



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:05 pm GMT

PDB ID : 2C6P  
Title : MEMBRANE-BOUND GLUTAMATE CARBOXYPEPTIDASE II (GCPII)  
IN COMPLEX WITH PHOSPHATE ANION  
Authors : Mesters, J.R.; Barinka, C.; Li, W.; Tsukamoto, T.; Majer, P.; Slusher, B.S.;  
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Deposited on : 2005-11-11  
Resolution : 2.39 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

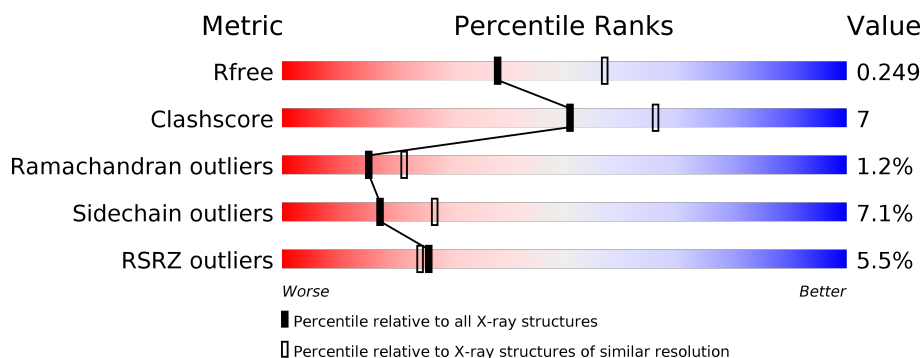
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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	707	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>.</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5374 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 II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	677	Total	C	N	O	S	0	0	0
			5155	3313	856	970	16			

- 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		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

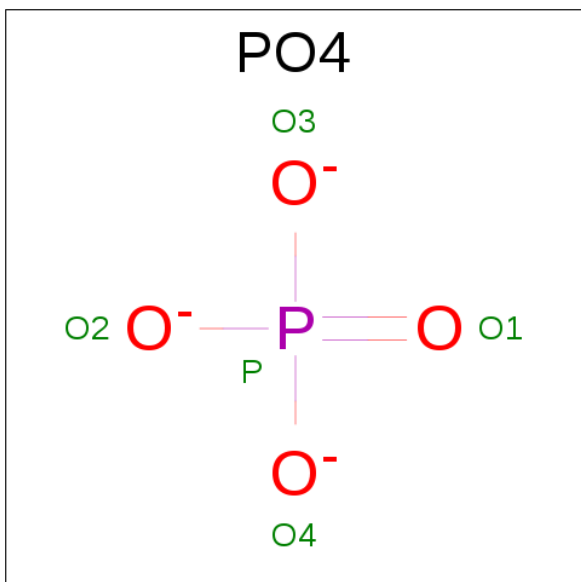


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

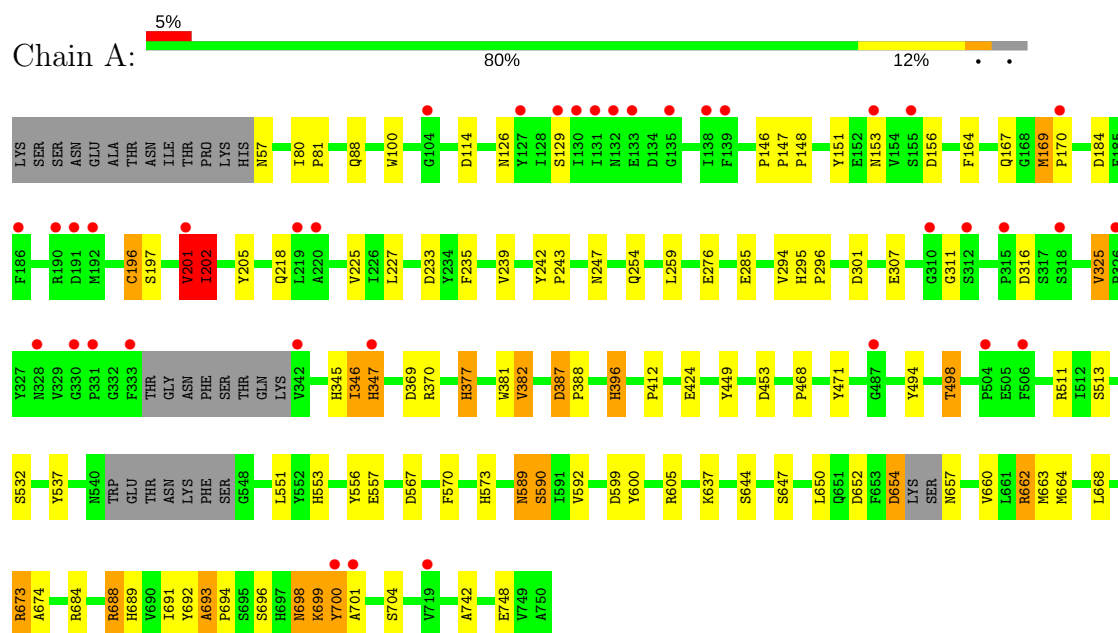
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	87	Total	O	0	0
			87	87		

