Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:51 pm BST

PDB ID	:	5T5F
Title	:	Neisseria meningitidis factor H binding protein in complex with monoclonal antibody JAR5
Authors	:	Malito, E.
Deposited on	:	2016-08-30
Resolution	:	2.98 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
https://www.wwpdb.org/validation/2017/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:

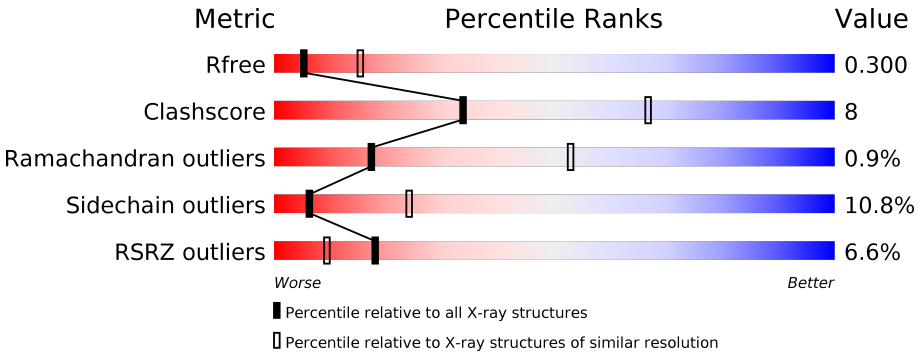
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.98 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}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 respectively. 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	253	11% 75% 12% • 11%
2	H	212	4% 66% 29% 5%
3	L	216	3% 73% 25% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5057 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 Factor H binding protein variant B24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1714	1064	309	340	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	256	LEU	-	expression tag	UNP Q6VRZ6

- Molecule 2 is a protein called Monoclonal antibody Jar5 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	212	Total	C	N	O	S	0	0	0
			1633	1046	265	314	8			

- Molecule 3 is a protein called Monoclonal antibody Jar5 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	216	Total	C	N	O	S	0	0	0
			1676	1049	285	334	8			

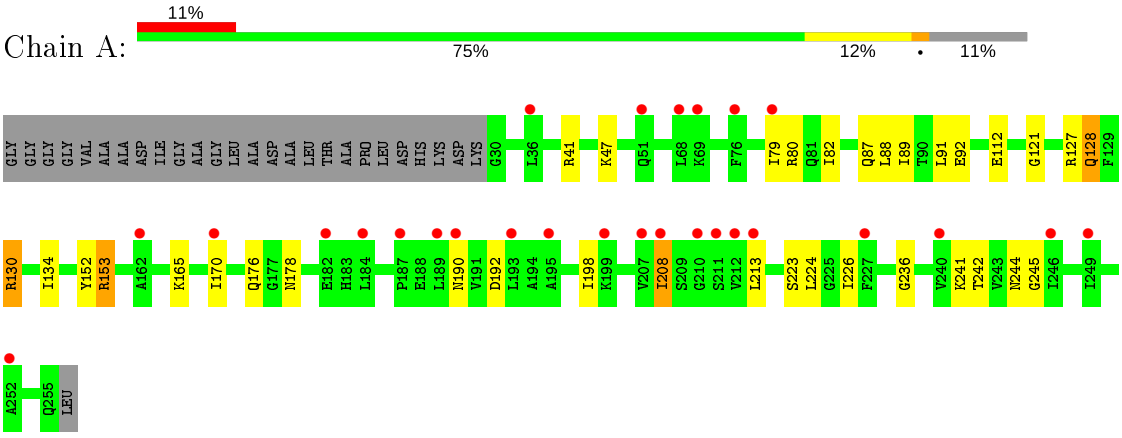
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	H	12	Total	O	0	0
			12	12		
4	L	11	Total	O	0	0
			11	11		

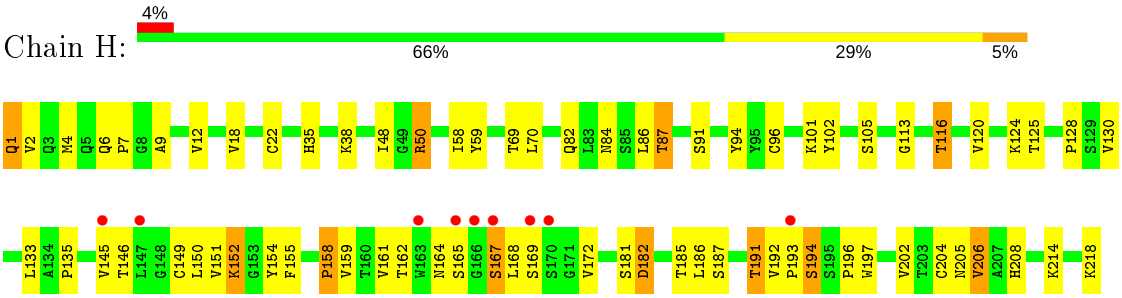
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

