



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:30 PM GMT

PDB ID : 4P44  
Title : X-ray structure of human glutamate carboxypeptidase II (GCP II) in complex with a phosphoramidate inhibitor JRB-4-81  
Authors : Novakova, Z.; Barinka, C.  
Deposited on : 2014-03-11  
Resolution : 1.75 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

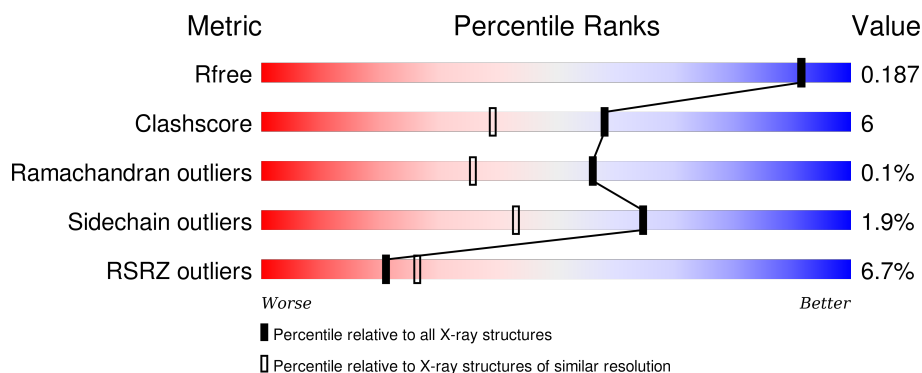
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	803	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6554 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	691	Total	C	N	O	S	0	43	0
			5734	3680	963	1069	22			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



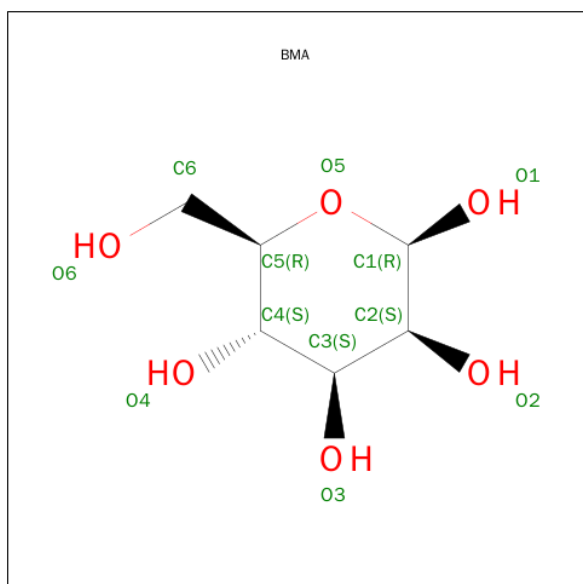
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		

- 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		

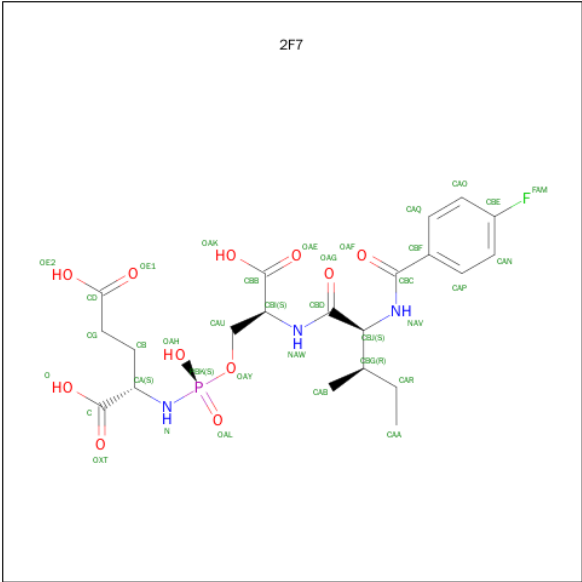
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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 N-(4-fluorobenzoyl)-L-alloisoleucyl-O-[(S)-{[(1S)-1,3-dicarboxypropyl]amino}(hydroxy)phosphoryl]-L-serine (three-letter code: 2F7) (formula: C<sub>21</sub>H<sub>29</sub>FN<sub>3</sub>O<sub>11</sub>P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	P		
8	A	1	37	21	1	3	11	1	0	0

