



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2017 – 08:57 AM EDT

PDB ID : 5JIH  
Title : Crystal structure of HER2 binding IgG1-Fc (Fcab STAB19)  
Authors : Humm, A.; Lobner, E.; Mlynek, G.; Obinger, C.; Djinovic-Carugo, K.  
Deposited on : 2016-04-22  
Resolution : 1.66 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](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-20029077  
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-20029077

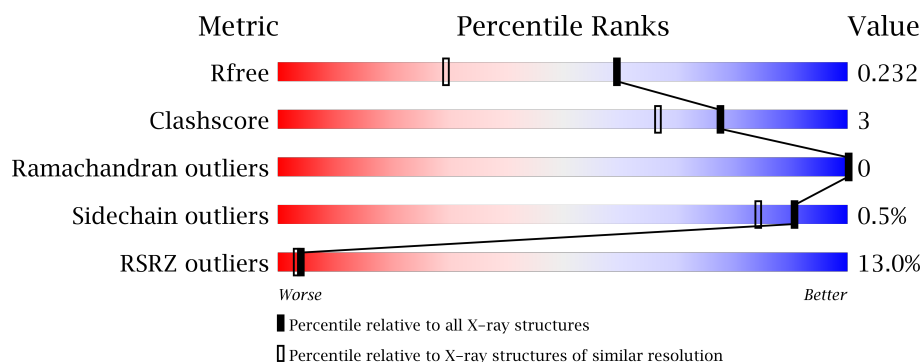
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.66 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	1368 (1.66-1.66)
Clashscore	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)
RSRZ outliers	101464	1371 (1.66-1.66)

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	227	<div> <div>4%</div> <div>90%</div> <div>7%</div> </div>
1	B	227	<div> <div>20%</div> <div>86%</div> <div>7%</div> <div>7%</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
2	NAG	A	505	-	-	-	X
5	FUC	A	508	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7144 atoms, of which 3340 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	212	Total	C	H	N	O	S	107	0	0
			3350	1082	1650	288	323	7			
1	B	212	Total	C	H	N	O	S	173	0	0
			3337	1082	1637	288	323	7			

There are 30 discrepancies between the modelled and reference sequences:

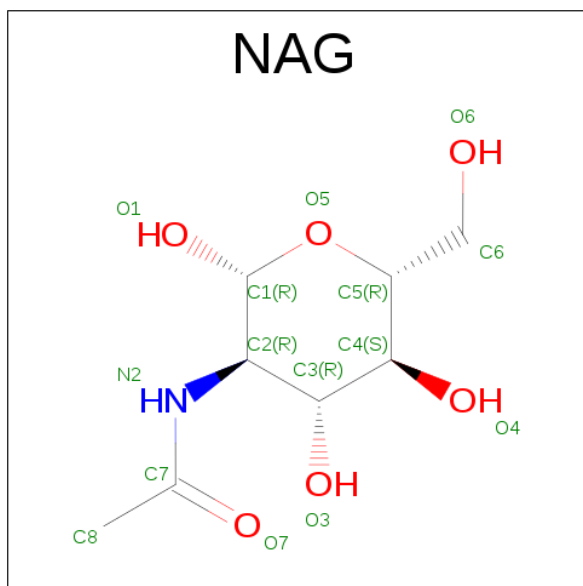
Chain	Residue	Modelled	Actual	Comment	Reference
A	358	TYR	LEU	engineered mutation	UNP P01857
A	359	LEU	THR	engineered mutation	UNP P01857
A	360	SER	LYS	engineered mutation	UNP P01857
A	361	ASP	ASN	engineered mutation	UNP P01857
A	362	SER	GLN	engineered mutation	UNP P01857
A	413	PRO	ASP	engineered mutation	UNP P01857
A	414	ARG	LYS	engineered mutation	UNP P01857
A	415	HIS	SER	engineered mutation	UNP P01857
A	415A	SER	-	insertion	UNP P01857
A	415B	GLU	-	insertion	UNP P01857
A	415C	THR	-	insertion	UNP P01857
A	415D	MET	-	insertion	UNP P01857
A	415E	ARG	-	insertion	UNP P01857
A	418	ALA	GLN	engineered mutation	UNP P01857
A	419	HIS	GLN	engineered mutation	UNP P01857
B	358	TYR	LEU	engineered mutation	UNP P01857
B	359	LEU	THR	engineered mutation	UNP P01857
B	360	SER	LYS	engineered mutation	UNP P01857
B	361	ASP	ASN	engineered mutation	UNP P01857
B	362	SER	GLN	engineered mutation	UNP P01857
B	413	PRO	ASP	engineered mutation	UNP P01857
B	414	ARG	LYS	engineered mutation	UNP P01857
B	415	HIS	SER	engineered mutation	UNP P01857
B	415A	SER	-	insertion	UNP P01857
B	415B	GLU	-	insertion	UNP P01857

