.16-1.65) 96.7 (49.71-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.46 (at 1.65Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.155 , 0.172 0.151 , 0.172	Depositor DCC
R_{free} test set	10365 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.054 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14549	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: ZN, B3N, GOL, K

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	0.49	0/3343	0.58	0/4548
1	B	0.53	0/3416	0.59	0/4648
1	C	0.52	0/3467	0.60	0/4713
1	D	0.50	0/3329	0.59	0/4528
All	All	0.51	0/13555	0.59	0/18437

There are no bond length outliers.

There are no bond angle outliers.

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	3226	0	3145	14	0
1	B	3310	0	3222	16	0
1	C	3352	0	3277	17	0
1	D	3218	0	3130	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	44	0	49	1	0
4	B	44	0	49	1	0
4	C	44	0	49	0	0
4	D	44	0	49	0	0
5	A	18	0	24	0	0
5	B	18	0	23	3	0
5	C	24	0	32	0	0
5	D	24	0	32	4	0
6	A	330	0	0	0	0
6	B	293	0	0	2	0
6	C	303	0	0	0	0
6	D	245	0	0	2	0
All	All	14549	0	13081	66	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 2.

All (66) 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:368[B]:ILE:HG21	1:C:387:LEU:CD2	2.01	0.89
1:B:368[A]:ILE:HG21	1:B:387:LEU:CD2	2.03	0.89
1:C:368[B]:ILE:HG21	1:C:387:LEU:HD22	1.61	0.83
1:C:368[B]:ILE:CG2	1:C:387:LEU:HD22	2.13	0.78
1:B:368[A]:ILE:HG21	1:B:387:LEU:HD22	1.66	0.76
1:B:368[A]:ILE:CG2	1:B:387:LEU:HD22	2.17	0.75
1:C:35:TYR:CE1	1:C:368[B]:ILE:HG23	2.22	0.73
5:D:800:GOL:H11	6:D:2024:HOH:O	1.88	0.73
1:B:368[A]:ILE:CG2	1:B:387:LEU:CD2	2.70	0.69
1:C:35:TYR:CE1	1:C:368[A]:ILE:HG23	2.28	0.68
1:C:368[B]:ILE:CG2	1:C:387:LEU:CD2	2.69	0.68
1:B:35:TYR:CE1	1:B:368[A]:ILE:HG23	2.29	0.68
1:B:35:TYR:CE1	1:B:368[B]:ILE:HG23	2.31	0.66
1:D:358:ILE:HG23	1:D:362:LYS:HD3	1.79	0.64
1:A:368[B]:ILE:HG21	1:A:387:LEU:CD2	2.30	0.62
1:D:247:LEU:HD23	1:D:262[B]:ILE:HD11	1.83	0.61
1:A:121:ALA:HB1	1:A:334:LEU:HD11	1.82	0.60
1:B:140:TRP:HZ2	5:B:800:GOL:H2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:HG23	1:A:362:LYS:HD3	1.85	0.58
1:D:140:TRP:HZ2	5:D:800:GOL:H31	1.69	0.58
1:D:25:TYR:HB2	5:D:800:GOL:H12	1.86	0.57
1:D:247:LEU:HD23	1:D:262[B]:ILE:CD1	2.35	0.56
1:A:368[B]:ILE:CG2	1:A:387:LEU:HD22	2.37	0.55
1:C:368[A]:ILE:CG2	1:C:387:LEU:HD22	2.36	0.55
1:D:35:TYR:CE1	1:D:368:ILE:HG23	2.41	0.55
5:D:800:GOL:C1	6:D:2024:HOH:O	2.51	0.53
5:B:800:GOL:H11	6:B:2029:HOH:O	2.08	0.53
1:B:368[B]:ILE:CG2	1:B:387:LEU:HD22	2.39	0.53
1:C:35:TYR:CD1	1:C:368[A]:ILE:HG23	2.45	0.52
1:D:271:ILE:HD12	1:D:434:LEU:HD11	1.93	0.51
1:C:368[B]:ILE:HG21	1:C:387:LEU:HD21	1.89	0.51
1:D:368:ILE:HG21	1:D:387:LEU:CD2	2.41	0.51
1:A:121:ALA:CB	1:A:334:LEU:HD11	2.40	0.51
1:B:368[A]:ILE:HG21	1:B:387:LEU:HD21	1.88	0.51
1:D:208:VAL:CG2	1:D:262[B]:ILE:HD11	2.41	0.50
1:B:35:TYR:CD1	1:B:368[B]:ILE:HG23	2.47	0.50
1:A:368[B]:ILE:HG21	1:A:387:LEU:HD22	1.92	0.49
1:A:368[B]:ILE:CG2	1:A:387:LEU:CD2	2.91	0.49
1:C:282[B]:CYS:SG	1:C:323:ILE:HD11	2.53	0.48
1:D:208:VAL:HG21	1:D:262[B]:ILE:HD11	1.96	0.48
1:D:368:ILE:CG2	1:D:387:LEU:HD22	2.44	0.47
1:B:187:LEU:HD21	1:B:294:ILE:HD12	1.96	0.47
1:C:368[A]:ILE:HG21	1:C:387:LEU:CD2	2.44	0.47
1:C:50:ASP:HB2	1:C:54:ARG:HD3	1.96	0.47
1:A:165:VAL:HG11	1:A:203:VAL:CG2	2.45	0.46
1:A:35:TYR:CE1	1:A:368[B]:ILE:HG23	2.50	0.46
1:C:271:ILE:HD12	1:C:434[A]:LEU:HD12	1.98	0.46
1:C:368[A]:ILE:HG22	1:C:387:LEU:HD22	1.95	0.45
1:D:368:ILE:CG2	1:D:387:LEU:CD2	2.95	0.45
1:B:368[B]:ILE:HG21	1:B:387:LEU:CD2	2.45	0.45
1:B:368[B]:ILE:HG22	1:B:387:LEU:HD22	1.97	0.45
1:C:368[A]:ILE:CG2	1:C:387:LEU:CD2	2.96	0.44
1:C:187:LEU:HD21	1:C:294:ILE:HD12	1.98	0.44
1:B:368[B]:ILE:CG2	1:B:387:LEU:CD2	2.96	0.44
5:B:800:GOL:C1	6:B:2029:HOH:O	2.65	0.44
1:A:251:GLU:HB2	1:A:294:ILE:HG23	1.98	0.44
1:D:282[B]:CYS:SG	1:D:323:ILE:HD11	2.58	0.43
1:D:429:ASP:O	1:D:433:GLN:HG2	2.18	0.43
1:B:142:HIS:NE2	4:B:700:B3N:N3	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:THR:HB	1:C:202:ARG:HH21	1.84	0.42
1:A:142:HIS:NE2	4:A:700:B3N:N3	2.59	0.42
1:A:35:TYR:CZ	1:A:373:PRO:HD3	2.56	0.41
1:A:35:TYR:CE1	1:A:368[A]:ILE:HG23	2.56	0.41
1:D:37:LEU:HD21	1:D:368:ILE:HD11	2.04	0.40
1:A:282[B]:CYS:SG	1:A:323:ILE:HD11	2.62	0.40
1:B:35:TYR:CZ	1:B:373:PRO:HD3	2.56	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	398/446 (89%)	392 (98%)	6 (2%)	0	100	100
1	B	406/446 (91%)	399 (98%)	7 (2%)	0	100	100
1	C	412/446 (92%)	405 (98%)	7 (2%)	0	100	100
1	D	396/446 (89%)	390 (98%)	6 (2%)	0	100	100
All	All	1612/1784 (90%)	1586 (98%)	26 (2%)	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	355/391 (91%)	349 (98%)	6 (2%)	60	39
1	B	363/391 (93%)	359 (99%)	4 (1%)	73	57
1	C	369/391 (94%)	366 (99%)	3 (1%)	81	70
1	D	353/391 (90%)	348 (99%)	5 (1%)	67	46
All	All	1440/1564 (92%)	1422 (99%)	18 (1%)	69	50

