

# Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 01:28 pm GMT

PDB ID : 2XY9

Title : Human Angiotensin converting enzyme in complex with phosphinic tripeptide Authors : Akif, M.; Schwager, S.L.; Anthony, C.S.; Czarny, B.; Beau, F.; Dive, V.;

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Deposited on : 2010-11-16

Resolution : 1.97 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.orgA user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

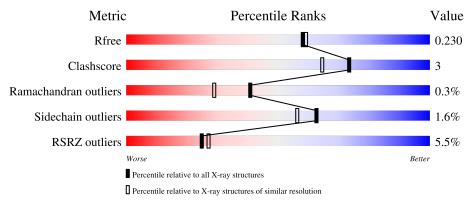
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.97 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
$R_{free}$	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	A	585	90%	9%	
2	В	4	100%		_

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	
3	ACT	A	1625	_	_	X	_	



## 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 5355 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.

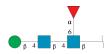
• Molecule 1 is a protein called ANGIOTENSIN-CONVERTING ENZYME.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	Λ	581	Total	С	N	О	S	0	0	0
1	A	301	4738	3042	809	863	24	0	0	U

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	624	ALA	-	expression tag	UNP P12821

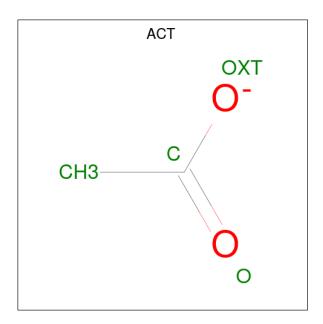
• Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

• Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).





Mol	Chain	Residues	Ato	ms	ZeroOcc	AltConf
3	A	1	Total 4	C O 2	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

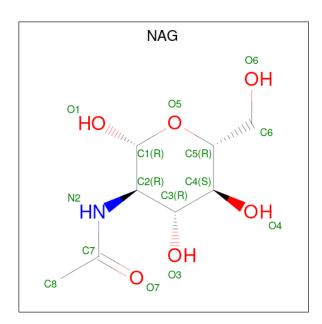
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0

• Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

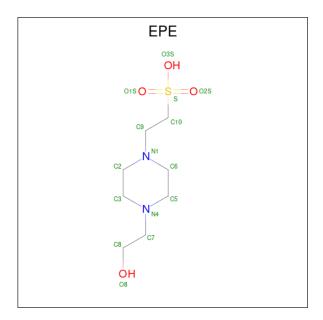
 $\bullet$  Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $\rm C_8H_{15}NO_6).$ 





Mol	Chain	Residues	A	tor	ns		ZeroOcc	AltConf
6	A	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).

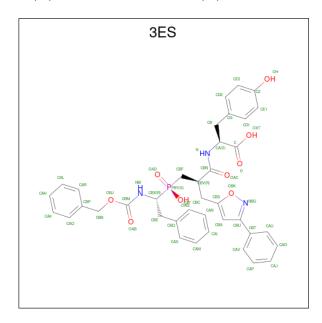


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	А	1	Total	С	N	О	S	0	0
'	11	1	15	8	2	4	1		

• Molecule 8 is  $[(2S)-2-({3-[HYDROXYL(2-PHENYL-(1R)-1-{[(BENZYLOXY)](2S)-2-({3-[HYDROXYL(2-PHENYL-(1R)-1-CARBONYL]-AMINO}ETHYL)PHOSPHINYL]-2-[(3-PHENYL-1R)-1-PHENYL-1R]-2-[(3-PHENYL-1R)-1-PHENYL-1R]-2-[(3-PHENYL-1R)-1-PHENYL-1R]-2-[(3-PHENYL-1R)-1-PHENYL-1R]-2-[(3-PHENYL-1R)-2-[(3-PHENYL-1R)-1-PHENYL-1R]-2-[(3-PHENYL-1R)-1-PHENYL-1R]-2-[(3-PHENYL-1R)-1-PHENYL-1R]-2-[(3-PHENYL-1R)-1-PHENYL-1R]-2-[(3-PHENYL-1R)-1-PHENYL-1R]-2-[(3-PHENYL-1R)-1-[(3-PHENYL-1R)-1-[(3-PHENYL-1R)-1R]-2-[(3-PHENYL-1R)-1-[(3-PHENYL-1R)-1R]-2-[(3-$ 



