



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:55 AM GMT

PDB ID : 2JBJ  
Title : MEMBRANE-BOUND GLUTAMATE CARBOXYPEPTIDASE II (GCP II)  
IN COMPLEX WITH 2-PMPA (2-PHOSPHONOMETHYL-PENTANEDIO  
IC ACID)  
Authors : Mesters, J.R.; Henning, K.; Hilgenfeld, R.  
Deposited on : 2006-12-07  
Resolution : 2.19 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 (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

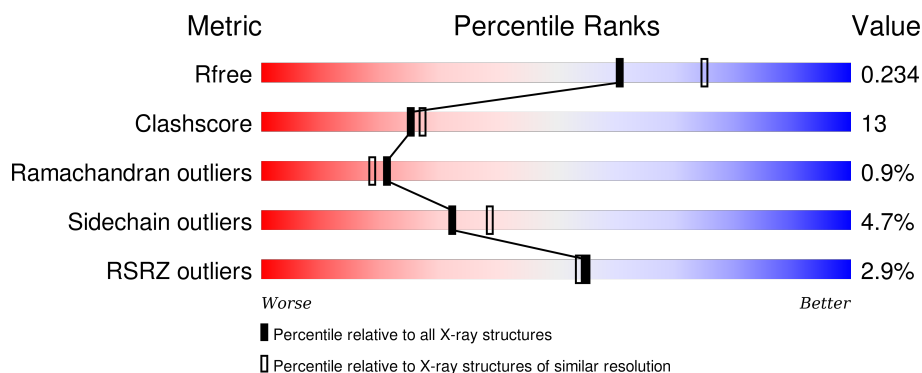
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	707	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>...</div> </div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5914 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called GLUTAMATE CARBOXYPEPTIDASE 2.

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

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

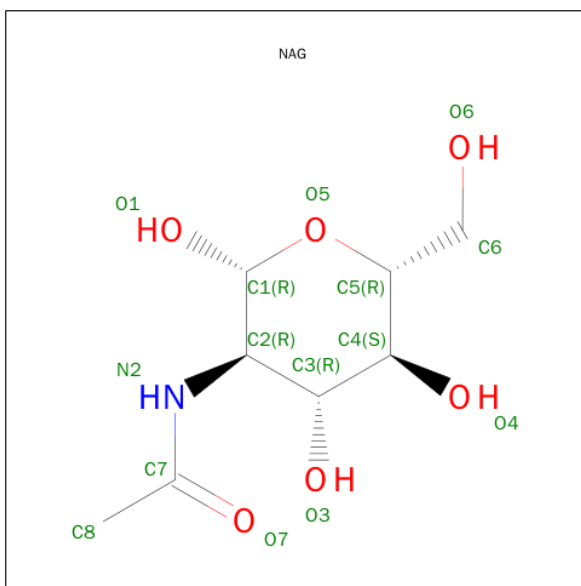
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 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<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

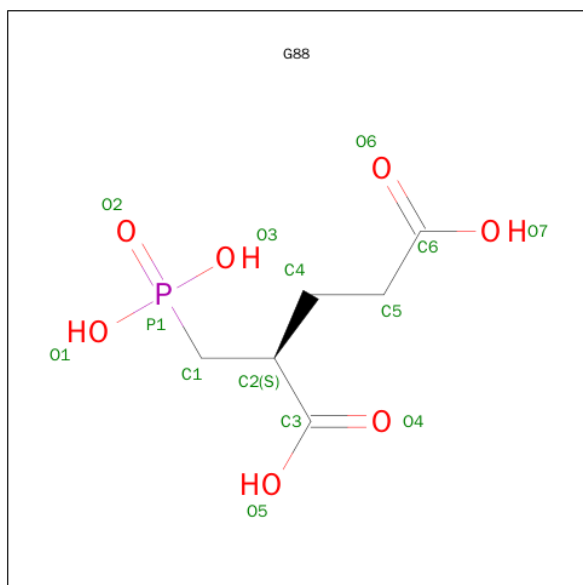


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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-(PHOSPHONOMETHYL)PENTANEDIOIC ACID (three-letter code: G88) (formula: C<sub>6</sub>H<sub>11</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O	P	0	0
			14	6	7	1		

