



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:22 PM GMT

PDB ID : 4OME
Title : X-ray structure of human glutamate carboxypeptidase II in complex with DC-CBL, a urea based inhibitor with distal carborane moiety
Authors : Barinka, C.; Ptacek, J.; Novakova, Z.; Byun, Y.
Deposited on : 2014-01-27
Resolution : 1.79 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

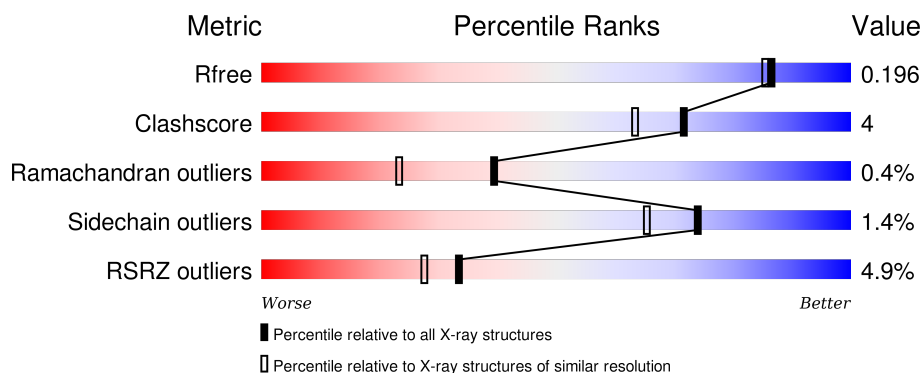
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	<div> <div>5%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>

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	804	-	-	-	X
3	NAG	A	803	-	-	-	X
4	NAG	A	808	-	-	-	X
5	NAG	A	811	-	-	-	X
5	MAN	A	814	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 6515 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	692	Total	C	N	O	S	0	40	0
			5714	3672	954	1065	23			

- 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		

- 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		

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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		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	4	Total	C	N	O	0	0
			50	28	2	20		

- 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		

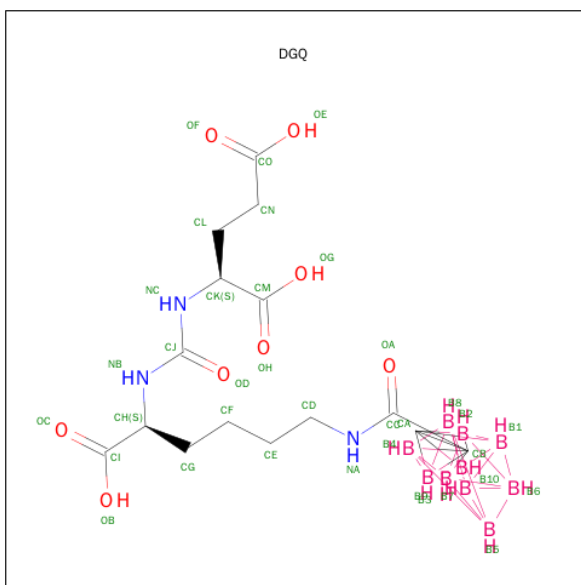
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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 (S)-2-(3-((S)-1-CARBOXY-5-(1,2-DICARBA-CLOSO-DODECARBORANYL AMIDO) PENTYL)UREIDO)PENTANEDIOIC ACID (three-letter code: DGQ) (formula: C₁₅H₃₁B₁₀N₃O₈).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	B	C	N	O	0	0
			36	10	15	3	8		

