



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:04 am GMT

PDB ID : 4KX9  
Title : Crystal structure of human aminopeptidase A complexed with arginine  
Authors : Yang, Y.; Liu, C.; Lin, Y.Y.; Li, F.  
Deposited on : 2013-05-24  
Resolution : 2.25 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 : 1.7.2 (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

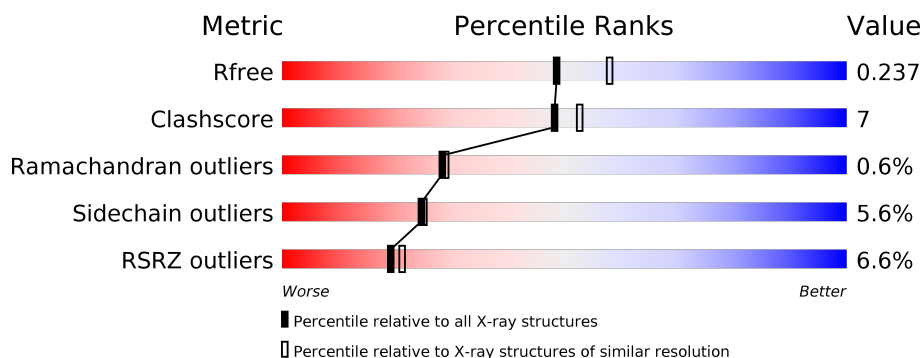
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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	888	<div> <div>7%</div> <div>83%</div> <div>14%</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
6	ARG	A	1018	-	-	X	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8011 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 Glutamyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	875	Total	C	N	O	S	0	2	0
			7160	4586	1192	1357	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	ARG	GLN	NATURAL VARIANTS	UNP Q07075
A	218	ALA	VAL	NATURAL VARIANTS	UNP Q07075
A	958	HIS	-	EXPRESSION TAG	UNP Q07075
A	959	HIS	-	EXPRESSION TAG	UNP Q07075
A	960	HIS	-	EXPRESSION TAG	UNP Q07075
A	961	HIS	-	EXPRESSION TAG	UNP Q07075
A	962	HIS	-	EXPRESSION TAG	UNP Q07075
A	963	HIS	-	EXPRESSION TAG	UNP Q07075

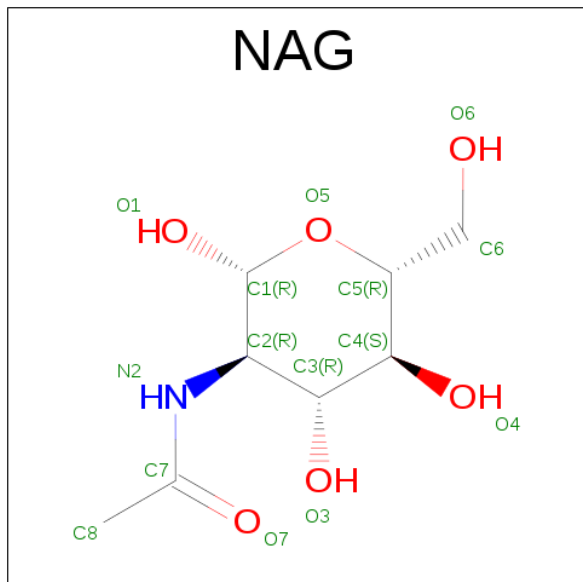
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

