



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2017 – 07:28 PM EDT

PDB ID : 4ZMJ
Title : Crystal Structure of Ligand-Free BG505 SOSIP.664 HIV-1 Env Trimer
Authors : Kwon, Y.D.; Kwong, P.D.
Deposited on : unknown
Resolution : 3.31 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 ⓘ 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

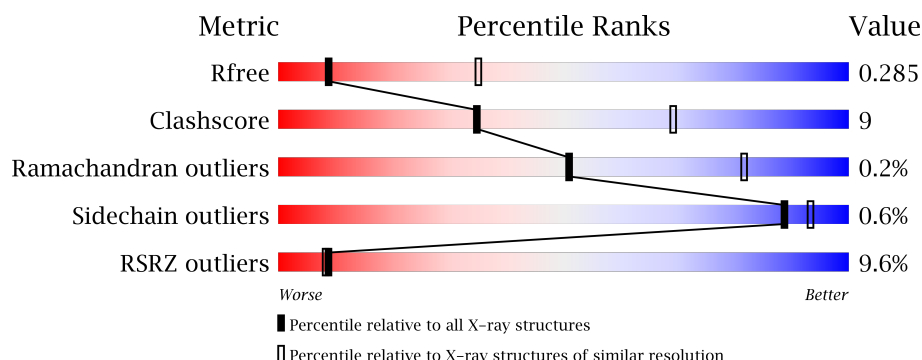
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1002 (3.38-3.26)
Clashscore	112137	1066 (3.38-3.26)
Ramachandran outliers	110173	1048 (3.38-3.26)
Sidechain outliers	110143	1047 (3.38-3.26)
RSRZ outliers	101464	1007 (3.38-3.26)

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	G	481	
2	B	153	

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	B	701	-	-	-	X
3	NAG	G	601	-	-	-	X
3	NAG	G	610	-	-	-	X
3	NAG	G	620	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4856 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	450	Total	C	N	O	S	0	0	0
			3543	2224	626	665	28			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	508	ARG	-	expression tag	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	123	Total	C	N	O	S	0	0	0
			975	613	169	187	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

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



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

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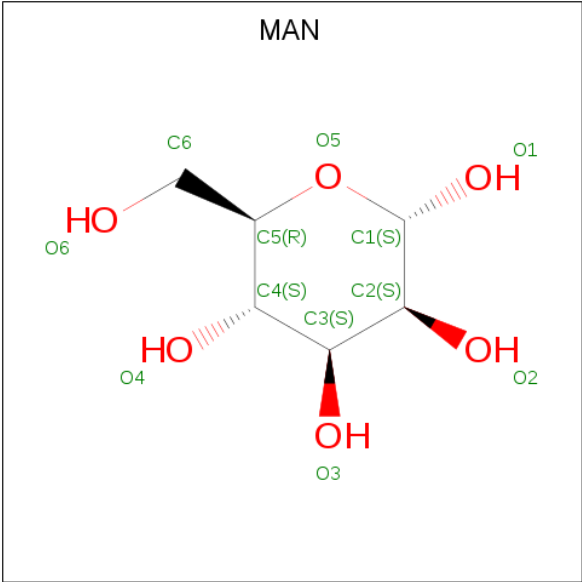
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	107.18Å 107.18Å 103.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.08 – 3.31 47.55 – 3.31	Depositor EDS
% Data completeness (in resolution range)	63.7 (35.08-3.31) 63.8 (47.55-3.31)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.266 , 0.285 0.267 , 0.285	Depositor DCC
R_{free} test set	322 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	88.7	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.099 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	4856	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	G	0.29	0/3617	0.61	0/4911
2	B	0.22	0/992	0.38	0/1345
All	All	0.28	0/4609	0.57	0/6256

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	G	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	354	GLY	Peptide
1	G	431	GLY	Peptide
1	G	494	LEU	Peptide
1	G	57	ASP	Peptide

5.2 Too-close contacts [i](#)

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	G	3543	0	3481	79	2
2	B	975	0	946	18	1
3	B	42	0	39	0	0
3	G	252	0	230	5	1
4	G	11	0	8	0	0
5	G	33	0	29	0	0
All	All	4856	0	4733	90	2

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 9.

