



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2021 – 02:06 PM EST

PDB ID : 7JMT
Title : Crystal structure of schistosome BCL-2 bound to ABT-737
Authors : Smith, N.A.; Smith, B.J.; Lee, E.F.; Colman, P.M.; Fairlie, W.D.
Deposited on : 2020-08-02
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.17
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) : 2.17

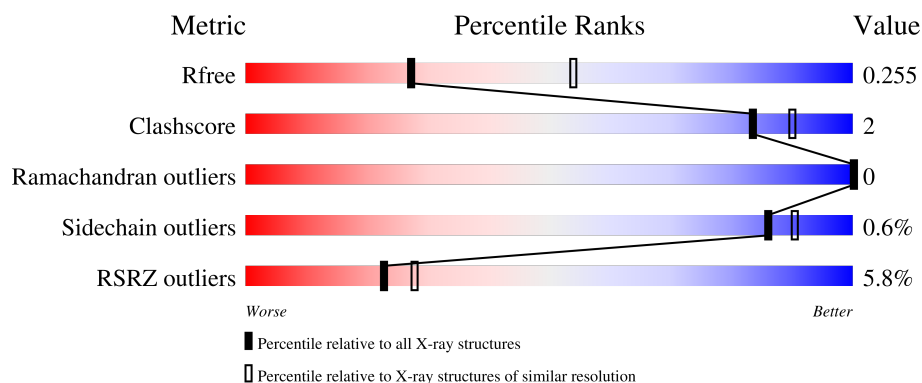
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	210	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>6%</div> <div>23%</div> </div> </div>
1	B	210	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>•</div> <div>26%</div> </div> </div>
1	C	210	<div> <div>•</div> <div> <div></div> <div>75%</div> <div>•</div> <div>21%</div> </div> </div>
1	D	210	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>•</div> <div>26%</div> </div> </div>
1	E	210	<div> <div>10%</div> <div> <div></div> <div>70%</div> <div>•</div> <div>26%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	210	<div><div></div><div></div><div></div><div></div></div> <div><div>4%</div><div>69%</div><div>8%</div><div>23%</div></div>

2 Entry composition [i](#)

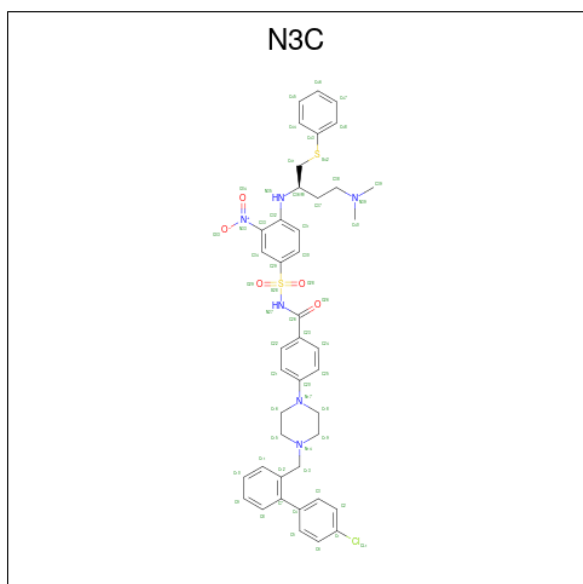
There are 3 unique types of molecules in this entry. The entry contains 15190 atoms, of which 7371 are hydrogens and 0 are deuteriums.

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 BCL-2 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	161	Total	C	H	N	O	S	0	0	0
			2496	812	1228	215	237	4			
1	B	156	Total	C	H	N	O	S	0	0	0
			2305	764	1113	196	228	4			
1	C	165	Total	C	H	N	O	S	0	0	0
			2564	832	1264	219	245	4			
1	D	156	Total	C	H	N	O	S	0	0	0
			2383	780	1165	203	231	4			
1	E	156	Total	C	H	N	O	S	0	0	0
			2367	779	1157	202	225	4			
1	F	161	Total	C	H	N	O	S	0	0	0
			2431	806	1168	214	239	4			

- Molecule 2 is 4-{4-[(4'-CHLOROBIPHENYL-2-YL)METHYL]PIPERAZIN-1-YL}-N-{[4-({(1R)-3-(DIMETHYLAMINO)-1-[(PHENYLTHIO)METHYL]PROPYL}AMINO)-3-NITROPHENYL]SULFONYL}BENZAMIDE (three-letter code: N3C) (formula: C₄₂H₄₅ClN₆O₅S₂) (labeled as "Ligand of Interest" by depositor).

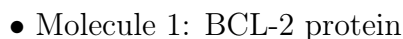
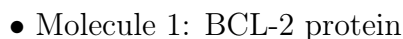


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	H	N	O	S	0	0
			102	42	1	46	6	5	2		
2	B	1	Total	C	Cl	H	N	O	S	0	0
			102	42	1	46	6	5	2		
2	C	1	Total	C	Cl	H	N	O	S	0	0
			102	42	1	46	6	5	2		
2	D	1	Total	C	Cl	H	N	O	S	0	0
			102	42	1	46	6	5	2		
2	E	1	Total	C	Cl	H	N	O	S	0	0
			102	42	1	46	6	5	2		
2	F	1	Total	C	Cl	H	N	O	S	0	0
			102	42	1	46	6	5	2		

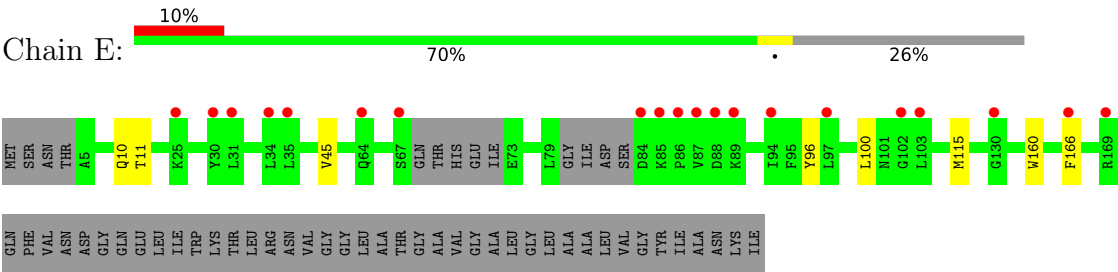
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	4	Total	O	0	0
			4	4		
3	C	7	Total	O	0	0
			7	7		
3	D	5	Total	O	0	0
			5	5		
3	E	2	Total	O	0	0
			2	2		
3	F	3	Total	O	0	0
			3	3		

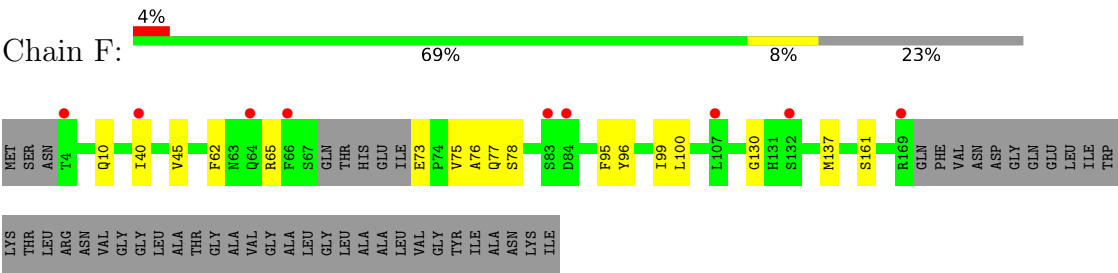
- Molecule 1: BCL-2 protein



● Molecule 1: BCL-2 protein



● Molecule 1: BCL-2 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.02Å 67.79Å 100.91Å 90.00° 118.79° 90.00°	Depositor
Resolution (Å)	86.47 – 2.75 86.47 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (86.47-2.75) 99.0 (86.47-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.234 , 0.255 0.234 , 0.255	Depositor DCC
R_{free} test set	1547 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.032 for -h-l,k,h 0.032 for l,k,-h-l 0.005 for h,-k,-h-l 0.005 for -h-l,-k,l 0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15190	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9279e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: N3C

