



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:22 PM UTC

PDB ID : 8C7R / pdb_00008c7r
Title : Crystal structure of rat autotaxin and compound MEY-003
Authors : Eymery, M.C.; McCarthy, A.A.
Deposited on : 2023-01-17
Resolution : 2.53 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

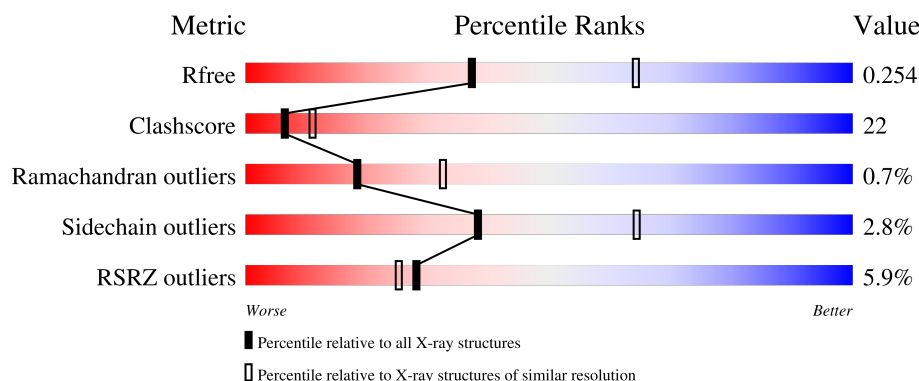
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	862	5% 54% 34% • 10%
2	B	2	100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6494 atoms, of which 46 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	775	Total	C	N	O	S	0	0	0
			6262	3971	1078	1164	49			

There are 27 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	?	-	GLU	deletion	UNP Q64610
A	?	-	ALA	deletion	UNP Q64610
A	?	-	GLU	deletion	UNP Q64610
A	?	-	THR	deletion	UNP Q64610
A	?	-	GLY	deletion	UNP Q64610
A	?	-	LYS	deletion	UNP Q64610
A	?	-	PHE	deletion	UNP Q64610
A	?	-	ARG	deletion	UNP Q64610
A	?	-	GLY	deletion	UNP Q64610
A	?	-	SER	deletion	UNP Q64610
A	?	-	LYS	deletion	UNP Q64610
A	?	-	HIS	deletion	UNP Q64610
A	?	-	GLU	deletion	UNP Q64610
A	?	-	ASN	deletion	UNP Q64610
A	?	-	LYS	deletion	UNP Q64610
A	?	-	LYS	deletion	UNP Q64610
A	?	-	ASN	deletion	UNP Q64610
A	?	-	LEU	deletion	UNP Q64610
A	?	-	ASN	deletion	UNP Q64610
A	?	-	GLY	deletion	UNP Q64610
A	?	-	SER	deletion	UNP Q64610
A	?	-	VAL	deletion	UNP Q64610
A	?	-	GLU	deletion	UNP Q64610
A	?	-	PRO	deletion	UNP Q64610

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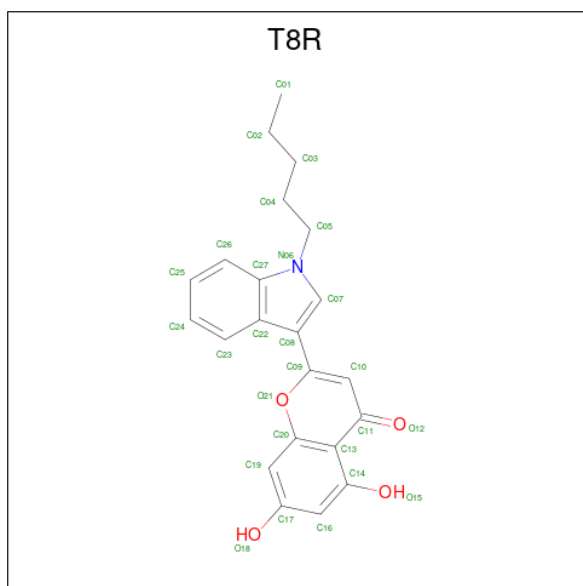
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP Q64610

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



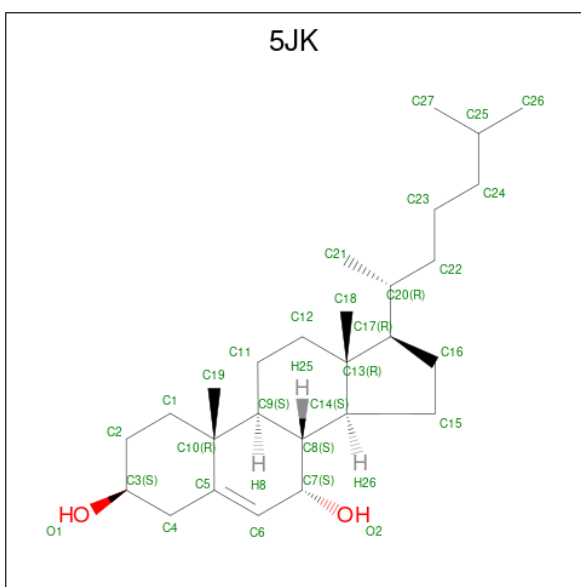
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 5,7-bis(oxidanyl)-2-(1-pentylindol-3-yl)chromen-4-one (CCD ID: T8R) (formula: C₂₂H₂₁NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	22	1	4		

- Molecule 4 is 7alpha-hydroxycholesterol (CCD ID: 5JK) (formula: C₂₇H₄₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			75	27	46	2		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		

- Molecule 6 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	I	0	0
			4	4		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	94	Total	O	0	0
			94	94		

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

Chain B:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.53Å 61.84Å 63.85Å 104.01° 98.43° 93.27°	Depositor
Resolution (Å)	43.64 – 2.53 43.64 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.2 (43.64-2.53) 98.2 (43.64-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.205 , 0.254 0.205 , 0.254	Depositor DCC
R_{free} test set	2005 reflections (7.68%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6494	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5JK, CA, T8R, NAG, IOD, ZN

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	0.31	2/6440 (0.0%)	0.51	3/8736 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	549	ARG	CZ-NH2	5.71	1.40	1.33
1	A	548	SER	C-N	-5.16	1.19	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	LYS	CA-CB-CG	-8.73	96.64	114.10
1	A	71	PRO	CA-N-CD	-5.76	103.44	111.50
1	A	71	PRO	N-CD-CG	-5.52	97.17	103.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	549	ARG	Sidechain

