



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:13 PM GMT

PDB ID : 4KXA  
Title : Crystal structure of human aminopeptidase A complexed with aspartate and calcium  
Authors : Yang, Y.; Liu, C.; Lin, Y.Y.; Li, F.  
Deposited on : 2013-05-24  
Resolution : 2.40 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

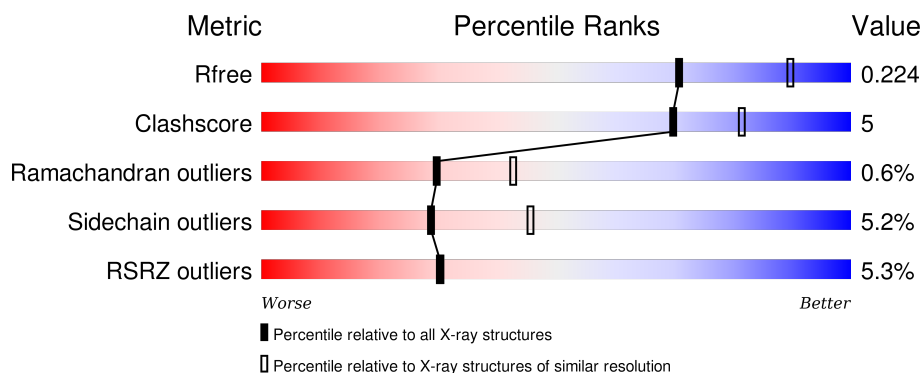
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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>5%</div> <div>84%</div> <div>13% ..</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
7	ASP	A	1019	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7901 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
			7159	4584	1192	1358	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 CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

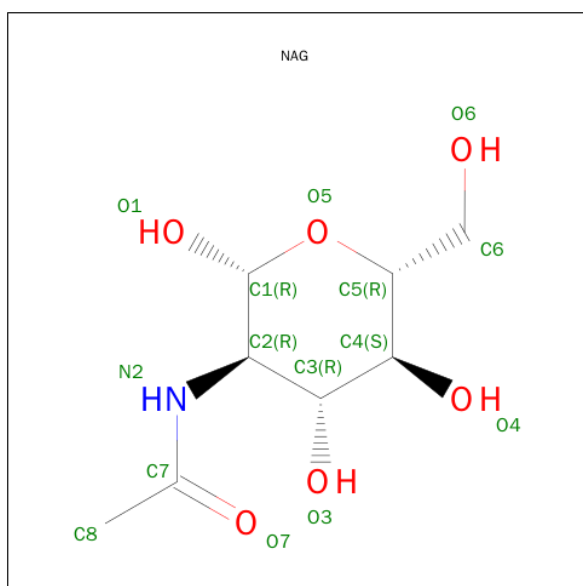
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

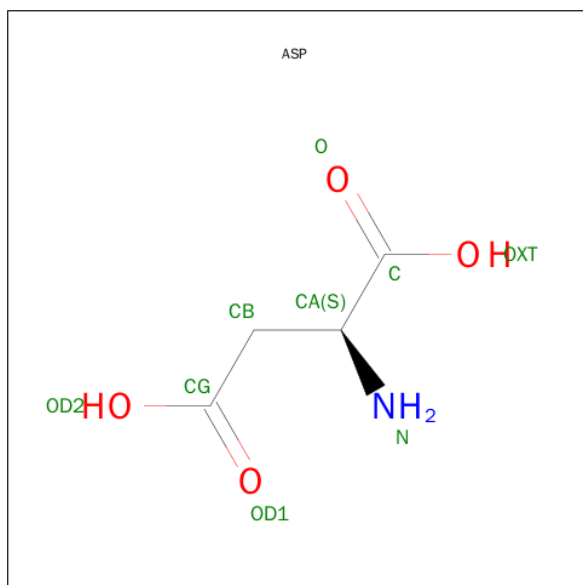


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 7 is ASPARTIC ACID (three-letter code: ASP) (formula:  $C_4H_7NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			9	4	1	4		

