



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:01 PM GMT

PDB ID : 4NGP
Title : Crystal Structure of Glutamate Carboxypeptidase II in a complex with urea-based inhibitor
Authors : Tykvart, J.; Pachl, P.
Deposited on : 2013-11-02
Resolution : 1.63 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

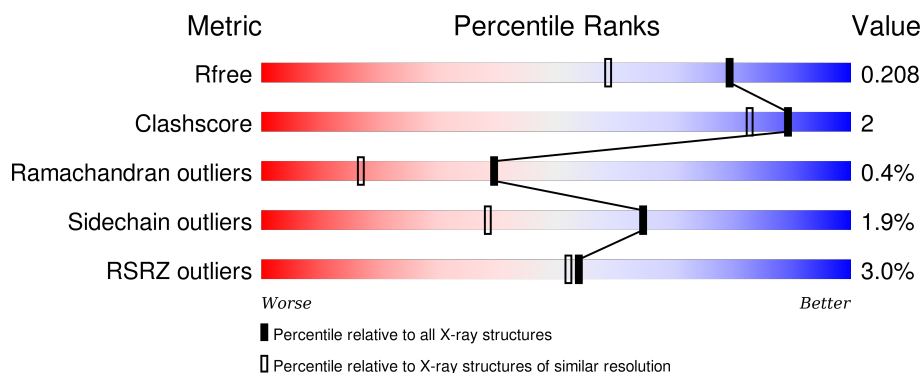
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.63 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	1953 (1.66-1.62)
Clashscore	102246	2091 (1.66-1.62)
Ramachandran outliers	100387	2052 (1.66-1.62)
Sidechain outliers	100360	2052 (1.66-1.62)
RSRZ outliers	91569	1955 (1.66-1.62)

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	739	

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	806	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	807	-	-	-	X
4	MAN	A	810	-	-	-	X
4	MAN	A	811	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6474 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	695	Total	C	N	O	S	0	13	0
			5593	3605	937	1032	19			

There are 32 discrepancies between the modelled and reference sequences:

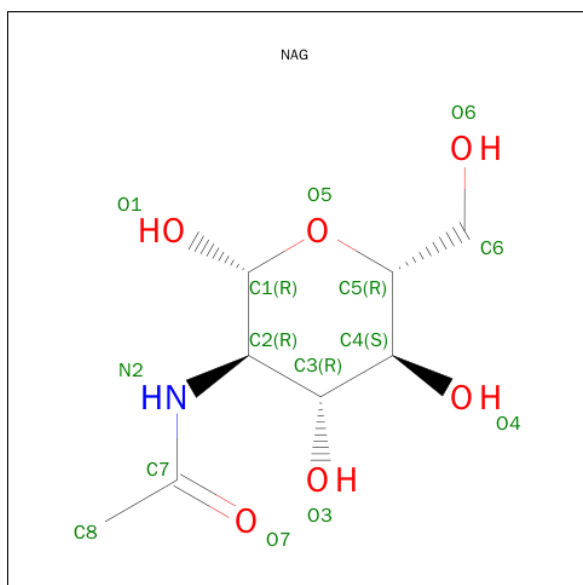
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ARG	-	EXPRESSION TAG	UNP Q04609
A	13	SER	-	EXPRESSION TAG	UNP Q04609
A	14	GLY	-	EXPRESSION TAG	UNP Q04609
A	15	LEU	-	EXPRESSION TAG	UNP Q04609
A	16	ASN	-	EXPRESSION TAG	UNP Q04609
A	17	ASP	-	EXPRESSION TAG	UNP Q04609
A	18	ILE	-	EXPRESSION TAG	UNP Q04609
A	19	PHE	-	EXPRESSION TAG	UNP Q04609
A	20	GLU	-	EXPRESSION TAG	UNP Q04609
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is SUGAR (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		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

