



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2025 – 12:42 pm GMT

PDB ID : 9F6R / pdb_00009f6r
Title : Crystal structure of human acetylcholinesterase in complex with the uncharged hybrid reactivator quinoline-3-hydroxy-pyridinaldoxime
Authors : Dias, J.; Nachon, F.
Deposited on : 2024-05-02
Resolution : 2.75 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

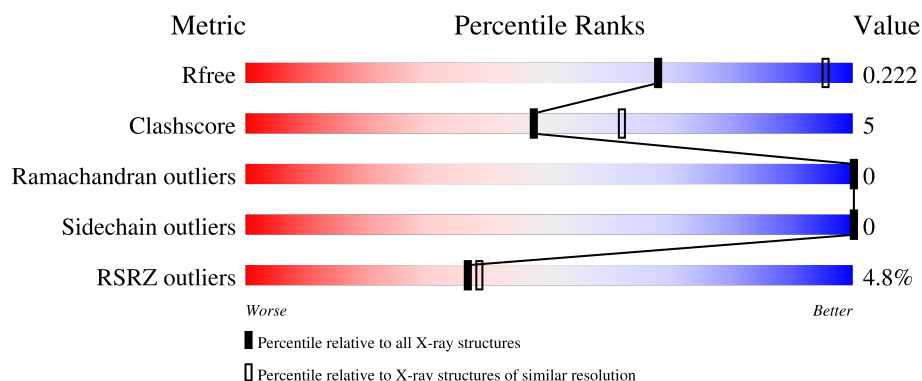
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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	543	<div> <div>4%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	B	543	<div> <div>5%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
2	C	3	<div> <div>33%</div> <div>67%</div> </div>
3	D	4	<div> <div>100%</div> </div>
4	H	2	<div> <div>50%</div> <div>50%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NA	A	660	-	-	-	X
10	NA	B	677	-	-	-	X
11	MG	A	701	-	-	-	X
12	A1AAJ	B	613	X	-	-	-
4	SIA	H	2	X	-	-	-
9	CL	B	643	-	-	-	X

2 Entry composition [i](#)

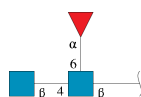
There are 14 unique types of molecules in this entry. The entry contains 9318 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylcholinesterase.

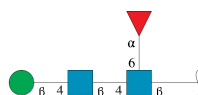
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	9	0
			4241	2723	741	764	13			
1	B	534	Total	C	N	O	S	0	1	0
			4164	2673	728	750	13			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



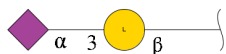
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



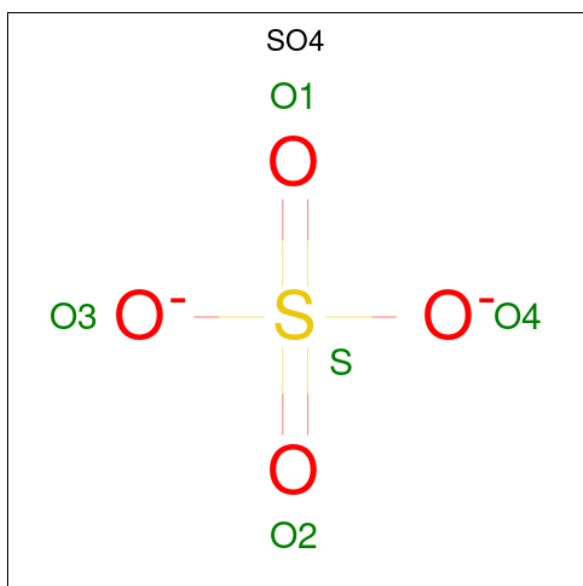
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-L-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	2	Total	C	N	O	0	0	0
			31	17	1	13			

- 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		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

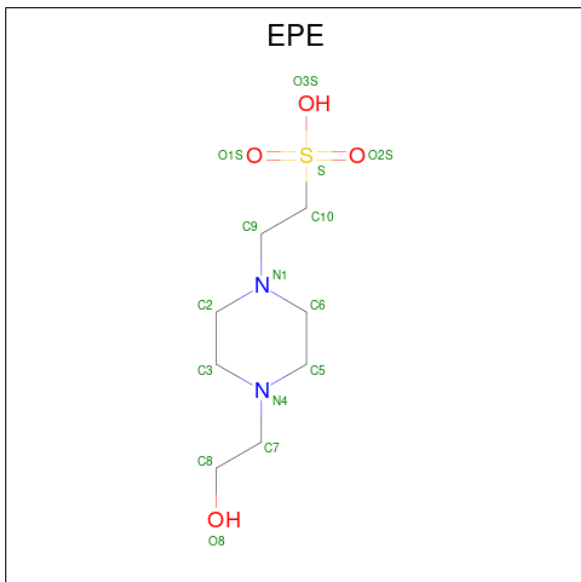
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



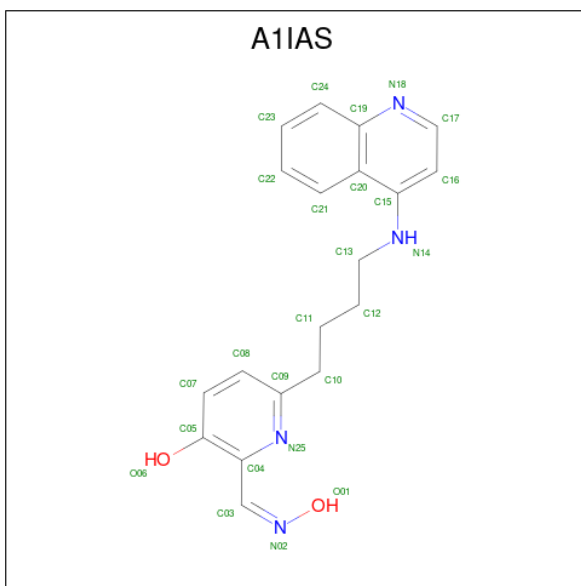
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total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

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 8 is 2-[({Z})-hydroxyiminomethyl]-6-[4-(quinolin-4-ylamino)butyl]pyridin-3-ol (CCD ID: A1IAS) (formula: $C_{19}H_{20}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	1
			25	19	4	2		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	19	Total	Cl	0	0
			19	19		
9	B	24	Total	Cl	0	0
			24	24		

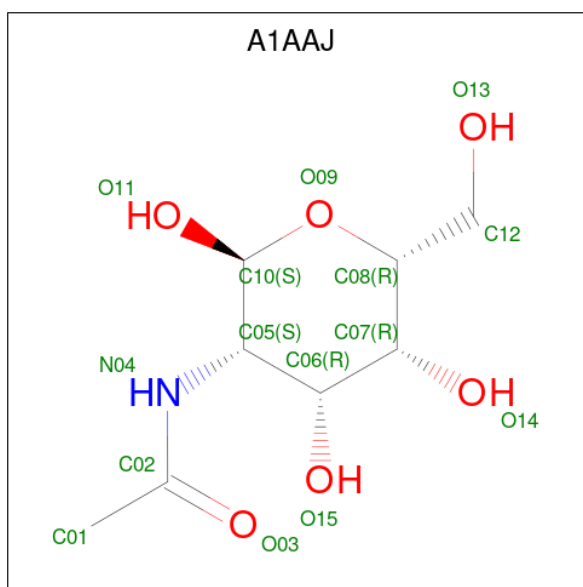
- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	46	Total	Na	0	0
			46	46		
10	B	36	Total	Na	0	0
			36	36		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

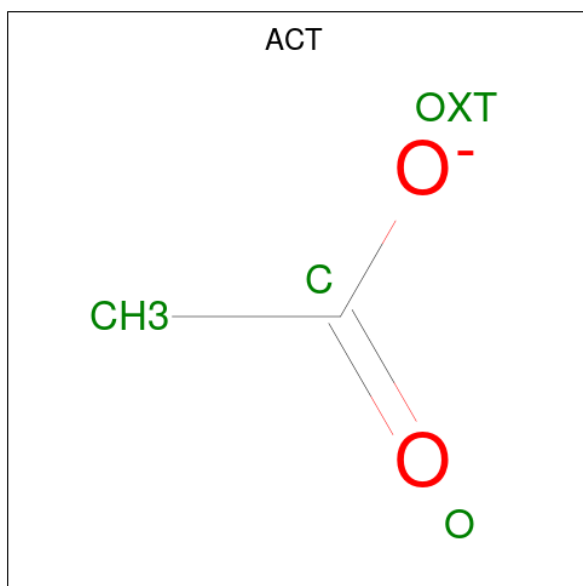
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	13	Total	Mg	0	0
			13	13		
11	B	3	Total	Mg	0	0
			3	3		

- Molecule 12 is N-Acetyl-D-Talosamine (CCD ID: A1AAJ) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 13 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			4	2	2		

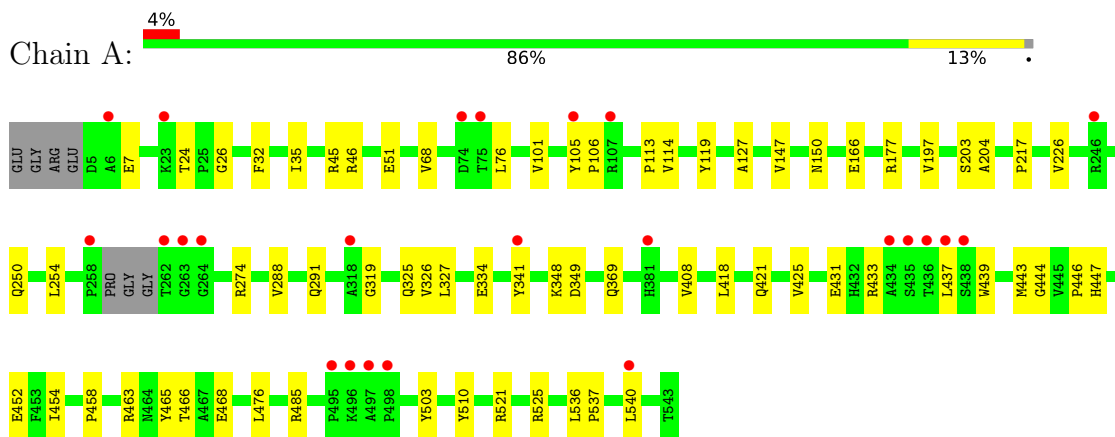
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	200	Total 200	O 200	0	0
14	B	171	Total 171	O 171	0	0

