



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 24, 2018 – 01:46 PM EDT

PDB ID : 6F9R  
Title : Crystal structure of human Angiotensin-1 converting enzyme N-domain in complex with Sampatrilat-Asp.  
Authors : Cozier, G.E.; Acharya, K.R.  
Deposited on : 2017-12-15  
Resolution : 1.85 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031021  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031021

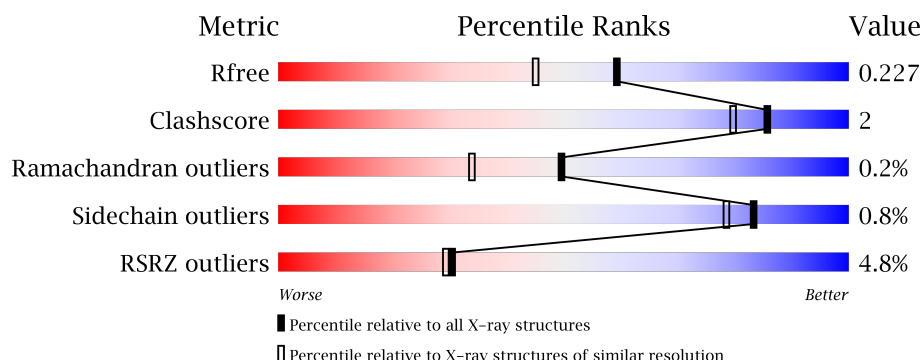
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	111664	2111 (1.86-1.86)
Clashscore	122126	2258 (1.86-1.86)
Ramachandran outliers	120053	2234 (1.86-1.86)
Sidechain outliers	120020	2234 (1.86-1.86)
RSRZ outliers	108989	2075 (1.86-1.86)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	629	<div> <div>5%</div> <div>91%</div> <div>5%</div> </div>
1	B	629	<div> <div>4%</div> <div>89%</div> <div>7%</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
12	ACT	A	717	-	-	X	-
2	NAG	B	702	-	-	-	X
4	BMA	A	706	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 21728 atoms, of which 10253 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	607	Total	C	H	N	O	S	0	8	0
			9780	3206	4779	862	914	19			
1	B	604	Total	C	H	N	O	S	0	54	0
			10442	3425	5102	917	979	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	conflict	UNP P12821
A	25	GLN	ASN	conflict	UNP P12821
A	82	GLN	ASN	conflict	UNP P12821
A	117	GLN	ASN	conflict	UNP P12821
A	289	GLN	ASN	conflict	UNP P12821
A	545	ARG	GLN	conflict	UNP P12821
A	576	LEU	PRO	conflict	UNP P12821
A	629	LEU	-	expression tag	UNP P12821
B	9	GLN	ASN	conflict	UNP P12821
B	25	GLN	ASN	conflict	UNP P12821
B	82	GLN	ASN	conflict	UNP P12821
B	117	GLN	ASN	conflict	UNP P12821
B	289	GLN	ASN	conflict	UNP P12821
B	545	ARG	GLN	conflict	UNP P12821
B	576	LEU	PRO	conflict	UNP P12821
B	629	LEU	-	expression tag	UNP P12821

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



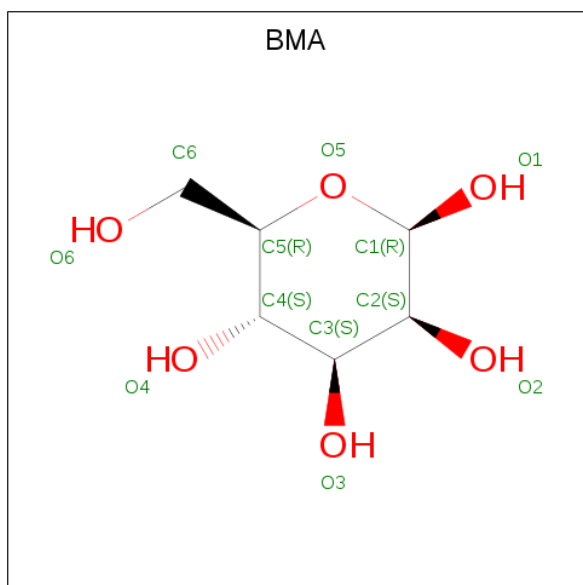
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
2	A	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
2	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
2	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
2	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
2	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
2	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
2	B	1	Total	C	H	N	O	0	0
			25	8	11	1	5		
2	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 3 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			20	6	10	4		
3	A	1	Total	C	H	O	0	0
			20	6	10	4		
3	B	1	Total	C	H	O	0	0
			20	6	10	4		
3	B	1	Total	C	H	O	0	0
			20	6	10	4		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).