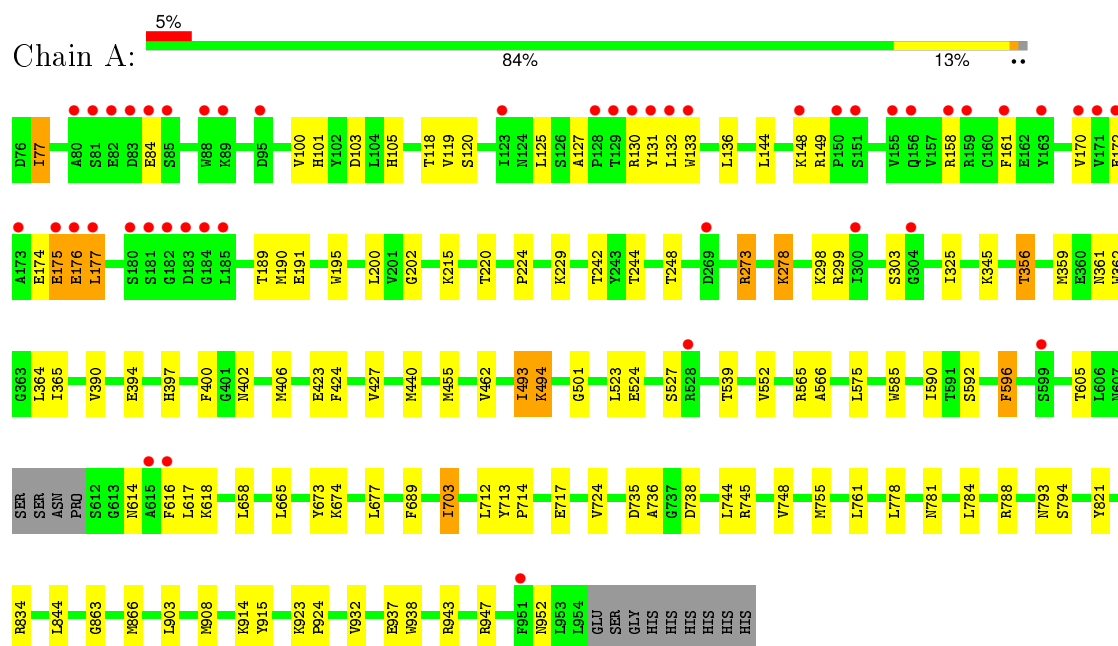
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	507	Total	O	0	0
			507	507		

### 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: Glutamyl aminopeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.09 Å   142.09 Å   237.41 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	48.57 – 2.40 48.57 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.57-2.40) 97.2 (48.57-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.152   ,   0.224 0.156   ,   0.224	Depositor DCC
$R_{free}$ test set	2838 reflections (5.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 54380 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7901	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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, CA, 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	0.35	0/7344	0.54	0/9985

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 [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	7159	0	6949	64	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	112	0	100	0	0
5	A	28	0	26	0	0
6	A	84	0	74	4	0
7	A	9	0	3	1	0
8	A	507	0	0	9	0
All	All	7901	0	7152	66	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 5.

