



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:37 AM UTC

PDB ID : 2F19 / pdb_00002f19
Title : THREE-DIMENSIONAL STRUCTURE OF TWO CRYSTAL FORMS OF
FAB R19.9, FROM A MONOCLONAL ANTI-ARSONATE ANTIBODY
Authors : Lascombe, M.B.; Alzari, P.M.; Poljak, R.J.; Nisonoff, A.
Deposited on : 1992-05-27
Resolution : 2.80 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

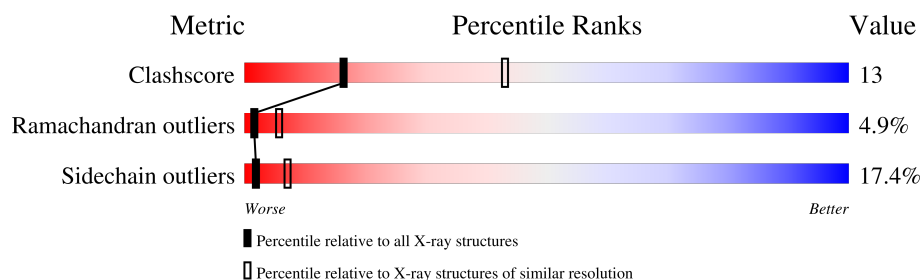
1 Overall quality at a glance

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)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	214	
2	H	221	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3320 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 IGG2B-KAPPA R19.9 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1663	1027	284	345	7			

- Molecule 2 is a protein called IGG2B-KAPPA R19.9 FAB (HEAVY CHAIN).

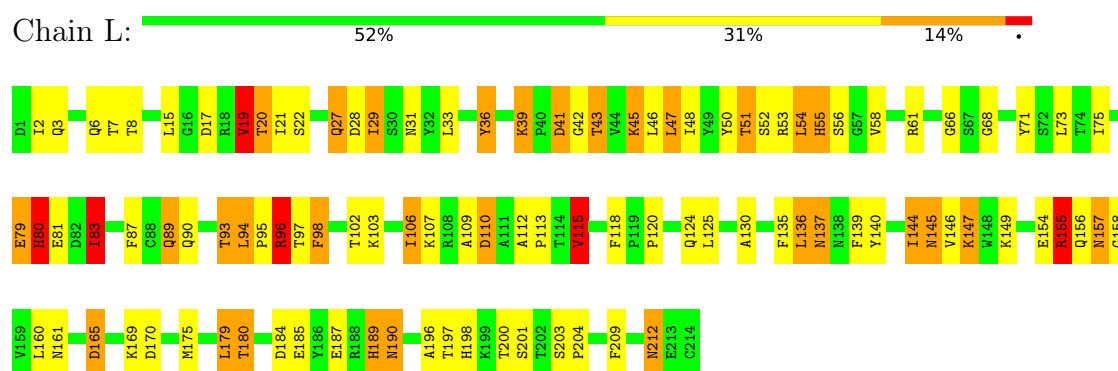
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1657	1047	270	332	8			

3 Residue-property plots

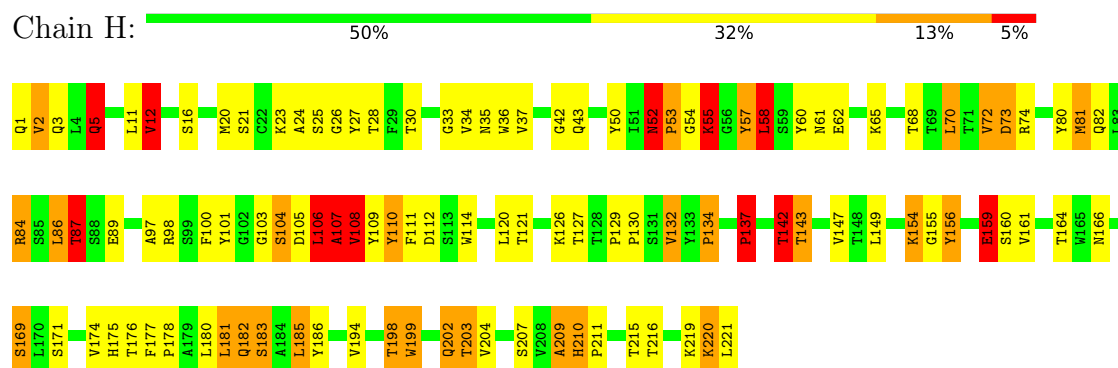
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: IGG2B-KAPPA R19.9 FAB (LIGHT CHAIN)



