



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2025 – 12:31 PM EDT

PDB ID : 9CF7 / pdb\_00009cf7  
Title : Germline-targeting HIV-1 gp120 engineered outer domain eODgt8 in complex with Fab eOD-PL01.1  
Authors : Sarkar, A.; Stanfield, R.L.; Wilson, I.A.  
Deposited on : 2024-06-27  
Resolution : 3.55 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

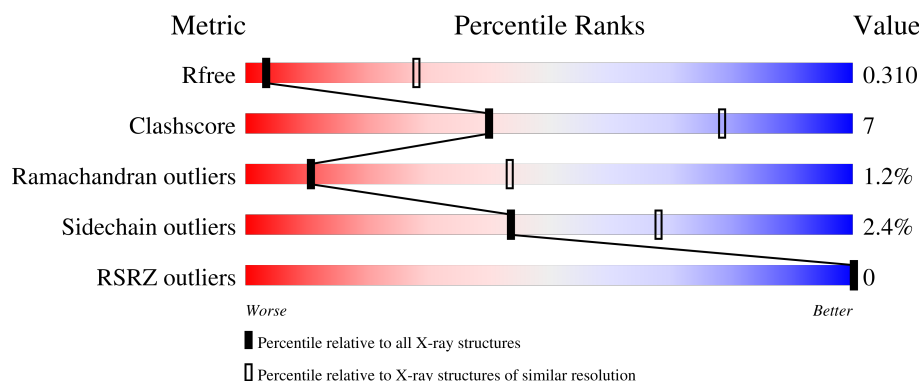
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.55 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))
$R_{free}$	164625	1261 (3.62-3.50)
Clashscore	180529	1351 (3.62-3.50)
Ramachandran outliers	177936	1336 (3.62-3.50)
Sidechain outliers	177891	1337 (3.62-3.50)
RSRZ outliers	164620	1260 (3.62-3.50)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	C	183	
2	H	222	
3	L	214	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4505 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 Germline-targeting HIV-1 gp120 engineered outer domain eODgt8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	167	Total	C	N	O	S	0	0	0
			1274	802	224	240	8			

- Molecule 2 is a protein called Fab eOD-PL01.1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1589	1005	265	315	4			

- Molecule 3 is a protein called Fab eOD-PL01.1 kappa light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1614	1002	276	331	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

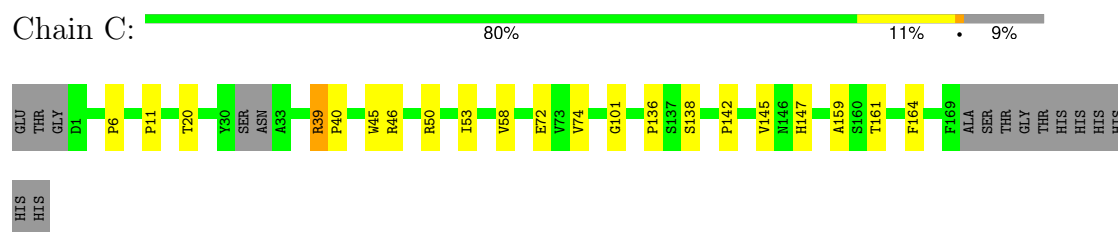


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

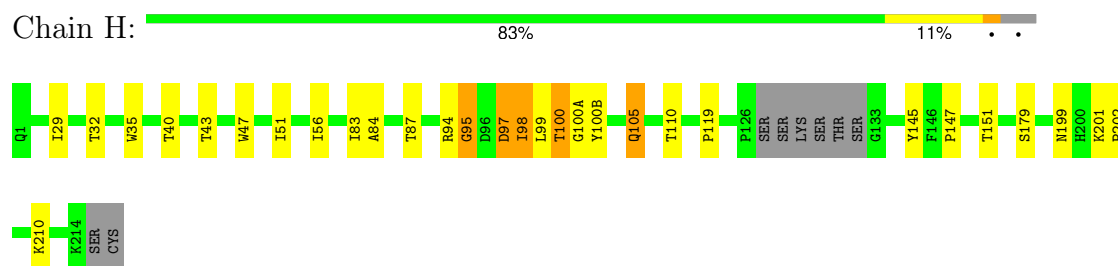
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

