



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:40 AM UTC

PDB ID : 1F4W / pdb_00001f4w
Title : CRYSTAL STRUCTURE OF AN ANTI-CARBOHYDRATE ANTIBODY
DIRECTED AGAINST VIBRIO CHOLERAЕ O1 IN COMPLEX WITH
ANTIGEN
Authors : Alzari, P.M.; Souchon, H.
Deposited on : 2000-06-10
Resolution : 2.30 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

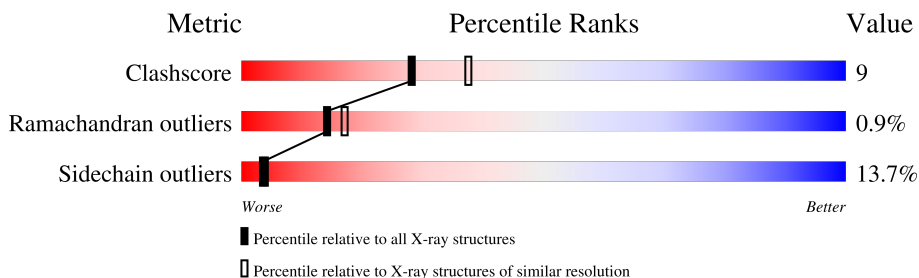
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	210	
2	H	216	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3205 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 ANTIBODY S-20-4, FAB FRAGMENT, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	210	Total	C	N	O	S	0	0	0
			1556	977	254	319	6			

- Molecule 2 is a protein called ANTIBODY S-20-4, FAB FRAGMENT, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1598	1011	257	322	8			

- Molecule 3 is water.

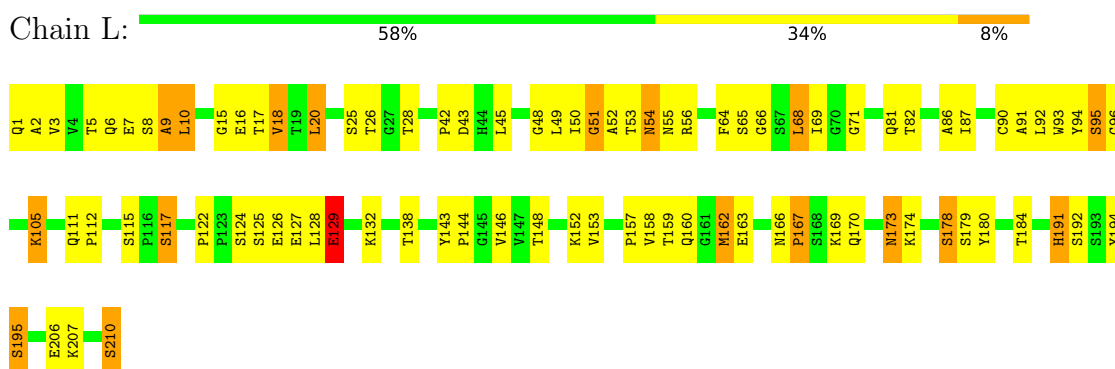
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	28	Total	O	0	0
			28	28		
3	H	23	Total	O	0	0
			23	23		

3 Residue-property plots

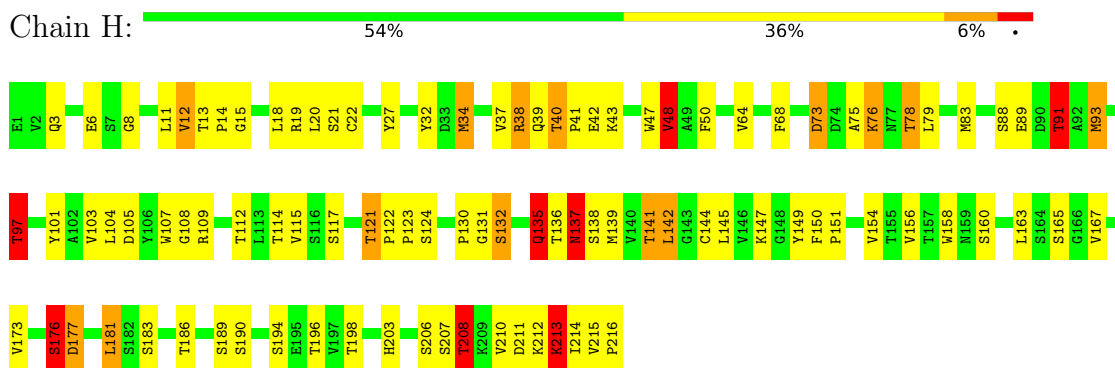
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: ANTIBODY S-20-4, FAB FRAGMENT, LIGHT CHAIN



