



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:14 AM UTC

PDB ID : 9GBM / pdb_00009gbm
Title : Human Angiotensin-1 converting enzyme C-domain in complex with a diprolyl inhibitor- SG3
Authors : Gregory, K.S.; Cozier, G.E.; Acharya, K.R.
Deposited on : 2024-07-31
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

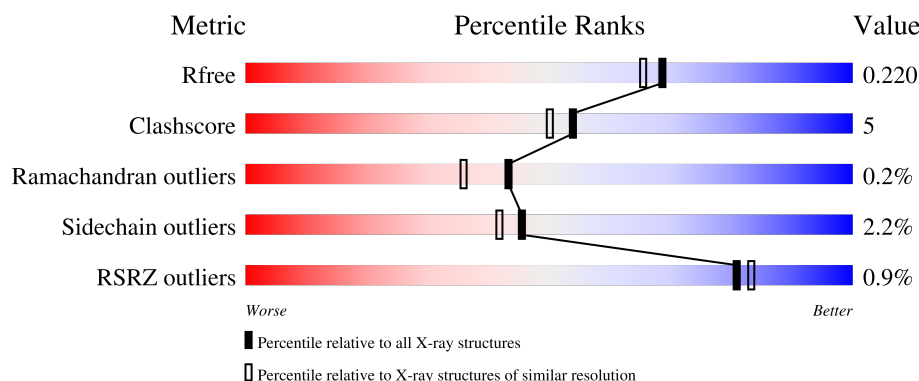
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

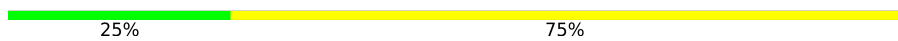
The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	597	
2	B	4	

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
4	PEG	A	702	-	-	X	-
7	CL	A	706	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5146 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.

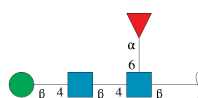
- Molecule 1 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	8	0
			4713	3019	804	866	24			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	GLY	GLU	engineered mutation	UNP P12821
A	90	GLN	ASN	engineered mutation	UNP P12821
A	155	GLN	ASN	engineered mutation	UNP P12821
A	337	GLN	ASN	engineered mutation	UNP P12821
A	586	GLN	ASN	engineered mutation	UNP P12821

- Molecule 2 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.

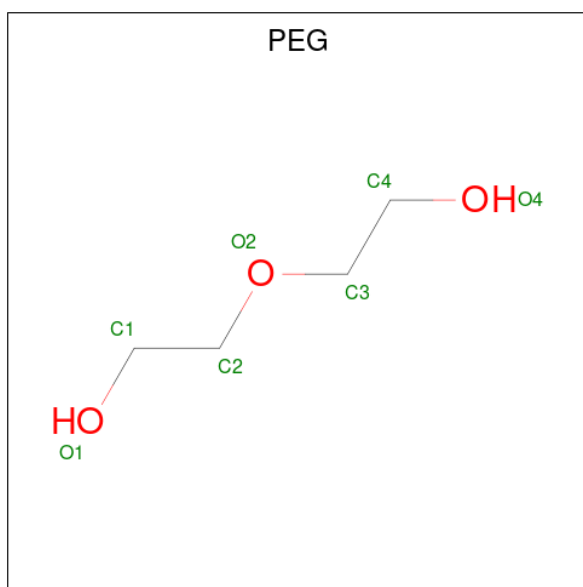


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

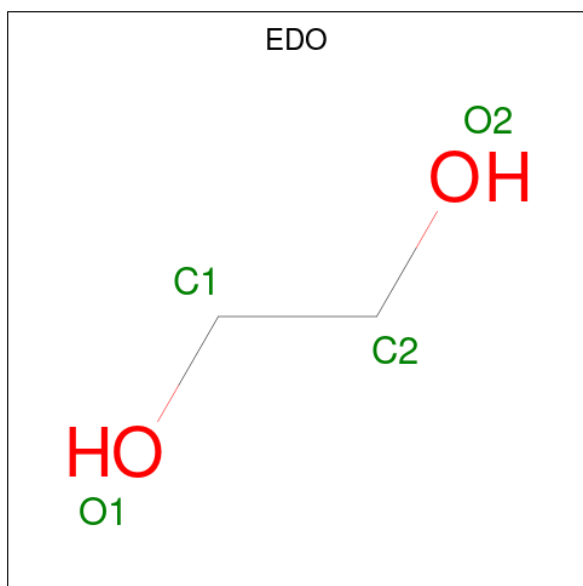
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



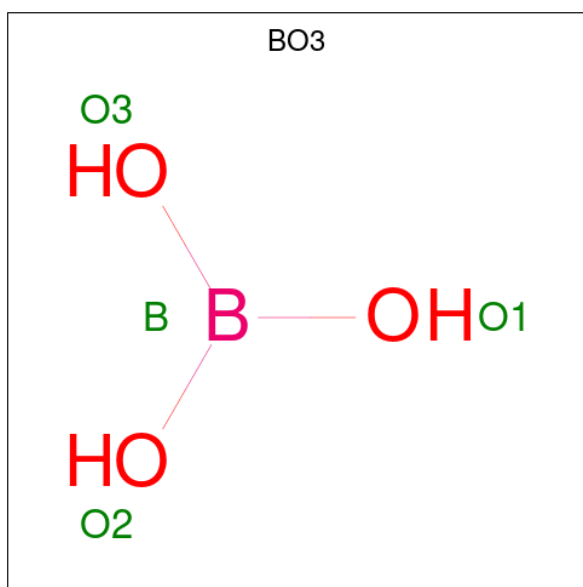
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is BORIC ACID (CCD ID: BO3) (formula: BH_3O_3).