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	0.60	0/1292	0.84	0/1750
1	B	0.58	0/1214	0.80	0/1649
1	C	0.63	0/1326	0.85	0/1799
1	D	0.60	0/1241	0.84	0/1682
1	E	0.59	0/1233	0.81	0/1672
1	F	0.60	0/1287	0.85	0/1744
All	All	0.60	0/7593	0.83	0/10296

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

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	1268	1228	1241	7	1
1	B	1192	1113	1126	3	0
1	C	1300	1264	1271	3	1
1	D	1218	1165	1172	2	1
1	E	1210	1157	1165	5	0
1	F	1263	1168	1221	11	1
2	A	56	46	45	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	56	46	45	2	0
2	C	56	46	45	1	0
2	D	56	46	45	1	0
2	E	56	46	45	1	0
2	F	56	46	45	2	0
3	A	11	0	0	0	0
3	B	4	0	0	0	0
3	C	7	0	0	0	0
3	D	5	0	0	0	0
3	E	2	0	0	0	0
3	F	3	0	0	0	0
All	All	7819	7371	7466	37	2

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 (37) 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:E:100:LEU:HD22	1:E:115:MET:HG3	1.76	0.68
1:F:73:GLU:CB	1:F:76:ALA:HB3	2.34	0.57
1:F:10:GLN:HG3	1:F:45:VAL:HG13	1.89	0.55
1:B:10:GLN:HG3	1:B:45:VAL:HG13	1.90	0.53
1:F:96:TYR:CZ	1:F:100:LEU:HD11	2.44	0.52
1:F:96:TYR:CE2	1:F:100:LEU:HD11	2.45	0.52
1:F:95:PHE:O	1:F:99:ILE:HG12	2.11	0.51
1:A:96:TYR:CZ	1:A:100:LEU:HD11	2.46	0.50
1:E:10:GLN:CG	1:E:45:VAL:HG13	2.41	0.50
1:F:62:PHE:HA	2:F:1001:N3C:H45	1.95	0.49
1:F:75:VAL:HA	1:F:78:SER:OG	2.13	0.49
1:E:96:TYR:O	1:E:100:LEU:HG	2.13	0.48
1:D:96:TYR:CE2	1:D:100:LEU:HD11	2.49	0.48
2:E:1001:N3C:H191	2:E:1001:N3C:C11	2.44	0.47
1:E:10:GLN:HG3	1:E:45:VAL:HG13	1.97	0.47
1:A:5:ALA:HB1	1:A:9:LEU:HD23	1.96	0.47
1:A:96:TYR:CE2	1:A:100:LEU:HD11	2.50	0.47
1:F:73:GLU:O	1:F:77:GLN:HG2	2.14	0.47
2:B:1001:N3C:O34	2:B:1001:N3C:C44	2.63	0.46
1:C:58:LEU:HD21	1:C:167:SER:HA	1.97	0.46
1:C:110:GLY:HA3	2:C:1001:N3C:HN27	1.81	0.46
2:D:1001:N3C:H47	2:D:1001:N3C:C22	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1001:N3C:H403	2:B:1001:N3C:H371	1.77	0.44
1:B:10:GLN:CG	1:B:45:VAL:HG13	2.47	0.43
1:E:11:THR:HG22	1:E:160:TRP:CZ2	2.54	0.42
1:A:55:LEU:HD21	1:A:116:PHE:CG	2.54	0.42
1:B:14:LEU:HA	1:B:52:ILE:HD11	2.02	0.42
1:A:99:ILE:HG21	1:A:118:PHE:CE1	2.54	0.42
1:D:10:GLN:HG3	1:D:45:VAL:HG13	2.01	0.42
1:F:137:MET:C	1:F:137:MET:SD	2.98	0.42
1:A:73:GLU:N	1:A:74:PRO:CD	2.83	0.42
1:C:72:ILE:HD12	1:C:121:ILE:HG21	2.01	0.42
1:F:40:ILE:N	1:F:40:ILE:HD12	2.35	0.42
1:A:110:GLY:HA3	2:A:1001:N3C:HN27	1.85	0.41
2:A:1001:N3C:C23	2:A:1001:N3C:H47	2.50	0.41
1:F:75:VAL:O	1:F:76:ALA:C	2.59	0.41
2:F:1001:N3C:H382	2:F:1001:N3C:H412	1.92	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:GLY:O	1:F:130:GLY:O[2_545]	1.69	0.51
1:A:17:SER:OG	1:D:152:ASN:OD1[1_454]	2.01	0.19

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	157/210 (75%)	156 (99%)	1 (1%)	0	100	100
1	B	152/210 (72%)	151 (99%)	1 (1%)	0	100	100
1	C	163/210 (78%)	162 (99%)	1 (1%)	0	100	100
1	D	152/210 (72%)	152 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	150/210 (71%)	148 (99%)	2 (1%)	0	100	100
1	F	157/210 (75%)	155 (99%)	2 (1%)	0	100	100
All	All	931/1260 (74%)	924 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/180 (76%)	137 (100%)	0	100	100
1	B	125/180 (69%)	125 (100%)	0	100	100
1	C	142/180 (79%)	141 (99%)	1 (1%)	84	89
1	D	131/180 (73%)	130 (99%)	1 (1%)	81	88
1	E	128/180 (71%)	127 (99%)	1 (1%)	81	88
1	F	136/180 (76%)	134 (98%)	2 (2%)	65	78
All	All	799/1080 (74%)	794 (99%)	5 (1%)	86	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	166	PHE
1	D	169	ARG
1	E	166	PHE
1	F	65	ARG
1	F	161	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	C	63	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	N3C	B	1001	-	59,61,61	1.93	7 (11%)	78,85,85	1.89	11 (14%)
2	N3C	D	1001	-	59,61,61	1.89	6 (10%)	78,85,85	1.83	14 (17%)
2	N3C	F	1001	-	59,61,61	1.79	6 (10%)	78,85,85	1.96	20 (25%)
2	N3C	A	1001	-	59,61,61	2.06	7 (11%)	78,85,85	2.04	15 (19%)
2	N3C	C	1001	-	59,61,61	2.16	7 (11%)	78,85,85	1.93	14 (17%)
2	N3C	E	1001	-	59,61,61	1.81	7 (11%)	78,85,85	2.18	17 (21%)

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	N3C	B	1001	-	-	13/43/55/55	0/6/6/6
2	N3C	D	1001	-	-	12/43/55/55	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	N3C	F	1001	-	-	5/43/55/55	0/6/6/6
2	N3C	A	1001	-	-	8/43/55/55	0/6/6/6
2	N3C	C	1001	-	-	8/43/55/55	0/6/6/6
2	N3C	E	1001	-	-	10/43/55/55	0/6/6/6