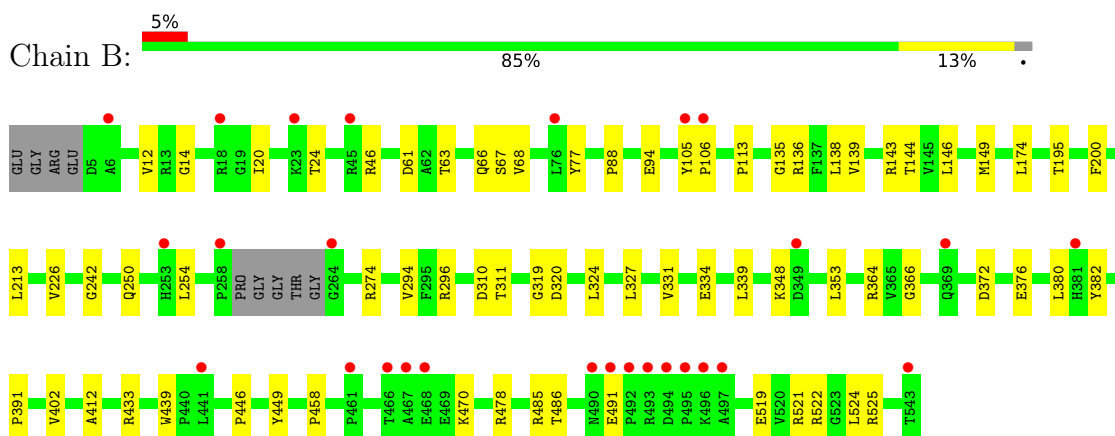
3 Residue-property plots [i](#)

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: Acetylcholinesterase



- Molecule 1: Acetylcholinesterase



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

MAG1
MAG2
BGA3
FUC4

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-L-galactopyranose

Chain H:  50%  50%

GIV1
STR2

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	210.74Å 210.74Å 114.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.98 – 2.75 68.98 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.8 (68.98-2.75) 98.9 (68.98-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.196 , 0.217 0.200 , 0.222	Depositor DCC
R_{free} test set	2001 reflections (2.65%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9318	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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: SO4, GIV, GOL, NA, MG, BMA, SIA, EPE, OAS, ACT, A1IAS, CL, FUC, NAG, A1AAJ

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	0.11	0/4368	0.28	0/5970
1	B	0.10	0/4285	0.27	0/5855
All	All	0.11	0/8653	0.27	0/11825

There are no bond length outliers.

There are no bond angle outliers.

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	4241	0	4117	43	0
1	B	4164	0	4042	48	0
2	C	38	0	34	0	0
3	D	49	0	43	0	0
4	H	31	0	27	2	0
5	A	65	0	0	0	0
5	B	60	0	0	0	0
6	A	54	0	72	2	0
6	B	30	0	40	2	0
7	A	15	0	18	2	0
7	B	15	0	18	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	25	0	0	0	0
9	A	19	0	0	1	0
9	B	24	0	0	4	0
10	A	46	0	0	0	0
10	B	36	0	0	0	0
11	A	13	0	0	0	0
11	B	3	0	0	0	0
12	B	15	0	0	0	0
13	B	4	0	3	0	0
14	A	200	0	0	2	0
14	B	171	0	0	5	0
All	All	9318	0	8414	95	0

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

All (95) 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:433[B]:ARG:NH1	1:A:444:GLY:O	2.23	0.72
1:B:113:PRO:HG3	1:B:485:ARG:HG2	1.71	0.71
1:A:452:GLU:OE1	1:A:465:TYR:OH	2.08	0.71
1:A:24:THR:HG22	1:A:26:GLY:H	1.57	0.68
1:A:466:THR:HG22	1:A:468:GLU:H	1.58	0.68
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.77	0.66
6:A:622:GOL:H11	7:A:623:EPE:H52	1.79	0.65
9:A:627:CL:CL	14:A:957:HOH:O	2.52	0.64
1:B:20:ILE:HB	1:B:63:THR:HG22	1.80	0.64
1:A:431:GLU:OE2	1:A:521:ARG:NH1	2.28	0.63
14:B:812:HOH:O	4:H:2:SIA:O1B	2.16	0.61
1:B:319:GLY:HA2	6:B:616:GOL:H31	1.81	0.61
1:B:525:ARG:NH1	14:B:701:HOH:O	2.32	0.60
1:B:106:PRO:HD2	1:B:143:ARG:HH21	1.68	0.59
1:A:46:ARG:O	1:A:274:ARG:NH1	2.36	0.59
1:B:12:VAL:HG23	1:B:14:GLY:H	1.67	0.59
1:B:138:LEU:HD23	1:B:146:LEU:HD12	1.85	0.58
1:B:46:ARG:O	1:B:274:ARG:NH1	2.36	0.57
1:B:412:ALA:HB2	1:B:524:LEU:HD23	1.85	0.57
1:B:310:ASP:OD1	1:B:311:THR:N	2.34	0.57
1:B:68:VAL:HG11	1:B:88:PRO:HB3	1.85	0.57
1:A:250:GLN:HG2	1:A:288:VAL:HG22	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ARG:NH1	14:B:702:HOH:O	2.32	0.56
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.88	0.56
1:B:226:VAL:HG22	1:B:327:LEU:HB3	1.87	0.55
1:B:213:LEU:HD22	1:B:324:LEU:HD21	1.89	0.54
1:B:61:ASP:OD1	1:B:63:THR:OG1	2.23	0.54
1:A:334:GLU:OE2	1:A:447:HIS:HD2	1.91	0.53
1:B:66:GLN:HG3	1:B:67:SER:H	1.72	0.53
1:A:348:LYS:NZ	1:A:349:ASP:OD1	2.36	0.52
1:A:203:OAS:HB3	1:A:447:HIS:HE1	1.73	0.52
1:B:380:LEU:O	1:B:382:TYR:N	2.41	0.51
1:A:203:OAS:HB3	1:A:447:HIS:CE1	2.45	0.51
1:B:135:GLY:HA3	1:B:146:LEU:HD13	1.91	0.51
1:A:101:VAL:HG22	1:A:147:VAL:HG22	1.93	0.51
1:B:46:ARG:NH2	1:B:94:GLU:OE2	2.34	0.51
1:B:521:ARG:NH1	14:B:716:HOH:O	2.43	0.50
1:B:446:PRO:HG2	1:B:449:TYR:CD2	2.46	0.50
1:B:433:ARG:NH2	1:B:439:TRP:O	2.38	0.50
1:B:486:THR:HG21	1:B:491:GLU:HG3	1.94	0.50
1:B:478:ARG:HD2	9:B:624:CL:CL	2.48	0.49
9:B:625:CL:CL	9:B:628:CL:CL	3.04	0.49
1:A:463:ARG:NH1	14:A:810:HOH:O	2.45	0.49
1:A:466:THR:HG22	1:A:468:GLU:N	2.27	0.49
1:B:106:PRO:O	1:B:143:ARG:NH2	2.46	0.49
1:A:439[A]:TRP:HB3	1:A:443:MET:HE2	1.95	0.48
1:A:45:ARG:NH1	1:A:51:GLU:OE2	2.46	0.48
1:A:76:LEU:HD22	1:A:341:TYR:CE1	2.48	0.48
1:A:433[B]:ARG:NH2	1:A:437[B]:LEU:HD21	2.29	0.48
1:B:174:LEU:HD13	4:H:2:SIA:H8	1.95	0.47
1:A:291:GLN:HE22	1:A:369:GLN:HG3	1.79	0.47
1:A:433[B]:ARG:HH21	1:A:437[B]:LEU:HD21	1.79	0.47
1:B:294:VAL:HG12	1:B:366:GLY:HA2	1.97	0.47
1:A:105:TYR:HB3	1:A:106:PRO:HD3	1.98	0.46
1:A:119:TYR:HE2	1:A:150:ASN:HA	1.80	0.46
7:A:623:EPE:O8	1:B:522:ARG:NH1	2.45	0.46
1:B:242:GLY:HA3	7:B:617:EPE:H101	1.97	0.46
1:B:339:LEU:HD21	1:B:402:VAL:HG21	1.97	0.46
1:A:408:VAL:HG11	1:A:525:ARG:HG3	1.97	0.45
1:A:226:VAL:HG22	1:A:327:LEU:HB3	1.98	0.45
1:B:478:ARG:NH1	14:B:715:HOH:O	2.42	0.45
1:A:7:GLU:H	1:A:7:GLU:CD	2.23	0.44
1:A:425:VAL:O	1:A:503:TYR:N	2.41	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:PRO:O	1:B:470:LYS:HE3	2.17	0.44
1:A:166:GLU:OE1	1:A:274:ARG:NH2	2.50	0.44
1:A:458:PRO:HA	1:A:465:TYR:CD1	2.53	0.44
1:B:320:ASP:H	6:B:616:GOL:H11	1.81	0.44
1:B:331:VAL:HG22	1:B:334:GLU:CD	2.42	0.44
1:A:114:VAL:HB	1:A:197:VAL:HG22	2.00	0.43
1:A:177:ARG:CZ	1:A:217:PRO:HB2	2.48	0.43
1:A:319:GLY:O	1:A:421:GLN:NE2	2.51	0.43
1:A:540:LEU:HD22	1:A:540:LEU:H	1.83	0.43
1:B:77:TYR:CZ	1:B:348:LYS:HG2	2.53	0.43
1:B:24:THR:HG22	1:B:136:ARG:HD3	2.00	0.43
1:A:203:OAS:OG	1:A:204:ALA:N	2.48	0.43
1:A:510:TYR:CZ	1:A:521:ARG:HB2	2.53	0.43
1:B:105:TYR:HB3	1:B:106:PRO:HD3	2.00	0.43
1:A:536:LEU:HB3	1:A:537:PRO:HD3	2.01	0.43
1:A:68:VAL:HG13	1:A:127:ALA:HB2	1.99	0.42
1:A:32:PHE:HB3	1:A:35:ILE:HD11	2.01	0.42
1:B:200:PHE:CB	1:B:226:VAL:HB	2.49	0.42
1:B:372:ASP:O	1:B:376:GLU:HG3	2.18	0.42
1:B:296:ARG:HA	1:B:296:ARG:HD3	1.84	0.42
1:B:439:TRP:NE1	1:B:449:TYR:OH	2.41	0.42
1:B:519:GLU:OE2	1:B:521:ARG:NE	2.42	0.42
1:A:325:GLN:HE22	6:A:614:GOL:H12	1.84	0.42
1:B:149:MET:HE2	1:B:149:MET:HB3	1.94	0.41
1:A:444:GLY:O	1:A:446:PRO:HD3	2.20	0.41
1:A:250:GLN:HE21	1:A:254:LEU:HD21	1.85	0.41
1:A:454:ILE:HD13	1:A:476:LEU:HB3	2.02	0.41
1:B:77:TYR:CE2	9:B:643:CL:CL	3.11	0.41
1:B:139:VAL:HG13	1:B:144:THR:O	2.21	0.41
1:B:195:THR:HG22	9:B:640:CL:CL	2.57	0.41
1:A:326:VAL:HG21	1:A:418:LEU:HD13	2.02	0.40
1:B:250:GLN:O	1:B:254:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	540/543 (99%)	515 (95%)	25 (5%)	0	100	100
1	B	530/543 (98%)	502 (95%)	28 (5%)	0	100	100
All	All	1070/1086 (98%)	1017 (95%)	53 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	441/437 (101%)	441 (100%)	0	100	100
1	B	433/437 (99%)	433 (100%)	0	100	100
All	All	874/874 (100%)	874 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	228	GLN
1	A	250	GLN
1	A	284	HIS
1	A	291	GLN
1	A	317	ASN
1	A	447	HIS
1	A	474	GLN
1	A	509	GLN
1	B	387	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	OAS	B	203	1	7,8,9	0.50	0	5,9,11	0.33	0
1	OAS	A	203	1,10	7,8,9	0.49	0	5,9,11	0.35	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
1	OAS	B	203	1	-	0/5/7/9	-
1	OAS	A	203	1,10	-	3/5/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	203	OAS	OAC-C1A-OG-CB
1	A	203	OAS	C2A-C1A-OG-CB
1	A	203	OAS	C-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	203	OAS	3	0

