



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:24 pm GMT

PDB ID : 2XEI  
Title : Human glutamate carboxypeptidase II in complex with Antibody- Recruiting Molecule ARM-P2  
Authors : Zhang, A.X.; Murelli, R.P.; Barinka, C.; Michel, J.; Cocleaza, A.; Jorgensen, W.L.; Lubkowski, J.; Spiegel, D.A.  
Deposited on : 2010-05-14  
Resolution : 1.69 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

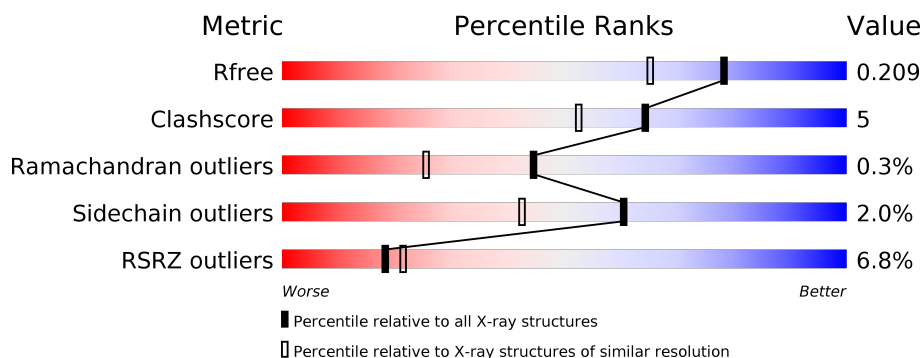
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.69 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	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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	709	<div> <div>7%</div> <div>86%</div> <div>11%</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
4	CL	A	1754	-	-	-	X
5	NAG	A	1756	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	1761	-	-	-	X
7	MAN	A	1766	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6491 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 GLUTAMATE CARBOXYPEPTIDASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	694	Total	C	N	O	S	0	39	0
			5714	3674	957	1062	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ARG	-	EXPRESSION TAG	UNP Q04609
A	43	SER	-	EXPRESSION TAG	UNP Q04609

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

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

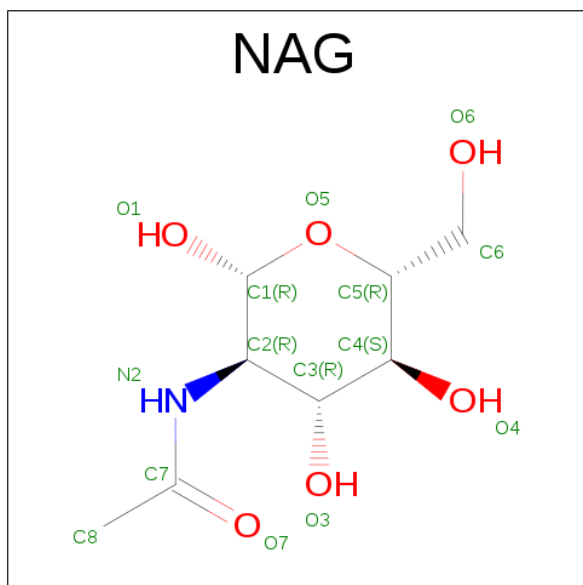
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

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

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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

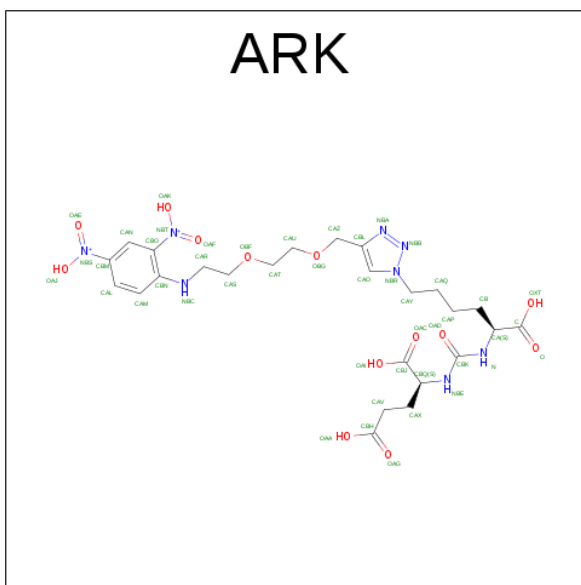


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is N-((1S)-5-[4-({2-[2-({2,4-BIS[HYDROXY(OXO)AMMONIO]PHENYL}AMINO)ETHOXY]ETHOXY}METHYL)-1H-1,2,3-TRIAZOL-1-YL]-1-CARBOXYPENTYL}CARBAMOYL)-L-GLUTAMIC ACID (three-letter code: ARK) (formula:  $C_{25}H_{36}N_8O_{13}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	19	1
			92	50	16	26		