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	N3C	C29-S28	-11.02	1.59	1.76
2	A	1001	N3C	C29-S28	-10.81	1.59	1.76
2	B	1001	N3C	C29-S28	-10.07	1.60	1.76
2	D	1001	N3C	C29-S28	-9.05	1.62	1.76
2	F	1001	N3C	C29-S28	-8.02	1.64	1.76
2	E	1001	N3C	C29-S28	-7.26	1.65	1.76
2	E	1001	N3C	C7-C4	-7.26	1.36	1.49
2	D	1001	N3C	C7-C4	-7.03	1.36	1.49
2	C	1001	N3C	S28-N27	-6.32	1.51	1.64
2	A	1001	N3C	S28-N27	-6.26	1.51	1.64
2	C	1001	N3C	C7-C4	-6.13	1.38	1.49
2	F	1001	N3C	C7-C4	-5.60	1.39	1.49
2	A	1001	N3C	C7-C4	-5.49	1.39	1.49
2	C	1001	N3C	C26-N27	-5.47	1.32	1.39
2	B	1001	N3C	C7-C4	-5.45	1.39	1.49
2	E	1001	N3C	S28-N27	-5.39	1.53	1.64
2	F	1001	N3C	S28-N27	-5.28	1.53	1.64
2	D	1001	N3C	S28-N27	-4.91	1.54	1.64
2	B	1001	N3C	S28-N27	-4.87	1.54	1.64
2	B	1001	N3C	C43-S42	-4.53	1.67	1.76
2	F	1001	N3C	C26-N27	-4.36	1.33	1.39
2	A	1001	N3C	C26-N27	-4.21	1.34	1.39
2	D	1001	N3C	C43-S42	-3.71	1.68	1.76
2	E	1001	N3C	C43-S42	-3.56	1.69	1.76
2	C	1001	N3C	C43-S42	-3.39	1.69	1.76
2	A	1001	N3C	C43-S42	-3.27	1.69	1.76
2	E	1001	N3C	C26-N27	-3.13	1.35	1.39
2	C	1001	N3C	C33-N33	-3.05	1.40	1.45
2	F	1001	N3C	C43-S42	-2.90	1.70	1.76
2	D	1001	N3C	C26-N27	-2.89	1.35	1.39
2	B	1001	N3C	C26-N27	-2.81	1.35	1.39
2	B	1001	N3C	C1-CL1	2.71	1.80	1.74
2	F	1001	N3C	C33-N33	-2.70	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	N3C	C33-N33	-2.62	1.41	1.45
2	E	1001	N3C	C33-N33	-2.55	1.41	1.45
2	B	1001	N3C	C33-N33	-2.47	1.41	1.45
2	C	1001	N3C	C41-S42	-2.29	1.76	1.81
2	D	1001	N3C	C33-N33	-2.18	1.41	1.45
2	A	1001	N3C	O29-S28	2.07	1.45	1.43
2	E	1001	N3C	C41-S42	-2.05	1.77	1.81

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	N3C	O29-S28-O28	-10.16	107.06	119.55
2	C	1001	N3C	O29-S28-O28	-9.95	107.32	119.55
2	A	1001	N3C	O29-S28-O28	-9.94	107.33	119.55
2	F	1001	N3C	O29-S28-O28	-9.15	108.31	119.55
2	B	1001	N3C	O29-S28-O28	-8.88	108.64	119.55
2	E	1001	N3C	O29-S28-O28	-8.68	108.88	119.55
2	B	1001	N3C	C33-C32-N35	-5.91	117.35	123.42
2	E	1001	N3C	O29-S28-C29	5.65	114.92	107.97
2	E	1001	N3C	C34-C29-S28	5.41	125.13	119.08
2	E	1001	N3C	C18-N17-C16	5.37	123.38	111.52
2	A	1001	N3C	C33-C32-N35	-5.32	117.96	123.42
2	B	1001	N3C	C37-C36-N35	-5.26	103.11	110.53
2	B	1001	N3C	C18-N17-C16	5.22	123.05	111.52
2	A	1001	N3C	C18-N17-C16	5.17	122.94	111.52
2	F	1001	N3C	C18-N17-C16	5.13	122.83	111.52
2	E	1001	N3C	C41-S42-C43	5.07	113.44	103.79
2	C	1001	N3C	O28-S28-C29	5.01	114.13	107.97
2	C	1001	N3C	C18-N17-C16	4.59	121.66	111.52
2	E	1001	N3C	C30-C29-C34	-4.54	115.04	120.62
2	A	1001	N3C	C37-C36-N35	-4.51	104.17	110.53
2	A	1001	N3C	O29-S28-C29	4.49	113.50	107.97
2	C	1001	N3C	C41-S42-C43	4.42	112.22	103.79
2	E	1001	N3C	C33-C32-N35	-4.41	118.89	123.42
2	D	1001	N3C	O29-S28-C29	4.33	113.30	107.97
2	B	1001	N3C	C30-C29-S28	4.18	124.31	119.77
2	D	1001	N3C	C18-N17-C16	4.15	120.68	111.52
2	A	1001	N3C	C41-S42-C43	3.97	111.35	103.79
2	C	1001	N3C	O29-S28-C29	3.89	112.76	107.97
2	F	1001	N3C	C26-N27-S28	-3.85	118.39	123.36
2	E	1001	N3C	C5-C4-C7	-3.83	114.70	120.91
2	A	1001	N3C	O34-N33-C33	3.80	125.53	119.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	N3C	O26-C26-N27	3.71	125.63	121.08
2	C	1001	N3C	C29-S28-N27	-3.64	100.47	105.97
2	E	1001	N3C	C19-C18-N17	-3.51	103.87	110.70
2	B	1001	N3C	C41-S42-C43	3.43	110.32	103.79
2	F	1001	N3C	C12-C13-N14	3.41	118.71	112.75
2	F	1001	N3C	C30-C29-C34	-3.39	116.45	120.62
2	F	1001	N3C	C33-C34-C29	3.35	122.74	119.13
2	E	1001	N3C	C33-C34-C29	3.27	122.65	119.13
2	D	1001	N3C	C12-C13-N14	3.27	118.47	112.75
2	F	1001	N3C	C41-S42-C43	3.24	109.96	103.79
2	D	1001	N3C	C33-C34-C29	3.11	122.48	119.13
2	E	1001	N3C	C8-C7-C12	3.11	121.96	118.96
2	E	1001	N3C	O28-S28-C29	3.03	111.70	107.97
2	B	1001	N3C	C23-C26-N27	3.03	119.75	116.09
2	A	1001	N3C	C13-N14-C15	-3.00	104.39	111.06
2	C	1001	N3C	C30-C29-S28	2.83	122.85	119.77
2	D	1001	N3C	C30-C29-S28	2.82	122.84	119.77
2	F	1001	N3C	C8-C7-C12	2.82	121.68	118.96
2	F	1001	N3C	C25-C20-N17	-2.80	117.51	121.38
2	D	1001	N3C	C16-C15-N14	-2.76	104.97	110.64
2	E	1001	N3C	C23-C26-N27	2.72	119.38	116.09
2	F	1001	N3C	C34-C29-S28	2.69	122.09	119.08
2	F	1001	N3C	C5-C4-C7	-2.68	116.57	120.91
2	F	1001	N3C	O28-S28-N27	2.66	114.22	106.74
2	B	1001	N3C	C34-C29-S28	-2.66	116.10	119.08
2	E	1001	N3C	C31-C30-C29	2.61	122.15	119.45
2	F	1001	N3C	C19-N14-C15	-2.58	103.02	108.83
2	F	1001	N3C	O29-S28-C29	2.57	111.13	107.97
2	F	1001	N3C	C33-C32-N35	-2.54	120.81	123.42
2	C	1001	N3C	C33-C34-C29	2.48	121.80	119.13
2	D	1001	N3C	O28-S28-C29	2.47	111.01	107.97
2	D	1001	N3C	C18-C19-N14	2.43	115.63	110.64
2	C	1001	N3C	C13-N14-C15	-2.42	105.68	111.06
2	C	1001	N3C	C33-C32-N35	-2.40	120.95	123.42
2	D	1001	N3C	C29-S28-N27	-2.38	102.37	105.97
2	A	1001	N3C	O28-S28-N27	2.36	113.39	106.74
2	D	1001	N3C	C23-C26-N27	2.36	118.95	116.09
2	C	1001	N3C	C15-C16-N17	2.36	115.28	110.70
2	A	1001	N3C	C5-C4-C7	-2.33	117.14	120.91
2	F	1001	N3C	C13-N14-C15	-2.31	105.93	111.06
2	A	1001	N3C	C26-N27-S28	-2.29	120.40	123.36
2	E	1001	N3C	C15-C16-N17	2.28	115.13	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	N3C	O26-C26-C23	-2.24	116.94	120.94
2	E	1001	N3C	C5-C4-C3	2.22	122.02	117.59
2	C	1001	N3C	C23-C26-N27	2.22	118.78	116.09
2	F	1001	N3C	C16-C15-N14	2.21	115.19	110.64
2	C	1001	N3C	C13-N14-C19	2.21	115.97	111.06
2	F	1001	N3C	C21-C20-N17	2.20	124.41	121.38
2	B	1001	N3C	C34-C33-C32	-2.19	119.54	121.53
2	F	1001	N3C	C13-N14-C19	2.14	115.82	111.06
2	A	1001	N3C	C13-N14-C19	2.11	115.76	111.06
2	B	1001	N3C	O29-S28-N27	2.10	112.66	106.74
2	D	1001	N3C	C30-C29-C34	-2.07	118.07	120.62
2	E	1001	N3C	C18-C19-N14	-2.07	106.40	110.64
2	A	1001	N3C	C12-C13-N14	2.06	116.36	112.75
2	D	1001	N3C	C8-C7-C12	2.06	120.94	118.96
2	D	1001	N3C	C4-C7-C12	-2.05	117.34	122.71
2	C	1001	N3C	O28-S28-N27	2.02	112.43	106.74
2	A	1001	N3C	C29-S28-N27	-2.02	102.92	105.97
2	F	1001	N3C	C37-C38-N39	2.01	119.99	113.83

