



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:22 AM UTC

PDB ID : 1A7Q / pdb_00001a7q
Title : FV FRAGMENT OF MOUSE MONOCLONAL ANTIBODY D1.3 (BALB/C, IGG1, K) HIGH AFFINITY EXPRESSED VARIANT CONTAINING SER26L->GLY, ILE29L->THR, GLU81L->ASP, THR97L->SER, PRO240H->LEU, ASP258H->ALA, LYS281H->GLU, ASN283H->ASP AND LEU312H->VAL
Authors : Marks, C.; Henrick, K.; Winter, G.
Deposited on : 1998-03-16
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

<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

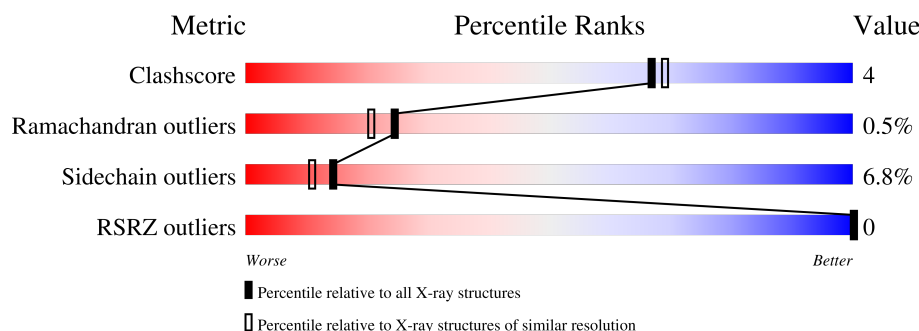
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	L	106	
2	H	116	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1728 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 IGG1-KAPPA D1.3 FV (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	106	Total	C	N	O	S	0	0	0
			791	503	128	158	2			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	VAL	GLU	conflict	GB 545862
L	26	GLY	SER	variant	GB 545862
L	29	THR	ILE	variant	GB 545862
L	50	TYR	LYS	conflict	GB 545862
L	51	THR	ALA	conflict	GB 545862
L	52	THR	GLN	conflict	GB 545862
L	56	ALA	ASP	conflict	GB 545862
L	81	ASP	GLU	variant	GB 545862
L	?	-	PRO	deletion	GB 545862
L	96	ARG	TRP	conflict	GB 545862
L	97	SER	THR	variant	GB 545862

- Molecule 2 is a protein called IGG1-KAPPA D1.3 FV (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	116	Total	C	N	O	S	0	0	0
			890	558	153	175	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	240	LEU	PRO	variant	GB 896294
H	258	ALA	ASP	variant	GB 896294
H	281	GLU	LYS	variant	GB 896294
H	283	ASP	ASN	variant	GB 896294

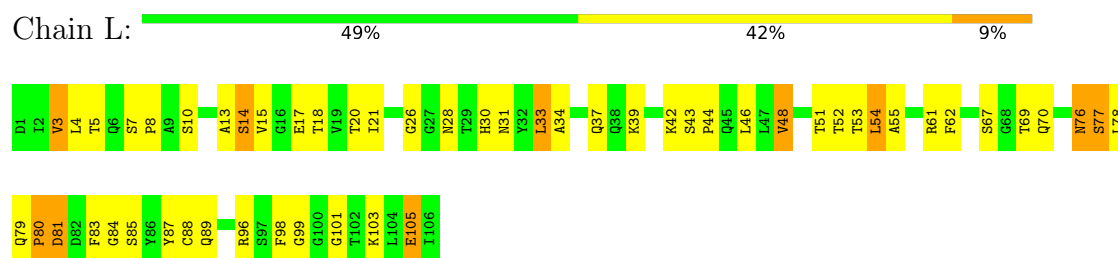
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	23	Total 23	O 23	0	0
3	H	24	Total 24	O 24	0	0

