



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:57 PM GMT

PDB ID : 4NAQ  
Title : Crystal structure of porcine aminopeptidase-N complexed with poly-alanine  
Authors : Chen, L.; Lin, Y.L.; Peng, G.; Li, F.  
Deposited on : 2013-10-22  
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

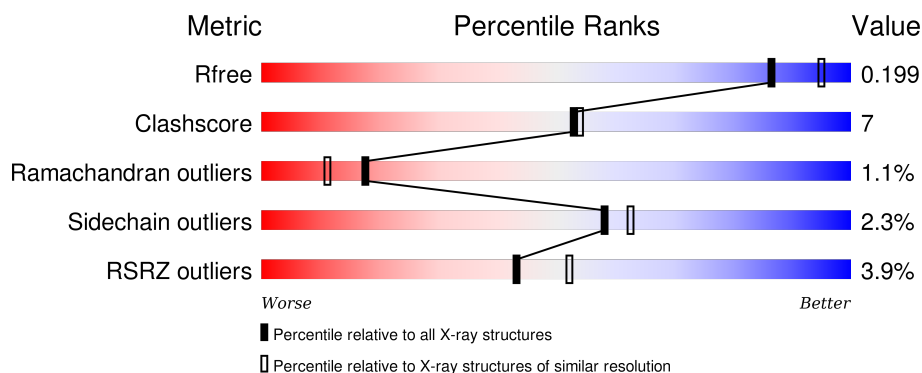
# 1 Overall quality at a glance

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	907	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
2	B	7	<div> <div>43%</div> <div>100%</div> <div>43%</div> <div>14%</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
4	NAG	A	1003	-	-	-	X
4	NAG	A	1007	-	-	-	X
5	SO4	A	1019	-	-	-	X
5	SO4	A	1022	-	-	-	X
5	SO4	A	1023	-	-	-	X
5	SO4	A	1025	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8330 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	901	Total	C	N	O	S	0	1	0
			7240	4621	1210	1379	30			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	PHE	LEU	CONFLICT	UNP P15145
A	384	GLN	GLU	CONFLICT	UNP P15145
A	964	SER	-	EXPRESSION TAG	UNP P15145
A	965	HIS	-	EXPRESSION TAG	UNP P15145
A	966	HIS	-	EXPRESSION TAG	UNP P15145
A	967	HIS	-	EXPRESSION TAG	UNP P15145
A	968	HIS	-	EXPRESSION TAG	UNP P15145
A	969	HIS	-	EXPRESSION TAG	UNP P15145
A	970	HIS	-	EXPRESSION TAG	UNP P15145

- Molecule 2 is a protein called poly A peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			36	21	7	8			

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

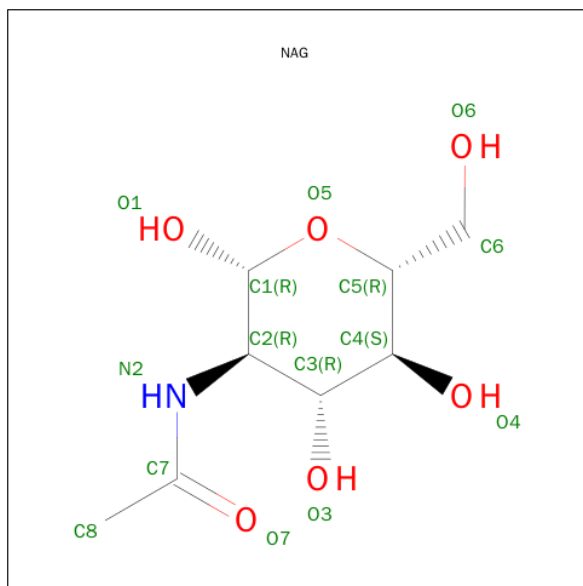
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

*Continued on next page...*

Continued from previous page...

