



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2018 – 09:39 am GMT

PDB ID : 1DFB
Title : STRUCTURE OF A HUMAN MONOCLONAL ANTIBODY FAB FRAGMENT AGAINST GP41 OF HUMAN IMMUNODEFICIENCY VIRUS TYPE I
Authors : He, X.M.; Rueker, F.; Casale, E.; Carter, D.C.
Deposited on : 1992-03-27
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

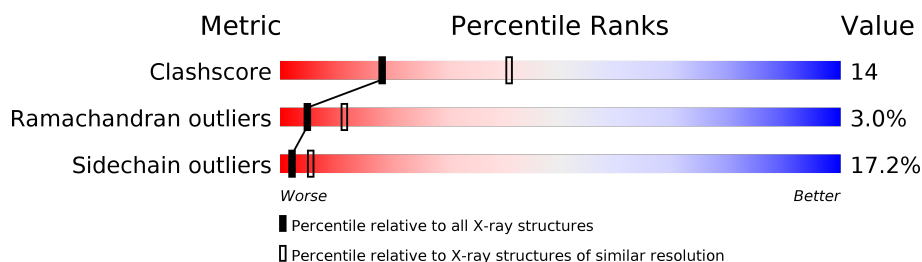
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	122078	2755 (2.70-2.70)
Ramachandran outliers	120005	2715 (2.70-2.70)
Sidechain outliers	119972	2715 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	212	
2	H	229	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3354 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 3D6 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1636	1024	274	332	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	31	ARG	PRO	CONFLICT	GB 468243
L	34	ALA	PRO	CONFLICT	GB 468243
L	43	VAL	ALA	CONFLICT	GB 468243
L	76	SER	THR	CONFLICT	GB 468243
L	87	TYR	PHE	CONFLICT	GB 468243
L	90	GLN	HIS	CONFLICT	GB 468243
L	?	-	ARG	DELETION	GB 468243
L	93	SER	PRO	CONFLICT	GB 468243
L	94	TYR	TRP	CONFLICT	GB 468243
L	95	SER	THR	CONFLICT	GB 468243
L	98	PRO	GLN	CONFLICT	GB 468243
L	103	ASP	GLU	CONFLICT	GB 468243

- Molecule 2 is a protein called IGG1-KAPPA 3D6 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	229	Total	C	N	O	S	0	0	0
			1718	1083	288	338	9			

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.60Å 74.70Å 105.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3354	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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	1.05	2/1672 (0.1%)	1.92	47/2268 (2.1%)
2	H	1.12	3/1760 (0.2%)	2.07	65/2391 (2.7%)
All	All	1.09	5/3432 (0.1%)	2.00	112/4659 (2.4%)

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	2
2	H	0	2
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	211	VAL	CA-CB	5.86	1.67	1.54
1	L	60	SER	CA-CB	5.82	1.61	1.52
1	L	15	VAL	CA-CB	5.80	1.67	1.54
2	H	167	TRP	CG-CD2	-5.73	1.33	1.43
2	H	116	TRP	CG-CD2	-5.06	1.35	1.43

