



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:00 PM UTC

PDB ID : 1RMF / pdb_00001rmf
Title : STRUCTURES OF A MONOCLONAL ANTI-ICAM-1 ANTIBODY R6.5
FRAGMENT AT 2.8 ANGSTROMS RESOLUTION
Authors : Jedrzejas, M.J.; Luo, M.
Deposited on : 1994-12-16
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

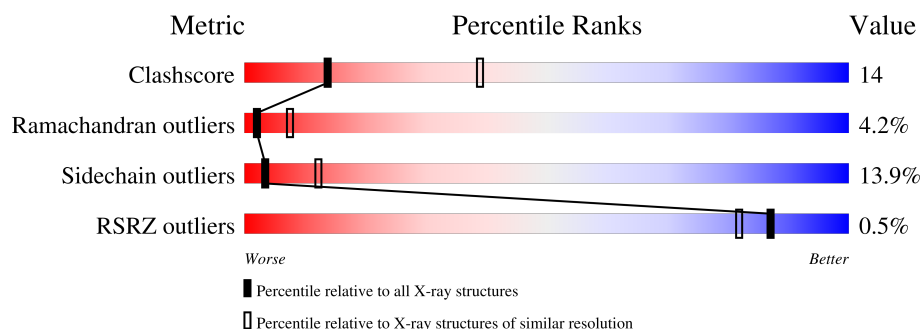
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	219	
2	H	216	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4208 atoms, of which 850 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 IGG2A-KAPPA R6.5 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	219	Total	C	H	N	O	S	0	0	0
			2095	1052	404	290	342	7			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	7	SER	THR	conflict	PIR S16112
L	36	ASN	THR	conflict	PIR S16112
L	39	HIS	TYR	conflict	PIR S16112
L	45	SER	PRO	conflict	PIR S16112
L	48	ALA	SER	conflict	PIR S16112
L	51	LEU	PRO	conflict	PIR S16112
L	55	LYS	ARG	conflict	PIR S16112
L	94	SER	PHE	conflict	PIR S16112
L	96	SER	GLY	conflict	PIR S16112
L	101	LEU	TYR	conflict	PIR S16112
L	108	LYS	ARG	conflict	PIR S16112

- Molecule 2 is a protein called IGG2A-KAPPA R6.5 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	216	Total	C	H	N	O	S	0	0	0
			1996	1034	368	265	324	5			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	6	GLN	GLU	conflict	GB 2852989
H	30	ILE	THR	conflict	GB 2852989
H	33	ALA	PRO	conflict	GB 2852989
H	34	ILE	MET	conflict	GB 2852989
H	39	GLU	GLN	conflict	GB 2852989

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Chain	Residue	Modelled	Actual	Comment	Reference
H	53	ALA	THR	conflict	GB 2852989
H	55	SER	TYR	conflict	GB 2852989
H	57	ASP	ASN	conflict	GB 2852989
H	62	GLN	ARG	conflict	GB 2852989
H	63	LYS	ASN	conflict	GB 2852989
H	77	ASN	SER	conflict	GB 2852989
H	81	LEU	MET	conflict	GB 2852989
H	99	GLY	-	insertion	GB 2852989
H	100	GLY	-	insertion	GB 2852989
H	101	TRP	-	insertion	GB 2852989
H	103	LEU	ASN	conflict	GB 2852989
H	?	-	ASP	deletion	GB 2852989
H	?	-	GLY	deletion	GB 2852989
H	?	-	TYR	deletion	GB 2852989
H	?	-	TYR	deletion	GB 2852989
H	105	SER	GLY	conflict	GB 2852989
H	107	ASP	ALA	conflict	GB 2852989
H	114	THR	LEU	conflict	GB 2852989
H	115	LEU	VAL	conflict	GB 2852989
H	119	SER	ALA	conflict	GB 2852989
H	128	THR	TYR	conflict	GB 2852989
H	146	VAL	CYS	conflict	GB 2852989