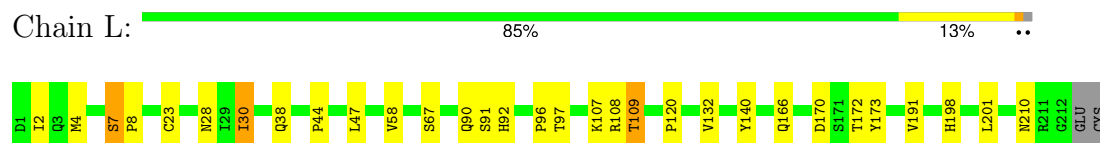
- Molecule 1: Germline-targeting HIV-1 gp120 engineered outer domain eODgt8



- Molecule 2: Fab eOD-PL01.1 heavy chain



- Molecule 3: Fab eOD-PL01.1 kappa light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.77Å 166.77Å 100.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.55 – 3.55 38.55 – 3.55	Depositor EDS
% Data completeness (in resolution range)	94.2 (38.55-3.55) 94.2 (38.55-3.55)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.265 , 0.299 0.269 , 0.310	Depositor DCC
$R_{free}$ test set	472 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	120.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 123.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: 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	C	0.47	0/1303	0.91	0/1769
2	H	0.48	0/1628	0.86	0/2227
3	L	0.48	0/1646	0.86	0/2235
All	All	0.48	0/4577	0.87	0/6231

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	C	1274	0	1234	12	0
2	H	1589	0	1564	25	0
3	L	1614	0	1578	24	0
4	C	28	0	26	0	0
All	All	4505	0	4402	57	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 7.

All (57) 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:L:108:ARG:NH2	3:L:172:THR:HG22	1.56	1.20
3:L:108:ARG:NH2	3:L:172:THR:CG2	2.36	0.87
3:L:108:ARG:HH22	3:L:172:THR:HG22	1.38	0.85
2:H:97:ASP:C	2:H:99:LEU:H	1.97	0.72
2:H:100:THR:HA	3:L:91:SER:OG	1.95	0.66
2:H:29:ILE:HA	2:H:35:TRP:CZ2	2.31	0.64
2:H:151:THR:HB	2:H:199:ASN:HB2	1.79	0.64
2:H:47:TRP:CD2	3:L:96:PRO:HD2	2.35	0.61
2:H:97:ASP:C	2:H:99:LEU:N	2.60	0.60
3:L:108:ARG:HH21	3:L:172:THR:HG22	1.56	0.59
2:H:100:THR:HG23	2:H:100(A):GLY:N	2.20	0.57
3:L:108:ARG:HG2	3:L:109:THR:H	1.71	0.56
2:H:97:ASP:O	2:H:99:LEU:N	2.40	0.54
3:L:107:LYS:HG3	3:L:140:TYR:OH	2.06	0.54
2:H:100:THR:HG23	2:H:100(A):GLY:H	1.73	0.54
1:C:46:ARG:CZ	2:H:98:ILE:HD11	2.38	0.54
3:L:108:ARG:NE	3:L:170:ASP:O	2.41	0.53
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.90	0.52
3:L:108:ARG:HG2	3:L:109:THR:N	2.24	0.52
1:C:11:PRO:O	1:C:101:GLY:HA2	2.10	0.51
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.92	0.51
3:L:47:LEU:HA	3:L:58:VAL:HG21	1.93	0.51
1:C:136:PRO:HB3	1:C:161:THR:HG22	1.94	0.50
3:L:4:MET:HE3	3:L:23:CYS:SG	2.52	0.49
2:H:83:ILE:HG22	2:H:84:ALA:N	2.29	0.48
1:C:39:ARG:HD3	1:C:138:SER:HB2	1.96	0.47
2:H:201:LYS:N	2:H:202:PRO:CD	2.77	0.47
2:H:95:GLY:HA2	2:H:100(B):TYR:HA	1.96	0.47
2:H:87:THR:HG23	2:H:110:THR:HA	1.97	0.47
3:L:198:HIS:HB3	3:L:201:LEU:HG	1.97	0.46
1:C:39:ARG:HH11	1:C:39:ARG:HB3	1.81	0.45
1:C:45:TRP:CZ3	1:C:58:VAL:HG12	2.51	0.45
2:H:40:THR:HB	2:H:43:THR:HB	1.98	0.45
2:H:35:TRP:CZ3	2:H:94:ARG:HD3	2.53	0.44
3:L:28:ASN:OD1	3:L:30:ILE:HD13	2.18	0.44
3:L:2:ILE:HD12	3:L:2:ILE:N	2.33	0.44
1:C:50:ARG:HH21	3:L:30:ILE:HG12	1.82	0.43
2:H:147:PRO:HD2	2:H:202:PRO:HB3	1.99	0.43
1:C:142:PRO:HA	1:C:145:VAL:HG12	2.00	0.43
2:H:94:ARG:NH1	2:H:95:GLY:O	2.51	0.43
3:L:90:GLN:HA	3:L:90:GLN:OE1	2.19	0.43
1:C:20:THR:O	1:C:20:THR:OG1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:108:ARG:CG	3:L:109:THR:H	2.32	0.42
2:H:105:GLN:NE2	2:H:105:GLN:H	2.18	0.42
2:H:201:LYS:N	2:H:202:PRO:HD2	2.34	0.42
1:C:40:PRO:HG3	1:C:164:PHE:CD2	2.55	0.42
2:H:100:THR:CG2	2:H:100(A):GLY:H	2.33	0.41
2:H:100:THR:CG2	2:H:100(A):GLY:N	2.83	0.41
1:C:46:ARG:O	1:C:50:ARG:HG3	2.21	0.41
3:L:108:ARG:CD	3:L:170:ASP:O	2.69	0.41
3:L:191:VAL:HG22	3:L:210:ASN:OD1	2.21	0.41
2:H:51:ILE:HG13	2:H:56:ILE:O	2.21	0.41
3:L:7:SER:HA	3:L:8:PRO:HA	1.91	0.41
3:L:38:GLN:NE2	3:L:44:PRO:HD3	2.35	0.41
3:L:166:GLN:CG	3:L:173:TYR:CZ	3.04	0.41
1:C:6:PRO:HG2	1:C:159:ALA:HB3	2.03	0.40
2:H:99:LEU:O	2:H:100(A):GLY:N	2.54	0.40