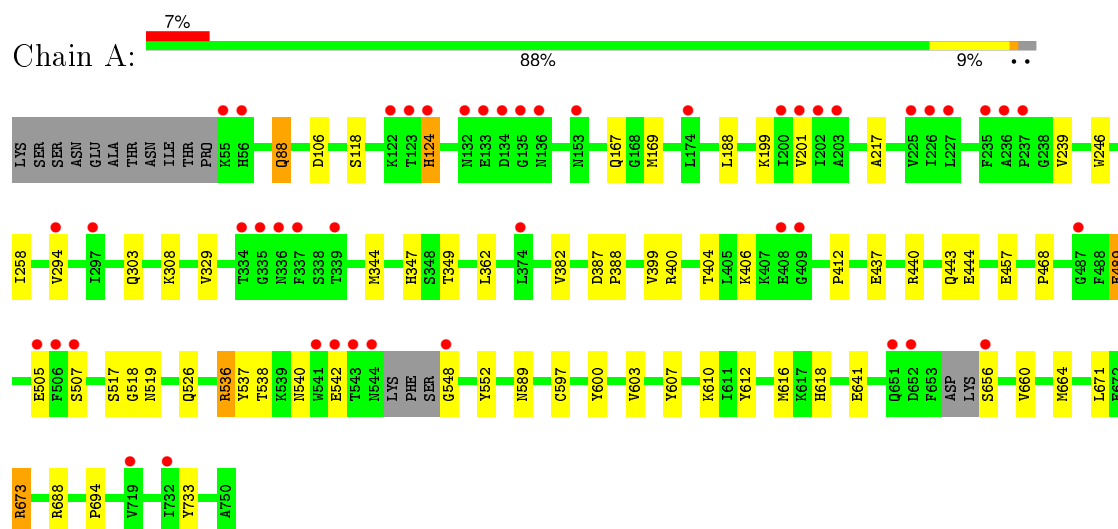
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	603	Total	O	0	0
			603	603		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Glutamate carboxypeptidase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.50Å 130.49Å 158.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.51 – 1.75 29.51 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.51-1.75) 99.9 (29.51-1.75)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.163 , 0.187 0.163 , 0.187	Depositor DCC
$R_{free}$ test set	5288 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 105760 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6554	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, 2F7, 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	0.94	1/5972 (0.0%)	0.81	7/8089 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	399	VAL	CB-CG2	5.16	1.63	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	688[A]	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	A	688[B]	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	A	440	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	673	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	A	673	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	536[A]	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	536[B]	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5734	0	5586	58	0
2	A	154	0	138	5	0
3	A	11	0	9	0	0
4	A	11	0	10	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	37	0	24	12	0
9	A	603	0	0	16	0
All	All	6554	0	5767	69	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 6.

