



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:59 PM GMT

PDB ID : 4GWN
Title : Crystal structure of human mature meprin beta
Authors : Arolas, J.L.; Broder, C.; Jefferson, T.; Guevara, T.; Sterchi, E.E.; Bode, W.;
Stocker, W.; Becker-Paul, C.; Gomis-Ruth, F.X.
Deposited on : 2012-09-03
Resolution : 3.00 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

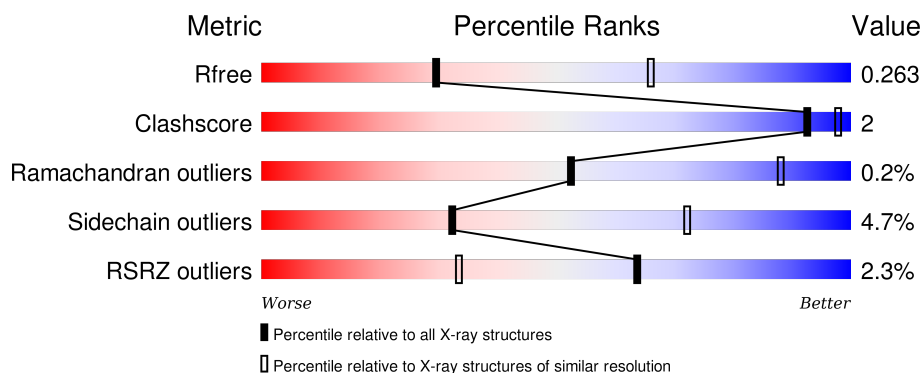
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	553	

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	CD	A	701	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4598 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 Meprin A subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4271	2685	741	824	21			

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cd	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	7	Total	C	N	O	0	0
			81	46	2	33		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

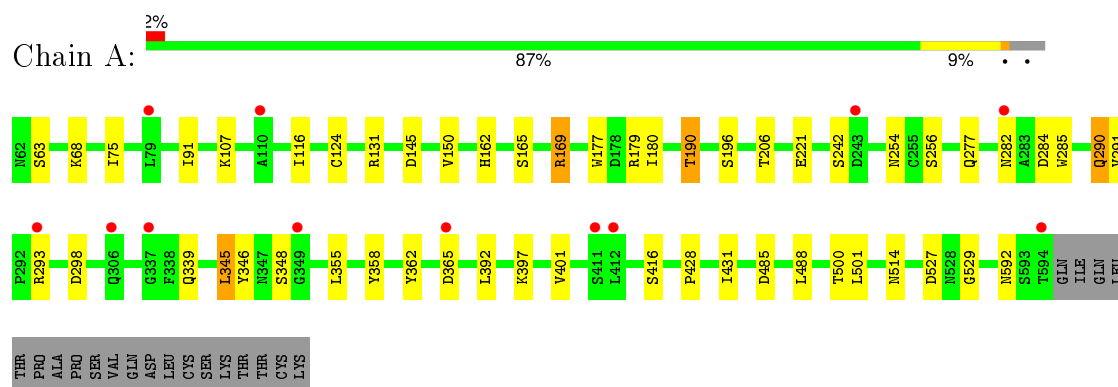


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		

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: Meprin A subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	74.96 Å 74.96 Å 502.65 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.16 – 3.00 48.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.16-3.00) 99.9 (48.16-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.01 Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.196 , 0.238 0.219 , 0.263	Depositor DCC
R_{free} test set	711 reflections (3.96%)	DCC
Wilson B-factor (Å ²)	88.1	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 81.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 17972 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4598	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, NA, CD, FUC, 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	0.41	0/4379	0.61	0/5935

There are no bond length outliers.

There are no bond angle outliers.

