



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:10 PM GMT

PDB ID : 1CBV  
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 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/ValidationPDFNotes.html>

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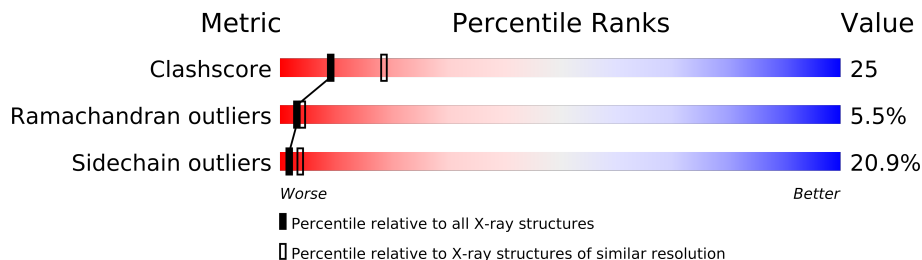
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	3	
2	L	219	
3	H	219	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3408 atoms, of which 0 are hydrogen and 0 are deuterium.

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

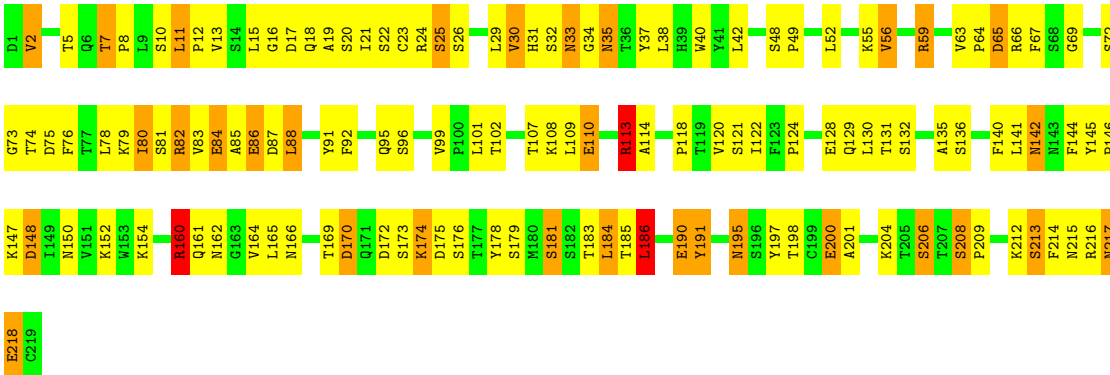
- Molecule 1: DNA (5'-D(\*TP\*TP\*T)-3')

Chain D: 



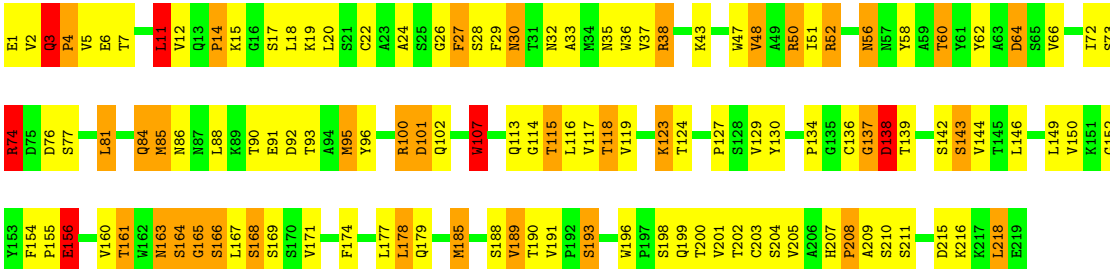
- Molecule 2: PROTEIN (FAB (BV04-01) AUTOANTIBODY-LIGHT CHAIN)

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 will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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	10.89	40/66 (60.6%)	7.28	35/98 (35.7%)
2	L	1.20	7/1732 (0.4%)	1.70	33/2350 (1.4%)
3	H	1.20	5/1694 (0.3%)	1.73	35/2313 (1.5%)
All	All	1.91	52/3492 (1.5%)	1.99	103/4761 (2.2%)

