



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:26 PM GMT

PDB ID : 2C6C  
Title : MEMBRANE-BOUND GLUTAMATE CARBOXYPEPTIDASE II (GCPII)  
IN COMPLEX WITH GPI-18431 (S)-2-(4-IODOBENZYLPHOSPHONOME  
THYL)-PENTANEDIOICACID  
Authors : Mesters, J.R.; Barinka, C.; Li, W.; Tsukamoto, T.; Majer, P.; Slusher, B.S.;  
Konvalinka, J.; Hilgenfeld, R.  
Deposited on : 2005-11-09  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

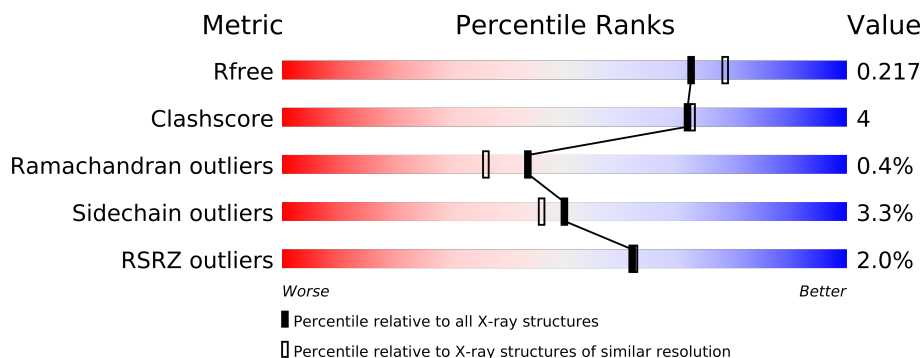
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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  $\geq 3$ , 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	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	NAG	A	1757	-	X
6	NAG	A	1759	-	X
6	NAG	A	1760	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5703 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 II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	682	Total	C	N	O	S	0	0	0
			5330	3434	886	993	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		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

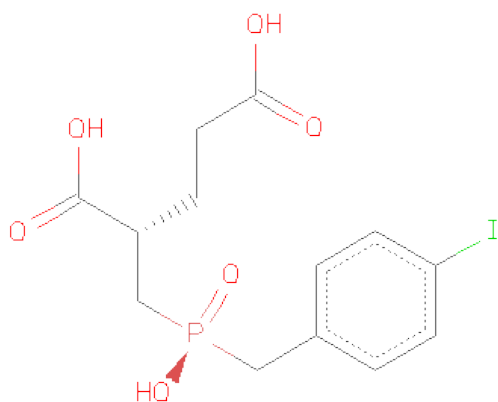


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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 (2S)-2-{[HYDROXY(4-IOBOBENZYL)PHOSPHORYL]METHYL}PENTANEDIOICACID (three-letter code: 24I) (formula: C<sub>13</sub>H<sub>16</sub>IO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	I	O	P	0	0
			21	13	1	6	1		

- Molecule 9 is water.

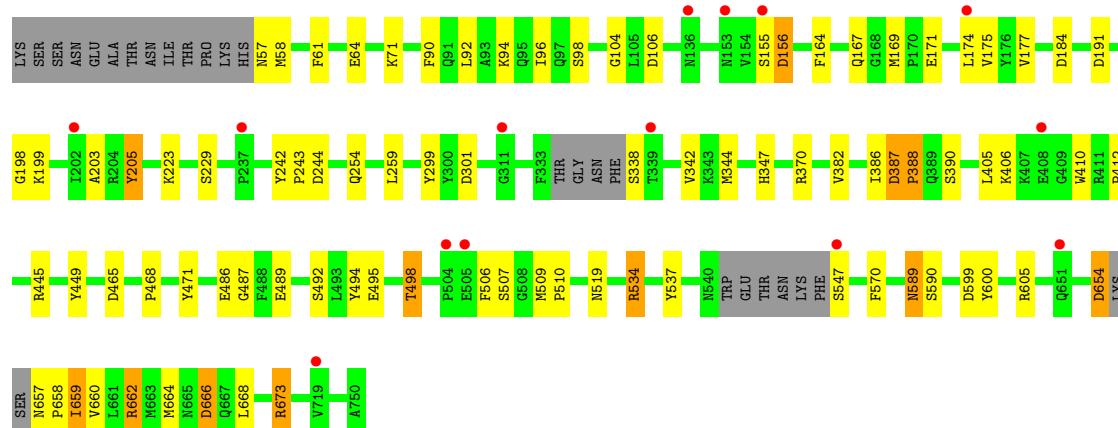
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	186	Total	O	0	0
			186	186		

