



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:21 PM UTC

PDB ID : 4ZG6 / pdb_00004zg6
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

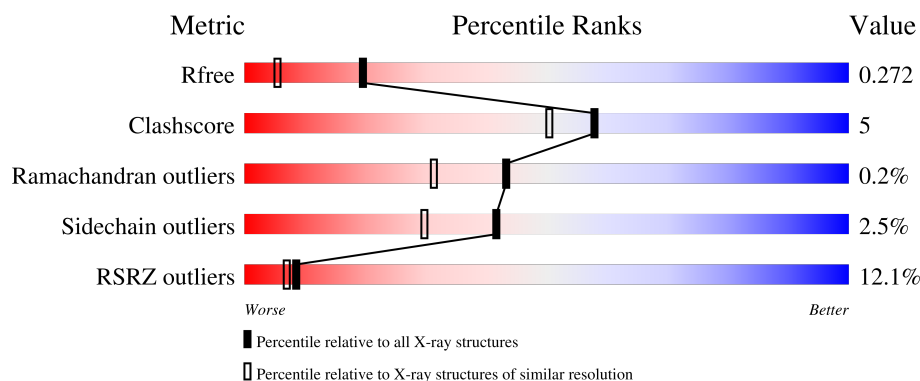
1 Overall quality at a glance

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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	855	13% 77% 9% 12%
1	B	855	8% 82% 6% 12%
2	C	3	100%
2	D	3	67% 33%

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
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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

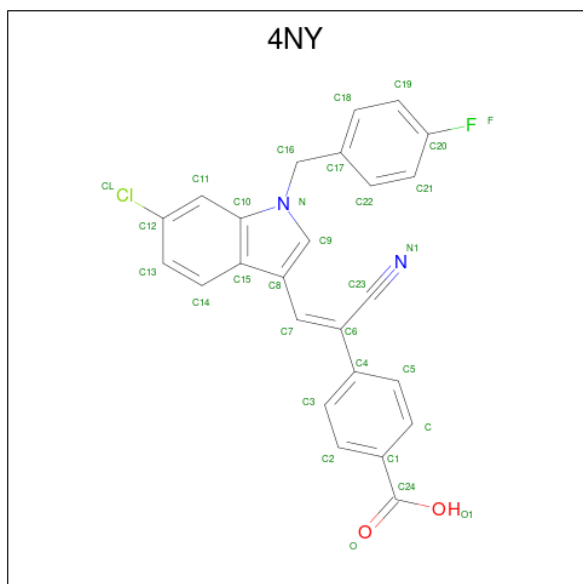
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		
5	B	2	Total	Na	0	0
			2	2		

- Molecule 6 is GLYCEROL (CCD ID: 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 (CCD ID: 4NY) (formula: C₂₅H₁₆ClFN₂O₂).



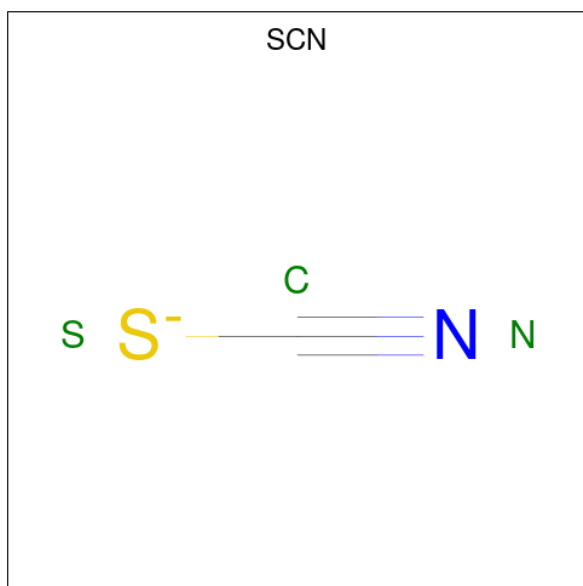
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	Cl	F	N	O	0	0
			31	25	1	1	2	2		

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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 (CCD ID: SCN) (formula: CNS).



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

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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

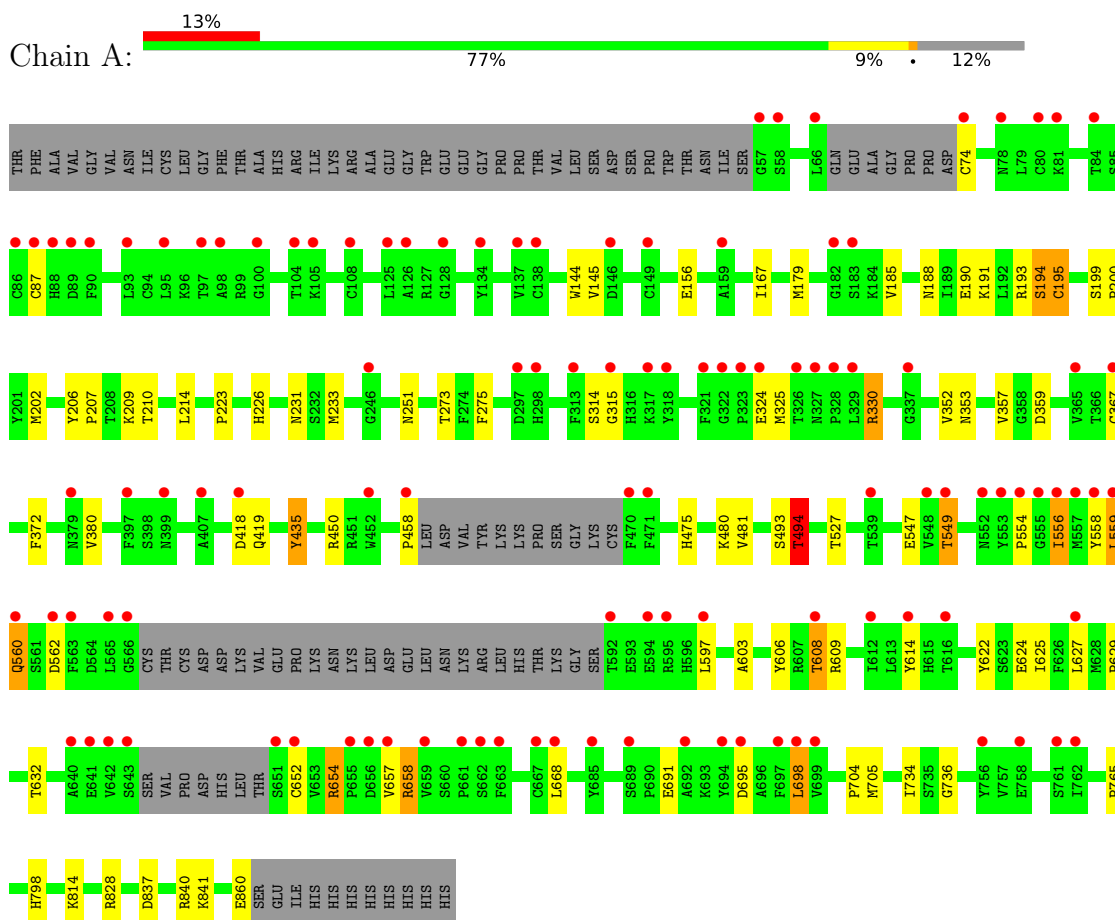
- Molecule 9 is water.