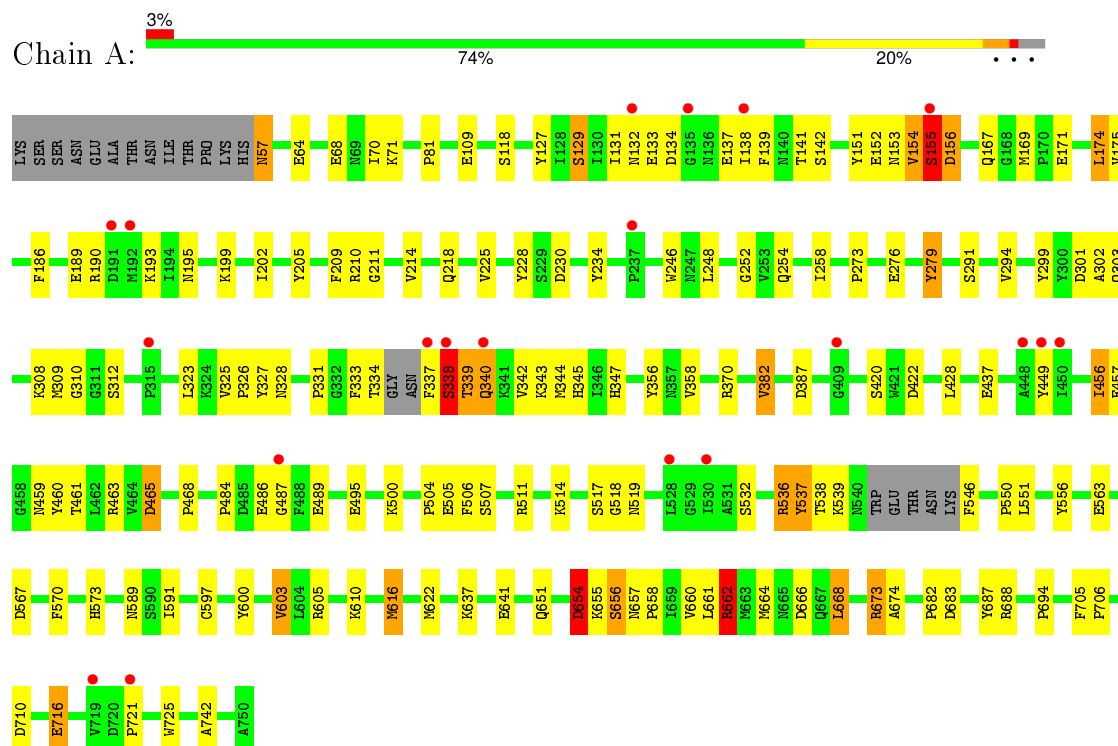
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	402	Total	O	0	0
			402	402		

### 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 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.75Å 130.98Å 159.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.02 – 2.19 32.53 – 2.19	Depositor EDS
% Data completeness (in resolution range)	96.1 (101.02-2.19) 96.1 (32.53-2.19)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.192 , 0.238 0.190 , 0.234	Depositor DCC
$R_{free}$ test set	1344 reflections (2.63%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 52510 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5914	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, CA, G88, 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	1.12	3/5468 (0.1%)	1.00	15/7431 (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	1	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	597	CYS	CB-SG	5.60	1.91	1.82
1	A	603	VAL	CB-CG2	-5.10	1.42	1.52
1	A	279	TYR	CE2-CZ	5.07	1.45	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	662	ARG	NE-CZ-NH1	10.51	125.55	120.30
1	A	662	ARG	NE-CZ-NH2	-10.11	115.25	120.30
1	A	654	ASP	CB-CG-OD2	-8.54	110.61	118.30
1	A	370	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	A	387	ASP	CB-CG-OD2	6.67	124.30	118.30
1	A	339	THR	N-CA-C	-6.21	94.23	111.00
1	A	156	ASP	N-CA-C	5.73	126.47	111.00
1	A	514	LYS	CD-CE-NZ	-5.69	98.61	111.70
1	A	654	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	668	LEU	CB-CG-CD1	5.65	120.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	210	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	A	688	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	428	LEU	CB-CG-CD1	5.10	119.67	111.00
1	A	710	ASP	CB-CG-OD1	5.10	122.89	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	156	ASP	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	SER	Peptide
1	A	155	SER	Peptide
1	A	338	SER	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5318	0	5004	127	0
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	5	0
6	A	42	0	39	2	0
7	A	50	0	43	3	0
8	A	14	0	8	0	0
9	A	402	0	0	39	0
All	All	5914	0	5169	134	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 13.

