W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 09:29 am GMT

PDB ID	:	4QGT
Title	:	The Crystal Structure of Human IgG Fc Domain with Enhanced Aromatic Sequon
Authors	:	Kong, L.; Connelly, S.C.; Wilson, I.A.
Deposited on	:	2014-05-25
Resolution	:	2.99 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

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 2.99 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		0.329
Clashscore		11
Ramachandran outliers		0.7%
Sidechain outliers		0.5%
RSRZ outliers		16.0%

Worse ◄─────────────────────► Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
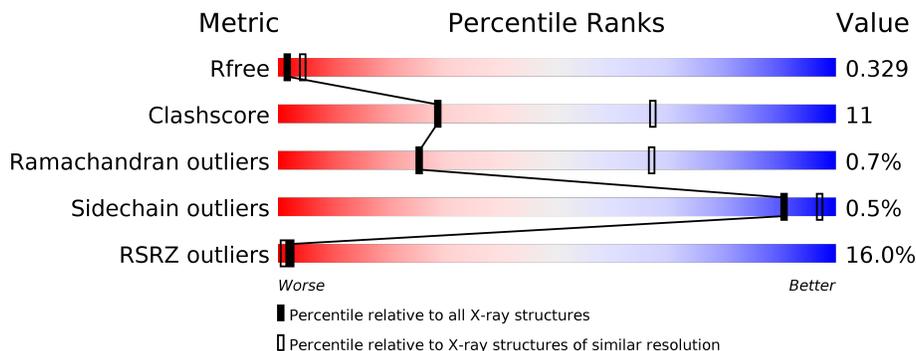
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	233	16% / 63% 24% • 12%
1	B	233	12% / 71% 18% 11%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 3463 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 Hepatitis B virus receptor binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total 1637	C 1044	N 274	O 312	S 7	0	0	0
1	B	207	Total 1654	C 1054	N 278	O 315	S 7	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	PHE	-	EXPRESSION TAG	UNP Q6PYX1
A	295	PHE	GLN	ENGINEERED MUTATION	UNP Q6PYX1
A	296	ALA	TYR	ENGINEERED MUTATION	UNP Q6PYX1
B	215	PHE	-	EXPRESSION TAG	UNP Q6PYX1
B	295	PHE	GLN	ENGINEERED MUTATION	UNP Q6PYX1
B	296	ALA	TYR	ENGINEERED MUTATION	UNP Q6PYX1

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total 64	C 36	N 3	O 25	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	8	Total 99	C 56	N 4	O 39	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1   C2

HO

O1

OH

O2
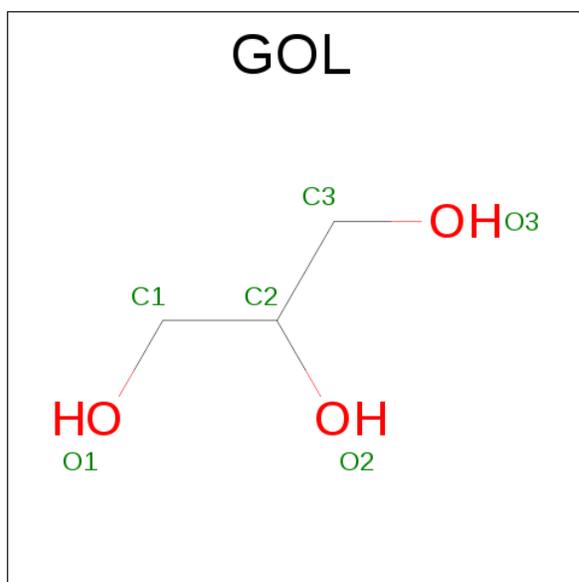
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 6	C 3	O 3	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	O 2	0	0
5	B	1	Total 1	O 1	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 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: Hepatitis B virus receptor binding protein

Chain A:

• Molecule 1: Hepatitis B virus receptor binding protein

Chain B:
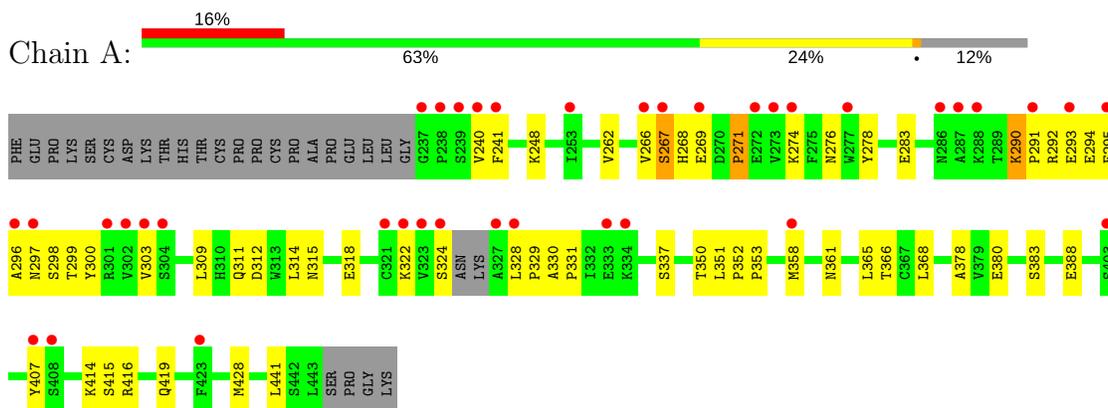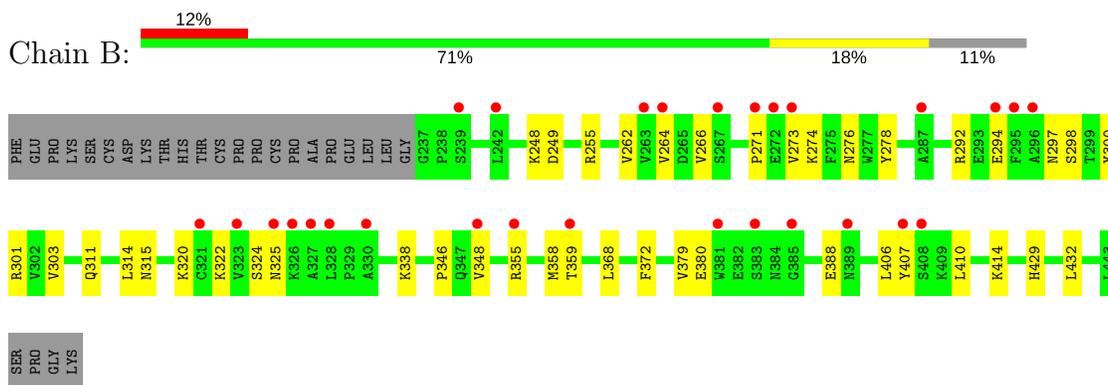
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.07Å 49.19Å 75.54Å 90.00° 104.21° 90.00°	Depositor
Resolution (Å)	46.85 – 2.99 46.85 – 2.99	Depositor EDS
% Data completeness (in resolution range)	87.9 (46.85-2.99) 88.0 (46.85-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.298 , 0.326 0.302 , 0.329	Depositor DCC
R_{free} test set	517 reflections (5.17%)	DCC
Wilson B-factor (Å^2)	69.3	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.5	EDS
L-test for twinning[2]	$< |L| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	3463	wwPDB-VP
Average B, all atoms (Å^2)	77.0	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 48.10 % 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 9.0296e-05. 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, 0.333 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, GOL, BMA, NAG, FUC

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	0.26	0/1682	0.45	0/2290
1	B	0.22	0/1700	0.40	0/2315
All	All	0.24	0/3382	0.42	0/4605

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	1637	0	1603	44	0
1	B	1654	0	1621	31	0
2	A	64	0	55	3	0
3	B	99	0	85	1	0
4	B	6	0	8	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
All	All	3463	0	3372	75	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 11.

The worst 5 of 75 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:297:ASN:HD21	2:A:501:NAG:C1	1.02	1.54
1:A:297:ASN:ND2	2:A:501:NAG:C1	1.87	1.37
1:B:358:MET:O	1:B:414:LYS:NZ	1.62	1.32
1:A:358:MET:O	1:A:414:LYS:NZ	1.94	1.00
1:A:268:HIS:O	1:A:269:GLU:HB2	1.81	0.81

There are no symmetry-related clashes.

