WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:12 PM GMT

PDB ID	:	1NWT
Title	:	Crystal structure of human cartilage gp39 (HC-gp39) in complex with chitopentaose
Authors	:	Fusetti, F.; Pijning, T.; Kalk, K.H.; Bos, E.; Dijkstra, B.W.
Deposited on	:	2003-02-06
Resolution	:	2.50 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

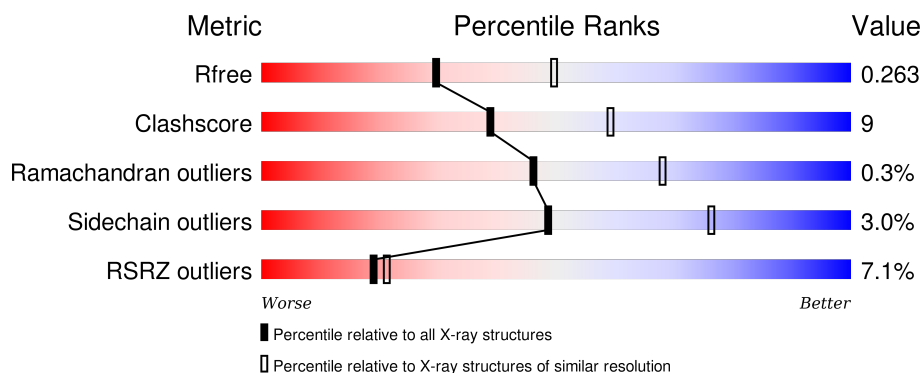|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.50 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	Percentile Ranks	Value
Rfree		0.263
Clashscore		9
Ramachandran outliers		0.3%
Sidechain outliers		3.0%
RSRZ outliers		7.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures
❚ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=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	362	5% / 83% / 15% / •
1	B	362	10% / 77% / 21% / •
1	C	362	8% / 83% / 16% / •
1	D	362	5% / 81% / 17% / •

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	NAG	A	-3	-	-	-	X
3	NAG	C	-3	-	-	-	X
3	NAG	C	1	-	-	X	-
4	NAG	B	-3	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12269 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 Chitinase-3 like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2838	1816	483	528	11			
1	B	362	Total	C	N	O	S	0	0	0
			2839	1816	483	529	11			
1	C	362	Total	C	N	O	S	0	0	0
			2839	1816	483	529	11			
1	D	362	Total	C	N	O	S	0	0	0
			2845	1819	486	529	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	ILE	THR	CONFLICT	UNP P36222
B	311	ILE	THR	CONFLICT	UNP P36222
C	311	ILE	THR	CONFLICT	UNP P36222
D	311	ILE	THR	CONFLICT	UNP P36222

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

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

- Molecule 3 is a polymer of unknown type called SUGAR (NAG-NAG-NAG-NAG-NAG-NA G).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	6	Total 85	C 48	N 6	O 31	0	0
3	C	6	Total 85	C 48	N 6	O 31	0	0
3	D	6	Total 85	C 48	N 6	O 31	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	5	Total 71	C 40	N 5	O 26	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	128	Total 128	O 128	0	0
5	B	83	Total 83	O 83	0	0
5	C	104	Total 104	O 104	0	0
5	D	155	Total 155	O 155	0	0

