



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:51 AM UTC

PDB ID : 3SGE / pdb_00003sge
Title : Crystal structure of mAb 17.2 in complex with R13 peptide
Authors : Pizarro, J.C.; Boulot, G.; Hontebeyrie, M.; Bentley, G.A.
Deposited on : 2011-06-14
Resolution : 1.89 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

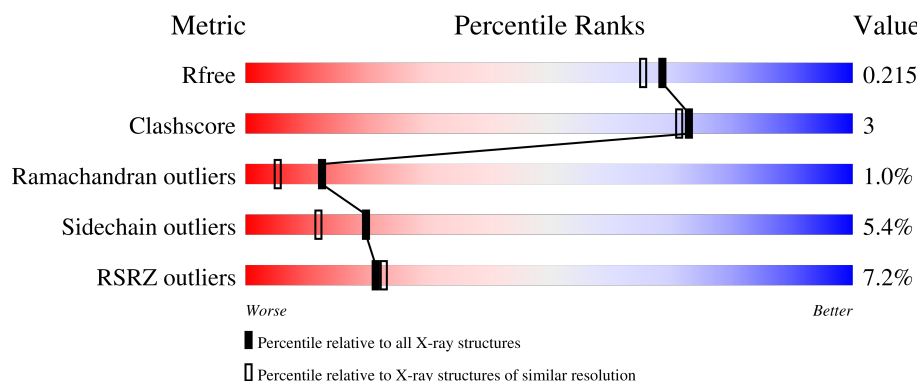
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	2% 89% 9% .
1	L	219	10% 90% 9% .
2	H	217	11% 87% 12% .
2	J	217	6% 86% 12% .
3	K	13	8% 54% 31% 15%

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Mol	Chain	Length	Quality of chain
3	M	13	8% 62% 23% 15%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7628 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	219	Total	C	N	O	S	0	1	0
			1706	1067	288	344	7			
1	I	219	Total	C	N	O	S	0	0	0
			1699	1063	285	344	7			

- Molecule 2 is a protein called Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	2	0
			1652	1036	278	328	10			
2	J	217	Total	C	N	O	S	0	1	0
			1654	1038	281	325	10			

- Molecule 3 is a protein called R13 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	11	Total	C	N	O	S	0	1	0
			91	54	11	25	1			
3	M	11	Total	C	N	O	S	0	0	0
			86	51	11	23	1			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

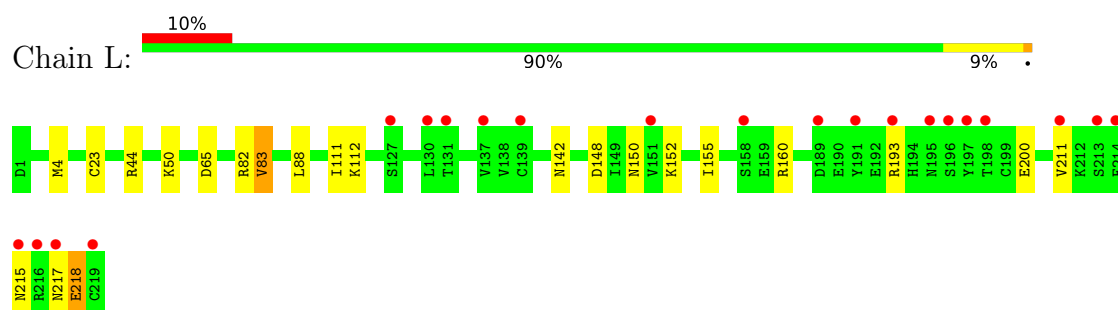
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	153	Total 153	O 153	0	0
5	H	170	Total 170	O 170	0	0
5	I	221	Total 221	O 221	0	0
5	J	168	Total 168	O 168	0	0
5	K	12	Total 12	O 12	0	0
5	M	14	Total 14	O 14	0	0

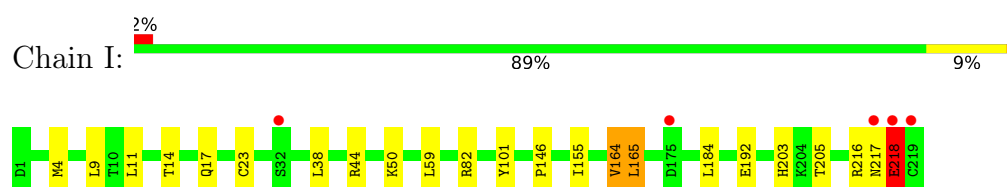
3 Residue-property plots [i](#)

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.