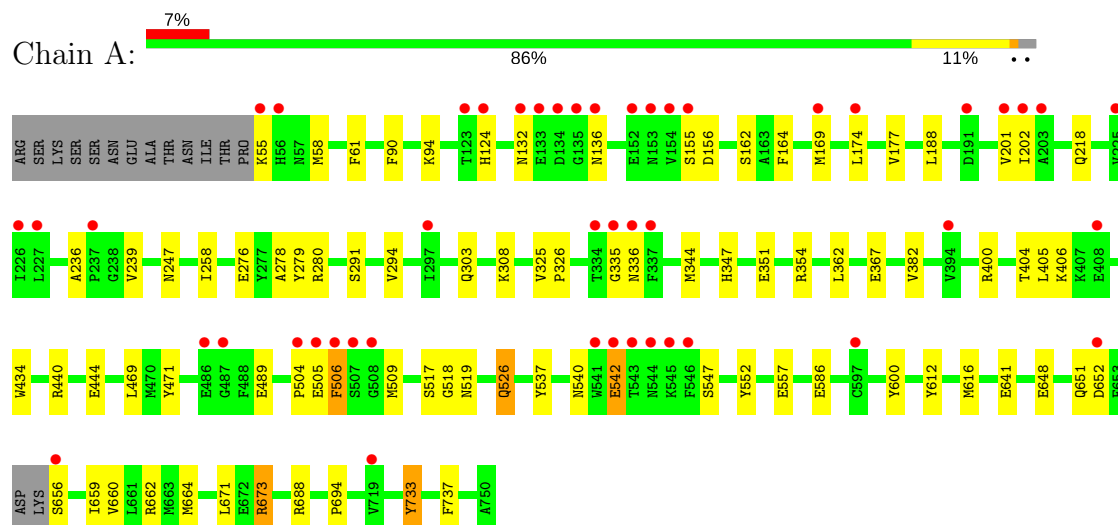
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	505	Total O 505 505	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 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: GLUTAMATE CARBOXYPEPTIDASE 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.50Å 130.04Å 158.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.69 29.49 – 1.69	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.00-1.69) 97.8 (29.49-1.69)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.4.0057	Depositor
R, $R_{free}$	0.159 , 0.185 0.190 , 0.209	Depositor DCC
$R_{free}$ test set	1693 reflections (1.48%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6491	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, CA, ARK, MAN

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	1.02	7/5989 (0.1%)	0.89	7/8113 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	557	GLU	CB-CG	-6.35	1.40	1.52
1	A	526	GLN	CB-CG	6.13	1.69	1.52
1	A	164	PHE	CE2-CZ	5.85	1.48	1.37
1	A	733	TYR	CD1-CE1	5.31	1.47	1.39
1	A	434	TRP	CE3-CZ3	5.08	1.47	1.38
1	A	737	PHE	CD2-CE2	5.07	1.49	1.39
1	A	162	SER	CB-OG	5.06	1.48	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	688[A]	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	688[B]	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	440	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	354	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	A	471	TYR	CB-CG-CD2	-5.58	117.66	121.00
1	A	673	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5714	0	5583	54	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	84	0	75	1	0
6	A	42	0	39	2	0
7	A	50	0	43	0	0
8	A	92	0	66	2	0
9	A	505	0	0	12	1
All	All	6491	0	5806	57	1