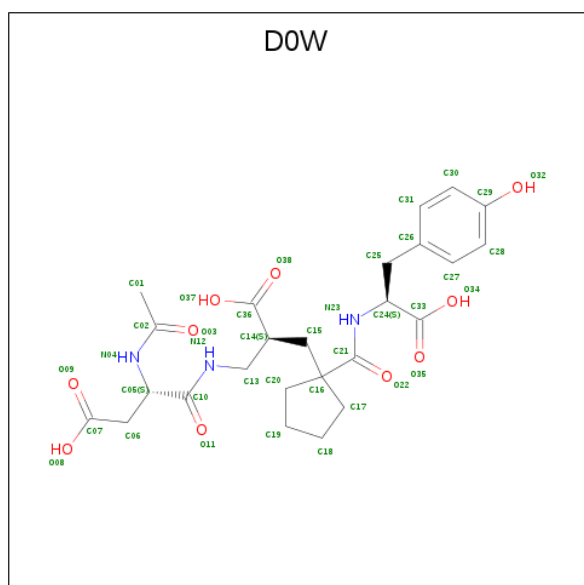


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			21	6	10	5		
4	B	1	Total	C	H	O	0	0
			21	6	10	5		

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

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

- Molecule 6 is Sampatrilat-Asp (three-letter code: D0W) (formula: C<sub>25</sub>H<sub>33</sub>N<sub>3</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	0
			68	25	30	3	10		
6	B	1	Total	C	H	N	O	0	0
			68	25	30	3	10		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

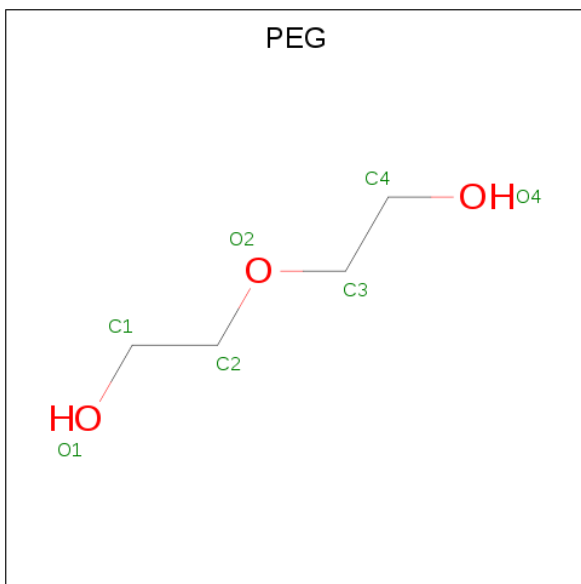
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

