Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:04 PM GMT

PDB ID	:	3SGD
Title	:	Crystal structure of the mouse mAb 17.2
Authors	:	Pizarro, J.C.; Boulot, G.; Hontebeyrie, M.; Bentley, G.A.
Deposited on	:	2011-06-14
Resolution	:	2.31 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:

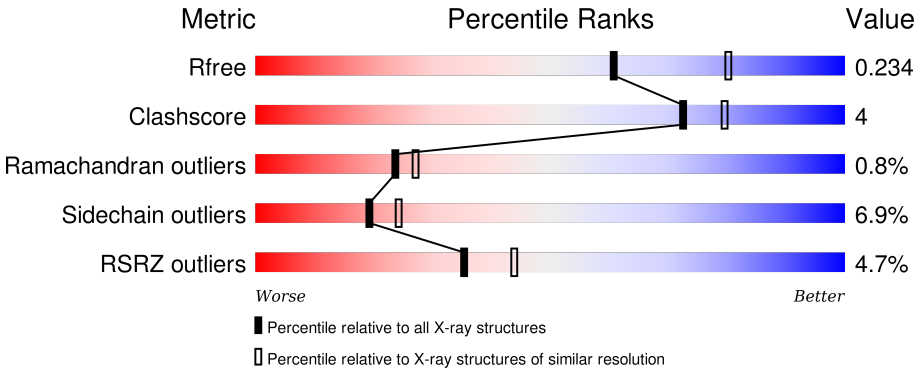
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.31 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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	I	219	% 89% 9% ·
1	L	219	6% 84% 15% ·
2	H	217	6% 85% 13% ·
2	J	217	6% 83% 15% ·

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7304 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 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	218	Total	C	N	O	S	0	2	0
			1700	1064	285	345	6			
1	I	218	Total	C	N	O	S	0	2	0
			1700	1065	284	345	6			

- Molecule 2 is a protein called Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	4	0
			1668	1048	281	329	10			
2	J	216	Total	C	N	O	S	0	0	0
			1636	1027	277	323	9			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	1	Total	Ca	0	0
			1	1		
3	L	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

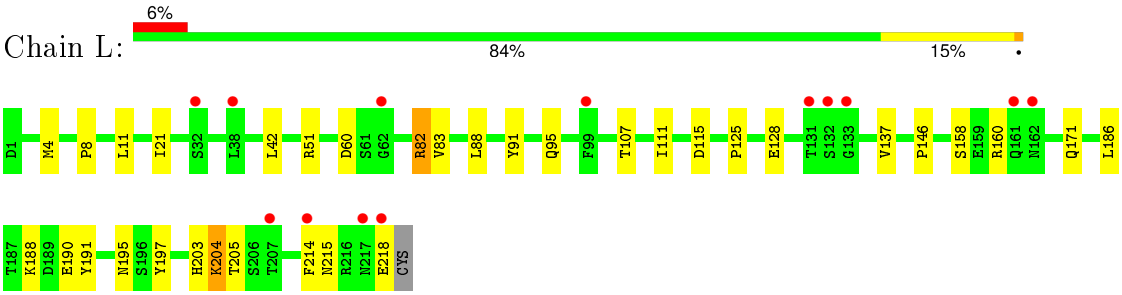
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	120	Total	O	0	0
			120	120		
4	H	128	Total	O	0	0
			128	128		
4	I	177	Total	O	0	0
			177	177		
4	J	172	Total	O	0	0
			172	172		

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.

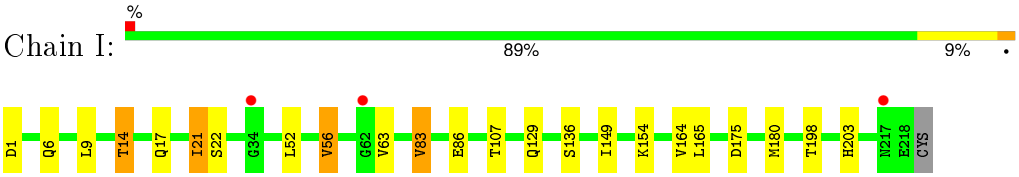
- Molecule 1: Light Chain

Chain L:



