



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:24 pm GMT

PDB ID : 2PVV  
Title : Structure of human glutamate carboxypeptidase II (GCP II) in complex with L-serine-O-sulfate  
Authors : Barinka, C.; Lubkowski, J.  
Deposited on : 2007-05-10  
Resolution : 2.11 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

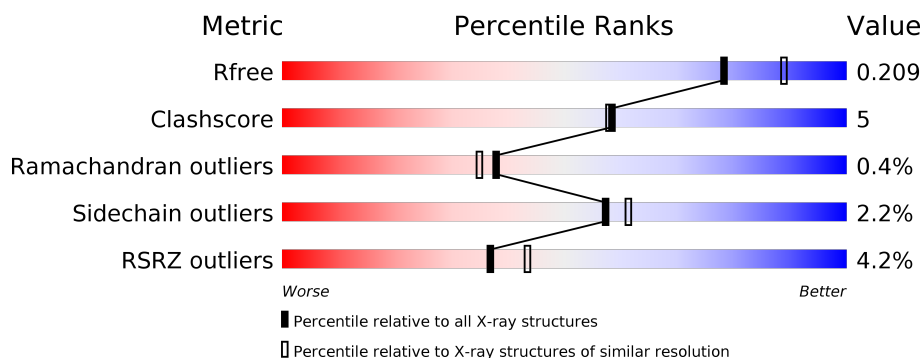
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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))
$R_{free}$	100719	4988 (2.14-2.10)
Clashscore	112137	5557 (2.14-2.10)
Ramachandran outliers	110173	5504 (2.14-2.10)
Sidechain outliers	110143	5505 (2.14-2.10)
RSRZ outliers	101464	5021 (2.14-2.10)

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  $\geq 3$ , 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>4%</div> <div>84%</div> <div>14%</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
2	NAG	A	1758	-	-	-	X
2	NAG	A	1761	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1757	-	-	-	X
4	MAN	A	1765	X	-	-	-
8	OSE	A	1768	X	-	-	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6329 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	694	Total	C	N	O	S	0	17	0
			5628	3619	944	1046	19			

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		
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: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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 (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		

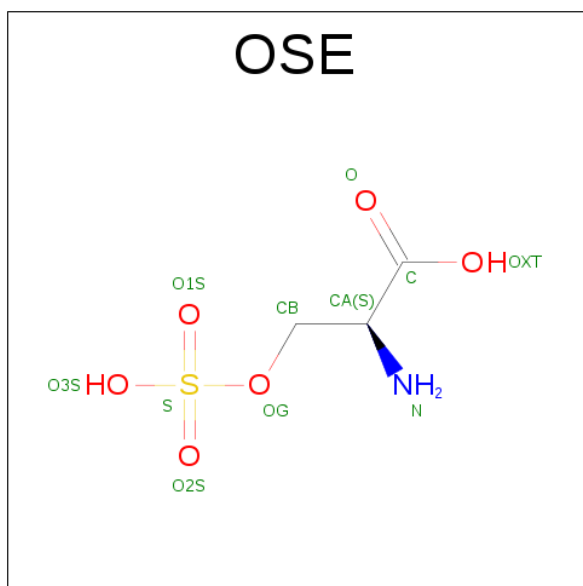
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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 Cl 1 1	0	0

- Molecule 8 is O-SULFO-L-SERINE (three-letter code: OSE) (formula:  $C_3H_7NO_6S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			11	3	1	6	1		

