



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:54 AM GMT

PDB ID : 2OOT
Title : A High Resolution Structure of Ligand-free Human Glutamate Carboxypeptidase II
Authors : Barinka, C.; Lubkowski, J.
Deposited on : 2007-01-26
Resolution : 1.64 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

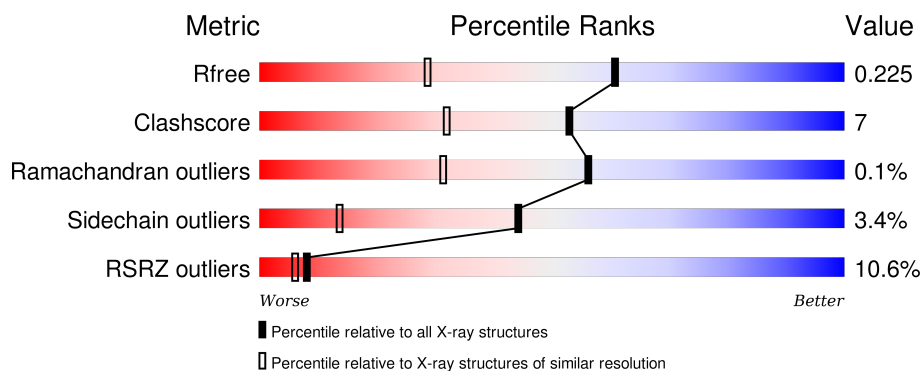
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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}	91344	1953 (1.66-1.62)
Clashscore	102246	2091 (1.66-1.62)
Ramachandran outliers	100387	2052 (1.66-1.62)
Sidechain outliers	100360	2052 (1.66-1.62)
RSRZ outliers	91569	1955 (1.66-1.62)

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	709	<div> <div>10%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1757	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	A	1766	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6511 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	686	Total	C	N	O	S	0	47	0
			5784	3701	974	1088	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ARG	-	CLONING ARTIFACT	UNP Q04609
A	43	SER	-	CLONING ARTIFACT	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		

- 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		
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		

- 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	0	0
			1	1		

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

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

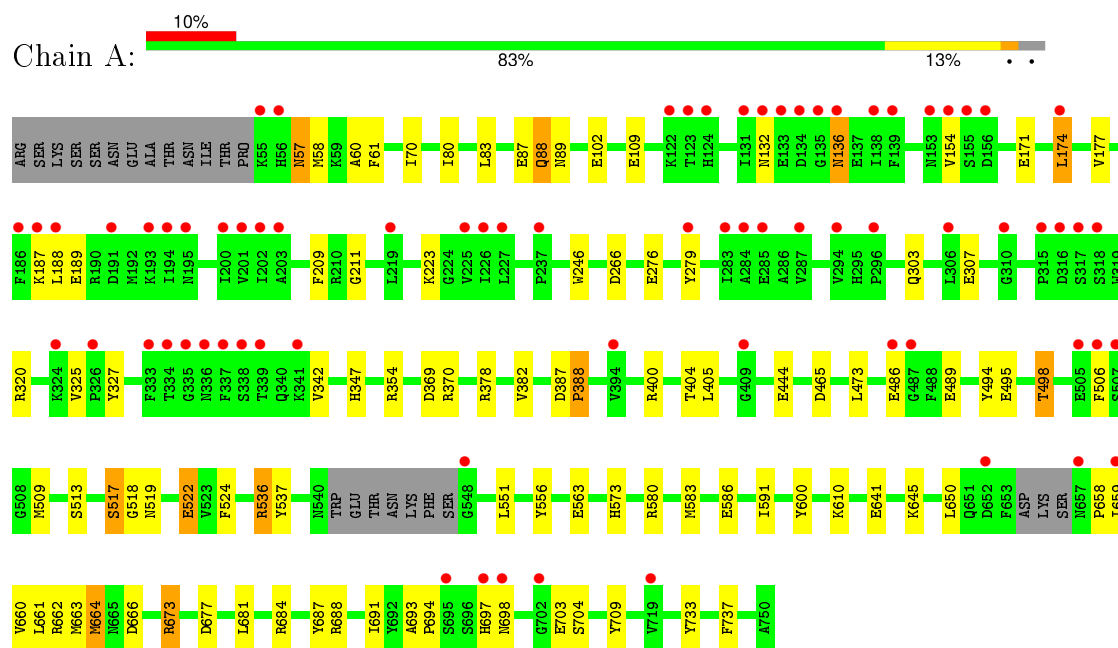
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	560	Total 561	O 561	0	1

