



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 11:27 PM GMT

PDB ID : 2JBK
Title : MEMBRANE-BOUND GLUTAMATE CARBOXYPEPTIDASE II (GCPII)
IN COMPLEX WITH QUISQUALIC ACID (QUISQUALATE, ALPHA-AM
INO-3,5-DIOXO-1,2,4-OXADIAZOLIDINE-2-PROPANOICACID)
Authors : Mesters, J.R.; Henning, K.; Hilgenfeld, R.
Deposited on : 2006-12-07
Resolution : 2.99 Å(reported)

This is a wwPDB validation summary 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>

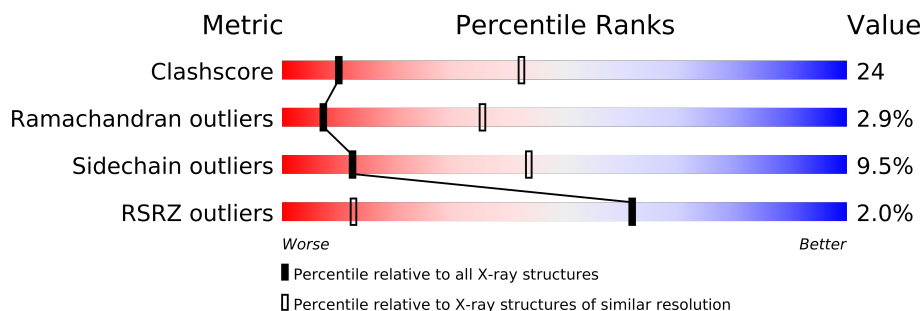
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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. 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	707	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5532 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	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).

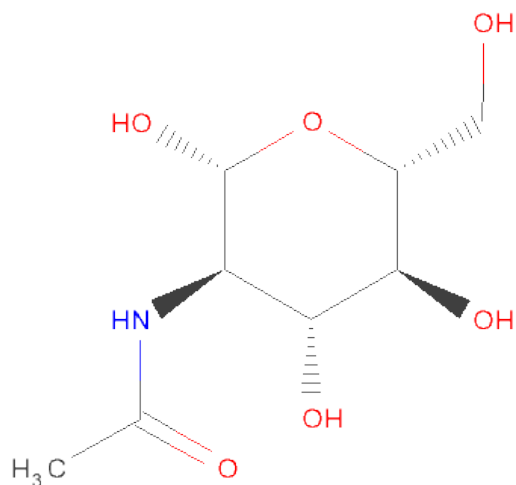
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 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		
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:

$C_8H_{15}NO_6$).

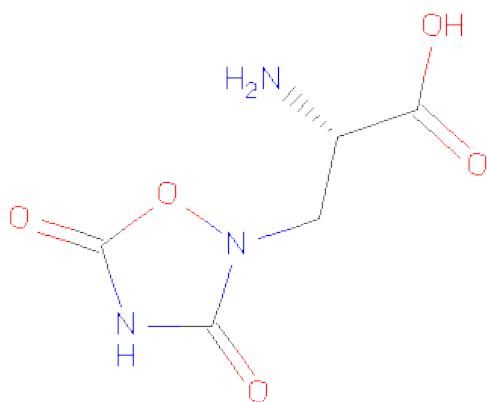


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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		

- Molecule 8 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (three-letter code: QUS) (formula: $C_5H_7N_3O_5$).



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		

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) 93.3 (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.	DCC
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 , 32.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 20723 reflections	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.

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 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	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	84	0	75	7	0
6	A	42	0	39	4	0
7	A	50	0	43	0	1
8	A	13	0	6	2	0
9	A	21	0	0	13	0
All	All	5532	0	5167	253	1

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 24.

The worst 5 of 253 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:HA	1:A:620:GLN:NE2	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	Distance(Å)	Clash(Å)
1:A:276:GLU:OE2	7:A:1762:BMA:O2[2_565]	2.19	0.01

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	681/707 (96%)	587 (86%)	74 (11%)	20 (3%)	7 35

