



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:24 PM UTC

PDB ID : 1DFB / pdb_00001dfb
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 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
Xtrriage (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

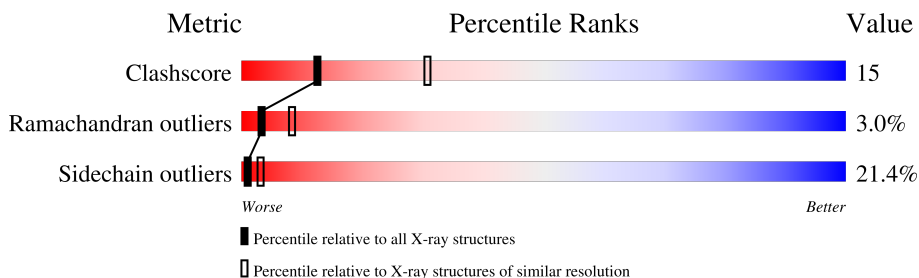
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (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 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	212	 42% 40% 15% •
2	H	229	 49% 36% 14% •

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
			Total	C	N	O	S			
1	L	212	1636	1024	274	332	6	0	0	0

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).

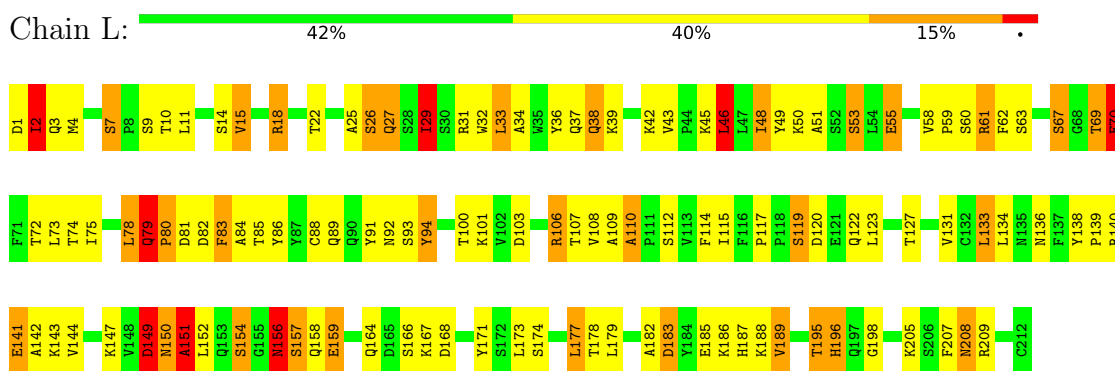
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	229	1718	1083	288	338	9	0	0	0

3 Residue-property plots

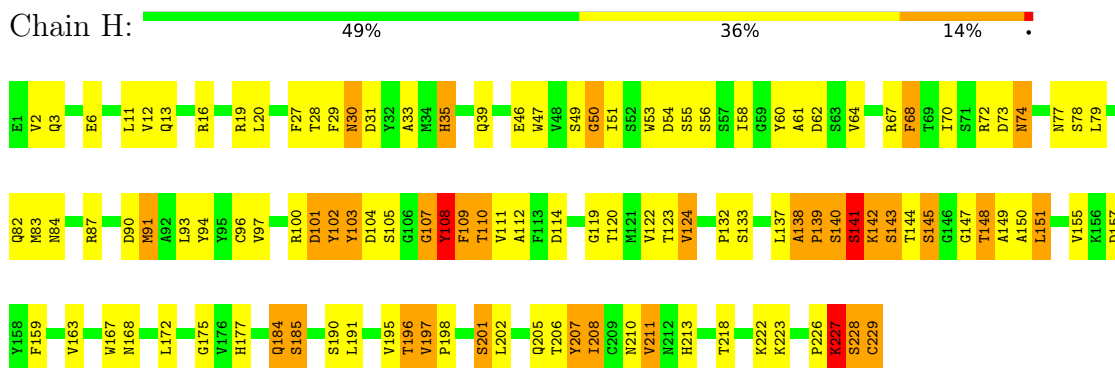
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: IGG1-KAPPA 3D6 FAB (LIGHT CHAIN)



