



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:03 am GMT

PDB ID : 5AM9  
Title : Crystal structure of the Angiotensin-1 converting enzyme N-domain in complex with amyloid-beta 10-16  
Authors : Masuyer, G.; Larmuth, K.M.; Douglas, R.G.; Sturrock, E.D.; Acharya, K.R.  
Deposited on : 2015-03-10  
Resolution : 1.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

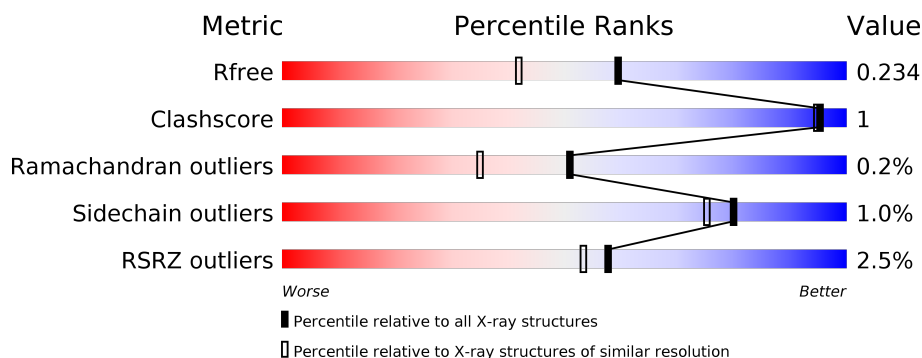
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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>2%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div>• •</div> </div>
1	B	629	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div></div> </div> <div>• •</div> </div>
1	C	629	<div> <div>%</div> <div> <div></div> <div>93%</div> <div></div> </div> <div>• • •</div> </div>
1	D	629	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> <div>•</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	A	1102	-	-	-	X
10	NAG	B	1102	-	-	-	X
10	NAG	D	1102	-	-	-	X
11	NAG	A	1104	-	-	-	X
12	PEG	A	1201	-	-	-	X
12	PEG	A	1203	-	-	-	X
12	PEG	B	1201	-	-	-	X
12	PEG	C	1202	-	-	-	X
12	PEG	C	1203	-	-	-	X
12	PEG	D	1204	-	-	-	X
13	P6G	A	1202	-	-	-	X
13	P6G	B	1203	-	-	-	X
13	P6G	B	1204	-	-	-	X
2	GLN	D	915	-	-	-	X
3	LYS	A	916	-	-	-	X
3	LYS	D	916	-	-	-	X

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 22178 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	603	Total	C	N	O	S	0	1	0
			4924	3164	844	897	19			
1	B	605	Total	C	N	O	S	0	3	0
			4962	3188	855	900	19			
1	C	611	Total	C	N	O	S	0	3	0
			5006	3214	858	914	20			
1	D	609	Total	C	N	O	S	0	3	0
			4995	3207	859	910	19			

There are 35 discrepancies between the modelled and reference sequences:

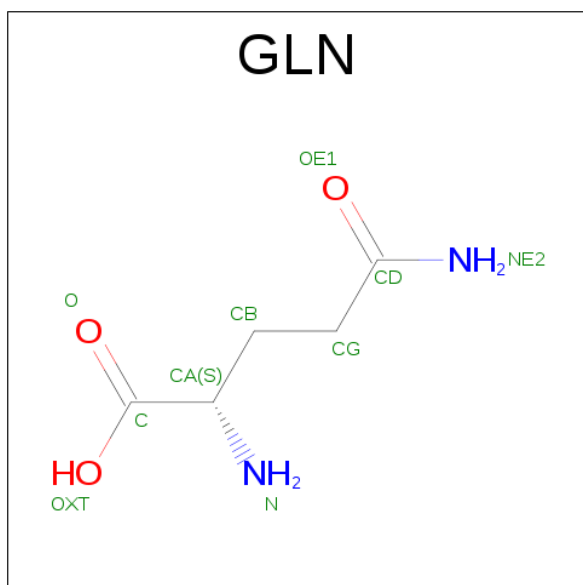
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
A	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
A	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821
B	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
B	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
B	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821
C	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
C	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
C	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
C	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821

*Continued on next page...*

Continued from previous page...

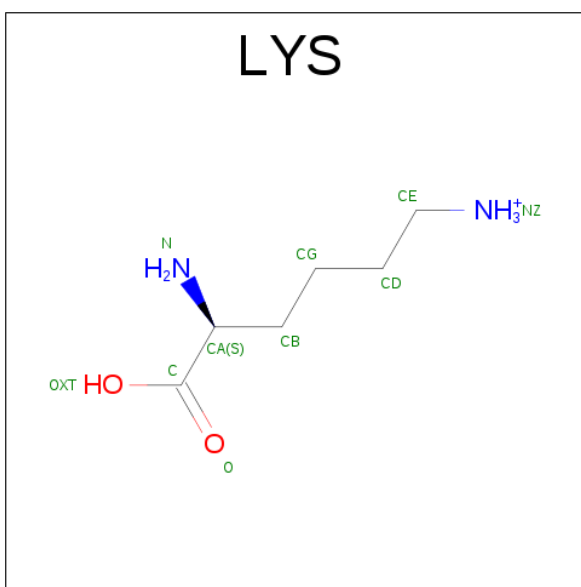
Chain	Residue	Modelled	Actual	Comment	Reference
C	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821
C	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
C	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
C	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
C	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821
D	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
D	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
D	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
D	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
D	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821
D	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
D	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
D	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
D	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821

- Molecule 2 is GLUTAMINE (three-letter code: GLN) (formula:  $C_5H_{10}N_2O_3$ ).