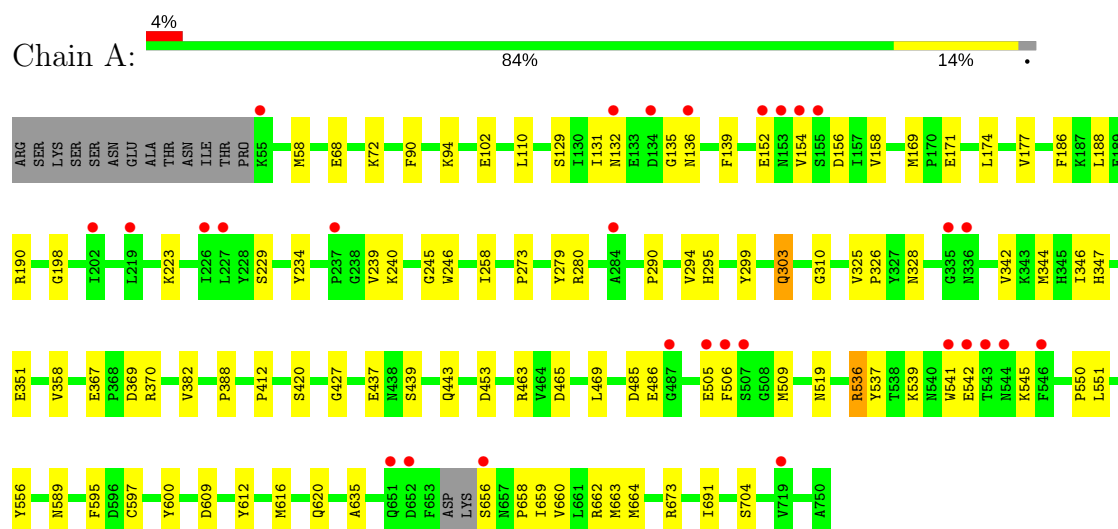
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	510	Total O 510 510	0	0

### 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 the various outlier classes 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, $\alpha$ , $\beta$ , $\gamma$	101.62Å 130.22Å 158.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.11 29.53 – 2.11	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-2.11) 98.5 (29.53-2.11)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.49 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.174 , 0.212 0.171 , 0.209	Depositor DCC
$R_{free}$ test set	3059 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6329	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, NAG, CL, CA, OSE, 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	1.02	4/5826 (0.1%)	0.85	2/7895 (0.0%)

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
4	A	1	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	GLU	CG-CD	6.45	1.61	1.51
1	A	158	VAL	CB-CG1	6.05	1.65	1.52
1	A	597	CYS	CB-SG	5.86	1.92	1.82
1	A	635	ALA	CA-CB	5.19	1.63	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	370	ARG	NE-CZ-NH1	5.76	123.18	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1765	MAN	C1

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	5628	0	5471	59	0
2	A	84	0	75	3	0
3	A	42	0	39	2	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	11	0	4	1	0
9	A	510	0	0	15	0
All	All	6329	0	5632	63	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 5.