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	N3C	C33-C32-N35-C36
2	B	1001	N3C	C37-C36-C41-S42
2	B	1001	N3C	C36-C37-C38-N39
2	E	1001	N3C	C32-C33-N33-O34
2	E	1001	N3C	C34-C33-N33-O34
2	F	1001	N3C	C36-C37-C38-N39
2	A	1001	N3C	C12-C13-N14-C19
2	D	1001	N3C	C12-C13-N14-C15
2	D	1001	N3C	C12-C13-N14-C19
2	F	1001	N3C	C37-C38-N39-C40
2	F	1001	N3C	C37-C38-N39-C39
2	A	1001	N3C	C12-C13-N14-C15
2	E	1001	N3C	C37-C38-N39-C40
2	D	1001	N3C	N35-C36-C37-C38
2	D	1001	N3C	C37-C38-N39-C40
2	E	1001	N3C	C36-C41-S42-C43
2	D	1001	N3C	C37-C38-N39-C39
2	F	1001	N3C	C12-C13-N14-C19
2	B	1001	N3C	C34-C29-S28-O29

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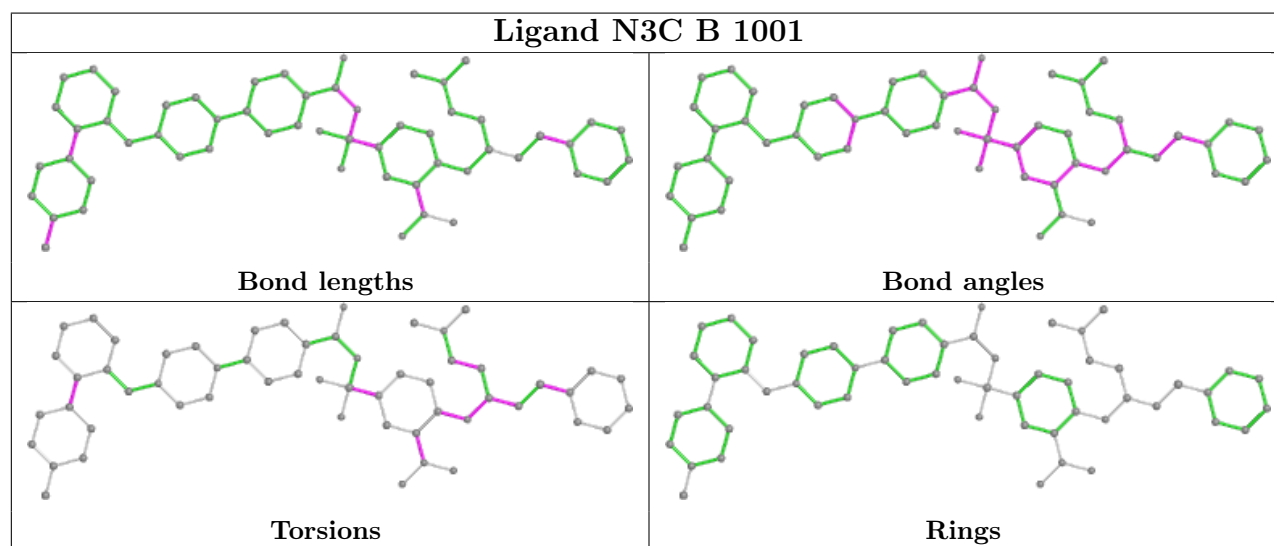
Mol	Chain	Res	Type	Atoms
2	B	1001	N3C	C30-C29-S28-O29
2	C	1001	N3C	C36-C37-C38-N39
2	D	1001	N3C	C41-C36-C37-C38
2	A	1001	N3C	N35-C36-C37-C38
2	B	1001	N3C	C5-C4-C7-C12
2	B	1001	N3C	C34-C33-N33-O34
2	E	1001	N3C	C5-C4-C7-C12
2	B	1001	N3C	C3-C4-C7-C12
2	E	1001	N3C	C3-C4-C7-C12
2	D	1001	N3C	C5-C4-C7-C12
2	C	1001	N3C	C12-C13-N14-C19
2	A	1001	N3C	C3-C4-C7-C12
2	D	1001	N3C	C3-C4-C7-C12
2	E	1001	N3C	C33-C32-N35-C36
2	B	1001	N3C	C44-C43-S42-C41
2	B	1001	N3C	C3-C4-C7-C8
2	B	1001	N3C	C5-C4-C7-C8
2	D	1001	N3C	C44-C43-S42-C41
2	D	1001	N3C	C5-C4-C7-C8
2	F	1001	N3C	C34-C33-N33-O34
2	A	1001	N3C	C5-C4-C7-C12
2	E	1001	N3C	C5-C4-C7-C8
2	D	1001	N3C	C48-C43-S42-C41
2	B	1001	N3C	C48-C43-S42-C41
2	E	1001	N3C	C3-C4-C7-C8
2	C	1001	N3C	C44-C43-S42-C41
2	A	1001	N3C	C3-C4-C7-C8
2	D	1001	N3C	C3-C4-C7-C8
2	C	1001	N3C	C3-C4-C7-C12
2	E	1001	N3C	C37-C38-N39-C39
2	C	1001	N3C	C48-C43-S42-C41
2	B	1001	N3C	C41-C36-N35-C32
2	A	1001	N3C	C44-C43-S42-C41
2	C	1001	N3C	C5-C4-C7-C12
2	C	1001	N3C	C3-C4-C7-C8
2	C	1001	N3C	C5-C4-C7-C8
2	A	1001	N3C	C5-C4-C7-C8