All (134) 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:657:ASN:ND2	1:A:660:VAL:HG23	1.71	1.05
1:A:651:GLN:CG	9:A:2143:HOH:O	2.05	1.03
1:A:616:MET:HE3	1:A:616:MET:HA	1.44	0.98
7:A:1767:MAN:H61	9:A:2399:HOH:O	1.66	0.95
1:A:589:ASN:HB2	9:A:2264:HOH:O	1.65	0.95
1:A:563:GLU:HG2	9:A:2255:HOH:O	1.70	0.91
1:A:657:ASN:ND2	1:A:660:VAL:CG2	2.36	0.88
7:A:1766:BMA:H5	9:A:2396:HOH:O	1.75	0.86
1:A:134:ASP:CA	9:A:2036:HOH:O	2.31	0.77
1:A:133:GLU:CA	9:A:2035:HOH:O	2.33	0.74
1:A:57:ASN:N	9:A:2001:HOH:O	2.21	0.73
1:A:133:GLU:N	9:A:2035:HOH:O	2.21	0.73
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.69	0.73
1:A:657:ASN:HD22	1:A:660:VAL:CG2	2.00	0.72
1:A:109:GLU:HG2	9:A:2020:HOH:O	1.89	0.72
1:A:338:SER:HB2	1:A:339:THR:HB	1.72	0.71
1:A:660:VAL:O	1:A:664:MET:HG2	1.90	0.71
1:A:154:VAL:CA	9:A:2055:HOH:O	2.39	0.70
1:A:654:ASP:OD1	1:A:656:SER:HB3	1.92	0.69
5:A:1755:NAG:H61	5:A:1756:NAG:C1	2.22	0.69
1:A:616:MET:HA	1:A:616:MET:CE	2.22	0.69
1:A:337:PHE:N	9:A:2154:HOH:O	2.27	0.68
1:A:167:GLN:HG2	1:A:347:HIS:HA	1.77	0.67
7:A:1767:MAN:H2	9:A:2398:HOH:O	1.96	0.66
1:A:193:LYS:CB	9:A:2034:HOH:O	2.44	0.65
1:A:716:GLU:CD	1:A:716:GLU:H	2.00	0.65
1:A:138:ILE:N	1:A:138:ILE:HD13	2.11	0.64
1:A:151:TYR:C	1:A:153:ASN:H	1.99	0.64
1:A:486:GLU:CG	9:A:2220:HOH:O	2.45	0.64
1:A:174:LEU:HD22	1:A:342:VAL:HG21	1.79	0.64
1:A:132:ASN:HD22	1:A:138:ILE:HD11	1.63	0.63
5:A:1762:NAG:H83	9:A:2217:HOH:O	1.98	0.63
1:A:337:PHE:O	1:A:339:THR:N	2.32	0.62
1:A:657:ASN:HD22	1:A:660:VAL:HG21	1.62	0.62
1:A:131:ILE:HD11	1:A:171:GLU:OE2	1.99	0.62
1:A:68:GLU:CG	9:A:2010:HOH:O	2.47	0.62
1:A:657:ASN:HD21	1:A:660:VAL:HG23	1.62	0.61
1:A:151:TYR:C	1:A:153:ASN:N	2.49	0.61
1:A:637:LYS:NZ	1:A:641:GLU:OE1	2.32	0.61
1:A:616:MET:HE3	1:A:622:MET:SD	2.41	0.60
1:A:189:GLU:CB	9:A:2081:HOH:O	2.49	0.60
1:A:456:ILE:HD12	1:A:573:HIS:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ILE:O	1:A:456:ILE:HG12	1.99	0.60
1:A:682:PRO:O	1:A:683:ASP:HB2	2.00	0.60
1:A:591:ILE:HG23	1:A:661:LEU:HD21	1.82	0.60