- Molecule 2: IGG1-KAPPA 3D6 FAB (HEAVY CHAIN)



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	3354	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

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	1.32	8/1672 (0.5%)	2.27	92/2268 (4.1%)
2	H	1.37	10/1760 (0.6%)	2.32	89/2391 (3.7%)
All	All	1.35	18/3432 (0.5%)	2.30	181/4659 (3.9%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	211	VAL	CA-CB	10.23	1.67	1.54
1	L	15	VAL	CA-CB	9.18	1.67	1.54
2	H	213	HIS	CD2-NE2	-7.18	1.29	1.37
2	H	124	VAL	CA-CB	7.11	1.62	1.54
1	L	196	HIS	CD2-NE2	-6.88	1.30	1.37
1	L	187	HIS	CD2-NE2	-6.82	1.30	1.37
1	L	131	VAL	CA-CB	6.81	1.62	1.54
2	H	35	HIS	CD2-NE2	-6.51	1.30	1.37
2	H	28	THR	CA-CB	5.99	1.60	1.52
1	L	29	ILE	CA-CB	5.90	1.61	1.54
1	L	196	HIS	CG-ND1	-5.74	1.31	1.38
1	L	115	ILE	CA-CB	5.59	1.64	1.55
2	H	167	TRP	CG-CD2	-5.47	1.33	1.43
2	H	208	ILE	CA-CB	-5.36	1.47	1.54
2	H	177	HIS	CD2-NE2	-5.32	1.32	1.37
2	H	197	VAL	CA-CB	-5.28	1.50	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	18	ARG	CA-CB	5.12	1.60	1.53
2	H	51	ILE	CA-CB	5.03	1.61	1.54