The worst 5 of 90 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:G:270:VAL:HG23	1:G:348:GLN:HG3	1.64	0.78
1:G:301:ASN:HB3	1:G:323:ILE:HB	1.64	0.77
1:G:270:VAL:HG12	1:G:288:PHE:HA	1.69	0.74
1:G:50:THR:O	1:G:103:GLN:NE2	2.16	0.73
1:G:138:ILE:HG23	1:G:139:THR:HG23	1.71	0.72

All (2) 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:G:136:ASN:ND2	3:G:610:NAG:O3[5_564]	2.16	0.04
1:G:187:SER:OG	2:B:660:LEU:O[2_774]	2.16	0.04

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	G	444/481 (92%)	411 (93%)	32 (7%)	1 (0%)	51 81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	119/153 (78%)	105 (88%)	14 (12%)	0	100	100
All	All	563/634 (89%)	516 (92%)	46 (8%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	57	ASP

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	G	402/428 (94%)	401 (100%)	1 (0%)	94	97
2	B	105/129 (81%)	103 (98%)	2 (2%)	62	82
All	All	507/557 (91%)	504 (99%)	3 (1%)	89	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	138	ILE
2	B	598	CYS
2	B	625	ASN

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

Mol	Chain	Res	Type
2	B	575	GLN

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 ⓘ

25 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	B	701	2	14,14,15	0.19	0	15,19,21	0.50	0
3	NAG	B	702	2	14,14,15	0.23	0	15,19,21	0.39	0
3	NAG	B	703	2	14,14,15	0.28	0	15,19,21	0.41	0
3	NAG	G	601	1	14,14,15	0.19	0	15,19,21	0.50	0
3	NAG	G	602	1,3	14,14,15	0.23	0	15,19,21	0.62	0
3	NAG	G	603	3,4	14,14,15	0.30	0	15,19,21	0.47	0
4	BMA	G	604	3,5	11,11,12	0.67	0	13,15,17	0.83	0
5	MAN	G	605	4	11,11,12	0.60	0	13,15,17	1.21	2 (15%)
5	MAN	G	606	5,4	11,11,12	0.72	0	13,15,17	1.05	1 (7%)
5	MAN	G	607	5	11,11,12	0.73	0	13,15,17	1.35	2 (15%)
3	NAG	G	608	1	14,14,15	0.46	0	15,19,21	1.30	1 (6%)
3	NAG	G	609	1	14,14,15	0.26	0	15,19,21	0.42	0
3	NAG	G	610	1	14,14,15	0.37	0	15,19,21	0.63	0
3	NAG	G	611	1	14,14,15	0.20	0	15,19,21	0.47	0
3	NAG	G	612	1	14,14,15	0.23	0	15,19,21	0.62	0
3	NAG	G	613	1	14,14,15	0.33	0	15,19,21	0.49	0
3	NAG	G	614	1	14,14,15	0.22	0	15,19,21	0.52	0
3	NAG	G	615	1	14,14,15	0.20	0	15,19,21	0.46	0
3	NAG	G	616	1	14,14,15	0.24	0	15,19,21	0.46	0
3	NAG	G	617	1,3	14,14,15	0.19	0	15,19,21	0.51	0
3	NAG	G	618	3	14,14,15	0.22	0	15,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	619	1	14,14,15	0.21	0	15,19,21	0.46	0
3	NAG	G	620	1	14,14,15	0.29	0	15,19,21	0.87	1 (6%)
3	NAG	G	621	1,3	14,14,15	0.28	0	15,19,21	0.46	0
3	NAG	G	622	3	14,14,15	0.31	0	15,19,21	0.59	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
3	NAG	B	701	2	-	0/6/23/26	0/1/1/1
3	NAG	B	702	2	-	0/6/23/26	0/1/1/1
3	NAG	B	703	2	-	0/6/23/26	0/1/1/1
3	NAG	G	601	1	-	0/6/23/26	0/1/1/1
3	NAG	G	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	603	3,4	-	0/6/23/26	0/1/1/1
4	BMA	G	604	3,5	-	0/2/19/22	0/1/1/1
5	MAN	G	605	4	-	0/2/19/22	0/1/1/1
5	MAN	G	606	5,4	-	0/2/19/22	0/1/1/1
5	MAN	G	607	5	-	0/2/19/22	1/1/1/1
3	NAG	G	608	1	-	0/6/23/26	0/1/1/1
3	NAG	G	609	1	-	0/6/23/26	0/1/1/1
3	NAG	G	610	1	-	0/6/23/26	0/1/1/1
3	NAG	G	611	1	-	0/6/23/26	0/1/1/1
3	NAG	G	612	1	-	0/6/23/26	0/1/1/1
3	NAG	G	613	1	-	0/6/23/26	0/1/1/1
3	NAG	G	614	1	-	0/6/23/26	0/1/1/1
3	NAG	G	615	1	-	0/6/23/26	0/1/1/1
3	NAG	G	616	1	-	0/6/23/26	0/1/1/1
3	NAG	G	617	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	618	3	-	0/6/23/26	0/1/1/1
3	NAG	G	619	1	-	0/6/23/26	0/1/1/1
3	NAG	G	620	1	-	0/6/23/26	0/1/1/1
3	NAG	G	621	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	622	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	606	MAN	O2-C2-C3	-2.62	105.02	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	607	MAN	O2-C2-C3	-2.31	105.64	110.17
5	G	605	MAN	O2-C2-C3	-2.23	105.79	110.17
5	G	605	MAN	C1-O5-C5	2.68	115.85	112.17
3	G	620	NAG	C1-O5-C5	2.71	115.90	112.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	607	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	602	NAG	2	0
3	G	603	NAG	3	0
3	G	608	NAG	1	0
3	G	610	NAG	0	1
3	G	617	NAG	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 [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, 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	G	450/481 (93%)	0.68	46 (10%) 7 6	40, 84, 145, 192	0
2	B	123/153 (80%)	0.61	9 (7%) 16 15	42, 103, 144, 179	0
All	All	573/634 (90%)	0.66	55 (9%) 9 8	40, 89, 146, 192	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	619	LEU	6.2
1	G	411	ASN	5.9
1	G	231	LYS	5.4
1	G	136	ASN	5.3
1	G	72	HIS	5.1

