



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:30 pm GMT

PDB ID : 3Q2W
Title : Crystal structure of mouse N-cadherin ectodomain
Authors : Jin,X.; Shapiro, L.
Deposited on : 2010-12-20
Resolution : 3.20 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

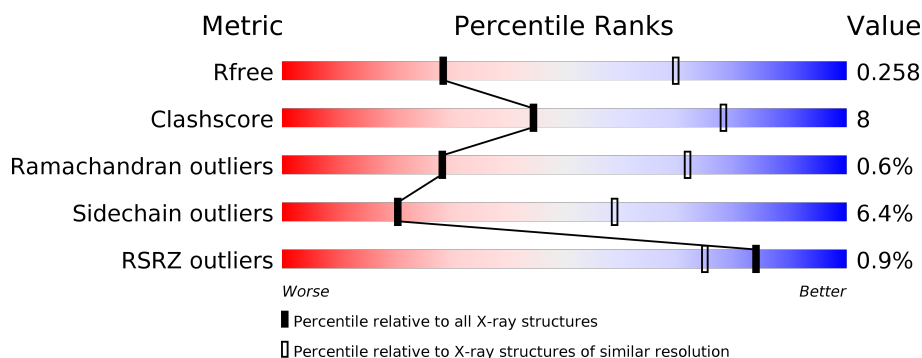
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	559	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;">%</div> <div style="position: absolute; top: 10px; left: 0; width: 100%;">77%18%..</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
3	MAN	A	701	X	-	-	-
3	MAN	A	702	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	A	706	X	-	-	-
3	MAN	A	707	-	-	-	X
3	MAN	A	709	X	-	-	-
4	NAG	A	801	X	-	-	-
4	NAG	A	804	X	-	-	X
4	NAG	A	807	X	-	-	-
5	NAG	A	805	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4451 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 Cadherin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	1	0
			4181	2630	715	824	12			

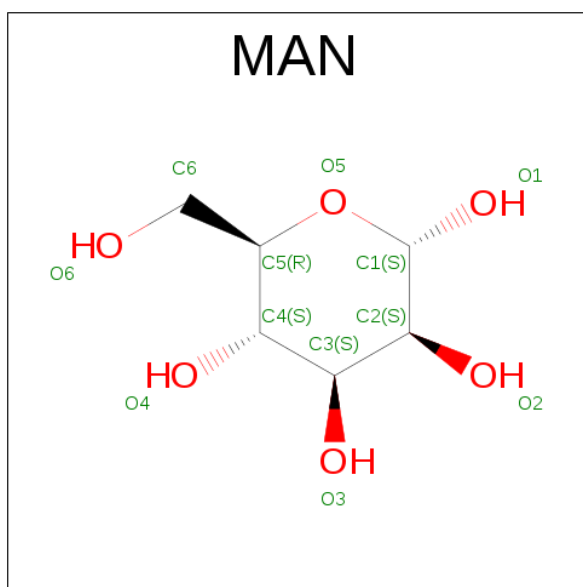
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	ASN	TYR	CONFLICT	UNP P15116
A	408	LYS	GLN	CONFLICT	UNP P15116
A	465	THR	ALA	CONFLICT	UNP P15116
A	554	HIS	-	EXPRESSION TAG	UNP P15116
A	555	HIS	-	EXPRESSION TAG	UNP P15116
A	556	HIS	-	EXPRESSION TAG	UNP P15116
A	557	HIS	-	EXPRESSION TAG	UNP P15116
A	558	HIS	-	EXPRESSION TAG	UNP P15116
A	559	HIS	-	EXPRESSION TAG	UNP P15116

