



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:47 PM UTC

PDB ID : 1CBV / pdb_00001cbv
Title : AN AUTOANTIBODY TO SINGLE-STRANDED DNA: COMPARISON OF
THE THREE-DIMENSIONAL STRUCTURES OF THE UNLIGANDED
FAB AND A DEOXYNUCLEOTIDE-FAB COMPLEX
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Deposited on : 1993-03-16
Resolution : 2.66 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

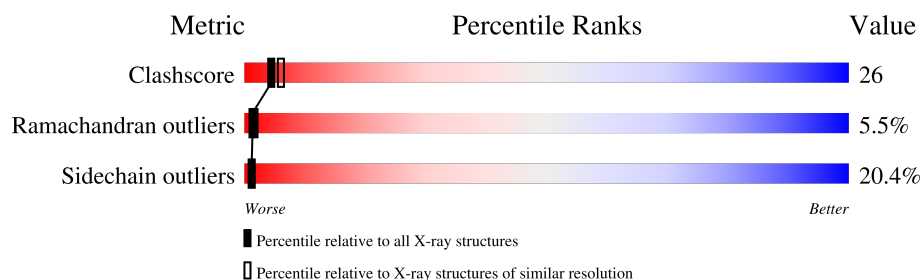
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)

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	D	3	33% 67%
2	L	219	32% 49% 16% •
3	H	219	38% 41% 16% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3408 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 DNA chain called DNA (5'-D(*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	3	Total	C	N	O	P	0	0	0
			61	30	6	22	3			

- Molecule 2 is a protein called PROTEIN (FAB (BV04-01) AUTOANTIBODY-LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	219	Total	C	N	O	S	0	0	0
			1694	1056	289	342	7			

- Molecule 3 is a protein called PROTEIN (FAB (BV04-01) AUTOANTIBODY-HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1653	1038	275	330	10			

3 Residue-property plots [i](#)

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.

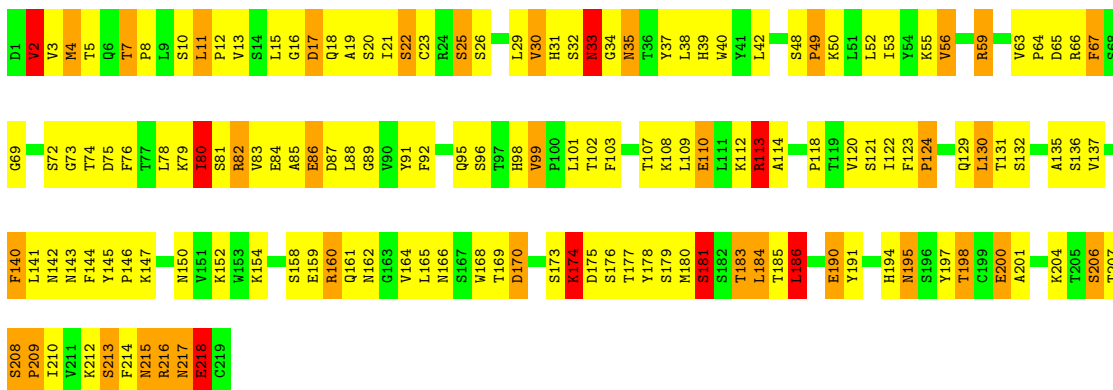
- Molecule 1: DNA (5'-D(*TP*TP*T)-3')

Chain D: 

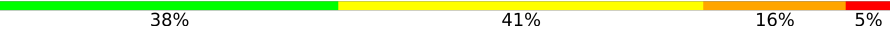
T1
T2
T3

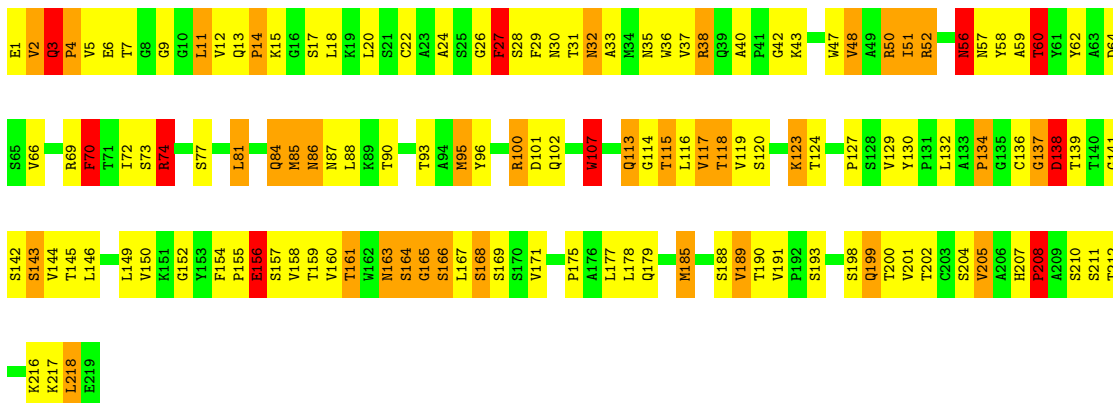
- Molecule 2: PROTEIN (FAB (BV04-01) AUTOANTIBODY-LIGHT CHAIN)

