



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 31, 2016 – 10:18 PM EDT

PDB ID : 5AMC  
Title : Crystal structure of the Angiotensin-1 converting enzyme N-domain in complex with amyloid-beta fluorogenic fragment 4-10  
Authors : Masuyer, G.; Larmuth, K.M.; Douglas, R.G.; Sturrock, E.D.; Acharya, K.R.  
Deposited on : 2015-03-10  
Resolution : 1.65 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  
<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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20027107

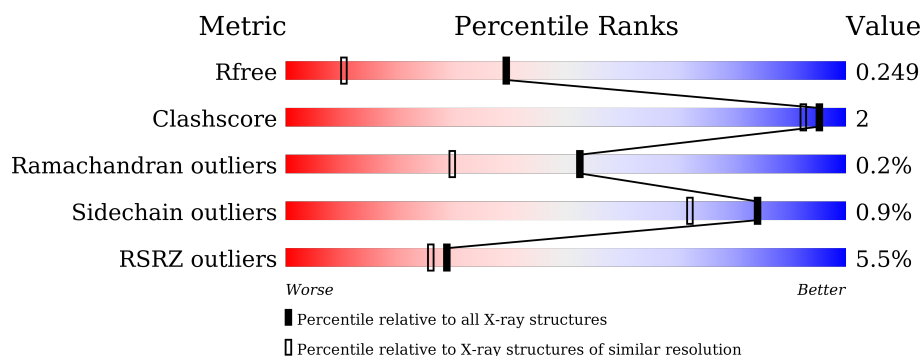
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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>92%</div> <div>• •</div> </div>
2	B	629	<div> <div>6%</div> <div>92%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PEG	A	1620	-	-	-	X
10	PEG	A	1622	-	-	-	X
10	PEG	B	1622	-	-	-	X
10	PEG	B	1623	-	-	-	X
12	NAG	B	1617	-	-	-	X
13	P6G	B	1621	-	-	-	X
3	GLY	A	906	-	-	-	X
3	GLY	B	906	-	-	-	X
4	NIY	A	907	-	-	-	X
4	NIY	B	907	-	-	-	X
8	NAG	A	1614	-	-	-	X
8	NAG	B	1615	-	-	-	X

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 11113 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	607	Total	C	N	O	S	0	3	0
			4969	3190	852	908	19			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	13	GLU	ASP	CONFLICT	UNP P12821
A	14	ASP	GLU	CONFLICT	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

- Molecule 2 is a protein called ANGIOTENSIN-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	607	Total	C	N	O	S	0	1	0
			4951	3181	849	902	19			

There are 9 discrepancies between the modelled and reference sequences:

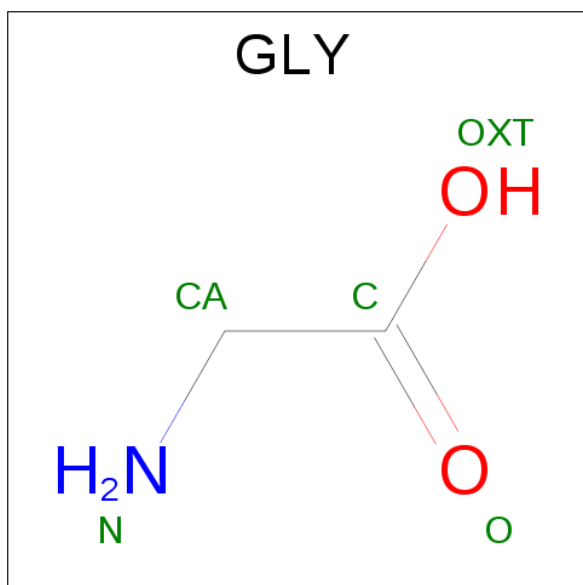
Chain	Residue	Modelled	Actual	Comment	Reference
B	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821

*Continued on next page...*

Continued from previous page...

