Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 10:11 PM EDT

PDB ID	:	1QBM
Title	:	FAB E8B ANTIBODY, X-RAY STRUCTURE AT 2.37 ANGSTROMS RESOLUTION
Authors	:	Mylvaganam, S.E.; Paterson, Y.; Getzoff, E.D.
Deposited on	:	1998-05-01
Resolution	:	2.37 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

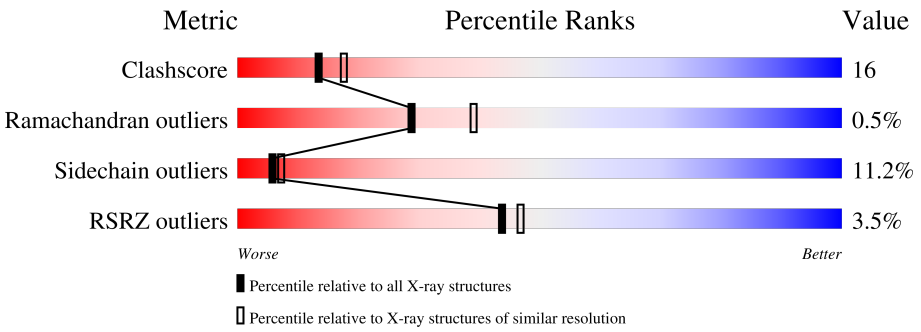
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

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

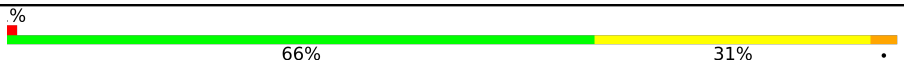
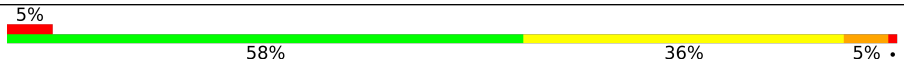
The reported resolution of this entry is 2.37 Å.

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	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 of 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	L	214	
2	H	219	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3444 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 E8B ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	214	1664	1038	282	337	7	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	85	SER	THR	conflict	GB 2072141
L	89	GLN	HIS	conflict	GB 2072141
L	106	ILE	VAL	conflict	GB 2072141
L	118	PHE	LEU	conflict	GB 2072141

- Molecule 2 is a protein called E8B ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	219	1653	1044	268	334	7	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	3	GLN	LYS	conflict	PIR S49220
H	5	GLN	LEU	conflict	PIR S49220
H	6	GLN	GLU	conflict	PIR S49220
H	14	PRO	SER	conflict	PIR S49220
H	43	LYS	GLN	conflict	PIR S49220
H	55	SER	ASN	conflict	PIR S49220
H	57	ASN	GLU	conflict	PIR S49220
H	58	THR	ILE	conflict	PIR S49220
H	66	ASP	GLY	conflict	PIR S49220
H	67	LYS	THR	conflict	PIR S49220
H	76	SER	THR	conflict	PIR S49220
H	?	-	VAL	deletion	PIR S49220

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ARG	deletion	PIR S49220
H	97	ALA	ARG	conflict	PIR S49220
H	100	ASP	GLY	conflict	PIR S49220
H	101	TYR	SER	conflict	PIR S49220
H	102	GLY	SER	conflict	PIR S49220
H	103	ASN	GLN	conflict	PIR S49220
H	104	PHE	GLU	conflict	PIR S49220
H	105	ASP	PRO	conflict	PIR S49220
H	119	GLU	LYS	conflict	PIR S49220
H	132	THR	SER	conflict	PIR S49220
H	135	LEU	GLN	conflict	PIR S49220
H	136	LYS	THR	conflict	PIR S49220
H	137	SER	ASN	conflict	PIR S49220
H	195	GLN	GLU	conflict	PIR S49220
H	218	ASN	ASP	conflict	PIR S49220

- Molecule 3 is water.

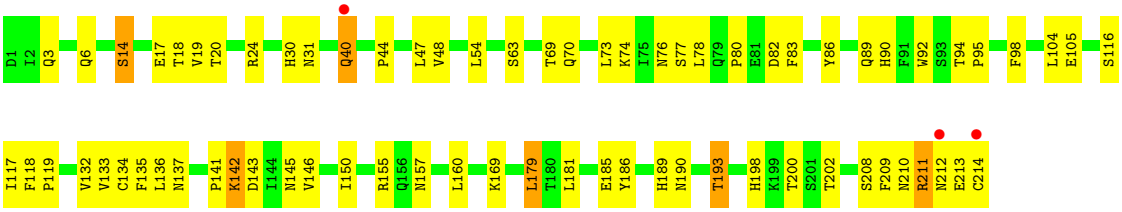
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	L	81	81	81	0	0
			Total	O		
3	H	46	46	46	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

