



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:51 PM GMT

PDB ID : 1VGE
Title : TR1.9 FAB FRAGMENT OF A HUMAN IGG1 KAPPA AUTOANTIBODY
Authors : Chacko, S.; Padlan, E.A.
Deposited on : 1996-01-04
Resolution : 2.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

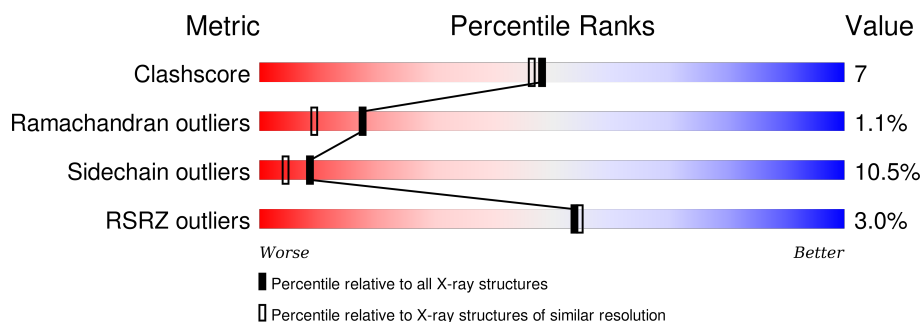
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 $\leq 5\%$. 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	L	214	<div> <div></div> <div>74%21%..</div> </div>
2	H	225	<div> <div>4%</div> <div>70%22%7%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3534 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 TR1.9 FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1632	1020	274	332	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	VAL	-	INSERTION	EMBL X95747
L	4	MET	-	INSERTION	EMBL X95747
L	11	LEU	VAL	CONFLICT	EMBL X95747
L	20	ASN	THR	CONFLICT	EMBL X95747
L	22	ALA	THR	CONFLICT	EMBL X95747
L	32	ALA	TRP	CONFLICT	EMBL X95747
L	45	ARG	LYS	CONFLICT	EMBL X95747
L	50	ASP	SER	CONFLICT	EMBL X95747
L	53	ASN	SER	CONFLICT	EMBL X95747
L	55	GLU	GLN	CONFLICT	EMBL X95747
L	72	THR	SER	CONFLICT	EMBL X95747
L	83	PHE	SER	CONFLICT	EMBL X95747
L	85	ILE	THR	CONFLICT	EMBL X95747
L	91	PHE	ALA	CONFLICT	EMBL X95747
L	94	TYR	PHE	CONFLICT	EMBL X95747
L	96	LEU	TYR	CONFLICT	EMBL X95747
L	100	GLY	GLN	CONFLICT	EMBL X95747
L	191	VAL	LEU	CONFLICT	EMBL X95747

- Molecule 2 is a protein called TR1.9 FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	225	Total	C	N	O	S	0	0	0
			1686	1063	286	330	7			

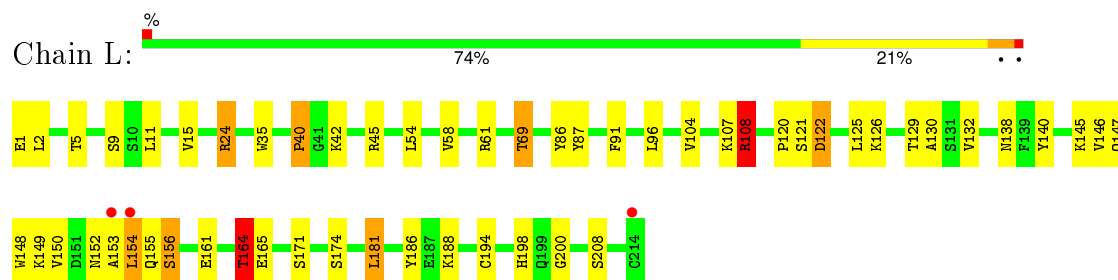
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	113	Total 113	O 113	0	0
3	L	103	Total 103	O 103	0	0

