



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:51 PM GMT

PDB ID : 4JO1
Title : Crystal structure of rabbit mAb R56 Fab in complex with V3 crown of HIV-1 JR-FL gp120
Authors : Pan, R.M.; Kong, X.P.
Deposited on : 2013-03-16
Resolution : 2.03 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

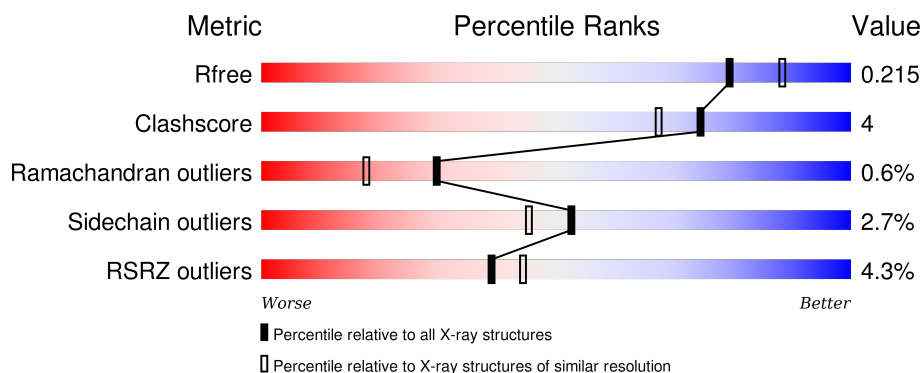
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	L	216	<div> <div></div> <div>93% 6% .</div> </div>
1	M	216	<div> <div></div> <div>91% 8% .</div> </div>
2	H	213	<div> <div>9%</div> <div>89% 10%</div> </div>
2	I	213	<div> <div>8%</div> <div>90% 9%</div> </div>
3	P	23	<div> <div></div> <div>43% 57%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	23	 A horizontal bar chart showing the quality of chain Q. The bar is divided into two segments: a green segment on the left representing 43% and a grey segment on the right representing 57%. The percentages are written below the corresponding segments.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7252 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 monoclonal anti-HIV-1 gp120 V3 antibody R56 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1596	988	265	334	9			
1	M	216	Total	C	N	O	S	0	0	0
			1596	988	265	334	9			

- Molecule 2 is a protein called monoclonal anti-HIV-1 gp120 V3 antibody R56 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	0	0
			1551	970	257	313	11			
2	I	213	Total	C	N	O	S	0	0	0
			1551	970	257	313	11			

- Molecule 3 is a protein called gp120.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	0	0	0
			74	46	16	12			
3	Q	10	Total	C	N	O	0	0	0
			74	46	16	12			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Ca	0	0
			1	1		
4	I	1	Total	Ca	0	0
			1	1		
4	L	2	Total	Ca	0	0
			2	2		
4	M	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	198	Total 198	O 198	0	0
5	H	195	Total 195	O 195	0	0
5	P	6	Total 6	O 6	0	0
5	M	197	Total 197	O 197	0	0
5	I	199	Total 199	O 199	0	0
5	Q	10	Total 10	O 10	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.

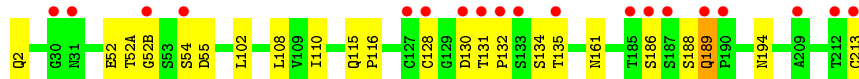
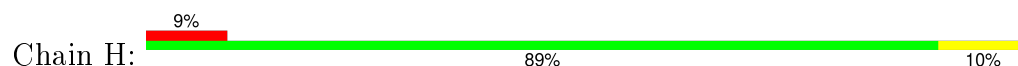
- Molecule 1: monoclonal anti-HIV-1 gp120 V3 antibody R56 light chain



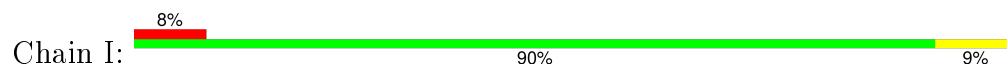
- Molecule 1: monoclonal anti-HIV-1 gp120 V3 antibody R56 light chain



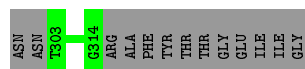
- Molecule 2: monoclonal anti-HIV-1 gp120 V3 antibody R56 heavy chain



- Molecule 2: monoclonal anti-HIV-1 gp120 V3 antibody R56 heavy chain



- Molecule 3: gp120



- Molecule 3: gp120



ASN	ASN	G314	ARG
ASN	ASN	G314	ALA
ASN	ASN	G314	PHE
ASN	ASN	G314	TYR
ASN	ASN	G314	THR
ASN	ASN	G314	GLY
ASN	ASN	G314	GLU
ASN	ASN	G314	ILE
ASN	ASN	G314	GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.51Å 74.35Å 84.44Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	36.23 – 2.03 43.76 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.5 (36.23-2.03) 99.5 (43.76-2.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.03Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.181 , 0.223 0.172 , 0.215	Depositor DCC
R_{free} test set	2834 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.4	EDS
Estimated twinning fraction	0.136 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 56041 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7252	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% 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