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	Ca	0	0
			12	12		

- Molecule 3 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

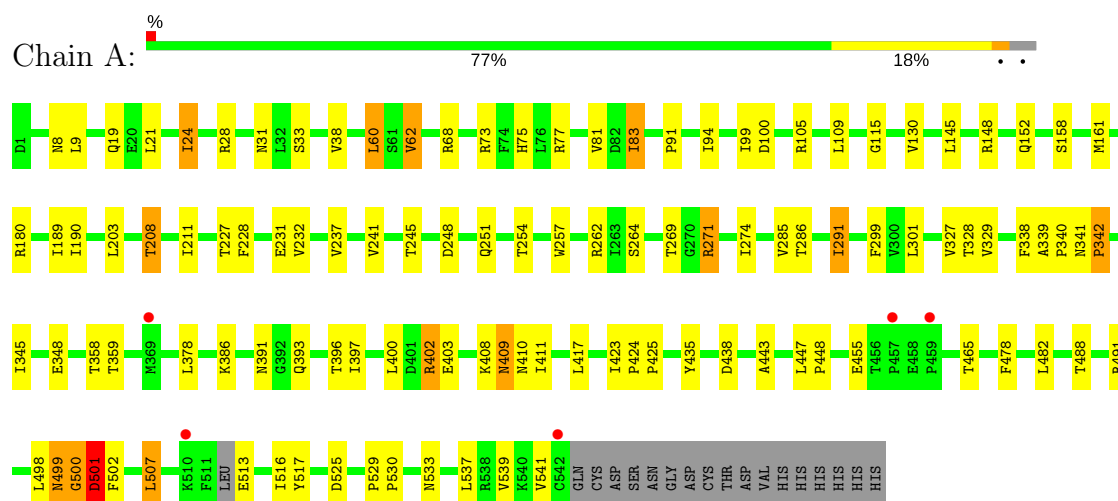
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	61	Total	O	0	0
			61	61		

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 the various outlier classes 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: Cadherin-2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	91.37Å 111.65Å 262.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 3.20 29.31 – 3.11	Depositor EDS
% Data completeness (in resolution range)	89.9 (19.95-3.20) 88.0 (29.31-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 3.11Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.230 , 0.267 0.219 , 0.258	Depositor DCC
R_{free} test set	1030 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 26.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4451	wwPDB-VP
Average B, all atoms (Å ²)	61.0	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, 0.333 respectively for untwinned datasets, and 0.375, 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: CA, NAG, 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	0.34	0/4275	0.57	2/5866 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	1	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	501	ASP	N-CA-CB	-11.10	90.62	110.60
1	A	501	ASP	N-CA-C	8.53	134.03	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	805	NAG	C1

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	4181	0	4091	65	0
2	A	12	0	0	0	0
3	A	99	0	90	0	0
4	A	42	0	39	0	0
5	A	56	0	50	0	0
6	A	61	0	0	0	0
All	All	4451	0	4270	65	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 8.