1:A:654:ASP:OD1	1:A:656:SER:CB	2.50	0.59
5:A:1755:NAG:H82	9:A:2012:HOH:O	2.01	0.59
1:A:589:ASN:CB	9:A:2264:HOH:O	2.36	0.58
1:A:563:GLU:CG	9:A:2255:HOH:O	2.39	0.57
1:A:171:GLU:HA	1:A:342:VAL:O	2.05	0.57
1:A:246:TRP:CD1	6:A:1761:NAG:H83	2.41	0.56
1:A:131:ILE:HG22	1:A:137:GLU:HG3	1.88	0.56
1:A:209:PHE:CE2	1:A:211:GLY:HA3	2.40	0.56
1:A:539:LYS:CD	9:A:2248:HOH:O	2.53	0.56
1:A:308:LYS:O	1:A:333:PHE:HB3	2.05	0.56
1:A:460:TYR:CE1	1:A:500:LYS:HD3	2.41	0.56
1:A:505:GLU:CA	9:A:2223:HOH:O	2.53	0.56
5:A:1756:NAG:H81	9:A:2383:HOH:O	2.06	0.55
1:A:225:VAL:O	1:A:294:VAL:HA	2.06	0.55
1:A:234:TYR:O	1:A:550:PRO:HB3	2.06	0.55
1:A:309:MET:HE2	1:A:328:ASN:O	2.06	0.55
1:A:616:MET:CE	1:A:622:MET:SD	2.96	0.54
1:A:459:ASN:OD1	6:A:1761:NAG:H2	2.07	0.54
1:A:337:PHE:O	1:A:338:SER:C	2.46	0.54
1:A:171:GLU:HB3	1:A:343:LYS:HG3	1.90	0.54
1:A:666:ASP:OD2	9:A:2322:HOH:O	2.18	0.53
1:A:129:SER:HA	1:A:139:PHE:O	2.09	0.53
1:A:468:PRO:HG2	1:A:603:VAL:HG21	1.90	0.53
1:A:138:ILE:O	5:A:1758:NAG:H82	2.08	0.53
1:A:175:VAL:HG23	1:A:199:LYS:HG3	1.91	0.53
1:A:109:GLU:HB2	9:A:2089:HOH:O	2.08	0.53
1:A:228:TYR:CE1	1:A:230:ASP:HB2	2.44	0.53
1:A:457:GLU:OE2	1:A:538:THR:OG1	2.23	0.53
1:A:456:ILE:HD12	1:A:573:HIS:HE1	1.74	0.52
1:A:279:TYR:HD2	9:A:2129:HOH:O	1.93	0.52
1:A:662:ARG:HD2	9:A:2322:HOH:O	2.10	0.51
1:A:495:GLU:CB	9:A:2098:HOH:O	2.58	0.51
1:A:248:LEU:HD11	1:A:252:GLY:HA3	1.92	0.51
1:A:57:ASN:HD22	1:A:57:ASN:N	2.10	0.50
1:A:457:GLU:HG3	1:A:538:THR:HA	1.92	0.49
1:A:310:GLY:O	1:A:328:ASN:HB3	2.13	0.49
1:A:326:PRO:O	1:A:327:TYR:HB2	2.13	0.49
1:A:465:ASP:OD1	1:A:465:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:SER:C	9:A:2225:HOH:O	2.52	0.48
1:A:334:THR:C	9:A:2152:HOH:O	2.52	0.48
1:A:273:PRO:HB3	1:A:437:GLU:HB2	1.96	0.48
1:A:463:ARG:HD3	1:A:536:ARG:CZ	2.44	0.48
1:A:70:ILE:HG21	1:A:573:HIS:HB3	1.96	0.47
1:A:141:THR:HG22	1:A:301:ASP:HB3	1.96	0.47
1:A:687:TYR:CZ	1:A:694:PRO:HG2	2.49	0.47
1:A:656:SER:O	1:A:658:PRO:HD3	2.14	0.47
1:A:489:GLU:H	1:A:489:GLU:CD	2.18	0.47
1:A:721:PRO:O	1:A:725:TRP:HD1	1.98	0.47