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	6262	0	6003	269	2
2	B	28	0	25	2	0
3	A	27	0	0	2	0
4	A	29	46	0	1	0
5	A	2	0	0	0	0
6	A	4	0	0	0	0
7	A	2	0	0	0	0
8	A	94	0	0	6	0
All	All	6448	46	6028	271	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (271) 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:749:GLU:OE1	8:A:1001:HOH:O	1.61	1.19
1:A:424:MET:HB3	1:A:426:GLN:HE21	1.12	1.15
1:A:456:LYS:HD3	1:A:457:PRO:HD2	1.34	1.09
1:A:499:LYS:HG2	1:A:500:VAL:N	1.72	1.00
1:A:499:LYS:HG2	1:A:500:VAL:H	1.27	1.00
1:A:645:PRO:HG2	1:A:648:LEU:HD12	1.49	0.94
1:A:76:ASP:OD2	1:A:78:LEU:N	2.02	0.93
1:A:698:VAL:HG23	1:A:701:MET:HE1	1.51	0.90
1:A:199:PRO:HG2	1:A:502:PRO:HG3	1.50	0.90
1:A:456:LYS:HD3	1:A:457:PRO:CD	2.04	0.88
1:A:166:ILE:HD12	1:A:351:VAL:HG11	1.55	0.87
1:A:673:LYS:H	1:A:673:LYS:HD3	1.41	0.86
1:A:78:LEU:HD11	1:A:274:PHE:HB2	1.59	0.84
1:A:424:MET:HB3	1:A:426:GLN:NE2	1.92	0.84
1:A:173:PHE:CE1	1:A:178:MET:HE2	2.12	0.83
1:A:593:GLU:OE1	8:A:1002:HOH:O	1.97	0.82
1:A:363:ASP:OD2	1:A:368:ARG:NH2	2.13	0.81
1:A:456:LYS:CD	1:A:457:PRO:HD2	2.11	0.79
1:A:415:LYS:HG3	1:A:416:PRO:HD2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:ARG:HG2	1:A:718:VAL:HG23	1.66	0.78
1:A:103:THR:OG1	1:A:105:ASP:OD1	2.02	0.75
1:A:112:ASN:HD21	1:A:114:GLU:HG2	1.51	0.74
1:A:704:MET:HE2	1:A:708:PHE:HE2	1.53	0.73
1:A:178:MET:HE3	1:A:486:VAL:HG21	1.70	0.72
2:B:2:NAG:O7	2:B:2:NAG:O3	2.07	0.72
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.25	0.72
1:A:390:GLY:HA3	1:A:445:LEU:HB2	1.72	0.70
1:A:645:PRO:CG	1:A:648:LEU:HD12	2.21	0.70
1:A:243:LEU:HD23	1:A:243:LEU:O	1.92	0.70
1:A:782:ASP:OD1	1:A:783:LYS:HG2	1.92	0.70
1:A:202:ARG:HH11	1:A:504:GLU:HG2	1.57	0.70
1:A:415:LYS:HG3	1:A:416:PRO:CD	2.21	0.69
1:A:515:LEU:HA	1:A:537:ASN:HD22	1.56	0.69
1:A:395:LYS:O	1:A:399:ASN:HB2	1.93	0.69
1:A:179:LYS:O	1:A:181:GLY:N	2.25	0.68
1:A:704:MET:HE2	1:A:708:PHE:CE2	2.28	0.68
1:A:673:LYS:H	1:A:673:LYS:CD	2.07	0.68
1:A:181:GLY:CA	1:A:184:VAL:HG22	2.23	0.68
1:A:646:GLU:HA	1:A:649:THR:HG23	1.77	0.67
1:A:483:MET:HE2	1:A:483:MET:HA	1.76	0.67
1:A:66:GLN:HA	1:A:66:GLN:OE1	1.94	0.66
1:A:698:VAL:HG23	1:A:701:MET:CE	2.24	0.66
1:A:449:ARG:HG3	1:A:450:ARG:HG3	1.77	0.66
1:A:638:GLN:O	1:A:638:GLN:HG3	1.94	0.66
1:A:394:ALA:HB1	1:A:399:ASN:ND2	2.12	0.65
1:A:112:ASN:ND2	1:A:114:GLU:HG2	2.11	0.64
1:A:258:PRO:HG2	1:A:261:ILE:HG12	1.79	0.64
1:A:329:ARG:HG2	1:A:329:ARG:HH11	1.62	0.64
1:A:468:CYS:N	8:A:1006:HOH:O	2.30	0.64
1:A:704:MET:HE1	1:A:712:TRP:CG	2.33	0.63
1:A:149:GLU:OE2	1:A:149:GLU:HA	1.97	0.63
1:A:184:VAL:HB	1:A:329:ARG:HG2	1.80	0.63
1:A:64:GLU:HG3	1:A:66:GLN:H	1.62	0.63
1:A:324:MET:C	1:A:327:PRO:HD2	2.24	0.62
1:A:721:LYS:HE3	1:A:725:SER:OG	1.98	0.62
1:A:526:THR:OG1	1:A:827:ARG:HD3	1.99	0.62
1:A:150:GLU:OE2	1:A:535:ARG:NH2	2.33	0.62
1:A:206:PRO:HB3	1:A:389:LEU:HD22	1.82	0.62
1:A:795:LEU:HD21	1:A:819:MET:HA	1.82	0.62
1:A:536:THR:HG22	1:A:537:ASN:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:LYS:HD3	1:A:858:TYR:CD1	2.35	0.61
1:A:845:TYR:O	1:A:849:LEU:HG	2.01	0.61
1:A:425:LYS:HD3	1:A:442:ASP:HA	1.82	0.61
1:A:549:ARG:HG3	1:A:550:PRO:HD2	1.82	0.61
1:A:665:ASN:OD1	1:A:667:LEU:HB2	2.01	0.61
1:A:231:SER:O	1:A:391:ARG:NH2	2.29	0.60
1:A:733:ILE:O	1:A:769:SER:HA	2.00	0.60
1:A:604:LEU:HD11	1:A:836:ASP:HB2	1.83	0.60
1:A:74:ARG:HD3	1:A:84:SER:HB3	1.81	0.60
1:A:665:ASN:OD1	1:A:668:ALA:N	2.33	0.60
1:A:856:HIS:HD2	1:A:858:TYR:CZ	2.20	0.60
1:A:273:PHE:HA	1:A:304:ALA:HB3	1.84	0.59
1:A:704:MET:HE1	1:A:712:TRP:CD2	2.38	0.59
1:A:823:THR:HG23	1:A:855:LEU:HD11	1.85	0.59
1:A:769:SER:HB3	1:A:793:PHE:CZ	2.38	0.59
1:A:173:PHE:CZ	1:A:178:MET:HE2	2.38	0.59
1:A:593:GLU:HG2	1:A:594:ARG:N	2.17	0.59
1:A:495:LYS:HD3	1:A:498:THR:HG21	1.85	0.58
1:A:499:LYS:CG	1:A:500:VAL:H	2.10	0.58
1:A:181:GLY:HA2	1:A:184:VAL:HG22	1.84	0.58
1:A:199:PRO:HD3	1:A:499:LYS:HE2	1.84	0.58
1:A:197:HIS:O	1:A:499:LYS:HG3	2.04	0.58
1:A:370:GLU:HG2	1:A:420:PHE:HE1	1.68	0.58
1:A:744:GLY:HA2	1:A:832:LEU:HD21	1.86	0.58
1:A:679:PHE:HB3	1:A:700:ASN:ND2	2.19	0.58
1:A:324:MET:O	1:A:327:PRO:HD2	2.04	0.58
