



Full wwPDB X-ray Structure Validation Report

Dec 12, 2024 – 04:07 PM EST

PDB ID : 7G61
Title : Crystal Structure of rat Autotaxin in complex with (2S)-6-chloro-2-[[6-(oxetan-3-ylsulfonyl)-5,7-dihydropyrrolo[3,4-d]pyrimidin-2-yl]amino]-2,3-dihydro-1H-indene-4-carbonitrile, i.e. SMILES N#Cc1cc(Cl)cc2c1C[C@H](C2)Nc1nc2c(cn1)CN(C2)S(=O)(=O)C1COC1 with IC50=0.00466106 microM
Authors : Stihle, M.; Benz, J.; Hunziker, D.; Pinard, E.; Rudolph, M.G.
Deposited on : 2023-06-05
Resolution : 1.83 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

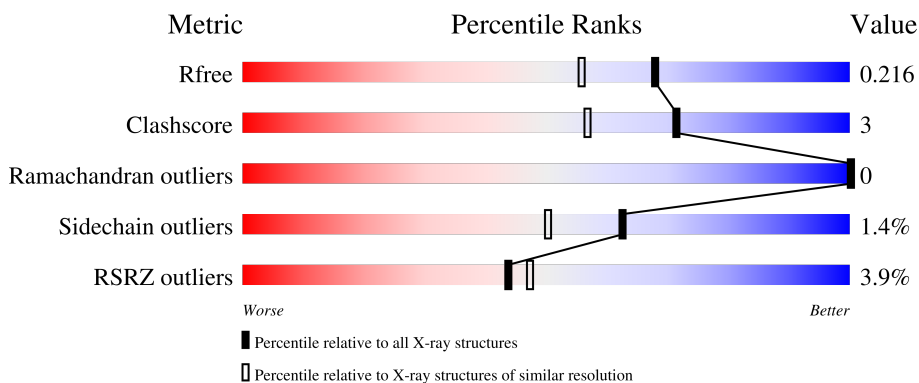
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


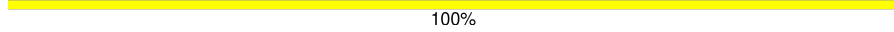
The reported resolution of this entry is 1.83 Å.

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}	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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	846	
2	B	8	

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 7603 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.

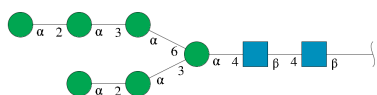
- Molecule 1 is a protein called Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	804	6664	4244	1138	1226	56	0	30	0

There are 14 discrepancies between the modelled and reference sequences:

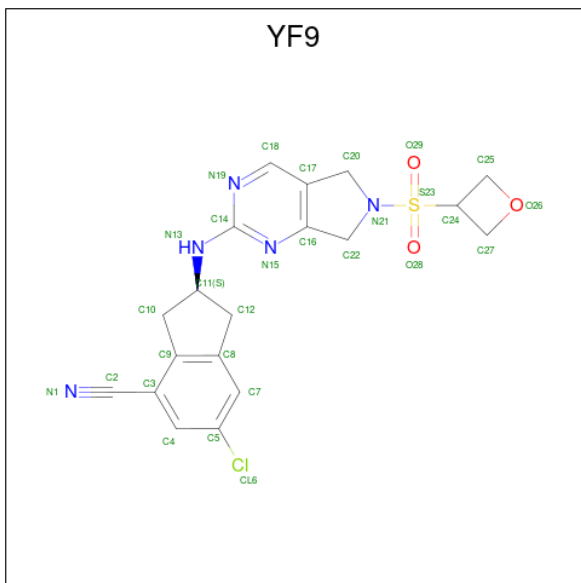
Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ALA	ASN	engineered mutation	UNP Q64610
A	410	ALA	ASN	engineered mutation	UNP Q64610
A	591	THR	ARG	engineered mutation	UNP Q64610
A	863	GLY	-	expression tag	UNP Q64610
A	864	GLY	-	expression tag	UNP Q64610
A	865	ARG	-	expression tag	UNP Q64610
A	866	HIS	-	expression tag	UNP Q64610
A	867	HIS	-	expression tag	UNP Q64610
A	868	HIS	-	expression tag	UNP Q64610
A	869	HIS	-	expression tag	UNP Q64610
A	870	HIS	-	expression tag	UNP Q64610
A	871	HIS	-	expression tag	UNP Q64610
A	872	HIS	-	expression tag	UNP Q64610
A	873	HIS	-	expression tag	UNP Q64610

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]alpha-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
			Total	C	N	O			
2	B	8	94	52	2	40	0	0	0

