Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:05 PM GMT

PDB ID	:	4KHT
Title	:	Triple helix bundle of GP41 complexed with fab 8066
Authors	:	Li, M.; Gustchina, A,; Wlodawer, A.
Deposited on	:	2013-05-01
Resolution	:	2.82 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:

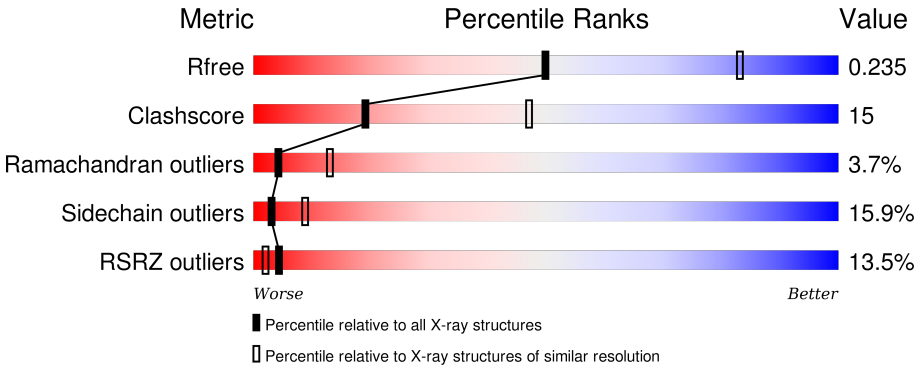
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.82 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	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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	67	19% 66% 22% 10%
2	H	245	11% 55% 28% 13%
3	L	213	13% 58% 31% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3691 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 Gp41 helix.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	66	Total	C	N	O	S	0	0	0
			525	333	95	95	2			

- Molecule 2 is a protein called 8066 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	1	0
			1603	1017	263	317	6			

- Molecule 3 is a protein called 8066 light chain.

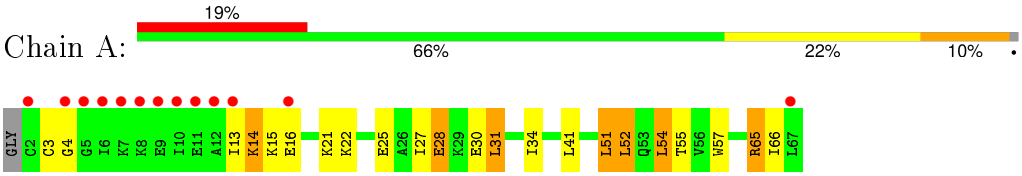
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	209	Total	C	N	O	S	0	0	0
			1563	978	258	322	5			

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.

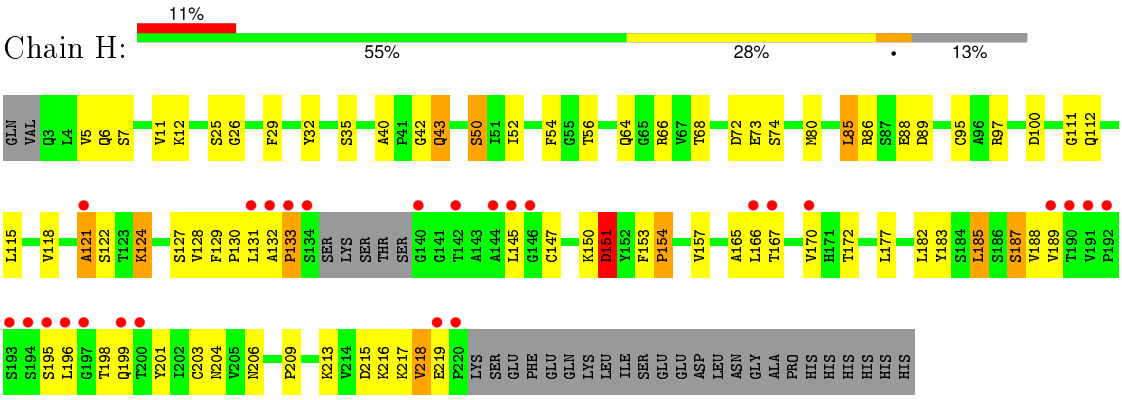
- Molecule 1: Gp41 helix

Chain A:



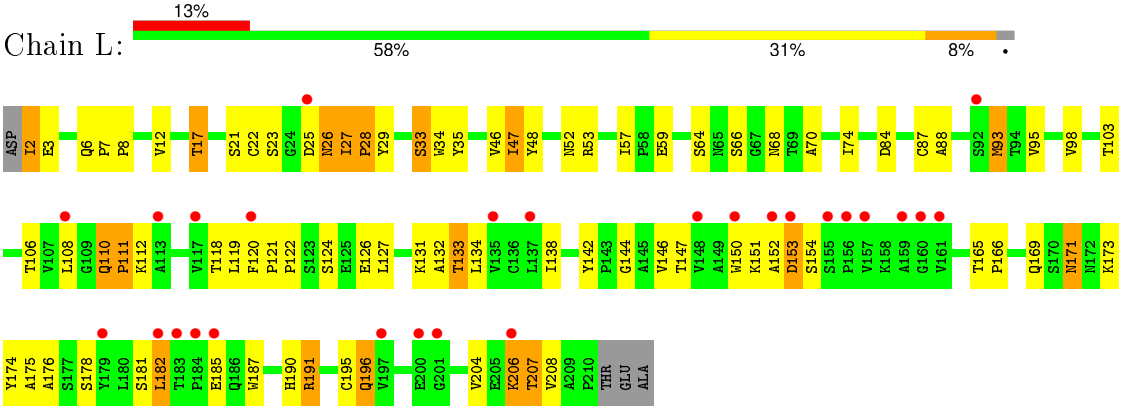
- Molecule 2: 8066 heavy chain

Chain H:



- Molecule 3: 8066 light chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	104.42Å 104.42Å 97.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.56 – 2.82 45.99 – 2.82	Depositor EDS
% Data completeness (in resolution range)	93.6 (35.56-2.82) 90.1 (45.99-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.215 , 0.266 0.230 , 0.235	Depositor DCC
R_{free} test set	695 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	79.0	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 99.0	EDS
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 14228 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3691	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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

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	0.50	0/527	0.66	1/702 (0.1%)
2	H	0.56	0/1646	0.68	1/2244 (0.0%)
3	L	0.45	0/1603	0.62	0/2195
All	All	0.50	0/3776	0.66	2/5141 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	52	LEU	CA-CB-CG	-5.79	101.99	115.30
2	H	185	LEU	CA-CB-CG	5.77	128.58	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	525	0	571	17	0
2	H	1603	0	1552	47	0
3	L	1563	0	1496	54	0
All	All	3691	0	3619	111	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 15.