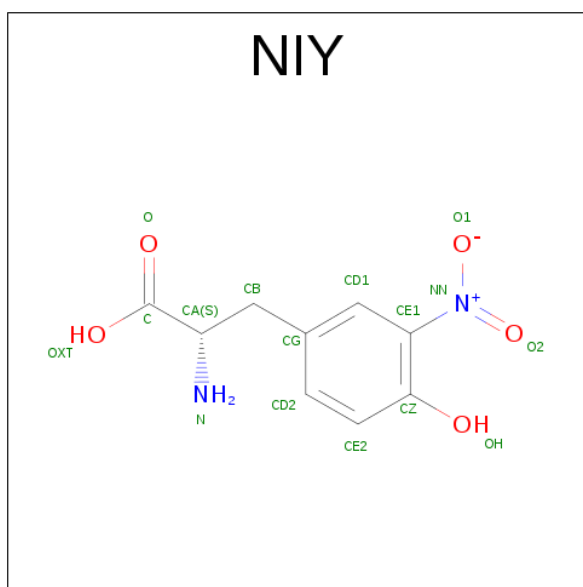
Chain	Residue	Modelled	Actual	Comment	Reference
B	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
B	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
B	629	LEU	ARG	ENGINEERED MUTATION	UNP P12821

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula:  $C_2H_5NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			4	2	1	1		
3	B	1	Total	C	N	O	0	0
			4	2	1	1		

- Molecule 4 is META-NITRO-TYROSINE (three-letter code: NIY) (formula:  $C_9H_{10}N_2O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	9	2	5		
4	B	1	Total	C	N	O	0	0
			16	9	2	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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

*Continued on next page...*

*Continued from previous page...*

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

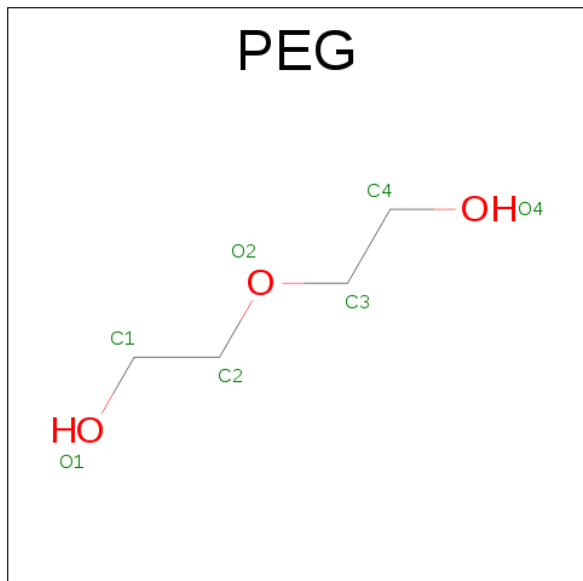
- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 9 is a polymer of unknown type called SUGAR (4-MER).

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

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



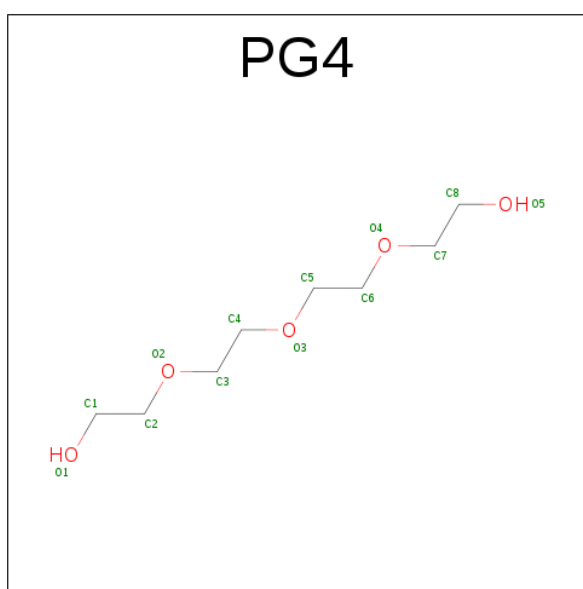
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		
10	A	1	Total	C	O	0	0
			7	4	3		

*Continued on next page...*

Continued from previous page...