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	4271	0	4031	17	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	56	0	50	0	0
5	A	81	0	70	1	0
6	A	28	0	26	0	0
7	A	116	0	97	0	0
8	A	38	0	34	0	0
9	A	6	0	8	0	0
All	All	4598	0	4316	18	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 (18) 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:345:LEU:HD11	1:A:355:LEU:HD22	1.76	0.66
1:A:346:TYR:HB3	1:A:416:SER:HB2	1.88	0.56
1:A:358:TYR:HB2	1:A:401:VAL:HB	1.91	0.53
1:A:277:GLN:HG3	1:A:285:TRP:HB2	1.96	0.48
1:A:339:GLN:HB2	1:A:392:LEU:HB2	1.96	0.48
5:A:705:NAG:H61	5:A:708:NAG:HN2	1.78	0.47
1:A:485:ASP:HA	1:A:488:LEU:HD12	1.97	0.46
1:A:179:ARG:HD3	1:A:221:GLU:HB2	1.98	0.45
1:A:75:ILE:HG21	1:A:116:ILE:HD12	1.99	0.44
1:A:162:HIS:O	1:A:165:SER:HB2	2.19	0.43
1:A:177:TRP:HA	1:A:180:ILE:HD12	2.01	0.43
1:A:293:ARG:HD2	1:A:348:SER:HB2	2.01	0.43
1:A:290:GLN:HG2	1:A:291:VAL:N	2.33	0.42
1:A:428:PRO:HG2	1:A:431:ILE:HD11	2.02	0.41
1:A:362:TYR:HB2	1:A:397:LYS:HG3	2.02	0.41
1:A:501:LEU:HB3	1:A:514:ASN:HB3	2.01	0.41
1:A:91:ILE:HA	1:A:150:VAL:HG11	2.03	0.41
1:A:169:ARG:HG2	1:A:190:THR:HG23	2.04	0.40

There are no symmetry-related clashes.

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	531/553 (96%)	500 (94%)	30 (6%)	1 (0%)	52 88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	529	GLY

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	473/492 (96%)	451 (95%)	22 (5%)	32 72

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	SER
1	A	68	LYS
1	A	107	LYS
1	A	124	CYS
1	A	131	ARG
1	A	145	ASP
1	A	169	ARG
1	A	190	THR
1	A	196	SER
1	A	206	THR
1	A	242	SER
1	A	254	ASN
1	A	256	SER
1	A	282	ASN
1	A	284	ASP
1	A	290	GLN
1	A	298	ASP
1	A	345	LEU
1	A	365	ASP
1	A	500	THR
1	A	527	ASP
1	A	592	ASN

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	304	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 ⓘ