- Molecule 3 is (2R)-6-chloro-2-[[6-(oxetane-3-sulfonyl)-6,7-dihydro-5H-pyrrolo[3,4-d]pyrimidin-2-yl]amino]-2,3-dihydro-1H-indene-4-carbonitrile (three-letter code: YF9) (formula: C₁₉H₁₈ClN₅O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
3	A	1	29	19	1	5	3	1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	2	2	2	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
5	A	1	1	1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Zn 1 1	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0

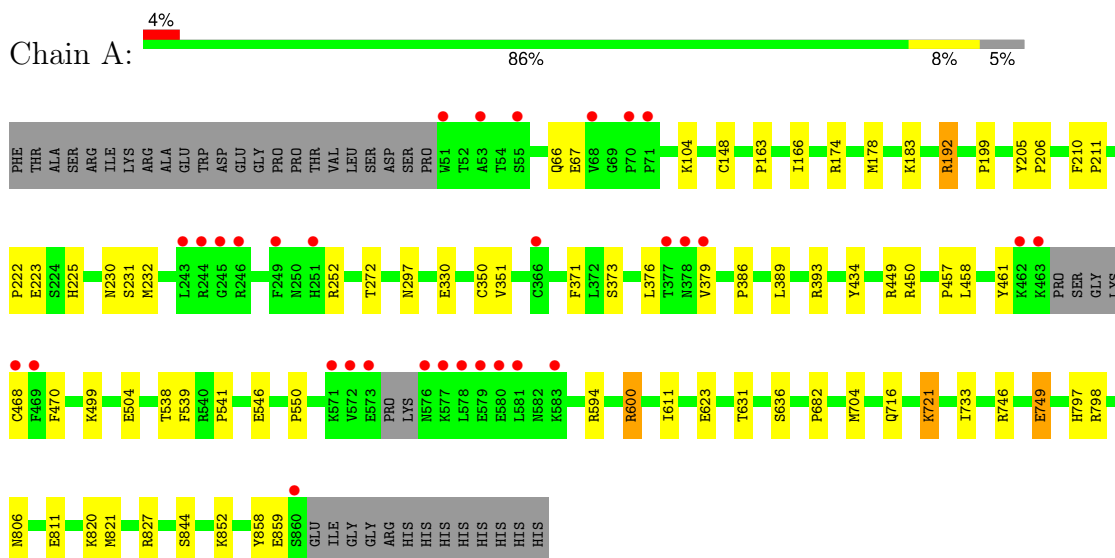
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	796	Total O 799 799	0	4

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]alpha-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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.95Å 91.73Å 119.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.83 – 1.83 68.83 – 1.83	Depositor EDS
% Data completeness (in resolution range)	86.9 (68.83-1.83) 86.9 (68.83-1.83)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.83Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.163 , 0.206 0.174 , 0.216	Depositor DCC
R_{free} test set	4070 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtrriage
Anisotropy	0.056	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7603	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, CA, K, ZN, NA, YF9, ACT

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	0.88	7/6931 (0.1%)	0.98	10/9391 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	GLU	CD-OE1	12.11	1.39	1.25
1	A	504	GLU	CD-OE2	7.51	1.33	1.25
1	A	223	GLU	CD-OE2	7.44	1.33	1.25
1	A	504	GLU	CD-OE1	6.86	1.33	1.25
1	A	811	GLU	CD-OE2	6.31	1.32	1.25
1	A	330	GLU	CD-OE1	5.56	1.31	1.25
1	A	859	GLU	CD-OE1	5.39	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	A	174	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	192	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	148[A]	CYS	CB-CA-C	-6.25	97.90	110.40
1	A	148[B]	CYS	CB-CA-C	-6.25	97.90	110.40
1	A	798	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	393	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	148[A]	CYS	N-CA-CB	5.31	120.16	110.60
1	A	148[B]	CYS	N-CA-CB	5.31	120.16	110.60
1	A	252	ARG	NE-CZ-NH1	-5.14	117.73	120.30

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	6664	0	6488	41	0
2	B	94	0	79	0	0
3	A	29	0	0	0	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	12	0	9	2	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	799	0	0	12	0
All	All	7603	0	6576	43	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 3.