All (69) 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	1.29	1.28
1:A:597[B]:CYS:SG	1:A:671:LEU:HD22	2.12	0.90
1:A:536[A]:ARG:HH12	8:A:818:2F7:H19	1.36	0.89
1:A:597[B]:CYS:SG	1:A:671:LEU:CD2	2.60	0.88
1:A:733:TYR:HE2	9:A:989:HOH:O	1.60	0.83
1:A:656[B]:SER:O	9:A:901:HOH:O	1.97	0.81
1:A:88:GLN:HE21	1:A:88:GLN:H	1.29	0.81
1:A:641:GLU:HG3	9:A:1322:HOH:O	1.82	0.79
8:A:818:2F7:H23	8:A:818:2F7:H25	1.49	0.78
1:A:536[A]:ARG:NH1	8:A:818:2F7:H19	2.00	0.75
1:A:457:GLU:OE2	1:A:536[A]:ARG:NH2	2.21	0.72
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.25	0.71
8:A:818:2F7:OAK	8:A:818:2F7:OAG	2.09	0.71
1:A:457:GLU:CD	1:A:536[A]:ARG:NH2	2.46	0.69
8:A:818:2F7:H23	8:A:818:2F7:NAV	2.07	0.68
8:A:818:2F7:H23	8:A:818:2F7:H26	1.75	0.67
1:A:603[A]:VAL:HG13	1:A:607:TYR:CZ	2.30	0.67
1:A:437:GLU:OE1	9:A:902:HOH:O	2.12	0.66
1:A:88:GLN:NE2	1:A:88:GLN:H	1.97	0.63
1:A:400:ARG:O	1:A:404[B]:THR:HG23	1.99	0.62
1:A:412:PRO:HA	1:A:589:ASN:HD21	1.63	0.62
2:A:802:NAG:H81	9:A:1212:HOH:O	1.99	0.61
1:A:457:GLU:HG2	1:A:536[A]:ARG:CZ	2.33	0.59
1:A:597[B]:CYS:SG	1:A:671:LEU:HD23	2.44	0.58
2:A:809:NAG:C8	9:A:1184:HOH:O	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603[A]:VAL:CG1	1:A:607:TYR:CE2	2.88	0.56
1:A:656[B]:SER:CB	9:A:901:HOH:O	2.53	0.55
1:A:536[A]:ARG:NH1	8:A:818:2F7:CAB	2.69	0.55
1:A:468:PRO:HG2	1:A:603[B]:VAL:HG21	1.90	0.54
1:A:517:SER:HB2	1:A:694:PRO:HG3	1.90	0.53
2:A:809:NAG:H83	9:A:1184:HOH:O	2.08	0.53
1:A:597[B]:CYS:HG	1:A:671:LEU:HD22	1.74	0.53
1:A:362:LEU:CD1	1:A:406:LYS:HD2	2.40	0.52
1:A:258:ILE:HD13	1:A:294:VAL:HB	1.90	0.52
1:A:603[A]:VAL:HG13	1:A:607:TYR:CE2	2.47	0.48
8:A:818:2F7:CBB	8:A:818:2F7:OAG	2.62	0.48
1:A:124:HIS:CE1	1:A:347:HIS:CE1	3.01	0.48
1:A:188:LEU:CD2	1:A:329[A]:VAL:HG11	2.42	0.48
1:A:603[A]:VAL:CG1	1:A:607:TYR:CZ	2.97	0.48
1:A:167:GLN:NE2	1:A:349[A]:THR:HG22	2.29	0.48
1:A:540:ASN:OD1	1:A:542:GLU:HG2	2.15	0.47
1:A:457:GLU:OE2	1:A:538:THR:OG1	2.23	0.47
1:A:308:LYS:HB2	9:A:1281:HOH:O	2.15	0.47
1:A:468:PRO:CG	1:A:603[B]:VAL:HG21	2.44	0.46
1:A:489:GLU:CD	1:A:489:GLU:H	2.19	0.46
8:A:818:2F7:H26	8:A:818:2F7:H25	1.16	0.45
1:A:443[A]:GLN:HG3	1:A:444:GLU:CD	2.37	0.45
1:A:618:HIS:HE1	9:A:1132:HOH:O	2.00	0.45
1:A:526[A]:GLN:NE2	9:A:1467:HOH:O	2.46	0.45
2:A:803:NAG:H83	9:A:1183:HOH:O	2.17	0.45
8:A:818:2F7:OAK	8:A:818:2F7:CBD	2.65	0.44
1:A:199:LYS:NZ	9:A:1219:HOH:O	2.49	0.44
1:A:733:TYR:CE2	9:A:989:HOH:O	2.47	0.44
1:A:610:LYS:NZ	9:A:1489:HOH:O	2.50	0.44
1:A:548:GLY:HA3	8:A:818:2F7:H21	1.99	0.43
1:A:517:SER:OG	1:A:518:GLY:N	2.51	0.43
1:A:552:TYR:CG	8:A:818:2F7:H24	2.53	0.43
1:A:201[A]:VAL:HG21	1:A:217:ALA:HB1	2.00	0.43
1:A:457:GLU:CD	1:A:536[A]:ARG:HH22	2.22	0.43
1:A:457:GLU:CG	1:A:536[A]:ARG:CZ	2.96	0.43
1:A:246:TRP:CD1	2:A:807:NAG:H83	2.54	0.43
1:A:188:LEU:HD21	1:A:329[A]:VAL:HG11	2.00	0.42
1:A:347:HIS:HE1	9:A:1283:HOH:O	2.03	0.42
1:A:457:GLU:CD	1:A:536[A]:ARG:CZ	2.87	0.41
1:A:258:ILE:HD13	1:A:294:VAL:CB	2.51	0.41
1:A:169:MET:HA	1:A:344:MET:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASP:OD1	1:A:406:LYS:HE3	2.21	0.41
1:A:118:SER:HA	1:A:349[B]:THR:O	2.21	0.40
1:A:387:ASP:HA	1:A:388:PRO:HA	1.90	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	725/707 (102%)	710 (98%)	14 (2%)	1 (0%)	56 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	629/603 (104%)	617 (98%)	12 (2%)	65 43

