



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:17 PM BST

PDB ID : 4ZG6
Title : Structural basis for inhibition of human autotaxin by four novel compounds
Authors : Stein, A.J.; Bain, G.; Hutchinson, J.H.; Evans, J.F.
Deposited on : 2015-04-22
Resolution : 1.80 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 : 2.13.1
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) : 2.13.1

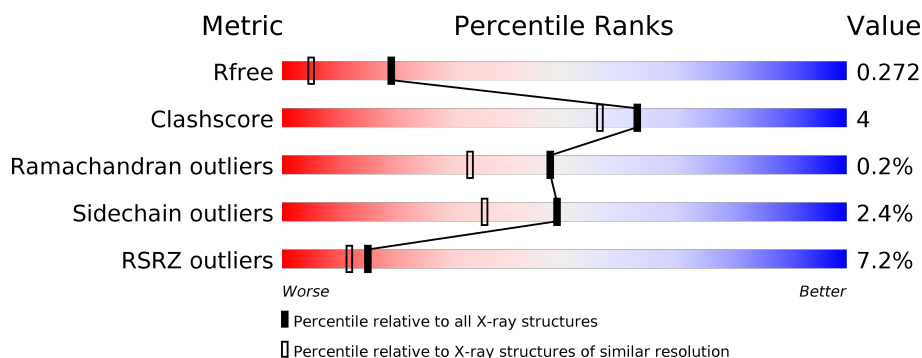
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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	855	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>9%</div> <div>12%</div> </div> </div>
1	B	855	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>6%</div> <div>12%</div> </div> </div>
2	C	3	<div> <div></div> <div>100%</div> </div>
2	D	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	909	-	-	X	-
6	GOL	B	909	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12830 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	754	Total	C	N	O	S	0	7	0
			6004	3826	1019	1115	44			
1	B	756	Total	C	N	O	S	0	6	0
			6014	3829	1025	1112	48			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	411	ALA	ASN	engineered mutation	UNP Q13822
A	864	HIS	-	expression tag	UNP Q13822
A	865	HIS	-	expression tag	UNP Q13822
A	866	HIS	-	expression tag	UNP Q13822
A	867	HIS	-	expression tag	UNP Q13822
A	868	HIS	-	expression tag	UNP Q13822
A	869	HIS	-	expression tag	UNP Q13822
A	870	HIS	-	expression tag	UNP Q13822
A	871	HIS	-	expression tag	UNP Q13822
B	411	ALA	ASN	engineered mutation	UNP Q13822
B	864	HIS	-	expression tag	UNP Q13822
B	865	HIS	-	expression tag	UNP Q13822
B	866	HIS	-	expression tag	UNP Q13822
B	867	HIS	-	expression tag	UNP Q13822
B	868	HIS	-	expression tag	UNP Q13822
B	869	HIS	-	expression tag	UNP Q13822
B	870	HIS	-	expression tag	UNP Q13822
B	871	HIS	-	expression tag	UNP Q13822

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

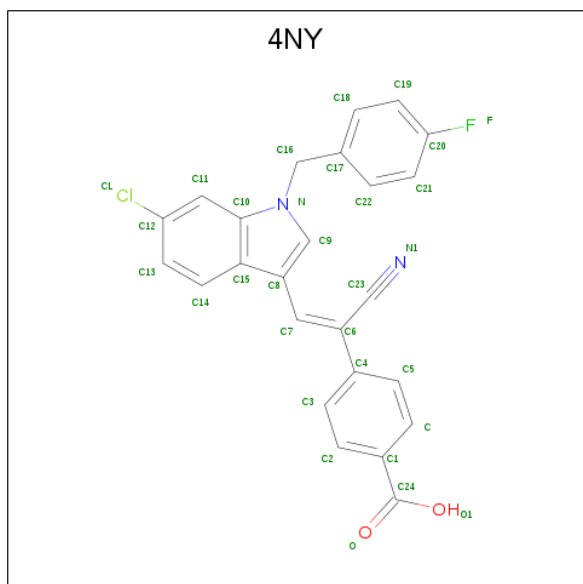
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is 4-{(Z)-2-[6-chloro-1-(4-fluorobenzyl)-1H-indol-3-yl]-1-cyanoethenyl}benzoic acid (three-letter code: 4NY) (formula: C₂₅H₁₆ClFN₂O₂).



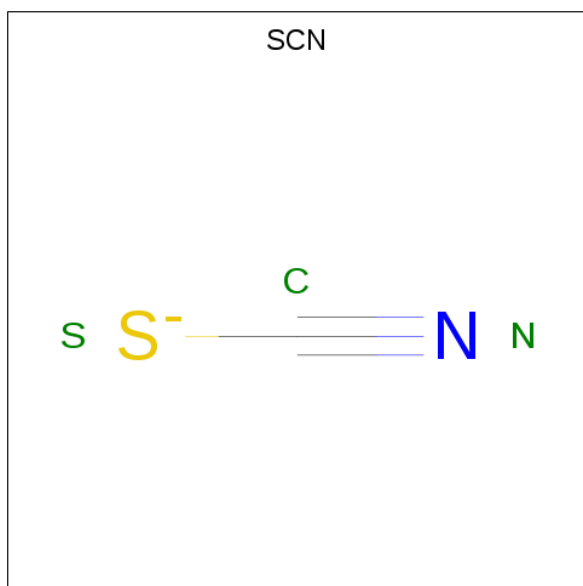
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	Cl	F	N	O	0	0
			31	25	1	1	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	Cl	F	N	O	
			31	25	1	1	2	2	
									0
									0

- Molecule 8 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	S	0	0
			3	1	1	1		
8	A	1	Total	C	N	S	0	0
			3	1	1	1		
8	A	1	Total	C	N	S	0	0
			3	1	1	1		
8	A	1	Total	C	N	S	0	0
			3	1	1	1		
8	A	1	Total	C	N	S	0	0
			3	1	1	1		
8	A	1	Total	C	N	S	0	0
			3	1	1	1		
8	B	1	Total	C	N	S	0	0
			3	1	1	1		
8	B	1	Total	C	N	S	0	0
			3	1	1	1		
8	B	1	Total	C	N	S	0	0
			3	1	1	1		

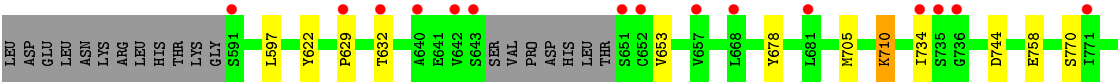
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total 3	C 1	N 1	S 1	0	0
8	B	1	Total 3	C 1	N 1	S 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	293	Total 293	O 293	0	0
9	B	321	Total 321	O 321	0	0



● Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.62Å 70.49Å 107.37Å 104.65° 99.27° 99.86°	Depositor
Resolution (Å)	34.69 – 1.80 34.69 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (34.69-1.80) 96.0 (34.69-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.220 , 0.265 0.227 , 0.272	Depositor DCC
R_{free} test set	7755 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12830	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 92.22 % 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 1.0268e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, BMA, NAG, NA, CA, 4NY, SCN

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	0.59	1/6195 (0.0%)	0.72	2/8424 (0.0%)
1	B	0.57	0/6203	0.74	3/8433 (0.0%)
All	All	0.58	1/12398 (0.0%)	0.73	5/16857 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	PRO	N-CD	5.55	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	ASP	CB-CG-OD1	5.75	123.48	118.30
1	B	195[A]	CYS	CA-CB-SG	5.75	124.34	114.00
1	B	195[B]	CYS	CA-CB-SG	5.75	124.34	114.00
1	B	744	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	748	ASP	CB-CG-OD2	-5.07	113.74	118.30

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	6004	0	5667	64	0
1	B	6014	0	5668	32	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	6	0	7	4	0
6	B	6	0	7	5	0
7	A	31	0	15	3	0
7	B	31	0	15	5	0
8	A	21	0	0	1	0
8	B	15	0	0	2	0
9	A	293	0	0	7	0
9	B	321	0	0	7	0
All	All	12830	0	11447	102	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 4.

All (102) 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:A:559:LEU:O	1:A:562:ASP:HB2	1.62	0.99
1:A:353:ASN:HD21	1:A:494:THR:HG23	1.28	0.97
1:A:251[B]:ASN:OD1	9:A:1002:HOH:O	1.82	0.97
1:A:494:THR:HG21	9:A:1202:HOH:O	1.72	0.88
1:A:353:ASN:HD21	1:A:494:THR:CG2	1.86	0.88
1:B:844:ARG:NH1	9:B:1002:HOH:O	2.07	0.87
1:A:353:ASN:ND2	1:A:494:THR:HG23	1.90	0.86
7:A:910:4NY:O1	9:A:1003:HOH:O	1.94	0.85
1:B:231:ASN:ND2	6:B:909:GOL:O1	2.10	0.84
1:A:556:ILE:HG23	1:A:657:VAL:HG11	1.63	0.79
1:A:559:LEU:N	1:A:562:ASP:OD2	2.14	0.79
1:B:251[B]:ASN:OD1	9:B:1001:HOH:O	2.01	0.78
1:A:231:ASN:ND2	6:A:909:GOL:O1	2.12	0.78
1:A:559:LEU:HB2	1:A:562:ASP:OD2	1.84	0.77
1:A:209:LYS:HG3	8:A:915:SCN:N	2.00	0.76
8:B:912:SCN:S	9:B:1002:HOH:O	2.48	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:THR:HG23	1:A:606:TYR:O	1.91	0.69
1:B:480:LYS:O	1:B:860:GLU:HG3	1.92	0.68
1:A:556:ILE:HG23	1:A:657:VAL:CG1	2.24	0.68
1:A:549:THR:HG21	1:A:608:THR:H	1.58	0.67
1:A:475:HIS:CD2	9:A:1001:HOH:O	2.46	0.67
1:B:128:GLY:O	1:B:291:GLN:HG2	1.95	0.67
1:A:314:SER:C	1:A:325:MET:HE1	2.15	0.66
1:A:156:GLU:OE2	9:A:1004:HOH:O	2.14	0.64
1:B:149[B]:CYS:SG	1:B:497:TYR:HE1	2.22	0.63
1:A:475:HIS:HE1	6:A:909:GOL:H11	1.64	0.63
1:B:149[B]:CYS:SG	1:B:497:TYR:CE1	2.94	0.60
1:B:209:LYS:HG3	8:B:914:SCN:N	2.16	0.59
1:A:559:LEU:O	1:A:562:ASP:CB	2.44	0.59
1:B:223:PRO:HA	1:B:226:HIS:CE1	2.38	0.59
1:A:475:HIS:CE1	6:A:909:GOL:H11	2.38	0.58
1:B:210:THR:HB	6:B:909:GOL:H12	1.84	0.58
1:B:527:THR:OG1	1:B:828[A]:ARG:HD3	2.03	0.58
1:A:273:THR:HG22	1:A:275:PHE:H	1.70	0.56
1:A:223:PRO:HA	1:A:226:HIS:CE1	2.40	0.56
1:A:372:PHE:CE1	1:A:458:PRO:HA	2.40	0.55
1:B:217[B]:LEU:HD11	9:B:1040:HOH:O	2.05	0.55
1:B:567:CYS:SG	1:B:653:VAL:HB	2.46	0.55
1:A:273:THR:O	9:A:1005:HOH:O	2.18	0.55
1:B:231:ASN:HD21	6:B:909:GOL:C1	2.19	0.55
1:A:652:CYS:SG	1:A:654:ARG:HG2	2.47	0.55
1:B:217[B]:LEU:CD1	7:B:910:4NY:CL	2.91	0.54
1:A:695:ASP:HA	1:A:698:LEU:HD23	1.91	0.53
1:B:190:GLU:OE2	1:B:193:ARG:NH1	2.41	0.53
1:A:559:LEU:CB	1:A:562:ASP:OD2	2.55	0.53
1:B:210:THR:CB	6:B:909:GOL:H12	2.39	0.53
1:A:549:THR:CG2	1:A:606:TYR:O	2.56	0.52
1:B:217[B]:LEU:HD21	9:B:1040:HOH:O	2.09	0.52
1:A:554:PRO:HB2	1:A:658:ARG:HB3	1.91	0.52
1:A:609:ARG:NH1	1:A:624:GLU:OE1	2.35	0.51
7:B:910:4NY:O1	9:B:1003:HOH:O	2.19	0.51
1:A:179:MET:CE	1:A:193:ARG:HD2	2.40	0.51
1:A:558:TYR:O	1:A:657:VAL:CG1	2.59	0.50
1:A:144:TRP:O	1:A:191:LYS:NZ	2.45	0.50
1:B:123:ASP:O	1:B:127:ARG:HG2	2.12	0.50
1:B:217[B]:LEU:HD12	7:B:910:4NY:CL	2.49	0.50
1:B:359:ASP:HB3	7:B:910:4NY:CL	2.50	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:909:GOL:H31	9:B:1266:HOH:O	2.13	0.49
1:B:770:SER:HB2	1:B:794:PHE:CZ	2.48	0.49
1:A:190:GLU:O	1:A:194[A]:SER:OG	2.28	0.49
1:A:559:LEU:O	1:A:562:ASP:N	2.43	0.48
1:A:558:TYR:O	1:A:657:VAL:HG13	2.14	0.48
1:B:622:TYR:HA	1:B:629:PRO:HA	1.95	0.48
1:A:190:GLU:OE2	1:A:193:ARG:NH1	2.47	0.48
1:A:480:LYS:O	1:A:860:GLU:HG3	2.13	0.47
1:B:678:TYR:O	1:B:710:LYS:HE2	2.15	0.47
1:A:179:MET:HE2	1:A:193:ARG:HD2	1.96	0.47
1:A:622:TYR:HA	1:A:629:PRO:HA	1.97	0.47
1:A:185:VAL:O	1:A:330:ARG:CG	2.63	0.46
1:A:74:CYS:SG	1:A:87:CYS:N	2.88	0.46
1:A:191:LYS:O	1:A:195:CYS:HB2	2.17	0.45
1:A:359:ASP:HB3	7:A:910:4NY:CL	2.53	0.45
1:A:210:THR:OG1	6:A:909:GOL:H12	2.17	0.45
1:B:206:TYR:CD1	1:B:207:PRO:HA	2.52	0.45
1:B:470:PHE:O	1:B:471:PHE:HB3	2.15	0.45
1:A:559:LEU:O	1:A:560:GLN:C	2.55	0.45
1:B:377:LEU:HB2	1:B:380:VAL:HG23	1.99	0.45
1:A:837:ASP:OD2	1:A:840:ARG:HD2	2.18	0.44
1:B:273:THR:HG22	1:B:275:PHE:H	1.82	0.44
1:B:389:THR:HG22	1:B:477:PHE:CZ	2.52	0.44
1:A:167:ILE:HD12	1:A:352:VAL:HG11	1.99	0.44
1:A:608:THR:HG22	1:A:625:ILE:HG13	1.99	0.44
1:A:705:MET:HA	1:A:798:HIS:NE2	2.32	0.43
1:A:315:GLY:N	1:A:325:MET:HE1	2.34	0.43
1:A:704:PRO:HG2	1:A:765:PRO:HD3	2.01	0.43
1:B:632:THR:O	1:B:734:ILE:HA	2.19	0.43
7:B:910:4NY:C23	7:B:910:4NY:C9	2.97	0.43
1:A:206:TYR:CD1	1:A:207:PRO:HA	2.54	0.42
1:A:185:VAL:O	1:A:330:ARG:HG2	2.20	0.42
1:A:527:THR:OG1	1:A:828[A]:ARG:HD3	2.20	0.42
1:A:632:THR:O	1:A:734:ILE:HA	2.19	0.41
1:A:559:LEU:CA	1:A:562:ASP:OD2	2.68	0.41
1:A:547:GLU:HG2	1:A:603:ALA:HB1	2.01	0.41
1:A:840:ARG:HG3	9:A:1179:HOH:O	2.20	0.41
1:A:614:TYR:O	1:A:658:ARG:NH1	2.53	0.41
1:B:183:SER:N	1:B:190:GLU:HG3	2.36	0.41
1:A:145:VAL:HB	1:A:188:ASN:OD1	2.21	0.40
1:A:450:ARG:NH1	1:A:481:VAL:HG13	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:910:4NY:C9	7:A:910:4NY:C23	3.00	0.40
1:A:185:VAL:O	1:A:330:ARG:HG3	2.21	0.40
1:A:207:PRO:HD3	1:A:435:TYR:CE1	2.57	0.40
1:B:705:MET:HA	1:B:798:HIS:NE2	2.36	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	751/855 (88%)	721 (96%)	29 (4%)	1 (0%)	51	36
1	B	752/855 (88%)	725 (96%)	25 (3%)	2 (0%)	41	27
All	All	1503/1710 (88%)	1446 (96%)	54 (4%)	3 (0%)	47	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	556	ILE
1	B	78	ASN
1	B	471	PHE

