



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:07 PM UTC

PDB ID : 7G4A / pdb_00007g4a
Title : Crystal Structure of rat Autotaxin in complex with (3-chloro-5-methylsulfonylphenyl)methyl 2-(1H-benzotriazole-5-carbonyl)-2,7-diazaspiro[3.5]nonane-7-carboxylate, i.e. SMILES c1c(cc(cc1S(=O)(=O)C)COC(=O)N1CCC2(CC1)CN(C2)C(=O)c1ccc2c(c1)N=NN2)Cl with IC50=0.332347 microM
Authors : Stihle, M.; Benz, J.; Hunziker, D.; Mattei, P.; Rudolph, M.G.
Deposited on : 2023-06-05
Resolution : 2.67 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	:	4-5-2 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

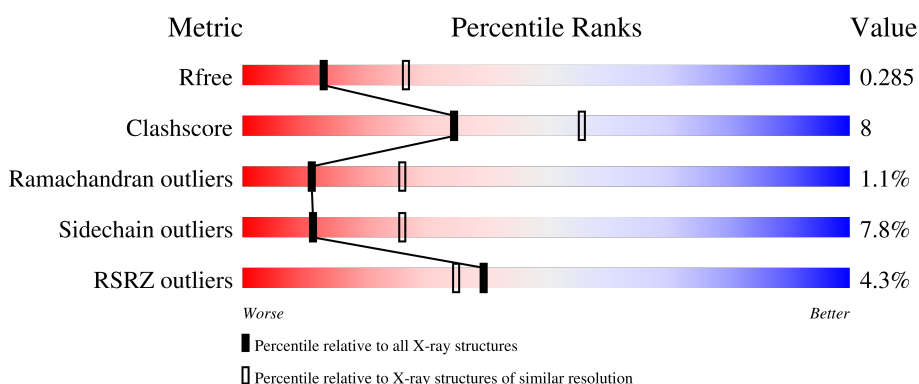
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	4% 71% 23% 5%
2	B	9	11% 89%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6785 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.

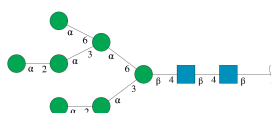
- Molecule 1 is a protein called Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	806	Total	C	N	O	S	0	0	0
			6508	4126	1122	1211	49			

There are 14 discrepancies between the modelled and reference sequences:

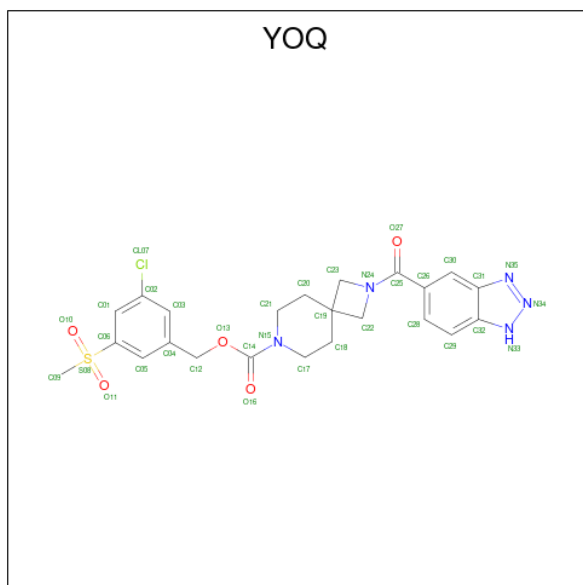
Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ALA	ASN	engineered mutation	UNP Q64610
A	410	ALA	ASN	engineered mutation	UNP Q64610
A	591	THR	ARG	engineered mutation	UNP Q64610
A	863	GLY	-	expression tag	UNP Q64610
A	864	GLY	-	expression tag	UNP Q64610
A	865	ARG	-	expression tag	UNP Q64610
A	866	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-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



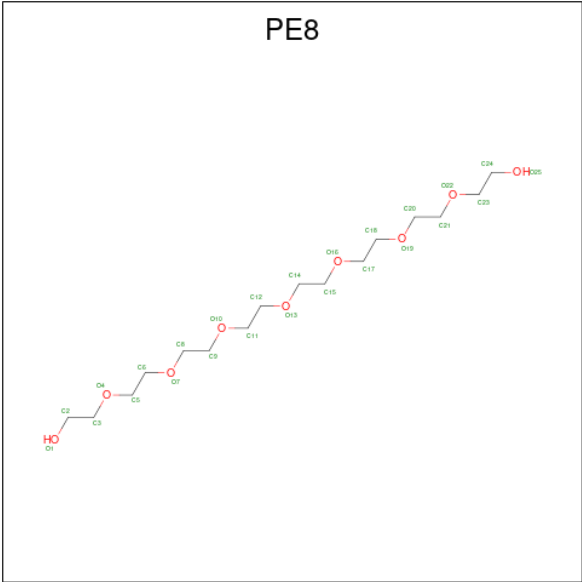
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 3 is [3-chloro-5-(methanesulfonyl)phenyl]methyl 2-(1H-benzotriazole-5-carbonyl)-2,7-diazaspiro[3.5]nonane-7-carboxylate (CCD ID: YOQ) (formula: C₂₃H₂₄ClN₅O₅S) (labeled as "Ligand of Interest" by depositor).