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	C	1	1,2	14,14,15	0.70	0	17,19,21	1.16	1 (5%)
2	NAG	C	2	2	14,14,15	0.73	0	17,19,21	1.56	4 (23%)
2	FUC	C	3	2	10,10,11	0.76	0	14,14,16	0.98	0
3	NAG	D	1	1,3	14,14,15	0.79	0	17,19,21	1.87	5 (29%)
3	NAG	D	2	3	14,14,15	0.76	0	17,19,21	2.02	5 (29%)
3	BMA	D	3	3	11,11,12	0.78	0	15,15,17	3.13	7 (46%)
3	FUC	D	4	3	10,10,11	0.74	0	14,14,16	1.09	1 (7%)
4	GIV	H	1	12,4	11,11,12	1.49	2 (18%)	15,15,17	2.17	7 (46%)
4	SIA	H	2	4	20,20,21	3.46	10 (50%)	24,28,31	3.58	10 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	FUC	D	4	3	-	-	0/1/1/1
4	GIV	H	1	12,4	-	0/2/19/22	0/1/1/1
4	SIA	H	2	4	2/2/8/9	8/18/34/38	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	SIA	O10-C10	7.81	1.40	1.23
4	H	2	SIA	C2-C1	5.84	1.57	1.52
4	H	2	SIA	O1A-C1	5.83	1.39	1.22
4	H	2	SIA	C4-C5	5.16	1.57	1.53
4	H	2	SIA	C7-C6	4.84	1.59	1.53
4	H	2	SIA	C10-N5	4.50	1.49	1.34
4	H	2	SIA	C6-C5	3.36	1.58	1.53
4	H	2	SIA	O1B-C1	3.08	1.40	1.30
4	H	1	GIV	C1-C2	2.86	1.58	1.52
4	H	1	GIV	C2-C3	2.47	1.56	1.52
4	H	2	SIA	C11-C10	2.16	1.55	1.50
4	H	2	SIA	C5-N5	2.06	1.49	1.45

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2	SIA	O10-C10-N5	-9.98	103.60	121.95
3	D	3	BMA	C1-O5-C5	9.89	125.59	112.19
4	H	2	SIA	O1B-C1-O1A	-7.62	106.78	124.09
4	H	2	SIA	O10-C10-C11	-6.14	110.65	122.06
4	H	2	SIA	O1A-C1-C2	-5.74	109.01	122.57
3	D	1	NAG	C2-N2-C7	5.56	130.82	122.90
3	D	2	NAG	C2-N2-C7	5.35	130.52	122.90
4	H	1	GIV	O3-C3-C2	4.34	118.30	109.99
4	H	2	SIA	C5-N5-C10	-3.88	113.73	123.18
4	H	2	SIA	C6-O6-C2	3.66	119.17	111.34
3	D	3	BMA	C3-C4-C5	3.61	116.68	110.24
2	C	2	NAG	C4-C3-C2	3.58	116.26	111.02
3	D	2	NAG	C4-C3-C2	3.34	115.91	111.02
4	H	1	GIV	C1-C2-C3	-3.11	105.85	109.67
4	H	2	SIA	O9-C9-C8	-3.05	104.42	111.07
3	D	3	BMA	O5-C5-C4	3.00	118.13	110.83
4	H	2	SIA	O1B-C1-C2	-3.00	104.47	113.03
4	H	1	GIV	O3-C3-C4	-2.97	103.48	110.35
4	H	1	GIV	C6-C5-C4	-2.96	106.08	113.00
3	D	1	NAG	C4-C3-C2	2.95	115.34	111.02
4	H	1	GIV	O5-C5-C6	2.88	111.72	107.20
4	H	2	SIA	O8-C8-C7	-2.67	102.61	109.10
2	C	2	NAG	C3-C4-C5	2.54	114.77	110.24
3	D	2	NAG	C1-O5-C5	-2.54	108.75	112.19
4	H	2	SIA	O6-C2-C3	2.53	113.94	110.46
3	D	3	BMA	O3-C3-C2	-2.45	105.30	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	O5-C1-C2	-2.33	107.61	111.29
4	H	1	GIV	O2-C2-C1	-2.33	104.39	109.15
3	D	3	BMA	O4-C4-C3	-2.30	105.04	110.35
2	C	2	NAG	C2-N2-C7	2.28	126.15	122.90
3	D	4	FUC	C1-O5-C5	2.28	117.94	112.78
4	H	1	GIV	O2-C2-C3	-2.20	105.72	110.14
3	D	1	NAG	O5-C5-C6	2.20	110.66	107.20
2	C	1	NAG	O4-C4-C3	-2.20	105.27	110.35
3	D	2	NAG	O7-C7-N2	2.15	125.90	121.95
3	D	3	BMA	C1-C2-C3	2.14	112.30	109.67
3	D	1	NAG	C1-C2-N2	2.07	114.03	110.49
3	D	1	NAG	C3-C4-C5	2.07	113.94	110.24
3	D	3	BMA	C2-C3-C4	2.07	114.48	110.89
3	D	2	NAG	O5-C1-C2	-2.06	108.04	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	2	SIA	C8
4	H	2	SIA	C7

All (18) torsion outliers are listed below:

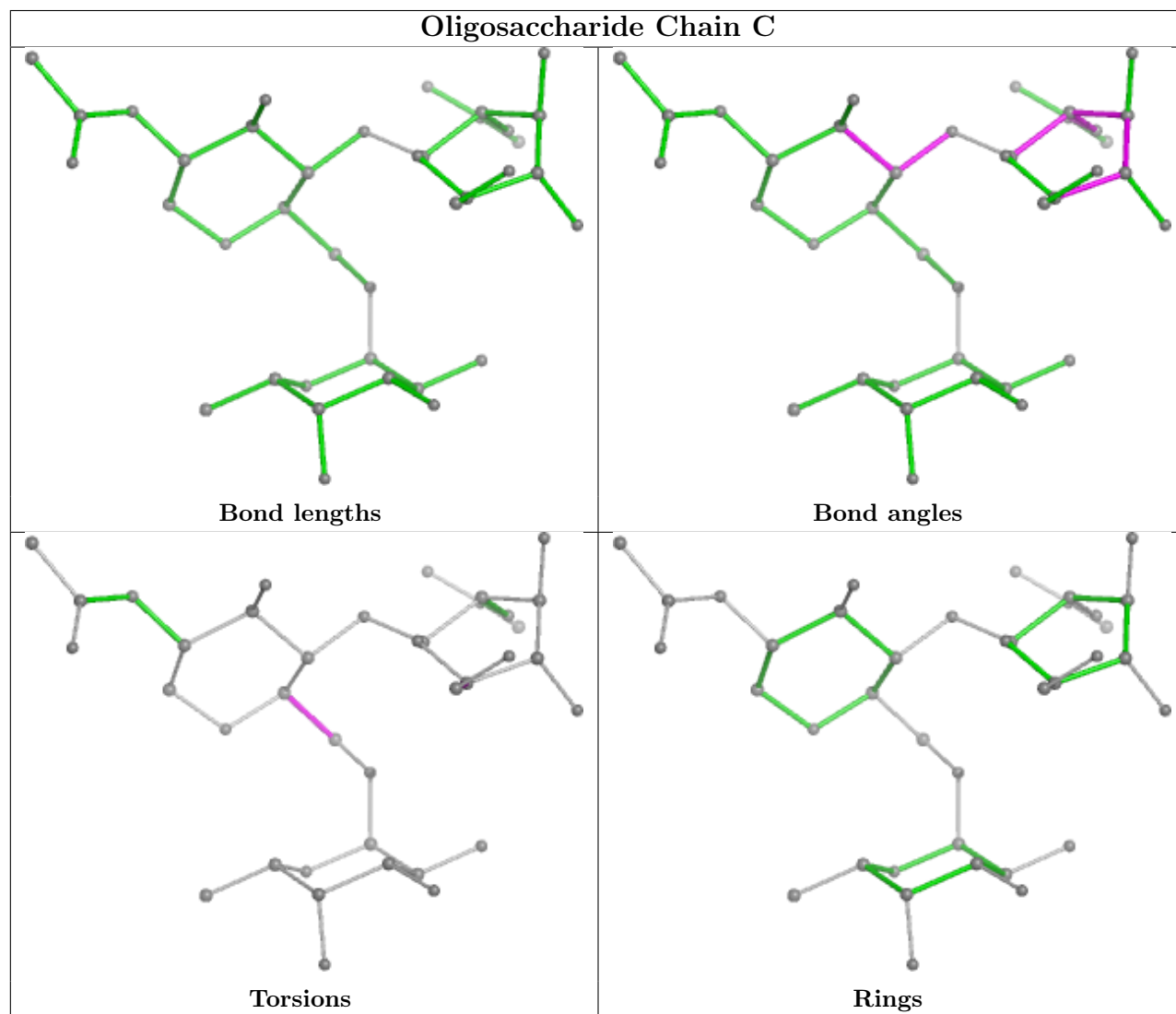
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C3-C2-N2-C7
4	H	2	SIA	O10-C10-N5-C5
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
4	H	2	SIA	O7-C7-C8-O8
4	H	2	SIA	C6-C7-C8-O8
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
4	H	2	SIA	C4-C5-N5-C10
3	D	2	NAG	C1-C2-N2-C7
4	H	2	SIA	C6-C5-N5-C10
4	H	2	SIA	O7-C7-C8-C9
4	H	2	SIA	C6-C7-C8-C9
3	D	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
4	H	2	SIA	O1B-C1-C2-C3

There are no ring outliers.

