



Full wwPDB X-ray Structure Validation Report i

May 14, 2014 – 12:11 AM EDT

PDB ID : 4OC2
Title : X-ray structure of of human glutamate carboxypeptidase II (GCPII) in a complex with CEIBzL, a urea-based inhibitor N 2 -{[(1S)-1-carboxybut-3-yn-1-yl] carbamoyl}-N 6 -(4-iodobenzoyl)-L-lysine
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Deposited on : 2014-01-08
Resolution : 1.65 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

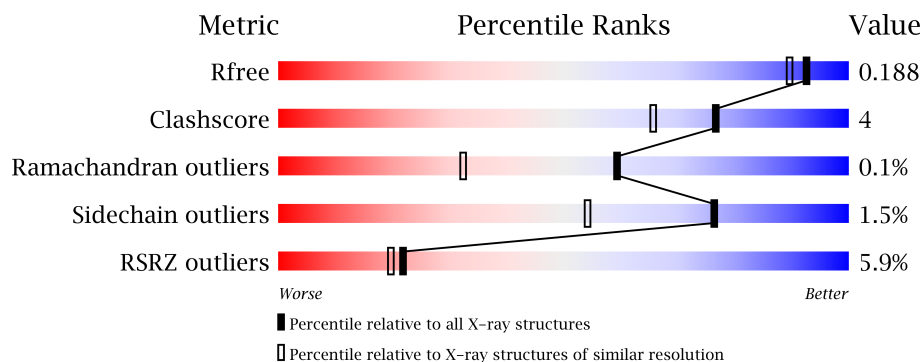
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.65 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	1404 (1.68-1.64)
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)
RSRZ outliers	66119	1404 (1.68-1.64)

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 ≥ 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
5	NAG	A	808	-	X
5	NAG	A	809	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 6674 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	62	0
			5900	3793	988	1096	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		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			24	14	1	9		

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

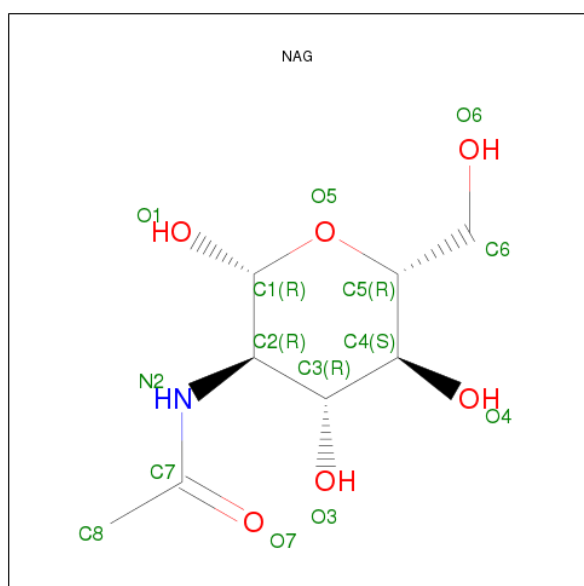
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			38	22	2	14		

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 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
			39	22	2	15		

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 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		

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

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

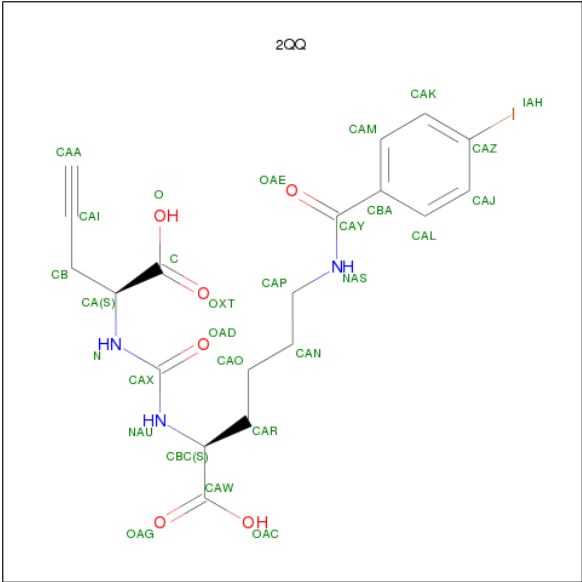
- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 11 is N 2 -{[(1S)-1-CARBOXYBUT-3-YN-1-YL]CARBAMOYL}-N 6 -(4-IO DOB ENZOYL)-L-LYSINE (three-letter code: 2QQ) (formula: C₁₉H₂₂IN₃O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	I	N	O	0	0
			29	19	1	3	6		

