



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:14 PM GMT

PDB ID : 4BXK  
Title : Crystal structure of the Angiotensin-1 converting enzyme N-domain in complex with a domain-specific inhibitor  
Authors : Douglas, R.G.; Sharma, R.K.; Masuyer, G.; Lubbe, L.; Zamora, I.; Acharya, K.R.; Chibale, K.; Sturrock, E.D.  
Deposited on : 2013-07-12  
Resolution : 2.20 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.

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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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

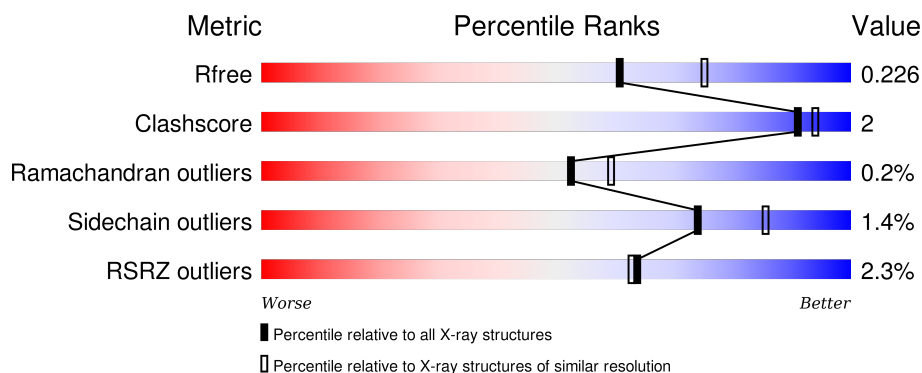
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

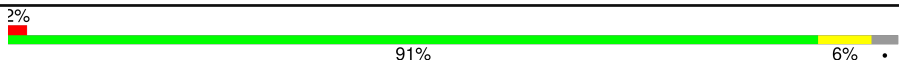
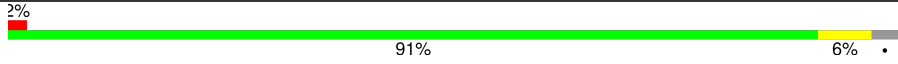
The reported resolution of this entry is 2.20 Å.

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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	
1	B	629	

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
2	PEG	A	702	-	-	-	X
3	P6G	A	704	-	-	-	X
3	P6G	B	709	-	-	-	X
6	NAG	B	1614	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 10657 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.

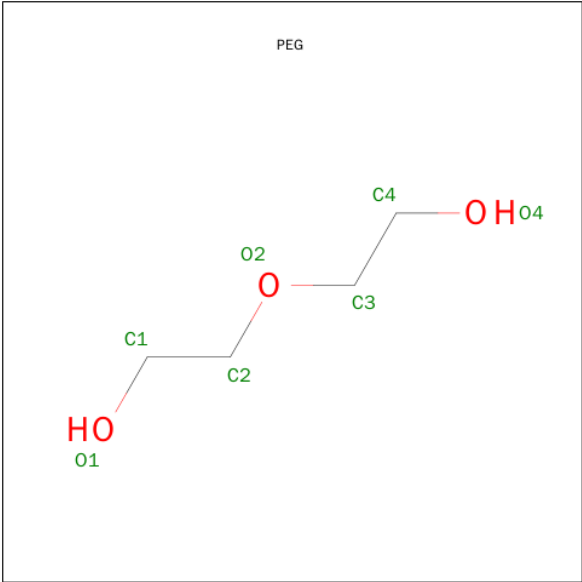
- Molecule 1 is a protein called ANGIOTENSIN-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	3	0
			4965	3188	853	905	19			
1	B	607	Total	C	N	O	S	0	2	0
			4954	3184	848	903	19			

There are 18 discrepancies between the modelled and reference sequences:

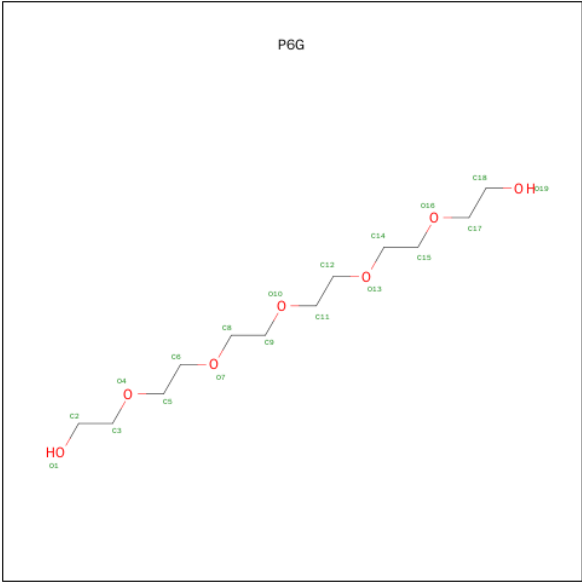
Chain	Residue	Modelled	Actual	Comment	Reference
A	629	LEU	-	EXPRESSION TAG	UNP P12821
A	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	131	GLN	ASN	ENGINEERED MUTATION	UNP P12821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

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



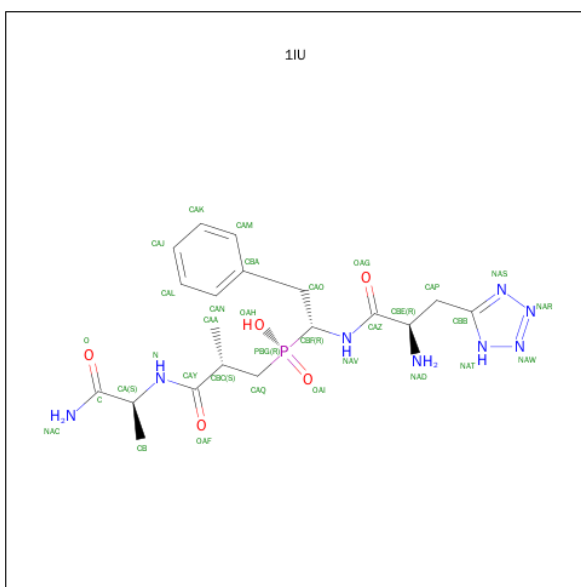
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 4 is [3-[[[(2S)-1-AZANYL-1-OXIDANYLIDENE-PROPAN-2-YL]AMINO]-2-METHYL-3-OXIDANYLIDENE-PROPYL]-[(1R)-1-[[[(2R)-2-AZANYL-3-(1H-1,2,3,4-TETRAZOL-5-YL)PROPANOYL]AMINO]-2-PHENYL-ETHYL]PHOSPHINIC ACID (three-letter code: 1IU) (formula: C<sub>19</sub>H<sub>29</sub>N<sub>8</sub>O<sub>5</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			33	19	8	5	1		
4	B	1	Total	C	N	O	P	0	0
			33	19	8	5	1		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

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

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

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

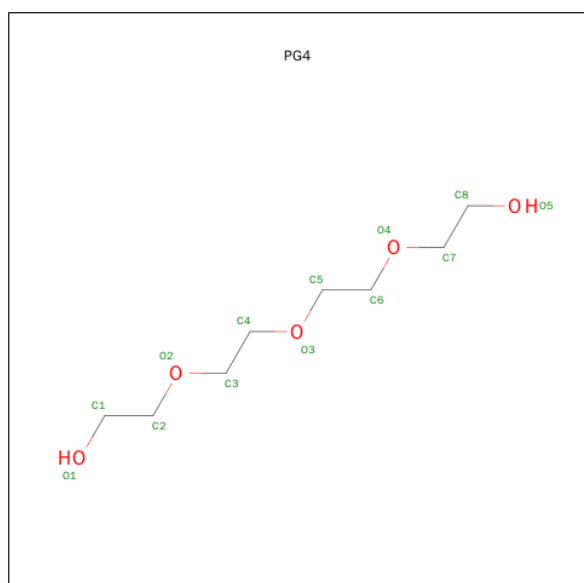
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