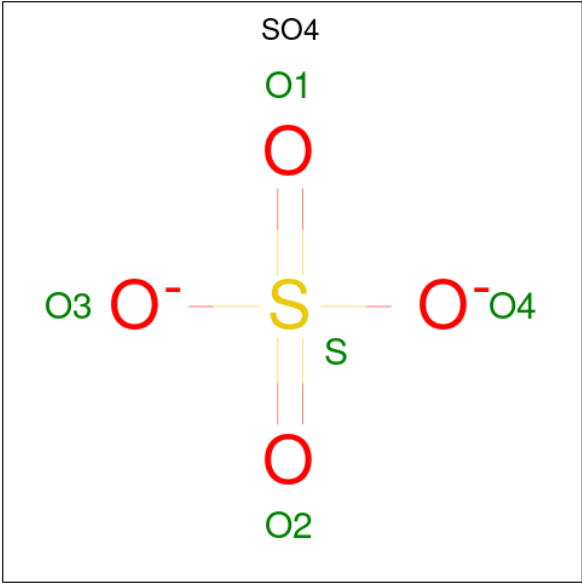
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			35	23	1	5	5	1		

- Molecule 4 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: C₁₆H₃₄O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			25	16	9		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

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

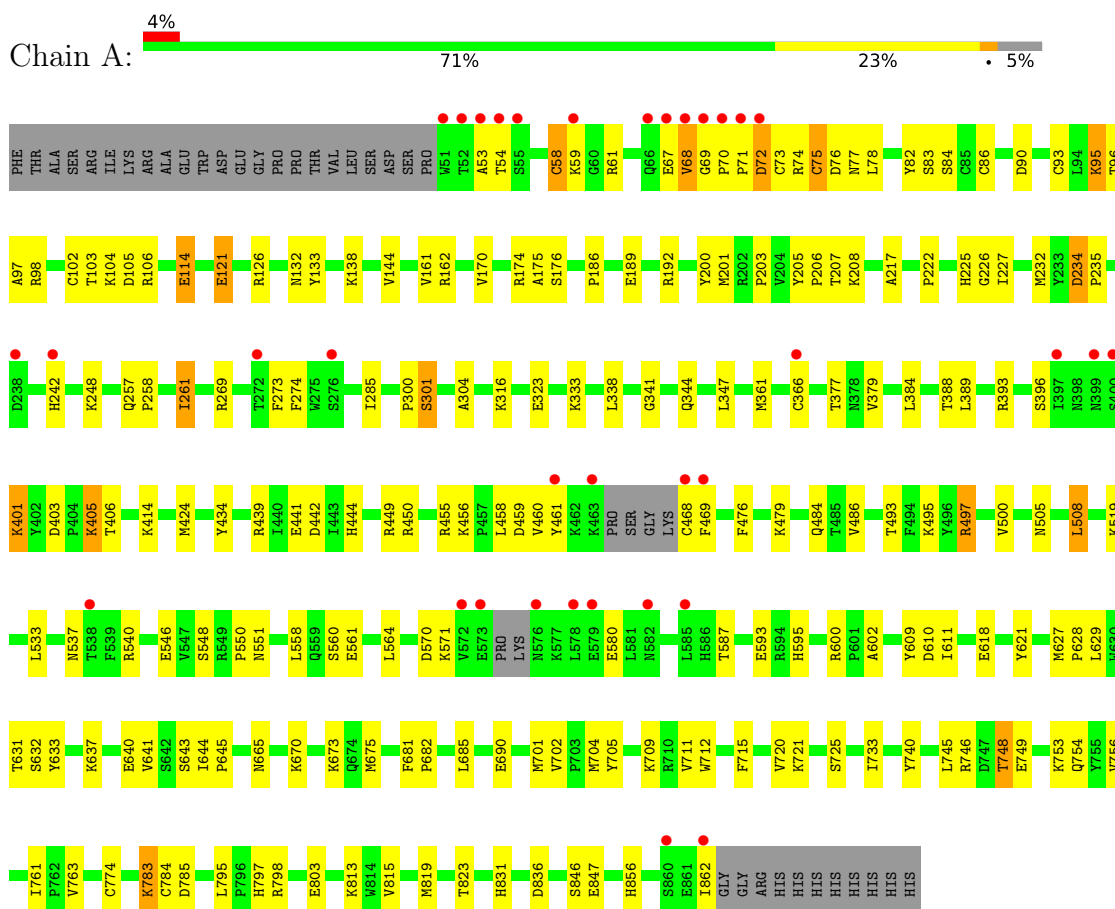
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	104	Total 104	O 104	0	0

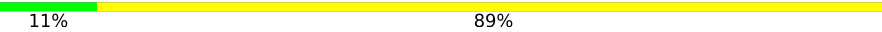
3 Residue-property plots [i](#)

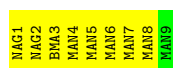
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.81Å 93.17Å 119.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.58 – 2.67 46.58 – 2.67	Depositor EDS
% Data completeness (in resolution range)	88.1 (46.58-2.67) 82.1 (46.58-2.67)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.69Å)	Xtriage
Refinement program	PHENIX dev_1019	Depositor
R, R_{free}	0.211 , 0.294 0.212 , 0.285	Depositor DCC
R_{free} test set	1294 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.815	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6785	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: NAG, CA, ZN, PE8, MAN, YOQ, SO4, BMA

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	0.58	0/6690	0.94	17/9073 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ASP	CA-C-N	7.10	126.93	119.05
1	A	234	ASP	C-N-CA	7.10	126.93	119.05
1	A	629	LEU	N-CA-C	-6.97	104.92	113.50
1	A	627	MET	CA-C-N	-6.89	113.21	120.03
1	A	627	MET	C-N-CA	-6.89	113.21	120.03
1	A	798	ARG	CA-C-N	6.83	127.42	120.04
1	A	798	ARG	C-N-CA	6.83	127.42	120.04
1	A	175	ALA	N-CA-C	6.10	118.71	111.33
1	A	424	MET	N-CA-C	-5.78	101.93	110.48
1	A	580	GLU	N-CA-C	-5.69	106.30	113.18
1	A	519	LYS	CA-C-N	5.66	126.55	119.98
1	A	519	LYS	C-N-CA	5.66	126.55	119.98
1	A	69	GLY	CA-C-N	5.37	125.91	120.38
1	A	69	GLY	C-N-CA	5.37	125.91	120.38
1	A	644	ILE	CA-C-N	5.35	125.34	119.89
1	A	644	ILE	C-N-CA	5.35	125.34	119.89
1	A	486	VAL	N-CA-C	5.19	117.08	108.99

