



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2017 – 09:17 AM EDT

PDB ID : 5ERD  
Title : Crystal structure of human Desmoglein-2 ectodomain  
Authors : Brasch, J.; Harrison, O.J.; Shapiro, L.  
Deposited on : unknown  
Resolution : 2.90 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](mailto: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.

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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 : rb-20029824  
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) : rb-20029824

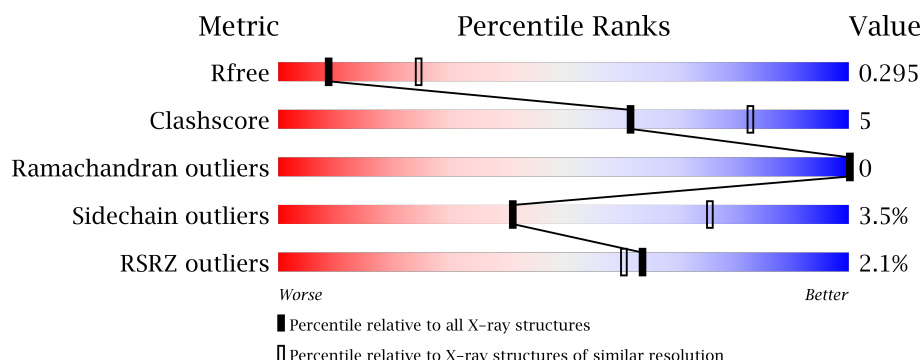
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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  $\geq 3$ , 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>0.1%</div> <div>87%</div> <div>11%</div> <div>0.1%</div> </div>
1	B	559	<div> <div>3%</div> <div>89%</div> <div>11%</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
5	MAN	A	615	-	-	-	X
6	CA	B	914	-	-	-	X
6	CA	B	916	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18333 atoms, of which 8981 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.

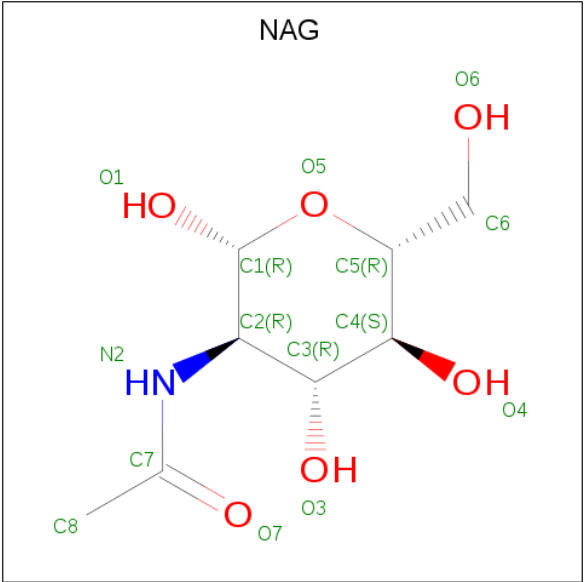
- Molecule 1 is a protein called Desmoglein-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	554	Total	C	H	N	O	S	0	2	0
			8661	2756	4295	726	873	11			
1	B	559	Total	C	H	N	O	S	0	1	0
			8735	2782	4325	740	877	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	554	HIS	-	expression tag	UNP Q14126
A	555	HIS	-	expression tag	UNP Q14126
A	556	HIS	-	expression tag	UNP Q14126
A	557	HIS	-	expression tag	UNP Q14126
A	558	HIS	-	expression tag	UNP Q14126
A	559	HIS	-	expression tag	UNP Q14126
B	554	HIS	-	expression tag	UNP Q14126
B	555	HIS	-	expression tag	UNP Q14126
B	556	HIS	-	expression tag	UNP Q14126
B	557	HIS	-	expression tag	UNP Q14126
B	558	HIS	-	expression tag	UNP Q14126
B	559	HIS	-	expression tag	UNP Q14126

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



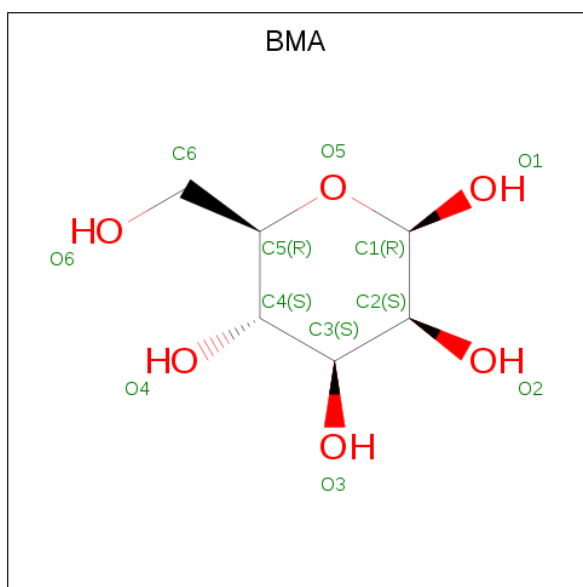
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