- Molecule 2: ANTIBODY S-20-4, FAB FRAGMENT, 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	45.67Å 113.32Å 46.21Å 90.00° 100.69° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3205	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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	1.07	0/1592	2.23	68/2180 (3.1%)
2	H	1.14	1/1641 (0.1%)	2.22	78/2252 (3.5%)
All	All	1.10	1/3233 (0.0%)	2.23	146/4432 (3.3%)

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
2	H	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	216	PRO	N-CD	5.66	1.55	1.47

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	56	ARG	CD-NE-CZ	20.34	152.87	124.40
1	L	8	SER	CA-C-O	9.90	130.91	120.42
2	H	48	VAL	N-CA-CB	-9.29	95.89	111.23
1	L	18	VAL	CB-CA-C	-9.02	96.85	110.55
1	L	50	ILE	CA-C-O	-8.71	110.91	120.67
1	L	55	ASN	CA-CB-CG	8.68	121.28	112.60
2	H	8	GLY	CA-C-N	-8.43	111.89	121.83
2	H	8	GLY	C-N-CA	-8.43	111.89	121.83
2	H	12	VAL	O-C-N	-8.36	113.67	122.95
2	H	21	SER	CA-CB-OG	-8.32	94.46	111.10
1	L	90	CYS	CA-C-O	-8.25	111.83	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	97	THR	CB-CA-C	-8.19	91.38	109.56
2	H	21	SER	CA-C-O	-8.04	112.02	121.11
2	H	208	THR	N-CA-CB	-8.03	96.76	111.37
2	H	37	VAL	CA-C-O	-8.01	111.99	121.28
1	L	65	SER	CA-C-O	-7.84	112.87	121.33
2	H	21	SER	O-C-N	7.75	133.27	123.19
1	L	55	ASN	OD1-CG-ND2	-7.67	114.93	122.60
2	H	3	GLN	CB-CA-C	7.60	122.94	109.65
1	L	81	GLN	CA-C-N	7.52	130.35	120.28
1	L	81	GLN	C-N-CA	7.52	130.35	120.28
2	H	210	VAL	CA-C-O	-7.44	112.48	120.36
1	L	191	HIS	CA-CB-CG	-7.35	106.45	113.80
1	L	91	ALA	CA-C-N	7.10	132.80	123.00
1	L	91	ALA	C-N-CA	7.10	132.80	123.00
1	L	178	SER	CA-CB-OG	-7.10	96.91	111.10
2	H	32	TYR	CA-C-O	7.08	129.16	121.16
1	L	125	SER	CB-CA-C	-6.97	99.22	110.79
2	H	105	ASP	CA-CB-CG	6.94	119.54	112.60
2	H	211	ASP	CA-CB-CG	-6.92	105.68	112.60
2	H	91	THR	N-CA-CB	6.91	120.36	109.71
2	H	117	SER	CA-CB-OG	-6.91	97.29	111.10
2	H	150	PHE	CA-CB-CG	-6.78	107.02	113.80
1	L	86	ALA	CA-C-O	-6.74	113.93	120.94
2	H	97	THR	N-CA-CB	6.72	124.02	111.53
2	H	68	PHE	CA-CB-CG	6.65	120.45	113.80
1	L	124	SER	CA-C-O	-6.63	113.90	121.72
2	H	32	TYR	N-CA-C	6.55	120.36	109.95
2	H	124	SER	N-CA-C	-6.55	99.63	110.17