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	A	141	HIS
1	A	151	PHE
1	A	233	PHE
1	A	251	GLU
1	A	301	TYR
1	B	80	GLU
1	B	141	HIS
1	B	151	PHE
1	B	301	TYR
1	C	141	HIS
1	C	151	PHE
1	C	301	TYR
1	D	81	GLU
1	D	141	HIS
1	D	151	PHE
1	D	233	PHE
1	D	301	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 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	B3N	A	700	2	22,22,22	2.93	8 (36%)	26,27,27	1.05	2 (7%)
5	GOL	A	801	-	5,5,5	0.79	0	5,5,5	1.10	0
5	GOL	D	800	-	5,5,5	1.01	0	5,5,5	1.31	0
5	GOL	A	800	-	5,5,5	0.81	0	5,5,5	1.17	0
4	B3N	D	700	2	22,22,22	2.92	8 (36%)	26,27,27	1.00	2 (7%)
4	B3N	B	701	-	22,22,22	3.31	7 (31%)	26,27,27	1.18	4 (15%)
5	GOL	B	801	-	5,5,5	0.83	0	5,5,5	1.22	0
4	B3N	B	700	2	22,22,22	2.87	7 (31%)	26,27,27	1.09	2 (7%)
4	B3N	C	701	-	22,22,22	3.32	7 (31%)	26,27,27	1.16	4 (15%)
5	GOL	D	802	-	5,5,5	0.72	0	5,5,5	1.01	0
5	GOL	C	802	-	5,5,5	0.67	0	5,5,5	0.92	0
5	GOL	C	803	-	5,5,5	0.77	0	5,5,5	1.27	0
5	GOL	B	800	-	5,5,5	1.03	0	5,5,5	1.07	0
4	B3N	C	700	2	22,22,22	2.86	7 (31%)	26,27,27	1.03	1 (3%)
5	GOL	D	803	-	5,5,5	0.76	0	5,5,5	0.83	0
5	GOL	A	802	-	5,5,5	0.72	0	5,5,5	0.84	0
5	GOL	D	801	-	5,5,5	0.84	0	5,5,5	0.99	0
5	GOL	C	800	-	5,5,5	0.81	0	5,5,5	1.35	0
4	B3N	D	701	-	22,22,22	3.24	8 (36%)	26,27,27	1.08	2 (7%)
5	GOL	C	801	-	5,5,5	0.76	0	5,5,5	1.10	0
4	B3N	A	701	-	22,22,22	3.29	8 (36%)	26,27,27	1.06	2 (7%)
5	GOL	B	802	-	5,5,5	0.81	0	5,5,5	0.63	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
4	B3N	A	700	2	-	2/20/20/20	0/1/1/1
5	GOL	A	801	-	-	0/4/4/4	-
5	GOL	D	800	-	-	3/4/4/4	-
5	GOL	A	800	-	-	1/4/4/4	-
4	B3N	D	700	2	-	0/20/20/20	0/1/1/1
4	B3N	B	701	-	-	4/20/20/20	0/1/1/1
5	GOL	B	801	-	-	2/4/4/4	-
4	B3N	B	700	2	-	0/20/20/20	0/1/1/1
4	B3N	C	701	-	-	4/20/20/20	0/1/1/1
5	GOL	D	802	-	-	0/4/4/4	-
5	GOL	C	802	-	-	1/4/4/4	-
5	GOL	C	803	-	-	2/4/4/4	-
5	GOL	B	800	-	-	3/4/4/4	-
4	B3N	C	700	2	-	1/20/20/20	0/1/1/1
5	GOL	D	803	-	-	0/4/4/4	-
5	GOL	A	802	-	-	1/4/4/4	-
5	GOL	D	801	-	-	1/4/4/4	-
5	GOL	C	800	-	-	2/4/4/4	-
4	B3N	D	701	-	-	5/20/20/20	0/1/1/1
5	GOL	C	801	-	-	0/4/4/4	-
4	B3N	A	701	-	-	4/20/20/20	0/1/1/1
5	GOL	B	802	-	-	0/4/4/4	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	B3N	C1-N3	10.38	1.43	1.32
4	A	701	B3N	C1-N3	10.24	1.43	1.32
4	C	701	B3N	C1-N3	10.22	1.43	1.32
4	D	701	B3N	C1-N3	10.00	1.43	1.32
4	D	700	B3N	C1-N3	8.40	1.41	1.32
4	C	700	B3N	C1-N3	8.15	1.41	1.32
4	A	700	B3N	C1-N3	8.00	1.41	1.32
4	B	700	B3N	C1-N3	7.64	1.40	1.32
4	C	701	B3N	C13-N12	7.18	1.49	1.33
4	B	701	B3N	C13-N12	6.90	1.48	1.33
4	D	701	B3N	C13-N12	6.69	1.48	1.33
4	A	701	B3N	C13-N12	6.66	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	B3N	C13-N12	6.38	1.47	1.33
4	B	700	B3N	C13-N12	6.32	1.47	1.33
4	D	700	B3N	C13-N12	6.11	1.47	1.33
4	C	700	B3N	C13-N12	5.83	1.46	1.33
4	B	700	B3N	O4-N3	-5.14	1.27	1.40
4	C	700	B3N	O4-N3	-5.05	1.27	1.40
4	A	700	B3N	O4-N3	-5.03	1.27	1.40
4	D	700	B3N	O4-N3	-5.02	1.27	1.40
4	D	701	B3N	O4-N3	-4.80	1.27	1.40
4	B	701	B3N	O4-N3	-4.74	1.28	1.40
4	C	701	B3N	O4-N3	-4.73	1.28	1.40
4	A	701	B3N	O4-N3	-4.72	1.28	1.40
4	A	701	B3N	C17-N20	4.46	1.48	1.37
4	B	700	B3N	C17-N20	4.42	1.47	1.37
4	D	701	B3N	C17-N20	4.33	1.47	1.37
4	C	701	B3N	C17-N20	4.23	1.47	1.37
4	B	701	B3N	C17-N20	4.23	1.47	1.37
4	A	700	B3N	C15-C14	4.22	1.46	1.39
4	C	700	B3N	C17-N20	4.21	1.47	1.37
4	C	701	B3N	C15-C14	4.12	1.46	1.39
4	A	701	B3N	C15-C14	4.09	1.46	1.39
4	A	700	B3N	C17-N20	4.05	1.47	1.37
4	D	701	B3N	C15-C14	3.94	1.46	1.39
4	D	700	B3N	C15-C14	3.92	1.46	1.39
4	D	700	B3N	C17-N20	3.91	1.46	1.37
4	B	701	B3N	C15-C14	3.88	1.45	1.39
4	B	700	B3N	C15-C14	3.72	1.45	1.39
4	C	700	B3N	C15-C14	3.34	1.45	1.39
4	B	701	B3N	C19-C18	3.20	1.44	1.38
4	C	701	B3N	C19-C18	2.98	1.44	1.38
4	A	701	B3N	C18-C17	2.98	1.45	1.39
4	B	701	B3N	C18-C17	2.92	1.45	1.39
4	C	700	B3N	C18-C17	2.83	1.44	1.39
4	C	701	B3N	C18-C17	2.81	1.44	1.39
4	A	701	B3N	C19-C18	2.78	1.43	1.38
4	D	701	B3N	C18-C17	2.76	1.44	1.39
4	D	700	B3N	C18-C17	2.76	1.44	1.39
4	D	701	B3N	C19-C18	2.73	1.43	1.38
4	A	700	B3N	C18-C17	2.61	1.44	1.39
4	B	700	B3N	C18-C17	2.57	1.44	1.39
4	B	700	B3N	C19-C18	2.54	1.43	1.38
4	C	700	B3N	C19-C18	2.50	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	B3N	C19-C18	2.38	1.43	1.38
4	D	700	B3N	C16-C17	2.17	1.43	1.39
4	A	700	B3N	C16-C17	2.15	1.43	1.39
4	D	700	B3N	C19-C18	2.08	1.42	1.38
4	A	701	B3N	C16-C17	2.08	1.43	1.39
4	D	701	B3N	C16-C17	2.02	1.43	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	700	B3N	O2-C1-N3	-3.40	119.10	123.27
4	A	700	B3N	O2-C1-N3	-3.02	119.56	123.27
4	B	700	B3N	C6-C5-C1	2.93	121.49	113.26
4	A	701	B3N	O2-C1-N3	-2.82	119.81	123.27
4	D	700	B3N	O2-C1-N3	-2.81	119.83	123.27
4	C	700	B3N	C6-C5-C1	2.73	120.91	113.26
4	D	701	B3N	O2-C1-N3	-2.71	119.94	123.27
4	A	700	B3N	C6-C5-C1	2.61	120.58	113.26
4	D	701	B3N	C6-C5-C1	2.45	120.12	113.26
4	D	700	B3N	C6-C5-C1	2.44	120.10	113.26
4	C	701	B3N	C6-C5-C1	2.36	119.89	113.26
4	A	701	B3N	C6-C5-C1	2.33	119.80	113.26
4	B	701	B3N	C9-C10-N12	2.32	118.86	112.21
4	C	701	B3N	O2-C1-N3	-2.21	120.56	123.27
4	C	701	B3N	C9-C10-N12	2.20	118.51	112.21
4	B	701	B3N	O2-C1-N3	-2.17	120.61	123.27
4	B	701	B3N	C14-C13-N12	2.16	121.73	117.09
4	B	701	B3N	C6-C5-C1	2.06	119.05	113.26
4	C	701	B3N	O23-C13-C14	-2.00	117.37	120.94