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	19	ARG	NE-CZ-NH1	11.57	126.09	120.30
2	H	72	ARG	NE-CZ-NH1	10.63	125.61	120.30
2	H	100	ARG	NE-CZ-NH1	10.46	125.53	120.30
2	H	19	ARG	NE-CZ-NH2	-10.22	115.19	120.30
2	H	72	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	L	91	TYR	CB-CG-CD1	-9.37	115.38	121.00
1	L	131	VAL	CG1-CB-CG2	-9.18	96.21	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	108	TYR	CB-CG-CD1	-9.11	115.53	121.00
2	H	95	TYR	CB-CG-CD2	-8.93	115.64	121.00
1	L	35	TRP	CD1-CG-CD2	8.69	113.25	106.30
2	H	191	LEU	CA-CB-CG	8.47	134.77	115.30
2	H	36	TRP	CD1-CG-CD2	8.46	113.07	106.30
2	H	139	PRO	CA-C-N	-8.36	98.80	117.20
1	L	46	LEU	CA-CB-CG	8.21	134.19	115.30
1	L	24	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	L	32	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	L	18	ARG	CA-CB-CG	7.97	130.93	113.40
2	H	116	TRP	CD1-CG-CD2	7.91	112.63	106.30
1	L	152	LEU	CA-CB-CG	7.79	133.22	115.30
2	H	139	PRO	O-C-N	7.74	135.08	122.70
2	H	167	TRP	CD1-CG-CD2	7.68	112.44	106.30
2	H	47	TRP	CD1-CG-CD2	7.66	112.43	106.30
2	H	102	TYR	CA-CB-CG	-7.58	98.99	113.40
2	H	148	THR	O-C-N	7.47	134.65	122.70
2	H	167	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	L	35	TRP	CE2-CD2-CG	-7.42	101.37	107.30
2	H	47	TRP	CE2-CD2-CG	-7.41	101.38	107.30
2	H	116	TRP	CE2-CD2-CG	-7.38	101.40	107.30
2	H	36	TRP	CE2-CD2-CG	-7.33	101.44	107.30
2	H	207	TYR	CB-CG-CD1	-7.27	116.64	121.00
2	H	100	ARG	N-CA-C	-7.11	91.80	111.00
1	L	32	TRP	CE2-CD2-CG	-6.97	101.72	107.30
2	H	122	VAL	CG1-CB-CG2	-6.93	99.81	110.90
2	H	53	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	L	151	ALA	CA-C-N	6.89	132.36	117.20
2	H	137	LEU	N-CA-C	-6.85	92.51	111.00
2	H	6	GLU	CA-CB-CG	6.77	128.29	113.40
1	L	7	SER	N-CA-CB	6.66	120.50	110.50
1	L	4	MET	CA-CB-CG	6.49	124.34	113.30
2	H	201	SER	N-CA-CB	-6.49	100.77	110.50
1	L	146	TRP	CE2-CD2-CG	-6.34	102.23	107.30
1	L	29	ILE	CA-CB-CG2	6.31	123.53	110.90
2	H	176	VAL	CG1-CB-CG2	-6.31	100.80	110.90
2	H	228	SER	CA-C-N	-6.20	103.56	117.20
1	L	151	ALA	O-C-N	-6.20	112.78	122.70
1	L	106	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	H	36	TRP	CG-CD1-NE1	-6.10	104.00	110.10
2	H	60	TYR	CB-CG-CD1	-6.10	117.34	121.00
2	H	79	LEU	CA-CB-CG	6.10	129.33	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	102	TYR	CA-C-N	-6.10	103.79	117.20
2	H	91	MET	CA-CB-CG	-6.02	103.06	113.30
1	L	86	TYR	CB-CG-CD2	-6.02	117.39	121.00
2	H	55	SER	N-CA-CB	-6.01	101.49	110.50
1	L	130	VAL	CA-CB-CG1	-5.94	101.99	110.90
1	L	78	LEU	CA-CB-CG	5.92	128.92	115.30
2	H	74	ASN	CA-C-N	5.92	130.23	117.20
1	L	69	THR	N-CA-CB	-5.91	99.07	110.30
2	H	147	GLY	CA-C-N	-5.85	104.33	117.20
1	L	144	VAL	CB-CA-C	-5.81	100.36	111.40
2	H	105	SER	N-CA-C	-5.80	95.34	111.00
1	L	27	GLN	CA-CB-CG	5.75	126.05	113.40
1	L	29	ILE	CA-CB-CG1	-5.69	100.18	111.00
2	H	140	SER	CA-C-N	-5.69	104.68	117.20
1	L	27	GLN	CB-CG-CD	5.67	126.35	111.60
2	H	151	LEU	O-C-N	-5.67	113.56	123.20
1	L	138	TYR	CB-CG-CD1	-5.66	117.61	121.00
2	H	148	THR	CA-C-N	-5.65	104.77	117.20
1	L	35	TRP	CB-CG-CD1	-5.61	119.71	127.00
2	H	120	THR	OG1-CB-CG2	5.60	122.88	110.00
1	L	36	TYR	CB-CG-CD2	-5.59	117.65	121.00
2	H	200	SER	CA-C-N	-5.46	105.18	117.20
2	H	53	TRP	CD1-CG-CD2	5.45	110.66	106.30