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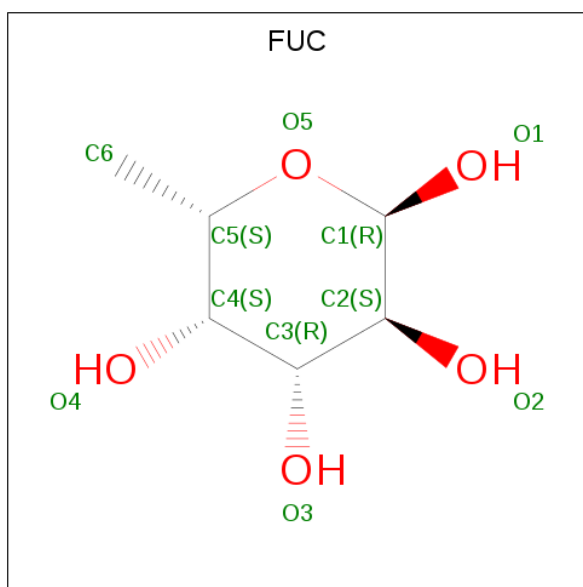
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



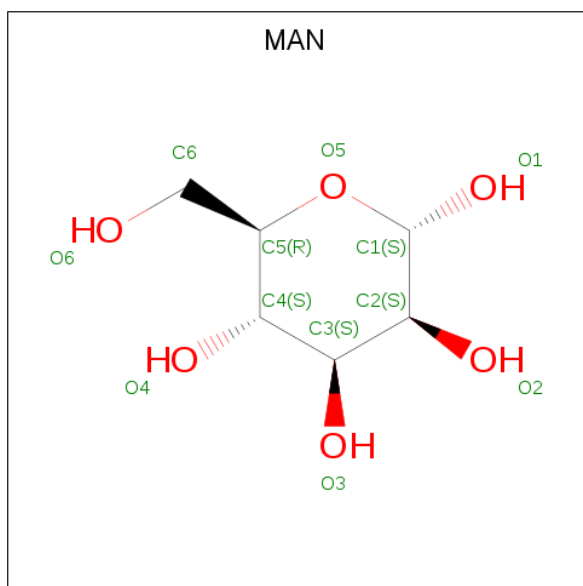
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			21	6	10	5		
3	A	1	Total	C	H	O	0	0
			21	6	10	5		
3	A	1	Total	C	H	O	0	0
			21	6	10	5		
3	B	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).



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

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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
			22	6	11	5		

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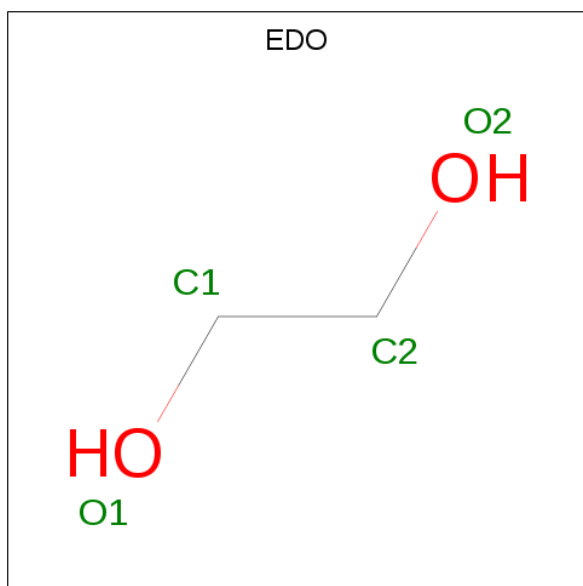
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			22	6	11	5		
5	B	1	Total	C	H	O	0	0
			22	6	11	5		
5	B	1	Total	C	H	O	0	0
			22	6	11	5		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	11	Total	Ca	0	0
			11	11		
6	A	11	Total	Ca	0	0
			11	11		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	98	Total	O	0	0
			98	98		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	94	Total	O	0	0
			94	94		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.97Å 114.48Å 226.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.39 – 2.90 84.39 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (84.39-2.90) 86.4 (84.39-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.91Å)	Xtriage
Refinement program	PHENIX dev_1810	Depositor
R, $R_{free}$	0.241 , 0.287 0.241 , 0.295	Depositor DCC
$R_{free}$ test set	2314 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	18333	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BMA, NAG, CA, EDO, 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	0.40	1/4455 (0.0%)	0.55	4/6049 (0.1%)
1	B	0.38	0/4501	0.53	5/6112 (0.1%)
All	All	0.39	1/8956 (0.0%)	0.54	9/12161 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	525	ASP	CB-CG	5.06	1.62	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	218	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	248	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	525	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	138	ASP	CB-CG-OD1	5.54	123.28	118.30