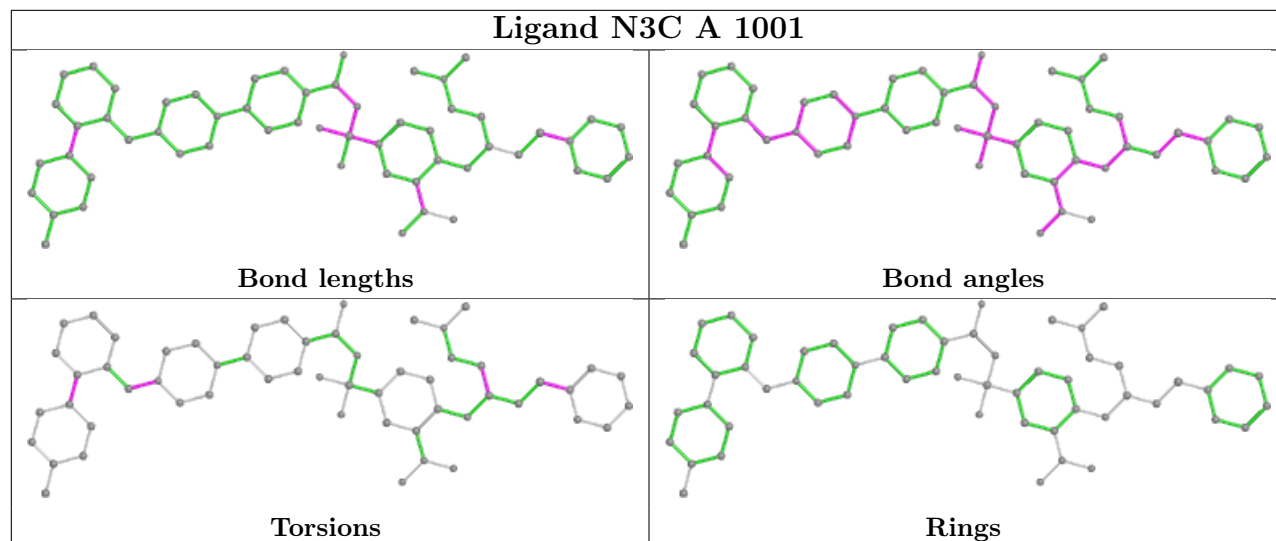
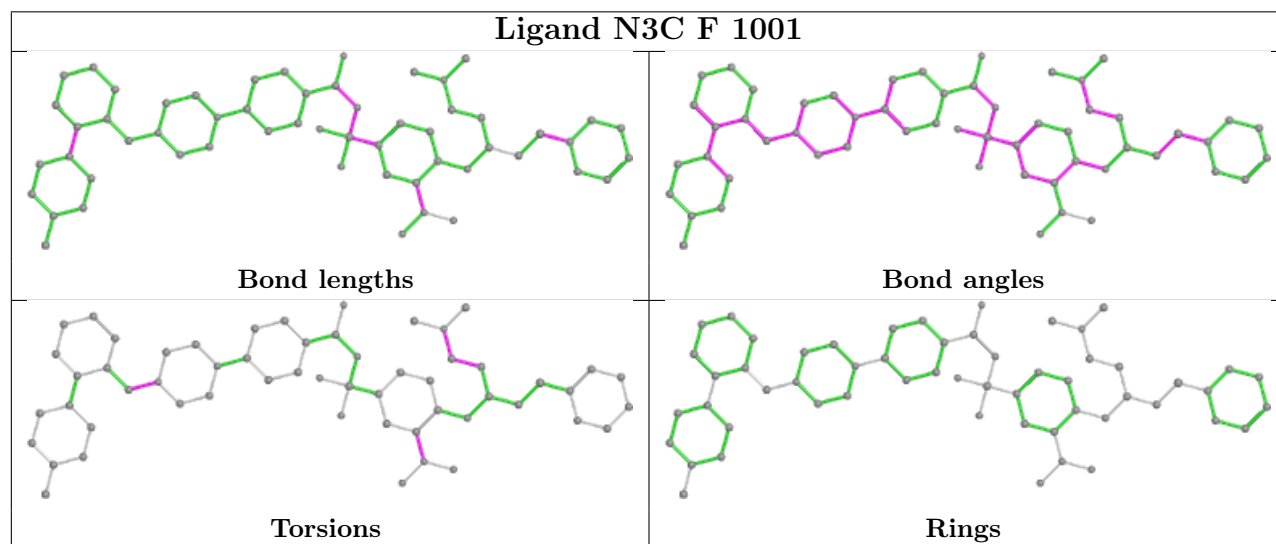
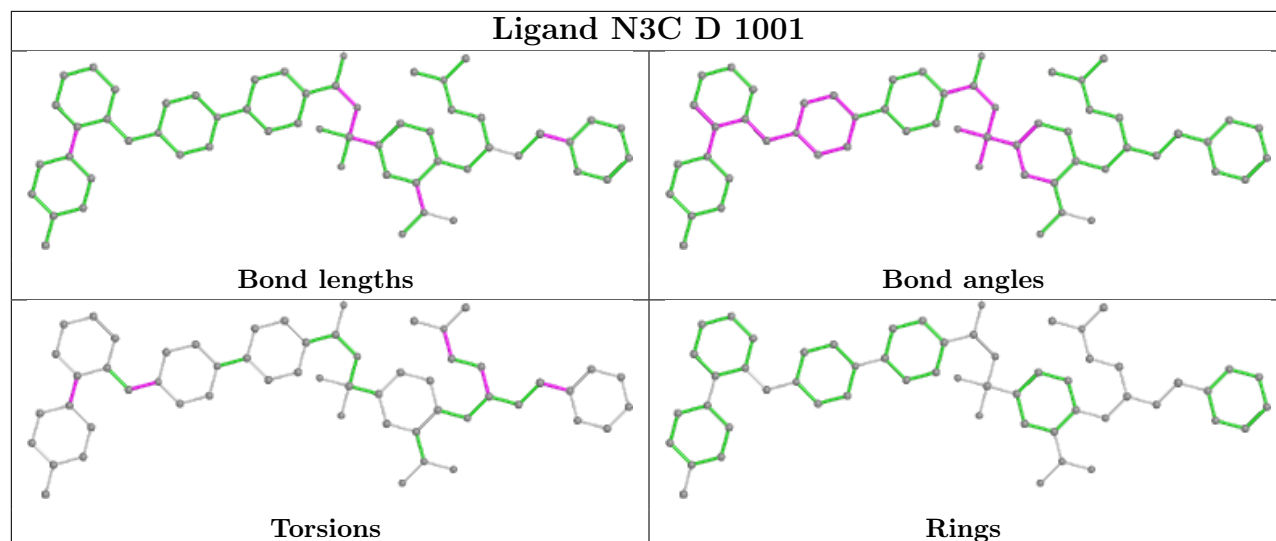
There are no ring outliers.