All (43) 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:199:PRO:HG3	1:A:499[B]:LYS:HE3	1.72	0.71
1:A:373:SER:HA	1:A:379:VAL:HG21	1.74	0.68
1:A:623:GLU:OE1	9:A:1101:HOH:O	2.12	0.66
1:A:231:SER:C	1:A:232[A]:MET:HG3	2.18	0.63
1:A:163:PRO:HB3	1:A:350:CYS:O	2.01	0.61
1:A:297:ASN:ND2	9:A:1112:HOH:O	2.34	0.61
1:A:449:ARG:O	1:A:450[A]:ARG:HB2	2.00	0.60
1:A:178[B]:MET:HE2	1:A:192:ARG:HD2	1.83	0.60
1:A:820:LYS:HG2	1:A:858[B]:TYR:CZ	2.37	0.60
6:A:1005:ACT:H1	9:A:1220:HOH:O	2.07	0.55
1:A:178[B]:MET:CE	1:A:192:ARG:HD2	2.36	0.54
1:A:371:PHE:CE1	1:A:457:PRO:HA	2.42	0.54
1:A:230:ASN:ND2	9:A:1103:HOH:O	2.20	0.54
1:A:600[A]:ARG:HH21	1:A:600[A]:ARG:CG	2.21	0.52
1:A:821[B]:MET:HA	1:A:821[B]:MET:HE2	1.92	0.51
1:A:376:LEU:HB2	1:A:379:VAL:HG22	1.93	0.51
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.47	0.50
1:A:550:PRO:HB2	1:A:611:ILE:HG12	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:SER:O	1:A:721[A]:LYS:NZ	2.46	0.49
1:A:749:GLU:HG3	9:A:1607:HOH:O	2.12	0.49
1:A:820:LYS:HG2	1:A:858[B]:TYR:CE1	2.48	0.49
1:A:468:CYS:HA	9:A:1771:HOH:O	2.12	0.49
1:A:820:LYS:HG2	1:A:858[B]:TYR:CE2	2.48	0.48
1:A:539:PHE:O	1:A:541:PRO:HD3	2.13	0.48
1:A:600[A]:ARG:CG	1:A:600[A]:ARG:NH2	2.73	0.48
1:A:166:ILE:HD12	1:A:351:VAL:HG11	1.96	0.48
6:A:1006:ACT:C	9:A:1103:HOH:O	2.61	0.48
1:A:594:ARG:NH2	9:A:1130:HOH:O	2.46	0.48
1:A:538:THR:O	9:A:1102:HOH:O	2.20	0.47
1:A:682:PRO:HB3	1:A:716:GLN:HB3	1.96	0.47
1:A:600[A]:ARG:HD2	1:A:611:ILE:HD11	1.97	0.45
1:A:806:ASN:HB2	9:A:1601:HOH:O	2.18	0.43
1:A:272:THR:HB	9:A:1385:HOH:O	2.19	0.43
1:A:704:MET:HA	1:A:797:HIS:NE2	2.34	0.43
1:A:470:PHE:C	1:A:470:PHE:CD1	2.92	0.42
1:A:827[B]:ARG:HG2	1:A:852:LYS:HB3	2.00	0.42
1:A:206:PRO:HD3	1:A:434:TYR:CE1	2.55	0.41
1:A:820:LYS:HE2	1:A:858[B]:TYR:CD2	2.56	0.41
1:A:746:ARG:NH2	9:A:1107:HOH:O	2.28	0.41
1:A:631:THR:O	1:A:733:ILE:HA	2.21	0.41
1:A:205:TYR:CD1	1:A:206:PRO:HA	2.55	0.40
1:A:458:LEU:HA	1:A:461:TYR:CE2	2.57	0.40
1:A:210:PHE:N	1:A:211:PRO:CD	2.85	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	828/846 (98%)	800 (97%)	28 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	757/765 (99%)	745 (98%)	12 (2%)	58 44

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	67	GLU
1	A	104	LYS
1	A	183	LYS
1	A	386	PRO
1	A	389	LEU
1	A	600[A]	ARG
1	A	600[B]	ARG
1	A	721[A]	LYS
1	A	721[B]	LYS
1	A	749	GLU
1	A	844	SER

