



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2014 – 05:08 PM EDT

PDB ID : 4OC3
Title : X-ray structure of of human glutamate carboxypeptidase II (GCPII) in a complex with CFIBzL, a urea-based inhibitor N 2 -{[(1S)-1-carboxy-2-(furan-2-yl)ethyl]carbamoyl}-N 6 -(4-iodobenzoyl)-L-lysine
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Deposited on : 2014-01-08
Resolution : 1.79 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>

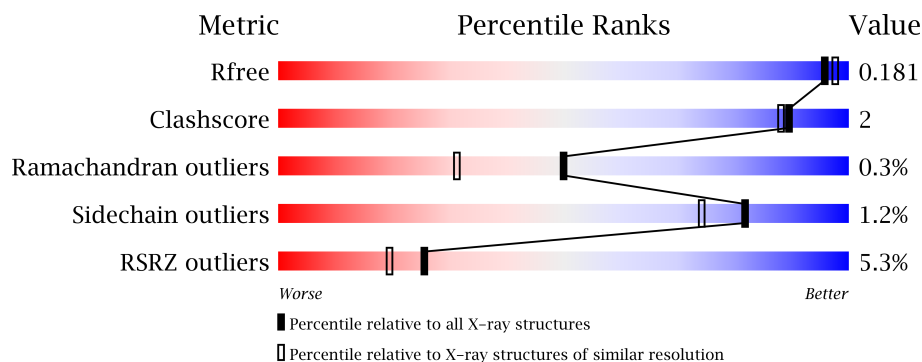
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.79 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	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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
3	NAG	A	807	-	X
3	NAG	A	808	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6495 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	70	0
			5899	3784	988	1103	24			

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

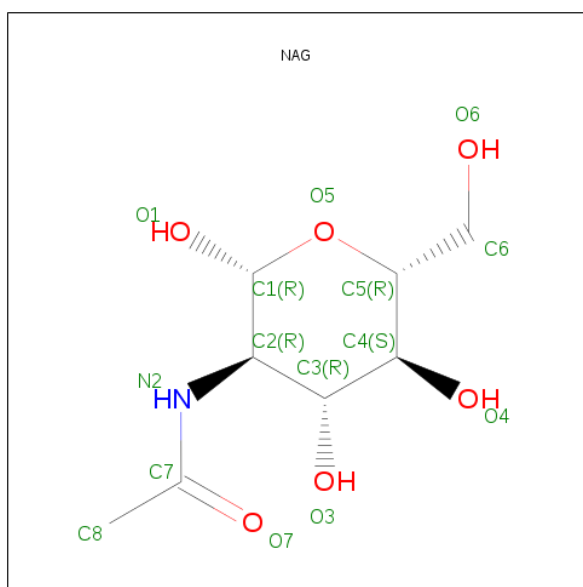
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	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 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	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 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

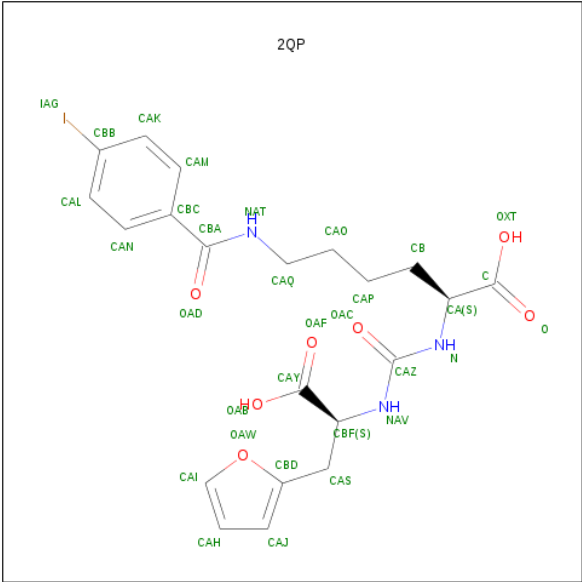
- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 10 is N 2 -{[(1S)-1-CARBOXY-2-(FURAN-2-YL)ETHYL]CARBAMOYL}-N 6 -(4-IODOBENZOYL)-L-LYSINE (three-letter code: 2QP) (formula: C₂₁H₂₄IN₃O₇).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	I	N	O	0	0
			32	21	1	3	7		