### 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 II



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.57Å 130.37Å 159.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.14 – 2.39 47.18 – 2.39	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.14-2.39) 97.3 (47.18-2.39)	Depositor EDS
$R_{merge}$	0.00	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.198 , 0.251 0.203 , 0.249	Depositor DCC
$R_{free}$ test set	1067 reflections (2.65%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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, PO4, CA

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	0.77	0/5299	0.89	19/7204 (0.3%)

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
1	A	0	3

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	662	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	A	369	ASP	CB-CG-OD2	7.04	124.64	118.30
1	A	202	ILE	N-CA-C	6.85	129.50	111.00
1	A	301	ASP	CB-CG-OD2	6.73	124.35	118.30
1	A	370	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	688	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	A	233	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	316	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	599	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	662	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	673	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	114	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	387	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	201	VAL	C-N-CA	5.58	135.66	121.70
1	A	156	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	370	ARG	NE-CZ-NH2	-5.23	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	184	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	652	ASP	CB-CG-OD2	5.07	122.87	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	VAL	Peptide
1	A	346	ILE	Peptide
1	A	699	LYS	Peptide

## 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	5155	0	4747	66	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	56	0	50	0	0
6	A	28	0	26	0	0
7	A	39	0	34	0	0
8	A	5	0	0	0	0
9	A	87	0	0	12	1
All	All	5374	0	4857	66	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 7.