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	DT	N1-C6	-33.78	1.14	1.38
1	D	2	DT	N1-C6	-32.69	1.15	1.38
1	D	3	DT	N1-C6	-31.89	1.16	1.38
1	D	1	DT	C5-C6	19.02	1.47	1.34
1	D	2	DT	C2-O2	18.70	1.37	1.22
1	D	2	DT	C5-C6	18.23	1.47	1.34
1	D	3	DT	C2-O2	17.71	1.36	1.22
1	D	3	DT	C5-C6	17.60	1.46	1.34
1	D	1	DT	C2'-C1'	-17.07	1.35	1.52
1	D	1	DT	C2-O2	16.52	1.35	1.22
1	D	3	DT	C2'-C1'	-13.11	1.39	1.52
1	D	1	DT	C3'-O3'	-12.38	1.27	1.44
1	D	3	DT	C4'-C3'	11.81	1.65	1.53
1	D	2	DT	C3'-O3'	-10.87	1.29	1.44
1	D	3	DT	N1-C2	10.27	1.46	1.38
1	D	1	DT	OP3-P	10.17	1.73	1.61
2	L	86	GLU	CD-OE2	9.89	1.36	1.25
1	D	2	DT	C4'-C3'	9.81	1.63	1.53
1	D	2	DT	N3-C4	-9.21	1.31	1.38
1	D	3	DT	C4-C5	-8.89	1.36	1.45
1	D	1	DT	C4-C5	-8.89	1.36	1.45
1	D	2	DT	C4-C5	-8.75	1.37	1.45
2	L	110	GLU	CD-OE1	8.70	1.35	1.25
1	D	2	DT	N1-C2	8.55	1.44	1.38
1	D	3	DT	C3'-O3'	-8.46	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	DT	C5-C7	-8.23	1.45	1.50
1	D	2	DT	C4'-O4'	8.15	1.53	1.45
1	D	3	DT	N3-C4	-7.79	1.32	1.38
1	D	1	DT	N3-C4	-7.68	1.32	1.38
1	D	1	DT	O3'-P	7.49	1.70	1.61
2	L	200	GLU	CD-OE2	7.29	1.33	1.25
2	L	218	GLU	CD-OE2	7.21	1.33	1.25
1	D	3	DT	O4'-C1'	7.18	1.50	1.42
3	H	4	PRO	N-CD	7.14	1.57	1.47
3	H	6	GLU	CD-OE1	7.04	1.33	1.25
1	D	3	DT	C5-C7	-6.98	1.45	1.50
2	L	190	GLU	CD-OE2	6.90	1.33	1.25
1	D	1	DT	C4'-C3'	6.87	1.60	1.53
1	D	2	DT	C2'-C1'	-6.72	1.45	1.52
3	H	1	GLU	CD-OE2	6.52	1.32	1.25
1	D	3	DT	C4-O4	6.48	1.29	1.23
1	D	3	DT	C3'-C2'	6.33	1.59	1.52
3	H	91	GLU	CD-OE2	6.22	1.32	1.25
1	D	2	DT	C3'-C2'	6.17	1.59	1.52
1	D	2	DT	C5-C7	-6.01	1.46	1.50
2	L	128	GLU	CD-OE2	5.87	1.32	1.25
1	D	1	DT	P-OP1	-5.41	1.39	1.49
1	D	1	DT	N1-C2	5.39	1.42	1.38
3	H	156	GLU	CD-OE2	5.28	1.31	1.25
1	D	2	DT	O3'-P	5.13	1.67	1.61
1	D	2	DT	C4-O4	5.08	1.27	1.23
2	L	84	GLU	CD-OE2	5.07	1.31	1.25