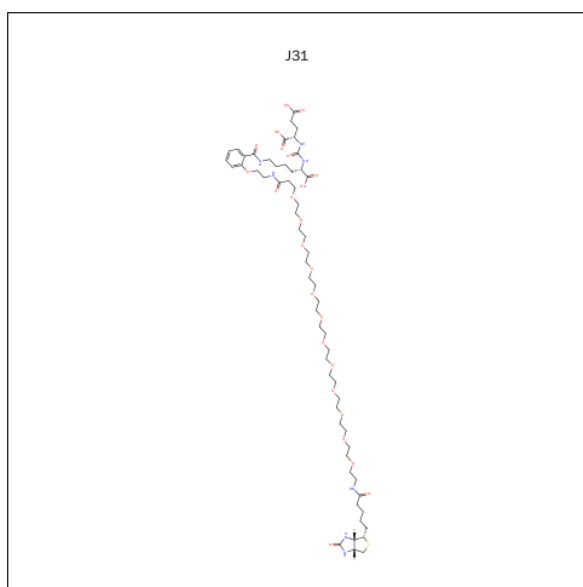
- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is N-[(1S)-1-CARBOXY-5-{[2-({4,44-DIOXO-48-[(3AS,4S,6AR)-2-OXOHEXA HYDRO-1H-THIENO[3,4-D]IMIDAZOL-4-YL]-7,10,13,16,19,22,25,28,31,34,37,40-DODEC AOX-3,43-DIAZAOCTATETRACONT-1-YL}OXY)BENZOYL]AMINO}PENTYL]CAR BAMOYL}-L-GLUTAMIC ACID (three-letter code: J31) (formula: C₅₈H₉₇N₇O₂₄S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			42	26	4	12		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

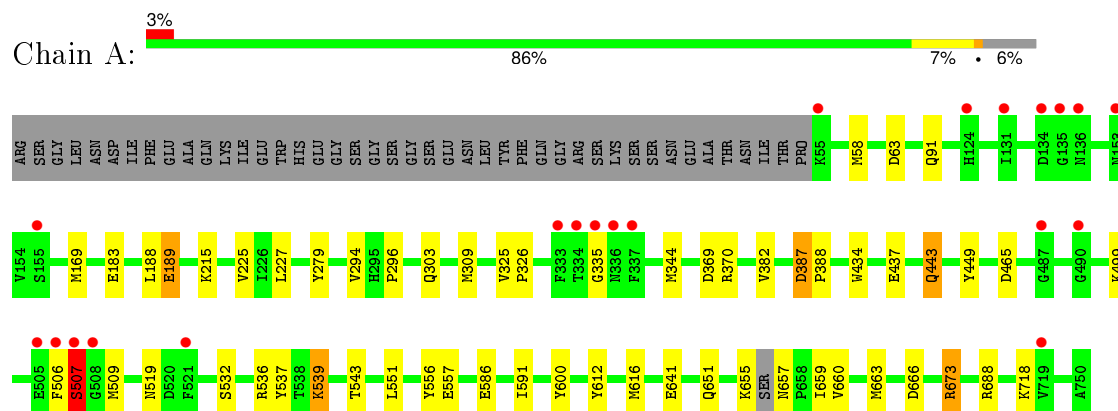
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	620	Total	O	0	3
			623	623		

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, α , β , γ	102.07Å 130.41Å 160.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.35 – 1.63 45.57 – 1.63	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.35-1.63) 98.3 (45.57-1.63)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.178 , 0.205 0.185 , 0.208	Depositor DCC
R_{free} test set	6475 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 129484 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6474	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, CL, CA, J31, 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	1.02	4/5777 (0.1%)	1.01	11/7831 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437	GLU	CD-OE2	-5.89	1.19	1.25
1	A	434	TRP	CE3-CZ3	5.77	1.48	1.38
1	A	183	GLU	CD-OE1	5.64	1.31	1.25
1	A	557	GLU	CD-OE2	-5.25	1.19	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	A	370	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	A	387	ASP	CB-CG-OD1	-7.92	111.17	118.30
1	A	673	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	673	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	465	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	309	MET	CG-SD-CE	-6.20	90.28	100.20
1	A	536	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	63	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	369	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	666	ASP	CB-CG-OD1	5.04	122.84	118.30