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	656/772 (85%)	631 (96%)	25 (4%)	33	18
1	B	657/772 (85%)	649 (99%)	8 (1%)	71	65
All	All	1313/1544 (85%)	1280 (98%)	33 (2%)	49	34

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

Mol	Chain	Res	Type
1	A	194[A]	SER
1	A	194[B]	SER
1	A	195	CYS
1	A	214	LEU
1	A	233	MET
1	A	324	GLU
1	A	330	ARG
1	A	367	CYS
1	A	382	ASP
1	A	390	LEU
1	A	493	SER
1	A	494	THR
1	A	549	THR
1	A	559	LEU
1	A	597	LEU
1	A	627	LEU
1	A	654	ARG
1	A	658	ARG
1	A	668	LEU
1	A	691	GLU
1	A	698	LEU
1	A	814	LYS
1	A	828[A]	ARG
1	A	828[B]	ARG
1	A	840	ARG
1	B	106	ASP
1	B	451	ARG
1	B	493	SER
1	B	567	CYS
1	B	597	LEU
1	B	710	LYS
1	B	758	GLU
1	B	844	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	ASN
1	A	747	HIS
1	B	231	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 ⓘ

6 monosaccharides 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	NAG	C	1	1,2	14,14,15	1.06	2 (14%)	17,19,21	1.31	2 (11%)
2	NAG	C	2	2	14,14,15	1.02	1 (7%)	17,19,21	1.43	4 (23%)
2	BMA	C	3	2	11,11,12	0.49	0	15,15,17	0.84	1 (6%)
2	NAG	D	1	1,2	14,14,15	0.93	0	17,19,21	0.93	0
2	NAG	D	2	2	14,14,15	0.82	1 (7%)	17,19,21	1.58	4 (23%)
2	BMA	D	3	2	11,11,12	0.43	0	15,15,17	0.96	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	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	O5-C1	-3.47	1.38	1.43
2	D	2	NAG	O5-C1	-2.70	1.39	1.43
2	C	1	NAG	C2-N2	-2.11	1.42	1.46
2	C	1	NAG	C3-C2	2.01	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C1-C2	-3.64	105.54	111.29
2	D	2	NAG	C1-O5-C5	3.39	116.79	112.19
2	C	2	NAG	O7-C7-C8	-2.81	116.83	122.06
2	C	2	NAG	C8-C7-N2	2.72	120.70	116.10
2	D	2	NAG	O4-C4-C5	-2.59	102.87	109.30
2	C	3	BMA	C1-O5-C5	2.49	115.57	112.19
2	D	2	NAG	C1-C2-N2	-2.49	106.24	110.49
2	C	2	NAG	C1-C2-N2	-2.37	106.43	110.49
2	C	2	NAG	O4-C4-C5	-2.32	103.55	109.30
2	D	2	NAG	O7-C7-C8	-2.19	117.99	122.06
2	C	1	NAG	O5-C5-C6	2.03	110.39	107.20