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 (57) 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:660[A]:VAL:O	1:A:664[A]:MET:HG2	1.41	1.20
1:A:90[B]:PHE:CZ	1:A:94:LYS:HD2	1.92	1.02
1:A:58:MET:CE	1:A:586:GLU:HG2	2.15	0.76
1:A:656[B]:SER:O	9:A:2402:HOH:O	2.04	0.75
1:A:641:GLU:HG3	9:A:2386:HOH:O	1.89	0.71
1:A:400:ARG:O	1:A:404[B]:THR:HG23	1.92	0.69
1:A:733:TYR:HE2	9:A:2477:HOH:O	1.74	0.69
1:A:308:LYS:HB2	9:A:2202:HOH:O	1.93	0.69
1:A:58:MET:HE1	1:A:586:GLU:HG2	1.75	0.67
1:A:177:VAL:HG12	1:A:188:LEU:HD11	1.77	0.66
1:A:90[B]:PHE:CE2	1:A:94:LYS:HD2	2.31	0.65
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.36	0.60
1:A:504:PRO:HB2	1:A:505:GLU:OE1	2.01	0.60
1:A:278:ALA:HB3	1:A:280[A]:ARG:NH1	2.16	0.60
1:A:155:SER:O	1:A:156:ASP:HB2	2.03	0.58
1:A:58:MET:HE2	1:A:586:GLU:HG2	1.83	0.56
1:A:540:ASN:OD1	1:A:542:GLU:HG3	2.05	0.56
1:A:505:GLU:OE1	1:A:505:GLU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:PHE:HB2	1:A:509:MET:HG3	1.88	0.55
1:A:239[A]:VAL:HG22	1:A:247:ASN:ND2	2.22	0.54
1:A:218[B]:GLN:NE2	1:A:291:SER:OG	2.41	0.53
1:A:276[A]:GLU:HB2	9:A:2165:HOH:O	2.08	0.53
6:A:1757:NAG:H83	9:A:2222:HOH:O	2.07	0.53
8:A:1770[A]:ARK:NBC	8:A:1770[A]:ARK:OAF	2.43	0.51
1:A:367:GLU:OE1	1:A:662[A]:ARG:NH1	2.39	0.51
1:A:648:GLU:O	1:A:651[B]:GLN:HG2	2.11	0.51
1:A:660[A]:VAL:O	1:A:664[A]:MET:CG	2.35	0.50
1:A:552:TYR:CE1	8:A:1770[B]:ARK:HB1C	2.47	0.50
5:A:1761:NAG:H83	9:A:2285:HOH:O	2.14	0.48
1:A:239[A]:VAL:HG22	1:A:247:ASN:CG	2.34	0.48
1:A:132:ASN:HD21	1:A:136:ASN:HD22	1.61	0.48
1:A:90[B]:PHE:CE2	1:A:94:LYS:CD	2.98	0.47
1:A:124:HIS:ND1	6:A:1757:NAG:H61	2.31	0.46
1:A:656[B]:SER:CB	9:A:2402:HOH:O	2.63	0.46
1:A:526:GLN:NE2	9:A:2309:HOH:O	2.43	0.45
1:A:258:ILE:HD13	1:A:294:VAL:HB	1.98	0.45
1:A:656[B]:SER:OG	9:A:2402:HOH:O	2.20	0.45
1:A:506:PHE:HB2	1:A:509:MET:CG	2.47	0.44
1:A:236:ALA:O	1:A:239[A]:VAL:HG13	2.18	0.44
1:A:347:HIS:HE1	9:A:2058:HOH:O	1.99	0.44
1:A:58:MET:HE1	1:A:586:GLU:CG	2.47	0.44
1:A:505:GLU:CB	1:A:506:PHE:CE2	3.02	0.43
1:A:469:LEU:HD21	1:A:671:LEU:HD23	2.00	0.43
1:A:325:VAL:HB	1:A:326:PRO:HD2	2.01	0.43
1:A:659[B]:ILE:HA	1:A:659[B]:ILE:HD12	1.75	0.43
1:A:347:HIS:CE1	9:A:2058:HOH:O	2.72	0.42
1:A:169:MET:HA	1:A:344:MET:O	2.20	0.42
1:A:517:SER:HB2	1:A:694:PRO:HG3	2.00	0.42
1:A:444:GLU:HA	1:A:444:GLU:OE1	2.20	0.42
1:A:489:GLU:CD	1:A:489:GLU:H	2.23	0.42
1:A:61:PHE:HB2	1:A:405[A]:LEU:HD11	2.02	0.41
1:A:174[A]:LEU:HG	1:A:202:ILE:HG22	2.03	0.41
1:A:517:SER:OG	1:A:518:GLY:N	2.52	0.41
1:A:177:VAL:CG1	1:A:201[B]:VAL:HG22	2.52	0.40
1:A:362:LEU:HD11	1:A:406:LYS:HG3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2260:HOH:O	9:A:2478:HOH:O[2_565]	2.19	0.01