1:A:281:HIS:NE2	1:A:308:GLU:OE1	2.37	0.57
1:A:593:GLU:OE2	1:A:593:GLU:N	2.37	0.57
1:A:559:GLN:CD	1:A:559:GLN:H	2.10	0.57
1:A:135:VAL:HA	1:A:140:GLU:O	2.04	0.57
1:A:499:LYS:CG	1:A:500:VAL:N	2.58	0.57
1:A:685:LEU:HD22	1:A:685:LEU:N	2.20	0.57
1:A:845:TYR:CZ	1:A:849:LEU:HD21	2.38	0.57
1:A:310:PRO:HB2	1:A:324:MET:HE1	1.86	0.56
1:A:833:THR:HB	1:A:835:LEU:HG	1.88	0.56
1:A:148:CYS:SG	1:A:190:LYS:HE3	2.45	0.56
1:A:508:LEU:O	1:A:512:MET:HG3	2.05	0.56
1:A:793:PHE:CD1	1:A:795:LEU:HG	2.40	0.56
1:A:682:PRO:HB3	1:A:716:GLN:HB3	1.88	0.56
1:A:426:GLN:H	1:A:426:GLN:CD	2.15	0.55
1:A:431:ARG:HD3	1:A:823:THR:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:ILE:HD11	8:A:1027:HOH:O	2.07	0.55
1:A:220:LEU:CD2	1:A:523:ASN:HA	2.36	0.55
1:A:199:PRO:CD	1:A:499:LYS:HE2	2.36	0.55
1:A:142:HIS:ND1	1:A:340:ASP:OD2	2.38	0.55
1:A:229:GLY:O	1:A:232:MET:HE2	2.07	0.55
1:A:370:GLU:HG2	1:A:420:PHE:CE1	2.41	0.55
1:A:749:GLU:HA	1:A:752:ILE:HD12	1.88	0.55
1:A:202:ARG:NH1	1:A:504:GLU:HG2	2.21	0.54
1:A:513:CYS:HB2	1:A:520:PRO:HG3	1.89	0.54
1:A:384:LEU:HD12	1:A:391:ARG:O	2.08	0.54
1:A:69:GLY:O	1:A:70:PRO:C	2.50	0.54
1:A:120:SER:HG	1:A:122:ASP:CG	2.17	0.53
1:A:142:HIS:HB2	1:A:145:ASP:OD2	2.09	0.53
1:A:67:GLU:O	1:A:67:GLU:HG2	2.08	0.53
1:A:493:THR:HB	1:A:515:LEU:CD2	2.39	0.53
1:A:111:ARG:HD3	1:A:122:ASP:OD2	2.09	0.53
1:A:246:ARG:HA	1:A:249:PHE:HD2	1.73	0.53
1:A:717:ARG:CG	1:A:718:VAL:HG23	2.39	0.52
1:A:180:LYS:HD3	1:A:180:LYS:C	2.34	0.52
1:A:199:PRO:HD3	1:A:499:LYS:CE	2.40	0.52
1:A:220:LEU:HD21	1:A:523:ASN:HA	1.92	0.51
1:A:100:TRP:CZ3	1:A:116:ALA:HB1	2.46	0.51
1:A:698:VAL:HA	1:A:701:MET:CE	2.40	0.51
1:A:399:ASN:ND2	1:A:402:TYR:HB3	2.25	0.51
1:A:483:MET:HE2	1:A:483:MET:CA	2.39	0.51
1:A:820:LYS:HD3	1:A:858:TYR:CG	2.45	0.51
1:A:333:LYS:O	1:A:337:GLN:HG3	2.10	0.51
1:A:325:THR:O	1:A:329:ARG:HG3	2.10	0.51
1:A:550:PRO:HG3	1:A:600:ARG:NH1	2.26	0.51
1:A:355:PHE:HB3	1:A:488:VAL:HB	1.93	0.50
1:A:378:ASN:HD22	1:A:401:LYS:HD3	1.76	0.50
1:A:134:GLN:HB3	1:A:140:GLU:HG3	1.94	0.50
1:A:748:THR:HG23	1:A:751:GLU:H	1.75	0.50
1:A:199:PRO:N	1:A:499:LYS:HE2	2.26	0.50
1:A:309:GLN:HB2	1:A:331:ILE:HD11	1.93	0.50
1:A:378:ASN:OD1	1:A:381:ASP:HB2	2.11	0.50
1:A:232:MET:HB2	1:A:241:PHE:HB3	1.94	0.50
1:A:793:PHE:CE2	1:A:819:MET:HE3	2.47	0.49
1:A:541:PRO:HB2	1:A:845:TYR:CD2	2.47	0.49
1:A:703:PRO:HG2	1:A:764:PRO:CD	2.43	0.49
1:A:225:HIS:CE1	1:A:227:ILE:HB	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:PRO:HA	1:A:225:HIS:NE2	2.27	0.49
1:A:536:THR:HG22	1:A:537:ASN:N	2.27	0.49
1:A:570:ASP:OD2	1:A:653:ARG:HD2	2.13	0.49
1:A:684:TYR:C	1:A:685:LEU:HD22	2.36	0.49
1:A:648:LEU:HD21	1:A:693:TYR:CE1	2.48	0.49
1:A:704:MET:HE1	1:A:712:TRP:CD1	2.47	0.49
1:A:133:TYR:O	1:A:137:CYS:HB2	2.13	0.49
2:B:2:NAG:HO3	2:B:2:NAG:C7	2.22	0.48
1:A:78:LEU:O	1:A:82:TYR:HD1	1.95	0.48
1:A:793:PHE:CD1	1:A:793:PHE:C	2.91	0.48
1:A:300:PRO:HG2	1:A:303:TYR:CE1	2.48	0.48
1:A:456:LYS:HD3	1:A:457:PRO:N	2.27	0.48
1:A:513:CYS:CB	1:A:520:PRO:HG3	2.43	0.48
1:A:665:ASN:HD21	1:A:668:ALA:HB2	1.78	0.48
1:A:217:ALA:HA	3:A:901:T8R:C02	2.44	0.48
1:A:770:ILE:HD13	1:A:826:VAL:HG22	1.95	0.48
1:A:237:PHE:CE2	1:A:252:ARG:HD2	2.49	0.48
1:A:830:GLU:OE2	1:A:852:LYS:HE2	2.14	0.48
1:A:481:ASN:HA	1:A:484:GLN:HG2	1.96	0.48
1:A:536:THR:CG2	1:A:537:ASN:H	2.25	0.48
1:A:703:PRO:HG2	1:A:764:PRO:HD3	1.96	0.48
1:A:698:VAL:HA	1:A:701:MET:HE2	1.95	0.47
1:A:493:THR:HB	1:A:515:LEU:HD23	1.96	0.47
1:A:171:ASP:O	1:A:311:ASP:N	2.47	0.47
1:A:482:SER:C	1:A:483:MET:HE2	2.39	0.47
1:A:756:VAL:HB	1:A:759:SER:OG	2.15	0.47
1:A:260:TRP:NE1	4:A:902:5JK:O2	2.48	0.47
1:A:513:CYS:HB3	1:A:518:LEU:O	2.15	0.47
1:A:626:LEU:O	1:A:664:GLN:NE2	2.40	0.47
1:A:792:SER:HB2	1:A:824:ALA:O	2.15	0.47
1:A:281:HIS:CE1	1:A:308:GLU:OE1	2.68	0.46
1:A:402:TYR:CD2	1:A:407:ILE:HD11	2.50	0.46
1:A:174:ARG:NH1	1:A:482:SER:HB2	2.31	0.46
1:A:268:VAL:HG21	1:A:518:LEU:HD21	1.96	0.46
1:A:388:THR:HG22	1:A:476:PHE:CZ	2.50	0.46
1:A:597:LEU:HD12	1:A:731:ASN:HB2	1.96	0.46
1:A:364:VAL:HG22	1:A:450:ARG:HA	1.96	0.46
1:A:133:TYR:OH	1:A:138:LYS:HE3	2.16	0.46
