Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:31 AM GMT

PDB ID	:	3MA9
Title	:	Crystal structure of gp41 derived protein complexed with fab 8066
Authors	:	Li, M.; Gustchina, E.; Louis, J.; Gustchina, A.; Wlodawer, A.; Clore, M.
Deposited on	:	2010-03-23
Resolution	:	2.05 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

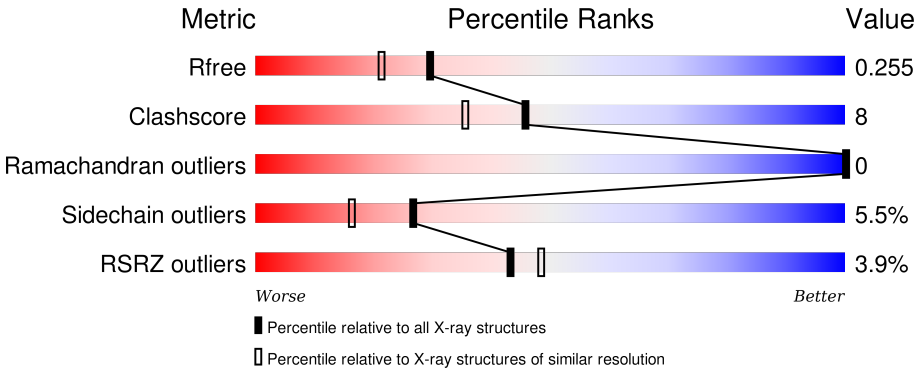
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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 <=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	217	3% 73% 16% • 9%
2	H	245	5% 76% 11% • 13%
3	L	213	2% 83% 14% ••

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5243 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 Transmembrane glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	2	0
			1637	1027	297	309	4			

- Molecule 2 is a protein called Fab8066 FAB ANTIBODY FRAGMENT, Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	1	0
			1599	1014	262	317	6			

- Molecule 3 is a protein called Fab8066 FAB ANTIBODY FRAGMENT, Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	209	Total	C	N	O	S	0	0	0
			1563	978	258	322	5			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Na	0	0
			1	1		
4	L	1	Total	Na	0	0
			1	1		

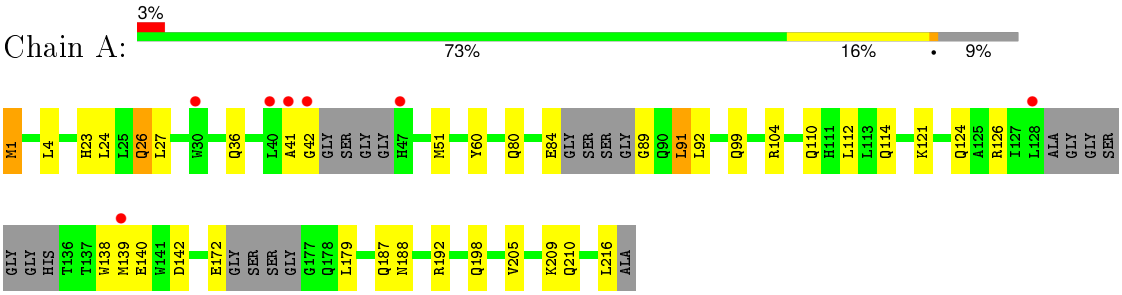
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	109	Total	O	0	0
			109	109		
5	H	177	Total	O	0	0
			177	177		
5	L	156	Total	O	0	0
			156	156		

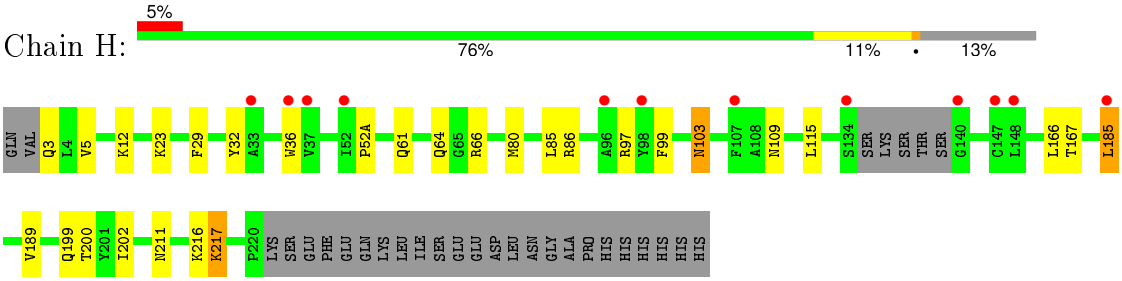
3 Residue-property plots (i)

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.