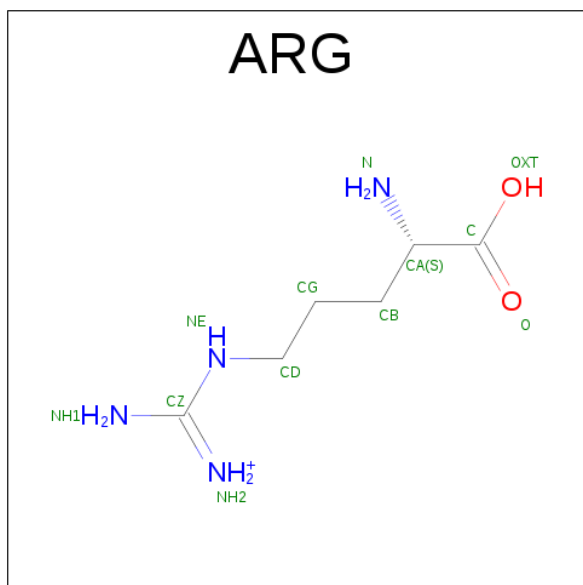


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			42	24	3	15		
5	A	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 6 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			12	6	4	2		

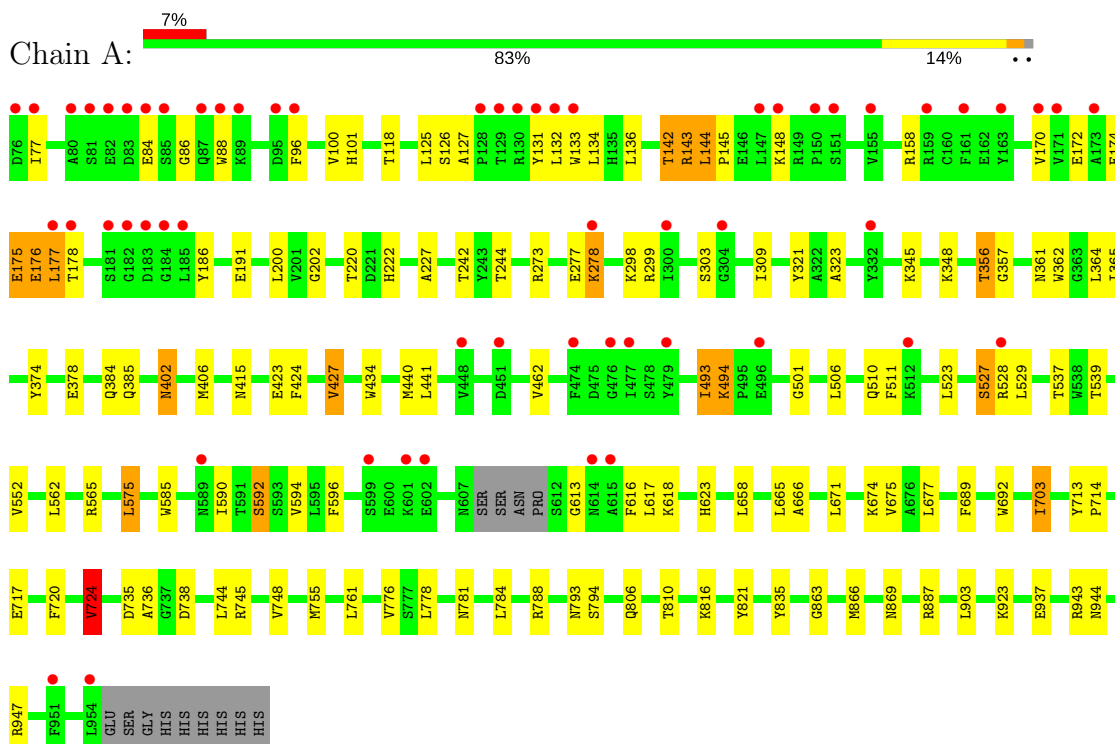
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	614	Total	O	0	0
			614	614		

### 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 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: Glutamyl aminopeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.27Å 142.27Å 237.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.59 – 2.25 45.55 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.59-2.25) 99.4 (45.55-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.163 , 0.234 0.174 , 0.237	Depositor DCC
$R_{free}$ test set	3403 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.9	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG

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	0.38	0/7345	0.57	1/9986 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	724	VAL	CB-CA-C	-5.91	100.17	111.40

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	7160	0	6957	92	0
2	A	1	0	0	0	0
3	A	112	0	100	4	0
4	A	28	0	26	0	0
5	A	84	0	74	5	0
6	A	12	0	12	13	0
7	A	614	0	0	19	0
All	All	8011	0	7169	101	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 7.

