Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2023 – 06:05 PM EDT

PDB ID	:	8DKF
Title	:	Antibody DH1030.1 Fab fragment
Authors	:	Gobeil, S.; Acharya, P.
Deposited on	:	2022-07-05
Resolution	:	1.79 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

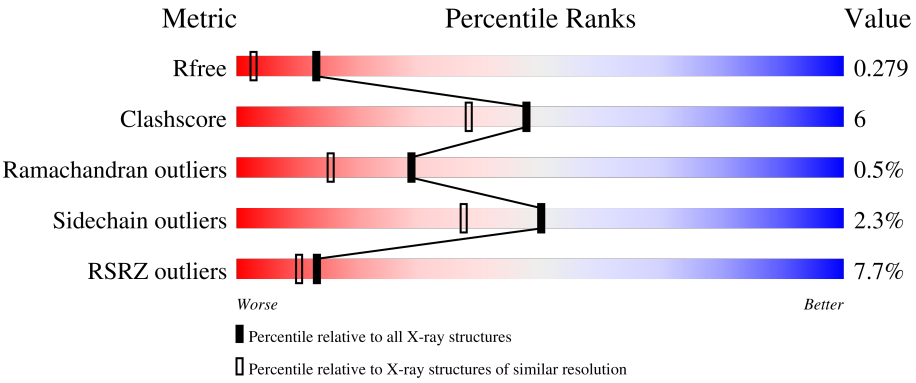
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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	A	230	5% 83% 13%
1	H	230	5% 86% 10%
2	B	219	8% 85% 13%
2	L	219	12% 83% 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7234 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 DH1030.1 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	225	Total	C	N	O	S	0	0	0
			1725	1083	300	336	6			
1	A	225	Total	C	N	O	S	0	0	0
			1719	1080	297	336	6			

- Molecule 2 is a protein called DH1030.1 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	217	Total	C	N	O	S	0	1	0
			1682	1055	288	334	5			
2	B	217	Total	C	N	O	S	0	1	0
			1679	1052	287	335	5			

- Molecule 3 is water.

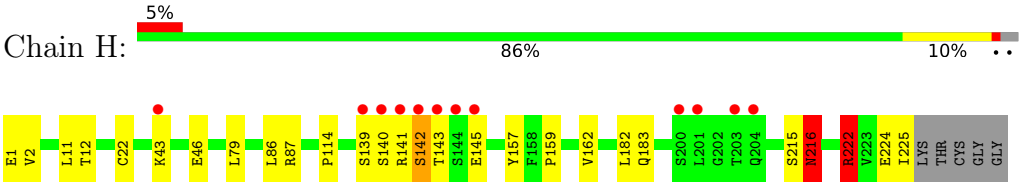
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	118	Total	O	0	0
			118	118		
3	L	98	Total	O	0	0
			98	98		
3	A	110	Total	O	0	0
			110	110		
3	B	103	Total	O	0	0
			103	103		

3 Residue-property plots

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.

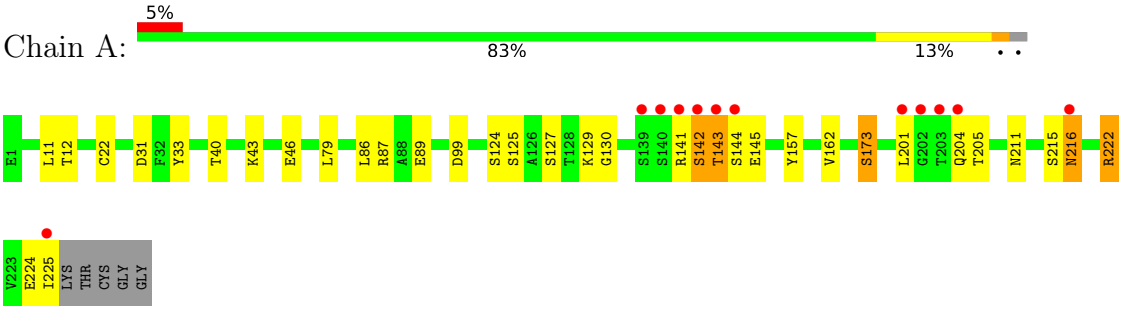
• Molecule 1: DH1030.1 Heavy chain

Chain H:



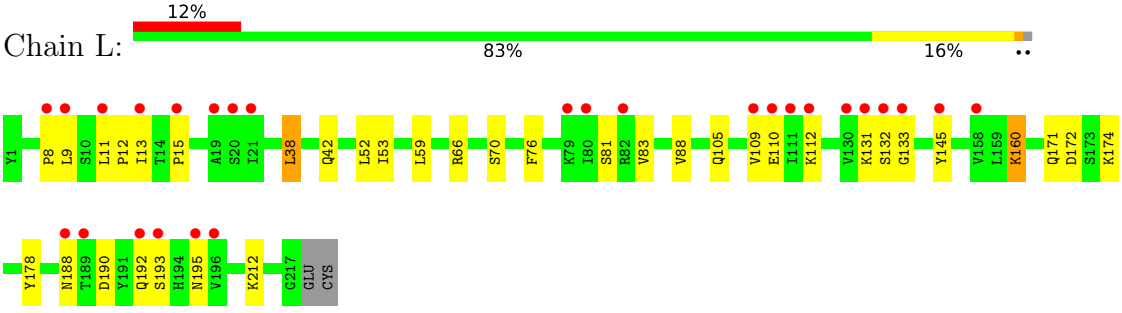
• Molecule 1: DH1030.1 Heavy chain

Chain A:



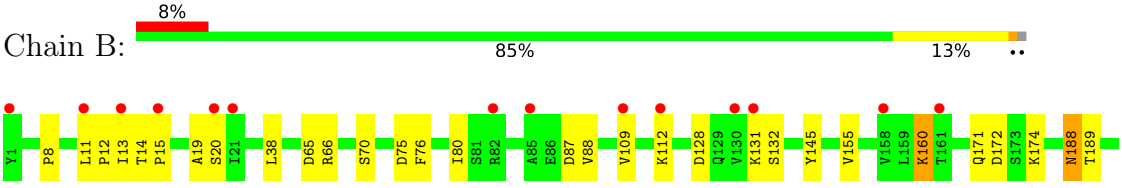
• Molecule 2: DH1030.1 Light chain

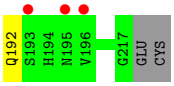
Chain L:



• Molecule 2: DH1030.1 Light chain

Chain B:




Q192
S193
H194
N195
V196
G217
GLU
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.19Å 103.12Å 109.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.52 – 1.79 43.52 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.52-1.79) 98.4 (43.52-1.79)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.239 , 0.274 0.240 , 0.279	Depositor DCC
R_{free} test set	1990 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7234	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 94.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9306e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.50	1/1763 (0.1%)	0.66	0/2403
1	H	0.51	3/1769 (0.2%)	0.68	4/2410 (0.2%)
2	B	0.31	0/1721	0.57	0/2342
2	L	0.34	0/1724	0.58	1/2345 (0.0%)
All	All	0.43	4/6977 (0.1%)	0.62	5/9500 (0.1%)

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	A	0	1
1	H	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	ASN	CB-CG	-13.02	1.21	1.51
1	H	216	ASN	CB-CG	-10.62	1.26	1.51
1	H	222	ARG	CZ-NH1	8.84	1.44	1.33
1	H	222	ARG	CZ-NH2	7.79	1.43	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	222	ARG	NE-CZ-NH2	-7.45	116.57	120.30
2	L	131	LYS	CB-CG-CD	-6.69	94.22	111.60
1	H	222	ARG	NH1-CZ-NH2	5.66	125.63	119.40
1	H	216	ASN	CA-CB-CG	-5.60	101.09	113.40
1	H	222	ARG	NE-CZ-NH1	-5.06	117.77	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ARG	Sidechain
1	H	222	ARG	Sidechain

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	A	1719	0	1657	23	0
1	H	1725	0	1668	17	0
2	B	1679	0	1633	23	0
2	L	1682	0	1641	20	0
3	A	110	0	0	1	0
3	B	103	0	0	1	0
3	H	118	0	0	2	0
3	L	98	0	0	0	0
All	All	7234	0	6599	82	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 6.

