



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 15, 2019 – 07:35 PM EDT

PDB ID : 2JBK
Title : membrane-bound glutamate carboxypeptidase II (GCPH) in complex with quisqualic acid (quisqualate, alpha-amino-3,5-dioxo-1,2,4-oxadiazolidine-2-panoic acid)
Authors : Mesters, J.R.; Henning, K.; Hilgenfeld, R.
Deposited on : 2006-12-07
Resolution : 2.99 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.3.2
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.3.2

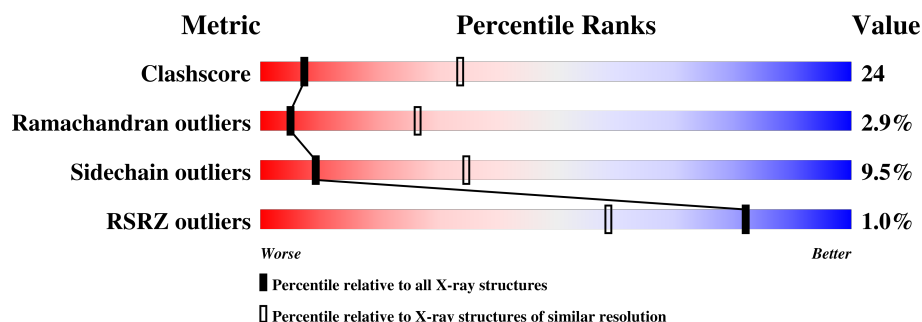
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.99 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))
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (3.00-3.00)

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. 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	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5532 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GLUTAMATE CARBOXYPEPTIDASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	S	0	0	0
			5318	3430	881	990	17			

- 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).

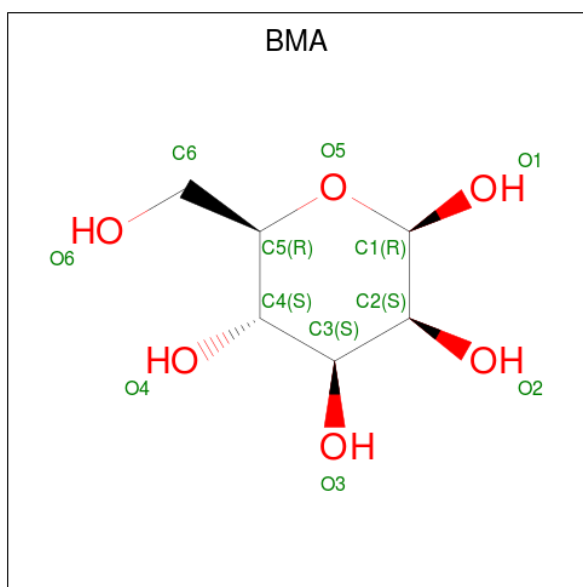
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



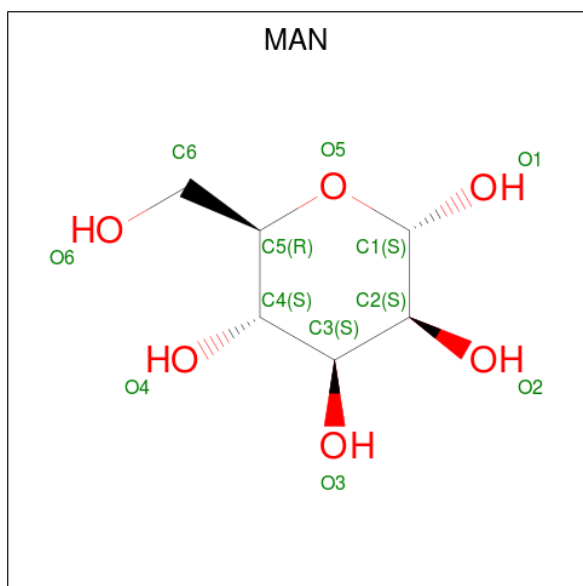
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1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