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		

- 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		
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		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	783	Total 783	O 783	0	0
7	B	5	Total 5	O 5	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	260.16Å 62.74Å 81.49Å 90.00° 100.28° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 47.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.10) 99.5 (47.55-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.145 , 0.198 0.148 , 0.199	Depositor DCC
$R_{free}$ test set	3797 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.3	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 75417 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, NAG, SO4

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	0.43	0/7428	0.60	0/10123
2	B	0.97	0/35	1.38	0/46
All	All	0.43	0/7463	0.60	0/10169

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	3	ALA	Peptide

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7240	0	6992	87	0
2	B	36	0	37	19	0
3	A	140	0	125	2	0
4	A	70	0	65	0	0
5	A	55	0	0	4	0
6	A	1	0	0	0	0
7	A	783	0	0	16	0
7	B	5	0	0	4	0
All	All	8330	0	7219	98	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 (98) 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:383:HIS:CE1	2:B:3:ALA:HB3	1.74	1.21
1:A:413:GLU:OE2	2:B:4:ALA:HA	1.42	1.17
1:A:881:TRP:CE3	1:A:918:PHE:HZ	1.87	0.91
1:A:870:GLN:HE21	1:A:905:ARG:HE	1.23	0.86
1:A:286:ASN:HB3	7:A:1799:HOH:O	1.75	0.86
1:A:383:HIS:ND1	2:B:3:ALA:HB3	1.91	0.85
1:A:376:ARG:HG3	7:A:1800:HOH:O	1.75	0.84
1:A:373:ASN:HD21	1:A:820:ASN:HD22	1.26	0.79
1:A:861:ASN:OD1	1:A:901:GLY:HA3	1.83	0.77
2:B:7:ALA:HB2	7:B:103:HOH:O	1.82	0.77
1:A:622:ASN:H	1:A:654:ASN:HD21	1.35	0.70
1:A:243:ASN:HD21	1:A:276:ALA:H	1.41	0.69
1:A:881:TRP:HZ2	1:A:927:PHE:HD1	1.40	0.69
1:A:864:ALA:O	1:A:905:ARG:NH1	2.26	0.68
1:A:413:GLU:CD	2:B:4:ALA:HA	2.14	0.68
1:A:208:GLN:HE21	1:A:209:SER:HA	1.59	0.68
2:B:3:ALA:HB1	2:B:4:ALA:O	1.93	0.67
1:A:373:ASN:HD21	1:A:820:ASN:ND2	1.91	0.67
1:A:881:TRP:CZ3	1:A:918:PHE:HZ	2.13	0.66
1:A:888:TYR:OH	1:A:895:PHE:CD1	2.47	0.65
1:A:881:TRP:CE3	1:A:918:PHE:CZ	2.78	0.65
1:A:176:GLU:HG3	7:A:1861:HOH:O	1.96	0.65
2:B:7:ALA:CB	7:B:103:HOH:O	2.44	0.64
1:A:884:LEU:HA	1:A:888:TYR:CE1	2.33	0.64
1:A:881:TRP:CZ2	1:A:927:PHE:HD1	2.16	0.63
1:A:468:ASP:HB2	5:A:1024:SO4:O2	1.99	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:LYS:HG3	7:A:1862:HOH:O	1.99	0.62
1:A:704:LEU:O	1:A:905:ARG:HG2	1.99	0.62
1:A:383:HIS:CE1	2:B:3:ALA:CB	2.68	0.61
1:A:921:ASN:HB2	7:A:1619:HOH:O	1.99	0.61
1:A:764:GLN:HE21	1:A:764:GLN:H	1.48	0.61
1:A:881:TRP:HZ2	1:A:927:PHE:CD1	2.18	0.60
1:A:881:TRP:CZ3	1:A:918:PHE:CZ	2.89	0.60
1:A:433:GLY:HA2	2:B:6:ALA:O	2.02	0.60
1:A:383:HIS:CD2	2:B:2:ALA:O	2.56	0.59
1:A:433:GLY:HA2	2:B:7:ALA:HA	1.84	0.58
1:A:448:HIS:HE1	1:A:468:ASP:OD2	1.86	0.58