## 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	728/709 (103%)	713 (98%)	13 (2%)	2 (0%)	44 25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	VAL
1	A	335	GLY

### 5.3.2 Protein sidechains [i](#)

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	629/605 (104%)	617 (98%)	12 (2%)	62 45

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	303	GLN
1	A	336	ASN
1	A	351	GLU

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Mol	Chain	Res	Type
1	A	506	PHE
1	A	519	ASN
1	A	537	TYR
1	A	542	GLU
1	A	547	SER
1	A	600	TYR
1	A	652	ASP
1	A	673	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	303	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

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	$\# Z  > 2$
5	NAG	A	1755	1,5	14,14,15	0.51	0	15,19,21	1.53	3 (20%)
5	NAG	A	1756	5	14,14,15	0.76	0	15,19,21	1.83	5 (33%)
5	NAG	A	1758	1,5	14,14,15	0.73	0	15,19,21	1.65	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	1761	1,5	14,14,15	0.82	0	15,19,21	1.33	2 (13%)
5	NAG	A	1762	5	14,14,15	0.57	0	15,19,21	1.43	1 (6%)
7	NAG	A	1763	1,7	14,14,15	1.06	1 (7%)	15,19,21	1.51	2 (13%)
7	NAG	A	1764	7	14,14,15	0.86	1 (7%)	15,19,21	1.55	4 (26%)
7	BMA	A	1765	7	11,11,12	0.57	0	13,15,17	1.14	1 (7%)
7	MAN	A	1766	7	11,11,12	0.73	0	13,15,17	1.18	0
5	NAG	A	1767	5	14,14,15	0.52	0	15,19,21	1.31	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
5	NAG	A	1755	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1756	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1758	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1761	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1762	5	-	0/6/23/26	0/1/1/1
7	NAG	A	1763	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1764	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1765	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1766	7	-	0/2/19/22	0/1/1/1
5	NAG	A	1767	5	-	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)
7	A	1764	NAG	O5-C1	-2.19	1.40	1.43
7	A	1763	NAG	C1-C2	2.61	1.56	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1763	NAG	O5-C1-C2	-4.27	105.53	111.47
7	A	1765	BMA	O3-C3-C2	-3.41	103.81	110.02
5	A	1755	NAG	O5-C1-C2	-3.30	106.88	111.47
5	A	1755	NAG	C2-N2-C7	-2.99	118.59	122.94
5	A	1756	NAG	O5-C1-C2	-2.94	107.38	111.47
5	A	1761	NAG	O5-C1-C2	-2.81	107.56	111.47
7	A	1764	NAG	C3-C4-C5	-2.70	105.45	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1758	NAG	O3-C3-C4	-2.53	104.85	110.36
7	A	1764	NAG	O5-C1-C2	-2.42	108.11	111.47
5	A	1755	NAG	O3-C3-C4	-2.34	105.26	110.36
7	A	1764	NAG	C4-C3-C2	-2.23	107.74	111.02
5	A	1758	NAG	O7-C7-C8	-2.20	118.05	122.06
5	A	1756	NAG	O7-C7-C8	-2.13	118.18	122.06
7	A	1764	NAG	O6-C6-C5	-2.12	104.21	111.34
7	A	1763	NAG	C6-C5-C4	-2.09	108.11	113.00
5	A	1758	NAG	O4-C4-C3	-2.07	105.84	110.36
5	A	1767	NAG	O4-C4-C5	2.18	114.79	109.28
5	A	1767	NAG	C1-O5-C5	2.19	115.19	112.17
5	A	1758	NAG	C8-C7-N2	2.22	120.12	116.11
5	A	1756	NAG	C8-C7-N2	2.33	120.32	116.11
5	A	1761	NAG	C2-N2-C7	2.53	126.63	122.94
5	A	1756	NAG	O4-C4-C5	2.73	116.16	109.28
5	A	1762	NAG	C8-C7-N2	2.95	121.44	116.11
5	A	1758	NAG	C1-O5-C5	3.09	116.43	112.17
5	A	1756	NAG	C2-N2-C7	3.14	127.53	122.94