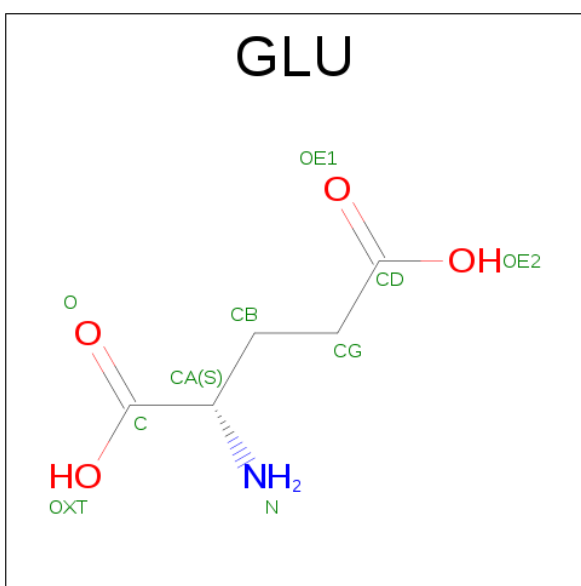
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	5	2	2		
2	D	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 3 is LYSINE (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ).



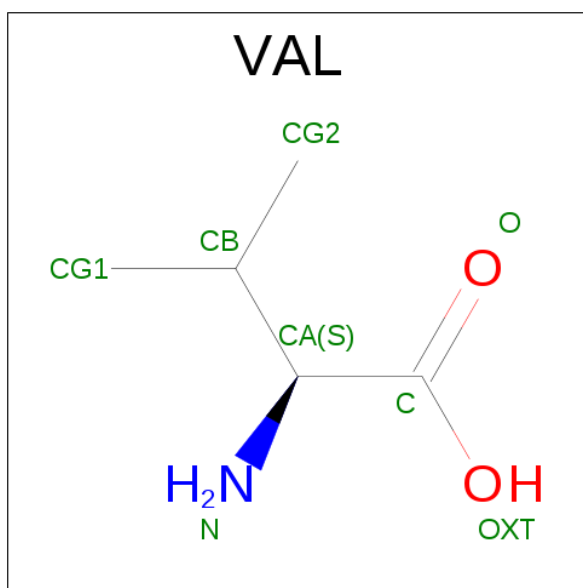
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	2	2		
3	D	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 4 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			9	5	1	3		
4	C	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 5 is VALINE (three-letter code: VAL) (formula:  $C_5H_{11}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			8	5	1	2		
5	C	1	Total	C	N	O	0	0
			8	5	1	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		
6	A	1	Total	Zn	0	0
			1	1		
6	D	1	Total	Zn	0	0
			1	1		
6	C	1	Total	Zn	0	0
			1	1		

- 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		
7	A	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0
8	D	1	Total Na 1 1	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total C N O 24 14 1 9	0	0

- Molecule 10 is a polymer of unknown type called SUGAR (2-MER).

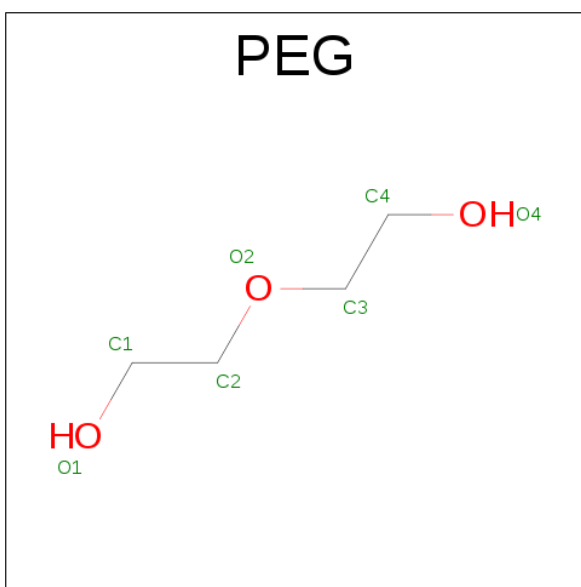
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	2	Total C N O 28 16 2 10	0	0
10	B	2	Total C N O 28 16 2 10	0	0
10	C	2	Total C N O 28 16 2 10	0	0
10	D	2	Total C N O 28 16 2 10	0	0

- Molecule 11 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	3	Total C N O 39 22 2 15	0	0
11	B	3	Total C N O 39 22 2 15	0	0

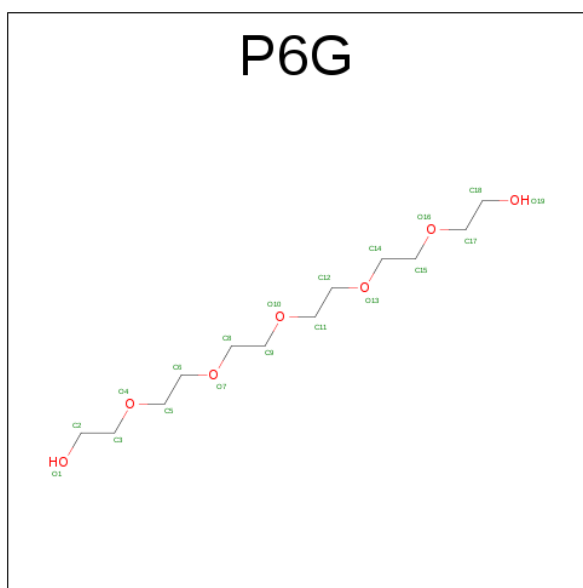
- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).





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

- Molecule 13 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			19	12	7		
13	B	1	Total	C	O	0	0
			19	12	7		
13	B	1	Total	C	O	0	0
			19	12	7		
13	D	1	Total	C	O	0	0
			19	12	7		

- Molecule 14 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	B	1	Total	Ca	0	0
			1	1		
14	C	1	Total	Ca	0	0
			1	1		

- Molecule 15 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	B	2	Total	C	N	O	0	0
			24	14	1	9		
15	C	2	Total	C	N	O	0	0
			24	14	1	9		
15	D	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 16 is a polymer of unknown type called SUGAR (4-MER).

