Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:35 PM GMT

PDB ID	:	5AAM
Title	:	Structure of a redesigned cross-reactive antibody to dengue virus with increased in vivo potency
Authors	:	Wong, Y.H.; Robinson, L.N.; Lescar, J.; Sasisekharan, R.
Deposited on	:	2015-07-27
Resolution	:	2.49 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 (1)) were used in the production of this report:

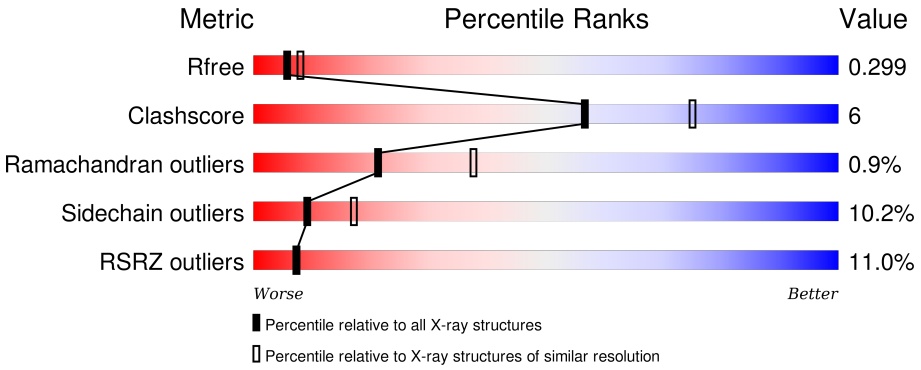
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.49 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	251	5% 73% 15% • 9%
1	B	251	% 71% 17% • 10%
2	C	115	34% 60% 22% • 17%
2	J	115	14% 68% 15% • 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5137 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 SCFV513.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1775	1113	306	346	10			
1	B	227	Total	C	N	O	S	0	0	0
			1773	1113	306	344	10			

- Molecule 2 is a protein called ENVELOPE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	95	Total	C	N	O	S	0	0	0
			725	458	123	140	4			
2	J	96	Total	C	N	O	S	0	0	0
			737	467	124	142	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	292	MET	-	EXPRESSION TAG	UNP U3N5N6
C	401	HIS	-	EXPRESSION TAG	UNP U3N5N6
C	402	HIS	-	EXPRESSION TAG	UNP U3N5N6
C	403	HIS	-	EXPRESSION TAG	UNP U3N5N6
C	404	HIS	-	EXPRESSION TAG	UNP U3N5N6
C	405	HIS	-	EXPRESSION TAG	UNP U3N5N6
C	406	HIS	-	EXPRESSION TAG	UNP U3N5N6
C	357	LEU	PHE	CONFLICT	UNP U3N5N6
C	384	ASN	ASP	CONFLICT	UNP U3N5N6
J	292	MET	-	EXPRESSION TAG	UNP U3N5N6
J	401	HIS	-	EXPRESSION TAG	UNP U3N5N6
J	402	HIS	-	EXPRESSION TAG	UNP U3N5N6
J	403	HIS	-	EXPRESSION TAG	UNP U3N5N6
J	404	HIS	-	EXPRESSION TAG	UNP U3N5N6
J	405	HIS	-	EXPRESSION TAG	UNP U3N5N6
J	406	HIS	-	EXPRESSION TAG	UNP U3N5N6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	357	LEU	PHE	CONFLICT	UNP U3N5N6
J	384	ASN	ASP	CONFLICT	UNP U3N5N6

- Molecule 3 is water.