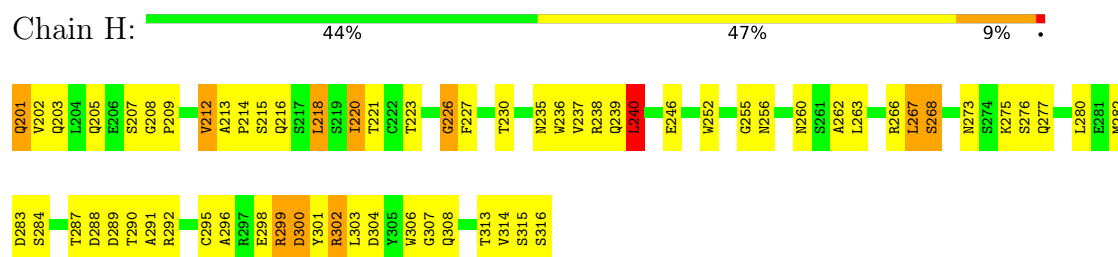
3 Residue-property plots

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: IGG1-KAPPA D1.3 FV (LIGHT CHAIN)



- Molecule 2: IGG1-KAPPA D1.3 FV (HEAVY CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.31Å 90.31Å 56.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00 6.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.00) 93.6 (6.00-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.01Å)	Xtriage
Refinement program	CCP4	Depositor
R, R_{free}	0.178 , (Not available) 0.177 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 81.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1728	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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

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	1.51	2/812 (0.2%)	2.59	61/1108 (5.5%)
2	H	1.50	2/909 (0.2%)	2.79	94/1236 (7.6%)
All	All	1.50	4/1721 (0.2%)	2.70	155/2344 (6.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	303	LEU	N-CA	6.30	1.55	1.46
1	L	51	THR	CA-CB	6.01	1.63	1.53
1	L	85	SER	N-CA	5.70	1.52	1.45
2	H	308	GLN	N-CA	5.13	1.52	1.46