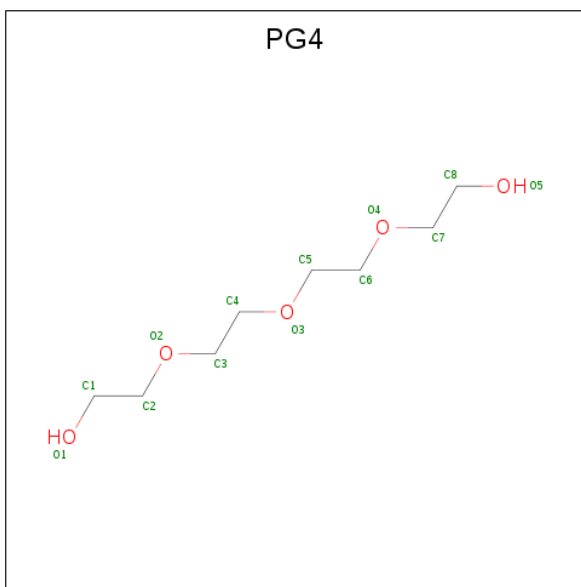
- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			17	4	10	3		
8	B	1	Total	C	H	O	0	0
			17	4	10	3		
8	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



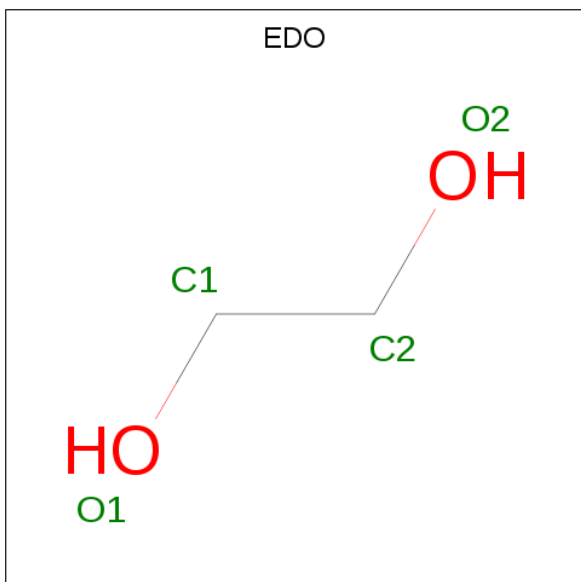


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

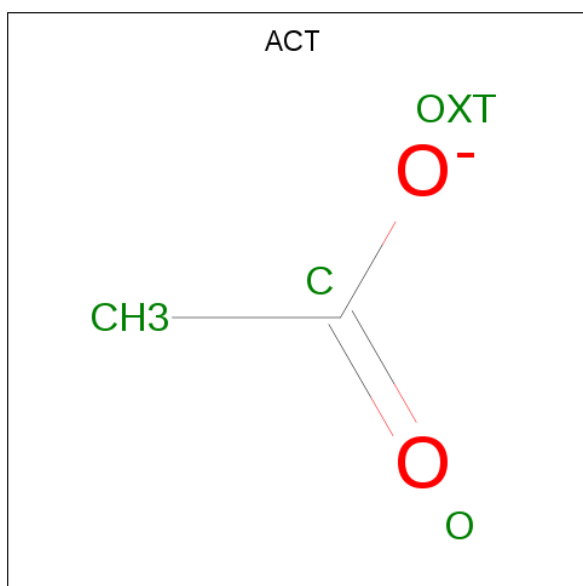
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	2	Total	Mg	0	0
			2	2		
10	A	1	Total	Mg	0	0
			1	1		

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



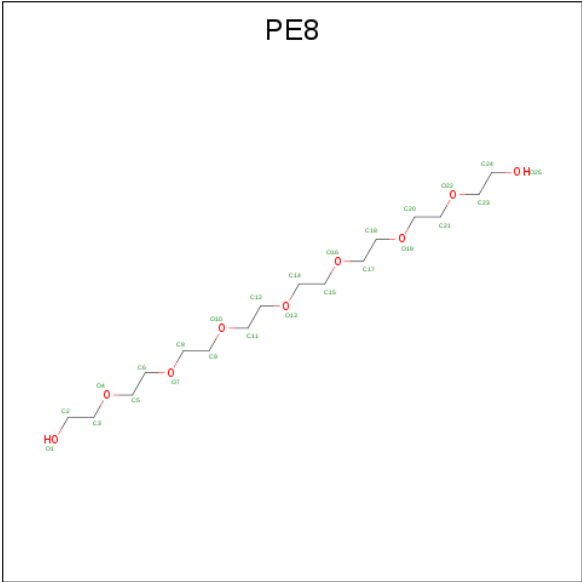
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			10	2	6	2		
11	B	1	Total	C	H	O	0	0
			10	2	6	2		
11	B	1	Total	C	H	O	0	0
			10	2	6	2		
11	B	1	Total	C	H	O	0	0
			10	2	6	2		
11	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 12 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			7	2	3	2		
12	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 13 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula:  $C_{16}H_{34}O_9$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	H	O	0	0
			59	16	34	9		