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3	DT	O4'-C4'-C3'	-31.42	87.15	106.00
1	D	1	DT	C5-C6-N1	18.86	135.02	123.70
1	D	3	DT	C5'-C4'-C3'	17.40	145.42	114.10
1	D	2	DT	C5-C6-N1	17.12	133.97	123.70
1	D	1	DT	C6-N1-C2	-16.04	113.28	121.30
1	D	3	DT	C5-C6-N1	15.44	132.97	123.70
1	D	2	DT	C6-N1-C2	-14.18	114.21	121.30
1	D	2	DT	C4'-C3'-C2'	-13.11	91.31	103.10
1	D	3	DT	O4'-C1'-N1	-13.07	98.85	108.00
1	D	3	DT	C6-N1-C2	-12.25	115.18	121.30
1	D	3	DT	C4'-C3'-C2'	-11.73	92.55	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	DT	O4'-C1'-C2'	-11.18	96.95	105.90
1	D	1	DT	C6-C5-C7	10.57	129.24	122.90
3	H	38	ARG	NE-CZ-NH2	10.47	125.54	120.30
1	D	1	DT	P-O3'-C3'	10.35	132.12	119.70
2	L	82	ARG	CD-NE-CZ	10.32	138.04	123.60
1	D	2	DT	C5'-C4'-C3'	10.29	132.63	114.10
2	L	186	LEU	CA-CB-CG	10.19	138.72	115.30
1	D	1	DT	C4-C5-C6	-9.76	112.14	118.00
1	D	1	DT	C3'-C2'-C1'	9.67	114.11	102.50
2	L	200	GLU	CA-CB-CG	9.42	134.12	113.40
3	H	52	ARG	NE-CZ-NH2	9.32	124.96	120.30
1	D	2	DT	C4-C5-C6	-9.29	112.43	118.00
1	D	3	DT	C4-C5-C6	-9.17	112.50	118.00
2	L	113	ARG	NE-CZ-NH1	8.88	124.74	120.30
2	L	65	ASP	CB-CG-OD1	8.39	125.86	118.30
1	D	1	DT	C5'-C4'-C3'	7.82	128.17	114.10
3	H	138	ASP	CB-CG-OD1	7.79	125.31	118.30
1	D	2	DT	C6-N1-C1'	7.76	132.04	120.40
3	H	74	ARG	NE-CZ-NH2	-7.72	116.44	120.30
3	H	6	GLU	CA-CB-CG	7.67	130.26	113.40
3	H	50	ARG	CD-NE-CZ	7.62	134.27	123.60
1	D	2	DT	C1'-O4'-C4'	-7.52	102.58	110.10
2	L	59	ARG	NE-CZ-NH2	7.50	124.05	120.30
3	H	74	ARG	CD-NE-CZ	7.38	133.93	123.60
1	D	2	DT	C6-C5-C7	7.35	127.31	122.90
3	H	74	ARG	NE-CZ-NH1	7.33	123.96	120.30
3	H	38	ARG	CG-CD-NE	7.30	127.13	111.80
3	H	38	ARG	NE-CZ-NH1	-7.28	116.66	120.30
3	H	107	TRP	CB-CA-C	7.25	124.89	110.40
2	L	148	ASP	CB-CG-OD2	7.19	124.77	118.30
3	H	101	ASP	CB-CG-OD2	7.17	124.76	118.30
3	H	116	LEU	CA-CB-CG	7.11	131.65	115.30
2	L	172	ASP	CB-CG-OD2	7.10	124.69	118.30
3	H	152	GLY	N-CA-C	7.10	130.85	113.10
3	H	215	ASP	CB-CG-OD2	7.06	124.65	118.30
1	D	1	DT	C6-N1-C1'	7.05	130.97	120.40
1	D	1	DT	N3-C2-O2	-7.04	118.08	122.30
3	H	107	TRP	CA-CB-CG	7.03	127.05	113.70
2	L	152	LYS	CA-CB-CG	6.97	128.73	113.40
1	D	2	DT	N3-C4-O4	-6.95	115.73	119.90
2	L	190	GLU	CA-CB-CG	6.86	128.50	113.40
1	D	2	DT	O4'-C1'-N1	6.84	112.79	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3	DT	C6-N1-C1'	6.83	130.64	120.40
2	L	24	ARG	NE-CZ-NH2	6.73	123.66	120.30
2	L	82	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	D	2	DT	P-O3'-C3'	6.66	127.69	119.70
2	L	88	LEU	CA-CB-CG	6.53	130.33	115.30
2	L	191	TYR	CB-CG-CD2	6.53	124.92	121.00
2	L	170	ASP	CB-CA-C	6.47	123.34	110.40
1	D	1	DT	C4'-C3'-C2'	-6.41	97.33	103.10
1	D	1	DT	O4'-C1'-N1	-6.36	103.55	108.00
2	L	86	GLU	CA-CB-CG	6.29	127.24	113.40
3	H	161	THR	CA-CB-CG2	6.24	121.14	112.40
1	D	3	DT	O4'-C1'-C2'	-6.13	101.00	105.90
2	L	175	ASP	CB-CG-OD1	6.10	123.79	118.30
2	L	86	GLU	CG-CD-OE1	6.09	130.47	118.30
1	D	1	DT	O3'-P-O5'	-6.00	92.60	104.00
2	L	59	ARG	NE-CZ-NH1	-5.93	117.34	120.30
3	H	100	ARG	NE-CZ-NH2	5.88	123.24	120.30
3	H	11	LEU	CA-CB-CG	5.88	128.82	115.30
2	L	35	ASN	CA-CB-CG	-5.85	100.52	113.40