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates i

8 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	B	1	2,1	14,14,15	1.21	1 (7%)	17,19,21	1.51	2 (11%)
2	NAG	B	2	2	14,14,15	1.51	2 (14%)	17,19,21	3.28	5 (29%)
2	MAN	B	3	2	11,11,12	1.46	2 (18%)	15,15,17	2.44	6 (40%)
2	MAN	B	4	2	11,11,12	1.79	5 (45%)	15,15,17	2.23	2 (13%)
2	MAN	B	5	2	11,11,12	1.32	1 (9%)	15,15,17	1.37	4 (26%)
2	MAN	B	6	2	11,11,12	1.50	3 (27%)	15,15,17	1.76	4 (26%)
2	MAN	B	7	2	11,11,12	1.50	3 (27%)	15,15,17	1.97	4 (26%)
2	MAN	B	8	2	11,11,12	1.65	2 (18%)	15,15,17	1.68	2 (13%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	MAN	B	3	2	-	1/2/19/22	1/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1
2	MAN	B	5	2	-	2/2/19/22	0/1/1/1
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1
2	MAN	B	7	2	-	2/2/19/22	0/1/1/1
2	MAN	B	8	2	-	1/2/19/22	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C6-C5	3.24	1.62	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	MAN	C2-C3	3.21	1.57	1.52
2	B	2	NAG	O6-C6	3.16	1.55	1.42
2	B	1	NAG	O5-C1	2.99	1.48	1.43
2	B	4	MAN	C2-C3	2.83	1.56	1.52
2	B	3	MAN	C2-C3	2.83	1.56	1.52
2	B	6	MAN	O5-C1	2.81	1.48	1.43
2	B	7	MAN	C1-C2	2.73	1.58	1.52
2	B	7	MAN	O2-C2	2.66	1.48	1.43
2	B	3	MAN	O3-C3	2.58	1.49	1.43
2	B	4	MAN	O5-C5	2.38	1.48	1.43
2	B	8	MAN	C1-C2	2.27	1.57	1.52
2	B	4	MAN	O5-C1	2.19	1.47	1.43
2	B	6	MAN	O5-C5	2.17	1.47	1.43
2	B	4	MAN	C4-C5	2.14	1.57	1.53
2	B	7	MAN	C4-C5	2.08	1.57	1.53
2	B	4	MAN	O3-C3	2.03	1.48	1.43
2	B	6	MAN	C4-C3	2.03	1.57	1.52
2	B	5	MAN	C2-C3	2.01	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	10.76	126.61	112.19
2	B	4	MAN	C1-O5-C5	6.37	120.72	112.19
2	B	3	MAN	O2-C2-C1	-5.59	96.42	109.22
2	B	2	NAG	C3-C4-C5	4.89	119.09	110.23
2	B	8	MAN	O3-C3-C2	4.24	118.71	110.05
2	B	7	MAN	O2-C2-C1	3.96	118.29	109.22
2	B	4	MAN	O3-C3-C2	3.93	118.07	110.05
2	B	1	NAG	O5-C1-C2	-3.86	105.32	111.29
2	B	6	MAN	O3-C3-C2	-3.75	102.40	110.05
2	B	3	MAN	C1-C2-C3	3.62	114.91	109.64
2	B	6	MAN	O5-C5-C6	3.53	114.52	107.66
2	B	2	NAG	O5-C5-C6	3.28	114.05	107.66
2	B	3	MAN	O5-C5-C6	3.26	114.00	107.66
2	B	8	MAN	O5-C5-C6	3.23	113.96	107.66
2	B	5	MAN	O5-C1-C2	-2.90	103.86	110.79
2	B	7	MAN	C1-O5-C5	2.79	115.93	112.19
2	B	7	MAN	O5-C5-C4	2.66	117.31	110.83
2	B	3	MAN	O2-C2-C3	2.53	115.39	110.15
2	B	2	NAG	O7-C7-C8	-2.43	117.72	122.05
2	B	3	MAN	C2-C3-C4	-2.34	106.74	110.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	MAN	C1-C2-C3	-2.30	106.29	109.64
2	B	5	MAN	C3-C4-C5	2.28	114.36	110.23
2	B	1	NAG	O4-C4-C5	-2.26	103.75	109.32
2	B	3	MAN	O3-C3-C2	2.25	114.64	110.05
2	B	6	MAN	C1-O5-C5	2.24	115.19	112.19
2	B	5	MAN	O4-C4-C5	2.06	114.40	109.32
2	B	6	MAN	C1-C2-C3	-2.03	106.68	109.64
2	B	2	NAG	O7-C7-N2	2.03	125.57	121.98
2	B	5	MAN	O4-C4-C3	-2.00	105.66	110.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