1:A:234:HIS:HE1	1:A:262:THR:OG1	1.87	0.58
1:A:399:TRP:CZ3	5:A:1025:SO4:O1	2.59	0.55
7:A:1784:HOH:O	2:B:7:ALA:CB	2.55	0.55
1:A:708:ARG:HD2	1:A:905:ARG:HD2	1.89	0.55
1:A:618:LEU:HD12	1:A:631:TYR:OH	2.07	0.55
2:B:5:ALA:HB2	7:B:101:HOH:O	2.07	0.55
1:A:919:LYS:C	1:A:921:ASN:H	2.09	0.55
1:A:351:ASN:HB2	1:A:354:LEU:O	2.08	0.54
1:A:939:GLU:HG2	7:A:1611:HOH:O	2.07	0.53
1:A:919:LYS:O	1:A:921:ASN:N	2.42	0.53
1:A:622:ASN:H	1:A:654:ASN:ND2	2.06	0.53
1:A:563:LEU:HD11	1:A:570:VAL:CG2	2.39	0.53
1:A:881:TRP:CZ2	1:A:927:PHE:CD1	2.96	0.53
1:A:395:THR:O	1:A:506:ASN:HA	2.10	0.52
1:A:637:ARG:NH2	1:A:640:GLN:HE22	2.07	0.51
1:A:338:GLN:HE22	1:A:381:ILE:HG23	1.76	0.50
1:A:392:ASN:HD22	1:A:392:ASN:N	2.09	0.49
1:A:614:ASP:N	1:A:614:ASP:OD1	2.45	0.49
1:A:708:ARG:NH1	7:A:1312:HOH:O	2.46	0.49
1:A:419:HIS:NE2	5:A:1020:SO4:O2	2.44	0.49
1:A:881:TRP:CH2	1:A:895:PHE:CE2	3.01	0.49
1:A:373:ASN:ND2	1:A:820:ASN:HD22	2.03	0.49
1:A:208:GLN:HE21	1:A:209:SER:CA	2.27	0.48
1:A:888:TYR:CD1	1:A:888:TYR:N	2.81	0.48
2:B:1:ALA:O	2:B:2:ALA:HB3	2.15	0.47
1:A:764:GLN:NE2	1:A:764:GLN:H	2.12	0.47
1:A:754:ILE:HG22	1:A:792:THR:HG21	1.98	0.46
1:A:708:ARG:HD3	7:A:1165:HOH:O	2.15	0.46
1:A:861:ASN:HD21	1:A:898:LEU:HA	1.81	0.46
1:A:587:ILE:HG22	1:A:618:LEU:HB3	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ARG:HG2	1:A:170:MET:HE1	1.99	0.45
1:A:302:ASN:ND2	5:A:1026:SO4:O4	2.39	0.45
1:A:737:TRP:CZ3	1:A:754:ILE:HD11	2.52	0.45
1:A:370:SER:O	1:A:373:ASN:HB3	2.17	0.45
1:A:102:LYS:HG3	7:A:1861:HOH:O	2.17	0.44
2:B:4:ALA:O	2:B:5:ALA:CB	2.66	0.44
7:A:1571:HOH:O	2:B:1:ALA:HB3	2.17	0.43
1:A:208:GLN:HA	1:A:209:SER:HA	1.80	0.43
3:A:1014:NAG:H82	7:A:1863:HOH:O	2.18	0.43
1:A:112:PRO:HD3	1:A:167:PRO:HG3	2.00	0.43
1:A:134:LEU:HG	1:A:142:VAL:HG21	2.00	0.43
1:A:448:HIS:HD2	1:A:449:PRO:O	2.02	0.43
1:A:884:LEU:HA	1:A:888:TYR:CD1	2.54	0.43
1:A:255:GLU:HB3	7:A:1704:HOH:O	2.18	0.43
1:A:881:TRP:CZ2	1:A:895:PHE:CE2	3.07	0.42
1:A:588:LYS:HE2	1:A:611:THR:HG22	2.02	0.42
1:A:286:ASN:HB3	1:A:296:ARG:HG2	2.02	0.42
1:A:106:ARG:NH1	3:A:1004:NAG:O3	2.41	0.42
1:A:618:LEU:CD1	7:A:1215:HOH:O	2.68	0.42
1:A:364:PHE:CE1	1:A:369:SER:HB2	2.54	0.42
1:A:689:TYR:CD1	1:A:748:TYR:HB3	2.54	0.42
1:A:881:TRP:CH2	1:A:895:PHE:CZ	3.08	0.42
1:A:108:LEU:HD12	1:A:109:CYS:N	2.34	0.42
1:A:243:ASN:ND2	1:A:276:ALA:H	2.12	0.41
2:B:4:ALA:O	2:B:5:ALA:HB2	2.21	0.41
1:A:919:LYS:C	1:A:921:ASN:N	2.74	0.41
1:A:432:PRO:HB2	2:B:7:ALA:HB1	2.03	0.41
1:A:387:HIS:HA	1:A:390:PHE:O	2.20	0.41
1:A:803:GLN:NE2	7:A:1768:HOH:O	2.54	0.41
1:A:361:ALA:HA	7:A:1800:HOH:O	2.21	0.40
2:B:1:ALA:C	7:B:104:HOH:O	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	900/907 (99%)	863 (96%)	31 (3%)	6 (1%)	26	21
2	B	5/7 (71%)	0	1 (20%)	4 (80%)	0	0
All	All	905/914 (99%)	863 (95%)	32 (4%)	10 (1%)	17	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	A	894	SER
1	A	920	LYS
2	B	2	ALA
2	B	5	ALA
2	B	6	ALA
2	B	3	ALA
1	A	889	GLY
1	A	924	ASP
1	A	892	SER