Chain L: 



- Molecule 3: PROTEIN (FAB (BV04-01) AUTOANTIBODY-HEAVY CHAIN)

Chain H: 



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	63.50Å 99.20Å 36.60Å 90.00° 95.30° 90.00°	Depositor
Resolution (Å)	6.00 – 2.66	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.66)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR, PROLSQ	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3408	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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	D	4.67	15/66 (22.7%)	4.66	21/98 (21.4%)
2	L	1.40	6/1732 (0.3%)	2.07	67/2350 (2.9%)
3	H	1.42	6/1694 (0.4%)	2.14	73/2313 (3.2%)
All	All	1.54	27/3492 (0.8%)	2.19	161/4761 (3.4%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	DT	OP3-P	12.45	1.73	1.48
1	D	1	DT	N1-C6	-11.92	1.14	1.38
1	D	2	DT	N1-C6	-11.54	1.15	1.38
1	D	3	DT	N1-C6	-11.26	1.16	1.38
1	D	1	DT	C2'-C1'	-8.88	1.35	1.52
1	D	2	DT	C2-O2	7.58	1.37	1.22
3	H	4	PRO	N-CD	7.21	1.57	1.47
1	D	3	DT	C2-O2	7.18	1.36	1.22
3	H	164	SER	CA-CB	-6.91	1.46	1.53
1	D	3	DT	C2'-C1'	-6.90	1.39	1.52
1	D	1	DT	C2-O2	6.71	1.35	1.22
1	D	1	DT	C5-C6	6.71	1.47	1.34
1	D	2	DT	C5-C6	6.43	1.47	1.34
3	H	156	GLU	C-O	6.23	1.31	1.24
1	D	3	DT	C5-C6	6.21	1.46	1.34
1	D	3	DT	C4'-C3'	6.21	1.65	1.52
1	D	1	DT	O3'-P	5.99	1.70	1.61
2	L	86	GLU	CD-OE2	5.88	1.36	1.25
3	H	138	ASP	N-CA	5.84	1.53	1.46
3	H	134	PRO	C-O	5.29	1.30	1.24
2	L	80	ILE	N-CA	5.25	1.52	1.46
1	D	2	DT	C4'-C3'	5.21	1.63	1.52
2	L	186	LEU	CA-CB	-5.20	1.45	1.53
2	L	110	GLU	CD-OE1	5.20	1.35	1.25
3	H	160	VAL	N-CA	5.10	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	3	VAL	C-O	5.07	1.29	1.24
2	L	152	LYS	N-CA	5.04	1.52	1.46

