



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:33 PM UTC

PDB ID : 2FGW / pdb_00002fgw
Title : X-RAY STRUCTURES OF FRAGMENTS FROM BINDING AND NON-BINDING VERSIONS OF A HUMANIZED ANTI-CD18 ANTIBODY: STRUCTURAL INDICATIONS OF THE KEY ROLE OF VH RESIDUES 59 TO 65
Authors : Eigenbrot, C.; Kessler, J.
Deposited on : 1994-01-16
Resolution : 3.00 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) : **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

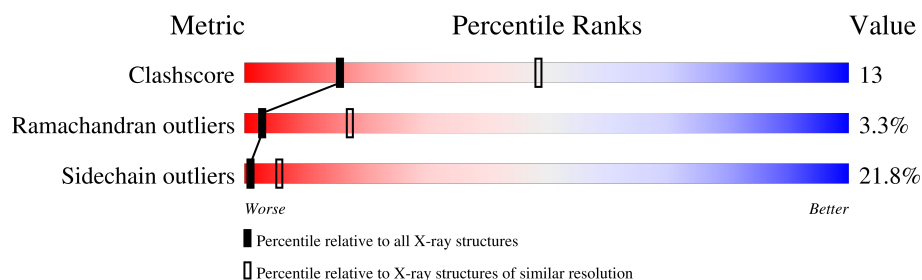
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	214	44% 41% 13% .
2	H	232	39% 38% 13% 5% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3282 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 H52 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1649	1029	277	337	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	14	SER	PHE	conflict	EMBL X95750
L	28	ASP	SER	conflict	EMBL X95750
L	30	ASN	SER	conflict	EMBL X95750
L	31	ASN	SER	conflict	EMBL X95750
L	50	TYR	ALA	conflict	EMBL X95750
L	51	THR	ALA	conflict	EMBL X95750
L	53	THR	SER	conflict	EMBL X95750
L	55	HIS	GLN	conflict	EMBL X95750
L	71	TYR	PHE	conflict	EMBL X95750
L	91	GLY	SER	conflict	EMBL X95750
L	92	ASN	HIS	conflict	EMBL X95750
L	93	THR	SER	conflict	EMBL X95750
L	94	LEU	THR	conflict	EMBL X95750
L	96	PRO	TYR	conflict	EMBL X95750
L	103	LYS	ASN	conflict	EMBL X95750
L	104	VAL	LEU	conflict	EMBL X95750

- Molecule 2 is a protein called H52 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	40	0	0
			1633	1024	277	322	10			

3 Residue-property plots

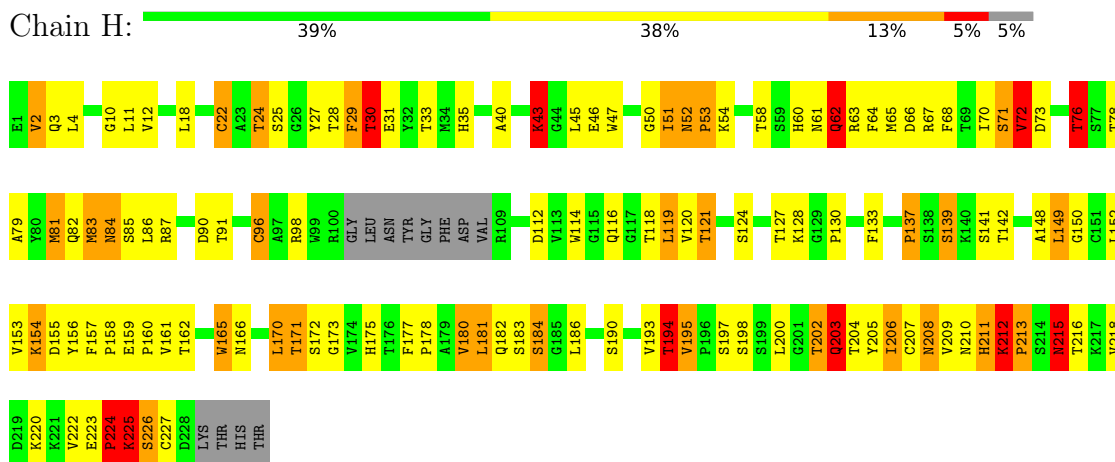
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: H52 FAB (LIGHT CHAIN)