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

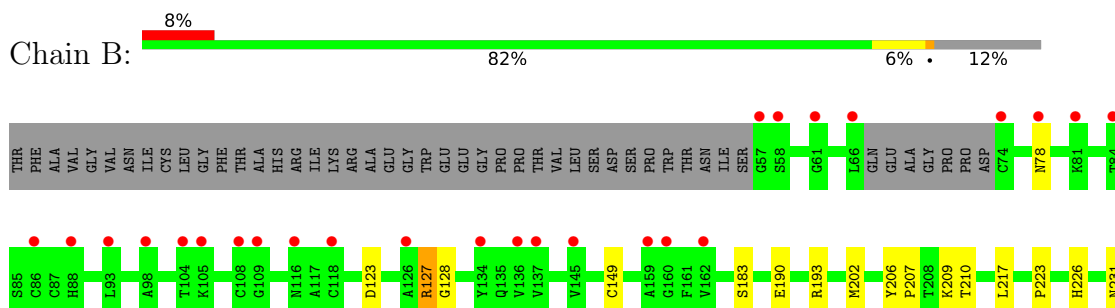
3 Residue-property plots

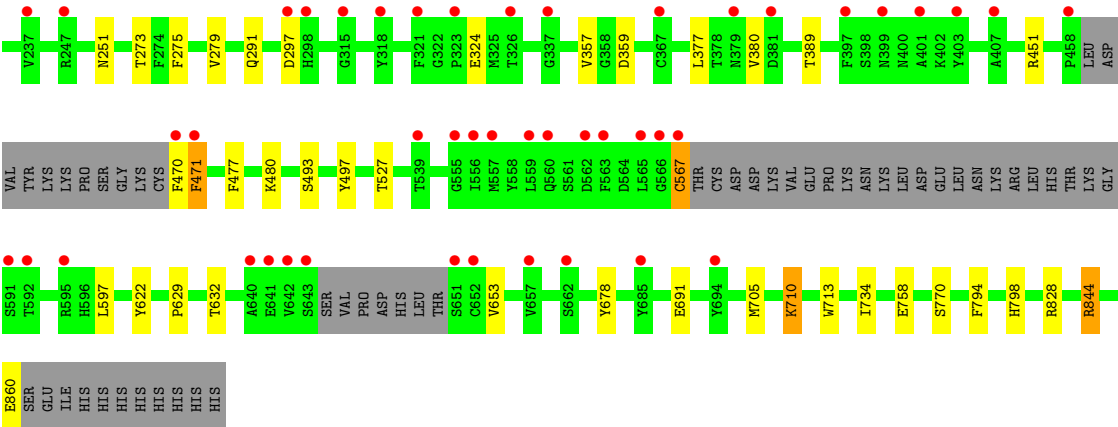
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2





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

Chain C: 100%



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

Chain D: 67% 33%



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 (4.83%)	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)	0.38 , 38.2	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	0.97	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: 4NY, NAG, BMA, CA, NA, ZN, SCN, GOL

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	0.79	3/6195 (0.0%)	0.91	4/8424 (0.0%)
1	B	0.77	0/6203	0.91	2/8433 (0.0%)
All	All	0.78	3/12398 (0.0%)	0.91	6/16857 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	PRO	N-CD	5.63	1.55	1.47
1	A	199	SER	C-O	-5.12	1.18	1.24
1	A	199	SER	C-N	5.01	1.40	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	THR	CB-CA-C	6.34	120.69	109.65
1	A	736	GLY	CA-C-N	5.50	125.97	120.14
1	A	736	GLY	C-N-CA	5.50	125.97	120.14
1	B	297	ASP	N-CA-C	5.35	117.53	111.11
1	A	435	TYR	N-CA-C	5.16	115.82	108.54
1	B	279	VAL	N-CA-C	5.05	116.38	110.62

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	67	0
1	B	6014	0	5668	34	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	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (107) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LYS:HG3	8:A:915:SCN:N	2.00	0.76
1:A:314:SER:C	1:A:325:MET:HE1	2.13	0.73
8:B:912:SCN:S	9:B:1002:HOH:O	2.48	0.70
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217[B]:LEU:HD12	7:B:910:4NY:CL	2.49	0.50
1:A:559:LEU:O	1:A:560:GLN:C	2.55	0.49
1:B:359:ASP:HB3	7:B:910:4NY:CL	2.50	0.49
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:179:MET:HE3	1:A:193:ARG:HD2	1.95	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:315:GLY:N	1:A:325:MET:HE1	2.29	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:202:MET:HE1	1:A:357:VAL:CG2	2.45	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:B:377:LEU:HB2	1:B:380:VAL:HG23	1.99	0.45
1:A:179:MET:HE3	1:A:193:ARG:CD	2.46	0.44
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:B:705:MET:HE1	1:B:713:TRP:CE2	2.54	0.43
1:A:705:MET:HA	1:A:798:HIS:NE2	2.32	0.43
1:A:418:ASP:O	1:A:419:GLN:C	2.62	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:B:202:MET:HE1	1:B:357:VAL:CG2	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	48	34
1	B	752/855 (88%)	725 (96%)	25 (3%)	2 (0%)	36	25
All	All	1503/1710 (88%)	1446 (96%)	54 (4%)	3 (0%)	43	31

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 ⓘ

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%)	632 (96%)	24 (4%)	30	18
1	B	657/772 (85%)	647 (98%)	10 (2%)	57	49
All	All	1313/1544 (85%)	1279 (97%)	34 (3%)	42	28

All (34) 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	380	VAL
1	A	493	SER
1	A	494	THR
1	A	549	THR
1	A	559	LEU
1	A	560	GLN
1	A	597	LEU
1	A	608	THR
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	841	LYS
1	B	127	ARG
1	B	324	GLU
1	B	451	ARG

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Mol	Chain	Res	Type
1	B	493	SER
1	B	567	CYS
1	B	597	LEU
1	B	691	GLU
1	B	710	LYS
1	B	758	GLU
1	B	844	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	ASN
1	A	747	HIS
1	B	119	HIS
1	B	485	GLN

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](#)