3	H	138	ASP	CA-CB-CG	5.85	126.28	113.40
2	L	35	ASN	N-CA-C	5.85	126.79	111.00
3	H	178	LEU	CA-CB-CG	5.81	128.67	115.30
1	D	3	DT	C6-C5-C7	5.78	126.37	122.90
2	L	86	GLU	OE1-CD-OE2	-5.77	116.38	123.30
3	H	100	ARG	CA-CB-CG	5.76	126.07	113.40
2	L	59	ARG	CA-CB-CG	5.74	126.02	113.40
1	D	2	DT	O5'-P-OP2	5.73	117.58	110.70
3	H	160	VAL	CB-CA-C	5.71	122.25	111.40
3	H	52	ARG	NE-CZ-NH1	-5.69	117.46	120.30
3	H	64	ASP	CB-CG-OD1	-5.69	113.18	118.30
2	L	179	SER	CB-CA-C	5.66	120.86	110.10
2	L	191	TYR	CB-CG-CD1	-5.64	117.61	121.00
2	L	110	GLU	CA-CB-CG	5.63	125.80	113.40
2	L	82	ARG	CA-CB-CG	5.60	125.71	113.40
3	H	38	ARG	CA-CB-CG	5.50	125.49	113.40
2	L	170	ASP	CB-CG-OD2	5.49	123.24	118.30
2	L	160	ARG	NE-CZ-NH2	5.49	123.05	120.30
3	H	76	ASP	CB-CG-OD2	5.39	123.15	118.30
3	H	142	SER	N-CA-CB	-5.39	102.42	110.50
3	H	92	ASP	CB-CG-OD1	5.31	123.08	118.30
3	H	92	ASP	CB-CG-OD2	-5.28	113.55	118.30
2	L	218	GLU	CA-CB-CG	5.26	124.97	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	209	ALA	CB-CA-C	5.26	117.99	110.10
3	H	207	HIS	CA-CB-CG	5.25	122.53	113.60
2	L	86	GLU	CB-CG-CD	5.18	128.19	114.20
3	H	164	SER	CA-CB-OG	5.15	125.11	111.20
2	L	110	GLU	CG-CD-OE2	5.08	128.45	118.30
3	H	4	PRO	N-CA-C	-5.06	98.94	112.10
2	L	113	ARG	CA-CB-CG	5.05	124.51	113.40
3	H	19	LYS	N-CA-CB	5.05	119.69	110.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	61	0	35	5	0
2	L	1694	0	1638	80	0
3	H	1653	0	1600	93	0
All	All	3408	0	3273	168	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (168) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:150:VAL:HB	3:H:185:MET:HG3	1.67	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:139:THR:HB	3:H:193:SER:OG	1.87	0.74
2:L:113:ARG:HD3	2:L:114:ALA:O	1.87	0.74
3:H:129:VAL:HG12	3:H:150:VAL:HG22	1.70	0.73
3:H:93:THR:HG23	3:H:118:THR:HA	1.69	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
3:H:58:TYR:HD1	3:H:74:ARG:HD2	1.55	0.68
2:L:154:LYS:HB2	2:L:198:THR:HB	1.74	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
3:H:36:TRP:HE1	3:H:81:LEU:HD22	1.61	0.65
2:L:118:PRO:HB3	2:L:144:PHE:HB3	1.78	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
3:H:26:GLY:O	3:H:28:SER:N	2.35	0.60
2:L:184:LEU:HD22	2:L:186:LEU:HD13	1.84	0.60
2:L:140:PHE:CD1	2:L:181:SER:HB3	2.36	0.60
2:L:31:HIS:ND1	2:L:37:TYR:HE2	2.00	0.59
2:L:21:ILE:HG23	2:L:107:THR:HG21	1.83	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
3:H:129:VAL:HA	3:H:149:LEU:O	2.05	0.57
2:L:52:LEU:O	2:L:63:VAL:HG21	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
3:H:12:VAL:HG21	3:H:88:LEU:HD13	1.87	0.56
2:L:56:VAL:O	2:L:69:GLY:HA3	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:H	3:H:11:LEU:HD22	1.71	0.55
3:H:24:ALA:HB3	3:H:29:PHE:CE2	2.42	0.55
2:L:147:LYS:HD2	2:L:178:TYR:CE2	2.41	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
2:L:140:PHE:CE1	2:L:181:SER:HB3	2.43	0.53
3:H:165:GLY:O	3:H:167:LEU:HD13	2.08	0.53
2:L:5:THR:O	2:L:23:CYS:HA	2.09	0.53
2:L:8:PRO:O	2:L:107:THR:HG23	2.09	0.52
3:H:51:ILE:HG13	3:H:60:THR:OG1	2.09	0.52
3:H:171:VAL:HA	3:H:188:SER:O	2.09	0.52