All (101) 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:356:THR:HG21	6:A:1018:ARG:HD3	1.11	1.08
1:A:378:GLU:HG3	7:A:1520:HOH:O	1.70	0.91
1:A:244:THR:HB	7:A:1695:HOH:O	1.72	0.88
1:A:761:LEU:HD22	1:A:793:ASN:HD21	1.35	0.88
1:A:356:THR:CG2	6:A:1018:ARG:HD3	2.02	0.87
1:A:142:THR:HG21	7:A:1308:HOH:O	1.74	0.85
1:A:356:THR:HG21	6:A:1018:ARG:CD	2.03	0.85
5:A:1013:NAG:H83	5:A:1013:NAG:H3	1.59	0.83
1:A:887:ARG:HH12	6:A:1018:ARG:HD2	1.46	0.80
5:A:1013:NAG:C8	5:A:1013:NAG:H3	2.13	0.79
1:A:356:THR:CG2	6:A:1018:ARG:HH11	1.96	0.79
1:A:77:ILE:HD13	1:A:143:ARG:HA	1.66	0.76
1:A:273:ARG:HD2	7:A:1559:HOH:O	1.84	0.76
1:A:356:THR:HG23	6:A:1018:ARG:NH1	2.02	0.75
1:A:501:GLY:HA3	1:A:523:LEU:HD23	1.69	0.74
1:A:118:THR:HG22	1:A:191:GLU:HG2	1.68	0.74
1:A:793:ASN:HB3	7:A:1550:HOH:O	1.88	0.73
1:A:423:GLU:O	1:A:427:VAL:HG12	1.90	0.72
1:A:158:ARG:HB2	1:A:174:GLU:HG2	1.72	0.71
1:A:511:PHE:CZ	7:A:1444:HOH:O	2.44	0.69
1:A:356:THR:HG23	6:A:1018:ARG:HH11	1.59	0.65
1:A:736:ALA:O	1:A:745:ARG:NH1	2.23	0.64
1:A:101:HIS:CD2	1:A:242:THR:HG23	2.34	0.63
1:A:511:PHE:HZ	7:A:1444:HOH:O	1.80	0.62
1:A:735:ASP:OD1	1:A:781:ASN:HB2	1.99	0.62
1:A:869:ASN:HB2	7:A:1571:HOH:O	1.99	0.62
1:A:277:GLU:HA	7:A:1358:HOH:O	2.00	0.61
3:A:1005:NAG:H83	3:A:1005:NAG:H3	1.82	0.61
5:A:1013:NAG:H83	5:A:1013:NAG:C3	2.31	0.61
1:A:101:HIS:HD2	1:A:242:THR:HG23	1.67	0.60
6:A:1018:ARG:HD2	7:A:1108:HOH:O	2.01	0.60
1:A:585:TRP:HZ3	1:A:594:VAL:HG23	1.66	0.60
1:A:244:THR:HG22	1:A:278:LYS:HA	1.83	0.59
1:A:703:ILE:HD12	1:A:713:TYR:CE2	2.37	0.59
1:A:923:LYS:HG3	7:A:1441:HOH:O	2.03	0.59
1:A:356:THR:CG2	6:A:1018:ARG:NH1	2.62	0.59
1:A:537:THR:HA	1:A:575:LEU:HD23	1.85	0.58
1:A:402:ASN:HD22	1:A:402:ASN:N	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LYS:HB2	7:A:1698:HOH:O	2.06	0.56
1:A:77:ILE:CD1	1:A:143:ARG:HA	2.35	0.56
1:A:175:GLU:O	1:A:176:GLU:HB3	2.05	0.56
1:A:131:TYR:CE2	1:A:172:GLU:HB3	2.40	0.56
1:A:565:ARG:CZ	1:A:937:GLU:HG3	2.37	0.55
6:A:1018:ARG:NH2	7:A:1106:HOH:O	2.39	0.55
1:A:585:TRP:CZ3	1:A:594:VAL:HG23	2.42	0.55
1:A:887:ARG:HH12	6:A:1018:ARG:CD	2.17	0.55
1:A:944:ASN:HB3	7:A:1631:HOH:O	2.06	0.55
5:A:1013:NAG:C3	5:A:1013:NAG:C8	2.86	0.54
1:A:717:GLU:HG2	1:A:755:MET:O	2.09	0.53
1:A:100:VAL:O	1:A:242:THR:HG22	2.09	0.53
1:A:177:LEU:HD13	1:A:178:THR:H	1.75	0.52
1:A:356:THR:HG21	6:A:1018:ARG:HH11	1.71	0.52