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3	DT	C5'-C4'-C3'	20.35	145.42	114.90
3	H	138	ASP	CA-CB-CG	13.68	126.28	112.60
1	D	3	DT	O4'-C4'-C3'	-12.17	87.15	105.40
2	L	35	ASN	CA-CB-CG	-12.08	100.52	112.60
1	D	2	DT	C5'-C4'-C3'	11.82	132.63	114.90
3	H	32	ASN	CA-CB-CG	10.14	122.74	112.60
2	L	200	GLU	CA-CB-CG	10.01	134.12	114.10
2	L	82	ARG	CD-NE-CZ	9.74	138.04	124.40
2	L	86	GLU	CB-CG-CD	9.17	128.19	112.60
3	H	57	ASN	CA-CB-CG	9.14	121.74	112.60
2	L	103	PHE	CA-CB-CG	9.00	122.80	113.80
1	D	1	DT	C5'-C4'-C3'	8.85	128.17	114.90
2	L	33	ASN	CA-CB-CG	8.80	121.40	112.60
3	H	207	HIS	CA-CB-CG	8.73	122.53	113.80
1	D	2	DT	C6-N1-C1'	8.46	132.04	119.35
3	H	107	TRP	CB-CA-C	8.44	124.89	109.71
2	L	194	HIS	CA-CB-CG	-8.40	105.39	113.80
1	D	1	DT	C3'-C2'-C1'	8.34	114.11	101.60
1	D	1	DT	C5-C6-N1	8.15	135.02	122.80
3	H	6	GLU	CA-CB-CG	8.08	130.26	114.10
1	D	1	DT	P-O3'-C3'	7.95	132.12	120.20
1	D	1	DT	C6-N1-C1'	7.75	130.97	119.35
3	H	160	VAL	CB-CA-C	7.73	122.25	110.96
1	D	1	DT	O3'-P-O5'	-7.60	92.60	104.00
3	H	86	ASN	CA-CB-CG	-7.55	105.05	112.60
1	D	3	DT	C6-N1-C1'	7.53	130.64	119.35
2	L	35	ASN	N-CA-C	7.51	126.79	110.80
3	H	152	GLY	N-CA-C	7.46	130.85	113.18
1	D	2	DT	C5-C6-N1	7.45	133.97	122.80
1	D	2	DT	C4'-C3'-C2'	-7.40	91.31	102.40
3	H	70	PHE	CA-CB-CG	7.38	121.18	113.80
2	L	152	LYS	CA-CB-CG	7.32	128.73	114.10
2	L	198	THR	CA-CB-OG1	-7.28	98.68	109.60
2	L	190	GLU	CA-CB-CG	7.20	128.50	114.10
2	L	140	PHE	CA-CB-CG	7.15	120.95	113.80
2	L	218	GLU	CB-CG-CD	7.15	124.75	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	56	ASN	OD1-CG-ND2	-7.14	115.46	122.60
3	H	107	TRP	CA-CB-CG	7.08	127.05	113.60
3	H	50	ARG	CD-NE-CZ	7.05	134.27	124.40
3	H	38	ARG	NE-CZ-NH2	7.04	125.54	119.20
3	H	164	SER	CA-CB-OG	7.01	125.11	111.10
3	H	38	ARG	CG-CD-NE	6.88	127.13	112.00
3	H	6	GLU	CB-CG-CD	6.83	124.22	112.60
3	H	74	ARG	CD-NE-CZ	6.80	133.93	124.40
1	D	3	DT	C5-C6-N1	6.78	132.97	122.80
3	H	120	SER	CA-C-O	-6.77	113.16	120.75
3	H	156	GLU	CA-C-O	-6.67	110.97	120.51
1	D	2	DT	N1-C1'-C2'	-6.61	103.58	113.50
3	H	205	VAL	N-CA-C	6.61	116.92	106.88
2	L	123	PHE	CA-CB-CG	6.59	120.39	113.80
2	L	207	THR	CA-C-O	6.59	126.39	119.14
2	L	195	ASN	CA-CB-CG	-6.58	106.02	112.60
3	H	3	GLN	CB-CG-CD	6.57	123.78	112.60
2	L	86	GLU	CA-CB-CG	6.57	127.24	114.10
1	D	3	DT	C4'-C3'-C2'	-6.57	92.55	102.40
3	H	4	PRO	N-CA-C	-6.57	98.94	112.47
3	H	157	SER	CA-C-O	6.52	128.74	121.11
3	H	113	GLN	OE1-CD-NE2	-6.51	116.09	122.60
3	H	57	ASN	OD1-CG-ND2	-6.50	116.10	122.60
2	L	186	LEU	CA-CB-CG	6.41	138.72	116.30
3	H	52	ARG	NE-CZ-NH2	6.40	124.96	119.20
1	D	3	DT	O4'-C1'-N1	-6.37	98.85	108.40
3	H	157	SER	N-CA-C	6.35	119.54	109.50
2	L	177	THR	CA-CB-OG1	-6.35	100.07	109.60
2	L	195	ASN	N-CA-C	6.34	121.26	111.56
3	H	9	GLY	CA-C-O	-6.33	115.81	121.64
1	D	2	DT	O4'-C1'-C2'	-6.30	96.95	106.40
2	L	89	GLY	O-C-N	6.26	129.00	123.80
3	H	161	THR	CA-CB-CG2	6.26	121.14	110.50
3	H	205	VAL	N-CA-CB	-6.26	104.09	111.60
2	L	39	HIS	CA-CB-CG	6.21	120.01	113.80
2	L	207	THR	N-CA-C	-6.18	105.89	113.50
3	H	31	THR	CA-CB-OG1	-6.11	100.43	109.60
3	H	199	GLN	CB-CG-CD	6.11	122.98	112.60
2	L	17	ASP	CA-CB-CG	6.03	118.63	112.60
3	H	217	LYS	CA-C-O	-6.03	114.05	120.92
2	L	2	VAL	CB-CA-C	6.03	119.47	111.21
3	H	212	THR	CA-CB-OG1	-6.01	100.59	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	VAL	CA-C-O	-5.99	113.42	121.02