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	800	GOL	C1-C2-C3-O3
5	C	800	GOL	C1-C2-C3-O3
5	D	800	GOL	O1-C1-C2-C3
5	D	800	GOL	C1-C2-C3-O3
4	D	701	B3N	C1-C5-C6-C7
4	C	701	B3N	N12-C10-C9-C8
4	B	701	B3N	N12-C10-C9-C8
4	D	701	B3N	N12-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
4	B	701	B3N	C5-C6-C7-C8
4	D	701	B3N	C5-C6-C7-C8
4	C	701	B3N	C5-C6-C7-C8
4	D	701	B3N	C6-C7-C8-C9
5	B	801	GOL	C1-C2-C3-O3
5	C	802	GOL	C1-C2-C3-O3
5	C	803	GOL	O1-C1-C2-C3
4	B	701	B3N	C6-C7-C8-C9
4	A	701	B3N	C1-C5-C6-C7
5	D	800	GOL	O1-C1-C2-O2
4	C	701	B3N	C9-C10-N12-C13
4	A	701	B3N	C5-C6-C7-C8
5	B	800	GOL	O1-C1-C2-O2
4	D	701	B3N	C7-C8-C9-C10
5	B	800	GOL	O2-C2-C3-O3
4	A	701	B3N	C6-C7-C8-C9
5	A	802	GOL	C1-C2-C3-O3
5	B	801	GOL	O1-C1-C2-O2
5	C	800	GOL	O1-C1-C2-O2
4	C	700	B3N	N12-C10-C9-C8
4	B	701	B3N	C1-C5-C6-C7
4	A	701	B3N	C7-C8-C9-C10
4	C	701	B3N	C1-C5-C6-C7
4	A	700	B3N	C5-C6-C7-C8
4	A	700	B3N	N12-C10-C9-C8
5	A	800	GOL	O1-C1-C2-C3
5	C	803	GOL	C1-C2-C3-O3
5	D	801	GOL	O1-C1-C2-C3

There are no ring outliers.

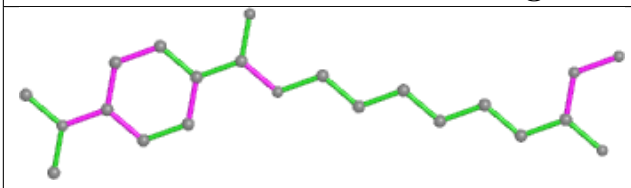
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	700	B3N	1	0
5	D	800	GOL	4	0
4	B	700	B3N	1	0
5	B	800	GOL	3	0

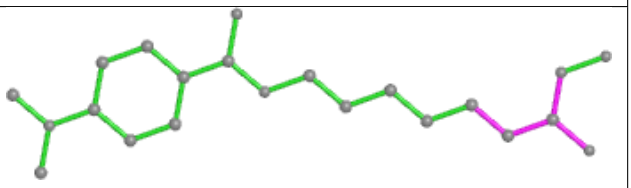
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

