



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 08:55 AM EST

PDB ID : 2FGW  
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 : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

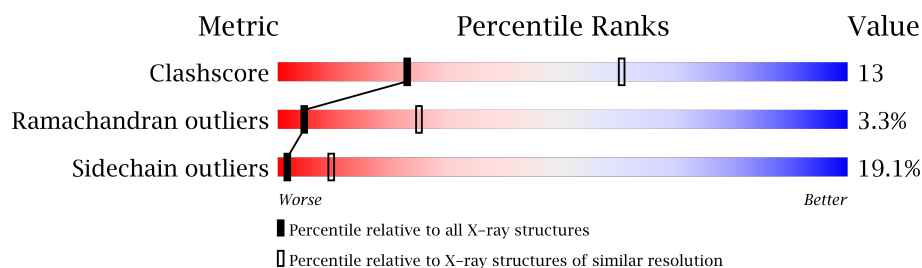
# 1 Overall quality at a glance

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	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	214	
2	H	232	

## 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).

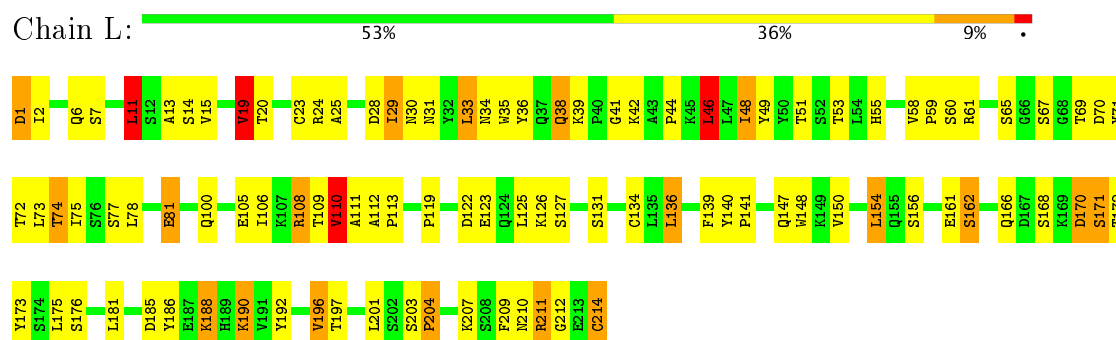
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	40	0	0
			1633	1024	277	322	10			

### 3 Residue-property plots [i](#)

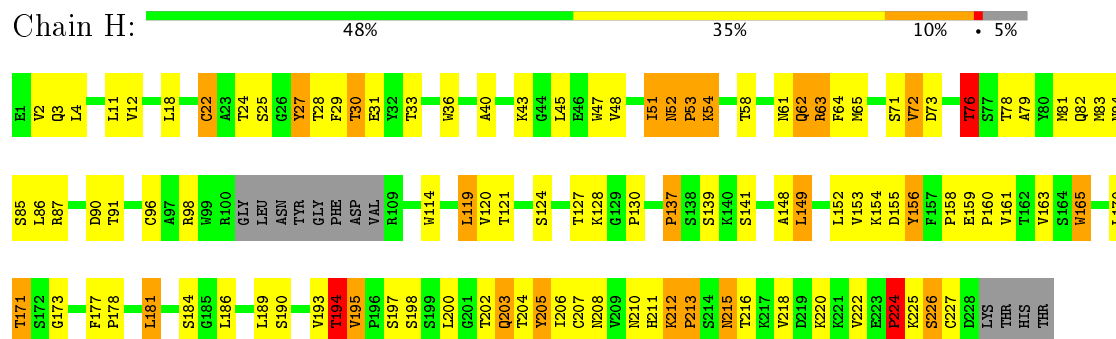
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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	0.97	0/1685	1.88	42/2291 (1.8%)
2	H	1.02	2/1671 (0.1%)	1.91	40/2274 (1.8%)
All	All	0.99	2/3356 (0.1%)	1.89	82/4565 (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
1	L	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	165	TRP	CG-CD2	-5.13	1.34	1.43
2	H	114	TRP	CG-CD2	-5.08	1.35	1.43