### 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 II

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.13Å 131.19Å 161.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 24.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (25.00-2.00) 94.3 (24.87-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.190 , 0.225 0.198 , 0.217	Depositor DCC
$R_{free}$ test set	1022 reflections (1.49%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.0	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 69679 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5703	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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, NAG, CL, CA, 24I, 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	1.08	3/5478 (0.1%)	0.98	16/7438 (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
7	A	1	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	590	SER	CA-CB	-6.60	1.43	1.52
1	A	449	TYR	CE2-CZ	-5.99	1.30	1.38
1	A	445	ARG	NE-CZ	-5.12	1.26	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	662	ARG	NE-CZ-NH1	11.17	125.89	120.30
1	A	184	ASP	CB-CG-OD2	9.16	126.55	118.30
1	A	666	ASP	CB-CG-OD2	8.23	125.71	118.30
1	A	301	ASP	CB-CG-OD2	7.68	125.21	118.30
1	A	387	ASP	CB-CG-OD2	7.61	125.15	118.30
1	A	673	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	A	244	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	465	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	662	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	106	ASP	CB-CG-OD2	6.31	123.98	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	599	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	156	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	534	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	191	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	370	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	659	ILE	N-CA-C	-5.02	97.44	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1765	MAN	C1

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	5330	0	5061	45	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	56	0	50	0	0
6	A	56	0	52	1	0
7	A	50	0	43	1	0
8	A	21	0	13	0	0
9	A	186	0	0	2	0
All	All	5703	0	5219	47	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 4.

All (47) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:657:ASN:ND2	1:A:660:VAL:HG23	1.49	1.26

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:657:ASN:HD22	1:A:660:VAL:CG2	1.68	1.07
1:A:657:ASN:HD22	1:A:660:VAL:HG23	0.84	0.98
1:A:660:VAL:O	1:A:664:MET:HG2	1.67	0.94
1:A:494:TYR:O	1:A:498:THR:HG23	1.72	0.88
1:A:494:TYR:O	1:A:498:THR:CG2	2.24	0.85
1:A:666:ASP:OD2	9:A:2140:HOH:O	1.99	0.80
1:A:412:PRO:HA	1:A:589:ASN:OD1	1.84	0.77
1:A:654:ASP:O	1:A:657:ASN:N	2.25	0.70
1:A:509:MET:HB2	1:A:510:PRO:HD2	1.79	0.64
7:A:1763:NAG:H62	7:A:1764:NAG:H83	1.79	0.63
1:A:662:ARG:HD2	9:A:2140:HOH:O	1.98	0.63
1:A:71:LYS:HG3	1:A:570:PHE:CE2	2.34	0.62
1:A:171:GLU:HA	1:A:342:VAL:O	1.98	0.62
1:A:509:MET:HB2	1:A:510:PRO:CD	2.30	0.62
1:A:169:MET:HA	1:A:344:MET:O	2.03	0.59
1:A:494:TYR:O	1:A:498:THR:HG22	2.01	0.59
1:A:654:ASP:N	1:A:654:ASP:OD1	2.37	0.58
1:A:155:SER:O	1:A:156:ASP:HB2	2.04	0.56
1:A:205:TYR:CE1	1:A:254:GLN:HB3	2.42	0.54
1:A:494:TYR:CE2	1:A:498:THR:HG21	2.45	0.52
1:A:487:GLY:N	1:A:489:GLU:OE2	2.40	0.52
1:A:242:TYR:CG	1:A:243:PRO:HA	2.45	0.51
1:A:657:ASN:ND2	1:A:660:VAL:CG2	2.42	0.51
1:A:657:ASN:ND2	1:A:660:VAL:H	2.10	0.49
1:A:492:SER:OG	1:A:495:GLU:HG3	2.13	0.48
1:A:386:ILE:O	1:A:390:SER:HB3	2.13	0.48
1:A:175:VAL:HG23	1:A:199:LYS:HG2	1.95	0.47
1:A:104:GLY:O	1:A:406:LYS:HD2	2.14	0.47
1:A:657:ASN:OD1	1:A:658:PRO:HD2	2.15	0.46
1:A:659:ILE:HD13	1:A:659:ILE:HA	1.70	0.45
1:A:164:PHE:CG	1:A:259:LEU:HD21	2.50	0.45
1:A:177:VAL:CG2	1:A:203:ALA:HB2	2.48	0.44
1:A:198:GLY:O	1:A:223:LYS:HD3	2.16	0.44
1:A:405:LEU:HD23	1:A:405:LEU:N	2.33	0.44
1:A:167:GLN:HG2	1:A:347:HIS:HA	2.00	0.43
1:A:660:VAL:O	1:A:664:MET:CG	2.54	0.43
1:A:468:PRO:HA	1:A:471:TYR:CD1	2.54	0.43
1:A:64:GLU:O	1:A:64:GLU:HG3	2.19	0.43
1:A:509:MET:CB	1:A:510:PRO:CD	2.93	0.43
1:A:58:MET:O	1:A:61:PHE:HB3	2.20	0.42
1:A:92:LEU:O	1:A:96:ILE:HG12	2.20	0.41
1:A:90:PHE:CZ	1:A:94:LYS:CD	3.04	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:229:SER:O	1:A:299:TYR:HB3	2.21	0.41
1:A:387:ASP:HA	1:A:388:PRO:HA	1.89	0.40
6:A:1757:NAG:HO6	6:A:1757:NAG:HO3	1.64	0.40
1:A:406:LYS:HA	1:A:410:TRP:O	2.21	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	674/707 (95%)	647 (96%)	24 (4%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	506	PHE
1	A	507	SER
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	547/603 (91%)	529 (97%)	18 (3%)	50	46