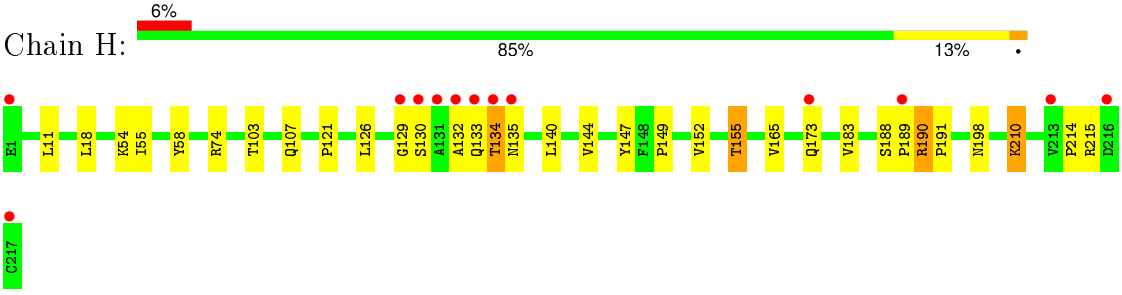
- Molecule 1: Light Chain

Chain I:



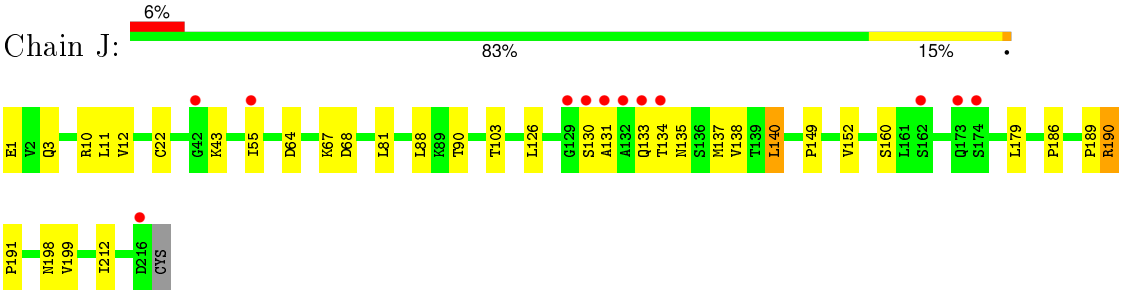
- Molecule 2: Heavy Chain

Chain H:



- Molecule 2: Heavy Chain

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.76Å 65.46Å 91.03Å 90.00° 98.18° 90.00°	Depositor
Resolution (Å)	18.93 – 2.31 18.82 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.8 (18.93-2.31) 98.8 (18.82-2.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.03 (at 2.30Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, R_{free}	0.172 , 0.235 0.171 , 0.234	Depositor DCC
R_{free} test set	2082 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 41489 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7304	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	I	0.53	0/1745	0.74	0/2369
1	L	0.49	0/1746	0.71	0/2371
2	H	0.51	0/1720	0.76	0/2345
2	J	0.50	0/1674	0.82	0/2284
All	All	0.51	0/6885	0.76	0/9369

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	I	1700	0	1650	9	0
1	L	1700	0	1649	16	0
2	H	1668	0	1643	18	0
2	J	1636	0	1609	15	0
3	I	1	0	0	0	0
3	L	2	0	0	0	0
4	H	128	0	0	0	0
4	I	177	0	0	0	0
4	J	172	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	120	0	0	1	0
All	All	7304	0	6551	56	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 4.