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	6508	0	6254	96	0
2	B	105	0	88	0	0
3	A	35	0	0	1	0
4	A	25	0	34	3	0
5	A	5	0	0	0	0
6	A	1	0	0	0	0
7	A	2	0	0	0	0
8	A	104	0	0	4	0
All	All	6785	0	6376	98	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 8.

All (98) 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:93:CYS:SG	8:A:1099:HOH:O	2.28	0.89
1:A:61:ARG:NH1	1:A:73:CYS:O	2.19	0.75
1:A:54:THR:HA	1:A:73:CYS:HB3	1.69	0.74
1:A:333:LYS:NZ	8:A:1003:HOH:O	2.23	0.72
1:A:53:ALA:H	1:A:71:PRO:HB2	1.56	0.70
1:A:258:PRO:HG2	1:A:261:ILE:HG13	1.76	0.67
1:A:795:LEU:HD21	1:A:819:MET:HG2	1.77	0.67
1:A:174:ARG:NH1	1:A:361:MET:O	2.31	0.63
1:A:205:TYR:OH	1:A:444:HIS:NE2	2.22	0.61
1:A:226:GLY:O	1:A:439:ARG:NH1	2.33	0.61
1:A:637:LYS:HG3	1:A:725:SER:HA	1.84	0.60
1:A:97:ALA:O	8:A:1001:HOH:O	2.15	0.60
1:A:595:HIS:HB3	1:A:633:TYR:HA	1.83	0.60
1:A:570:ASP:N	1:A:570:ASP:OD1	2.35	0.59
1:A:341:GLY:HA2	1:A:344:GLN:HG3	1.84	0.59
1:A:595:HIS:O	1:A:632:SER:OG	2.18	0.59
3:A:901:YOQ:C17	4:A:902:PE8:H241	2.33	0.58
1:A:458:LEU:HA	1:A:461:TYR:CE2	2.38	0.58
1:A:468:CYS:SG	1:A:469:PHE:N	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ASP:OD1	1:A:405:LYS:NZ	2.30	0.57
1:A:745:LEU:HD23	1:A:831:HIS:HB3	1.87	0.56
1:A:68:VAL:HG23	1:A:74:ARG:HG2	1.87	0.56
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.41	0.55
1:A:675:MET:HG2	1:A:756:VAL:HG22	1.88	0.55
1:A:225:HIS:CE1	1:A:227:ILE:HB	2.41	0.55
1:A:323:GLU:OE1	1:A:323:GLU:N	2.36	0.55
1:A:58:CYS:SG	1:A:86:CYS:HB2	2.47	0.54
1:A:269:ARG:HB3	1:A:300:PRO:HA	1.90	0.53
1:A:274:PHE:CD2	4:A:902:PE8:H202	2.44	0.53
1:A:189:GLU:OE2	1:A:192:ARG:NH1	2.38	0.52
1:A:550:PRO:HB3	1:A:609:TYR:CZ	2.45	0.52
1:A:201:MET:HE3	1:A:505:ASN:HB3	1.91	0.51
1:A:403:ASP:O	1:A:406:THR:OG1	2.23	0.51
1:A:564:LEU:HB3	1:A:665:ASN:HA	1.92	0.51
1:A:740:TYR:OH	1:A:763:VAL:O	2.22	0.51
1:A:740:TYR:HB3	1:A:753:LYS:HD3	1.92	0.51
1:A:711:VAL:HG13	1:A:815:VAL:HG13	1.94	0.50
1:A:206:PRO:O	1:A:208:LYS:N	2.38	0.50
1:A:550:PRO:HB2	1:A:611:ILE:HG12	1.93	0.50
1:A:631:THR:O	1:A:733:ILE:HA	2.13	0.49
1:A:495:LYS:HG3	1:A:533:LEU:O	2.13	0.49
1:A:401:LYS:HB2	1:A:401:LYS:NZ	2.28	0.49
1:A:105:ASP:OD1	1:A:106:ARG:N	2.45	0.49
1:A:144:VAL:HG21	1:A:186:PRO:HB2	1.96	0.48
4:A:902:PE8:H112	4:A:902:PE8:H82	1.58	0.48
1:A:641:VAL:HG22	1:A:685:LEU:HD21	1.96	0.48
1:A:455:ARG:NH2	1:A:456:LYS:HE2	2.28	0.47
1:A:449:ARG:O	1:A:450:ARG:HB2	2.14	0.47
1:A:643:SER:O	1:A:645:PRO:HD3	2.15	0.46
1:A:206:PRO:HD3	1:A:434:TYR:CE1	2.50	0.46
1:A:285:ILE:HD12	1:A:338:LEU:HD13	1.96	0.46
1:A:393:ARG:HB3	1:A:441:GLU:HG2	1.98	0.46
1:A:95:LYS:HE2	1:A:114:GLU:HA	1.96	0.46
1:A:341:GLY:O	1:A:344:GLN:HB2	2.16	0.45
1:A:61:ARG:O	1:A:75:CYS:HB2	2.17	0.45
1:A:704:MET:HE1	1:A:712:TRP:CE2	2.52	0.45
1:A:456:LYS:NZ	1:A:458:LEU:HD21	2.32	0.45
1:A:414:LYS:HD3	1:A:414:LYS:HA	1.74	0.45
1:A:82:TYR:C	1:A:84:SER:H	2.25	0.45
1:A:257:GLN:HA	1:A:258:PRO:HD2	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASP:O	1:A:78:LEU:N	2.48	0.45
1:A:551:ASN:HB2	1:A:610:ASP:OD1	2.16	0.45
1:A:546:GLU:OE2	1:A:600:ARG:NH2	2.49	0.44
1:A:133:TYR:OH	1:A:138:LYS:NZ	2.50	0.44
1:A:621:TYR:HA	1:A:628:PRO:HA	1.98	0.44
1:A:162:ARG:HD2	1:A:301:SER:OG	2.18	0.44
1:A:72:ASP:OD1	1:A:72:ASP:N	2.51	0.44
1:A:200:TYR:HE2	1:A:484:GLN:HE21	1.63	0.44
1:A:774:CYS:HB2	1:A:784:CYS:HB2	1.45	0.44
1:A:347:LEU:HD23	1:A:347:LEU:HA	1.84	0.44
1:A:458:LEU:HA	1:A:461:TYR:CZ	2.53	0.43
1:A:76:ASP:C	1:A:78:LEU:H	2.25	0.43
1:A:681:PHE:CD1	1:A:682:PRO:HD2	2.54	0.43
1:A:602:ALA:HB3	1:A:836:ASP:HB3	2.00	0.43
1:A:715:PHE:O	1:A:720:VAL:HG23	2.19	0.43
1:A:600:ARG:HD2	1:A:611:ILE:HD11	2.02	0.42
1:A:704:MET:HA	1:A:797:HIS:NE2	2.35	0.42
1:A:455:ARG:HB3	1:A:459:ASP:OD2	2.19	0.42
1:A:98:ARG:NH1	1:A:106:ARG:HG2	2.35	0.42
1:A:497:ARG:HH11	1:A:497:ARG:HB3	1.84	0.42
1:A:222:PRO:HD2	8:A:1055:HOH:O	2.19	0.42
1:A:388:THR:HG22	1:A:476:PHE:CZ	2.54	0.42
1:A:746:ARG:HH12	1:A:748:THR:HG22	1.84	0.42
1:A:102:CYS:N	1:A:132:ASN:HD21	2.18	0.42
1:A:234:ASP:HA	1:A:235:PRO:HD3	1.77	0.42
1:A:721:LYS:HA	1:A:721:LYS:HD2	1.84	0.42
1:A:500:VAL:HG21	1:A:533:LEU:HD11	2.01	0.41
1:A:705:TYR:O	1:A:709:LYS:HG3	2.20	0.41
1:A:126:ARG:HE	1:A:126:ARG:HB3	1.50	0.41
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.86	0.41
1:A:273:PHE:HA	1:A:304:ALA:HB3	2.03	0.41
1:A:558:LEU:N	1:A:561:GLU:OE1	2.44	0.41
1:A:393:ARG:NH1	1:A:441:GLU:OE2	2.54	0.40
1:A:823:THR:HG21	1:A:856:HIS:O	2.21	0.40
1:A:82:TYR:O	1:A:84:SER:N	2.54	0.40
1:A:217:ALA:O	1:A:258:PRO:HA	2.20	0.40
1:A:756:VAL:HB	1:A:761:ILE:HB	2.02	0.40
1:A:702:VAL:HG23	1:A:704:MET:HE3	2.03	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	800/846 (95%)	731 (91%)	60 (8%)	9 (1%)	11	26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	77	ASN
1	A	121	GLU
1	A	207	THR
1	A	83	SER
1	A	366	CYS
1	A	783	LYS
1	A	203	PRO
1	A	70	PRO