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)
1:A:377:HIS:CE1	1:A:388:PRO:HB3	1.96	0.99
1:A:692:TYR:O	1:A:693:ALA:CB	2.10	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ASP:C	9:A:2059:HOH:O	2.06	0.91
1:A:377:HIS:HD2	1:A:424:GLU:CG	1.85	0.90
1:A:654:ASP:HB2	9:A:2060:HOH:O	1.73	0.88
1:A:377:HIS:CD2	1:A:424:GLU:HB3	2.15	0.81
1:A:692:TYR:O	1:A:693:ALA:HB3	1.86	0.76
1:A:377:HIS:HD2	1:A:424:GLU:CD	1.92	0.73
1:A:692:TYR:O	1:A:693:ALA:HB2	1.90	0.71
1:A:657:ASN:CB	9:A:2059:HOH:O	2.39	0.69
1:A:295:HIS:ND1	1:A:296:PRO:HD2	2.08	0.69
1:A:377:HIS:HD2	1:A:424:GLU:CB	2.05	0.69
1:A:377:HIS:HE1	1:A:388:PRO:HB3	1.58	0.69
1:A:377:HIS:CD2	1:A:424:GLU:CB	2.77	0.68
1:A:494:TYR:O	1:A:498:THR:CG2	2.43	0.66
1:A:657:ASN:HB3	9:A:2059:HOH:O	1.94	0.66
1:A:377:HIS:CD2	1:A:424:GLU:CD	2.70	0.65
1:A:657:ASN:N	9:A:2059:HOH:O	2.32	0.62
1:A:377:HIS:CE1	1:A:388:PRO:CB	2.78	0.61
1:A:494:TYR:O	1:A:498:THR:HG23	2.01	0.61
1:A:377:HIS:CD2	1:A:424:GLU:CG	2.77	0.61
1:A:688:ARG:HD3	9:A:2073:HOH:O	2.00	0.59
1:A:657:ASN:ND2	1:A:660:VAL:HG23	2.16	0.59
1:A:377:HIS:ND1	1:A:388:PRO:HB3	2.15	0.59
1:A:654:ASP:CB	9:A:2060:HOH:O	2.38	0.59
1:A:654:ASP:N	1:A:654:ASP:OD1	2.37	0.58
1:A:377:HIS:ND1	1:A:388:PRO:HG3	2.20	0.57
1:A:100:TRP:HE1	1:A:396:HIS:HD2	1.50	0.56
1:A:126:ASN:OD1	1:A:347:HIS:HB2	2.05	0.56
1:A:494:TYR:O	1:A:498:THR:HG22	2.05	0.55
1:A:345:HIS:CG	9:A:2015:HOH:O	2.60	0.54
1:A:205:TYR:CE1	1:A:254:GLN:HB3	2.44	0.52
1:A:377:HIS:CD2	1:A:424:GLU:OE1	2.63	0.52
1:A:567:ASP:OD2	1:A:570:PHE:HA	2.11	0.50
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.92	0.50
1:A:227:LEU:O	1:A:296:PRO:HA	2.10	0.50
1:A:381:TRP:HD1	1:A:553:HIS:CD2	2.31	0.48
1:A:699:LYS:HB3	9:A:2042:HOH:O	2.12	0.48
1:A:164:PHE:CE2	1:A:259:LEU:HD11	2.47	0.48
1:A:126:ASN:OD1	1:A:346:ILE:HA	2.13	0.48
1:A:689:HIS:HD2	1:A:691:ILE:H	1.62	0.48
1:A:201:VAL:O	1:A:225:VAL:HA	2.15	0.47
1:A:307:GLU:HA	1:A:325:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:LYS:HA	9:A:2075:HOH:O	2.14	0.47
1:A:377:HIS:ND1	1:A:388:PRO:CB	2.79	0.46
1:A:650:LEU:HA	1:A:664:MET:CE	2.45	0.46
1:A:704:SER:HA	9:A:2076:HOH:O	2.16	0.46
1:A:80:ILE:HD12	1:A:88:GLN:HG2	1.97	0.46
1:A:235:PHE:HA	1:A:247:ASN:OD1	2.15	0.45
1:A:468:PRO:HA	1:A:471:TYR:CE1	2.52	0.45
1:A:225:VAL:HB	1:A:294:VAL:HG22	1.97	0.45
1:A:412:PRO:HA	1:A:589:ASN:OD1	2.18	0.45
1:A:449:TYR:O	1:A:532:SER:HA	2.17	0.44
1:A:225:VAL:O	1:A:294:VAL:HA	2.18	0.44
1:A:148:PRO:HG2	1:A:151:TYR:CD2	2.53	0.43
1:A:169:MET:N	1:A:170:PRO:CD	2.82	0.43
1:A:242:TYR:CG	1:A:243:PRO:HA	2.53	0.43
1:A:387:ASP:HA	1:A:388:PRO:HA	1.86	0.43
1:A:81:PRO:HA	1:A:382:VAL:O	2.19	0.43
1:A:674:ALA:HB1	1:A:742:ALA:HA	2.01	0.41
1:A:196:CYS:O	1:A:197:SER:C	2.58	0.41
1:A:590:SER:OG	1:A:592:VAL:O	2.37	0.40
1:A:694:PRO:HA	9:A:2075:HOH:O	2.21	0.40
1:A:146:PRO:HA	1:A:147:PRO:HD2	1.95	0.40
1:A:657:ASN:HD22	1:A:660:VAL:CG2	2.35	0.40
1:A:684:ARG:NH2	1:A:694:PRO:O	2.49	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:2020:HOH:O	9:A:2083:HOH:O[2_565]	2.02	0.18