 $\label{eq:henvelson} HENYLISOXAZOL-5-YL)METHYL]-1-OXO-PROPYL\\AMINO)-3-(4-HYDROXY-PHENYL) \ (three-letter code: 3ES) \ (formula: $C_{38}H_{38}N_3O_9P).$ 



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
Q	Λ	1	Total	С	N	О	Р	0	0	
0	A	1	51	38	3	9	1	U	U	
Q	Λ	1	Total	С	N	О	Р	0	0	
0	A	1	51	38	3	9	1	U		

#### • Molecule 9 is water.

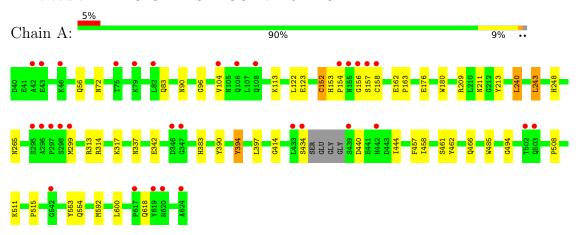
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	430	Total O 430 430	0	0



## 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: ANGIOTENSIN-CONVERTING ENZYME



• 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: 100%





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	58.73Å 86.09Å 134.81Å	Donositon
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.65 - 1.97	Depositor
Resolution (A)	45.65 - 1.97	EDS
% Data completeness	97.8 (45.65-1.97)	Depositor
(in resolution range)	97.8 (45.65-1.97)	EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.35 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
D D.	0.199 , 0.232	Depositor
$R, R_{free}$	0.199 , 0.230	DCC
$R_{free}$ test set	2442 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.1	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 42.9	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5355	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities 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: FUC, NAG, EPE, BMA, ZN, ACT, CL, 3ES

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	Bond	$\mathbf{lengths}$	Bond angles		
MIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.37	0/4878	0.51	0/6635	

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	A	4738	0	4571	31	0
2	В	49	0	43	0	0
3	A	4	0	3	2	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	14	0	13	0	0
7	A	15	0	17	0	0
8	A	102	0	71	0	0
9	A	430	0	0	4	0
All	All	5355	0	4718	31	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 3.



All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 4 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}\ ({\rm \AA})$	overlap (Å)
1:A:176:GLU:HG2	9:A:2143:HOH:O	1.85	0.75
1:A:123:GLU:HA	3:A:1625:ACT:H3	1.74	0.70
1:A:96:GLY:HA3	1:A:122:LEU:HD22	1.80	0.64
1:A:153:HIS:CE1	1:A:180:TRP:CZ2	2.86	0.64
1:A:90:ASN:ND2	9:A:2049:HOH:O	2.31	0.62
1:A:240:LEU:HD22	1:A:458:ILE:HG13	1.84	0.58
1:A:153:HIS:HB3	1:A:154:PRO:HD2	1.85	0.58
1:A:240:LEU:HD21	1:A:592:MET:SD	2.43	0.57
1:A:153:HIS:HB3	1:A:154:PRO:CD	2.35	0.56
1:A:313:ARG:O	1:A:317:LYS:HG2	2.07	0.55
1:A:457:PHE:CE2	1:A:461:SER:HB3	2.43	0.54
1:A:153:HIS:CE1	1:A:180:TRP:CE2	2.96	0.53
1:A:299:MET:HE1	1:A:434:SER:N	2.24	0.52
1:A:56:GLN:HB3	9:A:2013:HOH:O	2.10	0.51
1:A:152:CYS:CB	1:A:158:CYS:SG	3.00	0.50
1:A:553:TYR:O	1:A:554:GLN:HB2	2.12	0.49
1:A:104:VAL:HG13	1:A:113:LYS:HG2	1.95	0.47
1:A:265:ASN:ND2	1:A:618:GLN:OE1	2.41	0.46
1:A:394:TYR:HB2	1:A:397:LEU:HD12	1.98	0.46
1:A:211:ASN:HB2	3:A:1625:ACT:H2	1.98	0.46
1:A:440:ASP:O	1:A:444:ILE:HG12	2.17	0.45
1:A:248:HIS:HE1	1:A:494:GLY:O	2.00	0.45
1:A:209:ARG:HA	1:A:213:TYR:O	2.18	0.43
1:A:511:LYS:O	1:A:515:PRO:HD2	2.19	0.43
1:A:162:GLU:HA	1:A:163:PRO:HA	1.77	0.43
1:A:383:HIS:HA	1:A:414:GLY:HA3	2.01	0.43
1:A:243:LEU:HD13	1:A:600:LEU:HB2	2.01	0.41
1:A:462:TYR:O	1:A:466:GLN:HG2	2.21	0.41
1:A:485:TRP:CD2	1:A:508:PRO:HG3	2.56	0.41
1:A:83:GLN:HB3	9:A:2042:HOH:O	2.20	0.40
1:A:152:CYS:HA	1:A:157:SER:O	2.21	0.40