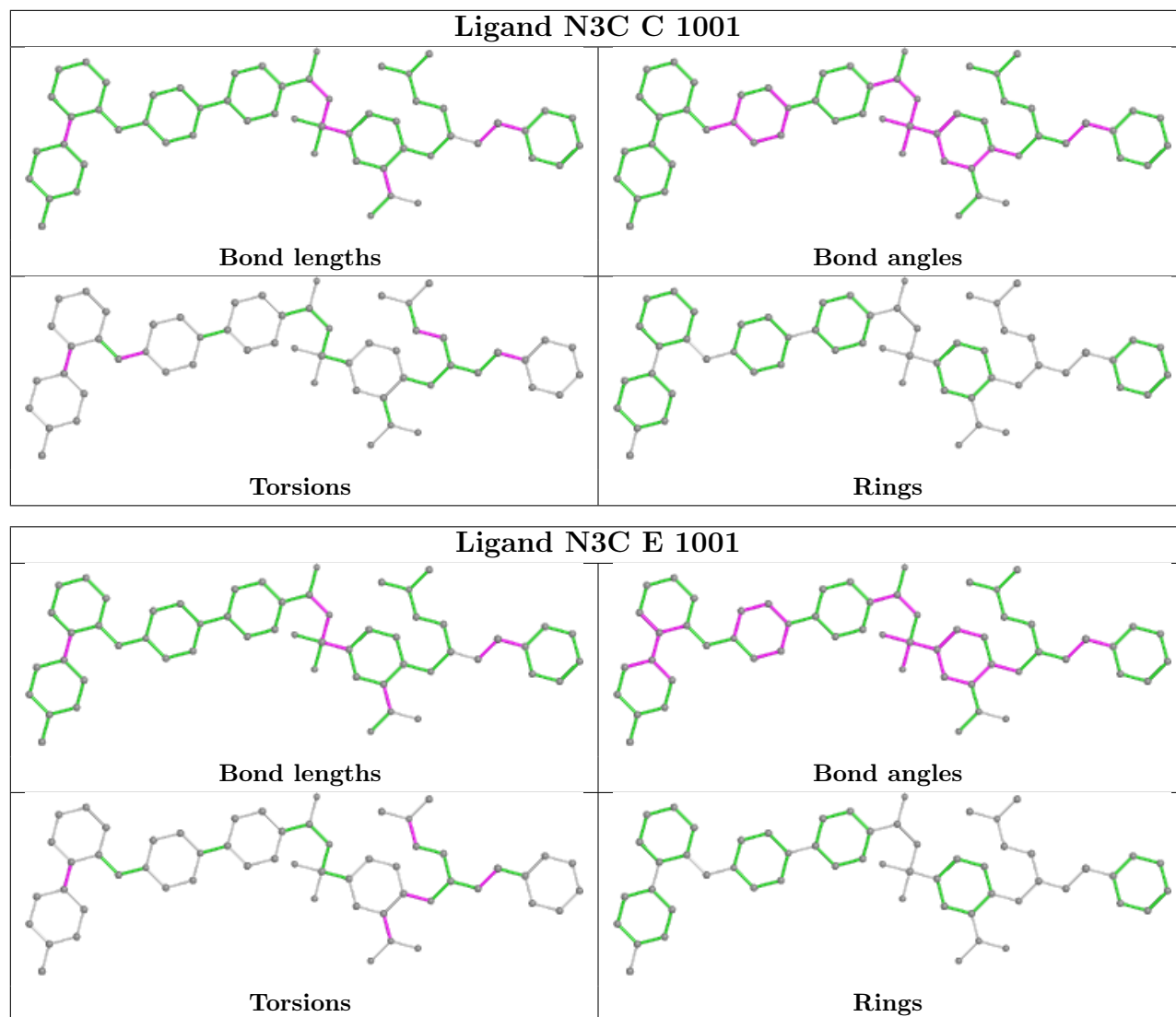
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	N3C	2	0
2	D	1001	N3C	1	0
2	F	1001	N3C	2	0
2	A	1001	N3C	2	0
2	C	1001	N3C	1	0
2	E	1001	N3C	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	161/210 (76%)	0.39	5 (3%)	49	58	36, 63, 105, 121	0
1	B	156/210 (74%)	0.59	14 (8%)	9	11	49, 92, 136, 229	0
1	C	165/210 (78%)	0.34	3 (1%)	68	76	43, 61, 94, 130	0
1	D	156/210 (74%)	0.35	4 (2%)	56	65	44, 62, 111, 131	0
1	E	156/210 (74%)	0.72	20 (12%)	3	4	53, 94, 137, 149	0
1	F	161/210 (76%)	0.54	9 (5%)	24	29	45, 78, 124, 138	0
All	All	955/1260 (75%)	0.49	55 (5%)	23	28	36, 73, 126, 229	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	169	ARG	5.5
1	E	86	PRO	5.2
1	F	4	THR	4.8
1	E	87	VAL	4.7
1	E	102	GLY	4.2
1	A	87	VAL	4.1
1	B	67	SER	3.9
1	B	97	LEU	3.9
1	D	87	VAL	3.7
1	D	84	ASP	3.6
1	F	64	GLN	3.4
1	B	104	PHE	3.3
1	E	30	TYR	3.3
1	F	107	LEU	3.3
1	F	84	ASP	3.3
1	F	66	PHE	3.2
1	E	85	LYS	3.2
1	E	84	ASP	3.1
1	F	169	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	127	SER	3.1
1	B	9	LEU	3.0
1	B	94	ILE	3.0
1	B	89	LYS	2.9
1	B	84	ASP	2.9
1	E	64	GLN	2.9
1	D	81	ILE	2.9
1	B	132	SER	2.9
1	E	88	ASP	2.7
1	C	67	SER	2.6
1	F	132	SER	2.6
1	A	81	ILE	2.6
1	E	130	GLY	2.6
1	E	67	SER	2.5
1	B	131	HIS	2.5
1	E	97	LEU	2.5
1	E	166	PHE	2.5
1	E	34	LEU	2.4
1	B	128	LYS	2.4
1	E	89	LYS	2.4
1	A	34	LEU	2.3
1	D	82	ASP	2.3
1	B	64	GLN	2.3
1	F	83	SER	2.2
1	A	94	ILE	2.2
1	A	9	LEU	2.2
1	F	40	ILE	2.2
1	E	35	LEU	2.2
1	E	94	ILE	2.1
1	C	107	LEU	2.1
1	B	62	PHE	2.1
1	B	100	LEU	2.1
1	E	31	LEU	2.0
1	E	103	LEU	2.0
1	E	25	LYS	2.0
1	C	89	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