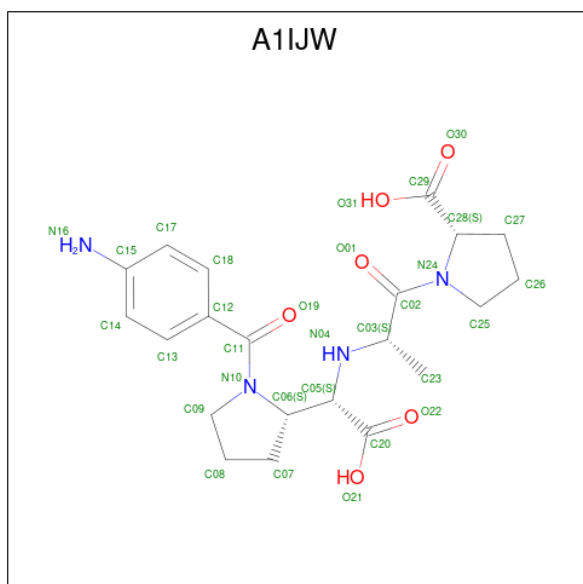


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total B O 4 1 3	0	0

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

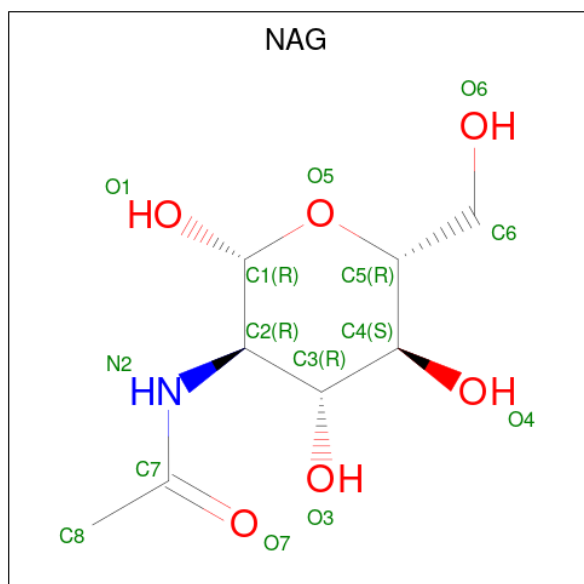
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Cl 2 2	0	0

- Molecule 8 is (2S)-1-[(2S)-2-[[[(1S)-1-[(2S)-1-(4-aminophenyl)carbonylpyrrolidin-2-yl]-2-oxidanyl-2-oxidanylidene-ethyl]amino]propanoyl]pyrrolidine-2-carboxylic acid (CCD ID: A1IJW) (formula: C₂₁H₂₈N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			31	21	4	6		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		

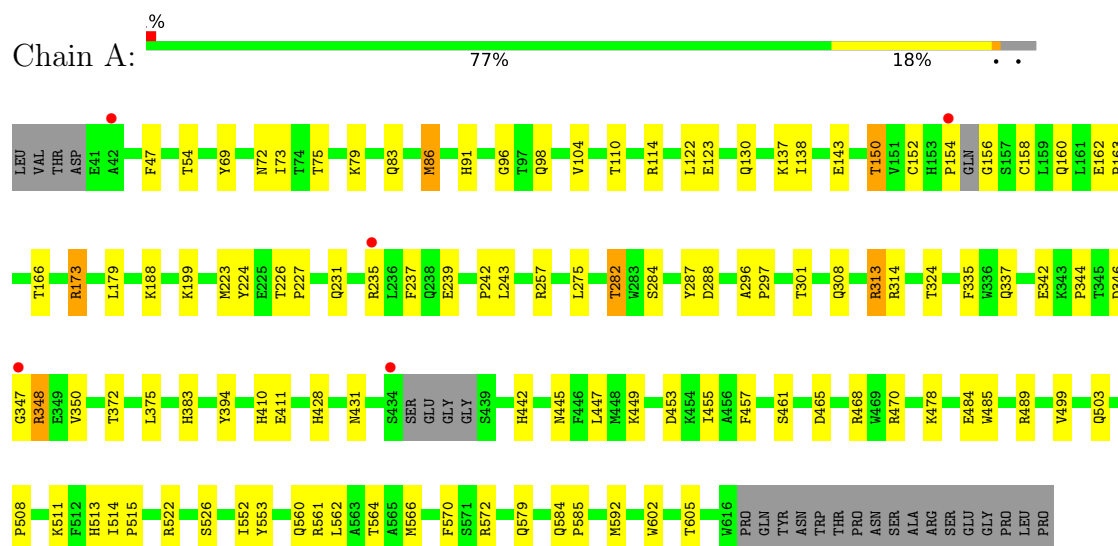
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	321	Total	O	0	0
			321	321		

3 Residue-property plots

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

- Molecule 1: Angiotensin-converting enzyme



- Molecule 2: 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.89Å 84.13Å 132.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.15 – 1.90 71.05 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (71.15-1.90) 99.8 (71.05-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.168 , 0.217 0.170 , 0.220	Depositor DCC
R_{free} test set	2396 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5146	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: BO3, FUC, BMA, NAG, EDO, CL, PEG, A1IJW, 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	0.97	2/4847 (0.0%)	1.53	45/6584 (0.7%)