All (111) 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:127:SER:HB2	2:H:150:LYS:HB2	1.61	0.83
3:L:27:ILE:HB	3:L:29:TYR:HE1	1.50	0.76
2:H:199:GLN:HB2	2:H:201:TYR:OH	1.88	0.73
3:L:22:CYS:HB3	3:L:70:ALA:HB3	1.69	0.72
3:L:28:PRO:HB2	3:L:29:TYR:HA	1.71	0.72
1:A:55:THR:HG22	2:H:54:PHE:HZ	1.56	0.71
2:H:199:GLN:HB2	2:H:201:TYR:CZ	2.29	0.68
1:A:3:CYS:SG	1:A:4:GLY:N	2.71	0.62
2:H:172:THR:HG22	2:H:187:SER:HB2	1.82	0.61
2:H:86:ARG:HG3	2:H:88:GLU:HG2	1.84	0.60
2:H:121:ALA:HB1	2:H:122:SER:OG	2.03	0.58
2:H:204:ASN:ND2	2:H:215:ASP:OD1	2.32	0.58
1:A:51:LEU:O	1:A:55:THR:HG23	2.04	0.57
1:A:27:ILE:O	1:A:30:GLU:N	2.37	0.57
2:H:177:LEU:HB2	2:H:183:TYR:CE1	2.40	0.57
1:A:55:THR:HG22	2:H:54:PHE:CZ	2.38	0.56
2:H:128:VAL:O	2:H:216:LYS:NZ	2.39	0.56
3:L:48:TYR:O	3:L:52:ASN:HB2	2.06	0.55
1:A:14:LYS:HD3	1:A:15:LYS:HD2	1.88	0.55
3:L:110:GLN:HE21	3:L:111:PRO:HD2	1.70	0.55
2:H:29:PHE:HA	2:H:32:TYR:CD2	2.41	0.55
3:L:124:SER:HA	3:L:127:LEU:HD12	1.89	0.55
3:L:133:THR:HB	3:L:181:SER:HA	1.89	0.55
3:L:206:LYS:NZ	3:L:207:THR:H	2.05	0.55
3:L:34:TRP:HD1	3:L:47:ILE:CG2	2.20	0.54
2:H:6:GLN:OE1	2:H:111:GLY:HA3	2.07	0.54
2:H:130:PRO:HD3	2:H:216:LYS:NZ	2.22	0.54
3:L:28:PRO:HB2	3:L:29:TYR:CA	2.38	0.54
3:L:152:ALA:O	3:L:154:SER:N	2.39	0.54
3:L:26:ASN:O	3:L:27:ILE:HG13	2.08	0.54
3:L:34:TRP:CZ3	3:L:87:CYS:HB3	2.43	0.53
3:L:27:ILE:HB	3:L:29:TYR:CE1	2.39	0.53
3:L:2:ILE:HD11	3:L:26:ASN:HB3	1.90	0.53
2:H:203:CYS:N	2:H:216:LYS:O	2.31	0.53
3:L:138:ILE:H	3:L:138:ILE:HD12	1.74	0.52
3:L:34:TRP:HD1	3:L:47:ILE:HG22	1.75	0.52
2:H:145:LEU:HD12	2:H:218:VAL:HB	1.91	0.52
3:L:110:GLN:HG3	3:L:111:PRO:HD2	1.92	0.52
3:L:153:ASP:HB2	3:L:190:HIS:HB3	1.92	0.52
3:L:33:SER:HB2	3:L:35:TYR:CE2	2.45	0.51
3:L:7:PRO:O	3:L:103:THR:OG1	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:151:ASP:OD2	2:H:151:ASP:N	2.44	0.50
2:H:166:LEU:HD21	2:H:189:VAL:HG11	1.93	0.50
1:A:57:TRP:CD1	2:H:52:ILE:HD11	2.47	0.49
2:H:11:VAL:HG23	2:H:209:PRO:HB3	1.93	0.49
1:A:25:GLU:HA	1:A:28:GLU:CD	2.33	0.48
1:A:57:TRP:HD1	2:H:52:ILE:HD11	1.78	0.48
3:L:169:GLN:HE21	3:L:175:ALA:HB2	1.78	0.48
3:L:112:LYS:HG3	3:L:142:TYR:O	2.14	0.48
2:H:54:PHE:HB2	2:H:56:THR:HG23	1.94	0.48
3:L:151:LYS:HG3	3:L:196:GLN:HE22	1.79	0.48
2:H:124:LYS:HE2	2:H:124:LYS:HB3	1.70	0.47
2:H:170:VAL:HG22	2:H:189:VAL:HG22	1.96	0.47
3:L:151:LYS:HB3	3:L:151:LYS:HE3	1.64	0.47
3:L:171:ASN:OD1	3:L:171:ASN:N	2.48	0.47
2:H:6:GLN:H	2:H:112:GLN:CD	2.19	0.46
2:H:11:VAL:O	2:H:12:LYS:HD2	2.16	0.46
2:H:130:PRO:HD3	2:H:216:LYS:HZ3	1.79	0.46