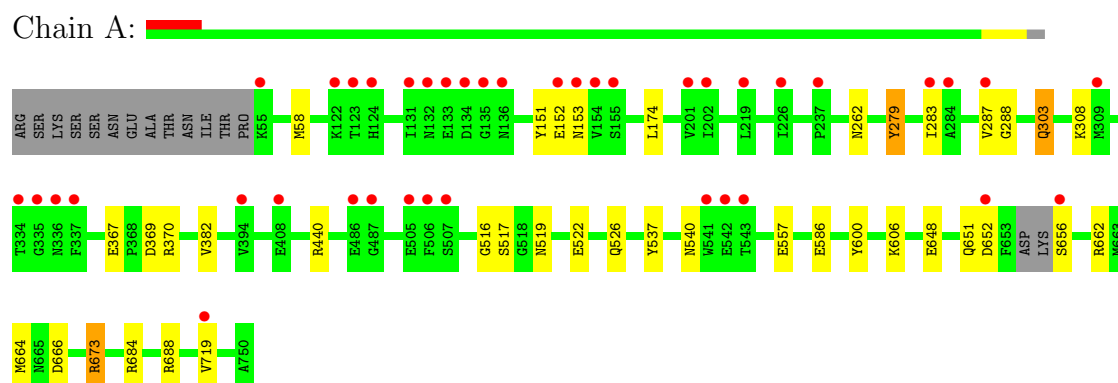
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	534	Total	O	0	1
			534	534		

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



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.34Å 130.25Å 159.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.47 – 1.65 29.47 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.47-1.65) 98.3 (29.47-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.165 , 0.188 0.166 , 0.188	Depositor DCC
R_{free} test set	2494 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 124081 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6674	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, 2QQ, FUC, 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	0.87	2/6179 (0.0%)	0.83	6/8365 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	557	GLU	CB-CG	-5.78	1.41	1.52
1	A	664	MET	CB-CG	5.28	1.68	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	A	370	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	440	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	684[A]	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	A	684[B]	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	A	673	ARG	NE-CZ-NH2	-5.55	117.53	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	5900	0	0	22	1
2	A	28	0	25	1	0
3	A	24	0	22	0	0
4	A	38	0	34	1	0
5	A	28	0	26	0	0
6	A	39	0	34	0	0
7	A	50	0	43	0	0
8	A	2	0	0	0	0
9	A	1	0	0	0	0
10	A	1	0	0	0	0
11	A	29	0	0	0	0
12	A	534	0	0	10	3
All	All	6674	0	184	24	3

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 4.

All (24) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:151[A]:TYR:O	1:A:153:ASN:N	1.94	1.00
1:A:648:GLU:O	1:A:651[B]:GLN:NE2	2.03	0.91
1:A:606[B]:LYS:N	1:A:606[B]:LYS:CD	2.51	0.70
1:A:606[B]:LYS:CE	12:A:1400:HOH:O	2.44	0.66
4:A:806:NAG:H83	12:A:1221:HOH:O	1.99	0.62
1:A:606[B]:LYS:CG	12:A:1400:HOH:O	2.52	0.58
1:A:283[B]:ILE:C	1:A:283[B]:ILE:CD1	2.74	0.56
1:A:262[B]:ASN:ND2	1:A:287:VAL:CG1	2.70	0.55
1:A:516:GLY:O	1:A:526[B]:GLN:NE2	2.40	0.54
1:A:308:LYS:NZ	12:A:1370:HOH:O	2.42	0.53
1:A:517:SER:OG	1:A:522:GLU:OE2	2.25	0.52
1:A:651[B]:GLN:NE2	1:A:652:ASP:CG	2.64	0.51
1:A:688[B]:ARG:CZ	12:A:1008:HOH:O	2.58	0.51
1:A:369:ASP:OD2	1:A:662[B]:ARG:NH2	2.43	0.51
1:A:688[B]:ARG:NH2	12:A:968:HOH:O	2.46	0.47
1:A:666:ASP:OD2	12:A:1111:HOH:O	2.19	0.47
1:A:656[B]:SER:O	1:A:656[B]:SER:OG	2.33	0.46
1:A:58:MET:CE	1:A:586:GLU:CG	2.93	0.46
1:A:367:GLU:OE1	1:A:662[A]:ARG:NH1	2.51	0.43
1:A:288:GLY:N	12:A:1416:HOH:O	2.52	0.42
1:A:303:GLN:NE2	12:A:1061:HOH:O	2.51	0.42
1:A:283[B]:ILE:O	1:A:283[B]:ILE:CD1	2.67	0.42
2:A:802:NAG:H81	12:A:1138:HOH:O	2.21	0.41