There are no symmetry-related clashes.



### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	577/585 (99%)	561 (97%)	14 (2%)	2 (0%)	41 29

#### All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	156	GLY

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed Rotameric		Outliers	Percentiles
1	A	505/510 (99%)	497 (98%)	8 (2%)	62 56

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	CYS
1	A	240	LEU
1	A	243	LEU
1	A	314	ARG
1	A	337	ASN
1	A	342	GLU
1	A	390	TYR
1	A	394	TYR



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	87	GLN
1	A	90	ASN
1	A	248	HIS
1	A	539	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

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	Chain	n Res	s Link	Bond lengths			Bond angles		
MIOI	Type		ries	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
2	NAG	В	1	2,1	14,14,15	0.48	0	17,19,21	0.62	0	
2	NAG	В	2	2	14,14,15	0.50	0	17,19,21	0.71	0	
2	BMA	В	3	2	11,11,12	0.51	0	15,15,17	0.95	0	
2	FUC	В	4	2	10,10,11	0.63	0	14,14,16	0.58	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.

$\mid \mathbf{M} \mid$	[ol	$\mathbf{Type}$	Chain	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
6	2	NAG	В	1	2,1	-	0/6/23/26	0/1/1/1
6	2	NAG	В	2	2	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

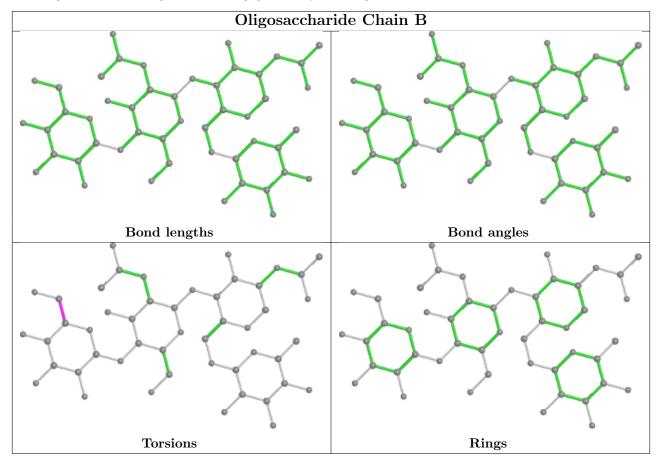
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	3	BMA	C4-C5-C6-O6
2	В	3	BMA	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 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	Trmo	Chain	Dag	Link	Bo	Bond lengths			Bond angles		
MIOI	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
7	EPE	A	1634	-	15,15,15	0.84	1 (6%)	18,20,20	1.98	6 (33%)	
6	NAG	A	1631	1	14,14,15	0.52	0	17,19,21	0.95	2 (11%)	
3	ACT	A	1625	-	3,3,3	0.79	0	3,3,3	0.88	0	
8	3ES	A	1636	-	48,55,55	1.50	3 (6%)	55,75,75	1.45	7 (12%)	
8	3ES	A	1635	5	48,55,55	1.23	3 (6%)	55,75,75	0.89	2 (3%)	

