Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:21 PM GMT

PDB ID	:	1F90
Title	:	FAB FRAGMENT OF MONOCLONAL ANTIBODY (LNKB-2) AGAINST HUMAN INTERLEUKIN-2 IN COMPLEX WITH ANTIGENIC PEPTIDE
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Deposited on	:	2000-07-06
Resolution	:	2.60 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 (i) symbol.

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

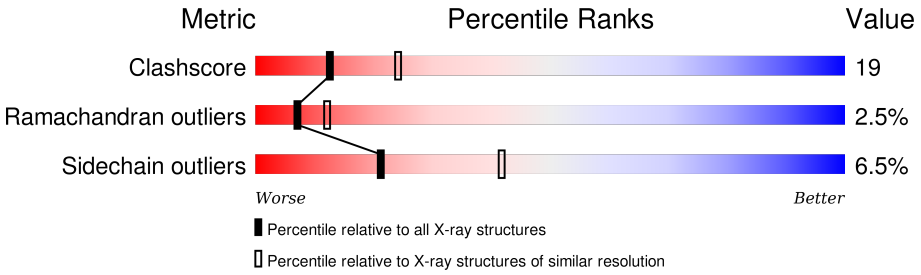
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.60 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	219	65% 30% 5%
2	H	220	60% 33% 7%
3	E	9	78% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3543 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 FAB FRAGMENT OF MONOCLONAL ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	219	Total	C	N	O	S	0	0	0
			1700	1059	290	344	7			

- Molecule 2 is a protein called FAB FRAGMENT OF MONOCLONAL ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1680	1067	271	335	7			

- Molecule 3 is a protein called ANTIGENIC NONAPEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	0	0	0
			74	48	11	15			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	3	Total	O	0	0
			3	3		
4	H	34	Total	O	0	0
			34	34		
4	L	52	Total	O	0	0
			52	52		

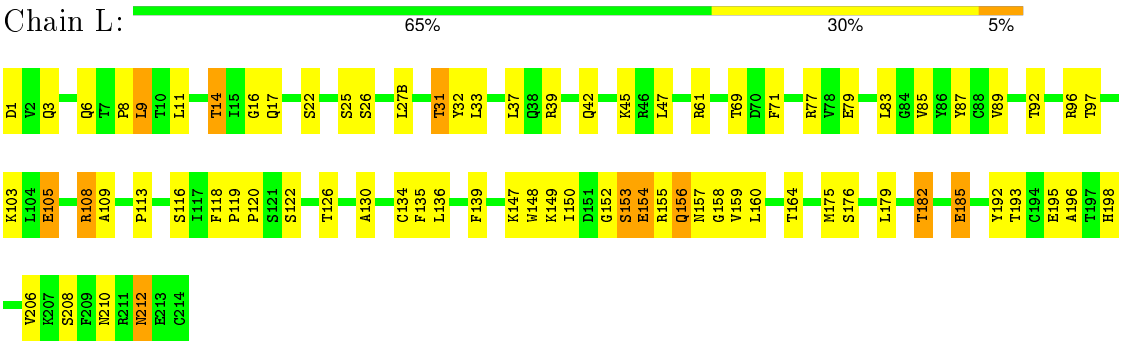
3 Residue-property plots (i)

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.

Note EDS was not executed.

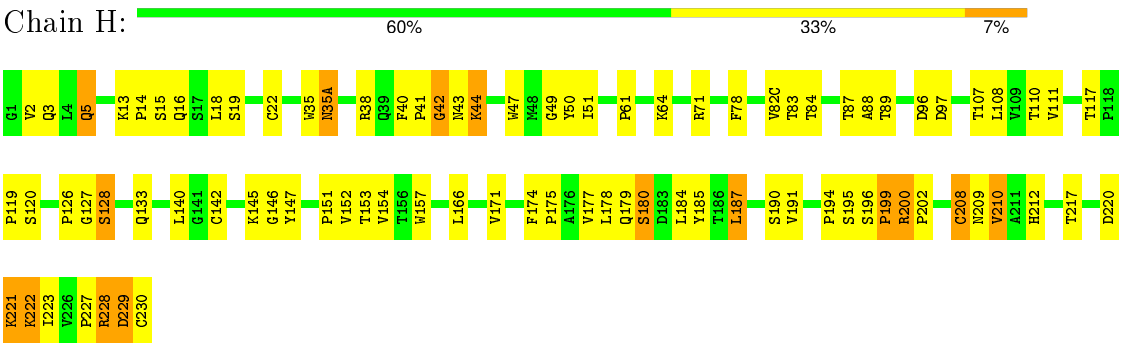
- Molecule 1: FAB FRAGMENT OF MONOCLONAL ANTIBODY

Chain L:



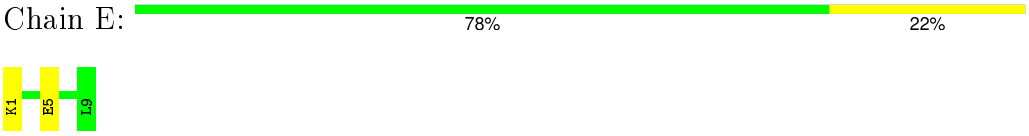
- Molecule 2: FAB FRAGMENT OF MONOCLONAL ANTIBODY

Chain H:



- Molecule 3: ANTIGENIC NONAPEPTIDE

Chain E:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.83Å 72.76Å 72.15Å 90.00° 106.98° 90.00°	Depositor
Resolution (Å)	99.00 – 2.60	Depositor
% Data completeness (in resolution range)	95.5 (99.00-2.60)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.165 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3543	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

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	L	0.37	0/1736	0.65	0/2355
2	H	0.39	0/1728	0.68	0/2370
3	E	0.47	0/74	0.57	0/98
All	All	0.38	0/3538	0.66	0/4823

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	L	1700	0	1651	67	0
2	H	1680	0	1625	72	0
3	E	74	0	82	1	0
4	E	3	0	0	0	0
4	H	34	0	0	2	0
4	L	52	0	0	4	0
All	All	3543	0	3358	132	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 19.