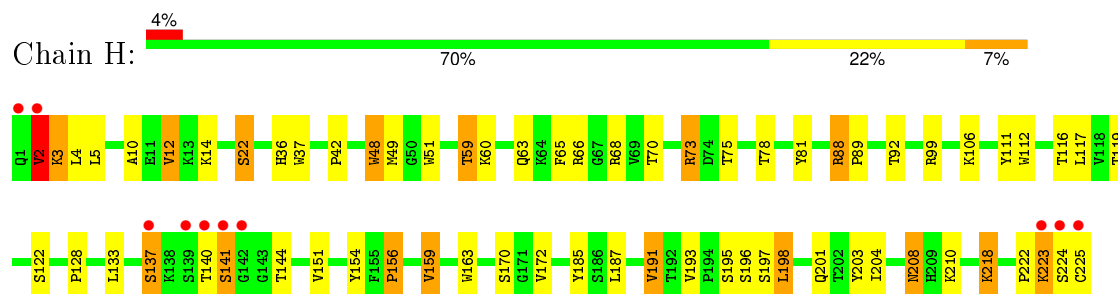
3 Residue-property plots [i](#)

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: TR1.9 FAB



• Molecule 2: TR1.9 FAB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.93 Å 62.78 Å 84.79 Å 90.00° 107.19° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 38.45 – 1.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 57.2 (38.45-1.98)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.98 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available) 0.169 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 91.9	EDS
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 20569 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3534	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.85	0/1666	1.55	16/2259 (0.7%)
2	H	0.87	0/1729	1.71	39/2349 (1.7%)
All	All	0.86	0/3395	1.64	55/4608 (1.2%)

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
2	H	0	1

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	99	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	L	108	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	L	148	TRP	CD1-CG-CD2	9.55	113.94	106.30
1	L	108	ARG	NE-CZ-NH2	-9.19	115.71	120.30
2	H	112	TRP	CD1-CG-CD2	8.87	113.39	106.30
2	H	73	ARG	NE-CZ-NH1	8.50	124.55	120.30
2	H	163	TRP	CD1-CG-CD2	8.12	112.79	106.30
2	H	68	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	L	164	THR	N-CA-CB	-7.86	95.36	110.30
1	L	148	TRP	CE2-CD2-CG	-7.75	101.10	107.30
2	H	2	VAL	N-CA-C	-7.32	91.23	111.00
2	H	137	SER	N-CA-C	-7.31	91.27	111.00
1	L	181	LEU	CA-CB-CG	7.28	132.05	115.30
1	L	35	TRP	CD1-CG-CD2	7.10	111.98	106.30
1	L	35	TRP	CE2-CD2-CG	-7.07	101.65	107.30
2	H	112	TRP	CE2-CD2-CG	-7.01	101.69	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	163	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	L	87	TYR	CB-CG-CD1	-6.97	116.82	121.00
2	H	159	VAL	CG1-CB-CG2	-6.74	100.11	110.90
2	H	48	TRP	CD1-CG-CD2	6.74	111.69	106.30
2	H	37	TRP	CE2-CD2-CG	-6.55	102.06	107.30
2	H	48	TRP	CE2-CD2-CG	-6.52	102.09	107.30
2	H	88	ARG	NE-CZ-NH2	-6.41	117.09	120.30
2	H	4	LEU	CA-CB-CG	6.24	129.66	115.30
2	H	68	ARG	NE-CZ-NH1	6.21	123.41	120.30
2	H	224	SER	CA-C-N	-6.10	103.78	117.20
2	H	37	TRP	CD1-CG-CD2	6.04	111.14	106.30
2	H	60	LYS	CA-CB-CG	-5.96	100.30	113.40
1	L	45	ARG	NE-CZ-NH2	-5.91	117.34	120.30
2	H	88	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	L	1	GLU	CA-CB-CG	5.85	126.26	113.40
2	H	51	TRP	CE2-CD2-CG	-5.80	102.66	107.30
2	H	73	ARG	CA-CB-CG	5.79	126.14	113.40
1	L	186	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	L	69	THR	N-CA-CB	-5.76	99.36	110.30
2	H	99	ARG	NE-CZ-NH1	5.66	123.13	120.30
2	H	4	LEU	N-CA-C	-5.64	95.78	111.00
1	L	148	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	L	154	LEU	CA-CB-CG	5.45	127.84	115.30
2	H	51	TRP	CD1-CG-CD2	5.44	110.65	106.30
2	H	12	VAL	CB-CA-C	-5.42	101.10	111.40
2	H	78	THR	N-CA-CB	-5.42	100.01	110.30
2	H	75	THR	N-CA-CB	-5.40	100.03	110.30
2	H	2	VAL	CA-CB-CG1	5.40	119.00	110.90
2	H	112	TRP	CG-CD1-NE1	-5.37	104.73	110.10
2	H	191	VAL	CG1-CB-CG2	-5.37	102.31	110.90
1	L	86	TYR	CB-CG-CD2	-5.33	117.81	121.00
2	H	224	SER	O-C-N	5.30	131.19	122.70
2	H	163	TRP	CG-CD1-NE1	-5.24	104.86	110.10
2	H	223	LYS	CA-CB-CG	5.18	124.79	113.40
2	H	133	LEU	N-CA-C	-5.12	97.18	111.00
2	H	185	TYR	CB-CG-CD1	-5.07	117.96	121.00
2	H	208	ASN	CB-CG-ND2	5.03	128.78	116.70
2	H	141	SER	N-CA-C	5.01	124.54	111.00
2	H	196	SER	N-CA-CB	-5.01	102.98	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	111	TYR	Sidechain