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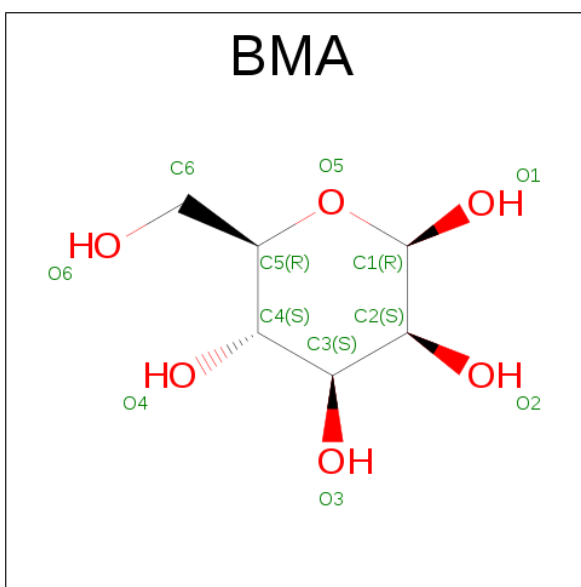
Chain	Residue	Modelled	Actual	Comment	Reference
B	415C	THR	-	insertion	UNP P01857
B	415D	MET	-	insertion	UNP P01857
B	415E	ARG	-	insertion	UNP P01857
B	418	ALA	GLN	engineered mutation	UNP P01857
B	419	HIS	GLN	engineered mutation	UNP P01857

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



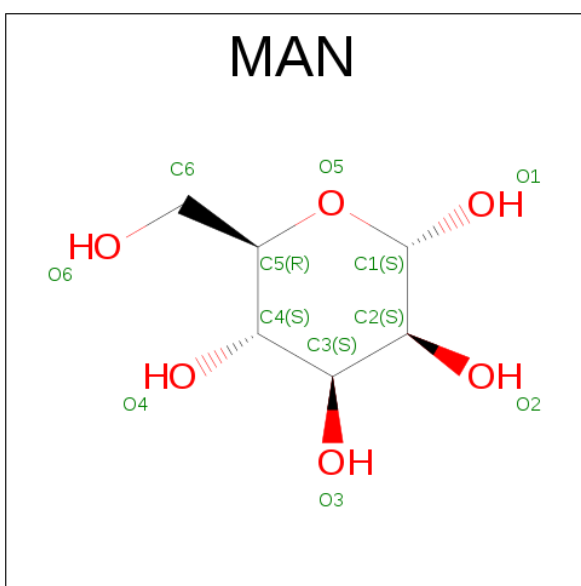
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O		0	0
			14	8	1	5			
2	A	1	Total	C	N	O		0	0
			14	8	1	5			
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	N	O		0	0
			14	8	1	5			
2	B	1	Total	C	N	O		0	0
			14	8	1	5			
2	B	1	Total	C	H	N	O	0	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	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



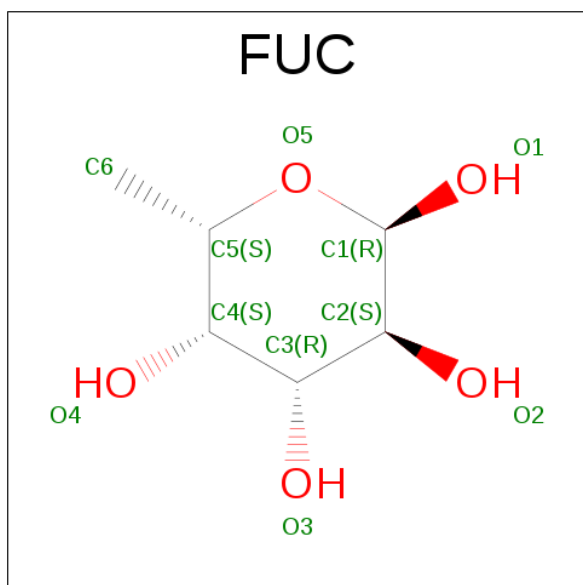
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



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

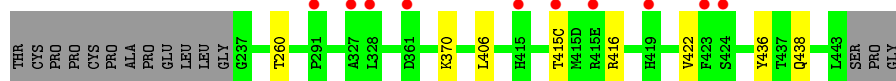
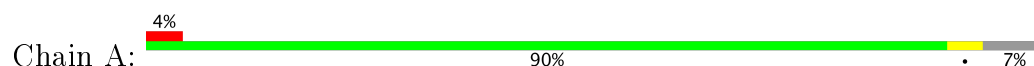
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	134	Total	O	0	0
			134	134		
6	B	96	Total	O	0	0
			96	96		