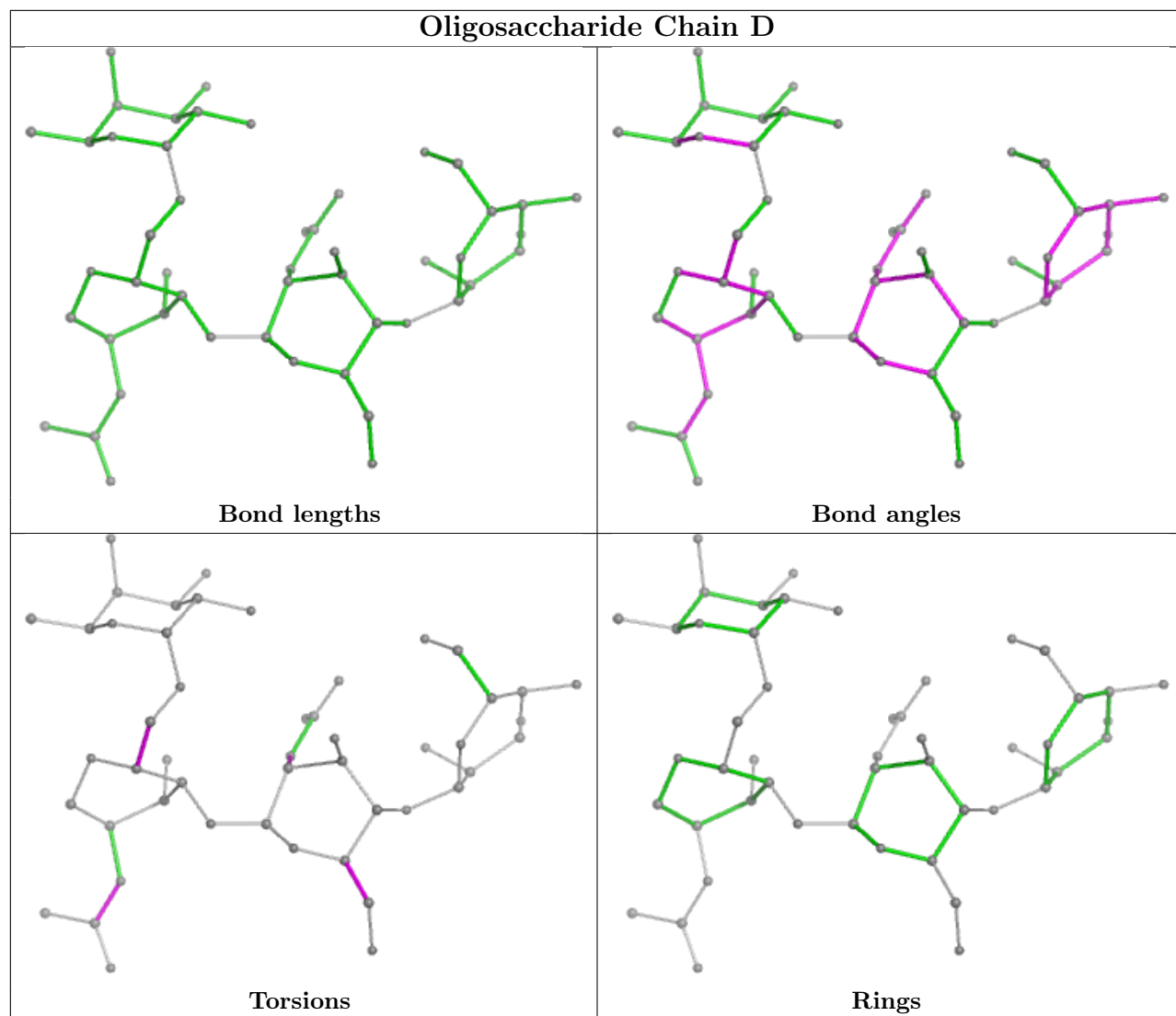
1 monomer is involved in 2 short contacts:

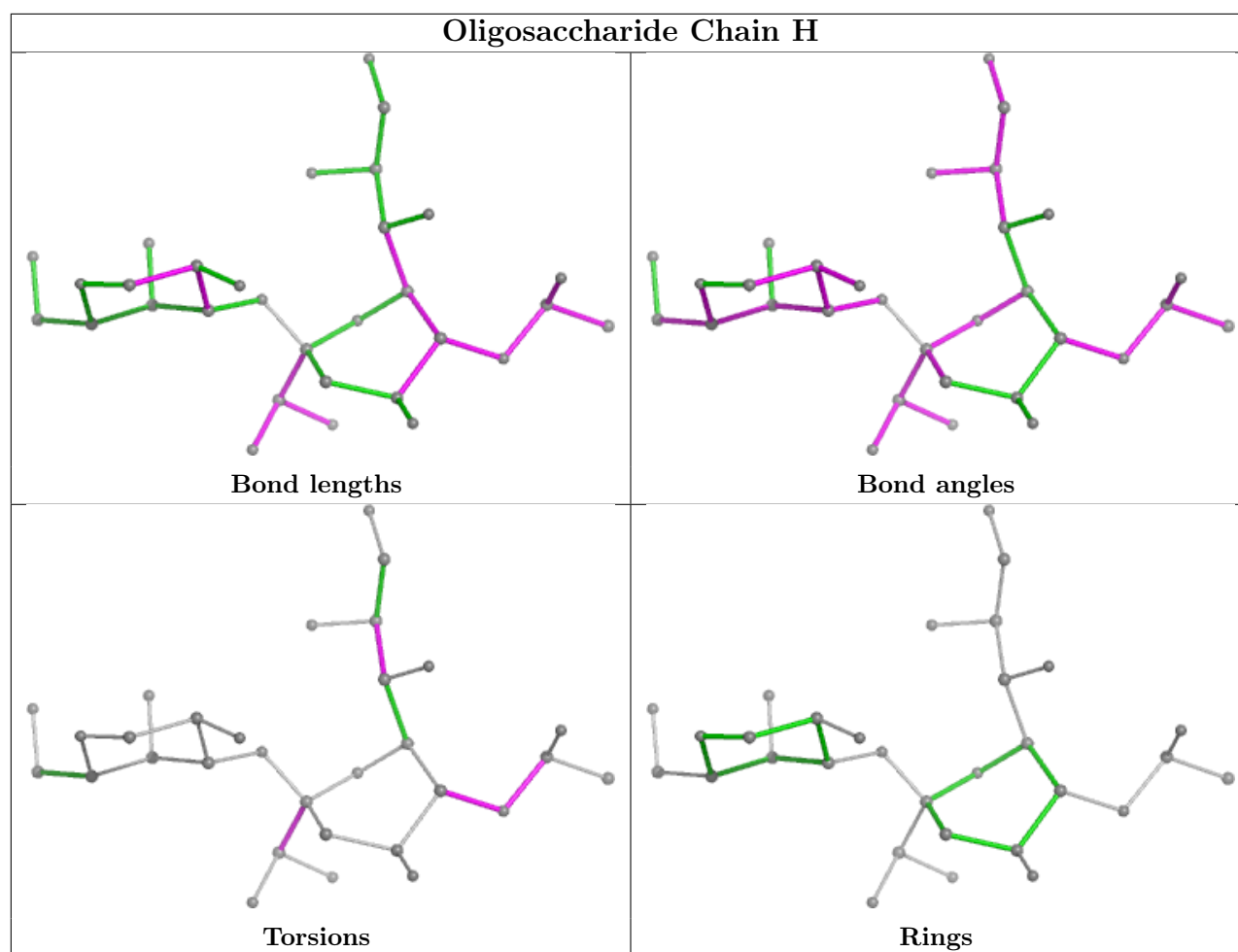
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	SIA	2	0