All (65) 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:251:GLN:O	1:A:254:THR:HG22	1.63	0.97
1:A:501:ASP:OD2	1:A:502:PHE:HD2	1.59	0.83
1:A:499:ASN:HD21	1:A:502:PHE:HB2	1.50	0.77
1:A:499:ASN:HD22	1:A:499:ASN:H	1.31	0.77
1:A:339:ALA:HB3	1:A:340:PRO:HD3	1.66	0.76
1:A:501:ASP:OD2	1:A:502:PHE:CD2	2.39	0.75
1:A:498:LEU:HB2	1:A:502:PHE:O	1.92	0.69
1:A:411:ILE:HG22	1:A:435:TYR:HA	1.75	0.68
1:A:499:ASN:H	1:A:499:ASN:ND2	1.91	0.68
1:A:499:ASN:N	1:A:499:ASN:ND2	2.38	0.68
1:A:299:PHE:HB2	1:A:327:VAL:HB	1.78	0.65
1:A:443:ALA:HB1	1:A:533:ASN:HB2	1.80	0.62
1:A:341:ASN:HB3	1:A:342:PRO:HD3	1.83	0.61
1:A:28:ARG:CG	1:A:28:ARG:HH11	2.13	0.60
1:A:447:LEU:HB3	1:A:448:PRO:HD3	1.84	0.59
1:A:409:ASN:HD22	1:A:410:ASN:H	1.48	0.59
1:A:478:PHE:CE2	1:A:525:ASP:HB3	2.40	0.57
1:A:73:ARG:HD3	1:A:75[B]:HIS:NE2	2.19	0.56
1:A:248:ASP:HB3	1:A:257:TRP:CD1	2.40	0.56
1:A:8:ASN:HB3	1:A:99:ILE:HD11	1.87	0.56
1:A:391:ASN:HB3	1:A:393:GLN:HG3	1.87	0.56
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.72	0.55
1:A:488:THR:HG22	1:A:491:ARG:NH2	2.22	0.55
1:A:109:LEU:H	1:A:109:LEU:HD12	1.72	0.54
1:A:359:THR:HG22	1:A:393:GLN:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HD12	1:A:285:VAL:HG22	1.89	0.54
1:A:152:GLN:HE22	1:A:161:MET:HG2	1.73	0.54
1:A:105:ARG:HG2	1:A:203:LEU:HB3	1.90	0.54
1:A:455:GLU:HG3	1:A:541:VAL:HG11	1.91	0.53
1:A:271:ARG:HG2	1:A:291:ILE:HG22	1.90	0.51
1:A:396:THR:HG21	1:A:400:LEU:HD11	1.92	0.50
1:A:499:ASN:HD22	1:A:499:ASN:N	1.93	0.50
1:A:345:ILE:HG13	1:A:358:THR:HG21	1.95	0.49
1:A:73:ARG:HD3	1:A:75[B]:HIS:CE1	2.47	0.49
1:A:24:ILE:HD11	1:A:60:LEU:HD13	1.95	0.48
1:A:28:ARG:CG	1:A:28:ARG:NH1	2.77	0.47
1:A:423:ILE:HB	1:A:424:PRO:HD3	1.96	0.47
1:A:19:GLN:HB3	1:A:62:VAL:HG23	1.95	0.47
1:A:402:ARG:HE	1:A:438:ASP:HB2	1.81	0.46
1:A:9:LEU:HD21	1:A:21:LEU:HD22	1.97	0.46
1:A:189:ILE:HD13	1:A:208:THR:HG23	1.98	0.45
1:A:529:PRO:HA	1:A:530:PRO:HD3	1.85	0.45
1:A:158:SER:HB3	1:A:161:MET:SD	2.56	0.45
1:A:499:ASN:ND2	1:A:500:GLY:H	2.15	0.45
1:A:77:ARG:HH21	1:A:91:PRO:HB2	1.82	0.45
1:A:499:ASN:HD22	1:A:500:GLY:H	1.64	0.44
1:A:507:LEU:H	1:A:507:LEU:CD1	2.31	0.44
1:A:33:SER:HB3	1:A:83:ILE:HD12	2.00	0.44
1:A:341:ASN:CB	1:A:342:PRO:HD3	2.47	0.43
1:A:115:GLY:O	1:A:211:ILE:HA	2.18	0.43
1:A:478:PHE:HE2	1:A:525:ASP:HB3	1.84	0.43
1:A:21:LEU:HD21	1:A:62:VAL:HG22	2.00	0.43
1:A:386:LYS:HD2	1:A:397:ILE:HD11	2.00	0.43
1:A:378:LEU:HD12	1:A:417:LEU:HG	2.00	0.43
1:A:513:GLU:N	1:A:517:TYR:HH	2.17	0.43
1:A:537:LEU:HD22	1:A:539:VAL:HG22	2.00	0.43
1:A:68:ARG:HD3	1:A:100:ASP:HB2	2.01	0.42
1:A:339:ALA:CB	1:A:340:PRO:HD3	2.44	0.42
1:A:228:PHE:HE1	1:A:245:THR:HG22	1.84	0.42
1:A:130:VAL:HG21	1:A:190:ILE:HG13	2.02	0.41
1:A:291:ILE:HD11	1:A:329:VAL:HG11	2.01	0.41
1:A:231:GLU:HA	1:A:328:THR:O	2.21	0.41
1:A:232:VAL:HG13	1:A:241:VAL:HG13	2.03	0.41
1:A:423:ILE:O	1:A:425:PRO:HD3	2.21	0.41
1:A:262:ARG:HH12	1:A:264:SER:HA	1.86	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	538/559 (96%)	491 (91%)	44 (8%)	3 (1%)	28 72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ASP
1	A	500	GLY
1	A	342	PRO

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	472/491 (96%)	442 (94%)	30 (6%)	20 59