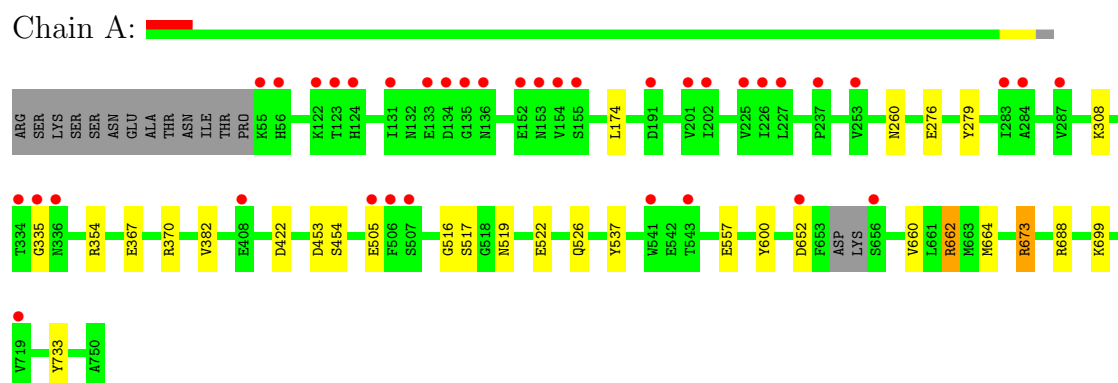
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	363	Total	O	0	0
			363	363		

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	101.57Å 130.43Å 159.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.52 – 1.79 29.53 – 1.79	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.52-1.79) 97.3 (29.53-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.02 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.161 , 0.181 0.162 , 0.181	Depositor DCC
R_{free} test set	1429 reflections (1.51%)	DCC
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 96068 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6495	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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, 2QP, CL, CA, 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	0.95	1/6216 (0.0%)	0.82	6/8413 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	557	GLU	CB-CG	-6.17	1.40	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	673	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	174[A]	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	174[B]	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	422	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	370	ARG	NE-CZ-NH2	-5.06	117.77	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	5899	0	0	13	0
2	A	28	0	25	0	0
3	A	42	0	39	1	0
4	A	38	0	34	0	0
5	A	39	0	34	0	0
6	A	50	0	43	0	0
7	A	2	0	0	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
10	A	32	0	0	0	0
11	A	363	0	0	7	0
All	All	6495	0	175	14	0

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 2.

All (14) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:260[A]:ASN:ND2	11:A:1217:HOH:O	1.64	1.24
1:A:688[B]:ARG:NH2	11:A:1257:HOH:O	2.09	0.85
1:A:660[A]:VAL:O	1:A:664[A]:MET:CG	2.35	0.75
1:A:308:LYS:NZ	11:A:1204:HOH:O	2.34	0.60
1:A:516:GLY:O	1:A:526[B]:GLN:NE2	2.41	0.54
1:A:276:GLU:OE2	1:A:354:ARG:NH2	2.42	0.53
1:A:367:GLU:OE1	1:A:662[A]:ARG:NH1	2.42	0.52
1:A:733:TYR:CE2	11:A:1154:HOH:O	2.54	0.51
3:A:803:NAG:H83	11:A:1094:HOH:O	2.12	0.48
1:A:699[A]:LYS:NZ	11:A:1120:HOH:O	2.48	0.45
1:A:662[B]:ARG:NE	11:A:939:HOH:O	2.49	0.45
1:A:453:ASP:O	1:A:454[A]:SER:C	2.57	0.43
1:A:517:SER:OG	1:A:522[A]:GLU:OE2	2.37	0.43

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	756/709 (107%)	735 (97%)	19 (2%)	2 (0%)	50 31

All (2) Ramachandran outliers are listed below:

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

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	658/605 (109%)	650 (99%)	8 (1%)	82 74

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	505	GLU
1	A	519	ASN
1	A	537	TYR
1	A	600	TYR
1	A	652	ASP
1	A	662[A]	ARG
1	A	662[B]	ARG
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 ⓘ