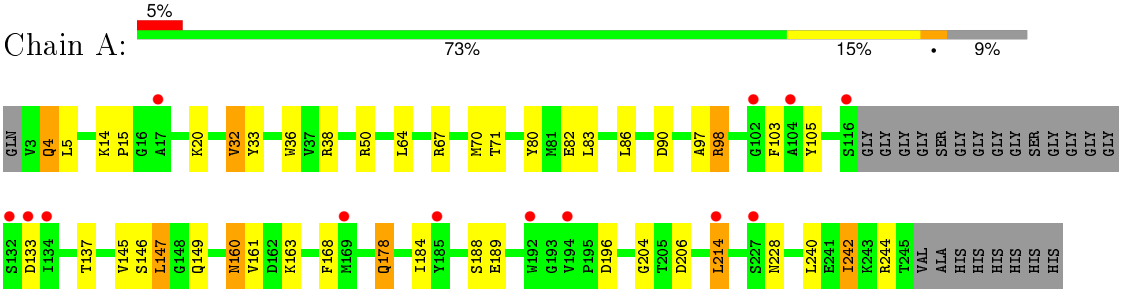
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	49	Total O 49 49	0	0
3	B	56	Total O 56 56	0	0
3	C	11	Total O 11 11	0	0
3	J	11	Total O 11 11	0	0

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.

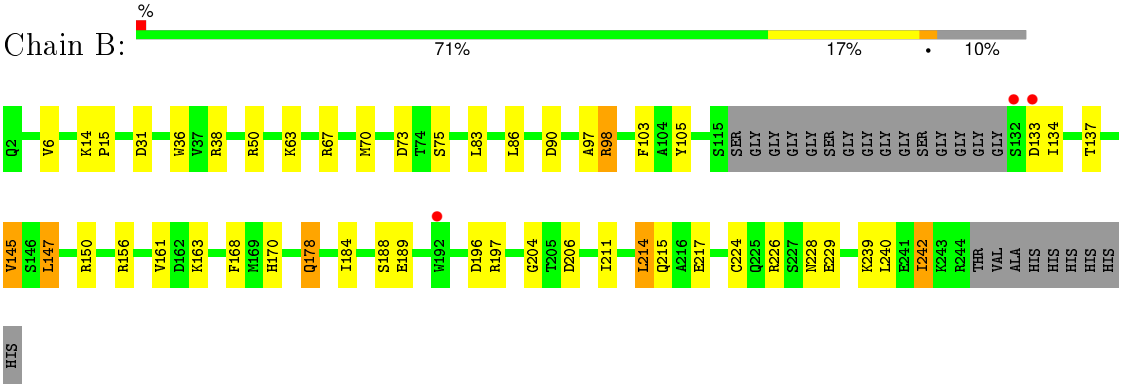
- Molecule 1: SCFV513

Chain A:



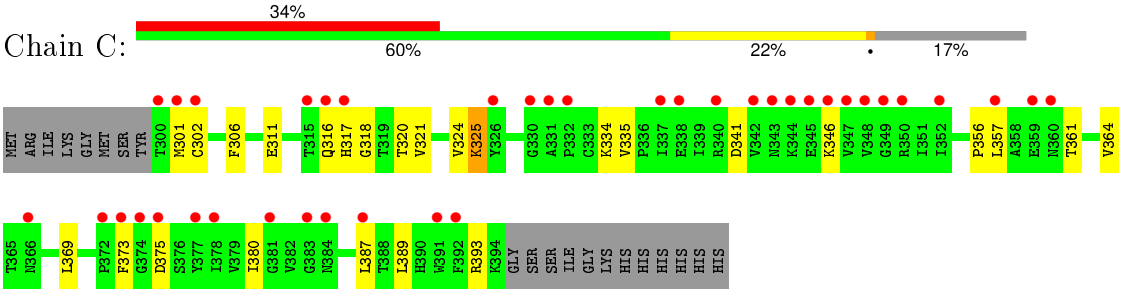
- Molecule 1: SCFV513

Chain B:



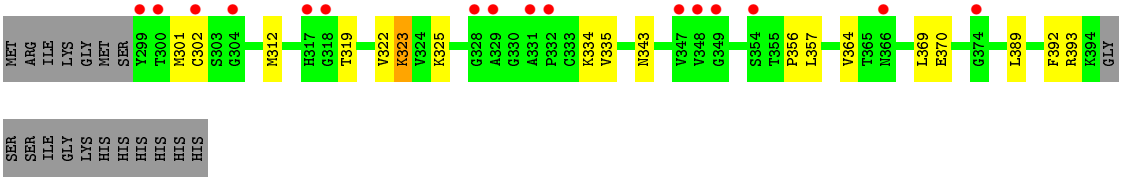
- Molecule 2: ENVELOPE PROTEIN

Chain C:



- Molecule 2: ENVELOPE PROTEIN

Chain J:


MET
ARG
ILE
LYS
GLY
MET
SER
Y299
T300
M301
C302
S303
G304
M312
H317
G318
T319
V322
K323
V324
K325
G328
A329
G330
A331
P332
C333
K334
V335
N343
V347
V348
G349
S354
T355
P356
L357
V364
T365
N366
L369
E370
G374
L389
F392
R393
K394
GLY
SER
SER
ILE
GLY
LYS
HIS
HIS
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HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.64Å 55.89Å 87.05Å 90.00° 104.58° 90.00°	Depositor
Resolution (Å)	29.55 – 2.49 29.55 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.55-2.49) 98.4 (29.55-2.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.51Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.0	Depositor
R, R_{free}	0.220 , 0.270 0.236 , 0.299	Depositor DCC
R_{free} test set	1188 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	68.7	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 59.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 23183 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5137	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.52	0/1815	0.75	0/2460
1	B	0.51	0/1813	0.77	0/2457
2	C	0.52	0/738	0.76	0/999
2	J	0.50	0/751	0.73	0/1017
All	All	0.51	0/5117	0.76	0/6933

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	1775	0	1710	27	0
1	B	1773	0	1713	23	0
2	C	725	0	732	9	0
2	J	737	0	741	7	0
3	A	49	0	0	0	0
3	B	56	0	0	3	0
3	C	11	0	0	0	0
3	J	11	0	0	0	0
All	All	5137	0	4896	60	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 (60) 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:67:ARG:NH2	1:A:90:ASP:OD2	2.19	0.75
1:B:67:ARG:NH2	1:B:90:ASP:OD2	2.20	0.74
1:B:105:TYR:HE1	2:J:325:LYS:HZ2	1.39	0.68
1:A:214:LEU:HD21	1:A:240:LEU:HD21	1.82	0.60
1:B:214:LEU:HD21	1:B:240:LEU:HD21	1.85	0.59
1:A:38:ARG:NH2	1:A:64:LEU:HD21	2.17	0.59
2:C:335:VAL:HB	2:C:356:PRO:HB2	1.88	0.55
2:C:380:ILE:HB	2:C:387:LEU:HB2	1.88	0.55
1:A:178:GLN:NE2	1:B:178:GLN:NE2	2.54	0.55
2:J:335:VAL:HB	2:J:356:PRO:HB2	1.88	0.54
2:J:301:MET:HA	2:J:334:LYS:HB2	1.90	0.53
2:C:301:MET:HA	2:C:334:LYS:HB2	1.91	0.52
2:C:306:PHE:HA	2:C:325:LYS:O	2.11	0.50
1:A:71:THR:OG1	1:A:80:TYR:HB2	2.12	0.50
1:B:6:VAL:HG23	3:B:2002:HOH:O	2.12	0.50
1:A:36:TRP:HD1	1:A:70:MET:CE	2.24	0.49
1:B:97:ALA:HB1	1:B:103:PHE:HB3	1.95	0.48
1:B:147:LEU:HD13	1:B:242:ILE:HD12	1.96	0.48
1:A:33:TYR:OH	2:C:311:GLU:HB2	2.14	0.48
2:C:341:ASP:HB2	2:C:346:LYS:HB2	1.96	0.48
1:B:31:ASP:HB3	2:J:323:LYS:HG2	1.96	0.47
1:A:32:VAL:HG11	1:A:98:ARG:HG3	1.96	0.47
