



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:15 PM GMT

PDB ID : 4BZS  
Title : Human angiotensin converting enzyme N-domain in complex with K-26  
Authors : Kramer, G.J.; Mohd, A.; Schwager, S.L.U.; MAsuyer, G.; Acharya, K.R.;  
Sturrock, E.D.; Bachmann, B.O.  
Deposited on : 2013-07-29  
Resolution : 2.10 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 (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

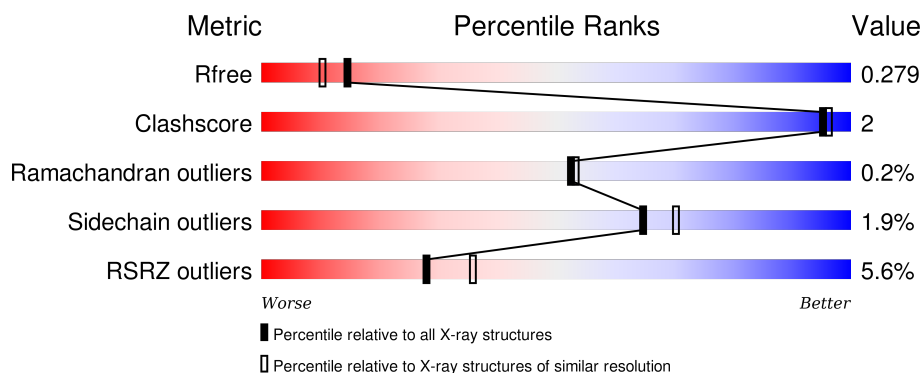
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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
6	PEG	B	704	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 10447 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	612	Total	C	N	O	S	4	0	0
			4980	3197	855	909	19			
1	B	610	Total	C	N	O	S	1	0	0
			4961	3186	853	903	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	629	LEU	-	EXPRESSION TAG	UNP P12821
A	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
B	629	LEU	-	EXPRESSION TAG	UNP P12821
B	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821

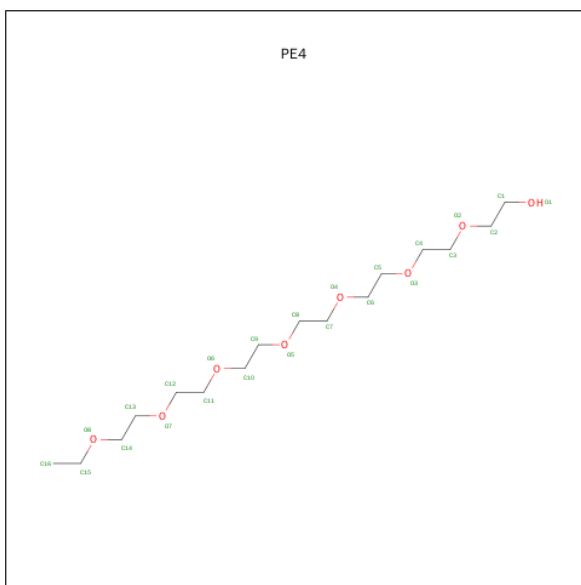
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

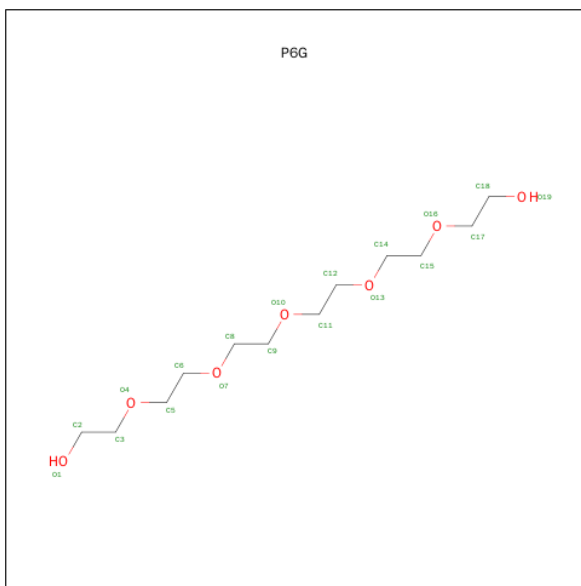
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $\text{C}_{12}\text{H}_{26}\text{O}_7$ ).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $\text{C}_4\text{H}_{10}\text{O}_3$ ).