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	729/765 (95%)	672 (92%)	57 (8%)	11	26

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	CYS
1	A	67	GLU

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Mol	Chain	Res	Type
1	A	68	VAL
1	A	72	ASP
1	A	75	CYS
1	A	90	ASP
1	A	95	LYS
1	A	96	THR
1	A	103	THR
1	A	104	LYS
1	A	114	GLU
1	A	121	GLU
1	A	161	VAL
1	A	170	VAL
1	A	176	SER
1	A	232	MET
1	A	242	HIS
1	A	248	LYS
1	A	261	ILE
1	A	301	SER
1	A	316	LYS
1	A	377	THR
1	A	379	VAL
1	A	384	LEU
1	A	389	LEU
1	A	396	SER
1	A	401	LYS
1	A	405	LYS
1	A	442	ASP
1	A	460	VAL
1	A	479	LYS
1	A	493	THR
1	A	497	ARG
1	A	508	LEU
1	A	537	ASN
1	A	540	ARG
1	A	548	SER
1	A	560	SER
1	A	571	LYS
1	A	587	THR
1	A	593	GLU
1	A	618	GLU
1	A	640	GLU
1	A	670	LYS

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Mol	Chain	Res	Type
1	A	673	LYS
1	A	690	GLU
1	A	701	MET
1	A	748	THR
1	A	749	GLU
1	A	754	GLN
1	A	783	LYS
1	A	785	ASP
1	A	803	GLU
1	A	813	LYS
1	A	846	SER
1	A	847	GLU
1	A	862	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	HIS
1	A	484	GLN
1	A	537	ASN
1	A	754	GLN
1	A	779	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](#)