1:A:155:GLU:O	1:A:350:CYS:HB2	2.15	0.46
1:A:421:LYS:HG3	1:A:422:PRO:HD2	1.97	0.46
1:A:782:ASP:CG	1:A:783:LYS:HE3	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LYS:HG3	1:A:416:PRO:N	2.28	0.46
1:A:628:PRO:HG2	1:A:680:LEU:HD12	1.98	0.46
1:A:144:VAL:HB	1:A:187:ASN:OD1	2.16	0.45
1:A:180:LYS:CG	1:A:180:LYS:O	2.65	0.45
1:A:298:GLU:O	1:A:300:PRO:HD3	2.15	0.45
1:A:142:HIS:HD1	1:A:340:ASP:CG	2.23	0.45
1:A:703:PRO:O	1:A:767:TYR:OH	2.24	0.45
1:A:393:ARG:HG2	1:A:394:ALA:N	2.31	0.45
1:A:740:TYR:OH	1:A:763:VAL:O	2.29	0.45
1:A:371:PHE:CE2	1:A:457:PRO:HA	2.51	0.45
1:A:716:GLN:NE2	8:A:1015:HOH:O	2.50	0.45
1:A:368:ARG:HB3	1:A:451:TRP:CD2	2.51	0.45
1:A:738:PHE:CZ	1:A:764:PRO:HG3	2.52	0.45
1:A:134:GLN:HG3	1:A:344:GLN:HG3	1.99	0.45
1:A:184:VAL:HG23	1:A:185:MET:CG	2.47	0.45
1:A:166:ILE:CD1	1:A:351:VAL:HG11	2.37	0.45
1:A:602:ALA:HB3	1:A:836:ASP:HB3	1.98	0.45
1:A:738:PHE:O	1:A:747:ASP:HB2	2.17	0.44
1:A:227:ILE:HA	1:A:232:MET:HE1	1.98	0.44
1:A:612:LEU:HB2	1:A:619:SER:OG	2.17	0.44
1:A:383:THR:OG1	1:A:395:LYS:NZ	2.49	0.44
1:A:329:ARG:HH11	1:A:329:ARG:CG	2.30	0.44
1:A:606:ARG:HA	1:A:606:ARG:HD2	1.58	0.44
1:A:625:PHE:CD1	1:A:625:PHE:N	2.85	0.44
1:A:844:SER:OG	1:A:847:GLU:HG3	2.18	0.44
1:A:71:PRO:HD2	1:A:72:ASP:H	1.82	0.44
1:A:71:PRO:O	1:A:72:ASP:C	2.59	0.44
1:A:112:ASN:CG	1:A:114:GLU:HG2	2.43	0.44
1:A:311:ASP:OD1	1:A:361:MET:HE1	2.17	0.44
1:A:806:ASN:OD1	1:A:806:ASN:N	2.42	0.44
1:A:181:GLY:HA3	1:A:184:VAL:HG22	1.96	0.44
1:A:621:TYR:HA	1:A:628:PRO:HA	2.00	0.44
1:A:185:MET:HA	1:A:332:ASP:CG	2.43	0.43
1:A:206:PRO:HD3	1:A:434:TYR:CE1	2.53	0.43
1:A:665:ASN:ND2	1:A:668:ALA:HB2	2.34	0.43
1:A:679:PHE:HA	1:A:700:ASN:O	2.18	0.43
1:A:133:TYR:HB3	1:A:344:GLN:OE1	2.18	0.43
1:A:171:ASP:HB3	1:A:311:ASP:HB2	2.00	0.43
1:A:335:VAL:O	1:A:339:MET:HG2	2.19	0.43
1:A:300:PRO:HG2	1:A:303:TYR:HE1	1.83	0.43
1:A:372:LEU:HD22	1:A:411:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ASN:OD1	1:A:481:ASN:N	2.52	0.43
1:A:647:HIS:CD2	1:A:648:LEU:HG	2.53	0.43
1:A:201:MET:HE1	1:A:356:VAL:CG2	2.49	0.43
1:A:512:MET:HE1	3:A:901:T8R:C01	2.48	0.43
1:A:248:LYS:HE2	1:A:249:PHE:CE2	2.54	0.42
1:A:165:LEU:O	1:A:302:VAL:HA	2.19	0.42
1:A:634:THR:O	1:A:635:ILE:HD13	2.19	0.42
1:A:67:GLU:O	1:A:67:GLU:CG	2.67	0.42
1:A:149:GLU:OE2	1:A:149:GLU:CA	2.66	0.42
1:A:627:MET:HE2	1:A:627:MET:HB2	1.46	0.42
1:A:638:GLN:O	1:A:638:GLN:CG	2.63	0.42
1:A:323:GLU:H	1:A:323:GLU:CD	2.28	0.42
1:A:412:THR:O	1:A:414:LYS:HG2	2.20	0.42
1:A:210:PHE:HB2	1:A:230:ASN:OD1	2.19	0.42
1:A:319:PRO:HG2	1:A:320:PHE:CE2	2.55	0.42
1:A:607:THR:OG1	1:A:624:ILE:HG13	2.19	0.42
1:A:366:CYS:HA	8:A:1038:HOH:O	2.18	0.42
1:A:184:VAL:HA	1:A:329:ARG:NH1	2.34	0.41
1:A:384:LEU:HD13	1:A:392:ILE:HG12	2.01	0.41
1:A:570:ASP:HA	1:A:693:TYR:HE1	1.84	0.41
1:A:655:ASP:HB2	1:A:697:LEU:HD22	2.03	0.41
1:A:794:ILE:HD13	1:A:832:LEU:HD12	2.01	0.41
1:A:209:THR:HG22	1:A:213:LEU:HD12	2.01	0.41
1:A:748:THR:HG22	1:A:751:GLU:CD	2.45	0.41
1:A:857:THR:O	1:A:858:TYR:HB2	2.20	0.41
1:A:143:TRP:HH2	1:A:191:LEU:HG	1.86	0.41
1:A:74:ARG:O	1:A:85:CYS:HA	2.20	0.41
1:A:112:ASN:OD1	1:A:114:GLU:HG2	2.19	0.41
1:A:364:VAL:HG12	1:A:470:PHE:HE2	1.86	0.41
1:A:536:THR:O	1:A:537:ASN:C	2.64	0.41
1:A:430:LYS:HD2	1:A:430:LYS:HA	1.83	0.41
1:A:76:ASP:CG	1:A:77:ASN:N	2.79	0.40
1:A:101:GLU:HB3	1:A:132:ASN:ND2	2.36	0.40
1:A:220:LEU:HD23	1:A:523:ASN:HA	2.03	0.40
1:A:378:ASN:O	1:A:380:ASP:N	2.54	0.40
1:A:215:THR:OG1	1:A:222:PRO:HD3	2.21	0.40
1:A:550:PRO:HB3	1:A:611:ILE:HD13	2.03	0.40
1:A:684:TYR:HB2	1:A:685:LEU:HD22	2.02	0.40
1:A:79:CYS:C	1:A:85:CYS:SG	3.04	0.40
1:A:178:MET:HE1	1:A:188:ILE:HG21	2.03	0.40
1:A:810:ASP:OD2	1:A:810:ASP:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:PRO:HG3	1:A:483:MET:O	2.20	0.40
1:A:685:LEU:N	1:A:685:LEU:CD2	2.83	0.40
1:A:311:ASP:OD1	1:A:361:MET:CE	2.70	0.40
1:A:515:LEU:HA	1:A:537:ASN:ND2	2.30	0.40
1:A:551:ASN:O	1:A:610:ASP:HA	2.21	0.40
1:A:650:ASN:HD22	1:A:650:ASN:HA	1.61	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:NH1	1:A:555:ILE:O[1_656]	2.15	0.05
1:A:265:LYS:NZ	1:A:778:THR:OG1[1_655]	2.17	0.03