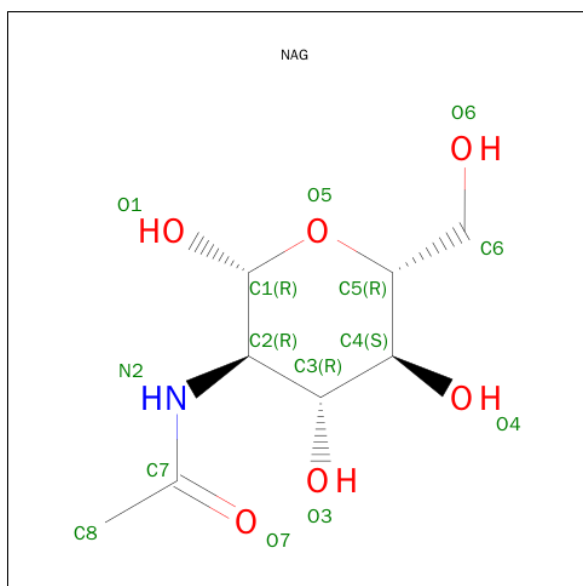
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Cl	0	0
			1	1		
9	A	1	Total	Cl	0	0
			1	1		

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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

- Molecule 11 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			14	8	1	5		

- 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 water.

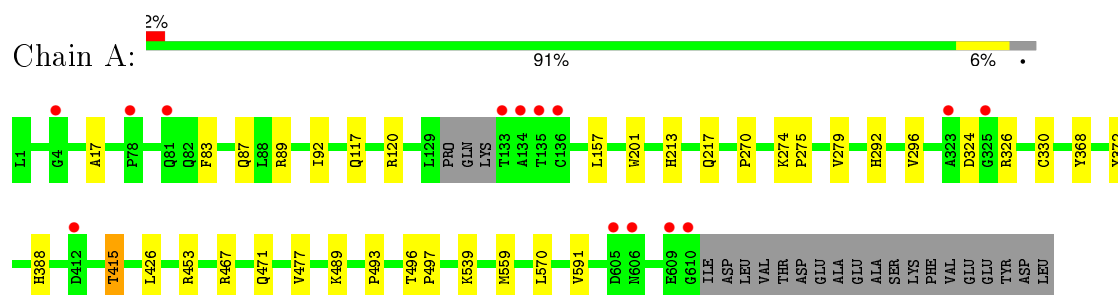
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	243	Total	O	0	0
			243	243		
13	B	166	Total	O	0	0
			166	166		



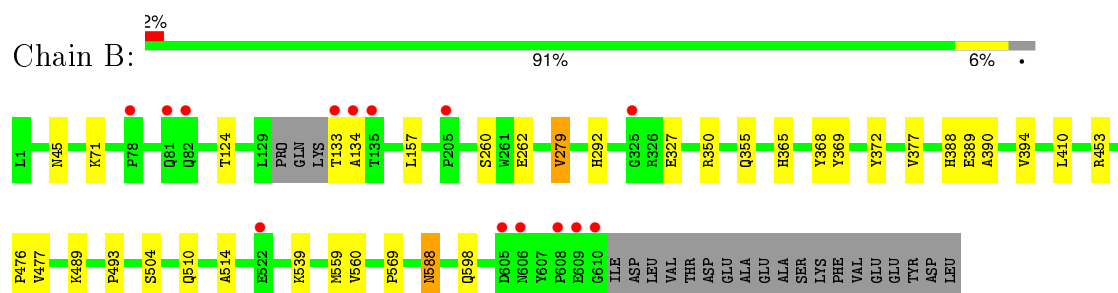
### 3 Residue-property plots [i](#)

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 1: ANGIOTENSIN-CONVERTING ENZYME



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.14Å 77.25Å 82.87Å 88.43° 64.28° 75.29°	Depositor
Resolution (Å)	29.69 – 2.20 29.67 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.4 (29.69-2.20) 88.4 (29.67-2.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.187 , 0.220 0.193 , 0.226	Depositor DCC
$R_{free}$ test set	3660 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 73011 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10657	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, PG4, FUC, P6G, 1IU, 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	0.40	0/5127	0.56	0/6985
1	B	0.39	0/5116	0.55	0/6971
All	All	0.39	0/10243	0.56	0/13956