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	L	1632	0	1585	26	0
2	H	1686	0	1656	23	0
3	H	113	0	0	2	0
3	L	103	0	0	4	0
All	All	3534	0	3241	48	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 7.

All (48) 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:H:12:VAL:HG22	2:H:156:PRO:HG3	1.60	0.82
2:H:195:SER:HA	2:H:198:LEU:HD23	1.75	0.69
1:L:122:ASP:HA	3:L:862:HOH:O	1.95	0.67
2:H:197:SER:HB3	2:H:201:GLN:HG3	1.78	0.66
1:L:150:VAL:O	1:L:154:LEU:HB2	1.96	0.66
2:H:36:HIS:HD2	2:H:48:TRP:HE1	1.47	0.63
2:H:198:LEU:HD12	2:H:222:PRO:HG3	1.84	0.60
2:H:63:GLN:HE22	2:H:66:ARG:HH11	1.48	0.59
2:H:63:GLN:NE2	2:H:66:ARG:HH11	2.01	0.57
2:H:151:VAL:HG11	2:H:159:VAL:HG11	1.90	0.53
2:H:92:THR:HG23	2:H:119:THR:HA	1.91	0.53
1:L:91:PHE:O	2:H:106:LYS:HG2	2.09	0.53
1:L:125:LEU:HD12	3:L:862:HOH:O	2.10	0.52
2:H:36:HIS:CD2	2:H:48:TRP:HE1	2.27	0.51
2:H:10:ALA:O	2:H:210:LYS:NZ	2.44	0.51
2:H:172:VAL:HG22	2:H:191:VAL:HG12	1.92	0.51
1:L:108:ARG:HG2	1:L:171:SER:HB2	1.92	0.51
2:H:128:PRO:HB3	2:H:154:TYR:HB3	1.93	0.50
2:H:2:VAL:O	2:H:3:LYS:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:172:VAL:HG22	2:H:191:VAL:CG1	2.42	0.49
2:H:193:VAL:HG21	2:H:203:TYR:OH	2.13	0.48
1:L:40:PRO:HB2	1:L:165:GLU:HG3	1.96	0.48
1:L:11:LEU:HD12	1:L:104:VAL:HG22	1.95	0.48
1:L:149:LYS:HA	1:L:155:GLN:HA	1.96	0.46
2:H:204:ILE:HA	2:H:218:LYS:O	2.16	0.46
1:L:91:PHE:HA	1:L:96:LEU:HD22	1.98	0.45
1:L:156:SER:HB2	3:L:873:HOH:O	2.16	0.44
1:L:108:ARG:HD2	1:L:140:TYR:CG	2.52	0.44
2:H:49:MET:HG2	2:H:65:PHE:CE2	2.53	0.44
1:L:198:HIS:CD2	1:L:200:GLY:H	2.35	0.44
2:H:59:THR:HG22	3:H:920:HOH:O	2.18	0.44
1:L:149:LYS:HB3	1:L:152:ASN:O	2.19	0.43
2:H:187:LEU:HA	3:H:758:HOH:O	2.18	0.43
2:H:88:ARG:HH11	2:H:88:ARG:HG3	1.83	0.43
1:L:40:PRO:CB	1:L:165:GLU:HG3	2.49	0.42
1:L:54:LEU:HD13	1:L:58:VAL:HB	2.01	0.42
1:L:42:LYS:HB3	1:L:42:LYS:HE2	1.55	0.42
1:L:107:LYS:HE3	1:L:107:LYS:HB3	1.88	0.42
1:L:146:VAL:HG13	1:L:194:CYS:SG	2.60	0.41
1:L:120:PRO:HD3	1:L:132:VAL:HG22	2.03	0.41
1:L:152:ASN:HD22	1:L:153:ALA:N	2.18	0.41
2:H:22:SER:HB3	2:H:81:TYR:CD2	2.56	0.41
1:L:5:THR:HG22	1:L:24:ARG:NH1	2.36	0.41
1:L:164:THR:HG22	1:L:174:SER:H	1.84	0.41
1:L:145:LYS:HB2	1:L:145:LYS:HE3	1.81	0.40
1:L:125:LEU:HD21	1:L:130:ALA:HB2	2.03	0.40
1:L:149:LYS:HD3	1:L:155:GLN:HB3	2.01	0.40
1:L:138:ASN:ND2	3:L:766:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	199 (94%)	12 (6%)	1 (0%)	34	26
2	H	223/225 (99%)	209 (94%)	10 (4%)	4 (2%)	11	4
All	All	435/439 (99%)	408 (94%)	22 (5%)	5 (1%)	17	9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	2	VAL
1	L	188	LYS
2	H	141	SER
2	H	140	THR
2	H	3	LYS