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

Mol	Chain	Res	Type
1	A	88	GLN
1	A	124	HIS
1	A	239[A]	VAL
1	A	239[B]	VAL
1	A	303	GLN
1	A	489	GLU
1	A	505	GLU
1	A	507	SER
1	A	519	ASN
1	A	537	TYR
1	A	600	TYR
1	A	673	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	167	GLN
1	A	303	GLN
1	A	347	HIS
1	A	544	ASN
1	A	589	ASN
1	A	618	HIS
1	A	651	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues 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	0.53	0	15,19,21	0.87	0
2	NAG	A	802	2	14,14,15	0.61	0	15,19,21	1.47	1 (6%)
2	NAG	A	803	1	14,14,15	0.70	0	15,19,21	1.97	3 (20%)
2	NAG	A	804	1,2	14,14,15	0.73	0	15,19,21	1.05	0
2	NAG	A	805	2	14,14,15	0.48	0	15,19,21	1.04	1 (6%)
2	NAG	A	806	1	14,14,15	0.48	0	15,19,21	2.69	3 (20%)
2	NAG	A	807	1	14,14,15	0.72	0	15,19,21	1.58	2 (13%)
2	NAG	A	808	1,2	14,14,15	0.86	1 (7%)	15,19,21	0.80	0
2	NAG	A	809	2	14,14,15	0.55	0	15,19,21	1.29	1 (6%)
2	NAG	A	810	1,2	14,14,15	0.71	0	15,19,21	1.13	1 (6%)
2	NAG	A	811	3,2	14,14,15	0.67	0	15,19,21	1.22	1 (6%)
4	MAN	A	813	3	11,11,12	0.56	0	14,15,17	1.12	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	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	803	1	-	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	806	1	-	0/6/23/26	0/1/1/1
2	NAG	A	807	1	-	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
2	NAG	A	810	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	811	3,2	-	0/6/23/26	0/1/1/1
4	MAN	A	813	3	-	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	2.09	1.28	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	803	NAG	C2-N2-C7	-2.85	119.38	123.04
2	A	811	NAG	C3-C4-C5	-2.82	105.28	110.20
2	A	807	NAG	O3-C3-C4	-2.32	105.12	110.34
2	A	806	NAG	C4-C3-C2	-2.26	107.71	111.23
2	A	806	NAG	C6-C5-C4	-2.10	107.84	113.02
2	A	803	NAG	C3-C4-C5	2.11	113.88	110.20
2	A	805	NAG	O4-C4-C5	2.43	115.67	109.24
4	A	813	MAN	O5-C5-C6	2.53	112.83	107.35
2	A	810	NAG	C1-O5-C5	2.65	115.61	112.25
2	A	809	NAG	C8-C7-N2	2.92	121.69	116.11
2	A	802	NAG	C2-N2-C7	3.82	127.95	123.04
2	A	807	NAG	C1-O5-C5	4.31	117.72	112.25
2	A	803	NAG	C1-O5-C5	5.93	119.77	112.25
2	A	806	NAG	C1-O5-C5	9.69	124.55	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	NAG	1	0
2	A	803	NAG	1	0
2	A	807	NAG	1	0
2	A	809	NAG	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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
2	NAG	A	801	1,2	14,14,15	0.53	0	15,19,21	0.87	0
2	NAG	A	802	2	14,14,15	0.61	0	15,19,21	1.47	1 (6%)
2	NAG	A	803	1	14,14,15	0.70	0	15,19,21	1.97	3 (20%)
2	NAG	A	804	1,2	14,14,15	0.73	0	15,19,21	1.05	0
2	NAG	A	805	2	14,14,15	0.48	0	15,19,21	1.04	1 (6%)
2	NAG	A	806	1	14,14,15	0.48	0	15,19,21	2.69	3 (20%)
2	NAG	A	807	1	14,14,15	0.72	0	15,19,21	1.58	2 (13%)
2	NAG	A	808	1,2	14,14,15	0.86	1 (7%)	15,19,21	0.80	0
2	NAG	A	809	2	14,14,15	0.55	0	15,19,21	1.29	1 (6%)
2	NAG	A	810	1,2	14,14,15	0.71	0	15,19,21	1.13	1 (6%)
2	NAG	A	811	3,2	14,14,15	0.67	0	15,19,21	1.22	1 (6%)
3	BMA	A	812	2,4	11,11,12	0.66	0	14,15,17	1.17	2 (14%)
4	MAN	A	813	3	11,11,12	0.56	0	14,15,17	1.12	1 (7%)
8	2F7	A	818	5	26,37,37	3.55	8 (30%)	35,51,51	2.94	16 (45%)

