



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:40 PM GMT

PDB ID : 4MCS  
Title : A high resolution structure of human glutamate carboxypeptidase II (GCP II)  
His475Tyr variant in complex with glutamic acid  
Authors : Ptacek, J.; Barinka, C.; Sacha, P.; Navratil, M.  
Deposited on : 2013-08-21  
Resolution : 1.83 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

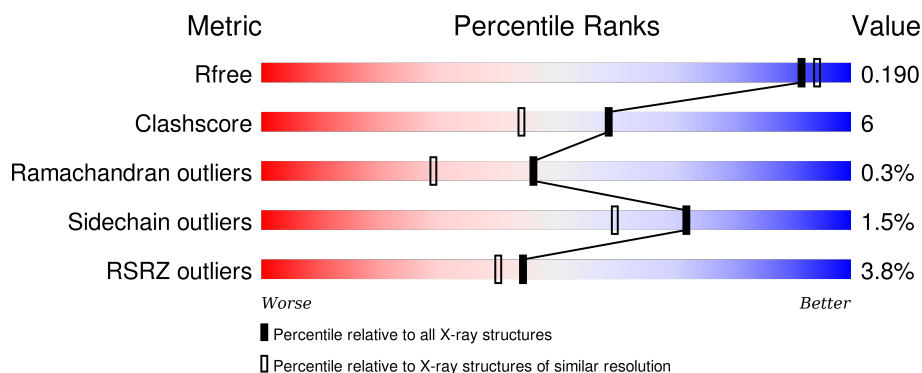
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.83 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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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	757	

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	802	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6485 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
			Total	C	N	O	S			
1	A	691	5702	3667	951	1063	21	0	45	0

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	INITIATING METHIONINE	UNP Q04609
A	-5	LYS	-	EXPRESSION TAG	UNP Q04609
A	-4	LEU	-	EXPRESSION TAG	UNP Q04609
A	-3	CYS	-	EXPRESSION TAG	UNP Q04609
A	-2	ILE	-	EXPRESSION TAG	UNP Q04609
A	-1	LEU	-	EXPRESSION TAG	UNP Q04609
A	0	LEU	-	EXPRESSION TAG	UNP Q04609
A	1	ALA	-	EXPRESSION TAG	UNP Q04609
A	2	VAL	-	EXPRESSION TAG	UNP Q04609
A	3	VAL	-	EXPRESSION TAG	UNP Q04609
A	4	ALA	-	EXPRESSION TAG	UNP Q04609
A	5	PHE	-	EXPRESSION TAG	UNP Q04609
A	6	VAL	-	EXPRESSION TAG	UNP Q04609
A	7	GLY	-	EXPRESSION TAG	UNP Q04609
A	8	LEU	-	EXPRESSION TAG	UNP Q04609
A	9	SER	-	EXPRESSION TAG	UNP Q04609
A	10	LEU	-	EXPRESSION TAG	UNP Q04609
A	11	GLY	-	EXPRESSION TAG	UNP Q04609
A	12	ARG	-	EXPRESSION TAG	UNP Q04609
A	13	SER	-	EXPRESSION TAG	UNP Q04609
A	14	GLY	-	EXPRESSION TAG	UNP Q04609
A	15	LEU	-	EXPRESSION TAG	UNP Q04609
A	16	ASN	-	EXPRESSION TAG	UNP Q04609
A	17	ASP	-	EXPRESSION TAG	UNP Q04609
A	18	ILE	-	EXPRESSION TAG	UNP Q04609
A	19	PHE	-	EXPRESSION TAG	UNP Q04609
A	20	GLU	-	EXPRESSION TAG	UNP Q04609