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(\AA^2)	Q<0.9
3	NAG	G	620	14/15	0.59	0.58	3.31	112,127,141,154	0
3	NAG	B	701	14/15	0.64	0.47	2.44	144,157,164,167	0
3	NAG	G	601	14/15	0.63	0.58	1.86	85,105,115,117	0
3	NAG	G	610	14/15	0.68	0.63	1.24	139,150,159,160	0
3	NAG	G	617	14/15	0.73	0.27	0.24	104,126,135,137	0
3	NAG	G	616	14/15	0.75	0.38	0.10	102,126,135,147	0
3	NAG	G	621	14/15	0.82	0.30	-0.32	92,103,113,120	0
5	MAN	G	607	11/12	0.71	0.28	-0.62	97,119,129,134	0
3	NAG	G	619	14/15	0.90	0.23	-0.89	83,102,113,117	0
3	NAG	G	602	14/15	0.91	0.19	-2.01	36,60,81,81	0
3	NAG	B	702	14/15	0.49	0.42	-	121,152,162,169	0
3	NAG	G	609	14/15	0.81	0.21	-	64,118,130,145	0
3	NAG	G	608	14/15	0.85	0.38	-	101,119,127,138	0
3	NAG	G	613	14/15	0.70	0.28	-	93,142,161,172	0
3	NAG	G	603	14/15	0.91	0.19	-	92,102,117,125	0
5	MAN	G	606	11/12	0.73	0.34	-	127,157,166,167	0
3	NAG	G	618	14/15	0.72	0.35	-	116,141,169,181	0
3	NAG	G	612	14/15	0.78	0.31	-	109,134,167,177	0
3	NAG	G	622	14/15	0.84	0.52	-	122,141,152,159	0
3	NAG	G	615	14/15	0.82	0.44	-	111,122,129,131	0
5	MAN	G	605	11/12	0.69	0.33	-	86,135,151,161	0
3	NAG	G	614	14/15	0.74	0.30	-	79,96,111,111	0
3	NAG	B	703	14/15	0.68	0.39	-	121,131,147,153	0
3	NAG	G	611	14/15	0.79	0.24	-	82,110,127,127	0
4	BMA	G	604	11/12	0.76	0.23	-	117,131,147,151	0

6.5 Other polymers [i](#)

There are no such residues in this entry.