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	239	GLN	OE1-CD-NE2	11.82	134.42	122.60
2	H	302	ARG	NE-CZ-NH2	-11.32	109.01	119.20
2	H	284	SER	N-CA-CB	-10.71	95.42	111.71
2	H	268	SER	N-CA-CB	10.68	130.47	111.13
2	H	227	PHE	CA-C-O	10.68	132.70	121.38
2	H	266	ARG	NE-CZ-NH2	-10.05	110.16	119.20
1	L	67	SER	CA-C-O	-9.82	110.77	121.28
1	L	81	ASP	CA-CB-CG	9.77	122.36	112.60
1	L	52	THR	CA-C-O	-9.47	108.48	118.90
2	H	304	ASP	CA-C-O	-9.37	108.64	119.60
2	H	201	GLN	N-CA-CB	-8.99	95.21	110.50
2	H	282	MET	CA-C-O	8.92	131.25	120.28
1	L	53	THR	CA-CB-OG1	-8.80	96.40	109.60
2	H	298	GLU	CA-C-O	8.77	130.17	120.70
1	L	83	PHE	CB-CA-C	8.66	125.40	109.46
1	L	79	GLN	CB-CA-C	8.61	121.89	108.63
2	H	268	SER	CB-CA-C	-8.58	92.70	109.68
2	H	302	ARG	NE-CZ-NH1	8.56	130.06	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	263	LEU	N-CA-CB	-8.34	98.11	110.53
1	L	76	ASN	CA-CB-CG	-8.32	104.28	112.60
2	H	267	LEU	CA-C-O	-8.23	111.86	121.16
2	H	256	ASN	OD1-CG-ND2	-8.19	114.41	122.60
2	H	315	SER	N-CA-CB	-8.11	99.00	111.56
1	L	80	PRO	CA-C-N	8.08	134.22	120.72
1	L	80	PRO	C-N-CA	8.08	134.22	120.72
1	L	18	THR	CA-CB-OG1	-8.07	97.50	109.60
1	L	67	SER	O-C-N	7.94	131.23	123.29
2	H	273	ASN	CA-C-O	-7.91	112.17	120.55
2	H	313	THR	CA-CB-OG1	-7.90	97.76	109.60
2	H	299	ARG	CD-NE-CZ	-7.89	113.35	124.40
1	L	62	PHE	CA-C-O	-7.86	112.08	120.80
1	L	4	LEU	O-C-N	7.80	133.12	123.21
1	L	21	ILE	CB-CA-C	7.78	122.21	110.62
1	L	54	LEU	CA-C-O	-7.76	112.54	121.47
2	H	235	ASN	CA-C-O	-7.75	112.14	121.28
2	H	273	ASN	O-C-N	7.61	130.19	122.12
2	H	201	GLN	O-C-N	-7.60	110.84	123.00
1	L	76	ASN	OD1-CG-ND2	7.56	130.16	122.60
2	H	256	ASN	CA-CB-CG	-7.53	105.07	112.60
2	H	203	GLN	CB-CG-CD	7.42	125.21	112.60
2	H	209	PRO	CA-C-O	-7.32	109.68	118.90
2	H	255	GLY	CA-C-O	-7.28	111.16	119.10
1	L	33	LEU	CD1-CG-CD2	7.27	126.80	110.80
1	L	77	SER	CA-C-O	7.27	130.91	120.51
2	H	208	GLY	O-C-N	7.23	129.00	121.77
2	H	295	CYS	CA-C-O	7.21	129.31	121.16
2	H	218	LEU	CA-CB-CG	7.06	141.01	116.30
2	H	268	SER	O-C-N	7.05	131.66	123.41
2	H	306	TRP	CE3-CZ3-CH2	-6.96	112.05	121.10
2	H	201	GLN	CA-CB-CG	-6.91	100.28	114.10
2	H	302	ARG	CD-NE-CZ	-6.75	114.94	124.40
1	L	98	PHE	CA-C-O	-6.72	113.56	121.16
2	H	267	LEU	N-CA-C	6.71	120.63	109.95
1	L	48	VAL	CA-C-O	-6.69	114.19	121.28
2	H	302	ARG	O-C-N	6.67	130.63	123.56
1	L	3	VAL	CA-CB-CG2	6.65	121.70	110.40
1	L	89	GLN	OE1-CD-NE2	-6.64	115.96	122.60
2	H	216	GLN	OE1-CD-NE2	6.64	129.24	122.60
1	L	31	ASN	CA-CB-CG	-6.60	106.00	112.60
1	L	96	ARG	NE-CZ-NH2	-6.59	113.27	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	287	THR	CA-CB-OG1	-6.54	99.79	109.60
2	H	292	ARG	O-C-N	6.47	130.58	123.27
1	L	76	ASN	CA-C-O	-6.40	113.39	120.69
2	H	266	ARG	NE-CZ-NH1	6.38	127.88	121.50
1	L	10	SER	CB-CA-C	-6.37	95.42	109.56
2	H	213	ALA	N-CA-CB	-6.37	101.45	110.04
2	H	275	LYS	CB-CA-C	6.34	121.89	109.72
1	L	13	ALA	CA-C-O	-6.32	114.50	121.33
2	H	260	ASN	CA-C-N	6.32	129.08	120.54
2	H	260	ASN	C-N-CA	6.32	129.08	120.54
2	H	238	ARG	NE-CZ-NH2	-6.25	113.58	119.20
2	H	304	ASP	O-C-N	6.24	131.22	122.36
2	H	212	VAL	CA-C-O	6.21	127.59	121.19
1	L	84	GLY	CA-C-N	-6.17	112.93	122.87
1	L	84	GLY	C-N-CA	-6.17	112.93	122.87
2	H	223	THR	CA-C-O	-6.13	113.75	120.43
2	H	201	GLN	CB-CA-C	6.10	121.70	110.10