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	1.07	2 (14%)	17,19,21	1.29	2 (11%)
2	NAG	C	2	2	14,14,15	0.98	1 (7%)	17,19,21	1.47	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	C	3	2	11,11,12	0.48	0	15,15,17	0.80	1 (6%)
2	NAG	D	1	1,2	14,14,15	0.95	0	17,19,21	0.89	0
2	NAG	D	2	2	14,14,15	0.79	1 (7%)	17,19,21	1.60	4 (23%)
2	BMA	D	3	2	11,11,12	0.41	0	15,15,17	0.87	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	-	1/6/23/26	0/1/1/1
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	-3.29	1.38	1.43
2	D	2	NAG	O5-C1	-2.56	1.39	1.43
2	C	1	NAG	C2-N2	-2.14	1.42	1.46
2	C	1	NAG	C3-C2	2.04	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	-3.72	105.54	111.29
2	D	2	NAG	C1-O5-C5	3.44	116.79	112.19
2	C	2	NAG	O7-C7-C8	-2.93	116.83	122.05
2	C	2	NAG	C8-C7-N2	2.77	120.70	116.12
2	D	2	NAG	C1-C2-N2	-2.66	106.24	110.43
2	D	2	NAG	O4-C4-C5	-2.62	102.87	109.32
2	C	2	NAG	C1-C2-N2	-2.54	106.43	110.43
2	C	3	BMA	C1-O5-C5	2.52	115.57	112.19
2	C	2	NAG	O4-C4-C5	-2.35	103.55	109.32
2	D	2	NAG	O7-C7-C8	-2.28	117.99	122.05
2	C	1	NAG	C2-N2-C7	2.02	125.60	122.90

There are no chirality outliers.

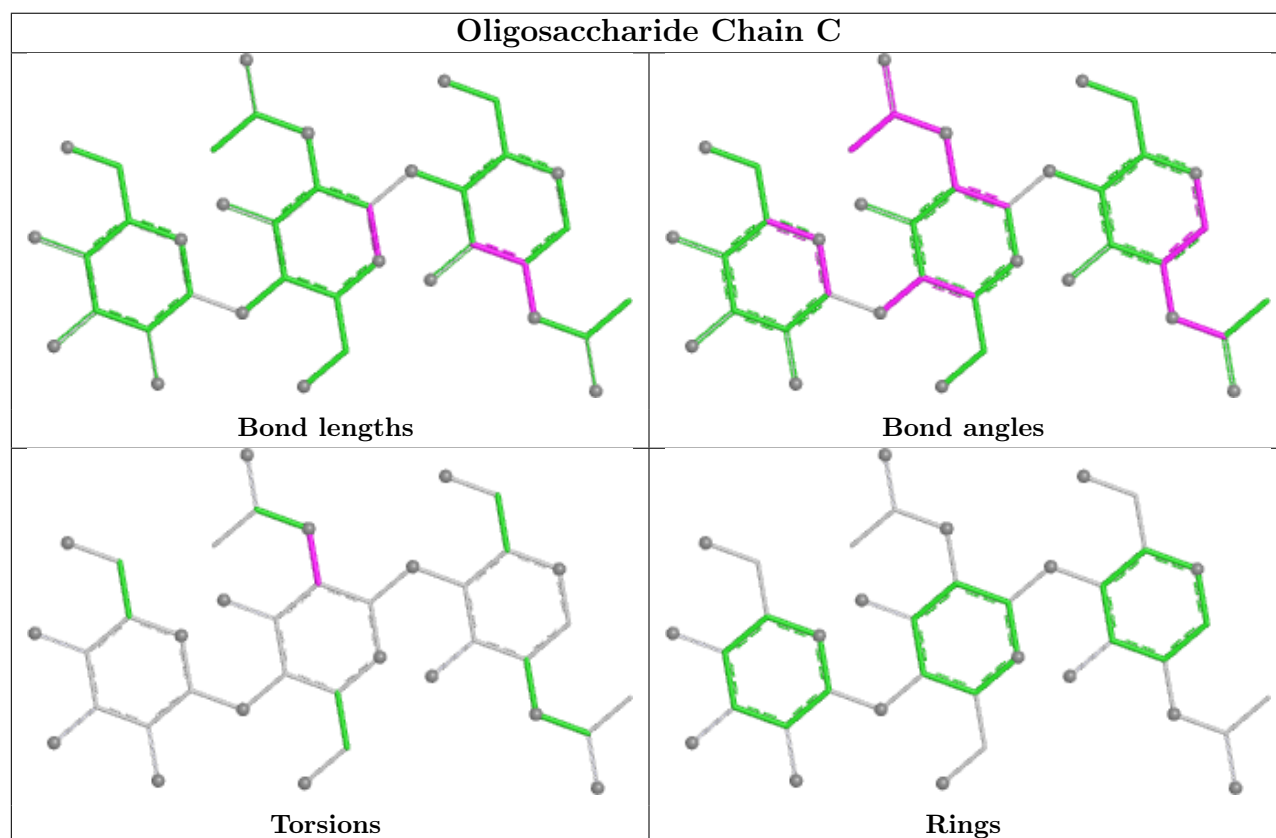
All (1) torsion outliers are listed below:

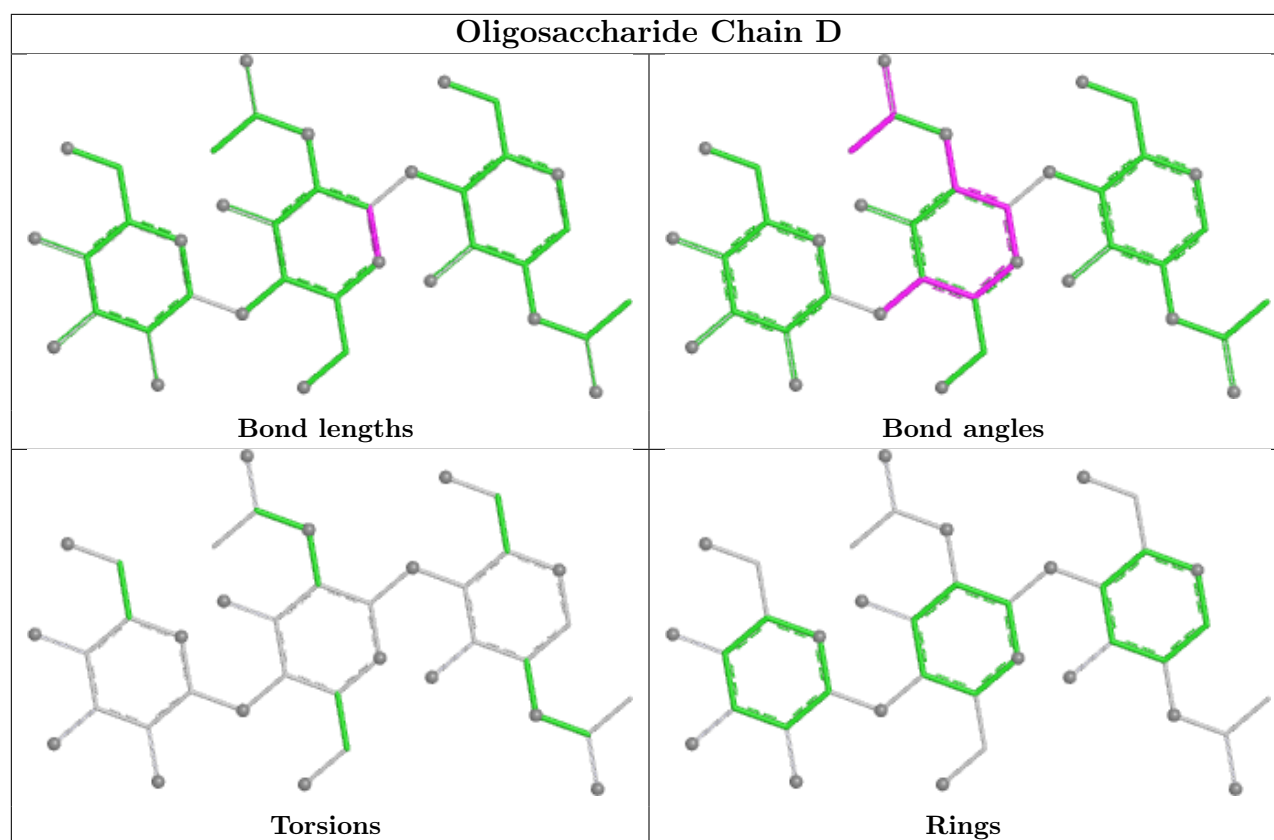
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C1-C2-N2-C7