• Molecule 2: IGG2B-KAPPA R19.9 FAB (HEAVY CHAIN)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.30Å 80.80Å 75.10Å 90.00° 96.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3320	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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	1.04	5/1697 (0.3%)	1.99	58/2301 (2.5%)
2	H	0.99	3/1699 (0.2%)	2.01	60/2316 (2.6%)
All	All	1.02	8/3396 (0.2%)	2.00	118/4617 (2.6%)

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
1	L	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	210	HIS	CD2-NE2	-6.58	1.30	1.37
1	L	55	HIS	CD2-NE2	-6.54	1.30	1.37
1	L	198	HIS	CD2-NE2	-6.38	1.30	1.37
1	L	80	HIS	CD2-NE2	-6.35	1.30	1.37
1	L	189	HIS	CD2-NE2	-6.33	1.30	1.37
1	L	115	VAL	CA-CB	6.22	1.62	1.54
2	H	175	HIS	CD2-NE2	-6.00	1.31	1.37
2	H	210	HIS	CG-ND1	-5.22	1.32	1.38

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	110	ASP	CA-CB-CG	10.35	122.95	112.60
2	H	199	TRP	O-C-N	-8.83	114.20	121.80
2	H	154	LYS	N-CA-C	8.79	123.78	109.72
1	L	98	PHE	CA-CB-CG	8.40	122.20	113.80
1	L	22	SER	N-CA-C	8.19	122.26	109.07
1	L	165	ASP	CA-CB-CG	8.18	120.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	161	ASN	N-CA-C	8.16	122.60	110.52
2	H	5	GLN	OE1-CD-NE2	-8.16	114.44	122.60
1	L	17	ASP	N-CA-C	8.11	121.23	110.53
1	L	154	GLU	N-CA-C	8.11	122.48	110.48
2	H	101	TYR	N-CA-C	7.84	121.55	110.50
2	H	156	TYR	N-CA-C	7.69	121.34	110.50
1	L	41	ASP	CA-C-O	7.34	131.00	120.51
2	H	132	VAL	N-CA-C	7.28	117.88	108.12
2	H	73	ASP	CA-CB-CG	7.27	119.87	112.60
1	L	19	VAL	CB-CA-C	-7.20	99.89	110.62
1	L	170	ASP	N-CA-C	7.01	121.14	112.59
2	H	72	VAL	N-CA-CB	-7.00	98.84	111.92
1	L	51	THR	CA-CB-OG1	-6.99	99.12	109.60
2	H	98	ARG	CB-CG-CD	-6.85	95.55	111.30
2	H	215	THR	CA-CB-OG1	-6.74	99.48	109.60
2	H	108	VAL	CA-CB-CG1	-6.71	99.00	110.40
1	L	89	GLN	OE1-CD-NE2	-6.70	115.91	122.60
2	H	159	GLU	N-CA-C	6.65	121.25	113.20
2	H	58	LEU	N-CA-C	6.62	119.13	109.07
2	H	68	THR	N-CA-C	6.60	120.58	109.76
1	L	51	THR	CA-CB-CG2	6.59	121.70	110.50
1	L	137	ASN	OD1-CG-ND2	-6.54	116.06	122.60
2	H	37	VAL	O-C-N	-6.48	116.26	123.26
2	H	209	ALA	N-CA-C	6.35	119.13	108.02
1	L	96	ARG	CB-CG-CD	6.32	125.83	111.30
2	H	215	THR	CA-CB-CG2	6.27	121.16	110.50
2	H	203	THR	CA-CB-OG1	-6.24	100.25	109.60
2	H	110	TYR	CA-CB-CG	6.18	125.02	113.90
2	H	129	PRO	CA-C-N	6.17	126.52	119.92
2	H	129	PRO	C-N-CA	6.17	126.52	119.92
1	L	27	GLN	N-CA-C	6.14	118.49	108.55
2	H	143	THR	N-CA-C	6.09	123.77	110.80
2	H	72	VAL	N-CA-C	6.09	118.67	108.81
1	L	198	HIS	CB-CG-CD2	-6.08	123.29	131.20
1	L	96	ARG	CA-CB-CG	6.08	126.26	114.10
1	L	212	ASN	CA-C-N	6.06	133.12	121.54
1	L	212	ASN	C-N-CA	6.06	133.12	121.54
1	L	109	ALA	CA-C-O	-6.05	114.50	121.15
1	L	209	PHE	CA-CB-CG	6.02	119.82	113.80
1	L	42	GLY	CA-C-O	6.02	127.05	120.97
1	L	87	PHE	CA-CB-CG	5.99	119.79	113.80
1	L	17	ASP	CA-CB-CG	5.97	118.57	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	72	VAL	CA-CB-CG2	-5.91	100.36	110.40