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	5593	0	5460	28	0
2	A	28	0	26	0	0
3	A	84	0	75	0	0
4	A	61	0	52	0	0
5	A	39	0	34	0	0
6	A	42	0	34	0	0
7	A	2	0	0	0	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
10	A	623	0	0	10	0
All	All	6474	0	5681	28	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 2.

All (28) 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:443:GLN:HG2	10:A:1516:HOH:O	1.73	0.87
1:A:91:GLN:HG2	10:A:1499:HOH:O	1.77	0.85
1:A:58:MET:HE1	1:A:586:GLU:HG2	1.71	0.72
1:A:215:LYS:HE2	10:A:1437:HOH:O	1.93	0.67
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.30	0.66
1:A:688[B]:ARG:NH1	10:A:1139:HOH:O	2.29	0.65
1:A:651:GLN:O	1:A:655:LYS:NZ	2.33	0.60
1:A:659[B]:ILE:O	1:A:663[B]:MET:HG3	2.04	0.58
1:A:506:PHE:O	1:A:507:SER:O	2.22	0.57
1:A:58:MET:CE	1:A:586:GLU:HG2	2.35	0.55
1:A:506:PHE:CB	1:A:509:MET:HG3	2.37	0.54
1:A:718:LYS:HE3	10:A:995:HOH:O	2.08	0.53
1:A:169:MET:HA	1:A:344:MET:O	2.08	0.52
1:A:189:GLU:HG3	10:A:1299:HOH:O	2.10	0.51
1:A:543:THR:HG22	1:A:543:THR:O	2.13	0.48
1:A:325:VAL:HB	1:A:326:PRO:HD2	1.95	0.48
1:A:641:GLU:HG3	10:A:1418:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:MET:HE1	10:A:943:HOH:O	2.17	0.45
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.99	0.43
1:A:591[A]:ILE:HD12	10:A:931:HOH:O	2.18	0.43
1:A:507:SER:C	1:A:509:MET:H	2.23	0.42
1:A:657[A]:ASN:CG	1:A:660[A]:VAL:HG23	2.40	0.42
1:A:227:LEU:O	1:A:296:PRO:HA	2.20	0.41
1:A:539:LYS:HE2	10:A:1128:HOH:O	2.20	0.41
1:A:225:VAL:O	1:A:294:VAL:HA	2.21	0.41
1:A:449:TYR:O	1:A:532:SER:HA	2.21	0.40
1:A:387:ASP:HA	1:A:388:PRO:HA	1.94	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	703/739 (95%)	682 (97%)	18 (3%)	3 (0%)	39 17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	GLY
1	A	507	SER
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	598/629 (95%)	587 (98%)	11 (2%)	66	41

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	LEU
1	A	189	GLU
1	A	303	GLN
1	A	443	GLN
1	A	499	LYS
1	A	507	SER
1	A	519	ASN
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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