1:A:674:LYS:HD3	5:A:1007:NAG:H62	1.91	0.51
1:A:348:LYS:HZ3	1:A:365:ILE:HD13	1.75	0.51
1:A:177:LEU:HB3	1:A:186:TYR:OH	2.11	0.51
1:A:299:ARG:HD2	1:A:323:ALA:HB1	1.92	0.50
1:A:96:PHE:HB2	1:A:126:SER:HB2	1.94	0.50
1:A:143:ARG:HD3	1:A:191:GLU:CD	2.32	0.50
1:A:616:PHE:HE2	1:A:618:LYS:HG3	1.77	0.50
1:A:493:ILE:O	1:A:494:LYS:HB2	2.12	0.49
1:A:361:ASN:HB2	1:A:364:LEU:O	2.13	0.49
1:A:321:TYR:HA	3:A:1004:NAG:H82	1.95	0.48
1:A:592:SER:HB2	7:A:1612:HOH:O	2.13	0.48
1:A:784:LEU:O	1:A:788:ARG:HG3	2.13	0.48
1:A:175:GLU:O	1:A:176:GLU:CB	2.61	0.47
1:A:943:ARG:HH12	1:A:947:ARG:HH11	1.61	0.47
1:A:863:GLY:HA2	1:A:866:MET:HB2	1.97	0.47
1:A:348:LYS:NZ	1:A:365:ILE:HD13	2.29	0.47
3:A:1005:NAG:C8	3:A:1005:NAG:H3	2.44	0.47
1:A:816:LYS:HE3	7:A:1647:HOH:O	2.15	0.47
6:A:1018:ARG:CD	7:A:1108:HOH:O	2.59	0.47
1:A:131:TYR:CD2	1:A:172:GLU:HB3	2.50	0.46
1:A:713:TYR:HB3	1:A:714:PRO:HD3	1.97	0.46
1:A:937:GLU:HG2	7:A:1511:HOH:O	2.15	0.46
1:A:385:GLN:HA	1:A:434:TRP:CZ3	2.50	0.46
1:A:689:PHE:HA	1:A:744:LEU:HD13	1.98	0.46
1:A:96:PHE:CB	1:A:126:SER:HB2	2.46	0.46
1:A:720:PHE:O	1:A:724:VAL:HG22	2.17	0.45
1:A:527:SER:C	1:A:529:LEU:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:THR:OG1	1:A:191:GLU:C	2.55	0.44
1:A:125:LEU:HD21	1:A:127:ALA:O	2.17	0.44
1:A:806:GLN:O	1:A:810:THR:HG22	2.18	0.44
1:A:493:ILE:HG12	1:A:527:SER:OG	2.18	0.43
1:A:356:THR:HB	1:A:357:GLY:H	1.69	0.43
1:A:671:LEU:HD11	1:A:675:VAL:HG11	2.01	0.43
1:A:424:PHE:CG	1:A:440:MET:HG2	2.54	0.43
1:A:374:TYR:CE1	1:A:384:GLN:HB2	2.54	0.42
1:A:776:VAL:HG23	7:A:1396:HOH:O	2.18	0.42
1:A:133:TRP:HB3	1:A:170:VAL:HG22	2.02	0.42
1:A:441:LEU:HD21	1:A:623:HIS:HB3	2.02	0.42
1:A:202:GLY:O	1:A:220:THR:HA	2.20	0.41
1:A:143:ARG:HD3	1:A:191:GLU:OE1	2.19	0.41
1:A:144:LEU:HD23	1:A:145:PRO:O	2.21	0.41
1:A:692:TRP:CH2	1:A:724:VAL:HG13	2.55	0.41
1:A:309:ILE:CD1	1:A:323:ALA:HA	2.51	0.41
1:A:222:HIS:CD2	1:A:227:ALA:HA	2.56	0.40
1:A:562:LEU:HA	1:A:562:LEU:HD12	1.98	0.40
1:A:321:TYR:CA	3:A:1004:NAG:H82	2.50	0.40
1:A:86:GLY:HA3	1:A:88:TRP:CZ3	2.57	0.40
1:A:493:ILE:HG13	1:A:529:LEU:HD12	2.04	0.40
1:A:666:ALA:HA	1:A:671:LEU:O	2.21	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	873/888 (98%)	839 (96%)	29 (3%)	5 (1%)	28	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	613	GLY
1	A	176	GLU
1	A	552	VAL
1	A	175	GLU
1	A	494	LYS

