



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2017 – 11:52 AM EDT

PDB ID : 5IW6
Title : anti-CD20 monoclonal antibody Fc fragment
Authors : Tang, C.; Chen, Z.
Deposited on : unknown
Resolution : 2.34 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : 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

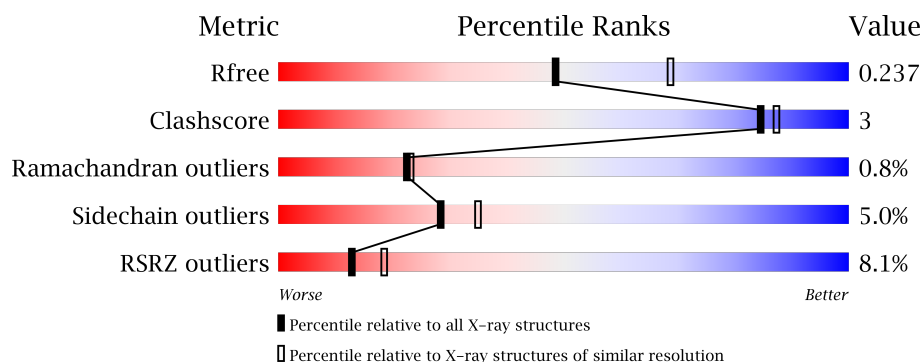
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (2.36-2.32)

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	209	<div> <div>4%</div> <div>94%</div> <div>5%</div> </div>
2	B	205	<div> <div>12%</div> <div>83%</div> <div>12%</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
3	NAG	A	505	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3486 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1655	1053	279	316	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	379	GLU	ASP	engineered mutation	UNP P01857
A	381	MET	LEU	engineered mutation	UNP P01857

- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	199	Total	C	N	O	S	0	1	1
			1524	974	250	293	7			

There are 2 discrepancies between the modelled and reference sequences:

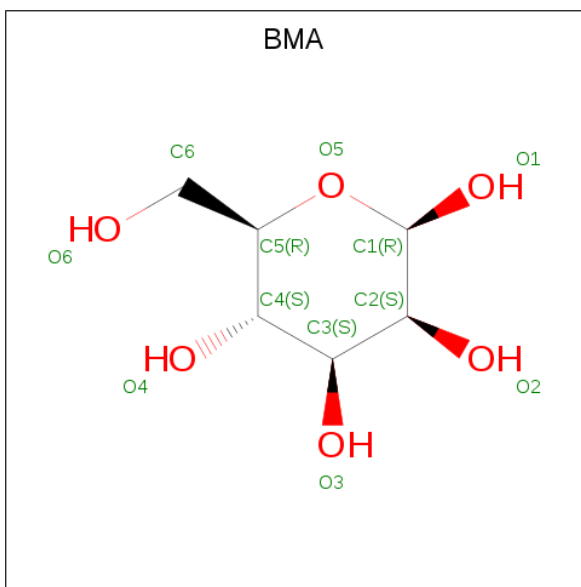
Chain	Residue	Modelled	Actual	Comment	Reference
B	379	GLU	ASP	engineered mutation	UNP P01857
B	381	MET	LEU	engineered mutation	UNP P01857

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



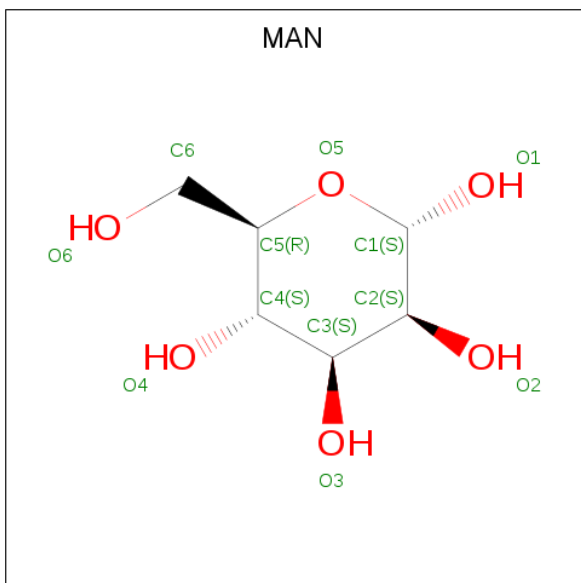
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