5.3.2 Protein sidechains ⓘ

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	185/185 (100%)	167 (90%)	18 (10%)	10	5
2	H	187/187 (100%)	166 (89%)	21 (11%)	7	4
All	All	372/372 (100%)	333 (90%)	39 (10%)	8	4

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	LEU
1	L	9	SER
1	L	15	VAL
1	L	24	ARG
1	L	40	PRO
1	L	61	ARG
1	L	69	THR
1	L	108	ARG
1	L	121	SER
1	L	122	ASP
1	L	126	LYS

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Mol	Chain	Res	Type
1	L	129	THR
1	L	147	GLN
1	L	156	SER
1	L	161	GLU
1	L	164	THR
1	L	181	LEU
1	L	208	SER
2	H	2	VAL
2	H	5	LEU
2	H	14	LYS
2	H	22	SER
2	H	42	PRO
2	H	59	THR
2	H	70	THR
2	H	73	ARG
2	H	89	PRO
2	H	116	THR
2	H	117	LEU
2	H	122	SER
2	H	137	SER
2	H	144	THR
2	H	156	PRO
2	H	170	SER
2	H	198	LEU
2	H	208	ASN
2	H	218	LYS
2	H	223	LYS
2	H	225	CYS

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

Mol	Chain	Res	Type
1	L	20	ASN
1	L	89	GLN
1	L	137	ASN
1	L	138	ASN
1	L	152	ASN
1	L	198	HIS
1	L	210	ASN
2	H	44	GLN
2	H	63	GLN
2	H	180	GLN

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Mol	Chain	Res	Type
2	H	208	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 carbohydrates 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%)	-0.59	3 (1%) 78 78	11, 26, 58, 102	0
2	H	225/225 (100%)	-0.50	10 (4%) 38 39	13, 26, 77, 100	0
All	All	439/439 (100%)	-0.54	13 (2%) 54 55	11, 26, 67, 102	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	2	VAL	7.3
2	H	141	SER	6.0
1	L	214	CYS	5.6
2	H	1	GLN	5.5
2	H	224	SER	5.0
1	L	153	ALA	4.7
2	H	140	THR	4.7
2	H	223	LYS	4.2
1	L	154	LEU	3.9
2	H	142	GLY	3.8
2	H	225	CYS	3.3
2	H	139	SER	3.3
2	H	137	SER	2.9

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.