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
5	A	1761	NAG	1	0

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
6	NAG	A	1757	1	14,14,15	0.86	0	15,19,21	1.96	4 (26%)
6	NAG	A	1759	1	14,14,15	0.46	0	15,19,21	1.53	2 (13%)
6	NAG	A	1760	1	14,14,15	0.80	0	15,19,21	2.07	5 (33%)
8	ARK	A	1770[A]	2	34,47,47	3.50	9 (26%)	35,61,61	2.03	11 (31%)
8	ARK	A	1770[B]	-	34,47,47	3.31	7 (20%)	35,61,61	1.86	8 (22%)

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
6	NAG	A	1757	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1759	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1760	1	-	0/6/23/26	0/1/1/1
8	ARK	A	1770[A]	2	-	0/31/47/47	0/2/2/2
8	ARK	A	1770[B]	-	-	0/31/47/47	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1770[A]	ARK	NBA-NBB	-6.99	1.24	1.34
8	A	1770[B]	ARK	NBA-NBB	-6.59	1.25	1.34
8	A	1770[B]	ARK	CBM-NBS	-6.06	1.33	1.45
8	A	1770[A]	ARK	CBM-NBS	-5.73	1.34	1.45
8	A	1770[B]	ARK	NBB-NBR	-4.89	1.24	1.34
8	A	1770[A]	ARK	NBB-NBR	-4.80	1.25	1.34
8	A	1770[A]	ARK	CAZ-CBL	-3.84	1.40	1.50
8	A	1770[B]	ARK	CAZ-CBL	-3.43	1.41	1.50
8	A	1770[A]	ARK	CAO-CBL	-2.05	1.33	1.36
8	A	1770[B]	ARK	CB-CA	2.92	1.57	1.53
8	A	1770[A]	ARK	CB-CA	3.21	1.57	1.53
8	A	1770[A]	ARK	CAX-CBQ	3.88	1.58	1.53
8	A	1770[B]	ARK	OAF-NBT	10.52	1.41	1.22
8	A	1770[B]	ARK	OAE-NBS	10.55	1.42	1.22
8	A	1770[A]	ARK	OAF-NBT	10.97	1.42	1.22
8	A	1770[A]	ARK	OAE-NBS	11.66	1.44	1.22



All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1770[A]	ARK	CB-CA-N	-5.24	102.26	110.22
6	A	1757	NAG	C2-N2-C7	-4.04	117.05	122.94
8	A	1770[A]	ARK	CAX-CBQ-CBJ	-3.97	106.52	112.28
6	A	1760	NAG	O3-C3-C4	-3.58	102.57	110.36
6	A	1757	NAG	C1-C2-N2	-3.13	105.13	110.49
8	A	1770[B]	ARK	CAV-CAX-CBQ	-2.90	107.40	113.19
8	A	1770[B]	ARK	CAO-CBL-NBA	-2.86	107.12	111.41
8	A	1770[A]	ARK	CAY-NBR-CAO	-2.70	123.26	129.76
8	A	1770[A]	ARK	CBO-CBN-NBC	-2.61	118.81	123.53
6	A	1759	NAG	C3-C4-C5	-2.56	105.71	110.22
8	A	1770[A]	ARK	CB-CA-C	-2.45	108.73	112.28
6	A	1760	NAG	C6-C5-C4	-2.43	107.31	113.00
8	A	1770[B]	ARK	CAX-CBQ-CBJ	-2.43	108.76	112.28
6	A	1760	NAG	C1-C2-N2	-2.37	106.43	110.49
6	A	1760	NAG	C2-N2-C7	-2.30	119.58	122.94
8	A	1770[A]	ARK	CAN-CBM-NBS	-2.20	116.93	118.81
8	A	1770[A]	ARK	CAO-CBL-NBA	-2.17	108.16	111.41
8	A	1770[B]	ARK	N-CBK-NBE	2.23	118.42	115.14
6	A	1757	NAG	C8-C7-N2	2.34	120.34	116.11
8	A	1770[B]	ARK	CAL-CBM-NBS	2.41	121.25	119.41
8	A	1770[B]	ARK	CAN-CBO-NBT	2.50	118.72	115.82
8	A	1770[A]	ARK	OAE-NBS-CBM	2.54	122.84	118.80
8	A	1770[A]	ARK	OBG-CAZ-CBL	2.68	118.77	110.95
6	A	1757	NAG	C1-O5-C5	2.90	116.17	112.17
8	A	1770[A]	ARK	NBA-NBB-NBR	3.93	110.28	107.31
6	A	1759	NAG	C1-O5-C5	4.13	117.86	112.17
6	A	1760	NAG	C1-O5-C5	4.45	118.30	112.17
8	A	1770[B]	ARK	OBG-CAZ-CBL	4.76	124.83	110.95
8	A	1770[A]	ARK	CAL-CBM-NBS	5.11	123.30	119.41
8	A	1770[B]	ARK	NBA-NBB-NBR	6.07	111.89	107.31