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

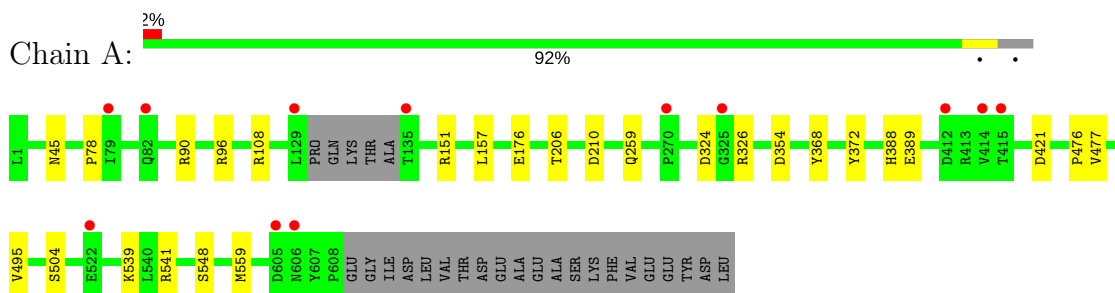
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	367	Total	O	0	0
			367	367		
17	B	407	Total	O	0	0
			407	407		
17	C	465	Total	O	0	0
			465	465		
17	D	403	Total	O	0	0
			403	403		
17	A	3	Total	O	0	0
			3	3		
17	B	1	Total	O	0	0
			1	1		
17	C	2	Total	O	0	0
			2	2		
17	D	1	Total	O	0	0
			1	1		

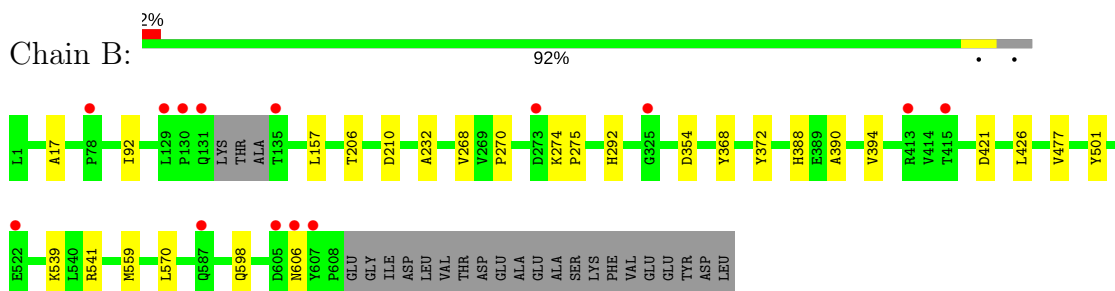
### 3 Residue-property plots [i](#)

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.

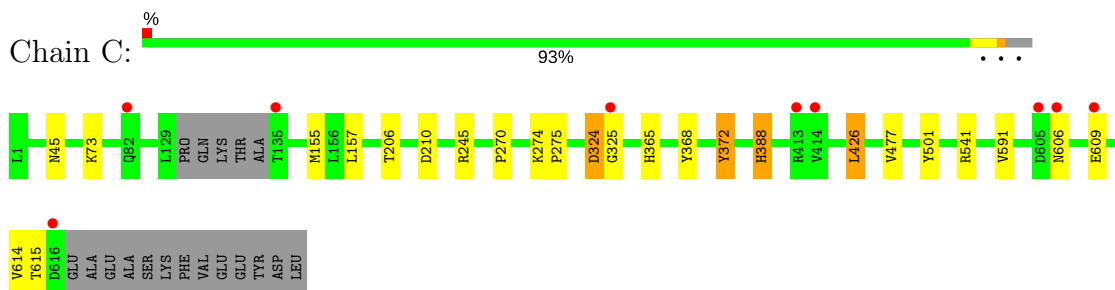
#### ● Molecule 1: ANGIOTENSIN-CONVERTING ENZYME



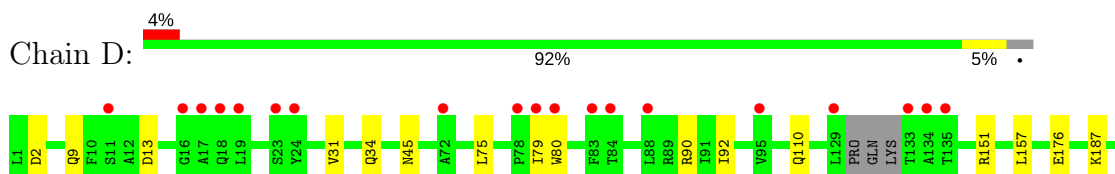
#### ● Molecule 1: ANGIOTENSIN-CONVERTING ENZYME

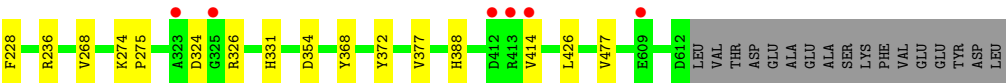


#### ● Molecule 1: ANGIOTENSIN-CONVERTING ENZYME



#### ● Molecule 1: ANGIOTENSIN-CONVERTING ENZYME





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.35Å 101.80Å 113.95Å 85.04° 85.55° 81.88°	Depositor
Resolution (Å)	113.27 – 1.80 30.37 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (113.27-1.80) 94.6 (30.37-1.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.197 , 0.229 0.204 , 0.234	Depositor DCC
$R_{free}$ test set	14478 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	22178	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.56 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.9036e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: ZN, BMA, NAG, CL, NA, CA, FUC, P6G, FUL, PEG, MAN

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	0.54	0/5083	0.73	7/6926 (0.1%)
1	B	0.56	0/5124	0.70	2/6978 (0.0%)
1	C	0.58	0/5167	0.74	3/7036 (0.0%)
1	D	0.58	0/5157	0.72	4/7023 (0.1%)
All	All	0.57	0/20531	0.72	16/27963 (0.1%)

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	C	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	C	541	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	B	541	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	326	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	354	ASP	CB-CG-OD1	6.01	123.71	118.30
1	D	151	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	354	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	326	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	426	LEU	CA-CB-CG	-5.53	102.58	115.30
1	C	541	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	151	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	541	ARG	NE-CZ-NH2	-5.29	117.66	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	354	ASP	CB-CG-OD1	5.24	123.02	118.30
1	D	90	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	236	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	108	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	324	ASP	Peptide