2	H	262	ALA	CA-C-O	-6.08	114.10	120.55
1	L	34	ALA	CA-C-O	6.05	128.54	121.46
1	L	103	LYS	CA-CB-CG	6.03	126.16	114.10
2	H	240	LEU	N-CA-CB	5.99	118.12	110.04
2	H	202	VAL	CA-C-O	-5.98	113.95	120.71
1	L	37	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	L	30	HIS	CA-CB-CG	-5.91	107.89	113.80
2	H	255	GLY	CA-C-N	-5.84	111.78	120.94
2	H	255	GLY	C-N-CA	-5.84	111.78	120.94
2	H	308	GLN	CG-CD-NE2	5.82	125.14	116.40
1	L	84	GLY	O-C-N	5.82	131.70	123.67
2	H	209	PRO	O-C-N	5.81	130.33	122.37
2	H	256	ASN	CB-CG-ND2	5.79	125.08	116.40
2	H	218	LEU	N-CA-CB	-5.76	100.89	111.37
2	H	236	TRP	CA-C-N	5.75	130.93	122.94
2	H	236	TRP	C-N-CA	5.75	130.93	122.94
1	L	14	SER	CA-C-O	-5.73	114.62	121.56
1	L	101	GLY	O-C-N	5.71	127.78	122.47
1	L	99	GLY	N-CA-C	-5.70	103.67	112.85
2	H	215	SER	CA-CB-OG	-5.69	99.71	111.10
1	L	46	LEU	CA-C-O	-5.69	114.79	121.16
2	H	283	ASP	O-C-N	5.69	129.31	122.94
1	L	39	LYS	CB-CA-C	5.68	119.18	109.80
1	L	20	THR	CA-CB-OG1	-5.68	101.08	109.60
1	L	26	GLY	N-CA-C	-5.67	106.71	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	61	ARG	N-CA-CB	5.66	120.29	110.39
2	H	239	GLN	CA-CB-CG	-5.65	102.80	114.10
2	H	203	GLN	CB-CA-C	5.63	120.81	109.38
2	H	299	ARG	NH1-CZ-NH2	5.63	126.62	119.30
1	L	78	LEU	O-C-N	5.61	129.81	122.97
1	L	14	SER	O-C-N	5.60	130.33	123.10
2	H	260	ASN	N-CA-CB	-5.59	101.14	109.69
2	H	237	VAL	CA-C-N	-5.57	113.45	122.81
2	H	237	VAL	C-N-CA	-5.57	113.45	122.81
2	H	205	GLN	OE1-CD-NE2	-5.56	117.04	122.60
2	H	288	ASP	CB-CA-C	5.55	120.62	110.36
2	H	252	TRP	CA-C-N	5.54	127.07	120.14
2	H	252	TRP	C-N-CA	5.54	127.07	120.14
2	H	226	GLY	CA-C-O	-5.51	112.89	119.06
2	H	263	LEU	N-CA-C	5.51	120.16	113.38
1	L	17	GLU	O-C-N	-5.50	116.58	122.85
1	L	28	ASN	OD1-CG-ND2	-5.50	117.10	122.60
2	H	300	ASP	O-C-N	5.50	129.62	122.86
2	H	230	THR	CA-CB-OG1	-5.47	101.39	109.60
2	H	296	ALA	O-C-N	5.47	129.81	123.41
1	L	39	LYS	CA-C-N	5.47	128.87	121.05
1	L	39	LYS	C-N-CA	5.47	128.87	121.05
2	H	268	SER	CA-C-N	-5.46	115.34	122.94
2	H	268	SER	C-N-CA	-5.46	115.34	122.94
2	H	267	LEU	N-CA-CB	-5.43	102.17	110.85
1	L	5	THR	CA-C-O	-5.41	114.52	120.36
2	H	306	TRP	CZ3-CH2-CZ2	5.35	128.46	121.50
2	H	263	LEU	CA-C-N	5.33	128.82	120.82
2	H	263	LEU	C-N-CA	5.33	128.82	120.82
1	L	42	LYS	CB-CA-C	5.33	120.71	109.79
2	H	307	GLY	N-CA-C	-5.32	104.04	112.66
2	H	301	TYR	N-CA-C	5.31	118.96	111.52
2	H	263	LEU	CA-C-O	5.26	125.14	119.15
2	H	290	THR	CA-CB-OG1	-5.23	101.76	109.60
2	H	221	THR	CA-C-O	-5.22	114.69	120.38
1	L	87	TYR	CA-C-O	-5.21	114.67	120.66
2	H	304	ASP	CB-CG-OD1	5.18	130.32	118.40
1	L	96	ARG	NE-CZ-NH1	5.18	126.68	121.50
1	L	55	ALA	CA-C-O	5.17	127.72	121.88
2	H	289	ASP	N-CA-C	-5.16	106.76	113.16
1	L	88	CYS	N-CA-C	-5.15	101.76	109.95
2	H	246	GLU	CA-C-N	5.14	128.15	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	246	GLU	C-N-CA	5.14	128.15	120.95
1	L	79	GLN	CG-CD-OE1	5.13	131.06	120.80
1	L	69	THR	CA-CB-CG2	5.12	119.20	110.50
2	H	299	ARG	N-CA-CB	-5.06	102.23	110.59
1	L	4	LEU	CA-C-O	-5.05	115.36	120.71
1	L	37	GLN	CA-C-O	-5.03	115.38	120.71
2	H	220	ILE	CB-CG1-CD1	-5.03	103.25	113.80
1	L	105	GLU	O-C-N	5.02	129.72	123.19
2	H	277	GLN	O-C-N	5.02	129.39	123.27
1	L	53	THR	CB-CA-C	-5.00	101.68	109.84
1	L	5	THR	CA-CB-OG1	-5.00	102.09	109.60