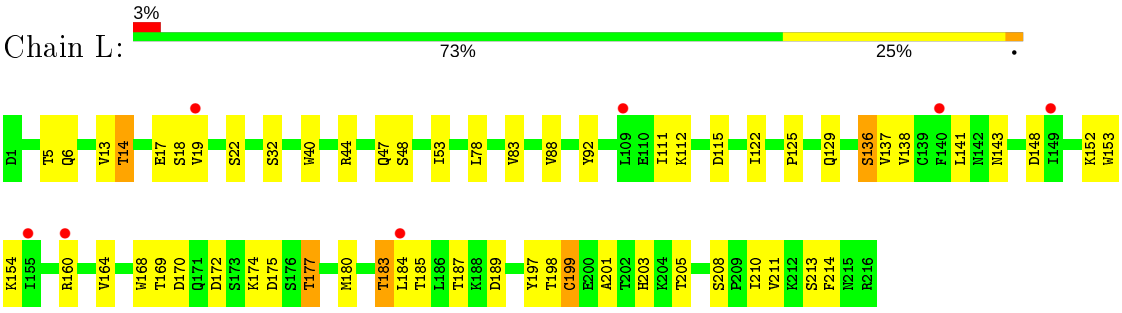
- Molecule 1: Factor H binding protein variant B24



- Molecule 2: Monoclonal antibody Jar5 heavy chain



- Molecule 3: Monoclonal antibody Jar5 light chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	65.37Å 146.49Å 218.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.70 – 2.98 59.70 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (59.70-2.98) 99.9 (59.70-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.223 , 0.273 0.246 , 0.300	Depositor DCC
R_{free} test set	1047 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	64.9	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 65.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5057	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.45	0/1737	0.70	0/2328
2	H	0.59	0/1681	0.79	0/2298
3	L	0.52	0/1716	0.74	0/2330
All	All	0.52	0/5134	0.74	0/6956

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	A	1714	0	1704	22	0
2	H	1633	0	1599	39	0
3	L	1676	0	1617	25	0
4	A	11	0	0	0	0
4	H	12	0	0	0	0
4	L	11	0	0	0	0
All	All	5057	0	4920	84	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 8.