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Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	-	EXPRESSION TAG	UNP Q04609
A	22	GLN	-	EXPRESSION TAG	UNP Q04609
A	23	LYS	-	EXPRESSION TAG	UNP Q04609
A	24	ILE	-	EXPRESSION TAG	UNP Q04609
A	25	GLU	-	EXPRESSION TAG	UNP Q04609
A	26	TRP	-	EXPRESSION TAG	UNP Q04609
A	27	HIS	-	EXPRESSION TAG	UNP Q04609
A	28	GLU	-	EXPRESSION TAG	UNP Q04609
A	29	GLY	-	EXPRESSION TAG	UNP Q04609
A	30	SER	-	EXPRESSION TAG	UNP Q04609
A	31	GLY	-	EXPRESSION TAG	UNP Q04609
A	32	SER	-	EXPRESSION TAG	UNP Q04609
A	33	GLY	-	EXPRESSION TAG	UNP Q04609
A	34	SER	-	EXPRESSION TAG	UNP Q04609
A	35	GLU	-	EXPRESSION TAG	UNP Q04609
A	36	ASN	-	EXPRESSION TAG	UNP Q04609
A	37	LEU	-	EXPRESSION TAG	UNP Q04609
A	38	TYR	-	EXPRESSION TAG	UNP Q04609
A	39	PHE	-	EXPRESSION TAG	UNP Q04609
A	40	GLN	-	EXPRESSION TAG	UNP Q04609
A	41	GLY	-	EXPRESSION TAG	UNP Q04609
A	42	ARG	-	EXPRESSION TAG	UNP Q04609
A	43	SER	-	EXPRESSION TAG	UNP Q04609
A	475	TYR	HIS	ENGINEERED MUTATION	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:  $C_8H_{15}NO_6$ ).



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		

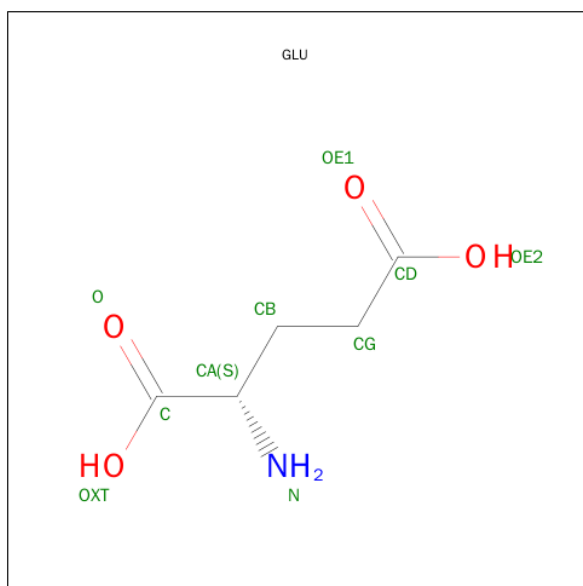
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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).

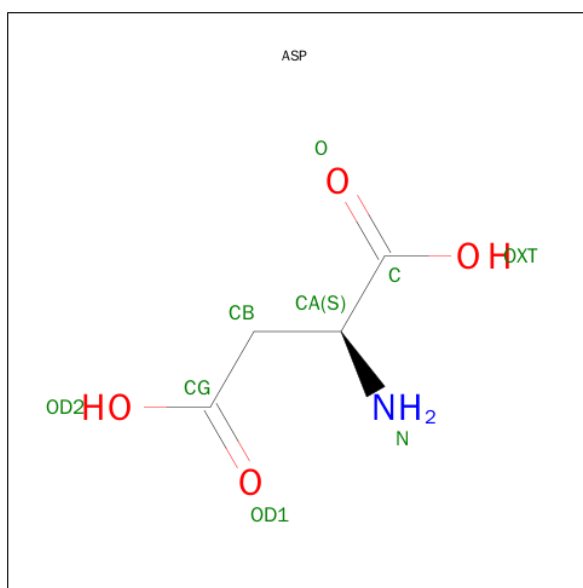
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Cl		0	0
			1	1			

- Molecule 8 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $C_5H_9NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 9 is ASPARTIC ACID (three-letter code: ASP) (formula:  $C_4H_7NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			9	4	1	4		