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

- 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		
7	B	2	Total	C	N	O	0	0
			24	14	1	9		

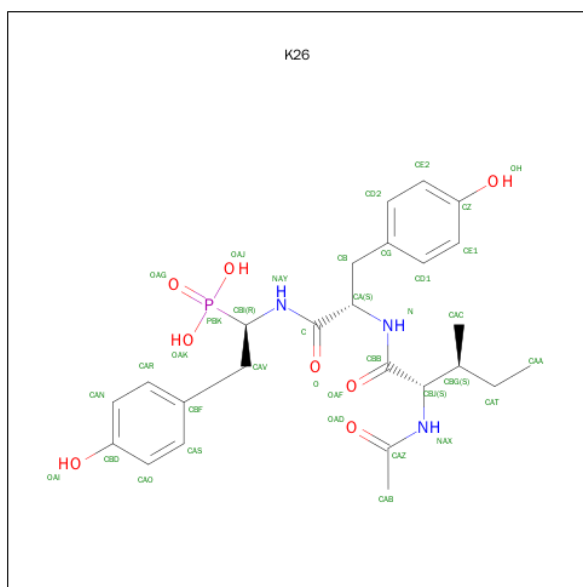
- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

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 (3-MER).

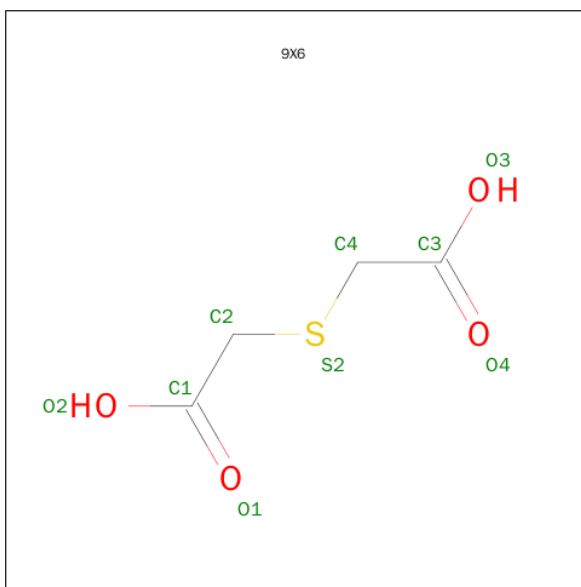
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	3	Total	C	N	O	0	0
			39	22	2	15		
9	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 10 is N-ACETYL-L-ILE-L-TYR-(R)-1-AMINO-2-(4-HYDROXYPHENYL)ETHYLPHOSPHONIC ACID (three-letter code: K26) (formula:  $C_{25}H_{34}N_3O_8P$ ).



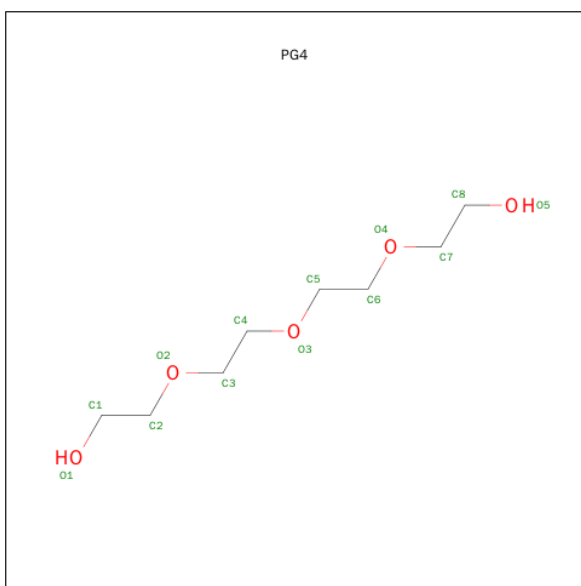
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	P	0	0
			37	25	3	8	1		
10	B	1	Total	C	N	O	P	0	0
			37	25	3	8	1		