3	H	100	ARG	CA-CB-CG	5.99	126.07	114.10
3	H	199	GLN	OE1-CD-NE2	-5.98	116.62	122.60
2	L	59	ARG	CA-CB-CG	5.96	126.02	114.10
3	H	59	ALA	CA-C-N	5.90	130.62	122.77
3	H	59	ALA	C-N-CA	5.90	130.62	122.77
3	H	3	GLN	CA-C-O	5.87	128.20	120.16
1	D	1	DT	C2'-C3'-O3'	5.87	120.30	111.50
2	L	80	ILE	CB-CA-C	5.85	119.22	111.21
2	L	110	GLU	CA-CB-CG	5.85	125.80	114.10
2	L	124	PRO	CA-C-N	5.82	126.01	119.90
2	L	124	PRO	C-N-CA	5.82	126.01	119.90
3	H	159	THR	CA-C-N	-5.81	115.57	123.12
3	H	159	THR	C-N-CA	-5.81	115.57	123.12
2	L	82	ARG	CA-CB-CG	5.81	125.71	114.10
3	H	86	ASN	OD1-CG-ND2	5.80	128.40	122.60
3	H	161	THR	CA-CB-OG1	-5.75	100.98	109.60
3	H	56	ASN	CB-CA-C	5.72	118.31	111.22
3	H	38	ARG	CA-CB-CG	5.69	125.49	114.10
3	H	158	VAL	CA-C-O	-5.68	115.71	121.67
3	H	1	GLU	CB-CG-CD	5.67	122.25	112.60
3	H	38	ARG	N-CA-CB	5.67	119.54	110.46
3	H	69	ARG	N-CA-C	-5.67	104.48	111.40
1	D	2	DT	C5'-C4'-O4'	-5.67	100.90	109.40
2	L	159	GLU	N-CA-C	5.66	118.44	110.23
2	L	137	VAL	CA-C-O	-5.65	113.86	120.75
3	H	60	THR	N-CA-CB	-5.63	101.24	110.42
2	L	89	GLY	N-CA-C	-5.62	102.94	111.42
3	H	117	VAL	CB-CA-C	5.57	118.23	110.99
3	H	2	VAL	N-CA-C	-5.55	105.11	110.72
2	L	49	PRO	CB-CA-C	5.54	118.24	110.98
2	L	98	HIS	ND1-CE1-NE2	5.50	113.90	108.40
2	L	183	THR	N-CA-CB	5.50	119.14	110.23
2	L	175	ASP	N-CA-C	-5.48	105.85	112.54
3	H	159	THR	CA-C-O	-5.48	114.43	120.24
2	L	218	GLU	CA-CB-CG	5.44	124.97	114.10
3	H	132	LEU	O-C-N	5.42	129.40	123.27
2	L	99	VAL	N-CA-C	-5.42	103.97	108.63
2	L	179	SER	CB-CA-C	5.40	120.86	109.79
2	L	59	ARG	NE-CZ-NH2	5.39	124.05	119.20
3	H	161	THR	N-CA-CB	-5.39	101.63	110.52
2	L	35	ASN	OD1-CG-ND2	5.38	127.98	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	13	GLN	N-CA-C	-5.37	102.67	110.08
2	L	2	VAL	N-CA-C	-5.35	100.73	108.87
1	D	1	DT	C6-N1-C2	-5.35	113.28	121.30
3	H	69	ARG	N-CA-CB	5.34	118.03	110.13
3	H	56	ASN	CA-CB-CG	5.32	117.92	112.60
2	L	158	SER	CA-C-N	5.31	128.25	120.71
2	L	158	SER	C-N-CA	5.31	128.25	120.71
2	L	89	GLY	CA-C-O	-5.28	116.87	121.04
2	L	170	ASP	CB-CA-C	5.26	123.34	111.78
2	L	86	GLU	CG-CD-OE1	5.25	130.47	118.40
3	H	141	GLY	CA-C-N	5.24	127.55	120.38
3	H	141	GLY	C-N-CA	5.24	127.55	120.38
2	L	130	LEU	CB-CA-C	5.23	119.47	110.79
3	H	69	ARG	O-C-N	5.22	128.49	122.17
3	H	207	HIS	CB-CA-C	5.22	119.21	110.55
2	L	143	ASN	N-CA-C	5.21	117.53	111.02
2	L	113	ARG	CA-CB-CG	5.21	124.51	114.10
3	H	27	PHE	CA-CB-CG	5.18	118.98	113.80
3	H	113	GLN	CB-CG-CD	5.17	121.39	112.60
2	L	53	ILE	CA-C-O	-5.17	114.88	120.67
3	H	13	GLN	OE1-CD-NE2	-5.16	117.44	122.60
3	H	208	PRO	CB-CA-C	5.15	120.06	111.56
2	L	4	MET	N-CA-CB	5.14	118.00	109.88
3	H	1	GLU	CA-CB-CG	5.13	124.36	114.10
2	L	181	SER	N-CA-C	5.13	117.14	108.02
2	L	194	HIS	ND1-CG-CD2	5.12	111.22	106.10
3	H	217	LYS	N-CA-C	-5.12	102.47	110.10
3	H	2	VAL	O-C-N	5.12	127.10	121.83
2	L	112	LYS	N-CA-CB	5.12	117.79	110.06
3	H	142	SER	N-CA-CB	-5.09	102.42	110.06
3	H	145	THR	CA-CB-OG1	-5.07	102.00	109.60
2	L	198	THR	CA-C-N	5.05	129.97	123.00
2	L	198	THR	C-N-CA	5.05	129.97	123.00
2	L	67	PHE	CB-CA-C	5.05	118.08	109.75
3	H	143	SER	CA-C-O	-5.04	115.54	121.44
2	L	22	SER	N-CA-C	5.04	117.11	108.90
2	L	110	GLU	N-CA-C	-5.04	102.57	110.17
2	L	209	PRO	CB-CA-C	5.03	117.67	111.23
2	L	174	LYS	CA-C-O	-5.03	113.32	120.51
2	L	110	GLU	CB-CG-CD	5.01	121.12	112.60
2	L	99	VAL	CA-C-O	-5.00	115.37	119.47