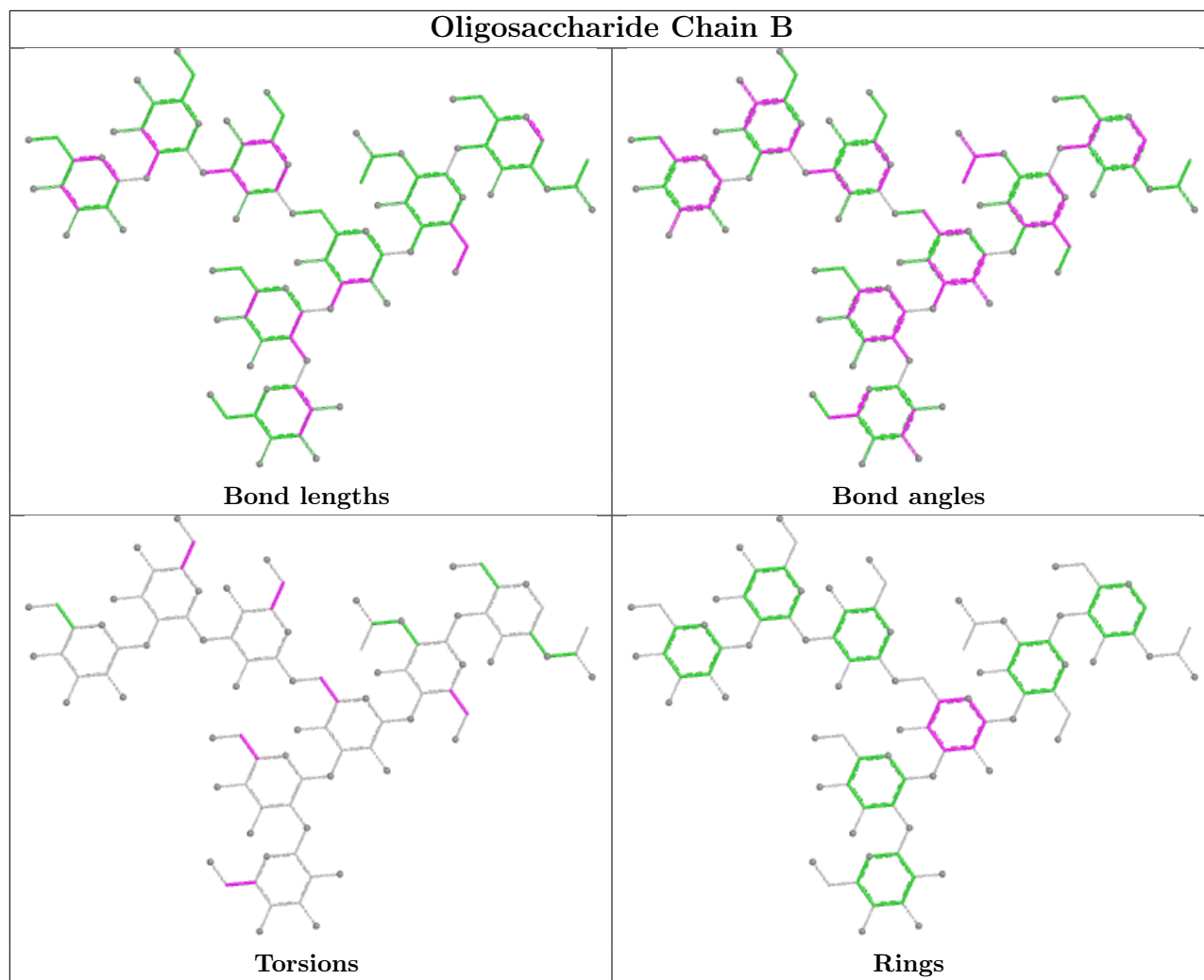
Mol	Chain	Res	Type	Atoms
2	B	7	MAN	C4-C5-C6-O6
2	B	7	MAN	O5-C5-C6-O6
2	B	5	MAN	O5-C5-C6-O6
2	B	5	MAN	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	3	MAN	C4-C5-C6-O6
2	B	8	MAN	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	MAN	C1-C2-C3-C4-C5-O5

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 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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
3	YF9	A	1001	-	28,33,33	2.76	15 (53%)	34,50,50	3.29	7 (20%)
6	ACT	A	1006	7	3,3,3	1.34	0	3,3,3	0.88	0
6	ACT	A	1004	-	3,3,3	1.53	0	3,3,3	0.75	0
6	ACT	A	1005	-	3,3,3	1.01	0	3,3,3	0.52	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
3	YF9	A	1001	-	-	1/16/40/40	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	YF9	C7-C8	-6.15	1.29	1.39
3	A	1001	YF9	C25-C24	4.78	1.60	1.53
3	A	1001	YF9	C10-C9	-4.75	1.45	1.51
3	A	1001	YF9	C4-C5	-4.72	1.30	1.38
3	A	1001	YF9	C20-N21	-4.10	1.43	1.48
3	A	1001	YF9	C27-C24	4.08	1.59	1.53
3	A	1001	YF9	C7-C5	3.68	1.44	1.38
3	A	1001	YF9	O28-S23	3.02	1.46	1.43
3	A	1001	YF9	C14-N15	2.63	1.42	1.34
3	A	1001	YF9	C14-N13	-2.48	1.31	1.34
3	A	1001	YF9	C14-N19	2.45	1.38	1.34
3	A	1001	YF9	C18-C17	-2.41	1.33	1.37
3	A	1001	YF9	C12-C8	-2.32	1.46	1.50
3	A	1001	YF9	C22-N21	2.15	1.51	1.48
3	A	1001	YF9	C3-C2	2.03	1.47	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	YF9	O29-S23-O28	-10.05	111.60	119.17
3	A	1001	YF9	C3-C4-C5	-9.80	115.05	119.44
3	A	1001	YF9	O29-S23-C24	9.50	119.93	107.82
3	A	1001	YF9	C4-C5-CL6	-4.28	113.80	119.17
3	A	1001	YF9	C7-C5-C4	3.70	126.13	121.64
3	A	1001	YF9	O29-S23-N21	-3.24	104.18	107.44
3	A	1001	YF9	O28-S23-N21	2.19	109.65	107.44