3 Residue-property plots ⓘ

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.
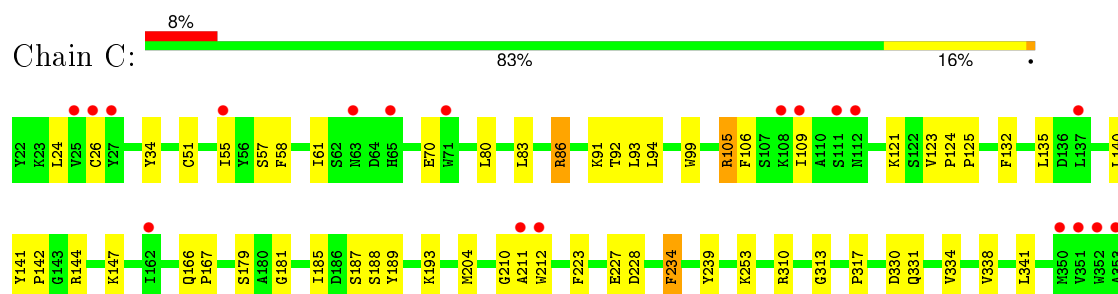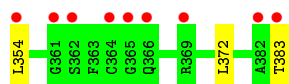
- Molecule 1: Chitinase-3 like protein 1
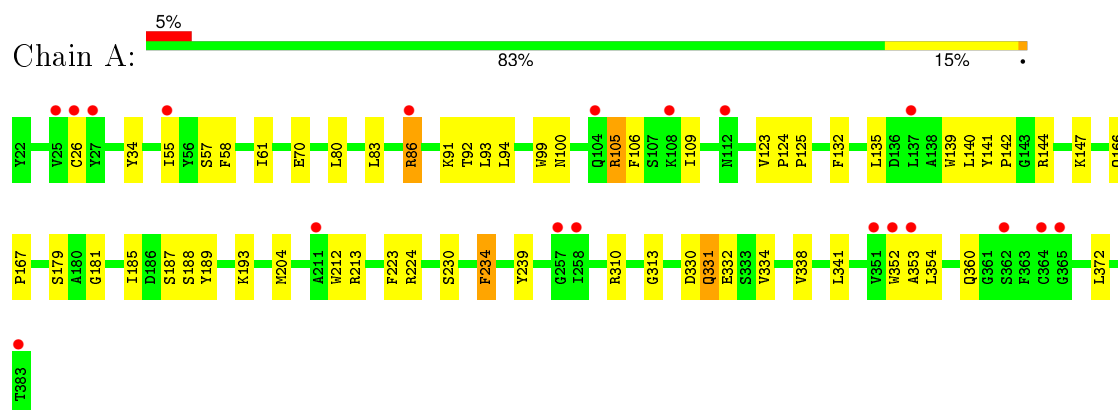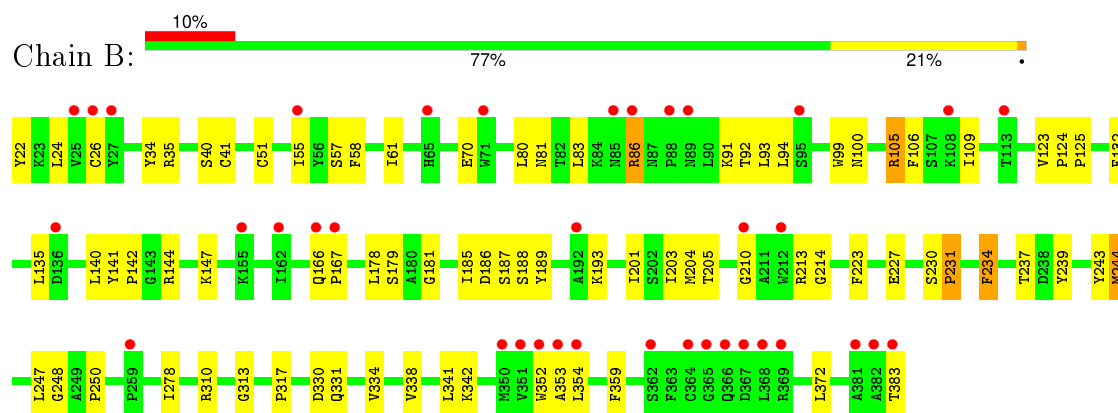
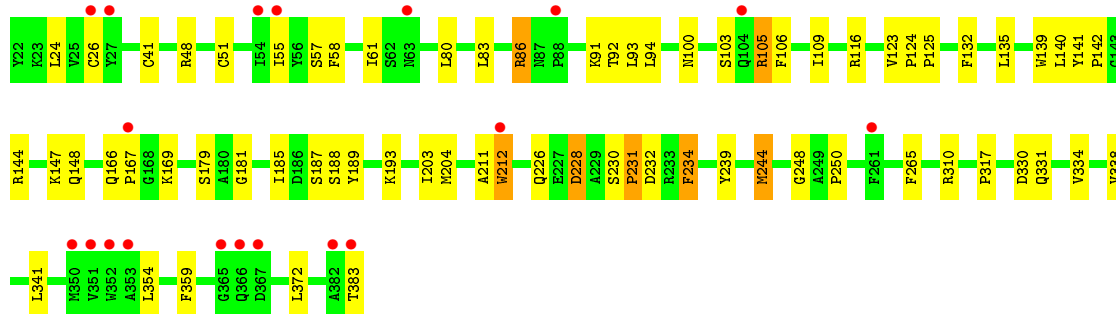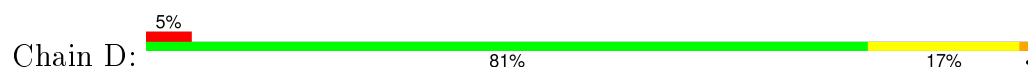- Molecule 1: Chitinase-3 like protein 1