2	H	121	THR	CB-CA-C	6.55	118.87	110.16
1	L	65	SER	CA-C-N	-6.52	115.97	121.58
1	L	65	SER	C-N-CA	-6.52	115.97	121.58
1	L	25	SER	CA-C-O	6.46	127.33	119.38
1	L	173	ASN	CA-CB-CG	-6.46	106.14	112.60
2	H	215	VAL	CA-C-O	6.45	128.60	119.95
2	H	156	VAL	CA-C-O	-6.43	113.64	120.39
2	H	147	LYS	N-CA-CB	-6.42	100.10	111.08
1	L	117	SER	N-CA-C	-6.41	98.28	108.73
2	H	121	THR	CA-CB-CG2	6.31	121.22	110.50
1	L	184	THR	N-CA-C	-6.28	101.22	110.52
2	H	75	ALA	CA-C-N	-6.23	112.89	122.60
2	H	75	ALA	C-N-CA	-6.23	112.89	122.60
2	H	6	GLU	CA-C-N	-6.11	111.95	122.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	6	GLU	C-N-CA	-6.11	111.95	122.10
2	H	11	LEU	O-C-N	-6.07	116.41	123.27
1	L	9	ALA	O-C-N	6.07	130.27	123.48
2	H	6	GLU	O-C-N	6.06	129.84	123.06
2	H	213	LYS	CA-CB-CG	6.06	126.21	114.10
1	L	8	SER	O-C-N	-6.04	115.26	122.15
1	L	3	VAL	N-CA-CB	6.03	119.48	111.64
2	H	48	VAL	CB-CA-C	6.02	121.16	111.29
1	L	90	CYS	N-CA-CB	-5.97	101.30	110.85
2	H	123	PRO	CA-C-O	-5.95	114.81	122.13
1	L	66	GLY	CA-C-O	-5.94	115.64	121.76
2	H	37	VAL	CA-C-N	-5.94	112.83	122.81
2	H	37	VAL	C-N-CA	-5.94	112.83	122.81
2	H	154	VAL	N-CA-CB	5.90	122.85	111.93
1	L	7	GLU	N-CA-C	-5.86	102.24	110.50
1	L	195	SER	CA-C-N	-5.73	114.92	123.00
1	L	195	SER	C-N-CA	-5.73	114.92	123.00
1	L	69	ILE	CB-CA-C	-5.73	102.33	110.12
2	H	177	ASP	CA-CB-CG	-5.72	106.88	112.60
2	H	38	ARG	NE-CZ-NH1	5.70	127.20	121.50
1	L	15	GLY	N-CA-C	-5.68	107.93	114.69
1	L	129	GLU	CA-CB-CG	5.66	125.42	114.10
2	H	108	GLY	CA-C-N	5.65	130.15	120.72
2	H	108	GLY	C-N-CA	5.65	130.15	120.72
1	L	8	SER	N-CA-CB	-5.64	101.81	110.16
2	H	64	VAL	O-C-N	5.62	127.57	121.78
2	H	198	THR	CA-C-O	-5.62	114.19	120.66
1	L	195	SER	O-C-N	5.62	130.13	123.27
2	H	141	THR	CB-CA-C	5.62	119.43	109.72
2	H	109	ARG	N-CA-CB	-5.61	101.08	110.39
1	L	64	PHE	CA-CB-CG	-5.60	108.20	113.80
2	H	147	LYS	CA-C-O	5.59	127.42	121.11
1	L	42	PRO	CA-C-N	5.57	132.18	121.54
1	L	42	PRO	C-N-CA	5.57	132.18	121.54
1	L	17	THR	CA-CB-OG1	-5.57	101.25	109.60
1	L	174	LYS	N-CA-C	-5.54	102.56	110.59
2	H	27	TYR	CA-C-O	-5.53	115.36	121.28
1	L	51	GLY	O-C-N	-5.52	118.80	123.60
1	L	18	VAL	CA-C-O	-5.50	115.89	121.67
2	H	14	PRO	N-CA-CB	5.49	108.08	103.25
1	L	90	CYS	CA-CB-SG	-5.47	101.81	114.40
