

wwPDB X-ray Structure Validation Summary Report (i)

Feb 7, 2022 – 03:20 pm GMT

PDB ID	:	7Q27
Title	:	Crystal structure of Angiotensin-1 converting enzyme C-domain in complex
		with dual ACE/NEP inhibitor AD011
Authors	:	Cozier, G.E.; Acharya, K.R.
Deposited on		
Resolution	:	1.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

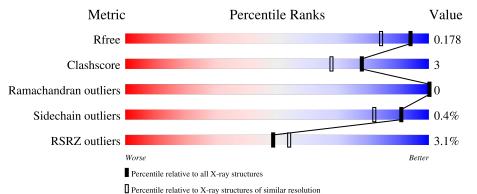
MolProbity		4 09b 467
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	А	597	^{3%} 92%	6% ·				
2	В	4	50%	50%				

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
9	BO3	А	711[A]	-	-	Х	-



2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 10818 atoms, of which 4975 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.

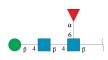
• Molecule 1 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	A	586	Total 9796	C 3179	Н 4817	N 853	O 920	S 27	0	29	0

There are 5 discrepancies between the modelled and reference sequences:

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

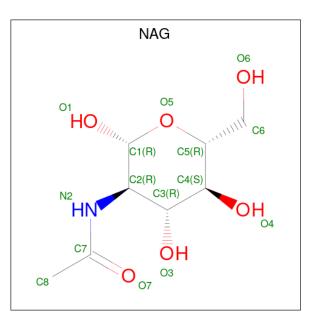
• Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopy ranose.



Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	Trace
2	В	4	Total 93	C 28	Н 44	N 2	0 19	0	0	0

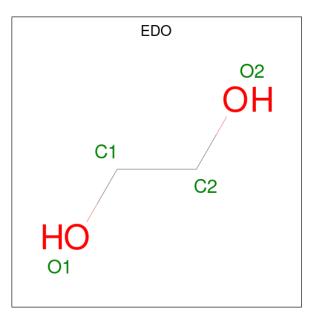
• Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	Δ	1	Total	С	Η	Ν	Ο	0	0
J	A	1	28	8	14	1	5	0	0

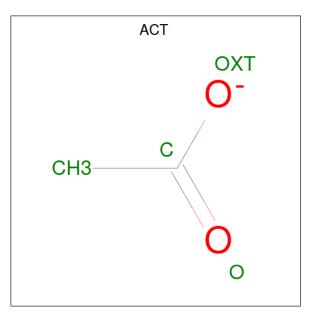
• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total C H O 20 4 12 4	0	1
4	А	1	Total C H O 10 2 6 2	0	0
4	А	1	Total C H O 10 2 6 2	0	0



• Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



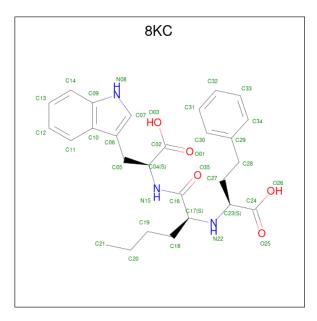
[Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
	5	А	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{H} & \text{C} \\ 7 & 2 & 3 & 2 \end{array}$) 2	0	0

• Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

• Molecule 7 is $(2 \{S\})-2-[[(2 \{S\})-1-[[(2 \{S\})-3-(1 \{H\}-indol-3-yl)-1-oxidanyl-1-oxidanylidene -propan-2-yl]amino]-1-oxidanylidene-hexan-2-yl]amino]-4-phenyl-butanoic acid (three-letter code: 8KC) (formula: C₂₇H₃₃N₃O₅) (labeled as "Ligand of Interest" by depositor).$



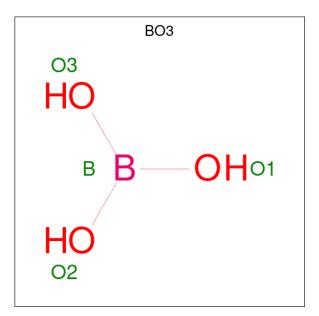


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
7	А	1	Total 66	С 27		N 3	O 5	0	0

• Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Μ	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
8		А	2	Total Cl 2 2	0	0

• Molecule 9 is BORIC ACID (three-letter code: BO3) (formula: BH₃O₃).

