



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:39 PM GMT

PDB ID : 3UJI
Title : Crystal structure of anti-HIV-1 V3 Fab 2558 in complex with MN peptide
Authors : Kong, X.P.
Deposited on : 2011-11-07
Resolution : 1.60 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
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4113 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 Light chain of anti-HIV-1 V3 monoclonal antibody 2558.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	208	Total	C	N	O	S	0	0	0
			1554	977	252	320	5			

- Molecule 2 is a protein called Fab region of the heavy chain of anti-HIV-1 V3 monoclonal antibody 2558.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1650	1055	264	324	7			

- Molecule 3 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	18	Total	C	N	O	0	0	0
			154	99	32	23			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	Ca	0	0
			1	1		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	3	Total	C	N	O	0	0
			38	22	2	14		

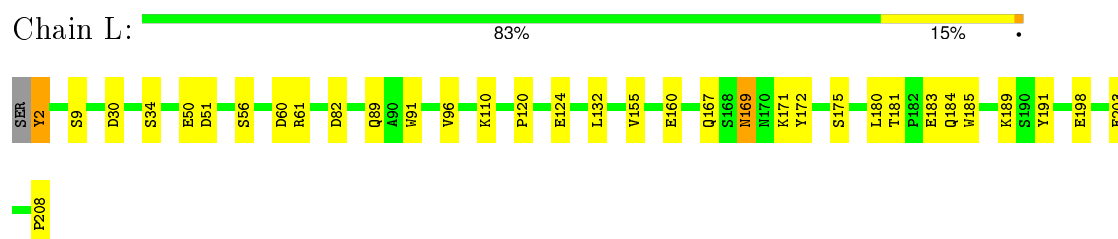
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	372	Total 372	O 372	0	0
6	H	324	Total 324	O 324	0	0
6	P	20	Total 20	O 20	0	0

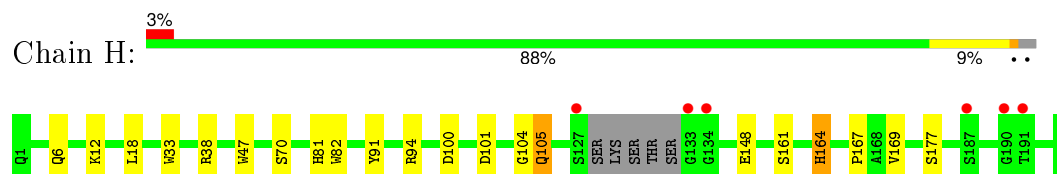
3 Residue-property plots [i](#)

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.

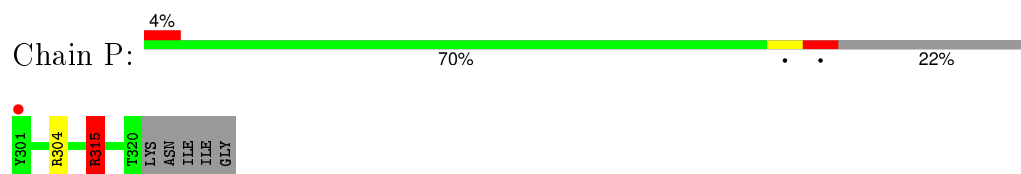
- Molecule 1: Light chain of anti-HIV-1 V3 monoclonal antibody 2558



- Molecule 2: Fab region of the heavy chain of anti-HIV-1 V3 monoclonal antibody 2558



