



# Full wwPDB X-ray Structure Validation Report

May 14, 2014 – 10:31 AM EDT

PDB ID : 4OC0  
Title : X-ray structure of of human glutamate carboxypeptidase II (GCPII) in a complex with CCIBzL, a urea-based inhibitor N 2 -[(1-carboxycyclopropyl)carbamoyl]-N 6 -(4-iodobenzoyl)-L-lysine  
Authors : Pavlicek, J.; Ptacek, J.; Cerny, J.; Byun, Y.; Skultetyova, L.; Pomper, M.; Lubkowski, J.; Barinka, C.  
Deposited on : 2014-01-08  
Resolution : 1.85 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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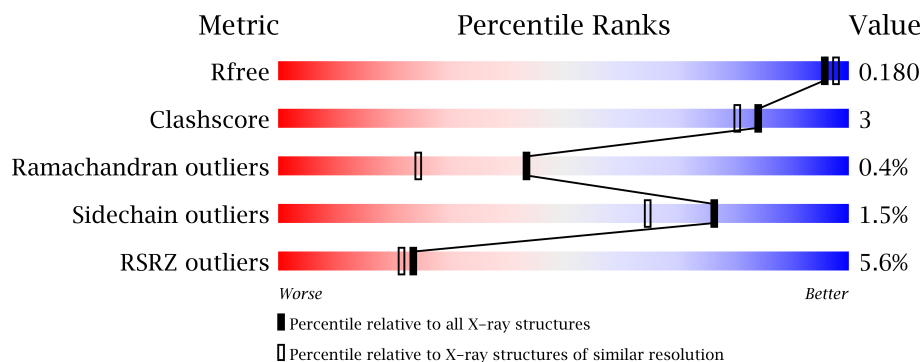
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22978

# 1 Overall quality at a glance


The reported resolution of this entry is 1.85 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))
$R_{free}$	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	709	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	806	-	X
3	NAG	A	807	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6490 atoms, of which 0 are hydrogen and 0 are deuterium.

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	64	0
			5832	3758	969	1082	23			

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

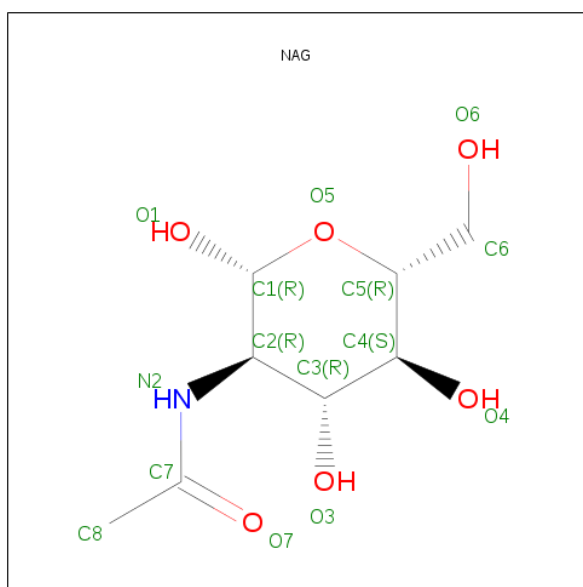
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

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

There are 6 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
A	42	ARG	-	EXPRESSION TAG	UNP Q04609
A	43	SER	-	EXPRESSION TAG	UNP Q04609
A	42	ARG	-	EXPRESSION TAG	UNP Q04609
A	43	SER	-	EXPRESSION TAG	UNP Q04609

- Molecule 3 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
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

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

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

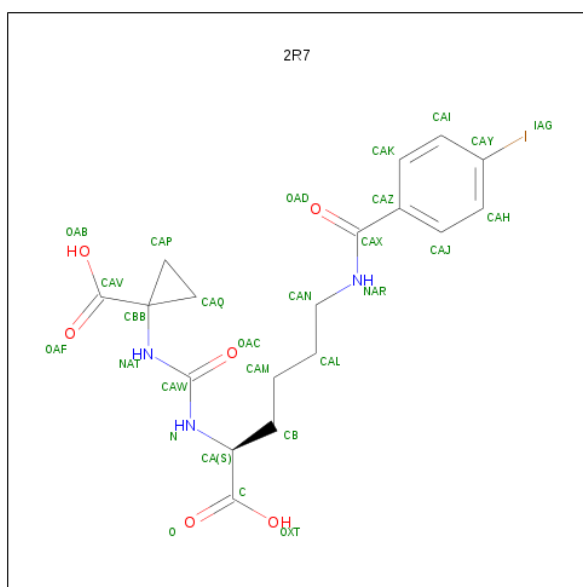
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is N 2 -[(1-CARBOXYCYCLOPROPYL)CARBAMOYL]-N 6 -(4-IODOBENZ OYL)-L-LYSINE (three-letter code: 2R7) (formula: C<sub>18</sub>H<sub>22</sub>IN<sub>3</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C I N O 28 18 1 3 6	0	0

- Molecule 9 is water.