24 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	$\# Z > 2$
4	NAG	A	703	1,4	14,14,15	0.34	0	15,19,21	0.81	0
4	NAG	A	704	4	14,14,15	0.30	0	15,19,21	0.55	0
5	NAG	A	705	1,5	14,14,15	0.28	0	15,19,21	0.66	0
5	FUC	A	706	5	10,10,11	0.42	0	14,14,16	1.31	1 (7%)
5	FUC	A	707	5	10,10,11	0.50	0	14,14,16	1.20	2 (14%)
5	NAG	A	708	5	14,14,15	0.30	0	15,19,21	0.37	0
5	BMA	A	709	5	11,11,12	0.33	0	14,15,17	0.98	1 (7%)
5	MAN	A	710	5	11,11,12	0.40	0	14,15,17	0.98	2 (14%)
5	MAN	A	711	5	11,11,12	0.42	0	14,15,17	0.88	1 (7%)
7	NAG	A	713	1,7	14,14,15	0.22	0	15,19,21	0.79	1 (6%)
7	NAG	A	714	7	14,14,15	0.27	0	15,19,21	0.82	1 (6%)
7	BMA	A	715	7	11,11,12	0.30	0	14,15,17	0.59	0
7	MAN	A	716	7	11,11,12	0.31	0	14,15,17	0.83	0
7	MAN	A	717	7	11,11,12	0.31	0	14,15,17	1.04	1 (7%)
7	MAN	A	718	7	11,11,12	0.33	0	14,15,17	0.93	1 (7%)
7	MAN	A	719	7	11,11,12	0.34	0	14,15,17	0.71	1 (7%)
7	MAN	A	720	7	11,11,12	0.33	0	14,15,17	1.05	1 (7%)
7	MAN	A	721	7	11,11,12	0.29	0	14,15,17	0.92	1 (7%)
7	MAN	A	722	7	11,11,12	0.43	0	14,15,17	0.97	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	723	1,4	14,14,15	0.29	0	15,19,21	0.89	1 (6%)
4	NAG	A	724	4	14,14,15	0.37	0	15,19,21	0.72	1 (6%)
8	NAG	A	725	1,8	14,14,15	0.29	0	15,19,21	0.98	1 (6%)
8	FUC	A	726	8	10,10,11	0.47	0	14,14,16	1.36	2 (14%)
8	NAG	A	727	8	14,14,15	0.30	0	15,19,21	0.68	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
4	NAG	A	703	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	704	4	-	0/6/23/26	0/1/1/1
5	NAG	A	705	1,5	-	0/6/23/26	0/1/1/1
5	FUC	A	706	5	-	0/0/17/20	0/1/1/1
5	FUC	A	707	5	-	0/0/17/20	0/1/1/1
5	NAG	A	708	5	-	0/6/23/26	0/1/1/1
5	BMA	A	709	5	-	0/2/19/22	0/1/1/1
5	MAN	A	710	5	-	0/2/19/22	0/1/1/1
5	MAN	A	711	5	-	0/2/19/22	0/1/1/1
7	NAG	A	713	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	714	7	-	0/6/23/26	0/1/1/1
7	BMA	A	715	7	-	0/2/19/22	0/1/1/1
7	MAN	A	716	7	-	0/2/19/22	0/1/1/1
7	MAN	A	717	7	-	0/2/19/22	0/1/1/1
7	MAN	A	718	7	-	0/2/19/22	0/1/1/1
7	MAN	A	719	7	-	0/2/19/22	0/1/1/1
7	MAN	A	720	7	-	0/2/19/22	0/1/1/1
7	MAN	A	721	7	-	0/2/19/22	0/1/1/1
7	MAN	A	722	7	-	0/2/19/22	0/1/1/1
4	NAG	A	723	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	724	4	-	0/6/23/26	0/1/1/1
8	NAG	A	725	1,8	-	0/6/23/26	0/1/1/1
8	FUC	A	726	8	-	0/0/17/20	0/1/1/1
8	NAG	A	727	8	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	719	MAN	C1-O5-C5	2.10	114.91	112.25
4	A	723	NAG	C1-O5-C5	2.11	114.92	112.25
4	A	724	NAG	C2-N2-C7	2.18	125.83	123.04
7	A	722	MAN	C1-C2-C3	2.19	112.14	109.54
8	A	727	NAG	C1-O5-C5	2.23	115.08	112.25
5	A	710	MAN	C1-C2-C3	2.31	112.27	109.54
5	A	711	MAN	C1-O5-C5	2.38	115.26	112.25
8	A	726	FUC	C1-C2-C3	2.38	112.36	109.54
7	A	713	NAG	C1-O5-C5	2.48	115.40	112.25
5	A	707	FUC	C1-C2-C3	2.55	112.56	109.54
5	A	710	MAN	C1-O5-C5	2.63	115.59	112.25
7	A	722	MAN	C1-O5-C5	2.70	115.67	112.25
7	A	714	NAG	C1-O5-C5	2.72	115.69	112.25
7	A	718	MAN	C1-O5-C5	3.05	116.12	112.25
7	A	721	MAN	C1-O5-C5	3.08	116.15	112.25
8	A	725	NAG	C1-O5-C5	3.23	116.34	112.25
5	A	709	BMA	C1-O5-C5	3.27	116.39	112.25
7	A	720	MAN	C1-O5-C5	3.27	116.39	112.25
5	A	707	FUC	C1-O5-C5	3.41	117.65	112.38
7	A	717	MAN	C1-O5-C5	3.67	116.90	112.25
8	A	726	FUC	C1-O5-C5	4.24	118.93	112.38
5	A	706	FUC	C1-O5-C5	4.47	119.28	112.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	705	NAG	1	0
5	A	708	NAG	1	0