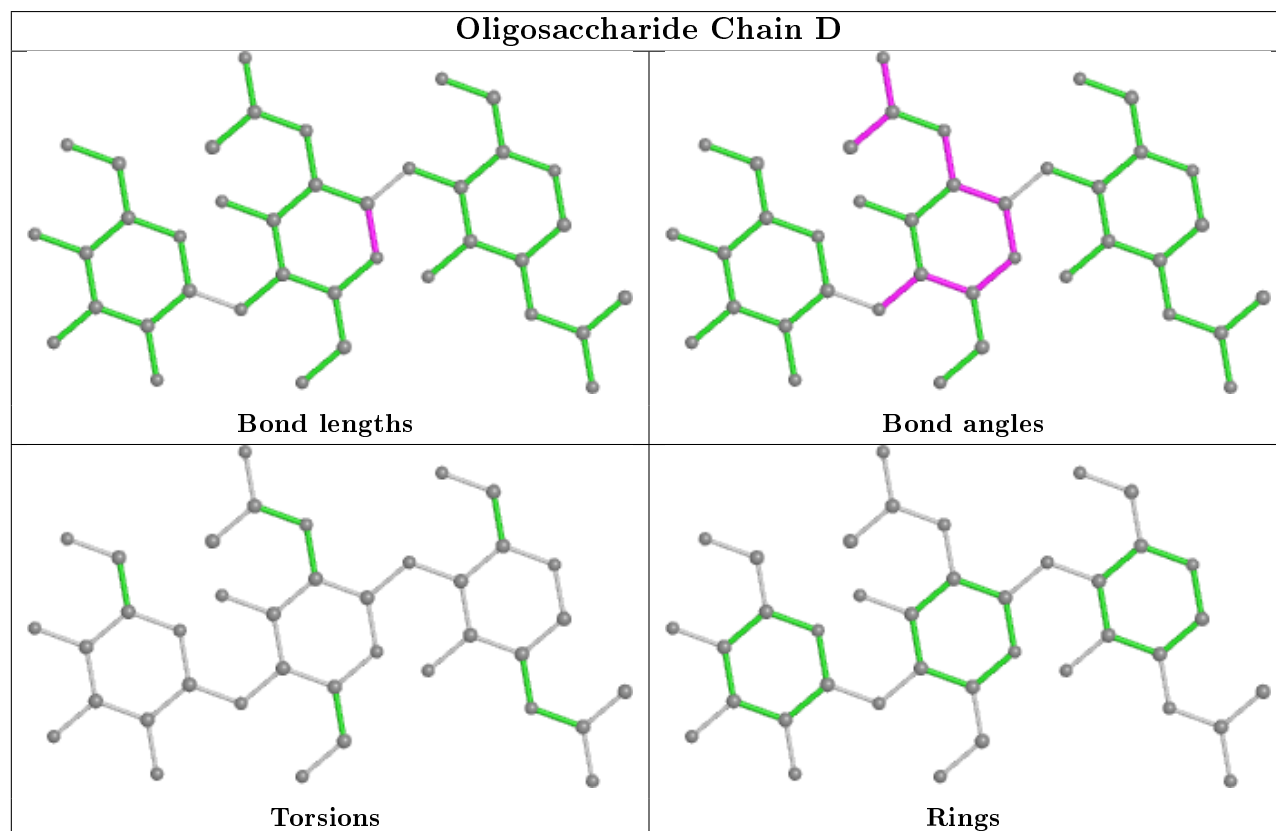
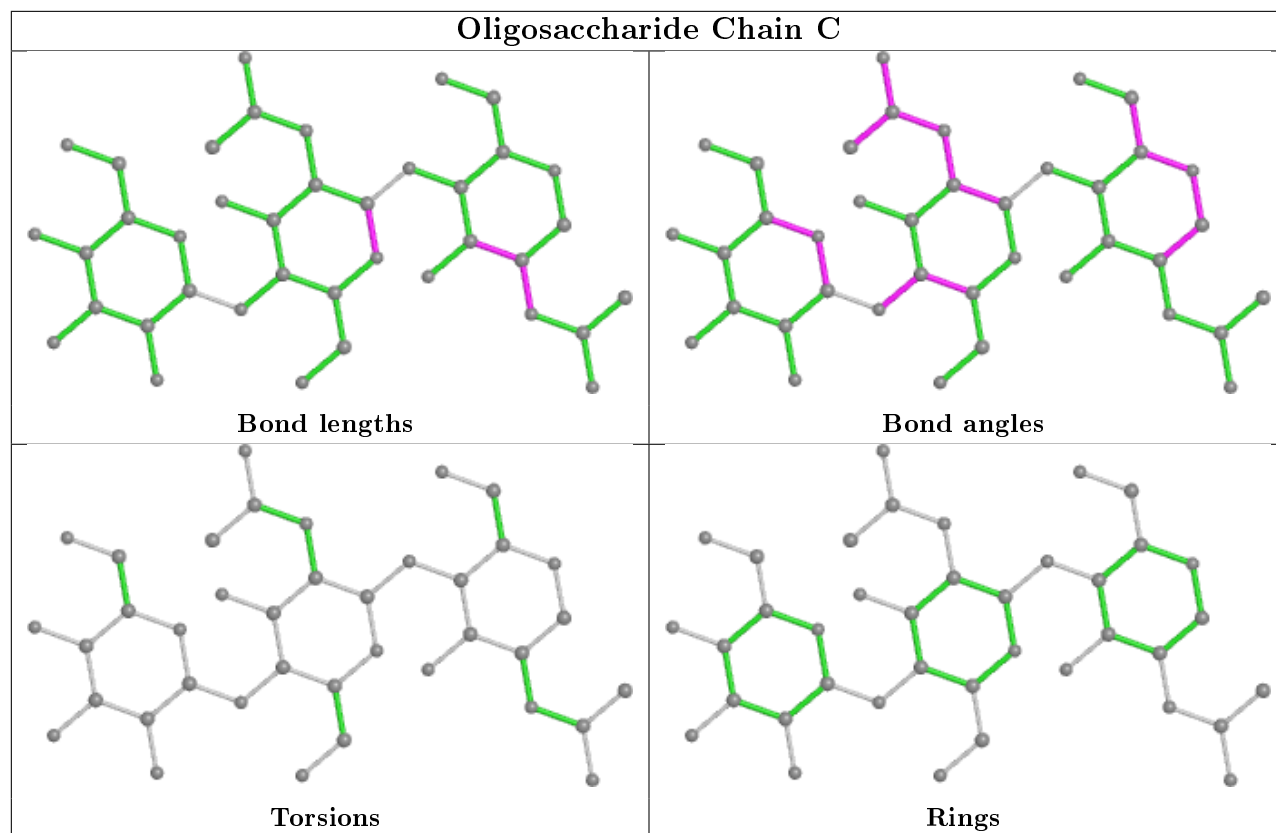
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 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	$\# Z > 2$
8	SCN	B	911	-	1,2,2	0.30	0	0,1,1	0.00	-
6	GOL	A	909	-	5,5,5	0.49	0	5,5,5	1.55	1 (20%)
8	SCN	B	912	-	1,2,2	0.77	0	0,1,1	0.00	-
8	SCN	A	916	-	1,2,2	0.06	0	0,1,1	0.00	-
8	SCN	A	915	-	1,2,2	0.32	0	0,1,1	0.00	-
8	SCN	A	912	-	1,2,2	0.63	0	0,1,1	0.00	-
8	SCN	B	913	-	1,2,2	0.01	0	0,1,1	0.00	-
8	SCN	A	911	-	1,2,2	0.47	0	0,1,1	0.00	-
8	SCN	B	914	-	1,2,2	0.01	0	0,1,1	0.00	-
8	SCN	A	914	-	1,2,2	0.20	0	0,1,1	0.00	-
7	4NY	A	910	-	31,34,34	2.56	5 (16%)	36,48,48	1.85	6 (16%)
7	4NY	B	910	-	31,34,34	2.57	7 (22%)	36,48,48	2.00	9 (25%)
8	SCN	A	917	-	1,2,2	0.06	0	0,1,1	0.00	-
8	SCN	A	913	-	1,2,2	0.41	0	0,1,1	0.00	-
8	SCN	B	915	-	1,2,2	0.27	0	0,1,1	0.00	-
6	GOL	B	909	-	5,5,5	0.50	0	5,5,5	1.49	1 (20%)