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	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	HIS	CE1-NE2	6.83	1.39	1.32
1	A	585	PRO	CA-CB	5.41	1.61	1.53

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	605	THR	CA-CB-OG1	-9.88	94.78	109.60
1	A	301	THR	CA-CB-OG1	-9.15	95.87	109.60
1	A	561	ARG	CG-CD-NE	-8.51	93.29	112.00
1	A	137	LYS	CB-CG-CD	7.84	129.33	111.30
1	A	75	THR	CA-CB-OG1	-7.75	97.98	109.60
1	A	372	THR	CA-CB-OG1	-7.58	98.23	109.60
1	A	188	LYS	N-CA-CB	7.49	121.80	110.19
1	A	503	GLN	CA-C-N	-7.45	110.79	122.86
1	A	503	GLN	C-N-CA	-7.45	110.79	122.86
1	A	235	ARG	CB-CA-C	-6.76	99.36	110.85
1	A	226	THR	CA-CB-OG1	-6.75	99.48	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	THR	CA-CB-OG1	-6.75	99.48	109.60
1	A	428	HIS	CA-CB-CG	-6.69	107.11	113.80
1	A	570	PHE	CA-CB-CG	6.67	120.47	113.80
1	A	86	MET	CG-SD-CE	6.64	115.51	100.90
1	A	166	THR	CA-CB-OG1	-6.24	100.24	109.60
1	A	173	ARG	CD-NE-CZ	6.01	132.82	124.40
1	A	337	GLN	CB-CA-C	-6.00	98.14	110.38
1	A	313	ARG	N-CA-CB	5.98	118.92	110.12
1	A	110	THR	CA-CB-OG1	-5.92	100.72	109.60
1	A	98	GLN	CB-CA-C	-5.89	100.83	110.85
1	A	98	GLN	N-CA-CB	5.87	118.85	110.16
1	A	237	PHE	N-CA-CB	-5.82	101.57	110.12
1	A	478	LYS	N-CA-CB	5.79	120.17	110.32
1	A	239	GLU	CB-CG-CD	-5.77	102.80	112.60
1	A	297	PRO	N-CA-C	-5.75	102.78	111.41
1	A	465	ASP	CA-C-N	-5.66	112.69	120.28
1	A	465	ASP	C-N-CA	-5.66	112.69	120.28
1	A	237	PHE	CA-CB-CG	-5.65	108.15	113.80
1	A	468	ARG	CG-CD-NE	-5.59	99.71	112.00
1	A	453	ASP	CB-CA-C	5.56	120.04	110.86
1	A	561	ARG	CB-CA-C	-5.49	102.03	110.81
1	A	114	ARG	N-CA-CB	-5.43	102.12	110.16
1	A	522	ARG	CD-NE-CZ	-5.41	116.82	124.40
1	A	572	ARG	CB-CA-C	-5.41	100.99	109.22
1	A	150	THR	CA-CB-OG1	-5.34	101.59	109.60
1	A	513	HIS	CA-CB-CG	-5.29	108.51	113.80
1	A	314	ARG	CB-CG-CD	5.26	123.39	111.30
1	A	602	TRP	CA-C-N	5.24	127.30	120.28
1	A	602	TRP	C-N-CA	5.24	127.30	120.28
1	A	484	GLU	CB-CG-CD	-5.11	103.92	112.60
1	A	257	ARG	CD-NE-CZ	5.05	131.47	124.40
1	A	47	PHE	CA-CB-CG	-5.04	108.75	113.80
1	A	347	GLY	CA-C-N	5.02	128.79	121.31
1	A	347	GLY	C-N-CA	5.02	128.79	121.31