All (3) 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)
12:A:1111:HOH:O	12:A:1365:HOH:O[2_565]	1.98	0.22
12:A:1225:HOH:O	12:A:1359:HOH:O[2_565]	2.05	0.15
1:A:152:GLU:OE2	12:A:1335:HOH:O[7_545]	2.18	0.02

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%)	729 (97%)	20 (3%)	1 (0%)	59 32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	641 (98%)	11 (2%)	73 48

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	LEU
1	A	279[A]	TYR
1	A	279[B]	TYR
1	A	303	GLN

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Mol	Chain	Res	Type
1	A	519	ASN
1	A	537	TYR
1	A	540	ASN
1	A	600	TYR
1	A	673	ARG
1	A	719[A]	VAL
1	A	719[B]	VAL

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 ⓘ

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	$\# Z > 2$
2	NAG	A	801	1,2	12,14,15	0.82	1 (8%)	15,19,21	1.74	3 (20%)
2	NAG	A	802	2	12,14,15	0.83	0	15,19,21	1.49	2 (13%)
3	NAG	A	803	1,3	12,14,15	0.59	0	15,19,21	1.48	2 (13%)
3	FUC	A	804	3	9,10,11	0.82	0	10,14,16	0.65	0
4	NAG	A	805	1,4	12,14,15	0.94	1 (8%)	15,19,21	1.51	3 (20%)
4	NAG	A	806	4	12,14,15	0.43	0	15,19,21	1.87	4 (26%)
4	FUC	A	807	4	9,10,11	0.80	0	10,14,16	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	810	1,6	12,14,15	1.41	3 (25%)	15,19,21	1.58	4 (26%)
6	NAG	A	811	6	12,14,15	0.64	0	15,19,21	1.31	3 (20%)
6	BMA	A	812	6	10,11,12	0.67	0	11,15,17	1.22	2 (18%)
7	NAG	A	813	1,7	12,14,15	0.83	0	15,19,21	1.21	3 (20%)
7	NAG	A	814	7	12,14,15	0.62	0	15,19,21	1.85	4 (26%)
7	BMA	A	815	7	10,11,12	0.49	0	11,15,17	1.18	1 (9%)
7	MAN	A	816	7	10,11,12	0.73	0	11,15,17	1.82	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
3	NAG	A	803	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	804	3	-	0/0/17/20	0/1/1/1
4	NAG	A	805	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	806	4	-	0/6/23/26	0/1/1/1
4	FUC	A	807	4	-	0/0/17/20	0/1/1/1
6	NAG	A	810	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	811	6	-	0/6/23/26	0/1/1/1
6	BMA	A	812	6	-	0/2/19/22	0/1/1/1
7	NAG	A	813	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	814	7	-	0/6/23/26	0/1/1/1
7	BMA	A	815	7	-	0/2/19/22	0/1/1/1
7	MAN	A	816	7	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	810	NAG	O7-C7	2.80	1.30	1.23
6	A	810	NAG	C2-N2	2.68	1.49	1.46
4	A	805	NAG	O5-C5	-2.14	1.42	1.45
6	A	810	NAG	O5-C5	-2.10	1.42	1.45
2	A	801	NAG	O5-C5	-2.08	1.42	1.45