### 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	797/802 (99%)	779 (98%)	18 (2%)	58	62

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	206	GLN
1	A	277	TYR
1	A	287	GLU
1	A	335	LYS
1	A	376	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	513	TRP
1	A	568	SER
1	A	644	GLN
1	A	716	LYS
1	A	764	GLN
1	A	815	GLN
1	A	853	LYS
1	A	858	SER
1	A	861	ASN
1	A	867	VAL
1	A	883	LYS
1	A	923	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	A	208	GLN
1	A	234	HIS
1	A	243	ASN
1	A	338	GLN
1	A	367	GLN
1	A	392	ASN
1	A	448	HIS
1	A	654	ASN
1	A	722	GLN
1	A	764	GLN
1	A	796	ASN
1	A	800	GLN
1	A	815	GLN
1	A	820	ASN
1	A	839	ASN
1	A	870	GLN
1	A	897	ASN
1	A	951	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 ⓘ

10 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	1001	1,3	14,14,15	0.54	0	15,19,21	1.03	1 (6%)
3	NAG	A	1002	3	14,14,15	0.55	0	15,19,21	1.46	3 (20%)
3	NAG	A	1004	1,3	14,14,15	0.62	0	15,19,21	1.02	1 (6%)
3	NAG	A	1005	3	14,14,15	0.47	0	15,19,21	2.45	3 (20%)
3	NAG	A	1008	1,3	14,14,15	0.47	0	15,19,21	1.43	1 (6%)
3	NAG	A	1009	3	14,14,15	0.46	0	15,19,21	1.40	1 (6%)
3	NAG	A	1010	1,3	14,14,15	0.50	0	15,19,21	2.13	3 (20%)
3	NAG	A	1011	3	14,14,15	0.51	0	15,19,21	0.97	1 (6%)
3	NAG	A	1013	1,3	14,14,15	0.44	0	15,19,21	1.20	1 (6%)
3	NAG	A	1014	3	14,14,15	0.43	0	15,19,21	1.86	2 (13%)