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



Oligosaccharide Chain D





5.6 Ligand geometry [i](#)

Of 185 ligands modelled in this entry, 141 are monoatomic - leaving 44 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	$\# Z > 2$
6	GOL	A	622	-	5,5,5	0.33	0	5,5,5	0.41	0
5	SO4	A	606	-	4,4,4	0.61	0	6,6,6	0.06	0
8	A1IAS	A	624[A]	10	27,27,27	1.86	7 (25%)	33,35,35	1.39	5 (15%)
6	GOL	A	619	-	5,5,5	0.32	0	5,5,5	0.39	0
5	SO4	A	607	-	4,4,4	0.61	0	6,6,6	0.08	0
6	GOL	A	617	-	5,5,5	0.32	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	604	-	4,4,4	0.61	0	6,6,6	0.05	0
5	SO4	B	605	-	4,4,4	0.60	0	6,6,6	0.09	0
5	SO4	B	612	-	4,4,4	0.61	0	6,6,6	0.07	0
5	SO4	B	603	-	4,4,4	0.61	0	6,6,6	0.08	0
5	SO4	A	603	-	4,4,4	0.59	0	6,6,6	0.11	0
5	SO4	A	608	-	4,4,4	0.60	0	6,6,6	0.07	0
6	GOL	B	618	-	5,5,5	0.33	0	5,5,5	0.37	0
5	SO4	A	612	10	4,4,4	0.60	0	6,6,6	0.07	0
6	GOL	A	615	-	5,5,5	0.32	0	5,5,5	0.38	0
6	GOL	B	616	-	5,5,5	0.33	0	5,5,5	0.34	0
5	SO4	A	613	-	4,4,4	0.60	0	6,6,6	0.08	0
5	SO4	B	602	-	4,4,4	0.61	0	6,6,6	0.07	0
5	SO4	A	609	-	4,4,4	0.60	0	6,6,6	0.07	0
5	SO4	A	610	-	4,4,4	0.60	0	6,6,6	0.05	0
6	GOL	B	619	-	5,5,5	0.34	0	5,5,5	0.36	0
6	GOL	A	614	-	5,5,5	0.34	0	5,5,5	0.31	0
7	EPE	A	623	-	15,15,15	0.83	1 (6%)	18,20,20	0.64	0
5	SO4	B	610	-	4,4,4	0.60	0	6,6,6	0.06	0
5	SO4	B	601	-	4,4,4	0.60	0	6,6,6	0.11	0
5	SO4	A	601	-	4,4,4	0.60	0	6,6,6	0.09	0
5	SO4	B	606	-	4,4,4	0.60	0	6,6,6	0.07	0
6	GOL	B	615	-	5,5,5	0.32	0	5,5,5	0.37	0
5	SO4	B	608	-	4,4,4	0.60	0	6,6,6	0.06	0
5	SO4	B	607	-	4,4,4	0.62	0	6,6,6	0.06	0
12	A1AAJ	B	613	4	15,15,15	2.95	7 (46%)	21,21,21	3.46	10 (47%)
6	GOL	A	618	10	5,5,5	0.33	0	5,5,5	0.32	0
5	SO4	A	605	-	4,4,4	0.61	0	6,6,6	0.08	0
13	ACT	B	620	-	3,3,3	1.05	0	3,3,3	1.29	0
5	SO4	B	609	-	4,4,4	0.60	0	6,6,6	0.06	0
5	SO4	B	611	10	4,4,4	0.60	0	6,6,6	0.07	0
6	GOL	A	616	-	5,5,5	0.35	0	5,5,5	0.35	0
5	SO4	A	604	-	4,4,4	0.59	0	6,6,6	0.12	0
6	GOL	A	620	-	5,5,5	0.33	0	5,5,5	0.38	0
5	SO4	A	611	-	4,4,4	0.60	0	6,6,6	0.08	0
6	GOL	B	614	-	5,5,5	0.32	0	5,5,5	0.37	0
7	EPE	B	617	-	15,15,15	0.85	1 (6%)	18,20,20	0.54	0
5	SO4	A	602	-	4,4,4	0.60	0	6,6,6	0.05	0
6	GOL	A	621	-	5,5,5	0.34	0	5,5,5	0.36	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
6	GOL	A	614	-	-	0/4/4/4	-
6	GOL	B	618	-	-	0/4/4/4	-
7	EPE	A	623	-	-	2/9/19/19	0/1/1/1
6	GOL	A	615	-	-	0/4/4/4	-
6	GOL	B	616	-	-	0/4/4/4	-
6	GOL	A	622	-	-	0/4/4/4	-
8	A1IAS	A	624[A]	10	-	6/11/11/11	0/3/3/3
6	GOL	A	616	-	-	0/4/4/4	-
6	GOL	A	619	-	-	4/4/4/4	-
6	GOL	A	620	-	-	0/4/4/4	-
6	GOL	A	617	-	-	0/4/4/4	-
6	GOL	B	614	-	-	0/4/4/4	-
6	GOL	B	615	-	-	0/4/4/4	-
7	EPE	B	617	-	-	5/9/19/19	0/1/1/1
12	A1AAJ	B	613	4	1/1/6/7	3/6/26/26	0/1/1/1
6	GOL	A	621	-	-	0/4/4/4	-
6	GOL	A	618	10	-	0/4/4/4	-
6	GOL	B	619	-	-	0/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	613	A1AAJ	O03-C02	8.29	1.42	1.23
12	B	613	A1AAJ	C02-N04	4.35	1.49	1.34
8	A	624[A]	A1IAS	C04-C03	3.67	1.54	1.47
8	A	624[A]	A1IAS	C15-N14	3.37	1.44	1.36
8	A	624[A]	A1IAS	C10-C09	3.24	1.58	1.51
12	B	613	A1AAJ	C05-N04	3.24	1.51	1.45
8	A	624[A]	A1IAS	C16-C17	2.97	1.44	1.38
12	B	613	A1AAJ	C07-C06	2.92	1.59	1.52
12	B	613	A1AAJ	C10-C05	2.71	1.56	1.52
8	A	624[A]	A1IAS	C04-N25	2.62	1.37	1.35
7	B	617	EPE	C10-S	2.53	1.81	1.77
8	A	624[A]	A1IAS	C03-N02	2.45	1.32	1.27
7	A	623	EPE	C10-S	2.39	1.80	1.77
12	B	613	A1AAJ	C06-C05	2.36	1.57	1.53
8	A	624[A]	A1IAS	O01-N02	-2.16	1.35	1.40
12	B	613	A1AAJ	C07-C08	2.14	1.57	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	613	A1AAJ	O03-C02-N04	-7.98	107.28	121.95
12	B	613	A1AAJ	O03-C02-C01	-7.08	108.91	122.06
12	B	613	A1AAJ	O09-C10-C05	6.56	116.11	109.52
8	A	624[A]	A1IAS	C04-N25-C09	4.41	122.93	117.91
12	B	613	A1AAJ	O15-C06-C05	-3.84	101.90	109.66
12	B	613	A1AAJ	C07-C06-C05	3.82	115.93	110.34
12	B	613	A1AAJ	O09-C08-C12	3.34	114.75	106.44
12	B	613	A1AAJ	C10-O09-C08	3.24	119.77	113.66
12	B	613	A1AAJ	C05-N04-C02	-3.13	115.57	123.18
12	B	613	A1AAJ	O15-C06-C07	-2.93	103.58	110.35
12	B	613	A1AAJ	C10-C05-N04	2.92	114.11	110.73
8	A	624[A]	A1IAS	O01-N02-C03	2.39	116.09	111.86
8	A	624[A]	A1IAS	C08-C09-N25	-2.24	119.57	122.41
8	A	624[A]	A1IAS	C10-C09-N25	2.03	118.97	115.95
8	A	624[A]	A1IAS	C12-C13-N14	2.02	116.91	111.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	B	613	A1AAJ	C08

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	619	GOL	C1-C2-C3-O3
6	A	619	GOL	O2-C2-C3-O3
7	A	623	EPE	C8-C7-N4-C5
7	A	623	EPE	S-C10-C9-N1
7	B	617	EPE	S-C10-C9-N1
7	B	617	EPE	C9-C10-S-O2S
8	A	624[A]	A1IAS	N02-C03-C04-C05
8	A	624[A]	A1IAS	N02-C03-C04-N25
12	B	613	A1AAJ	O03-C02-N04-C05
12	B	613	A1AAJ	C10-C05-N04-C02
8	A	624[A]	A1IAS	C11-C12-C13-N14
12	B	613	A1AAJ	C01-C02-N04-C05
7	B	617	EPE	C9-C10-S-O3S
8	A	624[A]	A1IAS	C09-C10-C11-C12
7	B	617	EPE	N4-C7-C8-O8
6	A	619	GOL	O1-C1-C2-O2
7	B	617	EPE	C9-C10-S-O1S
8	A	624[A]	A1IAS	C04-C03-N02-O01
8	A	624[A]	A1IAS	C12-C13-N14-C15

Continued on next page...

Continued from previous page...