All (84) 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:152:TYR:HE1	1:A:170:ILE:HG22	1.26	0.99
2:H:159:VAL:HG22	2:H:186:LEU:HD21	1.50	0.93
2:H:146:THR:HG22	2:H:191:THR:HB	1.59	0.84
1:A:152:TYR:HE1	1:A:170:ILE:CG2	1.91	0.82
1:A:152:TYR:CE1	1:A:170:ILE:HG22	2.14	0.81
2:H:159:VAL:CG2	2:H:186:LEU:HD21	2.14	0.76
3:L:172:ASP:OD1	3:L:174:LYS:HG2	1.90	0.71
2:H:193:PRO:HD2	2:H:196:PRO:HG2	1.76	0.67
1:A:89:ILE:HD11	2:H:105:SER:HB3	1.75	0.67
2:H:151:VAL:HG11	2:H:159:VAL:HG21	1.78	0.66
1:A:242:THR:HG22	1:A:245:GLY:O	1.97	0.65
1:A:152:TYR:CE1	1:A:170:ILE:CG2	2.77	0.63
2:H:4:MET:HB3	2:H:113:GLY:HA2	1.80	0.63
2:H:7:PRO:O	2:H:116:THR:HB	2.01	0.61
3:L:129:GLN:HE22	3:L:136:SER:HB2	1.65	0.60
1:A:153:ARG:HH12	1:A:165:LYS:HB3	1.65	0.60
2:H:4:MET:HG3	2:H:22:CYS:SG	2.42	0.60
1:A:80:ARG:HE	1:A:92:GLU:HG2	1.66	0.60
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.84	0.60
2:H:159:VAL:HG22	2:H:186:LEU:CD2	2.28	0.59
1:A:170:ILE:HD13	1:A:198:ILE:HD11	1.84	0.59
1:A:242:THR:HG23	1:A:244:ASN:H	1.68	0.59
3:L:44:ARG:HB2	3:L:47:GLN:NE2	2.19	0.57
1:A:47:LYS:HB3	1:A:79:ILE:HG13	1.88	0.55
2:H:159:VAL:HG12	2:H:208:HIS:HD2	1.71	0.55
2:H:9:ALA:HB2	2:H:158:PRO:HD3	1.88	0.55
3:L:40:TRP:HB2	3:L:53:ILE:HB	1.89	0.54
2:H:205:ASN:HD21	2:H:214:LYS:HG2	1.72	0.54
1:A:82:ILE:HG12	1:A:91:LEU:HD21	1.88	0.54
3:L:6:GLN:HE22	3:L:92:TYR:HA	1.73	0.54
2:H:6:GLN:HB3	2:H:116:THR:HG22	1.90	0.53
2:H:133:LEU:HD13	3:L:138:VAL:HG11	1.90	0.53
2:H:128:PRO:HB2	2:H:151:VAL:HG13	1.91	0.53
1:A:128:GLN:HE21	1:A:130:ARG:HG2	1.74	0.51
3:L:13:VAL:HG21	3:L:83:VAL:HG21	1.93	0.51
3:L:154:LYS:HB2	3:L:198:THR:HG23	1.93	0.50
3:L:169:THR:HG22	3:L:170:ASP:O	2.12	0.50
1:A:112:GLU:OE2	1:A:127:ARG:HD2	2.12	0.50
2:H:145:VAL:HG23	2:H:194:SER:HA	1.94	0.49
3:L:198:THR:HB	3:L:213:SER:CB	2.42	0.49
3:L:198:THR:HB	3:L:213:SER:HB2	1.93	0.49
3:L:44:ARG:HB2	3:L:47:GLN:HE21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:133:LEU:HD11	2:H:150:LEU:HB2	1.95	0.49
2:H:4:MET:HB3	2:H:113:GLY:CA	2.43	0.49
2:H:161:VAL:HG22	2:H:206:VAL:HB	1.94	0.49
1:A:134:ILE:HD13	1:A:236:GLY:HA2	1.94	0.48
2:H:87:THR:O	2:H:120:VAL:HG11	2.14	0.48
2:H:1:GLN:HG3	2:H:2:VAL:N	2.29	0.48
1:A:170:ILE:HD12	1:A:176:GLN:O	2.13	0.48
2:H:152:LYS:HA	2:H:185:THR:HG23	1.96	0.48
3:L:154:LYS:HB2	3:L:198:THR:CG2	2.45	0.46
2:H:151:VAL:HB	2:H:186:LEU:HG	1.96	0.46
1:A:47:LYS:HB3	1:A:79:ILE:CG1	2.46	0.46
3:L:14:THR:O	3:L:17:GLU:HB2	2.16	0.45
3:L:122:ILE:HD13	3:L:199:CYS:HB2	1.99	0.45
3:L:143:ASN:HA	3:L:177:THR:CG2	2.47	0.45
3:L:125:PRO:HD3	3:L:137:VAL:HG22	1.98	0.44
1:A:198:ILE:HD13	1:A:208:ILE:HB	2.00	0.44
2:H:38:LYS:HG3	2:H:94:TYR:CE2	2.53	0.44
1:A:192:ASP:HB2	1:A:213:LEU:HB2	1.99	0.44
3:L:160:ARG:HG2	3:L:184:LEU:HD21	1.99	0.44
2:H:159:VAL:HG12	2:H:208:HIS:CD2	2.50	0.44
2:H:101:LYS:HE2	2:H:102:TYR:CZ	2.52	0.43
3:L:201:ALA:HB3	3:L:210:ILE:HB	2.00	0.43
1:A:208:ILE:HG23	1:A:224:LEU:HB2	2.01	0.42
3:L:203:HIS:CD2	3:L:205:THR:HG22	2.54	0.42
1:A:47:LYS:HD2	1:A:79:ILE:HG12	2.01	0.42
3:L:153:TRP:NE1	3:L:164:VAL:HG21	2.34	0.42
3:L:138:VAL:HG23	3:L:183:THR:HG23	2.01	0.42
2:H:164:ASN:HB3	2:H:167:SER:HB2	2.02	0.42
2:H:197:TRP:HZ3	2:H:202:VAL:H	1.68	0.41
2:H:154:TYR:OH	2:H:186:LEU:HD23	2.20	0.41
2:H:35:HIS:CE1	2:H:50:ARG:HB2	2.55	0.41
2:H:130:VAL:HA	2:H:150:LEU:O	2.20	0.41
2:H:58:ILE:HG23	2:H:70:LEU:HD12	2.03	0.41
2:H:35:HIS:O	2:H:96:CYS:HA	2.20	0.41
2:H:125:THR:HA	2:H:155:PHE:O	2.21	0.41
2:H:50:ARG:HD2	2:H:59:TYR:HB2	2.02	0.41
3:L:175:ASP:CG	3:L:177:THR:HB	2.41	0.41
3:L:197:TYR:HB2	3:L:214:PHE:CE1	2.56	0.41
1:A:198:ILE:HD12	1:A:226:ILE:HD11	2.01	0.40
2:H:18:VAL:O	2:H:82:GLN:HA	2.21	0.40
3:L:13:VAL:O	3:L:111:ILE:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:86:LEU:HB3	2:H:120:VAL:HG21	2.01	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	224/253 (88%)	216 (96%)	7 (3%)	1 (0%)	34 70
2	H	208/212 (98%)	188 (90%)	16 (8%)	4 (2%)	8 33
3	L	214/216 (99%)	206 (96%)	7 (3%)	1 (0%)	29 66
All	All	646/681 (95%)	610 (94%)	30 (5%)	6 (1%)	17 53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	GLY
2	H	181	SER
3	L	115	ASP
2	H	135	PRO
2	H	182	ASP
2	H	158	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	177/192 (92%)	166 (94%)	11 (6%)	18 50
2	H	184/184 (100%)	159 (86%)	25 (14%)	3 15
3	L	192/192 (100%)	168 (88%)	24 (12%)	4 18
All	All	553/568 (97%)	493 (89%)	60 (11%)	6 24