## 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	4924	0	4688	10	0
1	B	4962	0	4737	12	0
1	C	5006	0	4780	19	0
1	D	4995	0	4775	13	0
2	A	9	0	7	0	0
2	D	9	0	7	1	0
3	A	10	0	13	2	0
3	D	10	0	13	0	0
4	B	9	0	5	0	0
4	C	9	0	5	0	0
5	B	8	0	9	1	0
5	C	8	0	9	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	24	0	22	0	0
10	A	28	0	25	0	0
10	B	28	0	25	0	0
10	C	28	0	25	0	0
10	D	28	0	25	0	0
11	A	39	0	34	0	0
11	B	39	0	34	0	0
12	A	21	0	30	0	0
12	B	21	0	30	0	0
12	C	28	0	40	2	0
12	D	28	0	40	0	0
13	A	19	0	26	0	0
13	B	38	0	52	1	0
13	D	19	0	26	1	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
15	B	24	0	22	0	0
15	C	24	0	22	0	0
15	D	24	0	22	0	0
16	C	49	0	43	0	0
16	D	49	0	43	0	0
17	A	370	0	0	3	0
17	B	408	0	0	0	0
17	C	467	0	0	3	0
17	D	404	0	0	2	0
All	All	22178	0	19634	57	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 1.

All (57) 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:C:155[A]:MET:HA	1:C:155[A]:MET:HE2	1.43	1.00
1:C:155[A]:MET:HE2	1:C:155[A]:MET:CA	2.05	0.75
1:C:365:HIS:HD1	1:C:388:HIS:CD2	2.08	0.71
1:C:206:THR:HG23	1:C:210:ASP:OD2	1.94	0.68
1:C:365:HIS:HD1	1:C:388:HIS:HD2	1.39	0.66
1:B:501:TYR:CD1	5:B:912:VAL:HG12	2.31	0.66
1:C:155[A]:MET:HA	1:C:155[A]:MET:CE	2.19	0.65
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.79	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:916:LYS:HE2	17:A:2293:HOH:O	1.97	0.64
1:A:206:THR:HG23	1:A:210:ASP:OD2	1.98	0.63
1:C:501:TYR:CD1	5:C:912:VAL:HG12	2.38	0.59
1:C:157:LEU:HD11	1:C:477:VAL:HG13	1.83	0.59
1:D:157:LEU:HD11	1:D:477:VAL:HG13	1.85	0.58
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.86	0.57
12:C:1201:PEG:H41	17:C:2379:HOH:O	2.04	0.56
1:B:206:THR:HG23	1:B:210:ASP:OD2	2.06	0.56
1:A:539:LYS:HE3	1:A:559:MET:O	2.07	0.54
1:B:270:PRO:HD3	1:B:426:LEU:HD22	1.89	0.53
1:D:176:GLU:OE1	17:D:2144:HOH:O	2.18	0.53
1:B:17:ALA:HB1	1:B:92:ILE:HD11	1.92	0.52
1:C:270:PRO:HD3	1:C:426:LEU:HD22	1.92	0.51
1:C:426:LEU:O	1:C:426:LEU:HG	2.09	0.51
1:D:331:HIS:CE1	2:D:915:GLN:HG3	2.46	0.50
1:C:155[A]:MET:HE1	1:C:615:THR:HG23	1.95	0.49
1:D:13:ASP:HA	1:D:79:ILE:HD13	1.95	0.48
1:D:268:VAL:HG12	1:D:426:LEU:HD11	1.95	0.48
1:A:389:GLU:HB2	1:A:504:SER:HB2	1.96	0.47
1:B:390:ALA:O	1:B:394:VAL:HG23	2.14	0.47
1:C:155[A]:MET:CE	1:C:614:VAL:HG23	2.45	0.47
1:C:73:LYS:NZ	17:C:2086:HOH:O	2.44	0.47
1:C:606:ASN:O	1:C:609:GLU:O	2.33	0.46
1:A:90:ARG:NH2	17:A:2086:HOH:O	2.48	0.46
1:C:324:ASP:N	1:C:325:GLY:HA2	2.30	0.46
1:D:274:LYS:HB3	1:D:275:PRO:CD	2.46	0.45
1:C:274:LYS:HB3	1:C:275:PRO:CD	2.47	0.45
1:D:110:GLN:OE1	17:D:2077:HOH:O	2.21	0.45
1:D:228:PHE:CZ	13:D:1201:P6G:H142	2.51	0.45
1:D:324:ASP:OD1	1:D:326:ARG:HB2	2.16	0.45
1:B:292:HIS:CE1	13:B:1203:P6G:H51	2.52	0.45
1:A:495:VAL:O	1:A:495:VAL:HG12	2.18	0.44
1:B:232:ALA:CB	1:B:268:VAL:HG12	2.47	0.44
1:C:245:ARG:HG2	1:C:591:VAL:HG11	2.00	0.43
12:C:1201:PEG:C4	17:C:2379:HOH:O	2.65	0.43
1:D:31:VAL:O	1:D:34:GLN:HG3	2.19	0.43
1:B:274:LYS:HB3	1:B:275:PRO:HD2	2.00	0.43
1:A:259:GLN:HE21	3:A:916:LYS:NZ	2.17	0.43
1:D:268:VAL:CG1	1:D:426:LEU:HD11	2.49	0.42
1:B:570:LEU:HD23	1:B:570:LEU:C	2.40	0.42
1:B:539:LYS:HE3	1:B:559:MET:O	2.19	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ARG:HG2	1:C:591:VAL:CG1	2.50	0.42
1:A:176:GLU:OE1	17:A:2156:HOH:O	2.21	0.42
1:A:157:LEU:HD13	1:A:476:PRO:HB2	2.02	0.42
1:A:90:ARG:NE	1:A:548:SER:O	2.54	0.41
1:B:270:PRO:HD3	1:B:426:LEU:CD2	2.50	0.41
1:D:9[A]:GLN:NE2	1:D:75:LEU:HD21	2.35	0.41
1:C:372:TYR:OH	1:C:388:HIS:HE1	2.04	0.41
1:D:80:TRP:HB2	1:D:92:ILE:HG21	2.03	0.41