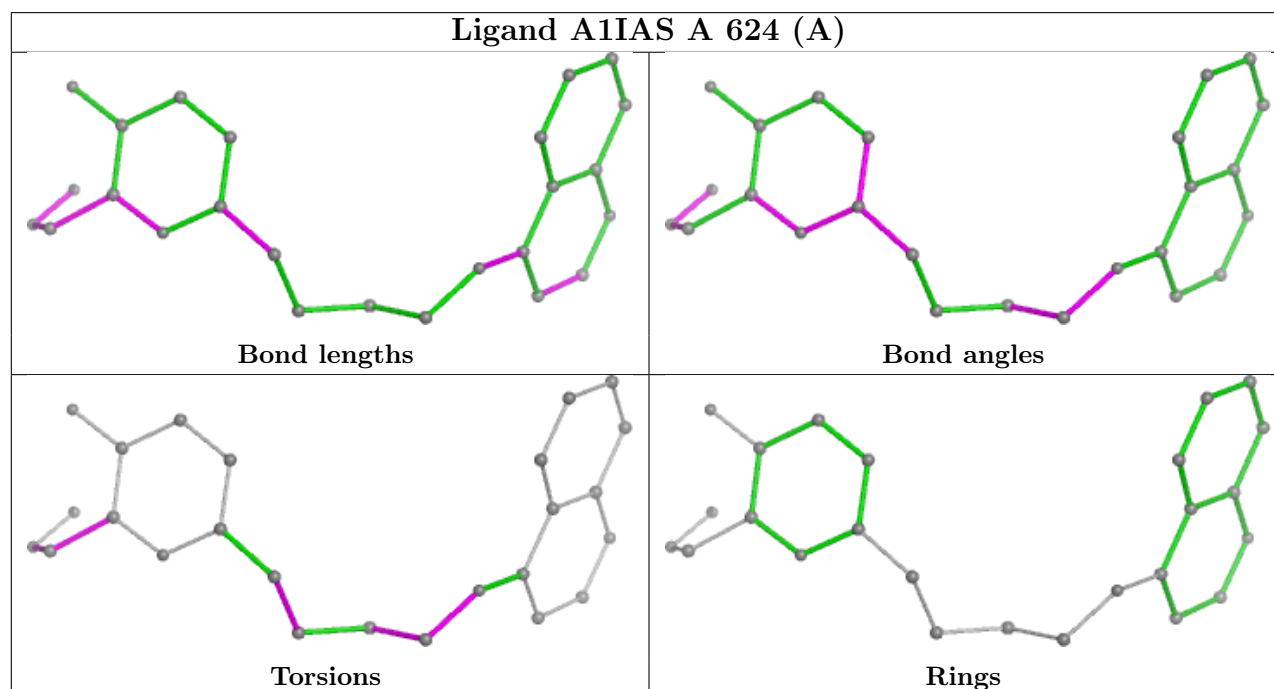
Mol	Chain	Res	Type	Atoms
6	A	619	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	622	GOL	1	0
6	B	616	GOL	2	0
6	A	614	GOL	1	0
7	A	623	EPE	2	0
7	B	617	EPE	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 [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	535/543 (98%)	0.21	24 (4%)	39 40	40, 78, 106, 132	10 (1%)
1	B	533/543 (98%)	0.22	27 (5%)	34 36	47, 83, 112, 160	1 (0%)
All	All	1068/1086 (98%)	0.22	51 (4%)	36 38	40, 80, 109, 160	11 (1%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	436[A]	THR	16.5
1	A	435[A]	SER	11.9
1	A	437[A]	LEU	7.3
1	A	258	PRO	5.9
1	B	381[A]	HIS	5.7
1	A	105	TYR	5.2
1	B	490	ASN	5.0
1	B	105	TYR	4.4
1	A	434[A]	ALA	4.3
1	B	76	LEU	4.2
1	B	495	PRO	4.0
1	A	6	ALA	3.8
1	A	23	LYS	3.6
1	B	492	PRO	3.6
1	B	258	PRO	3.6
1	B	264	GLY	3.5
1	A	341	TYR	3.4
1	A	496	LYS	3.1
1	A	381[A]	HIS	3.1
1	B	6	ALA	3.0
1	B	543	THR	2.9
1	A	438[A]	SER	2.9
1	B	493	ARG	2.8
1	B	491	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	264	GLY	2.8
1	B	349	ASP	2.8
1	A	498	PRO	2.8
1	A	497	ALA	2.7
1	A	75	THR	2.7
1	A	495	PRO	2.7
1	B	106	PRO	2.7
1	B	494	ASP	2.6
1	A	263	GLY	2.6
1	B	467	ALA	2.6
1	B	369	GLN	2.5
1	B	441	LEU	2.5
1	A	262	THR	2.5
1	B	466	THR	2.4
1	A	74	ASP	2.4
1	A	540	LEU	2.4
1	A	246	ARG	2.3
1	A	318	ALA	2.3
1	B	496	LYS	2.2
1	B	497	ALA	2.2
1	B	18	ARG	2.2
1	B	468	GLU	2.2
1	B	45	ARG	2.2
1	A	107	ARG	2.1
1	B	461	PRO	2.1
1	B	253	HIS	2.1
1	B	23	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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.

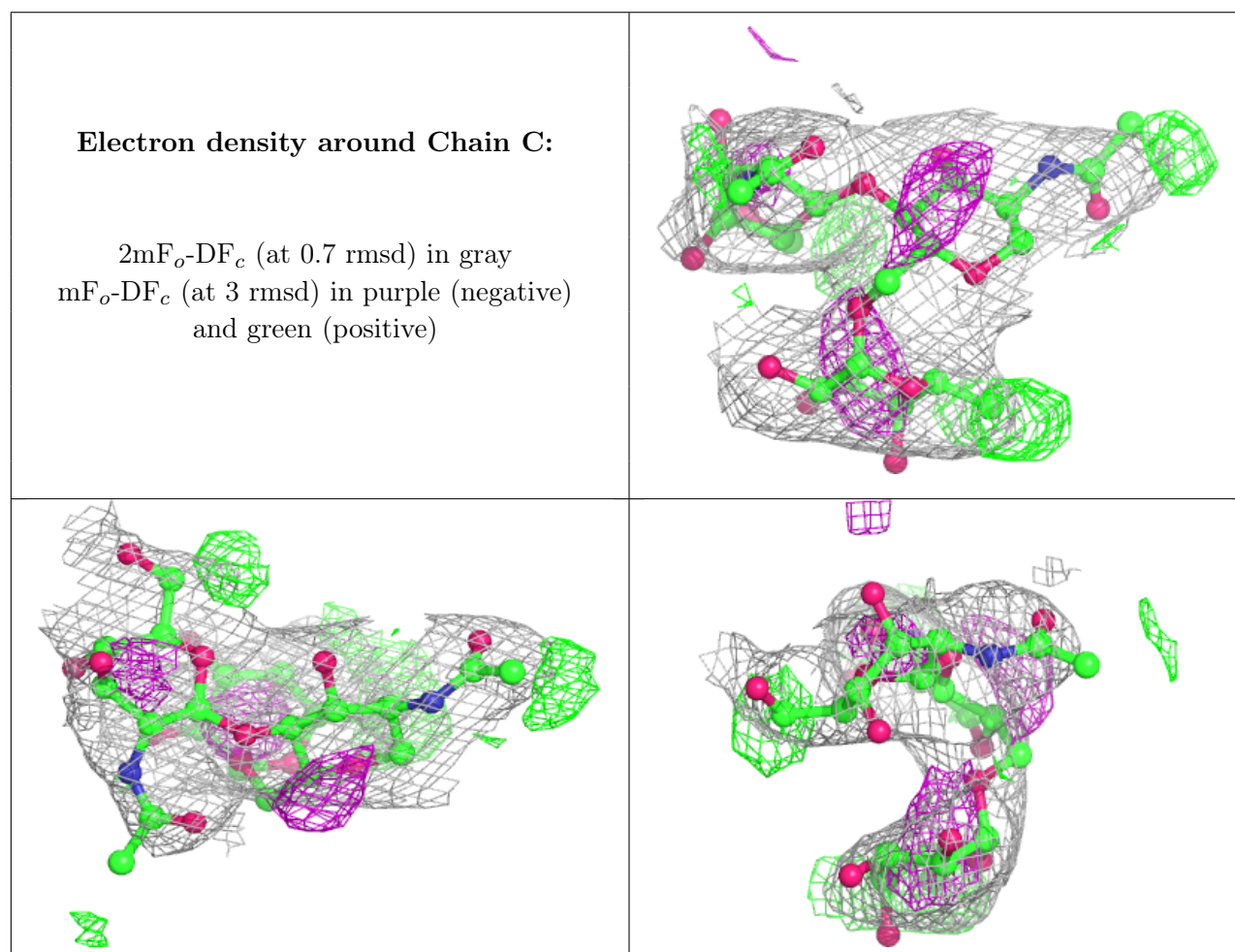
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OAS	A	203	9/10	0.95	0.12	68,72,89,91	0
1	OAS	B	203	9/10	0.97	0.10	65,69,86,87	0

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.

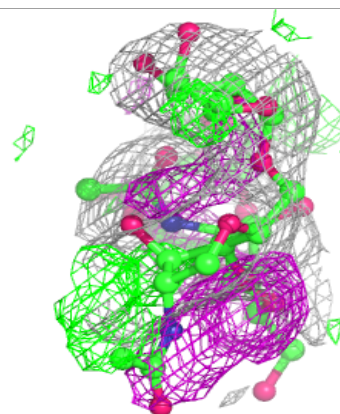
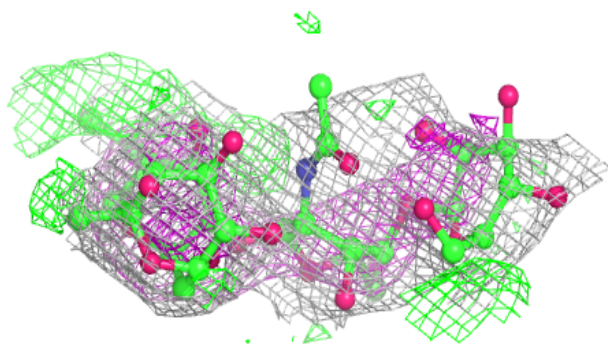
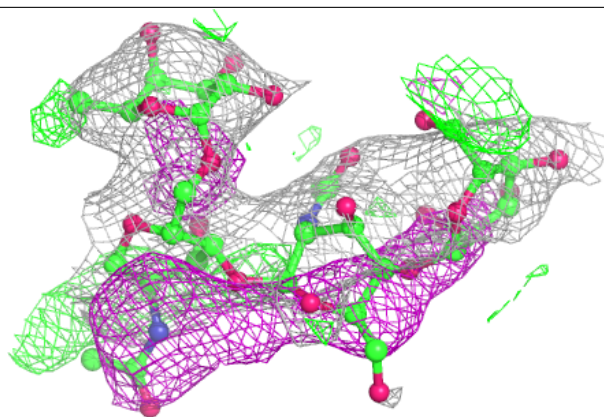
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	D	3	11/12	0.15	0.23	149,154,163,169	0
2	FUC	C	3	10/11	0.62	0.21	105,135,139,144	0
3	NAG	D	2	14/15	0.64	0.23	119,141,150,159	0
3	FUC	D	4	10/11	0.68	0.19	103,131,133,139	0
3	NAG	D	1	14/15	0.70	0.26	107,116,132,133	0
2	NAG	C	2	14/15	0.70	0.19	111,131,142,146	0
2	NAG	C	1	14/15	0.88	0.16	98,111,121,132	0
4	GIV	H	1	11/12	-	-	80,98,103,114	0
4	SIA	H	2	20/21	-	-	73,91,108,111	0