1:A:589:ASN:CG	9:A:2264:HOH:O	2.50	0.46
1:A:129:SER:HB3	1:A:137:GLU:HG2	1.96	0.46
1:A:186:PHE:O	1:A:190:ARG:HB2	2.15	0.46
1:A:546:PHE:N	9:A:2243:HOH:O	2.48	0.46
1:A:64:GLU:HG3	1:A:64:GLU:O	2.15	0.46
1:A:132:ASN:ND2	1:A:138:ILE:HD11	2.29	0.46
1:A:258:ILE:HD13	1:A:294:VAL:HB	1.98	0.46
1:A:487:GLY:HA2	1:A:489:GLU:OE2	2.17	0.45
1:A:299:TYR:HA	1:A:302:ALA:HB3	1.98	0.45
1:A:674:ALA:HB1	1:A:742:ALA:HA	1.99	0.45
1:A:449:TYR:O	1:A:532:SER:HA	2.17	0.45
1:A:205:TYR:CE1	1:A:254:GLN:HB3	2.52	0.45
1:A:517:SER:HB2	1:A:694:PRO:HG3	1.99	0.44
1:A:127:TYR:O	1:A:345:HIS:HD2	2.00	0.44
1:A:276:GLU:H	1:A:276:GLU:HG2	1.66	0.44
1:A:517:SER:OG	1:A:518:GLY:N	2.50	0.44
1:A:155:SER:O	1:A:156:ASP:CB	2.66	0.44
1:A:214:VAL:O	1:A:218:GLN:HB2	2.18	0.43
1:A:461:THR:HA	1:A:537:TYR:CE2	2.53	0.43
1:A:655:LYS:HB2	9:A:2317:HOH:O	2.18	0.43
1:A:308:LYS:O	1:A:333:PHE:CB	2.66	0.43
1:A:504:PRO:HG3	1:A:511:ARG:NH2	2.33	0.43
1:A:81:PRO:HA	1:A:382:VAL:O	2.18	0.43
1:A:155:SER:O	1:A:156:ASP:CG	2.57	0.43
1:A:507:SER:CA	9:A:2225:HOH:O	2.66	0.42
1:A:169:MET:HA	1:A:344:MET:O	2.19	0.42
1:A:610:LYS:CG	9:A:2151:HOH:O	2.67	0.42
1:A:487:GLY:CA	1:A:489:GLU:OE2	2.68	0.42
1:A:218:GLN:OE1	1:A:291:SER:N	2.34	0.42
1:A:358:VAL:HB	1:A:420:SER:HB3	2.02	0.42
1:A:195:ASN:HB3	9:A:2083:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ASP:OD2	1:A:570:PHE:HA	2.19	0.41
1:A:705:PHE:N	1:A:706:PRO:CD	2.83	0.41
1:A:334:THR:HG22	9:A:2152:HOH:O	2.19	0.41
1:A:325:VAL:HB	1:A:326:PRO:HD2	2.03	0.41
1:A:174:LEU:O	1:A:331:PRO:HA	2.21	0.41
1:A:71:LYS:HG3	1:A:570:PHE:CE2	2.56	0.41
1:A:486:GLU:CB	9:A:2220:HOH:O	2.69	0.40
1:A:131:ILE:O	1:A:340:GLN:HB3	2.22	0.40
1:A:308:LYS:O	1:A:333:PHE:HA	2.21	0.40
1:A:356:TYR:O	1:A:422:ASP:HB2	2.22	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	681/707 (96%)	640 (94%)	35 (5%)	6 (1%)	21	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	VAL
1	A	338	SER
1	A	506	PHE
1	A	152	GLU
1	A	155	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	536/603 (89%)	511 (95%)	25 (5%)	32	39