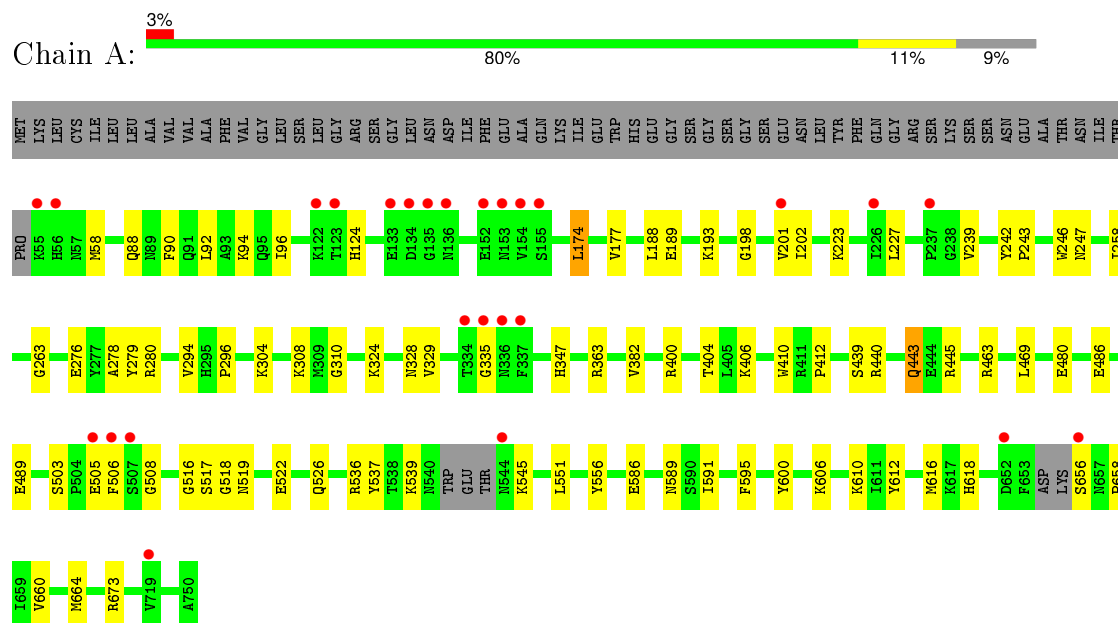
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	584	Total	O	0	0
			584	584		

### 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, $\alpha$ , $\beta$ , $\gamma$	101.55Å 130.40Å 158.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.53 – 1.83 28.53 – 1.83	Depositor EDS
% Data completeness (in resolution range)	93.0 (28.53-1.83) 93.0 (28.53-1.83)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.159 , 0.191 0.158 , 0.190	Depositor DCC
$R_{free}$ test set	1734 reflections (2.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 86607 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6485	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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, 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	0.91	0/5994	0.77	4/8114 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	440	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	445	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	A	174[A]	LEU	CA-CB-CG	5.09	127.00	115.30
1	A	174[B]	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	5702	0	5586	64	2
2	A	84	0	75	3	0
3	A	42	0	39	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	10	0	5	0	0
9	A	9	0	3	1	0
10	A	584	0	0	25	3
All	All	6485	0	5751	68	3

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 6.