1	L	87	TYR	CB-CG-CD2	-5.44	117.73	121.00
1	L	7	SER	CB-CA-C	-5.44	99.77	110.10
1	L	35	TRP	CG-CD1-NE1	-5.43	104.67	110.10
2	H	103	TYR	CA-CB-CG	-5.43	103.09	113.40
1	L	26	SER	N-CA-C	5.42	125.63	111.00
1	L	18	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	L	35	TRP	CG-CD2-CE3	5.38	138.74	133.90
2	H	207	TYR	CD1-CG-CD2	5.36	123.79	117.90
2	H	150	ALA	O-C-N	5.35	131.25	122.70
1	L	199	LEU	CA-CB-CG	5.30	127.50	115.30
1	L	139	PRO	CA-N-CD	-5.30	104.08	111.50
2	H	141	SER	N-CA-C	-5.29	96.72	111.00
1	L	173	LEU	CA-CB-CG	5.28	127.44	115.30
2	H	102	TYR	CG-CD1-CE1	-5.28	117.08	121.30
1	L	25	ALA	CA-C-N	5.27	128.80	117.20
2	H	157	ASP	CA-C-N	-5.27	105.60	117.20
2	H	151	LEU	CA-CB-CG	5.27	127.41	115.30
2	H	122	VAL	N-CA-C	-5.24	96.87	111.00
2	H	144	THR	CA-CB-CG2	5.24	119.73	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	152	LEU	N-CA-C	-5.21	96.92	111.00
1	L	32	TRP	CG-CD1-NE1	-5.18	104.92	110.10
2	H	36	TRP	CG-CD2-CE3	5.18	138.56	133.90
2	H	87	ARG	CB-CG-CD	-5.17	98.15	111.60
1	L	49	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	L	191	ALA	CB-CA-C	-5.17	102.35	110.10
2	H	151	LEU	CA-C-N	5.16	126.53	116.20
1	L	190	TYR	CB-CG-CD1	-5.14	117.92	121.00
2	H	142	LYS	C-N-CA	5.14	134.55	121.70
1	L	171	TYR	CB-CG-CD1	-5.14	117.92	121.00
2	H	100	ARG	CA-C-N	-5.13	105.92	117.20
2	H	222	LYS	CA-CB-CG	5.13	124.68	113.40
1	L	133	LEU	CA-CB-CG	5.12	127.08	115.30
2	H	84	ASN	CB-CG-ND2	5.09	128.93	116.70
2	H	94	TYR	CB-CG-CD1	-5.09	117.94	121.00
2	H	111	VAL	CA-CB-CG1	-5.09	103.26	110.90
1	L	2	ILE	CA-C-N	-5.09	106.01	117.20
2	H	228	SER	O-C-N	5.08	130.83	122.70
2	H	60	TYR	O-C-N	5.04	130.77	122.70
1	L	2	ILE	O-C-N	5.01	130.71	122.70
2	H	147	GLY	O-C-N	5.01	130.71	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	102	TYR	Sidechain
2	H	108	TYR	Sidechain
1	L	7	SER	Peptide
1	L	94	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	1636	0	1591	44	0
2	H	1718	0	1668	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3354	0	3259	95	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 (95) 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:101:ASP:HA	2:H:110:THR:HA	1.29	1.10
1:L:2:ILE:HG12	1:L:29:ILE:HD11	1.49	0.93
1:L:159:GLU:HG2	1:L:173:LEU:HD21	1.62	0.80
2:H:139:PRO:HB3	2:H:151:LEU:HB2	1.70	0.73
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.38	0.71
1:L:61:ARG:HH12	1:L:79:GLN:HB2	1.58	0.69
1:L:38:GLN:O	1:L:84:ALA:HB1	1.98	0.64
2:H:19:ARG:HH11	2:H:19:ARG:HG3	1.62	0.62
2:H:101:ASP:HA	2:H:110:THR:CA	2.18	0.61
1:L:120:ASP:HA	1:L:123:LEU:HD12	1.83	0.61
2:H:141:SER:HB3	2:H:145:SER:OG	2.00	0.60
2:H:227:LYS:HD3	2:H:228:SER:H	1.66	0.60
2:H:206:THR:HG23	2:H:223:LYS:HE3	1.84	0.59
2:H:168:ASN:HB2	2:H:172:LEU:HB2	1.83	0.59
1:L:80:PRO:HA	1:L:83:PHE:CE2	2.38	0.59
1:L:46:LEU:HD22	1:L:55:GLU:HG3	1.85	0.59
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.21	0.58
2:H:139:PRO:HB3	2:H:151:LEU:HD12	1.85	0.57
2:H:12:VAL:O	2:H:124:VAL:HA	2.04	0.57
1:L:38:GLN:HE22	2:H:39:GLN:HE22	1.50	0.57
2:H:30:ASN:O	2:H:53:TRP:HB2	2.04	0.57
1:L:61:ARG:NH1	1:L:79:GLN:HB2	2.19	0.57
1:L:154:SER:HB3	1:L:156:ASN:HD21	1.69	0.57
1:L:110:ALA:HB2	1:L:198:GLY:O	2.04	0.57
1:L:80:PRO:HA	1:L:83:PHE:HE2	1.69	0.57