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	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1002	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1004	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1005	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1008	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1009	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1010	1,3	-	0/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1011	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1013	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1014	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1010	NAG	C2-N2-C7	-3.40	118.68	123.04
3	A	1005	NAG	C6-C5-C4	-2.76	106.21	113.02
3	A	1004	NAG	C2-N2-C7	-2.60	119.69	123.04
3	A	1014	NAG	C4-C3-C2	-2.58	107.21	111.23
3	A	1002	NAG	C2-N2-C7	-2.41	119.94	123.04
3	A	1010	NAG	O3-C3-C4	-2.12	105.58	110.34
3	A	1002	NAG	C3-C4-C5	2.05	113.78	110.20
3	A	1011	NAG	C8-C7-N2	2.27	120.46	116.11
3	A	1001	NAG	C1-O5-C5	2.95	115.99	112.25
3	A	1005	NAG	C3-C4-C5	3.26	115.88	110.20
3	A	1002	NAG	C4-C3-C2	3.70	116.98	111.23
3	A	1013	NAG	C1-O5-C5	3.81	117.09	112.25
3	A	1009	NAG	C1-O5-C5	4.42	117.85	112.25
3	A	1008	NAG	C1-O5-C5	4.84	118.39	112.25
3	A	1014	NAG	C1-O5-C5	5.54	119.28	112.25
3	A	1010	NAG	C1-O5-C5	6.29	120.23	112.25
3	A	1005	NAG	C1-O5-C5	8.23	122.70	112.25

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
3	A	1004	NAG	1	0
3	A	1014	NAG	1	0

## 5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	1003	1	14,14,15	0.34	0	15,19,21	1.56	2 (13%)
4	NAG	A	1006	1	14,14,15	0.52	0	15,19,21	1.01	1 (6%)
4	NAG	A	1007	1	14,14,15	0.50	0	15,19,21	1.58	2 (13%)
4	NAG	A	1012	1	14,14,15	0.48	0	15,19,21	1.20	1 (6%)
4	NAG	A	1015	1	14,14,15	0.48	0	15,19,21	1.16	1 (6%)
5	SO4	A	1016	-	4,4,4	1.73	0	6,6,6	0.54	0
5	SO4	A	1017	-	4,4,4	0.43	0	6,6,6	0.27	0
5	SO4	A	1018	-	4,4,4	0.41	0	6,6,6	0.08	0
5	SO4	A	1019	-	4,4,4	0.48	0	6,6,6	0.48	0
5	SO4	A	1020	-	4,4,4	0.39	0	6,6,6	0.18	0
5	SO4	A	1021	-	4,4,4	0.42	0	6,6,6	0.17	0
5	SO4	A	1022	-	4,4,4	0.41	0	6,6,6	0.16	0
5	SO4	A	1023	-	4,4,4	0.39	0	6,6,6	0.11	0
5	SO4	A	1024	-	4,4,4	0.37	0	6,6,6	0.22	0
5	SO4	A	1025	-	4,4,4	0.55	0	6,6,6	0.54	0
5	SO4	A	1026	-	4,4,4	0.35	0	6,6,6	0.16	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	1003	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1012	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1015	1	-	0/6/23/26	0/1/1/1
5	SO4	A	1016	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1017	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1018	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1019	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1020	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1021	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1022	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	1023	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1024	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1025	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1026	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1007	NAG	C2-N2-C7	-2.23	120.17	123.04
4	A	1006	NAG	C1-O5-C5	2.02	114.82	112.25
4	A	1003	NAG	C2-N2-C7	2.28	125.97	123.04
4	A	1012	NAG	C1-O5-C5	3.32	116.46	112.25
4	A	1015	NAG	C1-O5-C5	3.84	117.12	112.25
4	A	1003	NAG	C1-O5-C5	4.27	117.67	112.25
4	A	1007	NAG	C1-O5-C5	4.78	118.31	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1020	SO4	1	0
5	A	1024	SO4	1	0
5	A	1025	SO4	1	0
5	A	1026	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	901/907 (99%)	-0.06	28 (3%)	52	61	22, 44, 81, 159	0
2	B	7/7 (100%)	5.97	7 (100%)	0	0	31, 39, 65, 72	0
All	All	908/914 (99%)	-0.02	35 (3%)	43	52	22, 44, 81, 159	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	885	PHE	12.1
1	A	889	GLY	11.1
1	A	890	GLY	10.6
2	B	2	ALA	9.5
2	B	3	ALA	8.9
1	A	925	VAL	8.5
1	A	923	MET	7.5
1	A	888	TYR	7.4
1	A	892	SER	6.8
1	A	93	ALA	6.0
1	A	924	ASP	5.8
2	B	5	ALA	5.5
2	B	4	ALA	5.2
2	B	6	ALA	4.6
2	B	1	ALA	4.3
1	A	886	GLN	4.2
1	A	891	GLY	4.1
1	A	882	LYS	4.0
1	A	895	PHE	4.0
1	A	926	GLY	3.9
2	B	7	ALA	3.8
1	A	927	PHE	3.8
1	A	881	TRP	3.6
1	A	884	LEU	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	781	GLU	3.4
1	A	932	ARG	3.3
1	A	893	PHE	3.0
1	A	94	ASP	2.8
1	A	197	ASN	2.7
1	A	922	ASN	2.7
1	A	918	PHE	2.6
1	A	887	ASP	2.6
1	A	949	LYS	2.5
1	A	928	GLY	2.4
1	A	196	GLY	2.3