12 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	0.80	1 (8%)	15,19,21	0.99	1 (6%)
2	NAG	A	802	2	12,14,15	0.88	0	15,19,21	1.45	2 (13%)
4	NAG	A	804	1,4	12,14,15	0.92	1 (8%)	15,19,21	1.18	1 (6%)
4	NAG	A	805	4	12,14,15	0.59	0	15,19,21	1.50	2 (13%)
4	FUC	A	806	4	9,10,11	0.84	0	10,14,16	1.44	1 (10%)
5	NAG	A	809	1,5	12,14,15	1.13	1 (8%)	15,19,21	1.59	3 (20%)
5	NAG	A	810	5	12,14,15	0.60	0	15,19,21	1.02	1 (6%)
5	BMA	A	811	5	10,11,12	0.79	0	11,15,17	1.45	2 (18%)
6	NAG	A	812	1,6	12,14,15	0.86	0	15,19,21	1.67	4 (26%)
6	NAG	A	813	6	12,14,15	0.74	0	15,19,21	1.63	4 (26%)
6	BMA	A	814	6	10,11,12	0.46	0	11,15,17	0.88	0
6	MAN	A	815	6	10,11,12	0.74	0	11,15,17	1.94	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
4	NAG	A	804	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	805	4	-	0/6/23/26	0/1/1/1
4	FUC	A	806	4	-	0/0/17/20	0/1/1/1
5	NAG	A	809	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	810	5	-	0/6/23/26	0/1/1/1
5	BMA	A	811	5	-	0/2/19/22	0/1/1/1
6	NAG	A	812	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	813	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	A	814	6	-	0/2/19/22	0/1/1/1
6	MAN	A	815	6	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	804	NAG	O5-C5	-2.31	1.41	1.45
2	A	801	NAG	O5-C5	-2.24	1.42	1.45
5	A	809	NAG	O7-C7	2.11	1.28	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	815	MAN	O5-C5-C6	5.25	112.48	106.98
2	A	802	NAG	C2-N2-C7	3.97	128.20	123.39
4	A	805	NAG	O5-C5-C6	3.94	111.12	106.98
5	A	809	NAG	O5-C5-C4	-3.78	105.86	110.65
6	A	812	NAG	O5-C5-C6	3.63	110.78	106.98
4	A	806	FUC	O5-C5-C6	3.61	113.91	108.03
6	A	813	NAG	O5-C5-C4	-3.14	106.67	110.65
6	A	812	NAG	C2-N2-C7	-3.06	119.69	123.39
5	A	811	BMA	O5-C5-C4	3.00	114.46	110.65
4	A	804	NAG	C3-C2-N2	-2.85	107.35	111.62
5	A	809	NAG	C3-C2-N2	-2.74	107.51	111.62
6	A	815	MAN	O3-C3-C2	2.70	114.64	109.74
6	A	812	NAG	O4-C4-C5	-2.69	102.13	109.25
6	A	813	NAG	C3-C4-C5	-2.65	105.41	110.17
6	A	813	NAG	C8-C7-N2	2.52	120.88	116.12
6	A	813	NAG	O6-C6-C5	-2.33	103.24	111.37
5	A	810	NAG	O7-C7-C8	-2.25	117.73	122.04
5	A	811	BMA	C3-C4-C5	2.24	114.18	110.17
4	A	805	NAG	O5-C5-C4	-2.18	107.88	110.65
6	A	812	NAG	C3-C4-C5	-2.14	106.32	110.17
5	A	809	NAG	O4-C4-C3	-2.08	105.70	110.36
2	A	801	NAG	O5-C5-C6	2.02	109.10	106.98
2	A	802	NAG	C3-C2-N2	-2.01	108.61	111.62

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	0.79	0	15,19,21	1.88	5 (33%)
3	NAG	A	807	1	12,14,15	0.50	0	15,19,21	1.85	2 (13%)
3	NAG	A	808	1	12,14,15	0.68	0	15,19,21	2.23	4 (26%)
10	2QP	A	820	7	33,33,33	2.02	9 (27%)	43,43,43	3.02	17 (39%)

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	807	1	-	0/6/23/26	0/1/1/1
3	NAG	A	808	1	-	0/6/23/26	0/1/1/1
10	2QP	A	820	7	-	0/31/32/32	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	820	2QP	CBB-IAG	5.97	2.26	2.10
10	A	820	2QP	CBC-CBA	4.55	1.59	1.50
10	A	820	2QP	CAJ-CBD	-3.33	1.31	1.39
10	A	820	2QP	CAK-CAM	3.16	1.44	1.38
10	A	820	2QP	OAW-CAI	3.12	1.42	1.35
10	A	820	2QP	CBF-CAY	2.56	1.59	1.52
10	A	820	2QP	CAL-CAN	2.49	1.43	1.38
10	A	820	2QP	CAS-CBD	2.23	1.54	1.50
10	A	820	2QP	CAH-CAI	-2.07	1.32	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	820	2QP	OAW-CAI-CAH	-7.14	105.73	111.35
3	A	808	NAG	O5-C5-C6	6.69	114.00	106.98
10	A	820	2QP	CAK-CBB-CAL	-6.69	109.92	120.66
10	A	820	2QP	CAQ-NAT-CBA	6.67	137.31	122.16
10	A	820	2QP	CBC-CBA-NAT	6.18	131.41	117.13
10	A	820	2QP	OAD-CBA-NAT	-5.82	110.16	122.55
3	A	807	NAG	O5-C5-C6	5.76	113.02	106.98
10	A	820	2QP	CAM-CAK-CBB	4.51	126.48	119.56
10	A	820	2QP	CAM-CBC-CAN	-4.05	113.03	118.62
10	A	820	2QP	CAL-CBB-IAG	3.94	125.65	119.69
3	A	803	NAG	O5-C5-C6	3.75	110.91	106.98
10	A	820	2QP	OAW-CBD-CAS	3.50	125.36	116.30
10	A	820	2QP	CAN-CAL-CBB	3.49	124.91	119.56
10	A	820	2QP	OAD-CBA-CBC	-3.29	115.26	120.98
10	A	820	2QP	CB-CA-N	-3.27	104.17	110.94
10	A	820	2QP	CAK-CBB-IAG	3.14	124.44	119.69
3	A	808	NAG	C2-N2-C7	-3.06	119.70	123.39
3	A	803	NAG	O5-C5-C4	-3.05	106.79	110.65
10	A	820	2QP	N-CAZ-NAV	2.88	119.78	114.93
3	A	803	NAG	C2-N2-C7	-2.84	119.96	123.39
3	A	807	NAG	C6-C5-C4	-2.83	106.12	113.04
10	A	820	2QP	CAM-CBC-CBA	2.81	129.29	120.57
10	A	820	2QP	CAO-CAQ-NAT	-2.80	103.85	112.20
3	A	808	NAG	C3-C4-C5	-2.56	105.57	110.17
10	A	820	2QP	CAL-CAN-CBC	2.47	123.66	120.76
3	A	803	NAG	O3-C3-C2	-2.46	104.14	109.16
3	A	808	NAG	O7-C7-C8	-2.43	117.38	122.04
3	A	803	NAG	C8-C7-N2	2.16	120.21	116.12

