



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:32 AM GMT

PDB ID : 2F19
Title : THREE-DIMENSIONAL STRUCTURE OF TWO CRYSTAL FORMS OF
FAB R19.9, FROM A MONOCLONAL ANTI-ARSONATE ANTIBODY
Authors : Lascombe, M.B.; Alzari, P.M.; Poljak, R.J.; Nisonoff, A.
Deposited on : 1992-05-27
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

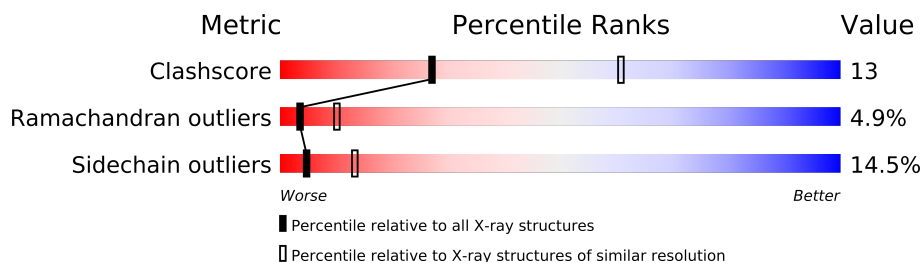
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	214	
2	H	221	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3320 atoms, of which 0 are hydrogen and 0 are deuterium.

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 IGG2B-KAPPA R19.9 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1663	1027	284	345	7			

- Molecule 2 is a protein called IGG2B-KAPPA R19.9 FAB (HEAVY CHAIN).

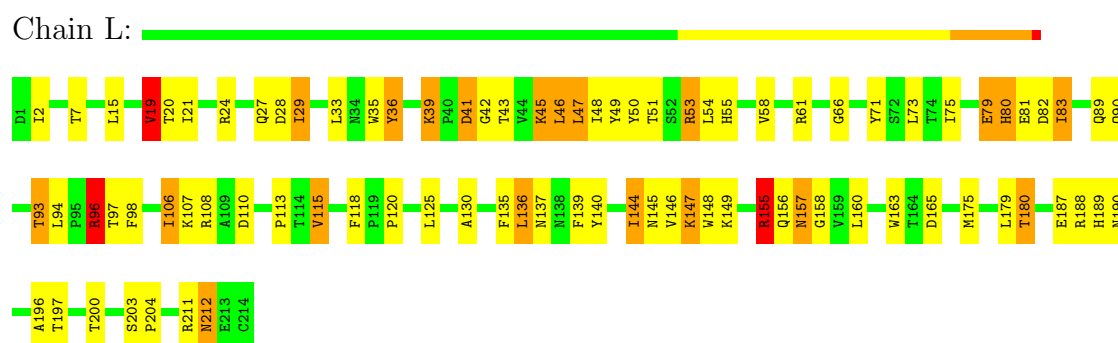
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1657	1047	270	332	8			

3 Residue-property plots

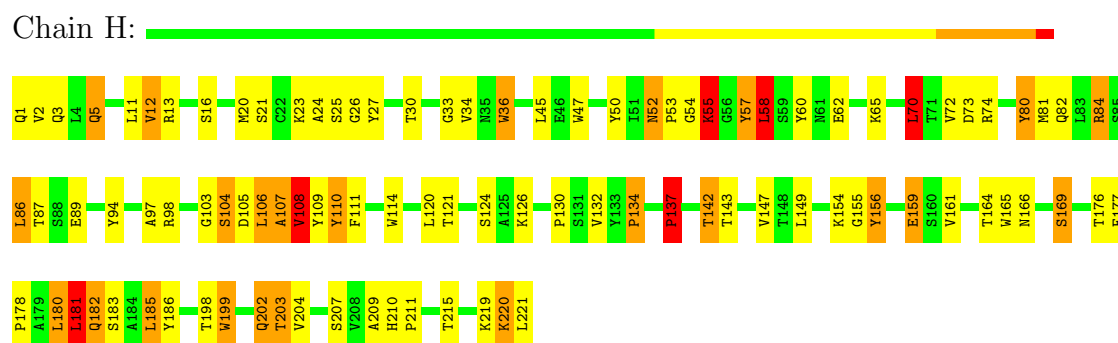
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: IGG2B-KAPPA R19.9 FAB (LIGHT CHAIN)