• Molecule 2: H52 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 3	Depositor
Cell constants a, b, c, α , β , γ	101.00 Å 101.00 Å 45.50 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3282	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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	1.27	4/1685 (0.2%)	2.16	69/2291 (3.0%)
2	H	1.34	10/1671 (0.6%)	2.30	89/2274 (3.9%)
All	All	1.30	14/3356 (0.4%)	2.23	158/4565 (3.5%)

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	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	60	HIS	CD2-NE2	-7.48	1.29	1.37
2	H	121	THR	CA-CB	7.45	1.64	1.53
2	H	211	HIS	CD2-NE2	-7.29	1.29	1.37
1	L	198	HIS	CD2-NE2	-6.89	1.30	1.37
2	H	35	HIS	CD2-NE2	-6.37	1.30	1.37
2	H	175	HIS	CD2-NE2	-5.84	1.31	1.37
2	H	47	TRP	CA-CB	-5.79	1.44	1.53
1	L	136	LEU	CA-CB	-5.66	1.45	1.53
2	H	211	HIS	CG-ND1	-5.33	1.32	1.38
1	L	189	HIS	CD2-NE2	-5.30	1.32	1.37
2	H	165	TRP	NE1-CE2	-5.28	1.31	1.37
1	L	120	PRO	CA-CB	-5.27	1.47	1.53
2	H	175	HIS	CA-C	-5.26	1.46	1.52
2	H	133	PHE	CA-CB	-5.24	1.46	1.54