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	600/629 (95%)	589 (98%)	8 (1%)	3 (0%)	32	17
1	B	604/629 (96%)	594 (98%)	10 (2%)	0	100	100
1	C	610/629 (97%)	599 (98%)	10 (2%)	1 (0%)	51	35
1	D	608/629 (97%)	594 (98%)	13 (2%)	1 (0%)	51	35
All	All	2422/2516 (96%)	2376 (98%)	41 (2%)	5 (0%)	51	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	45	ASN
1	D	45	ASN
1	A	45	ASN
1	A	78	PRO
1	A	324	ASP

### 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	517/541 (96%)	512 (99%)	5 (1%)	80	75
1	B	521/541 (96%)	515 (99%)	6 (1%)	75	69
1	C	527/541 (97%)	524 (99%)	3 (1%)	89	87
1	D	526/541 (97%)	519 (99%)	7 (1%)	73	66
All	All	2091/2164 (97%)	2070 (99%)	21 (1%)	80	75

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	A	421	ASP
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS
1	B	421	ASP
1	B	598	GLN
1	B	606	ASN
1	C	368	TYR
1	C	372	TYR
1	C	388	HIS
1	D	2	ASP
1	D	187	LYS
1	D	368	TYR
1	D	372	TYR
1	D	377	VAL
1	D	388	HIS
1	D	414	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	25	GLN
1	C	388	HIS
1	D	18	GLN
1	D	22	GLN
1	D	82	GLN
1	D	110	GLN

### 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 ⓘ

30 carbohydrates 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	$\# Z  > 2$
9	NAG	A	1100	1,9	14,14,15	0.43	0	15,19,21	0.98	0
9	FUL	A	1101	9	9,10,11	0.54	0	13,14,16	1.37	2 (15%)
10	NAG	A	1102	1,10	14,14,15	0.64	0	15,19,21	1.05	1 (6%)
10	NAG	A	1103	10	14,14,15	0.48	0	15,19,21	1.37	1 (6%)
11	NAG	A	1104	1,11	14,14,15	0.42	0	15,19,21	0.79	0
11	NAG	A	1105	11	14,14,15	0.39	0	15,19,21	0.92	0
11	MAN	A	1106	11	11,11,12	0.58	0	13,15,17	1.08	2 (15%)
15	NAG	B	1100	1,15	14,14,15	0.73	0	15,19,21	1.44	3 (20%)
15	FUC	B	1101	15	9,10,11	0.49	0	13,14,16	1.57	2 (15%)
10	NAG	B	1102	1,10	14,14,15	0.50	0	15,19,21	1.29	2 (13%)
10	NAG	B	1103	10	14,14,15	0.59	0	15,19,21	1.21	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	B	1104	1,11	14,14,15	0.43	0	15,19,21	1.04	1 (6%)
11	NAG	B	1105	11	14,14,15	0.50	0	15,19,21	1.17	0
11	MAN	B	1106	11	11,11,12	0.83	1 (9%)	13,15,17	2.15	4 (30%)
15	NAG	C	1100	1,15	14,14,15	0.68	0	15,19,21	1.62	3 (20%)
15	FUC	C	1101	15	9,10,11	0.77	0	13,14,16	2.19	2 (15%)
10	NAG	C	1102	1,10	14,14,15	0.44	0	15,19,21	1.46	2 (13%)
10	NAG	C	1103	10	14,14,15	0.48	0	15,19,21	1.16	0
16	NAG	C	1104	1,16	14,14,15	0.55	0	15,19,21	1.08	0
16	NAG	C	1105	16	14,14,15	0.48	0	15,19,21	1.14	1 (6%)
16	BMA	C	1106	16	11,11,12	0.53	0	13,15,17	0.93	1 (7%)
16	FUC	C	1107	16	9,10,11	0.64	0	13,14,16	1.32	2 (15%)
15	NAG	D	1100	1,15	14,14,15	0.62	0	15,19,21	1.03	0
15	FUC	D	1101	15	9,10,11	0.70	0	13,14,16	1.86	3 (23%)
10	NAG	D	1102	1,10	14,14,15	0.50	0	15,19,21	0.99	1 (6%)
10	NAG	D	1103	10	14,14,15	0.43	0	15,19,21	1.16	2 (13%)
16	NAG	D	1104	1,16	14,14,15	0.68	0	15,19,21	0.91	0
16	NAG	D	1105	16	14,14,15	0.37	0	15,19,21	0.91	1 (6%)
16	BMA	D	1106	16	11,11,12	0.54	0	13,15,17	0.79	1 (7%)
16	FUC	D	1107	16	9,10,11	0.45	0	13,14,16	0.87	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	1100	1,9	-	0/6/23/26	0/1/1/1
9	FUL	A	1101	9	-	0/0/17/20	0/1/1/1
10	NAG	A	1102	1,10	-	0/6/23/26	0/1/1/1
10	NAG	A	1103	10	-	0/6/23/26	0/1/1/1
11	NAG	A	1104	1,11	-	0/6/23/26	0/1/1/1
11	NAG	A	1105	11	-	0/6/23/26	0/1/1/1
11	MAN	A	1106	11	-	0/2/19/22	0/1/1/1
15	NAG	B	1100	1,15	-	0/6/23/26	0/1/1/1
15	FUC	B	1101	15	-	0/0/17/20	0/1/1/1
10	NAG	B	1102	1,10	-	0/6/23/26	0/1/1/1
10	NAG	B	1103	10	-	0/6/23/26	0/1/1/1
11	NAG	B	1104	1,11	-	0/6/23/26	0/1/1/1
11	NAG	B	1105	11	-	0/6/23/26	0/1/1/1
11	MAN	B	1106	11	-	0/2/19/22	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	C	1100	1,15	-	0/6/23/26	0/1/1/1
15	FUC	C	1101	15	-	0/0/17/20	0/1/1/1
10	NAG	C	1102	1,10	-	0/6/23/26	0/1/1/1
10	NAG	C	1103	10	-	0/6/23/26	0/1/1/1
16	NAG	C	1104	1,16	-	0/6/23/26	0/1/1/1
16	NAG	C	1105	16	-	0/6/23/26	0/1/1/1
16	BMA	C	1106	16	-	0/2/19/22	0/1/1/1
16	FUC	C	1107	16	-	0/0/17/20	0/1/1/1
15	NAG	D	1100	1,15	-	0/6/23/26	0/1/1/1
15	FUC	D	1101	15	-	0/0/17/20	0/1/1/1
10	NAG	D	1102	1,10	-	0/6/23/26	0/1/1/1
10	NAG	D	1103	10	-	0/6/23/26	0/1/1/1
16	NAG	D	1104	1,16	-	0/6/23/26	0/1/1/1
16	NAG	D	1105	16	-	0/6/23/26	0/1/1/1
16	BMA	D	1106	16	-	0/2/19/22	0/1/1/1
16	FUC	D	1107	16	-	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1106	MAN	C2-C3	2.06	1.55	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1102	NAG	O5-C1-C2	-4.30	105.49	111.47
15	C	1100	NAG	C1-C2-N2	-3.11	105.18	110.49
15	B	1100	NAG	O7-C7-N2	-2.94	116.26	121.92
16	D	1105	NAG	C1-C2-N2	-2.93	105.49	110.49
10	D	1103	NAG	C1-C2-N2	-2.74	105.81	110.49
15	B	1100	NAG	C2-N2-C7	-2.66	119.06	122.94
10	A	1102	NAG	O5-C1-C2	-2.58	107.88	111.47
10	B	1102	NAG	O5-C1-C2	-2.29	108.28	111.47
15	C	1100	NAG	O3-C3-C4	-2.27	105.42	110.36
15	D	1101	FUC	O3-C3-C4	-2.24	105.47	110.36
16	C	1106	BMA	C2-C3-C4	-2.16	107.12	110.88
15	B	1101	FUC	C1-C2-C3	-2.07	107.03	109.65
16	D	1106	BMA	C1-C2-C3	2.02	112.21	109.65
11	B	1104	NAG	C2-N2-C7	2.04	125.92	122.94
10	D	1103	NAG	C4-C3-C2	2.13	114.14	111.02
16	C	1107	FUC	O3-C3-C2	2.22	114.07	110.02
9	A	1101	FUL	O5-C5-C4	2.23	113.29	109.62