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	89	GLN	OE1-CD-NE2	-10.91	111.69	122.60
2	H	139	PRO	O-C-N	10.70	135.08	123.10
1	L	183	ASP	CA-CB-CG	10.54	123.14	112.60
2	H	114	ASP	CA-CB-CG	10.13	122.73	112.60
2	H	73	ASP	CA-CB-CG	10.06	122.66	112.60
2	H	100	ARG	N-CA-C	-9.63	91.80	108.56
1	L	156	ASN	OD1-CG-ND2	-9.17	113.43	122.60
2	H	148	THR	O-C-N	9.07	134.65	122.59
1	L	69	THR	N-CA-CB	-9.02	99.07	110.98
2	H	151	LEU	O-C-N	-8.86	113.56	123.48
2	H	157	ASP	N-CA-C	8.58	120.95	110.91
2	H	74	ASN	CA-CB-CG	-8.55	104.05	112.60
1	L	18	ARG	CA-CB-CG	8.42	130.93	114.10
2	H	84	ASN	CB-CG-ND2	8.35	128.93	116.40
2	H	109	PHE	N-CA-C	8.32	122.46	109.07
2	H	102	TYR	CA-CB-CG	-8.28	98.99	113.90
1	L	208	ASN	OD1-CG-ND2	-8.28	114.32	122.60
1	L	27	GLN	CB-CG-CD	8.09	126.35	112.60
2	H	31	ASP	N-CA-C	8.08	122.96	113.18
2	H	74	ASN	CA-C-O	-7.95	110.83	119.97
1	L	150	ASN	OD1-CG-ND2	-7.91	114.69	122.60
1	L	9	SER	N-CA-C	-7.91	102.74	111.36
2	H	77	ASN	OD1-CG-ND2	-7.89	114.70	122.60
1	L	79	GLN	OE1-CD-NE2	-7.85	114.75	122.60
2	H	137	LEU	N-CA-C	-7.67	92.51	107.62
1	L	29	ILE	CA-CB-CG2	7.66	123.53	110.50
1	L	89	GLN	CG-CD-NE2	7.62	127.83	116.40
1	L	152	LEU	N-CA-C	-7.58	96.92	108.67
2	H	184	GLN	OE1-CD-NE2	-7.50	115.10	122.60
2	H	122	VAL	N-CA-C	-7.46	96.87	107.75
1	L	168	ASP	CA-CB-CG	7.42	120.02	112.60
2	H	56	SER	N-CA-C	7.41	121.42	112.38
2	H	55	SER	N-CA-CB	-7.38	101.49	112.78
1	L	2	ILE	O-C-N	7.38	130.71	122.67
1	L	151	ALA	O-C-N	-7.37	112.78	122.59
2	H	138	ALA	N-CA-C	7.37	119.07	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	154	SER	N-CA-C	7.37	121.69	109.46
2	H	150	ALA	O-C-N	7.34	131.25	122.96
1	L	207	PHE	CA-CB-CG	7.28	121.08	113.80
2	H	105	SER	N-CA-C	-7.26	95.34	110.80
2	H	84	ASN	OD1-CG-ND2	-7.18	115.42	122.60
1	L	156	ASN	CB-CG-ND2	7.15	127.13	116.40
1	L	158	GLN	OE1-CD-NE2	-7.12	115.48	122.60
2	H	6	GLU	CA-CB-CG	7.09	128.29	114.10
2	H	163	VAL	N-CA-C	-7.07	97.99	108.45
1	L	26	SER	N-CA-C	6.96	125.63	110.80
1	L	75	ILE	N-CA-C	-6.86	98.57	108.17
1	L	144	VAL	CB-CA-C	-6.83	100.36	110.33
2	H	142	LYS	CA-C-N	6.81	134.55	121.54
2	H	142	LYS	C-N-CA	6.81	134.55	121.54
2	H	175	GLY	N-CA-C	-6.80	106.60	114.69
2	H	120	THR	OG1-CB-CG2	6.79	122.88	109.30
1	L	22	THR	CA-CB-OG1	-6.78	99.43	109.60
1	L	131	VAL	CG1-CB-CG2	-6.63	96.21	110.80
1	L	83	PHE	N-CA-C	-6.61	97.76	108.41
2	H	141	SER	N-CA-C	-6.61	96.72	110.80
2	H	228	SER	O-C-N	6.58	130.83	123.40
2	H	3	GLN	CB-CG-CD	-6.53	101.50	112.60
2	H	159	PHE	O-C-N	-6.50	116.77	121.84
2	H	205	GLN	N-CA-C	6.50	119.32	110.55
