wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:50 PM GMT

PDB ID	:	1MCO
Title	:	THREE-DIMENSIONAL STRUCTURE OF A HUMAN IMMUNOGLOBULIN WITH A HINGE DELETION
Authors	:	Guddat, L.W.; Edmundson, A.B.
Deposited on	:	1993-02-25
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

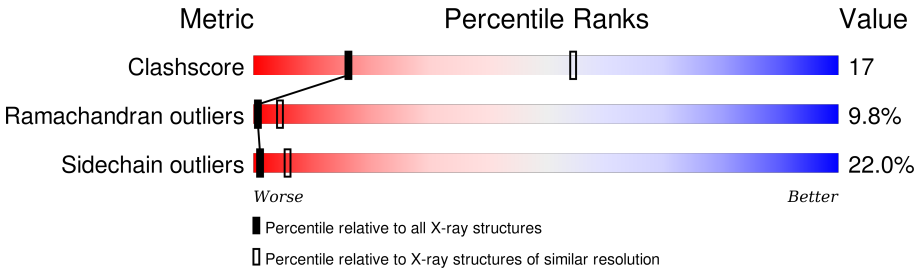
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	216	49% 35% 12% 5%
2	H	428	43% 30% 17% 10%

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
4	GUP	H	437	X	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5041 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 IGG1 MCG INTACT ANTIBODY (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1606	999	266	336	5			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	20	ILE	PHE	CONFLICT	PIR S14675
L	23	THR	SER	CONFLICT	PIR S14675
L	29	VAL	ILE	CONFLICT	PIR S14675
L	31	GLY	ASN	CONFLICT	PIR S14675
L	39	GLN	ARG	CONFLICT	PIR S14675
L	42	ALA	PRO	CONFLICT	PIR S14675
L	48	VAL	LEU	CONFLICT	PIR S14675
L	49	ILE	MET	CONFLICT	PIR S14675
L	54	ASN	THR	CONFLICT	PIR S14675
L	62	ASP	ASN	CONFLICT	PIR S14675
L	94	GLU	ALA	CONFLICT	PIR S14675
L	97	ASP	ASN	CONFLICT	PIR S14675
L	98	ASN	SER	CONFLICT	PIR S14675
L	99	PHE	LEU	CONFLICT	PIR S14675
L	100	VAL	ILE	CONFLICT	PIR S14675
L	103	THR	GLY	CONFLICT	PIR S14675
L	106	LYS	ARG	CONFLICT	PIR S14675
L	107	VAL	LEU	CONFLICT	PIR S14675
L	116	ASN	ALA	CONFLICT	PIR S14675
L	118	THR	SER	CONFLICT	PIR S14675
L	136	GLU	LEU	CONFLICT	PIR S14675
L	156	GLY	SER	CONFLICT	PIR S14675
L	167	LYS	THR	CONFLICT	PIR S14675

- Molecule 2 is a protein called IGG1 MCG INTACT ANTIBODY (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	428	Total	C	N	O	S	0	0	0
			3305	2108	551	635	11			

There are 67 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	GLN	DELETION	GB 243866
H	13	LYS	ARG	CONFLICT	GB 243866
H	16	GLU	GLN	CONFLICT	GB 243866
H	17	ALA	THR	CONFLICT	GB 243866
H	27	ASP	-	INSERTION	GB 243866
H	28	SER	PHE	CONFLICT	GB 243866
H	29	ILE	THR	CONFLICT	GB 243866
H	30	ASN	PHE	CONFLICT	GB 243866
H	32	ILE	-	INSERTION	GB 243866
H	33	LEU	ASP	CONFLICT	GB 243866
H	34	TYR	PHE	CONFLICT	GB 243866
H	36	TRP	MET	CONFLICT	GB 243866
H	37	SER	ASN	CONFLICT	GB 243866
H	39	ILE	VAL	CONFLICT	GB 243866
H	45	LYS	ARG	CONFLICT	GB 243866
H	52	TYR	PHE	CONFLICT	GB 243866
H	?	-	ARG	DELETION	GB 243866
H	?	-	ASP	DELETION	GB 243866
H	54	TYR	LYS	CONFLICT	GB 243866
H	55	TYR	ALA	CONFLICT	GB 243866
H	56	SER	LYS	CONFLICT	GB 243866
H	58	SER	TYR	CONFLICT	GB 243866
H	?	-	THR	DELETION	GB 243866
H	?	-	GLU	DELETION	GB 243866
H	61	GLY	-	INSERTION	GB 243866
H	65	LEU	VAL	CONFLICT	GB 243866
H	67	SER	GLY	CONFLICT	GB 243866
H	71	ILE	MET	CONFLICT	GB 243866
H	72	SER	LEU	CONFLICT	GB 243866
H	74	ASN	ASP	CONFLICT	GB 243866
H	81	TYR	SER	CONFLICT	GB 243866
H	82	SER	LEU	CONFLICT	GB 243866
H	83	LYS	ARG	CONFLICT	GB 243866
H	100	VAL	GLU	CONFLICT	GB 243866
H	101	PRO	GLY	CONFLICT	GB 243866
H	102	LEU	HIS	CONFLICT	GB 243866
H	103	VAL	THR	CONFLICT	GB 243866

