



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 28, 2019 – 10:59 PM EST

PDB ID : 6C01
Title : Human ectonucleotide pyrophosphatase / phosphodiesterase 3 (ENPP3, NPP3, CD203c)
Authors : Gorelik, A.; Randriamihaja, A.; Illes, K.; Nagar, B.
Deposited on : 2017-12-27
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

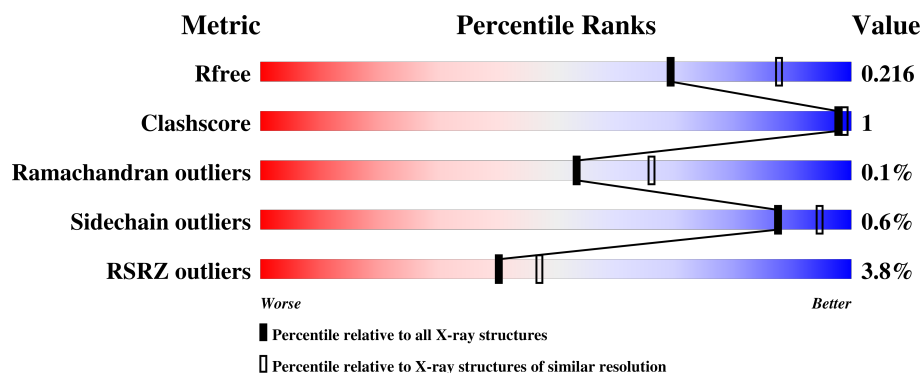
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)

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	838	<div> <div>4%</div> <div>95%</div> <div>..</div> </div>
1	B	838	<div> <div>3%</div> <div>94%</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
6	FUC	A	927	-	-	-	X
7	MAN	B	907	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 27890 atoms, of which 13140 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	819	Total	C	H	N	O	S	0	0	0
			12898	4202	6290	1125	1224	57			
1	B	807	Total	C	H	N	O	S	0	0	0
			12712	4145	6200	1106	1204	57			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ASP	-	expression tag	UNP O14638
A	39	ARG	-	expression tag	UNP O14638
A	40	HIS	-	expression tag	UNP O14638
A	41	HIS	-	expression tag	UNP O14638
A	42	HIS	-	expression tag	UNP O14638
A	43	HIS	-	expression tag	UNP O14638
A	44	HIS	-	expression tag	UNP O14638
A	45	HIS	-	expression tag	UNP O14638
A	46	LYS	-	expression tag	UNP O14638
A	47	LEU	-	expression tag	UNP O14638
B	38	ASP	-	expression tag	UNP O14638
B	39	ARG	-	expression tag	UNP O14638
B	40	HIS	-	expression tag	UNP O14638
B	41	HIS	-	expression tag	UNP O14638
B	42	HIS	-	expression tag	UNP O14638
B	43	HIS	-	expression tag	UNP O14638
B	44	HIS	-	expression tag	UNP O14638
B	45	HIS	-	expression tag	UNP O14638
B	46	LYS	-	expression tag	UNP O14638
B	47	LEU	-	expression tag	UNP O14638

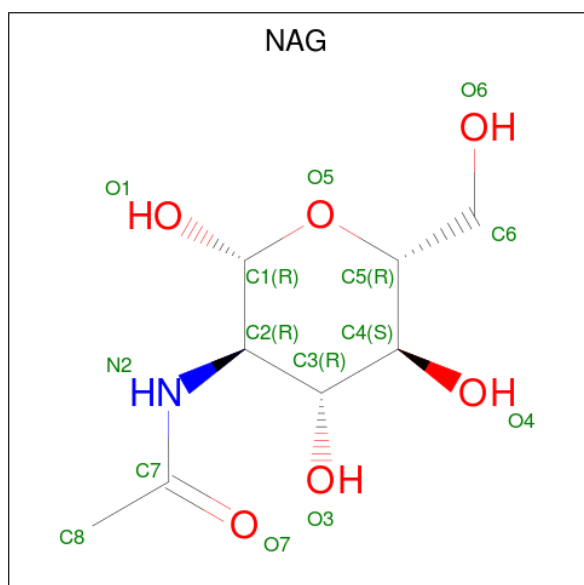
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

Continued on next page...

Continued from previous page...