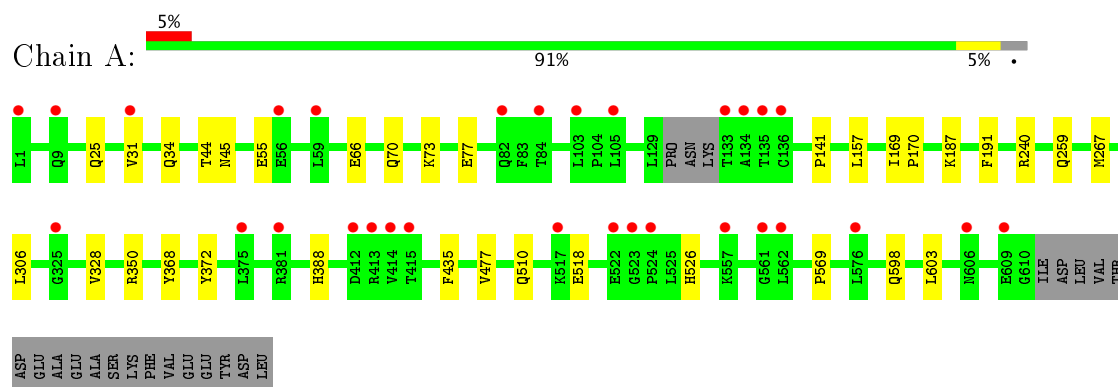
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	332	Total	O	0	6
			338	338		
14	B	407	Total	O	0	3
			410	410		

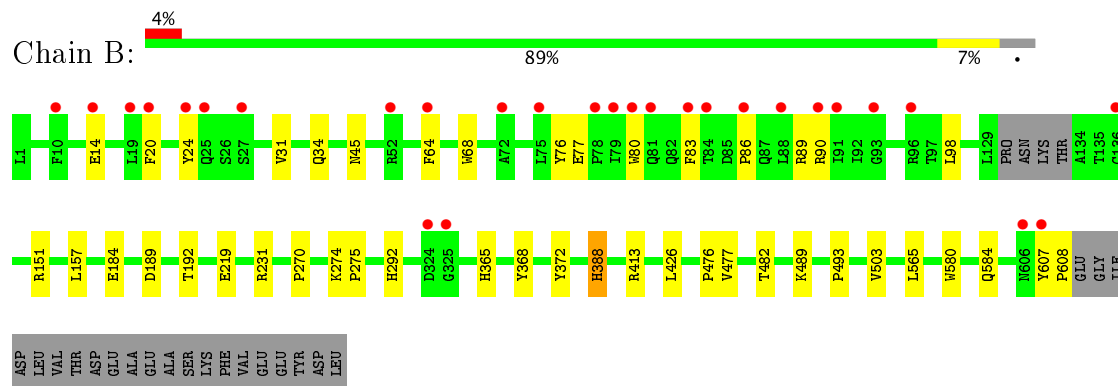
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 1: Angiotensin-converting enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.59Å 76.97Å 82.64Å 88.43° 64.40° 75.32°	Depositor
Resolution (Å)	44.39 – 1.85 56.01 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.6 (44.39-1.85) 98.6 (56.01-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 1.86Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.198 , 0.228 0.198 , 0.227	Depositor DCC
$R_{free}$ test set	2592 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21728	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: D0W, ZN, BMA, PE8, NAG, CL, MG, EDO, PG4, FUC, ACT, PEG