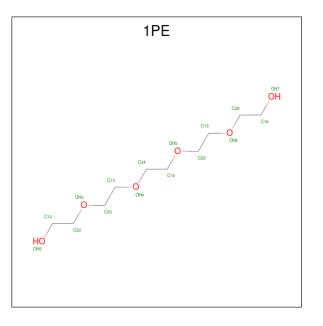




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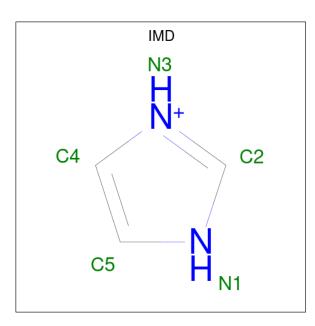
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	Total B H O 7 1 3 3	0	0
9	А	1	Total B H O 7 1 3 3	0	1
9	А	1	Total B H O 7 1 3 3	0	0
9	А	1	Total B H O 7 1 3 3	0	0
9	А	1	Total B H O 7 1 3 3	0	0

• Molecule 10 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	Λ	1	Total	С	Η	0	0	0
10	Л	1	38	10	22	6	0	0





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	А	1	Total 10	С 3	H5	N 2	0	0

• Molecule 12 is water.

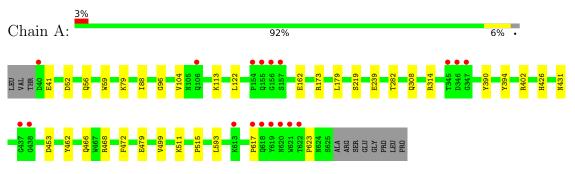
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	А	695	Total O 702 702	0	17



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: Angiotensin-converting enzyme



 \bullet Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alp ha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:	50%	50%
NAG1 NAG2 BMA3 FUC4		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	56.45Å 85.59Å 134.05Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.13 - 1.50	Depositor
Resolution (A)	52.03 - 1.50	EDS
% Data completeness	$100.0 \ (47.13 - 1.50)$	Depositor
(in resolution range)	$100.0\ (52.03-1.50)$	EDS
R _{merge}	0.22	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.91 (at 1.50 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
D D.	0.148 , 0.178	Depositor
R, R_{free}	0.149 , 0.178	DCC
R_{free} test set	2131 reflections (2.04%)	wwPDB-VP
Wilson B-factor $(Å^2)$	12.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10818	wwPDB-VP
Average B, all atoms $(Å^2)$	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, IMD, BO3, CL, ZN, BMA, 8KC, 1PE, NAG, EDO, FUC

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).

Mal	Chain	Chain Bond lengths			angles
	Mol Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.53	0/5156	0.69	0/7009

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 (i)

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	А	4979	4817	4775	27	1
2	В	49	44	43	0	0
3	А	14	14	13	0	0
4	А	16	24	24	0	0
5	А	4	3	3	1	0
6	А	1	0	0	0	0
7	А	35	31	0	0	0
8	А	2	0	0	0	0
9	А	20	15	15	2	0
10	А	16	22	22	0	0
11	А	5	5	5	1	0
12	А	702	0	0	13	0
All	All	5843	4975	4900	29	1



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 29 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:308[A]:GLN:NE2	12:A:801:HOH:O	1.96	0.98
1:A:59:TRP:CE2	1:A:88:ILE:HD11	2.18	0.77
1:A:219[A]:SER:OG	9:A:711[A]:BO3:O3	2.08	0.72
11:A:716:IMD:H4	12:A:844:HOH:O	1.96	0.64
1:A:59:TRP:CD2	1:A:88:ILE:HD11	2.34	0.63

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:HIS:HD1	1:A:479[A]:GLU:OE2[1_455]	1.56	0.04

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	А	614/597~(103%)	603~(98%)	11 (2%)	0	100 100	

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	541/520~(104%)	539~(100%)	2~(0%)	91 82		

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	390	TYR
1	А	394	TYR

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	Iol Type Chain Res				Bo	ond leng	\mathbf{ths}	Bond angles		
	Type	Chain	nes	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	NAG	В	1	1,2	$14,\!14,\!15$	0.48	0	$17,\!19,\!21$	0.44	0
2	NAG	В	2	2	14,14,15	0.46	0	17,19,21	0.43	0
2	BMA	В	3	2	11,11,12	1.13	0	$15,\!15,\!17$	0.99	1 (6%)
2	FUC	В	4	2	10,10,11	0.90	0	14,14,16	0.91	1 (7%)

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.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	В	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	В	2	2	-	2/6/23/26	0/1/1/1
2	BMA	В	3	2	-	0/2/19/22	0/1/1/1
2	FUC	В	4	2	-	-	0/1/1/1

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	3	BMA	C1-O5-C5	2.41	115.46	112.19
2	В	4	FUC	O2-C2-C1	2.00	113.25	109.15

There are no chirality outliers.