All (68) 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	1.42	1.16
1:A:412:PRO:HA	1:A:589[B]:ASN:HD21	1.29	0.94
1:A:658[A]:PRO:HB3	10:A:1261:HOH:O	1.69	0.90
1:A:400:ARG:O	1:A:404[B]:THR:HG23	1.80	0.82
1:A:363[B]:ARG:NH2	10:A:1461:HOH:O	2.11	0.79
1:A:508:GLY:O	10:A:1463:HOH:O	2.01	0.79
1:A:463:ARG:HH21	1:A:545:LYS:HE3	1.55	0.71
1:A:276[B]:GLU:OE1	10:A:1187:HOH:O	2.11	0.69
1:A:363[B]:ARG:HD2	10:A:1460:HOH:O	1.93	0.68
1:A:480:GLU:HG3	10:A:1468:HOH:O	1.96	0.66
1:A:463:ARG:NH2	1:A:545:LYS:HG3	2.11	0.65
1:A:505:GLU:HG3	1:A:606[A]:LYS:HD2	1.80	0.63
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.35	0.62
1:A:58:MET:CE	1:A:586[A]:GLU:HG2	2.30	0.61
2:A:802:NAG:H81	10:A:1155:HOH:O	2.01	0.60
9:A:819:ASP:N	10:A:1435:HOH:O	2.35	0.59
2:A:809:NAG:C8	10:A:1117:HOH:O	2.51	0.58
1:A:58:MET:HE1	1:A:586[A]:GLU:HG2	1.86	0.58
1:A:506:PHE:CE1	1:A:606[B]:LYS:NZ	2.74	0.56
1:A:88:GLN:HG2	10:A:1114:HOH:O	2.06	0.56
2:A:809:NAG:H83	10:A:1117:HOH:O	2.06	0.54
1:A:526[A]:GLN:NE2	10:A:1441:HOH:O	2.34	0.54
1:A:586[B]:GLU:HG2	10:A:1180:HOH:O	2.09	0.52
1:A:439:SER:O	1:A:443[A]:GLN:HB2	2.10	0.52
1:A:443[B]:GLN:HG3	1:A:443[B]:GLN:O	2.05	0.52
1:A:88:GLN:CG	10:A:1114:HOH:O	2.58	0.52
1:A:443[B]:GLN:NE2	10:A:935:HOH:O	2.44	0.51
1:A:188:LEU:HD21	1:A:329:VAL:HG11	1.93	0.50
1:A:239[A]:VAL:HG22	1:A:247:ASN:ND2	2.27	0.49
1:A:618:HIS:HE1	10:A:1046:HOH:O	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:PRO:HA	1:A:589[B]:ASN:ND2	2.11	0.49
1:A:90:PHE:CZ	1:A:94:LYS:HD2	2.48	0.49
1:A:610:LYS:NZ	10:A:1466:HOH:O	2.46	0.48
1:A:198:GLY:O	1:A:223:LYS:HE2	2.14	0.48
1:A:591[A]:ILE:HD12	10:A:1459:HOH:O	2.14	0.47
1:A:347:HIS:HE1	10:A:1245:HOH:O	1.97	0.47
1:A:124:HIS:CD2	1:A:347:HIS:CG	3.03	0.47
1:A:276[B]:GLU:HB2	10:A:1071:HOH:O	2.15	0.45
1:A:242:TYR:CG	1:A:243:PRO:HA	2.52	0.45
1:A:517:SER:OG	1:A:518:GLY:N	2.49	0.44
1:A:658[B]:PRO:HA	10:A:1261:HOH:O	2.17	0.44
1:A:516:GLY:O	1:A:526[B]:GLN:NE2	2.48	0.43
1:A:278:ALA:HB3	1:A:280[A]:ARG:NH1	2.34	0.43
1:A:486:GLU:OE1	10:A:1157:HOH:O	2.20	0.43
1:A:188:LEU:CD2	1:A:329:VAL:HG11	2.48	0.43
1:A:258:ILE:HD13	1:A:294:VAL:HB	2.01	0.43
1:A:503:SER:HB3	1:A:506:PHE:O	2.17	0.43
1:A:177:VAL:CG1	1:A:201[B]:VAL:HG22	2.49	0.43
1:A:188:LEU:HD21	1:A:329:VAL:CG1	2.48	0.43
1:A:310:GLY:O	1:A:328:ASN:HB3	2.19	0.43
1:A:304:LYS:HE3	10:A:1144:HOH:O	2.19	0.42
1:A:406:LYS:HA	1:A:410:TRP:O	2.19	0.42
1:A:58:MET:HE2	1:A:586[A]:GLU:HG2	2.00	0.42
1:A:469:LEU:O	1:A:595:PHE:HA	2.20	0.42
1:A:92:LEU:O	1:A:96:ILE:HG12	2.19	0.42
1:A:308:LYS:HB2	10:A:1243:HOH:O	2.20	0.42
1:A:489:GLU:CD	1:A:489:GLU:H	2.23	0.41
1:A:324:LYS:HD2	1:A:324:LYS:HA	1.88	0.41
1:A:258:ILE:HD12	1:A:294:VAL:HG21	2.02	0.41
1:A:246:TRP:CD1	3:A:807:NAG:H83	2.55	0.41
1:A:174[A]:LEU:HG	1:A:202:ILE:HG22	2.03	0.41
1:A:551:LEU:HD22	1:A:556:TYR:HB2	2.03	0.41
1:A:227:LEU:O	1:A:296:PRO:HA	2.20	0.41
1:A:58:MET:HE1	1:A:586[A]:GLU:CG	2.50	0.41
1:A:263:GLY:HA2	1:A:522:GLU:OE1	2.21	0.41
1:A:243:PRO:HD3	10:A:1443:HOH:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656[B]:SER:O	10:A:1261:HOH:O[4_566]	1.92	0.28
10:A:1122:HOH:O	10:A:1445:HOH:O[2_565]	1.93	0.27
1:A:656[B]:SER:OG	10:A:1261:HOH:O[4_566]	2.01	0.19