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	98	SER
1	A	174	LEU
1	A	205	TYR
1	A	338	SER
1	A	388	PRO
1	A	486	GLU
1	A	498	THR
1	A	519	ASN
1	A	534	ARG
1	A	537	TYR
1	A	547	SER
1	A	589	ASN
1	A	600	TYR
1	A	605	ARG
1	A	654	ASP
1	A	668	LEU
1	A	673	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	136	ASN
1	A	303	GLN
1	A	657	ASN

### 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 ⓘ

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
5	NAG	A	1755	1,5	12,14,15	0.69	0	15,19,21	2.17	3 (20%)
5	NAG	A	1756	5	12,14,15	0.62	0	15,19,21	1.41	1 (6%)
5	NAG	A	1761	1,5	12,14,15	1.15	1 (8%)	15,19,21	1.20	1 (6%)
5	NAG	A	1762	5	12,14,15	0.69	0	15,19,21	0.99	0
7	NAG	A	1763	1,7	12,14,15	0.97	1 (8%)	15,19,21	1.31	2 (13%)
7	NAG	A	1764	7	12,14,15	1.06	1 (8%)	15,19,21	1.60	4 (26%)
7	MAN	A	1765	1,7	10,11,12	0.78	0	11,15,17	2.83	4 (36%)
7	MAN	A	1766	7	10,11,12	0.80	0	11,15,17	1.75	3 (27%)

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	1755	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1756	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1761	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1762	5	-	0/6/23/26	0/1/1/1
7	NAG	A	1763	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1764	7	-	0/6/23/26	0/1/1/1
7	MAN	A	1765	1,7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	A	1766	7	-	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)
7	A	1764	NAG	C2-N2	-2.83	1.43	1.46
7	A	1763	NAG	O5-C5	-2.42	1.40	1.45
5	A	1761	NAG	C2-N2	-2.04	1.43	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1755	NAG	O5-C5-C6	6.56	113.86	106.98

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1765	MAN	O5-C5-C6	6.54	113.85	106.98
7	A	1766	MAN	O5-C5-C6	4.34	111.53	106.98
5	A	1756	NAG	C3-C2-N2	-4.07	105.57	111.76
7	A	1765	MAN	C6-C5-C4	-3.83	103.74	113.00
7	A	1765	MAN	O5-C5-C4	3.55	115.16	110.65
7	A	1765	MAN	O3-C3-C4	-3.34	102.86	110.35
5	A	1761	NAG	C3-C2-N2	-3.34	106.68	111.76
7	A	1764	NAG	C3-C4-C5	-3.07	104.73	110.20
7	A	1766	MAN	C4-C3-C2	-2.66	106.94	110.50
7	A	1763	NAG	O4-C4-C5	-2.53	102.62	109.28
5	A	1755	NAG	O4-C4-C3	-2.49	104.76	110.35
7	A	1766	MAN	O3-C3-C2	2.35	114.24	109.94
7	A	1764	NAG	C3-C2-N2	-2.27	108.30	111.76
5	A	1755	NAG	O5-C5-C4	2.12	113.34	110.65
7	A	1764	NAG	C4-C3-C2	-2.08	106.22	111.32
7	A	1763	NAG	O5-C5-C6	2.06	109.15	106.98
7	A	1764	NAG	C8-C7-N2	2.06	120.14	116.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1765	MAN	C1