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1106	MAN	C1-O5-C5	2.25	115.26	112.17
10	C	1102	NAG	C1-O5-C5	2.33	115.38	112.17
15	D	1101	FUC	O5-C1-C2	2.33	114.44	110.79
11	A	1106	MAN	C1-C2-C3	2.49	112.81	109.65
15	B	1100	NAG	C8-C7-N2	2.56	120.73	116.11
10	D	1102	NAG	C1-O5-C5	2.58	115.72	112.17
16	C	1105	NAG	C2-N2-C7	2.82	127.06	122.94
10	B	1102	NAG	C1-O5-C5	2.90	116.16	112.17
16	C	1107	FUC	O2-C2-C3	2.95	115.97	110.17
10	B	1103	NAG	C4-C3-C2	2.95	115.35	111.02
11	B	1106	MAN	C2-C3-C4	3.17	116.40	110.88
15	B	1101	FUC	C1-O5-C5	3.19	119.45	112.39
15	C	1100	NAG	C4-C3-C2	3.48	116.11	111.02
9	A	1101	FUL	C1-O5-C5	3.53	120.20	112.39
11	B	1106	MAN	C3-C4-C5	3.72	116.78	110.22
11	B	1106	MAN	C1-O5-C5	3.88	117.51	112.17
11	B	1106	MAN	C1-C2-C3	4.20	114.98	109.65
10	A	1103	NAG	C1-O5-C5	4.23	118.00	112.17
15	D	1101	FUC	C1-C2-C3	4.65	115.54	109.65
15	C	1101	FUC	O5-C1-C2	4.86	118.41	110.79
15	C	1101	FUC	C1-C2-C3	5.51	116.63	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 12 are monoatomic - leaving 26 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	$\# Z  > 2$
12	PEG	A	1200	-	6,6,6	0.45	0	5,5,5	0.38	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	PEG	A	1201	-	6,6,6	0.48	0	5,5,5	0.52	0
13	P6G	A	1202	-	18,18,18	0.50	0	17,17,17	0.41	0
12	PEG	A	1203	-	6,6,6	0.43	0	5,5,5	0.48	0
2	GLN	A	915	-	8,8,9	1.64	1 (12%)	6,9,11	0.79	0
3	LYS	A	916	-	4,9,9	0.49	0	3,10,10	0.75	0
12	PEG	B	1201	-	6,6,6	0.53	0	5,5,5	0.29	0
12	PEG	B	1202	-	6,6,6	0.67	0	5,5,5	0.60	0
13	P6G	B	1203	-	18,18,18	0.62	0	17,17,17	0.65	0
13	P6G	B	1204	-	18,18,18	0.45	0	17,17,17	0.38	0
12	PEG	B	1205	-	6,6,6	0.43	0	5,5,5	0.45	0
4	GLU	B	911	-	5,8,9	1.69	1 (20%)	2,9,11	1.68	0
5	VAL	B	912	-	3,7,7	0.18	0	3,9,9	0.41	0
12	PEG	C	1200	-	6,6,6	0.44	0	5,5,5	0.25	0
12	PEG	C	1201	-	6,6,6	0.55	0	5,5,5	0.65	0
12	PEG	C	1202	-	6,6,6	0.53	0	5,5,5	0.37	0
12	PEG	C	1203	-	6,6,6	0.53	0	5,5,5	0.77	0
4	GLU	C	911	-	5,8,9	1.02	0	2,9,11	1.46	0
5	VAL	C	912	-	3,7,7	0.33	0	3,9,9	0.15	0
12	PEG	D	1200	-	6,6,6	0.40	0	5,5,5	0.41	0
13	P6G	D	1201	-	18,18,18	0.72	0	17,17,17	1.09	2 (11%)
12	PEG	D	1202	-	6,6,6	0.49	0	5,5,5	0.59	0
12	PEG	D	1203	-	6,6,6	0.45	0	5,5,5	0.45	0
12	PEG	D	1204	-	6,6,6	0.48	0	5,5,5	0.40	0
2	GLN	D	915	-	8,8,9	1.75	1 (12%)	6,9,11	1.00	0
3	LYS	D	916	-	4,9,9	0.84	0	3,10,10	0.67	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
12	PEG	A	1200	-	-	0/4/4/4	0/0/0/0
12	PEG	A	1201	-	-	0/4/4/4	0/0/0/0
13	P6G	A	1202	-	-	0/16/16/16	0/0/0/0
12	PEG	A	1203	-	-	0/4/4/4	0/0/0/0
2	GLN	A	915	-	-	0/5/7/9	0/0/0/0
3	LYS	A	916	-	-	0/5/9/9	0/0/0/0
12	PEG	B	1201	-	-	0/4/4/4	0/0/0/0
12	PEG	B	1202	-	-	0/4/4/4	0/0/0/0
13	P6G	B	1203	-	-	0/16/16/16	0/0/0/0
13	P6G	B	1204	-	-	0/16/16/16	0/0/0/0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PEG	B	1205	-	-	0/4/4/4	0/0/0/0
4	GLU	B	911	-	-	0/3/7/9	0/0/0/0
5	VAL	B	912	-	-	0/4/8/8	0/0/0/0
12	PEG	C	1200	-	-	0/4/4/4	0/0/0/0
12	PEG	C	1201	-	-	0/4/4/4	0/0/0/0
12	PEG	C	1202	-	-	0/4/4/4	0/0/0/0
12	PEG	C	1203	-	-	0/4/4/4	0/0/0/0
4	GLU	C	911	-	-	0/3/7/9	0/0/0/0
5	VAL	C	912	-	-	0/4/8/8	0/0/0/0
12	PEG	D	1200	-	-	0/4/4/4	0/0/0/0
13	P6G	D	1201	-	-	0/16/16/16	0/0/0/0
12	PEG	D	1202	-	-	0/4/4/4	0/0/0/0
12	PEG	D	1203	-	-	0/4/4/4	0/0/0/0
12	PEG	D	1204	-	-	0/4/4/4	0/0/0/0
2	GLN	D	915	-	-	0/5/7/9	0/0/0/0
3	LYS	D	916	-	-	0/5/9/9	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	911	GLU	CA-C	3.55	1.54	1.50
