



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:46 PM UTC

PDB ID : 1NBV / pdb_00001nbv
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 : 2.00 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

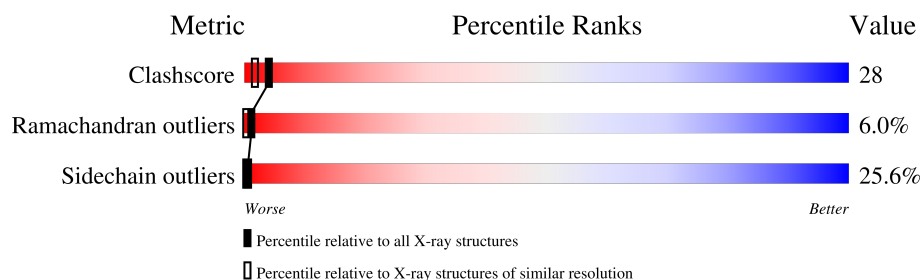
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	219	
2	H	219	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3347 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 IGG2B-KAPPA BV04-01 FAB (LIGHT CHAIN).

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

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	39	HIS	TYR	conflict	PIR S16112
L	51	LEU	PRO	conflict	PIR S16112
L	55	LYS	ARG	conflict	PIR S16112
L	94	SER	PHE	conflict	PIR S16112
L	96	SER	GLY	conflict	PIR S16112
L	101	LEU	TYR	conflict	PIR S16112
L	105	ALA	GLY	conflict	PIR S16112
L	108	LYS	ARG	conflict	PIR S16112
L	111	LEU	ILE	conflict	PIR S16112

- Molecule 2 is a protein called IGG2B-KAPPA BV04-01 FAB (HEAVY CHAIN).

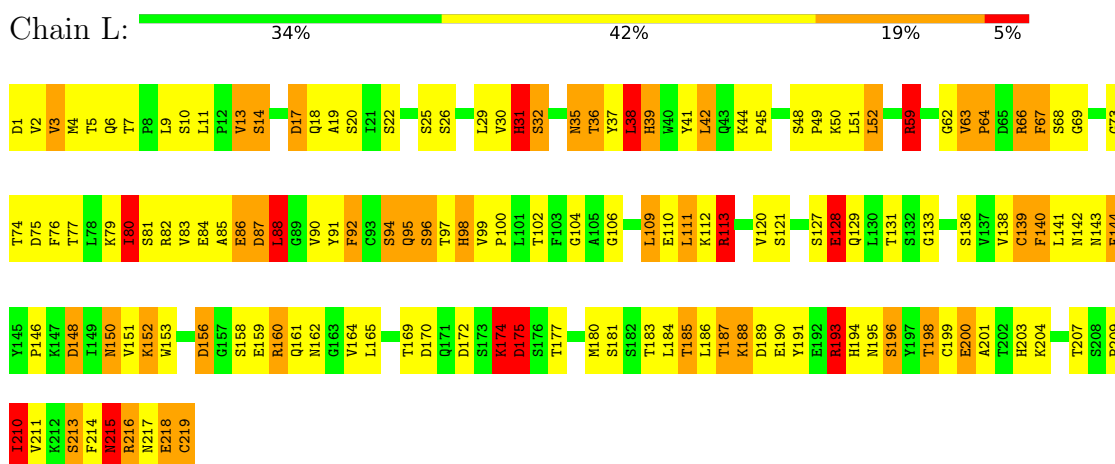
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1653	1038	275	330	10			