There are no chirality outliers.

All (1) torsion outliers are listed below:

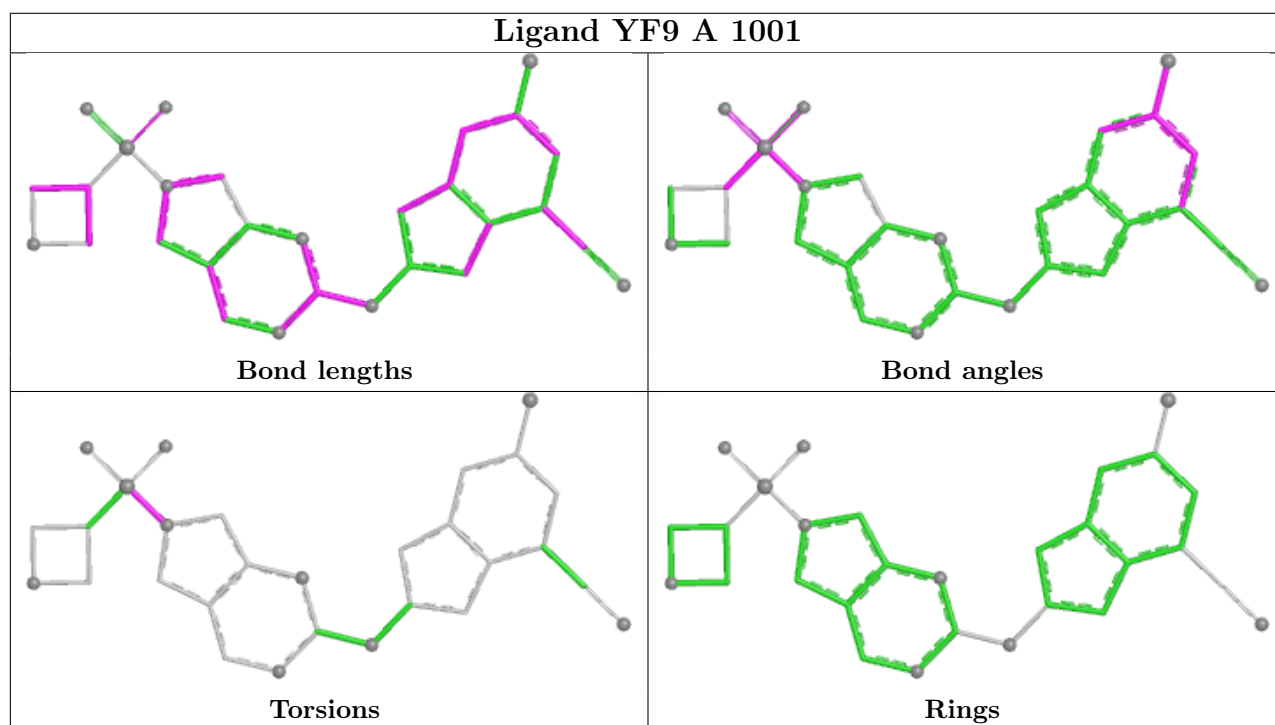
Mol	Chain	Res	Type	Atoms
3	A	1001	YF9	C22-N21-S23-O29

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1006	ACT	1	0
6	A	1005	ACT	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

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	804/846 (95%)	-0.19	31 (3%) 44 47	8, 21, 54, 114	30 (3%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	572	VAL	6.9
1	A	469	PHE	5.9
1	A	578	LEU	5.8
1	A	581	LEU	5.2
1	A	51	TRP	4.8
1	A	573	GLU	4.8
1	A	463	LYS	4.2
1	A	468	CYS	3.9
1	A	860	SER	3.8
1	A	70	PRO	3.7
1	A	577	LYS	3.7
1	A	243	LEU	3.5
1	A	246	ARG	3.4
1	A	68	VAL	3.3
1	A	571	LYS	3.3
1	A	462	LYS	3.2
1	A	71	PRO	3.0
1	A	580	GLU	2.9
1	A	249	PHE	2.8
1	A	576	ASN	2.8
1	A	378	ASN	2.7
1	A	55	SER	2.7
1	A	583	LYS	2.6
1	A	244	ARG	2.6
1	A	379	VAL	2.5
1	A	53	ALA	2.4
1	A	366	CYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	579	GLU	2.3
1	A	245	GLY	2.3
1	A	251	HIS	2.2
1	A	377	THR	2.1