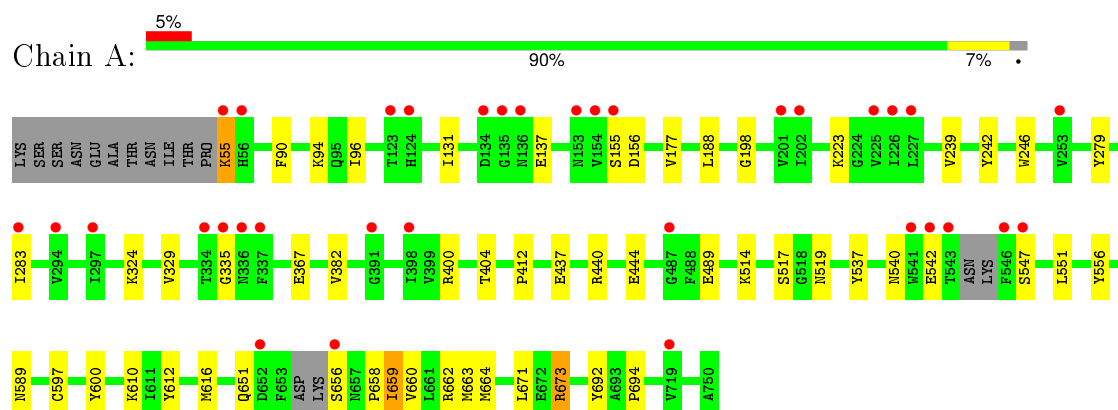
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	574	Total O 574 574	0	0

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	101.32Å 130.56Å 158.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.43 – 1.79 28.43 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (28.43-1.79) 99.4 (28.43-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.157 , 0.184 0.172 , 0.196	Depositor DCC
R_{free} test set	4859 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.8	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 97196 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6515	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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, CA, DGQ, 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	0.77	0/5958	0.75	2/8070 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	440	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	A	673	ARG	NE-CZ-NH1	6.19	123.39	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	5714	0	5569	44	2
2	A	56	0	50	3	0
3	A	42	0	39	2	0
4	A	39	0	34	2	0
5	A	50	0	43	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	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	574	0	0	17	3
All	All	6515	0	5754	50	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 4.