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	0.41	0/1628	0.81	3/2229 (0.1%)
1	M	0.41	0/1628	0.64	3/2229 (0.1%)
2	H	0.42	0/1587	0.58	0/2174
2	I	0.41	0/1587	0.59	0/2174
3	P	0.38	0/75	0.50	0/99
3	Q	0.31	0/75	0.53	0/99
All	All	0.41	0/6580	0.66	6/9004 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	107	ARG	NE-CZ-NH1	-18.76	110.92	120.30
1	L	107	ARG	NE-CZ-NH2	17.54	129.07	120.30
1	M	107	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	L	107	ARG	CD-NE-CZ	8.39	135.35	123.60
1	M	107	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	M	107	ARG	CD-NE-CZ	5.15	130.81	123.60

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	1596	0	1514	14	0
1	M	1596	0	1514	14	0
2	H	1551	0	1510	10	0
2	I	1551	0	1510	14	0
3	P	74	0	79	0	0
3	Q	74	0	79	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	L	2	0	0	0	0
4	M	1	0	0	0	0
5	H	195	0	0	5	0
5	I	199	0	0	7	0
5	L	198	0	0	5	1
5	M	197	0	0	4	1
5	P	6	0	0	0	0
5	Q	10	0	0	0	0
All	All	7252	0	6206	51	1

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 4.

All (51) 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)
2:H:52(A):THR:O	5:H:516:HOH:O	1.89	0.91
1:L:138:LYS:NZ	5:L:523:HOH:O	1.94	0.83
2:I:211:SER:HB3	2:I:212:THR:HA	1.60	0.82
1:M:137:ASN:OD1	5:M:553:HOH:O	1.98	0.80
2:I:52:GLU:OE1	2:I:54:SER:OG	2.03	0.77
1:M:63:LYS:NZ	5:M:522:HOH:O	2.16	0.77
2:I:130:ASP:OD2	5:I:498:HOH:O	2.05	0.74
2:I:2:GLN:OE1	2:I:2:GLN:N	2.23	0.72
2:H:161:ASN:OD1	5:H:513:HOH:O	2.07	0.71
2:H:2:GLN:N	2:H:2:GLN:OE1	2.24	0.70
2:I:31:ASN:ND2	5:I:439:HOH:O	2.25	0.68
1:L:63:LYS:NZ	5:L:541:HOH:O	2.27	0.68
2:I:128:CYS:O	5:I:583:HOH:O	2.11	0.67
1:L:137:ASN:OD1	5:L:532:HOH:O	2.12	0.67
2:H:186:SER:O	5:H:565:HOH:O	2.13	0.66
2:H:52:GLU:OE1	2:H:54:SER:OG	2.16	0.64
2:H:188:SER:HB3	5:H:503:HOH:O	1.97	0.62
2:H:52(B):GLY:HA2	5:H:516:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:53:SER:N	5:I:532:HOH:O	2.34	0.60
1:M:211:CYS:HA	2:I:128:CYS:HB3	1.84	0.60
2:I:211:SER:CB	2:I:212:THR:HA	2.32	0.59
1:M:2:GLN:NE2	1:M:95(C):ASP:H	2.05	0.55
1:L:2:GLN:N	1:L:2:GLN:NE2	2.56	0.54
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.89	0.54
1:L:2:GLN:NE2	1:L:95(C):ASP:H	2.06	0.54
1:M:2:GLN:NE2	1:M:2:GLN:N	2.56	0.53
1:M:37:GLN:HB2	1:M:47:LEU:HD11	1.91	0.52
1:L:2:GLN:NE2	5:L:552:HOH:O	2.43	0.52
1:M:60:SER:OG	5:M:537:HOH:O	2.20	0.50
2:I:32:ASN:HB3	5:I:533:HOH:O	2.12	0.49
1:L:2:GLN:N	1:L:2:GLN:CD	2.65	0.49
1:M:2:GLN:N	1:M:2:GLN:CD	2.65	0.49
1:M:167:SER:HB3	5:M:573:HOH:O	2.13	0.48
2:H:189:GLN:HE21	2:H:189:GLN:H	1.60	0.48
2:I:32:ASN:HB3	5:I:483:HOH:O	2.13	0.48
1:M:35:TRP:CE2	1:M:73:PHE:HB2	2.50	0.47
1:L:63:LYS:HE3	5:L:440:HOH:O	2.14	0.46
1:L:35:TRP:CE2	1:L:73:PHE:HB2	2.51	0.46
1:L:4:LEU:HD13	1:L:88:CYS:SG	2.57	0.45
2:I:146:LEU:HD13	2:I:174:GLY:O	2.17	0.45
1:M:63:LYS:HB3	1:M:63:LYS:HE3	1.80	0.44
2:I:108:LEU:HD21	2:I:110:ILE:HD11	2.00	0.43
1:M:81:ASP:OD2	1:M:167:SER:HB2	2.18	0.43
1:L:63:LYS:HB3	1:L:63:LYS:HE3	1.82	0.43
1:L:113:PRO:HB3	1:L:139:TYR:HB3	2.02	0.42
1:L:54:LEU:HD11	1:L:60:SER:HA	2.01	0.42
1:M:4:LEU:HD13	1:M:88:CYS:SG	2.60	0.41
1:M:113:PRO:HB3	1:M:139:TYR:HB3	2.02	0.41
2:H:108:LEU:HD21	2:H:110:ILE:HD11	2.02	0.41
2:I:172:SER:O	5:I:594:HOH:O	2.22	0.41
2:H:115:GLN:HA	2:H:116:PRO:HD3	1.96	0.40