2	H	198	THR	N-CA-C	-5.86	106.26	113.41
1	L	83	ILE	CA-C-O	5.81	128.01	120.69
1	L	96	ARG	NE-CZ-NH1	5.80	127.30	121.50
1	L	56	SER	N-CA-C	5.80	118.76	110.24
1	L	201	SER	N-CA-C	5.80	117.83	108.32
2	H	160	SER	N-CA-C	5.76	118.81	107.98
2	H	107	ALA	N-CA-C	5.75	123.06	110.80
2	H	174	VAL	N-CA-C	5.73	116.19	108.17
1	L	6	GLN	CA-CB-CG	-5.71	102.67	114.10
1	L	190	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	L	54	LEU	N-CA-C	5.71	117.98	109.25
1	L	102	THR	CA-C-N	-5.69	115.15	123.00
1	L	102	THR	C-N-CA	-5.69	115.15	123.00
1	L	20	THR	CA-C-O	5.68	126.26	120.24
2	H	171	SER	CA-C-O	5.67	126.48	119.79
2	H	112	ASP	CA-CB-CG	5.66	118.26	112.60
1	L	80	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	L	68	GLY	O-C-N	-5.60	115.42	122.70
1	L	112	ALA	N-CA-C	5.60	116.87	109.93
2	H	107	ALA	CA-C-N	5.57	132.00	121.97
2	H	107	ALA	C-N-CA	5.57	132.00	121.97
1	L	22	SER	CA-C-O	5.56	126.44	120.38
1	L	212	ASN	O-C-N	5.56	130.05	122.82
1	L	184	ASP	N-CA-C	5.54	117.40	111.36
2	H	108	VAL	CA-CB-CG2	5.54	119.82	110.40
2	H	12	VAL	N-CA-C	5.51	116.31	108.42
1	L	52	SER	N-CA-C	5.51	121.22	113.02
1	L	198	HIS	CB-CG-ND1	5.50	130.95	122.70
2	H	61	ASN	N-CA-C	-5.47	101.76	109.96
1	L	3	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	L	137	ASN	CB-CG-ND2	5.45	124.57	116.40
1	L	124	GLN	CG-CD-NE2	5.45	124.57	116.40
2	H	53	PRO	N-CA-C	5.42	120.67	113.57
2	H	52	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	L	137	ASN	N-CA-C	5.41	118.55	109.95
1	L	145	ASN	OD1-CG-ND2	-5.40	117.20	122.60
2	H	2	VAL	N-CA-C	5.39	120.56	109.34
1	L	155	ARG	N-CA-C	5.39	117.17	108.34
2	H	106	LEU	N-CA-C	-5.38	101.45	109.96
2	H	127	THR	N-CA-C	5.37	118.35	110.30
2	H	203	THR	CA-CB-CG2	5.36	119.61	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	42	GLY	N-CA-C	5.34	118.06	110.74
1	L	103	LYS	CB-CG-CD	-5.34	99.03	111.30
2	H	110	TYR	N-CA-C	-5.33	99.45	110.80
1	L	8	THR	O-C-N	-5.32	116.97	123.30
2	H	100	PHE	CA-CB-CG	5.32	119.12	113.80
2	H	87	THR	CA-CB-OG1	-5.31	101.64	109.60
1	L	31	ASN	N-CA-C	5.30	119.33	112.86
2	H	103	GLY	O-C-N	5.30	129.59	122.70
2	H	35	ASN	OD1-CG-ND2	-5.28	117.33	122.60
2	H	43	GLN	OE1-CD-NE2	-5.27	117.33	122.60
2	H	108	VAL	N-CA-CB	5.26	119.91	111.23
2	H	142	THR	N-CA-C	5.25	121.98	110.80
2	H	160	SER	CA-C-O	5.22	127.42	121.58
2	H	114	TRP	O-C-N	-5.21	116.59	123.16
2	H	52	ASN	CA-C-N	5.20	124.70	119.19
2	H	52	ASN	C-N-CA	5.20	124.70	119.19
2	H	183	SER	N-CA-C	5.18	117.57	108.56
1	L	43	THR	O-C-N	5.17	128.74	122.94
2	H	42	GLY	CA-C-O	5.13	124.67	118.97
1	L	27	GLN	CB-CG-CD	-5.11	103.91	112.60
2	H	87	THR	CA-CB-CG2	5.10	119.17	110.50
2	H	175	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	L	103	LYS	CA-CB-CG	5.04	124.19	114.10
1	L	137	ASN	CA-CB-CG	5.04	117.64	112.60
1	L	179	LEU	N-CA-C	5.04	116.85	111.36
2	H	194	VAL	CA-C-N	5.02	125.02	119.90
2	H	194	VAL	C-N-CA	5.02	125.02	119.90
2	H	74	ARG	O-C-N	5.02	129.26	122.59