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	76	THR	CA-CB-OG1	-12.02	91.57	109.60
2	H	155	ASP	N-CA-C	11.84	127.39	112.24
2	H	224	PRO	N-CA-C	10.24	133.57	112.47
2	H	194	THR	CA-C-O	9.26	130.33	120.33
1	L	67	SER	CA-CB-OG	-9.23	92.63	111.10
2	H	76	THR	CA-CB-CG2	8.97	125.75	110.50
2	H	171	THR	N-CA-CB	-8.87	99.21	111.00
2	H	84	ASN	CA-CB-CG	8.52	121.11	112.60
2	H	154	LYS	N-CA-C	8.24	123.44	110.17
2	H	66	ASP	CA-CB-CG	8.09	120.69	112.60
2	H	29	PHE	O-C-N	8.06	130.47	122.09
1	L	38	GLN	CA-CB-CG	8.05	130.20	114.10
2	H	50	GLY	CA-C-O	-8.05	114.23	121.47
2	H	215	ASN	CA-CB-CG	7.95	120.55	112.60
2	H	51	ILE	CB-CA-C	-7.75	97.30	110.71
2	H	206	ILE	N-CA-C	7.68	118.97	107.75
1	L	90	GLN	OE1-CD-NE2	-7.67	114.93	122.60
1	L	105	GLU	CA-CB-CG	-7.59	98.92	114.10
2	H	150	GLY	CA-C-O	-7.54	114.29	121.38
1	L	30	ASN	N-CA-C	7.49	121.99	112.86
1	L	189	HIS	CA-CB-CG	7.45	121.25	113.80
2	H	223	GLU	CA-C-N	7.41	129.10	119.84
2	H	223	GLU	C-N-CA	7.41	129.10	119.84
1	L	161	GLU	CA-CB-CG	7.29	128.69	114.10
1	L	102	THR	CA-CB-OG1	-7.19	98.81	109.60
2	H	52	ASN	CB-CG-ND2	7.18	127.17	116.40
1	L	2	ILE	N-CA-CB	-7.05	102.53	110.99
1	L	210	ASN	CA-CB-CG	6.99	119.59	112.60
2	H	58	THR	CA-CB-OG1	-6.95	99.17	109.60
2	H	202	THR	N-CA-C	-6.92	104.12	114.64
2	H	81	MET	CA-CB-CG	-6.88	100.34	114.10
1	L	38	GLN	CA-C-O	6.86	128.57	120.20
2	H	211	HIS	CB-CG-CD2	-6.86	122.28	131.20
2	H	175	HIS	CB-CG-CD2	-6.85	122.29	131.20
2	H	35	HIS	CB-CG-CD2	-6.79	122.38	131.20
1	L	137	ASN	CA-CB-CG	6.77	119.37	112.60
1	L	140	TYR	O-C-N	-6.76	116.56	121.84
1	L	6	GLN	CA-C-O	6.63	127.74	120.71
1	L	52	SER	N-CA-C	6.63	121.03	112.41
2	H	225	LYS	CA-C-O	-6.62	111.04	120.51
2	H	166	ASN	CA-CB-CG	-6.57	106.03	112.60
2	H	170	LEU	CA-C-O	6.53	127.33	120.54
1	L	29	ILE	N-CA-CB	-6.47	101.21	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	224	PRO	N-CA-CB	-6.47	96.46	103.25
1	L	11	LEU	N-CA-CB	-6.46	99.50	111.52
1	L	198	HIS	CB-CG-CD2	-6.44	122.83	131.20
1	L	21	ILE	N-CA-C	-6.43	99.12	108.71
2	H	10	GLY	CA-C-O	-6.42	115.97	121.04
2	H	51	ILE	N-CA-CB	6.42	121.98	111.45
1	L	143	GLU	N-CA-C	6.36	118.53	108.67
2	H	160	PRO	N-CA-C	6.32	128.53	112.10
2	H	46	GLU	CA-C-O	-6.30	113.99	121.11
2	H	118	THR	O-C-N	-6.28	116.07	123.41
2	H	133	PHE	O-C-N	-6.25	116.43	121.80
2	H	112	ASP	N-CA-C	6.24	119.36	111.69
1	L	124	GLN	CA-C-O	-6.15	114.36	120.82
2	H	165	TRP	O-C-N	6.15	131.01	123.21
1	L	28	ASP	O-C-N	6.13	131.05	122.77
1	L	212	GLY	CA-C-N	6.12	133.22	121.54
1	L	212	GLY	C-N-CA	6.12	133.22	121.54
2	H	67	ARG	N-CA-C	6.06	120.80	113.41
1	L	3	GLN	CB-CG-CD	-6.05	102.32	112.60
1	L	118	PHE	CA-C-N	6.03	126.59	120.38
1	L	118	PHE	C-N-CA	6.03	126.59	120.38
