



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:30 PM GMT

PDB ID : 4P45
Title : X-ray structure of human glutamate carboxypeptidase II (GCP II) in complex with a phosphoramidate inhibitor JRB-4-73
Authors : Novakova, Z.; Barinka, C.
Deposited on : 2014-03-11
Resolution : 1.87 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

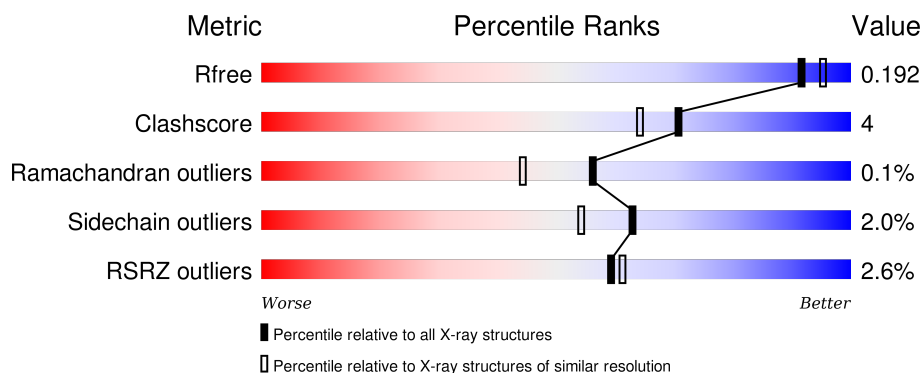
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.87 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	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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 ≥ 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

Continued on next page...

Continued from previous page...

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

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 6634 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	690	Total	C	N	O	S	0	49	0
			5779	3708	969	1081	21			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



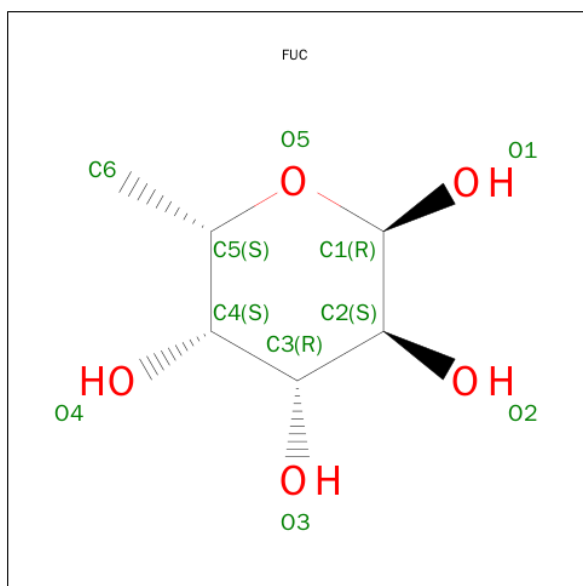
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

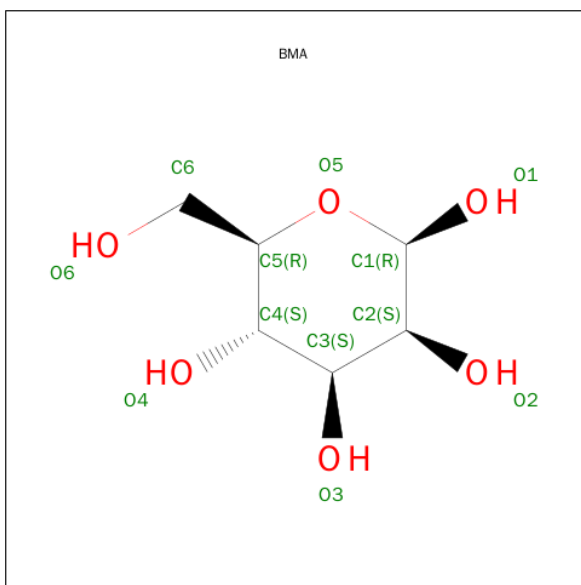
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