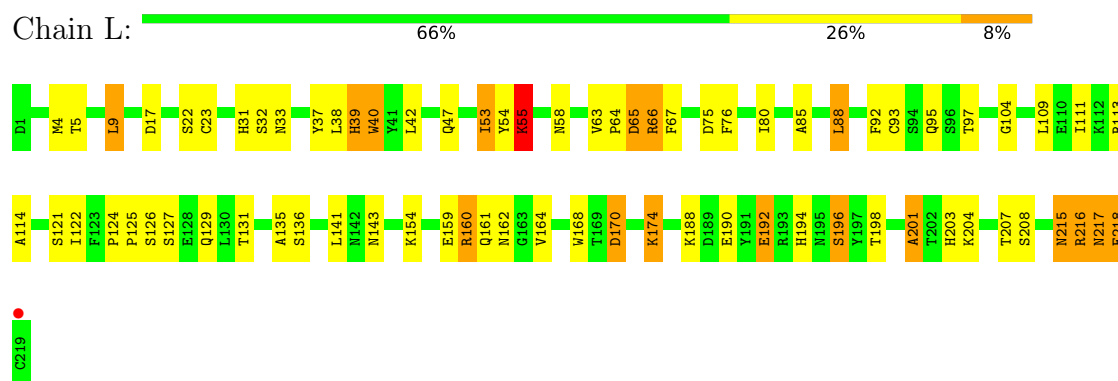
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	21	Total	H	O	0	0
			63	42	21		
3	H	18	Total	H	O	0	0
			54	36	18		

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: IGG2A-KAPPA R6.5 FAB (LIGHT CHAIN)



- Molecule 2: IGG2A-KAPPA R6.5 FAB (HEAVY CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	40.36Å 137.76Å 91.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.50 – 2.80 6.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.50-2.80) 80.3 (6.50-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.69Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , (Not available) 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.06 , 209.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4208	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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	1.23	9/1728 (0.5%)	1.77	31/2342 (1.3%)
2	H	1.35	10/1668 (0.6%)	1.98	54/2278 (2.4%)
All	All	1.29	19/3396 (0.6%)	1.88	85/4620 (1.8%)

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	4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	210	THR	CA-C	9.28	1.63	1.52
1	L	203	HIS	CD2-NE2	-7.91	1.29	1.37
2	H	35	HIS	CD2-NE2	-7.80	1.29	1.37
2	H	58	THR	CA-CB	7.37	1.66	1.53
1	L	39	HIS	CD2-NE2	-6.91	1.30	1.37
2	H	205	HIS	CD2-NE2	-6.51	1.30	1.37
2	H	170	HIS	CD2-NE2	-6.45	1.30	1.37
2	H	41	HIS	CD2-NE2	-6.19	1.31	1.37
1	L	31	HIS	CD2-NE2	-6.17	1.31	1.37
2	H	35	HIS	CG-ND1	-5.99	1.31	1.38
1	L	194	HIS	CD2-NE2	-5.76	1.31	1.37
1	L	194	HIS	CG-ND1	-5.71	1.31	1.38
2	H	127	VAL	CA-CB	5.35	1.61	1.54
2	H	136	ASP	CA-CB	5.34	1.60	1.53
1	L	39	HIS	CG-ND1	-5.34	1.32	1.38
1	L	192	GLU	CA-CB	-5.24	1.45	1.53
1	L	63	VAL	CA-CB	5.23	1.60	1.54
1	L	135	ALA	CA-CB	-5.11	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	209	SER	C-N	5.05	1.39	1.33