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	L	791	0	735	4	0
2	H	890	0	842	8	0
3	H	24	0	0	0	0
3	L	23	0	0	0	0
All	All	1728	0	1577	12	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 (12) 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:L:48:VAL:HG22	1:L:54:LEU:HD23	1.68	0.74
2:H:220:ILE:HD12	2:H:280:LEU:HD23	1.86	0.57
2:H:240:LEU:HD22	2:H:291:ALA:HB2	1.89	0.55
2:H:300:ASP:HB2	2:H:302:ARG:NH1	2.28	0.48
2:H:214:PRO:HD2	2:H:316:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:299:ARG:NH1	2:H:302:ARG:NH2	2.66	0.43
1:L:7:SER:HA	1:L:8:PRO:C	2.44	0.42
2:H:212:VAL:O	2:H:314:VAL:HA	2.20	0.42
1:L:43:SER:HA	1:L:44:PRO:HD3	1.84	0.42
2:H:267:LEU:HD22	2:H:280:LEU:HD11	2.03	0.41
1:L:15:VAL:HG21	1:L:80:PRO:HG3	2.02	0.41
2:H:201:GLN:O	2:H:226:GLY:HA3	2.22	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	L	104/106 (98%)	101 (97%)	2 (2%)	1 (1%)	12	8
2	H	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
All	All	218/222 (98%)	211 (97%)	6 (3%)	1 (0%)	24	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	77	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	L	82/88 (93%)	75 (92%)	7 (8%)	10	7
2	H	95/99 (96%)	90 (95%)	5 (5%)	20	18
All	All	177/187 (95%)	165 (93%)	12 (7%)	14	11

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	VAL
1	L	14	SER
1	L	33	LEU
1	L	70	GLN
1	L	76	ASN
1	L	81	ASP
1	L	105	GLU
2	H	207	SER
2	H	218	LEU
2	H	240	LEU
2	H	268	SER
2	H	276	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	30	HIS
1	L	45	GLN

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 oligosaccharides 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 [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	106/106 (100%)	-0.98	0 100 100	11, 21, 32, 38	11 (10%)
2	H	116/116 (100%)	-1.04	0 100 100	11, 20, 29, 32	11 (9%)
All	All	222/222 (100%)	-1.02	0 100 100	11, 21, 31, 38	22 (9%)

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.