- Molecule 1: Chitinase-3 like protein 1

• Molecule 1: Chitinase-3 like protein 1

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	128.32Å 128.32Å 108.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.50 29.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.92-2.50) 98.0 (29.92-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.253 0.231 , 0.263	Depositor DCC
R_{free} test set	8129 reflections (13.55%)	DCC
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.8	EDS
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 67403 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12269	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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 47.30 % 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 1.0122e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, NDG

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	0.29	0/2914	0.56	0/3951
1	B	0.30	0/2915	0.56	0/3952
1	C	0.30	0/2915	0.57	0/3952
1	D	0.30	0/2921	0.56	0/3959
All	All	0.30	0/11665	0.56	0/15814

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	2838	0	2742	47	0
1	B	2839	0	2742	54	0
1	C	2839	0	2742	41	0
1	D	2845	0	2753	55	0
2	A	28	0	25	0	0
2	B	28	0	25	1	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	85	0	75	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	85	0	75	8	0
3	D	85	0	75	8	0
4	B	71	0	63	10	0
5	A	128	0	0	5	0
5	B	83	0	0	1	0
5	C	104	0	0	3	0
5	D	155	0	0	6	0
All	All	12269	0	11367	208	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 9.

The worst 5 of 208 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:86:ARG:HB3	1:A:86:ARG:HH11	1.35	0.92
1:B:86:ARG:HH11	1:B:86:ARG:HB3	1.35	0.92
1:D:86:ARG:HB3	1:D:86:ARG:HH11	1.35	0.91
1:C:86:ARG:HH11	1:C:86:ARG:HB3	1.35	0.89
1:D:231:PRO:HG2	1:D:232:ASP:H	1.38	0.86

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	360/362 (99%)	344 (96%)	16 (4%)	0	100	100
1	B	360/362 (99%)	343 (95%)	16 (4%)	1 (0%)	46	68
1	C	360/362 (99%)	343 (95%)	16 (4%)	1 (0%)	46	68
1	D	360/362 (99%)	342 (95%)	16 (4%)	2 (1%)	30	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1440/1448 (99%)	1372 (95%)	64 (4%)	4 (0%)	46 68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	211	ALA
1	D	212	TRP
1	D	231	PRO
1	B	231	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	298/302 (99%)	291 (98%)	7 (2%)	58 83
1	B	298/302 (99%)	289 (97%)	9 (3%)	48 76
1	C	298/302 (99%)	288 (97%)	10 (3%)	44 72
1	D	299/302 (99%)	289 (97%)	10 (3%)	45 73
All	All	1193/1208 (99%)	1157 (97%)	36 (3%)	48 76

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	86	ARG
1	C	193	LYS
1	D	244	MET
1	C	105	ARG
1	C	227	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	171	GLN

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Mol	Chain	Res	Type
1	C	226	GLN
1	D	171	GLN
1	B	345	GLN
1	D	226	GLN

5.3.3　RNA (i)

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)