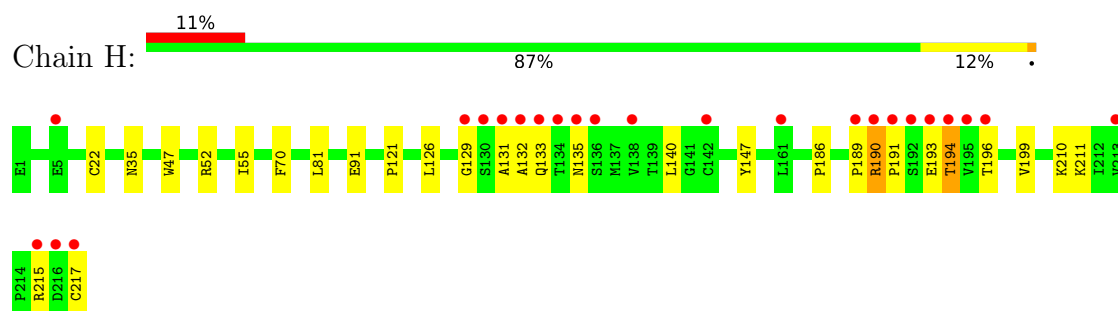
• Molecule 1: Light Chain



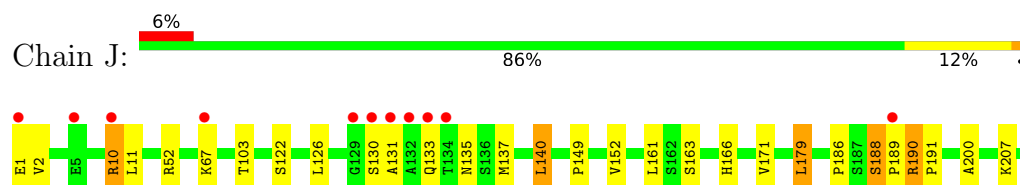
• Molecule 1: Light Chain



• Molecule 2: Heavy Chain



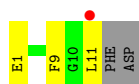
• Molecule 2: Heavy Chain



• Molecule 3: R13 peptide



● Molecule 3: R13 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.00Å 68.21Å 92.12Å 90.00° 98.37° 90.00°	Depositor
Resolution (Å)	29.69 – 1.89 29.69 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.69-1.89) 91.1 (29.69-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.89Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, R_{free}	0.179 , 0.211 0.181 , 0.215	Depositor DCC
R_{free} test set	3714 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7628	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 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	0.86	0/1737	1.09	1/2357 (0.0%)
1	L	0.79	0/1748	1.09	4/2371 (0.2%)
2	H	0.85	0/1696	1.09	1/2312 (0.0%)
2	J	0.86	1/1695 (0.1%)	1.12	5/2311 (0.2%)
3	K	0.93	0/95	1.70	4/125 (3.2%)
3	M	0.82	0/86	1.27	1/113 (0.9%)
All	All	0.84	1/7057 (0.0%)	1.11	16/9589 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	188	SER	CA-C	5.01	1.58	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	103	THR	N-CA-C	7.25	122.33	112.68
1	I	164	VAL	N-CA-CB	7.12	119.53	110.99
3	K	1	GLU	CA-C-N	6.80	134.53	121.54
3	K	1	GLU	C-N-CA	6.80	134.53	121.54
1	L	142	ASN	N-CA-C	6.70	120.74	109.76
3	M	9	PHE	CA-CB-CG	5.68	119.48	113.80
3	K	9	PHE	CA-CB-CG	5.62	119.42	113.80
1	L	83	VAL	N-CA-CB	5.52	118.74	110.13
1	L	217	ASN	CA-C-N	5.33	131.72	121.54
1	L	217	ASN	C-N-CA	5.33	131.72	121.54
2	J	122	SER	N-CA-C	-5.25	100.69	109.24
2	H	70	PHE	CA-CB-CG	5.24	119.04	113.80
2	J	1	GLU	CA-C-N	5.22	131.37	121.97
2	J	1	GLU	C-N-CA	5.22	131.37	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	179	LEU	N-CA-CB	-5.16	102.71	111.69
3	K	4	ASP	CA-CB-CG	5.15	117.75	112.60

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	1699	0	1647	11	0
1	L	1706	0	1656	4	0
2	H	1652	0	1624	11	0
2	J	1654	0	1634	18	0
3	K	91	0	69	0	0
3	M	86	0	67	1	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
5	H	170	0	0	0	0
5	I	221	0	0	1	0
5	J	168	0	0	1	0
5	K	12	0	0	0	0
5	L	153	0	0	0	0
5	M	14	0	0	0	0
All	All	7628	0	6697	43	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 3.