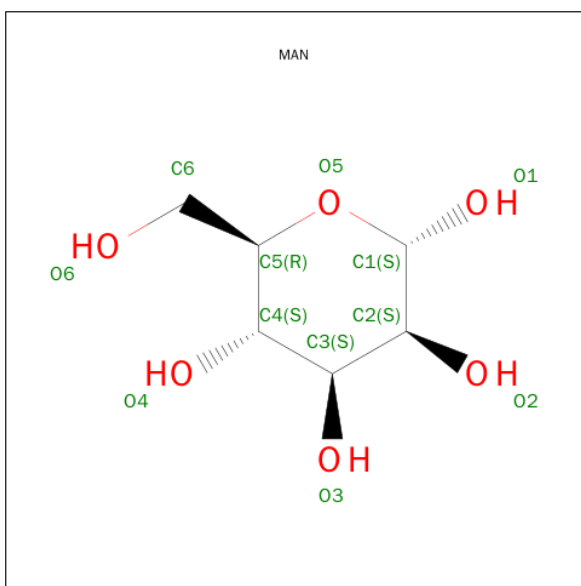
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



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

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

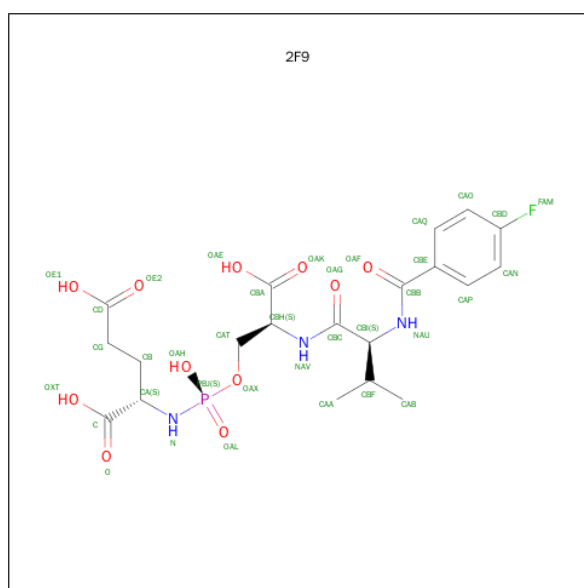
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is N-(4-fluorobenzoyl)-L-valyl-O-[(S)-{[(1S)-1,3-dicarboxypropyl]amino}(hydrox y)phosphoryl]-L-serine (three-letter code: 2F9) (formula: C₂₀H₂₇FN₃O₁₁P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	A	1	Total	C	F	N	O	P	0	0
			36	20	1	3	11	1		

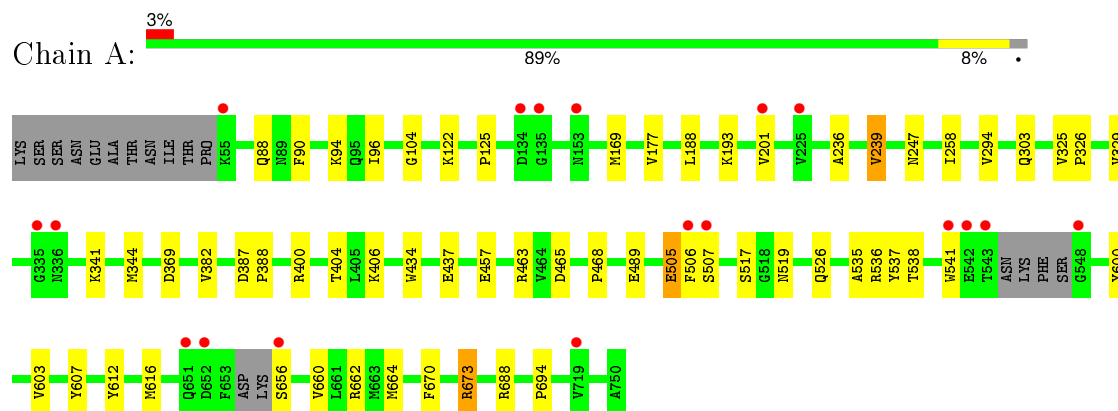
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	594	Total	O	0	0
			594	594		

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 ($\text{RSRZ} > 2$). 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, α , β , γ	101.44Å 130.31Å 158.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.18 – 1.87 28.18 – 1.87	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.18-1.87) 99.8 (28.18-1.87)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.162 , 0.193 0.162 , 0.192	Depositor DCC
R_{free} test set	4333 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 86835 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6634	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 2F9, FUC, 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	2/6018 (0.0%)	0.75	3/8150 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	TRP	CE3-CZ3	5.78	1.48	1.38
1	A	670	PHE	CE1-CZ	5.11	1.47	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	465	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	673	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	5779	0	5616	47	0
2	A	168	0	147	5	0
3	A	20	0	20	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	22	0	19	0	0
5	A	11	0	10	0	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	36	0	23	0	0
10	A	594	0	0	16	0
All	All	6634	0	5835	52	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 4.