3 Residue-property plots

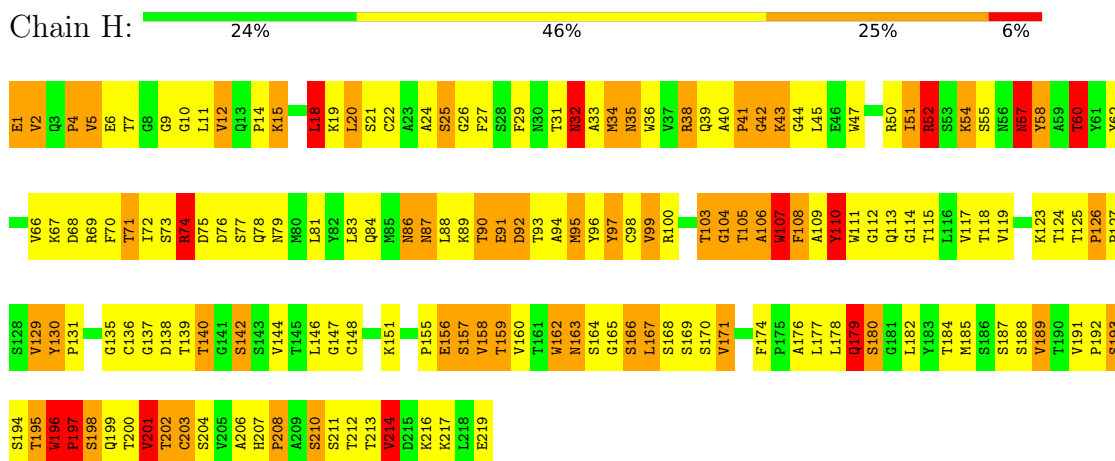
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: IGG2B-KAPPA BV04-01 FAB (LIGHT CHAIN)



• Molecule 2: IGG2B-KAPPA BV04-01 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 1	Depositor
Cell constants a, b, c, α , β , γ	58.40Å 43.70Å 41.50Å 83.40° 89.40° 84.40°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.246 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3347	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	L	1.52	7/1732 (0.4%)	2.18	72/2350 (3.1%)
2	H	1.51	9/1694 (0.5%)	2.28	87/2313 (3.8%)
All	All	1.51	16/3426 (0.5%)	2.23	159/4663 (3.4%)

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
2	H	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	105	THR	N-CA	10.98	1.53	1.46
1	L	104	GLY	N-CA	10.01	1.54	1.44
1	L	63	VAL	N-CA	7.03	1.54	1.46
2	H	34	MET	N-CA	6.88	1.54	1.45
1	L	3	VAL	N-CA	6.22	1.53	1.46
1	L	215	ASN	CA-C	6.12	1.59	1.52
2	H	196	TRP	CA-CB	5.97	1.62	1.53
1	L	32	SER	N-CA	5.90	1.53	1.46
2	H	60	THR	N-CA	5.88	1.53	1.45
1	L	31	HIS	CA-CB	-5.79	1.44	1.53
2	H	76	ASP	C-N	-5.72	1.25	1.33
2	H	11	LEU	C-N	-5.64	1.28	1.33
2	H	137	GLY	N-CA	5.44	1.53	1.45
1	L	158	SER	C-N	-5.29	1.28	1.33
2	H	196	TRP	C-O	5.26	1.31	1.25
2	H	192	PRO	N-CD	5.08	1.54	1.47