- Molecule 11 is THIODIGLYCOLIC ACID (three-letter code: 9X6) (formula:  $C_4H_6O_4S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	O	S	0	0
			9	4	4	1		
11	B	1	Total	C	O	S	0	0
			9	4	4	1		

- Molecule 12 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



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

- Molecule 13 is water.

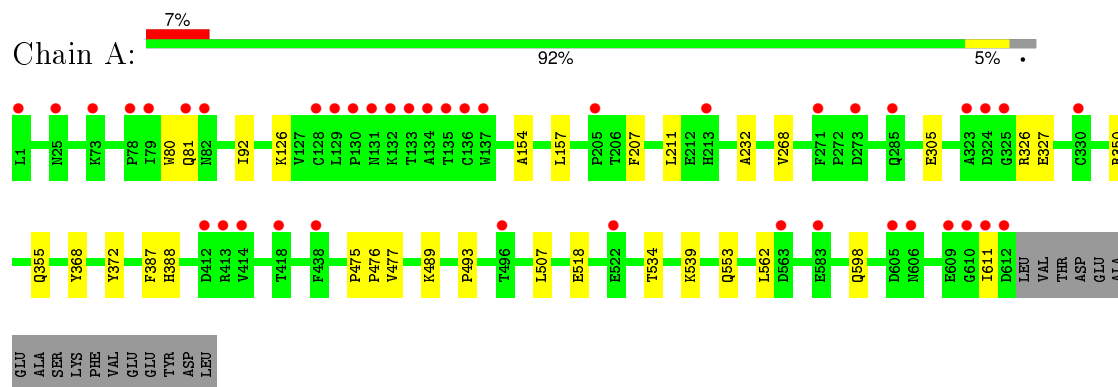


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	65	Total 65	O 65	0	0
13	B	96	Total 96	O 96	0	0

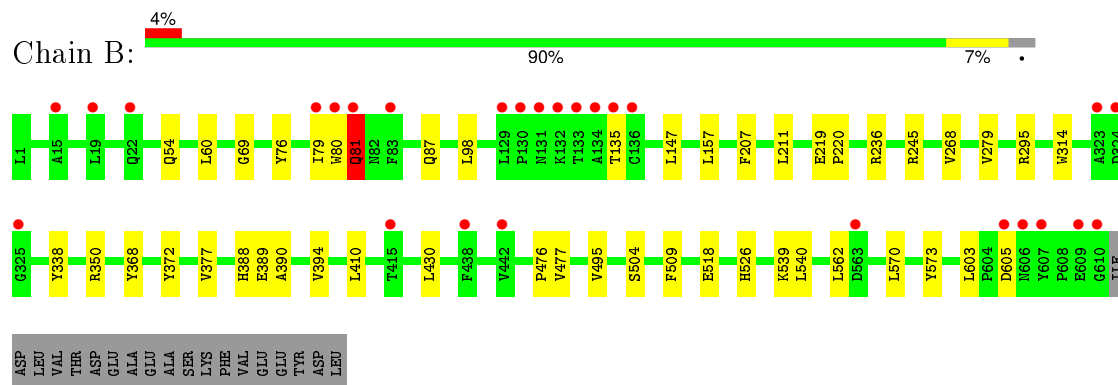
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	73.00Å 77.32Å 82.07Å 88.69° 64.53° 75.29°	Depositor
Resolution (Å)	36.61 – 2.10 36.58 – 2.10	Depositor EDS
% Data completeness (in resolution range)	83.5 (36.61-2.10) 81.8 (36.58-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.233 , 0.277 0.235 , 0.279	Depositor DCC
$R_{free}$ test set	3837 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.7	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 76412 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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, PE4, K26, 9X6, PG4, 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	0.29	1/5137 (0.0%)	0.45	1/7002 (0.0%)
1	B	0.28	0/5118	0.46	0/6976
All	All	0.29	1/10255 (0.0%)	0.46	1/13978 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	LYS	CG-CD	-6.45	1.30	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ILE	CB-CG1-CD1	-5.70	97.95	113.90