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	211	LYS	N-CA-C	17.81	138.33	110.20
1	L	161	GLN	N-CA-C	13.96	131.96	109.76
2	H	105	SER	N-CA-C	11.69	125.30	108.00
2	H	210	THR	N-CA-C	10.32	123.83	108.14
2	H	55	SER	N-CA-C	8.57	121.91	108.79
2	H	209	SER	N-CA-C	8.52	120.87	108.86
2	H	64	PHE	N-CA-C	8.29	122.97	113.02
2	H	103	LEU	N-CA-C	-8.26	97.22	109.62
2	H	104	LEU	N-CA-C	8.26	128.39	110.80
1	L	217	ASN	OD1-CG-ND2	-8.20	114.40	122.60
2	H	21	SER	N-CA-C	8.16	122.42	110.59
2	H	210	THR	CA-C-N	7.61	132.30	121.42
2	H	210	THR	C-N-CA	7.61	132.30	121.42
2	H	136	ASP	N-CA-C	-7.60	103.32	112.59
2	H	44	SER	N-CA-C	-7.47	100.46	110.55
2	H	58	THR	N-CA-C	-6.86	96.19	110.80
1	L	55	LYS	N-CA-C	-6.85	96.20	110.80
2	H	61	ASN	N-CA-C	-6.71	96.80	108.69
2	H	215	LYS	O-C-N	6.66	130.49	122.96
1	L	143	ASN	N-CA-C	6.60	120.19	111.28
2	H	136	ASP	CA-CB-CG	6.59	119.19	112.60
1	L	203	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	L	208	SER	N-CA-C	-6.43	101.44	110.31
2	H	212	VAL	N-CA-C	6.43	118.94	108.97
2	H	113	THR	N-CA-C	6.42	120.78	111.02
1	L	216	ARG	CA-C-N	6.37	133.70	121.54
1	L	216	ARG	C-N-CA	6.37	133.70	121.54
1	L	164	VAL	N-CA-CB	-6.36	103.59	110.53
2	H	170	HIS	CB-CG-CD2	-6.30	123.02	131.20
1	L	66	ARG	N-CA-C	6.25	120.52	113.02
2	H	191	SER	N-CA-C	6.22	119.72	111.75
1	L	47	GLN	OE1-CD-NE2	-6.18	116.42	122.60
2	H	194	TRP	CA-C-N	6.14	127.51	119.84
2	H	194	TRP	C-N-CA	6.14	127.51	119.84
1	L	196	SER	O-C-N	6.07	129.86	123.06
1	L	129	GLN	N-CA-C	-6.02	106.07	113.41
1	L	170	ASP	CA-CB-CG	5.92	118.53	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	215	LYS	CA-CB-CG	-5.87	102.36	114.10
2	H	59	ASN	N-CA-C	-5.78	99.92	108.99
1	L	215	ASN	OD1-CG-ND2	-5.77	116.83	122.60
2	H	35	HIS	CB-CG-CD2	-5.68	123.82	131.20
2	H	170	HIS	CA-CB-CG	5.66	119.46	113.80
1	L	39	HIS	CB-CG-CD2	-5.65	123.86	131.20
1	L	33	ASN	CA-CB-CG	5.63	118.23	112.60
2	H	172	PHE	CA-CB-CG	-5.61	108.19	113.80
2	H	43	LYS	N-CA-C	5.58	122.68	110.80
1	L	160	ARG	CA-CB-CG	5.57	125.24	114.10
2	H	161	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	L	164	VAL	N-CA-C	5.52	116.18	108.89
2	H	172	PHE	N-CA-C	5.50	117.88	110.29
1	L	194	HIS	CB-CG-CD2	-5.50	124.06	131.20
1	L	201	ALA	N-CA-C	5.48	118.42	109.59
2	H	197	GLN	CA-C-O	5.48	127.92	121.40
2	H	41	HIS	CB-CG-CD2	-5.48	124.08	131.20
2	H	156	VAL	N-CA-CB	-5.44	101.75	111.92
1	L	39	HIS	CA-C-O	-5.39	115.50	121.33
2	H	58	THR	N-CA-CB	5.39	119.61	110.49
1	L	162	ASN	O-C-N	-5.39	116.38	122.10
2	H	113	THR	CB-CA-C	-5.39	103.89	111.65
1	L	40	TRP	CG-CD2-CE3	5.38	139.28	133.90
2	H	101	TRP	CD1-CG-CD2	5.29	114.76	106.30
1	L	33	ASN	OD1-CG-ND2	-5.28	117.32	122.60
2	H	8	GLY	CA-C-O	-5.26	114.00	121.52
2	H	6	GLN	OE1-CD-NE2	-5.22	117.38	122.60
2	H	101	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	L	95	GLN	O-C-N	-5.19	117.24	123.31
2	H	177	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	L	65	ASP	CA-CB-CG	5.18	117.78	112.60
1	L	9	LEU	N-CA-C	-5.18	105.08	111.40
2	H	181	TYR	N-CA-C	5.17	118.11	110.46
2	H	194	TRP	O-C-N	-5.17	116.06	122.16
2	H	78	THR	N-CA-C	5.15	117.30	108.90
2	H	114	THR	O-C-N	5.12	129.40	122.59
2	H	156	VAL	N-CA-C	-5.10	100.55	108.81
2	H	208	SER	O-C-N	-5.07	115.85	122.59
2	H	36	TRP	CE2-CD2-CG	-5.07	101.12	107.20
2	H	5	GLN	CA-CB-CG	5.07	124.23	114.10
2	H	113	THR	OG1-CB-CG2	5.06	119.42	109.30
2	H	105	SER	CB-CA-C	-5.05	109.27	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	135	GLY	CA-C-O	5.04	124.66	119.27
1	L	168	TRP	CE2-CD2-CG	-5.03	101.16	107.20
2	H	205	HIS	CB-CG-CD2	-5.03	124.66	131.20
2	H	6	GLN	N-CA-C	-5.03	103.77	110.55
1	L	124	PRO	CA-C-N	5.02	125.30	119.93
1	L	124	PRO	C-N-CA	5.02	125.30	119.93