• Molecule 2: IGG2B-KAPPA R19.9 FAB (HEAVY CHAIN)



4 Data and refinement statistics

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	43.30Å 80.80Å 75.10Å 90.00° 96.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3320	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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	0.82	0/1697	1.69	31/2301 (1.3%)
2	H	0.80	0/1699	1.73	39/2316 (1.7%)
All	All	0.81	0/3396	1.71	70/4617 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	3

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	L	96	ARG	NE-CZ-NH1	14.01	127.30	120.30
1	L	155	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	L	108	ARG	NE-CZ-NH1	9.52	125.06	120.30
2	H	165	TRP	CD1-CG-CD2	8.84	113.37	106.30
2	H	199	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	L	163	TRP	CD1-CG-CD2	8.07	112.75	106.30
2	H	108	VAL	CA-CB-CG1	-7.93	99.00	110.90
1	L	148	TRP	CD1-CG-CD2	7.82	112.56	106.30
2	H	47	TRP	CD1-CG-CD2	7.62	112.39	106.30
1	L	35	TRP	CD1-CG-CD2	7.52	112.32	106.30
2	H	199	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	L	24	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	L	53	ARG	NE-CZ-NH1	7.42	124.01	120.30
2	H	74	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	L	35	TRP	CE2-CD2-CG	-7.27	101.49	107.30
1	L	163	TRP	CE2-CD2-CG	-7.26	101.49	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	84	ARG	NE-CZ-NH2	-7.25	116.68	120.30
2	H	165	TRP	CE2-CD2-CG	-7.23	101.52	107.30
2	H	36	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	L	155	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	L	148	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	L	212	ASN	CA-C-N	-7.06	101.66	117.20
2	H	72	VAL	CA-CB-CG2	-7.03	100.36	110.90
2	H	13	ARG	NE-CZ-NH1	6.95	123.78	120.30
2	H	156	TYR	CB-CG-CD2	-6.92	116.85	121.00
2	H	47	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	L	51	THR	CA-CB-CG2	6.64	121.70	112.40
2	H	84	ARG	NE-CZ-NH1	6.57	123.59	120.30
2	H	114	TRP	CE2-CD2-CG	-6.50	102.10	107.30
2	H	36	TRP	CD1-CG-CD2	6.45	111.46	106.30
1	L	96	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	L	83	ILE	CA-C-N	-6.31	103.33	117.20
2	H	180	LEU	CA-CB-CG	6.28	129.74	115.30
2	H	215	THR	CA-CB-CG2	6.26	121.16	112.40
1	L	41	ASP	CA-C-N	-6.23	103.75	116.20
2	H	98	ARG	CB-CG-CD	-6.17	95.55	111.60
2	H	181	LEU	CA-CB-CG	6.14	129.43	115.30
2	H	110	TYR	CA-CB-CG	6.12	125.02	113.40
1	L	46	LEU	CA-CB-CG	6.10	129.33	115.30
1	L	19	VAL	CB-CA-C	-6.06	99.89	111.40
2	H	45	LEU	CA-CB-CG	6.05	129.21	115.30
2	H	108	VAL	CA-CB-CG2	5.95	119.82	110.90