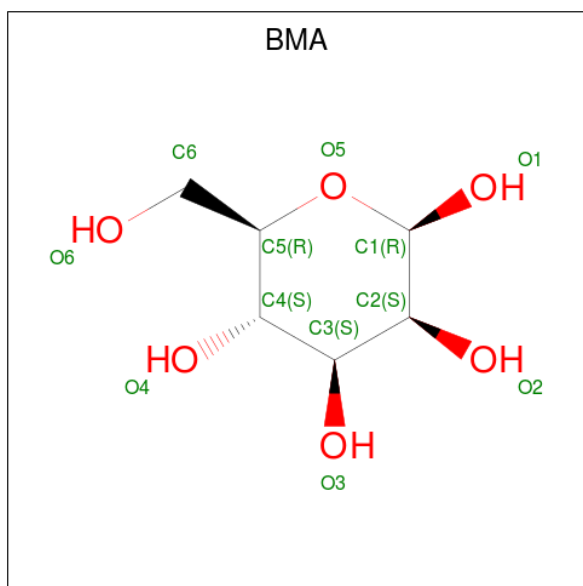
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

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



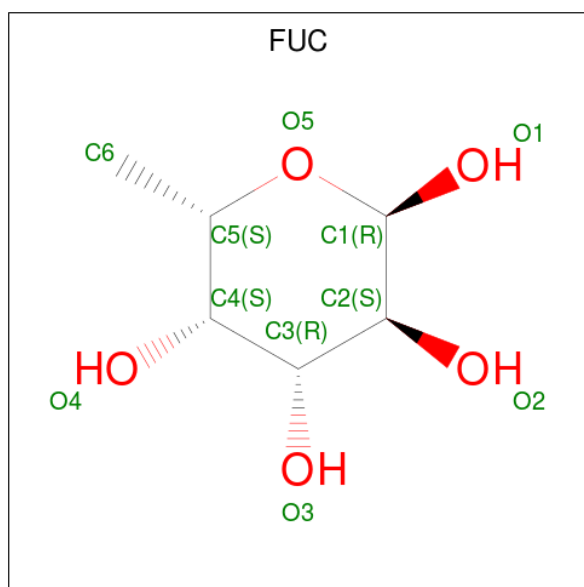
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			22	6	11	5		
5	A	1	Total	C	H	O	0	0
			22	6	11	5		
5	A	1	Total	C	H	O	0	0
			21	6	10	5		
5	A	1	Total	C	H	O	0	0
			21	6	10	5		

Continued on next page...

Continued from previous page...

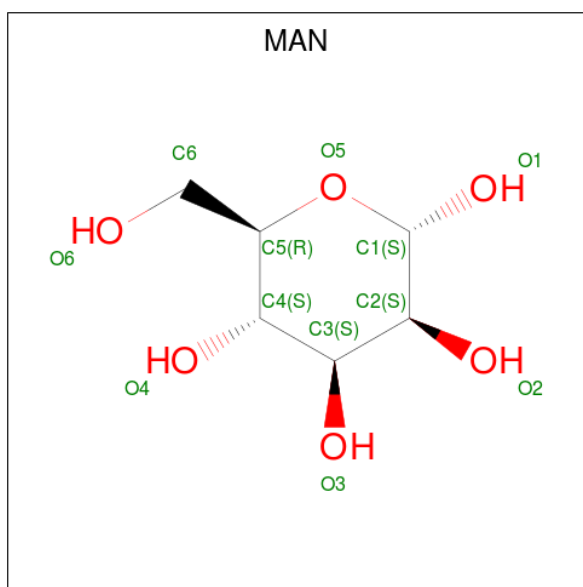
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			21	6	10	5		
5	B	1	Total	C	H	O	0	0
			22	6	11	5		
5	B	1	Total	C	H	O	0	0
			20	6	9	5		

- Molecule 6 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			21	6	11	4		
6	A	1	Total	C	H	O	0	0
			21	6	11	4		
6	A	1	Total	C	H	O	0	0
			21	6	11	4		
6	A	1	Total	C	H	O	0	0
			21	6	11	4		
6	B	1	Total	C	H	O	0	0
			21	6	11	4		
6	B	1	Total	C	H	O	0	0
			21	6	11	4		
6	B	1	Total	C	H	O	0	0
			21	6	11	4		