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	31	ASN
1	A	38	VAL
1	A	60	LEU
1	A	62	VAL
1	A	81	VAL
1	A	83	ILE
1	A	94	ILE

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Mol	Chain	Res	Type
1	A	145	LEU
1	A	148	ARG
1	A	180	ARG
1	A	208	THR
1	A	227	THR
1	A	237	VAL
1	A	269	THR
1	A	271	ARG
1	A	286	THR
1	A	291	ILE
1	A	301	LEU
1	A	338	PHE
1	A	348	GLU
1	A	402	ARG
1	A	403	GLU
1	A	408	LYS
1	A	409	ASN
1	A	465	THR
1	A	482	LEU
1	A	499	ASN
1	A	507	LEU
1	A	516	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	45	GLN
1	A	111	GLN
1	A	320	GLN
1	A	335	ASN
1	A	383	ASN
1	A	409	ASN
1	A	442	ASN
1	A	460	ASN
1	A	463	ASN
1	A	496	ASN
1	A	499	ASN
1	A	504	GLN
1	A	533	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 ⓘ

4 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$
5	NAG	A	802	1,5	14,14,15	0.59	0	15,19,21	0.88	0
5	NAG	A	803	5	14,14,15	0.59	0	15,19,21	1.00	1 (6%)
5	NAG	A	805	1,5	14,14,15	0.47	0	15,19,21	1.42	2 (13%)
5	NAG	A	806	5	14,14,15	0.52	0	15,19,21	1.10	2 (13%)

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
5	NAG	A	802	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	803	5	-	0/6/23/26	0/1/1/1
5	NAG	A	805	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	806	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	805	NAG	C2-N2-C7	2.11	126.02	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	806	NAG	C4-C3-C2	2.14	114.15	111.02
5	A	806	NAG	C1-O5-C5	2.81	116.03	112.17
5	A	803	NAG	C1-O5-C5	2.82	116.05	112.17
5	A	805	NAG	C1-O5-C5	4.83	118.82	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	805	NAG	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	MAN	A	701	1	11,11,12	0.72	0	13,15,17	1.24	2 (15%)
3	MAN	A	702	1	11,11,12	0.45	0	13,15,17	2.41	3 (23%)
3	MAN	A	703	1	11,11,12	0.72	0	13,15,17	1.61	3 (23%)
3	MAN	A	705	1	11,11,12	0.75	0	13,15,17	1.74	3 (23%)
3	MAN	A	706	1	11,11,12	0.59	0	13,15,17	0.60	0
3	MAN	A	707	1	11,11,12	0.63	0	13,15,17	0.66	0
3	MAN	A	708	1	11,11,12	0.60	0	13,15,17	1.07	1 (7%)
3	MAN	A	709	1	11,11,12	0.62	0	13,15,17	0.63	0
3	MAN	A	710	1	11,11,12	0.91	1 (9%)	13,15,17	1.39	1 (7%)
4	NAG	A	801	1	14,14,15	0.59	0	15,19,21	1.61	2 (13%)
4	NAG	A	804	1	14,14,15	0.46	0	15,19,21	1.32	2 (13%)
4	NAG	A	807	1	14,14,15	0.43	0	15,19,21	1.18	1 (6%)