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	108	ARG	NE-CZ-NH1	11.81	126.20	120.30
1	L	148	TRP	CD1-CG-CD2	11.53	115.52	106.30
2	H	76	THR	CA-CB-CG2	9.53	125.75	112.40
1	L	46	LEU	CA-CB-CG	9.49	137.13	115.30
2	H	205	TYR	CB-CG-CD1	-9.22	115.47	121.00
1	L	108	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	L	35	TRP	CD1-CG-CD2	8.75	113.30	106.30
1	L	173	TYR	CB-CG-CD1	-8.69	115.79	121.00
1	L	148	TRP	CE2-CD2-CG	-8.30	100.66	107.30
2	H	76	THR	CA-CB-OG1	-8.30	91.57	109.00
2	H	224	PRO	N-CA-C	8.26	133.57	112.10
1	L	61	ARG	NE-CZ-NH2	-7.92	116.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	47	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	L	38	GLN	CA-CB-CG	7.64	130.20	113.40
2	H	81	MET	CA-CB-CG	-7.62	100.34	113.30
2	H	36	TRP	CD1-CG-CD2	7.60	112.38	106.30
2	H	114	TRP	CD1-CG-CD2	7.50	112.30	106.30
2	H	194	THR	CA-C-N	-7.45	100.81	117.20
2	H	51	ILE	CB-CA-C	-7.15	97.30	111.60
2	H	165	TRP	CD1-CG-CD2	7.12	112.00	106.30
2	H	156	TYR	CB-CG-CD2	-7.12	116.73	121.00
1	L	19	VAL	CG1-CB-CG2	-7.08	99.57	110.90
2	H	165	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	L	161	GLU	CA-CB-CG	6.95	128.69	113.40
1	L	211	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	L	28	ASP	CA-C-N	-6.89	102.03	117.20
2	H	36	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	L	67	SER	CA-CB-OG	-6.88	92.63	111.20
1	L	148	TRP	CG-CD1-NE1	-6.83	103.27	110.10
1	L	134	CYS	CA-CB-SG	6.81	126.25	114.00
1	L	192	TYR	CB-CG-CD2	-6.76	116.94	121.00
2	H	119	LEU	CA-CB-CG	6.61	130.51	115.30
1	L	35	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	L	105	GLU	CA-CB-CG	-6.58	98.92	113.40
1	L	196	VAL	CA-CB-CG2	-6.57	101.05	110.90
1	L	212	GLY	CA-C-N	-6.54	102.81	117.20
2	H	195	VAL	CA-CB-CG2	-6.49	101.16	110.90
2	H	165	TRP	CA-C-N	-6.36	103.22	117.20
2	H	160	PRO	N-CA-C	6.32	128.53	112.10
2	H	47	TRP	CE2-CD2-CG	-6.29	102.27	107.30
2	H	72	VAL	CA-CB-CG2	-6.26	101.51	110.90
2	H	114	TRP	CE2-CD2-CG	-6.22	102.33	107.30
1	L	1	ASP	CA-C-N	-6.16	103.65	117.20
1	L	24	ARG	NE-CZ-NH1	6.11	123.36	120.30
2	H	63	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	H	155	ASP	N-CA-C	6.07	127.39	111.00
1	L	170	ASP	CB-CG-OD1	6.00	123.70	118.30
2	H	189	LEU	CA-CB-CG	5.99	129.07	115.30
1	L	38	GLN	CA-C-N	-5.95	104.11	117.20
1	L	156	SER	CA-C-N	-5.91	104.38	116.20
2	H	171	THR	N-CA-CB	-5.84	99.21	110.30
2	H	27	TYR	CB-CG-CD1	-5.82	117.51	121.00
2	H	163	VAL	CG1-CB-CG2	-5.81	101.60	110.90
1	L	6	GLN	CA-C-N	-5.80	104.45	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	212	GLY	N-CA-C	-5.59	99.14	113.10
2	H	224	PRO	N-CA-CB	-5.58	96.46	102.60
2	H	181	LEU	CA-CB-CG	5.51	127.97	115.30
2	H	48	VAL	CG1-CB-CG2	-5.51	102.09	110.90
2	H	190	SER	CB-CA-C	-5.48	99.68	110.10
2	H	47	TRP	CG-CD1-NE1	-5.46	104.64	110.10
2	H	54	LYS	CA-C-N	5.46	129.21	117.20
1	L	11	LEU	N-CA-CB	-5.45	99.50	110.40
1	L	29	ILE	CA-CB-CG1	-5.41	100.73	111.00
2	H	190	SER	N-CA-CB	5.30	118.44	110.50
1	L	150	VAL	CA-CB-CG2	-5.26	103.01	110.90
1	L	28	ASP	O-C-N	5.22	131.05	122.70
1	L	110	VAL	CA-CB-CG1	-5.21	103.09	110.90
2	H	165	TRP	CB-CG-CD1	-5.20	120.24	127.00
2	H	165	TRP	O-C-N	5.20	131.01	122.70
1	L	81	GLU	CA-CB-CG	5.18	124.79	113.40
1	L	131	SER	CA-C-N	-5.17	105.83	117.20
1	L	33	LEU	CA-CB-CG	-5.14	103.48	115.30
1	L	71	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	L	35	TRP	CG-CD1-NE1	-5.11	104.99	110.10
2	H	114	TRP	CA-CB-CG	5.11	123.40	113.70
2	H	222	VAL	CA-CB-CG1	-5.09	103.27	110.90
1	L	136	LEU	CB-CG-CD2	-5.07	102.38	111.00
2	H	58	THR	CA-CB-CG2	5.06	119.49	112.40
1	L	175	LEU	CA-CB-CG	5.05	126.92	115.30
1	L	14	SER	CA-C-N	-5.04	106.11	117.20
1	L	110	VAL	CB-CA-C	-5.03	101.83	111.40
2	H	22	CYS	N-CA-C	-5.01	97.47	111.00