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	769/862 (89%)	722 (94%)	42 (6%)	5 (1%)	18	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	A	180	LYS
1	A	570	ASP
1	A	70	PRO
1	A	181	GLY

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	702/778 (90%)	682 (97%)	20 (3%)	38 64

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	67	GLU
1	A	110	VAL
1	A	170	VAL
1	A	193	SER
1	A	240	SER
1	A	313	SER
1	A	370	GLU
1	A	401	LYS
1	A	408	ILE
1	A	421	LYS
1	A	426	GLN
1	A	535	ARG
1	A	540	ARG
1	A	567	THR
1	A	571	LYS
1	A	646	GLU
1	A	651	CYS
1	A	667	LEU
1	A	857	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	378	ASN
1	A	399	ASN
1	A	426	GLN
1	A	537	ASN
1	A	551	ASN

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Mol	Chain	Res	Type
1	A	650	ASN
1	A	716	GLN
1	A	801	ASN
1	A	831	HIS

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 ⓘ

2 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	0.46	0	17,19,21	0.66	1 (5%)
2	NAG	B	2	2	14,14,15	0.28	0	17,19,21	0.54	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	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	2.24	115.19	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

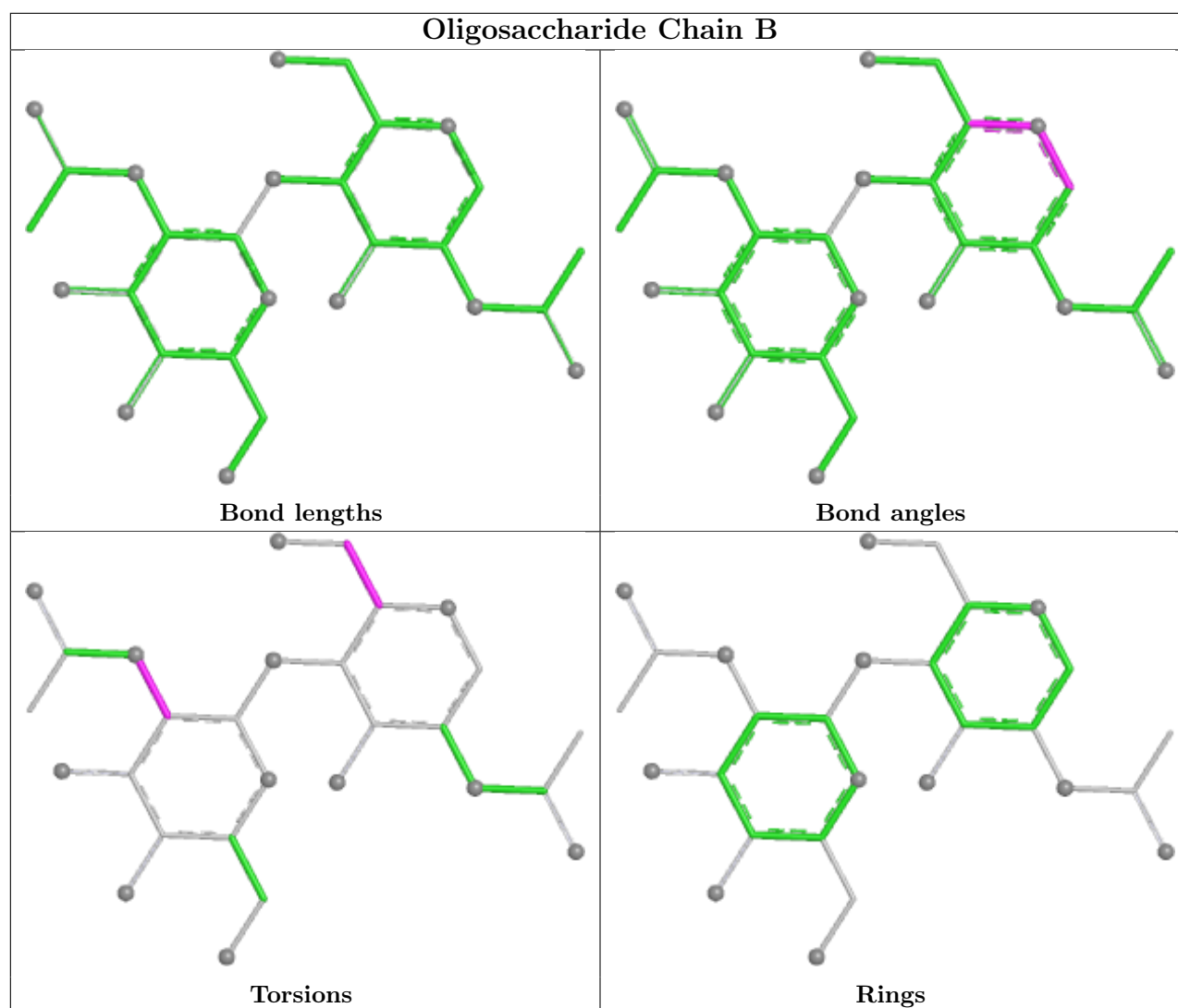
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	2	0