14 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	$\# Z > 2$
3	NAG	A	802	1,3	13,13,15	1.11	1 (7%)	13,17,21	1.30	2 (15%)
3	NAG	A	803	3	15,15,15	0.53	0	17,21,21	1.08	0
3	NAG	A	804	1,3	14,14,15	0.75	0	15,19,21	1.33	2 (13%)
3	NAG	A	805	3	14,14,15	0.63	0	15,19,21	1.13	1 (6%)
4	NAG	A	807	1,4	14,14,15	0.83	0	15,19,21	1.15	0
4	NAG	A	808	4	14,14,15	0.75	1 (7%)	15,19,21	1.22	1 (6%)
4	BMA	A	809	4	11,11,12	0.74	0	14,15,17	0.95	1 (7%)
4	MAN	A	810	4	11,11,12	0.75	0	14,15,17	1.18	2 (14%)
4	MAN	A	811	4	11,11,12	0.59	0	14,15,17	1.08	1 (7%)
5	NAG	A	812	1,5	13,13,15	0.97	0	13,17,21	2.13	6 (46%)
5	NAG	A	813	5	15,15,15	0.72	1 (6%)	17,21,21	0.99	1 (5%)
5	BMA	A	814	5	11,11,12	0.50	0	14,15,17	1.10	1 (7%)
3	NAG	A	815	1,3	14,14,15	0.80	1 (7%)	15,19,21	1.83	5 (33%)
3	NAG	A	816	3	14,14,15	0.63	0	15,19,21	1.93	3 (20%)

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	802	1,3	-	0/6/19/26	0/1/1/1
3	NAG	A	803	3	-	0/6/26/26	0/1/1/1
3	NAG	A	804	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	805	3	-	0/6/23/26	0/1/1/1
4	NAG	A	807	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	808	4	-	0/6/23/26	0/1/1/1
4	BMA	A	809	4	-	0/2/19/22	0/1/1/1
4	MAN	A	810	4	-	0/2/19/22	0/1/1/1
4	MAN	A	811	4	-	0/2/19/22	0/1/1/1
5	NAG	A	812	1,5	-	0/6/19/26	0/1/1/1
5	NAG	A	813	5	-	0/6/26/26	0/1/1/1
5	BMA	A	814	5	-	0/2/19/22	0/1/1/1
3	NAG	A	815	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	816	3	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	808	NAG	O5-C1	-2.25	1.39	1.43
5	A	813	NAG	C1-C2	-2.09	1.50	1.53
3	A	815	NAG	C3-C2	2.04	1.57	1.52
3	A	802	NAG	C1-C2	2.29	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	812	NAG	O5-C5-C4	-3.75	101.37	108.86
3	A	815	NAG	O3-C3-C4	-3.35	102.81	110.34
5	A	812	NAG	O6-C6-C5	-3.19	102.35	111.66
3	A	816	NAG	O7-C7-C8	-2.94	116.66	122.06
3	A	816	NAG	C6-C5-C4	-2.89	105.88	113.02
5	A	812	NAG	C3-C4-C5	-2.81	105.69	111.40
3	A	804	NAG	C2-N2-C7	-2.71	119.56	123.04
3	A	802	NAG	O3-C3-C2	-2.65	105.22	110.48
3	A	815	NAG	O7-C7-C8	-2.61	117.27	122.06
5	A	812	NAG	O7-C7-C8	-2.55	117.39	122.06
3	A	804	NAG	O4-C4-C3	-2.34	105.06	110.34
4	A	809	BMA	O3-C3-C2	-2.28	105.88	110.00
4	A	808	NAG	O4-C4-C5	-2.27	103.21	109.24
4	A	811	MAN	O2-C2-C1	-2.21	104.77	109.21
4	A	810	MAN	O3-C3-C4	-2.16	105.47	110.34
3	A	805	NAG	O3-C3-C2	-2.12	104.92	109.11
3	A	815	NAG	C3-C2-N2	2.08	115.55	110.56
4	A	810	MAN	C1-O5-C5	2.16	114.99	112.25
5	A	812	NAG	C8-C7-N2	2.31	120.53	116.11
5	A	813	NAG	O5-C5-C6	2.46	112.57	106.36
5	A	814	BMA	C6-C5-C4	2.48	119.12	113.02
3	A	815	NAG	C8-C7-N2	2.64	121.16	116.11
3	A	802	NAG	O5-C5-C6	2.95	110.20	106.51
5	A	812	NAG	O5-C5-C6	3.01	110.27	106.51
3	A	815	NAG	O3-C3-C2	3.24	115.53	109.11
3	A	816	NAG	C1-O5-C5	4.42	117.85	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	14,14,15	0.58	0	15,19,21	1.87	1 (6%)
2	NAG	A	806	1	14,14,15	0.94	0	15,19,21	1.51	3 (20%)
6	J31	A	817	7	33,42,92	0.87	2 (6%)	36,52,109	1.19	3 (8%)