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

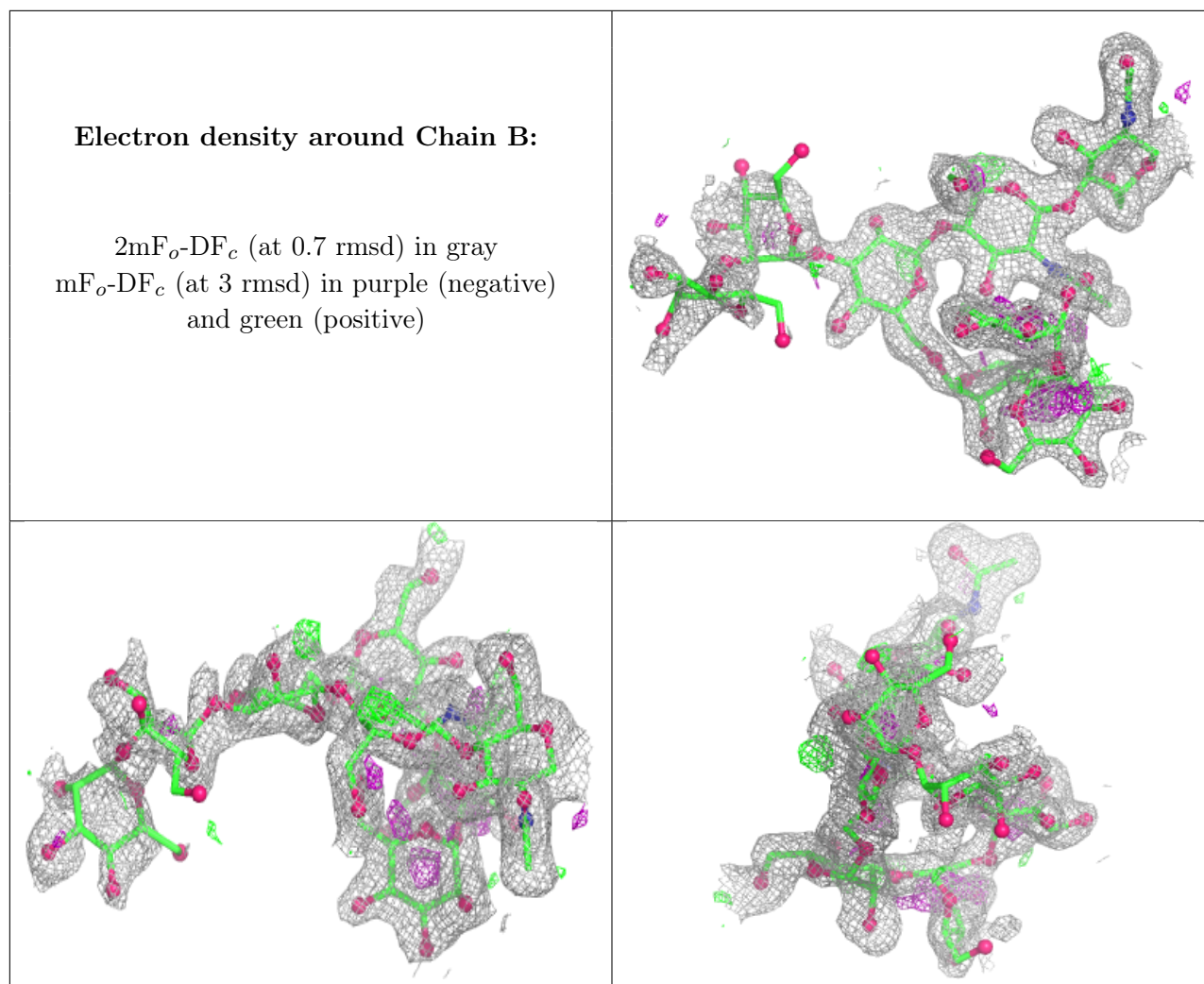
There are no non-standard protein/DNA/RNA residues in this entry.