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



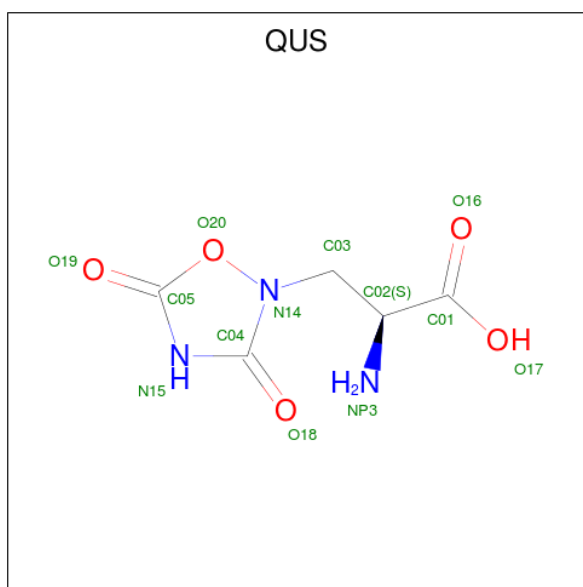
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (three-letter code: QUS) (formula: C₅H₇N₃O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			13	5	3	5		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	21	Total	O	0	0
			21	21		

i

● 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	103.14Å 130.76Å 159.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.99 49.38 – 2.99	Depositor EDS
% Data completeness (in resolution range)	93.2 (100.00-2.99) 93.2 (49.38-2.99)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.210 , (Not available) 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5532	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.13	9/5468 (0.2%)	1.05	14/7431 (0.2%)

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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	654	ASP	CB-CG	5.52	1.63	1.51
1	A	408	GLU	CB-CG	5.44	1.62	1.52
1	A	109	GLU	CD-OE2	5.36	1.31	1.25
1	A	101	LYS	CD-CE	5.19	1.64	1.51
1	A	171	GLU	CD-OE2	5.11	1.31	1.25

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	664	MET	CG-SD-CE	7.21	111.74	100.20
1	A	654	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	453	ASP	CB-CG-OD2	7.12	124.70	118.30
1	A	156	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	A	156	ASP	CB-CG-OD1	6.45	124.11	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	GLU	Peptide
1	A	338	SER	Peptide
1	A	506	PHE	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	5318	0	5004	251	1
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	154	0	138	11	0
6	A	11	0	9	0	1
7	A	11	0	10	0	0
8	A	13	0	6	2	0
9	A	21	0	0	13	0
All	All	5532	0	5167	253	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 24.

The worst 5 of 253 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)
5:A:1754:NAG:H3	9:A:2019:HOH:O	1.46	1.12
1:A:337:PHE:HB3	1:A:340:GLN:NE2	1.70	1.07
1:A:657:ASN:HD21	1:A:660:VAL:HG23	1.18	1.06
1:A:657:ASN:ND2	1:A:660:VAL:CG2	2.19	1.04
1:A:620:GLN:NE2	1:A:620:GLN:HA	1.71	1.02

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)
1:A:276:GLU:OE2	6:A:1762:BMA:O2[2_565]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	681/707 (96%)	587 (86%)	74 (11%)	20 (3%)	5	26

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	154	VAL
1	A	338	SER
1	A	505	GLU
1	A	192	MET

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	536/603 (89%)	485 (90%)	51 (10%)	9	35

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	ASP
1	A	509	MET
1	A	673	ARG
1	A	489	GLU
1	A	534	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	443	GLN
1	A	657	ASN
1	A	618	HIS
1	A	340	GLN
1	A	620	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	1751	1,5	14,14,15	1.01	1 (7%)	17,19,21	2.00	5 (29%)
5	NAG	A	1752	5	14,14,15	0.95	1 (7%)	17,19,21	2.79	6 (35%)
5	NAG	A	1753	1	14,14,15	1.35	3 (21%)	17,19,21	3.19	7 (41%)
5	NAG	A	1754	1,5	14,14,15	1.46	3 (21%)	17,19,21	2.95	9 (52%)
5	NAG	A	1755	5	14,14,15	1.09	1 (7%)	17,19,21	2.92	7 (41%)
5	NAG	A	1756	1	14,14,15	1.85	5 (35%)	17,19,21	2.74	8 (47%)
5	NAG	A	1757	1	14,14,15	1.09	1 (7%)	17,19,21	2.71	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1758	1,5	14,14,15	0.88	0	17,19,21	2.78	7 (41%)
5	NAG	A	1759	5	14,14,15	0.77	0	17,19,21	3.19	6 (35%)
5	NAG	A	1760	1,5	14,14,15	0.58	0	17,19,21	2.37	6 (35%)
5	NAG	A	1761	5,6	14,14,15	1.29	3 (21%)	17,19,21	3.55	7 (41%)
6	BMA	A	1762	5,7	11,11,12	1.06	1 (9%)	15,15,17	1.51	2 (13%)
7	MAN	A	1763	6	11,11,12	0.87	0	15,15,17	2.64	8 (53%)
8	QUS	A	1764	-	4,13,13	1.68	2 (50%)	0,18,18	0.00	-