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	803	1	-	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	806	1	-	0/6/23/26	0/1/1/1
2	NAG	A	807	1	-	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
2	NAG	A	810	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	811	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	812	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	813	3	-	0/2/19/22	0/1/1/1
8	2F7	A	818	5	-	0/35/46/46	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	818	2F7	PBK-OAH	-4.72	1.43	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	818	2F7	CBF-CBC	-4.26	1.41	1.50
8	A	818	2F7	FAM-CBE	-3.30	1.28	1.36
8	A	818	2F7	CBI-NAW	-2.95	1.42	1.46
2	A	808	NAG	O7-C7	2.09	1.28	1.23
8	A	818	2F7	CAO-CBE	2.11	1.41	1.37
8	A	818	2F7	CB-CA	2.70	1.57	1.53
8	A	818	2F7	PBK-N	8.24	1.70	1.61
8	A	818	2F7	PBK-OAL	12.98	1.61	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	818	2F7	CBJ-CBD-NAW	-5.87	103.49	116.44
8	A	818	2F7	CBF-CBC-NAV	-5.52	107.10	116.93
8	A	818	2F7	CAU-CBI-NAW	-5.22	98.17	111.14
8	A	818	2F7	OAL-PBK-N	-3.22	107.32	113.08
2	A	803	NAG	C2-N2-C7	-2.85	119.38	123.04
2	A	811	NAG	C3-C4-C5	-2.82	105.28	110.20
8	A	818	2F7	CAO-CAQ-CBF	-2.67	117.67	120.76
2	A	807	NAG	O3-C3-C4	-2.32	105.12	110.34
2	A	806	NAG	C4-C3-C2	-2.26	107.71	111.23
3	A	812	BMA	O3-C3-C2	-2.15	106.12	110.00
2	A	806	NAG	C6-C5-C4	-2.10	107.84	113.02
8	A	818	2F7	CAP-CBF-CBC	-2.05	114.09	120.60
2	A	803	NAG	C3-C4-C5	2.11	113.88	110.20
8	A	818	2F7	FAM-CBE-CAO	2.13	122.07	118.52
8	A	818	2F7	CAQ-CAO-CBE	2.23	120.75	118.35
3	A	812	BMA	C1-C2-C3	2.24	112.19	109.54
2	A	805	NAG	O4-C4-C5	2.43	115.67	109.24
8	A	818	2F7	CBI-NAW-CBD	2.52	127.36	123.43
4	A	813	MAN	O5-C5-C6	2.53	112.83	107.35
2	A	810	NAG	C1-O5-C5	2.65	115.61	112.25
8	A	818	2F7	OAG-CBD-NAW	2.74	128.28	122.93
2	A	809	NAG	C8-C7-N2	2.92	121.69	116.11
8	A	818	2F7	OAF-CBC-NAV	3.42	128.61	122.44
8	A	818	2F7	OAG-CBD-CBJ	3.46	127.80	120.68
2	A	802	NAG	C2-N2-C7	3.82	127.95	123.04
8	A	818	2F7	CBG-CBJ-CBD	3.83	118.67	111.72
2	A	807	NAG	C1-O5-C5	4.31	117.72	112.25
8	A	818	2F7	OAY-CAU-CBI	4.36	111.30	108.17
8	A	818	2F7	CBG-CBJ-NAV	5.79	123.99	111.12
2	A	803	NAG	C1-O5-C5	5.93	119.77	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	818	2F7	CBJ-NAV-CBC	7.35	136.57	121.43
2	A	806	NAG	C1-O5-C5	9.69	124.55	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	NAG	1	0
2	A	803	NAG	1	0
2	A	807	NAG	1	0
2	A	809	NAG	2	0