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	0.37	0/5175	0.49	0/7046
1	B	0.39	0/5527	0.52	0/7527
All	All	0.38	0/10702	0.51	0/14573

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	5001	4779	4761	16	0
1	B	5340	5102	5069	28	0
2	A	70	60	60	1	0
2	B	84	74	72	3	0
3	A	20	20	20	1	0
3	B	20	20	20	0	0
4	A	11	10	10	0	0
4	B	11	10	10	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	38	30	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	38	30	0	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	7	10	10	0	0
8	B	14	20	20	1	0
9	A	13	18	18	0	0
10	A	1	0	0	0	0
10	B	2	0	0	0	0
11	A	4	6	6	0	0
11	B	16	24	24	0	0
12	A	8	6	6	2	0
13	B	25	34	34	1	0
14	A	338	0	0	7	0
14	B	410	0	0	5	0
All	All	11475	10253	10140	51	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 2.

The worst 5 of 51 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:526:HIS:ND1	14:A:805:HOH:O	2.21	0.73
1:B:90[A]:ARG:NH2	14:B:803:HOH:O	2.22	0.71
2:B:707:NAG:H3	2:B:707:NAG:H83	1.77	0.64
1:A:518:GLU:OE2	14:A:802:HOH:O	2.15	0.64
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.85	0.59

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	611/629 (97%)	597 (98%)	13 (2%)	1 (0%)	49	34
1	B	654/629 (104%)	641 (98%)	12 (2%)	1 (0%)	49	34
All	All	1265/1258 (101%)	1238 (98%)	25 (2%)	2 (0%)	49	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	B	45	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	529/541 (98%)	524 (99%)	5 (1%)	81	75
1	B	564/541 (104%)	561 (100%)	3 (0%)	90	87
All	All	1093/1082 (101%)	1085 (99%)	8 (1%)	83	81

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	388	HIS
1	B	388	HIS
1	B	368	TYR
1	A	372	TYR
1	A	598	GLN