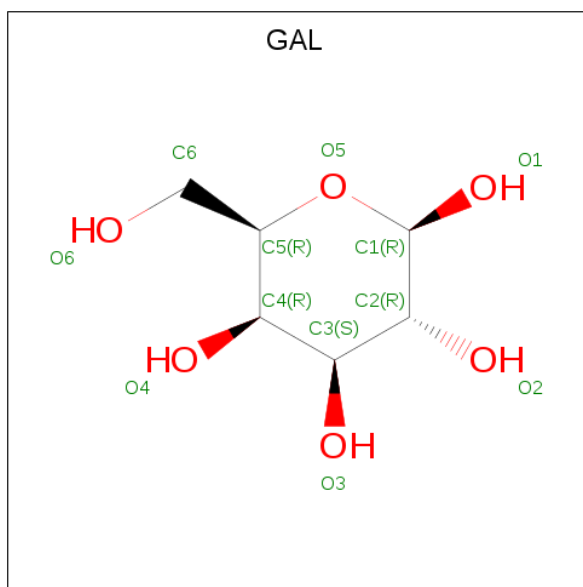
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

- Molecule 6 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C₆H₁₂O₆).



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

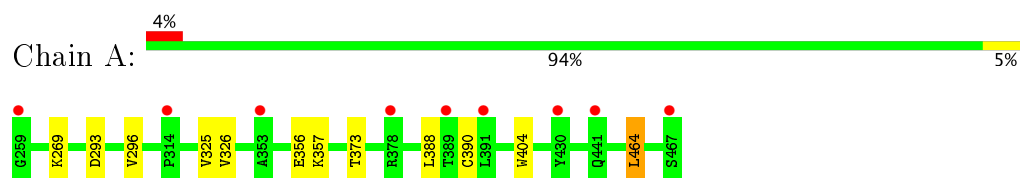
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	68	Total	O	0	0
			68	68		
7	B	39	Total	O	0	0
			39	39		

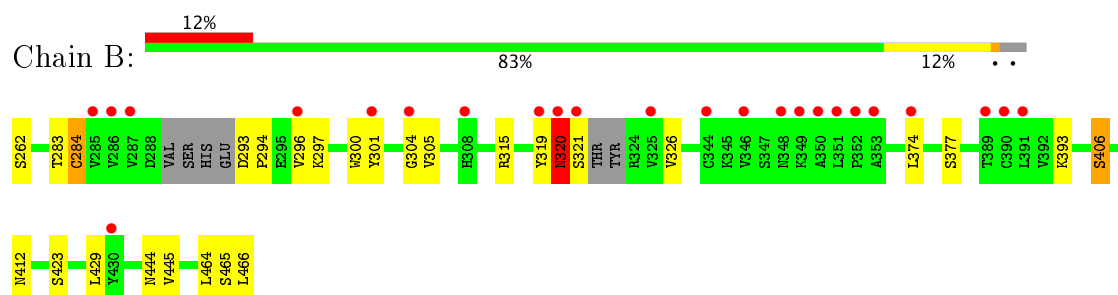
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ig gamma-1 chain C region



- Molecule 2: Ig gamma-1 chain C region



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.45Å 80.00Å 139.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.34 30.31 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.34) 99.6 (30.31-2.34)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.224 , 0.259 0.233 , 0.237	Depositor DCC
R_{free} test set	1229 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3486	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, GAL, BMA, NAG

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	0.49	0/1701	0.66	0/2319
2	B	0.53	0/1567	0.65	0/2144
All	All	0.51	0/3268	0.65	0/4463

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	1655	0	1607	4	0
2	B	1524	0	1430	14	0
3	A	56	0	49	0	0
3	B	56	0	49	1	0
4	A	22	0	17	0	0
4	B	22	0	17	0	0
5	A	11	0	9	0	0
5	B	11	0	9	0	0
6	A	11	0	10	0	0
6	B	11	0	10	0	0
7	A	68	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	39	0	0	0	0
All	All	3486	0	3207	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 3.

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)
2:B:319:TYR:CB	2:B:320:ASN:HB3	2.20	0.72
2:B:293:ASP:N	2:B:294:PRO:HD3	2.09	0.68
2:B:320:ASN:CG	2:B:321:SER:N	2.52	0.62
1:A:373:THR:HB	1:A:464:LEU:HG	1.82	0.61
2:B:320:ASN:OD1	2:B:321:SER:N	2.34	0.60
2:B:293:ASP:N	2:B:294:PRO:CD	2.65	0.60
2:B:301:TYR:HB3	2:B:304:GLY:O	2.02	0.59
1:A:356:GLU:O	1:A:357:LYS:HD3	2.06	0.56
2:B:445:VAL:HA	2:B:465:SER:HB3	1.90	0.52
2:B:406:SER:OG	2:B:445:VAL:O	2.26	0.49
2:B:429:LEU:HD12	2:B:429:LEU:C	2.34	0.48
7:A:602:HOH:O	2:B:393:LYS:NZ	2.39	0.48
2:B:283:THR:HG21	3:B:505:NAG:O6	2.16	0.46
2:B:284:CYS:HB2	2:B:300:TRP:CZ2	2.52	0.44
2:B:319:TYR:CB	2:B:320:ASN:CB	2.93	0.44
1:A:390:CYS:HB2	1:A:404:TRP:CZ2	2.53	0.43
1:A:269:LYS:HE3	7:A:608:HOH:O	2.19	0.42
2:B:296:VAL:HG12	2:B:297:LYS:N	2.35	0.41