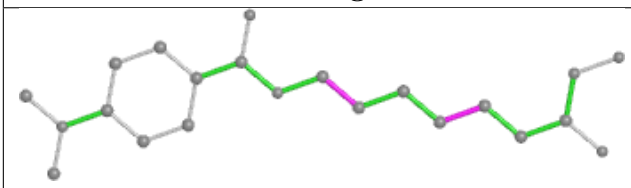
Ligand B3N A 700



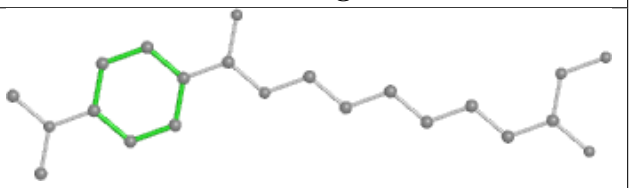
Bond lengths



Bond angles

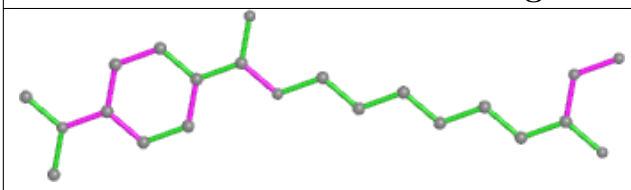


Torsions

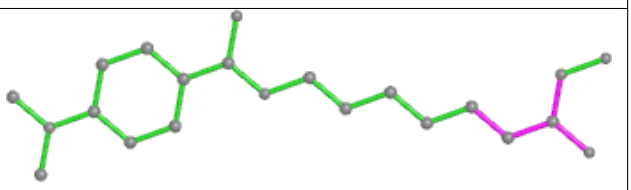


Rings

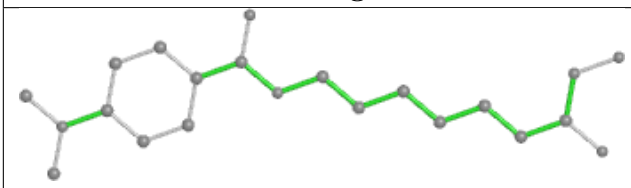
Ligand B3N D 700



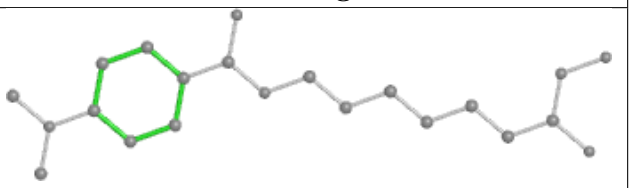
Bond lengths



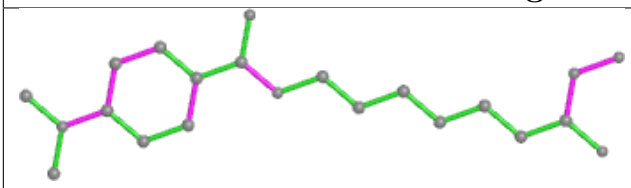
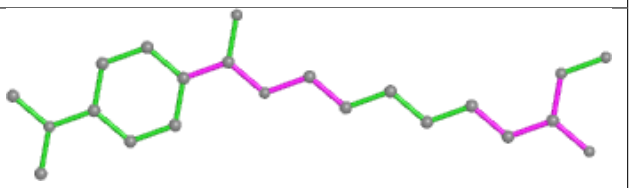
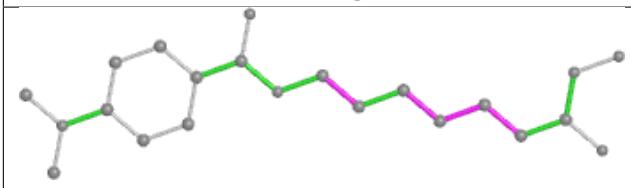
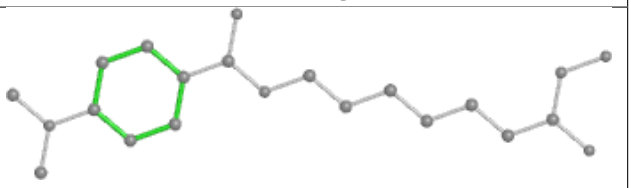
Bond angles

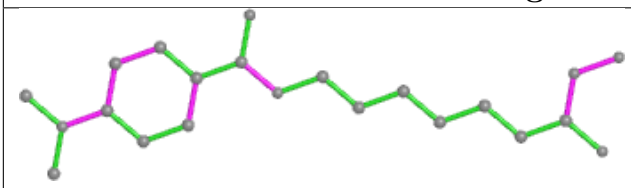
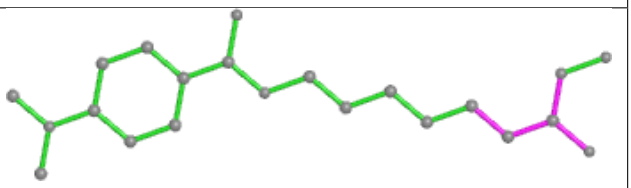
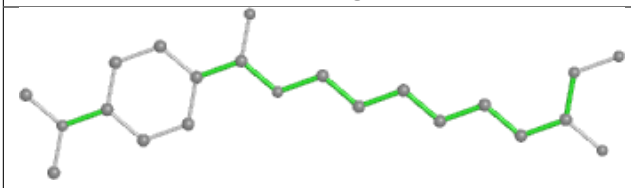
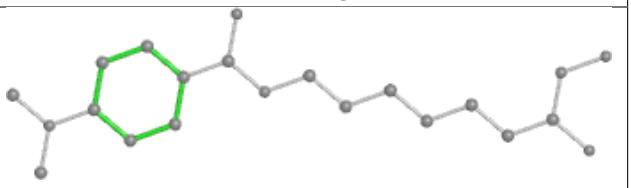


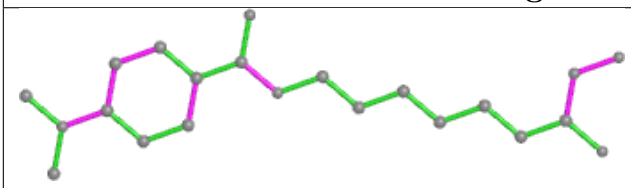
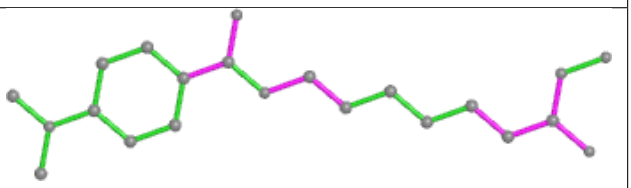
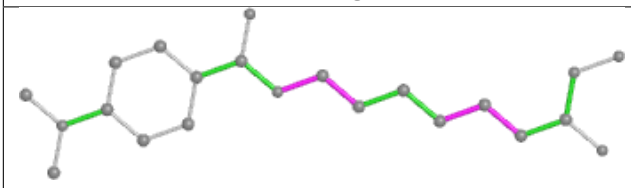
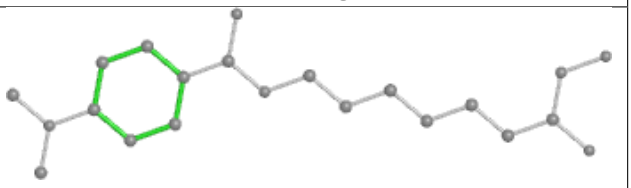
Torsions



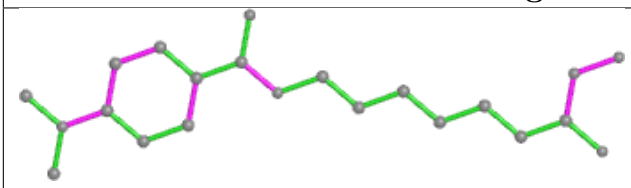
Rings

Ligand B3N B 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

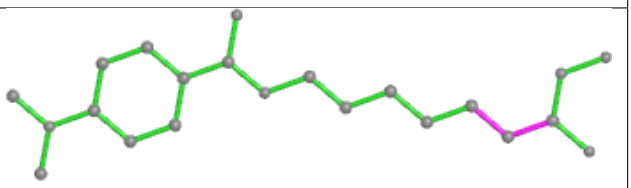
Ligand B3N B 700	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand B3N C 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