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	4980	0	4752	13	0
1	B	4961	0	4735	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	13	0	17	0	0
5	A	19	0	26	0	0
6	A	7	0	10	0	0
6	B	21	0	30	0	0
7	A	24	0	22	0	0
7	B	24	0	22	0	0
8	A	28	0	25	1	0
8	B	28	0	25	0	0
9	A	39	0	34	0	0
9	B	39	0	33	0	0
10	A	37	0	31	0	0
10	B	37	0	30	0	0
11	A	9	0	4	0	0
11	B	9	0	4	1	0
12	B	7	0	9	0	0
13	A	65	0	0	1	0
13	B	96	0	0	0	0
All	All	10447	0	9809	32	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 (32) 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:598:GLN:NE2	13:A:2064:HOH:O	2.19	0.65
1:A:326:ARG:HD3	8:A:803:NAG:H82	1.86	0.56
1:B:76:TYR:HD1	1:B:79:ILE:HD11	1.76	0.51
1:B:477:VAL:HG12	1:B:603:LEU:HD21	1.93	0.51
1:A:305:GLU:HG3	1:A:534:THR:HG22	1.93	0.50
1:B:69:GLY:HA3	1:B:98:LEU:HD21	1.94	0.50
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.93	0.49
1:B:509:PHE:CE2	1:B:570:LEU:HD13	2.48	0.49
1:B:279:VAL:HG11	1:B:410:LEU:HD13	1.95	0.49
1:B:495:VAL:O	1:B:495:VAL:HG12	2.13	0.49
1:B:157:LEU:HD13	1:B:476:PRO:HB2	1.96	0.48
1:A:207:PHE:CE2	1:A:211:LEU:HD11	2.49	0.48
1:A:518:GLU:HG3	1:A:539:LYS:HD2	1.95	0.47
1:A:350:ARG:H	1:A:355:GLN:HE21	1.62	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:TRP:O	1:B:81:GLN:CG	2.65	0.44
1:A:489:LYS:O	1:A:493:PRO:HD2	2.18	0.44
1:B:518:GLU:HG3	1:B:539:LYS:HD2	1.98	0.44
1:B:389:GLU:HB2	1:B:504:SER:HB2	2.00	0.43
1:A:154:ALA:HB1	1:A:611:ILE:HG21	2.00	0.43
1:A:80:TRP:O	1:A:81:GLN:HB2	2.19	0.43
1:B:390:ALA:O	1:B:394:VAL:HG23	2.19	0.43
1:A:232:ALA:CB	1:A:268:VAL:HG12	2.49	0.42
1:B:207:PHE:CE2	1:B:211:LEU:HD11	2.54	0.42
1:B:80:TRP:O	1:B:81:GLN:CB	2.68	0.42
1:A:387:PHE:CE1	1:A:507:LEU:HD21	2.56	0.41
1:B:268:VAL:HG21	1:B:430:LEU:HD11	2.03	0.41
1:B:526:HIS:HA	1:B:573:TYR:CE2	2.56	0.41
1:A:475:PRO:HA	1:A:476:PRO:HD3	1.93	0.41
1:B:338:TYR:CD1	1:B:377:VAL:HG23	2.56	0.41
1:B:219:GLU:HB3	1:B:220:PRO:HD3	2.03	0.40
1:B:295:ARG:HD2	1:B:314:TRP:CH2	2.56	0.40
11:B:1612:9X6:C3	11:B:1612:9X6:O1	2.69	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	610/629 (97%)	589 (97%)	21 (3%)	0	100	100
1	B	608/629 (97%)	592 (97%)	14 (2%)	2 (0%)	46	45
All	All	1218/1258 (97%)	1181 (97%)	35 (3%)	2 (0%)	52	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	135	THR
1	B	81	GLN