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 [i](#)

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	A	917	-	1,2,2	0.05	0	0,1,1	-	-
7	4NY	B	910	-	34,34,34	2.41	5 (14%)	47,48,48	2.68	17 (36%)
8	SCN	B	913	-	1,2,2	0.02	0	0,1,1	-	-
8	SCN	A	912	-	1,2,2	0.62	0	0,1,1	-	-
6	GOL	A	909	-	5,5,5	0.53	0	5,5,5	1.67	2 (40%)
7	4NY	A	910	-	34,34,34	2.46	5 (14%)	47,48,48	2.41	12 (25%)
8	SCN	A	916	-	1,2,2	0.05	0	0,1,1	-	-
8	SCN	B	915	-	1,2,2	0.27	0	0,1,1	-	-
8	SCN	B	914	-	1,2,2	0.02	0	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SCN	A	911	-	1,2,2	0.47	0	0,1,1	-	-
8	SCN	B	911	-	1,2,2	0.30	0	0,1,1	-	-
8	SCN	A	913	-	1,2,2	0.41	0	0,1,1	-	-
8	SCN	B	912	-	1,2,2	0.76	0	0,1,1	-	-
8	SCN	A	915	-	1,2,2	0.32	0	0,1,1	-	-
8	SCN	A	914	-	1,2,2	0.20	0	0,1,1	-	-
6	GOL	B	909	-	5,5,5	0.52	0	5,5,5	1.59	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
6	GOL	A	909	-	-	1/4/4/4	-
7	4NY	B	910	-	-	7/18/18/18	0/4/4/4
7	4NY	A	910	-	-	1/18/18/18	0/4/4/4
6	GOL	B	909	-	-	3/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	910	4NY	C23-C6	-11.56	1.26	1.44
7	B	910	4NY	C23-C6	-11.51	1.26	1.44
7	A	910	4NY	C15-C10	5.43	1.48	1.41
7	B	910	4NY	C15-C10	5.06	1.47	1.41
7	A	910	4NY	C15-C8	2.91	1.49	1.45
7	B	910	4NY	C12-CL	2.62	1.80	1.74
7	A	910	4NY	C7-C8	2.54	1.51	1.43
7	B	910	4NY	C15-C8	2.41	1.48	1.45
7	B	910	4NY	C7-C8	2.17	1.49	1.43
7	A	910	4NY	C12-CL	2.16	1.79	1.74

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	910	4NY	C8-C9-N	-7.98	107.25	110.62
7	B	910	4NY	C10-N-C9	7.18	112.78	108.49
7	B	910	4NY	C10-C15-C8	-6.68	102.00	106.79
7	A	910	4NY	C8-C9-N	-6.52	107.87	110.62
7	A	910	4NY	C10-C15-C8	-6.32	102.26	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	910	4NY	C10-N-C9	5.95	112.04	108.49
7	B	910	4NY	C5-C4-C6	-5.93	114.05	121.20
7	A	910	4NY	C3-C4-C6	-5.71	114.32	121.20
7	B	910	4NY	C15-C8-C9	4.16	109.71	106.28
7	B	910	4NY	C3-C4-C6	3.83	125.81	121.20
7	A	910	4NY	C5-C4-C6	3.81	125.78	121.20
7	A	910	4NY	C11-C10-C15	-3.74	117.24	122.29
7	B	910	4NY	C11-C10-C15	-3.49	117.58	122.29
7	A	910	4NY	C15-C8-C9	3.47	109.14	106.28
7	B	910	4NY	C7-C6-C23	3.44	124.72	120.18
7	A	910	4NY	C7-C6-C23	3.31	124.53	120.18
6	B	909	GOL	C3-C2-C1	-3.29	99.72	111.80
6	A	909	GOL	O3-C3-C2	-3.05	96.66	110.38
7	B	910	4NY	C4-C6-C7	-3.02	119.49	124.14
7	A	910	4NY	C21-C20-C19	-2.39	119.67	122.80
7	B	910	4NY	C21-C20-C19	-2.36	119.71	122.80
7	A	910	4NY	C16-N-C10	-2.31	122.81	126.13
7	B	910	4NY	C18-C19-C20	2.26	120.70	118.38
7	B	910	4NY	C17-C16-N	-2.25	109.36	112.78
7	B	910	4NY	C16-N-C10	-2.22	122.94	126.13
6	A	909	GOL	C3-C2-C1	-2.07	104.21	111.80
7	B	910	4NY	C14-C15-C10	2.05	121.60	119.24
7	B	910	4NY	C-C1-C24	-2.04	116.33	120.37
7	B	910	4NY	C14-C13-C12	2.03	121.29	119.24
7	A	910	4NY	C18-C19-C20	2.02	120.45	118.38
7	B	910	4NY	C9-C8-C7	-2.02	126.42	129.52
7	A	910	4NY	C9-C8-C7	-2.01	126.43	129.52

There are no chirality outliers.