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	4965	0	4726	25	0
1	B	4954	0	4718	19	0
2	A	21	0	30	0	0
2	B	14	0	20	0	0
3	A	13	0	17	0	0
3	B	19	0	26	2	0
4	A	33	0	28	0	0
4	B	33	0	28	2	0
5	A	24	0	22	0	0
6	A	28	0	25	0	0
6	B	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	49	0	43	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	B	10	0	13	1	0
11	B	14	0	12	0	0
12	B	39	0	34	0	0
13	A	243	0	0	7	0
13	B	166	0	0	1	0
All	All	10657	0	9767	44	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.

All (44) 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:B:260:SER:OG	1:B:262:GLU:OE1	1.86	0.93
1:B:350:ARG:H	1:B:355:GLN:HE21	1.36	0.73
1:A:17:ALA:HB1	1:A:92:ILE:CD1	2.26	0.66
1:A:87[B]:GLN:NE2	13:A:2008:HOH:O	2.32	0.63
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.81	0.62
1:B:453:ARG:NH2	10:B:704:PG4:O1	2.33	0.62
1:B:124:THR:HG22	1:B:327:GLU:HG2	1.81	0.61
1:A:87[B]:GLN:O	1:A:87[B]:GLN:CD	2.40	0.59
1:A:201:TRP:HZ3	1:A:497:PRO:HG2	1.67	0.58
1:A:87[B]:GLN:C	1:A:87[B]:GLN:CD	2.64	0.56
1:A:87[B]:GLN:C	1:A:87[B]:GLN:NE2	2.58	0.56
1:A:17:ALA:HB1	1:A:92:ILE:HD11	1.88	0.56
1:A:83:PHE:O	1:A:89:ARG:NH1	2.39	0.56
1:B:279:VAL:HG11	1:B:410:LEU:HD13	1.90	0.54
1:A:201:TRP:CZ3	1:A:497:PRO:HG2	2.43	0.53
1:B:292:HIS:HE2	3:B:709:P6G:H91	1.74	0.53
1:A:330:CYS:O	13:A:2150:HOH:O	2.19	0.52
1:A:415:THR:HG22	13:A:2181:HOH:O	2.09	0.52
1:A:467:ARG:HH11	1:A:471:GLN:HE22	1.57	0.52
1:B:588:ASN:HD22	1:B:588:ASN:N	2.09	0.51
1:B:539:LYS:HE3	1:B:559:MET:O	2.11	0.50
1:A:213[B]:HIS:ND1	13:A:2099:HOH:O	2.32	0.49
1:B:390:ALA:O	1:B:394:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LYS:HB3	1:A:275:PRO:CD	2.43	0.48
1:A:292:HIS:O	1:A:296:VAL:HG23	2.14	0.48
1:A:489:LYS:O	1:A:493:PRO:HD2	2.14	0.48
1:B:514:ALA:HB2	1:B:560:VAL:HG23	1.98	0.46
1:B:510:GLN:HG2	1:B:569:PRO:HG2	1.98	0.46
1:A:120:ARG:HB2	13:A:2018:HOH:O	2.16	0.45
1:A:539:LYS:HE3	1:A:559:MET:O	2.17	0.45
1:B:489:LYS:O	1:B:493:PRO:HD2	2.17	0.45
1:A:270:PRO:HD3	1:A:426:LEU:HD23	1.99	0.44
1:B:292:HIS:NE2	3:B:709:P6G:H62	2.33	0.44
1:A:157:LEU:HD11	1:A:477:VAL:HG13	2.00	0.44
1:A:217:GLN:NE2	13:A:2101:HOH:O	2.46	0.44
1:B:157:LEU:HD13	1:B:476:PRO:HB2	2.00	0.43
1:A:496:THR:HA	1:A:497:PRO:HD3	1.91	0.43
1:A:117:GLN:HG2	13:A:2043:HOH:O	2.20	0.42
1:B:598:GLN:NE2	13:B:2162:HOH:O	2.54	0.41
1:B:365:HIS:CE1	4:B:1001:1IU:HAP1	2.55	0.41
1:A:324:ASP:OD1	1:A:326:ARG:HB2	2.20	0.41
1:B:389:GLU:HB2	1:B:504:SER:HB2	2.03	0.41
1:B:369:TYR:OH	4:B:1001:1IU:NAT	2.53	0.41
1:A:570:LEU:C	1:A:570:LEU:HD23	2.41	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	606/629 (96%)	592 (98%)	14 (2%)	0	100	100
1	B	605/629 (96%)	591 (98%)	11 (2%)	3 (0%)	34	35
All	All	1211/1258 (96%)	1183 (98%)	25 (2%)	3 (0%)	52	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	ASN
1	B	134	ALA
1	B	377	VAL