All (50) 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:94[B]:LYS:HE3	10:A:1097:HOH:O	1.23	1.29
1:A:610:LYS:HE2	10:A:1081:HOH:O	1.69	0.93
1:A:658[A]:PRO:HB3	10:A:1252:HOH:O	1.71	0.89
1:A:610:LYS:CE	10:A:1081:HOH:O	2.27	0.80
1:A:597[B]:CYS:SG	1:A:671:LEU:CD2	2.72	0.77
1:A:597[B]:CYS:SG	1:A:671:LEU:HD22	2.24	0.77
4:A:809:NAG:H83	10:A:1113:HOH:O	1.86	0.75
2:A:802:NAG:H81	10:A:1149:HOH:O	1.88	0.73
1:A:400:ARG:O	1:A:404[B]:THR:HG23	1.89	0.73
1:A:659[A]:ILE:HD13	1:A:659[A]:ILE:N	2.02	0.73
1:A:131:ILE:HG22	1:A:137:GLU:HG2	1.81	0.61
1:A:177:VAL:HG12	1:A:188:LEU:HD11	1.82	0.59
1:A:188:LEU:HD21	1:A:329[A]:VAL:HG11	1.88	0.55
1:A:612:TYR:CZ	1:A:616:MET:HG3	2.42	0.54
1:A:437:GLU:OE1	10:A:1175:HOH:O	2.18	0.54
2:A:802:NAG:H83	10:A:1391:HOH:O	2.09	0.53
1:A:610:LYS:NZ	10:A:1081:HOH:O	2.36	0.52
1:A:198:GLY:O	1:A:223:LYS:HE2	2.14	0.48
1:A:610:LYS:NZ	10:A:1473:HOH:O	2.47	0.47
1:A:177:VAL:HG12	1:A:188:LEU:CD1	2.45	0.47
1:A:659[B]:ILE:O	1:A:663[B]:MET:HG3	2.14	0.46
1:A:489:GLU:CD	1:A:489:GLU:H	2.18	0.46
1:A:131:ILE:CG2	1:A:137:GLU:HG2	2.46	0.46
4:A:809:NAG:C8	10:A:1113:HOH:O	2.56	0.45
1:A:597[B]:CYS:SG	1:A:671:LEU:HD23	2.56	0.45
1:A:514[A]:LYS:HD2	1:A:692:TYR:HE1	1.81	0.45
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.99	0.45
2:A:802:NAG:C8	10:A:1149:HOH:O	2.58	0.45
1:A:412:PRO:HA	1:A:589[B]:ASN:OD1	2.17	0.45
1:A:246:TRP:CD1	3:A:807:NAG:H83	2.51	0.45
1:A:55:LYS:HE2	1:A:55:LYS:HB2	1.73	0.44
1:A:90:PHE:CE2	1:A:94[A]:LYS:HE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283[B]:ILE:HG22	10:A:1258:HOH:O	2.17	0.43
1:A:517:SER:HB2	1:A:694:PRO:HG3	2.00	0.43
1:A:155:SER:O	1:A:156:ASP:HB2	2.18	0.43
3:A:803:NAG:H83	10:A:1112:HOH:O	2.18	0.42
1:A:188:LEU:CD2	1:A:329[A]:VAL:HG11	2.50	0.42
1:A:597[B]:CYS:HG	1:A:671:LEU:HD22	1.82	0.42
1:A:660[A]:VAL:O	1:A:664[A]:MET:HG3	2.20	0.42
1:A:658[B]:PRO:HA	10:A:1252:HOH:O	2.20	0.41
1:A:658[A]:PRO:HG2	1:A:659[A]:ILE:HD13	2.01	0.41
1:A:367:GLU:OE1	1:A:662[A]:ARG:NH1	2.43	0.41
1:A:188:LEU:HD21	1:A:329[A]:VAL:CG1	2.48	0.41
1:A:242:TYR:OH	10:A:1406:HOH:O	1.85	0.41
1:A:96[B]:ILE:HD13	10:A:985:HOH:O	2.19	0.41
1:A:324:LYS:HA	1:A:324:LYS:HD3	1.90	0.41
1:A:540:ASN:OD1	1:A:542:GLU:HB3	2.21	0.40
1:A:444:GLU:HA	1:A:444:GLU:OE1	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)
10:A:1118:HOH:O	10:A:1438:HOH:O[2_565]	1.72	0.48
1:A:656[B]:SER:O	10:A:1252:HOH:O[4_566]	2.12	0.08
1:A:656[B]:SER:OG	10:A:1252:HOH:O[4_566]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	723/707 (102%)	703 (97%)	17 (2%)	3 (0%)	39 23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	GLY
1	A	382	VAL
1	A	547	SER

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	627/603 (104%)	617 (98%)	10 (2%)	70 59

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	239[A]	VAL
1	A	239[B]	VAL
1	A	519	ASN
1	A	537	TYR
1	A	600	TYR
1	A	651	GLN
1	A	659[A]	ILE
1	A	659[B]	ILE
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 ⓘ