All (43) 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:HD2	2:J:191:PRO:HA	1.52	0.91
2:H:190:ARG:HG2	2:H:191:PRO:HA	1.62	0.82
2:J:186:PRO:O	2:J:189:PRO:HD2	1.82	0.79
2:J:140:LEU:HD21	2:J:190:ARG:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:196:THR:HG22	2:H:211:LYS:HA	1.77	0.67
2:J:190:ARG:HH11	2:J:190:ARG:HB3	1.61	0.65
2:H:35:ASN:HD22	2:H:47:TRP:HE1	1.45	0.64
2:J:10:ARG:HB2	5:J:250:HOH:O	2.04	0.57
1:I:101:TYR:HE2	3:M:11:LEU:HD13	1.70	0.57
1:I:14:THR:H	1:I:17:GLN:HE21	1.55	0.52
2:J:200:ALA:HB2	2:J:207:LYS:HE2	1.94	0.50
1:L:44:ARG:HH12	1:L:50:LYS:HZ3	1.59	0.50
1:L:4:MET:HE3	1:L:23:CYS:SG	2.53	0.49
2:J:186:PRO:HB2	2:J:189:PRO:CD	2.43	0.48
1:I:14:THR:H	1:I:17:GLN:NE2	2.12	0.47
2:J:188:SER:OG	2:J:189:PRO:HD3	2.15	0.47
2:J:190:ARG:HH11	2:J:190:ARG:CB	2.27	0.47
2:J:186:PRO:C	2:J:189:PRO:HD2	2.40	0.47
2:H:129:GLY:HA2	2:H:215:ARG:HD3	1.96	0.46
2:H:186:PRO:O	2:H:189:PRO:HD2	2.16	0.46
1:L:155:ILE:HD12	1:L:160:ARG:HD2	1.97	0.46
1:I:44:ARG:HH12	1:I:50:LYS:HZ3	1.63	0.46
2:H:189:PRO:O	2:H:193:GLU:HB2	2.16	0.46
2:H:194:THR:HG23	2:H:196:THR:HG23	1.98	0.45
1:I:217:ASN:O	1:I:218:GLU:HB2	2.16	0.45
1:I:192:GLU:O	1:I:216:ARG:NH2	2.51	0.44
1:I:146:PRO:O	1:I:203:HIS:HE1	2.00	0.44
1:I:4:MET:HE3	1:I:23:CYS:SG	2.58	0.43
1:I:165:LEU:HG	2:J:171:VAL:HG11	2.00	0.43
2:J:11:LEU:HB2	2:J:149:PRO:HG3	2.01	0.43
2:J:140:LEU:HG	2:J:212:ILE:HG21	2.01	0.43
1:I:155:ILE:HD11	1:I:184:LEU:HD21	2.01	0.43
5:I:623:HOH:O	2:J:166:HIS:HD2	2.01	0.42
2:J:190:ARG:HD2	2:J:191:PRO:CA	2.36	0.42
1:L:88:LEU:HD12	1:L:111:ILE:HG12	2.01	0.42
2:J:186:PRO:HB2	2:J:189:PRO:HD3	2.01	0.42
2:J:135:ASN:HD22	2:J:137:MET:H	1.68	0.42
2:J:135:ASN:ND2	2:J:137:MET:H	2.17	0.42
2:H:121:PRO:HB3	2:H:147:TYR:HB3	2.01	0.41
1:I:203:HIS:HD2	1:I:205:THR:OG1	2.03	0.41
2:H:35:ASN:ND2	2:H:47:TRP:HE1	2.15	0.41
2:H:22:CYS:HB3	2:H:81:LEU:HB3	2.04	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	217/219 (99%)	214 (99%)	2 (1%)	1 (0%)	24	16
1	L	218/219 (100%)	215 (99%)	2 (1%)	1 (0%)	24	16
2	H	217/217 (100%)	204 (94%)	10 (5%)	3 (1%)	9	3
2	J	216/217 (100%)	206 (95%)	6 (3%)	4 (2%)	6	1
3	K	10/13 (77%)	8 (80%)	2 (20%)	0	100	100
3	M	9/13 (69%)	9 (100%)	0	0	100	100
All	All	887/898 (99%)	856 (96%)	22 (2%)	9 (1%)	12	5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	218	GLU
1	I	218	GLU
2	J	2	VAL
2	J	130	SER
2	H	132	ALA
2	J	10	ARG
2	H	131	ALA
2	H	133	GLN
2	J	131	ALA

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	196/196 (100%)	188 (96%)	8 (4%)	27	19
1	L	197/196 (100%)	184 (93%)	13 (7%)	15	8
2	H	189/188 (100%)	179 (95%)	10 (5%)	20	12
2	J	189/188 (100%)	179 (95%)	10 (5%)	20	12
3	K	10/11 (91%)	8 (80%)	2 (20%)	1	0
3	M	9/11 (82%)	8 (89%)	1 (11%)	6	2
All	All	790/790 (100%)	746 (94%)	44 (6%)	20	11