2	H	52	ASN	OD1-CG-ND2	-6.03	116.57	122.60
2	H	60	HIS	CB-CG-CD2	-6.03	123.36	131.20
2	H	157	PHE	CA-CB-CG	-6.01	107.79	113.80
1	L	11	LEU	O-C-N	-6.01	116.54	123.33
1	L	17	ASP	CA-CB-CG	5.99	118.59	112.60
2	H	22	CYS	N-CA-C	-5.97	97.47	107.80
1	L	46	LEU	CA-CB-CG	5.95	137.13	116.30
2	H	70	ILE	O-C-N	-5.95	116.80	122.98
1	L	212	GLY	N-CA-C	-5.93	99.14	113.18
2	H	157	PHE	O-C-N	-5.92	114.51	121.32
2	H	195	VAL	N-CA-CB	-5.90	102.95	111.21
1	L	31	ASN	CA-CB-CG	5.88	118.48	112.60
2	H	96	CYS	N-CA-C	-5.87	101.32	110.42
2	H	171	THR	CB-CA-C	5.82	118.21	109.13
2	H	116	GLN	CB-CG-CD	5.79	122.45	112.60
2	H	211	HIS	CB-CG-ND1	5.79	131.38	122.70
1	L	170	ASP	CA-C-O	5.79	126.23	121.02
1	L	156	SER	N-CA-C	5.77	118.87	109.06
1	L	110	VAL	CB-CA-C	-5.76	101.83	111.29
1	L	148	TRP	CD1-CG-CD2	5.76	115.52	106.30
2	H	71	SER	N-CA-C	-5.76	100.31	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	139	PHE	CA-CB-CG	5.73	119.53	113.80
2	H	212	LYS	O-C-N	-5.73	115.33	120.71
1	L	198	HIS	CB-CG-ND1	5.70	131.25	122.70
2	H	30	THR	CA-CB-OG1	-5.70	101.05	109.60
1	L	156	SER	O-C-N	5.70	130.22	123.33
1	L	29	ILE	CA-CB-CG1	-5.69	100.73	110.40
2	H	43	LYS	N-CA-C	5.67	115.33	107.73
1	L	117	ILE	O-C-N	-5.67	117.36	123.14
1	L	213	GLU	N-CA-C	-5.66	98.75	110.80
2	H	190	SER	CB-CA-C	-5.66	99.68	109.86
2	H	181	LEU	N-CA-C	-5.62	101.58	109.96
2	H	119	LEU	O-C-N	-5.61	116.93	123.27
2	H	203	GLN	N-CA-C	5.59	117.02	108.52
1	L	175	LEU	CD1-CG-CD2	-5.57	98.55	110.80
2	H	62	GLN	N-CA-C	5.55	122.62	110.80
1	L	137	ASN	CA-C-O	5.51	126.65	120.70
1	L	196	VAL	CA-CB-CG2	-5.50	101.05	110.40
2	H	24	THR	CA-CB-OG1	-5.50	101.35	109.60
2	H	184	SER	CA-CB-OG	5.49	122.08	111.10
1	L	195	GLU	N-CA-C	5.49	118.72	107.69
1	L	148	TRP	CE2-CD2-CG	-5.45	100.66	107.20
1	L	195	GLU	CA-C-O	5.44	127.43	120.57
1	L	193	ALA	N-CA-C	5.43	117.52	108.99
2	H	195	VAL	CA-CB-CG2	-5.43	101.16	110.40
1	L	138	ASN	N-CA-C	5.38	118.67	111.24
2	H	180	VAL	CB-CA-C	-5.38	103.61	110.98
1	L	194	CYS	N-CA-CB	-5.37	102.27	110.65
2	H	203	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	L	81	GLU	CA-CB-CG	5.35	124.79	114.10
2	H	182	GLN	CB-CG-CD	-5.34	103.51	112.60
1	L	103	LYS	CA-C-O	-5.34	115.37	120.92
1	L	148	TRP	CG-CD1-NE1	-5.33	103.27	110.20
2	H	35	HIS	CA-CB-CG	-5.33	108.47	113.80
1	L	148	TRP	O-C-N	5.32	129.44	123.27
2	H	183	SER	O-C-N	5.32	127.62	122.09
2	H	162	THR	CA-CB-OG1	-5.32	101.62	109.60
2	H	154	LYS	CA-C-O	5.31	127.55	121.28
1	L	70	ASP	N-CA-C	5.31	117.55	108.90
2	H	29	PHE	CA-C-N	5.30	129.17	120.63
2	H	29	PHE	C-N-CA	5.30	129.17	120.63
2	H	58	THR	N-CA-C	5.30	117.06	108.26
2	H	58	THR	CA-CB-CG2	5.29	119.49	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	101	GLY	CA-C-O	-5.28	117.65	122.24