9 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	0.65	0	17,19,21	1.00	2 (11%)
2	NAG	B	2	2	14,14,15	0.58	0	17,19,21	1.83	3 (17%)
2	BMA	B	3	2	11,11,12	0.69	0	15,15,17	0.84	1 (6%)
2	MAN	B	4	2	11,11,12	0.53	0	15,15,17	1.53	3 (20%)
2	MAN	B	5	2	11,11,12	0.47	0	15,15,17	1.07	1 (6%)
2	MAN	B	6	2	11,11,12	0.52	0	15,15,17	1.02	1 (6%)
2	MAN	B	7	2	11,11,12	0.53	0	15,15,17	1.33	1 (6%)
2	MAN	B	8	2	11,11,12	0.49	0	15,15,17	1.02	1 (6%)
2	MAN	B	9	2	11,11,12	0.59	0	15,15,17	0.60	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	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	1/2/19/22	0/1/1/1
2	MAN	B	5	2	-	1/2/19/22	0/1/1/1
2	MAN	B	6	2	-	1/2/19/22	0/1/1/1
2	MAN	B	7	2	-	2/2/19/22	1/1/1/1
2	MAN	B	8	2	-	2/2/19/22	0/1/1/1
2	MAN	B	9	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	5.18	119.13	112.19
2	B	4	MAN	C1-O5-C5	4.47	118.18	112.19
2	B	7	MAN	C1-O5-C5	4.07	117.64	112.19
2	B	6	MAN	C1-O5-C5	3.13	116.38	112.19
2	B	5	MAN	C1-O5-C5	2.62	115.69	112.19
2	B	3	BMA	C1-C2-C3	2.54	113.34	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	MAN	C1-O5-C5	2.41	115.42	112.19
2	B	4	MAN	C1-C2-C3	2.21	112.86	109.64
2	B	1	NAG	C2-N2-C7	-2.14	120.03	122.90
2	B	2	NAG	C3-C4-C5	2.14	114.12	110.23
2	B	4	MAN	C3-C4-C5	2.10	114.05	110.23
2	B	1	NAG	O5-C1-C2	-2.03	108.15	111.29
2	B	2	NAG	C6-C5-C4	-2.01	108.08	113.02

There are no chirality outliers.

All (13) torsion outliers are listed below:

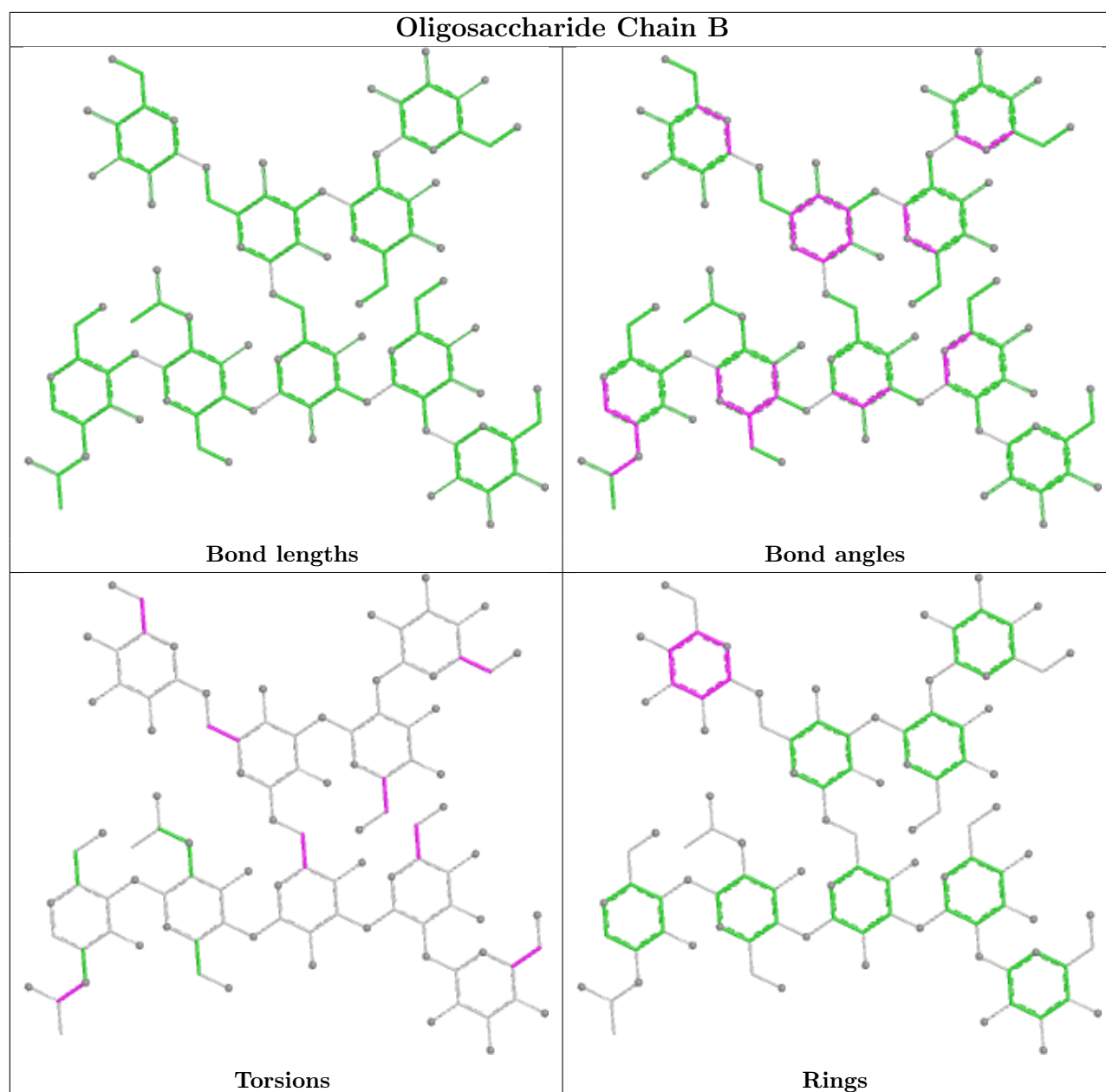
Mol	Chain	Res	Type	Atoms
2	B	9	MAN	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	8	MAN	O5-C5-C6-O6
2	B	8	MAN	C4-C5-C6-O6
2	B	9	MAN	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	7	MAN	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
2	B	5	MAN	O5-C5-C6-O6
2	B	6	MAN	C4-C5-C6-O6
2	B	7	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	7	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 ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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
5	SO4	A	903	-	4,4,4	0.28	0	6,6,6	0.18	0
3	YOQ	A	901	6	39,39,39	1.39	6 (15%)	49,59,59	1.50	4 (8%)
4	PE8	A	902	-	24,24,24	0.73	0	23,23,23	1.50	1 (4%)