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	ARG	Sidechain
1	A	470	ARG	Sidechain
1	A	489	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	4713	0	4549	45	0
2	B	49	0	43	0	0
3	A	1	0	0	0	0
4	A	7	0	10	4	0
5	A	4	0	6	0	0
6	A	4	0	3	0	0
7	A	2	0	0	2	0
8	A	31	0	0	0	0
9	A	14	0	13	0	0
10	A	321	0	0	6	0
All	All	5146	0	4624	46	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 (46) 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:282[A]:THR:HG23	10:A:802:HOH:O	1.44	1.13
7:A:706:CL:CL	10:A:1069:HOH:O	2.10	1.05
1:A:154:PRO:O	1:A:156:GLY:N	1.98	0.95
1:A:455:ILE:HD13	1:A:592:MET:HE2	1.57	0.84
1:A:346:ASP:OD1	1:A:348:ARG:HB3	1.79	0.82
1:A:284:SER:HB2	1:A:449:LYS:HE2	1.67	0.76
1:A:560:GLN:O	1:A:564:THR:HG23	1.97	0.65
1:A:179:LEU:HD11	1:A:499:VAL:HG23	1.80	0.64
1:A:449:LYS:HG2	4:A:702:PEG:H41	1.84	0.60
1:A:83:GLN:HA	1:A:86:MET:HE3	1.86	0.57
1:A:69:TYR:CE1	1:A:73:ILE:HG23	2.40	0.57
1:A:138:ILE:CD1	1:A:199:LYS:HG3	2.38	0.53
1:A:308:GLN:OE1	1:A:431:ASN:HB3	2.10	0.51
1:A:173:ARG:HH11	1:A:288:ASP:CG	2.19	0.51
1:A:143:GLU:HG3	10:A:877:HOH:O	2.11	0.50
1:A:173:ARG:NH1	1:A:288:ASP:OD1	2.44	0.49
1:A:231:GLN:HG3	10:A:919:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LEU:HD21	4:A:702:PEG:H32	1.94	0.49
1:A:275:LEU:N	1:A:275:LEU:HD22	2.29	0.48
1:A:344:PRO:HG2	1:A:350:VAL:HG11	1.95	0.48
1:A:150:THR:HG22	1:A:160:GLN:HG2	1.96	0.47
1:A:455:ILE:CD1	1:A:592:MET:HE2	2.36	0.47
1:A:96:GLY:HA3	1:A:122:LEU:HD11	1.96	0.47
1:A:287:TYR:OH	1:A:445:ASN:HB3	2.15	0.47
1:A:514:ILE:HB	1:A:515:PRO:CD	2.45	0.46
1:A:227:PRO:HD2	10:A:882:HOH:O	2.14	0.45
1:A:335:PHE:CD1	1:A:335:PHE:C	2.95	0.45
1:A:152:CYS:HA	1:A:158:CYS:HA	1.99	0.44
1:A:457:PHE:CE2	1:A:461:SER:HB3	2.53	0.43
1:A:449:LYS:CG	4:A:702:PEG:H41	2.47	0.43
1:A:552:ILE:O	1:A:553:TYR:C	2.60	0.43
1:A:449:LYS:NZ	4:A:702:PEG:H11	2.34	0.42
1:A:562:LEU:HB3	1:A:566:MET:HE2	2.00	0.42
1:A:179:LEU:HD11	1:A:499:VAL:CG2	2.47	0.42
1:A:485:TRP:CD2	1:A:508:PRO:HG3	2.55	0.41
1:A:411:GLU:HB2	1:A:526:SER:HB2	2.03	0.41
1:A:138:ILE:HD11	1:A:199:LYS:HG3	2.01	0.41
1:A:579:GLN:HA	1:A:584:GLN:O	2.21	0.41
1:A:162:GLU:HA	1:A:163:PRO:HA	1.84	0.41
1:A:223:MET:HE2	1:A:223:MET:HB3	1.82	0.41
1:A:511:LYS:O	1:A:515:PRO:HD2	2.20	0.40
1:A:282[A]:THR:HG21	10:A:1057:HOH:O	2.21	0.40
1:A:296:ALA:HB1	1:A:442:HIS:CE1	2.56	0.40
1:A:54:THR:OG1	1:A:91:HIS:HE1	2.05	0.40
1:A:224:TYR:OH	7:A:706:CL:CL	2.73	0.40
1:A:447:LEU:HD23	1:A:447:LEU:HA	1.95	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	573/597 (96%)	560 (98%)	12 (2%)	1 (0%)	43	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ASN

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	506/520 (97%)	494 (98%)	12 (2%)	43	38

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

Mol	Chain	Res	Type
1	A	79	LYS
1	A	104	VAL
1	A	123	GLU
1	A	130	GLN
1	A	242	PRO
1	A	243	LEU
1	A	282[A]	THR
1	A	282[B]	THR
1	A	342	GLU
1	A	348	ARG
1	A	394	TYR
1	A	410	HIS

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

Mol	Chain	Res	Type
1	A	91	HIS
1	A	195	GLN
1	A	442	HIS

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Mol	Chain	Res	Type
1	A	610	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 ⓘ

4 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	0.42	0	17,19,21	1.00	1 (5%)
2	NAG	B	2	2	14,14,15	0.69	0	17,19,21	1.34	2 (11%)
2	BMA	B	3	2	11,11,12	1.45	2 (18%)	15,15,17	1.84	5 (33%)
2	FUC	B	4	2	10,10,11	0.78	0	14,14,16	0.92	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
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	FUC	B	4	2	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	BMA	C2-C3	3.73	1.58	1.52
2	B	3	BMA	O5-C5	2.62	1.48	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BMA	O3-C3-C2	4.38	118.98	110.05
2	B	3	BMA	C3-C4-C5	-3.44	103.99	110.23
2	B	2	NAG	O3-C3-C2	-3.16	102.84	109.40
2	B	1	NAG	C2-N2-C7	2.86	126.74	122.90
2	B	3	BMA	O5-C5-C6	2.09	111.74	107.66
2	B	3	BMA	O2-C2-C3	2.04	114.37	110.15
2	B	2	NAG	O6-C6-C5	-2.01	104.49	111.33
2	B	3	BMA	C1-C2-C3	2.00	112.56	109.64

There are no chirality outliers.