All (82) 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:H:1:GLU:OE2	3:H:301:HOH:O	1.98	0.81
2:B:131:LYS:O	2:B:131:LYS:HG2	1.88	0.73
1:H:222:ARG:HD2	1:H:224:GLU:HG3	1.74	0.70
2:B:188:ASN:OD1	2:B:189:THR:N	2.25	0.69
2:L:172:ASP:OD1	2:L:174:LYS:N	2.26	0.66
1:A:142:SER:O	1:A:144:SER:N	2.28	0.65
1:H:215:SER:O	1:H:216:ASN:HB2	1.95	0.64
1:H:12:THR:HG21	1:H:86:LEU:HD13	1.81	0.63
2:B:172:ASP:OD1	2:B:174:LYS:N	2.28	0.63
2:B:88:VAL:HG21	2:B:171:GLN:HB3	1.80	0.62
1:H:222:ARG:CD	1:H:224:GLU:HG3	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:8:PRO:HG2	2:L:11:LEU:HG	1.83	0.60
2:L:53:ILE:HD13	2:L:59:LEU:HD23	1.82	0.60
2:L:88:VAL:HG21	2:L:171:GLN:HB3	1.82	0.60
2:B:128:ASP:OD2	3:B:301:HOH:O	2.15	0.59
1:A:225:ILE:H	1:A:225:ILE:HD12	1.66	0.59
2:L:53:ILE:CD1	2:L:59:LEU:HD23	2.33	0.58
1:H:2:VAL:HG12	1:H:114:PRO:HG3	1.87	0.55
1:A:225:ILE:HD12	1:A:225:ILE:N	2.22	0.55
2:L:15:PRO:HA	2:L:83:VAL:HG23	1.89	0.54
1:A:43:LYS:HE3	1:A:46:GLU:OE1	2.08	0.54
1:H:225:ILE:HD12	1:H:225:ILE:N	2.23	0.54
1:A:222:ARG:CD	1:A:224:GLU:HG3	2.39	0.53
2:B:8:PRO:HG2	2:B:11:LEU:HG	1.90	0.52
1:H:141:ARG:O	1:H:143:THR:N	2.40	0.52
2:B:160:LYS:HA	2:B:160:LYS:HE2	1.90	0.52
2:B:112:LYS:HA	2:B:145:TYR:OH	2.09	0.52
1:A:11:LEU:HD11	1:A:124:SER:HB3	1.90	0.51
2:B:160:LYS:HE2	2:B:160:LYS:CA	2.41	0.50
2:B:188:ASN:O	2:B:192:GLN:HG2	2.12	0.50
1:H:225:ILE:HD12	1:H:225:ILE:H	1.76	0.50
2:B:13:ILE:HD12	2:B:109:VAL:HG13	1.94	0.50
1:A:204:GLN:NE2	1:A:205:THR:HG22	2.27	0.50
1:A:215:SER:O	1:A:216:ASN:CB	2.58	0.49
2:L:132:SER:OG	2:L:133:GLY:N	2.45	0.49
2:B:80:ILE:HD12	2:B:80:ILE:N	2.27	0.49
2:B:66:ARG:NH2	2:B:87:ASP:OD1	2.41	0.48
1:A:142:SER:OG	1:A:145:GLU:HB2	2.14	0.47
2:B:112:LYS:HD3	2:B:145:TYR:OH	2.14	0.47
1:A:222:ARG:HD3	1:A:224:GLU:HG3	1.96	0.46
1:A:33:TYR:HB2	1:A:99:ASP:HB3	1.98	0.46
2:L:13:ILE:HD12	2:L:109:VAL:HG13	1.97	0.45
1:H:157:TYR:CE2	1:H:162:VAL:HG13	2.52	0.45
2:B:12:PRO:HB2	2:B:112:LYS:NZ	2.32	0.45
1:A:201:LEU:HD12	1:A:201:LEU:N	2.32	0.45