2	H	105	ASP	CB-CG-OD1	5.45	130.93	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	179	SER	CA-CB-OG	-5.43	100.23	111.10
1	L	20	LEU	CA-C-O	-5.42	114.96	120.71
2	H	190	SER	CA-C-N	5.41	127.80	120.44
2	H	190	SER	C-N-CA	5.41	127.80	120.44
1	L	195	SER	CA-CB-OG	-5.41	100.28	111.10
2	H	165	SER	N-CA-CB	5.41	118.99	110.23
2	H	105	ASP	CA-C-O	-5.39	114.04	120.56
2	H	50	PHE	CA-CB-CG	5.37	119.17	113.80
1	L	92	LEU	CA-C-O	5.36	126.22	120.38
2	H	6	GLU	CA-C-O	-5.35	114.94	121.36
1	L	122	PRO	CA-C-N	5.34	125.28	119.78
1	L	122	PRO	C-N-CA	5.34	125.28	119.78
1	L	191	HIS	CA-C-N	-5.33	113.87	122.24
1	L	191	HIS	C-N-CA	-5.33	113.87	122.24
1	L	25	SER	CA-C-N	5.32	129.11	120.60
1	L	25	SER	C-N-CA	5.32	129.11	120.60
2	H	47	TRP	N-CA-C	-5.30	102.64	110.48
2	H	34	MET	N-CA-C	5.29	117.73	109.52
2	H	158	TRP	CA-C-N	5.27	129.88	122.46
2	H	158	TRP	C-N-CA	5.27	129.88	122.46
2	H	101	TYR	O-C-N	-5.26	116.64	122.91
1	L	55	ASN	CB-CG-ND2	5.26	124.28	116.40
2	H	19	ARG	CD-NE-CZ	5.24	131.74	124.40
2	H	40	THR	CA-C-N	5.24	125.29	119.32
2	H	40	THR	C-N-CA	5.24	125.29	119.32
1	L	9	ALA	CA-C-O	-5.21	115.16	120.89
1	L	6	GLN	CG-CD-NE2	5.21	124.21	116.40
2	H	89	GLU	CG-CD-OE2	-5.20	106.44	118.40
1	L	184	THR	N-CA-CB	5.20	118.78	110.46
1	L	163	GLU	CA-CB-CG	5.20	124.49	114.10
2	H	15	GLY	N-CA-C	-5.18	108.92	115.08
2	H	145	LEU	CA-C-N	5.18	130.35	123.10
2	H	145	LEU	C-N-CA	5.18	130.35	123.10
2	H	91	THR	CA-CB-OG1	5.17	117.35	109.60
1	L	95	SER	N-CA-CB	-5.16	104.34	112.13
1	L	15	GLY	CA-C-O	5.16	124.79	119.27
2	H	144	CYS	CA-CB-SG	-5.16	102.54	114.40
1	L	170	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	L	105	LYS	CA-C-N	-5.13	115.64	122.72
1	L	105	LYS	C-N-CA	-5.13	115.64	122.72
2	H	173	VAL	N-CA-CB	5.11	121.06	112.47
1	L	6	GLN	CA-C-O	-5.11	115.63	121.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	167	PRO	CA-C-O	-5.10	115.76	121.32
2	H	147	LYS	N-CA-C	5.09	117.86	109.72
2	H	167	VAL	CA-C-O	-5.09	114.56	121.02
2	H	176	SER	CA-CB-OG	5.06	121.22	111.10
2	H	73	ASP	CA-CB-CG	-5.05	107.55	112.60
2	H	183	SER	CA-C-O	-5.05	115.33	120.99
2	H	112	THR	N-CA-C	5.04	117.78	109.76
1	L	138	THR	O-C-N	5.03	129.60	123.21
1	L	6	GLN	OE1-CD-NE2	-5.00	117.60	122.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	39	GLN	Mainchain
1	L	128	LEU	Mainchain