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Chain	Residue	Modelled	Actual	Comment	Reference
H	104	VAL	ALA	CONFLICT	GB 243866
H	105	ASN	ALA	CONFLICT	GB 243866
H	?	-	PHE	DELETION	GB 243866
H	?	-	ASP	DELETION	GB 243866
H	?	-	TYR	DELETION	GB 243866
H	111	THR	SER	CONFLICT	GB 243866
H	152	GLN	GLU	CONFLICT	GB 243866
H	214	ARG	LYS	CONFLICT	GB 243866
H	?	-	GLU	DELETION	GB 243866
H	?	-	PRO	DELETION	GB 243866
H	?	-	LYS	DELETION	GB 243866
H	?	-	SER	DELETION	GB 243866
H	?	-	CYS	DELETION	GB 243866
H	?	-	ASP	DELETION	GB 243866
H	?	-	LYS	DELETION	GB 243866
H	?	-	THR	DELETION	GB 243866
H	?	-	HIS	DELETION	GB 243866
H	?	-	THR	DELETION	GB 243866
H	?	-	CYS	DELETION	GB 243866
H	?	-	PRO	DELETION	GB 243866
H	?	-	PRO	DELETION	GB 243866
H	?	-	CYS	DELETION	GB 243866
H	?	-	PRO	DELETION	GB 243866
H	257	GLN	GLU	CONFLICT	GB 243866
H	268	GLN	GLU	CONFLICT	GB 243866
H	279	GLN	GLU	CONFLICT	GB 243866
H	297	ASN	ASP	CONFLICT	GB 243866
H	300	ASP	ASN	CONFLICT	GB 243866
H	341	GLU	ASP	CONFLICT	GB 243866
H	343	MET	LEU	CONFLICT	GB 243866

- Molecule 3 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	8	Total	C	N	O	0	0
			105	59	4	42		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	2	Total	C	N	O	0	0
			25	14	1	10		

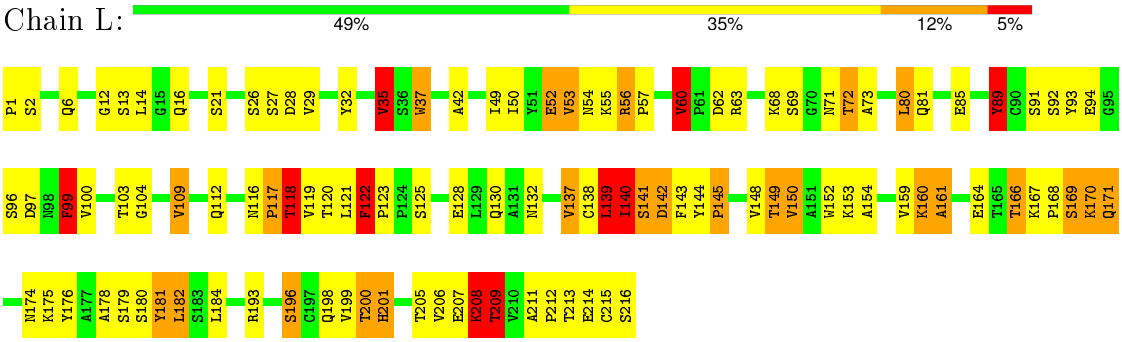
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