## 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	726 / 757 (96%)	708 (98%)	16 (2%)	2 (0%)	46 29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	GLY
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	630 / 643 (98%)	618 (98%)	12 (2%)	65 50

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189[A]	GLU
1	A	189[B]	GLU

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Mol	Chain	Res	Type
1	A	193	LYS
1	A	443[A]	GLN
1	A	443[B]	GLN
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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	303	GLN
1	A	618	HIS

### 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	$\# Z  > 2$
2	NAG	A	801	1,2	14,14,15	0.52	0	15,19,21	1.17	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	802	2	14,14,15	0.66	0	15,19,21	0.99	1 (6%)
2	NAG	A	804	1,2	14,14,15	0.50	0	15,19,21	1.21	1 (6%)
2	NAG	A	805	2	14,14,15	0.50	0	15,19,21	1.17	3 (20%)
2	NAG	A	808	1,2	14,14,15	0.78	1 (7%)	15,19,21	0.75	0
2	NAG	A	809	2	14,14,15	0.52	0	15,19,21	1.23	2 (13%)
4	NAG	A	810	1,4	14,14,15	0.56	0	15,19,21	1.52	3 (20%)
4	NAG	A	811	4	14,14,15	0.62	0	15,19,21	1.71	5 (33%)
4	BMA	A	812	4	11,11,12	0.45	0	14,15,17	1.46	2 (14%)
4	MAN	A	813	4	11,11,12	0.68	0	14,15,17	1.47	3 (21%)

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	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	802	2	-	0/6/23/26	0/1/1/1
2	NAG	A	804	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	805	2	-	0/6/23/26	0/1/1/1
2	NAG	A	808	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	809	2	-	0/6/23/26	0/1/1/1
4	NAG	A	810	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	811	4	-	0/6/23/26	0/1/1/1
4	BMA	A	812	4	-	0/2/19/22	0/1/1/1
4	MAN	A	813	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	808	NAG	O7-C7	2.12	1.28	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	811	NAG	C3-C4-C5	-3.58	103.96	110.20
4	A	812	BMA	O3-C3-C2	-3.23	104.17	110.00
4	A	811	NAG	C2-N2-C7	-3.19	118.95	123.04
4	A	810	NAG	O6-C6-C5	-2.84	101.95	111.33
4	A	810	NAG	C6-C5-C4	-2.41	107.06	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	813	MAN	C3-C4-C5	-2.25	106.27	110.20
2	A	801	NAG	O4-C4-C3	-2.17	105.45	110.34
4	A	811	NAG	C4-C3-C2	-2.15	107.88	111.23
4	A	811	NAG	O7-C7-C8	-2.09	118.23	122.06
2	A	805	NAG	C2-N2-C7	-2.06	120.39	123.04
2	A	805	NAG	C1-O5-C5	2.03	114.82	112.25
4	A	811	NAG	C8-C7-N2	2.34	120.58	116.11
2	A	809	NAG	C8-C7-N2	2.41	120.72	116.11
2	A	805	NAG	O4-C4-C5	2.45	115.74	109.24
2	A	802	NAG	C2-N2-C7	2.49	126.23	123.04
2	A	809	NAG	C1-O5-C5	2.62	115.58	112.25
4	A	813	MAN	O3-C3-C2	2.75	114.96	110.00
4	A	812	BMA	C1-C2-C3	2.78	112.83	109.54
2	A	804	NAG	C1-O5-C5	2.87	115.89	112.25
4	A	810	NAG	C1-O5-C5	3.55	116.75	112.25
4	A	813	MAN	O5-C5-C6	3.59	115.13	107.35

There are no chirality outliers.