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

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 38 ligands modelled in this entry, 7 are monoatomic - leaving 31 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	$\# Z  > 2$
2	NAG	A	701	1,3	14,14,15	0.28	0	17,19,21	0.72	0
3	FUC	A	702	2	9,10,11	1.11	1 (11%)	13,14,16	1.16	1 (7%)
2	NAG	A	703	1,3,2	14,14,15	0.30	0	17,19,21	0.47	0
2	NAG	A	704	2,4	14,14,15	0.21	0	17,19,21	0.68	1 (5%)
3	FUC	A	705	2	9,10,11	0.90	1 (11%)	13,14,16	0.98	1 (7%)
4	BMA	A	706	2	11,11,12	0.89	0	15,15,17	0.80	0
2	NAG	A	707	1,2	14,14,15	0.35	0	17,19,21	0.46	0
2	NAG	A	708	2	14,14,15	0.19	0	17,19,21	0.48	0
6	D0W	A	710	5	29,39,39	2.45	7 (24%)	35,54,54	1.33	3 (8%)
8	PEG	A	712	-	6,6,6	0.47	0	5,5,5	0.40	0
9	PG4	A	713	-	12,12,12	0.51	0	11,11,11	0.38	0
11	EDO	A	715	-	3,3,3	0.54	0	2,2,2	0.22	0
12	ACT	A	716	-	1,3,3	6.94	1 (100%)	0,3,3	0.00	-
12	ACT	A	717	-	1,3,3	7.56	1 (100%)	0,3,3	0.00	-
2	NAG	B	701	1,2	14,14,15	0.28	0	17,19,21	0.60	0
2	NAG	B	702	2	14,14,15	0.28	0	17,19,21	0.47	0
2	NAG	B	703	1,3,2	14,14,15	0.57	0	17,19,21	0.47	0
2	NAG	B	704	2,4	14,14,15	0.38	0	17,19,21	0.58	0
4	BMA	B	705	2	11,11,12	0.63	0	15,15,17	0.69	0
3	FUC	B	706	2	9,10,11	0.98	0	13,14,16	0.80	0
2	NAG	B	707	1,3,2	14,14,15	0.36	0	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUC	B	708	2	9,10,11	1.15	0	13,14,16	1.59	4 (30%)
2	NAG	B	709	2	14,14,15	0.24	0	17,19,21	0.52	0
6	D0W	B	711	5	29,39,39	2.52	7 (24%)	35,54,54	1.48	6 (17%)
8	PEG	B	713	-	6,6,6	0.44	0	5,5,5	0.36	0
8	PEG	B	714	-	6,6,6	0.47	0	5,5,5	0.41	0
11	EDO	B	717	-	3,3,3	0.50	0	2,2,2	0.24	0
11	EDO	B	718	-	3,3,3	0.50	0	2,2,2	0.33	0
11	EDO	B	719	-	3,3,3	0.51	0	2,2,2	0.17	0
11	EDO	B	720	-	3,3,3	0.54	0	2,2,2	0.15	0
13	PE8	B	721	-	24,24,24	0.51	0	23,23,23	0.41	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	A	701	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	702	2	-	0/0/17/20	0/1/1/1
2	NAG	A	703	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	A	704	2,4	-	0/6/23/26	0/1/1/1
3	FUC	A	705	2	-	0/0/17/20	0/1/1/1
4	BMA	A	706	2	-	0/2/19/22	0/1/1/1
2	NAG	A	707	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	708	2	-	0/6/23/26	0/1/1/1
6	D0W	A	710	5	-	0/34/53/53	0/2/2/2
8	PEG	A	712	-	-	0/4/4/4	0/0/0/0
9	PG4	A	713	-	-	0/10/10/10	0/0/0/0
11	EDO	A	715	-	-	0/1/1/1	0/0/0/0
12	ACT	A	716	-	-	0/0/0/0	0/0/0/0
12	ACT	A	717	-	-	0/0/0/0	0/0/0/0
2	NAG	B	701	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	702	2	-	0/6/23/26	0/1/1/1
2	NAG	B	703	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	B	704	2,4	-	0/6/23/26	0/1/1/1
4	BMA	B	705	2	-	0/2/19/22	0/1/1/1
3	FUC	B	706	2	-	0/0/17/20	0/1/1/1
2	NAG	B	707	1,3,2	-	0/6/23/26	0/1/1/1
3	FUC	B	708	2	-	0/0/17/20	0/1/1/1
2	NAG	B	709	2	-	0/6/23/26	0/1/1/1
6	D0W	B	711	5	-	0/34/53/53	0/2/2/2
8	PEG	B	713	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	B	714	-	-	0/4/4/4	0/0/0/0
11	EDO	B	717	-	-	0/1/1/1	0/0/0/0
11	EDO	B	718	-	-	0/1/1/1	0/0/0/0
11	EDO	B	719	-	-	0/1/1/1	0/0/0/0
11	EDO	B	720	-	-	0/1/1/1	0/0/0/0
13	PE8	B	721	-	-	0/22/22/22	0/0/0/0