2	H	107	GLY	N-CA-C	-6.49	105.78	111.95
1	L	79	GLN	CA-C-N	6.46	127.92	119.84
1	L	79	GLN	C-N-CA	6.46	127.92	119.84
2	H	155	VAL	N-CA-CB	-6.45	104.35	112.15
2	H	50	GLY	CA-C-O	-6.41	114.38	121.37
1	L	136	ASN	N-CA-C	6.41	124.44	110.80
1	L	58	VAL	N-CA-C	-6.34	103.18	108.63
1	L	187	HIS	CA-CB-CG	-6.33	107.47	113.80
2	H	60	TYR	O-C-N	6.29	130.77	123.41
2	H	122	VAL	N-CA-CB	-6.27	103.49	111.64
1	L	48	ILE	O-C-N	-6.24	116.32	123.00
1	L	147	LYS	O-C-N	-6.24	115.12	123.23
1	L	27	GLN	CG-CD-NE2	6.22	125.73	116.40
2	H	112	ALA	O-C-N	-6.18	115.69	123.17
2	H	147	GLY	O-C-N	6.16	130.71	122.70
2	H	103	TYR	O-C-N	-6.16	116.83	123.42
2	H	184	GLN	N-CA-C	6.15	118.85	110.55
2	H	30	ASN	CA-CB-CG	6.13	118.73	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	101	ASP	CA-C-N	-6.09	112.91	121.99
2	H	101	ASP	C-N-CA	-6.09	112.91	121.99
1	L	117	PRO	CA-C-N	6.08	126.11	119.90
1	L	117	PRO	C-N-CA	6.08	126.11	119.90
1	L	103	ASP	CA-CB-CG	6.05	118.65	112.60
1	L	45	LYS	CA-C-O	-6.02	114.07	120.40
1	L	29	ILE	CA-CB-CG1	-6.01	100.18	110.40
2	H	103	TYR	CA-CB-CG	-6.00	103.09	113.90
1	L	27	GLN	CA-CB-CG	5.97	126.05	114.10
1	L	92	ASN	N-CA-C	-5.96	104.16	112.45
2	H	133	SER	N-CA-C	-5.96	99.48	109.07
2	H	51	ILE	N-CA-C	5.95	116.20	108.35
1	L	143	LYS	CA-C-N	5.95	131.25	122.99
1	L	143	LYS	C-N-CA	5.95	131.25	122.99
1	L	186	LYS	CA-C-N	5.95	131.97	121.80
1	L	186	LYS	C-N-CA	5.95	131.97	121.80
2	H	139	PRO	N-CA-C	-5.94	101.83	110.80
1	L	205	LYS	CA-C-O	-5.93	114.42	120.71
1	L	149	ASP	N-CA-C	5.92	123.41	110.80
2	H	201	SER	N-CA-CB	-5.91	100.77	110.40
2	H	78	SER	CA-C-O	5.88	127.58	120.99
1	L	7	SER	CB-CA-C	-5.87	99.77	108.87
1	L	27	GLN	OE1-CD-NE2	-5.86	116.74	122.60
1	L	109	ALA	N-CA-C	-5.84	98.89	108.76
1	L	171	TYR	O-C-N	-5.81	115.60	123.15
2	H	51	ILE	O-C-N	-5.78	116.39	123.09
2	H	101	ASP	CA-CB-CG	5.76	118.36	112.60
1	L	25	ALA	O-C-N	-5.75	115.53	123.12
1	L	29	ILE	N-CA-CB	-5.74	104.64	112.28
2	H	87	ARG	CB-CG-CD	-5.72	98.15	111.30
2	H	138	ALA	CA-C-N	5.71	125.89	119.90
2	H	138	ALA	C-N-CA	5.71	125.89	119.90
2	H	110	THR	CA-CB-OG1	-5.70	101.06	109.60
2	H	112	ALA	N-CA-C	5.69	117.83	109.24
2	H	61	ALA	N-CA-C	-5.67	102.01	110.23
2	H	64	VAL	N-CA-CB	-5.65	101.90	111.23
1	L	53	SER	N-CA-C	5.65	118.78	110.30
2	H	96	CYS	O-C-N	-5.61	116.93	123.27
2	H	56	SER	O-C-N	-5.61	115.10	122.39
1	L	29	ILE	N-CA-C	-5.60	106.85	112.17
2	H	185	SER	N-CA-C	5.59	122.70	110.80
2	H	102	TYR	O-C-N	5.59	130.08	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	3	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	L	7	SER	N-CA-CB	5.55	120.50	110.72