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 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	5JK	A	902	-	32,32,32	4.40	15 (46%)	48,50,50	2.52	15 (31%)
3	T8R	A	901	-	29,30,30	2.62	16 (55%)	40,43,43	2.14	10 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5JK	A	902	-	-	0/10/71/71	0/4/4/4
3	T8R	A	901	-	-	4/8/9/9	0/4/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	5JK	C6-C5	16.58	1.59	1.33
4	A	902	5JK	C8-C7	9.16	1.63	1.53
4	A	902	5JK	C16-C15	6.36	1.71	1.54
4	A	902	5JK	C20-C17	-6.16	1.43	1.54
4	A	902	5JK	C15-C14	5.86	1.66	1.54
3	A	901	T8R	C19-C20	5.70	1.48	1.38
4	A	902	5JK	C13-C17	4.87	1.63	1.55
4	A	902	5JK	C12-C13	-4.74	1.45	1.54
4	A	902	5JK	C12-C11	4.57	1.62	1.53
3	A	901	T8R	C07-N06	4.30	1.43	1.36
3	A	901	T8R	C26-C27	3.94	1.45	1.39
4	A	902	5JK	O2-C7	-3.89	1.36	1.43
3	A	901	T8R	C05-N06	3.82	1.54	1.47
4	A	902	5JK	C10-C9	3.39	1.61	1.56
3	A	901	T8R	O21-C09	3.32	1.42	1.37
3	A	901	T8R	C23-C22	3.29	1.44	1.39
3	A	901	T8R	C22-C08	3.18	1.51	1.45
3	A	901	T8R	C10-C11	3.10	1.51	1.44
3	A	901	T8R	C19-C17	3.07	1.43	1.39
3	A	901	T8R	C16-C17	2.99	1.43	1.39
3	A	901	T8R	O21-C20	2.85	1.42	1.38
3	A	901	T8R	C16-C14	2.69	1.42	1.38
3	A	901	T8R	C27-N06	2.65	1.43	1.39
4	A	902	5JK	C8-C14	-2.61	1.48	1.53
3	A	901	T8R	C07-C08	2.61	1.42	1.37
3	A	901	T8R	O15-C14	2.59	1.41	1.36
4	A	902	5JK	C10-C5	-2.45	1.48	1.52
4	A	902	5JK	C22-C20	2.41	1.60	1.54
3	A	901	T8R	C25-C24	2.33	1.43	1.38
4	A	902	5JK	C8-C9	2.24	1.58	1.53
4	A	902	5JK	C4-C3	2.24	1.56	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	5JK	C7-C6-C5	-10.27	115.84	125.18
3	A	901	T8R	O21-C20-C19	5.96	124.28	115.83
3	A	901	T8R	O21-C09-C10	-5.87	115.56	123.84
4	A	902	5JK	C19-C10-C9	-4.55	106.55	111.66
4	A	902	5JK	C4-C5-C10	-4.55	110.60	116.42
3	A	901	T8R	C22-C08-C09	4.44	133.02	127.24
4	A	902	5JK	C13-C14-C8	4.27	119.33	113.93
3	A	901	T8R	C14-C13-C20	3.77	121.01	117.41
4	A	902	5JK	C1-C10-C9	-3.73	103.80	108.74
3	A	901	T8R	C20-C13-C11	-3.51	116.35	119.60
4	A	902	5JK	C10-C9-C8	-3.50	109.01	113.28
4	A	902	5JK	C1-C10-C5	3.50	114.77	108.74
4	A	902	5JK	C9-C10-C5	3.36	114.58	109.65
3	A	901	T8R	C20-O21-C09	3.33	125.66	119.73
4	A	902	5JK	C17-C13-C14	3.06	103.61	100.10
3	A	901	T8R	C22-C08-C07	-3.05	103.54	106.29
3	A	901	T8R	O21-C20-C13	-2.78	118.47	121.19
4	A	902	5JK	C13-C17-C20	-2.77	115.21	119.50
4	A	902	5JK	C22-C20-C17	-2.70	104.72	110.33
3	A	901	T8R	C19-C20-C13	-2.60	117.26	121.79
4	A	902	5JK	C18-C13-C12	-2.53	106.87	110.61
4	A	902	5JK	C2-C3-C4	2.41	113.68	110.29
4	A	902	5JK	C4-C5-C6	2.34	122.44	120.70
3	A	901	T8R	C27-C22-C08	2.33	109.02	106.76
4	A	902	5JK	C8-C7-C6	-2.22	108.16	111.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