There are no chirality outliers.

There are no planarity outliers.

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	D	61	0	35	5	0
2	L	1694	0	1638	84	0
3	H	1653	0	1600	98	0
All	All	3408	0	3273	177	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 26.

All (177) 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)
3:H:123:LYS:HD2	3:H:124:THR:H	1.20	1.05
3:H:52:ARG:NH1	3:H:56:ASN:HD22	1.69	0.91
3:H:51:ILE:HD13	3:H:74:ARG:HG2	1.53	0.90
3:H:171:VAL:HG22	3:H:189:VAL:HG23	1.60	0.83
1:D:1:DT:H3'	3:H:107:TRP:HZ3	1.45	0.82
3:H:58:TYR:CD1	3:H:74:ARG:HD2	2.15	0.81
3:H:26:GLY:HA3	3:H:100:ARG:HH12	1.48	0.77
3:H:52:ARG:HH11	3:H:56:ASN:HD22	1.29	0.76
3:H:139:THR:HB	3:H:193:SER:OG	1.87	0.74
3:H:150:VAL:HB	3:H:185:MET:HG3	1.67	0.74
2:L:113:ARG:HD3	2:L:114:ALA:O	1.87	0.74
3:H:93:THR:HG23	3:H:118:THR:HA	1.69	0.73
3:H:129:VAL:HG12	3:H:150:VAL:HG22	1.70	0.73
2:L:34:GLY:HA3	2:L:37:TYR:OH	1.88	0.73
3:H:161:THR:HB	3:H:204:SER:HB2	1.70	0.72
3:H:146:LEU:HB3	3:H:218:LEU:CD2	2.19	0.72
1:D:1:DT:H72	3:H:107:TRP:HB3	1.71	0.70
3:H:129:VAL:HG11	3:H:205:VAL:HG21	1.72	0.69
3:H:12:VAL:HG23	3:H:119:VAL:HG22	1.73	0.69
3:H:163:ASN:HB3	3:H:202:THR:HB	1.74	0.69
2:L:154:LYS:HB2	2:L:198:THR:HB	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:58:TYR:HD1	3:H:74:ARG:HD2	1.55	0.68
2:L:59:ARG:HG2	2:L:63:VAL:HB	1.76	0.68
3:H:3:GLN:HG3	3:H:5:VAL:HG23	1.76	0.67
2:L:118:PRO:HB3	2:L:144:PHE:HB3	1.78	0.65
3:H:36:TRP:HE1	3:H:81:LEU:HD22	1.61	0.65
3:H:123:LYS:HD2	3:H:124:THR:N	2.03	0.65
2:L:59:ARG:CG	2:L:63:VAL:HB	2.27	0.65
3:H:33:ALA:HB3	3:H:101:ASP:OD2	1.95	0.65
3:H:26:GLY:HA3	3:H:100:ARG:NH1	2.12	0.64
3:H:129:VAL:HG23	3:H:216:LYS:HG3	1.81	0.62
3:H:198:SER:HB2	3:H:199:GLN:OE1	1.99	0.62
2:L:166:ASN:O	3:H:177:LEU:HD11	2.00	0.62
2:L:140:PHE:CE2	3:H:188:SER:HB3	2.35	0.61
2:L:184:LEU:HD22	2:L:186:LEU:HD13	1.84	0.60
3:H:26:GLY:O	3:H:28:SER:N	2.35	0.60
2:L:140:PHE:CD1	2:L:181:SER:HB3	2.36	0.60
2:L:21:ILE:HG23	2:L:107:THR:HG21	1.83	0.59
2:L:31:HIS:ND1	2:L:37:TYR:HE2	2.00	0.59
2:L:52:LEU:HD11	2:L:91:TYR:HE1	1.67	0.59
2:L:18:GLN:HG3	2:L:79:LYS:NZ	2.19	0.57
2:L:206:SER:HB2	2:L:208:SER:O	2.04	0.57
2:L:31:HIS:CD2	2:L:32:SER:H	2.23	0.57
3:H:12:VAL:HG11	3:H:18:LEU:HG	1.87	0.57
3:H:50:ARG:NH1	3:H:101:ASP:OD2	2.37	0.57
2:L:52:LEU:O	2:L:63:VAL:HG21	2.05	0.57
3:H:129:VAL:HA	3:H:149:LEU:O	2.05	0.57
3:H:146:LEU:HB2	3:H:189:VAL:HG12	1.87	0.57
3:H:26:GLY:CA	3:H:100:ARG:HH12	2.16	0.56
2:L:56:VAL:O	2:L:69:GLY:HA3	2.05	0.56
3:H:12:VAL:HG21	3:H:88:LEU:HD13	1.87	0.56
2:L:198:THR:OG1	2:L:213:SER:HB3	2.06	0.56
3:H:48:VAL:HG12	3:H:66:VAL:HG11	1.88	0.56
3:H:167:LEU:O	3:H:169:SER:N	2.38	0.55
3:H:171:VAL:CG2	3:H:189:VAL:HG23	2.35	0.55