2	H	68	PHE	O-C-N	-5.54	116.71	123.19
1	L	72	THR	N-CA-CB	-5.54	101.24	111.53
1	L	1	ASP	CA-C-O	-5.53	111.39	120.80
2	H	91	MET	CA-CB-CG	-5.52	103.06	114.10
1	L	143	LYS	CB-CG-CD	-5.51	98.61	111.30
2	H	79	LEU	N-CA-C	-5.44	101.70	110.14
2	H	207	TYR	CA-CB-CG	-5.44	104.10	113.90
1	L	69	THR	CB-CA-C	5.44	118.19	109.27
2	H	144	THR	CA-CB-CG2	5.43	119.73	110.50
1	L	177	LEU	N-CA-C	-5.43	100.33	109.07
1	L	70	GLU	CB-CG-CD	5.42	121.81	112.60
2	H	196	THR	N-CA-C	-5.41	100.36	109.07
2	H	177	HIS	CB-CG-CD2	-5.40	124.19	131.20
1	L	110	ALA	CA-C-N	5.37	125.35	120.03
1	L	110	ALA	C-N-CA	5.37	125.35	120.03
1	L	187	HIS	O-C-N	-5.33	117.66	123.26
2	H	227	LYS	N-CA-C	-5.32	101.76	109.31
1	L	186	LYS	N-CA-C	-5.31	104.38	111.87
1	L	22	THR	N-CA-CB	-5.31	102.00	111.08
1	L	139	PRO	CA-N-CD	-5.30	104.08	111.50
1	L	3	GLN	CG-CD-NE2	5.29	124.34	116.40
2	H	222	LYS	CA-CB-CG	5.29	124.68	114.10
1	L	27	GLN	N-CA-C	-5.28	101.04	109.23
2	H	191	LEU	CA-CB-CG	5.28	134.77	116.30
2	H	101	ASP	N-CA-C	-5.27	106.85	113.28
1	L	94	TYR	N-CA-CB	-5.25	104.27	112.41
1	L	108	VAL	CA-C-O	5.23	127.11	121.36
2	H	108	TYR	N-CA-CB	-5.22	102.07	110.69
1	L	195	THR	CA-CB-OG1	-5.21	101.78	109.60
2	H	139	PRO	N-CA-CB	5.21	107.95	103.36
2	H	46	GLU	N-CA-C	-5.17	99.55	108.69
1	L	7	SER	N-CA-C	-5.15	101.19	109.58
1	L	79	GLN	N-CA-C	-5.14	102.68	110.50
1	L	122	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	L	4	MET	CA-CB-CG	5.12	124.34	114.10
1	L	158	GLN	CG-CD-NE2	5.12	124.07	116.40
1	L	46	LEU	CA-CB-CG	5.11	134.19	116.30
2	H	33	ALA	N-CA-C	-5.11	101.64	109.76
1	L	157	SER	N-CA-C	-5.11	101.66	108.86
2	H	111	VAL	CA-C-O	-5.11	114.74	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	210	ASN	OD1-CG-ND2	-5.10	117.50	122.60
2	H	103	TYR	N-CA-CB	-5.09	103.67	111.56
1	L	58	VAL	CA-C-N	5.08	125.37	119.93
1	L	58	VAL	C-N-CA	5.08	125.37	119.93
2	H	139	PRO	CA-N-CD	-5.08	104.89	112.00
2	H	222	LYS	CB-CG-CD	5.08	122.98	111.30
2	H	87	ARG	CA-CB-CG	5.07	124.24	114.10
1	L	106	ARG	O-C-N	-5.07	118.22	123.29
2	H	35	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	L	38	GLN	OE1-CD-NE2	-5.06	117.54	122.60
2	H	213	HIS	CB-CG-CD2	-5.05	124.63	131.20
2	H	105	SER	CA-CB-OG	5.05	121.20	111.10
1	L	119	SER	N-CA-C	-5.05	103.01	110.48
1	L	150	ASN	O-C-N	5.04	129.30	122.59
1	L	3	GLN	N-CA-C	-5.04	101.02	109.24
1	L	136	ASN	O-C-N	-5.04	115.89	122.59
1	L	208	ASN	CB-CG-ND2	5.04	123.96	116.40
1	L	182	ALA	O-C-N	-5.03	116.60	122.03
1	L	119	SER	CA-CB-OG	5.01	121.11	111.10