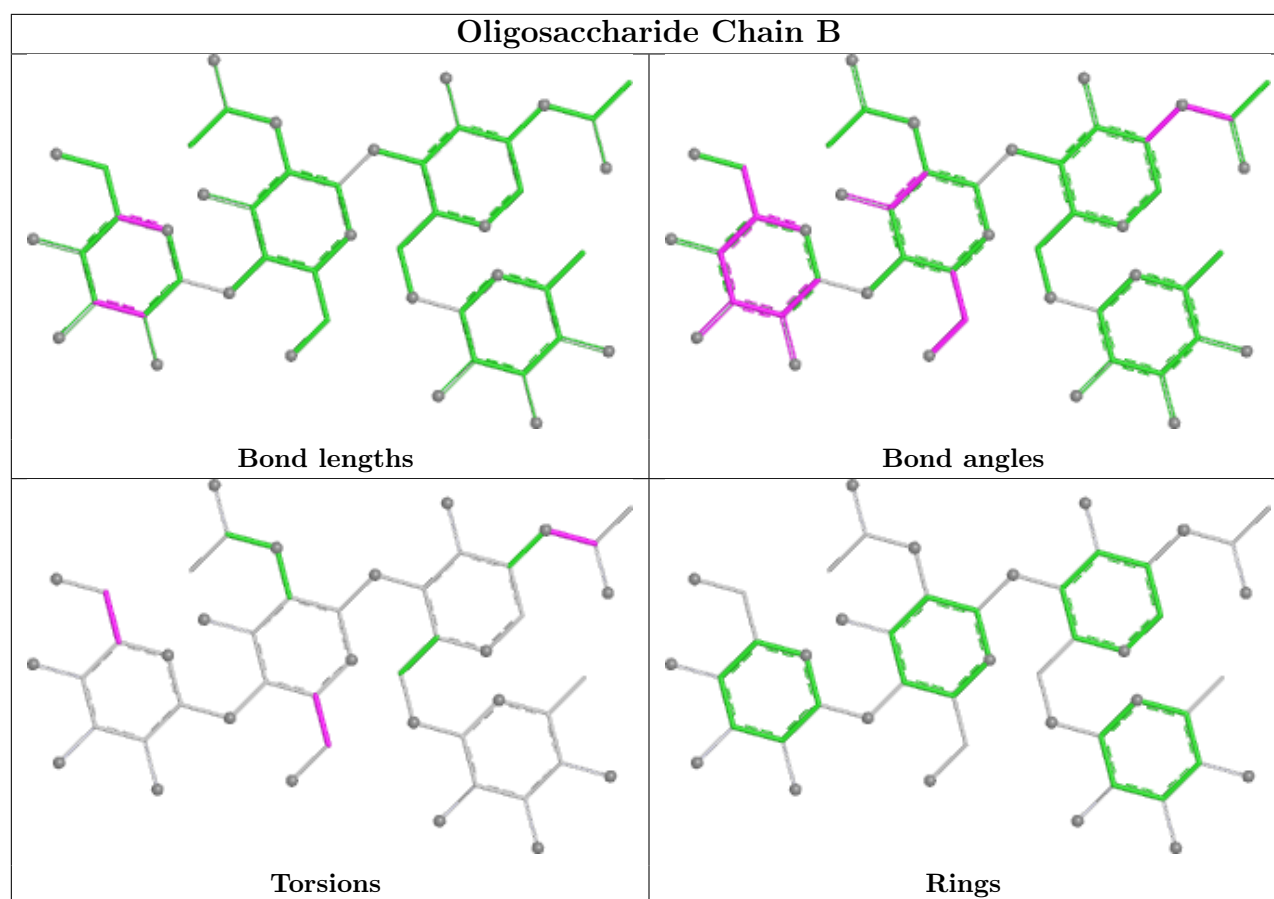
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	3	BMA	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	BO3	A	704	-	3,3,3	0.28	0	3,3,3	0.84	0
4	PEG	A	702	-	6,6,6	0.34	0	5,5,5	0.50	0
8	A1IJW	A	707	3	33,33,33	2.88	21 (63%)	41,47,47	2.44	17 (41%)
9	NAG	A	708	1	14,14,15	0.47	0	17,19,21	1.70	2 (11%)
5	EDO	A	703	-	3,3,3	0.22	0	2,2,2	0.59	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
9	NAG	A	708	1	-	2/6/23/26	0/1/1/1
5	EDO	A	703	-	-	1/1/1/1	-
8	A1IJW	A	707	3	-	3/32/52/52	0/3/3/3
4	PEG	A	702	-	-	4/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	707	A1IJW	C09-N10	5.88	1.59	1.47
8	A	707	A1IJW	C02-N24	5.65	1.47	1.34
8	A	707	A1IJW	C06-N10	-5.04	1.40	1.46
8	A	707	A1IJW	C25-N24	4.56	1.56	1.47
8	A	707	A1IJW	C11-N10	4.42	1.44	1.34
8	A	707	A1IJW	C27-C28	-3.81	1.44	1.53
8	A	707	A1IJW	C18-C12	3.66	1.45	1.39
8	A	707	A1IJW	C26-C27	3.22	1.64	1.51
8	A	707	A1IJW	C18-C17	2.97	1.43	1.38
8	A	707	A1IJW	C28-C29	2.87	1.58	1.52
8	A	707	A1IJW	C26-C25	-2.86	1.42	1.51
8	A	707	A1IJW	C12-C11	2.78	1.54	1.50
8	A	707	A1IJW	C15-N16	2.74	1.47	1.38
8	A	707	A1IJW	O30-C29	2.60	1.29	1.22
8	A	707	A1IJW	C08-C09	-2.58	1.43	1.51
8	A	707	A1IJW	C17-C15	2.39	1.45	1.40
8	A	707	A1IJW	O19-C11	-2.33	1.17	1.22
8	A	707	A1IJW	C05-N04	-2.28	1.43	1.46
8	A	707	A1IJW	C08-C07	2.27	1.61	1.51
8	A	707	A1IJW	O01-C02	-2.16	1.18	1.22
8	A	707	A1IJW	O22-C20	2.05	1.28	1.22