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	131	ALA	Peptide
2	H	181	TYR	Sidechain
2	H	194	TRP	Peptide
2	H	215	LYS	Mainchain

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	1691	404	1636	29	0
2	H	1628	368	1607	75	0
3	H	18	36	0	0	0
3	L	21	42	0	0	0
All	All	3358	850	3243	94	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 14.

All (94) 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:146:VAL:HG11	2:H:201:CYS:SG	1.97	1.04
1:L:23:CYS:SG	1:L:93:CYS:SG	2.54	1.01
2:H:59:ASN:HA	2:H:70:MET:HE2	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:202:ASN:HA	2:H:211:LYS:HB3	1.49	0.95
2:H:146:VAL:HG21	2:H:201:CYS:SG	2.20	0.81
2:H:13:ARG:HG2	2:H:14:PRO:HD2	1.61	0.81
2:H:4:LEU:HD22	2:H:22:CYS:SG	2.22	0.79
2:H:133:VAL:HB	2:H:137:THR:HB	1.69	0.74
2:H:146:VAL:CG1	2:H:201:CYS:SG	2.77	0.71
2:H:121:LYS:H	2:H:121:LYS:HD2	1.56	0.71
2:H:102:LEU:O	2:H:104:LEU:HD12	1.93	0.68
2:H:162:SER:H	2:H:202:ASN:HD21	1.42	0.67
1:L:54:TYR:HB2	2:H:104:LEU:HB2	1.77	0.67
2:H:48:ILE:HD11	2:H:81:LEU:HD11	1.77	0.65
2:H:51:ILE:HD13	2:H:72:VAL:HG13	1.79	0.63
2:H:127:VAL:HG11	2:H:203:VAL:HG11	1.81	0.62
2:H:6:GLN:HG2	2:H:96:CYS:SG	2.40	0.62
2:H:54:TYR:HD1	2:H:54:TYR:N	2.00	0.59
2:H:5:GLN:HG3	2:H:23:LYS:HD2	1.84	0.58
2:H:54:TYR:N	2:H:54:TYR:CD1	2.73	0.56
2:H:146:VAL:HG21	2:H:201:CYS:CB	2.36	0.56
1:L:192:GLU:O	1:L:218:GLU:HA	2.07	0.55
2:H:43:LYS:HB3	2:H:43:LYS:NZ	2.22	0.54
2:H:146:VAL:CB	2:H:201:CYS:SG	2.96	0.54
2:H:38:LYS:HG3	2:H:94:TYR:CE1	2.44	0.53
2:H:146:VAL:CG2	2:H:201:CYS:SG	2.94	0.53
2:H:160:TRP:HZ3	2:H:214:LYS:HE3	1.74	0.53
2:H:205:HIS:H	2:H:209:SER:HB2	1.75	0.52
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.27	0.52
1:L:55:LYS:HA	2:H:104:LEU:HD22	1.92	0.51
2:H:6:GLN:HB2	2:H:111:GLN:OE1	2.10	0.51
2:H:101:TRP:O	2:H:104:LEU:HA	2.10	0.51
1:L:39:HIS:O	1:L:93:CYS:HA	2.12	0.49
1:L:113:ARG:HD3	1:L:114:ALA:O	2.13	0.49
2:H:143:THR:HA	2:H:187:VAL:O	2.12	0.49
1:L:122:ILE:H	2:H:133:VAL:HG13	1.77	0.49
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.60	0.49
1:L:55:LYS:CA	2:H:104:LEU:HD22	2.42	0.49
2:H:59:ASN:HB2	2:H:68:ALA:O	2.13	0.48
1:L:54:TYR:CD2	2:H:104:LEU:HB2	2.48	0.48
2:H:33:ALA:HB2	2:H:53:ALA:HB3	1.96	0.48
2:H:59:ASN:ND2	2:H:68:ALA:HB3	2.29	0.48
2:H:139:GLY:O	2:H:140:SER:HB2	2.14	0.48