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
7	4NY	A	910	-	-	5/12/18/18	0/4/4/4
7	4NY	B	910	-	-	8/12/18/18	0/4/4/4
6	GOL	A	909	-	-	2/4/4/4	-
6	GOL	B	909	-	-	4/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	910	4NY	C23-C6	-11.96	1.26	1.44
7	B	910	4NY	C23-C6	-11.90	1.26	1.44
7	A	910	4NY	C8-C15	3.36	1.49	1.41
7	B	910	4NY	C10-N	-3.07	1.35	1.39
7	B	910	4NY	C8-C15	3.07	1.48	1.41
7	A	910	4NY	C1-C24	2.79	1.50	1.47
7	B	910	4NY	C12-CL	2.78	1.80	1.74
7	B	910	4NY	C1-C24	2.49	1.49	1.47
7	A	910	4NY	C12-CL	2.29	1.79	1.74
7	A	910	4NY	C10-N	-2.26	1.36	1.39
7	B	910	4NY	C16-N	-2.07	1.46	1.49
7	B	910	4NY	C14-C13	2.03	1.40	1.36

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	910	4NY	C5-C4-C6	-7.09	114.05	121.18
7	A	910	4NY	C3-C4-C6	-6.82	114.32	121.18
7	B	910	4NY	C3-C4-C6	4.59	125.81	121.18
7	A	910	4NY	C5-C4-C6	4.57	125.78	121.18
6	B	909	GOL	C3-C2-C1	-3.08	99.72	111.70
7	B	910	4NY	C-C1-C24	-3.01	116.33	120.37
6	A	909	GOL	O3-C3-C2	-2.82	96.66	110.20
7	A	910	4NY	C11-C10-C15	-2.42	117.24	120.92
7	B	910	4NY	C4-C6-C7	-2.41	119.49	123.99
7	A	910	4NY	C2-C1-C24	-2.39	117.16	120.37
7	A	910	4NY	C21-C20-C19	-2.38	119.67	122.83
7	B	910	4NY	C21-C20-C19	-2.35	119.71	122.83
7	B	910	4NY	C18-C19-C20	2.26	120.70	118.36
7	B	910	4NY	C11-C10-C15	-2.20	117.58	120.92
7	B	910	4NY	C13-C14-C15	-2.07	118.25	121.13
7	B	910	4NY	C17-C16-N	-2.05	109.36	112.71
7	A	910	4NY	C18-C19-C20	2.02	120.45	118.36

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	909	GOL	C1-C2-C3-O3
6	B	909	GOL	O2-C2-C3-O3
7	B	910	4NY	C5-C4-C6-C23
6	A	909	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

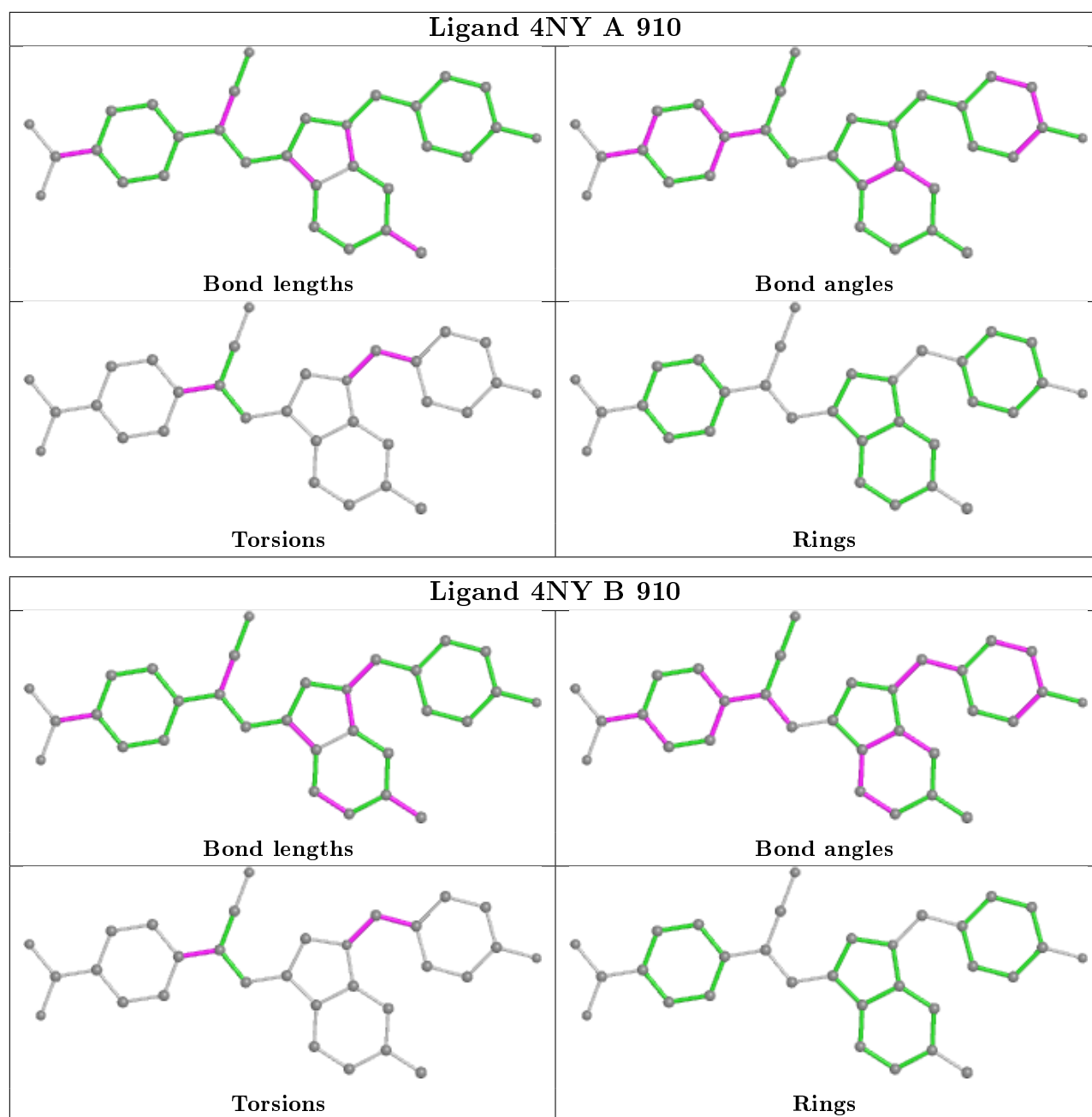
Mol	Chain	Res	Type	Atoms
6	B	909	GOL	O1-C1-C2-O2
7	B	910	4NY	C3-C4-C6-C7
7	B	910	4NY	C5-C4-C6-C7
7	B	910	4NY	C3-C4-C6-C23
7	A	910	4NY	C17-C16-N-C9
7	B	910	4NY	C17-C16-N-C9
7	B	910	4NY	N-C16-C17-C22
7	B	910	4NY	N-C16-C17-C18
7	A	910	4NY	N-C16-C17-C18
7	A	910	4NY	N-C16-C17-C22
7	A	910	4NY	C17-C16-N-C10
7	B	910	4NY	C17-C16-N-C10
6	A	909	GOL	O1-C1-C2-C3
6	B	909	GOL	O1-C1-C2-C3
7	A	910	4NY	C3-C4-C6-C7