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	175	ASP	CA-CB-CG	20.61	133.21	112.60
2	H	105	THR	N-CA-C	-16.54	95.22	108.78
1	L	215	ASN	CA-CB-CG	15.37	127.97	112.60
2	H	32	ASN	CA-CB-CG	12.15	124.75	112.60
1	L	162	ASN	CA-CB-CG	11.69	124.29	112.60
2	H	156	GLU	CA-CB-CG	11.12	136.34	114.10
2	H	86	ASN	CA-CB-CG	10.71	123.31	112.60
1	L	31	HIS	CA-CB-CG	10.31	124.11	113.80
1	L	144	PHE	CA-CB-CG	10.04	123.84	113.80
1	L	98	HIS	CA-CB-CG	9.88	123.68	113.80
2	H	57	ASN	CA-CB-CG	9.49	122.09	112.60
2	H	214	VAL	CB-CA-C	9.46	121.45	111.23
1	L	81	SER	N-CA-C	9.24	122.29	111.02
2	H	70	PHE	CA-CB-CG	9.02	122.82	113.80
1	L	79	LYS	CA-CB-CG	8.82	131.73	114.10
1	L	2	VAL	CB-CA-C	8.66	123.20	110.98
1	L	63	VAL	CB-CA-C	8.63	118.96	110.94
1	L	128	GLU	CA-CB-CG	8.54	131.19	114.10
2	H	110	TYR	CA-CB-CG	8.33	128.89	113.90
2	H	74	ARG	CD-NE-CZ	8.31	136.04	124.40
1	L	140	PHE	CA-CB-CG	8.27	122.07	113.80
2	H	1	GLU	CA-C-N	8.06	136.48	121.97
2	H	1	GLU	C-N-CA	8.06	136.48	121.97
1	L	109	LEU	CA-C-O	-8.06	112.16	120.54
2	H	35	ASN	CA-CB-CG	7.96	120.56	112.60
1	L	216	ARG	CD-NE-CZ	7.86	135.40	124.40
2	H	179	GLN	N-CA-CB	7.81	123.66	110.46
1	L	63	VAL	N-CA-C	-7.70	102.01	108.63
2	H	197	PRO	N-CA-C	7.65	132.00	112.10
1	L	210	ILE	N-CA-C	-7.59	99.81	109.30
1	L	215	ASN	N-CA-CB	7.52	123.32	110.68
2	H	75	ASP	CB-CA-C	7.48	122.15	111.82
2	H	126	PRO	CB-CA-C	7.38	119.92	110.92
1	L	3	VAL	CB-CA-C	7.32	122.38	111.26
2	H	213	THR	CA-CB-OG1	-7.32	98.63	109.60
2	H	10	GLY	N-CA-C	-7.29	100.59	110.43
2	H	137	GLY	N-CA-C	-7.18	96.15	113.18
2	H	163	ASN	N-CA-CB	7.14	121.57	110.21
1	L	142	ASN	CA-C-N	7.07	135.04	121.54
1	L	142	ASN	C-N-CA	7.07	135.04	121.54
1	L	187	THR	CA-CB-OG1	-7.05	99.02	109.60
2	H	130	TYR	CA-C-N	6.99	127.23	119.90
2	H	130	TYR	C-N-CA	6.99	127.23	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	164	SER	N-CA-C	-6.99	98.46	109.50
2	H	193	SER	CA-CB-OG	6.99	125.07	111.10
2	H	34	MET	CB-CA-C	6.95	123.91	109.38
2	H	138	ASP	CA-C-N	6.94	134.80	121.54
2	H	138	ASP	C-N-CA	6.94	134.80	121.54
1	L	194	HIS	CA-CB-CG	6.94	120.74	113.80
2	H	92	ASP	N-CA-C	-6.94	102.93	113.89
1	L	90	VAL	CB-CA-C	6.93	121.16	110.83
1	L	113	ARG	CA-CB-CG	6.77	127.64	114.10