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			22	6	11	5		
7	A	1	Total	C	H	O	0	0
			22	6	11	5		
7	B	1	Total	C	H	O	0	0
			22	6	11	5		
7	B	1	Total	C	H	O	0	0
			22	6	11	5		
7	B	1	Total	C	H	O	0	0
			22	6	11	5		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Na	0	0
			1	1		
8	A	1	Total	Na	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	527	Total	O	0	0
			527	527		
9	B	417	Total	O	0	0
			417	417		

- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.18Å 133.64Å 167.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.27 – 2.30 48.27 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (48.27-2.30) 83.3 (48.27-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.174 , 0.214 0.176 , 0.216	Depositor DCC
R_{free} test set	1918 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27890	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8911e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, NA, CA, 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	0.30	0/6806	0.47	0/9255
1	B	0.29	0/6707	0.47	0/9119
All	All	0.30	0/13513	0.47	0/18374

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

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	6608	6290	6290	11	1
1	B	6512	6200	6199	10	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	238	222	205	0	0
4	B	238	224	207	1	0
5	A	44	42	38	0	0
5	B	33	30	27	0	0
6	A	40	44	40	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	30	33	30	0	0
7	A	22	22	20	0	0
7	B	33	33	30	0	1
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	527	0	0	2	1
9	B	417	0	0	3	1
All	All	14750	13140	13086	22	2

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 1.

The worst 5 of 22 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:70:ARG:NH2	9:A:1001:HOH:O	2.18	0.76
1:B:102:ARG:NH2	1:B:115:CYS:SG	2.60	0.73
1:B:170:ARG:NH2	9:B:1002:HOH:O	2.23	0.70
1:A:225:ASP:OD1	1:A:226:ASN:N	2.34	0.59
1:A:195:LYS:NZ	1:A:510:GLU:OE1	2.40	0.54

All (2) 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)
1:A:326:SER:O	7:B:920:MAN:O6[4_566]	2.08	0.12
9:A:1321:HOH:O	9:B:1126:HOH:O[4_476]	2.09	0.11

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	817/838 (98%)	793 (97%)	23 (3%)	1 (0%)	53	66
1	B	801/838 (96%)	773 (96%)	28 (4%)	0	100	100
All	All	1618/1676 (96%)	1566 (97%)	51 (3%)	1 (0%)	53	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	662	PRO

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	740/758 (98%)	735 (99%)	5 (1%)	85	93
1	B	730/758 (96%)	726 (100%)	4 (0%)	90	96
All	All	1470/1516 (97%)	1461 (99%)	9 (1%)	87	94

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	808	ILE
1	B	370	LEU
1	B	221	HIS
1	A	370	LEU
1	B	164	PHE