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	711	D0W	C20-C16	-6.89	1.39	1.54
6	A	710	D0W	C20-C16	-6.84	1.39	1.54
6	A	710	D0W	O11-C10	-2.46	1.18	1.23
6	B	711	D0W	O11-C10	-2.10	1.19	1.23
3	A	705	FUC	C1-C2	2.25	1.57	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	711	D0W	C33-C24-N23	-5.01	101.53	112.39
6	A	710	D0W	C33-C24-N23	-3.37	105.08	112.39
6	B	711	D0W	C15-C14-C36	-3.21	107.52	112.70
3	A	705	FUC	O2-C2-C1	2.03	113.27	109.17
3	B	708	FUC	O5-C1-C2	2.06	113.99	110.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	NAG	1	0
3	A	702	FUC	1	0
6	A	710	D0W	1	0
12	A	717	ACT	2	0
2	B	707	NAG	3	0
6	B	711	D0W	1	0
8	B	714	PEG	1	0
13	B	721	PE8	1	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	607/629 (96%)	0.38	30 (4%) 29 28	17, 37, 68, 106	0
1	B	604/629 (96%)	0.24	28 (4%) 32 31	17, 30, 53, 83	0
All	All	1211/1258 (96%)	0.31	58 (4%) 30 29	17, 32, 63, 106	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	325	GLY	8.6
1	A	413	ARG	5.8
1	B	325	GLY	5.8
1	A	1	LEU	5.4
1	A	609	GLU	5.4

### 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](#)

There are no carbohydrates in this entry.

### 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<sup>th</sup> 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
4	BMA	A	706	11/12	0.62	0.45	84,105,126,130	0
12	ACT	A	716	4/4	0.65	0.19	50,61,63,69	0
2	NAG	B	702	14/15	0.67	0.42	61,98,133,155	0
3	FUC	B	706	10/11	0.69	0.27	44,57,75,79	20
2	NAG	A	707	14/15	0.74	0.27	51,72,89,93	26
12	ACT	A	717	4/4	0.74	0.21	35,42,53,65	0
2	NAG	B	709	14/15	0.75	0.19	47,67,84,94	27
4	BMA	B	705	11/12	0.75	0.18	57,73,87,99	0
3	FUC	A	702	10/11	0.76	0.24	56,70,84,97	0
2	NAG	A	708	14/15	0.76	0.25	74,90,124,133	0
11	EDO	A	715	4/4	0.78	0.30	55,66,68,74	0
3	FUC	A	705	10/11	0.80	0.35	60,77,93,99	0
2	NAG	A	704	14/15	0.80	0.34	68,85,99,109	0
2	NAG	B	701	14/15	0.82	0.31	47,63,83,89	0
11	EDO	B	719	4/4	0.84	0.21	53,64,70,70	0
3	FUC	B	708	10/11	0.84	0.15	48,73,102,108	0
11	EDO	B	717	4/4	0.85	0.12	45,54,65,68	0
8	PEG	A	712	7/7	0.86	0.14	48,59,87,87	0
8	PEG	B	714	7/7	0.87	0.35	37,59,71,76	0
2	NAG	A	703	14/15	0.88	0.25	50,69,83,88	0
11	EDO	B	720	4/4	0.88	0.27	52,62,71,71	0
13	PE8	B	721	25/25	0.89	0.12	38,54,67,69	0
2	NAG	B	707	14/15	0.89	0.13	32,45,66,69	0
11	EDO	B	718	4/4	0.90	0.12	41,50,60,61	0
9	PG4	A	713	13/13	0.90	0.14	33,51,70,71	0
2	NAG	A	701	14/15	0.91	0.11	35,53,73,88	0
2	NAG	B	703	14/15	0.92	0.12	33,46,60,63	0
8	PEG	B	713	7/7	0.92	0.10	35,46,60,67	0
2	NAG	B	704	14/15	0.93	0.16	32,51,58,61	0
6	D0W	B	711	38/38	0.93	0.13	20,32,66,79	0
10	MG	B	715	1/1	0.94	0.07	45,45,45,45	0
10	MG	B	716	1/1	0.94	0.14	43,43,43,43	0
6	D0W	A	710	38/38	0.96	0.11	17,27,65,85	0
5	ZN	B	710	1/1	0.97	0.14	28,28,28,28	0
7	CL	A	711	1/1	0.98	0.14	26,26,26,26	0
5	ZN	A	709	1/1	0.99	0.12	21,21,21,21	0
7	CL	B	712	1/1	0.99	0.17	24,24,24,24	0
10	MG	A	714	1/1	0.99	0.15	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.