1	L	189	ASP	CA-CB-CG	-6.76	105.84	112.60
2	H	97	TYR	CA-CB-CG	6.76	126.06	113.90
2	H	164	SER	CA-C-O	-6.73	113.24	121.11
2	H	174	PHE	CA-C-N	6.69	126.67	119.78
2	H	174	PHE	C-N-CA	6.69	126.67	119.78
2	H	163	ASN	O-C-N	6.68	130.94	122.93
2	H	159	THR	N-CA-C	6.58	118.23	107.23
2	H	129	VAL	N-CA-CB	-6.54	103.27	111.31
1	L	32	SER	CB-CA-C	6.53	123.41	110.42
1	L	67	PHE	CA-CB-CG	6.51	120.31	113.80
1	L	80	ILE	CA-C-N	6.49	129.81	120.79
1	L	80	ILE	C-N-CA	6.49	129.81	120.79
2	H	95	MET	CA-C-O	-6.49	113.36	120.43
2	H	12	VAL	CA-C-O	-6.48	115.52	120.96
1	L	200	GLU	CA-CB-CG	6.48	127.05	114.10
1	L	102	THR	CB-CA-C	6.44	121.31	109.71
1	L	188	LYS	CA-C-N	6.43	129.18	120.44
1	L	188	LYS	C-N-CA	6.43	129.18	120.44
2	H	54	LYS	N-CA-C	-6.39	103.44	111.11
2	H	76	ASP	N-CA-C	-6.38	100.46	109.96
2	H	196	TRP	CA-C-O	-6.36	114.63	119.59
1	L	160	ARG	CA-C-O	-6.34	111.44	120.51
1	L	113	ARG	CB-CA-C	6.32	121.05	110.43
2	H	4	PRO	N-CA-C	-6.32	101.27	111.19
1	L	79	LYS	N-CA-CB	6.24	120.81	110.63
2	H	66	VAL	O-C-N	6.24	128.21	121.78
2	H	95	MET	N-CA-C	-6.24	99.07	109.24
1	L	215	ASN	O-C-N	6.22	130.71	123.30
2	H	158	VAL	CA-C-O	-6.21	115.34	121.67
1	L	159	GLU	CA-CB-CG	6.20	126.50	114.10
2	H	92	ASP	N-CA-CB	6.17	119.84	110.95
2	H	139	THR	CA-C-O	-6.14	111.72	120.51
2	H	142	SER	N-CA-C	-6.12	105.97	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	218	GLU	N-CA-C	-6.08	106.46	114.31
1	L	185	THR	CB-CA-C	6.00	120.13	110.16
1	L	148	ASP	CA-CB-CG	6.00	118.60	112.60
1	L	88	LEU	CA-CB-CG	5.99	137.27	116.30
1	L	92	PHE	CA-CB-CG	5.96	119.76	113.80
2	H	144	VAL	CB-CA-C	5.96	119.70	110.28
2	H	60	THR	N-CA-CB	-5.96	100.44	111.52
2	H	87	ASN	CA-CB-CG	5.95	118.55	112.60
2	H	38	ARG	NE-CZ-NH2	5.94	124.55	119.20
1	L	86	GLU	CB-CG-CD	5.91	122.64	112.60
2	H	11	LEU	CA-C-N	5.87	129.82	121.96
2	H	11	LEU	C-N-CA	5.87	129.82	121.96
1	L	153	TRP	CB-CA-C	5.84	119.44	109.80
2	H	178	LEU	CA-C-N	-5.83	114.51	123.14
2	H	178	LEU	C-N-CA	-5.83	114.51	123.14
2	H	140	THR	CA-CB-OG1	-5.79	100.91	109.60
2	H	86	ASN	CB-CG-ND2	5.77	125.06	116.40
1	L	199	CYS	N-CA-CB	5.76	119.83	110.43
2	H	171	VAL	N-CA-CB	-5.75	104.45	110.72
2	H	21	SER	N-CA-C	5.74	118.85	108.69
2	H	103	THR	CA-C-O	-5.72	113.85	120.49