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

- Molecule 11 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



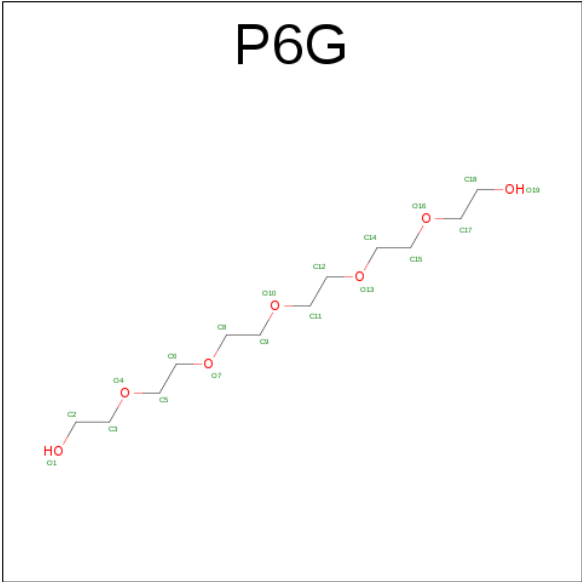
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 12 is a polymer of unknown type called SUGAR (3-MER).

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

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





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

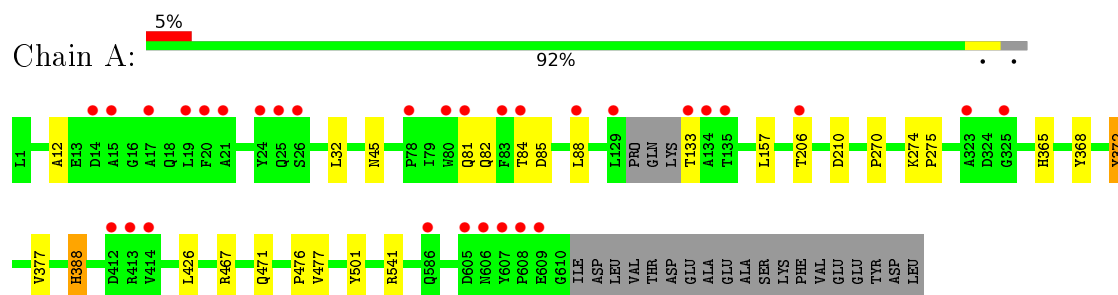
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	510	Total	O	0	0
			510	510		
14	B	376	Total	O	0	0
			376	376		

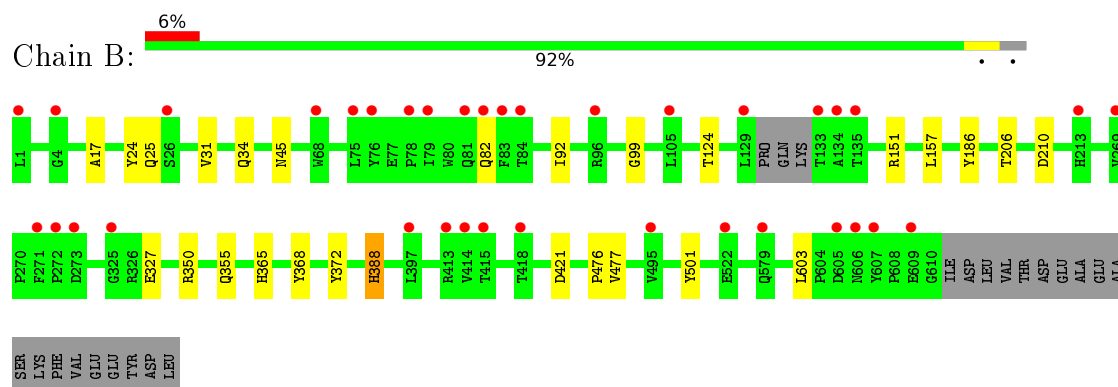
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: ANGIOTENSIN-CONVERTING ENZYME