2	H	13	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	L	96	ARG	CA-CB-CG	5.84	126.26	113.40
1	L	49	TYR	CB-CG-CD2	-5.83	117.50	121.00
2	H	114	TRP	CD1-CG-CD2	5.83	110.96	106.30
1	L	188	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	H	72	VAL	N-CA-CB	-5.75	98.84	111.50
2	H	165	TRP	CG-CD1-NE1	-5.67	104.43	110.10
2	H	94	TYR	CB-CG-CD2	-5.66	117.61	121.00
2	H	80	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	L	108	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	L	96	ARG	CB-CG-CD	5.47	125.83	111.60
2	H	199	TRP	CB-CG-CD1	-5.47	119.89	127.00
2	H	199	TRP	CG-CD1-NE1	-5.37	104.73	110.10
2	H	74	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	H	103	GLY	CA-C-N	-5.31	105.52	117.20
1	L	42	GLY	CA-C-N	-5.28	105.58	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	70	LEU	CA-CB-CG	5.27	127.42	115.30
1	L	148	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	L	41	ASP	CA-C-O	5.19	131.00	120.10
1	L	82	ASP	CB-CG-OD2	-5.18	113.63	118.30
2	H	74	ARG	CA-C-N	-5.16	105.86	117.20
2	H	203	THR	CA-CB-CG2	5.15	119.61	112.40
2	H	58	LEU	CA-CB-CG	5.14	127.12	115.30
1	L	163	TRP	CG-CD1-NE1	-5.13	104.97	110.10
2	H	47	TRP	CG-CD1-NE1	-5.12	104.98	110.10
2	H	124	SER	CA-C-N	-5.05	106.09	117.20
1	L	35	TRP	CG-CD2-CE3	5.05	138.44	133.90
1	L	211	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	203	SER	Peptide
1	L	36	TYR	Sidechain
1	L	50	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1663	0	1589	45	0
2	H	1657	0	1610	45	0
All	All	3320	0	3199	85	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (85) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:115:VAL:HB	1:L:136:LEU:HD13	1.66	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:164:THR:HG23	2:H:207:SER:HB2	1.67	0.75
1:L:36:TYR:CE1	1:L:46:LEU:HD23	2.25	0.72
1:L:19:VAL:HG23	1:L:75:ILE:HB	1.73	0.69
1:L:94:LEU:HD11	1:L:96:ARG:HH11	1.58	0.68
2:H:82:GLN:NE2	2:H:84:ARG:HE	1.96	0.64
2:H:12:VAL:HG11	2:H:86:LEU:HD23	1.82	0.61
1:L:160:LEU:HG	2:H:180:LEU:HD11	1.82	0.61
1:L:48:ILE:HG12	1:L:54:LEU:HD23	1.81	0.60
1:L:115:VAL:HA	1:L:135:PHE:O	2.02	0.59
1:L:45:LYS:HZ2	1:L:46:LEU:H	1.52	0.58
1:L:27:GLN:O	1:L:29:ILE:HG23	2.04	0.58
1:L:46:LEU:HD12	1:L:55:HIS:HB2	1.85	0.57
2:H:104:SER:OG	2:H:109:TYR:HB3	2.05	0.57
1:L:96:ARG:HD2	2:H:109:TYR:CE2	2.40	0.56
2:H:149:LEU:HD13	2:H:204:VAL:HG11	1.87	0.56
1:L:147:LYS:HE3	1:L:149:LYS:NZ	2.22	0.54
2:H:87:THR:HG22	2:H:89:GLU:H	1.72	0.54
1:L:61:ARG:NH1	1:L:79:GLU:HB2	2.22	0.54
2:H:156:TYR:HE2	2:H:159:GLU:HA	1.73	0.54
1:L:107:LYS:HA	1:L:140:TYR:OH	2.07	0.53
1:L:110:ASP:HB3	1:L:200:THR:HG22	1.91	0.53
1:L:190:ASN:HD21	1:L:212:ASN:HB2	1.74	0.53