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	203	SER	Peptide
1	L	36	TYR	Sidechain
1	L	50	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	1663	0	1589	45	0
2	H	1657	0	1610	45	0
All	All	3320	0	3199	85	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 13.

All (85) 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:146:VAL:HG11	1:L:175:MET:HE1	1.65	0.79
1:L:115:VAL:HB	1:L:136:LEU:HD13	1.66	0.77
2:H:164:THR:HG23	2:H:207:SER:HB2	1.67	0.75
1:L:36:TYR:CE1	1:L:46:LEU:HD23	2.25	0.72
1:L:19:VAL:HG23	1:L:75:ILE:HB	1.73	0.69
1:L:94:LEU:HD11	1:L:96:ARG:HH11	1.58	0.68
2:H:82:GLN:NE2	2:H:84:ARG:HE	1.96	0.64
2:H:12:VAL:HG11	2:H:86:LEU:HD23	1.82	0.61
1:L:160:LEU:HG	2:H:180:LEU:HD11	1.82	0.61
1:L:48:ILE:HG12	1:L:54:LEU:HD23	1.81	0.60
1:L:115:VAL:HA	1:L:135:PHE:O	2.02	0.59
1:L:45:LYS:HZ2	1:L:46:LEU:H	1.51	0.58
1:L:27:GLN:O	1:L:29:ILE:HG23	2.04	0.58
1:L:46:LEU:HD12	1:L:55:HIS:HB2	1.85	0.57
2:H:104:SER:OG	2:H:109:TYR:HB3	2.05	0.57
1:L:96:ARG:HD2	2:H:109:TYR:CE2	2.40	0.56
2:H:149:LEU:HD13	2:H:204:VAL:HG11	1.87	0.56
1:L:147:LYS:HE3	1:L:149:LYS:NZ	2.22	0.54
1:L:61:ARG:NH1	1:L:79:GLU:HB2	2.22	0.54
2:H:87:THR:HG22	2:H:89:GLU:H	1.72	0.54
2:H:156:TYR:HE2	2:H:159:GLU:HA	1.73	0.54
1:L:107:LYS:HA	1:L:140:TYR:OH	2.07	0.53
2:H:220:LYS:HZ2	2:H:220:LYS:HB2	1.72	0.53
1:L:110:ASP:HB3	1:L:200:THR:HG22	1.91	0.53
1:L:190:ASN:HD21	1:L:212:ASN:HB2	1.74	0.53
1:L:190:ASN:ND2	1:L:212:ASN:HB2	2.24	0.52
2:H:106:LEU:H	2:H:106:LEU:HD22	1.75	0.51
2:H:155:GLY:HA2	2:H:185:LEU:HB2	1.91	0.51
1:L:47:LEU:HB3	1:L:48:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:TRP:HB3	2:H:81:MET:HE2	1.93	0.51
2:H:30:THR:HA	2:H:53:PRO:HB2	1.92	0.51
1:L:15:LEU:CD2	1:L:106:ILE:HD11	2.41	0.50
2:H:97:ALA:HB1	2:H:111:PHE:HB3	1.93	0.50
2:H:185:LEU:HG	2:H:185:LEU:O	2.10	0.50
1:L:21:ILE:HD12	1:L:73:LEU:HD23	1.94	0.50
1:L:46:LEU:CD1	1:L:55:HIS:HB2	2.41	0.50
2:H:156:TYR:CE2	2:H:159:GLU:HA	2.47	0.50
2:H:198:THR:O	2:H:202:GLN:HB2	2.11	0.50
1:L:39:LYS:HE2	1:L:81:GLU:O	2.12	0.49
2:H:204:VAL:HG13	2:H:221:LEU:HB2	1.94	0.49
1:L:80:HIS:O	1:L:83:ILE:HG12	2.12	0.49