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	707	A1IJW	C14-C13-C12	-6.68	113.67	120.80
8	A	707	A1IJW	C18-C12-C13	5.61	125.70	118.57
8	A	707	A1IJW	C18-C17-C15	-4.96	114.60	120.66
8	A	707	A1IJW	C17-C15-C14	4.11	124.34	118.16
9	A	708	NAG	C1-C2-N2	-4.01	104.11	110.43
8	A	707	A1IJW	O01-C02-N24	-3.62	114.88	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	707	A1IJW	O31-C29-C28	3.42	124.49	113.34
9	A	708	NAG	C1-O5-C5	3.28	116.58	112.19
8	A	707	A1IJW	C23-C03-C02	-3.21	103.68	109.87
8	A	707	A1IJW	C18-C12-C11	-2.93	112.77	120.28
8	A	707	A1IJW	C27-C28-C29	-2.80	105.31	111.26
8	A	707	A1IJW	C27-C28-N24	2.56	106.77	103.02
8	A	707	A1IJW	C14-C15-N16	-2.33	116.61	120.90
8	A	707	A1IJW	C29-C28-N24	-2.29	107.94	112.54
8	A	707	A1IJW	O31-C29-O30	-2.28	118.92	124.08
8	A	707	A1IJW	C17-C18-C12	-2.27	118.38	120.80
8	A	707	A1IJW	C07-C06-N10	-2.25	100.77	102.66
8	A	707	A1IJW	O01-C02-C03	2.22	124.73	120.15
8	A	707	A1IJW	C13-C14-C15	2.06	123.18	120.66

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	707	A1IJW	N04-C05-C06-C07
9	A	708	NAG	C8-C7-N2-C2
9	A	708	NAG	O7-C7-N2-C2
4	A	702	PEG	O2-C3-C4-O4
4	A	702	PEG	O1-C1-C2-O2
8	A	707	A1IJW	C20-C05-C06-C07
4	A	702	PEG	C1-C2-O2-C3
4	A	702	PEG	C4-C3-O2-C2
8	A	707	A1IJW	N04-C05-C06-N10
5	A	703	EDO	O1-C1-C2-O2

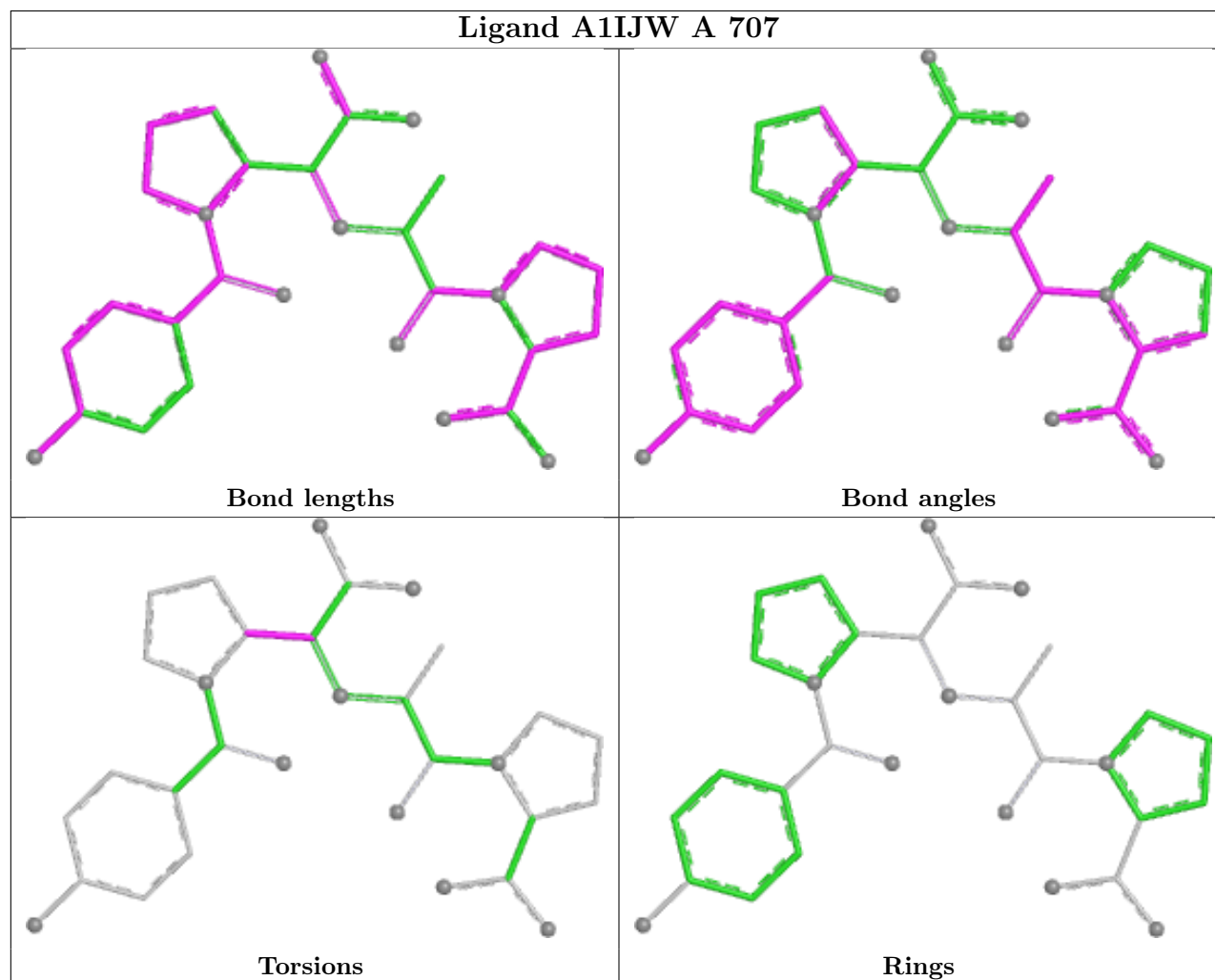
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	702	PEG	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	571/597 (95%)	-0.38	5 (0%) 81 83	9, 24, 47, 67	8 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	SER	2.8
1	A	347	GLY	2.8
1	A	154	PRO	2.8
1	A	235	ARG	2.2
1	A	42	ALA	2.1