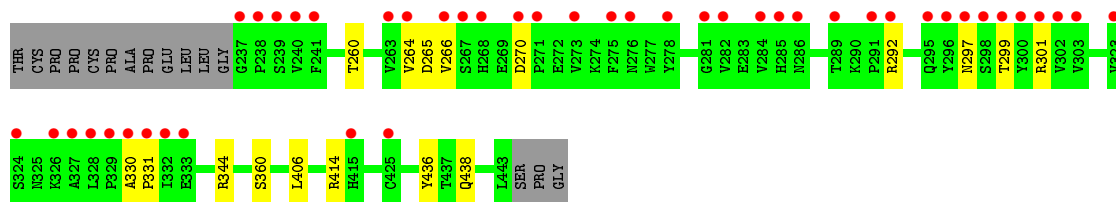
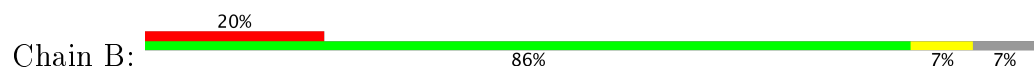
### 3 Residue-property plots [i](#)

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 1: 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, $\alpha$ , $\beta$ , $\gamma$	49.66 Å 79.47 Å 140.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.82 – 1.66 46.82 – 1.66	Depositor EDS
% Data completeness (in resolution range)	97.8 (46.82-1.66) 97.9 (46.82-1.66)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 1.66 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1894)	Depositor
R, $R_{free}$	0.198 , 0.231 0.197 , 0.232	Depositor DCC
$R_{free}$ test set	4662 reflections (7.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.13% 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: FUC, BMA, NAG, 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	0.65	0/1750	0.68	0/2386
1	B	0.61	0/1750	0.66	0/2386
All	All	0.63	0/3500	0.67	0/4772

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	1700	1650	1655	6	0
1	B	1700	1637	1655	12	0
2	A	56	28	49	5	0
2	B	42	14	37	4	0
3	A	11	0	8	0	0
3	B	11	0	8	0	0
4	A	22	0	18	0	0
4	B	22	0	19	1	0
5	A	10	11	10	4	0
6	A	134	0	0	2	0
6	B	96	0	0	3	0
All	All	3804	3340	3459	23	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 (23) 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:B:270:ASP:O	6:B:601:HOH:O	1.92	0.87
4:B:506:MAN:O3	6:B:602:HOH:O	1.99	0.78
1:B:344:ARG:NH1	6:B:603:HOH:O	2.15	0.67
2:A:501:NAG:H61	5:A:508:FUC:H3	1.76	0.67
1:B:260:THR:HG21	2:B:505:NAG:H81	1.81	0.62
2:A:501:NAG:H61	5:A:508:FUC:H5	1.83	0.61
2:A:501:NAG:H61	5:A:508:FUC:C3	2.33	0.58
1:A:436:TYR:CE2	1:A:438:GLN:HG3	2.40	0.56
1:B:360:SER:O	1:B:414:ARG:HD2	2.04	0.56
1:A:260:THR:HG21	2:A:505:NAG:H81	1.88	0.55
1:B:297:ASN:OD1	1:B:299:THR:HG22	2.09	0.53
1:B:436:TYR:CE2	1:B:438:GLN:HG3	2.44	0.52
1:A:422:VAL:O	6:A:601:HOH:O	2.19	0.50
1:A:415(C):THR:HA	1:A:416:ARG:HE	1.75	0.50
2:A:501:NAG:H61	5:A:508:FUC:C5	2.41	0.50
1:B:264:VAL:HG21	2:B:502:NAG:H2	1.94	0.50
1:B:330:ALA:HB1	1:B:331:PRO:HD2	1.97	0.46
1:A:406:LEU:HD12	1:A:406:LEU:C	2.36	0.46
1:A:370:LYS:HD3	6:A:636:HOH:O	2.16	0.45
1:B:264:VAL:HG12	1:B:265:ASP:N	2.34	0.42
1:B:301:ARG:HH22	2:B:505:NAG:H82	1.85	0.42
1:B:406:LEU:HD12	1:B:406:LEU:C	2.41	0.41
1:B:265:ASP:OD1	2:B:501:NAG:H83	2.21	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	210/227 (92%)	210 (100%)	0	0	100	100
1	B	210/227 (92%)	209 (100%)	1 (0%)	0	100	100
All	All	420/454 (92%)	419 (100%)	1 (0%)	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	197/209 (94%)	197 (100%)	0	100	100
1	B	197/209 (94%)	195 (99%)	2 (1%)	80	65
All	All	394/418 (94%)	392 (100%)	2 (0%)	91	84