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
8	3ES	A	1635	5	-	7/38/48/48	0/5/5/5
6	NAG	A	1631	1	-	0/6/23/26	0/1/1/1
8	3ES	A	1636	-	-	8/38/48/48	0/5/5/5
7	EPE	A	1634	-	-	0/9/19/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
8	A	1636	3ES	PBY-CBF	6.13	1.85	1.79
8	A	1636	3ES	CBB-CBP	-5.00	1.38	1.50
8	A	1635	3ES	CBB-CBP	-4.12	1.40	1.50
8	A	1635	3ES	CBA-CBS	-4.00	1.34	1.39
8	A	1636	3ES	CBA-CBS	-3.81	1.34	1.39
7	A	1634	EPE	C10-S	2.73	1.81	1.77
8	A	1635	3ES	PBY-CBF	2.50	1.82	1.79

All (17) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
8	A	1636	3ES	PBY-CBX-CBE	-4.67	103.10	110.99
7	A	1634	EPE	C5-N4-C3	4.58	119.13	108.83
8	A	1636	3ES	OAG-PBY-CBX	4.29	116.50	106.87
8	A	1636	3ES	OBJ-CBB-CBP	4.15	119.37	109.39
7	A	1634	EPE	C7-N4-C5	3.61	120.46	111.23
7	A	1634	EPE	C7-N4-C3	3.44	120.04	111.23
8	A	1636	3ES	OBJ-CBM-NBI	3.38	117.37	110.50
8	A	1636	3ES	PBY-CBX-NBI	2.88	115.59	109.18
8	A	1635	3ES	CBB-OBJ-CBM	2.74	122.04	115.93
7	A	1634	EPE	O2S-S-C10	2.67	110.13	106.92
7	A	1634	EPE	O3S-S-C10	2.44	109.72	105.77
8	A	1636	3ES	OBJ-CBM-OAB	-2.41	119.63	124.25
7	A	1634	EPE	C6-N1-C2	2.30	114.01	108.83
8	A	1636	3ES	CBE-CBX-NBI	-2.18	108.82	111.39
6	A	1631	NAG	C1-O5-C5	2.16	115.11	112.19
8	A	1635	3ES	OBJ-CBB-CBP	2.15	114.57	109.39
6	A	1631	NAG	C4-C3-C2	2.02	113.98	111.02

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1635	3ES	OAC-CBN-CBV-CBC
8	A	1635	3ES	N-CBN-CBV-CBC
8	A	1636	3ES	PBY-CBF-CBV-CBC
8	A	1635	3ES	N-CA-CB-CG
8	A	1636	3ES	CBS-CBC-CBV-CBF
8	A	1635	3ES	C-CA-CB-CG
8	A	1636	3ES	CA-CB-CG-CD2
8	A	1636	3ES	CA-CB-CG-CD1
8	A	1636	3ES	PBY-CBF-CBV-CBN
8	A	1635	3ES	OAC-CBN-CBV-CBF
8	A	1635	3ES	N-CBN-CBV-CBF
8	A	1636	3ES	NBI-CBX-PBY-OAD
8	A	1635	3ES	CBS-CBC-CBV-CBF
8	A	1636	3ES	N-CBN-CBV-CBC
8	A	1636	3ES	CBE-CBX-PBY-OAD

There are no ring outliers.

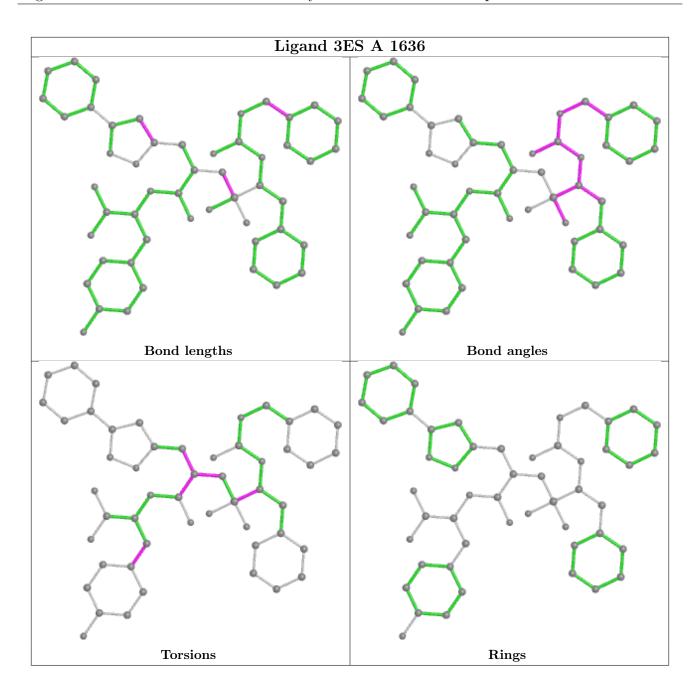
1 monomer is involved in 2 short contacts:



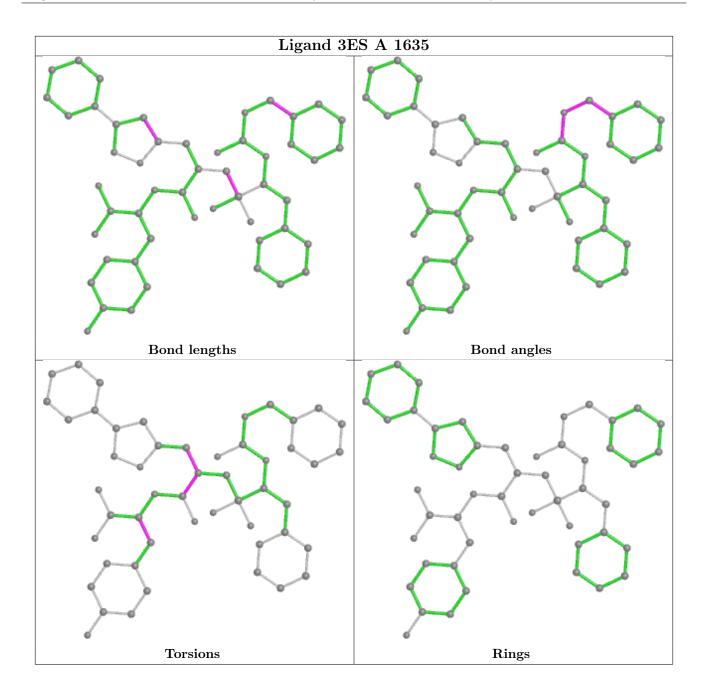
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1625	ACT	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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>	$\# \mathrm{RSRZ}{>}2$		$OWAB(Å^2)$	Q < 0.9
1	A	581/585 (99%)	0.21	32 (5%) 25	27	10, 20, 36, 49	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	GLY	7.8
1	A	157	SER	5.4
1	A	154	PRO	5.0
1	A	347	GLY	4.9
1	A	503	GLN	4.5
1	A	299	MET	4.5
1	A	298	SER	4.3
1	A	155	ASN	4.1
1	A	297	PRO	4.1
1	A	346	ASP	4.0
1	A	75	THR	3.8
1	A	296	ALA	3.4
1	A	295	SER	3.3
1	A	108	GLN	3.2
1	A	439	SER	3.2
1	A	46	LYS	3.0
1	A	620	ASN	2.9
1	A	79	LYS	2.7
1	A	619	TYR	2.6
1	A	106	GLN	2.6
1	A	104	VAL	2.5
1	A	624	ALA	2.5
1	A	617	PRO	2.5
1	A	502	THR	2.4
1	A	542	GLY	2.3
1	A	82	LEU	2.3
1	A	42	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	434	SER	2.2
1	A	433	LEU	2.2
1	A	442	HIS	2.2
1	A	158	CYS	2.1
1	A	43	GLU	2.0