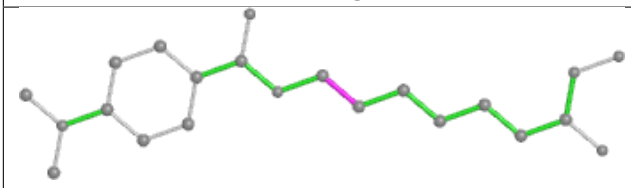
Ligand B3N C 700



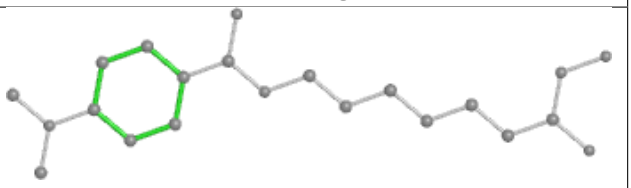
Bond lengths



Bond angles

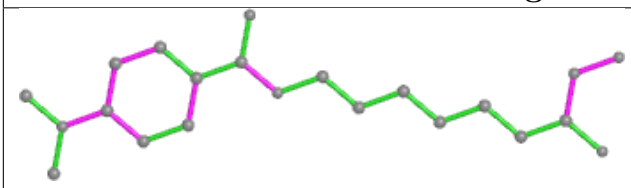


Torsions

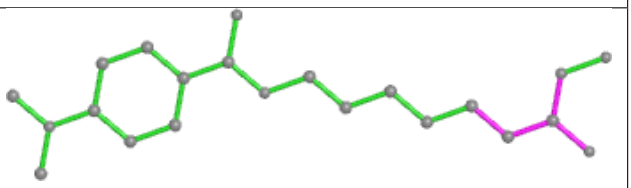


Rings

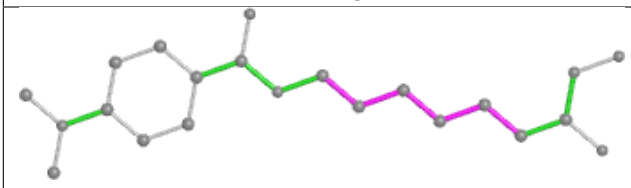
Ligand B3N D 701



Bond lengths



Bond angles



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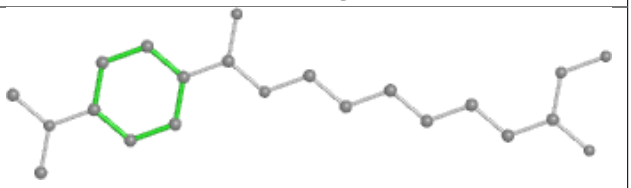
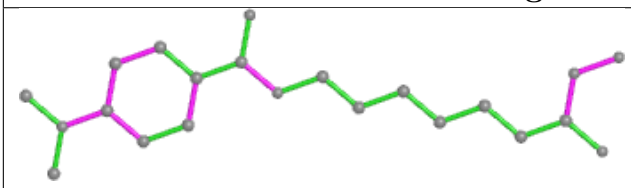
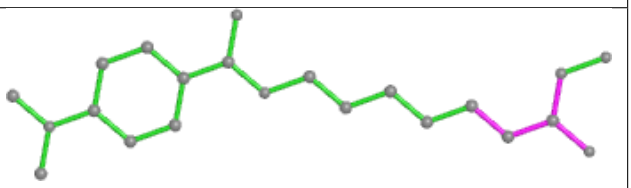


Rings

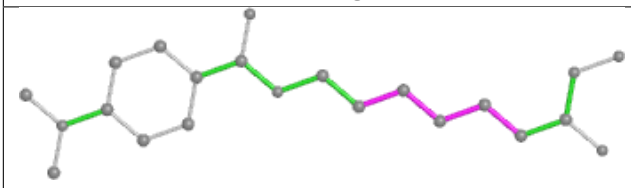
Ligand B3N A 701



Bond lengths



Bond angles



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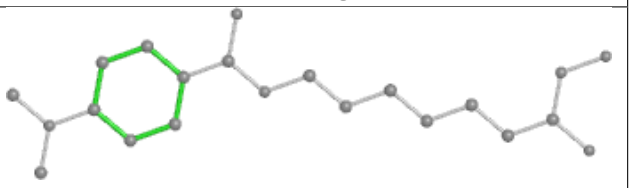

Rings

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	399/446 (89%)	-0.20	23 (5%)	23	22	13, 20, 49, 73	0
1	B	413/446 (92%)	-0.42	7 (1%)	70	73	12, 18, 38, 71	0
1	C	416/446 (93%)	-0.37	5 (1%)	79	81	12, 19, 40, 79	0
1	D	399/446 (89%)	-0.21	19 (4%)	30	29	13, 21, 51, 85	0
All	All	1627/1784 (91%)	-0.30	54 (3%)	46	47	12, 20, 44, 85	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	TYR	8.3
1	D	392	PHE	8.3
1	A	392	PHE	8.1
1	D	428	TYR	7.8
1	A	428	TYR	6.9
1	D	426	TYR	6.9
1	A	426	TYR	6.8
1	A	435	TYR	6.2
1	A	425	ILE	5.9
1	D	168	THR	5.8
1	A	434	LEU	5.3
1	D	432	TYR	5.2
1	D	425	ILE	5.1
1	D	434	LEU	4.7
1	D	435	TYR	4.4
1	A	168	THR	4.3
1	D	429	ASP	4.3
1	D	232	ILE	4.1
1	B	230	LEU	4.0
1	C	83	GLU	3.9
1	A	81	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	315	SER	3.4
1	D	383	PRO	3.4
1	D	402	ASP	3.4
1	A	433	GLN	3.3
1	D	315	SER	3.2
1	D	393	PRO	3.2
1	A	429	ASP	3.1
1	A	169	PRO	3.1
1	D	223	ASN	2.9
1	A	232	ILE	2.9
1	A	393	PRO	2.9
1	D	231	PRO	2.7
1	A	368[A]	ILE	2.6
1	A	83	GLU	2.6
1	D	412	LEU	2.6
1	B	425	ILE	2.5
1	A	427	ASP	2.4
1	B	177	GLN	2.4
1	C	425	ILE	2.4
1	A	404	ILE	2.4
1	A	223	ASN	2.3
1	A	412	LEU	2.3
1	B	231	PRO	2.3
1	D	222	TRP	2.2
1	D	81	GLU	2.2
1	C	224	MET	2.2
1	B	394	HIS	2.1
1	C	401	LEU	2.1
1	B	232	ILE	2.1
1	C	438	THR	2.1
1	B	222	TRP	2.1
1	A	402	ASP	2.0
1	A	383	PRO	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.