3 Residue-property plots [i](#)

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	101.76 Å 130.13 Å 158.87 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.64 27.41 – 1.64	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-1.64) 98.0 (27.41-1.64)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.64 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.228 0.204 , 0.225	Depositor DCC
R_{free} test set	3784 reflections (3.11%)	DCC
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 69.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 125315 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6511	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 2.81% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	0.96	5/5955 (0.1%)	0.92	13/8064 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	524	PHE	CE1-CZ	6.32	1.49	1.37
1	A	83	LEU	CG-CD2	6.11	1.74	1.51
1	A	737	PHE	CG-CD1	5.45	1.47	1.38
1	A	517	SER	CB-OG	5.09	1.48	1.42
1	A	102	GLU	CG-CD	5.02	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	A	673	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	673	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	370	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	A	688	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	662[A]	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	662[B]	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	677	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	A	369	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	174	LEU	CA-CB-CG	5.77	128.57	115.30
1	A	83	LEU	CB-CG-CD2	-5.35	101.90	111.00
1	A	580	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	666	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

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	5784	0	5588	76	0
2	A	56	0	50	1	0
3	A	56	0	52	1	0
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	561	0	0	16	0
All	All	6511	0	5733	77	0

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 7.

All (77) 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)
1:A:697[B]:HIS:O	1:A:698[B]:ASN:ND2	1.60	1.33
1:A:517:SER:OG	1:A:522[B]:GLU:OE2	1.80	0.98
1:A:494:TYR:O	1:A:498[A]:THR:HG23	1.67	0.95
1:A:89[B]:ASN:HD21	1:A:378:ARG:HH21	1.04	0.94
1:A:465[A]:ASP:OD1	1:A:536[A]:ARG:NH1	2.01	0.91
1:A:693[B]:ALA:HB2	8:A:1773:HOH:O	1.67	0.91
1:A:89[B]:ASN:ND2	1:A:378:ARG:HH21	1.74	0.83
1:A:660:VAL:O	1:A:664[B]:MET:HG2	1.78	0.82
1:A:684:ARG:NH2	1:A:694[B]:PRO:O	2.14	0.80
1:A:58:MET:HE1	1:A:586:GLU:HG2	1.67	0.76
1:A:58:MET:CE	1:A:586:GLU:HG2	2.16	0.76
1:A:697[B]:HIS:O	1:A:698[B]:ASN:CG	2.26	0.73
1:A:89[B]:ASN:HD21	1:A:378:ARG:NH2	1.83	0.70
1:A:641:GLU:HG3	8:A:2310:HOH:O	1.89	0.70