1	L	131	SER	CA-C-O	5.25	127.56	120.47
2	H	72	VAL	CA-CB-CG2	-5.23	101.51	110.40
2	H	47	TRP	CA-C-O	-5.21	115.30	121.66
1	L	202	SER	N-CA-C	5.20	118.72	112.38
2	H	208	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	L	133	VAL	N-CA-C	5.17	115.34	108.11
1	L	212	GLY	O-C-N	5.17	129.42	122.70
2	H	114	TRP	CA-CB-CG	5.16	123.40	113.60
1	L	134	CYS	CA-CB-SG	5.15	126.25	114.40
1	L	79	GLN	N-CA-C	-5.14	102.23	110.10
2	H	2	VAL	N-CA-CB	-5.13	103.22	110.26
1	L	132	VAL	N-CA-C	-5.13	102.12	108.89
2	H	142	THR	N-CA-C	-5.11	105.62	111.14
1	L	19	VAL	CG1-CB-CG2	-5.10	99.57	110.80
2	H	139	SER	N-CA-C	5.10	121.66	110.80
2	H	58	THR	N-CA-CB	-5.10	102.46	110.77
2	H	68	PHE	CA-C-O	-5.08	115.32	120.71
2	H	114	TRP	CE2-CD2-CE3	5.08	123.88	118.80
2	H	209	VAL	N-CA-CB	-5.08	105.21	111.00
1	L	7	SER	CA-CB-OG	-5.08	100.94	111.10
2	H	76	THR	N-CA-CB	-5.08	102.19	110.42
2	H	212	LYS	N-CA-C	5.08	120.37	113.16
2	H	112	ASP	CA-CB-CG	5.07	117.67	112.60
1	L	211	ARG	O-C-N	5.07	129.33	122.59
1	L	158	ASN	N-CA-C	-5.06	105.40	112.03
2	H	210	ASN	CA-CB-CG	5.06	117.66	112.60
2	H	211	HIS	O-C-N	5.02	129.54	123.01
2	H	211	HIS	CA-C-N	5.01	126.36	120.09
2	H	211	HIS	C-N-CA	5.01	126.36	120.09
1	L	195	GLU	N-CA-CB	-5.01	102.42	110.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	36	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	1649	0	1596	41	0
2	H	1633	0	1579	46	0
All	All	3282	0	3175	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)
2:H:137:PRO:HG3	2:H:149:LEU:HD23	1.53	0.91
1:L:19:VAL:HG23	1:L:75:ILE:HB	1.69	0.73
1:L:25:ALA:O	1:L:69:THR:HB	1.91	0.70
2:H:30:THR:HA	2:H:53:PRO:HB2	1.83	0.59
1:L:20:THR:HA	1:L:73:LEU:O	2.02	0.59
2:H:165:TRP:CH2	2:H:207:CYS:HB3	2.39	0.58
1:L:30:ASN:O	1:L:31:ASN:HB2	2.02	0.58
2:H:40:ALA:O	2:H:43:LYS:HB2	2.03	0.57
1:L:123:GLU:O	1:L:126:LYS:HB3	2.05	0.56
2:H:203:GLN:NE2	2:H:204:THR:H	2.03	0.56
2:H:137:PRO:HD3	2:H:149:LEU:HB3	1.88	0.56
2:H:212:LYS:HD3	2:H:212:LYS:H	1.71	0.56
2:H:195:VAL:HG21	2:H:205:TYR:CZ	2.41	0.55
1:L:170:ASP:O	1:L:172:THR:HG23	2.05	0.55
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.87	0.55
1:L:1:ASP:N	1:L:2:ILE:HD12	2.22	0.55
2:H:63:ARG:HH11	2:H:63:ARG:HG3	1.73	0.54
1:L:185:ASP:HA	1:L:188:LYS:HG2	1.89	0.54
2:H:82:GLN:NE2	2:H:84:ASN:HD21	2.05	0.54
2:H:153:VAL:HG11	2:H:161:VAL:HG11	1.90	0.54
2:H:173:GLY:O	2:H:193:VAL:HA	2.07	0.53
1:L:19:VAL:O	1:L:74:THR:HA	2.09	0.53
1:L:44:PRO:HG2	2:H:45:LEU:HD11	1.91	0.52
2:H:130:PRO:HB3	2:H:156:TYR:HB3	1.89	0.52
1:L:139:PHE:O	1:L:172:THR:HB	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:CYS:HB3	2:H:79:ALA:HB3	1.92	0.52
2:H:76:THR:HG23	2:H:78:THR:OG1	2.10	0.51