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

5.5 Carbohydrates ⓘ

11 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	0.59	0	15,19,21	1.57	4 (26%)
2	NAG	A	802	2	14,14,15	0.53	0	15,19,21	1.42	1 (6%)
2	NAG	A	804	1,2	14,14,15	0.71	0	15,19,21	1.09	2 (13%)
2	NAG	A	805	2	14,14,15	0.45	0	15,19,21	0.91	0
4	NAG	A	808	1,4	14,14,15	0.69	0	15,19,21	0.69	0
4	NAG	A	809	4	14,14,15	0.71	0	15,19,21	1.26	3 (20%)
4	BMA	A	810	4	11,11,12	0.65	0	14,15,17	1.00	0
5	NAG	A	811	1,5	14,14,15	0.62	0	15,19,21	1.66	2 (13%)
5	NAG	A	812	5	14,14,15	0.76	1 (7%)	15,19,21	1.72	3 (20%)
5	BMA	A	813	5	11,11,12	0.57	0	14,15,17	1.31	2 (14%)
5	MAN	A	814	5	11,11,12	0.71	0	14,15,17	1.38	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
4	NAG	A	808	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	809	4	-	0/6/23/26	0/1/1/1
4	BMA	A	810	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	811	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	812	5	-	0/6/23/26	0/1/1/1
5	BMA	A	813	5	-	0/2/19/22	0/1/1/1
5	MAN	A	814	5	-	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)
5	A	812	NAG	O5-C1	-2.21	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	812	NAG	C3-C4-C5	-3.74	103.67	110.20
2	A	801	NAG	C2-N2-C7	-2.91	119.30	123.04
5	A	813	BMA	O3-C3-C2	-2.74	105.05	110.00
2	A	804	NAG	O4-C4-C3	-2.54	104.61	110.34
5	A	812	NAG	C2-N2-C7	-2.46	119.87	123.04
4	A	809	NAG	O7-C7-C8	-2.44	117.59	122.06
2	A	801	NAG	O7-C7-C8	-2.24	117.96	122.06
4	A	809	NAG	C2-N2-C7	-2.19	120.22	123.04
2	A	801	NAG	C3-C4-C5	-2.14	106.47	110.20
2	A	804	NAG	C2-N2-C7	-2.05	120.40	123.04
5	A	811	NAG	O4-C4-C3	2.03	114.92	110.34
5	A	812	NAG	O4-C4-C3	2.06	114.99	110.34
5	A	814	MAN	O3-C3-C2	2.24	114.04	110.00
5	A	813	BMA	C1-C2-C3	2.39	112.37	109.54
4	A	809	NAG	C8-C7-N2	2.54	120.96	116.11
5	A	814	MAN	O5-C5-C6	2.57	112.91	107.35
2	A	801	NAG	C1-O5-C5	3.06	116.13	112.25
2	A	802	NAG	C2-N2-C7	3.95	128.11	123.04
5	A	811	NAG	C1-O5-C5	5.05	118.66	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	NAG	3	0
4	A	809	NAG	2	0

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	803	1	14,14,15	0.66	0	15,19,21	1.91	4 (26%)
3	NAG	A	806	1	14,14,15	0.40	0	15,19,21	2.47	2 (13%)
3	NAG	A	807	1	14,14,15	0.68	0	15,19,21	1.65	3 (20%)
9	DGQ	A	819	6	36,54,54	2.53	10 (27%)	86,155,155	1.35	11 (12%)

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
9	DGQ	A	819	6	-	0/26/479/479	0/0/19/19