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	1757	NAG	2	0
8	A	1770[A]	ARK	1	0
8	A	1770[B]	ARK	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	694/709 (97%)	0.17	47 (6%) 18 21	14, 25, 46, 71	1 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	506	PHE	5.3
1	A	507	SER	4.9
1	A	545	LYS	4.8
1	A	546	PHE	4.7
1	A	544	ASN	4.7
1	A	719	VAL	4.5
1	A	155	SER	4.4
1	A	55	LYS	4.4
1	A	656[A]	SER	4.2
1	A	153	ASN	4.1
1	A	542	GLU	4.0
1	A	226	ILE	3.7
1	A	134	ASP	3.6
1	A	652	ASP	3.5
1	A	201[A]	VAL	3.5
1	A	505	GLU	3.5
1	A	123	THR	3.4
1	A	541	TRP	3.4
1	A	136	ASN	3.3
1	A	56	HIS	3.2
1	A	336	ASN	3.2
1	A	227	LEU	3.2
1	A	154	VAL	3.2
1	A	543	THR	2.9
1	A	202	ILE	2.9
1	A	135	GLY	2.9
1	A	237	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	152	GLU	2.8
1	A	335	GLY	2.8
1	A	169	MET	2.7
1	A	504	PRO	2.7
1	A	225	VAL	2.7
1	A	124	HIS	2.6
1	A	394	VAL	2.6
1	A	487	GLY	2.6
1	A	508	GLY	2.6
1	A	486	GLU	2.5
1	A	174[A]	LEU	2.4
1	A	191	ASP	2.3
1	A	334	THR	2.3
1	A	337	PHE	2.2
1	A	597	CYS	2.2
1	A	203	ALA	2.1
1	A	408	GLU	2.1
1	A	133	GLU	2.1
1	A	297	ILE	2.1
1	A	132	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
5	NAG	A	1756	14/15	0.64	0.25	7.38	44,53,58,62	0
5	NAG	A	1761	14/15	0.89	0.13	4.27	27,30,39,44	0
7	MAN	A	1766	11/12	0.91	0.19	2.64	46,50,53,54	0
5	NAG	A	1758	14/15	0.88	0.14	1.58	38,40,46,52	0
7	NAG	A	1763	14/15	0.92	0.09	0.77	20,27,36,46	0
5	NAG	A	1755	14/15	0.94	0.10	-	32,40,46,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	A	1764	14/15	0.90	0.23	-	36,39,48,51	0
7	BMA	A	1765	11/12	0.90	0.16	-	35,38,42,43	0
5	NAG	A	1762	14/15	0.89	0.21	-	37,42,49,49	0
5	NAG	A	1767	14/15	0.83	0.28	-	56,61,67,68	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
4	CL	A	1754	1/1	0.99	0.17	2.09	8,8,8,8	0
8	ARK	A	1770[B]	46/46	0.92	0.17	1.98	14,33,54,54	46
6	NAG	A	1757	14/15	0.76	0.27	1.83	47,55,63,63	0
3	CA	A	1753	1/1	1.00	0.08	1.66	5,5,5,5	0
8	ARK	A	1770[A]	46/46	0.92	0.17	1.02	15,61,70,72	46
2	ZN	A	1751	1/1	0.99	0.13	0.30	7,7,7,7	0
2	ZN	A	1752	1/1	1.00	0.12	-0.80	6,6,6,6	0
6	NAG	A	1760	14/15	0.89	0.15	-	27,49,51,56	0
6	NAG	A	1759	14/15	0.81	0.21	-	59,65,70,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.