All (132) 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:200:ARG:HD2	2:H:202:PRO:HA	1.36	1.08
2:H:200:ARG:HH11	2:H:200:ARG:HB3	1.15	1.05
2:H:196:SER:HB2	2:H:199:PRO:HD3	1.42	0.99
2:H:140:LEU:HD11	2:H:200:ARG:HG3	1.47	0.96
2:H:200:ARG:HB3	2:H:200:ARG:NH1	1.80	0.95
1:L:182:THR:HG23	1:L:185:GLU:HB2	1.54	0.87
2:H:222:LYS:H	2:H:222:LYS:HD2	1.40	0.87
2:H:200:ARG:HH11	2:H:200:ARG:CB	1.88	0.85
2:H:140:LEU:HD13	2:H:223:ILE:HG21	1.59	0.82
2:H:194:PRO:O	2:H:199:PRO:HD2	1.79	0.82
1:L:1:ASP:HB3	4:L:252:HOH:O	1.82	0.79
1:L:9:LEU:HD22	1:L:9:LEU:H	1.47	0.79
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.64	0.79
1:L:149:LYS:HD3	1:L:153:SER:HA	1.66	0.77
1:L:61:ARG:CZ	1:L:79:GLU:HG3	2.15	0.77
2:H:42:GLY:HA3	2:H:44:LYS:HE3	1.67	0.74
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.24	0.72
2:H:178:LEU:HB2	2:H:185:TYR:CE1	2.25	0.72
1:L:31:THR:HG21	4:L:241:HOH:O	1.89	0.70
2:H:221:LYS:HA	2:H:221:LYS:HE2	1.74	0.69
1:L:120:PRO:HG2	1:L:130:ALA:HB1	1.75	0.69
2:H:142:CYS:HB2	2:H:157:TRP:CH2	2.29	0.68
1:L:148:TRP:O	1:L:155:ARG:HA	1.97	0.64
2:H:187:LEU:C	2:H:187:LEU:HD23	2.17	0.64
2:H:196:SER:HB2	2:H:199:PRO:CD	2.24	0.64
1:L:160:LEU:HD22	2:H:177:VAL:HG11	1.80	0.63
2:H:42:GLY:O	2:H:43:ASN:HB2	1.99	0.62
2:H:35(A):ASN:HD22	2:H:35(A):ASN:H	1.48	0.62
2:H:107:THR:HB	4:H:244:HOH:O	2.00	0.62
2:H:40:PHE:HB2	2:H:44:LYS:HG3	1.82	0.62
1:L:156:GLN:HG3	1:L:157:ASN:N	2.16	0.61
1:L:9:LEU:HD22	1:L:9:LEU:N	2.13	0.61
1:L:193:THR:HA	1:L:208:SER:HB3	1.82	0.61
1:L:108:ARG:HD3	1:L:109:ALA:O	2.01	0.60
2:H:146:GLY:HA2	2:H:184:LEU:HB3	1.83	0.59
1:L:119:PRO:HD2	2:H:228:ARG:NH2	2.18	0.59
1:L:27(B):LEU:O	1:L:92:THR:HG21	2.03	0.58
1:L:32:TYR:HD2	1:L:92:THR:HG22	1.69	0.57
2:H:194:PRO:HG2	2:H:199:PRO:CD	2.35	0.57
2:H:222:LYS:H	2:H:222:LYS:CD	2.14	0.56
1:L:27(B):LEU:HD12	1:L:71:PHE:CE2	2.41	0.56
1:L:147:LYS:HE2	1:L:155:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:108:LEU:HB3	4:H:253:HOH:O	2.05	0.55
2:H:140:LEU:HD13	2:H:223:ILE:CG2	2.34	0.55
1:L:61:ARG:NH2	1:L:79:GLU:HG3	2.20	0.55
1:L:16:GLY:HA2	1:L:77:ARG:HG2	1.88	0.55
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.88	0.55
1:L:156:GLN:HG2	1:L:179:LEU:HD11	1.89	0.54
1:L:32:TYR:CD2	1:L:92:THR:HG22	2.43	0.54
2:H:41:PRO:O	2:H:44:LYS:NZ	2.37	0.54
2:H:16:GLN:O	2:H:82(C):VAL:HG22	2.07	0.54
1:L:122:SER:O	1:L:126:THR:HG23	2.08	0.54
2:H:157:TRP:CZ3	2:H:208:CYS:HB2	2.43	0.54
2:H:35(A):ASN:ND2	2:H:35(A):ASN:N	2.55	0.54
2:H:84:THR:HG22	2:H:111:VAL:O	2.09	0.53
1:L:136:LEU:N	1:L:136:LEU:HD12	2.24	0.53
2:H:50:TYR:C	2:H:50:TYR:CD1	2.82	0.53
2:H:179:GLN:O	2:H:180:SER:HB2	2.09	0.53
1:L:103:LYS:HG2	1:L:105:GLU:OE1	2.09	0.52
1:L:9:LEU:H	1:L:9:LEU:CD2	2.21	0.52
1:L:25:SER:O	1:L:69:THR:HG23	2.10	0.52
1:L:152:GLY:O	1:L:154:GLU:N	2.43	0.51
1:L:120:PRO:CG	1:L:130:ALA:HB1	2.41	0.51
1:L:153:SER:O	1:L:155:ARG:N	2.44	0.50
2:H:14:PRO:O	2:H:15:SER:HB3	2.10	0.50
1:L:45:LYS:HB3	1:L:45:LYS:NZ	2.27	0.50
2:H:127:GLY:O	2:H:128:SER:CB	2.60	0.50
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.92	0.50
1:L:3:GLN:HG3	1:L:26:SER:HB3	1.94	0.50
2:H:71:ARG:HA	2:H:78:PHE:HA	1.94	0.50
1:L:175:MET:HG2	1:L:176:SER:N	2.27	0.49
2:H:35(A):ASN:N	2:H:35(A):ASN:HD22	2.09	0.49
1:L:195:GLU:CG	1:L:206:VAL:HG22	2.40	0.49
2:H:127:GLY:O	2:H:128:SER:HB2	2.13	0.49
1:L:14:THR:HG22	1:L:17:GLN:HG2	1.95	0.49
2:H:96:ASP:O	2:H:97:ASP:HB2	2.12	0.49
1:L:135:PHE:CE2	2:H:190:SER:HB3	2.48	0.49
2:H:133:GLN:N	2:H:133:GLN:CD	2.67	0.48
3:E:1:LYS:HE3	3:E:5:GLU:OE1	2.12	0.48
2:H:153:THR:O	2:H:210:VAL:HA	2.13	0.48
2:H:61:PRO:O	2:H:64:LYS:HG2	2.14	0.48