### 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	520/541 (96%)	513 (99%)	7 (1%)	76	87
1	B	519/541 (96%)	512 (99%)	7 (1%)	76	87
All	All	1039/1082 (96%)	1025 (99%)	14 (1%)	74	87

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	279	VAL
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	A	415	THR
1	A	453	ARG
1	A	591	VAL
1	B	71	LYS
1	B	133	THR
1	B	279	VAL
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS
1	B	588	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	217	GLN
1	A	285	GLN
1	A	371	GLN
1	A	471	GLN
1	A	491	HIS
1	A	494	ASN
1	A	600	HIS
1	B	25	GLN
1	B	355	GLN
1	B	371	GLN
1	B	491	HIS
1	B	588	ASN
1	B	598	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 ⓘ

13 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	$\# Z  > 2$
5	NAG	A	1612	1,5	14,14,15	0.58	0	15,19,21	0.99	0
5	FUC	A	1613	5	10,10,11	0.82	0	14,14,16	2.25	3 (21%)
6	NAG	A	1614	1,6	14,14,15	0.53	0	15,19,21	0.98	1 (6%)
6	NAG	A	1615	6	14,14,15	0.42	0	15,19,21	0.98	0
7	NAG	A	1616	1,7	14,14,15	0.52	0	15,19,21	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	A	1617	7	14,14,15	0.52	0	15,19,21	0.82	0
7	BMA	A	1618	7	11,11,12	0.44	0	14,15,17	1.23	1 (7%)
7	FUC	A	1619	7	10,10,11	0.61	0	14,14,16	0.63	0
6	NAG	B	1614	1,6	14,14,15	0.59	0	15,19,21	0.91	1 (6%)
6	NAG	B	1615	6	14,14,15	0.50	0	15,19,21	0.74	0
12	NAG	B	1616	1,12	14,14,15	0.46	0	15,19,21	1.17	1 (6%)
12	NAG	B	1617	12	14,14,15	0.50	0	15,19,21	0.71	0
12	BMA	B	1618	12	11,11,12	0.43	0	14,15,17	2.03	3 (21%)

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
5	NAG	A	1612	1,5	-	0/6/23/26	0/1/1/1
5	FUC	A	1613	5	-	0/0/17/20	0/1/1/1
6	NAG	A	1614	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1615	6	-	0/6/23/26	0/1/1/1
7	NAG	A	1616	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1617	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1618	7	-	0/2/19/22	0/1/1/1
7	FUC	A	1619	7	-	0/0/17/20	0/1/1/1
6	NAG	B	1614	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1615	6	-	0/6/23/26	0/1/1/1
12	NAG	B	1616	1,12	-	0/6/23/26	0/1/1/1
12	NAG	B	1617	12	-	0/6/23/26	0/1/1/1
12	BMA	B	1618	12	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1614	NAG	C4-C3-C2	2.11	114.52	111.23
6	A	1614	NAG	C1-O5-C5	2.30	115.17	112.25
12	B	1618	BMA	O5-C1-C2	2.92	115.60	110.86
5	A	1613	FUC	C3-C4-C5	2.96	114.71	109.72
12	B	1616	NAG	C1-O5-C5	2.96	116.01	112.25
7	A	1618	BMA	C1-C2-C3	3.38	113.54	109.54
5	A	1613	FUC	C2-C3-C4	3.51	117.00	111.04
12	B	1618	BMA	C1-O5-C5	4.76	118.30	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1618	BMA	C1-C2-C3	4.77	115.18	109.54
5	A	1613	FUC	C1-C2-C3	6.46	117.19	109.54