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.03Å 76.47Å 83.16Å 88.78° 64.25° 75.64°	Depositor
Resolution (Å)	74.53 – 1.65 30.81 – 1.65	Depositor EDS
% Data completeness (in resolution range)	91.7 (74.53-1.65) 90.0 (30.81-1.65)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.208 , 0.242 0.215 , 0.249	Depositor DCC
$R_{free}$ test set	8521 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 172483 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11113	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: ZN, BMA, NAG, CL, PG4, NIY, FUC, P6G, 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	0.51	0/5133	0.69	2/6991 (0.0%)
2	B	0.49	0/5109	0.66	1/6959 (0.0%)
All	All	0.50	0/10242	0.68	3/13950 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	151	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	A	541	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	541	ARG	NE-CZ-NH2	-5.23	117.68	120.30

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	4969	0	4744	16	0
2	B	4951	0	4724	15	0
3	A	4	0	2	0	0
3	B	4	0	2	0	0
4	A	16	0	6	1	0
4	B	16	0	7	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	24	0	22	0	0
7	B	24	0	22	0	0
8	A	28	0	25	0	0
8	B	28	0	25	0	0
9	A	49	0	43	0	0
10	A	21	0	30	0	0
10	B	21	0	30	0	0
11	B	10	0	13	0	0
12	B	39	0	34	0	0
13	B	19	0	26	0	0
14	A	510	0	0	2	0
14	B	376	0	0	0	0
All	All	11113	0	9755	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 2.

The worst 5 of 31 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:365:HIS:HD1	1:A:388:HIS:HD2	1.33	0.74
1:A:365:HIS:HD1	1:A:388:HIS:CD2	2.09	0.71
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.73	0.69
2:B:350:ARG:H	2:B:355:GLN:HE21	1.46	0.64
2:B:124:THR:HG22	2:B:327:GLU:CG	2.32	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	606/629 (96%)	594 (98%)	11 (2%)	1 (0%)	52	30
2	B	604/629 (96%)	593 (98%)	10 (2%)	1 (0%)	52	30
All	All	1210/1258 (96%)	1187 (98%)	21 (2%)	2 (0%)	52	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
2	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	523/541 (97%)	519 (99%)	4 (1%)	86	76
2	B	519/541 (96%)	514 (99%)	5 (1%)	82	68
All	All	1042/1082 (96%)	1033 (99%)	9 (1%)	84	72

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	82	GLN
2	B	421	ASP
2	B	372	TYR
1	A	372	TYR
2	B	368	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	471	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	388	HIS
2	B	355	GLN
1	A	371	GLN
2	B	87	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 ⓘ

15 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	$\# Z  > 2$
7	NAG	A	1612	1,7	14,14,15	0.73	0	15,19,21	1.31	3 (20%)
7	FUC	A	1613	7	10,10,11	0.64	0	13,14,16	2.20	3 (23%)
8	NAG	A	1614	1,8	14,14,15	0.38	0	15,19,21	0.89	1 (6%)
8	NAG	A	1615	8	14,14,15	0.41	0	15,19,21	0.95	2 (13%)
9	NAG	A	1616	1,9	14,14,15	0.44	0	15,19,21	0.53	0
9	NAG	A	1617	9	14,14,15	0.31	0	15,19,21	0.70	0
9	BMA	A	1618	9	11,11,12	0.30	0	15,15,17	0.78	0
9	FUC	A	1619	9	10,10,11	0.46	0	13,14,16	0.56	0
7	NAG	B	1613	2,7	14,14,15	0.47	0	15,19,21	1.25	2 (13%)
7	FUC	B	1614	7	10,10,11	0.64	0	13,14,16	2.02	3 (23%)
8	NAG	B	1615	8,2	14,14,15	0.46	0	15,19,21	0.64	0
8	NAG	B	1616	8	14,14,15	0.52	0	15,19,21	1.43	2 (13%)
12	NAG	B	1617	12,2	14,14,15	0.35	0	15,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	NAG	B	1618	12	14,14,15	0.34	0	15,19,21	0.97	0
12	BMA	B	1619	12	11,11,12	0.38	0	15,15,17	0.97	1 (6%)