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 ⓘ

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%)	12 44

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 ⓘ

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	$\# Z > 2$
5	NAG	A	1751	1,5	12,14,15	1.23	1 (8%)	15,19,21	2.42	4 (26%)
5	NAG	A	1752	5	12,14,15	0.87	0	15,19,21	3.12	7 (46%)
5	NAG	A	1754	1,5	12,14,15	1.41	2 (16%)	15,19,21	2.91	6 (40%)
5	NAG	A	1755	5	12,14,15	0.98	0	15,19,21	3.36	6 (40%)
5	NAG	A	1758	1,5	12,14,15	1.08	1 (8%)	15,19,21	3.16	7 (46%)
5	NAG	A	1759	5	12,14,15	0.92	0	15,19,21	2.92	4 (26%)
7	NAG	A	1760	1,7	12,14,15	0.64	0	15,19,21	2.48	6 (40%)
7	NAG	A	1761	7	12,14,15	1.32	2 (16%)	15,19,21	3.08	6 (40%)
7	BMA	A	1762	7	10,11,12	0.95	0	11,15,17	1.43	1 (9%)
7	MAN	A	1763	7	10,11,12	0.80	0	11,15,17	3.46	6 (54%)

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	-	0/6/23/26	0/1/1/1
5	NAG	A	1754	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1755	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1758	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1759	5	-	0/6/23/26	0/1/1/1
7	NAG	A	1760	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1761	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1762	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1763	7	-	0/2/19/22	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1761	NAG	O5-C5	-3.47	1.39	1.45
5	A	1754	NAG	C2-N2	3.26	1.50	1.46
5	A	1758	NAG	C2-N2	-2.70	1.43	1.46
5	A	1754	NAG	O7-C7	2.64	1.29	1.23
7	A	1761	NAG	C8-C7	2.61	1.56	1.50

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1759	NAG	C2-N2-C7	-9.30	107.48	123.09
5	A	1755	NAG	O5-C5-C4	-8.71	99.60	110.65
5	A	1752	NAG	O5-C5-C4	8.62	121.59	110.65
7	A	1761	NAG	C2-N2-C7	-8.44	108.92	123.09
5	A	1754	NAG	O5-C5-C6	7.64	115.00	106.98

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$
6	NAG	A	1753	1	12,14,15	1.13	1 (8%)	15,19,21	3.69	7 (46%)
6	NAG	A	1756	1	12,14,15	1.62	3 (25%)	15,19,21	2.79	5 (33%)
6	NAG	A	1757	1	12,14,15	0.79	0	15,19,21	2.59	7 (46%)
8	QUS	A	1764	-	9,13,13	0.97	1 (11%)	7,18,18	1.00	1 (14%)

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	1753	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1756	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1757	1	-	0/6/23/26	0/1/1/1
8	QUS	A	1764	-	-	0/6/8/8	0/0/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1756	NAG	C8-C7	2.58	1.56	1.50
6	A	1756	NAG	O7-C7	2.57	1.28	1.23
6	A	1756	NAG	O5-C5	2.24	1.49	1.45
8	A	1764	QUS	O18-C04	-2.12	1.18	1.23
6	A	1753	NAG	C6-C5	2.03	1.59	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1753	NAG	O5-C5-C6	11.40	118.94	106.98
6	A	1756	NAG	O5-C5-C6	8.19	115.58	106.98
6	A	1757	NAG	O5-C5-C6	5.96	113.24	106.98
6	A	1753	NAG	C3-C4-C5	-5.50	100.38	110.20
6	A	1757	NAG	C3-C2-N2	4.13	118.04	111.76

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	687/707 (97%)	-0.15	13 (1%) 64 13	35, 35, 35, 35	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	GLN	3.7
1	A	719	VAL	3.3
1	A	333	PHE	3.0
1	A	135	GLY	2.6
1	A	341	LYS	2.5

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
5	NAG	A	1759	14/15	0.21	-	35,35,35,35	0
5	NAG	A	1752	14/15	0.40	-	35,35,35,35	0
7	MAN	A	1763	11/12	0.15	-	35,35,35,35	0
5	NAG	A	1751	14/15	0.22	-	35,35,35,35	0
7	NAG	A	1760	14/15	0.15	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	A	1755	14/15	0.42	-	35,35,35,35	0
5	NAG	A	1754	14/15	0.24	-	35,35,35,35	0
7	BMA	A	1762	11/12	0.18	-	35,35,35,35	0
5	NAG	A	1758	14/15	0.15	-	35,35,35,35	0
7	NAG	A	1761	14/15	0.22	-	35,35,35,35	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
8	QUS	A	1764	13/13	0.19	-	35,35,35,35	0
6	NAG	A	1756	14/15	0.32	-	35,35,35,35	0
2	ZN	A	802	1/1	0.12	-	35,35,35,35	0
3	CA	A	803	1/1	0.12	-	35,35,35,35	0
4	CL	A	804	1/1	0.17	-	35,35,35,35	0
6	NAG	A	1753	14/15	0.38	-	35,35,35,35	0
6	NAG	A	1757	14/15	0.20	-	35,35,35,35	0
2	ZN	A	801	1/1	0.13	-	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.