2:H:166:ASN:HB2	2:H:169:SER:OG	2.13	0.49
2:H:33:GLY:HA3	2:H:50:TYR:CE1	2.48	0.48
2:H:132:VAL:HG12	2:H:219:LYS:HG3	1.96	0.47
1:L:137:ASN:HD21	2:H:177:PHE:HZ	1.62	0.47
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.95	0.47
2:H:1:GLN:HB3	2:H:26:GLY:HA3	1.97	0.47
1:L:125:LEU:CD2	1:L:130:ALA:HB2	2.45	0.46
1:L:155:ARG:NH2	1:L:158:GLY:HA3	2.30	0.46
1:L:96:ARG:HH12	2:H:104:SER:HB3	1.80	0.46
2:H:104:SER:HG	2:H:109:TYR:HB3	1.79	0.46
2:H:107:ALA:O	2:H:108:VAL:HG23	2.17	0.45
2:H:73:ASP:HB2	2:H:80:TYR:HE2	1.81	0.45
1:L:144:ILE:HD11	1:L:196:ALA:HB1	1.98	0.45
2:H:60:TYR:CE2	2:H:70:LEU:HD22	2.51	0.45
2:H:164:THR:CG2	2:H:207:SER:HB2	2.42	0.44
2:H:181:LEU:HA	2:H:186:TYR:HA	2.00	0.44
2:H:137:PRO:HD3	2:H:149:LEU:HD23	1.99	0.44
2:H:181:LEU:HD12	2:H:182:GLN:O	2.18	0.44
2:H:5:GLN:NE2	2:H:23:LYS:O	2.50	0.44
1:L:96:ARG:HD2	2:H:109:TYR:CZ	2.53	0.44
1:L:89:GLN:HB2	1:L:98:PHE:CD1	2.54	0.43
1:L:155:ARG:HH22	1:L:158:GLY:HA3	1.83	0.43
2:H:147:VAL:HG11	2:H:199:TRP:CE3	2.54	0.43
1:L:144:ILE:HD13	1:L:145:ASN:N	2.32	0.43
2:H:57:TYR:HB2	2:H:58:LEU:H	1.59	0.43
1:L:144:ILE:HD13	1:L:145:ASN:H	1.84	0.43
2:H:154:LYS:HB2	2:H:154:LYS:HE3	1.78	0.43
1:L:53:ARG:HG3	1:L:53:ARG:HH11	1.84	0.42
1:L:118:PHE:HE2	1:L:135:PHE:CD2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:LYS:N	2:H:55:LYS:HE3	2.34	0.42
1:L:66:GLY:HA3	1:L:71:TYR:CD2	2.54	0.42
1:L:90:GLN:HE21	1:L:97:THR:H	1.67	0.42
1:L:156:GLN:O	1:L:157:ASN:HB2	2.20	0.42
1:L:120:PRO:CG	1:L:130:ALA:HB1	2.50	0.42
1:L:125:LEU:HD23	1:L:130:ALA:HB2	2.00	0.41
1:L:47:LEU:HA	1:L:58:VAL:HG21	2.02	0.41
2:H:183:SER:N	2:H:185:LEU:HD23	2.35	0.41
2:H:181:LEU:HA	2:H:185:LEU:O	2.20	0.41
2:H:209:ALA:O	2:H:211:PRO:HD3	2.21	0.41
2:H:24:ALA:HB1	2:H:27:TYR:CE2	2.56	0.41
1:L:94:LEU:HA	1:L:95:PRO:C	2.45	0.41
2:H:52:ASN:ND2	2:H:54:GLY:H	2.19	0.40
1:L:2:ILE:CD1	1:L:93:THR:HB	2.52	0.40
2:H:130:PRO:HD3	2:H:210:HIS:ND1	2.37	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%)	189 (89%)	18 (8%)	5 (2%)	4	17
2	H	219/221 (99%)	181 (83%)	22 (10%)	16 (7%)	1	2
All	All	431/435 (99%)	370 (86%)	40 (9%)	21 (5%)	1	6