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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\# Z  > 2$
4	1IU	A	1001	8	29,34,34	2.54	7 (24%)	30,47,47	1.20	3 (10%)
2	PEG	A	701	-	6,6,6	0.51	0	5,5,5	0.40	0
2	PEG	A	702	-	6,6,6	0.49	0	5,5,5	0.25	0
2	PEG	A	703	-	6,6,6	0.39	0	5,5,5	0.38	0
3	P6G	A	704	-	12,12,18	0.50	0	11,11,17	0.35	0
4	1IU	B	1001	8	29,34,34	1.73	5 (17%)	30,47,47	1.09	2 (6%)
11	NAG	B	1612	1	14,14,15	0.73	1 (7%)	15,19,21	2.07	3 (20%)
2	PEG	B	701	-	6,6,6	0.50	0	5,5,5	0.33	0
10	PG4	B	704	-	9,9,12	0.41	0	8,8,11	0.30	0
3	P6G	B	709	-	18,18,18	0.63	0	17,17,17	0.60	0
2	PEG	B	711	-	6,6,6	0.40	0	5,5,5	0.34	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
4	1IU	A	1001	8	-	2/32/39/39	0/2/2/2
2	PEG	A	701	-	-	0/4/4/4	0/0/0/0
2	PEG	A	702	-	-	0/4/4/4	0/0/0/0
2	PEG	A	703	-	-	0/4/4/4	0/0/0/0
3	P6G	A	704	-	-	0/10/10/16	0/0/0/0
4	1IU	B	1001	8	-	0/32/39/39	0/2/2/2
11	NAG	B	1612	1	-	0/6/23/26	0/1/1/1
2	PEG	B	701	-	-	0/4/4/4	0/0/0/0
10	PG4	B	704	-	-	0/7/7/10	0/0/0/0
3	P6G	B	709	-	-	0/16/16/16	0/0/0/0
2	PEG	B	711	-	-	0/4/4/4	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	1IU	NAT-NAW	-8.11	1.22	1.34
4	A	1001	1IU	NAS-NAR	-7.63	1.23	1.34
4	B	1001	1IU	NAT-NAW	-5.27	1.26	1.34
4	B	1001	1IU	NAS-NAR	-3.72	1.29	1.34
4	A	1001	1IU	CAO-CBA	-3.58	1.42	1.51
4	B	1001	1IU	CAO-CBA	-3.58	1.42	1.51
4	A	1001	1IU	PBG-CAQ	-3.34	1.76	1.79
4	A	1001	1IU	NAW-NAR	-2.53	1.28	1.32
11	B	1612	NAG	C1-C2	-2.12	1.49	1.52
4	A	1001	1IU	CBC-CAY	2.05	1.55	1.51
4	B	1001	1IU	CBC-CAY	2.62	1.56	1.51
4	B	1001	1IU	PBG-OAI	3.77	1.56	1.49
4	A	1001	1IU	PBG-OAI	4.42	1.58	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1612	NAG	C3-C2-N2	-4.63	99.46	110.56
4	B	1001	1IU	OAH-PBG-OAI	-4.03	107.53	113.72
4	A	1001	1IU	OAH-PBG-OAI	-3.02	109.09	113.72
11	B	1612	NAG	O5-C5-C6	2.22	112.14	107.35
4	A	1001	1IU	CAP-CBE-CAZ	2.57	113.35	108.33
4	B	1001	1IU	CAP-CBE-CAZ	2.64	113.48	108.33
4	A	1001	1IU	NAT-NAW-NAR	2.65	111.11	109.59
11	B	1612	NAG	C4-C3-C2	5.03	119.05	111.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	1IU	CAP-CBE-CAZ-NAV
4	A	1001	1IU	OAG-CAZ-CBE-CAP