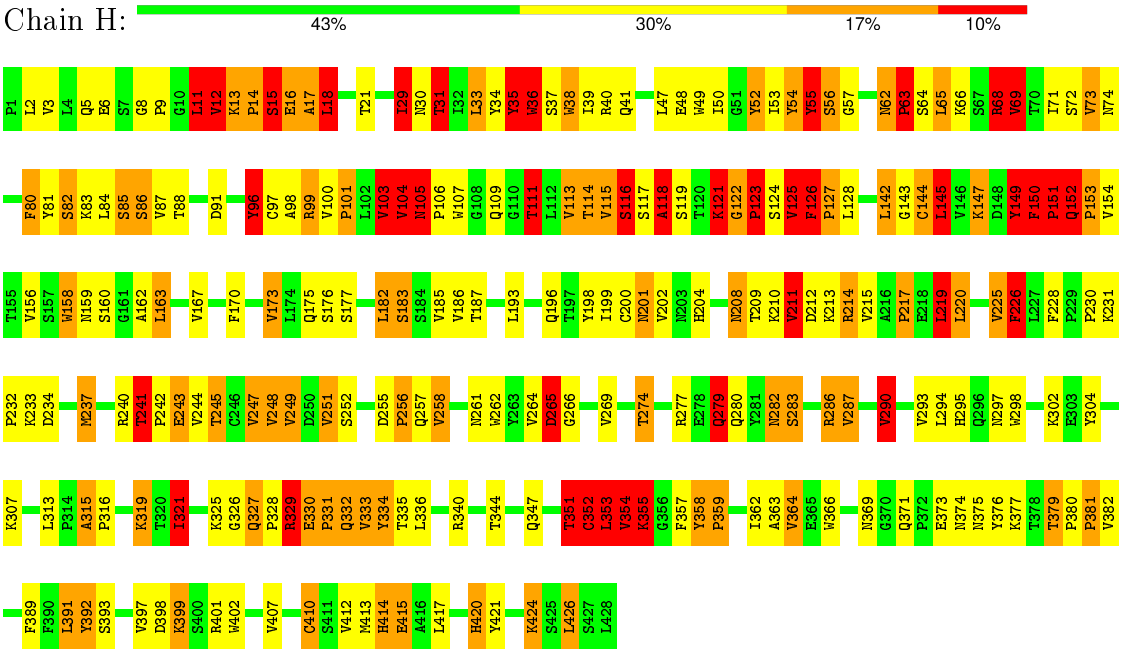
- Molecule 1: IGG1 MCG INTACT ANTIBODY (LIGHT CHAIN)

Chain L:



- Molecule 2: IGG1 MCG INTACT ANTIBODY (HEAVY CHAIN)

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	88.40Å 110.00Å 186.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.232 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5041	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, GUP, NAG, SIA, GAL, FUL, 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	L	0.95	2/1645 (0.1%)	2.06	73/2242 (3.3%)
2	H	1.09	17/3396 (0.5%)	2.47	227/4641 (4.9%)
All	All	1.05	19/5041 (0.4%)	2.35	300/6883 (4.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
2	H	0	10
4	H	1	0
All	All	1	12

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	85	SER	CA-CB	7.76	1.64	1.52
2	H	84	LEU	CA-CB	7.22	1.70	1.53
2	H	18	LEU	N-CA	6.62	1.59	1.46
2	H	243	GLU	CD-OE1	-6.51	1.18	1.25
2	H	84	LEU	CB-CG	6.04	1.70	1.52

The worst 5 of 300 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	290	VAL	CG1-CB-CG2	-23.59	73.15	110.90
2	H	290	VAL	CA-CB-CG1	-19.64	81.44	110.90
2	H	247	VAL	CG1-CB-CG2	-17.56	82.80	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	354	VAL	CG1-CB-CG2	-16.69	84.20	110.90
2	H	17	ALA	N-CA-CB	-15.06	89.02	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	437	GUP	C1

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	15	SER	Mainchain
2	H	17	ALA	Mainchain
2	H	54	TYR	Sidechain
2	H	96	TYR	Sidechain
1	L	144	TYR	Sidechain,Peptide

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	L	1606	0	1536	48	0
2	H	3305	0	3277	136	0
3	H	105	0	87	12	0
4	H	25	0	20	12	0
All	All	5041	0	4920	166	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 17.