### 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	787/797 (99%)	743 (94%)	44 (6%)	25	25

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	GLU
1	A	132	LEU
1	A	134	LEU
1	A	136	LEU
1	A	142	THR
1	A	143	ARG
1	A	144	LEU
1	A	148	LYS
1	A	177	LEU
1	A	200	LEU
1	A	278	LYS
1	A	298	LYS
1	A	303	SER
1	A	345	LYS
1	A	356	THR
1	A	362	TRP
1	A	402	ASN
1	A	406	MET
1	A	415	ASN
1	A	427	VAL
1	A	462	VAL
1	A	493	ILE

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Mol	Chain	Res	Type
1	A	506	LEU
1	A	510	GLN
1	A	527	SER
1	A	528	ARG
1	A	539	THR
1	A	575	LEU
1	A	590	ILE
1	A	592	SER
1	A	596	PHE
1	A	617	LEU
1	A	658	LEU
1	A	665	LEU
1	A	677	LEU
1	A	703	ILE
1	A	724	VAL
1	A	738	ASP
1	A	748	VAL
1	A	778	LEU
1	A	794	SER
1	A	821	TYR
1	A	835	TYR
1	A	903	LEU

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	101	HIS
1	A	105	HIS
1	A	402	ASN
1	A	415	ASN
1	A	510	GLN
1	A	792	GLN
1	A	793	ASN
1	A	874	ASN