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	65	ASP
1	L	82[A]	ARG
1	L	82[B]	ARG
1	L	83	VAL
1	L	112	LYS
1	L	148	ASP
1	L	150	ASN
1	L	152	LYS
1	L	193	ARG
1	L	200	GLU
1	L	211	VAL
1	L	215	ASN
1	L	218	GLU
2	H	52	ARG
2	H	91	GLU
2	H	126	LEU
2	H	135	ASN
2	H	140	LEU
2	H	190	ARG
2	H	194	THR
2	H	199	VAL
2	H	210	LYS
2	H	217	CYS
1	I	9	LEU
1	I	11	LEU
1	I	38	LEU
1	I	59	LEU
1	I	82	ARG
1	I	164	VAL
1	I	165	LEU

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Mol	Chain	Res	Type
1	I	218	GLU
2	J	52	ARG
2	J	67	LYS
2	J	126	LEU
2	J	133	GLN
2	J	140	LEU
2	J	152	VAL
2	J	161	LEU
2	J	163	SER
2	J	179	LEU
2	J	190	ARG
3	K	2[A]	GLU
3	K	2[B]	GLU
3	M	1	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	142	ASN
1	L	143	ASN
1	L	166	ASN
1	L	195	ASN
2	H	35	ASN
2	H	78	GLN
1	I	17	GLN
1	I	27	GLN
1	I	43	GLN
1	I	161	GLN
1	I	166	ASN
1	I	203	HIS
1	I	215	ASN
1	I	217	ASN
2	J	39	GLN
2	J	78	GLN
2	J	133	GLN
2	J	135	ASN
2	J	166	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [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, 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	I	219/219 (100%)	0.19	5 (2%) 61 65	4, 31, 49, 88	1 (0%)
1	L	219/219 (100%)	0.44	21 (9%) 13 14	5, 34, 75, 101	2 (0%)
2	H	217/217 (100%)	0.76	24 (11%) 10 11	3, 31, 63, 83	8 (3%)
2	J	217/217 (100%)	0.49	12 (5%) 30 32	3, 30, 50, 71	5 (2%)
3	K	11/13 (84%)	0.52	1 (9%) 15 15	24, 30, 68, 72	1 (9%)
3	M	11/13 (84%)	0.98	1 (9%) 15 15	29, 38, 65, 79	0
All	All	894/898 (99%)	0.48	64 (7%) 21 23	3, 31, 63, 101	17 (1%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	219	CYS	34.5
2	J	132	ALA	32.6
2	J	134	THR	29.2
2	H	132	ALA	24.1
2	J	217	CYS	24.0
2	H	134	THR	21.7
2	H	217	CYS	21.5
2	J	133	GLN	21.1
1	L	219	CYS	19.3
2	H	135	ASN	18.6
2	H	133	GLN	15.4
2	H	216	ASP	14.9
3	M	11	LEU	5.9
2	J	131	ALA	5.6
2	H	129	GLY	4.9
3	K	11	LEU	4.3
2	J	1	GLU	4.0
1	L	189	ASP	3.8
2	J	189	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	211	VAL	3.6
1	L	131	THR	3.6
2	H	130	SER	3.5
2	H	213	VAL	3.3
1	L	158	SER	3.3
2	H	138	VAL	3.3
2	H	194	THR	3.3
1	L	214	PHE	3.3
1	I	218	GLU	3.2
1	L	127	SER	3.0
2	H	196	THR	3.0
1	L	139	CYS	3.0
1	I	217	ASN	2.9
2	H	195	VAL	2.9
1	L	196	SER	2.8
2	J	130	SER	2.8
1	L	193	ARG	2.8
2	H	189	PRO	2.8
1	L	195	ASN	2.7
2	H	192	SER	2.7
2	H	193	GLU	2.6
2	H	136	SER	2.6
1	I	175	ASP	2.5
1	L	216	ARG	2.5
1	L	215	ASN	2.4
1	L	217	ASN	2.4
2	J	10	ARG	2.4
1	L	130	LEU	2.4
1	L	191	TYR	2.4
2	H	215	ARG	2.4
2	H	142	CYS	2.4
2	J	5	GLU	2.3
2	H	161	LEU	2.3
1	L	197	TYR	2.3
1	L	198	THR	2.3
2	J	67	LYS	2.3
2	J	129	GLY	2.3
1	I	32	SER	2.2
1	L	151	VAL	2.1
1	L	213	SER	2.1
1	L	137	VAL	2.1
2	H	191	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	131	ALA	2.1
2	H	190	ARG	2.0
2	H	5[A]	GLU	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	I	220	1/1	0.94	0.06	69,69,69,69	0
4	CA	L	220	1/1	0.96	0.06	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.