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	266	VAL
1	B	292	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

14 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$
2	NAG	A	501	1,2,5	14,14,15	0.27	0	15,19,21	1.58	2 (13%)
2	NAG	A	502	3,2	14,14,15	0.75	1 (7%)	15,19,21	0.80	0
3	BMA	A	503	2,4	11,11,12	1.12	1 (9%)	13,15,17	0.91	0
4	MAN	A	504	3,2	11,11,12	2.29	2 (18%)	13,15,17	2.66	5 (38%)
2	NAG	A	505	4	14,14,15	1.59	2 (14%)	15,19,21	1.26	2 (13%)
4	MAN	A	506	3,2	11,11,12	0.82	0	13,15,17	1.41	2 (15%)
2	NAG	A	507	4	14,14,15	0.63	1 (7%)	15,19,21	1.15	1 (6%)
5	FUC	A	508	2	9,10,11	1.82	2 (22%)	13,14,16	1.66	3 (23%)
2	NAG	B	501	1,2	14,14,15	0.28	0	15,19,21	0.68	1 (6%)
2	NAG	B	502	3,2	14,14,15	0.29	0	15,19,21	0.43	0
3	BMA	B	503	2,4	11,11,12	1.29	3 (27%)	13,15,17	1.23	2 (15%)
4	MAN	B	504	3,2	11,11,12	2.20	2 (18%)	13,15,17	1.60	2 (15%)
2	NAG	B	505	4	14,14,15	0.93	2 (14%)	15,19,21	1.12	1 (6%)
4	MAN	B	506	3	11,11,12	0.88	1 (9%)	13,15,17	1.15	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
2	NAG	A	501	1,2,5	-	0/6/23/26	0/1/1/1
2	NAG	A	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	503	2,4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	504	3,2	-	0/2/19/22	0/1/1/1
2	NAG	A	505	4	-	0/6/23/26	0/1/1/1
4	MAN	A	506	3,2	-	0/2/19/22	0/1/1/1
2	NAG	A	507	4	-	0/6/23/26	0/1/1/1
5	FUC	A	508	2	-	0/0/17/20	0/1/1/1
2	NAG	B	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	504	3,2	-	0/2/19/22	0/1/1/1
2	NAG	B	505	4	-	0/6/23/26	0/1/1/1
4	MAN	B	506	3	-	0/2/19/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	505	NAG	O5-C1	-4.10	1.37	1.43
3	A	503	BMA	O5-C1	-2.93	1.38	1.43
2	A	502	NAG	O5-C1	-2.47	1.39	1.43
3	B	503	BMA	O5-C1	-2.01	1.40	1.43
2	A	507	NAG	O5-C1	2.07	1.47	1.43
4	B	506	MAN	C4-C3	2.13	1.57	1.52
5	A	508	FUC	C2-C3	2.15	1.55	1.52
3	B	503	BMA	C2-C3	2.17	1.55	1.52
4	A	504	MAN	O2-C2	2.30	1.48	1.43
2	B	505	NAG	O5-C1	2.35	1.47	1.43
2	B	505	NAG	C1-C2	2.40	1.55	1.52
3	B	503	BMA	C1-C2	2.43	1.57	1.52
4	B	504	MAN	O2-C2	2.73	1.49	1.43
2	A	505	NAG	C1-C2	3.77	1.57	1.52
5	A	508	FUC	C1-C2	4.78	1.63	1.52
4	B	504	MAN	C2-C3	6.01	1.60	1.52
4	A	504	MAN	C2-C3	6.29	1.61	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	506	MAN	O2-C2-C3	-3.13	104.02	110.17
2	A	505	NAG	C1-O5-C5	-2.57	108.62	112.17
4	B	506	MAN	O2-C2-C3	-2.41	105.44	110.17
2	A	505	NAG	C1-C2-N2	-2.03	107.02	110.49
2	B	501	NAG	C1-O5-C5	2.06	115.01	112.17
2	A	501	NAG	C3-C4-C5	2.06	113.85	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	MAN	O2-C2-C3	2.10	114.31	110.17
3	B	503	BMA	C1-O5-C5	2.21	115.21	112.17
3	B	503	BMA	O3-C3-C2	2.35	114.31	110.02
4	A	506	MAN	C1-O5-C5	2.90	116.17	112.17
5	A	508	FUC	O2-C2-C1	2.96	115.19	109.18
4	B	504	MAN	O2-C2-C3	3.19	116.43	110.17
4	A	504	MAN	O5-C1-C2	3.24	115.86	110.79
5	A	508	FUC	C1-O5-C5	3.30	119.69	112.39
2	B	505	NAG	C1-O5-C5	3.40	116.86	112.17
5	A	508	FUC	C1-C2-C3	3.45	114.02	109.65
4	B	504	MAN	O3-C3-C2	3.49	116.38	110.02
2	A	507	NAG	C1-O5-C5	4.00	117.67	112.17
4	A	504	MAN	C1-O5-C5	4.14	117.87	112.17
4	A	504	MAN	C1-C2-C3	4.70	115.61	109.65
2	A	501	NAG	C1-O5-C5	4.74	118.71	112.17
4	A	504	MAN	O2-C2-C1	5.48	120.33	109.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	4	0
2	A	505	NAG	1	0
5	A	508	FUC	4	0
2	B	501	NAG	1	0
2	B	502	NAG	1	0
2	B	505	NAG	2	0
4	B	506	MAN	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