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	909	GOL	4	0
8	B	912	SCN	1	0
8	A	915	SCN	1	0
8	B	914	SCN	1	0
7	A	910	4NY	3	0
7	B	910	4NY	5	0
6	B	909	GOL	5	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	754/855 (88%)	0.34	59 (7%) 13 10	20, 37, 64, 81	0
1	B	756/855 (88%)	0.22	49 (6%) 18 15	19, 35, 60, 79	0
All	All	1510/1710 (88%)	0.28	108 (7%) 15 12	19, 36, 63, 81	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	470	PHE	7.1
1	B	643	SER	6.5
1	A	559	LEU	6.3
1	A	657	VAL	6.0
1	B	567	CYS	6.0
1	A	668	LEU	5.3
1	A	471	PHE	5.2
1	A	397	PHE	4.8
1	A	651	SER	4.7
1	B	84	THR	4.6
1	B	642	VAL	4.6
1	B	397	PHE	4.5
1	A	643	SER	4.2
1	A	563	PHE	4.2
1	A	558	TYR	3.9
1	B	58	SER	3.9
1	A	641	GLU	3.9
1	A	642	VAL	3.9
1	A	84	THR	3.8
1	A	104	THR	3.7
1	B	470	PHE	3.6
1	A	74	CYS	3.6
1	B	471	PHE	3.6
1	A	58	SER	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	323	PRO	3.5
1	A	681	LEU	3.5
1	B	401	ALA	3.5
1	A	690	PRO	3.3
1	A	562	ASP	3.3
1	B	167	ILE	3.3
1	A	83	TYR	3.3
1	A	692	ALA	3.3
1	A	555	GLY	3.2
1	A	557	MET	3.2
1	A	367	CYS	3.2
1	B	321	PHE	3.2
1	B	88	HIS	3.2
1	B	591	SER	3.2
1	A	82	SER	3.1
1	A	167	ILE	3.1
1	A	734	ILE	3.1
1	B	168	ILE	3.1
1	A	401	ALA	3.1
1	A	640	ALA	3.0
1	A	561	SER	3.0
1	B	74	CYS	3.0
1	A	560	GLN	3.0
1	B	104	THR	3.0
1	A	318	TYR	2.9
1	B	640	ALA	2.9
1	B	734	ILE	2.9
1	B	357	VAL	2.8
1	B	217[A]	LEU	2.8
1	A	398	SER	2.8
1	B	668	LEU	2.8
1	B	657	VAL	2.8
1	A	564	ASP	2.7
1	B	651	SER	2.7
1	B	75	ARG	2.7
1	B	559	LEU	2.7
1	B	355	ILE	2.7
1	A	759	GLY	2.6
1	B	557	MET	2.6
1	A	399	ASN	2.6
1	B	148	ASP	2.6
1	A	298	HIS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	398	SER	2.5
1	A	217[A]	LEU	2.5
1	B	564	ASP	2.5
1	A	689	SER	2.5
1	B	418	ASP	2.4
1	B	399	ASN	2.4
1	A	736	GLY	2.4
1	B	83	TYR	2.4
1	B	381	ASP	2.4
1	B	400	ASN	2.4
1	A	75	ARG	2.4
1	B	82	SER	2.3
1	B	563	PHE	2.3
1	B	566	GLY	2.3
1	A	632	THR	2.3
1	A	168	ILE	2.3
1	A	137	VAL	2.3
1	A	629	PRO	2.3
1	B	629	PRO	2.3
1	B	736	GLY	2.2
1	B	354	VAL	2.2
1	A	630	LEU	2.2
1	B	652	CYS	2.2
1	B	681	LEU	2.2
1	A	418	ASP	2.2
1	A	652	CYS	2.2
1	A	60	LYS	2.2
1	A	86	CYS	2.2
1	A	400	ASN	2.2
1	B	245	ARG	2.2
1	A	738	ILE	2.2
1	B	771	ILE	2.2
1	A	357	VAL	2.1
1	B	57	GLY	2.1
1	A	539	THR	2.1
1	A	737	PRO	2.1
1	B	735	SER	2.0
1	A	631	TRP	2.0
1	A	556	ILE	2.0
1	A	691	GLU	2.0
1	B	106	ASP	2.0
1	B	632	THR	2.0