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

Mol	Chain	Res	Type
1	A	57	ASN
1	A	118	SER
1	A	142	SER
1	A	155	SER
1	A	174	LEU
1	A	202	ILE
1	A	303	GLN
1	A	312	SER
1	A	323	LEU
1	A	340	GLN
1	A	456	ILE
1	A	465	ASP
1	A	484	PRO
1	A	519	ASN
1	A	536	ARG
1	A	537	TYR
1	A	600	TYR
1	A	605	ARG
1	A	616	MET
1	A	654	ASP
1	A	656	SER
1	A	662	ARG
1	A	668	LEU
1	A	673	ARG
1	A	716	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	GLN
1	A	618	HIS
1	A	657	ASN

### 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 ⓘ

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	1755	1,5	14,14,15	0.65	0	15,19,21	2.04	5 (33%)
5	NAG	A	1756	5	14,14,15	0.74	0	15,19,21	1.98	5 (33%)
5	NAG	A	1758	1,5	14,14,15	0.94	2 (14%)	15,19,21	1.51	2 (13%)
5	NAG	A	1759	5	14,14,15	0.71	0	15,19,21	1.85	2 (13%)
5	NAG	A	1762	1,5	14,14,15	1.07	0	15,19,21	1.64	1 (6%)
5	NAG	A	1763	5	14,14,15	0.60	0	15,19,21	1.86	2 (13%)
7	NAG	A	1764	1,7	14,14,15	0.78	0	15,19,21	1.56	4 (26%)
7	NAG	A	1765	7	14,14,15	0.76	0	15,19,21	1.56	2 (13%)
7	BMA	A	1766	7	11,11,12	0.82	0	14,15,17	1.87	4 (28%)
7	MAN	A	1767	7	11,11,12	0.59	0	14,15,17	1.58	2 (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
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	1758	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1759	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1762	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1763	5	-	0/6/23/26	0/1/1/1
7	NAG	A	1764	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1765	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1766	7	-	0/2/19/22	1/1/1/1
7	MAN	A	1767	7	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1758	NAG	C4-C5	2.10	1.57	1.53
5	A	1758	NAG	C1-C2	2.30	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1763	NAG	C2-N2-C7	-5.60	115.85	123.04
5	A	1755	NAG	C2-N2-C7	-5.45	116.04	123.04
5	A	1755	NAG	C3-C4-C5	-2.88	105.18	110.20
5	A	1755	NAG	O4-C4-C3	-2.81	104.02	110.34
7	A	1766	BMA	O3-C3-C4	-2.80	104.03	110.34
7	A	1764	NAG	C6-C5-C4	-2.56	106.70	113.02
7	A	1764	NAG	C2-N2-C7	-2.43	119.91	123.04
5	A	1756	NAG	O7-C7-N2	-2.17	117.44	121.86
5	A	1756	NAG	C4-C3-C2	2.01	114.36	111.23
5	A	1758	NAG	O4-C4-C5	2.04	114.64	109.24
5	A	1755	NAG	O5-C5-C6	2.14	111.98	107.35
7	A	1764	NAG	C4-C3-C2	2.25	114.72	111.23
7	A	1766	BMA	C3-C4-C5	2.34	114.27	110.20
7	A	1766	BMA	O5-C1-C2	2.34	114.66	110.86
7	A	1765	NAG	C8-C7-N2	2.37	120.65	116.11
5	A	1763	NAG	C1-O5-C5	2.40	115.29	112.25
5	A	1756	NAG	C8-C7-N2	2.61	121.10	116.11
5	A	1755	NAG	O3-C3-C2	2.68	114.42	109.11
7	A	1767	MAN	O2-C2-C1	2.94	115.10	109.21
7	A	1764	NAG	C1-O5-C5	3.05	116.12	112.25
5	A	1759	NAG	C4-C3-C2	3.48	116.64	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1758	NAG	C1-O5-C5	3.81	117.08	112.25
7	A	1767	MAN	O5-C5-C6	3.82	115.62	107.35
7	A	1765	NAG	C1-O5-C5	4.18	117.55	112.25
5	A	1756	NAG	C1-O5-C5	4.33	117.74	112.25
5	A	1756	NAG	C2-N2-C7	4.37	128.66	123.04
5	A	1759	NAG	C1-O5-C5	4.52	117.99	112.25
7	A	1766	BMA	C1-O5-C5	4.52	117.99	112.25
5	A	1762	NAG	C1-O5-C5	4.87	118.43	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1766	BMA	C1-C2-C3-C4-C5-O5

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1755	NAG	2	0
5	A	1756	NAG	2	0
5	A	1758	NAG	1	0
5	A	1762	NAG	1	0
7	A	1766	BMA	1	0
7	A	1767	MAN	2	0

## 5.6 Ligand geometry [i](#)

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	1757	1	14,14,15	0.78	0	15,19,21	1.93	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	1760	1	14,14,15	1.21	1 (7%)	15,19,21	2.43	3 (20%)
6	NAG	A	1761	1	14,14,15	0.68	1 (7%)	15,19,21	2.87	6 (40%)
8	G88	A	1768	2	6,13,13	5.56	2 (33%)	10,18,18	2.06	4 (40%)