All (12) 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
6	A	909	GOL	O1-C1-C2-O2
6	B	909	GOL	O1-C1-C2-O2
7	B	910	4NY	C5-C4-C6-C7
7	B	910	4NY	C3-C4-C6-C7
7	B	910	4NY	C5-C4-C6-C23
7	B	910	4NY	C3-C4-C6-C23
7	B	910	4NY	C-C1-C24-O
7	B	910	4NY	C2-C1-C24-O

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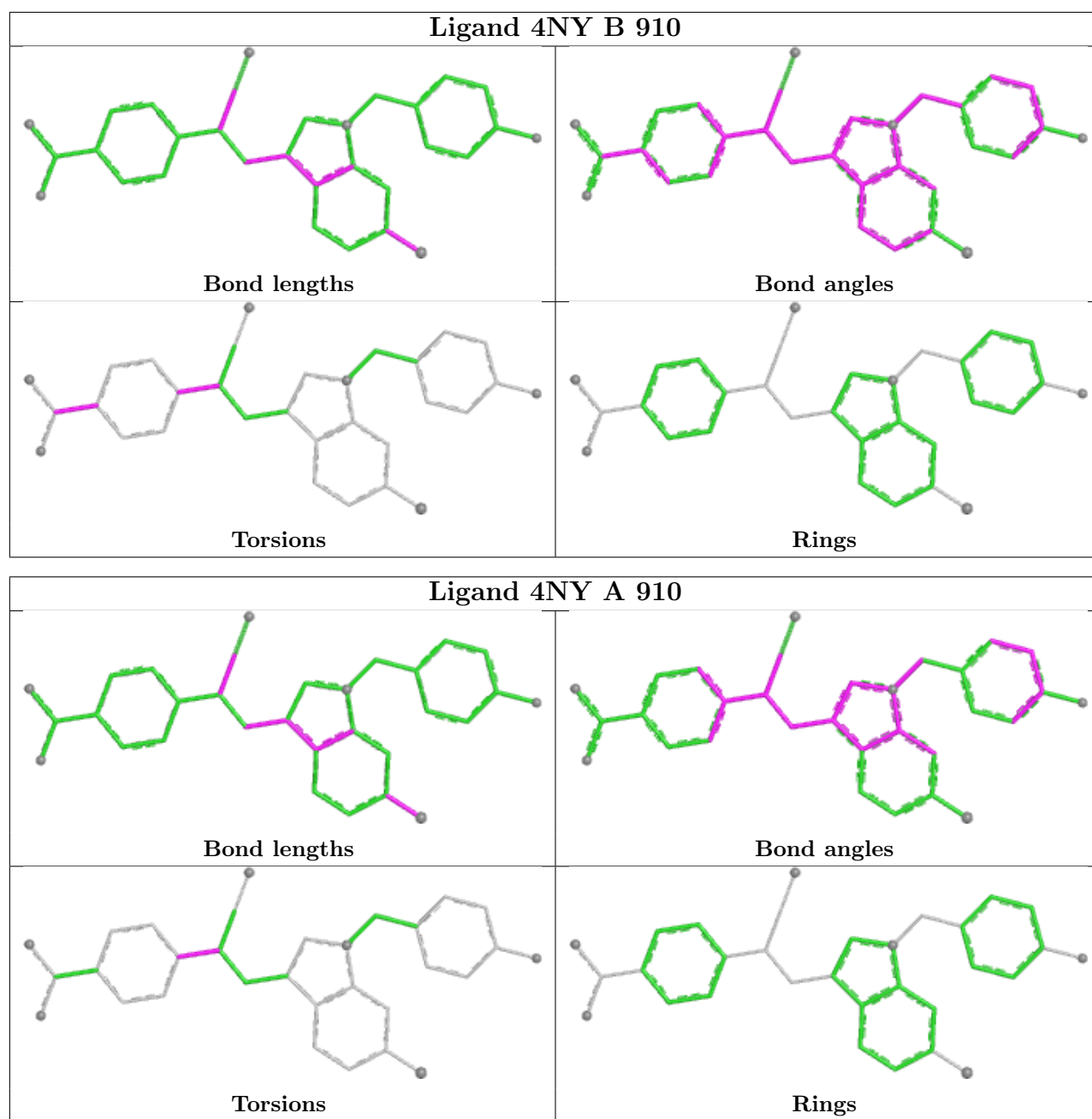
Mol	Chain	Res	Type	Atoms
7	A	910	4NY	C3-C4-C6-C7
7	B	910	4NY	C-C1-C24-O1