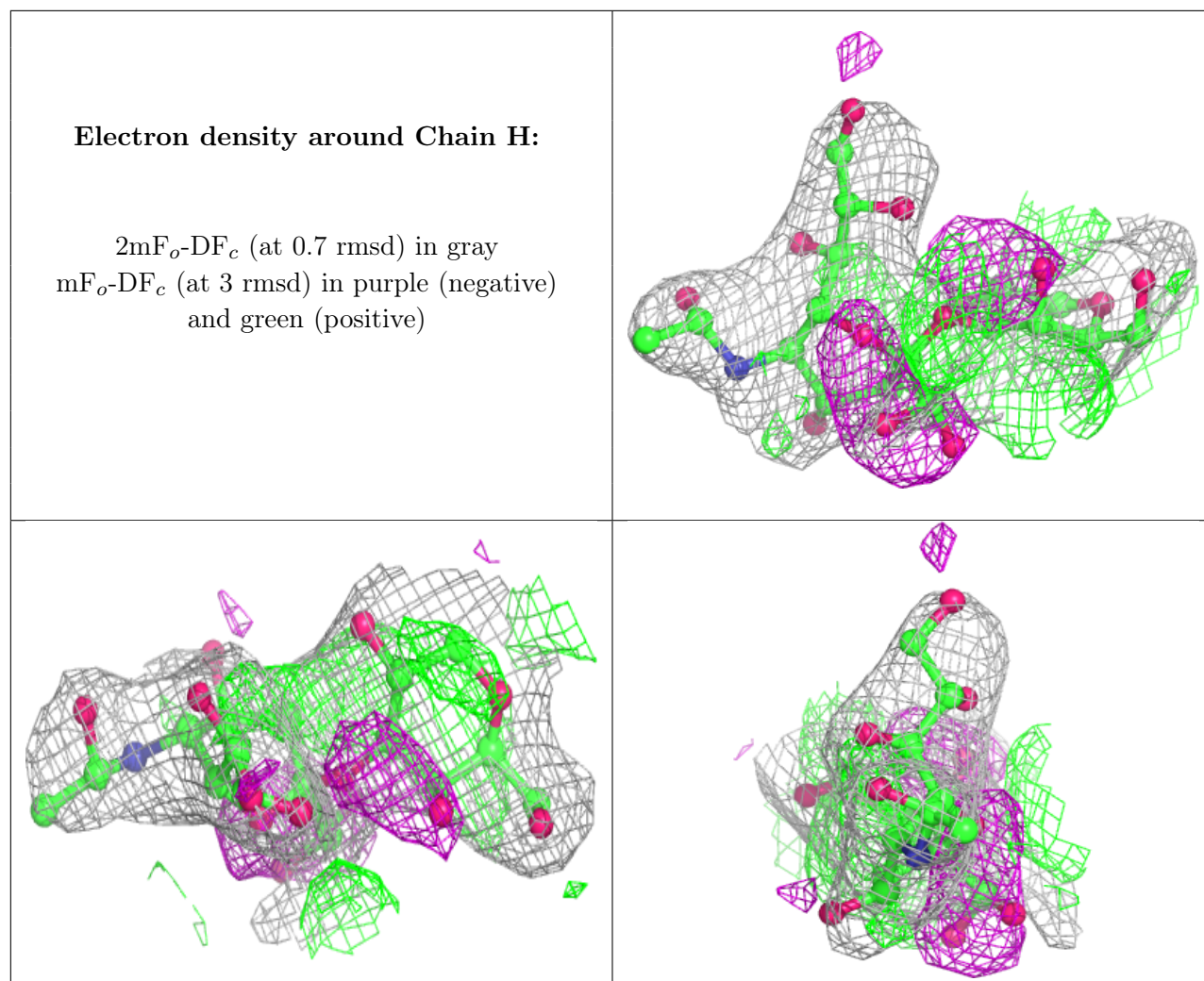
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

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





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
5	SO4	B	610	5/5	0.50	0.12	133,149,162,163	0
10	NA	A	686	1/1	0.52	0.39	110,110,110,110	0
10	NA	B	671	1/1	0.52	0.33	115,115,115,115	0
12	A1AAJ	B	613	15/15	0.54	0.28	99,110,116,117	0
7	EPE	A	623	15/15	0.55	0.27	126,135,163,171	0
10	NA	A	689	1/1	0.57	0.36	131,131,131,131	0
10	NA	B	657	1/1	0.58	0.34	115,115,115,115	0
10	NA	A	647	1/1	0.59	0.35	131,131,131,131	0
9	CL	B	633	1/1	0.61	0.38	119,119,119,119	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	B	619	6/6	0.62	0.24	114,116,119,120	0
9	CL	B	643	1/1	0.64	0.50	122,122,122,122	0
6	GOL	A	621	6/6	0.64	0.33	108,117,121,123	0
10	NA	B	646	1/1	0.64	0.20	110,110,110,110	0
5	SO4	B	608	5/5	0.65	0.10	157,157,168,171	0
5	SO4	A	606	5/5	0.65	0.13	116,119,140,143	0
11	MG	A	701	1/1	0.66	0.49	119,119,119,119	0
5	SO4	B	612	5/5	0.67	0.23	94,94,107,111	5
10	NA	A	684	1/1	0.67	0.24	125,125,125,125	0
6	GOL	B	618	6/6	0.67	0.18	116,124,128,130	0
10	NA	A	687	1/1	0.68	0.28	121,121,121,121	0
9	CL	A	637	1/1	0.69	0.19	142,142,142,142	0
5	SO4	B	609	5/5	0.70	0.10	127,132,136,144	0
10	NA	B	674	1/1	0.70	0.39	113,113,113,113	0
5	SO4	B	607	5/5	0.72	0.16	113,115,136,148	0
7	EPE	B	617	15/15	0.72	0.35	93,108,118,129	15
11	MG	A	691	1/1	0.72	0.27	102,102,102,102	0
10	NA	B	656	1/1	0.72	0.33	128,128,128,128	0
5	SO4	B	604	5/5	0.72	0.11	116,127,147,150	0
5	SO4	B	603	5/5	0.73	0.11	120,126,146,149	0
5	SO4	A	608	5/5	0.73	0.11	123,123,138,139	0
10	NA	A	649	1/1	0.73	0.15	117,117,117,117	0
5	SO4	A	611	5/5	0.74	0.12	99,109,123,124	5
10	NA	A	672	1/1	0.74	0.29	104,104,104,104	0
10	NA	B	677	1/1	0.74	0.47	107,107,107,107	0
10	NA	A	683	1/1	0.74	0.28	114,114,114,114	0
11	MG	A	699	1/1	0.74	0.38	112,112,112,112	0
5	SO4	A	604	5/5	0.74	0.17	100,115,133,136	0
6	GOL	A	618	6/6	0.74	0.24	113,119,123,124	0
5	SO4	A	607	5/5	0.75	0.10	119,123,139,144	0
9	CL	B	638	1/1	0.75	0.20	125,125,125,125	0
6	GOL	A	619	6/6	0.75	0.24	97,109,114,118	0
10	NA	B	676	1/1	0.76	0.32	123,123,123,123	0
6	GOL	A	620	6/6	0.76	0.22	104,111,118,122	0
9	CL	A	631	1/1	0.77	0.21	135,135,135,135	0
10	NA	B	659	1/1	0.77	0.23	103,103,103,103	0
5	SO4	A	613	5/5	0.78	0.12	104,106,115,122	5
10	NA	A	660	1/1	0.78	0.40	116,116,116,116	0
5	SO4	A	609	5/5	0.79	0.10	100,107,111,120	5
11	MG	A	698	1/1	0.80	0.24	107,107,107,107	0
5	SO4	B	605	5/5	0.80	0.12	107,119,139,141	0
6	GOL	B	615	6/6	0.80	0.23	97,103,104,107	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	NA	A	669	1/1	0.80	0.13	106,106,106,106	0
9	CL	B	629	1/1	0.81	0.31	124,124,124,124	0
10	NA	A	675	1/1	0.82	0.25	110,110,110,110	0
10	NA	A	682	1/1	0.82	0.31	105,105,105,105	0
9	CL	B	624	1/1	0.82	0.20	133,133,133,133	0
6	GOL	A	616	6/6	0.82	0.19	79,85,90,99	0
9	CL	A	630	1/1	0.83	0.23	122,122,122,122	0
10	NA	A	676	1/1	0.83	0.27	113,113,113,113	0
10	NA	B	667	1/1	0.83	0.20	127,127,127,127	0
11	MG	A	695	1/1	0.84	0.40	120,120,120,120	0
10	NA	A	646	1/1	0.84	0.11	114,114,114,114	0
6	GOL	B	614	6/6	0.84	0.20	98,100,103,105	0
9	CL	A	632	1/1	0.84	0.15	117,117,117,117	0
11	MG	B	681	1/1	0.84	0.18	96,96,96,96	0
10	NA	A	645	1/1	0.84	0.37	96,96,96,96	0
10	NA	A	656	1/1	0.85	0.28	93,93,93,93	0
11	MG	A	692	1/1	0.85	0.21	118,118,118,118	0
9	CL	B	640	1/1	0.85	0.30	113,113,113,113	0
9	CL	B	644	1/1	0.85	0.13	119,119,119,119	0
10	NA	A	666	1/1	0.86	0.35	108,108,108,108	0
10	NA	A	680	1/1	0.86	0.28	102,102,102,102	0
9	CL	B	637	1/1	0.86	0.22	118,118,118,118	0
11	MG	B	682	1/1	0.86	0.21	87,87,87,87	0
10	NA	B	655	1/1	0.86	0.32	97,97,97,97	0
5	SO4	A	605	5/5	0.87	0.10	102,111,134,144	0
9	CL	A	643	1/1	0.87	0.21	127,127,127,127	0
9	CL	B	635	1/1	0.87	0.16	110,110,110,110	0
11	MG	A	702	1/1	0.87	0.20	108,108,108,108	0
10	NA	A	679	1/1	0.87	0.24	80,80,80,80	0
9	CL	A	634	1/1	0.87	0.15	125,125,125,125	0
10	NA	A	671	1/1	0.87	0.32	106,106,106,106	0
10	NA	B	666	1/1	0.88	0.21	98,98,98,98	0
10	NA	A	662	1/1	0.88	0.19	97,97,97,97	0
10	NA	B	678	1/1	0.88	0.24	113,113,113,113	0
6	GOL	A	614	6/6	0.88	0.21	95,97,101,108	0
10	NA	B	673	1/1	0.88	0.42	131,131,131,131	0
10	NA	A	668	1/1	0.88	0.20	111,111,111,111	0
11	MG	A	697	1/1	0.88	0.16	105,105,105,105	0
10	NA	A	670	1/1	0.89	0.18	99,99,99,99	0
9	CL	B	639	1/1	0.89	0.18	115,115,115,115	0
11	MG	A	700	1/1	0.89	0.33	109,109,109,109	0
6	GOL	A	617	6/6	0.89	0.19	98,104,108,109	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	NA	B	650	1/1	0.90	0.35	85,85,85,85	0
10	NA	B	652	1/1	0.90	0.12	93,93,93,93	0
10	NA	A	657	1/1	0.90	0.24	108,108,108,108	0
10	NA	A	681	1/1	0.90	0.19	107,107,107,107	0
6	GOL	A	615	6/6	0.90	0.18	89,93,99,102	0
9	CL	A	642	1/1	0.90	0.26	105,105,105,105	0
10	NA	B	662	1/1	0.90	0.11	100,100,100,100	0
10	NA	A	673	1/1	0.90	0.19	115,115,115,115	0
10	NA	A	685	1/1	0.90	0.42	86,86,86,86	0
10	NA	B	668	1/1	0.90	0.23	118,118,118,118	0
10	NA	A	674	1/1	0.90	0.21	99,99,99,99	0
9	CL	B	634	1/1	0.90	0.16	115,115,115,115	0
9	CL	A	628	1/1	0.90	0.13	111,111,111,111	0
5	SO4	A	610	5/5	0.90	0.14	81,85,96,97	5
10	NA	B	679	1/1	0.91	0.34	94,94,94,94	0
11	MG	A	690	1/1	0.91	0.20	101,101,101,101	0
6	GOL	A	622	6/6	0.91	0.15	72,100,108,115	0
9	CL	A	640	1/1	0.91	0.17	120,120,120,120	0
10	NA	B	649	1/1	0.91	0.21	102,102,102,102	0
11	MG	A	696	1/1	0.91	0.19	102,102,102,102	0
8	A1IAS	A	624[A]	25/25	0.91	0.23	74,84,95,98	25
10	NA	B	669	1/1	0.91	0.22	98,98,98,98	0
10	NA	B	670	1/1	0.91	0.27	106,106,106,106	0
5	SO4	A	603	5/5	0.91	0.11	81,87,95,100	5
10	NA	B	653	1/1	0.91	0.22	86,86,86,86	0
9	CL	A	633	1/1	0.91	0.12	121,121,121,121	0
9	CL	A	629	1/1	0.91	0.17	111,111,111,111	0
10	NA	A	677	1/1	0.91	0.24	103,103,103,103	0
9	CL	B	632	1/1	0.91	0.25	121,121,121,121	0
5	SO4	B	601	5/5	0.92	0.12	87,92,104,118	0
10	NA	A	661	1/1	0.92	0.12	113,113,113,113	0
10	NA	B	661	1/1	0.92	0.20	107,107,107,107	0
10	NA	B	648	1/1	0.92	0.18	91,91,91,91	0
9	CL	A	638	1/1	0.92	0.11	125,125,125,125	0
10	NA	A	664	1/1	0.92	0.20	101,101,101,101	0
10	NA	A	654	1/1	0.92	0.24	89,89,89,89	0
10	NA	A	655	1/1	0.92	0.21	110,110,110,110	0
5	SO4	B	611	5/5	0.92	0.14	83,85,90,101	5
9	CL	B	642	1/1	0.92	0.20	109,109,109,109	0
10	NA	B	665	1/1	0.93	0.20	98,98,98,98	0
9	CL	B	622	1/1	0.93	0.20	104,104,104,104	0
9	CL	B	623	1/1	0.93	0.20	116,116,116,116	0