All (56) 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)
2:J:190:ARG:HH11	2:J:190:ARG:HG3	1.13	1.07
2:J:190:ARG:HH11	2:J:190:ARG:CG	1.84	0.89
2:J:186:PRO:O	2:J:189:PRO:HD2	1.72	0.89
2:J:190:ARG:NH1	2:J:190:ARG:HG3	1.90	0.74
2:H:190[B]:ARG:HG2	2:H:191:PRO:HA	1.79	0.64
2:H:190[B]:ARG:HH11	2:H:190[B]:ARG:HB3	1.62	0.64
2:H:155:THR:HG22	2:H:198:ASN:OD1	1.99	0.63
2:J:12:VAL:HG11	2:J:88:LEU:HD13	1.81	0.63
2:H:140:LEU:HD11	2:H:190[A]:ARG:HD2	1.82	0.60
2:J:190:ARG:CG	2:J:190:ARG:NH1	2.56	0.57
1:I:17:GLN:O	1:I:83:VAL:HG13	2.04	0.57
1:I:14:THR:HG22	1:I:17:GLN:HB2	1.87	0.57
1:I:129:GLN:NE2	1:I:136:SER:H	2.03	0.56
2:J:186:PRO:HB2	2:J:189:PRO:HD3	1.86	0.56
1:L:21:ILE:HG21	1:L:107:THR:HG21	1.87	0.55
1:I:129:GLN:HE22	1:I:136:SER:H	1.53	0.55
2:H:129:GLY:HA2	2:H:215:ARG:HD3	1.88	0.55
1:L:191:TYR:HA	1:L:197:TYR:OH	2.07	0.54
2:J:11:LEU:HB2	2:J:149:PRO:HG3	1.90	0.54
1:L:8:PRO:HD2	1:L:21:ILE:HG22	1.90	0.53
2:H:140:LEU:HD11	2:H:190[B]:ARG:HD3	1.91	0.53
1:L:128:GLU:OE1	2:H:210:LYS:HE3	2.09	0.52
1:L:146:PRO:O	1:L:203:HIS:HE1	1.93	0.51
1:L:195:ASN:O	1:L:215:ASN:HA	2.09	0.51
1:L:51:ARG:NH2	2:H:103:THR:HG22	2.24	0.51
2:H:11:LEU:HB2	2:H:149:PRO:HG3	1.93	0.51
1:I:21:ILE:HD13	1:I:107:THR:OG1	2.11	0.51
2:H:190[B]:ARG:NH1	2:H:190[B]:ARG:HB3	2.25	0.50
2:H:140:LEU:CD1	2:H:190[B]:ARG:HD3	2.42	0.50
2:H:133:GLN:HG2	2:H:134:THR:H	1.77	0.49
2:H:165:VAL:HG12	2:H:183:VAL:HG23	1.94	0.49
2:J:186:PRO:HB2	2:J:189:PRO:CD	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:149:ILE:HD12	1:I:203:HIS:CD2	2.50	0.47
1:L:88:LEU:HD11	1:L:171:GLN:HB2	1.95	0.47
1:L:125:PRO:HD3	1:L:137:VAL:HG22	1.95	0.47
2:J:135:ASN:HD22	2:J:137:MET:H	1.61	0.47
1:L:197:TYR:HB2	1:L:214:PHE:CE2	2.50	0.46
1:I:6:GLN:HE21	1:I:21:ILE:HD11	1.79	0.46
1:L:203:HIS:HD2	1:L:205:THR:OG1	2.00	0.45
2:J:67:LYS:O	2:J:68:ASP:HB2	2.16	0.45
2:H:121:PRO:HB3	2:H:147:TYR:HB3	1.98	0.45
2:J:140:LEU:HG	2:J:212:ILE:HG21	1.99	0.45
2:H:190[A]:ARG:HG2	2:H:191:PRO:HA	2.00	0.44
2:J:186:PRO:C	2:J:189:PRO:HD2	2.36	0.44
1:L:4:MET:HE2	1:L:95:GLN:HB3	2.00	0.44
2:H:144:VAL:HG11	2:H:152:VAL:HG11	2.00	0.43
2:J:22:CYS:HB3	2:J:81:LEU:HB3	2.00	0.43
2:J:190:ARG:HD2	2:J:191:PRO:HA	2.01	0.43
1:I:154:LYS:HB2	1:I:198:THR:HB	1.99	0.43
1:L:82:ARG:HG3	4:L:382:HOH:O	2.19	0.43
1:I:52:LEU:HA	1:I:63:VAL:HG21	2.02	0.42
2:H:190[B]:ARG:HH21	2:H:214:PRO:HG3	1.84	0.41
1:L:42:LEU:HD13	1:L:91:TYR:CZ	2.56	0.41
1:L:115:ASP:OD2	1:L:204:LYS:HE3	2.21	0.41
2:H:58:TYR:CD2	2:H:74:ARG:HD3	2.56	0.40
1:L:88:LEU:HD12	1:L:111:ILE:HG12	2.03	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	I	218/219 (100%)	216 (99%)	1 (0%)	1 (0%)	34 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	218/219 (100%)	214 (98%)	4 (2%)	0	100 100
2	H	219/217 (101%)	208 (95%)	8 (4%)	3 (1%)	14 13
2	J	214/217 (99%)	201 (94%)	10 (5%)	3 (1%)	14 13
All	All	869/872 (100%)	839 (96%)	23 (3%)	7 (1%)	24 27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	10	ARG
2	J	130	SER
2	H	189	PRO
2	H	132	ALA
2	H	134	THR
2	J	131	ALA
1	I	56	VAL