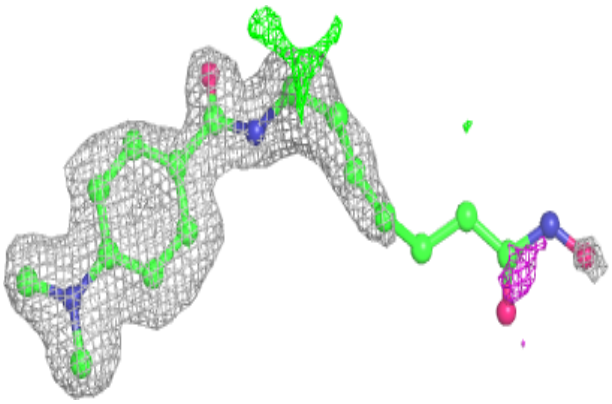
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	B3N	A	701	22/22	0.73	0.30	30,50,75,77	0
5	GOL	C	803	6/6	0.80	0.16	38,42,43,45	0
5	GOL	C	802	6/6	0.83	0.15	23,29,31,32	0
5	GOL	B	800	6/6	0.84	0.16	33,34,35,36	0
4	B3N	B	701	22/22	0.84	0.32	28,58,92,92	0
4	B3N	C	701	22/22	0.84	0.35	27,52,86,87	0
5	GOL	B	801	6/6	0.85	0.14	24,28,30,31	0
4	B3N	A	700	22/22	0.86	0.10	22,27,30,30	0
5	GOL	D	803	6/6	0.86	0.11	22,28,28,29	0
4	B3N	D	701	22/22	0.87	0.30	31,58,99,102	0
4	B3N	D	700	22/22	0.87	0.10	21,27,30,31	0
5	GOL	B	802	6/6	0.88	0.16	23,28,30,32	0
5	GOL	D	800	6/6	0.88	0.25	32,40,42,43	0
4	B3N	B	700	22/22	0.88	0.11	21,29,33,35	0
4	B3N	C	700	22/22	0.89	0.12	20,30,34,36	0
5	GOL	D	802	6/6	0.90	0.14	23,28,31,33	0
5	GOL	C	801	6/6	0.90	0.12	28,33,38,42	0
5	GOL	A	802	6/6	0.91	0.14	20,28,28,29	0
5	GOL	D	801	6/6	0.92	0.08	22,25,27,27	0
5	GOL	A	801	6/6	0.92	0.14	21,28,29,30	0
5	GOL	C	800	6/6	0.92	0.07	26,29,31,32	0
5	GOL	A	800	6/6	0.96	0.07	24,25,25,27	0
3	K	D	601	1/1	0.98	0.04	22,22,22,22	0
3	K	C	601	1/1	0.99	0.04	23,23,23,23	0
3	K	A	601	1/1	0.99	0.04	20,20,20,20	0
3	K	B	601	1/1	0.99	0.03	22,22,22,22	0
3	K	D	600	1/1	1.00	0.07	13,13,13,13	0
2	ZN	D	500	1/1	1.00	0.07	22,22,22,22	0
3	K	A	600	1/1	1.00	0.07	13,13,13,13	0
2	ZN	A	500	1/1	1.00	0.06	22,22,22,22	0
3	K	B	600	1/1	1.00	0.07	12,12,12,12	0
2	ZN	B	500	1/1	1.00	0.06	21,21,21,21	0
3	K	C	600	1/1	1.00	0.08	12,12,12,12	0
2	ZN	C	500	1/1	1.00	0.04	21,21,21,21	0

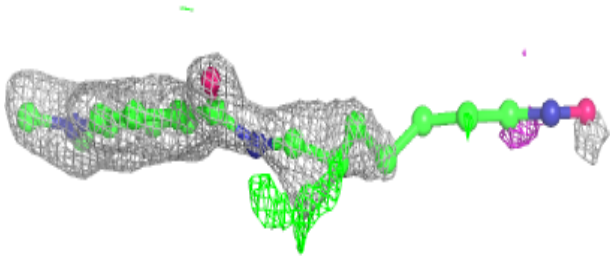
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

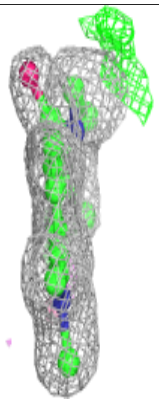
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around B3N A 701:

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

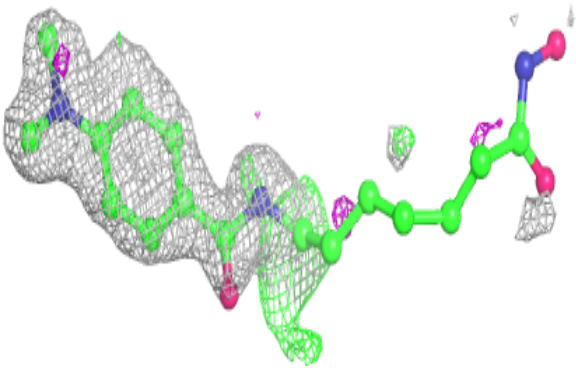


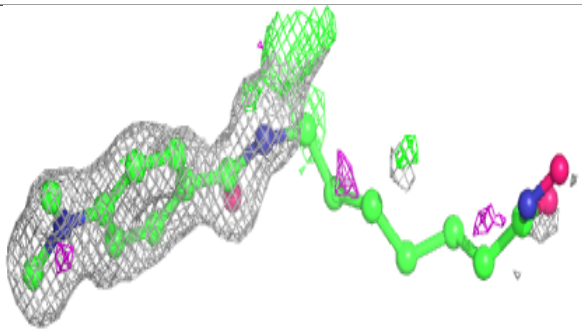


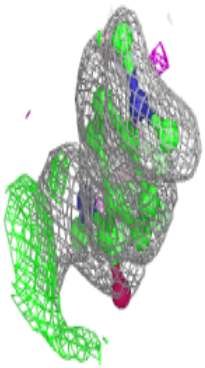


Electron density around B3N B 701:

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

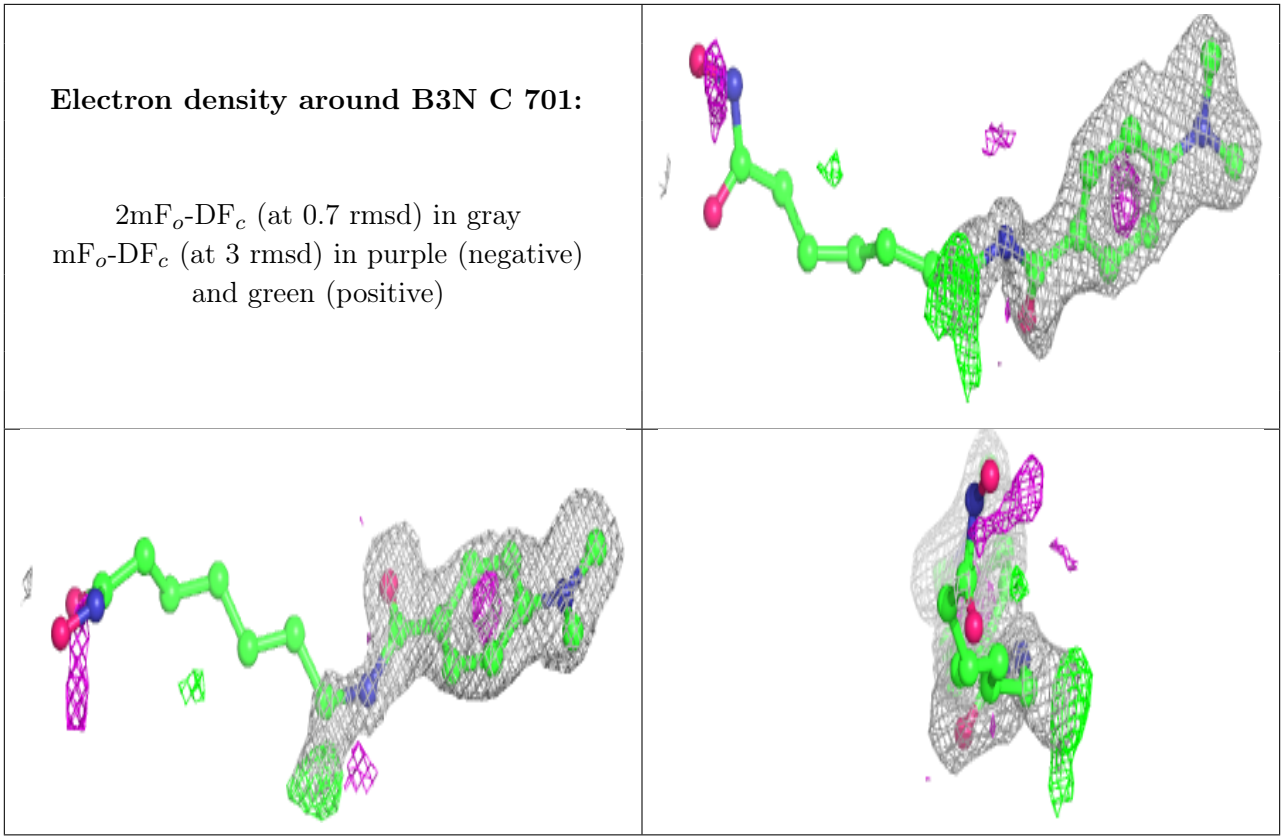






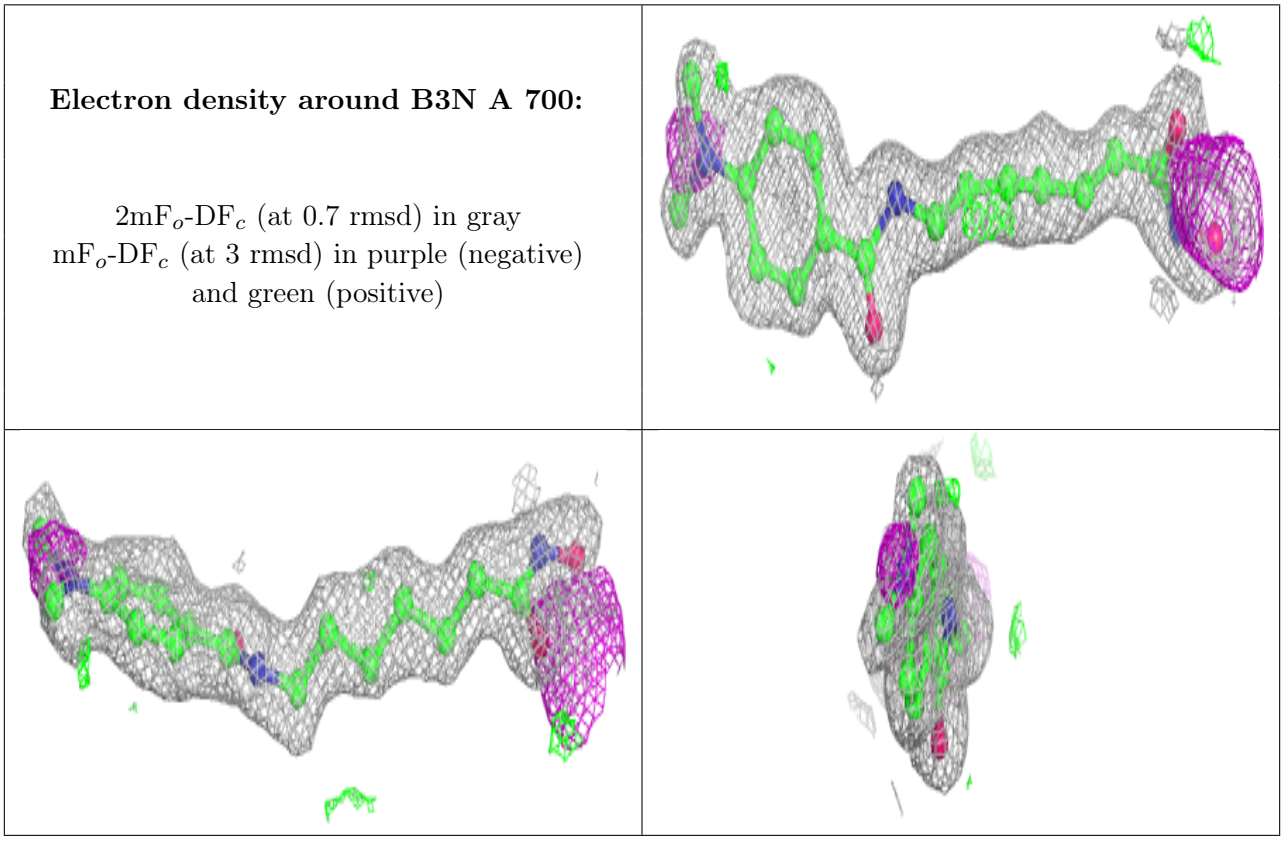
Electron density around B3N C 701:

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



Electron density around B3N A 700:

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



Electron density around B3N D 701:

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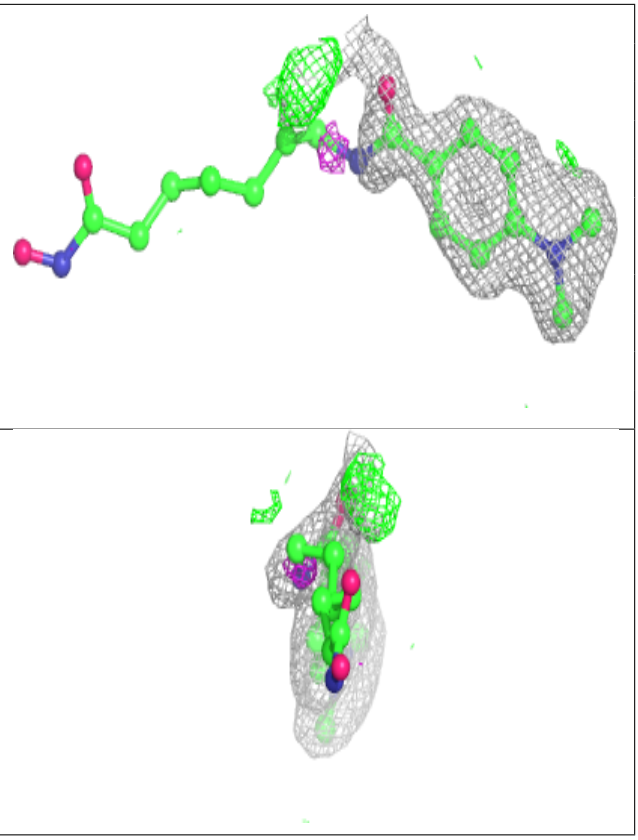
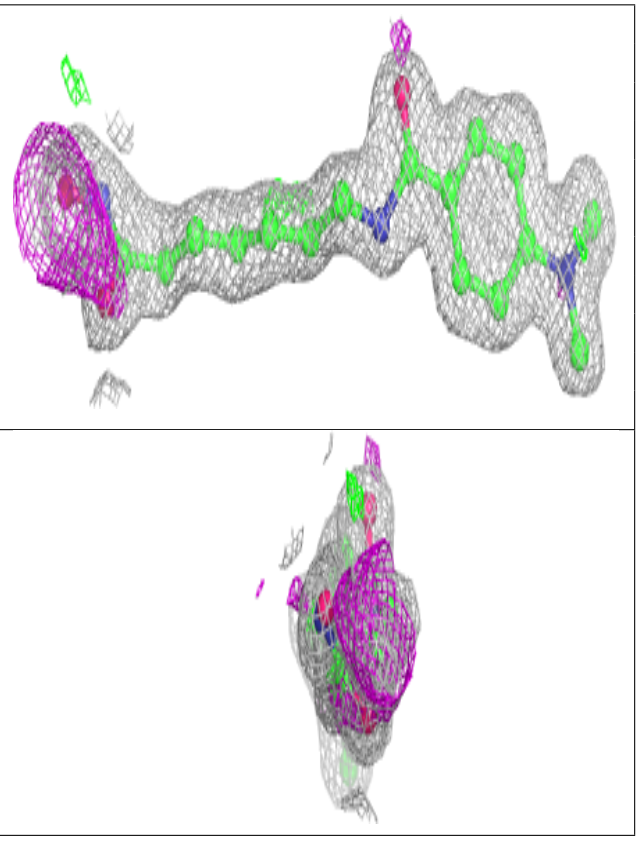
and green (positive)