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	910	4NY	5	0
6	A	909	GOL	4	0
7	A	910	4NY	3	0
8	B	914	SCN	1	0
8	B	912	SCN	1	0
8	A	915	SCN	1	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%)	0.86	111 (14%) 6 4	14, 37, 64, 81	7 (0%)
1	B	756/855 (88%)	0.65	71 (9%) 14 12	14, 35, 60, 79	6 (0%)
All	All	1510/1710 (88%)	0.75	182 (12%) 8 7	14, 36, 63, 81	13 (0%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	567	CYS	5.6
1	A	657	VAL	5.5
1	A	556	ILE	5.5
1	B	57	GLY	5.2
1	B	643	SER	5.2
1	B	78	ASN	4.9
1	A	58	SER	4.9
1	A	471	PHE	4.6
1	A	74	CYS	4.5
1	A	399	ASN	4.5
1	B	642	VAL	4.2
1	A	88	HIS	4.1
1	A	326	THR	4.0
1	A	104	THR	3.9
1	A	566	GLY	3.9
1	B	565	LEU	3.8
1	A	317	LYS	3.8
1	B	126	ALA	3.8
1	B	105	LYS	3.7
1	B	556	ILE	3.7
1	A	57	GLY	3.7
1	A	323	PRO	3.7
1	A	315	GLY	3.7
1	A	557	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	656	ASP	3.7
1	A	84	THR	3.7
1	B	84	THR	3.7
1	A	559	LEU	3.6
1	A	692	ALA	3.6
1	A	367	CYS	3.6
1	B	471	PHE	3.6
1	A	685	TYR	3.6
1	B	397	PHE	3.6
1	A	318	TYR	3.6
1	A	105	LYS	3.5
1	B	321	PHE	3.5
1	A	95	LEU	3.5
1	A	643	SER	3.4
1	A	549	THR	3.4
1	A	470	PHE	3.4
1	A	563	PHE	3.4
1	A	246	GLY	3.3
1	A	565	LEU	3.3
1	B	104	THR	3.3
1	A	321	PHE	3.3
1	B	592	THR	3.2
1	B	399	ASN	3.2
1	B	159	ALA	3.2
1	A	555	GLY	3.2
1	A	108	CYS	3.2
1	A	93	LEU	3.2
1	A	651	SER	3.2
1	A	659	VAL	3.1
1	B	470	PHE	3.1
1	A	694	TYR	3.1
1	A	397	PHE	3.1
1	A	592	THR	3.1
1	B	651	SER	3.1
1	B	559	LEU	3.0
1	B	563	PHE	3.0
1	B	58	SER	3.0
1	B	662	SER	3.0
1	B	81	LYS	3.0
1	A	595	ARG	2.9
1	B	109	GLY	2.9
1	A	298	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	554	PRO	2.9
1	A	86	CYS	2.9
1	B	337	GLY	2.9
1	A	328	PRO	2.9
1	A	458	PRO	2.9
1	A	126	ALA	2.9
1	A	87	CYS	2.9
1	A	652	CYS	2.9
1	A	324	GLU	2.8
1	A	662	SER	2.8
1	B	539	THR	2.8
1	B	557	MET	2.8
1	B	694	TYR	2.7
1	B	595	ARG	2.7
1	B	315	GLY	2.7
1	A	539	THR	2.7
1	A	663	PHE	2.7
1	B	86	CYS	2.7
1	B	108	CYS	2.7
1	A	698	LEU	2.7
1	B	66	LEU	2.7
1	A	642	VAL	2.7
1	B	401	ALA	2.6
1	A	329	LEU	2.6
1	B	657	VAL	2.6
1	A	667	CYS	2.6
1	B	652	CYS	2.6
1	B	318	TYR	2.6
1	A	562	ASP	2.6
1	A	641	GLU	2.6
1	A	98	ALA	2.6
1	A	183	SER	2.6
1	A	327	ASN	2.6
1	B	145	VAL	2.5
1	B	458	PRO	2.5
1	A	100	GLY	2.5
1	A	137	VAL	2.5
1	B	326	THR	2.5
1	B	74	CYS	2.5
1	B	134	TYR	2.5
1	A	125	LEU	2.5
1	A	627	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	88	HIS	2.5
1	B	93	LEU	2.4
1	B	641	GLU	2.4
1	A	548	VAL	2.4
1	A	379	ASN	2.4
1	B	379	ASN	2.4
1	A	558	TYR	2.4
1	A	697	PHE	2.4
1	A	297	ASP	2.4
1	A	616	THR	2.4
1	A	78	ASN	2.4
1	A	322	GLY	2.4
1	A	138	CYS	2.4
1	B	298	HIS	2.4
1	A	337	GLY	2.4
1	B	566	GLY	2.4
1	A	695	ASP	2.3
1	B	381	ASP	2.3
1	A	134	TYR	2.3
1	A	762	ILE	2.3
1	A	761	SER	2.3
1	A	560	GLN	2.3
1	B	685	TYR	2.3
1	A	407	ALA	2.3
1	A	655	PRO	2.3
1	A	365	VAL	2.3
1	A	90	PHE	2.3
1	B	403	TYR	2.3
1	B	323	PRO	2.3
1	B	61	GLY	2.3
1	B	137	VAL	2.3
1	B	162	VAL	2.3
1	A	80	CYS	2.3
1	B	247	ARG	2.2
1	B	98	ALA	2.2
1	B	407	ALA	2.2
1	B	116	ASN	2.2
1	A	97	THR	2.2
1	A	608	THR	2.2
1	B	160	GLY	2.2
1	B	555	GLY	2.2
1	B	640	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	612	ILE	2.2
1	A	81	LYS	2.2
1	B	367	CYS	2.2
1	B	560	GLN	2.2
1	A	418	ASP	2.2
1	A	661	PRO	2.2
1	A	313	PHE	2.2
1	A	640	ALA	2.2
1	A	553	TYR	2.1
1	A	758	GLU	2.1
1	A	452	TRP	2.1
1	A	66	LEU	2.1
1	A	668	LEU	2.1
1	A	159	ALA	2.1
1	A	552	ASN	2.1
1	A	89	ASP	2.1
1	B	591	SER	2.1
1	B	136	VAL	2.1
1	A	756	TYR	2.1
1	B	297	ASP	2.1
1	A	689	SER	2.1
1	A	182	GLY	2.1
1	A	699	VAL	2.1
1	A	149	CYS	2.1
1	A	597	LEU	2.1
1	B	562	ASP	2.1
1	A	594	GLU	2.0
1	B	237	VAL	2.0
1	B	118	CYS	2.0
1	A	146	ASP	2.0
1	A	128	GLY	2.0
1	A	614	TYR	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.

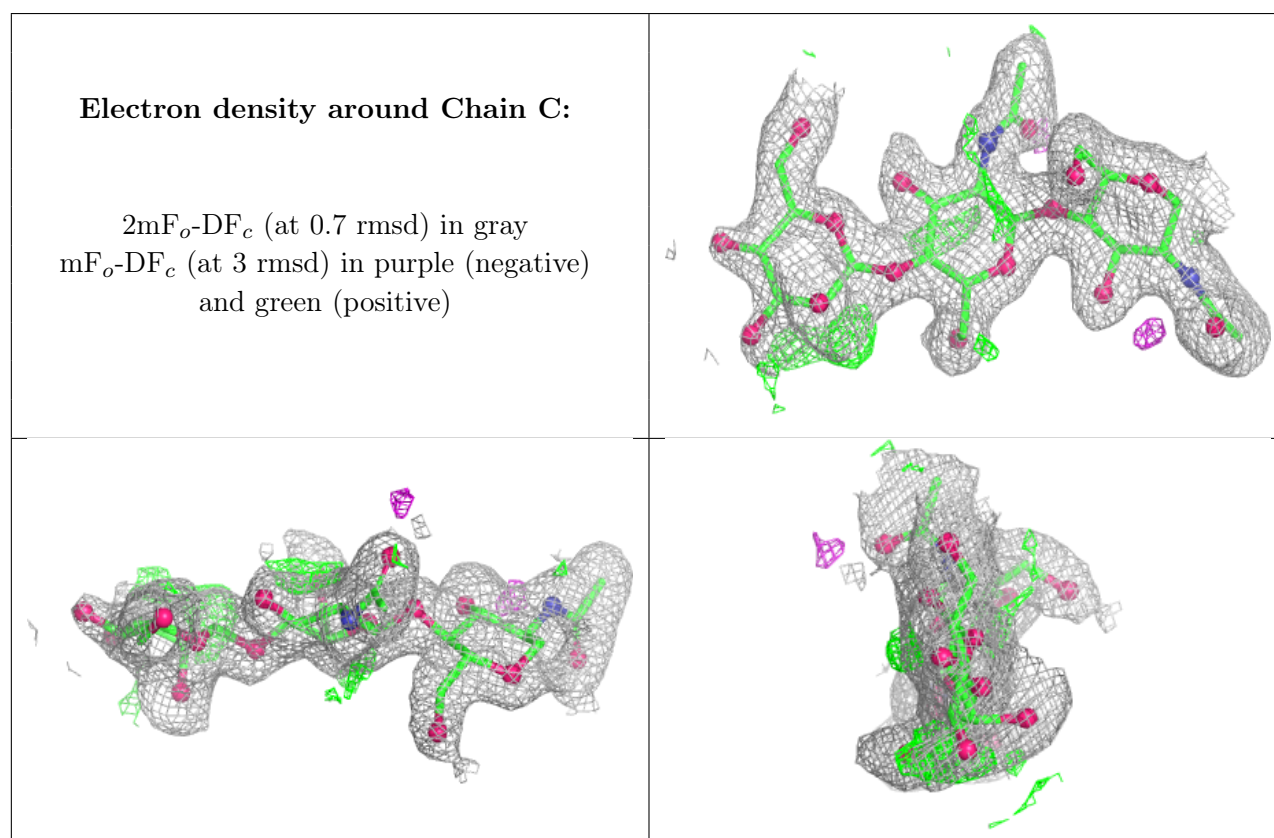
6.3 Carbohydrates [i](#)