### 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$
3	NAG	A	1002	1,3	14,14,15	0.46	0	15,19,21	0.83	0
3	NAG	A	1003	3	14,14,15	0.75	1 (7%)	15,19,21	1.48	2 (13%)
3	NAG	A	1004	1,3	14,14,15	0.59	0	15,19,21	1.53	3 (20%)
3	NAG	A	1005	3	14,14,15	0.60	0	15,19,21	1.62	2 (13%)
5	NAG	A	1007	1,5	14,14,15	0.55	0	15,19,21	1.07	1 (6%)
5	NAG	A	1008	5	14,14,15	0.72	0	15,19,21	1.09	1 (6%)
5	NAG	A	1009	5	14,14,15	0.56	0	15,19,21	1.12	1 (6%)
5	NAG	A	1011	1,5	14,14,15	0.46	0	15,19,21	1.22	1 (6%)
5	NAG	A	1012	5	14,14,15	0.60	0	15,19,21	1.95	3 (20%)
5	NAG	A	1013	5	14,14,15	0.66	0	15,19,21	2.68	9 (60%)
3	NAG	A	1014	1,3	14,14,15	0.50	0	15,19,21	2.27	4 (26%)
3	NAG	A	1015	3	14,14,15	0.53	0	15,19,21	1.01	1 (6%)
3	NAG	A	1016	1,3	14,14,15	0.61	0	15,19,21	0.63	0
3	NAG	A	1017	3	14,14,15	0.42	0	15,19,21	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
3	NAG	A	1002	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1003	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1004	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1005	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1007	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1008	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1009	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1011	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1012	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1013	5	-	0/6/23/26	0/1/1/1
3	NAG	A	1014	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1015	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1016	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1017	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	NAG	O7-C7	2.07	1.28	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1012	NAG	O5-C1-C2	-4.30	105.49	111.47
5	A	1008	NAG	O5-C1-C2	-3.29	106.89	111.47
3	A	1004	NAG	O5-C1-C2	-2.97	107.34	111.47
3	A	1014	NAG	C4-C3-C2	-2.95	106.69	111.02
5	A	1013	NAG	O5-C1-C2	-2.93	107.40	111.47
5	A	1013	NAG	O7-C7-C8	-2.82	116.92	122.06
3	A	1003	NAG	O5-C1-C2	-2.64	107.80	111.47
5	A	1013	NAG	C6-C5-C4	-2.19	107.87	113.00
3	A	1015	NAG	C4-C3-C2	2.01	113.96	111.02
3	A	1017	NAG	C1-O5-C5	2.04	114.97	112.17
5	A	1007	NAG	O4-C4-C5	2.12	114.62	109.28
3	A	1004	NAG	C1-O5-C5	2.19	115.19	112.17
5	A	1009	NAG	C1-C2-N2	2.31	114.43	110.49
5	A	1013	NAG	C3-C4-C5	2.33	114.33	110.22
5	A	1013	NAG	C8-C7-N2	2.45	120.52	116.11
3	A	1005	NAG	C8-C7-N2	2.64	120.87	116.11
3	A	1003	NAG	C1-O5-C5	2.89	116.15	112.17
5	A	1011	NAG	C1-O5-C5	3.23	116.62	112.17
5	A	1012	NAG	C1-C2-N2	3.37	116.24	110.49
3	A	1014	NAG	O4-C4-C5	3.42	117.89	109.28
5	A	1013	NAG	C1-C2-N2	3.55	116.56	110.49
3	A	1014	NAG	O4-C4-C3	3.56	118.11	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1013	NAG	C1-O5-C5	3.73	117.31	112.17
5	A	1013	NAG	C4-C3-C2	3.74	116.50	111.02
3	A	1004	NAG	C2-N2-C7	3.82	128.52	122.94
5	A	1012	NAG	C2-N2-C7	3.90	128.63	122.94
3	A	1005	NAG	C2-N2-C7	4.35	129.29	122.94
5	A	1013	NAG	C2-N2-C7	5.69	131.25	122.94
3	A	1014	NAG	C1-O5-C5	6.03	120.47	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1004	NAG	2	0
3	A	1005	NAG	2	0
5	A	1007	NAG	1	0
5	A	1013	NAG	4	0