3:H:167:LEU:HD23	3:H:191:VAL:HG23	1.91	0.52
2:L:17:ASP:O	2:L:83:VAL:HG23	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:131:THR:O	2:L:131:THR:HG22	2.11	0.50
2:L:101:LEU:HD23	3:H:47:TRP:HB2	1.92	0.50
1:D:1:DT:H3'	3:H:107:TRP:CZ3	2.36	0.50
3:H:167:LEU:HD23	3:H:191:VAL:CG2	2.41	0.50
2:L:38:LEU:HG	2:L:76:PHE:CG	2.46	0.50
3:H:84:GLN:NE2	3:H:86:ASN:OD1	2.45	0.50
3:H:38:ARG:HD3	3:H:96:TYR:OH	2.11	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
3:H:164:SER:O	3:H:165:GLY:C	2.51	0.49
2:L:141:LEU:HD21	2:L:201:ALA:HB2	1.94	0.49
2:L:164:VAL:HA	2:L:183:THR:O	2.12	0.49
2:L:25:SER:O	2:L:74:THR:HG23	2.13	0.49
2:L:2:VAL:HA	2:L:26:SER:OG	2.13	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:136:SER:HA	2:L:184:LEU:O	2.12	0.48
2:L:18:GLN:HG3	2:L:79:LYS:HZ1	1.78	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:N	3:H:11:LEU:HD22	2.29	0.48
3:H:163:ASN:O	3:H:201:VAL:HA	2.14	0.47
2:L:108:LYS:HE2	2:L:170:ASP:OD1	2.13	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
3:H:35:ASN:HD22	3:H:50:ARG:HB2	1.80	0.47
3:H:24:ALA:HB3	3:H:29:PHE:HE2	1.79	0.47
2:L:160:ARG:O	2:L:161:GLN:NE2	2.48	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:165:LEU:HD21	3:H:179:GLN:HB2	1.96	0.46
3:H:52:ARG:HH11	3:H:56:ASN:ND2	2.06	0.46
3:H:174:PHE:O	3:H:185:MET:HE2	2.16	0.46
3:H:37:VAL:HG22	3:H:47:TRP:HA	1.97	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:137:GLY:O	3:H:138:ASP:HB3	2.16	0.45
3:H:164:SER:O	3:H:166:SER:N	2.49	0.45
3:H:12:VAL:CG2	3:H:119:VAL:HG22	2.44	0.45
2:L:15:LEU:HD11	2:L:85:ALA:CA	2.47	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
3:H:20:LEU:HD21	3:H:117:VAL:HG21	1.98	0.44
3:H:146:LEU:HB3	3:H:218:LEU:HD23	1.99	0.44
2:L:122:ILE:HD13	2:L:213:SER:HA	1.99	0.44
2:L:59:ARG:HD3	2:L:63:VAL:O	2.18	0.44
2:L:18:GLN:HA	2:L:81:SER:O	2.17	0.44
2:L:15:LEU:HD11	2:L:85:ALA:HB2	1.99	0.44
2:L:19:ALA:HB3	2:L:80:ILE:HG23	1.98	0.44
3:H:3:GLN:HE21	3:H:5:VAL:HG21	1.82	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:40:TRP:CE2	2:L:78:LEU:HB2	2.52	0.44
2:L:141:LEU:C	2:L:142:ASN:HD22	2.21	0.44
3:H:73:SER:O	3:H:81:LEU:HD23	2.18	0.43
2:L:130:LEU:HA	2:L:130:LEU:HD23	1.88	0.43
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
3:H:14:PRO:HG3	3:H:119:VAL:HG12	2.01	0.43
2:L:59:ARG:NH1	2:L:67:PHE:O	2.50	0.43
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:H5'	1:D:3:DT:C6	2.54	0.42
2:L:190:GLU:O	2:L:191:TYR:C	2.57	0.42
2:L:120:VAL:HG22	2:L:141:LEU:HG	2.00	0.42
3:H:185:MET:HB2	3:H:185:MET:HE2	1.89	0.42
2:L:147:LYS:HD2	2:L:178:TYR:CD2	2.55	0.42
2:L:80:ILE:CD1	2:L:83:VAL:HG22	2.49	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:62:TYR:CE1	3:H:72:ILE:HG22	2.55	0.41
2:L:129:GLN:HA	3:H:130:TYR:CE1	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
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: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:85:MET:HE1	3:H:96:TYR:CZ	2.56	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%)	4	8
3	H	217/219 (99%)	176 (81%)	26 (12%)	15 (7%)	2	2
All	All	434/438 (99%)	356 (82%)	54 (12%)	24 (6%)	3	4