2	H	92	ASP	CA-CB-CG	5.68	118.28	112.60
2	H	124	THR	CA-CB-OG1	-5.67	101.09	109.60
2	H	201	VAL	CB-CA-C	5.62	117.42	110.73
1	L	185	THR	CA-C-O	5.61	126.31	120.30
2	H	104	GLY	CA-C-N	-5.61	116.99	123.04
2	H	104	GLY	C-N-CA	-5.61	116.99	123.04
1	L	59	ARG	NE-CZ-NH1	-5.60	115.90	121.50
1	L	104	GLY	N-CA-C	-5.60	101.91	112.10
1	L	204	LYS	CA-CB-CG	5.59	125.29	114.10
1	L	63	VAL	N-CA-CB	-5.57	104.27	110.23
2	H	193	SER	N-CA-CB	5.56	118.92	110.14
1	L	62	GLY	N-CA-C	5.55	123.26	115.43
1	L	162	ASN	OD1-CG-ND2	-5.54	117.06	122.60
2	H	105	THR	O-C-N	5.53	125.62	121.47
1	L	215	ASN	N-CA-C	-5.52	99.89	108.90
1	L	109	LEU	O-C-N	5.51	129.60	123.05
2	H	151	LYS	CA-C-N	5.50	132.19	121.41
2	H	151	LYS	C-N-CA	5.50	132.19	121.41
1	L	185	THR	CA-C-N	5.47	131.18	122.59
1	L	185	THR	C-N-CA	5.47	131.18	122.59
2	H	106	ALA	CA-C-N	5.43	131.91	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	106	ALA	C-N-CA	5.43	131.91	121.54
1	L	75	ASP	CA-CB-CG	5.42	118.02	112.60
1	L	193	ARG	CG-CD-NE	5.38	123.84	112.00
2	H	92	ASP	O-C-N	5.37	128.08	122.23
2	H	86	ASN	OD1-CG-ND2	-5.35	117.25	122.60
2	H	18	LEU	CA-CB-CG	5.28	134.77	116.30
2	H	163	ASN	N-CA-C	-5.25	99.96	108.41
2	H	103	THR	CA-C-N	-5.24	117.21	123.44
2	H	103	THR	C-N-CA	-5.24	117.21	123.44
1	L	87	ASP	N-CA-C	-5.23	107.07	113.50
1	L	193	ARG	CA-CB-CG	5.21	124.52	114.10
1	L	128	GLU	CB-CG-CD	5.20	121.44	112.60
2	H	108	PHE	CA-CB-CG	5.19	118.99	113.80
2	H	174	PHE	CB-CA-C	5.18	116.80	109.08
1	L	175	ASP	CB-CA-C	5.18	120.72	110.42
1	L	169	THR	CA-CB-CG2	5.16	119.28	110.50
1	L	59	ARG	CD-NE-CZ	-5.15	117.19	124.40
1	L	170	ASP	N-CA-C	-5.14	103.90	110.53
1	L	38	LEU	CA-C-O	-5.13	114.44	120.60
2	H	42	GLY	N-CA-C	-5.12	105.15	111.45
2	H	105	THR	CA-C-O	-5.11	114.98	117.94
1	L	5	THR	CA-CB-OG1	-5.10	101.95	109.60
2	H	1	GLU	CA-CB-CG	5.08	124.27	114.10
1	L	96	SER	CA-C-O	-5.08	113.60	119.59
2	H	162	TRP	O-C-N	5.07	129.77	123.28
1	L	214	PHE	CA-CB-CG	5.04	118.84	113.80
2	H	42	GLY	CA-C-N	5.03	131.14	121.54
2	H	42	GLY	C-N-CA	5.03	131.14	121.54
2	H	113	GLN	CB-CG-CD	5.02	121.14	112.60
1	L	64	PRO	N-CA-C	-5.02	103.56	111.34
2	H	125	THR	N-CA-C	-5.00	98.75	109.81
1	L	99	VAL	N-CA-CB	-5.00	104.21	111.21