All (52) 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	1.43	1.17
1:A:463:ARG:NH1	1:A:536[B]:ARG:HH12	1.42	1.17
1:A:463:ARG:NH1	1:A:536[B]:ARG:NH1	1.98	1.11
1:A:463:ARG:CZ	1:A:536[B]:ARG:NH1	2.28	0.96
1:A:88[B]:GLN:OE1	10:A:1286:HOH:O	1.98	0.81
1:A:463:ARG:HH12	1:A:536[B]:ARG:HH12	1.31	0.79
2:A:802:NAG:H81	10:A:1207:HOH:O	1.84	0.77
1:A:656[B]:SER:O	10:A:901:HOH:O	2.05	0.74
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.32	0.65
1:A:688[B]:ARG:NH2	10:A:1059:HOH:O	2.15	0.61
1:A:603[A]:VAL:HG13	1:A:607:TYR:CZ	2.40	0.56
1:A:517[A]:SER:HB2	1:A:694:PRO:HG3	1.86	0.56
1:A:603[A]:VAL:CG1	1:A:607:TYR:CE2	2.89	0.56
2:A:812:NAG:C8	10:A:1179:HOH:O	2.53	0.56
1:A:517[B]:SER:HB2	1:A:694:PRO:HG3	1.87	0.55
2:A:812:NAG:H83	10:A:1179:HOH:O	2.05	0.55
1:A:400:ARG:O	1:A:404[B]:THR:HG23	2.07	0.54
2:A:803:NAG:H83	10:A:1178:HOH:O	2.07	0.54
1:A:177:VAL:HG12	1:A:188:LEU:HD11	1.89	0.54
1:A:236:ALA:O	1:A:239[A]:VAL:HG13	2.07	0.54
1:A:526[A]:GLN:NE2	10:A:1447:HOH:O	2.37	0.53
1:A:535:ALA:C	1:A:536[B]:ARG:HG3	2.29	0.53
1:A:505:GLU:HG3	1:A:506:PHE:CD1	2.43	0.53
1:A:437:GLU:OE1	10:A:902:HOH:O	2.19	0.52
1:A:457[A]:GLU:OE2	1:A:538:THR:OG1	2.24	0.51
1:A:188:LEU:HD21	1:A:329[A]:VAL:HG11	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:MET:HA	1:A:344:MET:O	2.12	0.50
1:A:88[B]:GLN:CD	10:A:1286:HOH:O	2.45	0.49
1:A:188:LEU:CD2	1:A:329[A]:VAL:HG11	2.42	0.49
1:A:603[A]:VAL:CG1	1:A:607:TYR:CZ	2.97	0.48
1:A:96[B]:ILE:HD13	10:A:1073:HOH:O	2.13	0.47
1:A:94[B]:LYS:HE2	10:A:1328:HOH:O	2.15	0.46
1:A:94[B]:LYS:HE2	10:A:1467:HOH:O	2.15	0.45
1:A:239[A]:VAL:HG22	1:A:247:ASN:ND2	2.32	0.45
1:A:489:GLU:CD	1:A:489:GLU:H	2.21	0.45
1:A:505:GLU:HG3	1:A:506:PHE:CE1	2.52	0.44
1:A:656[B]:SER:CB	10:A:901:HOH:O	2.62	0.44
1:A:468:PRO:HG2	1:A:603[B]:VAL:HG21	2.00	0.43
1:A:258:ILE:HD13	1:A:294:VAL:HB	2.01	0.43
1:A:468:PRO:CG	1:A:603[B]:VAL:HG21	2.47	0.43
1:A:387:ASP:HA	1:A:388:PRO:HA	1.89	0.43
1:A:325:VAL:HB	1:A:326:PRO:HD2	1.99	0.43
1:A:177:VAL:HG13	1:A:201[B]:VAL:HG22	2.01	0.42
1:A:90:PHE:CZ	1:A:94[A]:LYS:HD2	2.54	0.42
1:A:177:VAL:HG12	1:A:188:LEU:CD1	2.50	0.42
1:A:104:GLY:O	1:A:406:LYS:HD3	2.20	0.42
1:A:656[B]:SER:OG	10:A:901:HOH:O	2.11	0.42
2:A:802:NAG:H83	10:A:1413:HOH:O	2.20	0.41
1:A:369:ASP:OD2	1:A:662[B]:ARG:NH2	2.34	0.41
1:A:177:VAL:CG1	1:A:201[B]:VAL:HG22	2.51	0.41
1:A:239[A]:VAL:HG22	1:A:247:ASN:CG	2.42	0.40
1:A:125:PRO:HG2	3:A:808:FUC:H63	2.04	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	730/707 (103%)	714 (98%)	15 (2%)	1 (0%)	56	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	634/603 (105%)	621 (98%)	13 (2%)	61	52