Continued on next page...

Continued from previous page...

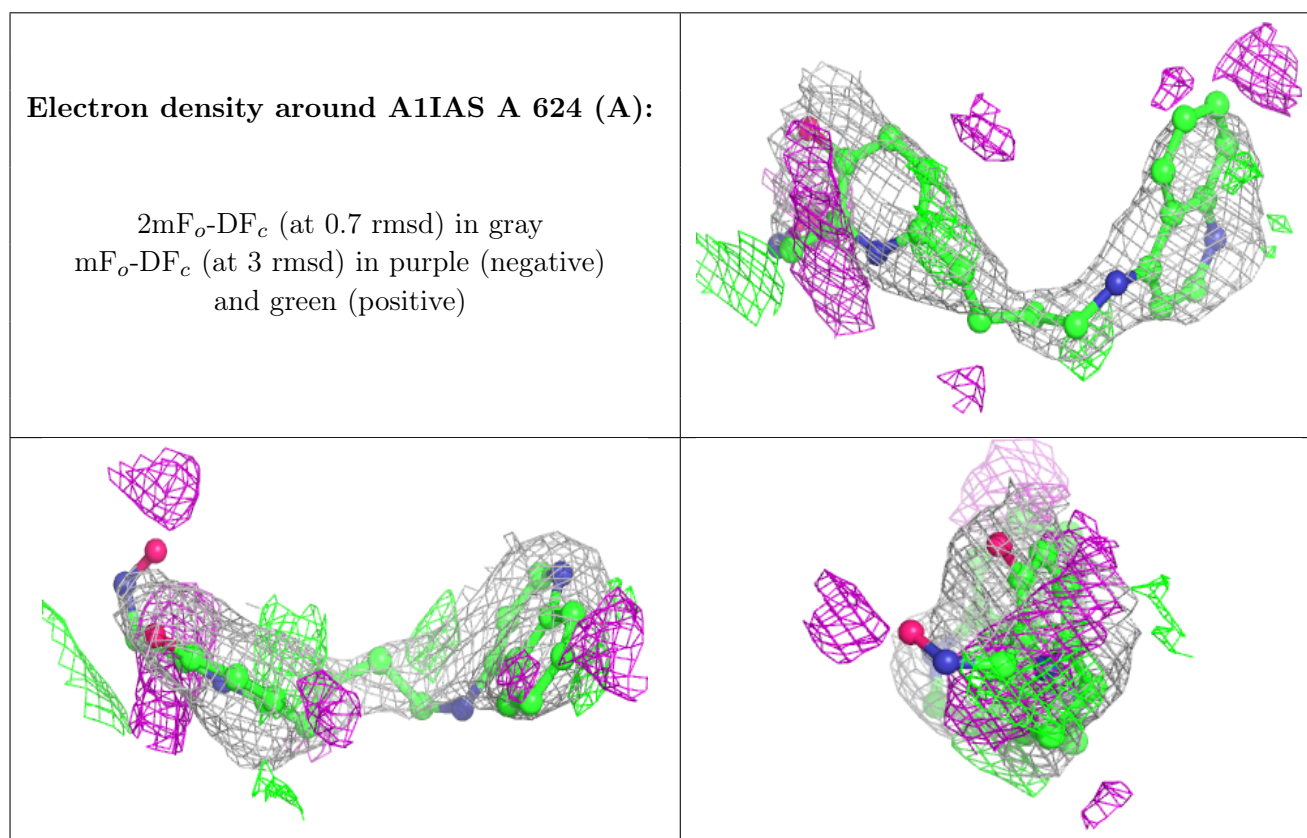
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	MG	A	694	1/1	0.93	0.25	101,101,101,101	0
9	CL	A	636	1/1	0.93	0.10	123,123,123,123	0
9	CL	B	627	1/1	0.93	0.24	104,104,104,104	0
5	SO4	A	601	5/5	0.93	0.08	101,103,116,120	0
9	CL	B	631	1/1	0.93	0.18	107,107,107,107	0
5	SO4	B	602	5/5	0.93	0.10	101,105,114,122	0
10	NA	A	665	1/1	0.93	0.33	116,116,116,116	0
10	NA	B	658	1/1	0.93	0.20	116,116,116,116	0
10	NA	A	650	1/1	0.93	0.19	87,87,87,87	0
9	CL	B	641	1/1	0.93	0.13	111,111,111,111	0
10	NA	B	647	1/1	0.93	0.16	88,88,88,88	0
10	NA	B	680	1/1	0.93	0.17	86,86,86,86	0
5	SO4	A	602	5/5	0.94	0.13	97,97,104,110	0
10	NA	B	645	1/1	0.94	0.15	107,107,107,107	0
10	NA	B	660	1/1	0.94	0.25	93,93,93,93	0
9	CL	B	636	1/1	0.94	0.09	120,120,120,120	0
9	CL	B	630	1/1	0.94	0.12	118,118,118,118	0
10	NA	B	664	1/1	0.94	0.16	79,79,79,79	0
9	CL	B	628	1/1	0.94	0.16	97,97,97,97	0
11	MG	A	693	1/1	0.94	0.14	105,105,105,105	0
10	NA	B	675	1/1	0.94	0.14	78,78,78,78	0
11	MG	B	683	1/1	0.94	0.23	104,104,104,104	0
10	NA	A	688	1/1	0.94	0.22	119,119,119,119	0
10	NA	A	678	1/1	0.95	0.14	97,97,97,97	0
9	CL	A	635	1/1	0.95	0.17	114,114,114,114	0
9	CL	B	621	1/1	0.95	0.18	105,105,105,105	0
5	SO4	A	612	5/5	0.95	0.14	81,82,94,98	5
10	NA	B	651	1/1	0.95	0.11	92,92,92,92	0
10	NA	A	652	1/1	0.95	0.12	90,90,90,90	0
9	CL	A	641	1/1	0.95	0.17	110,110,110,110	0
6	GOL	B	616	6/6	0.95	0.17	78,84,89,91	0
5	SO4	B	606	5/5	0.96	0.14	93,99,112,112	0
10	NA	A	644	1/1	0.96	0.18	101,101,101,101	0
10	NA	A	658	1/1	0.96	0.15	108,108,108,108	0
10	NA	A	651	1/1	0.96	0.11	77,77,77,77	0
9	CL	B	625	1/1	0.96	0.11	92,92,92,92	0
9	CL	B	626	1/1	0.96	0.14	112,112,112,112	0
10	NA	B	663	1/1	0.96	0.18	100,100,100,100	0
9	CL	A	626	1/1	0.96	0.13	105,105,105,105	0
10	NA	A	667	1/1	0.97	0.13	105,105,105,105	0
10	NA	A	648	1/1	0.97	0.15	107,107,107,107	0
10	NA	B	654	1/1	0.97	0.14	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	NA	A	663	1/1	0.97	0.16	83,83,83,83	0
10	NA	A	659	1/1	0.97	0.22	104,104,104,104	0
9	CL	A	625	1/1	0.97	0.17	96,96,96,96	0
10	NA	B	672	1/1	0.97	0.07	96,96,96,96	0
9	CL	A	639	1/1	0.97	0.11	114,114,114,114	0
13	ACT	B	620	4/4	0.97	0.13	81,82,84,85	0
10	NA	A	653	1/1	0.98	0.10	85,85,85,85	0
9	CL	A	627	1/1	0.99	0.07	107,107,107,107	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 ⓘ

There are no such residues in this entry.