5.2 Too-close contacts [i](#)

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	1556	0	1490	28	0
2	H	1598	0	1517	30	0
3	H	23	0	0	0	0
3	L	28	0	0	1	0
All	All	3205	0	3007	55	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 9.

All (55) 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:1:GLN:HG2	1:L:2:ALA:H	1.42	0.85
2:H:196:THR:HG23	2:H:213:LYS:HD3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:139:MET:HE3	2:H:186:THR:HG22	1.63	0.81
1:L:162:MET:HE2	1:L:162:MET:H	1.48	0.77
2:H:88:SER:O	2:H:91:THR:HG23	1.87	0.75
1:L:28:THR:HG23	1:L:71:GLY:HA2	1.75	0.67
2:H:122:PRO:HB3	2:H:208:THR:HG21	1.79	0.63
2:H:38:ARG:HD3	2:H:48:VAL:HG21	1.80	0.62
1:L:28:THR:HG23	1:L:71:GLY:CA	2.32	0.60
1:L:192:SER:O	1:L:210:SER:HA	2.02	0.58
2:H:130:PRO:HD3	2:H:142:LEU:HD12	1.85	0.58
2:H:206:SER:OG	2:H:208:THR:HB	2.04	0.58
2:H:151:PRO:O	2:H:203:HIS:HE1	1.87	0.58
1:L:126:GLU:OE2	2:H:212:LYS:NZ	2.38	0.56
1:L:94:TYR:O	1:L:95:SER:HB2	2.06	0.56
2:H:176:SER:O	2:H:177:ASP:HB2	2.06	0.55
1:L:166:ASN:O	3:L:228:HOH:O	2.19	0.53
1:L:153:VAL:HG23	1:L:158:VAL:CG2	2.39	0.52
1:L:93:TRP:CH2	1:L:96:GLY:HA2	2.46	0.51
2:H:91:THR:HG22	2:H:115:VAL:H	1.76	0.51
1:L:191:HIS:HB2	1:L:194:TYR:OH	2.11	0.50
1:L:169:LYS:HE3	1:L:173:ASN:OD1	2.11	0.49
2:H:139:MET:HE3	2:H:186:THR:CG2	2.39	0.49
2:H:20:LEU:HG	2:H:83:MET:HE2	1.93	0.49
2:H:12:VAL:HG12	2:H:13:THR:N	2.27	0.48
1:L:127:GLU:HG2	1:L:132:LYS:O	2.13	0.48
2:H:42:GLU:O	2:H:43:LYS:HB2	2.12	0.48
1:L:93:TRP:CZ2	1:L:96:GLY:HA2	2.48	0.48
1:L:52:ALA:O	1:L:53:THR:HB	2.13	0.48
1:L:51:GLY:HA3	2:H:103:VAL:HG22	1.96	0.47
2:H:142:LEU:HG	2:H:214:ILE:HG21	1.95	0.47
2:H:131:GLY:O	2:H:132:SER:C	2.58	0.47
1:L:143:TYR:HA	1:L:144:PRO:C	2.40	0.46
1:L:111:GLN:HB2	1:L:112:PRO:HD2	1.99	0.45
2:H:149:TYR:OH	2:H:181:LEU:HD13	2.17	0.45
2:H:97:THR:HG23	2:H:107:TRP:CG	2.52	0.45
1:L:129:GLU:OE1	1:L:129:GLU:HA	2.18	0.44
1:L:111:GLN:HB2	1:L:112:PRO:CD	2.48	0.44
1:L:160:GLN:HA	1:L:162:MET:HE1	2.00	0.43
2:H:97:THR:HG23	2:H:107:TRP:CD1	2.53	0.43
1:L:48:GLY:HA3	2:H:104:LEU:O	2.18	0.43
1:L:166:ASN:HA	1:L:167:PRO:HD3	1.89	0.43
1:L:53:THR:HG21	1:L:68:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:54:ASN:HD22	1:L:54:ASN:C	2.27	0.42
1:L:87:ILE:HD12	1:L:105:LYS:HG2	2.01	0.42
1:L:162:MET:HA	1:L:180:TYR:O	2.20	0.41
2:H:135:GLN:H	2:H:135:GLN:HG3	1.63	0.41
2:H:73:ASP:OD1	2:H:73:ASP:C	2.62	0.41
2:H:76:LYS:HB2	2:H:78:THR:HG23	2.03	0.41
2:H:91:THR:HB	2:H:114:THR:HA	2.01	0.41
2:H:40:THR:HB	2:H:41:PRO:HD2	2.03	0.41
2:H:93:MET:HE3	2:H:93:MET:HB2	1.73	0.41
2:H:137:ASN:HB2	2:H:138:SER:H	1.63	0.40
1:L:9:ALA:O	1:L:10:LEU:HD13	2.22	0.40
2:H:22:CYS:HB3	2:H:79:LEU:HB3	2.02	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	208/210 (99%)	200 (96%)	7 (3%)	1 (0%)	24	31
2	H	214/216 (99%)	203 (95%)	8 (4%)	3 (1%)	9	9
All	All	422/426 (99%)	403 (96%)	15 (4%)	4 (1%)	14	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	43	ASP
2	H	135	GLN
2	H	132	SER
2	H	137	ASN

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	172/177 (97%)	147 (86%)	25 (14%)	3	3
2	H	178/186 (96%)	155 (87%)	23 (13%)	4	4
All	All	350/363 (96%)	302 (86%)	48 (14%)	3	4

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	10	LEU
1	L	16	GLU
1	L	18	VAL
1	L	20	LEU
1	L	26	THR
1	L	45	LEU
1	L	49	LEU
1	L	54	ASN
1	L	68	LEU
1	L	82	THR
1	L	115	SER
1	L	117	SER
1	L	129	GLU
1	L	146	VAL
1	L	148	THR
1	L	152	LYS
1	L	157	PRO
1	L	159	THR
1	L	162	MET
1	L	178	SER
1	L	195	SER
1	L	206	GLU
1	L	207	LYS
1	L	210	SER
2	H	18	LEU
2	H	34	MET

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Mol	Chain	Res	Type
2	H	48	VAL
2	H	76	LYS
2	H	78	THR
2	H	91	THR
2	H	93	MET
2	H	97	THR
2	H	121	THR
2	H	135	GLN
2	H	136	THR
2	H	137	ASN
2	H	141	THR
2	H	142	LEU
2	H	160	SER
2	H	163	LEU
2	H	176	SER
2	H	181	LEU
2	H	189	SER
2	H	194	SER
2	H	207	SER
2	H	208	THR
2	H	213	LYS

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	54	ASN
1	L	55	ASN
1	L	131	ASN
1	L	191	HIS
2	H	82	GLN
2	H	137	ASN
2	H	203	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 [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.