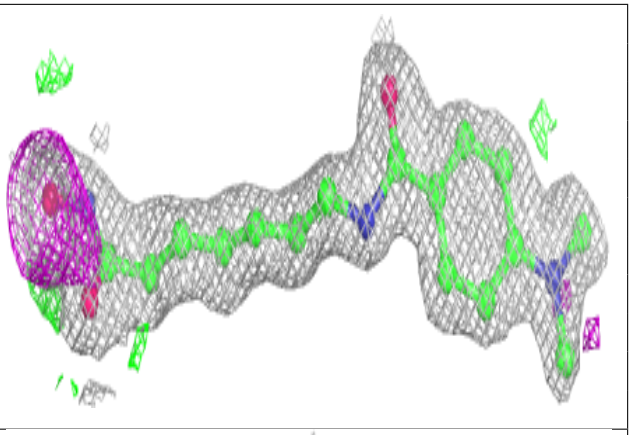
Electron density around B3N D 700:

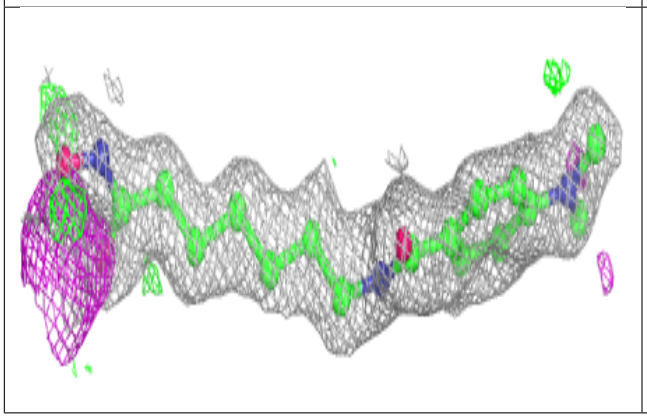
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

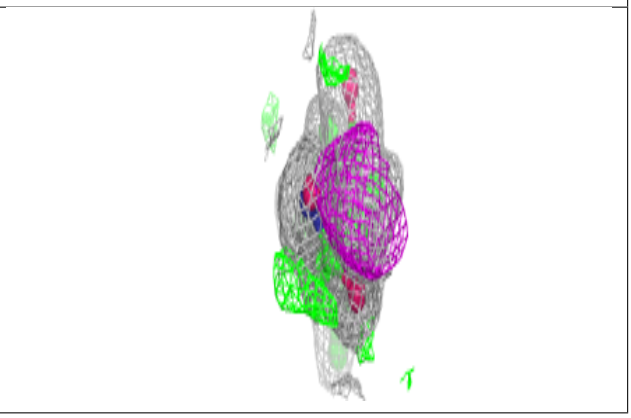


Electron density around B3N B 700:

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

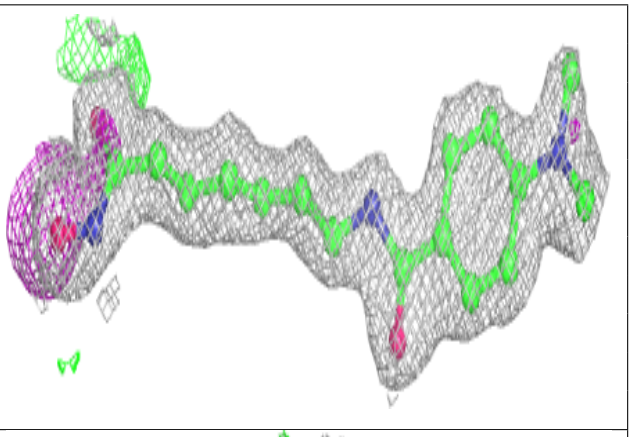


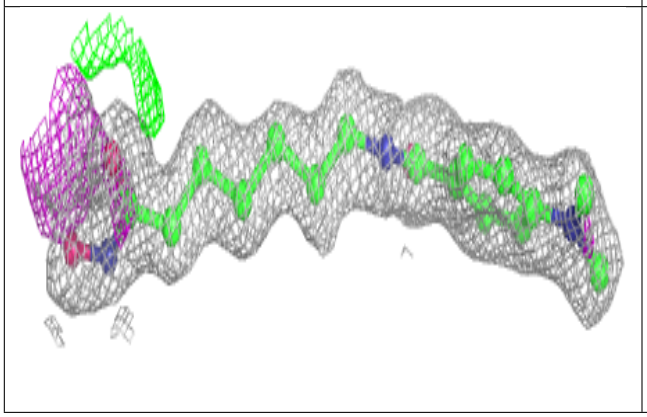


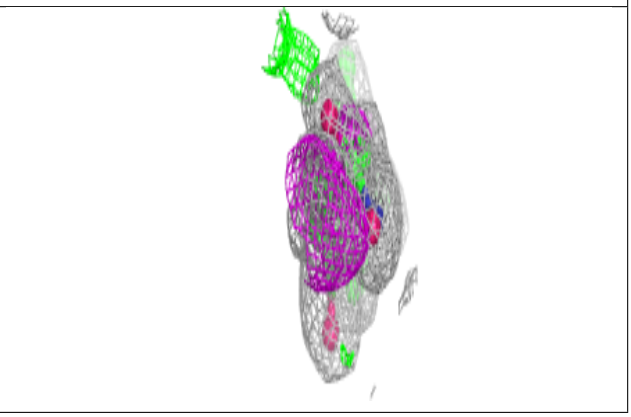


Electron density around B3N C 700:

$2mF_o$-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.