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	C	163/183 (89%)	147 (90%)	14 (9%)	2 (1%)	11	43
2	H	210/222 (95%)	188 (90%)	19 (9%)	3 (1%)	9	40
3	L	210/214 (98%)	196 (93%)	12 (6%)	2 (1%)	13	47
All	All	583/619 (94%)	531 (91%)	45 (8%)	7 (1%)	11	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	98	ILE
2	H	100	THR

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Mol	Chain	Res	Type
1	C	147	HIS
3	L	30	ILE
3	L	67	SER
1	C	53	ILE
2	H	95	GLY

### 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	C	137/150 (91%)	134 (98%)	3 (2%)	47	70
2	H	181/189 (96%)	176 (97%)	5 (3%)	38	64
3	L	187/189 (99%)	183 (98%)	4 (2%)	48	71
All	All	505/528 (96%)	493 (98%)	12 (2%)	44	68

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	39	ARG
1	C	72	GLU
1	C	74	VAL
2	H	32	THR
2	H	97	ASP
2	H	105	GLN
2	H	179	SER
2	H	210	LYS
3	L	7	SER
3	L	92	HIS
3	L	97	THR
3	L	109	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	114	ASN
2	H	3	GLN
2	H	39	GLN
2	H	53	HIS
2	H	58	ASN
2	H	105	GLN
3	L	37	GLN
3	L	38	GLN
3	L	49	ASN
3	L	79	GLN
3	L	138	ASN
3	L	160	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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 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	$\# Z  > 2$
4	NAG	C	201	1	14,14,15	0.42	0	17,19,21	1.22	2 (11%)
4	NAG	C	202	1	14,14,15	0.51	0	17,19,21	1.36	3 (17%)

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	NAG	C	201	1	-	3/6/23/26	0/1/1/1
4	NAG	C	202	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	201	NAG	C2-N2-C7	3.74	127.91	122.90
4	C	202	NAG	C1-O5-C5	3.58	116.98	112.19
4	C	201	NAG	C1-C2-N2	2.84	114.90	110.43
4	C	202	NAG	O5-C1-C2	2.75	115.54	111.29
4	C	202	NAG	C1-C2-N2	2.46	114.30	110.43

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	201	NAG	O5-C5-C6-O6
4	C	202	NAG	C8-C7-N2-C2
4	C	202	NAG	O7-C7-N2-C2
4	C	201	NAG	C4-C5-C6-O6
4	C	202	NAG	O5-C5-C6-O6
4	C	201	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	C	167/183 (91%)	-0.80	0 100 100	98, 141, 190, 248	0
2	H	214/222 (96%)	-0.71	0 100 100	120, 170, 209, 224	0
3	L	212/214 (99%)	-0.88	0 100 100	116, 158, 226, 238	0
All	All	593/619 (95%)	-0.80	0 100 100	98, 158, 215, 248	0

There are no RSRZ outliers to report.

### 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 oligosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	C	201	14/15	0.67	0.08	156,166,169,169	0
4	NAG	C	202	14/15	0.77	0.07	193,202,207,209	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.