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LYS
1	A	193	LYS
1	A	239[A]	VAL
1	A	239[B]	VAL
1	A	303	GLN
1	A	341	LYS
1	A	505	GLU
1	A	507	SER
1	A	519	ASN
1	A	537	TYR
1	A	541	TRP
1	A	600	TYR
1	A	673	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

15 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	0.62	0	15,19,21	0.90	1 (6%)
2	NAG	A	802	2	14,14,15	0.55	0	15,19,21	1.08	1 (6%)
2	NAG	A	803	1,3,2	14,14,15	0.76	0	15,19,21	1.20	1 (6%)
2	NAG	A	804	2	14,14,15	0.54	0	15,19,21	1.48	1 (6%)
3	FUC	A	805	2	10,10,11	0.63	0	14,14,16	1.18	2 (14%)
2	NAG	A	806	1,3,2	14,14,15	0.71	0	15,19,21	0.90	0
2	NAG	A	807	2	14,14,15	0.49	0	15,19,21	1.02	0
3	FUC	A	808	2	10,10,11	0.68	0	14,14,16	1.04	0
2	NAG	A	809	1	14,14,15	0.35	0	15,19,21	2.42	2 (13%)
2	NAG	A	810	1	14,14,15	0.61	0	15,19,21	1.63	3 (20%)
2	NAG	A	811	1,2	14,14,15	0.93	0	15,19,21	0.74	0
2	NAG	A	812	2,4	14,14,15	0.74	0	15,19,21	1.01	0
2	NAG	A	814	1,2	14,14,15	0.78	0	15,19,21	1.48	3 (20%)
2	NAG	A	815	2,4	14,14,15	0.67	0	15,19,21	1.39	1 (6%)
5	MAN	A	817	4	11,11,12	0.68	0	14,15,17	1.18	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	803	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	A	804	2	-	0/6/23/26	0/1/1/1
3	FUC	A	805	2	-	0/0/17/20	0/1/1/1
2	NAG	A	806	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	A	807	2	-	0/6/23/26	0/1/1/1
3	FUC	A	808	2	-	0/0/17/20	0/1/1/1
2	NAG	A	809	1	-	0/6/23/26	0/1/1/1
2	NAG	A	810	1	-	0/6/23/26	0/1/1/1
2	NAG	A	811	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	812	2,4	-	0/6/23/26	0/1/1/1
2	NAG	A	814	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	815	2,4	-	0/6/23/26	0/1/1/1
5	MAN	A	817	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	815	NAG	C3-C4-C5	-2.77	105.37	110.20
2	A	809	NAG	C4-C3-C2	-2.63	107.14	111.23
2	A	810	NAG	C2-N2-C7	-2.47	119.87	123.04
2	A	814	NAG	C2-N2-C7	-2.26	120.13	123.04
2	A	803	NAG	C2-N2-C7	-2.24	120.17	123.04
2	A	801	NAG	C2-N2-C7	-2.23	120.17	123.04
3	A	805	FUC	C1-C2-C3	-2.15	106.99	109.54
2	A	814	NAG	O4-C4-C5	-2.13	103.58	109.24
2	A	802	NAG	C2-N2-C7	2.23	125.90	123.04
3	A	805	FUC	C1-O5-C5	2.28	115.89	112.38
5	A	817	MAN	O5-C5-C6	2.37	112.47	107.35
2	A	810	NAG	O3-C3-C2	2.42	113.90	109.11
2	A	810	NAG	C1-O5-C5	3.77	117.04	112.25
2	A	814	NAG	C1-O5-C5	4.28	117.68	112.25
2	A	804	NAG	C1-O5-C5	4.54	118.01	112.25
2	A	809	NAG	C1-O5-C5	8.29	122.77	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	NAG	2	0
2	A	803	NAG	1	0
3	A	808	FUC	1	0
2	A	812	NAG	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	0.62	0	15,19,21	0.90	1 (6%)
2	NAG	A	802	2	14,14,15	0.55	0	15,19,21	1.08	1 (6%)
2	NAG	A	803	1,3,2	14,14,15	0.76	0	15,19,21	1.20	1 (6%)
2	NAG	A	804	2	14,14,15	0.54	0	15,19,21	1.48	1 (6%)
3	FUC	A	805	2	10,10,11	0.63	0	14,14,16	1.18	2 (14%)
2	NAG	A	806	1,3,2	14,14,15	0.71	0	15,19,21	0.90	0
2	NAG	A	807	2	14,14,15	0.49	0	15,19,21	1.02	0
3	FUC	A	808	2	10,10,11	0.68	0	14,14,16	1.04	0
2	NAG	A	809	1	14,14,15	0.35	0	15,19,21	2.42	2 (13%)
2	NAG	A	810	1	14,14,15	0.61	0	15,19,21	1.63	3 (20%)
2	NAG	A	811	1,2	14,14,15	0.93	0	15,19,21	0.74	0
2	NAG	A	812	2,4	14,14,15	0.74	0	15,19,21	1.01	0
4	BMA	A	813	2	11,11,12	0.54	0	14,15,17	0.96	1 (7%)
2	NAG	A	814	1,2	14,14,15	0.78	0	15,19,21	1.48	3 (20%)
2	NAG	A	815	2,4	14,14,15	0.67	0	15,19,21	1.39	1 (6%)
4	BMA	A	816	2,5	11,11,12	0.57	0	14,15,17	1.04	1 (7%)
5	MAN	A	817	4	11,11,12	0.68	0	14,15,17	1.18	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	2F9	A	822	6	25,36,36	3.23	7 (28%)	34,50,50	1.49	2 (5%)