2:H:72:ARG:HD3	2:H:74:ASN:HD21	1.72	0.55
1:L:31:ARG:HH12	1:L:67:SER:HA	1.72	0.55
2:H:104:ASP:HA	2:H:107:GLY:O	2.07	0.54
2:H:103:TYR:O	2:H:108:TYR:HA	2.07	0.54
2:H:151:LEU:HD22	2:H:195:VAL:CG2	2.39	0.53
1:L:134:LEU:HD13	1:L:173:LEU:HD22	1.90	0.53
2:H:139:PRO:HG2	2:H:226:PRO:HB3	1.91	0.52
2:H:35:HIS:HB2	2:H:97:VAL:CG2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:18:ARG:NH2	1:L:74:THR:HG21	2.24	0.52
1:L:38:GLN:NE2	2:H:39:GLN:HE22	2.07	0.52
1:L:134:LEU:N	1:L:134:LEU:HD12	2.25	0.51
2:H:142:LYS:HE3	2:H:145:SER:HA	1.92	0.51
1:L:149:ASP:HA	1:L:189:VAL:HG23	1.93	0.51
2:H:103:TYR:HB3	2:H:109:PHE:HD1	1.76	0.50
2:H:91:MET:HG3	2:H:124:VAL:H	1.76	0.50
1:L:138:TYR:HE1	1:L:164:GLN:HE22	1.59	0.50
1:L:37:GLN:HG3	1:L:86:TYR:CE2	2.47	0.50
1:L:114:PHE:HD2	1:L:133:LEU:HD13	1.77	0.50
1:L:78:LEU:HD12	1:L:82:ASP:HB2	1.93	0.50
2:H:140:SER:OG	2:H:143:SER:N	2.45	0.50
1:L:42:LYS:HG3	1:L:43:VAL:O	2.13	0.49
1:L:188:LYS:NZ	1:L:208:ASN:HB3	2.28	0.49
2:H:140:SER:OG	2:H:141:SER:N	2.46	0.48
1:L:18:ARG:HH21	1:L:74:THR:HG21	1.78	0.48
2:H:72:ARG:HD3	2:H:74:ASN:ND2	2.29	0.48
2:H:197:VAL:HG11	2:H:207:TYR:CE1	2.49	0.48
2:H:49:SER:HB3	2:H:70:ILE:HD12	1.95	0.47
2:H:11:LEU:HD12	2:H:12:VAL:N	2.30	0.47
2:H:91:MET:HG3	2:H:123:THR:HA	1.97	0.47
1:L:46:LEU:HD21	1:L:49:TYR:HD1	1.80	0.47
2:H:139:PRO:HB2	2:H:202:LEU:HD21	1.97	0.46
2:H:132:PRO:HD2	2:H:218:THR:HG21	1.97	0.46
1:L:70:GLU:HG2	1:L:70:GLU:O	2.14	0.46
2:H:35:HIS:CD2	2:H:50:GLY:HA3	2.50	0.45
1:L:59:PRO:HG3	1:L:61:ARG:HH21	1.80	0.45
1:L:38:GLN:HE22	2:H:39:GLN:NE2	2.14	0.45
2:H:142:LYS:HG3	2:H:145:SER:HB3	1.99	0.45
1:L:138:TYR:HE1	1:L:164:GLN:NE2	2.15	0.45
1:L:188:LYS:O	1:L:208:ASN:HA	2.17	0.44
1:L:59:PRO:HG2	1:L:62:PHE:HE1	1.82	0.44
1:L:142:ALA:HB2	1:L:196:HIS:ND1	2.33	0.44
2:H:142:LYS:HG3	2:H:145:SER:HA	1.99	0.44
1:L:36:TYR:O	1:L:86:TYR:HA	2.17	0.44
2:H:13:GLN:HB2	2:H:16:ARG:HG3	2.00	0.43
1:L:33:LEU:HG	1:L:34:ALA:N	2.32	0.43
1:L:50:LYS:HD3	2:H:103:TYR:CZ	2.54	0.43
2:H:94:TYR:O	2:H:119:GLY:HA2	2.19	0.43
1:L:80:PRO:HG2	1:L:81:ASP:OD2	2.19	0.42
1:L:33:LEU:HD11	1:L:88:CYS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:106:ARG:HG2	1:L:107:THR:H	1.85	0.42
2:H:168:ASN:ND2	2:H:172:LEU:HD12	2.34	0.42
1:L:85:THR:HA	1:L:100:THR:O	2.20	0.42
2:H:138:ALA:HB1	2:H:139:PRO:HD2	2.02	0.42
2:H:68:PHE:HA	2:H:82:GLN:O	2.19	0.42
2:H:35:HIS:HB2	2:H:97:VAL:HG22	2.00	0.42
1:L:32:TRP:HB3	1:L:91:TYR:HB2	2.01	0.42
1:L:39:LYS:H	1:L:42:LYS:HG2	1.84	0.42
2:H:184:GLN:OE1	2:H:190:SER:HB2	2.20	0.41
1:L:149:ASP:O	1:L:151:ALA:N	2.51	0.41
2:H:35:HIS:HA	2:H:50:GLY:HA2	2.02	0.41
2:H:148:THR:HG22	2:H:198:PRO:HA	2.03	0.41
2:H:139:PRO:HB3	2:H:151:LEU:CB	2.45	0.41
2:H:151:LEU:HD22	2:H:195:VAL:HG23	2.03	0.41
2:H:149:ALA:O	2:H:196:THR:HA	2.21	0.41
1:L:159:GLU:HA	1:L:174:SER:O	2.21	0.40
2:H:27:PHE:CE1	2:H:29:PHE:HA	2.56	0.40
2:H:53:TRP:CE3	2:H:54:ASP:HB3	2.56	0.40
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.55	0.40
2:H:93:LEU:HD11	2:H:119:GLY:HA3	2.04	0.40
2:H:142:LYS:CE	2:H:145:SER:HA	2.52	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	210/212 (99%)	187 (89%)	16 (8%)	7 (3%)	4	10
2	H	227/229 (99%)	198 (87%)	23 (10%)	6 (3%)	6	15
All	All	437/441 (99%)	385 (88%)	39 (9%)	13 (3%)	5	11