### 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	524/541 (97%)	518 (99%)	6 (1%)	80	85
1	B	521/541 (96%)	507 (97%)	14 (3%)	52	56
All	All	1045/1082 (97%)	1025 (98%)	20 (2%)	65	70

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	327	GLU
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	A	553	GLN
1	A	562	LEU
1	B	54	GLN
1	B	60	LEU
1	B	81	GLN
1	B	87	GLN
1	B	147	LEU
1	B	236	ARG
1	B	245	ARG
1	B	350	ARG
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS
1	B	540	LEU
1	B	562	LEU
1	B	605	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	GLN
1	A	355	GLN
1	A	553	GLN
1	A	568	GLN
1	A	582	GLN
1	B	81	GLN
1	B	367	GLN
1	B	526	HIS

### 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 ⓘ

14 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	801	1,7	14,14,15	0.48	0	15,19,21	0.79	0
7	FUC	A	802	7	10,10,11	0.58	0	14,14,16	0.79	0
8	NAG	A	803	1,8	14,14,15	0.51	0	15,19,21	0.90	1 (6%)
8	NAG	A	804	8	14,14,15	0.48	0	15,19,21	0.72	0
9	NAG	A	805	1,9	14,14,15	0.46	0	15,19,21	0.76	0
9	NAG	A	806	9	14,14,15	0.52	0	15,19,21	0.59	0
9	BMA	A	807	9	11,11,12	0.29	0	14,15,17	0.56	0
7	NAG	B	801	1,7	14,14,15	0.49	0	15,19,21	0.76	0
7	FUC	B	802	7	10,10,11	0.58	0	14,14,16	0.79	0
8	NAG	B	803	1,8	14,14,15	0.51	0	15,19,21	0.96	1 (6%)
8	NAG	B	804	8	14,14,15	0.46	0	15,19,21	0.77	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	B	805	1,9	14,14,15	0.48	0	15,19,21	0.62	0
9	NAG	B	806	9	14,14,15	0.44	0	15,19,21	0.75	0
9	BMA	B	807	9	11,11,12	0.33	0	14,15,17	0.68	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
7	NAG	A	801	1,7	-	0/6/23/26	0/1/1/1
7	FUC	A	802	7	-	0/0/17/20	0/1/1/1
8	NAG	A	803	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	804	8	-	0/6/23/26	0/1/1/1
9	NAG	A	805	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	806	9	-	0/6/23/26	0/1/1/1
9	BMA	A	807	9	-	0/2/19/22	0/1/1/1
7	NAG	B	801	1,7	-	0/6/23/26	0/1/1/1
7	FUC	B	802	7	-	0/0/17/20	0/1/1/1
8	NAG	B	803	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	804	8	-	0/6/23/26	0/1/1/1
9	NAG	B	805	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	806	9	-	0/6/23/26	0/1/1/1
9	BMA	B	807	9	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	803	NAG	C1-O5-C5	2.10	114.92	112.25
8	B	803	NAG	C1-O5-C5	2.71	115.68	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	803	NAG	1	0