3:H:11:LEU:HD22	3:H:11:LEU:H	1.71	0.55
2:L:147:LYS:HD2	2:L:178:TYR:CE2	2.41	0.55
3:H:24:ALA:HB3	3:H:29:PHE:CE2	2.42	0.55
2:L:81:SER:OG	2:L:82:ARG:N	2.41	0.54
3:H:2:VAL:O	3:H:3:GLN:HG2	2.07	0.54
3:H:164:SER:O	3:H:165:GLY:C	2.51	0.54
2:L:140:PHE:CE1	2:L:181:SER:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:5:THR:O	2:L:23:CYS:HA	2.09	0.53
3:H:165:GLY:O	3:H:167:LEU:HD13	2.08	0.53
2:L:8:PRO:O	2:L:107:THR:HG23	2.09	0.52
2:L:17:ASP:O	2:L:83:VAL:HG23	2.09	0.52
3:H:51:ILE:HG13	3:H:60:THR:OG1	2.09	0.52
3:H:167:LEU:HD23	3:H:191:VAL:HG23	1.91	0.52
3:H:171:VAL:HA	3:H:188:SER:O	2.09	0.52
2:L:195:ASN:ND2	2:L:217:ASN:OD1	2.43	0.52
3:H:95:MET:HA	3:H:115:THR:O	2.09	0.52
3:H:35:ASN:HD21	3:H:50:ARG:HD2	1.74	0.51
3:H:169:SER:HA	3:H:190:THR:O	2.10	0.51
3:H:163:ASN:HD22	3:H:202:THR:CB	2.24	0.51
2:L:101:LEU:HD23	3:H:47:TRP:HB2	1.92	0.50
2:L:131:THR:HG22	2:L:131:THR:O	2.11	0.50
1:D:1:DT:H3'	3:H:107:TRP:CZ3	2.36	0.50
2:L:38:LEU:HG	2:L:76:PHE:CG	2.46	0.50
3:H:167:LEU:HD23	3:H:191:VAL:CG2	2.41	0.50
3:H:38:ARG:HD3	3:H:96:TYR:OH	2.11	0.50
3:H:84:GLN:NE2	3:H:86:ASN:OD1	2.45	0.50
1:D:1:DT:OP2	3:H:52:ARG:HD3	2.12	0.50
2:L:96:SER:HB2	3:H:107:TRP:HE1	1.76	0.50
2:L:12:PRO:HG3	2:L:110:GLU:OE1	2.11	0.49
2:L:40:TRP:CE3	2:L:78:LEU:HD22	2.47	0.49
2:L:31:HIS:HD1	2:L:37:TYR:HE2	1.61	0.49
2:L:135:ALA:O	2:L:185:THR:HA	2.12	0.49
2:L:141:LEU:HD21	2:L:201:ALA:HB2	1.94	0.49
2:L:25:SER:O	2:L:74:THR:HG23	2.13	0.49
2:L:164:VAL:HA	2:L:183:THR:O	2.12	0.49
2:L:2:VAL:HA	2:L:26:SER:OG	2.13	0.49
2:L:141:LEU:C	2:L:142:ASN:HD22	2.21	0.49
2:L:40:TRP:HA	2:L:92:PHE:O	2.13	0.48
2:L:2:VAL:O	2:L:102:THR:HG21	2.13	0.48
2:L:136:SER:HA	2:L:184:LEU:O	2.12	0.48
3:H:38:ARG:HD3	3:H:96:TYR:CZ	2.49	0.48
3:H:136:CYS:O	3:H:138:ASP:N	2.41	0.48
3:H:5:VAL:O	3:H:22:CYS:HA	2.14	0.48
3:H:11:LEU:HD22	3:H:11:LEU:N	2.29	0.48
2:L:108:LYS:HE2	2:L:170:ASP:OD1	2.13	0.47
3:H:163:ASN:O	3:H:201:VAL:HA	2.14	0.47
3:H:17:SER:OG	3:H:86:ASN:ND2	2.47	0.47
3:H:129:VAL:HG11	3:H:205:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:160:ARG:O	2:L:161:GLN:NE2	2.48	0.47
2:L:190:GLU:O	2:L:191:TYR:C	2.57	0.47
3:H:24:ALA:HB3	3:H:29:PHE:HE2	1.79	0.47
3:H:35:ASN:HD22	3:H:50:ARG:HB2	1.80	0.47
2:L:29:LEU:HD11	2:L:38:LEU:HD23	1.96	0.47
2:L:124:PRO:HB3	2:L:214:PHE:CE2	2.50	0.47
3:H:143:SER:HA	3:H:191:VAL:O	2.16	0.46
3:H:14:PRO:O	3:H:15:LYS:HB2	2.15	0.46
3:H:146:LEU:HB3	3:H:218:LEU:HD22	1.96	0.46
3:H:51:ILE:HB	3:H:72:ILE:HD13	1.97	0.46
3:H:51:ILE:HD13	3:H:74:ARG:CG	2.37	0.46
3:H:129:VAL:CG1	3:H:205:VAL:HG11	2.45	0.46
2:L:18:GLN:HG3	2:L:79:LYS:HZ1	1.81	0.46
2:L:165:LEU:HD21	3:H:179:GLN:HB2	1.96	0.46
3:H:37:VAL:HG22	3:H:47:TRP:HA	1.97	0.46