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	201/233 (86%)	188 (94%)	10 (5%)	3 (2%)	12	48
1	B	205/233 (88%)	199 (97%)	6 (3%)	0	100	100
All	All	406/466 (87%)	387 (95%)	16 (4%)	3 (1%)	25	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	SER
1	A	290	LYS
1	A	271	PRO

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	190/215 (88%)	190 (100%)	0	100	100
1	B	192/215 (89%)	190 (99%)	2 (1%)	80	94
All	All	382/430 (89%)	380 (100%)	2 (0%)	91	97

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

Mol	Chain	Res	Type
1	B	298	SER
1	B	348	VAL

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 ⓘ

13 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	$\#|Z| > 2$
2	NAG	A	501	2	14,14,15	0.73	0	15,19,21	1.20	1 (6%)
2	NAG	A	502	2	14,14,15	0.75	0	15,19,21	1.03	1 (6%)
2	BMA	A	503	2	11,11,12	0.62	0	13,15,17	1.66	3 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	MAN	A	504	2	11,11,12	0.79	0	13,15,17	1.46	1 (7%)
2	NAG	A	505	2	14,14,15	0.93	0	15,19,21	1.29	1 (6%)
3	NAG	B	501	1,3	14,14,15	0.71	0	15,19,21	1.19	1 (6%)
3	NAG	B	502	3	14,14,15	0.74	0	15,19,21	1.03	1 (6%)
3	BMA	B	503	3	11,11,12	0.61	0	13,15,17	1.67	3 (23%)
3	MAN	B	504	3	11,11,12	0.61	0	13,15,17	1.42	1 (7%)
3	NAG	B	505	3	14,14,15	0.47	0	15,19,21	1.13	2 (13%)
3	MAN	B	506	3	11,11,12	0.80	0	13,15,17	1.45	1 (7%)
3	NAG	B	507	3	14,14,15	0.93	0	15,19,21	1.29	1 (6%)
3	FUC	B	508	3	9,10,11	0.62	0	13,14,16	1.23	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	2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
2	BMA	A	503	2	-	0/2/19/22	0/1/1/1
2	MAN	A	504	2	-	0/2/19/22	0/1/1/1
2	NAG	A	505	2	-	0/6/23/26	0/1/1/1
3	NAG	B	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	502	3	-	0/6/23/26	0/1/1/1
3	BMA	B	503	3	-	0/2/19/22	0/1/1/1
3	MAN	B	504	3	-	0/2/19/22	0/1/1/1
3	NAG	B	505	3	-	0/6/23/26	0/1/1/1
3	MAN	B	506	3	-	0/2/19/22	0/1/1/1
3	NAG	B	507	3	-	0/6/23/26	0/1/1/1
3	FUC	B	508	3	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	BMA	O3-C3-C4	-3.55	102.64	110.36
2	A	503	BMA	O3-C3-C4	-3.54	102.65	110.36
2	A	503	BMA	O6-C6-C5	-2.75	102.09	111.34
3	B	503	BMA	O6-C6-C5	-2.73	102.14	111.34
2	A	502	NAG	C8-C7-N2	-2.05	112.42	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	2	0
2	A	503	BMA	1	0
3	B	508	FUC	1	0

5.6 Ligand geometry (i)

1 ligand is 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	$\#|Z| > 2$
4	GOL	B	509	-	5,5,5	0.35	0	5,5,5	0.25	0

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
4	GOL	B	509	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	205/233 (87%)	1.06	38 (18%)	1	1	31, 67, 130, 143	0
1	B	207/233 (88%)	1.01	28 (13%)	3	1	31, 66, 106, 127	0
All	All	412/466 (88%)	1.04	66 (16%)	2	1	31, 67, 123, 143	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	VAL	8.6
1	B	271	PRO	7.3
1	A	297	ASN	7.2
1	B	327	ALA	6.9
1	B	273	VAL	6.6

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
3	NAG	B	507	14/15	0.82	0.31	1.49	66,90,109,110	0
2	NAG	A	505	14/15	0.82	0.30	1.01	81,105,130,142	0
3	NAG	B	502	14/15	0.91	0.17	-1.45	89,99,103,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
2	BMA	A	503	11/12	0.66	0.34	-	194,302,322,324	0
3	NAG	B	505	14/15	0.76	0.24	-	104,111,116,120	0
2	NAG	A	501	14/15	0.64	0.46	-	280,327,380,388	0
3	BMA	B	503	11/12	0.82	0.17	-	80,100,108,110	0
3	NAG	B	501	14/15	0.84	0.17	-	87,98,103,109	0
2	MAN	A	504	11/12	0.87	0.21	-	123,146,164,167	0
3	MAN	B	504	11/12	0.72	0.22	-	107,111,116,116	0
3	FUC	B	508	10/11	0.60	0.32	-	87,99,110,115	0
2	NAG	A	502	14/15	0.49	0.43	-	249,308,346,366	0
3	MAN	B	506	11/12	0.92	0.17	-	90,95,98,103	0

6.4 Ligands ⓘ

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	GOL	B	509	6/6	0.68	0.42	-	61,83,85,92	0

6.5 Other polymers ⓘ

There are no such residues in this entry.