All (66) 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)
6:A:1014:NAG:H3	6:A:1014:NAG:H83	1.54	0.88
1:A:175:GLU:O	1:A:176:GLU:HB3	1.77	0.84
1:A:229:LYS:HE3	8:A:1568:HOH:O	1.82	0.79
1:A:423:GLU:O	1:A:427:VAL:HG12	1.84	0.78
1:A:118:THR:HG22	1:A:191:GLU:HG2	1.64	0.78
1:A:501:GLY:HA3	1:A:523:LEU:HD23	1.65	0.77
6:A:1014:NAG:C8	6:A:1014:NAG:H3	2.16	0.75
1:A:736:ALA:O	1:A:745:ARG:NH1	2.18	0.73
1:A:248:THR:OG1	1:A:273:ARG:HG3	1.91	0.70
1:A:761:LEU:HD22	1:A:793:ASN:HD21	1.54	0.70
1:A:101:HIS:CD2	1:A:242:THR:HG23	2.30	0.66
1:A:361:ASN:HB2	1:A:364:LEU:O	1.96	0.65
1:A:735:ASP:OD1	1:A:781:ASN:HB2	1.96	0.65
1:A:195:TRP:HZ3	8:A:1569:HOH:O	1.80	0.64
1:A:244:THR:HG22	1:A:278:LYS:HA	1.81	0.62
1:A:674:LYS:HD3	6:A:1009:NAG:H62	1.81	0.60
1:A:717:GLU:HG2	1:A:755:MET:O	2.03	0.59
1:A:923:LYS:HG3	8:A:1478:HOH:O	2.02	0.58
1:A:175:GLU:O	1:A:176:GLU:CB	2.51	0.57
1:A:158:ARG:HB2	1:A:174:GLU:HG2	1.87	0.57
1:A:119:VAL:O	1:A:189:THR:HA	2.06	0.56
1:A:273:ARG:HD3	8:A:1499:HOH:O	2.09	0.52
1:A:703:ILE:HD12	1:A:713:TYR:CE2	2.46	0.51
1:A:215:LYS:HE2	8:A:1580:HOH:O	2.12	0.49
1:A:616:PHE:HE1	1:A:618:LYS:HG3	1.76	0.49
1:A:673:TYR:HH	1:A:938:TRP:HE1	1.60	0.49
1:A:149:ARG:HE	1:A:177:LEU:HD21	1.78	0.49
1:A:390:VAL:O	1:A:394:GLU:HG2	2.13	0.48
1:A:937:GLU:HG2	8:A:1449:HOH:O	2.14	0.47
1:A:130:ARG:NH2	1:A:172:GLU:OE1	2.48	0.47
1:A:77:ILE:HD11	1:A:144:LEU:N	2.30	0.47
1:A:713:TYR:HB3	1:A:714:PRO:HD3	1.97	0.46
1:A:131:TYR:CD2	1:A:172:GLU:HB3	2.50	0.46
1:A:105:HIS:HE1	1:A:248:THR:OG1	1.98	0.46
1:A:101:HIS:HD2	1:A:242:THR:HG23	1.75	0.46
1:A:493:ILE:O	1:A:494:LYS:HB2	2.16	0.46
1:A:455:MET:HE2	1:A:566:ALA:HB1	1.98	0.46
1:A:914:LYS:HD3	1:A:915:TYR:CE2	2.51	0.46
1:A:689:PHE:HA	1:A:744:LEU:HD13	1.98	0.46
1:A:424:PHE:CG	1:A:440:MET:HG2	2.52	0.45
1:A:793:ASN:HB3	8:A:1492:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HD21	1:A:127:ALA:O	2.17	0.45
1:A:402:ASN:HD22	1:A:402:ASN:N	2.15	0.44
1:A:943:ARG:HH12	1:A:947:ARG:HH11	1.66	0.44
1:A:359:MET:O	1:A:365:ILE:HG23	2.18	0.44
1:A:397:HIS:HA	1:A:400:PHE:O	2.18	0.44
1:A:585:TRP:CZ2	1:A:592:SER:HB2	2.53	0.43
1:A:161:PHE:CZ	1:A:170:VAL:HB	2.53	0.43
1:A:908:MET:SD	1:A:932:VAL:HG21	2.59	0.43
1:A:616:PHE:CE1	1:A:618:LYS:HG3	2.53	0.43
1:A:596:PHE:CD1	1:A:596:PHE:C	2.93	0.43
1:A:565:ARG:CZ	1:A:937:GLU:HG3	2.49	0.43
1:A:103:ASP:HB2	1:A:120:SER:HB2	2.01	0.43
1:A:133:TRP:CB	1:A:170:VAL:HG22	2.49	0.42
1:A:202:GLY:O	1:A:220:THR:HA	2.18	0.42
1:A:100:VAL:O	1:A:242:THR:HG22	2.19	0.42
1:A:215:LYS:CE	8:A:1580:HOH:O	2.68	0.41
1:A:175:GLU:HG3	1:A:176:GLU:O	2.21	0.41
1:A:585:TRP:CD1	1:A:617:LEU:CD2	3.03	0.41
1:A:952:ASN:HB3	6:A:1010:NAG:O4	2.20	0.41
1:A:863:GLY:HA2	1:A:866:MET:HB2	2.01	0.41
1:A:923:LYS:HB2	1:A:924:PRO:HD3	2.02	0.41
1:A:923:LYS:HA	1:A:923:LYS:HD2	1.91	0.40
1:A:784:LEU:O	1:A:788:ARG:HG3	2.20	0.40
1:A:834:ARG:HD2	8:A:1595:HOH:O	2.20	0.40
1:A:356:THR:HG21	7:A:1019:ASP:CG	2.42	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	873/888 (98%)	839 (96%)	29 (3%)	5 (1%)	30	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	GLU
1	A	552	VAL
1	A	176	GLU
1	A	494	LYS
1	A	224	PRO

### 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%)	746 (95%)	41 (5%)	29 45

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ILE
1	A	84	GLU
1	A	132	LEU
1	A	136	LEU
1	A	148	LYS
1	A	177	LEU
1	A	190	MET
1	A	200	LEU
1	A	273	ARG
1	A	278	LYS
1	A	298	LYS
1	A	299	ARG
1	A	303	SER
1	A	325	ILE
1	A	345	LYS
1	A	356	THR
1	A	362	TRP
1	A	406	MET
1	A	462	VAL
1	A	493	ILE