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

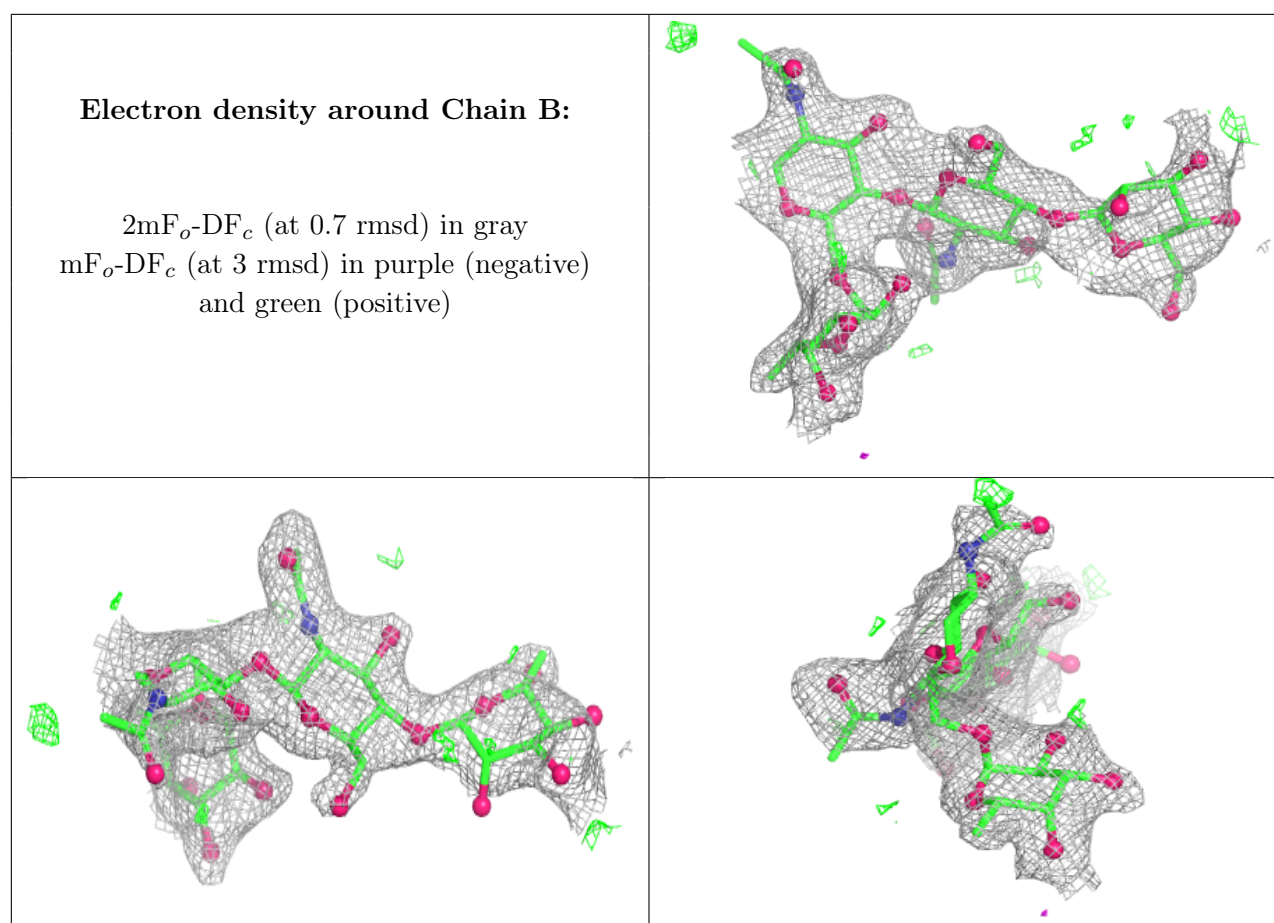
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	B	3	11/12	0.55	0.17	68,77,97,102	0
2	NAG	B	2	14/15	0.88	0.11	44,52,61,69	0
2	NAG	B	1	14/15	0.89	0.11	39,49,78,79	0
2	FUC	B	4	10/11	0.89	0.09	36,46,52,56	10