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	816	MAN	O5-C5-C6	5.37	112.61	106.98
4	A	806	NAG	O5-C5-C6	3.95	111.12	106.98
2	A	801	NAG	C2-N2-C7	-3.88	118.70	123.39
3	A	803	NAG	O5-C5-C6	3.82	110.99	106.98
2	A	801	NAG	O5-C5-C6	3.62	110.78	106.98
4	A	806	NAG	C2-N2-C7	3.45	127.57	123.39
7	A	814	NAG	C3-C4-C5	-3.40	104.07	110.17
2	A	802	NAG	C3-C2-N2	-3.36	106.58	111.62
2	A	802	NAG	C2-N2-C7	3.30	127.39	123.39
4	A	805	NAG	O5-C5-C6	3.27	110.41	106.98
7	A	814	NAG	C2-N2-C7	-3.25	119.47	123.39
6	A	810	NAG	O5-C5-C4	-3.19	106.61	110.65
4	A	805	NAG	C3-C2-N2	-3.04	107.06	111.62
4	A	806	NAG	C8-C7-N2	2.90	121.61	116.12
6	A	810	NAG	O4-C4-C3	-2.73	104.25	110.36
6	A	810	NAG	C3-C2-N2	-2.65	107.66	111.62
6	A	812	BMA	O5-C5-C4	2.53	113.86	110.65
7	A	814	NAG	C8-C7-N2	2.44	120.72	116.12
6	A	811	NAG	O5-C5-C6	2.42	109.52	106.98
7	A	813	NAG	C6-C5-C4	-2.37	107.25	113.04
2	A	801	NAG	O3-C3-C4	-2.37	105.07	110.36
4	A	806	NAG	O7-C7-C8	-2.31	117.62	122.04
7	A	814	NAG	O5-C5-C4	-2.30	107.73	110.65
7	A	813	NAG	C2-N2-C7	-2.22	120.71	123.39
7	A	815	BMA	O5-C5-C4	-2.21	107.85	110.65
7	A	813	NAG	O4-C4-C5	-2.20	103.43	109.25
6	A	810	NAG	C2-N2-C7	2.17	126.02	123.39
6	A	812	BMA	C3-C4-C5	2.13	114.00	110.17
6	A	811	NAG	C2-N2-C7	-2.13	120.82	123.39
7	A	816	MAN	O3-C3-C2	2.10	113.56	109.74
6	A	811	NAG	O4-C4-C5	-2.04	103.86	109.25
4	A	805	NAG	O5-C5-C4	-2.03	108.08	110.65
3	A	803	NAG	O3-C3-C2	-2.01	105.07	109.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	$\# Z > 2$
5	NAG	A	808	1	12,14,15	0.65	0	15,19,21	1.18	1 (6%)
5	NAG	A	809	1	12,14,15	0.72	0	15,19,21	2.08	3 (20%)
11	2QQ	A	821	8	29,29,29	1.93	6 (20%)	37,37,37	2.24	10 (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
5	NAG	A	808	1	-	0/6/23/26	0/1/1/1
5	NAG	A	809	1	-	0/6/23/26	0/1/1/1
11	2QQ	A	821	8	-	0/30/31/31	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	821	2QQ	CAZ-IAH	6.11	2.26	2.10
11	A	821	2QQ	CBA-CAY	4.63	1.59	1.50
11	A	821	2QQ	CAK-CAM	2.80	1.44	1.38
11	A	821	2QQ	CAJ-CAL	2.49	1.43	1.38
11	A	821	2QQ	CA-C	2.36	1.58	1.52
11	A	821	2QQ	CAM-CBA	2.31	1.43	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	821	2QQ	CAJ-CAZ-CAK	-6.78	109.76	120.66
5	A	809	NAG	O5-C5-C6	6.33	113.62	106.98
11	A	821	2QQ	CAK-CAZ-IAH	5.29	127.70	119.69
11	A	821	2QQ	CAL-CBA-CAM	-4.33	112.64	118.62
11	A	821	2QQ	CAM-CAK-CAZ	4.08	125.83	119.56
11	A	821	2QQ	CAL-CAJ-CAZ	3.90	125.55	119.56
5	A	808	NAG	O5-C5-C4	3.29	114.83	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	809	NAG	C3-C4-C5	-3.03	104.74	110.17
11	A	821	2QQ	CAJ-CAL-CBA	2.74	123.98	120.76
11	A	821	2QQ	CA-CB-CAI	2.54	117.36	113.58
11	A	821	2QQ	CA-N-CAX	-2.51	115.25	120.98
11	A	821	2QQ	CAR-CBC-NAU	-2.38	106.00	110.94
11	A	821	2QQ	OAE-CAY-NAS	-2.05	118.18	122.55
5	A	809	NAG	O7-C7-C8	-2.02	118.17	122.04