1:L:113:ARG:HD3	1:L:114:ALA:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:142:VAL:O	2:H:188:THR:HA	2.14	0.47
2:H:162:SER:H	2:H:202:ASN:ND2	2.11	0.47
1:L:141:LEU:HD21	1:L:201:ALA:HB2	1.97	0.47
2:H:35:HIS:HE1	2:H:54:TYR:OH	1.98	0.47
1:L:54:TYR:HD2	2:H:104:LEU:HB2	1.81	0.46
2:H:51:ILE:HA	2:H:57:ASP:OD1	2.15	0.46
2:H:19:LYS:HD3	2:H:80:TYR:CD1	2.50	0.46
2:H:102:LEU:C	2:H:104:LEU:N	2.73	0.46
2:H:101:TRP:HB3	2:H:102:LEU:H	1.62	0.46
1:L:55:LYS:N	2:H:104:LEU:HD22	2.31	0.45
1:L:121:SER:HB3	2:H:133:VAL:HG22	1.98	0.45
2:H:158:LEU:HA	2:H:202:ASN:O	2.16	0.45
2:H:35:HIS:HD2	2:H:47:TRP:NE1	2.15	0.45
2:H:194:TRP:CD2	2:H:195:PRO:HA	2.52	0.45
2:H:39:GLU:HB3	2:H:93:ILE:HB	1.99	0.45
1:L:122:ILE:O	2:H:133:VAL:HA	2.17	0.44
2:H:13:ARG:HG2	2:H:14:PRO:CD	2.39	0.44
2:H:2:VAL:HG13	2:H:27:TYR:CD1	2.53	0.44
1:L:40:TRP:HA	1:L:92:PHE:O	2.18	0.44
1:L:53:ILE:HA	1:L:58:ASN:O	2.18	0.44
1:L:55:LYS:HB2	2:H:104:LEU:HD13	2.00	0.44
2:H:12:VAL:O	2:H:117:VAL:HA	2.17	0.44
1:L:85:ALA:O	1:L:88:LEU:HD22	2.18	0.43
2:H:64:PHE:HA	2:H:67:LYS:HE3	1.99	0.43
2:H:73:ASP:HB2	2:H:80:TYR:HE2	1.82	0.43
1:L:64:PRO:HG2	1:L:67:PHE:HE1	1.84	0.43
2:H:209:SER:O	2:H:210:THR:HG23	2.17	0.43
2:H:54:TYR:HD1	2:H:54:TYR:H	1.67	0.43
1:L:196:SER:HB3	1:L:215:ASN:ND2	2.34	0.43
1:L:66:ARG:O	1:L:80:ILE:HA	2.19	0.42
2:H:29:PHE:CE2	2:H:77:ASN:HA	2.55	0.42
1:L:4:MET:HB2	1:L:104:GLY:HA2	2.02	0.42
2:H:177:GLN:NE2	2:H:177:GLN:HA	2.35	0.42
1:L:154:LYS:HB2	1:L:198:THR:HB	2.02	0.42
2:H:211:LYS:O	2:H:211:LYS:HE2	2.20	0.42
2:H:16:VAL:HG12	2:H:17:SER:H	1.85	0.42
2:H:68:ALA:HA	2:H:82:GLU:O	2.20	0.42
2:H:16:VAL:HG12	2:H:17:SER:N	2.35	0.41
2:H:177:GLN:HA	2:H:177:GLN:HE21	1.84	0.41
2:H:197:GLN:OE1	2:H:216:ILE:HG12	2.20	0.41
2:H:171:THR:CG2	2:H:183:LEU:HD21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:38:LEU:HD22	1:L:76:PHE:CG	2.55	0.41
1:L:37:TYR:HB2	1:L:97:THR:OG1	2.21	0.41
1:L:174:LYS:HE2	1:L:174:LYS:HB2	1.77	0.41
1:L:125:PRO:HG3	1:L:136:SER:O	2.21	0.40
2:H:125:PRO:HB3	2:H:151:TYR:HB3	2.03	0.40
2:H:128:THR:HA	2:H:129:PRO:HD3	1.80	0.40
2:H:121:LYS:H	2:H:121:LYS:CD	2.30	0.40
1:L:88:LEU:HD12	1:L:109:LEU:HD23	2.03	0.40
2:H:38:LYS:HG3	2:H:94:TYR:HE1	1.87	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	217/219 (99%)	193 (89%)	18 (8%)	6 (3%)	4	14
2	H	214/216 (99%)	175 (82%)	27 (13%)	12 (6%)	1	4
All	All	431/435 (99%)	368 (85%)	45 (10%)	18 (4%)	2	7