8	A	818	2F7	12	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	691/707 (97%)	0.11	46 (6%)	21 26	12, 23, 40, 74	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	TRP	10.5
1	A	544	ASN	6.0
1	A	543	THR	5.0
1	A	335	GLY	4.8
1	A	542	GLU	4.4
1	A	201[A]	VAL	4.4
1	A	55	LYS	4.2
1	A	507	SER	4.2
1	A	226	ILE	4.2
1	A	135	GLY	4.1
1	A	548	GLY	4.1
1	A	506	PHE	4.0
1	A	133	GLU	3.9
1	A	134	ASP	3.7
1	A	202	ILE	3.7
1	A	652	ASP	3.6
1	A	227	LEU	3.6
1	A	719	VAL	3.3
1	A	225	VAL	3.3
1	A	153	ASN	3.1
1	A	56	HIS	3.1
1	A	336	ASN	3.1
1	A	237	PRO	3.0
1	A	505	GLU	2.9
1	A	656[A]	SER	2.8
1	A	487	GLY	2.8
1	A	339	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	136	ASN	2.7
1	A	124	HIS	2.7
1	A	334	THR	2.7
1	A	235	PHE	2.6
1	A	123	THR	2.5
1	A	132	ASN	2.5
1	A	337	PHE	2.5
1	A	408	GLU	2.5
1	A	651	GLN	2.5
1	A	174	LEU	2.4
1	A	203	ALA	2.4
1	A	294	VAL	2.4
1	A	122	LYS	2.3
1	A	374	LEU	2.3
1	A	297	ILE	2.3
1	A	732	ILE	2.3
1	A	200	ILE	2.2
1	A	409	GLY	2.2
1	A	236	ALA	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	0.77	0.31	6.70	35,45,50,52	0
2	NAG	A	803	14/15	0.70	0.32	3.08	44,50,57,57	0
2	NAG	A	808	14/15	0.95	0.10	1.49	24,27,33,37	0
2	NAG	A	810	14/15	0.92	0.10	1.41	19,24,35,41	0
4	MAN	A	813	11/12	0.92	0.19	1.27	40,44,46,49	0
2	NAG	A	804	14/15	0.91	0.16	-	34,39,42,51	0
2	NAG	A	811	14/15	0.91	0.22	-	36,39,47,48	0
2	NAG	A	801	14/15	0.93	0.12	-	32,38,43,46	0
2	NAG	A	805	14/15	0.76	0.33	-	49,53,58,58	0
2	NAG	A	807	14/15	0.89	0.14	-	31,45,51,51	0
2	NAG	A	806	14/15	0.84	0.27	-	60,65,68,70	0
2	NAG	A	809	14/15	0.90	0.17	-	35,40,47,48	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 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
2	NAG	A	802	14/15	0.77	0.31	6.70	35,45,50,52	0
2	NAG	A	803	14/15	0.70	0.32	3.08	44,50,57,57	0
2	NAG	A	808	14/15	0.95	0.10	1.49	24,27,33,37	0
2	NAG	A	810	14/15	0.92	0.10	1.41	19,24,35,41	0
4	MAN	A	813	11/12	0.92	0.19	1.27	40,44,46,49	0
8	2F7	A	818	37/37	0.97	0.12	0.47	14,34,55,56	0
6	CA	A	816	1/1	1.00	0.06	-0.10	14,14,14,14	0
5	ZN	A	815	1/1	1.00	0.06	-1.14	17,17,17,17	0
7	CL	A	817	1/1	1.00	0.06	-1.93	20,20,20,20	0
5	ZN	A	814	1/1	1.00	0.05	-4.32	16,16,16,16	0
2	NAG	A	805	14/15	0.76	0.33	-	49,53,58,58	0
3	BMA	A	812	11/12	0.92	0.16	-	36,37,43,45	0
2	NAG	A	801	14/15	0.93	0.12	-	32,38,43,46	0
2	NAG	A	807	14/15	0.89	0.14	-	31,45,51,51	0
2	NAG	A	804	14/15	0.91	0.16	-	34,39,42,51	0
2	NAG	A	811	14/15	0.91	0.22	-	36,39,47,48	0
2	NAG	A	806	14/15	0.84	0.27	-	60,65,68,70	0
2	NAG	A	809	14/15	0.90	0.17	-	35,40,47,48	0

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

There are no such residues in this entry.