2:J:319:THR:HG22	2:J:370:GLU:HG3	1.95	0.47
1:A:4:GLN:OE1	1:A:5:LEU:N	2.44	0.47
1:B:36:TRP:HD1	1:B:70:MET:CE	2.28	0.47
1:A:97:ALA:HB1	1:A:103:PHE:HB3	1.98	0.46
1:B:170:HIS:O	1:B:224:CYS:HA	2.16	0.45
1:A:146:SER:O	1:A:149:GLN:HB2	2.17	0.45
2:J:312:MET:HE1	2:J:322:VAL:HG13	1.97	0.45
2:C:324:VAL:HG11	2:C:380:ILE:HG12	1.99	0.45
1:A:147:LEU:HD13	1:A:242:ILE:HD12	1.98	0.45
1:B:184:ILE:HA	1:B:189:GLU:O	2.17	0.45
1:A:98:ARG:HB3	1:A:105:TYR:HB2	1.99	0.45
2:C:373:PHE:HA	2:C:393:ARG:HB3	1.98	0.45
1:B:197:ARG:O	1:B:211:ILE:HA	2.17	0.44
3:B:2040:HOH:O	2:J:389:LEU:HA	2.16	0.44
1:A:147:LEU:CD1	1:A:242:ILE:HD12	2.47	0.44
1:A:244:ARG:HH22	1:B:215:GLN:NE2	2.16	0.44
1:B:147:LEU:CD1	1:B:242:ILE:HD12	2.47	0.44
1:B:145:VAL:HG12	1:B:214:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:CG1	1:A:214:LEU:HG	2.49	0.43
1:A:38:ARG:HH22	1:A:64:LEU:HD21	1.84	0.43
1:A:168:PHE:HB2	1:A:228:ASN:HB3	2.01	0.42
1:B:98:ARG:HB3	1:B:105:TYR:HB2	2.02	0.42
1:A:145:VAL:HG12	1:A:214:LEU:HG	2.01	0.42
1:A:15:PRO:HA	1:A:86:LEU:O	2.19	0.42
1:A:67:ARG:HH22	1:A:90:ASP:CG	2.23	0.42
1:A:163:LYS:HB2	1:A:228:ASN:HB2	2.02	0.42
1:A:184:ILE:HA	1:A:189:GLU:O	2.19	0.42
1:B:145:VAL:CG1	1:B:214:LEU:HG	2.50	0.42
1:B:168:PHE:HB2	1:B:228:ASN:HB3	2.01	0.41
1:B:226:ARG:HH22	1:B:229:GLU:HB3	1.85	0.41
1:B:134:ILE:HD12	3:B:2033:HOH:O	2.20	0.41
1:B:15:PRO:HA	1:B:86:LEU:O	2.20	0.41
1:B:163:LYS:HB2	1:B:228:ASN:HB2	2.03	0.41
1:A:160:ASN:H	1:A:160:ASN:HD22	1.68	0.41
1:A:105:TYR:CE1	2:C:325:LYS:HE3	2.56	0.41
1:A:32:VAL:HG11	1:A:98:ARG:CG	2.51	0.40
1:B:156:ARG:HG3	1:B:156:ARG:HH11	1.87	0.40
1:A:20:LYS:HB2	1:A:82:GLU:OE1	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	224/251 (89%)	214 (96%)	8 (4%)	2 (1%)	21 37
1	B	223/251 (89%)	215 (96%)	6 (3%)	2 (1%)	21 37
2	C	93/115 (81%)	80 (86%)	11 (12%)	2 (2%)	8 13
2	J	94/115 (82%)	84 (89%)	10 (11%)	0	100 100
All	All	634/732 (87%)	593 (94%)	35 (6%)	6 (1%)	21 37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	316	GLN
2	C	318	GLY
1	A	161	VAL
1	B	161	VAL
1	A	204	GLY
1	B	204	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	A	191/202 (95%)	175 (92%)	16 (8%)	14 25
1	B	191/202 (95%)	170 (89%)	21 (11%)	8 14
2	C	82/99 (83%)	71 (87%)	11 (13%)	5 9
2	J	83/99 (84%)	75 (90%)	8 (10%)	10 19
All	All	547/602 (91%)	491 (90%)	56 (10%)	9 17

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	14	LYS
1	A	32	VAL
1	A	50	ARG
1	A	83	LEU
1	A	98	ARG
1	A	133	ASP
1	A	137	THR
1	A	147	LEU
1	A	160	ASN
1	A	178	GLN
1	A	188	SER
1	A	196	ASP
1	A	206	ASP