2	D	915	GLN	CA-C	4.09	1.55	1.50
2	A	915	GLN	CA-C	4.29	1.55	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	1201	P6G	O10-C9-C8	2.03	119.72	110.41
13	D	1201	P6G	O16-C17-C18	2.24	120.47	110.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	916	LYS	2	0
13	B	1203	P6G	1	0
5	B	912	VAL	1	0
12	C	1201	PEG	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	912	VAL	1	0
13	D	1201	P6G	1	0
2	D	915	GLN	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	603/629 (95%)	-0.25	12 (1%) 65 61	16, 27, 46, 70	0
1	B	605/629 (96%)	-0.28	14 (2%) 61 57	16, 24, 41, 67	0
1	C	611/629 (97%)	-0.38	9 (1%) 74 70	15, 22, 39, 60	0
1	D	609/629 (96%)	-0.20	25 (4%) 38 32	16, 24, 50, 79	0
All	All	2428/2516 (96%)	-0.28	60 (2%) 58 53	15, 25, 45, 79	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	325	GLY	8.0
1	A	135	THR	7.3
1	D	134	ALA	7.3
1	A	415	THR	6.3
1	D	79	ILE	6.3
1	B	135	THR	5.2
1	A	325	GLY	4.9
1	D	135	THR	4.6
1	C	325	GLY	4.5
1	B	605	ASP	4.4
1	B	606	ASN	4.2
1	D	19	LEU	4.2
1	B	415	THR	4.1
1	D	133	THR	4.1
1	C	135	THR	4.1
1	B	130	PRO	4.1
1	A	606	ASN	4.0
1	D	83	PHE	3.9
1	C	414	VAL	3.8
1	B	325	GLY	3.7
1	D	88	LEU	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	414	VAL	3.2
1	B	129	LEU	3.2
1	C	605	ASP	3.2
1	A	412	ASP	3.0
1	D	80	TRP	3.0
1	B	607	TYR	3.0
1	B	131	GLN	2.9
1	D	609	GLU	2.8
1	D	414	VAL	2.8
1	C	609	GLU	2.8
1	D	413	ARG	2.8
1	B	78	PRO	2.7
1	A	522	GLU	2.7
1	A	129	LEU	2.6
1	D	95	VAL	2.6
1	A	79	ILE	2.6
1	C	606	ASN	2.6
1	B	413	ARG	2.5
1	A	605	ASP	2.5
1	B	273	ASP	2.4
1	B	587	GLN	2.4
1	D	78	PRO	2.4
1	D	412	ASP	2.4
1	C	413	ARG	2.3
1	D	323	ALA	2.3
1	D	24	TYR	2.3
1	D	16	GLY	2.2
1	D	129	LEU	2.2
1	A	270	PRO	2.2
1	D	18	GLN	2.2
1	B	522	GLU	2.2
1	D	23	SER	2.2
1	C	616	ASP	2.1
1	D	17	ALA	2.1
1	C	82	GLN	2.1
1	D	72	ALA	2.1
1	A	82	GLN	2.0
1	D	11	SER	2.0
1	D	84	THR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	NAG	A	1104	14/15	0.86	0.28	4.41	62,63,67,67	0
10	NAG	D	1102	14/15	0.81	0.25	4.06	41,45,51,58	0
10	NAG	B	1102	14/15	0.86	0.25	2.90	40,44,50,58	0
10	NAG	A	1102	14/15	0.86	0.24	2.29	39,41,47,54	0
15	NAG	B	1100	14/15	0.80	0.13	1.50	36,42,50,50	0
9	NAG	A	1100	14/15	0.81	0.13	1.45	44,50,58,58	0
15	NAG	C	1100	14/15	0.84	0.14	1.33	39,45,50,52	0
15	NAG	D	1100	14/15	0.82	0.13	1.16	38,44,49,52	0
11	NAG	B	1104	14/15	0.96	0.15	0.89	46,48,52,54	0
10	NAG	C	1102	14/15	0.91	0.14	0.75	34,37,40,46	0
16	NAG	D	1104	14/15	0.94	0.12	0.50	34,38,42,42	0
16	NAG	C	1104	14/15	0.93	0.09	0.06	32,33,36,39	0
16	BMA	D	1106	11/12	0.73	0.26	-	65,67,70,72	0
15	FUC	C	1101	10/11	0.55	0.35	-	58,63,67,68	0
10	NAG	A	1103	14/15	0.72	0.47	-	62,68,70,70	0
9	FUL	A	1101	10/11	0.75	0.21	-	63,66,66,68	0
16	FUC	D	1107	10/11	0.86	0.19	-	45,48,51,51	0
10	NAG	C	1103	14/15	0.74	0.37	-	49,54,63,67	0
11	NAG	B	1105	14/15	0.91	0.25	-	52,55,57,60	0
15	FUC	B	1101	10/11	0.71	0.31	-	58,64,67,68	0
16	NAG	C	1105	14/15	0.92	0.17	-	38,41,47,50	0
11	MAN	A	1106	11/12	0.70	0.31	-	70,74,76,76	0
16	FUC	C	1107	10/11	0.90	0.19	-	42,43,46,47	0
10	NAG	D	1103	14/15	0.74	0.44	-	63,69,74,75	0
11	MAN	B	1106	11/12	0.66	0.33	-	64,66,69,69	0
11	NAG	A	1105	14/15	0.81	0.38	-	67,70,72,75	0
15	FUC	D	1101	10/11	0.62	0.32	-	57,62,65,66	0
16	BMA	C	1106	11/12	0.78	0.18	-	46,48,53,54	0
10	NAG	B	1103	14/15	0.62	0.48	-	65,71,75,79	0
16	NAG	D	1105	14/15	0.89	0.17	-	46,52,56,61	0