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	156	ASN
2	H	140	SER
2	H	143	SER
1	L	26	SER
1	L	51	ALA
2	H	2	VAL
2	H	185	SER
1	L	151	ALA
2	H	141	SER
2	H	145	SER
1	L	149	ASP
1	L	150	ASN
1	L	80	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	188/188 (100%)	156 (83%)	32 (17%)	2	5
2	H	191/191 (100%)	158 (83%)	33 (17%)	2	5
All	All	379/379 (100%)	314 (83%)	65 (17%)	2	5

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	10	THR
1	L	11	LEU
1	L	18	ARG
1	L	27	GLN
1	L	29	ILE
1	L	33	LEU
1	L	46	LEU
1	L	53	SER
1	L	55	GLU
1	L	60	SER

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Mol	Chain	Res	Type
1	L	61	ARG
1	L	63	SER
1	L	67	SER
1	L	69	THR
1	L	70	GLU
1	L	73	LEU
1	L	78	LEU
1	L	93	SER
1	L	112	SER
1	L	119	SER
1	L	127	THR
1	L	133	LEU
1	L	140	ARG
1	L	141	GLU
1	L	156	ASN
1	L	159	GLU
1	L	166	SER
1	L	167	LYS
1	L	177	LEU
1	L	178	THR
1	L	183	ASP
1	L	189	VAL
2	H	3	GLN
2	H	5	VAL
2	H	6	GLU
2	H	16	ARG
2	H	19	ARG
2	H	49	SER
2	H	62	ASP
2	H	64	VAL
2	H	67	ARG
2	H	73	ASP
2	H	77	ASN
2	H	78	SER
2	H	79	LEU
2	H	91	MET
2	H	103	TYR
2	H	108	TYR
2	H	109	PHE
2	H	118	GLN
2	H	120	THR
2	H	133	SER

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Mol	Chain	Res	Type
2	H	144	THR
2	H	145	SER
2	H	151	LEU
2	H	154	LEU
2	H	164	THR
2	H	182	VAL
2	H	191	LEU
2	H	199	SER
2	H	200	SER
2	H	204	THR
2	H	208	ILE
2	H	227	LYS
2	H	229	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	89	GLN
1	L	92	ASN
1	L	153	GLN
1	L	156	ASN
1	L	197	GLN
2	H	35	HIS
2	H	39	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 carbohydrates 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

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.