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

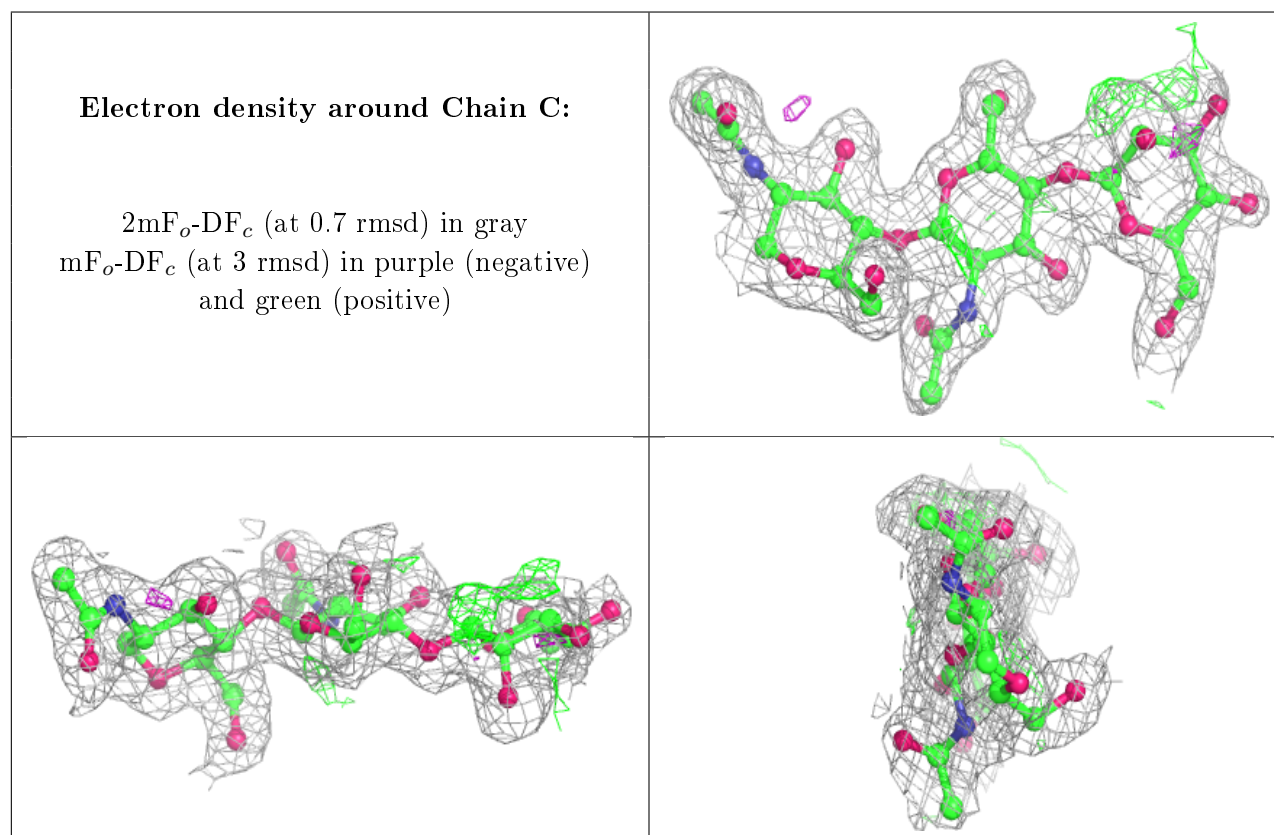
There are no non-standard protein/DNA/RNA residues in this entry.

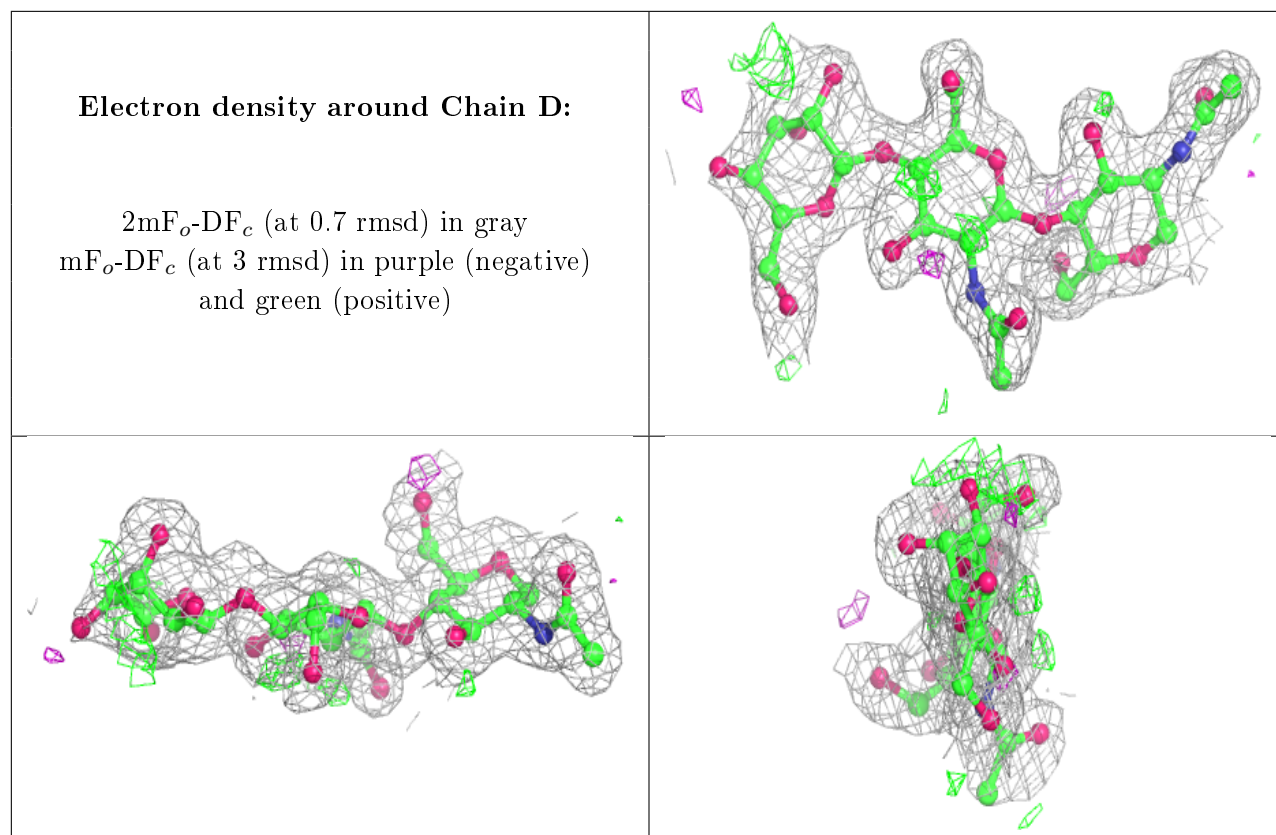
6.3 Carbohydrates [i](#)

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	BMA	C	3	11/12	0.74	0.26	48,54,64,64	0
2	BMA	D	3	11/12	0.85	0.22	53,58,64,69	0
2	NAG	C	2	14/15	0.90	0.14	30,41,45,48	0
2	NAG	D	2	14/15	0.91	0.16	29,38,45,48	0
2	NAG	D	1	14/15	0.95	0.07	21,24,28,31	0
2	NAG	C	1	14/15	0.96	0.07	22,24,27,31	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands ⓘ

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
8	SCN	A	913	3/3	0.83	0.18	55,55,59,67	0
7	4NY	A	910	31/31	0.84	0.15	36,44,63,66	0
7	4NY	B	910	31/31	0.87	0.14	37,46,61,66	0
5	NA	A	907	1/1	0.91	0.07	39,39,39,39	0
8	SCN	B	912	3/3	0.93	0.18	42,42,46,51	0
8	SCN	A	916	3/3	0.93	0.26	50,50,52,55	0
5	NA	B	908	1/1	0.95	0.05	37,37,37,37	0
8	SCN	A	917	3/3	0.95	0.18	54,54,56,56	0
6	GOL	B	909	6/6	0.95	0.14	29,38,39,48	0
6	GOL	A	909	6/6	0.96	0.12	29,35,36,38	0
8	SCN	B	911	3/3	0.96	0.07	37,37,42,43	0
8	SCN	B	913	3/3	0.96	0.14	52,52,55,56	0
8	SCN	A	912	3/3	0.97	0.09	43,43,44,48	0
8	SCN	A	911	3/3	0.97	0.06	40,40,41,45	0

Continued on next page...