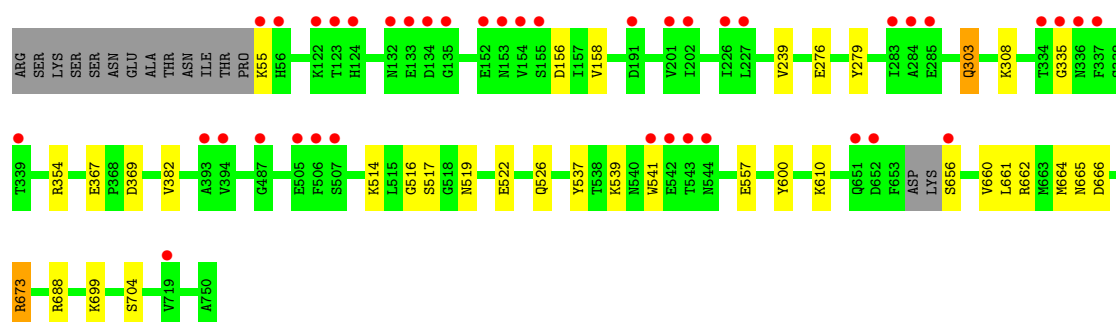
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	450	Total O 450 450	0	0

### 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 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 ( $RSRZ > 2$ ). 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

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.38Å 129.94Å 158.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.47 – 1.85 28.47 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (28.47-1.85) 99.2 (28.47-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.161 , 0.181 0.162 , 0.180	Depositor DCC
$R_{free}$ test set	1319 reflections (1.51%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 50.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 88925 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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.

## 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, 2R7, 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	0.91	2/6167 (0.0%)	0.78	1/8344 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	VAL	CB-CG1	6.73	1.67	1.52
1	A	557	GLU	CB-CG	-5.43	1.41	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	ARG	NE-CZ-NH2	-5.23	117.68	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5832	0	0	17	2
2	A	84	0	75	1	0
3	A	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	50	0	43	0	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	28	0	0	0	0
9	A	450	0	0	8	2
All	All	6490	0	157	18	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (18) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:688[B]:ARG:NH1	9:A:1236:HOH:O	2.02	0.90
1:A:660[A]:VAL:O	1:A:664[A]:MET:CG	2.36	0.73
1:A:276[B]:GLU:CG	9:A:1066:HOH:O	2.36	0.73
2:A:802:NAG:H81	9:A:1138:HOH:O	1.95	0.64
1:A:516:GLY:O	1:A:526[B]:GLN:NE2	2.33	0.62
1:A:517:SER:OG	1:A:522[A]:GLU:OE2	2.18	0.61
1:A:688[B]:ARG:NH1	9:A:969:HOH:O	2.35	0.60
1:A:308:LYS:NZ	9:A:1226:HOH:O	2.37	0.58
1:A:369:ASP:OD2	1:A:662[B]:ARG:NH2	2.44	0.51
1:A:367:GLU:OE1	1:A:662[A]:ARG:NH1	2.46	0.49
1:A:303:GLN:NE2	9:A:1061:HOH:O	2.46	0.49
1:A:610:LYS:NZ	9:A:1075:HOH:O	2.46	0.48
1:A:276[A]:GLU:OE2	1:A:354:ARG:NH2	2.51	0.44
1:A:514[B]:LYS:CE	1:A:704[B]:SER:OG	2.66	0.43
1:A:661[A]:LEU:O	1:A:665:ASN:N	2.51	0.43
1:A:699:LYS:NZ	9:A:1350:HOH:O	2.52	0.42

All (2) 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	Distance(Å)	Clash(Å)
1:A:656[B]:SER:O	9:A:1216:HOH:O[4_566]	2.09	0.11
1:A:666:ASP:OD2	9:A:939:HOH:O[2_565]	2.14	0.06

## 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	750/709 (106%)	732 (98%)	15 (2%)	3 (0%)	43 24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	541	TRP
1	A	335	GLY
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	652/605 (108%)	642 (98%)	10 (2%)	76 65