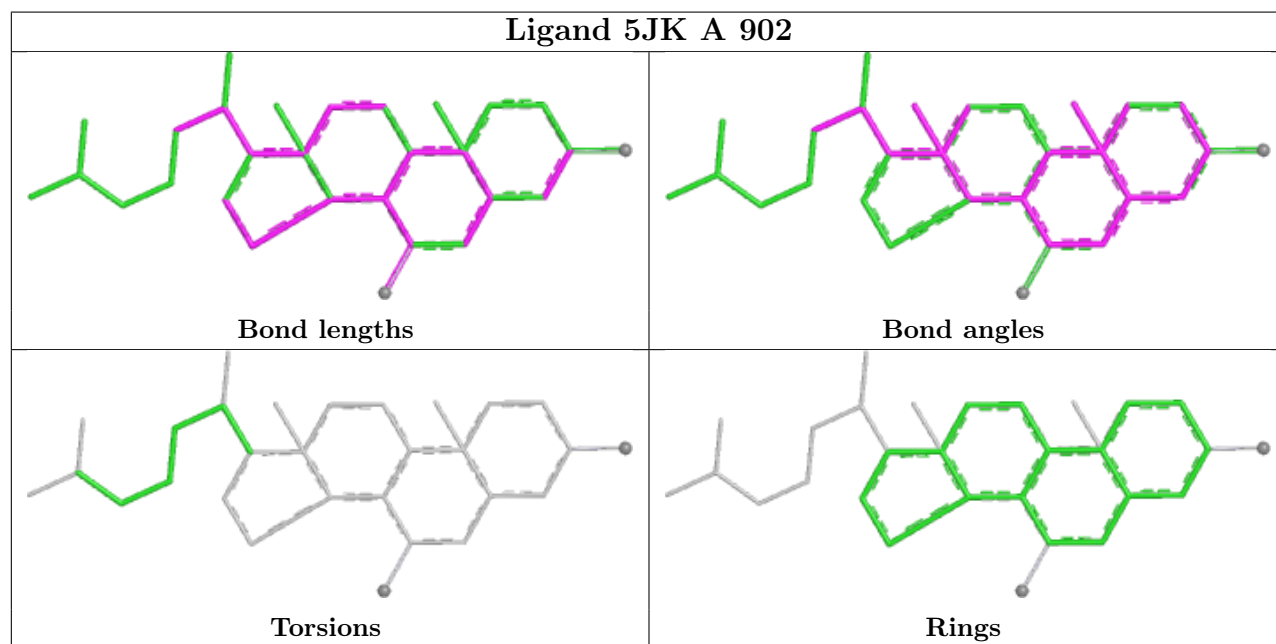
Mol	Chain	Res	Type	Atoms
3	A	901	T8R	C04-C05-N06-C07
3	A	901	T8R	C07-C08-C09-C10
3	A	901	T8R	C04-C05-N06-C27
3	A	901	T8R	C02-C03-C04-C05

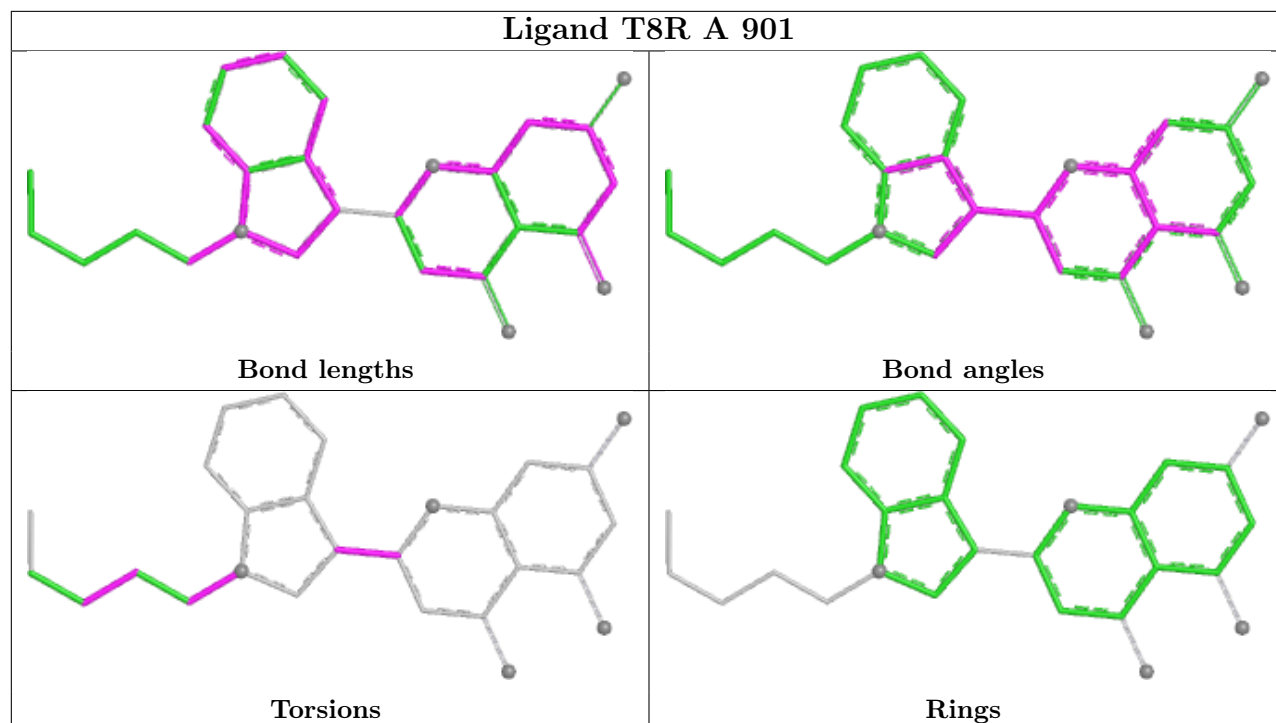
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	5JK	1	0
3	A	901	T8R	2	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	548:SER	C	549:ARG	N	1.19

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	775/862 (89%)	0.39	46 (5%) 28 25	23, 39, 71, 280	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	PRO	5.7
1	A	68	VAL	4.8
1	A	499	LYS	4.6
1	A	537	ASN	4.1
1	A	70	PRO	3.9
1	A	180	LYS	3.9
1	A	570	ASP	3.9
1	A	397	ILE	3.8
1	A	81	SER	3.7
1	A	76	ASP	3.7
1	A	72	ASP	3.6
1	A	399	ASN	3.4
1	A	73	CYS	3.3
1	A	181	GLY	3.3
1	A	396	SER	3.2
1	A	148	CYS	3.0
1	A	378	ASN	3.0
1	A	593	GLU	3.0
1	A	59	LYS	2.8
1	A	320	PHE	2.8
1	A	538	THR	2.8
1	A	688	SER	2.7
1	A	785	ASP	2.7
1	A	69	GLY	2.6
1	A	56	GLY	2.5
1	A	272	THR	2.5
1	A	400	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	571	LYS	2.3
1	A	648	LEU	2.3
1	A	125	SER	2.3
1	A	405	LYS	2.3
1	A	536	THR	2.2
1	A	793	PHE	2.2
1	A	197	HIS	2.2
1	A	91	GLU	2.2
1	A	594	ARG	2.2
1	A	110	VAL	2.1
1	A	549	ARG	2.1
1	A	346	ARG	2.1
1	A	545	ASP	2.1
1	A	192	ARG	2.1
1	A	182	SER	2.1
1	A	84	SER	2.0
1	A	313	SER	2.0
1	A	416	PRO	2.0
1	A	113	GLU	2.0