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	-	1/6/23/26	0/1/1/1
6	NAG	A	1760	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1761	1	-	0/6/23/26	0/1/1/1
8	G88	A	1768	2	-	0/8/14/14	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1761	NAG	C1-C2	2.14	1.55	1.52
6	A	1760	NAG	C1-C2	2.57	1.56	1.52
8	A	1768	G88	P1-O3	6.98	1.71	1.54
8	A	1768	G88	P1-O2	11.63	1.76	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1761	NAG	C4-C3-C2	-7.96	98.85	111.23
6	A	1757	NAG	C2-N2-C7	-4.35	117.45	123.04
6	A	1761	NAG	C3-C4-C5	-3.93	103.34	110.20
8	A	1768	G88	O2-P1-C1	-3.23	104.27	111.25
6	A	1760	NAG	C4-C3-C2	-2.97	106.62	111.23
8	A	1768	G88	C4-C2-C3	-2.49	105.84	111.95
6	A	1757	NAG	C1-O5-C5	-2.46	109.13	112.25
6	A	1761	NAG	C2-N2-C7	-2.45	119.89	123.04
8	A	1768	G88	O3-P1-O2	-2.17	106.85	112.40
6	A	1757	NAG	C4-C3-C2	2.25	114.73	111.23
6	A	1760	NAG	O3-C3-C2	2.38	113.83	109.11
6	A	1761	NAG	O3-C3-C2	2.83	114.72	109.11
6	A	1761	NAG	O4-C4-C5	2.85	116.79	109.24
6	A	1757	NAG	O5-C5-C6	3.51	114.95	107.35
8	A	1768	G88	O3-P1-C1	4.02	116.69	106.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1761	NAG	C1-O5-C5	4.16	117.53	112.25
6	A	1760	NAG	C1-O5-C5	7.92	122.30	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1757	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1761	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	687/707 (97%)	-0.02	20 (2%) 55 54	25, 41, 68, 75	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	SER	5.6
1	A	487	GLY	4.0
1	A	719	VAL	3.9
1	A	448	ALA	3.1
1	A	135	GLY	3.0
1	A	409	GLY	2.7
1	A	337	PHE	2.7
1	A	132	ASN	2.6
1	A	191	ASP	2.6
1	A	530	ILE	2.6
1	A	450	ILE	2.6
1	A	237	PRO	2.3
1	A	338	SER	2.3
1	A	721	PRO	2.3
1	A	340	GLN	2.3
1	A	192	MET	2.2
1	A	449	TYR	2.2
1	A	315	PRO	2.1
1	A	528	LEU	2.0
1	A	138	ILE	2.0

### 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 [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
5	NAG	A	1758	14/15	0.85	0.24	1.92	68,72,75,75	0
7	MAN	A	1767	11/12	0.93	0.13	1.67	75,75,75,75	0
7	NAG	A	1764	14/15	0.97	0.06	-1.19	29,43,58,62	0
5	NAG	A	1759	14/15	0.89	0.38	-	75,75,75,75	0
7	NAG	A	1765	14/15	0.88	0.13	-	67,72,75,75	0
5	NAG	A	1762	14/15	0.94	0.12	-	46,50,53,55	0
5	NAG	A	1756	14/15	0.78	0.37	-	72,75,75,75	0
5	NAG	A	1763	14/15	0.96	0.22	-	57,61,67,70	0
5	NAG	A	1755	14/15	0.95	0.14	-	53,60,66,72	0
7	BMA	A	1766	11/12	0.91	0.14	-	74,75,75,75	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
8	G88	A	1768	14/14	0.99	0.13	0.07	29,34,39,40	0
3	CA	A	1753	1/1	1.00	0.08	-0.49	30,30,30,30	0
4	CL	A	1754	1/1	0.99	0.15	-0.63	37,37,37,37	0
2	ZN	A	1751	1/1	1.00	0.07	-3.64	51,51,51,51	0
2	ZN	A	1752	1/1	0.99	0.07	-4.15	49,49,49,49	0
6	NAG	A	1760	14/15	0.62	0.35	-	75,75,75,75	0
6	NAG	A	1761	14/15	0.85	0.18	-	52,70,75,75	0
6	NAG	A	1757	14/15	0.83	0.31	-	73,75,75,75	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.