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	207/209 (99%)	205 (99%)	2 (1%)	0	100	100
2	B	194/205 (95%)	185 (95%)	6 (3%)	3 (2%)	12	9
All	All	401/414 (97%)	390 (97%)	8 (2%)	3 (1%)	22	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	315	ARG
2	B	320	ASN
2	B	305	VAL

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	190/194 (98%)	184 (97%)	6 (3%)	44	54
2	B	168/192 (88%)	156 (93%)	12 (7%)	17	18
All	All	358/386 (93%)	340 (95%)	18 (5%)	28	35

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	ASP
1	A	296	VAL
1	A	325	VAL
1	A	326	VAL
1	A	388	LEU
1	A	464	LEU
2	B	262	SER
2	B	284	CYS
2	B	320	ASN
2	B	326	VAL
2	B	374	LEU
2	B	377	SER
2	B	406	SER

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Mol	Chain	Res	Type
2	B	412	ASN
2	B	423	SER
2	B	444	ASN
2	B	464	LEU
2	B	466	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	ASN
1	A	457	ASN
1	A	461	GLN
2	B	299	ASN
2	B	348	ASN
2	B	412	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](#)

16 ligands 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	501	1,3	14,14,15	0.52	0	15,19,21	1.63	3 (20%)
3	NAG	A	502	3,4	14,14,15	0.58	0	15,19,21	1.20	1 (6%)
4	BMA	A	503	3,5,4	11,11,12	0.36	0	13,15,17	1.64	3 (23%)
4	BMA	A	504	3,4	11,11,12	0.79	0	13,15,17	1.64	2 (15%)
3	NAG	A	505	4,6	14,14,15	0.45	0	15,19,21	1.32	2 (13%)
5	MAN	A	506	3,4	11,11,12	0.70	0	13,15,17	1.34	1 (7%)
3	NAG	A	507	5	14,14,15	0.44	0	15,19,21	1.19	1 (6%)
6	GAL	A	508	3	11,11,12	0.62	0	13,15,17	1.00	0
3	NAG	B	501	3,2	14,14,15	0.62	0	15,19,21	1.45	2 (13%)
3	NAG	B	502	3,4	14,14,15	0.82	0	15,19,21	1.08	1 (6%)
4	BMA	B	503	3,5,4	11,11,12	0.47	0	13,15,17	1.46	3 (23%)
4	BMA	B	504	3,4	11,11,12	0.66	0	13,15,17	2.31	4 (30%)
3	NAG	B	505	4,6	14,14,15	0.81	0	15,19,21	1.47	2 (13%)
5	MAN	B	506	3,4	11,11,12	0.70	0	13,15,17	0.95	1 (7%)
3	NAG	B	507	5	14,14,15	0.57	0	15,19,21	1.12	1 (6%)
6	GAL	B	508	3	11,11,12	0.69	0	13,15,17	1.20	1 (7%)