31 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	NAG	A	-1	3	14,14,15	0.89	0	15,19,21	1.33	2 (13%)
3	NDG	A	-2	3	14,14,15	0.97	1 (7%)	15,19,21	1.23	3 (20%)
3	NAG	A	-3	3	14,14,15	0.51	0	15,19,21	0.76	1 (6%)
3	NAG	A	1	3	14,14,15	0.63	0	15,19,21	0.88	1 (6%)
3	NAG	A	2	3	14,14,15	0.63	0	15,19,21	0.69	1 (6%)
3	NAG	A	3	3	15,15,15	0.43	0	17,21,21	0.59	0
2	NAG	A	411	1,2	14,14,15	0.54	0	15,19,21	0.74	1 (6%)
2	NAG	A	412	2	14,14,15	0.53	0	15,19,21	0.96	1 (6%)
4	NAG	B	-1	4	14,14,15	0.92	1 (7%)	15,19,21	1.32	1 (6%)
4	NDG	B	-2	4	14,14,15	0.92	1 (7%)	15,19,21	1.06	1 (6%)
4	NAG	B	-3	4	14,14,15	0.56	0	15,19,21	0.69	1 (6%)
4	NAG	B	1	4	14,14,15	0.61	0	15,19,21	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NDG	B	2	4	15,15,15	0.59	0	17,21,21	0.53	0
2	NAG	B	421	1,2	14,14,15	0.52	0	15,19,21	0.83	1 (6%)
2	NAG	B	422	2	14,14,15	0.57	0	15,19,21	0.73	1 (6%)
3	NAG	C	-1	3	14,14,15	0.78	0	15,19,21	1.04	2 (13%)
3	NDG	C	-2	3	14,14,15	0.79	0	15,19,21	0.94	1 (6%)
3	NAG	C	-3	3	14,14,15	0.48	0	15,19,21	0.71	1 (6%)
3	NAG	C	1	3	14,14,15	0.65	0	15,19,21	0.89	1 (6%)
3	NAG	C	2	3	14,14,15	0.76	0	15,19,21	0.75	0
3	NAG	C	3	3	15,15,15	0.45	0	17,21,21	0.59	0
2	NAG	C	431	1,2	14,14,15	0.49	0	15,19,21	0.69	1 (6%)
2	NAG	C	432	2	14,14,15	0.51	0	15,19,21	0.66	0
3	NAG	D	-1	3	14,14,15	0.90	1 (7%)	15,19,21	1.31	1 (6%)
3	NDG	D	-2	3	14,14,15	1.03	1 (7%)	15,19,21	1.25	2 (13%)
3	NAG	D	-3	3	14,14,15	0.49	0	15,19,21	0.79	1 (6%)
3	NAG	D	1	3	14,14,15	0.64	0	15,19,21	0.91	1 (6%)
3	NAG	D	2	3	14,14,15	0.57	0	15,19,21	0.68	0
3	NAG	D	3	3	15,15,15	0.43	0	17,21,21	0.68	0
2	NAG	D	441	1,2	14,14,15	0.51	0	15,19,21	0.76	1 (6%)
2	NAG	D	442	2	14,14,15	0.52	0	15,19,21	0.91	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	NAG	A	-1	3	-	0/6/23/26	0/1/1/1
3	NDG	A	-2	3	-	0/6/23/26	0/1/1/1
3	NAG	A	-3	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1	3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
3	NAG	A	3	3	-	0/6/26/26	0/1/1/1
2	NAG	A	411	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	412	2	-	0/6/23/26	0/1/1/1
4	NAG	B	-1	4	-	0/6/23/26	0/1/1/1
4	NDG	B	-2	4	-	0/6/23/26	0/1/1/1
4	NAG	B	-3	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1	4	-	0/6/23/26	0/1/1/1
4	NDG	B	2	4	-	0/6/26/26	0/1/1/1
2	NAG	B	421	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	422	2	-	0/6/23/26	0/1/1/1
3	NAG	C	-1	3	-	0/6/23/26	0/1/1/1
3	NDG	C	-2	3	-	0/6/23/26	0/1/1/1
3	NAG	C	-3	3	-	0/6/23/26	0/1/1/1
3	NAG	C	1	3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	NAG	C	3	3	-	0/6/26/26	0/1/1/1
2	NAG	C	431	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	432	2	-	0/6/23/26	0/1/1/1
3	NAG	D	-1	3	-	0/6/23/26	0/1/1/1
3	NDG	D	-2	3	-	0/6/23/26	0/1/1/1
3	NAG	D	-3	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	NAG	D	3	3	-	0/6/26/26	0/1/1/1
2	NAG	D	441	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	442	2	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	-1	NAG	C1-C2	2.04	1.55	1.52
4	B	-1	NAG	C1-C2	2.32	1.55	1.52
3	A	-2	NDG	C1-C2	2.76	1.56	1.52
4	B	-2	NDG	C1-C2	2.77	1.56	1.52
3	D	-2	NDG	C1-C2	3.09	1.56	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	-1	NAG	C2-N2-C7	-3.09	119.07	123.04
3	A	-1	NAG	C2-N2-C7	-2.92	119.29	123.04
4	B	-1	NAG	C2-N2-C7	-2.81	119.44	123.04
2	D	442	NAG	C2-N2-C7	-2.74	119.52	123.04
2	B	421	NAG	C2-N2-C7	-2.71	119.55	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	-1	NAG	3	0
3	A	-2	NDG	3	0
3	A	1	NAG	3	0
3	A	2	NAG	2	0
4	B	-1	NAG	4	0
4	B	-2	NDG	3	0
4	B	-3	NAG	2	0
4	B	1	NAG	4	0
4	B	2	NDG	1	0
2	B	421	NAG	1	0
2	B	422	NAG	1	0
3	C	-1	NAG	1	0
3	C	1	NAG	7	0
3	C	2	NAG	2	0
3	D	-1	NAG	3	0
3	D	-2	NDG	1	0
3	D	1	NAG	4	0
3	D	3	NAG	2	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