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	2	VAL
2	H	104	SER
2	H	107	ALA

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Mol	Chain	Res	Type
2	H	108	VAL
2	H	142	THR
1	L	41	ASP
1	L	157	ASN
1	L	180	THR
2	H	55	LYS
2	H	105	ASP
2	H	110	TYR
2	H	203	THR
2	H	16	SER
2	H	169	SER
2	H	202	GLN
1	L	189	HIS
2	H	137	PRO
2	H	143	THR
2	H	182	GLN
2	H	134	PRO
1	L	28	ASP

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	192/192 (100%)	162 (84%)	30 (16%)	2	9
2	H	187/187 (100%)	151 (81%)	36 (19%)	1	5
All	All	379/379 (100%)	313 (83%)	66 (17%)	2	7

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	THR
1	L	19	VAL
1	L	20	THR
1	L	29	ILE
1	L	33	LEU

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Mol	Chain	Res	Type
1	L	39	LYS
1	L	43	THR
1	L	45	LYS
1	L	47	LEU
1	L	51	THR
1	L	79	GLU
1	L	80	HIS
1	L	83	ILE
1	L	93	THR
1	L	94	LEU
1	L	96	ARG
1	L	106	ILE
1	L	115	VAL
1	L	136	LEU
1	L	144	ILE
1	L	147	LYS
1	L	155	ARG
1	L	165	ASP
1	L	169	LYS
1	L	179	LEU
1	L	180	THR
1	L	185	GLU
1	L	187	GLU
1	L	197	THR
1	L	204	PRO
2	H	3	GLN
2	H	5	GLN
2	H	11	LEU
2	H	12	VAL
2	H	20	MET
2	H	21	SER
2	H	25	SER
2	H	28	THR
2	H	34	VAL
2	H	52	ASN
2	H	55	LYS
2	H	57	TYR
2	H	58	LEU
2	H	62	GLU
2	H	65	LYS
2	H	70	LEU
2	H	72	VAL

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Mol	Chain	Res	Type
2	H	81	MET
2	H	84	ARG
2	H	86	LEU
2	H	87	THR
2	H	106	LEU
2	H	120	LEU
2	H	121	THR
2	H	126	LYS
2	H	134	PRO
2	H	137	PRO
2	H	142	THR
2	H	159	GLU
2	H	161	VAL
2	H	176	THR
2	H	178	PRO
2	H	181	LEU
2	H	185	LEU
2	H	216	THR
2	H	220	LYS

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

Mol	Chain	Res	Type
1	L	37	GLN
1	L	38	GLN
1	L	137	ASN
1	L	198	HIS
1	L	210	ASN
1	L	212	ASN
2	H	5	GLN
2	H	39	GLN
2	H	52	ASN
2	H	82	GLN
2	H	175	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](#)

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.