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	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	502	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	503	3,5,4	-	0/2/19/22	0/1/1/1
4	BMA	A	504	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	505	4,6	-	0/6/23/26	0/1/1/1
5	MAN	A	506	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	507	5	-	0/6/23/26	0/1/1/1
6	GAL	A	508	3	-	0/2/19/22	0/1/1/1
3	NAG	B	501	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	502	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	503	3,5,4	-	0/2/19/22	0/1/1/1
4	BMA	B	504	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	505	4,6	-	0/6/23/26	0/1/1/1
5	MAN	B	506	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	507	5	-	0/6/23/26	0/1/1/1
6	GAL	B	508	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	BMA	C1-C2-C3	-6.33	101.63	109.65
4	A	504	BMA	C1-C2-C3	-4.77	103.61	109.65
3	A	505	NAG	O5-C1-C2	-4.05	105.84	111.47
4	A	503	BMA	C6-C5-C4	-3.54	104.72	113.00
5	A	506	MAN	O2-C2-C3	-3.39	103.52	110.17
3	B	505	NAG	O5-C1-C2	-3.33	106.83	111.47
3	A	502	NAG	O5-C1-C2	-2.57	107.89	111.47
4	B	503	BMA	O3-C3-C4	-2.44	105.04	110.36
5	B	506	MAN	O2-C2-C3	-2.41	105.44	110.17
4	A	504	BMA	O5-C1-C2	-2.31	107.16	110.79
4	A	503	BMA	O3-C3-C4	-2.23	105.50	110.36
4	B	504	BMA	O5-C1-C2	-2.12	107.47	110.79
3	A	501	NAG	O5-C1-C2	-2.10	108.55	111.47
3	A	505	NAG	O7-C7-C8	-2.03	118.36	122.06
6	B	508	GAL	C2-C3-C4	2.07	114.48	110.88
3	B	501	NAG	C1-C2-N2	2.10	114.07	110.49
4	B	503	BMA	C1-C2-C3	2.18	112.41	109.65
4	A	503	BMA	C3-C4-C5	2.35	114.36	110.22
4	B	503	BMA	C3-C4-C5	2.36	114.37	110.22
4	B	504	BMA	O2-C2-C1	2.71	114.69	109.18
3	B	507	NAG	C3-C4-C5	2.72	115.01	110.22
3	A	507	NAG	C1-O5-C5	2.87	116.12	112.17
4	B	504	BMA	C3-C4-C5	3.30	116.03	110.22
3	A	501	NAG	C8-C7-N2	3.40	122.24	116.11
3	B	502	NAG	C4-C3-C2	3.49	116.13	111.02
3	B	505	NAG	C4-C3-C2	3.56	116.24	111.02
3	A	501	NAG	C1-O5-C5	3.61	117.14	112.17
3	B	501	NAG	C1-O5-C5	4.23	117.99	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	505	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	209/209 (100%)	0.05	9 (4%) 36 47	31, 53, 86, 97	0
2	B	199/205 (97%)	0.53	24 (12%) 5 8	30, 59, 104, 118	0
All	All	408/414 (98%)	0.28	33 (8%) 13 18	30, 55, 95, 118	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	319	TYR	6.0
2	B	321	SER	5.0
1	A	467	SER	4.8
2	B	346	VAL	4.4
2	B	351	LEU	4.4
2	B	389	THR	4.1
2	B	320	ASN	3.7
2	B	287	VAL	3.6
2	B	325	VAL	3.5
2	B	344	CYS	3.5
2	B	348	ASN	3.4
2	B	374	LEU	3.4
1	A	259	GLY	3.3
2	B	352	PRO	3.2
2	B	353	ALA	3.1
2	B	349	LYS	2.9
2	B	350	ALA	2.8
1	A	389	THR	2.8
2	B	304	GLY	2.8
2	B	391	LEU	2.8
1	A	314	PRO	2.7
2	B	301	TYR	2.6
2	B	430	TYR	2.6
1	A	391	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	353	ALA	2.5
2	B	308	HIS	2.3
2	B	285	VAL	2.2
1	A	430	TYR	2.2
1	A	378	ARG	2.2
1	A	441	GLN	2.1
2	B	286	VAL	2.1
2	B	296	VAL	2.1
2	B	390	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	505	14/15	0.81	0.22	2.96	71,82,102,106	0
6	GAL	A	508	11/12	0.85	0.19	1.08	70,78,87,88	0
6	GAL	B	508	11/12	0.92	0.13	-1.08	70,77,79,85	0
3	NAG	A	507	14/15	0.86	0.35	-	104,113,119,121	0
4	BMA	B	504	11/12	0.82	0.29	-	89,91,94,97	0
4	BMA	A	503	11/12	0.93	0.13	-	70,74,77,81	0
3	NAG	B	501	14/15	0.54	0.43	-	108,118,129,132	0
4	BMA	B	503	11/12	0.85	0.15	-	81,92,95,97	0
3	NAG	B	507	14/15	0.79	0.31	-	85,109,114,115	0
5	MAN	B	506	11/12	0.86	0.22	-	89,95,101,101	0
3	NAG	B	505	14/15	0.89	0.27	-	75,81,90,91	0
3	NAG	B	502	14/15	0.68	0.33	-	89,109,118,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	MAN	A	506	11/12	0.86	0.17	-	82,87,91,98	0
3	NAG	A	502	14/15	0.94	0.12	-	70,77,88,93	0
3	NAG	A	501	14/15	0.92	0.12	-	80,85,93,95	0
4	BMA	A	504	11/12	0.82	0.17	-	81,84,89,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.