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	-	0/6/23/26	0/1/1/1
2	NAG	A	806	1	-	0/6/23/26	0/1/1/1
6	J31	A	817	7	-	0/36/46/110	0/1/1/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	817	J31	C5-N1	-2.74	1.42	1.46
6	A	817	J31	C9-C8	2.07	1.56	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	817	J31	C18-C13-C	-3.41	120.53	126.18
2	A	806	NAG	C3-C4-C5	-2.34	106.11	110.20
2	A	806	NAG	O3-C3-C2	-2.15	104.86	109.11
6	A	817	J31	N2-C7-N1	2.06	118.48	115.08
6	A	817	J31	O-C-C13	2.25	125.27	120.95
2	A	806	NAG	O5-C5-C6	3.57	115.08	107.35
2	A	801	NAG	C1-O5-C5	5.52	119.25	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	695/739 (94%)	0.09	21 (3%) 54 52	11, 21, 41, 65	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	507	SER	4.6
1	A	506	PHE	4.0
1	A	336	ASN	3.5
1	A	487	GLY	3.3
1	A	337	PHE	3.3
1	A	508	GLY	3.1
1	A	334	THR	3.0
1	A	153	ASN	2.9
1	A	135	GLY	2.9
1	A	719	VAL	2.9
1	A	134	ASP	2.8
1	A	505	GLU	2.8
1	A	136	ASN	2.7
1	A	131	ILE	2.4
1	A	55	LYS	2.3
1	A	155	SER	2.3
1	A	124	HIS	2.3
1	A	490	GLY	2.2
1	A	521	PHE	2.2
1	A	335	GLY	2.1
1	A	333	PHE	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 ⓘ

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(Å ²)	Q<0.9
4	MAN	A	811	11/12	0.77	0.23	3.31	46,51,59,66	0
4	NAG	A	807	14/15	0.93	0.08	2.34	18,24,32,43	0
4	MAN	A	810	11/12	0.89	0.14	2.07	41,44,48,51	0
5	NAG	A	812	13/15	0.91	0.10	1.32	24,26,29,37	0
3	NAG	A	802	13/15	0.85	0.14	0.12	33,36,40,41	0
4	BMA	A	809	11/12	0.91	0.11	-	37,40,44,45	0
3	NAG	A	803	15/15	0.89	0.24	-	48,51,58,67	0
3	NAG	A	805	14/15	0.78	0.28	-	35,43,50,57	0
3	NAG	A	816	14/15	0.77	0.32	-	53,57,64,65	0
5	BMA	A	814	11/12	0.65	0.30	-	59,63,66,70	0
3	NAG	A	804	14/15	0.93	0.12	-	26,32,37,43	0
3	NAG	A	815	14/15	0.87	0.11	-	26,38,42,48	0
4	NAG	A	808	14/15	0.92	0.14	-	31,36,45,48	0
5	NAG	A	813	15/15	0.94	0.11	-	27,37,44,50	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
2	NAG	A	806	14/15	0.80	0.24	2.28	38,48,65,67	0
6	J31	A	817	42/90	0.95	0.14	1.04	12,28,54,60	0
9	CA	A	821	1/1	1.00	0.08	-0.01	12,12,12,12	0
8	CL	A	820	1/1	0.99	0.11	-1.31	15,15,15,15	0
7	ZN	A	819	1/1	1.00	0.08	-2.25	14,14,14,14	0
7	ZN	A	818	1/1	1.00	0.08	-3.71	13,13,13,13	0
2	NAG	A	801	14/15	0.85	0.22	-	53,59,63,63	0

6.5 Other polymers

There are no such residues in this entry.