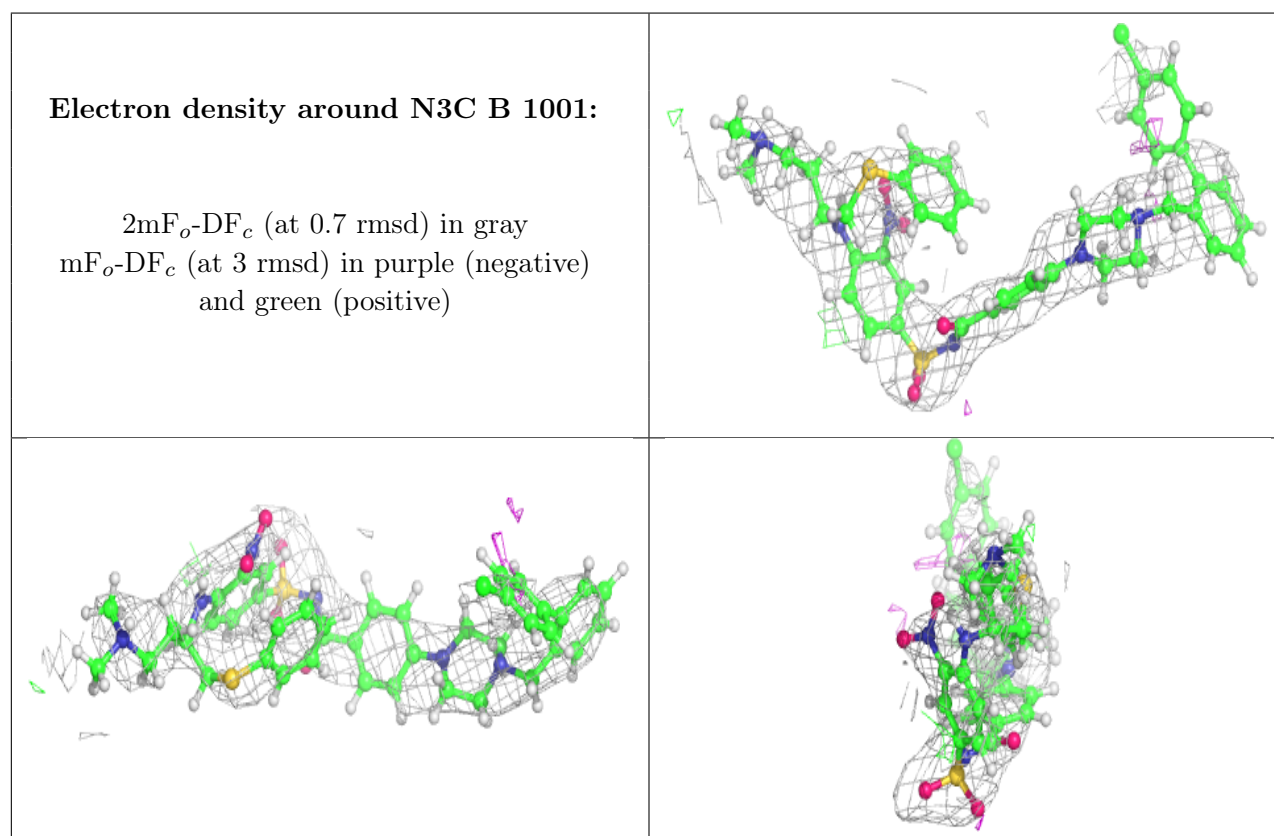
There are no monosaccharides in this entry.

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.

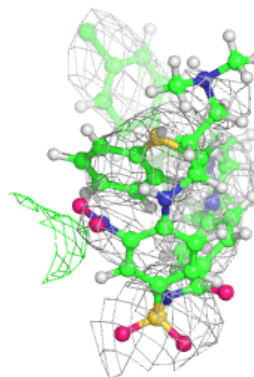
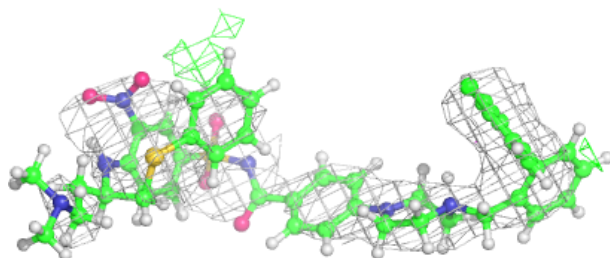
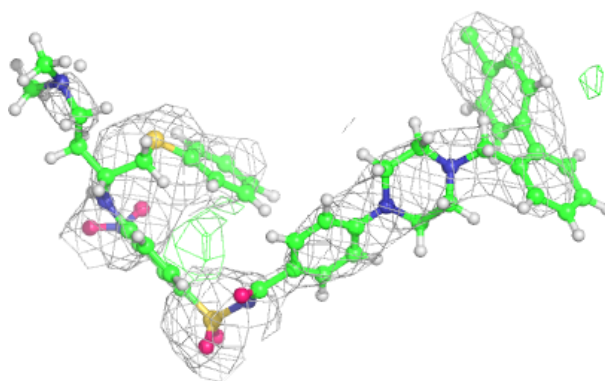
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	N3C	B	1001	56/56	0.82	0.35	96,123,154,161	0
2	N3C	E	1001	56/56	0.86	0.33	86,125,165,170	0
2	N3C	F	1001	56/56	0.89	0.28	67,100,158,175	0
2	N3C	C	1001	56/56	0.91	0.22	66,102,144,168	0
2	N3C	A	1001	56/56	0.95	0.19	46,68,89,102	0
2	N3C	D	1001	56/56	0.95	0.21	49,81,140,147	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.

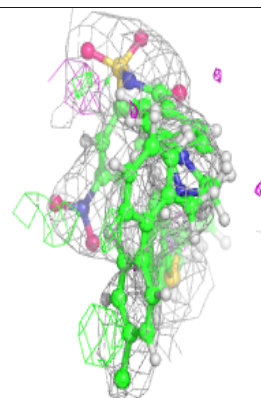
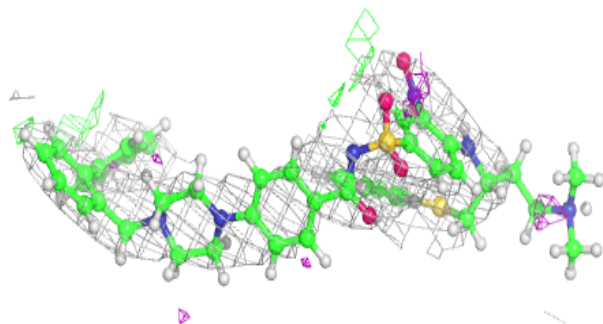
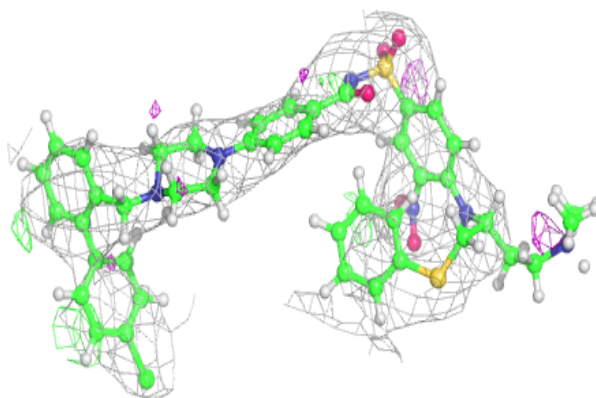