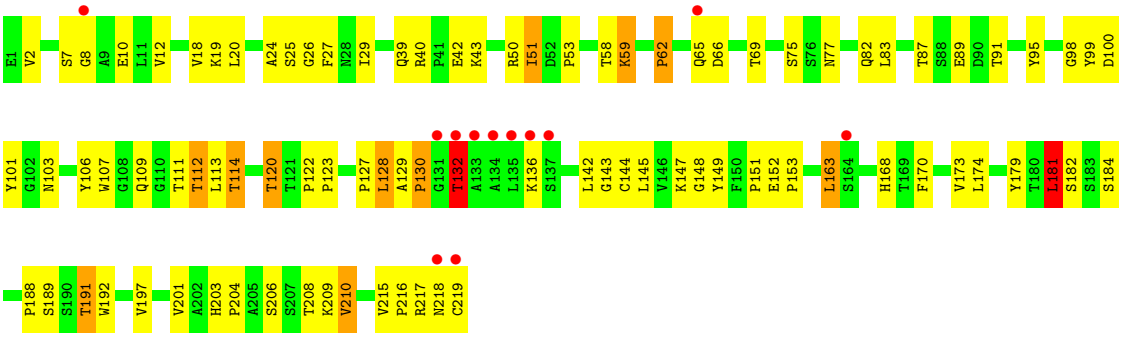
- Molecule 1: E8B ANTIBODY

Chain L:



- Molecule 2: E8B ANTIBODY

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.96Å 85.01Å 63.33Å 90.00° 105.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.37 9.97 – 2.37	Depositor EDS
% Data completeness (in resolution range)	82.8 (10.00-2.37) 82.9 (9.97-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.194 , 0.269 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 53.5	EDS
L-test for twinning[1]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3444	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]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 (i)

5.1 Standard geometry (i)

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	0.62	0/1705	0.84	0/2315
2	H	0.56	0/1696	0.90	4/2321 (0.2%)
All	All	0.59	0/3401	0.87	4/4636 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	132	THR	N-CA-C	7.31	130.75	111.00
2	H	130	PRO	N-CA-C	5.38	126.09	112.10
2	H	209	LYS	N-CA-C	-5.29	96.72	111.00
2	H	181	LEU	CA-CB-CG	5.12	127.08	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1664	0	1581	54	0
2	H	1653	0	1606	56	0
3	H	46	0	0	3	0
3	L	81	0	0	1	0
All	All	3444	0	3187	105	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 16.