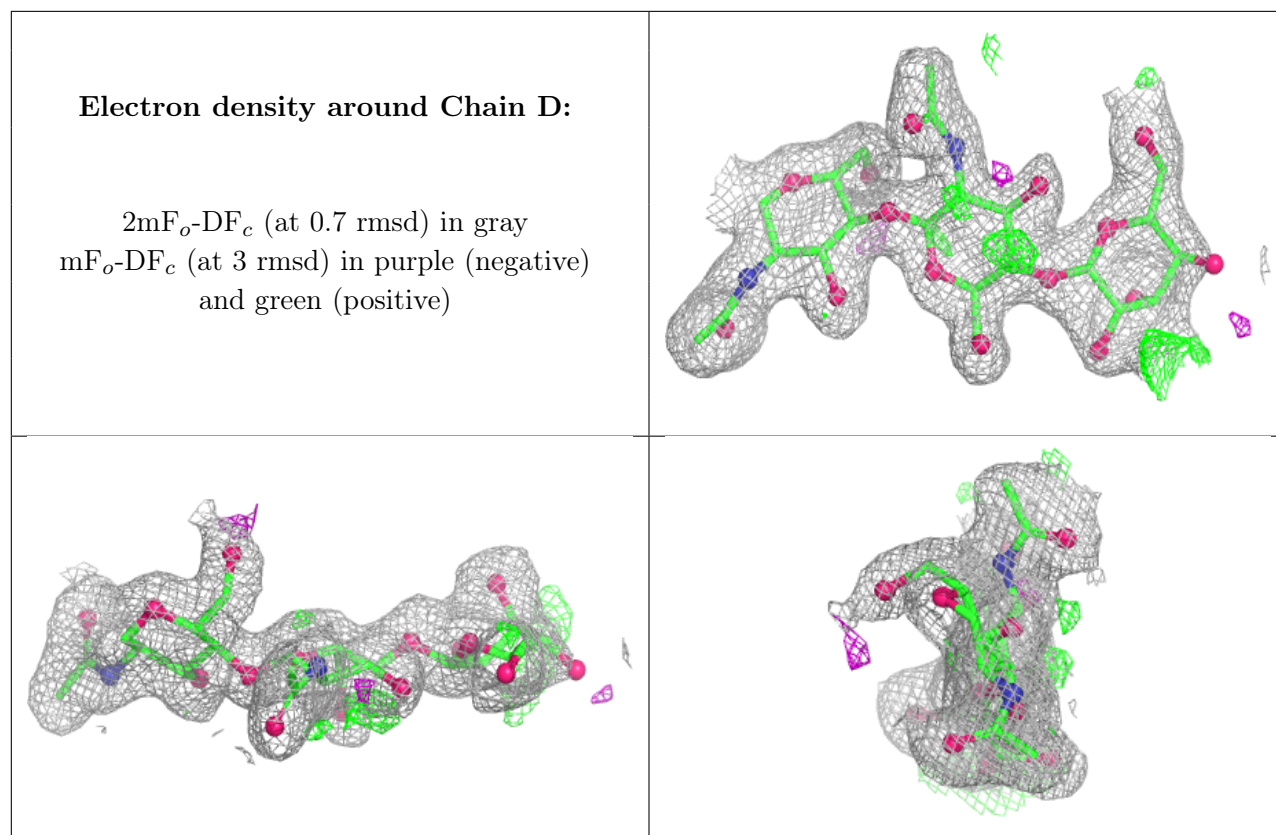
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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(Å ²)	Q<0.9
2	BMA	C	3	11/12	0.70	0.14	48,54,64,64	0
2	BMA	D	3	11/12	0.78	0.12	53,58,64,69	0
2	NAG	C	2	14/15	0.84	0.12	30,41,45,48	0
2	NAG	D	2	14/15	0.87	0.12	29,38,45,48	0
2	NAG	C	1	14/15	0.95	0.08	22,24,27,31	0
2	NAG	D	1	14/15	0.95	0.07	21,24,28,31	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 [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.