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Mol	Chain	Res	Type
1	A	524	GLU
1	A	527	SER
1	A	539	THR
1	A	575	LEU
1	A	590	ILE
1	A	596	PHE
1	A	605	THR
1	A	614	ASN
1	A	658	LEU
1	A	665	LEU
1	A	677	LEU
1	A	703	ILE
1	A	712	LEU
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	844	LEU
1	A	903	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	154	GLN
1	A	402	ASN
1	A	415	ASN
1	A	429	HIS
1	A	510	GLN
1	A	570	GLN
1	A	614	ASN
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$
4	NAG	A	1003	1,4	14,14,15	0.51	0	15,19,21	0.98	0
4	NAG	A	1004	4	14,14,15	0.46	0	15,19,21	0.76	0
4	NAG	A	1005	1,4	14,14,15	0.52	0	15,19,21	1.64	3 (20%)
4	NAG	A	1006	4	14,14,15	0.62	0	15,19,21	2.19	2 (13%)
6	NAG	A	1009	1,6	14,14,15	0.54	0	15,19,21	1.41	3 (20%)
6	NAG	A	1010	6	14,14,15	0.80	1 (7%)	15,19,21	1.98	4 (26%)
6	NAG	A	1011	6	14,14,15	0.69	0	15,19,21	0.92	0
6	NAG	A	1012	1,6	14,14,15	0.47	0	15,19,21	0.96	1 (6%)
6	NAG	A	1013	6	14,14,15	0.57	0	15,19,21	1.54	2 (13%)
6	NAG	A	1014	6	14,14,15	1.04	1 (7%)	15,19,21	2.53	6 (40%)
4	NAG	A	1015	1,4	14,14,15	0.64	0	15,19,21	2.23	4 (26%)
4	NAG	A	1016	4	14,14,15	0.49	0	15,19,21	1.05	1 (6%)
4	NAG	A	1017	1,4	14,14,15	0.52	0	15,19,21	0.73	0
4	NAG	A	1018	4	14,14,15	0.45	0	15,19,21	0.82	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	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1004	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1005	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1006	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1009	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1010	6	-	0/6/23/26	0/1/1/1
6	NAG	A	1011	6	-	0/6/23/26	0/1/1/1
6	NAG	A	1012	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1013	6	-	0/6/23/26	0/1/1/1
6	NAG	A	1014	6	-	0/6/23/26	0/1/1/1
4	NAG	A	1015	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1016	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1017	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1018	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1010	NAG	C1-C2	2.08	1.55	1.52
6	A	1014	NAG	O6-C6	2.84	1.54	1.42

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1015	NAG	C4-C3-C2	-3.19	106.27	111.23
6	A	1014	NAG	O7-C7-C8	-2.58	117.33	122.06
6	A	1009	NAG	O7-C7-C8	-2.49	117.49	122.06
6	A	1010	NAG	C6-C5-C4	-2.21	107.57	113.02
4	A	1005	NAG	C8-C7-N2	2.06	120.05	116.11
6	A	1009	NAG	C8-C7-N2	2.17	120.27	116.11
6	A	1012	NAG	C1-O5-C5	2.22	115.06	112.25
6	A	1009	NAG	C2-N2-C7	2.42	126.15	123.04
4	A	1015	NAG	O4-C4-C5	2.59	116.10	109.24
4	A	1016	NAG	C1-O5-C5	2.78	115.77	112.25
6	A	1014	NAG	C3-C4-C5	2.90	115.25	110.20
6	A	1014	NAG	C8-C7-N2	3.06	121.96	116.11
6	A	1013	NAG	C1-O5-C5	3.21	116.32	112.25
6	A	1014	NAG	C1-O5-C5	3.30	116.44	112.25
4	A	1005	NAG	C1-O5-C5	3.39	116.55	112.25
6	A	1013	NAG	C2-N2-C7	3.45	127.47	123.04
6	A	1010	NAG	C4-C3-C2	3.58	116.79	111.23
4	A	1005	NAG	O4-C4-C3	3.60	118.45	110.34
6	A	1010	NAG	C1-O5-C5	3.94	117.24	112.25
6	A	1014	NAG	C4-C3-C2	3.99	117.44	111.23
4	A	1015	NAG	O4-C4-C3	4.10	119.57	110.34
6	A	1010	NAG	C3-C4-C5	4.47	117.99	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1006	NAG	C2-N2-C7	5.03	129.50	123.04
4	A	1015	NAG	C1-O5-C5	5.87	119.70	112.25
4	A	1006	NAG	C1-O5-C5	5.95	119.80	112.25
6	A	1014	NAG	C2-N2-C7	6.41	131.27	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1009	NAG	1	0
6	A	1010	NAG	1	0
6	A	1014	NAG	2	0