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	46	0
2	H	1718	0	1668	59	0
All	All	3354	0	3259	101	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 15.

All (101) 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:20:LEU:HD22	2:H:83:MET:HE2	1.81	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:91:MET:HE2	2:H:123:THR:HG23	1.85	0.57
1:L:38:GLN:HE22	2:H:39:GLN:HE22	1.50	0.57
2:H:12:VAL:O	2:H:124:VAL:HA	2.04	0.57
1:L:61:ARG:NH1	1:L:79:GLN:HB2	2.19	0.57
2:H:30:ASN:O	2:H:53:TRP:HB2	2.04	0.57
1:L:110:ALA:HB2	1:L:198:GLY:O	2.04	0.57
1:L:154:SER:HB3	1:L:156:ASN:HD21	1.69	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:134:LEU:HD12	1:L:134:LEU:N	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:91:MET:HG3	2:H:124:VAL:H	1.76	0.50
2:H:103:TYR:HB3	2:H:109:PHE:HD1	1.76	0.50
1:L:37:GLN:HG3	1:L:86:TYR:CE2	2.47	0.50
1:L:138:TYR:HE1	1:L:164:GLN:HE22	1.59	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
1:L:46:LEU:HD21	1:L:49:TYR:HD1	1.80	0.47
2:H:91:MET:HG3	2:H:123:THR:HA	1.97	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:O	1:L:70:GLU:HG2	2.14	0.46
1:L:59:PRO:HG3	1:L:61:ARG:HH21	1.80	0.45
2:H:35:HIS:CD2	2:H:50:GLY:HA3	2.50	0.45
1:L:38:GLN:HE22	2:H:39:GLN:NE2	2.14	0.45
1:L:138:TYR:HE1	1:L:164:GLN:NE2	2.15	0.45
2:H:142:LYS:HG3	2:H:145:SER:HB3	1.99	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:185:GLU:CD	1:L:209:ARG:HH21	2.26	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:50:LYS:HD3	2:H:103:TYR:CZ	2.54	0.43
1:L:33:LEU:HG	1:L:34:ALA:N	2.32	0.43
1:L:141:GLU:N	1:L:141:GLU:CD	2.76	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
1:L:85:THR:HA	1:L:100:THR:O	2.20	0.42
2:H:168:ASN:ND2	2:H:172:LEU:HD12	2.34	0.42
2:H:35:HIS:HB2	2:H:97:VAL:HG22	2.00	0.42
2:H:68:PHE:HA	2:H:82:GLN:O	2.19	0.42
2:H:138:ALA:HB1	2:H:139:PRO:HD2	2.02	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
2:H:228:SER:C	2:H:229:CYS:SG	3.04	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:139:PRO:HB3	2:H:151:LEU:CB	2.45	0.41
2:H:148:THR:HG22	2:H:198:PRO:HA	2.03	0.41
2:H:151:LEU:HD22	2:H:195:VAL:HG23	2.03	0.41
2:H:201:SER:O	2:H:202:LEU:C	2.64	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 [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	210/212 (99%)	187 (89%)	16 (8%)	7 (3%)	3 7
2	H	227/229 (99%)	198 (87%)	23 (10%)	6 (3%)	4 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	437/441 (99%)	385 (88%)	39 (9%)	13 (3%)	3 8

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 [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	184/188 (98%)	144 (78%)	40 (22%)	1 3
2	H	31/191 (16%)	25 (81%)	6 (19%)	1 4
All	All	215/379 (57%)	169 (79%)	46 (21%)	1 3

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	10	THR
1	L	11	LEU
1	L	14	SER
1	L	15	VAL

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Mol	Chain	Res	Type
1	L	27	GLN
1	L	29	ILE
1	L	33	LEU
1	L	46	LEU
1	L	48	ILE
1	L	53	SER
1	L	55	GLU
1	L	60	SER
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	79	GLN
1	L	93	SER
1	L	101	LYS
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	157	SER
1	L	159	GLU
1	L	166	SER
1	L	167	LYS
1	L	177	LEU
1	L	178	THR
1	L	179	LEU
1	L	183	ASP
1	L	189	VAL
1	L	195	THR
2	H	58	ILE
2	H	62	ASP
2	H	208	ILE
2	H	211	VAL
2	H	227	LYS
2	H	229	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	122	GLN
1	L	153	GLN
1	L	156	ASN
1	L	158	GLN
1	L	196	HIS
2	H	39	GLN

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

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.