1:L:190:ASN:ND2	1:L:212:ASN:HB2	2.24	0.52
2:H:155:GLY:HA2	2:H:185:LEU:HB2	1.91	0.51
2:H:106:LEU:HD22	2:H:106:LEU:H	1.75	0.51
1:L:47:LEU:HB3	1:L:48:ILE:HG13	1.92	0.51
2:H:30:THR:HA	2:H:53:PRO:HB2	1.92	0.51
1:L:15:LEU:CD2	1:L:106:ILE:HD11	2.41	0.50
2:H:97:ALA:HB1	2:H:111:PHE:HB3	1.93	0.50
2:H:185:LEU:O	2:H:185:LEU:HG	2.10	0.50
1:L:46:LEU:CD1	1:L:55:HIS:HB2	2.41	0.50
1:L:21:ILE:HD12	1:L:73:LEU:HD23	1.94	0.50
2:H:156:TYR:CE2	2:H:159:GLU:HA	2.47	0.50
2:H:198:THR:O	2:H:202:GLN:HB2	2.11	0.50
1:L:39:LYS:HE2	1:L:81:GLU:O	2.12	0.49
2:H:204:VAL:HG13	2:H:221:LEU:HB2	1.94	0.49
2:H:166:ASN:HB2	2:H:169:SER:OG	2.13	0.49
1:L:80:HIS:O	1:L:83:ILE:HG12	2.12	0.49
2:H:33:GLY:HA3	2:H:50:TYR:CE1	2.48	0.48
2:H:132:VAL:HG12	2:H:219:LYS:HG3	1.96	0.47
1:L:137:ASN:HD21	2:H:177:PHE:HZ	1.62	0.47
2:H:1:GLN:HB3	2:H:26:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.95	0.47
1:L:146:VAL:HG11	1:L:175:MET:CE	2.45	0.47
2:H:36:TRP:HB3	2:H:81:MET:HE2	1.97	0.46
1:L:125:LEU:CD2	1:L:130:ALA:HB2	2.45	0.46
1:L:155:ARG:NH2	1:L:158:GLY:HA3	2.30	0.46
1:L:96:ARG:HH12	2:H:104:SER:HB3	1.80	0.46
2:H:104:SER:HG	2:H:109:TYR:HB3	1.79	0.46
2:H:107:ALA:O	2:H:108:VAL:HG23	2.17	0.45
2:H:73:ASP:HB2	2:H:80:TYR:HE2	1.81	0.45
2:H:60:TYR:CE2	2:H:70:LEU:HD22	2.51	0.45
1:L:144:ILE:HD11	1:L:196:ALA:HB1	1.98	0.45
1:L:146:VAL:HG11	1:L:175:MET:HE3	1.99	0.45
2:H:164:THR:CG2	2:H:207:SER:HB2	2.42	0.44
2:H:181:LEU:HA	2:H:186:TYR:HA	2.00	0.44
2:H:137:PRO:HD3	2:H:149:LEU:HD23	1.99	0.44
2:H:181:LEU:HD12	2:H:182:GLN:O	2.18	0.44
2:H:5:GLN:NE2	2:H:23:LYS:O	2.50	0.44
1:L:96:ARG:HD2	2:H:109:TYR:CZ	2.53	0.44
1:L:89:GLN:HB2	1:L:98:PHE:CD1	2.54	0.43
1:L:155:ARG:HH22	1:L:158:GLY:HA3	1.83	0.43
2:H:147:VAL:HG11	2:H:199:TRP:CE3	2.54	0.43
1:L:144:ILE:HD13	1:L:145:ASN:N	2.32	0.43
2:H:57:TYR:HB2	2:H:58:LEU:H	1.59	0.43
1:L:144:ILE:HD13	1:L:145:ASN:H	1.84	0.43
2:H:154:LYS:HE3	2:H:154:LYS:HB2	1.78	0.43
1:L:53:ARG:HG3	1:L:53:ARG:HH11	1.84	0.42
1:L:118:PHE:HE2	1:L:135:PHE:CD2	2.37	0.42
2:H:55:LYS:HE3	2:H:55:LYS:N	2.34	0.42
1:L:66:GLY:HA3	1:L:71:TYR:CD2	2.54	0.42
1:L:90:GLN:HE21	1:L:97:THR:H	1.67	0.42
1:L:156:GLN:O	1:L:157:ASN:HB2	2.20	0.42
1:L:120:PRO:CG	1:L:130:ALA:HB1	2.50	0.42
1:L:125:LEU:HD23	1:L:130:ALA:HB2	2.00	0.41
1:L:47:LEU:HA	1:L:58:VAL:HG21	2.02	0.41
2:H:183:SER:N	2:H:185:LEU:HD23	2.35	0.41
2:H:181:LEU:HA	2:H:185:LEU:O	2.20	0.41
2:H:209:ALA:O	2:H:211:PRO:HD3	2.21	0.41
2:H:24:ALA:HB1	2:H:27:TYR:CE2	2.56	0.41
2:H:220:LYS:HB2	2:H:220:LYS:HZ3	1.86	0.41
2:H:52:ASN:ND2	2:H:54:GLY:H	2.19	0.40
2:H:130:PRO:HD3	2:H:210:HIS:ND1	2.37	0.40
1:L:2:ILE:CD1	1:L:93:THR:HB	2.52	0.40