All (2) torsion outliers are listed below:

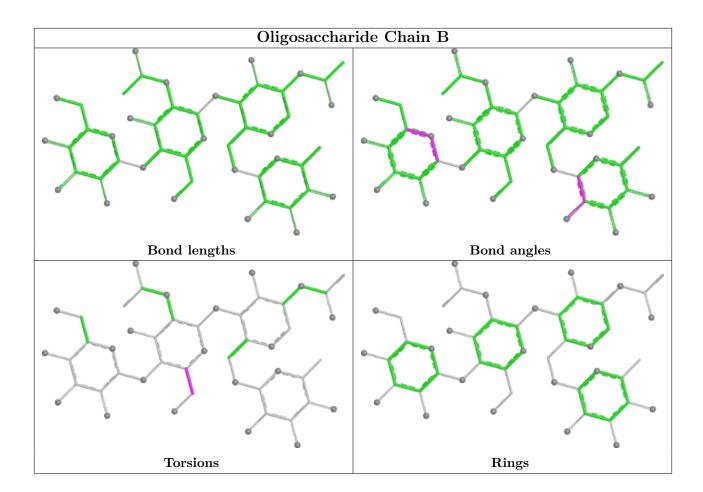
Mol	Chain	Res	Type	Atoms
2	В	2	NAG	C4-C5-C6-O6
2	В	2	NAG	O5-C5-C6-O6

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 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	Turne	Chain	Res	Link	В	ond leng	gths	B	ond ang	les
	Type	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BO3	А	711[A]	-	3,3,3	0.69	0	3,3,3	0.69	0
5	ACT	A	705	-	$1,\!3,\!3$	<mark>6.99</mark>	1 (100%)	$0,\!3,\!3$	-	-
3	NAG	А	701	1	14,14,15	0.33	0	17,19,21	0.50	0
4	EDO	А	703	-	3,3,3	0.46	0	2,2,2	0.27	0
9	BO3	А	710	-	3,3,3	0.65	0	3,3,3	0.55	0
9	BO3	А	713	-	3, 3, 3	0.29	0	3,3,3	0.13	0
4	EDO	А	704	-	3,3,3	0.54	0	2,2,2	0.81	0
10	1PE	А	715	-	$15,\!15,\!15$	0.48	0	14,14,14	0.52	0



Mol	Turne	Chain	Res	Link	B	ond leng	gths	В	ond ang	les
	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	EDO	А	702[B]	-	$3,\!3,\!3$	0.37	0	$2,\!2,\!2$	0.53	0
7	8KC	А	707	6	30,37,37	1.22	1 (3%)	34,49,49	1.16	2 (5%)
11	IMD	А	716	-	$3,\!5,\!5$	0.23	0	$4,\!5,\!5$	0.63	0
9	BO3	А	714	-	$3,\!3,\!3$	0.28	0	3,3,3	0.38	0
4	EDO	А	702[A]	-	$3,\!3,\!3$	0.44	0	2,2,2	0.55	0
9	BO3	А	712	-	$3,\!3,\!3$	0.32	0	3,3,3	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	А	701	1	-	0/6/23/26	0/1/1/1
4	EDO	А	703	-	-	0/1/1/1	-
4	EDO	А	704	-	-	1/1/1/1	-
10	1PE	А	715	-	-	0/13/13/13	-
4	EDO	А	702[B]	-	-	1/1/1/1	-
7	8KC	А	707	6	-	6/24/42/42	0/3/3/3
11	IMD	А	716	-	-	-	0/1/1/1
4	EDO	А	702[A]	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
5	А	705	ACT	CH3-C	6.99	1.57	1.48
7	А	707	8KC	C16-N15	4.12	1.43	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
7	А	707	8KC	C04-N15-C16	-3.91	117.33	123.19
7	А	707	8KC	C16-C17-N22	-2.20	105.74	110.51

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
4	А	702[A]	EDO	O1-C1-C2-O2
7	А	707	8KC	C05-C04-N15-C16
7	А	707	8KC	O35-C16-C17-N22

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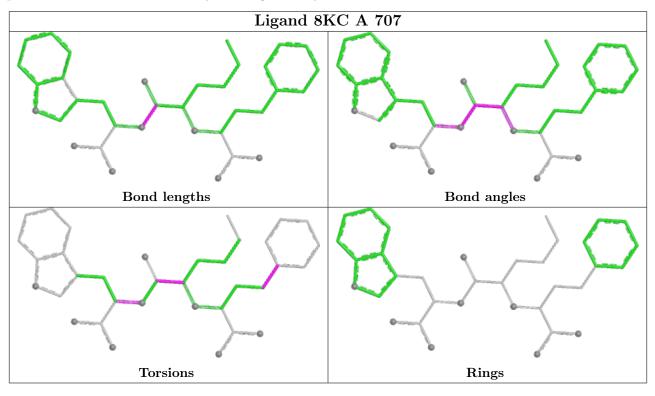
Mol	Chain	Res	Type	Atoms
7	А	707	8KC	N15-C16-C17-N22
7	А	707	8KC	C02-C04-N15-C16