All (105) 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:L:47:LEU:HD11	1:L:86:TYR:HE1	1.48	0.78
2:H:51:ILE:HG12	2:H:58:THR:HG22	1.64	0.77
2:H:151:PRO:O	2:H:203:HIS:HE1	1.67	0.76
2:H:123:PRO:HB3	2:H:149:TYR:HB3	1.72	0.71
1:L:70:GLN:HB2	3:L:251:HOH:O	1.91	0.70
1:L:186:TYR:CZ	1:L:211:ARG:HG3	2.27	0.69
2:H:112:THR:HG22	3:H:247:HOH:O	1.92	0.68
2:H:24:ALA:HB1	2:H:27:PHE:CE1	2.29	0.67
1:L:40:GLN:NE2	1:L:40:GLN:H	1.93	0.66
1:L:132:VAL:CG1	1:L:209:PHE:HE2	2.09	0.66
1:L:47:LEU:HD11	1:L:86:TYR:CE1	2.30	0.66
1:L:90:HIS:HD2	1:L:92:TRP:H	1.44	0.66
1:L:141:PRO:O	1:L:198:HIS:HE1	1.77	0.65
1:L:142:LYS:HD3	1:L:142:LYS:H	1.60	0.65
1:L:210:ASN:HB2	1:L:213:GLU:HB2	1.79	0.64
1:L:18:THR:HG23	1:L:76:ASN:HA	1.82	0.62
2:H:50:ARG:HH11	2:H:50:ARG:HG3	1.65	0.62
2:H:51:ILE:O	2:H:53:PRO:HD3	2.00	0.61
2:H:91:THR:HG23	2:H:114:THR:HA	1.84	0.60
1:L:136:LEU:HD12	1:L:136:LEU:N	2.17	0.59
1:L:214:CYS:SG	2:H:218:ASN:O	2.61	0.58
1:L:48:VAL:HG22	1:L:54:LEU:HD12	1.84	0.58
1:L:78:LEU:HD21	1:L:104:LEU:HD21	1.86	0.57
1:L:44:PRO:HD2	2:H:107:TRP:CE3	2.40	0.57
1:L:19:VAL:O	1:L:74:LYS:HA	2.05	0.56
2:H:123:PRO:CB	2:H:149:TYR:HB3	2.35	0.56
1:L:190:ASN:O	1:L:210:ASN:HA	2.07	0.55
2:H:2:VAL:HB	2:H:106:TYR:CE2	2.41	0.55
2:H:147:LYS:HG2	2:H:148:GLY:N	2.21	0.54
1:L:155:ARG:HG2	1:L:179:LEU:HD21	1.90	0.54
2:H:123:PRO:CA	2:H:149:TYR:HB3	2.37	0.54
2:H:114:THR:HG21	2:H:179:TYR:OH	2.08	0.54
1:L:20:THR:HA	1:L:73:LEU:O	2.08	0.54
1:L:70:GLN:HA	1:L:70:GLN:OE1	2.09	0.53
1:L:80:PRO:O	1:L:83:PHE:HD2	1.92	0.53
1:L:40:GLN:HE21	1:L:40:GLN:N	2.07	0.53
1:L:24:ARG:HA	1:L:69:THR:O	2.09	0.52
1:L:116:SER:O	1:L:134:CYS:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:ARG:HG3	2:H:50:ARG:NH1	2.25	0.51
1:L:136:LEU:HD21	1:L:146:VAL:HG22	1.92	0.51
1:L:118:PHE:CE1	1:L:135:PHE:CD2	2.99	0.51
2:H:181:LEU:C	2:H:181:LEU:HD12	2.31	0.50
1:L:132:VAL:HG13	1:L:209:PHE:HE2	1.74	0.50
1:L:210:ASN:CB	1:L:213:GLU:HB2	2.41	0.50
2:H:69:THR:HB	2:H:82:GLN:HB3	1.94	0.50
1:L:133:VAL:HG12	1:L:134:CYS:N	2.27	0.50
1:L:137:ASN:HD21	2:H:170:PHE:HZ	1.58	0.49
1:L:132:VAL:HG11	1:L:209:PHE:HE2	1.75	0.49
1:L:198:HIS:HD2	1:L:200:THR:OG1	1.95	0.49
1:L:185:GLU:O	1:L:189:HIS:HD2	1.95	0.49
1:L:40:GLN:NE2	1:L:40:GLN:N	2.61	0.49
2:H:87:THR:HG22	2:H:89:GLU:H	1.78	0.48
2:H:144:CYS:O	2:H:182:SER:HA	2.14	0.48
2:H:142:LEU:HD12	2:H:197:VAL:HG11	1.96	0.48
2:H:62:PRO:O	2:H:65:GLN:HG2	2.13	0.47
1:L:132:VAL:HG13	1:L:209:PHE:CE2	2.48	0.47
2:H:114:THR:HG22	2:H:174:LEU:HD22	1.97	0.47
2:H:10:GLU:HB2	2:H:113:LEU:CD1	2.45	0.47
1:L:30:HIS:O	1:L:31:ASN:HB2	2.14	0.46
1:L:14:SER:O	1:L:17:GLU:HB2	2.15	0.46
2:H:10:GLU:HB2	2:H:113:LEU:HD12	1.97	0.46
2:H:204:PRO:HA	3:H:262:HOH:O	2.15	0.46
2:H:40:ARG:HB2	2:H:43:LYS:HB2	1.98	0.45
2:H:188:PRO:HD2	2:H:191:THR:OG1	2.16	0.45
2:H:128:LEU:HB2	2:H:143:GLY:O	2.16	0.45
2:H:100:ASP:CG	2:H:101:TYR:H	2.20	0.45
2:H:29:ILE:HG12	2:H:77:ASN:OD1	2.17	0.44
2:H:201:VAL:HG22	2:H:210:VAL:HG13	1.99	0.44
1:L:90:HIS:HD2	1:L:92:TRP:N	2.12	0.44
2:H:127:PRO:O	2:H:127:PRO:HG2	2.18	0.44
2:H:65:GLN:HG3	2:H:66:ASP:N	2.33	0.44
1:L:78:LEU:HD23	1:L:82:ASP:HB2	2.00	0.44
2:H:39:GLN:HE21	2:H:95:TYR:HE2	1.64	0.44
2:H:122:PRO:HB3	2:H:208:THR:OG1	2.17	0.44
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.53	0.43
2:H:51:ILE:HG12	2:H:58:THR:CG2	2.41	0.43
2:H:168:HIS:HB2	2:H:184:SER:OG	2.18	0.43
2:H:217:ARG:C	2:H:219:CYS:H	2.21	0.43
2:H:163:LEU:HD12	2:H:163:LEU:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:8:GLY:O	2:H:111:THR:HG23	2.19	0.43
2:H:39:GLN:NE2	2:H:95:TYR:HE2	2.17	0.42
2:H:129:ALA:HA	2:H:130:PRO:HD3	1.71	0.42
1:L:117:ILE:HA	1:L:133:VAL:O	2.20	0.42
1:L:160:LEU:HD21	2:H:173:VAL:CG1	2.49	0.42
1:L:150:ILE:HD11	1:L:181:LEU:HD21	2.00	0.42
2:H:59:LYS:HA	3:H:220:HOH:O	2.19	0.42
2:H:192:TRP:CZ2	2:H:216:PRO:HG3	2.55	0.42
1:L:118:PHE:HE1	1:L:135:PHE:CD2	2.37	0.42
1:L:90:HIS:CE1	1:L:95:PRO:O	2.73	0.42
1:L:94:THR:OG1	2:H:59:LYS:HG2	2.20	0.42
1:L:193:THR:HB	1:L:208:SER:OG	2.20	0.42
2:H:128:LEU:HB2	2:H:143:GLY:C	2.40	0.42
1:L:40:GLN:H	1:L:40:GLN:CD	2.23	0.42
1:L:133:VAL:CG1	1:L:134:CYS:N	2.84	0.41
1:L:89:GLN:HB2	1:L:98:PHE:CE1	2.56	0.41
2:H:18:VAL:HG22	2:H:19:LYS:N	2.35	0.41
1:L:119:PRO:HB3	1:L:209:PHE:CE1	2.56	0.41
1:L:155:ARG:CG	1:L:179:LEU:HD21	2.49	0.41
1:L:19:VAL:HG11	1:L:104:LEU:HD11	2.03	0.41
2:H:98:GLY:O	2:H:99:TYR:HB3	2.21	0.41
2:H:147:LYS:HG2	2:H:148:GLY:H	1.85	0.40
2:H:203:HIS:CD2	2:H:206:SER:OG	2.74	0.40
2:H:20:LEU:HD22	2:H:111:THR:HG21	2.03	0.40
1:L:6:GLN:NE2	1:L:86:TYR:O	2.54	0.40
2:H:26:GLY:O	2:H:27:PHE:HB3	2.21	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	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
2	H	217/219 (99%)	198 (91%)	17 (8%)	2 (1%)	17	23
All	All	429/433 (99%)	399 (93%)	28 (6%)	2 (0%)	29	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	132	THR
2	H	120	THR