2:H:212:HIS:HB3	2:H:217:THR:HB	1.96	0.48
1:L:150:ILE:N	1:L:150:ILE:HD12	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:LEU:HD21	1:L:196:ALA:HB2	1.96	0.48
2:H:154:VAL:HG22	2:H:210:VAL:HB	1.96	0.48
2:H:87:THR:O	2:H:88:ALA:HB2	2.15	0.47
1:L:147:LYS:HD3	1:L:155:ARG:HH11	1.78	0.47
1:L:87:TYR:OH	2:H:43:ASN:HB3	2.14	0.47
1:L:89:VAL:HG23	1:L:97:THR:O	2.14	0.47
1:L:1:ASP:CG	4:L:220:HOH:O	2.52	0.46
1:L:152:GLY:C	1:L:154:GLU:H	2.18	0.46
1:L:147:LYS:HE2	1:L:155:ARG:HH12	1.79	0.46
1:L:150:ILE:HD13	1:L:156:GLN:HB2	1.98	0.46
2:H:126:PRO:HD3	2:H:140:LEU:CD2	2.45	0.46
2:H:194:PRO:HG2	2:H:199:PRO:HD2	1.97	0.46
2:H:166:LEU:HD12	2:H:166:LEU:N	2.31	0.46
2:H:120:SER:OG	2:H:145:LYS:HB3	2.16	0.46
2:H:171:VAL:HG22	2:H:191:VAL:HG23	1.97	0.45
2:H:35:TRP:N	2:H:35:TRP:CD1	2.85	0.45
1:L:119:PRO:HD2	2:H:228:ARG:HH22	1.80	0.45
2:H:178:LEU:HD12	2:H:184:LEU:O	2.16	0.45
1:L:160:LEU:HD22	2:H:177:VAL:CG1	2.47	0.45
2:H:84:THR:HA	2:H:111:VAL:HB	1.97	0.45
1:L:39:ARG:HB2	1:L:42:GLN:OE1	2.18	0.44
1:L:210:ASN:CB	1:L:212:ASN:HD21	2.31	0.44
2:H:18:LEU:HD12	2:H:19:SER:H	1.83	0.44
2:H:51:ILE:O	2:H:51:ILE:HG23	2.17	0.44
1:L:192:TYR:O	1:L:208:SER:HB2	2.17	0.44
1:L:6:GLN:HA	1:L:22:SER:O	2.18	0.44
1:L:8:PRO:HG3	1:L:11:LEU:HD13	2.01	0.43
2:H:229:ASP:HB3	2:H:230:CYS:H	1.45	0.43
1:L:37:LEU:HB2	1:L:47:LEU:HD11	2.01	0.43
2:H:133:GLN:O	2:H:195:SER:HB3	2.18	0.43
1:L:85:VAL:HG21	2:H:43:ASN:ND2	2.35	0.42
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.53	0.42
2:H:41:PRO:C	2:H:44:LYS:NZ	2.73	0.42
2:H:83:THR:C	2:H:111:VAL:HG11	2.40	0.42
1:L:1:ASP:OD1	4:L:220:HOH:O	2.21	0.42
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.90	0.42
1:L:152:GLY:C	1:L:154:GLU:N	2.73	0.42
1:L:113:PRO:HD3	1:L:198:HIS:ND1	2.34	0.42
1:L:32:TYR:H	1:L:92:THR:HG22	1.83	0.42
1:L:32:TYR:HB2	1:L:92:THR:HG22	2.02	0.42
2:H:13:LYS:HD3	2:H:13:LYS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:33:LEU:HD22	1:L:71:PHE:CD2	2.56	0.41
2:H:209:ASN:ND2	2:H:220:ASP:OD1	2.53	0.41
2:H:5:GLN:O	2:H:22:CYS:HA	2.21	0.41
1:L:210:ASN:HB3	1:L:212:ASN:HD21	1.87	0.40
2:H:174:PHE:HA	2:H:175:PRO:HD3	1.94	0.40
2:H:38:ARG:HA	2:H:89:THR:O	2.21	0.40
1:L:164:THR:HG23	2:H:174:PHE:CD1	2.56	0.40
1:L:116:SER:O	1:L:134:CYS:HA	2.22	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	L	217/219 (99%)	207 (95%)	6 (3%)	4 (2%)	11 21
2	H	218/220 (99%)	193 (88%)	18 (8%)	7 (3%)	5 8
3	E	7/9 (78%)	5 (71%)	2 (29%)	0	100 100
All	All	442/448 (99%)	405 (92%)	26 (6%)	11 (2%)	7 12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	128	SER
2	H	199	PRO
1	L	153	SER
1	L	212	ASN
2	H	2	VAL
2	H	228	ARG
1	L	158	GLY
1	L	154	GLU
2	H	180	SER

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Mol	Chain	Res	Type
2	H	227	PRO
2	H	42	GLY

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	196/196 (100%)	185 (94%)	11 (6%)	26 50
2	H	194/194 (100%)	179 (92%)	15 (8%)	16 31
3	E	9/9 (100%)	9 (100%)	0	100 100
All	All	399/399 (100%)	373 (94%)	26 (6%)	21 42

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	9	LEU
1	L	14	THR
1	L	31	THR
1	L	83	LEU
1	L	96	ARG
1	L	105	GLU
1	L	108	ARG
1	L	156	GLN
1	L	159	VAL
1	L	182	THR
1	L	185	GLU
2	H	3	GLN
2	H	5	GLN
2	H	35(A)	ASN
2	H	44	LYS
2	H	110	THR
2	H	117	THR
2	H	151	PRO
2	H	152	VAL
2	H	187	LEU

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Mol	Chain	Res	Type
2	H	200	ARG
2	H	208	CYS
2	H	210	VAL
2	H	221	LYS
2	H	222	LYS
2	H	229	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	124	GLN
1	L	156	GLN
1	L	212	ASN
2	H	3	GLN
2	H	5	GLN
2	H	35(A)	ASN
2	H	81	GLN
2	H	105	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.