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	44	0
All	All	3282	0	3175	83	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 (83) 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
1:L:30:ASN:O	1:L:31:ASN:HB2	2.02	0.59
2:H:165:TRP:CH2	2:H:207:CYS:HB3	2.39	0.58
2:H:40:ALA:O	2:H:43:LYS:HB2	2.03	0.57
2:H:203:GLN:NE2	2:H:204:THR:H	2.03	0.56
1:L:123:GLU:O	1:L:126:LYS:HB3	2.05	0.56
2:H:137:PRO:HD3	2:H:149:LEU:HB3	1.88	0.56
2:H:212:LYS:H	2:H:212:LYS:HD3	1.71	0.56
2:H:195:VAL:HG21	2:H:205:TYR:CZ	2.41	0.55
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.87	0.55
1:L:170:ASP:O	1:L:172:THR:HG23	2.05	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
2:H:82:GLN:NE2	2:H:84:ASN:HD21	2.05	0.54
1:L:185:ASP:HA	1:L:188:LYS:HG2	1.89	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:152:LEU:HG	2:H:154:LYS:HG3	1.95	0.48
2:H:130:PRO:HD2	2:H:216:THR:HG21	1.95	0.48
2:H:73:ASP:HB3	2:H:76:THR:HG22	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
2:H:2:VAL:HG13	2:H:27:TYR:CD2	2.50	0.47
1:L:162:SER:OG	2:H:177:PHE:HB3	2.14	0.47
1:L:188:LYS:NZ	1:L:188:LYS:HB2	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:62:GLN:CD	2:H:62:GLN:H	2.20	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
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.99	0.43
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.84	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:195:VAL:HG21	2:H:205:TYR:OH	2.18	0.43
2:H:2:VAL:HA	2:H:25:SER:O	2.18	0.43
1:L:136:LEU:HD11	1:L:196:VAL:HG21	2.00	0.43
1:L:11:LEU:HD21	1:L:19:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:13:ALA:HB3	1:L:78:LEU:CD1	2.49	0.41
2:H:61:ASN:HB3	2:H:64:PHE:HD2	1.85	0.41
1:L:190:LYS:HD2	1:L:210:ASN:HD22	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%)	7	34
2	H	216/232 (93%)	188 (87%)	19 (9%)	9 (4%)	3	18
All	All	428/446 (96%)	381 (89%)	33 (8%)	14 (3%)	4	25

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

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Mol	Chain	Res	Type
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%)	157 (83%)	33 (17%)	2	11
2	H	182/196 (93%)	144 (79%)	38 (21%)	1	6
All	All	372/386 (96%)	301 (81%)	71 (19%)	2	9

All (71) 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	23	CYS
1	L	29	ILE
1	L	33	LEU
1	L	34	ASN
1	L	38	GLN
1	L	46	LEU
1	L	48	ILE
1	L	65	SER
1	L	70	ASP
1	L	72	THR
1	L	74	THR
1	L	77	SER
1	L	81	GLU

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Mol	Chain	Res	Type
1	L	100	GLN
1	L	109	THR
1	L	110	VAL
1	L	122	ASP
1	L	154	LEU
1	L	162	SER
1	L	168	SER
1	L	171	SER
1	L	176	SER
1	L	181	LEU
1	L	188	LYS
1	L	190	LYS
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	51	ILE
2	H	52	ASN
2	H	53	PRO
2	H	71	SER
2	H	76	THR
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	178	PRO
2	H	181	LEU
2	H	186	LEU

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Mol	Chain	Res	Type
2	H	194	THR
2	H	198	SER
2	H	202	THR
2	H	203	GLN
2	H	210	ASN
2	H	212	LYS
2	H	213	PRO
2	H	215	ASN
2	H	218	VAL
2	H	220	LYS
2	H	224	PRO
2	H	227	CYS

Some 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	92	ASN
1	L	210	ASN
2	H	39	GLN
2	H	52	ASN
2	H	82	GLN
2	H	203	GLN
2	H	210	ASN
2	H	211	HIS

### 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.