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	188/188 (100%)	172 (92%)	16 (8%)	10	14
2	H	188/188 (100%)	162 (86%)	26 (14%)	3	4
All	All	376/376 (100%)	334 (89%)	42 (11%)	6	7

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	GLN
1	L	14	SER
1	L	40	GLN
1	L	63	SER
1	L	77	SER
1	L	105	GLU
1	L	142	LYS
1	L	143	ASP
1	L	145	ASN
1	L	157	ASN
1	L	169	LYS
1	L	179	LEU
1	L	193	THR
1	L	202	THR

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Mol	Chain	Res	Type
1	L	211	ARG
1	L	212	ASN
2	H	7	SER
2	H	12	VAL
2	H	25	SER
2	H	42	GLU
2	H	51	ILE
2	H	59	LYS
2	H	62	PRO
2	H	75	SER
2	H	83	LEU
2	H	103	ASN
2	H	109	GLN
2	H	112	THR
2	H	114	THR
2	H	120	THR
2	H	128	LEU
2	H	132	THR
2	H	136	LYS
2	H	145	LEU
2	H	152	GLU
2	H	153	PRO
2	H	163	LEU
2	H	181	LEU
2	H	189	SER
2	H	191	THR
2	H	210	VAL
2	H	215	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	40	GLN
1	L	90	HIS
1	L	137	ASN
1	L	198	HIS
1	L	210	ASN
1	L	212	ASN
2	H	39	GLN
2	H	57	ASN
2	H	103	ASN

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Mol	Chain	Res	Type
2	H	203	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	L	214/214 (100%)	-0.27	3 (1%)	75	77	13, 30, 52, 92	0
2	H	219/219 (100%)	0.09	12 (5%)	25	27	16, 38, 70, 100	0
All	All	433/433 (100%)	-0.08	15 (3%)	44	47	13, 33, 62, 100	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	133	ALA	6.4
2	H	219	CYS	5.6
2	H	135	LEU	4.1
2	H	137	SER	3.8
1	L	212	ASN	3.3
2	H	134	ALA	2.9
1	L	214	CYS	2.7
2	H	136	LYS	2.5
2	H	132	THR	2.5
2	H	8	GLY	2.5
1	L	40	GLN	2.3
2	H	131	GLY	2.3
2	H	164	SER	2.3
2	H	218	ASN	2.2
2	H	65	GLN	2.1

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 monosaccharides 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.