1:H:11:LEU:HB2	1:H:159:PRO:HG3	1.98	0.45
2:B:131:LYS:O	2:B:132:SER:OG	2.21	0.45
1:H:87:ARG:NH2	1:A:31:ASP:OD2	2.43	0.45
2:L:171:GLN:HG3	2:L:178:TYR:CZ	2.52	0.45
1:A:87:ARG:HB3	1:A:89:GLU:OE1	2.17	0.45
1:H:142:SER:O	1:H:142:SER:OG	2.29	0.44
2:L:42:GLN:HB2	2:L:52:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:THR:OG1	1:A:43:LYS:HG2	2.17	0.44
2:L:190:ASP:O	2:L:193:SER:HB3	2.18	0.44
1:A:12:THR:HG21	1:A:86:LEU:CD1	2.47	0.44
2:B:15:PRO:HD3	2:B:112:LYS:O	2.18	0.44
1:A:141:ARG:O	1:A:143:THR:N	2.51	0.44
2:L:188:ASN:O	2:L:192:GLN:HG2	2.18	0.43
1:A:12:THR:HG21	1:A:86:LEU:HD13	1.99	0.43
1:H:22:CYS:HB3	1:H:79:LEU:HB3	2.00	0.43
2:L:112[A]:LYS:HA	2:L:145:TYR:OH	2.18	0.43
2:B:12:PRO:HB2	2:B:112:LYS:CE	2.49	0.43
2:L:112[B]:LYS:HA	2:L:145:TYR:OH	2.18	0.42
2:L:160:LYS:CE	2:L:160:LYS:HA	2.49	0.42
1:A:22:CYS:HB3	1:A:79:LEU:HB3	2.01	0.42
1:A:173:SER:O	3:A:301:HOH:O	2.22	0.42
1:H:43:LYS:NZ	1:H:46:GLU:OE1	2.51	0.42
1:H:182:LEU:HD13	1:H:183:GLN:O	2.18	0.42
2:L:9:LEU:HD11	2:L:105:GLN:HE21	1.84	0.42
2:B:155:VAL:HG11	2:B:160:LYS:HE3	2.02	0.42
2:B:12:PRO:HB2	2:B:112:LYS:HE2	2.02	0.41
2:B:160:LYS:HA	2:B:160:LYS:CE	2.51	0.41
2:L:212:LYS:HA	2:L:212:LYS:HD3	1.88	0.41
1:H:141:ARG:NH1	3:H:310:HOH:O	2.52	0.41
1:A:204:GLN:OE1	1:A:204:GLN:HA	2.20	0.41
2:B:38:LEU:HD13	2:B:76:PHE:CD1	2.55	0.41
2:L:12:PRO:HA	2:L:110:GLU:HG3	2.03	0.41
1:A:157:TYR:CE2	1:A:162:VAL:HG13	2.56	0.40
2:B:13:ILE:HD13	2:B:19:ALA:HB2	2.04	0.40
2:L:38:LEU:HD13	2:L:76:PHE:CD1	2.56	0.40
2:L:66:ARG:HB2	2:L:81:SER:HB3	2.03	0.40
1:A:129:LYS:HG2	1:A:130:GLY:O	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	A	223/230 (97%)	212 (95%)	9 (4%)	2 (1%)	17 6
1	H	223/230 (97%)	211 (95%)	10 (4%)	2 (1%)	17 6
2	B	216/219 (99%)	207 (96%)	9 (4%)	0	100 100
2	L	216/219 (99%)	213 (99%)	3 (1%)	0	100 100
All	All	878/898 (98%)	843 (96%)	31 (4%)	4 (0%)	29 15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	THR
1	H	216	ASN
1	A	142	SER
1	H	142	SER