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

Mol	Chain	Res	Type
1	B	499	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 61 ligands modelled in this entry, 8 are monoatomic - leaving 53 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	$\# Z > 2$
4	NAG	A	904	1,4	14,14,15	0.30	0	17,19,21	0.58	0
4	NAG	A	905	4	14,14,15	0.23	0	17,19,21	0.50	0
5	BMA	A	906	4	11,11,12	0.91	0	15,15,17	0.79	0
4	NAG	A	907	1,4	14,14,15	0.39	0	17,19,21	0.48	0
4	NAG	A	908	5,4	14,14,15	0.49	0	17,19,21	0.50	0
4	NAG	A	909	1,4,6	14,14,15	0.30	0	17,19,21	0.59	0
6	FUC	A	910	4	9,10,11	0.91	0	13,14,16	0.86	0
4	NAG	A	911	4	14,14,15	0.42	0	17,19,21	0.39	0
4	NAG	A	912	1,4	14,14,15	0.19	0	17,19,21	0.68	0
4	NAG	A	913	5,4	14,14,15	0.49	0	17,19,21	0.45	0
5	BMA	A	914	4	11,11,12	0.75	0	15,15,17	0.71	0
7	MAN	A	915	5	11,11,12	0.95	0	15,15,17	1.22	1 (6%)
6	FUC	A	916	4	9,10,11	0.64	0	13,14,16	0.73	0
5	BMA	A	917	4,7	11,11,12	0.64	0	15,15,17	0.90	0
4	NAG	A	918	1,4,6	14,14,15	0.26	0	17,19,21	0.42	0
4	NAG	A	919	5,4	14,14,15	0.26	0	17,19,21	0.39	0
6	FUC	A	920	4	9,10,11	0.83	0	13,14,16	0.83	0
4	NAG	A	921	1,4,6	14,14,15	0.39	0	17,19,21	0.58	0
4	NAG	A	922	4	14,14,15	0.24	0	17,19,21	0.48	0
5	BMA	A	923	4,7	11,11,12	1.10	1 (9%)	15,15,17	0.79	0
7	MAN	A	924	5	11,11,12	1.13	2 (18%)	15,15,17	1.13	2 (13%)
4	NAG	A	925	1,4	14,14,15	0.45	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	926	5,4	14,14,15	0.23	0	17,19,21	0.50	0
6	FUC	A	927	4	9,10,11	1.50	2 (22%)	13,14,16	1.46	1 (7%)
4	NAG	A	928	1,4,6	14,14,15	0.35	0	17,19,21	0.38	0
4	NAG	A	929	4	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	A	930	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	B	904	1,4	14,14,15	0.22	0	17,19,21	0.51	0
4	NAG	B	905	4	14,14,15	0.23	0	17,19,21	0.58	0
5	BMA	B	906	4,7	11,11,12	0.80	0	15,15,17	0.68	0
7	MAN	B	907	5	11,11,12	0.87	1 (9%)	15,15,17	1.21	2 (13%)
4	NAG	B	908	1,4	14,14,15	0.29	0	17,19,21	0.49	0
4	NAG	B	909	5,4	14,14,15	0.37	0	17,19,21	0.43	0
6	FUC	B	910	4	9,10,11	0.92	0	13,14,16	0.84	0
4	NAG	B	911	1,4,6	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	B	912	4	14,14,15	0.27	0	17,19,21	0.65	0
5	BMA	B	913	4	11,11,12	1.11	1 (9%)	15,15,17	0.89	1 (6%)
4	NAG	B	914	1,4	14,14,15	0.32	0	17,19,21	0.62	0
4	NAG	B	915	5,4	14,14,15	0.59	1 (7%)	17,19,21	0.74	0
6	FUC	B	916	4	9,10,11	0.54	0	13,14,16	0.87	0
4	NAG	B	917	1,4,6	14,14,15	0.33	0	17,19,21	0.55	0
4	NAG	B	918	4	14,14,15	0.34	0	17,19,21	0.39	0
7	MAN	B	919	5	11,11,12	0.87	0	15,15,17	1.09	1 (6%)
7	MAN	B	920	5	11,11,12	0.93	0	15,15,17	0.91	0
5	BMA	B	921	4,7	11,11,12	0.42	0	15,15,17	0.73	0
4	NAG	B	922	1,4	14,14,15	0.36	0	17,19,21	0.49	0
4	NAG	B	923	5,4	14,14,15	0.17	0	17,19,21	0.50	0
6	FUC	B	924	4	9,10,11	0.81	0	13,14,16	1.06	1 (7%)