- Molecule 3: Envelope glycoprotein gp160



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.35Å 73.10Å 88.66Å 90.00° 121.98° 90.00°	Depositor
Resolution (Å)	50.00 – 1.60 17.76 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-1.60) 99.1 (17.76-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.161 , 0.194 0.161 , 0.193	Depositor DCC
R_{free} test set	3660 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 72546 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4113	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, 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	L	1.47	7/1592 (0.4%)	1.47	13/2175 (0.6%)
2	H	1.35	5/1696 (0.3%)	1.28	6/2310 (0.3%)
3	P	1.30	0/158	1.45	2/210 (1.0%)
All	All	1.41	12/3446 (0.3%)	1.38	21/4695 (0.4%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	61	ARG	CZ-NH1	7.31	1.42	1.33
2	H	82	TRP	CD2-CE2	6.50	1.49	1.41
2	H	164	HIS	CA-CB	-6.34	1.40	1.53
1	L	50	GLU	CD-OE1	6.07	1.32	1.25
1	L	34	SER	CA-CB	5.95	1.61	1.52
2	H	33	TRP	CD2-CE2	5.83	1.48	1.41
1	L	175	SER	CB-OG	-5.25	1.35	1.42
2	H	148	GLU	CD-OE1	5.22	1.31	1.25
1	L	191	TYR	CG-CD1	5.20	1.46	1.39
1	L	9	SER	CB-OG	-5.08	1.35	1.42
2	H	177	SER	CB-OG	5.05	1.48	1.42
1	L	91	TRP	CD2-CE2	5.03	1.47	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	82	ASP	CB-CG-OD2	-8.99	110.21	118.30
1	L	61	ARG	NE-CZ-NH2	8.95	124.78	120.30
1	L	51	ASP	CB-CG-OD1	7.55	125.09	118.30
1	L	61	ARG	NE-CZ-NH1	-7.06	116.77	120.30
2	H	101	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	L	180	LEU	CB-CG-CD1	-6.30	100.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	94	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	L	124	GLU	OE1-CD-OE2	6.14	130.67	123.30
1	L	60	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	L	198	GLU	OE1-CD-OE2	5.97	130.46	123.30
2	H	38	ARG	NE-CZ-NH2	5.79	123.19	120.30
2	H	101	ASP	CB-CG-OD1	5.66	123.39	118.30
1	L	82	ASP	OD1-CG-OD2	5.61	133.95	123.30
1	L	110	LYS	CD-CE-NZ	-5.59	98.84	111.70
1	L	60	ASP	N-CA-C	5.48	125.81	111.00
3	P	304	ARG	NE-CZ-NH2	5.42	123.01	120.30
2	H	100	ASP	CB-CG-OD2	-5.36	113.48	118.30
3	P	315	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	L	172	TYR	CB-CG-CD2	-5.30	117.82	121.00
2	H	12	LYS	CD-CE-NZ	-5.15	99.85	111.70
1	L	30	ASP	CB-CG-OD1	5.14	122.92	118.30

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	L	1554	0	1509	16	0
2	H	1650	0	1585	13	0
3	P	154	0	158	4	0
4	L	1	0	0	0	0
5	H	38	0	34	2	0
6	H	324	0	0	3	1
6	L	372	0	0	2	3
6	P	20	0	0	0	1
All	All	4113	0	3286	31	4

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 5.

All (31) 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:P:315:ARG:HH11	3:P:315:ARG:HG3	1.08	1.16
2:H:6:GLN:H	2:H:105:GLN:HE22	1.10	0.98
1:L:181:THR:H	1:L:184:GLN:HE21	1.06	0.97
2:H:105:GLN:HE21	2:H:105:GLN:H	1.15	0.91
3:P:315:ARG:NH1	3:P:315:ARG:HG3	1.86	0.81
3:P:315:ARG:CG	3:P:315:ARG:HH11	1.91	0.81
2:H:70:SER:OG	2:H:81:HIS:HE1	1.79	0.66
2:H:6:GLN:HE21	2:H:104:GLY:HA3	1.63	0.64
2:H:6:GLN:H	2:H:105:GLN:NE2	1.91	0.64
1:L:167:GLN:HE21	1:L:169:ASN:HD21	1.46	0.63
1:L:203:GLU:OE1	6:L:308:HOH:O	2.16	0.61
1:L:2:TYR:N	5:H:402:NAG:HO6	2.00	0.60
1:L:2:TYR:N	5:H:401:NAG:HO3	1.98	0.60
1:L:181:THR:H	1:L:184:GLN:NE2	1.90	0.58
2:H:164:HIS:ND1	6:H:570:HOH:O	2.33	0.55
1:L:181:THR:N	1:L:184:GLN:HE21	1.90	0.52
2:H:164:HIS:CD2	6:H:488:HOH:O	2.63	0.50
1:L:167:GLN:HE21	1:L:169:ASN:ND2	2.10	0.49
1:L:181:THR:OG1	1:L:184:GLN:HG3	2.13	0.49
2:H:105:GLN:N	2:H:105:GLN:HE21	1.97	0.48
1:L:120:PRO:HD3	1:L:132:LEU:CD2	2.44	0.47
2:H:105:GLN:NE2	2:H:105:GLN:H	1.98	0.47
1:L:169:ASN:C	1:L:169:ASN:HD22	2.17	0.47
2:H:18:LEU:HD12	6:H:409:HOH:O	2.16	0.45
3:P:315:ARG:CG	3:P:315:ARG:NH1	2.60	0.45
1:L:185:TRP:CZ2	1:L:208:PRO:HA	2.52	0.45
2:H:6:GLN:HE22	2:H:91:TYR:HA	1.82	0.43
1:L:169:ASN:ND2	1:L:171:LYS:H	2.17	0.42
1:L:184:GLN:NE2	6:L:345:HOH:O	2.39	0.41
1:L:96:VAL:HB	2:H:47:TRP:CG	2.56	0.41
1:L:160:GLU:HB3	2:H:169:VAL:HG21	2.02	0.41