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	4366	4295	4297	39	2
1	B	4410	4325	4325	30	1
2	A	112	112	97	17	0
2	B	126	126	112	15	0
3	A	33	30	30	1	0
3	B	11	10	10	1	0
4	A	10	11	10	2	0
5	A	33	33	30	0	0
5	B	33	33	29	2	1
6	A	11	0	0	0	0
6	B	11	0	0	0	0
7	A	4	6	5	0	0
8	A	98	0	0	5	0
8	B	94	0	0	2	0
All	All	9352	8981	8945	92	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 92 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)
2:A:605:NAG:C6	2:A:606:NAG:H2	2.04	0.88
1:A:133:ASN:OD1	1:A:134:ALA:N	2.13	0.82
2:B:907:NAG:O6	3:B:908:BMA:O5	1.98	0.81
2:A:605:NAG:O6	2:A:606:NAG:O7	2.00	0.80
2:B:913:NAG:H82	2:B:913:NAG:H3	1.65	0.79

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASN:O	5:B:901:MAN:O4[1_554]	1.67	0.53
1:A:158:TYR:OH	1:A:484:VAL:O[2_555]	1.97	0.23
1:B:158:TYR:OH	1:B:484:VAL:O[2_454]	2.01	0.19

## 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	554/559 (99%)	527 (95%)	27 (5%)	0	100	100
1	B	558/559 (100%)	527 (94%)	31 (6%)	0	100	100
All	All	1112/1118 (100%)	1054 (95%)	58 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	494/497 (99%)	479 (97%)	15 (3%)	46	80
1	B	498/497 (100%)	478 (96%)	20 (4%)	36	71
All	All	992/994 (100%)	957 (96%)	35 (4%)	41	75

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	VAL
1	B	225	ASN
1	B	544	CYS
1	B	25	HIS
1	B	32	ARG