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	MAN	A	701	1	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	A	702	1	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	A	703	1	-	0/2/19/22	0/1/1/1
3	MAN	A	705	1	-	0/2/19/22	0/1/1/1
3	MAN	A	706	1	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	A	707	1	-	0/2/19/22	0/1/1/1
3	MAN	A	708	1	-	0/2/19/22	0/1/1/1
3	MAN	A	709	1	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	A	710	1	-	0/2/19/22	0/1/1/1
4	NAG	A	801	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	804	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	807	1	1/1/5/7	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	710	MAN	O6-C6	2.36	1.52	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	NAG	O5-C1-C2	-4.83	104.75	111.47
4	A	804	NAG	O5-C1-C2	-3.05	107.22	111.47
3	A	701	MAN	O5-C1-C2	-2.14	107.43	110.79
3	A	703	MAN	C1-O5-C5	2.11	115.08	112.17
4	A	801	NAG	C3-C4-C5	2.15	114.01	110.22
3	A	705	MAN	C1-C2-C3	2.19	112.42	109.65
3	A	703	MAN	C3-C4-C5	2.46	114.56	110.22
3	A	702	MAN	C3-C4-C5	2.61	114.81	110.22
4	A	804	NAG	C1-O5-C5	2.79	116.02	112.17
3	A	708	MAN	C1-O5-C5	2.83	116.07	112.17
3	A	701	MAN	C3-C4-C5	3.01	115.52	110.22
3	A	705	MAN	C2-C3-C4	3.06	116.21	110.88
3	A	702	MAN	O5-C1-C2	3.10	115.64	110.79
4	A	807	NAG	C1-O5-C5	3.62	117.15	112.17
3	A	710	MAN	C1-O5-C5	3.76	117.34	112.17
3	A	703	MAN	C1-C2-C3	3.99	114.71	109.65
3	A	705	MAN	C3-C4-C5	4.10	117.45	110.22
3	A	702	MAN	C1-O5-C5	7.54	122.56	112.17

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	807	NAG	C1
4	A	804	NAG	C1
4	A	801	NAG	C1
3	A	702	MAN	C1
3	A	706	MAN	C1
3	A	709	MAN	C1
3	A	701	MAN	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	541/559 (96%)	-0.37	5 (0%) 84 75	10, 53, 120, 159	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	542	CYS	2.8
1	A	459	PRO	2.7
1	A	369	MET	2.2
1	A	510	LYS	2.1
1	A	457	PRO	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
5	NAG	A	802	14/15	0.92	0.15	0.34	36,43,52,60	0
5	NAG	A	805	14/15	0.90	0.22	-0.66	93,105,107,113	0
5	NAG	A	803	14/15	0.86	0.26	-	42,64,80,81	0
5	NAG	A	806	14/15	0.76	0.26	-	91,115,130,133	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(Å ²)	Q<0.9
3	MAN	A	707	11/12	0.87	0.27	4.85	71,78,87,88	0
4	NAG	A	804	14/15	0.85	0.33	2.70	87,101,106,107	0
3	MAN	A	710	11/12	0.86	0.34	1.00	100,108,125,125	0
4	NAG	A	807	14/15	0.91	0.23	0.65	77,81,88,89	0
3	MAN	A	702	11/12	0.95	0.17	-0.16	36,40,55,56	0
2	CA	A	604	1/1	0.99	0.12	-0.49	14,14,14,14	0
2	CA	A	601	1/1	0.98	0.10	-0.67	26,26,26,26	0
3	MAN	A	701	11/12	0.95	0.14	-0.83	38,45,54,61	0
2	CA	A	606	1/1	0.98	0.12	-1.03	34,34,34,34	0
2	CA	A	605	1/1	0.97	0.10	-1.56	29,29,29,29	0
2	CA	A	610	1/1	0.96	0.10	-1.74	68,68,68,68	0
2	CA	A	602	1/1	0.99	0.08	-1.94	14,14,14,14	0
2	CA	A	603	1/1	0.98	0.07	-2.14	21,21,21,21	0
2	CA	A	608	1/1	0.97	0.11	-2.29	49,49,49,49	0
2	CA	A	612	1/1	0.95	0.04	-2.56	62,62,62,62	0
2	CA	A	607	1/1	0.93	0.07	-3.58	59,59,59,59	0
2	CA	A	609	1/1	0.86	0.07	-4.00	90,90,90,90	0
2	CA	A	611	1/1	0.98	0.05	-7.12	65,65,65,65	0
4	NAG	A	801	14/15	0.84	0.28	-	53,74,82,86	0
3	MAN	A	705	11/12	0.92	0.10	-	56,73,80,81	0
3	MAN	A	703	11/12	0.88	0.29	-	54,64,72,72	0
3	MAN	A	706	11/12	0.87	0.17	-	56,83,95,98	0
3	MAN	A	708	11/12	0.90	0.17	-	100,103,107,113	0
3	MAN	A	709	11/12	0.77	0.33	-	118,128,140,147	0

6.5 Other polymers [i](#)

There are no such residues in this entry.