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	156	ASP
1	A	239[A]	VAL
1	A	239[B]	VAL
1	A	303	GLN
1	A	519	ASN
1	A	537	TYR
1	A	539[A]	LYS
1	A	600	TYR
1	A	673	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z  > 2$
2	NAG	A	801	1,2	12,14,15	0.78	0	15,19,21	1.51	3 (20%)
2	NAG	A	802	2	12,14,15	0.84	0	15,19,21	1.47	2 (13%)
2	NAG	A	804	1,2	12,14,15	0.90	1 (8%)	15,19,21	1.17	2 (13%)
2	NAG	A	805	2	12,14,15	0.60	0	15,19,21	0.94	0
2	NAG	A	808	1,2	12,14,15	1.19	2 (16%)	15,19,21	1.84	3 (20%)
2	NAG	A	809	2	12,14,15	0.58	0	15,19,21	1.31	3 (20%)
4	NAG	A	810	1,4	12,14,15	0.75	0	15,19,21	1.22	2 (13%)
4	NAG	A	811	4	12,14,15	0.87	1 (8%)	15,19,21	1.85	5 (33%)
4	BMA	A	812	4	10,11,12	0.48	0	11,15,17	1.06	1 (9%)
4	MAN	A	813	4	10,11,12	0.81	0	11,15,17	1.89	2 (18%)

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
2	NAG	A	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	802	2	-	0/6/23/26	0/1/1/1
2	NAG	A	804	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	805	2	-	0/6/23/26	0/1/1/1
2	NAG	A	808	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	809	2	-	0/6/23/26	0/1/1/1
4	NAG	A	810	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	811	4	-	0/6/23/26	0/1/1/1
4	BMA	A	812	4	-	0/2/19/22	0/1/1/1
4	MAN	A	813	4	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	811	NAG	O5-C5	-2.58	1.41	1.45
2	A	808	NAG	O7-C7	2.27	1.28	1.23
2	A	804	NAG	O5-C5	-2.21	1.42	1.45
2	A	808	NAG	O5-C5	-2.04	1.42	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	808	NAG	O5-C5-C4	-5.35	103.86	110.65
4	A	813	MAN	O5-C5-C6	5.04	112.27	106.98
4	A	811	NAG	C3-C4-C5	-3.51	103.87	110.17
2	A	801	NAG	O5-C5-C6	3.26	110.40	106.98
2	A	809	NAG	O5-C5-C6	3.17	110.31	106.98
4	A	810	NAG	C6-C5-C4	-2.95	105.83	113.04
2	A	802	NAG	O5-C5-C4	-2.88	107.00	110.65
2	A	802	NAG	C3-C2-N2	-2.81	107.41	111.62
4	A	811	NAG	O5-C5-C6	2.81	109.93	106.98
4	A	813	MAN	O3-C3-C2	2.70	114.65	109.74
2	A	801	NAG	C3-C2-N2	-2.68	107.61	111.62
2	A	808	NAG	O4-C4-C3	-2.61	104.52	110.36
2	A	808	NAG	C3-C2-N2	-2.54	107.82	111.62
2	A	801	NAG	O4-C4-C3	-2.52	104.73	110.36
4	A	811	NAG	C2-N2-C7	-2.47	120.40	123.39
4	A	812	BMA	O3-C3-C2	-2.39	105.41	109.74
2	A	809	NAG	O7-C7-C8	-2.35	117.55	122.04
4	A	810	NAG	C2-N2-C7	-2.26	120.66	123.39
4	A	811	NAG	O4-C4-C3	2.19	115.25	110.36
2	A	804	NAG	C3-C2-N2	-2.18	108.35	111.62
2	A	809	NAG	C8-C7-N2	2.18	120.23	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	804	NAG	O4-C4-C3	-2.13	105.60	110.36
4	A	811	NAG	C8-C7-N2	2.04	119.97	116.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	NAG	A	803	1	12,14,15	0.74	0	15,19,21	1.69	2 (13%)
3	NAG	A	806	1	12,14,15	0.50	0	15,19,21	1.61	2 (13%)
3	NAG	A	807	1	12,14,15	0.76	0	15,19,21	1.32	2 (13%)
8	2R7	A	818	-	29,29,29	2.12	7 (24%)	40,40,40	2.34	11 (27%)