2:H:197:SER:O	2:H:200:LEU:HG	2.10	0.51
1:L:48:ILE:HA	1:L:53:THR:O	2.11	0.51
2:H:62:GLN:H	2:H:62:GLN:CD	2.20	0.49
1:L:190:LYS:HD3	1:L:211:ARG:H	1.77	0.49
1:L:41:GLY:O	1:L:42:LYS:HG3	2.12	0.49
1:L:13:ALA:HB3	1:L:78:LEU:HD12	1.92	0.49
2:H:127:THR:HG22	2:H:158:PRO:HD3	1.95	0.49
1:L:108:ARG:HH21	1:L:111:ALA:HB2	1.78	0.49
2:H:28:THR:HB	2:H:31:GLU:OE1	2.13	0.48
2:H:30:THR:O	2:H:54:LYS:HG3	2.13	0.48
2:H:73:ASP:HB3	2:H:76:THR:HG22	1.95	0.48
2:H:130:PRO:HD2	2:H:216:THR:HG21	1.95	0.48
2:H:152:LEU:HG	2:H:154:LYS:HG3	1.95	0.48
2:H:128:LYS:NZ	2:H:128:LYS:HB3	2.28	0.48
1:L:55:HIS:HB3	1:L:58:VAL:HG21	1.96	0.48
2:H:2:VAL:HG13	2:H:27:TYR:HD2	1.78	0.47
1:L:162:SER:OG	2:H:177:PHE:HB3	2.14	0.47
2:H:2:VAL:HG13	2:H:27:TYR:CD2	2.50	0.47
1:L:188:LYS:HB2	1:L:188:LYS:NZ	2.30	0.47
2:H:206:ILE:HG22	2:H:208:ASN:ND2	2.30	0.47
1:L:39:LYS:HB2	1:L:42:LYS:HD2	1.97	0.47
2:H:62:GLN:HA	2:H:65:MET:HB3	1.96	0.46
2:H:165:TRP:HB2	2:H:170:LEU:HB3	1.97	0.46
1:L:78:LEU:HD13	1:L:106:ILE:HD12	1.97	0.46
2:H:158:PRO:O	2:H:211:HIS:HE1	1.99	0.46
1:L:49:TYR:O	1:L:53:THR:HB	2.16	0.45
1:L:78:LEU:HD13	1:L:106:ILE:CD1	2.46	0.45
1:L:11:LEU:HD21	1:L:19:VAL:CG1	2.46	0.45
2:H:65:MET:HB3	2:H:65:MET:HE3	1.91	0.45
1:L:110:VAL:HG13	1:L:141:PRO:HD3	1.98	0.45
2:H:161:VAL:HG22	2:H:211:HIS:HB2	1.98	0.45
1:L:140:TYR:CE1	1:L:141:PRO:HG3	2.51	0.44
1:L:196:VAL:O	1:L:204:PRO:HA	2.16	0.44
2:H:225:LYS:O	2:H:226:SER:HB2	2.18	0.44
2:H:52:ASN:ND2	2:H:54:LYS:HB2	2.32	0.44
2:H:91:THR:HA	2:H:120:VAL:O	2.17	0.44
1:L:125:LEU:HD11	1:L:214:CYS:HB3	1.99	0.44
2:H:29:PHE:HE2	2:H:72:VAL:HG13	1.83	0.44
2:H:148:ALA:HB2	2:H:194:THR:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.84	0.43
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.99	0.43
1:L:112:ALA:HB1	1:L:201:LEU:HD13	1.99	0.43
1:L:119:PRO:HG3	1:L:209:PHE:CD2	2.54	0.43
2:H:2:VAL:HA	2:H:25:SER:O	2.18	0.43
2:H:195:VAL:HG21	2:H:205:TYR:OH	2.18	0.43
1:L:136:LEU:HD11	1:L:196:VAL:HG21	2.00	0.43
2:H:81:MET:HE2	2:H:81:MET:HB3	1.76	0.43
1:L:11:LEU:HD21	1:L:19:VAL:HG12	2.01	0.42
1:L:13:ALA:HB3	1:L:78:LEU:CD1	2.49	0.41
1:L:190:LYS:HD2	1:L:210:ASN:HD22	1.85	0.41
2:H:61:ASN:HB3	2:H:64:PHE:HD2	1.85	0.41
1:L:186:TYR:HE2	1:L:214:CYS:HB2	1.85	0.41
1:L:147:GLN:OE1	1:L:154:LEU:HD21	2.20	0.41
1:L:125:LEU:CD1	1:L:214:CYS:HB3	2.51	0.41
1:L:46:LEU:HD21	1:L:49:TYR:HB3	2.03	0.41
2:H:24:THR:HG23	2:H:27:TYR:CE2	2.56	0.40
1:L:166:GLN:HG2	1:L:171:SER:HA	2.03	0.40
2:H:137:PRO:CD	2:H:149:LEU:HB3	2.51	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%)	193 (91%)	14 (7%)	5 (2%)	4	24
2	H	216/232 (93%)	188 (87%)	19 (9%)	9 (4%)	2	13
All	All	428/446 (96%)	381 (89%)	33 (8%)	14 (3%)	3	17