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1001	1IU	2	0
10	B	704	PG4	1	0
3	B	709	P6G	2	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	607/629 (96%)	-0.35	14 (2%) 64 63	13, 24, 44, 79	0
1	B	607/629 (96%)	-0.24	14 (2%) 64 63	13, 28, 50, 70	0
All	All	1214/1258 (96%)	-0.29	28 (2%) 64 63	13, 26, 49, 79	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	325	GLY	6.2
1	B	135	THR	4.3
1	B	133	THR	4.2
1	A	78	PRO	4.0
1	B	134	ALA	3.9
1	B	81	GLN	3.5
1	A	610	GLY	3.5
1	B	325	GLY	3.2
1	B	78	PRO	2.8
1	A	133	THR	2.8
1	B	609	GLU	2.8
1	A	609	GLU	2.7
1	B	522	GLU	2.7
1	A	134	ALA	2.6
1	B	606	ASN	2.6
1	A	323	ALA	2.5
1	B	605	ASP	2.5
1	B	82	GLN	2.5
1	A	135	THR	2.5
1	A	605	ASP	2.3
1	A	81	GLN	2.3
1	A	606	ASN	2.3
1	B	608	PRO	2.2
1	B	610	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	4	GLY	2.1
1	A	136	CYS	2.0
1	A	412	ASP	2.0
1	B	205	PRO	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
6	NAG	B	1614	14/15	0.90	0.27	2.18	45,47,51,57	0
6	NAG	A	1614	14/15	0.86	0.22	1.22	42,45,47,49	0
5	NAG	A	1612	14/15	0.92	0.16	1.19	32,36,41,47	0
7	NAG	A	1616	14/15	0.95	0.13	0.39	37,39,42,42	0
12	BMA	B	1618	11/12	0.81	0.36	-	76,78,79,82	0
12	NAG	B	1617	14/15	0.90	0.40	-	66,70,71,74	0
7	NAG	A	1617	14/15	0.90	0.19	-	44,48,52,53	0
7	FUC	A	1619	10/11	0.83	0.22	-	42,43,45,45	0
6	NAG	A	1615	14/15	0.79	0.34	-	47,53,56,57	0
6	NAG	B	1615	14/15	0.85	0.42	-	61,64,65,66	0
12	NAG	B	1616	14/15	0.90	0.20	-	53,55,57,61	0
5	FUC	A	1613	10/11	0.77	0.34	-	53,56,58,59	0
7	BMA	A	1618	11/12	0.80	0.24	-	55,59,60,60	0

## 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. 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
2	PEG	A	702	7/7	0.77	0.21	7.13	56,58,59,59	0
3	P6G	B	709	19/19	0.76	0.15	4.11	33,39,42,42	0
3	P6G	A	704	13/19	0.83	0.17	3.02	42,43,48,48	0
2	PEG	B	711	7/7	0.86	0.15	1.65	34,35,42,43	0
10	PG4	B	704	10/13	0.93	0.13	0.88	37,37,39,39	0
11	NAG	B	1612	14/15	0.85	0.14	0.60	37,40,43,43	0
2	PEG	A	703	7/7	0.90	0.16	0.43	42,44,44,44	0
4	1IU	B	1001	33/33	0.97	0.11	0.07	14,17,23,23	0
4	1IU	A	1001	33/33	0.96	0.11	-0.26	18,20,26,26	0
9	CL	A	1621	1/1	0.99	0.07	-2.01	17,17,17,17	0
9	CL	B	1620	1/1	1.00	0.07	-3.36	22,22,22,22	0
8	ZN	A	1620	1/1	0.99	0.09	-	17,17,17,17	0
2	PEG	A	701	7/7	0.80	0.22	-	47,48,49,49	0
8	ZN	B	1619	1/1	1.00	0.09	-	14,14,14,14	0
2	PEG	B	701	7/7	0.79	0.23	-	42,46,46,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.