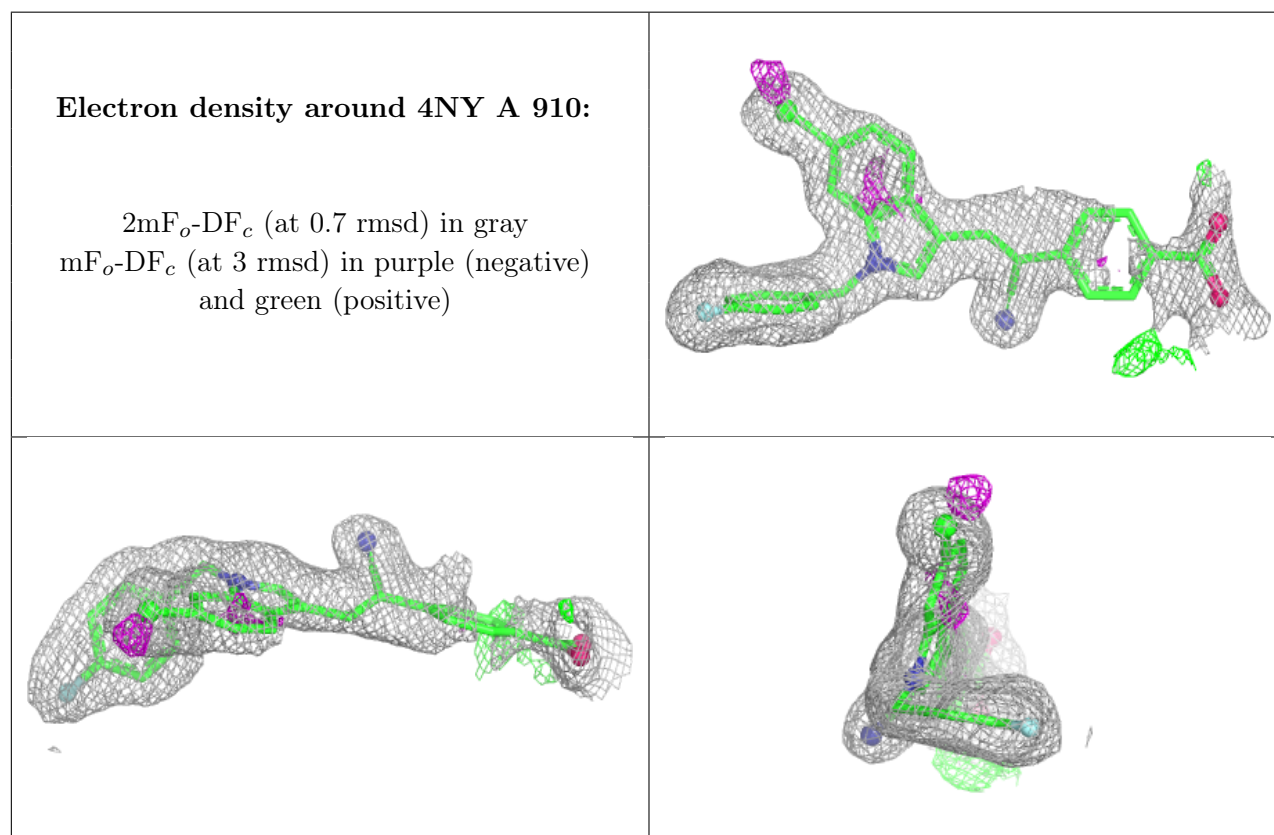
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SCN	A	913	3/3	0.85	0.16	55,55,59,67	0
8	SCN	A	916	3/3	0.86	0.23	50,50,52,55	0
6	GOL	A	909	6/6	0.88	0.14	29,35,36,38	0
7	4NY	A	910	31/31	0.89	0.12	36,44,63,66	0
6	GOL	B	909	6/6	0.90	0.15	29,38,39,48	0
7	4NY	B	910	31/31	0.90	0.11	37,46,61,66	0
8	SCN	A	917	3/3	0.90	0.18	54,54,56,56	0
5	NA	A	907	1/1	0.91	0.08	39,39,39,39	0
8	SCN	A	914	3/3	0.92	0.12	57,57,57,58	0
8	SCN	A	915	3/3	0.92	0.15	49,49,50,55	0
8	SCN	B	912	3/3	0.92	0.15	42,42,46,51	0
8	SCN	B	915	3/3	0.92	0.13	60,60,65,65	0
8	SCN	B	913	3/3	0.93	0.17	52,52,55,56	0
5	NA	B	908	1/1	0.93	0.06	37,37,37,37	0

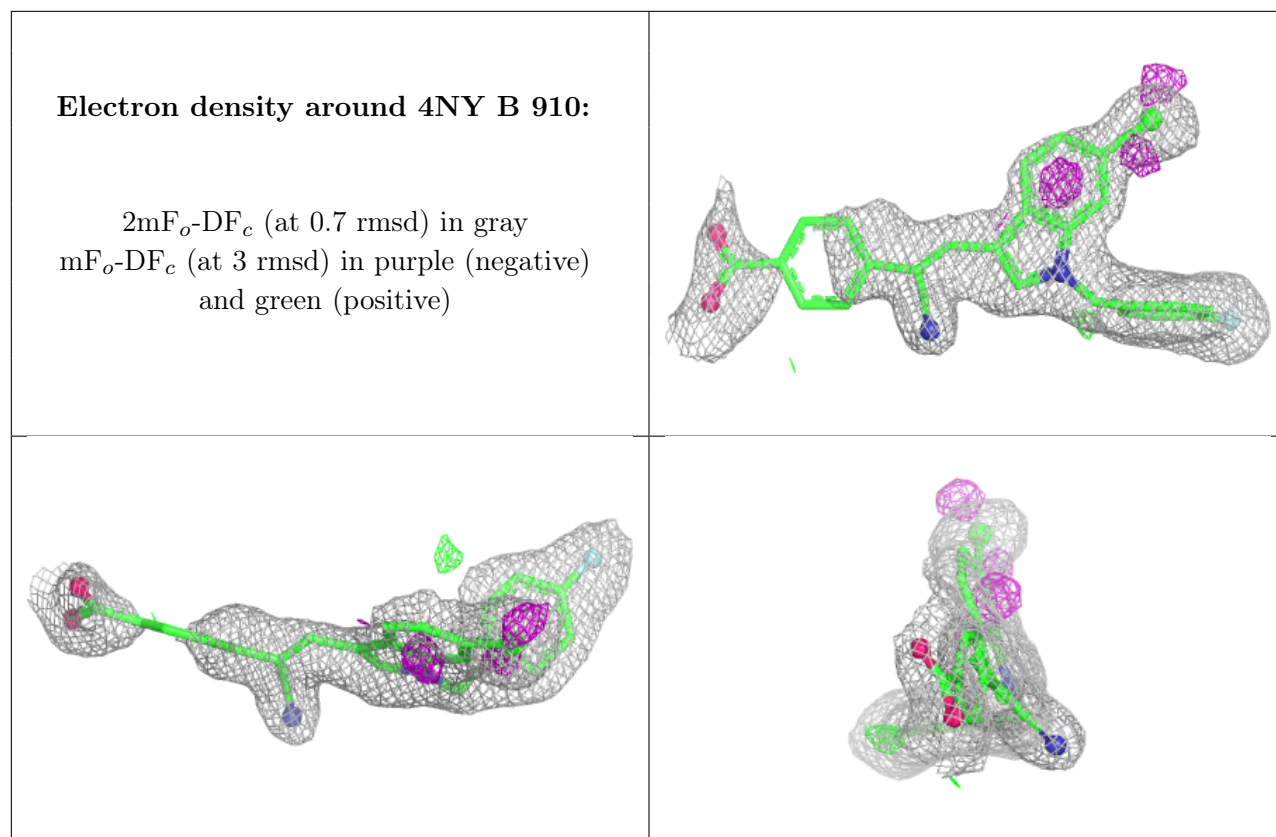
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SCN	A	912	3/3	0.94	0.13	43,43,44,48	0
8	SCN	B	914	3/3	0.95	0.15	45,45,48,51	0
8	SCN	B	911	3/3	0.95	0.11	37,37,42,43	0
8	SCN	A	911	3/3	0.96	0.10	40,40,41,45	0
5	NA	B	906	1/1	0.97	0.06	34,34,34,34	0
4	CA	B	907	1/1	0.97	0.05	25,25,25,25	0
5	NA	A	908	1/1	0.97	0.06	31,31,31,31	0
4	CA	A	906	1/1	0.98	0.04	28,28,28,28	0
3	ZN	B	904	1/1	0.99	0.09	40,40,40,40	0
3	ZN	B	905	1/1	0.99	0.03	31,31,31,31	0
3	ZN	A	904	1/1	0.99	0.12	39,39,39,39	0
3	ZN	A	905	1/1	0.99	0.05	34,34,34,34	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.