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are 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	$\# Z  > 2$
5	NAG	A	1007	1	14,14,15	0.58	0	15,19,21	0.89	1 (6%)
5	NAG	A	1008	1	14,14,15	0.51	0	15,19,21	1.51	1 (6%)
7	ASP	A	1019	-	2,8,8	0.23	0	0,10,10	0.00	-

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	1007	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1008	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ASP	A	1019	-	-	0/2/8/8	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1007	NAG	C4-C3-C2	2.06	114.43	111.23
5	A	1008	NAG	C2-N2-C7	4.32	128.59	123.04

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
7	A	1019	ASP	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	875/888 (98%)	-0.18	46 (5%) 30 30	27, 58, 107, 155	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	ASP	4.8
1	A	84	GLU	4.7
1	A	173	ALA	4.6
1	A	182	GLY	4.6
1	A	185	LEU	4.2
1	A	88	TRP	4.1
1	A	615	ALA	4.1
1	A	175	GLU	3.9
1	A	128	PRO	3.7
1	A	184	GLY	3.6
1	A	82	GLU	3.6
1	A	528	ARG	3.5
1	A	83	ASP	3.5
1	A	89	LYS	3.3
1	A	177	LEU	3.2
1	A	133	TRP	3.1
1	A	123	ILE	3.1
1	A	163	TYR	3.1
1	A	80	ALA	3.1
1	A	85	SER	3.1
1	A	129	THR	3.0
1	A	300	ILE	2.8
1	A	159	ARG	2.8
1	A	161	PHE	2.7
1	A	171	VAL	2.7
1	A	599	SER	2.7
1	A	81	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	170	VAL	2.6
1	A	172	GLU	2.6
1	A	131	TYR	2.6
1	A	130	ARG	2.6
1	A	951	PHE	2.5
1	A	616	PHE	2.5
1	A	132	LEU	2.5
1	A	148	LYS	2.4
1	A	180	SER	2.4
1	A	176	GLU	2.3
1	A	181	SER	2.3
1	A	158	ARG	2.2
1	A	150	PRO	2.1
1	A	156	GLN	2.1
1	A	95	ASP	2.1
1	A	151	SER	2.1
1	A	304	GLY	2.1
1	A	155	VAL	2.0
1	A	269	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
6	NAG	A	1012	14/15	0.98	0.14	0.63	70,91,105,108	0
6	NAG	A	1009	14/15	0.96	0.08	-0.91	79,106,121,122	0
4	NAG	A	1005	14/15	0.94	0.15	-	81,111,127,131	0
6	NAG	A	1011	14/15	0.85	0.25	-	123,160,173,182	0
4	NAG	A	1006	14/15	0.91	0.34	-	102,161,196,205	0
4	NAG	A	1015	14/15	0.96	0.26	-	66,90,112,115	0
6	NAG	A	1014	14/15	0.93	0.21	-	126,160,177,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	1018	14/15	0.91	0.25	-	110,137,156,163	0
6	NAG	A	1013	14/15	0.96	0.20	-	102,120,140,144	0
6	NAG	A	1010	14/15	0.95	0.19	-	112,143,157,159	0
4	NAG	A	1004	14/15	0.87	0.31	-	136,154,174,175	0
4	NAG	A	1003	14/15	0.96	0.13	-	74,103,128,144	0
4	NAG	A	1017	14/15	0.96	0.10	-	58,83,106,115	0
4	NAG	A	1016	14/15	0.92	0.39	-	120,134,157,166	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
7	ASP	A	1019	9/9	0.80	0.35	5.43	75,90,110,122	0
2	CA	A	1001	1/1	0.99	0.17	-0.11	50,50,50,50	1
3	ZN	A	1002	1/1	0.99	0.08	-2.69	103,103,103,103	0
5	NAG	A	1008	14/15	0.84	0.30	-	131,156,172,183	0
5	NAG	A	1007	14/15	0.70	0.31	-	132,159,172,176	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.