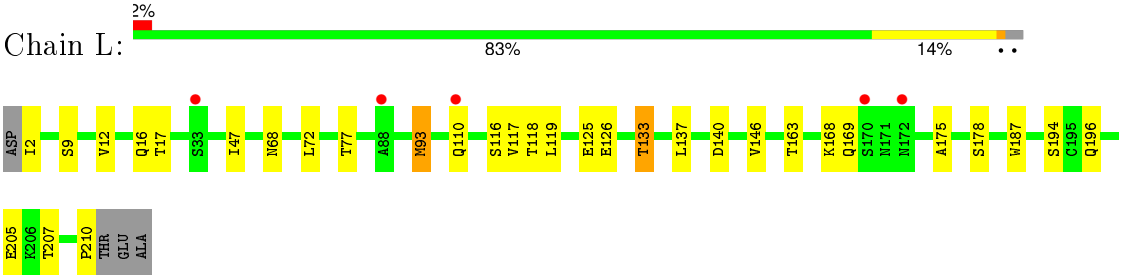
- Molecule 1: Transmembrane glycoprotein



- Molecule 2: Fab8066 FAB ANTIBODY FRAGMENT, Heavy Chain



- Molecule 3: Fab8066 FAB ANTIBODY FRAGMENT, Light Chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	41.53Å 124.70Å 133.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.45 – 2.05 29.45 – 2.04	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.45-2.05) 98.6 (29.45-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.5.0104	Depositor
R, R_{free}	0.193 , 0.245 0.199 , 0.255	Depositor DCC
R_{free} test set	1405 reflections (3.28%)	DCC
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 44446 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5243	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA

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	0.49	0/1658	0.55	0/2238
2	H	0.53	0/1642	0.63	1/2238 (0.0%)
3	L	0.47	0/1603	0.59	0/2195
All	All	0.50	0/4903	0.59	1/6671 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	185	LEU	CA-CB-CG	6.81	130.96	115.30

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	A	1637	0	1649	26	1
2	H	1599	0	1548	26	0
3	L	1563	0	1496	24	0
4	H	1	0	0	0	0
4	L	1	0	0	0	0
5	A	109	0	0	7	0
5	H	177	0	0	11	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	156	0	0	9	1
All	All	5243	0	4693	73	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 8.