4	NAG	B	925	1,4,6	14,14,15	0.31	0	17,19,21	0.43	0
4	NAG	B	926	4	14,14,15	0.37	0	17,19,21	0.48	0
4	NAG	B	927	1,4	14,14,15	0.39	0	17,19,21	0.78	0
4	NAG	B	928	4	14,14,15	0.32	0	17,19,21	0.40	0
4	NAG	B	929	1	14,14,15	0.78	1 (7%)	17,19,21	1.50	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	904	1,4	-	2/6/23/26	0/1/1/1
4	NAG	A	905	4	-	0/6/23/26	0/1/1/1
5	BMA	A	906	4	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	907	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	908	5,4	-	2/6/23/26	0/1/1/1
4	NAG	A	909	1,4,6	-	0/6/23/26	0/1/1/1
6	FUC	A	910	4	-	-	0/1/1/1
4	NAG	A	911	4	-	2/6/23/26	0/1/1/1
4	NAG	A	912	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	913	5,4	-	2/6/23/26	0/1/1/1
5	BMA	A	914	4	-	2/2/19/22	0/1/1/1
7	MAN	A	915	5	-	0/2/19/22	0/1/1/1
6	FUC	A	916	4	-	-	0/1/1/1
5	BMA	A	917	4,7	-	2/2/19/22	0/1/1/1
4	NAG	A	918	1,4,6	-	0/6/23/26	0/1/1/1
4	NAG	A	919	5,4	-	0/6/23/26	0/1/1/1
6	FUC	A	920	4	-	-	0/1/1/1
4	NAG	A	921	1,4,6	-	0/6/23/26	0/1/1/1
4	NAG	A	922	4	-	2/6/23/26	0/1/1/1
5	BMA	A	923	4,7	-	2/2/19/22	0/1/1/1
7	MAN	A	924	5	-	0/2/19/22	0/1/1/1
4	NAG	A	925	1,4	-	1/6/23/26	0/1/1/1
4	NAG	A	926	5,4	-	0/6/23/26	0/1/1/1
6	FUC	A	927	4	-	-	0/1/1/1
4	NAG	A	928	1,4,6	-	0/6/23/26	0/1/1/1
4	NAG	A	929	4	-	2/6/23/26	0/1/1/1
4	NAG	A	930	1	-	2/6/23/26	0/1/1/1
4	NAG	B	904	1,4	-	2/6/23/26	0/1/1/1
4	NAG	B	905	4	-	0/6/23/26	0/1/1/1
5	BMA	B	906	4,7	-	2/2/19/22	0/1/1/1
7	MAN	B	907	5	-	0/2/19/22	0/1/1/1
4	NAG	B	908	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	909	5,4	-	2/6/23/26	0/1/1/1
6	FUC	B	910	4	-	-	0/1/1/1
4	NAG	B	911	1,4,6	-	0/6/23/26	0/1/1/1
4	NAG	B	912	4	-	2/6/23/26	0/1/1/1
5	BMA	B	913	4	-	2/2/19/22	0/1/1/1
4	NAG	B	914	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	915	5,4	-	2/6/23/26	0/1/1/1
6	FUC	B	916	4	-	-	0/1/1/1
4	NAG	B	917	1,4,6	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	918	4	-	2/6/23/26	0/1/1/1
7	MAN	B	919	5	-	1/2/19/22	0/1/1/1
7	MAN	B	920	5	-	2/2/19/22	0/1/1/1
5	BMA	B	921	4,7	-	0/2/19/22	0/1/1/1
4	NAG	B	922	1,4	-	2/6/23/26	0/1/1/1
4	NAG	B	923	5,4	-	0/6/23/26	0/1/1/1
6	FUC	B	924	4	-	-	0/1/1/1
4	NAG	B	925	1,4,6	-	0/6/23/26	0/1/1/1
4	NAG	B	926	4	-	1/6/23/26	0/1/1/1
4	NAG	B	927	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	928	4	-	1/6/23/26	0/1/1/1
4	NAG	B	929	1	-	0/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	927	FUC	C1-C2	3.80	1.61	1.52
4	B	929	NAG	O5-C1	2.78	1.48	1.43
5	A	923	BMA	C1-C2	2.57	1.58	1.52
5	B	913	BMA	C4-C5	2.34	1.58	1.53
4	B	915	NAG	O5-C1	-2.13	1.40	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	929	NAG	C1-O5-C5	5.74	120.00	112.20
6	A	927	FUC	C1-C2-C3	4.21	114.83	109.66
7	A	915	MAN	C1-O5-C5	3.70	117.23	112.20
7	B	907	MAN	C1-O5-C5	3.48	116.93	112.20
7	B	919	MAN	C1-O5-C5	2.85	116.07	112.20