1:A:641:GLU:CG	8:A:2310:HOH:O	2.40	0.69
1:A:506:PHE:HB2	1:A:509:MET:HG3	1.75	0.69
1:A:266:ASP:N	8:A:2022:HOH:O	2.24	0.67
1:A:704[A]:SER:OG	8:A:2309:HOH:O	2.14	0.65
1:A:733:TYR:HE2	8:A:2038:HOH:O	1.82	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87[A]:GLU:HG2	1:A:88:GLN:HE21	1.63	0.62
1:A:703[B]:GLU:HB2	1:A:709:TYR:CD1	2.36	0.60
1:A:517:SER:HB2	1:A:694[A]:PRO:HG3	1.84	0.59
1:A:174:LEU:HD22	1:A:342:VAL:HG21	1.84	0.59
1:A:659:ILE:O	1:A:663[A]:MET:HG3	2.03	0.59
1:A:465[A]:ASP:OD2	1:A:513:SER:HB2	2.04	0.57
1:A:681:LEU:HD11	1:A:693[B]:ALA:HB3	1.87	0.57
1:A:87[A]:GLU:CD	1:A:87[A]:GLU:H	2.08	0.56
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.88	0.56
1:A:307:GLU:HA	1:A:325:VAL:HG22	1.87	0.55
1:A:465[A]:ASP:OD1	1:A:536[A]:ARG:NH2	2.39	0.55
1:A:684:ARG:NH1	1:A:694[B]:PRO:O	2.38	0.55
1:A:465[A]:ASP:OD1	1:A:536[A]:ARG:CZ	2.53	0.55
1:A:347:HIS:HE1	8:A:2065:HOH:O	1.90	0.54
1:A:693[B]:ALA:CB	8:A:1773:HOH:O	2.41	0.52
1:A:473:LEU:HG	1:A:583[B]:MET:SD	2.52	0.50
1:A:486:GLU:HG2	8:A:2107:HOH:O	2.11	0.49
1:A:494:TYR:CE2	1:A:498[A]:THR:HG21	2.47	0.49
1:A:80:ILE:HD12	1:A:88:GLN:HG2	1.95	0.48
1:A:154:VAL:HG22	8:A:2037:HOH:O	2.13	0.48
1:A:506:PHE:CB	1:A:509:MET:HG3	2.43	0.48
1:A:320:ARG:HG2	1:A:327:TYR:HB2	1.95	0.48
1:A:691:ILE:O	1:A:704[A]:SER:HA	2.15	0.47
1:A:684:ARG:CZ	1:A:694[B]:PRO:O	2.61	0.47
1:A:687:TYR:CZ	1:A:694[A]:PRO:HG2	2.50	0.47
1:A:209:PHE:CE2	1:A:211:GLY:HA3	2.50	0.47
1:A:473:LEU:HD23	1:A:583[B]:MET:CE	2.45	0.46
1:A:400:ARG:O	1:A:404[B]:THR:HG23	2.15	0.46
1:A:645[B]:LYS:HE3	8:A:2311:HOH:O	2.14	0.46
1:A:89[B]:ASN:HD22	1:A:89[B]:ASN:C	2.20	0.45
1:A:132:ASN:ND2	1:A:136:ASN:HB3	2.31	0.45
2:A:1756:NAG:H81	8:A:1991:HOH:O	2.16	0.45
1:A:276:GLU:OE2	1:A:354:ARG:NH2	2.46	0.44
1:A:650:LEU:HD12	1:A:664[A]:MET:HG2	1.98	0.44
1:A:87[A]:GLU:HG2	1:A:88:GLN:NE2	2.32	0.44
1:A:154:VAL:CG2	8:A:2037:HOH:O	2.66	0.44
1:A:591[A]:ILE:HG22	1:A:661:LEU:HD21	2.00	0.43
1:A:57:ASN:ND2	1:A:60:ALA:H	2.16	0.43
1:A:246:TRP:CD1	3:A:1760:NAG:H83	2.53	0.43
1:A:387:ASP:HA	1:A:388:PRO:HA	1.90	0.43
1:A:109[A]:GLU:OE2	8:A:1968:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:PRO:HA	1:A:661:LEU:HB3	2.01	0.43
1:A:681:LEU:HD11	1:A:693[B]:ALA:CB	2.48	0.42
1:A:663[B]:MET:HE2	1:A:663[B]:MET:HB2	1.89	0.42
1:A:320:ARG:HD2	8:A:2192:HOH:O	2.19	0.42
1:A:177:VAL:HG12	1:A:188:LEU:HD11	2.00	0.42
1:A:70:ILE:HG21	1:A:573:HIS:HB3	2.02	0.42
1:A:645[A]:LYS:HA	1:A:645[A]:LYS:HD3	1.85	0.42
1:A:444:GLU:HA	1:A:444:GLU:OE1	2.20	0.42
1:A:489:GLU:H	1:A:489:GLU:CD	2.24	0.41
1:A:517:SER:OG	1:A:518:GLY:N	2.52	0.41
1:A:61:PHE:HB2	1:A:405[A]:LEU:HD11	2.03	0.41
1:A:473:LEU:HD23	1:A:583[B]:MET:HE3	2.03	0.40
1:A:132:ASN:HD21	1:A:136:ASN:HB3	1.86	0.40
1:A:495:GLU:HG3	8:A:2288:HOH:O	2.20	0.40