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	87	GLN
1	A	88	LEU
1	A	128	GLN
1	A	130	ARG
1	A	153	ARG
1	A	178	ASN
1	A	190	ASN
1	A	208	ILE
1	A	223	SER
1	A	241	LYS
2	H	1	GLN
2	H	12	VAL
2	H	50	ARG
2	H	69	THR
2	H	84	ASN
2	H	87	THR
2	H	91	SER
2	H	116	THR
2	H	124	LYS
2	H	149	CYS
2	H	152	LYS
2	H	162	THR
2	H	165	SER
2	H	167	SER
2	H	168	LEU
2	H	169	SER
2	H	172	VAL
2	H	182	ASP
2	H	187	SER
2	H	191	THR
2	H	192	VAL
2	H	194	SER
2	H	204	CYS

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Mol	Chain	Res	Type
2	H	206	VAL
2	H	218	LYS
3	L	5	THR
3	L	14	THR
3	L	18	SER
3	L	19	VAL
3	L	22	SER
3	L	32	SER
3	L	48	SER
3	L	78	LEU
3	L	88	VAL
3	L	112	LYS
3	L	136	SER
3	L	141	LEU
3	L	148	ASP
3	L	152	LYS
3	L	168	TRP
3	L	177	THR
3	L	180	MET
3	L	183	THR
3	L	185	THR
3	L	187	THR
3	L	189	ASP
3	L	199	CYS
3	L	208	SER
3	L	211	VAL

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

Mol	Chain	Res	Type
2	H	1	GLN
2	H	82	GLN
2	H	164	ASN
2	H	205	ASN
3	L	6	GLN
3	L	47	GLN
3	L	203	HIS

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	136:GLY	C	143:SER	N	14.69

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	226/253 (89%)	0.99	27 (11%) 4 2	45, 81, 117, 128	0
2	H	212/212 (100%)	0.48	9 (4%) 36 21	31, 55, 99, 116	0
3	L	216/216 (100%)	0.56	7 (3%) 47 29	33, 60, 96, 105	0
All	All	654/681 (96%)	0.68	43 (6%) 18 9	31, 65, 110, 128	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	170	SER	8.0
2	H	167	SER	5.5
2	H	169	SER	4.8
1	A	210	GLY	4.2
3	L	155	ILE	4.0
2	H	165	SER	4.0
1	A	207	VAL	3.9
1	A	170	ILE	3.4
1	A	212	VAL	3.4
1	A	189	LEU	3.3
1	A	190	ASN	3.1
1	A	182	GLU	3.1
1	A	36	LEU	3.0
3	L	184	LEU	3.0
1	A	252	ALA	3.0
1	A	51	GLN	2.9
1	A	249	ILE	2.8
1	A	68	LEU	2.8
1	A	184	LEU	2.8
1	A	162	ALA	2.7
1	A	208	ILE	2.6
1	A	69	LYS	2.6
1	A	240	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	211	SER	2.5
3	L	160	ARG	2.5
2	H	145	VAL	2.5
1	A	193	LEU	2.5
2	H	166	GLY	2.5
3	L	109	LEU	2.5
2	H	193	PRO	2.4
1	A	199	LYS	2.4
2	H	163	TRP	2.3
1	A	187	PRO	2.3
3	L	149	ILE	2.3
3	L	19	VAL	2.3
1	A	195	ALA	2.3
1	A	79	ILE	2.3
1	A	246	ILE	2.1
2	H	147	LEU	2.1
3	L	140	PHE	2.1
1	A	227	PHE	2.1
1	A	213	LEU	2.0
1	A	76	PHE	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.