3:L:88:ALA:HA	3:L:98:VAL:O	2.16	0.46
3:L:46:VAL:O	3:L:47:ILE:HD12	2.15	0.45
2:H:188:VAL:HG11	3:L:120:PHE:HE2	1.81	0.45
2:H:29:PHE:CD1	2:H:73:GLU:HA	2.51	0.45
2:H:32:TYR:CD1	2:H:97:ARG:HD2	2.51	0.45
3:L:166:PRO:HB2	3:L:174:TYR:HD1	1.81	0.45
3:L:150:TRP:HZ2	3:L:178:SER:O	2.00	0.45
2:H:151:ASP:HB2	2:H:182:LEU:HD13	1.99	0.44
3:L:53:ARG:NH2	3:L:59:GLU:HG3	2.32	0.44
2:H:42:GLY:C	2:H:43:GLN:HG2	2.37	0.44
2:H:66:ARG:NH2	2:H:89:ASP:OD1	2.51	0.44
3:L:126:GLU:OE2	3:L:133:THR:HG22	2.17	0.44
1:A:54:LEU:HA	1:A:54:LEU:HD12	1.86	0.44
3:L:131:LYS:HD3	3:L:182:LEU:O	2.18	0.44
2:H:85:LEU:HB3	2:H:118:VAL:HG11	2.00	0.44
3:L:122:PRO:HB3	3:L:132:ALA:HB1	1.99	0.44
2:H:35:SER:OG	2:H:50:SER:OG	2.32	0.44
2:H:132:ALA:HB3	3:L:121:PRO:HG2	2.00	0.43
3:L:196:GLN:HB2	3:L:196:GLN:HE21	1.64	0.43
2:H:66:ARG:HH22	2:H:89:ASP:CG	2.21	0.43
2:H:153:PHE:HA	2:H:154:PRO:HA	1.77	0.43
3:L:171:ASN:C	3:L:173:LYS:H	2.21	0.43
3:L:121:PRO:HB3	3:L:208:VAL:HG21	2.01	0.43
3:L:7:PRO:HA	3:L:8:PRO:HD3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:88:GLU:CD	2:H:88:GLU:H	2.21	0.43
2:H:129:PHE:HE2	2:H:150:LYS:HG3	1.82	0.43
3:L:53:ARG:HB3	3:L:57:ILE:HB	2.01	0.43
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.55	0.43
3:L:166:PRO:HB2	3:L:174:TYR:CD1	2.53	0.42
3:L:28:PRO:CB	3:L:29:TYR:HA	2.45	0.42
2:H:131:LEU:HD13	3:L:120:PHE:CG	2.55	0.42
3:L:122:PRO:HD3	3:L:134:LEU:HG	2.01	0.42
3:L:110:GLN:HE21	3:L:111:PRO:CD	2.33	0.42
3:L:166:PRO:HA	3:L:175:ALA:O	2.20	0.42
2:H:72:ASP:OD2	2:H:74:SER:OG	2.31	0.42
3:L:181:SER:O	3:L:182:LEU:HD23	2.20	0.42
1:A:27:ILE:HA	1:A:30:GLU:OE2	2.20	0.42
3:L:144:GLY:O	3:L:146:VAL:HG12	2.20	0.41
1:A:65:ARG:C	1:A:66:ILE:HD13	2.40	0.41
3:L:68:ASN:H	3:L:68:ASN:HD22	1.68	0.41
2:H:121:ALA:HA	2:H:122:SER:HA	1.84	0.41
3:L:138:ILE:HB	3:L:176:ALA:HB3	2.02	0.41
3:L:169:GLN:NE2	3:L:175:ALA:HB2	2.36	0.41
2:H:151:ASP:HA	2:H:183:TYR:O	2.21	0.41
2:H:85:LEU:HD12	2:H:85:LEU:HA	1.91	0.41
1:A:22:LYS:HA	1:A:25:GLU:HB2	2.02	0.41
1:A:31:LEU:O	1:A:34:ILE:HB	2.21	0.40
2:H:40:ALA:HB3	2:H:43:GLN:HG3	2.02	0.40
3:L:17:THR:HA	3:L:74:ILE:O	2.20	0.40
1:A:51:LEU:HD23	1:A:51:LEU:HA	1.70	0.40
2:H:132:ALA:HA	2:H:133:PRO:HD3	1.69	0.40
1:A:65:ARG:O	1:A:66:ILE:HD13	2.21	0.40
3:L:110:GLN:HA	3:L:110:GLN:NE2	2.36	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	A	64/67 (96%)	56 (88%)	6 (9%)	2 (3%)	5 17
2	H	211/245 (86%)	190 (90%)	13 (6%)	8 (4%)	4 12
3	L	207/213 (97%)	172 (83%)	27 (13%)	8 (4%)	4 12
All	All	482/525 (92%)	418 (87%)	46 (10%)	18 (4%)	4 13