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	196	TRP	Mainchain

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	1694	0	1638	91	1
2	H	1653	0	1600	107	1
All	All	3347	0	3238	183	1

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 28.

All (183) 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:127:PRO:HD2	2:H:212:THR:HG21	1.50	0.91
1:L:1:ASP:HB2	1:L:100:PRO:HD2	1.59	0.84
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.58	0.83
2:H:22:CYS:HB3	2:H:81:LEU:HB3	1.62	0.80
1:L:95:GLN:HE21	1:L:97:THR:H	1.30	0.77
1:L:41:TYR:HE1	1:L:94:SER:HB3	1.51	0.76
2:H:159:THR:HB	2:H:206:ALA:HB3	1.69	0.75
1:L:218:GLU:O	1:L:219:CYS:HB3	1.86	0.75
1:L:200:GLU:HB2	1:L:211:VAL:HG12	1.69	0.74
1:L:95:GLN:HE22	1:L:98:HIS:H	1.37	0.73
1:L:95:GLN:NE2	1:L:97:THR:H	1.90	0.69
1:L:152:LYS:HE3	1:L:160:ARG:HH12	1.58	0.69
1:L:7:THR:HB	1:L:22:SER:HB3	1.73	0.69
2:H:9:GLY:HA2	2:H:18:LEU:HD11	1.73	0.69
2:H:2:VAL:HG11	2:H:26:GLY:HA3	1.76	0.68
1:L:128:GLU:HG2	2:H:216:LYS:NZ	2.08	0.68
2:H:24:ALA:C	2:H:26:GLY:H	2.01	0.68
1:L:96:SER:HG	2:H:107:TRP:CD1	2.11	0.67
2:H:6:GLU:OE1	2:H:112:GLY:HA3	1.95	0.67
1:L:31:HIS:HB2	1:L:37:TYR:HE1	1.59	0.66
2:H:14:PRO:O	2:H:15:LYS:HB2	1.97	0.64
2:H:34:MET:HG2	2:H:81:LEU:HD22	1.79	0.64
2:H:171:VAL:HG12	2:H:189:VAL:HG23	1.80	0.64
2:H:176:ALA:HB2	2:H:185:MET:HB2	1.79	0.64
2:H:4:PRO:HG3	2:H:100:ARG:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:93:THR:HA	2:H:117:VAL:O	1.98	0.64
2:H:147:GLY:HA2	2:H:187:SER:O	1.98	0.64
2:H:195:THR:O	2:H:199:GLN:HB2	1.97	0.64
2:H:193:SER:O	2:H:194:SER:C	2.42	0.63
1:L:184:LEU:HD21	1:L:186:LEU:HD21	1.80	0.63
2:H:163:ASN:HB3	2:H:202:THR:OG1	1.98	0.63
2:H:107:TRP:H	2:H:107:TRP:HE3	1.47	0.62
1:L:44:LYS:HE2	1:L:86:GLU:HG2	1.82	0.62
2:H:35:ASN:HD22	2:H:47:TRP:NE1	1.98	0.61
2:H:74:ARG:HG3	2:H:74:ARG:HH11	1.66	0.60
1:L:32:SER:O	1:L:35:ASN:ND2	2.35	0.60
1:L:200:GLU:CB	1:L:211:VAL:HG12	2.33	0.59
1:L:95:GLN:NE2	1:L:98:HIS:H	2.01	0.59
1:L:85:ALA:O	1:L:88:LEU:HB2	2.01	0.59
1:L:19:ALA:HB3	1:L:80:ILE:HG23	1.85	0.58
1:L:13:VAL:HG11	1:L:83:VAL:HG21	1.84	0.58
1:L:219:CYS:C	2:H:136:CYS:HB2	2.27	0.58
2:H:162:TRP:CE3	2:H:201:VAL:HG12	2.38	0.58
2:H:34:MET:CG	2:H:81:LEU:HD22	2.34	0.58
1:L:86:GLU:HG2	1:L:86:GLU:O	2.04	0.58
1:L:133:GLY:HA2	1:L:188:LYS:HB2	1.86	0.57
2:H:26:GLY:O	2:H:100:ARG:NH2	2.36	0.57
1:L:30:VAL:HG12	1:L:36:THR:HB	1.87	0.57
1:L:96:SER:OG	2:H:107:TRP:HB2	2.05	0.57