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	1757	1	12,14,15	0.42	0	15,19,21	2.02	2 (13%)
6	NAG	A	1758	1	12,14,15	0.99	0	15,19,21	1.17	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	1759	1	12,14,15	0.64	0	15,19,21	1.54	3 (20%)
6	NAG	A	1760	1	12,14,15	0.61	0	15,19,21	2.16	5 (33%)
8	24I	A	1767	2	21,21,21	1.21	3 (14%)	29,29,29	1.57	7 (24%)

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	1757	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1758	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1759	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1760	1	-	0/6/23/26	0/1/1/1
8	24I	A	1767	2	-	0/19/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1767	24I	P1-O2	3.01	1.62	1.54
8	A	1767	24I	P1-O1	2.33	1.57	1.50
8	A	1767	24I	C6-C8	-2.25	1.46	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1757	NAG	O5-C5-C6	6.38	113.68	106.98
6	A	1760	NAG	O5-C5-C6	5.34	112.58	106.98
6	A	1759	NAG	C2-N2-C7	-3.69	116.89	123.09
8	A	1767	24I	C2-C1-I	-2.97	115.14	119.69
8	A	1767	24I	O6-C14-C13	2.97	124.70	114.22
6	A	1760	NAG	O3-C3-C2	2.83	115.03	109.09
6	A	1760	NAG	C3-C2-N2	2.81	116.04	111.76
8	A	1767	24I	C3-C1-I	2.71	123.84	119.69
6	A	1760	NAG	O7-C7-C8	-2.61	116.96	122.04
8	A	1767	24I	O6-C14-O5	-2.49	116.97	123.30
8	A	1767	24I	C3-C5-C8	-2.48	117.40	121.05
6	A	1758	NAG	C3-C2-N2	-2.30	108.25	111.76
6	A	1759	NAG	O5-C5-C6	2.17	109.26	106.98
6	A	1760	NAG	C3-C4-C5	-2.17	106.33	110.20
6	A	1757	NAG	O7-C7-C8	-2.13	117.88	122.04

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1759	NAG	C4-C3-C2	-2.12	106.12	111.32
8	A	1767	24I	C6-P1-C7	-2.10	103.60	107.72
8	A	1767	24I	C4-C8-C5	2.04	121.61	118.16
6	A	1758	NAG	C8-C7-N2	-2.03	112.13	116.11

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1759	NAG	O7-C7-N2-C2

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, 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	682/707 (96%)	-0.17	14 (2%) 60 61	18, 33, 55, 74	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	719	VAL	3.6
1	A	155	SER	2.8
1	A	505	GLU	2.8
1	A	136	ASN	2.8
1	A	651	GLN	2.6
1	A	174	LEU	2.5
1	A	547	SER	2.5
1	A	339	THR	2.4
1	A	504	PRO	2.4
1	A	153	ASN	2.3
1	A	202	ILE	2.1
1	A	237	PRO	2.1
1	A	311	GLY	2.1
1	A	408	GLU	2.1

### 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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	1756	14/15	0.30	13.37	60,62,65,65	0
5	NAG	A	1761	14/15	0.21	7.20	42,46,49,53	0
7	MAN	A	1766	11/12	0.23	5.23	67,69,70,72	0
7	NAG	A	1763	14/15	0.12	3.78	28,31,41,44	0
7	MAN	A	1765	11/12	0.25	3.34	56,62,65,68	0
7	NAG	A	1764	14/15	0.24	3.15	44,48,54,57	0
5	NAG	A	1755	14/15	0.13	2.50	44,51,54,55	0
5	NAG	A	1762	14/15	0.26	0.49	57,61,65,66	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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	A	1759	14/15	0.36	8.50	75,78,80,81	0
6	NAG	A	1757	14/15	0.32	4.90	62,67,69,70	0
6	NAG	A	1760	14/15	0.18	2.91	45,56,60,62	0
6	NAG	A	1758	14/15	0.18	1.34	51,53,56,56	0
3	CA	A	1753	1/1	0.08	-0.33	20,20,20,20	0
8	24I	A	1767	21/21	0.08	-0.52	20,23,35,41	0
2	ZN	A	1752	1/1	0.06	-1.38	23,23,23,23	0
4	CL	A	1754	1/1	0.06	-1.53	27,27,27,27	0
2	ZN	A	1751	1/1	0.06	-1.63	23,23,23,23	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.