## 5.6 Ligand geometry

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$
10	K26	A	1001	2	37,38,38	1.60	4 (10%)	46,53,53	1.19	4 (8%)
11	9X6	A	1613	-	2,8,8	3.19	2 (100%)	3,9,9	1.75	1 (33%)
4	PE4	A	703	-	12,12,23	0.47	0	11,11,22	0.18	0
5	P6G	A	704	-	18,18,18	0.50	0	17,17,17	0.18	0
6	PEG	A	705	-	6,6,6	0.47	0	5,5,5	0.24	0
10	K26	B	1001	2	37,38,38	1.63	4 (10%)	46,53,53	1.24	3 (6%)
12	PG4	B	1611	-	6,6,12	0.45	0	5,5,11	0.20	0
11	9X6	B	1612	-	2,8,8	2.80	2 (100%)	3,9,9	3.03	1 (33%)
6	PEG	B	703	-	6,6,6	0.50	0	5,5,5	0.26	0
6	PEG	B	704	-	6,6,6	0.43	0	5,5,5	0.27	0
6	PEG	B	705	-	6,6,6	0.46	0	5,5,5	0.27	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
10	K26	A	1001	2	-	0/40/40/40	0/2/2/2
11	9X6	A	1613	-	-	0/2/6/6	0/0/0/0
4	PE4	A	703	-	-	0/10/10/21	0/0/0/0
5	P6G	A	704	-	-	0/16/16/16	0/0/0/0
6	PEG	A	705	-	-	0/4/4/4	0/0/0/0
10	K26	B	1001	2	-	0/40/40/40	0/2/2/2
12	PG4	B	1611	-	-	0/4/4/10	0/0/0/0
11	9X6	B	1612	-	-	0/2/6/6	0/0/0/0
6	PEG	B	703	-	-	0/4/4/4	0/0/0/0
6	PEG	B	704	-	-	0/4/4/4	0/0/0/0
6	PEG	B	705	-	-	0/4/4/4	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1001	K26	PBK-OAJ	-5.20	1.46	1.54
10	A	1001	K26	PBK-OAJ	-5.11	1.46	1.54
10	B	1001	K26	PBK-OAK	-5.03	1.46	1.54
10	A	1001	K26	PBK-OAK	-4.95	1.46	1.54
10	B	1001	K26	CAV-CBF	-4.11	1.41	1.51
10	A	1001	K26	CAV-CBF	-4.09	1.41	1.51
10	A	1001	K26	CB-CG	-3.98	1.41	1.51
10	B	1001	K26	CB-CG	-3.93	1.41	1.51
11	A	1613	9X6	C2-S2	-3.30	1.76	1.82
11	A	1613	9X6	C4-S2	-3.08	1.77	1.82
11	B	1612	9X6	C4-S2	-2.81	1.77	1.82
11	B	1612	9X6	C2-S2	-2.79	1.77	1.82