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	819	DGQ	CG-CH	-5.90	1.45	1.53
9	A	819	DGQ	CB-CC	-4.57	1.49	1.53
9	A	819	DGQ	B10-B1	-3.56	1.70	1.84
9	A	819	DGQ	CL-CK	-2.55	1.49	1.53
9	A	819	DGQ	B6-B1	-2.41	1.70	1.77
9	A	819	DGQ	CF-CG	-2.27	1.41	1.52
9	A	819	DGQ	B7-B1	-2.06	1.71	1.77
9	A	819	DGQ	CJ-NB	2.37	1.42	1.35
9	A	819	DGQ	CJ-NC	2.63	1.42	1.35
9	A	819	DGQ	CC-NA	10.40	1.43	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	819	DGQ	B4-CB-B2	-3.72	111.28	113.47
9	A	819	DGQ	B3-CB-B9	-3.39	111.47	113.47
9	A	819	DGQ	B10-CA-B1	-3.16	58.96	68.73
3	A	807	NAG	O3-C3-C4	-3.05	103.48	110.34
9	A	819	DGQ	CE-CF-CG	-2.45	104.96	113.66
9	A	819	DGQ	B4-CB-B3	-2.41	61.27	62.78
3	A	803	NAG	O3-C3-C4	-2.08	105.65	110.34
3	A	803	NAG	O5-C5-C6	2.02	111.72	107.35
3	A	806	NAG	O5-C5-C6	2.06	111.80	107.35
3	A	807	NAG	C8-C7-N2	2.09	120.11	116.11
9	A	819	DGQ	B7-B1-B10	2.15	62.01	57.64
3	A	803	NAG	C3-C4-C5	2.22	114.07	110.20
9	A	819	DGQ	B1-B10-CA	2.36	59.36	55.64
9	A	819	DGQ	OA-CC-CB	2.82	122.44	119.86
3	A	807	NAG	C1-O5-C5	3.25	116.38	112.25
9	A	819	DGQ	B7-B1-B2	3.36	112.53	107.37
9	A	819	DGQ	B6-B1-B10	3.51	112.41	106.48
9	A	819	DGQ	B10-B1-CA	3.82	61.67	55.64
3	A	803	NAG	C1-O5-C5	5.62	119.38	112.25
3	A	806	NAG	C1-O5-C5	8.47	122.99	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	803	NAG	1	0
3	A	807	NAG	1	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	692/707 (97%)	0.11	34 (4%)	33 27	13, 23, 44, 84	4 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	543	THR	7.2
1	A	656[A]	SER	4.4
1	A	542	GLU	4.4
1	A	55	LYS	4.1
1	A	201[A]	VAL	3.9
1	A	134	ASP	3.8
1	A	541	TRP	3.6
1	A	546	PHE	3.5
1	A	155	SER	3.4
1	A	335	GLY	3.2
1	A	227	LEU	3.2
1	A	336	ASN	3.1
1	A	153	ASN	3.1
1	A	226	ILE	2.8
1	A	487	GLY	2.7
1	A	719	VAL	2.7
1	A	337	PHE	2.7
1	A	56	HIS	2.7
1	A	225	VAL	2.6
1	A	294	VAL	2.6
1	A	297	ILE	2.5
1	A	652	ASP	2.5
1	A	547	SER	2.5
1	A	398	ILE	2.4
1	A	202	ILE	2.3
1	A	124	HIS	2.2
1	A	135	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	334	THR	2.2
1	A	136	ASN	2.2
1	A	154	VAL	2.2
1	A	123	THR	2.2
1	A	283[A]	ILE	2.1
1	A	391	GLY	2.1
1	A	253	VAL	2.0

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, 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	802	14/15	0.75	0.32	8.04	29,37,42,45	0
4	NAG	A	808	14/15	0.89	0.17	6.83	17,19,23,25	0
2	NAG	A	804	14/15	0.90	0.18	4.12	24,26,29,34	0
5	NAG	A	811	14/15	0.93	0.13	2.94	12,16,25,31	0
5	MAN	A	814	11/12	0.89	0.22	2.32	34,36,39,42	0
4	NAG	A	809	14/15	0.90	0.24	-	28,32,38,40	0
5	NAG	A	812	14/15	0.89	0.26	-	27,33,41,46	0
5	BMA	A	813	11/12	0.84	0.22	-	29,33,35,37	0
2	NAG	A	805	14/15	0.81	0.37	-	34,41,48,55	0
2	NAG	A	801	14/15	0.92	0.16	-	21,28,35,40	0
4	BMA	A	810	11/12	0.68	0.33	-	40,46,52,57	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, 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
3	NAG	A	803	14/15	0.76	0.32	3.60	35,39,54,56	0
9	DGQ	A	819	36/36	0.95	0.14	0.81	13,26,75,77	0
7	CA	A	817	1/1	1.00	0.03	-2.37	9,9,9,9	0
8	CL	A	818	1/1	1.00	0.04	-3.02	12,12,12,12	0
6	ZN	A	816	1/1	0.99	0.02	-4.41	10,10,10,10	0
6	ZN	A	815	1/1	1.00	0.03	-8.95	10,10,10,10	0
3	NAG	A	807	14/15	0.89	0.20	-	21,33,40,41	0
3	NAG	A	806	14/15	0.81	0.33	-	54,60,68,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.