1:L:193:ARG:HH11	1:L:193:ARG:HG3	1.69	0.57
1:L:95:GLN:NE2	1:L:97:THR:N	2.53	0.56
1:L:66:ARG:NH1	1:L:84:GLU:HG3	2.21	0.56
1:L:96:SER:HG	2:H:107:TRP:CG	2.22	0.56
2:H:35:ASN:HD22	2:H:47:TRP:HE1	1.53	0.56
2:H:198:SER:O	2:H:199:GLN:HG2	2.04	0.56
2:H:7:THR:O	2:H:20:LEU:HD13	2.05	0.56
1:L:165:LEU:HD11	2:H:177:LEU:HB3	1.87	0.56
2:H:1:GLU:O	2:H:2:VAL:HG23	2.05	0.56
1:L:80:ILE:HD11	1:L:87:ASP:OD2	2.06	0.56
2:H:60:THR:HG23	2:H:62:TYR:CE2	2.42	0.55
2:H:90:THR:C	2:H:92:ASP:H	2.14	0.55
1:L:174:LYS:HD3	1:L:175:ASP:HB3	1.88	0.55
1:L:200:GLU:HA	1:L:210:ILE:O	2.07	0.55
2:H:162:TRP:HA	2:H:202:THR:O	2.06	0.55
2:H:24:ALA:O	2:H:26:GLY:N	2.34	0.55
2:H:39:GLN:HG3	2:H:44:GLY:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:41:TYR:CE1	1:L:94:SER:HB3	2.37	0.54
1:L:91:TYR:O	1:L:106:GLY:HA2	2.06	0.54
1:L:88:LEU:HD21	1:L:111:LEU:HD22	1.88	0.54
1:L:164:VAL:HA	1:L:183:THR:O	2.08	0.54
2:H:126:PRO:HB3	2:H:212:THR:OG1	2.08	0.54
1:L:44:LYS:HE2	1:L:86:GLU:O	2.06	0.54
2:H:24:ALA:C	2:H:26:GLY:N	2.65	0.54
1:L:49:PRO:HG3	2:H:45:LEU:HD11	1.90	0.54
1:L:41:TYR:HA	1:L:50:LYS:O	2.09	0.53
1:L:6:GLN:OE1	1:L:92:PHE:HA	2.09	0.53
1:L:161:GLN:HG3	1:L:184:LEU:HD11	1.90	0.53
2:H:45:LEU:HD13	2:H:111:TRP:CH2	2.44	0.53
1:L:191:TYR:C	1:L:193:ARG:H	2.16	0.52
2:H:36:TRP:HD1	2:H:72:ILE:HD12	1.74	0.52
1:L:14:SER:O	1:L:17:ASP:HB2	2.10	0.52
2:H:105:THR:HG22	2:H:106:ALA:H	1.74	0.52
2:H:38:ARG:HB2	2:H:94:ALA:HB1	1.90	0.52
1:L:215:ASN:HB2	1:L:218:GLU:HG3	1.91	0.52
1:L:140:PHE:CE2	2:H:188:SER:HB3	2.46	0.51
2:H:160:VAL:HG23	2:H:185:MET:HE1	1.92	0.51
2:H:35:ASN:CG	2:H:50:ARG:HB3	2.36	0.51
1:L:29:LEU:O	1:L:36:THR:HA	2.11	0.51
1:L:140:PHE:CD2	2:H:188:SER:HB3	2.46	0.51
2:H:62:TYR:OH	2:H:71:THR:HA	2.10	0.51
2:H:197:PRO:C	2:H:199:GLN:H	2.19	0.50
2:H:32:ASN:ND2	2:H:100:ARG:NH1	2.59	0.50
2:H:35:ASN:ND2	2:H:47:TRP:HE1	2.08	0.50
2:H:1:GLU:HA	2:H:110:TYR:HE2	1.77	0.50
2:H:146:LEU:O	2:H:188:SER:HA	2.12	0.50
2:H:6:GLU:OE2	2:H:97:TYR:HA	2.12	0.49
2:H:4:PRO:HB3	2:H:22:CYS:SG	2.53	0.49
1:L:121:SER:O	1:L:139:CYS:HB2	2.12	0.49
2:H:9:GLY:HA2	2:H:18:LEU:CD1	2.42	0.49
2:H:67:LYS:O	2:H:68:ASP:HB2	2.12	0.49
1:L:64:PRO:HD2	1:L:67:PHE:HE1	1.77	0.49
1:L:69:GLY:HA2	1:L:77:THR:O	2.11	0.49
2:H:52:ARG:O	2:H:74:ARG:NH2	2.45	0.49
1:L:64:PRO:HD2	1:L:67:PHE:CE1	2.47	0.49
1:L:150:ASN:O	1:L:201:ALA:HA	2.13	0.48
2:H:5:VAL:O	2:H:22:CYS:HA	2.13	0.48