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	51	THR
2	H	62	GLN
2	H	139	SER
2	H	224	PRO
2	H	226	SER
1	L	60	SER
2	H	184	SER
2	H	215	ASN
1	L	127	SER
2	H	141	SER
2	H	137	PRO
1	L	110	VAL
1	L	204	PRO
2	H	213	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	190/190 (100%)	152 (80%)	38 (20%)	1	7
2	H	182/196 (93%)	139 (76%)	43 (24%)	1	4
All	All	372/386 (96%)	291 (78%)	81 (22%)	1	6

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	11	LEU
1	L	15	VAL
1	L	19	VAL
1	L	20	THR
1	L	23	CYS
1	L	29	ILE
1	L	33	LEU
1	L	34	ASN
1	L	38	GLN

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Mol	Chain	Res	Type
1	L	46	LEU
1	L	48	ILE
1	L	60	SER
1	L	65	SER
1	L	70	ASP
1	L	72	THR
1	L	74	THR
1	L	77	SER
1	L	81	GLU
1	L	100	GLN
1	L	103	LYS
1	L	109	THR
1	L	110	VAL
1	L	149	LYS
1	L	154	LEU
1	L	162	SER
1	L	168	SER
1	L	171	SER
1	L	175	LEU
1	L	176	SER
1	L	181	LEU
1	L	188	LYS
1	L	190	LYS
1	L	196	VAL
1	L	197	THR
1	L	203	SER
1	L	207	LYS
1	L	214	CYS
2	H	3	GLN
2	H	4	LEU
2	H	11	LEU
2	H	12	VAL
2	H	18	LEU
2	H	30	THR
2	H	33	THR
2	H	43	LYS
2	H	51	ILE
2	H	53	PRO
2	H	71	SER
2	H	72	VAL
2	H	76	THR
2	H	83	MET

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Mol	Chain	Res	Type
2	H	85	SER
2	H	87	ARG
2	H	90	ASP
2	H	96	CYS
2	H	98	ARG
2	H	119	LEU
2	H	121	THR
2	H	124	SER
2	H	149	LEU
2	H	159	GLU
2	H	171	THR
2	H	172	SER
2	H	178	PRO
2	H	180	VAL
2	H	181	LEU
2	H	186	LEU
2	H	194	THR
2	H	198	SER
2	H	202	THR
2	H	203	GLN
2	H	212	LYS
2	H	213	PRO
2	H	215	ASN
2	H	218	VAL
2	H	220	LYS
2	H	222	VAL
2	H	224	PRO
2	H	225	LYS
2	H	227	CYS

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	38	GLN
1	L	210	ASN
2	H	39	GLN
2	H	52	ASN
2	H	55	ASN
2	H	82	GLN
2	H	116	GLN
2	H	203	GLN
2	H	211	HIS

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.