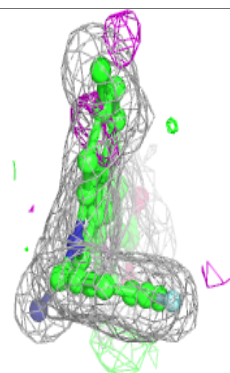
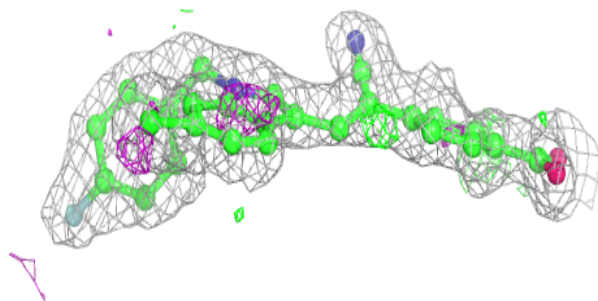
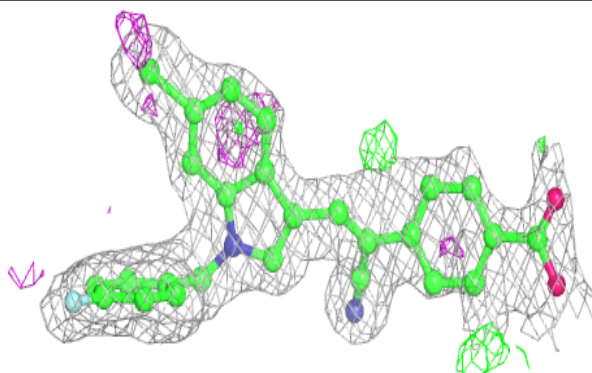
Continued from previous page...

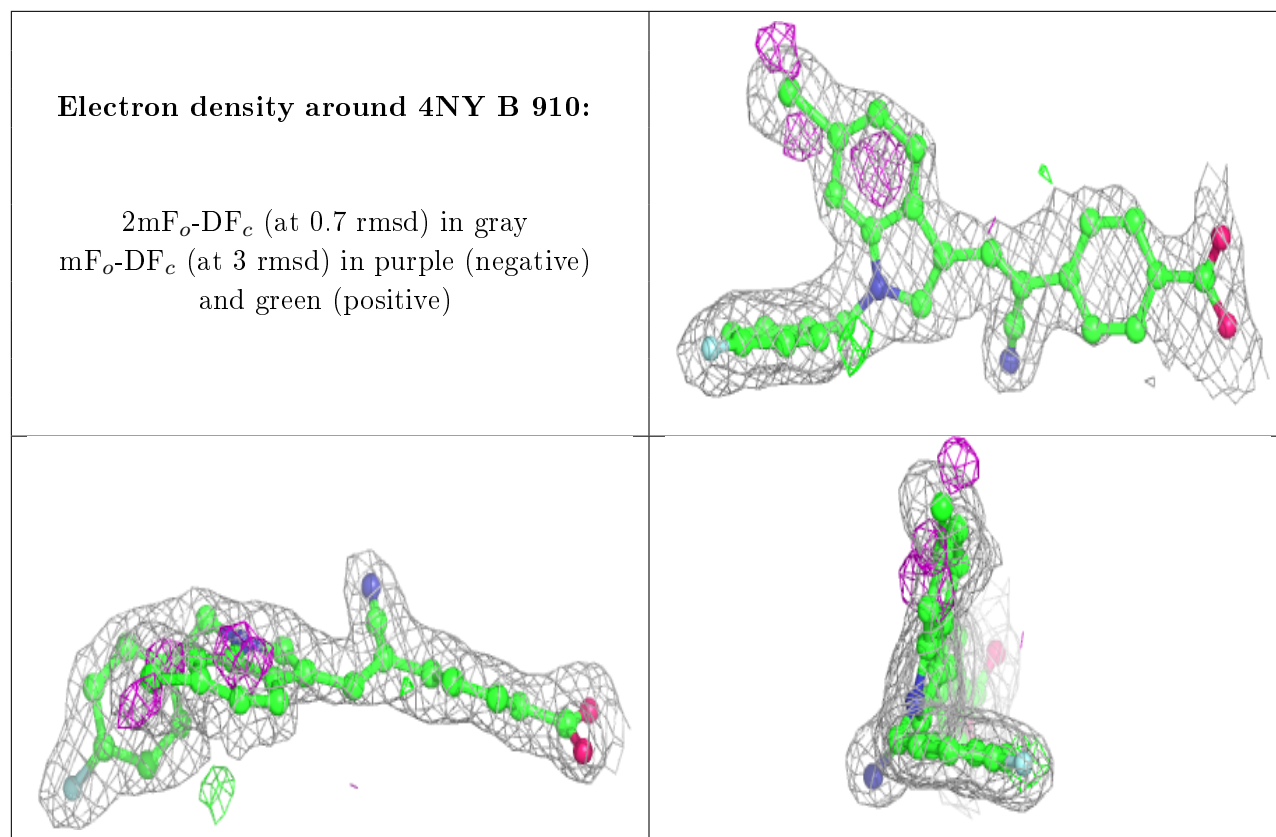
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	SCN	A	915	3/3	0.97	0.07	49,49,50,55	0
5	NA	B	906	1/1	0.97	0.05	34,34,34,34	0
8	SCN	B	915	3/3	0.97	0.09	60,60,65,65	0
8	SCN	A	914	3/3	0.98	0.07	57,57,57,58	0
4	CA	B	907	1/1	0.99	0.04	25,25,25,25	0
3	ZN	A	904	1/1	0.99	0.03	39,39,39,39	0
8	SCN	B	914	3/3	0.99	0.07	45,45,48,51	0
3	ZN	B	904	1/1	0.99	0.02	40,40,40,40	0
5	NA	A	908	1/1	0.99	0.03	31,31,31,31	0
4	CA	A	906	1/1	0.99	0.04	28,28,28,28	0
3	ZN	A	905	1/1	0.99	0.03	34,34,34,34	0
3	ZN	B	905	1/1	1.00	0.05	31,31,31,31	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 4NY A 910:

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.