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	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	A	804	2	-	0/6/23/26	0/1/1/1
3	FUC	A	805	2	-	0/0/17/20	0/1/1/1
2	NAG	A	806	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	A	807	2	-	0/6/23/26	0/1/1/1
3	FUC	A	808	2	-	0/0/17/20	0/1/1/1
2	NAG	A	809	1	-	0/6/23/26	0/1/1/1
2	NAG	A	810	1	-	0/6/23/26	0/1/1/1
2	NAG	A	811	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	812	2,4	-	0/6/23/26	0/1/1/1
4	BMA	A	813	2	-	0/2/19/22	0/1/1/1
2	NAG	A	814	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	815	2,4	-	0/6/23/26	0/1/1/1
4	BMA	A	816	2,5	-	0/2/19/22	0/1/1/1
5	MAN	A	817	4	-	0/2/19/22	0/1/1/1
9	2F9	A	822	6	-	0/33/44/44	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	822	2F9	CBE-CBB	-3.11	1.43	1.50
9	A	822	2F9	PBJ-OAH	-2.59	1.49	1.56
9	A	822	2F9	PBJ-N	-2.45	1.58	1.61
9	A	822	2F9	CB-CA	2.74	1.57	1.53
9	A	822	2F9	CBI-NAU	2.81	1.52	1.45
9	A	822	2F9	FAM-CBD	8.26	1.55	1.36
9	A	822	2F9	PBJ-OAL	11.38	1.59	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	815	NAG	C3-C4-C5	-2.77	105.37	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	809	NAG	C4-C3-C2	-2.63	107.14	111.23
2	A	810	NAG	C2-N2-C7	-2.47	119.87	123.04
2	A	814	NAG	C2-N2-C7	-2.26	120.13	123.04
2	A	803	NAG	C2-N2-C7	-2.24	120.17	123.04
2	A	801	NAG	C2-N2-C7	-2.23	120.17	123.04
3	A	805	FUC	C1-C2-C3	-2.15	106.99	109.54
2	A	814	NAG	O4-C4-C5	-2.13	103.58	109.24
9	A	822	2F9	CAN-CBD-CAO	-2.02	119.97	122.87
4	A	813	BMA	C3-C4-C5	2.19	114.01	110.20
2	A	802	NAG	C2-N2-C7	2.23	125.90	123.04
3	A	805	FUC	C1-O5-C5	2.28	115.89	112.38
4	A	816	BMA	C1-O5-C5	2.36	115.24	112.25
5	A	817	MAN	O5-C5-C6	2.37	112.47	107.35
2	A	810	NAG	O3-C3-C2	2.42	113.90	109.11
2	A	810	NAG	C1-O5-C5	3.77	117.04	112.25
2	A	814	NAG	C1-O5-C5	4.28	117.68	112.25
2	A	804	NAG	C1-O5-C5	4.54	118.01	112.25
9	A	822	2F9	OAX-CAT-CBH	6.69	112.97	108.17
2	A	809	NAG	C1-O5-C5	8.29	122.77	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	NAG	2	0
2	A	803	NAG	1	0
3	A	808	FUC	1	0
2	A	812	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, 95th 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 ²)	Q<0.9
1	A	690/707 (97%)	-0.23	18 (2%) 59 61	11, 23, 42, 71	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	TRP	9.0
1	A	543	THR	5.1
1	A	542	GLU	4.5
1	A	55	LYS	3.9
1	A	656[A]	SER	3.3
1	A	548	GLY	3.2
1	A	335	GLY	2.9
1	A	135	GLY	2.7
1	A	336	ASN	2.6
1	A	134	ASP	2.5
1	A	153	ASN	2.5
1	A	651	GLN	2.4
1	A	506	PHE	2.4
1	A	507	SER	2.3
1	A	201[A]	VAL	2.3
1	A	652	ASP	2.3
1	A	719	VAL	2.2
1	A	225	VAL	2.0