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Mol	Chain	Res	Type
1	A	214	LEU
1	A	242	ILE
1	B	14	LYS
1	B	38	ARG
1	B	50	ARG
1	B	63	LYS
1	B	73	ASP
1	B	75	SER
1	B	83	LEU
1	B	98	ARG
1	B	133	ASP
1	B	137	THR
1	B	145	VAL
1	B	147	LEU
1	B	150	ARG
1	B	178	GLN
1	B	188	SER
1	B	196	ASP
1	B	206	ASP
1	B	214	LEU
1	B	217	GLU
1	B	239	LYS
1	B	242	ILE
2	C	302	CYS
2	C	317	HIS
2	C	320	THR
2	C	321	VAL
2	C	325	LYS
2	C	357	LEU
2	C	361	THR
2	C	364	VAL
2	C	369	LEU
2	C	375	ASP
2	C	389	LEU
2	J	302	CYS
2	J	323	LYS
2	J	343	ASN
2	J	357	LEU
2	J	364	VAL
2	J	369	LEU
2	J	392	PHE
2	J	393	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	178	GLN
1	B	178	GLN
1	B	215	GLN
2	J	390	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

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	228/251 (90%)	0.33	13 (5%) 27 31	45, 73, 106, 128	1 (0%)
1	B	227/251 (90%)	0.01	3 (1%) 79 82	46, 67, 92, 127	1 (0%)
2	C	95/115 (82%)	2.10	39 (41%) 0 0	80, 130, 152, 163	1 (1%)
2	J	96/115 (83%)	1.09	16 (16%) 2 2	74, 114, 137, 145	1 (1%)
All	All	646/732 (88%)	0.59	71 (10%) 7 7	45, 79, 136, 163	4 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	348	VAL	7.4
2	C	349	GLY	7.3
2	C	384	ASN	6.7
2	C	343	ASN	6.2
2	C	317	HIS	6.1
2	C	344	LYS	5.7
2	J	348	VAL	5.7
2	C	331	ALA	5.6
1	B	132	SER	5.4
2	C	359	GLU	5.0
2	C	377	TYR	5.0
2	J	300	THR	4.6
2	C	360	ASN	4.4
2	J	328	GLY	4.4
2	C	366	ASN	4.4
2	J	329	ALA	4.1
1	A	134	ILE	4.1
2	C	381	GLY	4.1
2	J	317	HIS	3.9
2	J	299	TYR	3.8
2	C	330	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	316	GLN	3.6
1	A	133	ASP	3.5
1	A	194	VAL	3.5
2	C	332	PRO	3.5
2	J	366	ASN	3.4
2	C	342	VAL	3.4
2	C	345	GLU	3.2
1	A	116	SER	3.2
2	C	392	PHE	3.2
2	C	391	TRP	3.1
1	A	102	GLY	3.1
2	C	374	GLY	3.1
2	C	347	VAL	3.1
2	C	346	LYS	3.1
1	B	133	ASP	3.0
2	J	318	GLY	3.0
2	C	383	GLY	2.9
2	C	300	THR	2.9
2	J	332	PRO	2.8
2	J	331	ALA	2.8
2	C	302	CYS	2.8
2	J	347	VAL	2.6
1	A	104	ALA	2.6
2	C	340	ARG	2.6
2	C	373	PHE	2.6
2	C	372	PRO	2.6
1	B	192	TRP	2.5
2	J	354	SER	2.5
2	C	350	ARG	2.4
1	A	132	SER	2.4
2	J	349	GLY	2.4
2	C	301	MET	2.4
1	A	227	SER	2.4
2	J	374	GLY	2.3
2	C	337	ILE	2.3
2	C	352	ILE	2.3
2	C	375	ASP	2.3
2	C	357	LEU	2.3
1	A	192	TRP	2.2
2	J	302	CYS	2.2
2	C	326	TYR	2.2
1	A	214	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	169	MET	2.2
2	J	304	GLY	2.2
2	C	315	THR	2.2
2	C	378	ILE	2.1
2	C	387	LEU	2.1
2	C	338	GLU	2.1
1	A	17	ALA	2.1
1	A	185	TYR	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.