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
12	PEG	C	1202	7/7	0.79	0.22	31.03	51,52,56,56	0
3	LYS	D	916	10/10	0.86	0.19	6.49	21,25,33,33	0
12	PEG	C	1203	7/7	0.82	0.22	5.30	40,41,43,45	0
2	GLN	D	915	9/10	0.89	0.15	5.16	23,27,32,33	0
12	PEG	D	1204	7/7	0.80	0.23	4.97	52,53,53,54	0
12	PEG	A	1201	7/7	0.76	0.17	4.87	40,43,46,47	0
13	P6G	B	1203	19/19	0.85	0.13	4.44	38,41,52,55	0
13	P6G	B	1204	19/19	0.78	0.17	4.09	50,57,62,64	0
13	P6G	A	1202	19/19	0.82	0.14	2.93	37,43,49,50	0
3	LYS	A	916	10/10	0.91	0.14	2.87	23,25,34,34	0
12	PEG	A	1203	7/7	0.87	0.19	2.70	40,41,43,45	0
12	PEG	B	1201	7/7	0.82	0.22	2.31	53,54,56,57	0
12	PEG	C	1201	7/7	0.91	0.17	1.57	41,42,44,45	0
13	P6G	D	1201	19/19	0.86	0.13	1.35	29,36,49,51	0
4	GLU	B	911	9/10	0.91	0.10	1.15	22,23,26,27	0
12	PEG	A	1200	7/7	0.84	0.19	1.05	53,53,58,58	0
2	GLN	A	915	9/10	0.94	0.10	0.91	23,26,27,28	0
12	PEG	C	1200	7/7	0.93	0.14	0.44	46,46,50,51	0
5	VAL	B	912	8/8	0.96	0.10	0.34	19,22,23,25	0
4	GLU	C	911	9/10	0.96	0.08	-0.35	18,21,23,24	0
7	CL	C	1002	1/1	1.00	0.07	-1.07	17,17,17,17	0
7	CL	B	1002	1/1	1.00	0.05	-1.18	19,19,19,19	0
5	VAL	C	912	8/8	0.97	0.08	-1.48	19,21,23,23	0
7	CL	A	1002	1/1	1.00	0.06	-1.87	21,21,21,21	0
7	CL	D	1002	1/1	0.99	0.06	-2.53	20,20,20,20	0
8	NA	D	1003	1/1	0.97	0.06	-2.70	40,40,40,40	0
14	CA	C	1003	1/1	1.00	0.03	-3.84	25,25,25,25	0
14	CA	B	1003	1/1	0.99	0.04	-4.21	41,41,41,41	0
8	NA	A	1003	1/1	0.99	0.04	-4.36	30,30,30,30	0
12	PEG	D	1203	7/7	0.74	0.26	-	57,59,60,62	0
12	PEG	D	1200	7/7	0.86	0.20	-	56,57,58,59	0
6	ZN	A	1001	1/1	1.00	0.06	-	20,20,20,20	0
12	PEG	B	1202	7/7	0.78	0.23	-	43,44,46,47	0
6	ZN	B	1001	1/1	1.00	0.05	-	18,18,18,18	0
12	PEG	D	1202	7/7	0.81	0.18	-	51,53,53,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
12	PEG	B	1205	7/7	0.85	0.19	-	56,57,58,60	0
6	ZN	D	1001	1/1	1.00	0.06	-	19,19,19,19	0
6	ZN	C	1001	1/1	1.00	0.05	-	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.