3:H:52:ARG:HH11	3:H:56:ASN:ND2	2.06	0.46
3:H:35:ASN:HD21	3:H:50:ARG:HH11	1.64	0.46
2:L:80:ILE:HD11	2:L:83:VAL:HA	1.97	0.45
3:H:164:SER:O	3:H:166:SER:N	2.49	0.45
2:L:15:LEU:HD11	2:L:85:ALA:CA	2.47	0.45
3:H:12:VAL:CG2	3:H:119:VAL:HG22	2.44	0.45
2:L:173:SER:O	2:L:174:LYS:CB	2.64	0.45
2:L:66:ARG:NH1	2:L:84:GLU:HB2	2.31	0.45
2:L:7:THR:N	2:L:22:SER:O	2.49	0.44
2:L:168:TRP:CH2	2:L:180:MET:HE2	2.52	0.44
3:H:20:LEU:HD21	3:H:117:VAL:HG21	1.98	0.44
2:L:15:LEU:HD11	2:L:85:ALA:HB2	1.99	0.44
2:L:18:GLN:HA	2:L:81:SER:O	2.17	0.44
2:L:59:ARG:HD3	2:L:63:VAL:O	2.18	0.44
2:L:122:ILE:HD13	2:L:213:SER:HA	1.99	0.44
3:H:146:LEU:HB3	3:H:218:LEU:HD23	1.99	0.44
2:L:19:ALA:HB3	2:L:80:ILE:HG23	1.98	0.44
2:L:40:TRP:CE2	2:L:78:LEU:HB2	2.52	0.44
3:H:3:GLN:HE21	3:H:5:VAL:HG21	1.82	0.44
3:H:40:ALA:C	3:H:42:GLY:H	2.25	0.44
3:H:101:ASP:CG	3:H:107:TRP:HB2	2.43	0.44
3:H:185:MET:HB2	3:H:185:MET:HE2	1.66	0.44
3:H:26:GLY:C	3:H:100:ARG:HH22	2.26	0.43
2:L:130:LEU:HD23	2:L:130:LEU:HA	1.88	0.43
3:H:73:SER:O	3:H:81:LEU:HD23	2.18	0.43
3:H:137:GLY:O	3:H:138:ASP:HB3	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:11:LEU:HD12	2:L:109:LEU:CD2	2.48	0.43
3:H:150:VAL:HB	3:H:185:MET:CG	2.45	0.43
2:L:147:LYS:HG2	2:L:147:LYS:O	2.19	0.43
2:L:52:LEU:HA	2:L:63:VAL:HG21	2.01	0.43
2:L:59:ARG:NH1	2:L:67:PHE:O	2.50	0.43
3:H:14:PRO:HG3	3:H:119:VAL:HG12	2.01	0.43
2:L:215:ASN:O	2:L:216:ARG:C	2.62	0.42
2:L:55:LYS:O	2:L:56:VAL:HG12	2.19	0.42
3:H:114:GLY:O	3:H:115:THR:HB	2.18	0.42
1:D:3:DT:C6	1:D:3:DT:H5'	2.54	0.42
2:L:4:MET:HE2	2:L:95:GLN:HB3	2.01	0.42
2:L:120:VAL:HG22	2:L:141:LEU:HG	2.00	0.42
2:L:80:ILE:CD1	2:L:83:VAL:HG22	2.49	0.42
2:L:147:LYS:HD2	2:L:178:TYR:CD2	2.55	0.42
3:H:85:MET:HE1	3:H:96:TYR:CZ	2.54	0.42
2:L:140:PHE:HD1	2:L:181:SER:HB3	1.81	0.42
2:L:145:TYR:CD1	2:L:146:PRO:HA	2.55	0.42
3:H:70:PHE:CZ	3:H:85:MET:HE2	2.55	0.42
2:L:129:GLN:HA	3:H:130:TYR:CE1	2.55	0.41
3:H:62:TYR:CE1	3:H:72:ILE:HG22	2.55	0.41
2:L:63:VAL:HA	2:L:64:PRO:HD3	1.85	0.41
2:L:30:VAL:O	2:L:30:VAL:HG12	2.20	0.41
3:H:165:GLY:C	3:H:167:LEU:H	2.27	0.41
2:L:169:THR:HG22	2:L:170:ASP:O	2.21	0.41
3:H:154:PHE:CE1	3:H:155:PRO:HB3	2.55	0.41
2:L:191:TYR:HE1	2:L:197:TYR:CE2	2.38	0.41
2:L:21:ILE:HG12	2:L:107:THR:HG21	2.03	0.41
2:L:168:TRP:CZ2	2:L:180:MET:HE2	2.55	0.41
2:L:145:TYR:CG	2:L:146:PRO:HA	2.55	0.41
2:L:31:HIS:HD2	2:L:32:SER:H	1.66	0.41
2:L:12:PRO:HA	2:L:110:GLU:HG2	2.03	0.41
3:H:27:PHE:CD1	3:H:28:SER:N	2.89	0.40
3:H:86:ASN:O	3:H:87:ASN:C	2.65	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	
2	L	217/219 (99%)	180 (83%)	28 (13%)	9 (4%)	2	3
3	H	217/219 (99%)	176 (81%)	26 (12%)	15 (7%)	1	0
All	All	434/438 (99%)	356 (82%)	54 (12%)	24 (6%)	1	2