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, 95th 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 ²)	Q<0.9
1	A	694/709 (97%)	0.15	40 (5%)	22 20	16, 28, 51, 71	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	TRP	6.8
1	A	719[A]	VAL	5.8
1	A	55	LYS	5.4
1	A	153	ASN	5.4
1	A	506	PHE	5.2
1	A	335	GLY	4.8
1	A	287	VAL	4.8
1	A	505	GLU	4.6
1	A	133	GLU	4.5
1	A	136	ASN	4.4
1	A	135	GLY	4.4
1	A	656[A]	SER	4.4
1	A	542	GLU	4.3
1	A	334	THR	4.1
1	A	336	ASN	4.0
1	A	152	GLU	3.9
1	A	543	THR	3.8
1	A	155	SER	3.8
1	A	237	PRO	3.7
1	A	132	ASN	3.7
1	A	134	ASP	3.5
1	A	154	VAL	3.5
1	A	131[A]	ILE	3.3
1	A	337	PHE	3.2
1	A	201[A]	VAL	3.2
1	A	202	ILE	3.1
1	A	283[A]	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	486[A]	GLU	2.8
1	A	507[A]	SER	2.8
1	A	652	ASP	2.7
1	A	123	THR	2.6
1	A	124	HIS	2.5
1	A	122	LYS	2.4
1	A	226	ILE	2.4
1	A	487	GLY	2.4
1	A	394	VAL	2.3
1	A	219	LEU	2.2
1	A	408	GLU	2.2
1	A	284	ALA	2.2
1	A	309[A]	MET	2.1

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, 95th 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 ²)	Q<0.9
3	FUC	A	804	10/11	0.46	22.24	63,66,67,69	0
4	FUC	A	807	10/11	0.53	18.46	55,60,62,63	0
6	BMA	A	812	11/12	0.34	4.64	47,49,54,57	0
2	NAG	A	802	14/15	0.36	4.02	37,47,50,52	0
7	NAG	A	814	14/15	0.29	3.19	35,39,49,50	0
2	NAG	A	801	14/15	0.09	3.14	30,39,45,48	0
3	NAG	A	803	14/15	0.30	2.85	40,46,53,59	0
6	NAG	A	810	14/15	0.13	2.84	26,28,37,40	0
4	NAG	A	805	14/15	0.16	2.70	35,40,46,46	0
7	MAN	A	816	11/12	0.23	1.96	41,44,50,53	0
4	NAG	A	806	14/15	0.38	1.93	49,52,55,57	0
7	NAG	A	813	14/15	0.11	1.51	21,27,35,43	0
7	BMA	A	815	11/12	0.19	0.70	37,39,42,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	A	811	14/15	0.21	0.44	33,39,44,45	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, 95th 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(\AA^2)	Q<0.9
5	NAG	A	808	14/15	0.31	10.69	53,61,64,65	0
5	NAG	A	809	14/15	0.18	2.97	31,44,52,53	0
10	CL	A	820	1/1	0.15	0.44	26,26,26,26	0
9	CA	A	819	1/1	0.05	-0.10	17,17,17,17	0
11	2QQ	A	821	29/29	0.09	-0.51	22,28,43,44	0
8	ZN	A	818	1/1	0.04	-2.73	22,22,22,22	0
8	ZN	A	817	1/1	0.08	-4.51	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.