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	216	ARG
1	L	217	ASN
2	H	43	LYS
2	H	62	GLN
2	H	133	VAL
2	H	140	SER
2	H	162	SER
1	L	55	LYS
1	L	204	LYS

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Mol	Chain	Res	Type
2	H	58	THR
2	H	101	TRP
2	H	206	PRO
1	L	160	ARG
2	H	77	ASN
1	L	65	ASP
2	H	102	LEU
2	H	114	THR
2	H	195	PRO

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	196/196 (100%)	175 (89%)	21 (11%)	6	21
2	H	185/185 (100%)	153 (83%)	32 (17%)	2	7
All	All	381/381 (100%)	328 (86%)	53 (14%)	3	12

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	9	LEU
1	L	17	ASP
1	L	22	SER
1	L	32	SER
1	L	42	LEU
1	L	53	ILE
1	L	55	LYS
1	L	75	ASP
1	L	88	LEU
1	L	111	ILE
1	L	126	SER
1	L	127	SER
1	L	131	THR

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Mol	Chain	Res	Type
1	L	159	GLU
1	L	170	ASP
1	L	174	LYS
1	L	188	LYS
1	L	190	GLU
1	L	207	THR
1	L	218	GLU
2	H	5	GLN
2	H	10	GLU
2	H	11	LEU
2	H	14	PRO
2	H	25	SER
2	H	30	ILE
2	H	31	ASP
2	H	48	ILE
2	H	54	TYR
2	H	55	SER
2	H	58	THR
2	H	60	TYR
2	H	73	ASP
2	H	87	THR
2	H	111	GLN
2	H	121	LYS
2	H	127	VAL
2	H	137	THR
2	H	142	VAL
2	H	146	VAL
2	H	149	LYS
2	H	156	VAL
2	H	158	LEU
2	H	175	VAL
2	H	179	ASP
2	H	198	SER
2	H	206	PRO
2	H	210	THR
2	H	211	LYS
2	H	212	VAL
2	H	214	LYS
2	H	216	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	35	ASN
1	L	129	GLN
1	L	215	ASN
1	L	217	ASN
2	H	5	GLN
2	H	35	HIS
2	H	59	ASN
2	H	177	GLN
2	H	202	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 oligosaccharides 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	219/219 (100%)	-0.58	1 (0%) 87 82	2, 13, 21, 34	0
2	H	216/216 (100%)	-0.34	1 (0%) 87 82	4, 15, 24, 29	0
All	All	435/435 (100%)	-0.46	2 (0%) 87 82	2, 13, 24, 34	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	100	GLY	3.0
1	L	219	CYS	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 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.