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	802	NAG	1	0
2	A	809	NAG	2	0

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
3	NAG	A	803	1	14,14,15	0.58	0	15,19,21	2.34	3 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	806	1	14,14,15	0.53	0	15,19,21	1.14	3 (20%)
3	NAG	A	807	1	14,14,15	0.76	0	15,19,21	1.77	3 (20%)
8	GLU	A	818	-	3,9,9	0.60	0	2,11,11	0.21	0
9	ASP	A	819	-	2,8,8	0.12	0	0,10,10	0.00	-

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	803	1	-	0/6/23/26	0/1/1/1
3	NAG	A	806	1	-	0/6/23/26	0/1/1/1
3	NAG	A	807	1	-	0/6/23/26	0/1/1/1
8	GLU	A	818	-	-	0/3/9/9	0/0/0/0
9	ASP	A	819	-	-	0/2/8/8	0/0/0/0

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	NAG	C2-N2-C7	-4.27	117.56	123.04
3	A	803	NAG	C4-C3-C2	-3.95	105.09	111.23
3	A	807	NAG	O3-C3-C4	-2.86	103.89	110.34
3	A	807	NAG	O7-C7-C8	-2.51	117.45	122.06
3	A	806	NAG	C3-C4-C5	-2.09	106.55	110.20
3	A	806	NAG	C1-O5-C5	2.04	114.84	112.25
3	A	806	NAG	O5-C5-C6	2.68	113.14	107.35
3	A	807	NAG	C1-O5-C5	4.31	117.72	112.25
3	A	803	NAG	C1-O5-C5	6.12	120.02	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	807	NAG	1	0
9	A	819	ASP	1	0

## 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	691/757 (91%)	-0.27	26 (3%) 44 40	15, 28, 49, 70	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	LYS	4.2
1	A	544	ASN	4.0
1	A	506	PHE	3.6
1	A	155	SER	3.4
1	A	335	GLY	3.2
1	A	719	VAL	3.2
1	A	656[A]	SER	3.2
1	A	153	ASN	3.0
1	A	505	GLU	2.9
1	A	56	HIS	2.9
1	A	134	ASP	2.9
1	A	135	GLY	2.9
1	A	123	THR	2.8
1	A	136	ASN	2.8
1	A	226	ILE	2.7
1	A	201[A]	VAL	2.5
1	A	237	PRO	2.4
1	A	133	GLU	2.3
1	A	336	ASN	2.2
1	A	122	LYS	2.2
1	A	334	THR	2.2
1	A	152	GLU	2.2
1	A	337	PHE	2.1
1	A	507	SER	2.1
1	A	652	ASP	2.1
1	A	154	VAL	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	802	14/15	0.78	0.24	5.11	43,54,58,60	0
2	NAG	A	808	14/15	0.94	0.09	1.88	31,35,40,41	0
4	MAN	A	813	11/12	0.93	0.17	1.12	63,64,66,66	0
4	NAG	A	810	14/15	0.94	0.08	0.89	21,29,40,45	0
2	NAG	A	804	14/15	0.95	0.13	0.75	45,51,57,68	0
2	NAG	A	809	14/15	0.91	0.21	-	42,50,53,56	0
2	NAG	A	805	14/15	0.79	0.32	-	53,58,63,64	0
2	NAG	A	801	14/15	0.96	0.08	-	35,42,45,48	0
4	NAG	A	811	14/15	0.91	0.20	-	43,50,54,57	0
4	BMA	A	812	11/12	0.83	0.19	-	51,58,61,64	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	803	14/15	0.80	0.25	1.66	53,57,64,67	0
9	ASP	A	819	9/9	0.92	0.13	0.79	37,41,43,46	0
6	CA	A	816	1/1	1.00	0.06	0.22	18,18,18,18	0
8	GLU	A	818	10/10	0.98	0.09	-0.01	20,21,22,22	0
7	CL	A	817	1/1	1.00	0.08	-1.42	23,23,23,23	0
5	ZN	A	815	1/1	1.00	0.06	-2.53	20,20,20,20	0
5	ZN	A	814	1/1	1.00	0.07	-6.38	23,23,23,23	0
3	NAG	A	807	14/15	0.91	0.14	-	33,48,53,56	0
3	NAG	A	806	14/15	0.91	0.24	-	72,78,81,81	0

## 6.5 Other polymers

There are no such residues in this entry.