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
7	NAG	A	1612	1,7	-	0/6/23/26	0/1/1/1
7	FUC	A	1613	7	-	0/0/17/20	0/1/1/1
8	NAG	A	1614	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	1615	8	-	0/6/23/26	0/1/1/1
9	NAG	A	1616	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	1617	9	-	0/6/23/26	0/1/1/1
9	BMA	A	1618	9	-	0/2/19/22	0/1/1/1
9	FUC	A	1619	9	-	0/0/17/20	0/1/1/1
7	NAG	B	1613	2,7	-	0/6/23/26	0/1/1/1
7	FUC	B	1614	7	-	0/0/17/20	0/1/1/1
8	NAG	B	1615	8,2	-	0/6/23/26	0/1/1/1
8	NAG	B	1616	8	-	0/6/23/26	0/1/1/1
12	NAG	B	1617	12,2	-	0/6/23/26	0/1/1/1
12	NAG	B	1618	12	-	0/6/23/26	0/1/1/1
12	BMA	B	1619	12	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1613	NAG	O5-C5-C6	2.00	111.62	107.34
8	A	1615	NAG	C3-C4-C5	2.07	113.92	110.23
8	B	1616	NAG	C3-C4-C5	2.09	113.95	110.23
7	A	1612	NAG	C2-N2-C7	2.16	125.91	123.11
8	A	1615	NAG	C4-C3-C2	2.24	114.81	111.34

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

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z  > 2$
10	PEG	A	1620	-	6,6,6	0.50	0	5,5,5	0.52	0
10	PEG	A	1621	-	6,6,6	0.48	0	5,5,5	0.28	0
10	PEG	A	1622	-	6,6,6	0.49	0	5,5,5	0.42	0
3	GLY	A	906	4	3,3,4	0.81	0	0,2,4	0.00	-
4	NIY	A	907	3	11,16,16	5.29	2 (18%)	10,22,22	1.15	0
11	PG4	B	1611	-	9,9,12	0.41	0	8,8,11	0.38	0
10	PEG	B	1620	-	6,6,6	0.53	0	5,5,5	0.19	0
13	P6G	B	1621	-	18,18,18	0.73	0	17,17,17	0.64	0
10	PEG	B	1622	-	6,6,6	0.49	0	5,5,5	0.39	0
10	PEG	B	1623	-	6,6,6	0.51	0	5,5,5	0.22	0
3	GLY	B	906	4	3,3,4	0.79	0	0,2,4	0.00	-
4	NIY	B	907	3	11,16,16	5.27	2 (18%)	10,22,22	1.45	2 (20%)