All (73) 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:172:GLU:OE2	5:A:386:HOH:O	1.82	0.96
1:A:99:GLN:HE21	1:A:187:GLN:HE21	1.12	0.94
3:L:196:GLN:HG2	3:L:205:GLU:HG2	1.48	0.94
2:H:103:ASN:HD22	2:H:103:ASN:H	1.17	0.90
2:H:97:ARG:HH21	2:H:109:ASN:HD21	1.24	0.84
2:H:97:ARG:HE	2:H:109:ASN:HD22	1.28	0.82
3:L:163:THR:HG22	3:L:178:SER:OG	1.80	0.82
2:H:217:LYS:HG2	5:H:376:HOH:O	1.81	0.80
1:A:36:GLN:HE22	1:A:41:ALA:H	1.31	0.76
2:H:3:GLN:OE1	5:H:317:HOH:O	2.02	0.75
2:H:199:GLN:CA	5:H:380:HOH:O	2.40	0.70
3:L:196:GLN:HG2	3:L:205:GLU:CG	2.24	0.68
2:H:103:ASN:HD22	2:H:103:ASN:N	1.91	0.68
1:A:104:ARG:NH1	5:A:246:HOH:O	2.27	0.67
1:A:210:GLN:NE2	5:A:387:HOH:O	2.27	0.66
1:A:51:MET:SD	3:L:93:MET:HG3	2.37	0.64
2:H:200:THR:HG22	5:H:382:HOH:O	1.96	0.64
2:H:211:ASN:HB3	5:H:355:HOH:O	1.97	0.64
2:H:97:ARG:HE	2:H:109:ASN:ND2	1.97	0.61
1:A:23:HIS:HE1	2:H:99:PHE:O	1.83	0.60
2:H:97:ARG:HH21	2:H:109:ASN:ND2	1.96	0.60
3:L:16:GLN:O	3:L:77:THR:HG23	2.02	0.60
2:H:5:VAL:HG23	2:H:23:LYS:HE3	1.82	0.60
1:A:23:HIS:HD2	5:H:299:HOH:O	1.88	0.56
3:L:194:SER:HB3	3:L:207:THR:HG22	1.88	0.56
2:H:61:GLN:HB3	5:H:306:HOH:O	2.05	0.56
3:L:126:GLU:OE2	3:L:133:THR:CG2	2.53	0.56
3:L:169:GLN:HE21	3:L:175:ALA:HB2	1.72	0.54
3:L:126:GLU:OE2	3:L:133:THR:HG23	2.09	0.53
3:L:47:ILE:HD13	3:L:72:LEU:CD1	2.39	0.52
3:L:125:GLU:HB2	5:L:216:HOH:O	2.09	0.52
2:H:66:ARG:CD	5:H:400:HOH:O	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:12:VAL:HG13	3:L:16:GLN:HB3	1.91	0.51
2:H:66:ARG:HD3	5:H:400:HOH:O	2.12	0.50
1:A:198:GLN:HG3	5:A:410:HOH:O	2.12	0.50
3:L:17:THR:HG22	5:L:371:HOH:O	2.12	0.50
3:L:163:THR:HG21	5:L:402:HOH:O	2.12	0.49
3:L:2:ILE:N	5:L:360:HOH:O	2.45	0.49
3:L:163:THR:HG22	3:L:178:SER:HG	1.77	0.48
2:H:3:GLN:N	5:H:291:HOH:O	2.46	0.48
3:L:68:ASN:HB3	5:L:375:HOH:O	2.13	0.48
1:A:121:LYS:HA	1:A:124:GLN:HG2	1.95	0.47
1:A:42:GLY:H	1:A:126:ARG:HH21	1.60	0.47
1:A:205:VAL:O	1:A:209:LYS:HG3	2.12	0.47
1:A:84:GLU:HG2	5:A:308:HOH:O	2.13	0.47
3:L:194:SER:CB	3:L:207:THR:HG22	2.45	0.47
2:H:103:ASN:ND2	2:H:103:ASN:H	1.99	0.47
1:A:42:GLY:N	1:A:126:ARG:HH21	2.12	0.46
2:H:202:ILE:HG12	2:H:217:LYS:HD3	1.96	0.46
2:H:29:PHE:HA	2:H:32:TYR:CE2	2.50	0.46
3:L:116:SER:HB3	5:L:388:HOH:O	2.15	0.46
3:L:110:GLN:HB3	5:L:361:HOH:O	2.15	0.46
1:A:1[B]:MET:SD	1:A:4:LEU:HD12	2.55	0.46
3:L:187:TRP:CZ2	3:L:210:PRO:HA	2.51	0.46
1:A:26:GLN:HG2	2:H:99:PHE:CE1	2.51	0.45
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.52	0.45
1:A:110:GLN:HE22	1:A:114:GLN:HE21	1.65	0.44
1:A:188:ASN:O	1:A:192:ARG:HG2	2.18	0.43
3:L:140:ASP:H	3:L:169:GLN:HE22	1.67	0.43
2:H:166:LEU:HD21	2:H:189:VAL:HG11	2.00	0.43
1:A:89:GLY:N	5:A:393:HOH:O	2.51	0.43
1:A:110:GLN:NE2	1:A:114:GLN:HE21	2.16	0.43
1:A:4:LEU:HD13	1:A:91:LEU:HD13	2.01	0.42
3:L:118:THR:HG23	5:L:388:HOH:O	2.17	0.42
1:A:138:TRP:HA	1:A:138:TRP:HE3	1.84	0.42
2:H:23:LYS:HE2	5:H:253:HOH:O	2.19	0.42
1:A:138:TRP:HA	1:A:138:TRP:CE3	2.54	0.42
1:A:216:LEU:HA	5:A:439:HOH:O	2.20	0.42
2:H:29:PHE:CZ	2:H:52(A):PRO:HB3	2.55	0.41
3:L:9:SER:HB2	5:L:341:HOH:O	2.20	0.41
2:H:5:VAL:CG2	2:H:23:LYS:HE3	2.50	0.40