All (63) 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:660[A]:VAL:O	1:A:664[A]:MET:HG2	1.32	1.22
1:A:486:GLU:HG2	9:A:2025:HOH:O	1.68	0.94
1:A:620:GLN:NE2	9:A:2116:HOH:O	2.10	0.84
1:A:506:PHE:HB2	1:A:509:MET:HG3	1.69	0.74
1:A:177:VAL:HG12	1:A:188:LEU:HD11	1.73	0.71
1:A:367:GLU:OE1	1:A:662[A]:ARG:NH1	2.29	0.65
1:A:660[A]:VAL:O	1:A:664[A]:MET:CG	2.27	0.64
2:A:1767:NAG:H83	9:A:2140:HOH:O	1.98	0.62
1:A:412:PRO:HA	1:A:589:ASN:OD1	2.02	0.59
1:A:506:PHE:CB	1:A:509:MET:HG3	2.32	0.59
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.37	0.59
1:A:443:GLN:CG	9:A:2278:HOH:O	2.52	0.58
1:A:443:GLN:HG2	9:A:2278:HOH:O	2.05	0.57
1:A:152:GLU:OE2	9:A:1982:HOH:O	2.17	0.56
1:A:90:PHE:CE2	1:A:94:LYS:HE2	2.40	0.56
1:A:68:GLU:O	1:A:72:LYS:HG3	2.06	0.55
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.88	0.55
1:A:273:PRO:HB3	1:A:437:GLU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1762:NAG:H83	9:A:1986:HOH:O	2.08	0.53
1:A:229:SER:O	1:A:299:TYR:HB3	2.09	0.53
1:A:310:GLY:O	1:A:328:ASN:HB3	2.09	0.53
1:A:303:GLN:OE1	1:A:325:VAL:HG13	2.09	0.52
1:A:295:HIS:HB2	1:A:346:ILE:HD11	1.92	0.52
1:A:463:ARG:HH21	1:A:545:LYS:HE2	1.76	0.51
1:A:347:HIS:HE1	9:A:2104:HOH:O	1.94	0.51
1:A:169:MET:HA	1:A:344:MET:O	2.11	0.51
2:A:1762:NAG:C8	9:A:1986:HOH:O	2.58	0.51
1:A:131:ILE:HG12	1:A:135:GLY:HA2	1.95	0.49
3:A:1757:NAG:H83	9:A:1984:HOH:O	2.12	0.49
1:A:453:ASP:HB3	1:A:536[B]:ARG:HH12	1.76	0.49
1:A:536[B]:ARG:NH2	9:A:2272:HOH:O	2.39	0.48
1:A:506:PHE:HB2	1:A:509:MET:CG	2.41	0.48
1:A:186:PHE:O	1:A:190:ARG:HB2	2.13	0.47
1:A:132:ASN:HD21	1:A:136:ASN:HD22	1.62	0.47
1:A:132:ASN:ND2	1:A:136:ASN:HB2	2.29	0.47
1:A:485:ASP:O	9:A:1902:HOH:O	2.21	0.46
1:A:129:SER:HA	1:A:139:PHE:O	2.16	0.46
1:A:258:ILE:HD13	1:A:294:VAL:HB	1.98	0.45
1:A:659[B]:ILE:O	1:A:663[B]:MET:HG3	2.17	0.45
1:A:691:ILE:O	1:A:704:SER:HA	2.17	0.45
1:A:369:ASP:OD2	1:A:662[B]:ARG:NH2	2.31	0.45
1:A:656[B]:SER:O	1:A:658[B]:PRO:HD3	2.16	0.45
1:A:246:TRP:CD1	3:A:1760:NAG:H83	2.51	0.45
1:A:443:GLN:HG3	9:A:2278:HOH:O	2.17	0.44
1:A:439:SER:O	1:A:443:GLN:HB2	2.17	0.44
1:A:358:VAL:HB	1:A:420:SER:HB3	1.99	0.44
1:A:110:LEU:CD2	1:A:358:VAL:HG22	2.47	0.44
1:A:463:ARG:NH2	1:A:545:LYS:HE2	2.33	0.44
1:A:234:TYR:O	1:A:550:PRO:HB3	2.18	0.44
1:A:659[B]:ILE:HA	1:A:659[B]:ILE:HD13	1.86	0.43
1:A:325:VAL:HB	1:A:326:PRO:HD2	1.99	0.43
1:A:427:GLY:HA2	8:A:1768:OSE:O3S	2.19	0.43
1:A:258:ILE:CD1	1:A:290:PRO:HG3	2.49	0.43
1:A:68:GLU:OE2	1:A:72:LYS:HE3	2.19	0.42
1:A:505:GLU:HG2	1:A:506:PHE:CE1	2.54	0.42
1:A:609:ASP:OD2	9:A:2126:HOH:O	2.21	0.42
1:A:469:LEU:O	1:A:595:PHE:HA	2.19	0.42
1:A:154:VAL:HG22	9:A:2266:HOH:O	2.19	0.41
1:A:171:GLU:HA	1:A:342:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLY:O	1:A:223:LYS:HE2	2.20	0.41
1:A:240:LYS:O	1:A:245:GLY:HA3	2.21	0.40

There are no symmetry-related clashes.