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



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

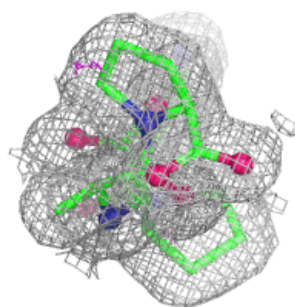
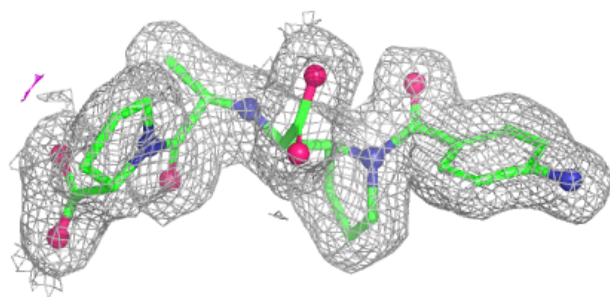
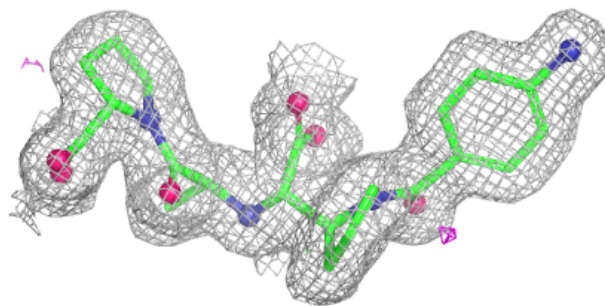
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	NAG	A	708	14/15	0.79	0.13	54,66,73,75	0
5	EDO	A	703	4/4	0.82	0.17	51,60,66,66	0
6	BO3	A	704	4/4	0.87	0.23	43,43,52,57	0
4	PEG	A	702	7/7	0.88	0.15	39,49,56,69	0
7	CL	A	706	1/1	0.97	0.11	36,36,36,36	0
8	A1IJW	A	707	31/31	0.98	0.04	13,17,20,22	0
7	CL	A	705	1/1	0.99	0.02	23,23,23,23	0
3	ZN	A	701	1/1	1.00	0.01	17,17,17,17	0

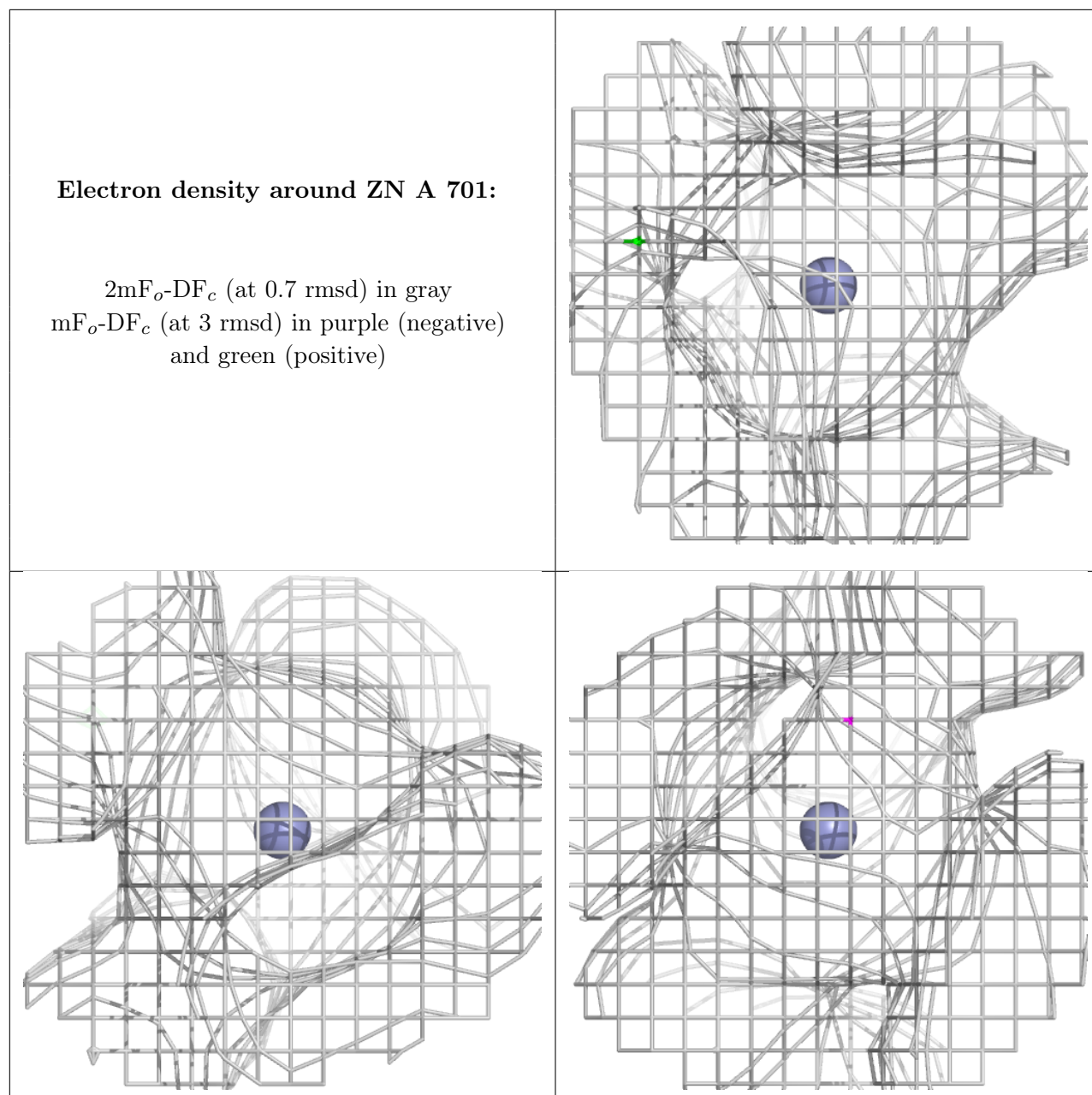
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

Electron density around A1IJW A 707:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.