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	I	197/196 (100%)	184 (93%)	13 (7%)	21 26
1	L	197/196 (100%)	186 (94%)	11 (6%)	26 35
2	H	191/188 (102%)	178 (93%)	13 (7%)	20 25
2	J	186/188 (99%)	168 (90%)	18 (10%)	10 11
All	All	771/768 (100%)	716 (93%)	55 (7%)	19 23

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

Mol	Chain	Res	Type
1	L	11	LEU
1	L	60	ASP
1	L	82	ARG
1	L	83	VAL

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Mol	Chain	Res	Type
1	L	158	SER
1	L	160	ARG
1	L	186	LEU
1	L	188	LYS
1	L	190	GLU
1	L	204	LYS
1	L	218	GLU
2	H	18	LEU
2	H	54	LYS
2	H	55	ILE
2	H	107	GLN
2	H	126	LEU
2	H	130	SER
2	H	135	ASN
2	H	155	THR
2	H	173	GLN
2	H	188	SER
2	H	190[A]	ARG
2	H	190[B]	ARG
2	H	210	LYS
1	I	1	ASP
1	I	9	LEU
1	I	14	THR
1	I	21	ILE
1	I	22[A]	SER
1	I	22[B]	SER
1	I	56	VAL
1	I	83	VAL
1	I	86	GLU
1	I	164	VAL
1	I	165	LEU
1	I	175	ASP
1	I	180	MET
2	J	1	GLU
2	J	3	GLN
2	J	43	LYS
2	J	55	ILE
2	J	64	ASP
2	J	90	THR
2	J	103	THR
2	J	126	LEU
2	J	133	GLN

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Mol	Chain	Res	Type
2	J	134	THR
2	J	138	VAL
2	J	140	LEU
2	J	152	VAL
2	J	160	SER
2	J	179	LEU
2	J	190	ARG
2	J	198	ASN
2	J	199	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	143	ASN
1	L	166	ASN
1	L	203	HIS
2	H	56	ASN
2	H	135	ASN
1	I	17	GLN
1	I	129	GLN
1	I	166	ASN
1	I	215	ASN
2	J	56	ASN
2	J	84	GLN
2	J	135	ASN

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

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	I	218/219 (99%)	-0.23	3 (1%)	78	83	16, 26, 44, 66	0
1	L	218/219 (99%)	0.19	13 (5%)	25	33	17, 35, 61, 129	0
2	H	217/217 (100%)	0.27	13 (5%)	25	33	17, 29, 68, 105	0
2	J	216/217 (99%)	-0.03	12 (5%)	28	36	18, 27, 50, 91	0
All	All	869/872 (99%)	0.05	41 (4%)	35	44	16, 29, 57, 129	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	217	CYS	13.7
2	H	134	THR	11.2
2	H	132	ALA	10.1
2	H	133	GLN	9.1
2	H	131	ALA	8.8
1	L	218	GLU	8.2
2	J	131	ALA	7.3
2	H	216	ASP	7.2
2	J	134	THR	6.0
2	H	135	ASN	5.3
2	H	130	SER	5.3
1	L	217	ASN	4.9
2	J	133	GLN	4.7
2	J	132	ALA	4.5
2	J	130	SER	4.3
1	L	62	GLY	3.9
1	L	207	THR	3.6
1	L	162	ASN	3.6
1	I	217	ASN	3.3
2	J	216	ASP	3.1
1	I	62	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	32	SER	3.0
1	L	133	GLY	2.9
1	L	38	LEU	2.9
2	H	129	GLY	2.8
2	J	173	GLN	2.8
1	L	131	THR	2.8
2	H	189	PRO	2.7
2	H	173	GLN	2.6
2	J	162	SER	2.5
1	L	99	PHE	2.5
2	J	42	GLY	2.4
1	I	34	GLY	2.4
2	J	55	ILE	2.4
2	H	213	VAL	2.3
1	L	214	PHE	2.3
2	H	1	GLU	2.3
2	J	174	SER	2.3
1	L	161	GLN	2.2
2	J	129	GLY	2.2
1	L	132	SER	2.2

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CA	L	221	1/1	0.96	0.07	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CA	L	220	1/1	0.83	0.06	-	64,64,64,64	0
3	CA	I	220	1/1	0.93	0.06	-	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.