## 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	706/709 (100%)	679 (96%)	24 (3%)	3 (0%)	38 35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	541	TRP
1	A	542	GLU
1	A	382	VAL

### 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	608/605 (100%)	594 (98%)	14 (2%)	56 59

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	MET
1	A	174	LEU
1	A	239	VAL
1	A	303	GLN
1	A	351	GLU
1	A	388	PRO
1	A	465	ASP
1	A	519	ASN
1	A	536[A]	ARG
1	A	536[B]	ARG
1	A	537	TYR
1	A	539	LYS
1	A	600	TYR
1	A	673	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	618	HIS

### 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](#)

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
2	NAG	A	1755	1,2	14,14,15	0.67	0	15,19,21	1.59	2 (13%)
2	NAG	A	1756	2	14,14,15	0.68	0	15,19,21	2.12	4 (26%)
2	NAG	A	1758	1,2	14,14,15	0.82	0	15,19,21	1.19	1 (6%)
2	NAG	A	1761	1,2	14,14,15	1.08	0	15,19,21	1.66	3 (20%)
2	NAG	A	1762	2	14,14,15	0.69	0	15,19,21	1.19	1 (6%)
4	NAG	A	1763	1,4	14,14,15	0.73	0	15,19,21	1.91	3 (20%)
4	NAG	A	1764	4	14,14,15	0.83	1 (7%)	15,19,21	1.39	3 (20%)
4	MAN	A	1765	4	11,11,12	1.10	1 (9%)	13,15,17	1.38	3 (23%)
4	MAN	A	1766	4	11,11,12	0.62	0	13,15,17	0.88	0
2	NAG	A	1767	2	14,14,15	0.40	0	15,19,21	1.55	5 (33%)

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
2	NAG	A	1756	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1758	1,2	-	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	MAN	A	1765	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	1766	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1767	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1765	MAN	O5-C1	-3.07	1.38	1.43
4	A	1764	NAG	O5-C1	-2.18	1.40	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1761	NAG	O5-C1-C2	-4.59	105.09	111.47
4	A	1763	NAG	O5-C1-C2	-4.12	105.75	111.47
2	A	1755	NAG	O4-C4-C3	-3.54	102.65	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1764	NAG	C3-C4-C5	-2.82	105.24	110.22
2	A	1755	NAG	O5-C1-C2	-2.68	107.75	111.47
4	A	1763	NAG	C2-N2-C7	-2.22	119.70	122.94
4	A	1765	MAN	O5-C1-C2	-2.21	107.33	110.79
4	A	1764	NAG	O7-C7-C8	-2.20	118.05	122.06
2	A	1758	NAG	O4-C4-C3	-2.19	105.60	110.36
4	A	1765	MAN	O3-C3-C2	-2.19	106.05	110.02
2	A	1767	NAG	O7-C7-C8	-2.18	118.09	122.06
2	A	1761	NAG	O6-C6-C5	-2.05	104.45	111.34
2	A	1767	NAG	C1-C2-N2	-2.03	107.02	110.49
2	A	1761	NAG	C2-N2-C7	2.16	126.09	122.94
2	A	1767	NAG	C2-N2-C7	2.25	126.23	122.94
2	A	1756	NAG	C3-C4-C5	2.27	114.22	110.22
2	A	1767	NAG	O4-C4-C5	2.28	115.02	109.28
4	A	1764	NAG	C8-C7-N2	2.33	120.31	116.11
4	A	1765	MAN	C1-O5-C5	2.86	116.11	112.17
2	A	1762	NAG	C8-C7-N2	2.98	121.48	116.11
2	A	1767	NAG	C8-C7-N2	3.21	121.90	116.11
2	A	1756	NAG	C4-C3-C2	3.44	116.06	111.02
2	A	1756	NAG	C1-O5-C5	3.98	117.66	112.17
4	A	1763	NAG	C1-O5-C5	4.68	118.62	112.17
2	A	1756	NAG	C2-N2-C7	5.23	130.58	122.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1765	MAN	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1762	NAG	2	0
2	A	1767	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	0.69	0	15,19,21	2.04	3 (20%)
3	NAG	A	1759	1	14,14,15	0.44	0	15,19,21	1.17	1 (6%)
3	NAG	A	1760	1	14,14,15	0.68	0	15,19,21	1.65	2 (13%)
8	OSE	A	1768	-	6,10,10	0.79	0	5,14,14	1.66	1 (20%)