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%)	0.08	37 (5%) 25 19	14, 26, 47, 65	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	719[A]	VAL	5.8
1	A	55	LYS	4.9
1	A	506	PHE	4.7
1	A	153	ASN	4.6
1	A	505	GLU	3.9
1	A	656[A]	SER	3.8
1	A	134	ASP	3.5
1	A	336	ASN	3.4
1	A	202	ILE	3.3
1	A	154	VAL	3.3
1	A	123	THR	3.2
1	A	124	HIS	3.2
1	A	237	PRO	3.2
1	A	135	GLY	3.2
1	A	133	GLU	3.1
1	A	201[A]	VAL	3.0
1	A	283[A]	ILE	3.0
1	A	541	TRP	3.0
1	A	155[A]	SER	2.9
1	A	507	SER	2.9
1	A	287	VAL	2.8
1	A	335	GLY	2.8
1	A	152	GLU	2.8
1	A	652	ASP	2.7
1	A	227	LEU	2.6
1	A	122	LYS	2.6
1	A	334	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	226	ILE	2.5
1	A	543	THR	2.5
1	A	136[A]	ASN	2.4
1	A	191	ASP	2.3
1	A	225	VAL	2.3
1	A	131[A]	ILE	2.2
1	A	284	ALA	2.2
1	A	253	VAL	2.2
1	A	56	HIS	2.2
1	A	408	GLU	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, 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
4	FUC	A	806	10/11	0.40	23.48	56,60,61,62	0
2	NAG	A	801	14/15	0.12	4.92	32,40,44,47	0
2	NAG	A	802	14/15	0.27	4.60	39,52,56,58	0
5	NAG	A	809	14/15	0.12	3.11	28,30,37,39	0
5	BMA	A	811	11/12	0.31	2.56	52,55,60,61	0
4	NAG	A	805	14/15	0.30	1.98	56,60,66,66	0
6	NAG	A	813	14/15	0.21	1.37	34,39,47,48	0
5	NAG	A	810	14/15	0.20	0.77	35,40,46,48	0
4	NAG	A	804	14/15	0.15	0.76	36,43,46,52	0
6	MAN	A	815	11/12	0.15	0.62	44,47,51,52	0
6	BMA	A	814	11/12	0.15	0.53	37,41,43,44	0
6	NAG	A	812	14/15	0.08	0.50	21,26,36,45	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(Å ²)	Q<0.9
3	NAG	A	807	14/15	0.23	8.66	55,63,68,69	0
3	NAG	A	808	14/15	0.20	3.72	32,49,54,58	0
3	NAG	A	803	14/15	0.30	1.69	43,49,53,56	0
9	CL	A	819	1/1	0.14	1.46	26,26,26,26	0
10	2QP	A	820	32/32	0.11	0.36	20,31,43,48	0
8	CA	A	818	1/1	0.04	-1.61	15,15,15,15	0
7	ZN	A	817	1/1	0.05	-2.50	19,19,19,19	0
7	ZN	A	816	1/1	0.07	-4.13	21,21,21,21	0

6.5 Other polymers

There are no such residues in this entry.