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	YOQ	A	901	6	-	3/23/45/45	0/5/5/5
4	PE8	A	902	-	-	17/22/22/22	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	YOQ	C28-C26	3.28	1.44	1.39
3	A	901	YOQ	C22-C19	2.85	1.57	1.54
3	A	901	YOQ	C23-N24	2.63	1.50	1.47
3	A	901	YOQ	C31-N35	-2.57	1.34	1.38
3	A	901	YOQ	O16-C14	2.34	1.24	1.21
3	A	901	YOQ	C14-N15	2.26	1.39	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	YOQ	O27-C25-N24	-5.32	113.97	122.35
3	A	901	YOQ	C26-C25-N24	5.01	124.92	118.66
3	A	901	YOQ	C05-C06-S08	2.63	121.13	119.02
3	A	901	YOQ	C23-N24-C22	-2.47	92.97	95.12
4	A	902	PE8	O19-C18-C17	2.16	120.20	110.35

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	YOQ	C26-C25-N24-C22
3	A	901	YOQ	O27-C25-N24-C22
4	A	902	PE8	C8-C9-O10-C11
4	A	902	PE8	O19-C20-C21-O22

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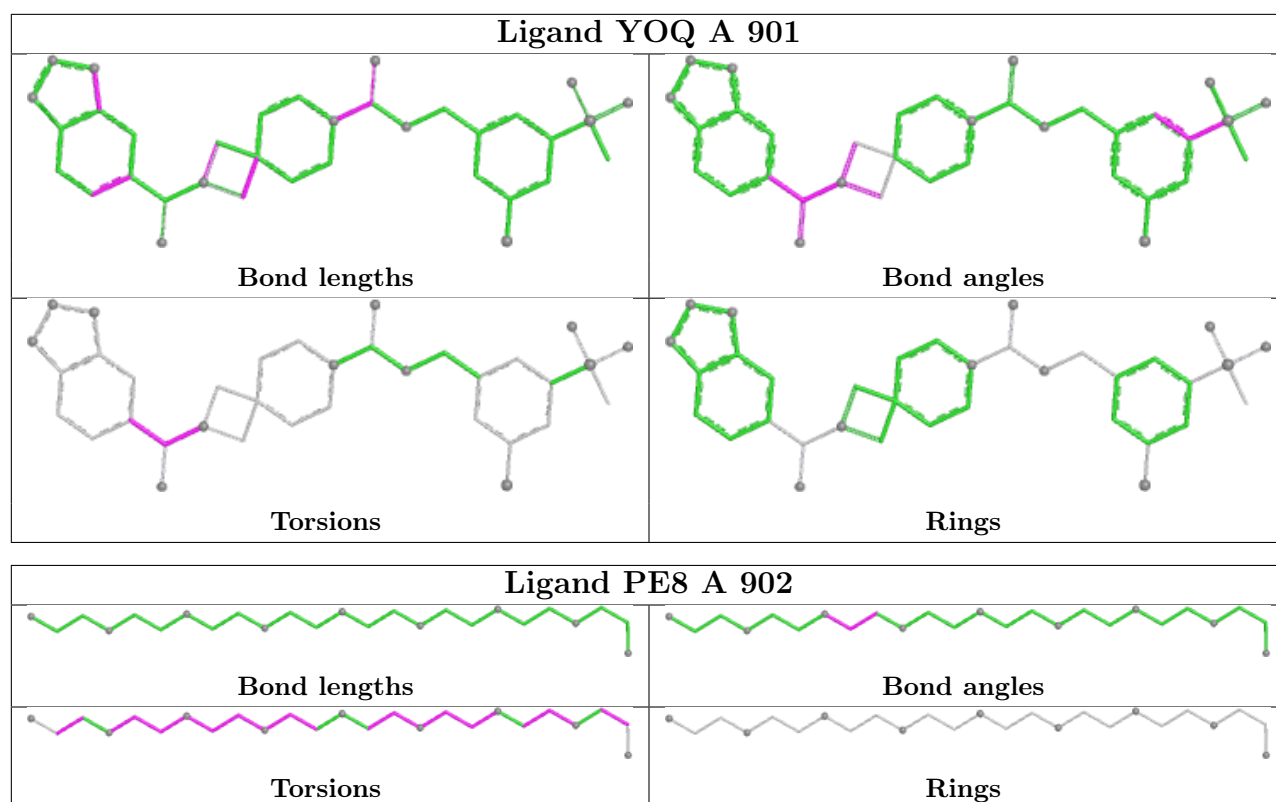
Mol	Chain	Res	Type	Atoms
4	A	902	PE8	O16-C17-C18-O19
4	A	902	PE8	O13-C14-C15-O16
4	A	902	PE8	O22-C23-C24-O25
4	A	902	PE8	O7-C8-C9-O10
4	A	902	PE8	O10-C11-C12-O13
4	A	902	PE8	C12-C11-O10-C9
4	A	902	PE8	C21-C20-O19-C18
4	A	902	PE8	C20-C21-O22-C23
4	A	902	PE8	C18-C17-O16-C15
4	A	902	PE8	O4-C5-C6-O7
4	A	902	PE8	O1-C2-C3-O4
4	A	902	PE8	C17-C18-O19-C20
4	A	902	PE8	C6-C5-O4-C3
3	A	901	YOQ	O27-C25-C26-C28
4	A	902	PE8	C9-C8-O7-C6
4	A	902	PE8	C14-C15-O16-C17