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(Å²)	Q<0.9
1	A	362/362 (100%)	0.09	19 (5%)	31	35	17, 31, 55, 78	0
1	B	362/362 (100%)	0.43	37 (10%)	9	9	20, 38, 60, 80	0
1	C	362/362 (100%)	0.18	28 (7%)	16	18	16, 33, 59, 81	0
1	D	362/362 (100%)	0.11	19 (5%)	31	35	16, 30, 60, 81	0
All	All	1448/1448 (100%)	0.20	103 (7%)	19	21	16, 33, 59, 81	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	365	GLY	5.0
1	C	383	THR	4.4
1	B	162	ILE	4.3
1	C	362	SER	4.2
1	B	166	GLN	4.1

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(Å²)	Q<0.9
4	NAG	B	-3	14/15	0.81	0.38	6.64	65,69,74,77	0
3	NAG	C	-3	14/15	0.84	0.31	5.10	20,26,30,36	14
3	NAG	A	-3	14/15	0.82	0.23	2.01	13,21,23,25	14
3	NAG	A	1	14/15	0.83	0.26	1.80	52,59,64,67	0
4	NDG	B	2	15/15	0.81	0.27	1.71	52,58,63,72	0
2	NAG	B	421	14/15	0.87	0.25	1.56	58,68,74,76	0
3	NAG	A	2	14/15	0.89	0.21	1.41	35,49,57,59	0
3	NAG	D	1	14/15	0.83	0.25	1.35	44,57,61,63	0
4	NAG	B	1	14/15	0.82	0.22	1.19	42,56,61,61	0
2	NAG	A	411	14/15	0.92	0.22	0.88	43,49,58,62	0
3	NAG	C	2	14/15	0.84	0.20	0.84	50,58,65,66	0
2	NAG	D	441	14/15	0.92	0.20	0.77	40,47,52,54	0
3	NAG	D	2	14/15	0.79	0.20	0.74	47,60,62,64	0
3	NAG	D	-3	14/15	0.90	0.18	0.72	10,12,17,18	14
3	NAG	C	1	14/15	0.88	0.20	0.50	49,53,55,56	0
3	NAG	A	-1	14/15	0.84	0.23	0.40	24,33,39,43	0
2	NAG	C	431	14/15	0.84	0.20	0.39	57,66,72,80	0
3	NAG	C	-1	14/15	0.90	0.21	0.34	27,33,37,42	0
3	NAG	D	-1	14/15	0.86	0.22	-0.04	22,32,39,42	0
4	NAG	B	-1	14/15	0.86	0.21	-0.06	25,38,43,43	0
4	NDG	B	-2	14/15	0.87	0.18	-0.18	34,39,47,54	0
3	NDG	D	-2	14/15	0.89	0.16	-0.44	18,27,31,35	0
3	NDG	C	-2	14/15	0.93	0.14	-0.62	20,34,41,42	0
3	NDG	A	-2	14/15	0.94	0.12	-0.96	12,28,35,37	0
2	NAG	D	442	14/15	0.85	0.48	-	62,71,74,75	0
3	NAG	C	3	15/15	0.57	0.29	-	52,54,60,60	15
2	NAG	C	432	14/15	0.77	0.38	-	84,89,91,95	0
2	NAG	A	412	14/15	0.76	0.42	-	74,82,86,90	0
2	NAG	B	422	14/15	0.79	0.42	-	80,83,86,87	0
3	NAG	D	3	15/15	0.75	0.28	-	41,50,54,55	15
3	NAG	A	3	15/15	0.74	0.26	-	32,36,41,46	15

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.