There are no symmetry-related clashes.

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	212/214 (99%)	189 (89%)	18 (8%)	5 (2%)	9	29
2	H	219/221 (99%)	181 (83%)	22 (10%)	16 (7%)	2	3
All	All	431/435 (99%)	370 (86%)	40 (9%)	21 (5%)	3	10

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	2	VAL
2	H	104	SER
2	H	107	ALA
2	H	108	VAL
2	H	142	THR
1	L	41	ASP
1	L	157	ASN
1	L	180	THR
2	H	55	LYS
2	H	105	ASP
2	H	110	TYR
2	H	203	THR
2	H	16	SER
2	H	169	SER
2	H	202	GLN
1	L	189	HIS
2	H	137	PRO
2	H	143	THR
2	H	182	GLN
2	H	134	PRO
1	L	28	ASP

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	192/192 (100%)	167 (87%)	25 (13%)	6	17
2	H	187/187 (100%)	157 (84%)	30 (16%)	3	10
All	All	379/379 (100%)	324 (86%)	55 (14%)	5	13

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	THR
1	L	19	VAL
1	L	20	THR
1	L	29	ILE
1	L	33	LEU
1	L	39	LYS
1	L	43	THR
1	L	45	LYS
1	L	47	LEU
1	L	79	GLU
1	L	80	HIS
1	L	93	THR
1	L	96	ARG
1	L	106	ILE
1	L	115	VAL
1	L	136	LEU
1	L	144	ILE
1	L	147	LYS
1	L	155	ARG
1	L	165	ASP
1	L	179	LEU
1	L	180	THR
1	L	187	GLU
1	L	197	THR
1	L	204	PRO
2	H	3	GLN
2	H	5	GLN
2	H	11	LEU
2	H	12	VAL

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Mol	Chain	Res	Type
2	H	20	MET
2	H	21	SER
2	H	25	SER
2	H	34	VAL
2	H	52	ASN
2	H	55	LYS
2	H	57	TYR
2	H	58	LEU
2	H	62	GLU
2	H	65	LYS
2	H	70	LEU
2	H	86	LEU
2	H	106	LEU
2	H	120	LEU
2	H	121	THR
2	H	126	LYS
2	H	134	PRO
2	H	137	PRO
2	H	142	THR
2	H	159	GLU
2	H	161	VAL
2	H	176	THR
2	H	178	PRO
2	H	181	LEU
2	H	185	LEU
2	H	220	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	137	ASN
1	L	198	HIS
1	L	212	ASN
2	H	5	GLN
2	H	52	ASN
2	H	82	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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.