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	1751	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1752	5	-	4/6/23/26	0/1/1/1
5	NAG	A	1753	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1754	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	1755	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1756	1	-	6/6/23/26	0/1/1/1
5	NAG	A	1757	1	-	6/6/23/26	0/1/1/1
5	NAG	A	1758	1,5	-	4/6/23/26	0/1/1/1
5	NAG	A	1759	5	-	1/6/23/26	0/1/1/1
5	NAG	A	1760	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	1761	5,6	-	4/6/23/26	0/1/1/1
6	BMA	A	1762	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	1763	6	-	0/2/19/22	0/1/1/1
8	QUS	A	1764	-	-	1/2/8/8	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1754	NAG	C1-C2	3.48	1.57	1.52
5	A	1756	NAG	O5-C1	3.05	1.48	1.43
5	A	1756	NAG	O5-C5	2.96	1.49	1.43
5	A	1757	NAG	O5-C1	2.70	1.48	1.43
5	A	1761	NAG	C8-C7	2.63	1.56	1.50

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1759	NAG	C2-N2-C7	-10.78	107.48	122.92
5	A	1761	NAG	C2-N2-C7	-9.77	108.92	122.92
5	A	1753	NAG	O5-C5-C6	7.45	118.94	107.15
5	A	1758	NAG	C2-N2-C7	-7.42	112.29	122.92
5	A	1761	NAG	C1-O5-C5	-6.74	103.04	112.20

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1752	NAG	C8-C7-N2-C2
5	A	1756	NAG	C8-C7-N2-C2
5	A	1756	NAG	O7-C7-N2-C2
8	A	1764	QUS	C01-C02-C03-N14
5	A	1758	NAG	C8-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1753	NAG	2	0
5	A	1754	NAG	5	0
5	A	1756	NAG	1	0
5	A	1757	NAG	1	0
5	A	1758	NAG	2	0
5	A	1759	NAG	1	0
6	A	1762	BMA	0	1
8	A	1764	QUS	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	687/707 (97%)	-0.22	7 (1%) 82 59	35, 35, 35, 35	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	GLN	2.8
1	A	719	VAL	2.7
1	A	310	GLY	2.3
1	A	155	SER	2.2
1	A	153	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	1756	14/15	0.85	0.30	35,35,35,35	0
5	NAG	A	1755	14/15	0.89	0.42	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	A	1753	14/15	0.91	0.36	35,35,35,35	0
5	NAG	A	1761	14/15	0.91	0.19	35,35,35,35	0
5	NAG	A	1754	14/15	0.92	0.28	35,35,35,35	0
6	BMA	A	1762	11/12	0.93	0.15	35,35,35,35	0
7	MAN	A	1763	11/12	0.93	0.15	35,35,35,35	0
5	NAG	A	1757	14/15	0.93	0.21	35,35,35,35	0
5	NAG	A	1759	14/15	0.93	0.22	35,35,35,35	0
5	NAG	A	1752	14/15	0.94	0.37	35,35,35,35	0
5	NAG	A	1760	14/15	0.95	0.14	35,35,35,35	0
5	NAG	A	1751	14/15	0.96	0.23	35,35,35,35	0
4	CL	A	804	1/1	0.97	0.16	35,35,35,35	0
8	QUS	A	1764	13/13	0.97	0.19	35,35,35,35	0
5	NAG	A	1758	14/15	0.97	0.18	35,35,35,35	0
2	ZN	A	802	1/1	0.98	0.11	35,35,35,35	0
2	ZN	A	801	1/1	0.98	0.12	35,35,35,35	0
3	CA	A	803	1/1	1.00	0.13	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.