## 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
3	NAG	A	1001	14/15	0.98	0.13	1.28	35,42,52,55	0
3	NAG	A	1004	14/15	0.98	0.09	0.59	28,34,46,49	0
3	NAG	A	1013	14/15	0.96	0.09	-1.07	51,62,79,80	0
3	NAG	A	1010	14/15	0.97	0.08	-1.74	32,38,45,48	0
3	NAG	A	1002	14/15	0.92	0.27	-	58,76,92,103	0
3	NAG	A	1005	14/15	0.95	0.24	-	51,60,79,91	0
3	NAG	A	1011	14/15	0.92	0.20	-	61,67,85,90	0
3	NAG	A	1008	14/15	0.86	0.20	-	59,73,86,94	0
3	NAG	A	1009	14/15	0.88	0.28	-	43,92,106,117	0
3	NAG	A	1014	14/15	0.82	0.21	-	75,94,101,105	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
5	SO4	A	1023	5/5	0.83	0.49	21.10	106,109,136,136	0
4	NAG	A	1003	14/15	0.95	0.16	11.83	43,53,68,72	0
5	SO4	A	1025	5/5	0.94	0.23	9.59	43,53,82,86	0
5	SO4	A	1019	5/5	0.94	0.19	6.34	70,70,84,89	0
4	NAG	A	1007	14/15	0.92	0.21	3.67	47,55,65,70	0
5	SO4	A	1022	5/5	0.89	0.18	2.50	84,85,106,107	0
5	SO4	A	1017	5/5	0.94	0.11	0.59	74,75,90,94	0
6	ZN	A	1027	1/1	0.86	0.14	-0.59	29,29,29,29	0
5	SO4	A	1018	5/5	0.96	0.11	-0.94	63,73,84,85	0
5	SO4	A	1016	5/5	0.98	0.06	-3.32	53,54,56,71	0
5	SO4	A	1026	5/5	0.94	0.21	-	82,88,94,98	0
5	SO4	A	1020	5/5	0.94	0.18	-	83,83,94,111	0
4	NAG	A	1015	14/15	0.76	0.40	-	94,100,107,114	0
5	SO4	A	1021	5/5	0.91	0.17	-	89,99,104,110	0
5	SO4	A	1024	5/5	0.95	0.10	-	70,88,101,112	0
4	NAG	A	1006	14/15	0.89	0.12	-	49,59,76,81	0
4	NAG	A	1012	14/15	0.87	0.16	-	69,84,94,96	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.