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	YOQ	1	0
4	A	902	PE8	3	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	806/846 (95%)	0.48	35 (4%) 40 35	24, 44, 88, 146	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	TRP	4.1
1	A	862	ILE	3.9
1	A	463	LYS	3.7
1	A	68	VAL	3.7
1	A	461	TYR	3.3
1	A	71	PRO	3.3
1	A	397	ILE	3.2
1	A	70	PRO	3.1
1	A	469	PHE	3.1
1	A	572	VAL	3.0
1	A	468	CYS	2.8
1	A	69	GLY	2.7
1	A	579	GLU	2.7
1	A	238	ASP	2.7
1	A	66	GLN	2.6
1	A	54	THR	2.6
1	A	366	CYS	2.6
1	A	52	THR	2.5
1	A	53	ALA	2.5
1	A	582	ASN	2.4
1	A	573	GLU	2.4
1	A	578	LEU	2.4
1	A	272	THR	2.4
1	A	59	LYS	2.3
1	A	860	SER	2.3
1	A	242	HIS	2.2
1	A	67	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	585	LEU	2.2
1	A	72	ASP	2.2
1	A	538	THR	2.1
1	A	576	ASN	2.1
1	A	276	SER	2.1
1	A	399	ASN	2.1
1	A	55	SER	2.0
1	A	400	SER	2.0

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

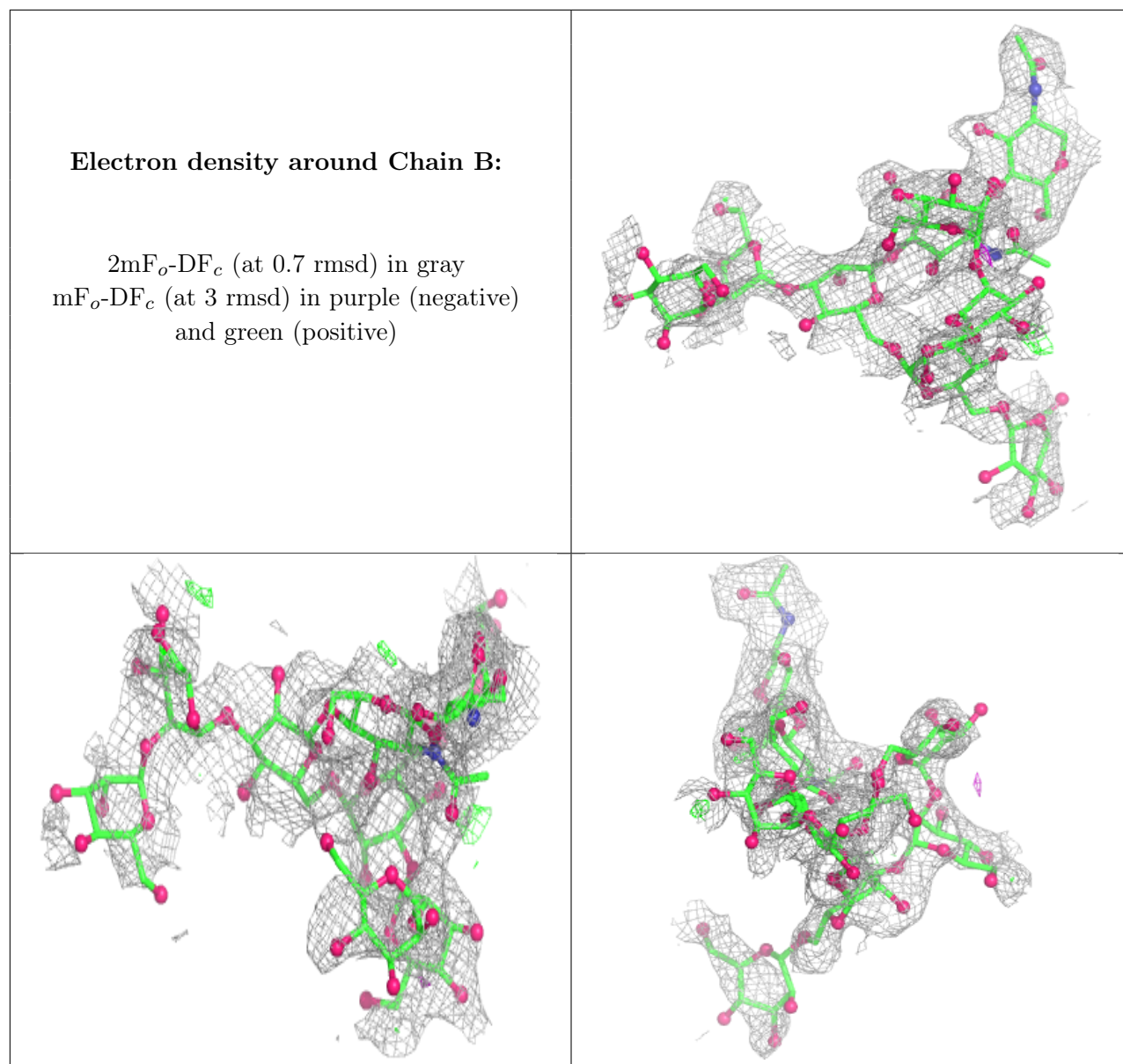
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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	MAN	B	4	11/12	0.45	0.16	115,122,139,146	0
2	MAN	B	8	11/12	0.49	0.19	136,142,147,151	0
2	MAN	B	7	11/12	0.58	0.19	138,147,151,152	0
2	BMA	B	3	11/12	0.59	0.14	98,107,116,129	0
2	MAN	B	5	11/12	0.67	0.21	107,115,121,121	0
2	MAN	B	6	11/12	0.68	0.21	106,116,119,124	0
2	MAN	B	9	11/12	0.68	0.20	145,149,154,156	0
2	NAG	B	2	14/15	0.80	0.12	37,53,68,85	0
2	NAG	B	1	14/15	0.92	0.08	24,38,43,45	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(Å ²)	Q<0.9
4	PE8	A	902	25/25	0.80	0.14	32,43,55,56	0
5	SO4	A	903	5/5	0.90	0.12	56,65,68,69	0
3	YOQ	A	901	35/35	0.92	0.10	27,37,51,58	0
7	CA	A	906	1/1	0.96	0.06	38,38,38,38	0
7	CA	A	905	1/1	0.99	0.05	28,28,28,28	0