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	725/709 (102%)	708 (98%)	16 (2%)	1 (0%)	56 31

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	625/605 (103%)	600 (96%)	25 (4%)	38	10

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	88	GLN
1	A	136	ASN
1	A	171	GLU
1	A	187	LYS
1	A	189	GLU
1	A	223	LYS
1	A	279[A]	TYR
1	A	279[B]	TYR
1	A	303	GLN
1	A	388	PRO
1	A	498[A]	THR
1	A	498[B]	THR
1	A	519	ASN
1	A	522[A]	GLU
1	A	522[B]	GLU
1	A	536[A]	ARG
1	A	536[B]	ARG
1	A	537	TYR
1	A	563	GLU
1	A	600	TYR
1	A	610	LYS
1	A	664[A]	MET
1	A	664[B]	MET
1	A	673	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	88	GLN
1	A	136	ASN
1	A	618	HIS

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Mol	Chain	Res	Type
1	A	620	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

8 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	1755	1,2	14,14,15	0.52	0	15,19,21	1.02	0
2	NAG	A	1756	2	14,14,15	0.65	0	15,19,21	0.99	1 (6%)
2	NAG	A	1761	1,2	14,14,15	0.81	1 (7%)	15,19,21	0.93	1 (6%)
2	NAG	A	1762	2	14,14,15	0.43	0	15,19,21	0.97	1 (6%)
4	NAG	A	1763	1,4	14,14,15	0.79	1 (7%)	15,19,21	0.96	1 (6%)
4	NAG	A	1764	4	14,14,15	0.69	1 (7%)	15,19,21	1.44	3 (20%)
4	BMA	A	1765	4	11,11,12	0.83	1 (9%)	14,15,17	0.97	1 (7%)
4	MAN	A	1766	4	11,11,12	0.46	0	14,15,17	0.96	1 (7%)

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	1755	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1756	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1761	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1762	2	-	0/6/23/26	0/1/1/1
4	NAG	A	1763	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1764	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1765	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1766	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	1765	BMA	O5-C1	-2.19	1.40	1.43
4	A	1764	NAG	O5-C1	-2.15	1.40	1.43
4	A	1763	NAG	C1-C2	2.11	1.55	1.52
2	A	1761	NAG	O7-C7	2.19	1.28	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1763	NAG	C6-C5-C4	-2.59	106.62	113.02
4	A	1764	NAG	O7-C7-C8	-2.43	117.61	122.06
4	A	1765	BMA	O3-C3-C2	-2.08	106.25	110.00
2	A	1762	NAG	C8-C7-N2	2.07	120.06	116.11
4	A	1766	MAN	C1-O5-C5	2.12	114.94	112.25
4	A	1764	NAG	C8-C7-N2	2.17	120.27	116.11
2	A	1761	NAG	C2-N2-C7	2.30	125.99	123.04
2	A	1756	NAG	C2-N2-C7	2.47	126.21	123.04
4	A	1764	NAG	C1-O5-C5	3.37	116.53	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1756	NAG	1	0

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	1757	1	14,14,15	0.52	0	15,19,21	1.80	3 (20%)
3	NAG	A	1758	1	14,14,15	0.78	1 (7%)	15,19,21	0.86	1 (6%)
3	NAG	A	1759	1	14,14,15	0.38	0	15,19,21	1.26	3 (20%)
3	NAG	A	1760	1	14,14,15	0.52	0	15,19,21	1.51	2 (13%)

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	1757	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1758	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1759	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1760	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1758	NAG	C1-C2	2.05	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1759	NAG	C4-C3-C2	-2.33	107.61	111.23
3	A	1759	NAG	C2-N2-C7	-2.06	120.39	123.04
3	A	1757	NAG	C8-C7-N2	2.06	120.04	116.11
3	A	1758	NAG	C1-O5-C5	2.37	115.25	112.25
3	A	1759	NAG	C1-O5-C5	2.77	115.77	112.25
3	A	1757	NAG	O5-C5-C6	3.08	114.02	107.35
3	A	1760	NAG	C3-C4-C5	3.11	115.61	110.20
3	A	1760	NAG	C1-O5-C5	3.62	116.85	112.25
3	A	1757	NAG	C1-O5-C5	5.25	118.91	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1760	NAG	1	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 ⓘ