All (1) 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)
5:L:524:HOH:O	5:M:534:HOH:O[2_556]	1.78	0.42

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%)	207 (97%)	7 (3%)	0	100	100
1	M	214/216 (99%)	207 (97%)	7 (3%)	0	100	100
2	H	211/213 (99%)	203 (96%)	5 (2%)	3 (1%)	14	4
2	I	211/213 (99%)	203 (96%)	6 (3%)	2 (1%)	21	10
3	P	8/23 (35%)	7 (88%)	1 (12%)	0	100	100
3	Q	8/23 (35%)	7 (88%)	1 (12%)	0	100	100
All	All	866/904 (96%)	834 (96%)	27 (3%)	5 (1%)	30	18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	132	PRO
2	I	211	SER
2	H	128	CYS
2	H	132	PRO
2	H	134	SER

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	183/183 (100%)	180 (98%)	3 (2%)	70	67
1	M	183/183 (100%)	179 (98%)	4 (2%)	60	53
2	H	178/178 (100%)	170 (96%)	8 (4%)	34	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	178/178 (100%)	173 (97%)	5 (3%)	51	44
3	P	8/18 (44%)	8 (100%)	0	100	100
3	Q	8/18 (44%)	8 (100%)	0	100	100
All	All	738/758 (97%)	718 (97%)	20 (3%)	52	45

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	GLN
1	L	4	LEU
1	L	54	LEU
2	H	55	ASP
2	H	102	LEU
2	H	130	ASP
2	H	131	THR
2	H	135	THR
2	H	189	GLN
2	H	194	ASN
2	H	213	CYS
1	M	2	GLN
1	M	4	LEU
1	M	54	LEU
1	M	130	VAL
2	I	55	ASP
2	I	102	LEU
2	I	135	THR
2	I	186	SER
2	I	189	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	137	ASN
2	H	2	GLN
2	H	189	GLN
1	M	137	ASN
2	I	2	GLN
2	I	31	ASN
2	I	189	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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are 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 ⓘ

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(Å ²)	Q<0.9
1	L	216/216 (100%)	-0.06	2 (0%) 85 89	16, 26, 45, 55	0
1	M	216/216 (100%)	-0.07	1 (0%) 91 93	15, 25, 46, 53	0
2	H	213/213 (100%)	0.25	19 (8%) 12 13	16, 27, 76, 121	0
2	I	213/213 (100%)	0.31	16 (7%) 17 20	15, 27, 69, 96	0
3	P	10/23 (43%)	0.10	0 100 100	19, 29, 53, 60	0
3	Q	10/23 (43%)	0.18	0 100 100	20, 29, 53, 60	0
All	All	878/904 (97%)	0.11	38 (4%) 39 44	15, 26, 53, 121	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	213	CYS	6.6
2	I	211	SER	6.2
2	I	212	THR	6.0
2	I	186	SER	6.0
2	H	30	GLY	5.6
2	H	131	THR	5.3
2	I	187	SER	5.2
2	H	132	PRO	5.0
2	I	213	CYS	4.9
2	H	128	CYS	4.7
2	H	130	ASP	4.3
2	I	130	ASP	4.3
2	I	54	SER	4.2
1	L	211	CYS	4.1
2	H	54	SER	4.1
2	I	134	SER	4.0
2	H	186	SER	4.0
2	I	135	THR	4.0
2	I	131	THR	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	185	THR	3.8
2	I	210	PRO	3.6
2	I	133	SER	3.2
2	H	189	GLN	3.1
2	I	53	SER	3.0
2	I	185	THR	2.9
2	H	133	SER	2.8
2	H	212	THR	2.8
1	L	126	ALA	2.7
2	H	187	SER	2.7
2	H	190	PRO	2.6
2	I	190	PRO	2.6
2	H	52(B)	GLY	2.5
2	H	31	ASN	2.5
2	H	127	CYS	2.4
2	H	135	THR	2.3
1	M	125	VAL	2.3
2	I	173	SER	2.2
2	H	209	ALA	2.2

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(Å ²)	Q<0.9
4	CA	L	301	1/1	1.00	0.10	0.07	21,21,21,21	0
4	CA	I	301	1/1	0.98	0.10	-0.75	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	M	301	1/1	1.00	0.08	-1.98	19,19,19,19	0
4	CA	H	301	1/1	0.99	0.09	-2.54	28,28,28,28	0
4	CA	L	302	1/1	0.99	0.07	-	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.