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	191/195 (98%)	187 (98%)	4 (2%)	53 42
1	H	192/195 (98%)	189 (98%)	3 (2%)	62 54
2	B	193/194 (100%)	186 (96%)	7 (4%)	35 20
2	L	193/194 (100%)	189 (98%)	4 (2%)	53 42
All	All	769/778 (99%)	751 (98%)	18 (2%)	50 37

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	139	SER
1	H	140	SER
1	H	145	GLU
2	L	38	LEU

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Mol	Chain	Res	Type
2	L	70	SER
2	L	160	LYS
2	L	195	ASN
1	A	125	SER
1	A	127	SER
1	A	173	SER
1	A	211	ASN
2	B	14	THR
2	B	20	SER
2	B	65	ASP
2	B	70	SER
2	B	75	ASP
2	B	160	LYS
2	B	188	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	211	ASN

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

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	225/230 (97%)	0.67	12 (5%) 26 21	21, 35, 67, 82	0
1	H	225/230 (97%)	0.64	12 (5%) 26 21	20, 33, 69, 84	0
2	B	217/219 (99%)	0.73	17 (7%) 13 10	23, 39, 64, 70	0
2	L	217/219 (99%)	0.84	27 (12%) 4 3	23, 38, 63, 73	0
All	All	884/898 (98%)	0.72	68 (7%) 13 10	20, 37, 65, 84	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	141	ARG	7.9
1	H	142	SER	6.8
1	A	144	SER	6.1
2	L	11	LEU	5.8
1	A	142	SER	5.8
1	H	144	SER	5.7
1	H	140	SER	5.4
1	H	203	THR	5.3
1	A	140	SER	5.0
2	L	131	LYS	4.6
2	L	82	ARG	4.4
2	B	11	LEU	4.3
2	B	13	ILE	4.2
2	L	13	ILE	4.2
2	L	130	VAL	4.2
2	B	196	VAL	4.1
1	A	139	SER	4.0
2	B	130	VAL	4.0
1	A	203	THR	4.0
2	L	193	SER	4.0
1	A	143	THR	3.9

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Mol	Chain	Res	Type	RSRZ
2	L	132	SER	3.9
1	A	202	GLY	3.8
1	H	204	GLN	3.6
2	L	195	ASN	3.5
2	L	158	VAL	3.4
1	A	204	GLN	3.4
2	L	21	ILE	3.3
1	H	139	SER	3.0
2	L	15	PRO	3.0
2	B	112	LYS	2.9
2	B	161	THR	2.8
2	B	131	LYS	2.8
2	B	15	PRO	2.7
1	H	143	THR	2.7
1	A	225	ILE	2.7
2	L	9	LEU	2.6
2	L	109	VAL	2.6
2	B	20	SER	2.6
2	L	80	ILE	2.6
2	L	192	GLN	2.6
2	B	82	ARG	2.5
2	L	145	TYR	2.5
1	A	141	ARG	2.5
2	L	189	THR	2.5
1	H	200	SER	2.4
2	B	109	VAL	2.4
1	H	201	LEU	2.4
2	B	193	SER	2.4
2	L	8	PRO	2.4
2	L	196	VAL	2.4
2	L	133	GLY	2.4
1	A	201	LEU	2.3
1	A	216	ASN	2.3
2	L	110	GLU	2.3
2	B	1	TYR	2.3
2	L	79	LYS	2.3
2	L	20	SER	2.3
2	L	19	ALA	2.3
2	B	158	VAL	2.2
2	B	21	ILE	2.2
1	H	43	LYS	2.1
2	L	112[A]	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	195	ASN	2.1
2	L	111	ILE	2.1
1	H	145	GLU	2.1
2	B	85	ALA	2.0
2	L	188	ASN	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 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.