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

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

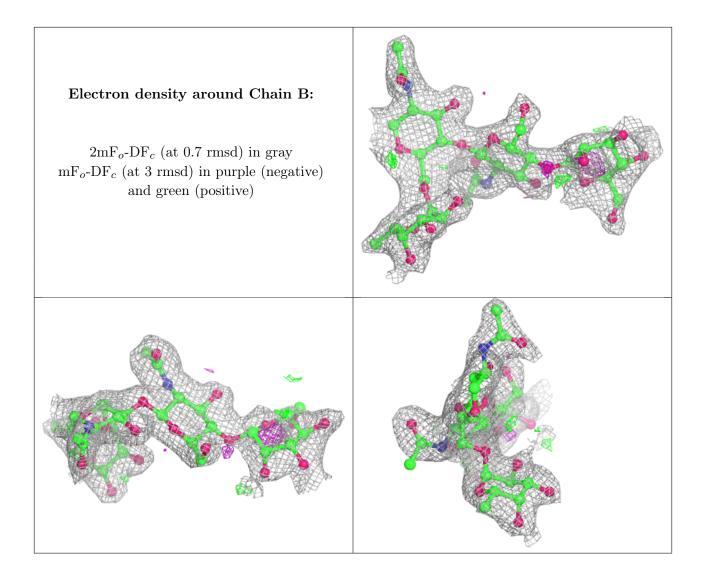
### 6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	BMA	В	3	11/12	0.64	0.26	55,57,57,57	0
2	NAG	В	2	14/15	0.83	0.17	47,49,51,54	0
2	NAG	В	1	14/15	0.86	0.16	42,44,44,46	0
2	FUC	В	4	10/11	0.92	0.13	43,43,44,44	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.





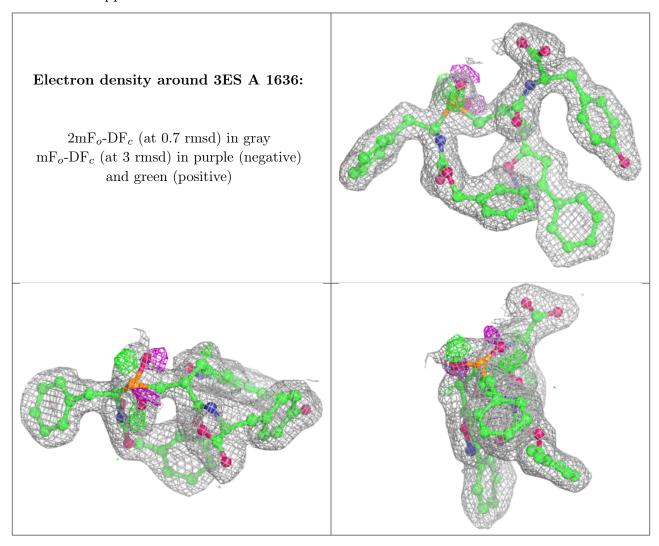
## 6.4 Ligands (i)

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.

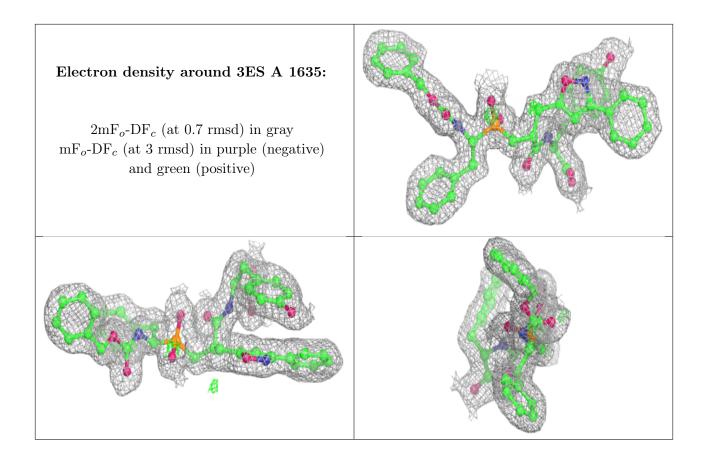
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
7	EPE	A	1634	15/15	0.56	0.33	62,62,64,64	15
6	NAG	A	1631	14/15	0.75	0.40	38,42,42,44	0
3	ACT	A	1625	4/4	0.89	0.15	18,18,18,18	0
8	3ES	A	1636	51/51	0.94	0.13	17,20,23,26	0
8	3ES	A	1635	51/51	0.97	0.15	9,13,18,20	0
4	$\operatorname{CL}$	A	1626	1/1	0.99	0.09	15,15,15,15	0
4	CL	A	1627	1/1	0.99	0.13	13,13,13,13	0
5	ZN	A	1628	1/1	1.00	0.06	14,14,14,14	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 (i)

There are no such residues in this entry.