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	686/709 (96%)	0.53	73 (10%) 8 6	14, 25, 51, 64	2 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	GLY	6.7
1	A	338	SER	5.8
1	A	337	PHE	5.7
1	A	219	LEU	5.3
1	A	548	GLY	5.2
1	A	226	ILE	5.1
1	A	55	LYS	5.1
1	A	155[A]	SER	5.1
1	A	133	GLU	4.6
1	A	202	ILE	4.6
1	A	719	VAL	4.4
1	A	153	ASN	4.3
1	A	335	GLY	4.3
1	A	134	ASP	4.3
1	A	283	ILE	4.0
1	A	334	THR	4.0
1	A	317	SER	4.0
1	A	227	LEU	3.9
1	A	225	VAL	3.9
1	A	507	SER	3.8
1	A	195	ASN	3.8
1	A	339	THR	3.7
1	A	186	PHE	3.7
1	A	336	ASN	3.6
1	A	194	ILE	3.5
1	A	506	PHE	3.5
1	A	132	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	697[A]	HIS	3.4
1	A	191	ASP	3.4
1	A	136	ASN	3.3
1	A	505	GLU	3.3
1	A	138	ILE	3.3
1	A	318	SER	3.3
1	A	487	GLY	3.2
1	A	123	THR	3.1
1	A	200	ILE	3.1
1	A	294	VAL	3.1
1	A	174	LEU	3.1
1	A	310	GLY	3.0
1	A	316	ASP	3.0
1	A	315	PRO	3.0
1	A	203	ALA	2.7
1	A	154	VAL	2.7
1	A	284	ALA	2.7
1	A	287	VAL	2.6
1	A	237	PRO	2.6
1	A	341	LYS	2.6
1	A	122	LYS	2.5
1	A	156	ASP	2.5
1	A	296	PRO	2.5
1	A	306	LEU	2.5
1	A	324	LYS	2.5
1	A	409	GLY	2.5
1	A	201	VAL	2.4
1	A	56	HIS	2.4
1	A	193	LYS	2.4
1	A	652	ASP	2.4
1	A	124	HIS	2.3
1	A	131	ILE	2.3
1	A	139	PHE	2.3
1	A	695[A]	SER	2.3
1	A	659	ILE	2.2
1	A	702[A]	GLY	2.2
1	A	698[A]	ASN	2.2
1	A	394	VAL	2.2
1	A	187	LYS	2.2
1	A	486	GLU	2.2
1	A	188	LEU	2.2
1	A	326	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	333	PHE	2.1
1	A	285	GLU	2.1
1	A	279[A]	TYR	2.0
1	A	657	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](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MAN	A	1766	11/12	0.90	0.18	2.96	43,46,49,51	0
4	NAG	A	1763	14/15	0.91	0.09	0.29	20,25,32,40	0
2	NAG	A	1756	14/15	0.64	0.28	-	38,47,51,54	0
4	BMA	A	1765	11/12	0.88	0.18	-	37,40,41,42	0
2	NAG	A	1755	14/15	0.92	0.12	-	31,37,43,46	0
2	NAG	A	1762	14/15	0.91	0.20	-	30,37,43,44	0
2	NAG	A	1761	14/15	0.90	0.11	-	27,29,35,39	0
4	NAG	A	1764	14/15	0.88	0.19	-	33,36,45,46	0

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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	1757	14/15	0.73	0.32	3.16	47,53,56,57	0
3	NAG	A	1758	14/15	0.77	0.20	1.23	41,48,51,52	0
5	ZN	A	1752	1/1	1.00	0.05	-1.36	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	CL	A	1754	1/1	1.00	0.03	-2.20	25,25,25,25	0
6	CA	A	1753	1/1	1.00	0.06	-2.31	14,14,14,14	0
5	ZN	A	1751	1/1	1.00	0.06	-2.90	21,21,21,21	0
3	NAG	A	1760	14/15	0.82	0.21	-	32,46,53,54	0
3	NAG	A	1759	14/15	0.67	0.34	-	70,73,75,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.