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

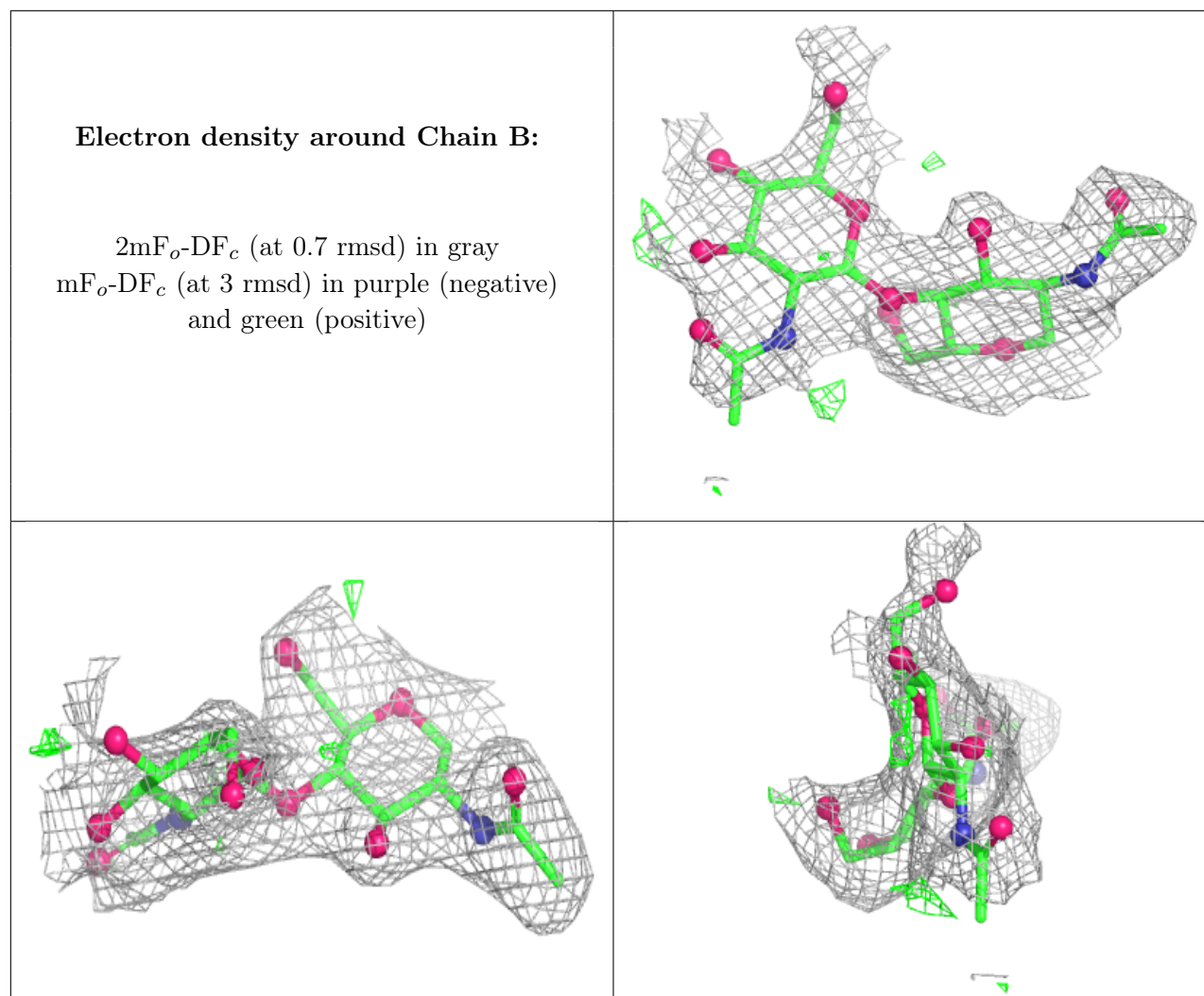
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	NAG	B	2	14/15	0.71	0.17	59,69,73,78	0
2	NAG	B	1	14/15	0.90	0.09	29,39,44,51	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($\text{\AA}^2$)	Q<0.9
4	5JK	A	902	29/29	0.81	0.15	30,42,61,68	75
3	T8R	A	901	27/27	0.85	0.15	42,44,48,53	0
5	ZN	A	904	1/1	0.93	0.09	90,90,90,90	0
7	CA	A	909	1/1	0.95	0.18	60,60,60,60	0
5	ZN	A	903	1/1	0.97	0.06	46,46,46,46	0
7	CA	A	910	1/1	0.97	0.05	40,40,40,40	0
6	IOD	A	907	1/1	0.99	0.13	72,72,72,72	0
6	IOD	A	908	1/1	0.99	0.17	71,71,71,71	0
6	IOD	A	905	1/1	0.99	0.05	50,50,50,50	0

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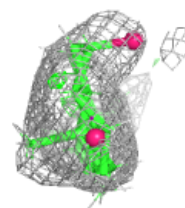
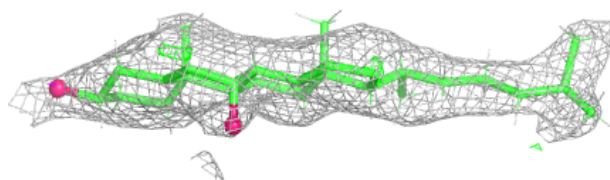
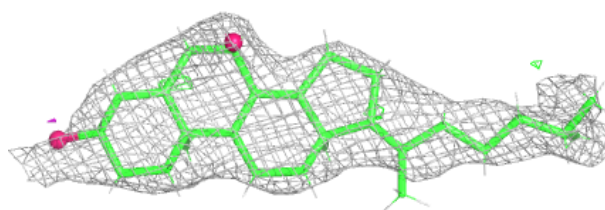
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	IOD	A	906	1/1	0.99	0.15	78,78,78,78	0

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.

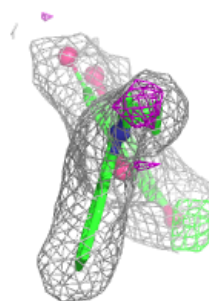
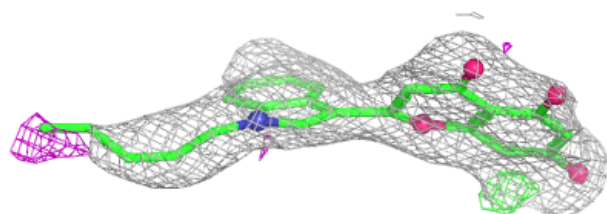
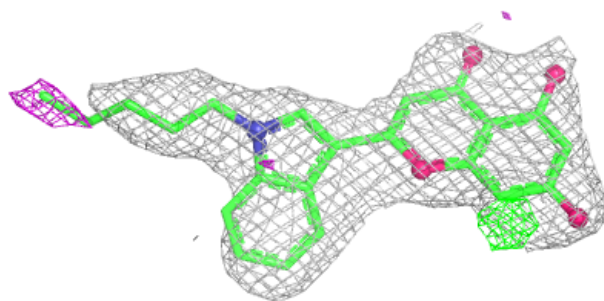
Electron density around 5JK A 902:

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



Electron density around T8R A 901:

$2mF_o-DF_c$ (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.