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

Mol	Chain	Res	Type
1	A	444	ASN

### 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](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 22 are monoatomic - leaving 29 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	$\# Z  > 2$
2	NAG	A	601	1	14,14,15	1.04	1 (7%)	15,19,21	2.26	3 (20%)
2	NAG	A	602	1,2	14,14,15	0.76	1 (7%)	15,19,21	1.59	3 (20%)
2	NAG	A	603	3,2	14,14,15	0.48	0	15,19,21	0.88	1 (6%)
3	BMA	A	604	2	11,11,12	2.91	8 (72%)	13,15,17	1.41	1 (7%)
2	NAG	A	605	1,2	14,14,15	2.11	1 (7%)	15,19,21	1.40	3 (20%)
2	NAG	A	606	3,2	14,14,15	2.00	2 (14%)	15,19,21	2.17	4 (26%)
3	BMA	A	607	2	11,11,12	3.05	8 (72%)	13,15,17	1.75	3 (23%)
2	NAG	A	608	1	14,14,15	0.91	1 (7%)	15,19,21	1.53	3 (20%)
2	NAG	A	609	1,2,4	14,14,15	1.10	1 (7%)	15,19,21	1.72	4 (26%)
2	NAG	A	610	3,2	14,14,15	0.88	2 (14%)	15,19,21	1.69	3 (20%)
3	BMA	A	611	2	11,11,12	2.44	6 (54%)	13,15,17	1.95	5 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FUC	A	612	2	9,10,11	1.43	2 (22%)	13,14,16	0.90	1 (7%)
5	MAN	A	613	1	11,11,12	0.85	0	13,15,17	2.11	3 (23%)
5	MAN	A	614	1	11,11,12	1.07	1 (9%)	13,15,17	2.62	3 (23%)
5	MAN	A	615	1	11,11,12	0.91	1 (9%)	13,15,17	1.54	4 (30%)
7	EDO	A	627	-	3,3,3	0.65	0	2,2,2	0.65	0
5	MAN	B	901	1	11,11,12	1.89	3 (27%)	13,15,17	2.61	5 (38%)
5	MAN	B	902	1	11,11,12	1.27	1 (9%)	13,15,17	2.27	4 (30%)
5	MAN	B	903	1	11,11,12	1.32	2 (18%)	13,15,17	2.15	4 (30%)
2	NAG	B	904	1,2	14,14,15	0.76	1 (7%)	15,19,21	2.13	3 (20%)
2	NAG	B	905	2	14,14,15	0.83	1 (7%)	15,19,21	0.87	0
2	NAG	B	906	1,2	14,14,15	0.79	0	15,19,21	2.02	3 (20%)
2	NAG	B	907	3,2	14,14,15	0.99	2 (14%)	15,19,21	1.59	3 (20%)
3	BMA	B	908	2	11,11,12	3.24	9 (81%)	13,15,17	1.46	2 (15%)
2	NAG	B	909	1,2	14,14,15	1.03	1 (7%)	15,19,21	1.06	0
2	NAG	B	910	2	14,14,15	1.40	2 (14%)	15,19,21	1.11	1 (6%)
2	NAG	B	911	1	14,14,15	0.36	0	15,19,21	0.56	0
2	NAG	B	912	1,2	14,14,15	1.01	2 (14%)	15,19,21	1.31	2 (13%)
2	NAG	B	913	2	14,14,15	0.77	1 (7%)	15,19,21	1.47	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
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	603	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	604	2	-	0/2/19/22	0/1/1/1
2	NAG	A	605	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	606	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	607	2	-	0/2/19/22	0/1/1/1
2	NAG	A	608	1	-	0/6/23/26	0/1/1/1
2	NAG	A	609	1,2,4	-	0/6/23/26	0/1/1/1
2	NAG	A	610	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	611	2	-	0/2/19/22	0/1/1/1
4	FUC	A	612	2	-	0/0/17/20	0/1/1/1
5	MAN	A	613	1	-	0/2/19/22	0/1/1/1
5	MAN	A	614	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	A	615	1	-	0/2/19/22	0/1/1/1
7	EDO	A	627	-	-	0/1/1/1	0/0/0/0
5	MAN	B	901	1	-	0/2/19/22	0/1/1/1
5	MAN	B	902	1	-	0/2/19/22	0/1/1/1
5	MAN	B	903	1	-	0/2/19/22	0/1/1/1
2	NAG	B	904	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	905	2	-	0/6/23/26	0/1/1/1
2	NAG	B	906	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	907	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	908	2	-	0/2/19/22	0/1/1/1
2	NAG	B	909	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	910	2	-	0/6/23/26	0/1/1/1
2	NAG	B	911	1	-	0/6/23/26	0/1/1/1
2	NAG	B	912	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	913	2	-	0/6/23/26	0/1/1/1

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	NAG	O5-C1	-7.64	1.31	1.43
5	B	901	MAN	O4-C4	-4.60	1.32	1.43
2	A	606	NAG	O5-C1	-3.32	1.38	1.43
3	A	611	BMA	C2-C3	-3.09	1.48	1.52
2	B	912	NAG	O5-C1	-3.05	1.38	1.43

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	606	NAG	C1-O5-C5	-5.67	104.35	112.17
3	A	607	BMA	C1-O5-C5	-4.60	105.82	112.17
2	B	906	NAG	C1-O5-C5	-4.21	106.36	112.17
3	A	604	BMA	C1-O5-C5	-4.19	106.39	112.17
2	B	910	NAG	C1-O5-C5	-3.53	107.31	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	605	NAG	6	0
2	A	606	NAG	6	0
2	A	608	NAG	3	0
2	A	609	NAG	4	0
2	A	610	NAG	4	0
3	A	611	BMA	1	0
4	A	612	FUC	2	0
5	B	901	MAN	1	1
5	B	903	MAN	1	0
2	B	904	NAG	4	0
2	B	906	NAG	4	0
2	B	907	NAG	3	0
3	B	908	BMA	1	0
2	B	911	NAG	1	0
2	B	913	NAG	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	554/559 (99%)	0.43	7 (1%) 77 76	47, 70, 98, 189	0
1	B	559/559 (100%)	0.44	16 (2%) 52 46	42, 72, 107, 135	0
All	All	1113/1118 (99%)	0.44	23 (2%) 64 60	42, 71, 104, 189	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	559	HIS	6.9
1	A	554	HIS	6.7
1	B	31	GLU	3.8
1	B	451	ILE	3.7
1	B	30	GLU	3.3