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	915	NAG	O5-C5-C6-O6
5	A	914	BMA	O5-C5-C6-O6
7	B	920	MAN	O5-C5-C6-O6
4	A	904	NAG	O5-C5-C6-O6
4	A	922	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	920	MAN	0	1
4	B	929	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 [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	819/838 (97%)	-0.04	33 (4%) 38 45	20, 36, 79, 139	0
1	B	807/838 (96%)	0.02	29 (3%) 42 49	21, 40, 88, 150	0
All	All	1626/1676 (97%)	-0.01	62 (3%) 40 47	20, 38, 83, 150	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	LEU	9.0
1	A	68	ASN	9.0
1	B	74	ALA	8.7
1	B	73	VAL	8.3
1	B	62	SER	7.7

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](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(\AA^2)	Q<0.9
4	NAG	A	911	14/15	0.60	0.34	87,94,111,113	0
4	NAG	A	922	14/15	0.63	0.36	100,108,128,129	0
6	FUC	A	927	10/11	0.66	0.43	81,90,104,108	0
4	NAG	B	927	14/15	0.67	0.27	62,74,86,90	0
7	MAN	A	915	11/12	0.70	0.28	82,86,101,102	0
5	BMA	A	906	11/12	0.72	0.20	69,75,88,90	0
5	BMA	A	914	11/12	0.73	0.23	77,86,100,103	0
4	NAG	B	929	14/15	0.73	0.36	74,85,101,102	0
5	BMA	B	913	11/12	0.74	0.24	78,83,100,100	0
4	NAG	A	921	14/15	0.75	0.20	72,88,106,106	0
4	NAG	B	912	14/15	0.75	0.27	81,85,101,102	0
4	NAG	A	928	14/15	0.76	0.20	56,72,86,86	0
6	FUC	A	910	10/11	0.76	0.40	87,90,108,109	0
4	NAG	A	930	14/15	0.76	0.38	72,85,101,102	0
4	NAG	B	928	14/15	0.76	0.38	86,92,109,111	0
4	NAG	B	918	14/15	0.77	0.33	95,104,124,125	0
6	FUC	A	920	10/11	0.78	0.21	91,94,113,113	0
6	FUC	B	910	10/11	0.78	0.36	78,81,97,98	0
5	BMA	A	923	11/12	0.79	0.15	52,63,75,76	0
5	BMA	B	906	11/12	0.79	0.19	72,80,95,96	0
4	NAG	A	929	14/15	0.80	0.28	89,97,115,116	0
7	MAN	B	907	11/12	0.80	0.46	91,97,115,116	0
6	FUC	B	916	10/11	0.81	0.20	84,87,104,105	0
5	BMA	A	917	11/12	0.82	0.23	77,82,98,98	0
4	NAG	B	905	14/15	0.82	0.30	67,81,96,101	0
4	NAG	A	925	14/15	0.83	0.12	43,61,76,77	0
4	NAG	B	917	14/15	0.84	0.21	63,80,93,96	0
7	MAN	B	919	11/12	0.87	0.13	52,59,69,71	0
4	NAG	A	905	14/15	0.88	0.34	65,77,92,93	0
4	NAG	B	909	14/15	0.89	0.14	46,56,67,71	0
7	MAN	A	924	11/12	0.89	0.17	56,65,76,79	0
4	NAG	A	908	14/15	0.89	0.14	47,57,68,71	0
4	NAG	A	926	14/15	0.90	0.17	67,73,88,90	0
4	NAG	B	926	14/15	0.90	0.20	73,79,95,95	0
4	NAG	B	911	14/15	0.90	0.18	51,68,80,82	0
4	NAG	A	904	14/15	0.90	0.13	41,52,62,65	0
4	NAG	B	922	14/15	0.91	0.10	38,47,55,57	0
6	FUC	B	924	10/11	0.91	0.14	69,74,85,89	0
4	NAG	A	909	14/15	0.91	0.20	50,66,84,87	0
4	NAG	B	923	14/15	0.91	0.14	48,56,69,69	0
8	NA	B	930	1/1	0.91	0.12	56,56,56,56	0
4	NAG	B	915	14/15	0.91	0.15	41,55,71,72	0
4	NAG	B	904	14/15	0.92	0.15	39,51,61,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	A	913	14/15	0.92	0.14	43,54,66,71	0
7	MAN	B	920	11/12	0.92	0.14	52,57,69,69	0
5	BMA	B	921	11/12	0.93	0.09	45,50,59,61	0
4	NAG	A	919	14/15	0.93	0.10	59,68,79,82	0
4	NAG	A	918	14/15	0.94	0.10	36,47,54,57	0
8	NA	A	931	1/1	0.94	0.16	58,58,58,58	0
4	NAG	B	925	14/15	0.95	0.10	52,64,75,77	0
6	FUC	A	916	10/11	0.95	0.10	44,48,57,58	0
4	NAG	A	907	14/15	0.95	0.12	28,42,52,53	0
4	NAG	B	908	14/15	0.95	0.12	25,39,47,52	0
4	NAG	B	914	14/15	0.97	0.15	18,27,32,35	0
4	NAG	A	912	14/15	0.98	0.14	22,29,36,36	0
2	ZN	B	902	1/1	0.99	0.15	33,33,33,33	0
2	ZN	A	902	1/1	0.99	0.16	34,34,34,34	0
2	ZN	A	901	1/1	0.99	0.16	28,28,28,28	0
3	CA	A	903	1/1	1.00	0.12	28,28,28,28	0
2	ZN	B	901	1/1	1.00	0.14	29,29,29,29	0
3	CA	B	903	1/1	1.00	0.14	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.