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	1001	K26	OAG-PBK-CBI	-6.17	101.13	113.97
10	A	1001	K26	OAG-PBK-CBI	-5.60	102.32	113.97
10	A	1001	K26	C-CA-N	-2.63	103.84	111.26
10	B	1001	K26	C-CA-N	-2.20	105.06	111.26
10	A	1001	K26	CG-CB-CA	-2.07	107.38	113.41
11	A	1613	9X6	C2-S2-C4	2.34	107.93	102.65
10	A	1001	K26	OAK-PBK-OAJ	2.75	115.83	107.57
10	B	1001	K26	OAK-PBK-OAJ	2.90	116.28	107.57
11	B	1612	9X6	C2-S2-C4	5.25	114.51	102.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	1612	9X6	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	612/629 (97%)	0.45	41 (6%)	21 28	22, 40, 70, 102	2 (0%)
1	B	610/629 (96%)	0.21	27 (4%)	38 47	22, 36, 61, 89	1 (0%)
All	All	1222/1258 (97%)	0.33	68 (5%)	28 36	22, 38, 65, 102	3 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	610	GLY	8.4
1	B	610	GLY	8.0
1	A	133	THR	7.6
1	A	134	ALA	6.8
1	A	132	LYS	6.6
1	A	131	ASN	6.3
1	A	413	ARG	6.0
1	B	130	PRO	5.8
1	A	325	GLY	5.5
1	A	130	PRO	5.2
1	A	129	LEU	5.1
1	B	135	THR	4.9
1	B	79	ILE	4.9
1	B	134	ALA	4.7
1	A	609	GLU	4.7
1	A	418	THR	4.5
1	B	325	GLY	4.3
1	A	136	CYS	4.2
1	A	82	ASN	4.2
1	A	412	ASP	4.0
1	A	273	ASP	3.9
1	A	135	THR	3.9
1	B	131	ASN	3.8
1	A	612	ASP	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	133	THR	3.7
1	B	605	ASP	3.6
1	A	81	GLN	3.5
1	A	1	LEU	3.5
1	B	324	ASP	3.4
1	B	129	LEU	3.3
1	A	330	CYS	3.3
1	B	609	GLU	3.2
1	A	606	ASN	3.2
1	A	324	ASP	3.2
1	A	128	CYS	3.2
1	B	80	TRP	3.1
1	B	22	GLN	3.0
1	A	78	PRO	3.0
1	B	132	LYS	3.0
1	A	79	ILE	2.9
1	A	323	ALA	2.8
1	B	415	THR	2.8
1	B	19	LEU	2.7
1	A	285	GLN	2.6
1	A	563	ASP	2.6
1	B	606	ASN	2.6
1	A	414	VAL	2.6
1	B	136	CYS	2.6
1	B	83	PHE	2.5
1	B	438	PHE	2.5
1	B	81	GLN	2.5
1	B	607	TYR	2.4
1	A	522	GLU	2.4
1	A	611	ILE	2.3
1	B	323	ALA	2.3
1	A	496	THR	2.3
1	B	15	ALA	2.2
1	A	205	PRO	2.2
1	B	442	VAL	2.2
1	A	583	GLU	2.2
1	A	213	HIS	2.2
1	A	271	PHE	2.2
1	A	137	TRP	2.1
1	B	563	ASP	2.1
1	A	605	ASP	2.1
1	A	73	LYS	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	438	PHE	2.0
1	A	25	ASN	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
7	NAG	A	801	14/15	0.88	0.14	0.41	50,53,59,64	0
7	NAG	B	801	14/15	0.84	0.15	0.30	47,50,55,60	0
9	NAG	B	805	14/15	0.86	0.14	0.09	56,58,62,62	0
8	NAG	B	803	14/15	0.90	0.13	-0.29	49,50,51,52	0
9	NAG	A	805	14/15	0.85	0.17	-	74,75,76,78	0
7	FUC	A	802	10/11	0.58	0.44	-	68,70,71,71	0
8	NAG	B	804	14/15	0.90	0.26	-	54,55,57,58	0
8	NAG	A	804	14/15	0.85	0.48	-	73,76,78,79	0
7	FUC	B	802	10/11	0.75	0.36	-	63,64,65,66	0
9	NAG	A	806	14/15	0.83	0.27	-	81,82,85,87	0
9	BMA	B	807	11/12	0.66	0.31	-	72,74,74,74	0
8	NAG	A	803	14/15	0.91	0.28	-	56,61,63,68	0
9	BMA	A	807	11/12	0.72	0.40	-	89,91,92,93	0
9	NAG	B	806	14/15	0.91	0.17	-	65,67,69,70	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
6	PEG	B	704	7/7	0.84	0.18	3.93	58,59,61,62	0
11	9X6	B	1612	9/9	0.86	0.21	1.64	41,43,44,47	0
5	P6G	A	704	19/19	0.80	0.17	1.41	53,56,57,57	0
4	PE4	A	703	13/24	0.86	0.13	0.99	43,45,51,51	0
11	9X6	A	1613	9/9	0.86	0.20	0.63	37,39,40,42	0
10	K26	B	1001	37/37	0.94	0.16	0.60	26,31,36,37	0
10	K26	A	1001	37/37	0.94	0.17	0.27	25,30,33,34	0
12	PG4	B	1611	7/13	0.89	0.13	-0.21	48,49,49,49	0
3	CL	B	702	1/1	0.99	0.10	-1.72	27,27,27,27	0
3	CL	A	702	1/1	0.99	0.05	-3.77	29,29,29,29	0
2	ZN	B	701	1/1	0.98	0.10	-	37,37,37,37	0
6	PEG	A	705	7/7	0.79	0.17	-	54,55,55,56	0
6	PEG	B	705	7/7	0.74	0.17	-	52,53,53,53	0
6	PEG	B	703	7/7	0.81	0.18	-	44,46,47,47	0
2	ZN	A	701	1/1	0.99	0.06	-	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.