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	MAN	B	7	11/12	0.54	0.17	78,90,93,97	0
2	MAN	B	3	11/12	0.66	0.15	56,61,71,75	0
2	MAN	B	8	11/12	0.67	0.16	39,78,91,97	0
2	MAN	B	4	11/12	0.74	0.15	49,54,62,63	0
2	MAN	B	5	11/12	0.83	0.15	39,52,59,61	0
2	NAG	B	2	14/15	0.88	0.10	24,30,39,48	0
2	MAN	B	6	11/12	0.89	0.12	30,44,49,50	0
2	NAG	B	1	14/15	0.97	0.05	14,15,18,19	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.

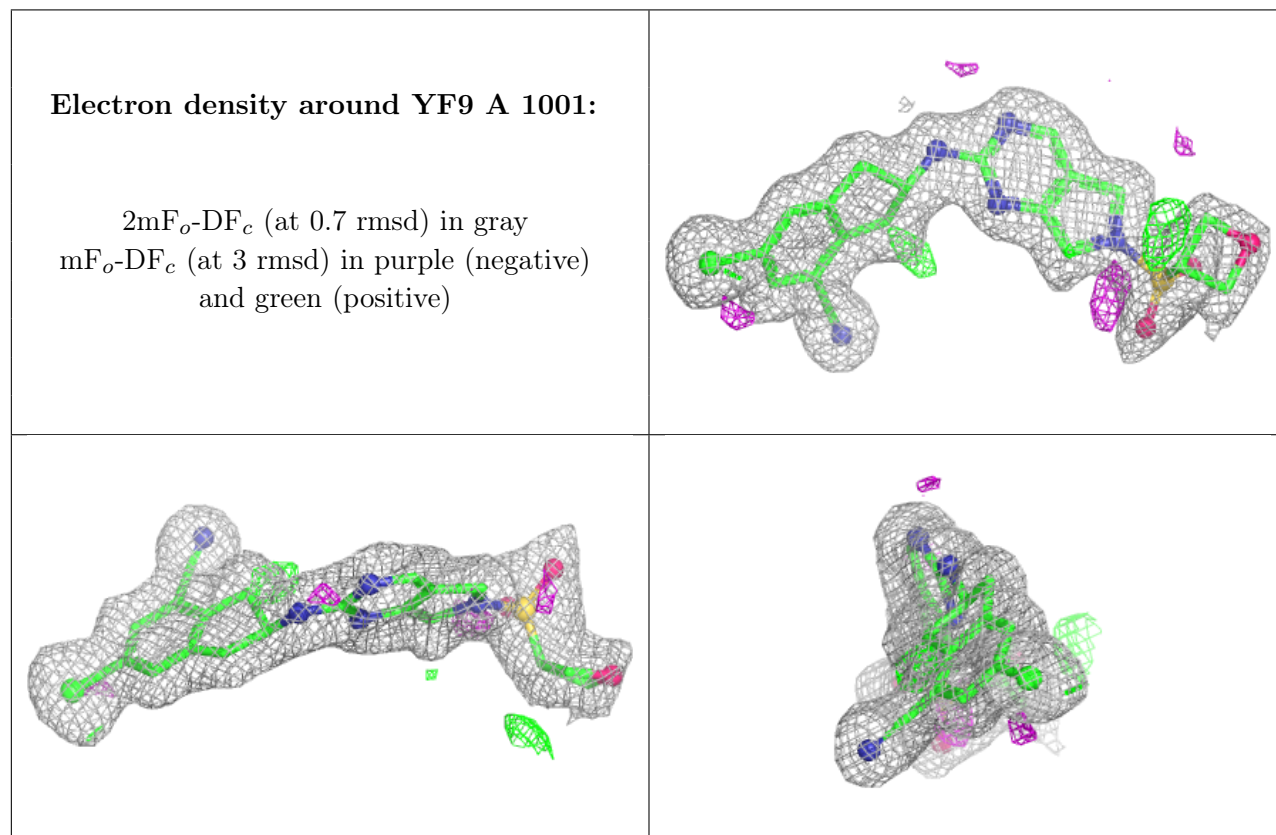


6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
6	ACT	A	1005	4/4	0.91	0.12	30,32,40,44	0
6	ACT	A	1004	4/4	0.92	0.09	24,30,32,33	0
3	YF9	A	1001	29/29	0.96	0.07	13,16,50,52	0
6	ACT	A	1006	4/4	0.96	0.13	29,46,49,56	0
8	NA	A	1008	1/1	0.96	0.06	31,31,31,31	0
4	CA	A	1002	1/1	0.99	0.07	25,25,25,25	0
5	K	A	1003	1/1	0.99	0.04	22,22,22,22	0
7	ZN	A	1007	1/1	1.00	0.01	17,17,17,17	0
4	CA	A	1009	1/1	1.00	0.01	13,13,13,13	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.