The worst 5 of 166 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)
3:H:432:BMA:HO3	4:H:437:GUP:C1	1.61	1.03
1:L:139:LEU:HG	2:H:147:LYS:HE3	1.60	0.84
2:H:226:PHE:CD2	3:H:432:BMA:H3	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:179:SER:HA	2:H:147:LYS:HE2	1.63	0.81
2:H:125:VAL:HG21	2:H:211:VAL:HG11	1.63	0.79

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	L	214/216 (99%)	164 (77%)	32 (15%)	18 (8%)	1 6
2	H	426/428 (100%)	304 (71%)	77 (18%)	45 (11%)	0 3
All	All	640/644 (99%)	468 (73%)	109 (17%)	63 (10%)	1 4

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	26	SER
1	L	52	GLU
1	L	96	SER
1	L	117	PRO
1	L	123	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	L	181/181 (100%)	143 (79%)	38 (21%)	1 7
2	H	383/383 (100%)	297 (78%)	86 (22%)	1 5
All	All	564/564 (100%)	440 (78%)	124 (22%)	1 6

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	74	ASN
2	H	145	LEU
2	H	377	LYS
2	H	80	PHE
2	H	109	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	196	GLN
2	H	201	ASN
2	H	327	GLN
2	H	109	GLN
2	H	175	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)

10 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	H	429	3,2	14,14,15	2.26	6 (42%)	15,19,21	4.43	9 (60%)
3	FUL	H	430	3	10,10,11	1.42	1 (10%)	14,14,16	1.07	1 (7%)
3	NAG	H	431	3	14,14,15	1.48	2 (14%)	15,19,21	3.79	6 (40%)
3	BMA	H	432	3,4	11,11,12	2.18	4 (36%)	14,15,17	4.52	9 (64%)
3	MAN	H	433	3	11,11,12	1.92	3 (27%)	14,15,17	2.79	6 (42%)
3	NAG	H	434	3	14,14,15	1.59	3 (21%)	15,19,21	2.64	5 (33%)
3	GAL	H	435	3	11,11,12	3.51	8 (72%)	14,15,17	4.18	10 (71%)
3	SIA	H	436	3	16,20,21	2.74	5 (31%)	18,28,31	2.92	7 (38%)
4	GUP	H	437	3,4	11,11,12	3.93	4 (36%)	14,15,17	5.47	7 (50%)
4	NAG	H	438	4	14,14,15	2.27	5 (35%)	15,19,21	3.09	8 (53%)

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	H	429	3,2	-	0/6/23/26	0/1/1/1
3	FUL	H	430	3	-	0/0/17/20	0/1/1/1
3	NAG	H	431	3	-	0/6/23/26	0/1/1/1
3	BMA	H	432	3,4	-	0/2/19/22	0/1/1/1
3	MAN	H	433	3	-	0/2/19/22	0/1/1/1
3	NAG	H	434	3	-	0/6/23/26	0/1/1/1
3	GAL	H	435	3	-	0/2/19/22	0/1/1/1
3	SIA	H	436	3	-	0/14/34/38	0/1/1/1
4	GUP	H	437	3,4	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	H	438	4	-	0/6/23/26	0/1/1/1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	438	NAG	C8-C7	-4.11	1.42	1.50
4	H	438	NAG	C2-N2	-3.90	1.39	1.46
3	H	433	MAN	O3-C3	-3.56	1.34	1.43
3	H	435	GAL	O4-C4	-3.08	1.35	1.43
4	H	438	NAG	C7-N2	-3.08	1.22	1.34

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	431	NAG	O3-C3-C4	-7.90	92.54	110.34
4	H	437	GUP	C1-C2-C3	-7.87	100.23	109.54
4	H	437	GUP	O5-C1-C2	-6.67	100.04	110.86
3	H	432	BMA	O3-C3-C2	-5.30	100.43	110.00
3	H	434	NAG	O4-C4-C3	-4.79	99.56	110.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	437	GUP	C1

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	431	NAG	1	0
3	H	432	BMA	5	0
3	H	433	MAN	1	0
3	H	435	GAL	4	0
3	H	436	SIA	3	0
4	H	437	GUP	6	0
4	H	438	NAG	6	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.