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:A:1[A]:MET:CE	1:A:60:TYR:OH[4_566]	2.13	0.07
5:H:269:HOH:O	5:L:312:HOH:O[1_655]	2.15	0.05

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	A	188/217 (87%)	185 (98%)	3 (2%)	0	100	100
2	H	211/245 (86%)	208 (99%)	3 (1%)	0	100	100
3	L	207/213 (97%)	203 (98%)	4 (2%)	0	100	100
All	All	606/675 (90%)	596 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	180/185 (97%)	167 (93%)	13 (7%)	18	9
2	H	178/207 (86%)	168 (94%)	10 (6%)	26	16
3	L	175/178 (98%)	168 (96%)	7 (4%)	38	29
All	All	533/570 (94%)	503 (94%)	30 (6%)	27	16

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1[A]	MET
1	A	1[B]	MET
1	A	24	LEU
1	A	26	GLN
1	A	27	LEU
1	A	80	GLN
1	A	91	LEU
1	A	92	LEU
1	A	112	LEU
1	A	139	MET
1	A	140	GLU
1	A	142	ASP
1	A	179	LEU
2	H	12	LYS
2	H	64	GLN
2	H	85	LEU
2	H	86	ARG
2	H	103	ASN
2	H	115	LEU
2	H	167	THR
2	H	185	LEU
2	H	216	LYS
2	H	217	LYS
3	L	93	MET
3	L	117	VAL
3	L	119	LEU
3	L	133	THR
3	L	137	LEU
3	L	146	VAL
3	L	168	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	10	GLN
1	A	11	GLN
1	A	23	HIS
1	A	36	GLN
1	A	110	GLN
1	A	187	GLN
1	A	197	GLN
1	A	202	GLN

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Mol	Chain	Res	Type
2	H	103	ASN
2	H	109	ASN
2	H	171	HIS
3	L	169	GLN
3	L	196	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

Of 2 ligands modelled in this entry, 2 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

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, 95^{th} 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	A	197/217 (90%)	0.06	7 (3%) 46 53	24, 33, 64, 92	0
2	H	214/245 (87%)	0.06	12 (5%) 28 32	25, 37, 58, 76	0
3	L	209/213 (98%)	-0.12	5 (2%) 62 68	29, 42, 62, 79	0
All	All	620/675 (91%)	-0.00	24 (3%) 43 48	24, 38, 62, 92	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	LEU	7.8
2	H	134	SER	7.2
2	H	140	GLY	4.4
1	A	47	HIS	3.5
1	A	41	ALA	3.3
2	H	185	LEU	3.1
2	H	148	LEU	3.0
2	H	33	ALA	2.9
2	H	52	ILE	2.9
2	H	147	CYS	2.9
2	H	107	PHE	2.9
1	A	40	LEU	2.8
1	A	42	GLY	2.6
2	H	96	ALA	2.6
2	H	37	VAL	2.5
3	L	110	GLN	2.5
2	H	98	TYR	2.5
3	L	88	ALA	2.4
3	L	170	SER	2.4
3	L	33	SER	2.2
1	A	30	TRP	2.0
2	H	36	TRP	2.0
1	A	139	MET	2.0

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Mol	Chain	Res	Type	RSRZ
3	L	172	ASN	2.0

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, 95^{th} 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	NA	H	245	1/1	0.97	0.17	0.50	35,35,35,35	0
4	NA	L	214	1/1	0.88	0.11	0.07	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.