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 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
6	NAG	A	712	1	14,14,15	0.34	0	15,19,21	0.50	0
6	NAG	A	728	1	14,14,15	0.34	0	15,19,21	0.90	1 (6%)
9	GOL	A	729	-	5,5,5	0.30	0	5,5,5	0.30	0

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
6	NAG	A	712	1	-	0/6/23/26	0/1/1/1
6	NAG	A	728	1	-	0/6/23/26	0/1/1/1
9	GOL	A	729	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	728	NAG	C1-O5-C5	3.22	116.34	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 [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	533/553 (96%)	0.16	12 (2%) 64 33	81, 106, 155, 176	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	ASP	3.5
1	A	306	GLN	3.1
1	A	349	GLY	3.1
1	A	594	THR	2.6
1	A	110	ALA	2.5
1	A	411	SER	2.3
1	A	293	ARG	2.3
1	A	282	ASN	2.2
1	A	412	LEU	2.2
1	A	243	ASP	2.1
1	A	79	LEU	2.1
1	A	337	GLY	2.0

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

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(\AA^2)	Q<0.9
4	NAG	A	703	14/15	0.77	0.24	-0.48	149,152,159,159	0
7	NAG	A	714	14/15	0.98	0.18	-0.52	100,106,110,113	0
5	FUC	A	707	10/11	0.92	0.21	-0.80	124,126,128,128	0
5	FUC	A	706	10/11	0.89	0.19	-	136,137,139,140	0
5	BMA	A	709	11/12	0.95	0.14	-	151,154,159,161	0
7	BMA	A	715	11/12	0.93	0.12	-	117,120,126,132	0
7	MAN	A	719	11/12	0.88	0.41	-	151,157,159,160	0
7	MAN	A	716	11/12	0.94	0.09	-	141,143,147,152	0
7	MAN	A	717	11/12	0.97	0.14	-	119,122,125,129	0
8	NAG	A	727	14/15	0.77	0.41	-	167,174,176,178	0
4	NAG	A	704	14/15	0.64	0.32	-	159,163,166,168	0
7	MAN	A	718	11/12	0.90	0.16	-	135,136,139,145	0
7	MAN	A	721	11/12	0.94	0.30	-	116,122,124,126	0
5	NAG	A	708	14/15	0.93	0.18	-	138,141,144,147	0
5	MAN	A	710	11/12	0.86	0.34	-	162,164,168,168	0
7	NAG	A	713	14/15	0.94	0.21	-	102,114,127,129	0
5	MAN	A	711	11/12	0.77	0.27	-	161,165,169,169	0
5	NAG	A	705	14/15	0.93	0.11	-	128,131,134,136	0
8	FUC	A	726	10/11	0.72	0.43	-	172,176,178,180	0
8	NAG	A	725	14/15	0.70	0.36	-	151,163,173,174	0
4	NAG	A	724	14/15	0.85	0.19	-	150,154,157,158	0
4	NAG	A	723	14/15	0.86	0.16	-	135,138,141,145	0
7	MAN	A	720	11/12	0.95	0.14	-	122,124,130,132	0
7	MAN	A	722	11/12	0.87	0.18	-	157,162,168,168	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(\AA^2)	Q<0.9
2	CD	A	701	1/1	0.98	0.24	2.15	110,110,110,110	0
3	NA	A	702	1/1	0.99	0.18	-0.44	99,99,99,99	0
9	GOL	A	729	6/6	0.89	0.29	-	82,84,84,84	0
6	NAG	A	712	14/15	0.73	0.45	-	163,165,166,167	0
6	NAG	A	728	14/15	0.53	0.40	-	179,181,186,186	0

6.5 Other polymers [i](#)

There are no such residues in this entry.