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	174	LYS
3	H	27	PHE
3	H	156	GLU
3	H	168	SER
2	L	33	ASN
2	L	35	ASN
2	L	65	ASP
2	L	73	GLY
2	L	218	GLU
3	H	30	ASN
3	H	43	LYS
3	H	165	GLY
3	H	210	SER
2	L	160	ARG
3	H	3	GLN
3	H	137	GLY
3	H	208	PRO
3	H	138	ASP
3	H	211	SER
3	H	127	PRO
3	H	134	PRO
2	L	16	GLY
2	L	30	VAL
3	H	4	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	
2	L	197/197 (100%)	156 (79%)	41 (21%)	1	1
3	H	186/186 (100%)	149 (80%)	37 (20%)	1	1
All	All	383/383 (100%)	305 (80%)	78 (20%)	1	1

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	2	VAL
2	L	7	THR
2	L	10	SER
2	L	11	LEU
2	L	13	VAL
2	L	20	SER
2	L	25	SER
2	L	33	ASN
2	L	42	LEU
2	L	48	SER
2	L	49	PRO
2	L	50	LYS
2	L	56	VAL
2	L	72	SER
2	L	75	ASP
2	L	80	ILE
2	L	86	GLU
2	L	87	ASP
2	L	88	LEU
2	L	99	VAL
2	L	113	ARG
2	L	121	SER
2	L	132	SER
2	L	150	ASN
2	L	162	ASN
2	L	176	SER
2	L	181	SER

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Mol	Chain	Res	Type
2	L	184	LEU
2	L	186	LEU
2	L	200	GLU
2	L	204	LYS
2	L	206	SER
2	L	208	SER
2	L	209	PRO
2	L	210	ILE
2	L	212	LYS
2	L	213	SER
2	L	215	ASN
2	L	216	ARG
2	L	217	ASN
2	L	218	GLU
3	H	3	GLN
3	H	7	THR
3	H	11	LEU
3	H	14	PRO
3	H	32	ASN
3	H	48	VAL
3	H	51	ILE
3	H	56	ASN
3	H	60	THR
3	H	64	ASP
3	H	70	PHE
3	H	74	ARG
3	H	77	SER
3	H	81	LEU
3	H	84	GLN
3	H	85	MET
3	H	90	THR
3	H	95	MET
3	H	102	GLN
3	H	107	TRP
3	H	113	GLN
3	H	115	THR
3	H	116	LEU
3	H	118	THR
3	H	123	LYS
3	H	144	VAL
3	H	156	GLU
3	H	163	ASN

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Mol	Chain	Res	Type
3	H	166	SER
3	H	168	SER
3	H	175	PRO
3	H	178	LEU
3	H	185	MET
3	H	189	VAL
3	H	200	THR
3	H	208	PRO
3	H	218	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	58	ASN
2	L	129	GLN
2	L	142	ASN
2	L	161	GLN
2	L	166	ASN
3	H	3	GLN
3	H	32	ASN
3	H	35	ASN
3	H	56	ASN
3	H	84	GLN
3	H	86	ASN
3	H	163	ASN

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

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.