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	803	1	-	0/6/23/26	0/1/1/1
3	NAG	A	806	1	-	0/6/23/26	0/1/1/1
3	NAG	A	807	1	-	0/6/23/26	0/1/1/1
8	2R7	A	818	-	-	0/31/35/35	0/1/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	818	2R7	CAQ-CBB	-6.94	1.43	1.51
8	A	818	2R7	CAY-IAG	3.96	2.21	2.10
8	A	818	2R7	CAZ-CAX	3.68	1.57	1.50
8	A	818	2R7	CBB-CAV	-3.46	1.44	1.53
8	A	818	2R7	O-C	2.47	1.30	1.22
8	A	818	2R7	CAI-CAK	2.34	1.43	1.38
8	A	818	2R7	CB-CA	2.16	1.58	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	818	2R7	CAQ-CBB-CAV	6.70	130.81	117.11
8	A	818	2R7	CAQ-CAP-CBB	-5.51	56.39	60.60
8	A	818	2R7	CB-CA-N	-4.94	100.73	110.94
8	A	818	2R7	CAV-CBB-NAT	-4.63	107.60	116.72
3	A	806	NAG	O5-C5-C6	4.54	111.74	106.98
8	A	818	2R7	CAP-CBB-NAT	-4.51	112.65	117.36
3	A	803	NAG	O5-C5-C6	4.40	111.59	106.98
8	A	818	2R7	CAI-CAY-CAH	-3.32	115.33	120.66
3	A	807	NAG	O5-C5-C6	3.04	110.17	106.98
8	A	818	2R7	CAP-CBB-CAQ	2.80	62.09	58.80
8	A	818	2R7	OAF-CAV-CBB	-2.64	116.37	122.88
8	A	818	2R7	CA-N-CAW	2.46	126.59	120.98
3	A	807	NAG	C2-N2-C7	-2.36	120.53	123.39
3	A	803	NAG	C2-N2-C7	-2.30	120.61	123.39
3	A	806	NAG	C6-C5-C4	-2.25	107.53	113.04
8	A	818	2R7	CAJ-CAH-CAY	2.17	122.89	119.56
8	A	818	2R7	CAI-CAY-IAG	2.01	122.73	119.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	694/709 (97%)	0.09	40 (5%)	22 20	20, 33, 57, 77	1 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	ASN	5.2
1	A	55	LYS	5.0
1	A	541	TRP	5.0
1	A	152	GLU	4.8
1	A	543	THR	4.4
1	A	135	GLY	4.2
1	A	719	VAL	4.1
1	A	133	GLU	4.1
1	A	335	GLY	4.0
1	A	134	ASP	3.7
1	A	505	GLU	3.6
1	A	542	GLU	3.5
1	A	124	HIS	3.5
1	A	202	ILE	3.4
1	A	656[A]	SER	3.3
1	A	123	THR	3.3
1	A	334	THR	3.2
1	A	132	ASN	3.1
1	A	201[A]	VAL	3.0
1	A	56	HIS	3.0
1	A	336	ASN	2.9
1	A	122	LYS	2.9
1	A	191	ASP	2.9
1	A	227	LEU	2.9
1	A	155	SER	2.6
1	A	285	GLU	2.6
1	A	226	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	506	PHE	2.6
1	A	154	VAL	2.6
1	A	337	PHE	2.5
1	A	284	ALA	2.5
1	A	652	ASP	2.4
1	A	394	VAL	2.3
1	A	507	SER	2.3
1	A	283[A]	ILE	2.3
1	A	487	GLY	2.2
1	A	393	ALA	2.1
1	A	651[A]	GLN	2.1
1	A	339	THR	2.0
1	A	544	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	802	14/15	0.29	5.19	47,59,62,66	0
2	NAG	A	801	14/15	0.12	2.87	37,46,52,54	0
2	NAG	A	808	14/15	0.13	2.51	34,37,42,44	0
4	MAN	A	813	11/12	0.26	1.94	53,57,61,61	0
2	NAG	A	805	14/15	0.38	1.73	64,67,73,73	0
2	NAG	A	804	14/15	0.14	1.06	45,50,53,59	0
4	NAG	A	811	14/15	0.23	0.64	43,49,57,59	0
2	NAG	A	809	14/15	0.22	0.14	42,48,51,56	0
4	BMA	A	812	11/12	0.18	0.11	49,51,53,54	0
4	NAG	A	810	14/15	0.08	-0.39	27,32,43,51	0



## 6.4 Ligands

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	806	14/15	0.34	4.72	66,74,78,78	0
3	NAG	A	807	14/15	0.19	2.47	37,54,63,63	0
3	NAG	A	803	14/15	0.36	1.76	50,59,63,64	0
8	2R7	A	818	28/28	0.12	-0.20	31,43,53,55	0
6	CA	A	816	1/1	0.07	-0.53	21,21,21,21	0
7	CL	A	817	1/1	0.10	-0.84	29,29,29,29	0
5	ZN	A	815	1/1	0.08	-2.08	25,25,25,25	0
5	ZN	A	814	1/1	0.08	-6.56	27,27,27,27	0

## 6.5 Other polymers

There are no such residues in this entry.