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
10	PEG	A	1620	-	-	0/4/4/4	0/0/0/0
10	PEG	A	1621	-	-	0/4/4/4	0/0/0/0
10	PEG	A	1622	-	-	0/4/4/4	0/0/0/0
3	GLY	A	906	4	-	0/0/1/2	0/0/0/0
4	NIY	A	907	3	-	0/7/12/12	0/1/1/1
11	PG4	B	1611	-	-	0/7/7/10	0/0/0/0
10	PEG	B	1620	-	-	0/4/4/4	0/0/0/0
13	P6G	B	1621	-	-	0/16/16/16	0/0/0/0
10	PEG	B	1622	-	-	0/4/4/4	0/0/0/0
10	PEG	B	1623	-	-	0/4/4/4	0/0/0/0
3	GLY	B	906	4	-	0/0/1/2	0/0/0/0
4	NIY	B	907	3	-	0/7/12/12	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	907	NIY	CB-CG	-5.70	1.37	1.51
4	A	907	NIY	CB-CG	-5.42	1.37	1.51
4	B	907	NIY	O2-NN	16.32	1.55	1.22
4	A	907	NIY	O2-NN	16.57	1.55	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	907	NIY	CG-CB-CA	-2.71	107.71	114.24
4	B	907	NIY	CB-CG-CD1	-2.26	116.03	120.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	907	NIY	1	0
4	B	907	NIY	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%)	0.16	31 (5%) 32 29	16, 26, 48, 73	0
2	B	607/629 (96%)	0.35	36 (5%) 26 23	16, 29, 48, 75	0
All	All	1214/1258 (96%)	0.26	67 (5%) 29 26	16, 28, 48, 75	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	325	GLY	6.0
2	B	133	THR	5.9
2	B	134	ALA	5.7
2	B	415	THR	5.7
1	A	78	PRO	5.6

### 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
8	NAG	A	1614	14/15	0.67	0.31	6.70	48,51,56,59	0
8	NAG	B	1615	14/15	0.77	0.29	2.98	42,44,49,56	0
12	NAG	B	1617	14/15	0.83	0.25	2.79	63,65,69,70	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
7	NAG	B	1613	14/15	0.86	0.13	1.09	42,48,54,60	0
9	NAG	A	1616	14/15	0.93	0.13	0.83	35,37,46,48	0
7	NAG	A	1612	14/15	0.84	0.13	0.80	34,41,50,50	0
8	NAG	B	1616	14/15	0.74	0.46	-	63,66,70,71	0
7	FUC	B	1614	10/11	0.65	0.33	-	61,66,70,71	0
12	NAG	B	1618	14/15	0.90	0.31	-	73,77,79,81	0
9	BMA	A	1618	11/12	0.82	0.20	-	59,61,63,63	0
7	FUC	A	1613	10/11	0.59	0.31	-	60,66,68,69	0
12	BMA	B	1619	11/12	0.76	0.32	-	82,83,85,87	0
8	NAG	A	1615	14/15	0.67	0.40	-	55,67,72,73	0
9	NAG	A	1617	14/15	0.92	0.17	-	42,48,54,56	0
9	FUC	A	1619	10/11	0.85	0.22	-	45,47,49,52	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( $\text{\AA}^2$ )	Q<0.9
10	PEG	B	1623	7/7	0.79	0.23	12.70	61,62,65,66	0
3	GLY	B	906	4/5	0.81	0.18	6.89	44,44,45,47	0
3	GLY	A	906	4/5	0.66	0.21	5.45	42,43,44,44	0
13	P6G	B	1621	19/19	0.64	0.17	4.63	35,45,49,50	0
10	PEG	A	1620	7/7	0.84	0.20	4.08	51,52,54,55	0
4	NIY	B	907	16/16	0.76	0.17	3.32	25,45,52,59	0
10	PEG	A	1622	7/7	0.73	0.17	2.97	40,42,45,46	0
10	PEG	B	1622	7/7	0.77	0.18	2.81	56,57,58,58	0
4	NIY	A	907	16/16	0.77	0.19	2.70	23,41,48,49	0
11	PG4	B	1611	10/13	0.85	0.15	1.86	40,45,47,47	0
6	CL	A	1611	1/1	0.99	0.06	-1.38	19,19,19,19	0
6	CL	B	1612	1/1	0.99	0.07	-2.03	23,23,23,23	0
5	ZN	A	1001	1/1	1.00	0.07	-	19,19,19,19	0
5	ZN	B	1001	1/1	1.00	0.06	-	20,20,20,20	0
10	PEG	A	1621	7/7	0.75	0.16	-	51,51,55,58	0
10	PEG	B	1620	7/7	0.85	0.15	-	39,40,43,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.