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	1759	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1760	1	-	0/6/23/26	0/1/1/1
8	OSE	A	1768	-	1/1/3/3	0/6/10/10	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1760	NAG	O7-C7-C8	-2.40	117.69	122.06
3	A	1757	NAG	C8-C7-N2	2.08	119.86	116.11
3	A	1757	NAG	C3-C4-C5	2.64	114.87	110.22
3	A	1759	NAG	C1-O5-C5	3.27	116.67	112.17
8	A	1768	OSE	O3S-S-O2S	3.57	121.45	108.79
3	A	1760	NAG	C1-O5-C5	4.21	117.97	112.17
3	A	1757	NAG	C1-O5-C5	6.28	120.83	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	1768	OSE	CA

There are no torsion outliers.



There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1757	NAG	1	0
3	A	1760	NAG	1	0
8	A	1768	OSE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	694/709 (97%)	-0.13	29 (4%)	37 43	14, 26, 50, 71	1 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	TRP	7.2
1	A	543	THR	4.6
1	A	335	GLY	4.0
1	A	153	ASN	3.9
1	A	544	ASN	3.5
1	A	284	ALA	3.5
1	A	155[A]	SER	3.5
1	A	542	GLU	3.3
1	A	55	LYS	3.0
1	A	227	LEU	2.9
1	A	656[A]	SER	2.8
1	A	505	GLU	2.7
1	A	336	ASN	2.7
1	A	134	ASP	2.6
1	A	237	PRO	2.6
1	A	152	GLU	2.5
1	A	226	ILE	2.4
1	A	219	LEU	2.4
1	A	507	SER	2.4
1	A	136	ASN	2.4
1	A	719	VAL	2.3
1	A	651	GLN	2.3
1	A	546	PHE	2.3
1	A	487	GLY	2.2
1	A	132	ASN	2.2
1	A	202	ILE	2.1
1	A	506	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	154	VAL	2.1
1	A	652	ASP	2.1

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	A	1758	14/15	0.83	0.21	4.30	47,49,54,59	0
2	NAG	A	1761	14/15	0.93	0.14	2.56	28,31,37,40	0
4	MAN	A	1766	11/12	0.94	0.15	0.88	50,52,55,57	0
4	NAG	A	1763	14/15	0.96	0.07	-0.19	16,26,37,42	0
2	NAG	A	1767	14/15	0.70	0.31	-	61,64,68,69	0
2	NAG	A	1762	14/15	0.92	0.17	-	35,42,48,49	0
2	NAG	A	1755	14/15	0.94	0.10	-	37,42,46,50	0
2	NAG	A	1756	14/15	0.74	0.31	-	46,55,60,61	0
4	MAN	A	1765	11/12	0.88	0.12	-	42,46,47,49	0
4	NAG	A	1764	14/15	0.92	0.20	-	37,42,46,54	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	A	1757	14/15	0.78	0.30	2.61	51,57,64,64	0
6	CA	A	1753	1/1	0.99	0.06	-0.41	16,16,16,16	0
7	CL	A	1754	1/1	1.00	0.12	-0.81	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	OSE	A	1768	11/11	0.99	0.08	-0.87	22,22,27,32	0
5	ZN	A	1752	1/1	1.00	0.07	-2.17	21,21,21,21	0
5	ZN	A	1751	1/1	1.00	0.08	-4.58	24,24,24,24	0
3	NAG	A	1759	14/15	0.78	0.26	-	68,73,76,76	0
3	NAG	A	1760	14/15	0.85	0.21	-	36,52,56,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.