## 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	669/707 (95%)	620 (93%)	41 (6%)	8 (1%)	15	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	ILE
1	A	693	ALA
1	A	698	ASN
1	A	701	ALA
1	A	311	GLY
1	A	347	HIS
1	A	700	TYR
1	A	382	VAL

### 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	504/603 (84%)	468 (93%)	36 (7%)	17	27

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	129	SER
1	A	153	ASN
1	A	167	GLN
1	A	169	MET
1	A	196	CYS
1	A	202	ILE
1	A	218	GLN
1	A	239	VAL
1	A	276	GLU
1	A	285	GLU
1	A	325	VAL
1	A	377	HIS

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Mol	Chain	Res	Type
1	A	396	HIS
1	A	498	THR
1	A	511	ARG
1	A	513	SER
1	A	537	TYR
1	A	557	GLU
1	A	573	HIS
1	A	589	ASN
1	A	590	SER
1	A	600	TYR
1	A	605	ARG
1	A	637	LYS
1	A	644	SER
1	A	647	SER
1	A	654	ASP
1	A	662	ARG
1	A	663	MET
1	A	668	LEU
1	A	673	ARG
1	A	696	SER
1	A	698	ASN
1	A	700	TYR
1	A	748	GLU

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	82	HIS
1	A	112	HIS
1	A	347	HIS
1	A	377	HIS
1	A	396	HIS
1	A	573	HIS
1	A	657	ASN
1	A	689	HIS
1	A	697	HIS
1	A	698	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 ⓘ

7 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	0.40	0	15,19,21	1.73	4 (26%)
5	NAG	A	1756	5	14,14,15	0.69	0	15,19,21	2.22	7 (46%)
5	NAG	A	1759	1,5	14,14,15	0.80	0	15,19,21	1.33	2 (13%)
5	NAG	A	1760	5	14,14,15	0.60	0	15,19,21	0.91	0
7	NAG	A	1761	1,7	14,14,15	0.76	1 (7%)	15,19,21	1.34	2 (13%)
7	NAG	A	1762	7	14,14,15	0.72	0	15,19,21	2.36	8 (53%)
7	BMA	A	1763	7	11,11,12	0.92	0	13,15,17	1.54	2 (15%)