Electron density around N3C E 1001:

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

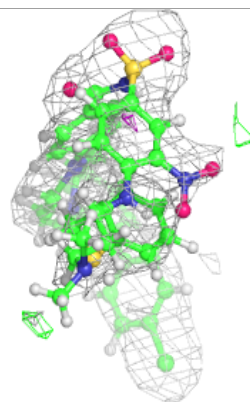
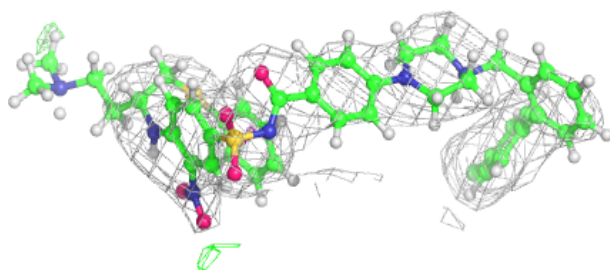
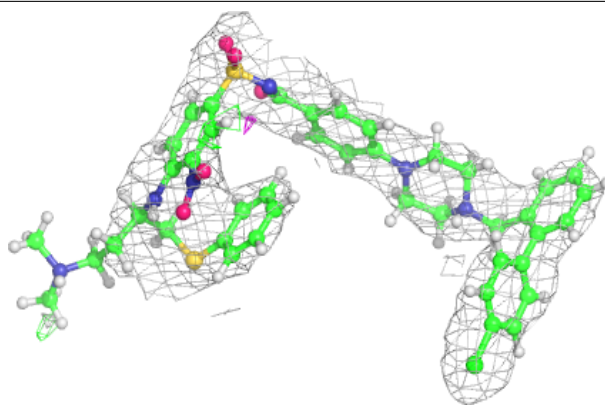
**Electron density around N3C F 1001:**

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

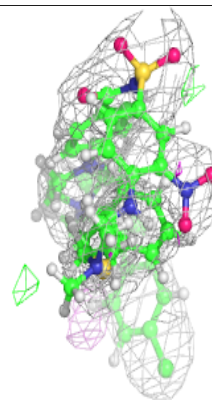
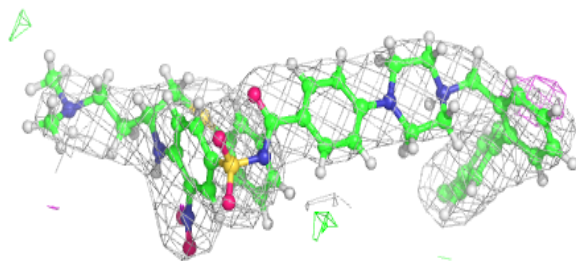
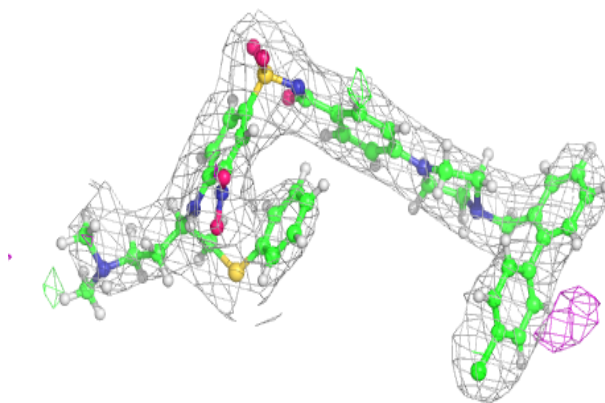


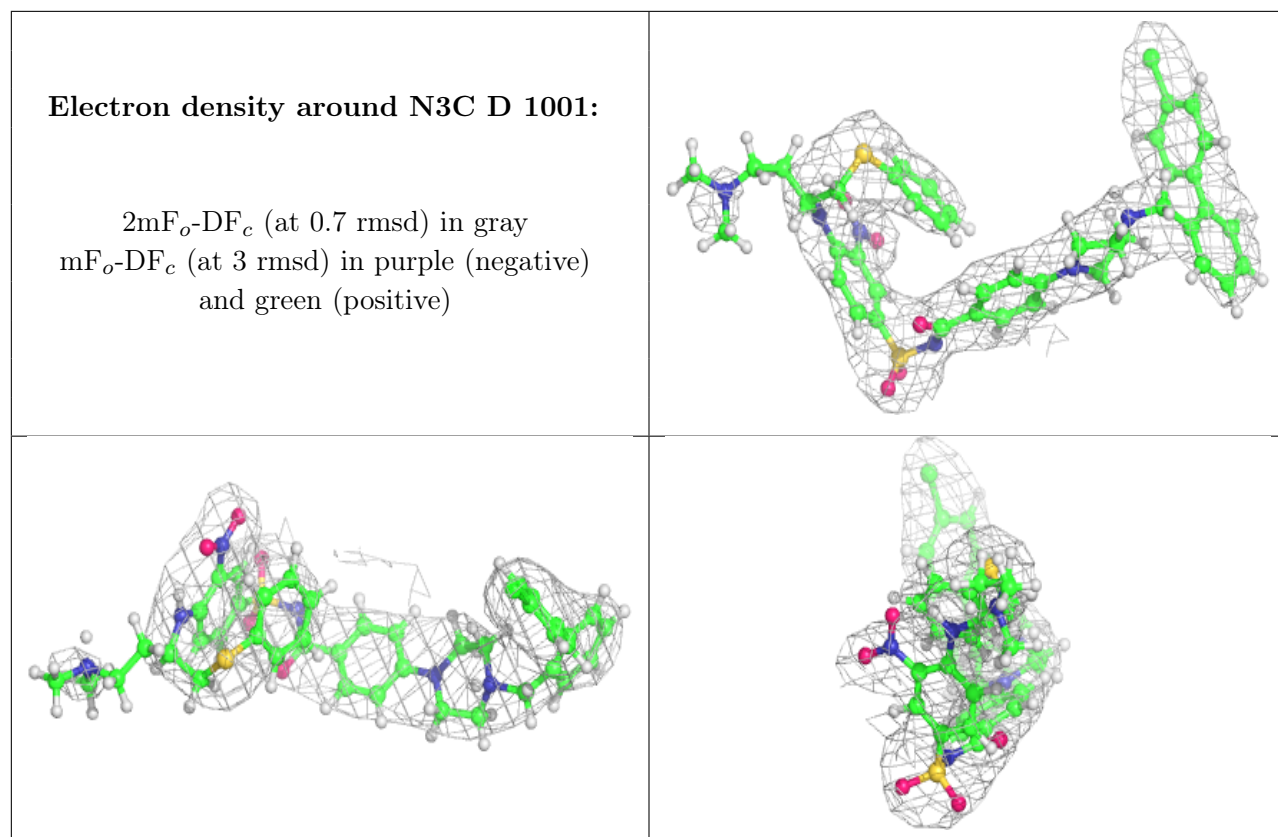
Electron density around N3C C 1001:

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

**Electron density around N3C A 1001:**

$2mF_o-DF_c$ (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.