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%)	155 (79%)	42 (21%)	1	3
3	H	186/186 (100%)	148 (80%)	38 (20%)	2	4
All	All	383/383 (100%)	303 (79%)	80 (21%)	1	3

All (80) 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	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	95	GLN
2	L	99	VAL
2	L	113	ARG
2	L	121	SER
2	L	132	SER
2	L	142	ASN
2	L	148	ASP
2	L	150	ASN
2	L	162	ASN
2	L	176	SER
2	L	181	SER
2	L	184	LEU
2	L	186	LEU
2	L	195	ASN
2	L	200	GLU
2	L	204	LYS
2	L	206	SER

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Mol	Chain	Res	Type
2	L	208	SER
2	L	209	PRO
2	L	212	LYS
2	L	213	SER
2	L	215	ASN
2	L	216	ARG
2	L	217	ASN
3	H	3	GLN
3	H	7	THR
3	H	11	LEU
3	H	14	PRO
3	H	30	ASN
3	H	32	ASN
3	H	48	VAL
3	H	56	ASN
3	H	60	THR
3	H	64	ASP
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	118	THR
3	H	123	LYS
3	H	143	SER
3	H	144	VAL
3	H	156	GLU
3	H	163	ASN
3	H	166	SER
3	H	168	SER
3	H	178	LEU
3	H	185	MET
3	H	189	VAL
3	H	193	SER
3	H	196	TRP
3	H	200	THR

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Mol	Chain	Res	Type
3	H	203	CYS
3	H	208	PRO
3	H	218	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	39	HIS
2	L	58	ASN
2	L	142	ASN
2	L	161	GLN
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 ⓘ

There are no RNA chains 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 will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.