### 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, 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	212/227 (93%)	0.38	10 (4%) 32 31	30, 47, 92, 160	13 (6%)
1	B	212/227 (93%)	1.21	45 (21%) 1 1	28, 62, 137, 224	18 (8%)
All	All	424/454 (93%)	0.80	55 (12%) 4 3	28, 52, 125, 224	31 (7%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	291	PRO	9.5
1	B	300	TYR	9.0
1	B	296	TYR	8.2
1	B	299	THR	8.1
1	B	264	VAL	6.4
1	B	330	ALA	6.1
1	B	273	VAL	6.1
1	A	419	HIS	6.0
1	B	303	VAL	5.7
1	B	282	VAL	5.4
1	B	328	LEU	5.4
1	B	302	VAL	5.4
1	B	237	GLY	4.4
1	B	297	ASN	4.4
1	B	295	GLN	4.3
1	B	238	PRO	4.3
1	B	332	ILE	4.2
1	B	324	SER	4.2
1	B	268	HIS	4.0
1	B	240	VAL	4.0
1	B	270	ASP	3.8
1	B	301	ARG	3.7
1	B	239	SER	3.6
1	B	327	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	271	PRO	3.5
1	B	281	GLY	3.5
1	A	327	ALA	3.3
1	B	285	HIS	3.3
1	A	415(C)	THR	3.2
1	B	266	VAL	3.2
1	B	329	PRO	3.2
1	B	289	THR	3.2
1	B	276	ASN	3.1
1	B	326	LYS	3.0
1	B	263	VAL	3.0
1	B	331	PRO	3.0
1	B	323	VAL	3.0
1	B	267	SER	2.8
1	B	241	PHE	2.8
1	B	275	PHE	2.8
1	B	298	SER	2.8
1	B	415	HIS	2.8
1	B	286	ASN	2.7
1	B	292	ARG	2.6
1	A	424	SER	2.6
1	B	333	GLU	2.5
1	A	328	LEU	2.5
1	B	425	CYS	2.4
1	A	291	PRO	2.3
1	A	423	PHE	2.3
1	A	415(E)	ARG	2.2
1	B	284	VAL	2.2
1	A	415	HIS	2.1
1	A	361	ASP	2.0
1	B	278	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

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(Å <sup>2</sup> )	Q<0.9
2	NAG	A	505	14/15	0.73	0.16	3.21	58,75,110,110	0
5	FUC	A	508	10/11	0.60	0.23	2.95	71,96,152,152	0
2	NAG	B	505	14/15	0.63	0.29	1.32	60,93,148,148	0
2	NAG	B	502	14/15	0.65	0.30	0.86	78,92,101,122	0
2	NAG	A	501	14/15	0.85	0.09	-0.78	48,58,100,101	0
4	MAN	B	504	11/12	0.89	0.10	-	66,76,83,87	0
4	MAN	A	504	11/12	0.79	0.12	-	37,48,54,82	0
2	NAG	A	507	14/15	0.60	0.26	-	107,141,219,219	0
3	BMA	A	503	11/12	0.94	0.07	-	40,44,50,52	0
2	NAG	A	502	14/15	0.93	0.10	-	43,47,51,55	0
3	BMA	B	503	11/12	0.81	0.13	-	61,64,86,93	0
4	MAN	A	506	11/12	0.90	0.09	-	55,66,83,107	0
4	MAN	B	506	11/12	0.78	0.15	-	72,80,101,102	0
2	NAG	B	501	14/15	0.62	0.38	-	81,175,181,186	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.