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	151	ASP
2	H	196	LEU
3	L	28	PRO
3	L	191	ARG
2	H	26	GLY
2	H	165	ALA
2	H	195	SER
2	H	121	ALA
3	L	93	MET
3	L	153	ASP
1	A	28	GLU
2	H	154	PRO
3	L	111	PRO
1	A	21	LYS
3	L	195	CYS
3	L	27	ILE
3	L	66	SER
2	H	133	PRO

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	56/56 (100%)	48 (86%)	8 (14%)	4 12
2	H	178/207 (86%)	153 (86%)	25 (14%)	4 12
3	L	175/178 (98%)	143 (82%)	32 (18%)	2 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	409/441 (93%)	344 (84%)	65 (16%)	3 9

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	14	LYS
1	A	16	GLU
1	A	31	LEU
1	A	41	LEU
1	A	51	LEU
1	A	54	LEU
1	A	65	ARG
2	H	5	VAL
2	H	7	SER
2	H	25	SER
2	H	43	GLN
2	H	50	SER
2	H	64	GLN
2	H	68	THR
2	H	80	MET
2	H	85	LEU
2	H	95	CYS
2	H	100	ASP
2	H	115	LEU
2	H	124	LYS
2	H	147	CYS
2	H	151	ASP
2	H	157	VAL
2	H	167	THR
2	H	185	LEU
2	H	187	SER
2	H	198	THR
2	H	206	ASN
2	H	213	LYS
2	H	217	LYS
2	H	218	VAL
2	H	219	GLU
3	L	2	ILE
3	L	3	GLU
3	L	6	GLN
3	L	12	VAL

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Mol	Chain	Res	Type
3	L	17	THR
3	L	21	SER
3	L	23	SER
3	L	25	ASP
3	L	26	ASN
3	L	33	SER
3	L	47	ILE
3	L	64	SER
3	L	84	ASP
3	L	93	MET
3	L	95	VAL
3	L	106	THR
3	L	108	LEU
3	L	110	GLN
3	L	118	THR
3	L	119	LEU
3	L	133	THR
3	L	147	THR
3	L	165	THR
3	L	171	ASN
3	L	182	LEU
3	L	185	GLU
3	L	187	TRP
3	L	191	ARG
3	L	196	GLN
3	L	204	VAL
3	L	206	LYS
3	L	207	THR

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

Mol	Chain	Res	Type
1	A	61	GLN
2	H	58	ASN
2	H	171	HIS
2	H	178	GLN
3	L	68	ASN
3	L	110	GLN
3	L	169	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

There are no ligands in this entry.

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	66/67 (98%)	1.02	13 (19%)	1	1	48, 127, 237, 268	0
2	H	214/245 (87%)	0.66	26 (12%)	6	3	49, 106, 221, 263	0
3	L	209/213 (98%)	0.69	27 (12%)	5	2	60, 156, 221, 283	0
All	All	489/525 (93%)	0.72	66 (13%)	4	2	48, 131, 225, 283	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	134	SER	11.3
3	L	184	PRO	10.0
1	A	5	GLY	8.3
2	H	132	ALA	7.9
2	H	133	PRO	6.9
3	L	182	LEU	6.5
1	A	6	ILE	6.4
2	H	199	GLN	6.3
2	H	220	PRO	6.1
3	L	159	ALA	6.0
2	H	193	SER	5.9
1	A	11	GLU	5.8
3	L	183	THR	5.4
2	H	191	VAL	5.3
3	L	185	GLU	5.0
3	L	148	VAL	4.9
3	L	160	GLY	4.9
1	A	67	LEU	4.8
1	A	4	GLY	4.7
2	H	192	PRO	4.5
3	L	179	TYR	4.4
2	H	131	LEU	4.4
2	H	140	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
2	H	194	SER	4.2
2	H	144	ALA	4.1
3	L	150	TRP	4.0
1	A	2	CYS	4.0
2	H	200	THR	3.6
2	H	190	THR	3.5
1	A	10	ILE	3.5
3	L	152	ALA	3.5
3	L	120	PHE	3.5
3	L	153	ASP	3.4
2	H	145	LEU	3.3
3	L	197	VAL	3.2
2	H	189	VAL	3.1
2	H	166	LEU	3.1
2	H	142	THR	3.1
2	H	170	VAL	3.0
1	A	8	LYS	3.0
3	L	135	VAL	3.0
2	H	167	THR	3.0
3	L	206	LYS	2.9
1	A	16	GLU	2.8
1	A	12	ALA	2.8
2	H	197	GLY	2.7
3	L	117	VAL	2.7
2	H	219	GLU	2.7
3	L	108	LEU	2.7
3	L	113	ALA	2.7
3	L	137	LEU	2.6
1	A	7	LYS	2.6
3	L	25	ASP	2.5
3	L	156	PRO	2.5
2	H	146	GLY	2.4
3	L	161	VAL	2.4
2	H	196	LEU	2.4
1	A	9	GLU	2.4
2	H	121	ALA	2.3
3	L	200	GLU	2.3
3	L	157	VAL	2.3
3	L	201	GLY	2.2
1	A	13	ILE	2.2
3	L	155	SER	2.1
2	H	195	SER	2.0

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Mol	Chain	Res	Type	RSRZ
3	L	92	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.