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, 95th 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(\AA^2)	Q<0.9
2	NAG	A	802	14/15	0.77	0.25	3.70	43,52,56,57	0
2	NAG	A	803	14/15	0.72	0.23	2.95	49,55,65,65	0
5	MAN	A	817	11/12	0.92	0.17	1.82	44,46,48,50	0
2	NAG	A	814	14/15	0.95	0.08	1.48	18,26,36,42	0
2	NAG	A	811	14/15	0.93	0.10	0.53	30,32,37,39	0
2	NAG	A	801	14/15	0.94	0.09	-	32,40,44,47	0
2	NAG	A	809	14/15	0.87	0.18	-	62,67,70,71	0
2	NAG	A	810	14/15	0.93	0.12	-	30,46,50,51	0
3	FUC	A	808	10/11	0.82	0.31	-	60,63,65,66	0
2	NAG	A	815	14/15	0.94	0.18	-	36,40,48,49	0
2	NAG	A	812	14/15	0.89	0.17	-	40,46,53,56	0
2	NAG	A	807	14/15	0.80	0.27	-	53,58,63,64	0
2	NAG	A	804	14/15	0.77	0.40	-	69,71,74,75	0
3	FUC	A	805	10/11	0.87	0.42	-	68,70,71,71	0
2	NAG	A	806	14/15	0.92	0.13	-	42,44,52,53	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, 95th 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(\AA^2)	Q<0.9
2	NAG	A	802	14/15	0.77	0.25	3.70	43,52,56,57	0
2	NAG	A	803	14/15	0.72	0.23	2.95	49,55,65,65	0
5	MAN	A	817	11/12	0.92	0.17	1.82	44,46,48,50	0
2	NAG	A	814	14/15	0.95	0.08	1.48	18,26,36,42	0
9	2F9	A	822	36/36	0.95	0.14	1.12	7,29,42,47	0
2	NAG	A	811	14/15	0.93	0.10	0.53	30,32,37,39	0
7	CA	A	820	1/1	1.00	0.05	-0.33	14,14,14,14	0
8	CL	A	821	1/1	1.00	0.04	-2.04	20,20,20,20	0
6	ZN	A	819	1/1	1.00	0.04	-2.13	16,16,16,16	0
6	ZN	A	818	1/1	1.00	0.04	-6.89	15,15,15,15	0
2	NAG	A	806	14/15	0.92	0.13	-	42,44,52,53	0
2	NAG	A	810	14/15	0.93	0.12	-	30,46,50,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	804	14/15	0.77	0.40	-	69,71,74,75	0
2	NAG	A	812	14/15	0.89	0.17	-	40,46,53,56	0
2	NAG	A	809	14/15	0.87	0.18	-	62,67,70,71	0
3	FUC	A	808	10/11	0.82	0.31	-	60,63,65,66	0
2	NAG	A	801	14/15	0.94	0.09	-	32,40,44,47	0
4	BMA	A	813	11/12	0.77	0.23	-	61,65,69,72	0
2	NAG	A	807	14/15	0.80	0.27	-	53,58,63,64	0
4	BMA	A	816	11/12	0.90	0.12	-	37,41,43,43	0
3	FUC	A	805	10/11	0.87	0.42	-	68,70,71,71	0
2	NAG	A	815	14/15	0.94	0.18	-	36,40,48,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.