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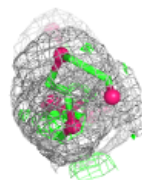
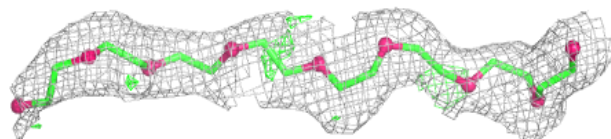
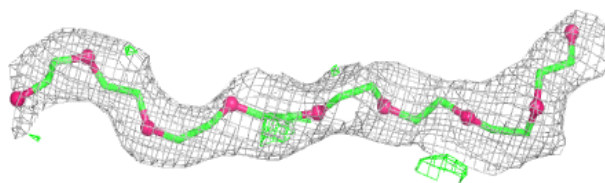
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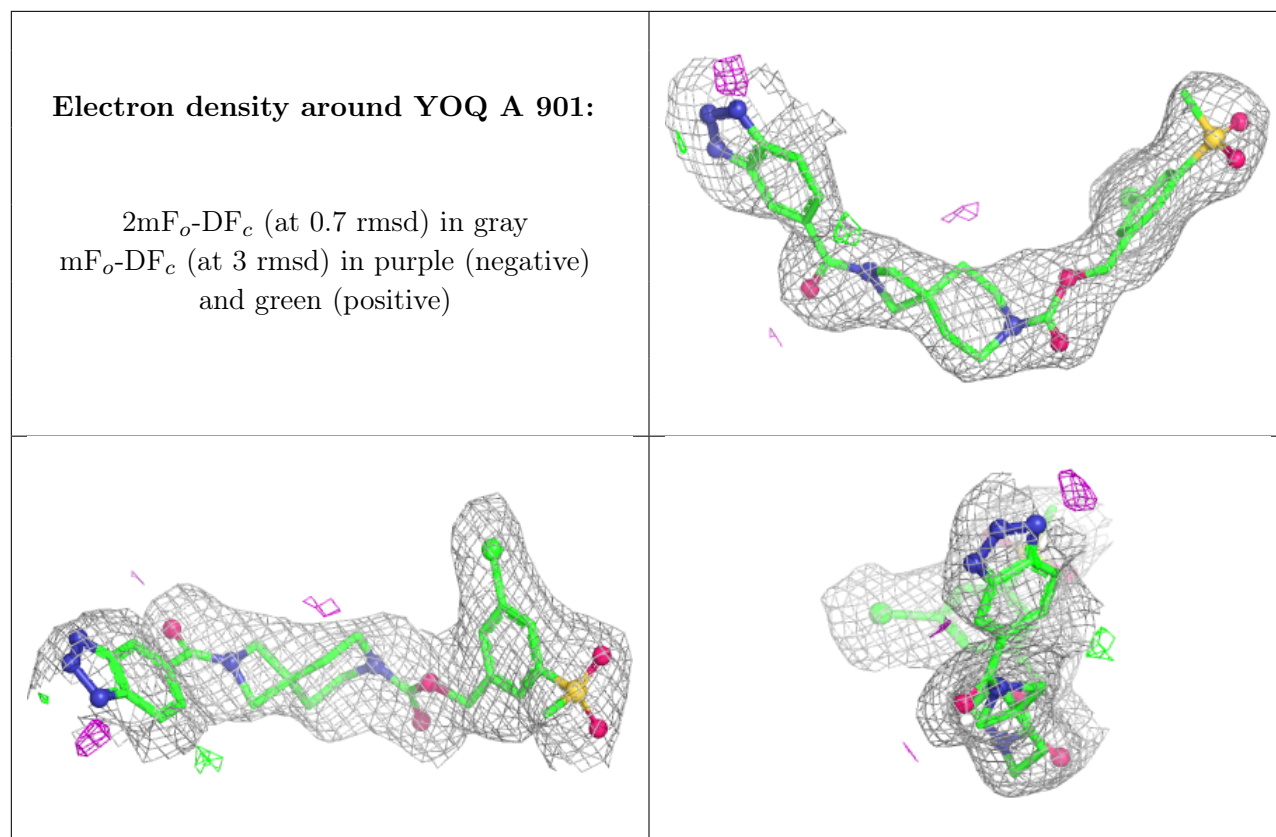
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ZN	A	904	1/1	0.99	0.06	30,30,30,30	0

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 PE8 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.