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	А	711[A]	BO3	2	0
5	А	705	ACT	1	0
11	А	716	IMD	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 then 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, 95^{th} 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	2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	586/597~(98%)	-0.20	18 (3%) 49	54	7, 15, 37, 70	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	619	TYR	5.8
1	А	155	GLN	5.3
1	А	620	ASN	4.3
1	А	617	PRO	4.1
1	А	437	GLY	3.8

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

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

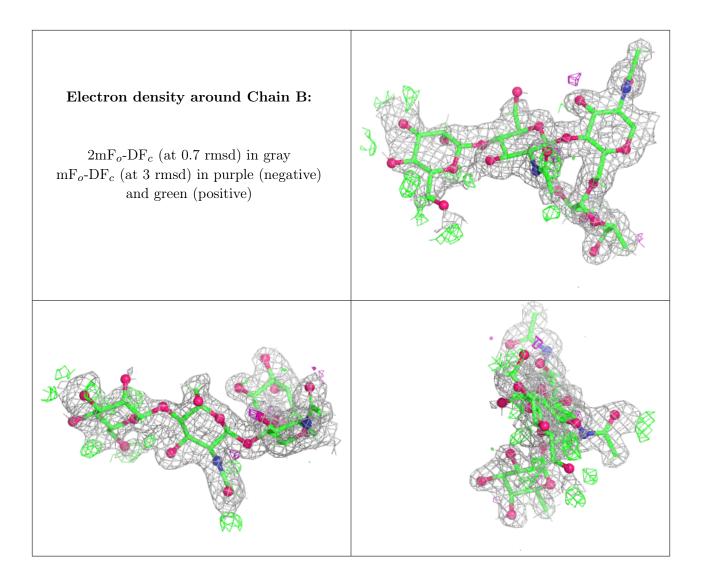
6.3 Carbohydrates (i)

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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	BMA	В	3	11/12	0.75	0.15	38,75,91,91	0
2	FUC	В	4	10/11	0.87	0.21	30,40,55,62	0
2	NAG	В	2	14/15	0.92	0.13	$25,\!41,\!59,\!101$	0
2	NAG	В	1	14/15	0.95	0.13	$20,\!34,\!46,\!50$	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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	EDO	А	704	4/4	0.79	0.12	$36,\!46,\!57,\!57$	0
9	BO3	А	714	4/4	0.81	0.27	$35,\!41,\!50,\!60$	0
5	ACT	А	705	4/4	0.83	0.22	40,48,57,57	0
9	BO3	А	711[A]	4/4	0.86	0.17	$16,\!17,\!21,\!25$	7
3	NAG	А	701	14/15	0.86	0.20	$36,\!46,\!58,\!73$	0
9	BO3	А	713	4/4	0.87	0.18	40,45,48,55	0
4	EDO	А	703	4/4	0.87	0.21	$39,\!47,\!55,\!58$	0
9	BO3	А	712	4/4	0.92	0.13	19,26,32,38	0
9	BO3	А	710	4/4	0.93	0.10	18,26,32,39	0

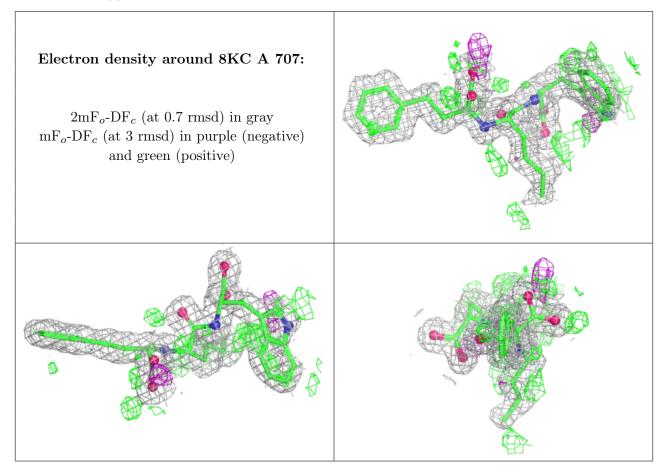
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
4	EDO	А	702[A]	4/4	0.95	0.14	10,21,38,46	10
4	EDO	А	702[B]	4/4	0.95	0.14	10,24,34,41	10
10	1PE	А	715	16/16	0.95	0.09	16,24,56,56	0
7	8KC	А	707	35/35	0.96	0.08	9,16,45,66	0
11	IMD	А	716	5/5	0.97	0.08	15,20,25,26	0
8	CL	А	708	1/1	0.99	0.07	12,12,12,12	0
8	CL	А	709	1/1	1.00	0.07	11,11,11,11	0
6	ZN	А	706	1/1	1.00	0.06	10,10,10,10	0

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



6.5 Other polymers (i)

There are no such residues in this entry.