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	NAG	A	1006	1	14,14,15	0.60	0	15,19,21	0.96	1 (6%)
4	NAG	A	1010	1	14,14,15	0.58	0	15,19,21	1.62	4 (26%)
6	ARG	A	1018	-	6,11,11	0.55	0	5,13,13	0.86	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	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1010	1	-	0/6/23/26	0/1/1/1
6	ARG	A	1018	-	-	0/7/11/11	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1010	NAG	O5-C1-C2	-2.49	108.01	111.47
4	A	1010	NAG	C1-C2-N2	2.15	114.17	110.49
4	A	1010	NAG	C3-C4-C5	2.22	114.14	110.22
4	A	1006	NAG	C4-C3-C2	2.32	114.42	111.02
4	A	1010	NAG	C2-N2-C7	4.29	129.21	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1018	ARG	13	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	875/888 (98%)	0.02	58 (6%) 19 21	21, 54, 102, 138	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	GLU	4.7
1	A	184	GLY	4.6
1	A	183	ASP	4.2
1	A	181	SER	3.8
1	A	951	PHE	3.5
1	A	182	GLY	3.3
1	A	151	SER	3.3
1	A	278	LYS	3.2
1	A	76	ASP	3.2
1	A	304	GLY	3.1
1	A	82	GLU	3.1
1	A	614	ASN	3.1
1	A	132	LEU	3.1
1	A	89	LYS	3.0
1	A	148	LYS	3.0
1	A	83	ASP	3.0
1	A	159	ARG	3.0
1	A	477	ILE	2.9
1	A	88	TRP	2.9
1	A	80	ALA	2.9
1	A	173	ALA	2.9
1	A	476	GLY	2.8
1	A	128	PRO	2.8
1	A	528	ARG	2.8
1	A	185	LEU	2.7
1	A	602	GLU	2.6
1	A	131	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	171	VAL	2.5
1	A	589	ASN	2.4
1	A	130	ARG	2.4
1	A	87	GLN	2.3
1	A	599	SER	2.3
1	A	601	LYS	2.3
1	A	150	PRO	2.3
1	A	300	ILE	2.3
1	A	170	VAL	2.3
1	A	85	SER	2.3
1	A	129	THR	2.2
1	A	615	ALA	2.2
1	A	332	TYR	2.2
1	A	474	PHE	2.2
1	A	954	LEU	2.2
1	A	496	GLU	2.2
1	A	512	LYS	2.2
1	A	96	PHE	2.2
1	A	163	TYR	2.2
1	A	161	PHE	2.2
1	A	81	SER	2.2
1	A	177	LEU	2.1
1	A	155	VAL	2.1
1	A	147	LEU	2.1
1	A	178	THR	2.1
1	A	448	VAL	2.1
1	A	133	TRP	2.1
1	A	479	TYR	2.0
1	A	77	ILE	2.0
1	A	95	ASP	2.0
1	A	451	ASP	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
5	NAG	A	1011	14/15	0.93	0.12	-0.01	63,88,106,164	0
5	NAG	A	1007	14/15	0.96	0.09	-0.91	62,93,114,121	0
3	NAG	A	1015	14/15	0.86	0.41	-	118,136,152,157	0
3	NAG	A	1014	14/15	0.96	0.28	-	54,78,103,114	0
3	NAG	A	1002	14/15	0.94	0.12	-	64,90,120,139	0
3	NAG	A	1017	14/15	0.87	0.23	-	107,135,145,147	0
5	NAG	A	1013	14/15	0.90	0.19	-	122,154,167,177	0
3	NAG	A	1016	14/15	0.96	0.11	-	51,78,97,108	0
3	NAG	A	1004	14/15	0.95	0.13	-	71,103,110,122	0
3	NAG	A	1003	14/15	0.87	0.27	-	127,143,164,166	0
5	NAG	A	1008	14/15	0.95	0.14	-	129,143,170,218	0
5	NAG	A	1012	14/15	0.92	0.20	-	90,118,137,139	0
5	NAG	A	1009	14/15	0.85	0.28	-	136,160,176,178	0
3	NAG	A	1005	14/15	0.79	0.30	-	134,151,164,178	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(Å <sup>2</sup> )	Q<0.9
6	ARG	A	1018	12/12	0.57	0.53	10.05	75,96,102,107	0
2	ZN	A	1001	1/1	1.00	0.09	-1.63	84,84,84,84	0
4	NAG	A	1006	14/15	0.70	0.35	-	108,143,167,172	0
4	NAG	A	1010	14/15	0.74	0.35	-	127,155,173,182	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.