All (4) 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)
6:L:296:HOH:O	6:L:405:HOH:O[3_545]	1.75	0.45
6:L:350:HOH:O	6:L:373:HOH:O[3_545]	1.94	0.26
6:H:409:HOH:O	6:P:255:HOH:O[4_445]	1.95	0.25
6:L:313:HOH:O	6:L:336:HOH:O[4_556]	2.08	0.12

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	L	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
2	H	214/223 (96%)	210 (98%)	4 (2%)	0	100	100
3	P	16/23 (70%)	16 (100%)	0	0	100	100
All	All	436/455 (96%)	428 (98%)	8 (2%)	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	L	176/177 (99%)	169 (96%)	7 (4%)	38	12
2	H	183/188 (97%)	180 (98%)	3 (2%)	70	47
3	P	15/19 (79%)	14 (93%)	1 (7%)	20	4
All	All	374/384 (97%)	363 (97%)	11 (3%)	50	21

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	TYR
1	L	56	SER
1	L	89	GLN
1	L	155	VAL
1	L	169	ASN

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Mol	Chain	Res	Type
1	L	183	GLU
1	L	189	LYS
2	H	105	GLN
2	H	161	SER
2	H	167	PRO
3	P	315	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	42	GLN
1	L	79	GLN
1	L	89	GLN
1	L	108	GLN
1	L	169	ASN
1	L	170	ASN
1	L	184	GLN
2	H	1	GLN
2	H	6	GLN
2	H	66	GLN
2	H	81	HIS
2	H	105	GLN
2	H	164	HIS

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](#)

3 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
5	NAG	H	401	2,5	14,14,15	1.03	1 (7%)	15,19,21	1.55	2 (13%)
5	NAG	H	402	5	14,14,15	1.62	2 (14%)	15,19,21	2.05	5 (33%)
5	FUC	H	403	5	10,10,11	0.97	0	14,14,16	1.94	6 (42%)

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
5	NAG	H	401	2,5	-	0/6/23/26	0/1/1/1
5	NAG	H	402	5	-	0/6/23/26	0/1/1/1
5	FUC	H	403	5	-	0/0/17/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	401	NAG	O7-C7	2.23	1.28	1.23
5	H	402	NAG	C2-N2	3.36	1.52	1.46
5	H	402	NAG	C8-C7	4.53	1.59	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	403	FUC	C1-C2-C3	-4.31	104.45	109.54
5	H	402	NAG	C2-N2-C7	-3.53	118.51	123.04
5	H	401	NAG	C3-C4-C5	-3.37	104.32	110.20
5	H	402	NAG	C3-C4-C5	-3.28	104.48	110.20
5	H	402	NAG	O5-C5-C6	-3.16	100.51	107.35
5	H	402	NAG	O7-C7-C8	-2.40	117.65	122.06
5	H	403	FUC	O4-C4-C3	-2.23	105.32	110.34
5	H	403	FUC	C3-C4-C5	-2.06	106.25	109.72
5	H	403	FUC	O2-C2-C3	2.15	114.45	110.12
5	H	403	FUC	C2-C3-C4	2.41	115.14	111.04
5	H	403	FUC	C1-O5-C5	2.68	116.52	112.38
5	H	401	NAG	C4-C3-C2	2.98	115.86	111.23
5	H	402	NAG	O7-C7-N2	3.86	129.73	121.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	401	NAG	1	0
5	H	402	NAG	1	0

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 [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	L	208/209 (99%)	-0.53	0	100 100	9, 15, 31, 53	0
2	H	218/223 (97%)	-0.40	6 (2%)	56 54	11, 17, 38, 71	0
3	P	18/23 (78%)	0.02	1 (5%)	28 25	12, 18, 42, 57	0
All	All	444/455 (97%)	-0.45	7 (1%)	74 74	9, 17, 34, 71	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	133	GLY	8.4
3	P	301	TYR	5.8
2	H	190	GLY	3.7
2	H	134	GLY	3.5
2	H	127	SER	3.3
2	H	191	THR	2.8
2	H	187	SER	2.7

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](#)

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
5	FUC	H	403	10/11	0.96	0.06	-1.07	19,21,24,25	0
5	NAG	H	401	14/15	0.97	0.04	-1.48	15,16,17,18	0
5	NAG	H	402	14/15	0.94	0.11	-	17,20,26,27	0

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
4	CA	L	209	1/1	1.00	0.02	-	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.