### 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. 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	MAN	A	615	11/12	0.84	0.38	2.55	98,118,134,158	0
6	CA	B	914	1/1	0.95	0.23	2.29	64,64,64,64	0
6	CA	B	916	1/1	0.97	0.24	2.29	46,46,46,46	0
5	MAN	A	613	11/12	0.90	0.30	1.98	98,123,141,148	0
5	MAN	B	901	11/12	0.82	0.29	1.77	92,116,139,157	0
6	CA	A	619	1/1	0.98	0.23	1.66	48,48,48,48	0
2	NAG	B	906	14/15	0.66	0.33	1.58	118,141,167,175	0
5	MAN	B	903	11/12	0.87	0.29	1.57	93,111,129,133	0
6	CA	B	921	1/1	0.92	0.23	1.22	51,51,51,51	0
5	MAN	A	614	11/12	0.86	0.30	1.00	109,129,150,155	0
6	CA	A	624	1/1	0.72	0.25	0.97	65,65,65,65	0
6	CA	B	923	1/1	0.93	0.23	0.89	77,77,77,77	0
6	CA	A	617	1/1	0.95	0.22	0.88	71,71,71,71	0
6	CA	A	618	1/1	0.94	0.20	0.82	71,71,71,71	0
6	CA	B	919	1/1	0.87	0.21	0.52	63,63,63,63	0
6	CA	B	915	1/1	0.74	0.20	0.45	79,79,79,79	0
2	NAG	B	904	14/15	0.89	0.24	0.40	86,110,129,138	0
6	CA	B	918	1/1	0.77	0.23	0.39	70,70,70,70	0
2	NAG	B	907	14/15	0.78	0.26	0.34	90,130,157,162	0
7	EDO	A	627	4/4	0.82	0.22	0.26	63,77,99,119	0
6	CA	B	920	1/1	0.89	0.21	0.19	69,69,69,69	0
6	CA	A	622	1/1	0.97	0.22	0.17	64,64,64,64	0
2	NAG	A	609	14/15	0.81	0.24	0.08	84,115,141,162	0
2	NAG	B	909	14/15	0.81	0.24	0.04	68,83,97,102	0
6	CA	B	922	1/1	0.94	0.20	-0.04	59,59,59,59	0
6	CA	A	626	1/1	0.84	0.20	-0.10	78,78,78,78	0
6	CA	A	616	1/1	0.91	0.18	-0.42	66,66,66,66	0
6	CA	A	623	1/1	0.55	0.17	-0.45	79,79,79,79	0
6	CA	A	620	1/1	0.86	0.17	-0.51	78,78,78,78	0
6	CA	B	924	1/1	0.91	0.17	-0.74	71,71,71,71	0
5	MAN	B	902	11/12	0.90	0.22	-0.80	77,99,115,134	0
2	NAG	A	602	14/15	0.87	0.19	-0.80	78,99,119,148	0
2	NAG	B	912	14/15	0.86	0.21	-1.00	87,120,146,162	0
2	NAG	A	605	14/15	0.85	0.17	-1.07	84,115,138,143	0
6	CA	B	917	1/1	0.77	0.16	-1.12	71,71,71,71	0
2	NAG	A	608	14/15	0.82	0.17	-1.17	80,114,137,146	0
6	CA	A	625	1/1	0.94	0.16	-1.19	58,58,58,58	0
6	CA	A	621	1/1	0.89	0.13	-1.26	58,58,58,58	0
3	BMA	A	611	11/12	0.84	0.17	-	60,77,94,99	0
2	NAG	A	610	14/15	0.83	0.19	-	112,129,149,154	0
2	NAG	B	913	14/15	0.77	0.20	-	93,128,157,162	0
3	BMA	A	604	11/12	0.76	0.18	-	71,84,95,111	0
3	BMA	B	908	11/12	0.53	0.28	-	70,87,104,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	601	14/15	0.71	0.21	-	113,165,199,201	0
3	BMA	A	607	11/12	0.61	0.28	-	65,84,101,111	0
2	NAG	A	606	14/15	0.75	0.17	-	68,126,154,161	0
2	NAG	A	603	14/15	0.67	0.24	-	89,117,145,153	0
4	FUC	A	612	10/11	0.83	0.36	-	116,140,167,174	0
2	NAG	B	911	14/15	0.79	0.21	-	97,138,173,175	0
2	NAG	B	905	14/15	0.87	0.16	-	91,116,139,144	0
2	NAG	B	910	14/15	0.70	0.29	-	65,82,98,102	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.