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	1759	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1760	5	-	0/6/23/26	0/1/1/1
7	NAG	A	1761	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1762	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1763	7	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1761	NAG	O5-C1	-2.51	1.39	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1755	NAG	O5-C1-C2	-4.21	105.61	111.47
7	A	1762	NAG	C4-C3-C2	-4.14	104.95	111.02
7	A	1761	NAG	O5-C1-C2	-3.62	106.44	111.47
5	A	1759	NAG	O4-C4-C3	-2.80	104.26	110.36
7	A	1762	NAG	O5-C1-C2	-2.67	107.75	111.47
5	A	1755	NAG	O4-C4-C3	-2.66	104.57	110.36
5	A	1759	NAG	O5-C1-C2	-2.64	107.80	111.47
5	A	1756	NAG	O5-C1-C2	-2.47	108.03	111.47
7	A	1763	BMA	O2-C2-C3	-2.39	105.49	110.17
5	A	1756	NAG	O7-C7-C8	-2.15	118.14	122.06
7	A	1762	NAG	O7-C7-C8	-2.01	118.39	122.06
5	A	1755	NAG	O6-C6-C5	2.29	119.06	111.34
7	A	1761	NAG	C1-O5-C5	2.44	115.53	112.17
5	A	1756	NAG	C1-O5-C5	2.45	115.55	112.17
7	A	1762	NAG	O4-C4-C3	2.51	115.83	110.36
5	A	1756	NAG	C2-N2-C7	2.65	126.81	122.94
7	A	1762	NAG	C8-C7-N2	2.74	121.06	116.11
5	A	1756	NAG	C3-C4-C5	2.77	115.09	110.22
5	A	1755	NAG	C1-O5-C5	2.85	116.09	112.17
7	A	1762	NAG	C1-C2-N2	2.91	115.45	110.49
7	A	1762	NAG	O3-C3-C4	3.45	117.87	110.36
5	A	1756	NAG	C4-C3-C2	3.82	116.62	111.02
7	A	1762	NAG	C1-O5-C5	3.95	117.60	112.17
5	A	1756	NAG	C8-C7-N2	3.98	123.29	116.11
7	A	1763	BMA	C1-C2-C3	4.18	114.95	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 4 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	$\# Z  > 2$
6	NAG	A	1757	1	14,14,15	0.90	0	15,19,21	1.99	4 (26%)
6	NAG	A	1758	1	14,14,15	0.64	0	15,19,21	2.14	1 (6%)
8	PO4	A	1764	2	4,4,4	1.01	0	6,6,6	0.79	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
6	NAG	A	1757	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1758	1	-	0/6/23/26	0/1/1/1
8	PO4	A	1764	2	-	0/0/0/0	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(°)
6	A	1757	NAG	O5-C1-C2	-2.83	107.53	111.47
6	A	1757	NAG	O3-C3-C4	2.22	115.19	110.36
6	A	1757	NAG	C1-C2-N2	3.16	115.89	110.49
6	A	1757	NAG	C1-O5-C5	4.47	118.32	112.17
6	A	1758	NAG	C1-O5-C5	6.83	121.58	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	677/707 (95%)	0.10	37 (5%) 26 24	23, 44, 86, 100	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	700	TYR	6.5
1	A	153	ASN	4.3
1	A	219	LEU	3.9
1	A	220	ALA	3.9
1	A	719	VAL	3.9
1	A	190	ARG	3.7
1	A	191	ASP	3.6
1	A	342	VAL	3.6
1	A	310	GLY	3.5
1	A	333	PHE	3.5
1	A	186	PHE	3.4
1	A	133	GLU	3.4
1	A	129	SER	3.4
1	A	132	ASN	3.2
1	A	138	ILE	3.0
1	A	155	SER	2.8
1	A	347	HIS	2.8
1	A	326	PRO	2.7
1	A	328	ASN	2.6
1	A	315	PRO	2.6
1	A	104	GLY	2.5
1	A	139	PHE	2.5
1	A	318	SER	2.4
1	A	487	GLY	2.4
1	A	170	PRO	2.3
1	A	331	PRO	2.3
1	A	701	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	127	TYR	2.2
1	A	312	SER	2.2
1	A	130	ILE	2.2
1	A	330	GLY	2.2
1	A	135	GLY	2.1
1	A	131	ILE	2.1
1	A	201	VAL	2.1
1	A	192	MET	2.1
1	A	506	PHE	2.0
1	A	504	PRO	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	1759	14/15	0.93	0.11	-0.58	52,55,59,61	0
7	NAG	A	1761	14/15	0.97	0.08	-1.93	34,40,52,57	0
5	NAG	A	1760	14/15	0.93	0.10	-	63,67,69,70	0
5	NAG	A	1755	14/15	0.94	0.18	-	53,57,61,67	0
7	BMA	A	1763	11/12	0.83	0.13	-	75,77,79,79	0
7	NAG	A	1762	14/15	0.93	0.12	-	63,69,71,73	0
5	NAG	A	1756	14/15	0.79	0.30	-	71,78,80,81	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	0.51	35,35,35,35	0
2	ZN	A	1752	1/1	0.99	0.13	-0.78	30,30,30,30	0
8	PO4	A	1764	5/5	0.99	0.12	-0.96	35,38,41,41	0
2	ZN	A	1751	1/1	1.00	0.11	-1.28	30,30,30,30	0
3	CA	A	1753	1/1	1.00	0.09	-1.34	25,25,25,25	0
6	NAG	A	1758	14/15	0.82	0.20	-	53,69,73,73	0
6	NAG	A	1757	14/15	0.72	0.25	-	74,77,79,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.