2:H:24:ALA:HB3	2:H:29:PHE:CD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:78:GLN:O	2:H:79:ASN:HB2	2.12	0.48
1:L:85:ALA:HA	1:L:88:LEU:HD22	1.95	0.48
2:H:69:ARG:HB3	2:H:86:ASN:O	2.14	0.48
1:L:195:ASN:OD1	1:L:216:ARG:HB3	2.13	0.48
1:L:49:PRO:HG2	2:H:111:TRP:CZ3	2.48	0.48
1:L:49:PRO:CG	2:H:45:LEU:HD11	2.43	0.48
2:H:38:ARG:HA	2:H:95:MET:O	2.13	0.47
1:L:165:LEU:CD2	2:H:184:THR:HB	2.45	0.47
2:H:35:ASN:ND2	2:H:50:ARG:HB3	2.29	0.47
2:H:163:ASN:OD1	2:H:163:ASN:C	2.57	0.47
1:L:44:LYS:HB3	1:L:45:PRO:HD2	1.96	0.47
2:H:105:THR:O	2:H:106:ALA:HB2	2.14	0.47
2:H:107:TRP:HE3	2:H:107:TRP:N	2.11	0.47
2:H:127:PRO:HD2	2:H:212:THR:CG2	2.32	0.47
2:H:51:ILE:HD13	2:H:74:ARG:HD2	1.96	0.47
1:L:201:ALA:O	1:L:209:PRO:HA	2.15	0.46
1:L:51:LEU:HD22	2:H:109:ALA:HA	1.98	0.46
1:L:216:ARG:C	1:L:218:GLU:H	2.22	0.46
1:L:38:LEU:HG	1:L:39:HIS:N	2.30	0.46
2:H:165:GLY:O	2:H:167:LEU:HD23	2.14	0.46
1:L:59:ARG:NH1	1:L:67:PHE:O	2.49	0.46
2:H:38:ARG:NH1	2:H:96:TYR:OH	2.47	0.46
1:L:31:HIS:HB2	1:L:37:TYR:CE1	2.47	0.45
1:L:193:ARG:HH11	1:L:193:ARG:CG	2.29	0.45
1:L:146:PRO:HD2	1:L:203:HIS:CE1	2.52	0.45
2:H:89:LYS:O	2:H:119:VAL:HG11	2.17	0.45
2:H:22:CYS:O	2:H:81:LEU:N	2.42	0.45
2:H:32:ASN:ND2	2:H:100:ARG:HH12	2.14	0.45
2:H:203:CYS:O	2:H:203:CYS:SG	2.76	0.44
1:L:195:ASN:ND2	1:L:217:ASN:OD1	2.38	0.44
1:L:128:GLU:HG2	2:H:216:LYS:HZ3	1.82	0.44
2:H:32:ASN:HB3	2:H:33:ALA:H	1.57	0.44
2:H:156:GLU:O	2:H:157:SER:CB	2.66	0.44
2:H:166:SER:C	2:H:167:LEU:HG	2.43	0.44
2:H:129:VAL:HG12	2:H:216:LYS:HG3	2.00	0.44
2:H:57:ASN:O	2:H:58:TYR:C	2.61	0.43
2:H:99:VAL:HG11	2:H:108:PHE:HB3	1.99	0.43
2:H:84:GLN:HG3	2:H:86:ASN:ND2	2.33	0.43
2:H:135:GLY:C	2:H:136:CYS:SG	3.00	0.43
1:L:11:LEU:HD23	1:L:109:LEU:CD2	2.49	0.43
2:H:130:TYR:HA	2:H:131:PRO:HD2	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:42:GLY:O	2:H:43:LYS:O	2.37	0.43
2:H:208:PRO:C	2:H:210:SER:H	2.26	0.43
1:L:37:TYR:HD1	1:L:97:THR:OG1	2.01	0.43
2:H:197:PRO:O	2:H:199:GLN:N	2.49	0.43
1:L:39:HIS:HE1	2:H:106:ALA:CB	2.32	0.42
1:L:59:ARG:HH11	1:L:59:ARG:HD3	1.57	0.42
1:L:42:LEU:CD1	1:L:44:LYS:HE3	2.48	0.42
2:H:176:ALA:CB	2:H:185:MET:HB2	2.48	0.42
1:L:129:GLN:OE1	1:L:136:SER:HB2	2.19	0.42
2:H:179:GLN:O	2:H:180:SER:CB	2.67	0.42
1:L:156:ASP:HA	1:L:196:SER:OG	2.20	0.42
1:L:190:GLU:O	1:L:193:ARG:HB3	2.20	0.42
1:L:172:ASP:OD1	1:L:174:LYS:HB3	2.19	0.42
1:L:91:TYR:CE1	1:L:109:LEU:HG	2.55	0.42
1:L:38:LEU:HD22	1:L:76:PHE:CG	2.55	0.42
1:L:42:LEU:HD11	1:L:44:LYS:HE3	2.02	0.42
2:H:212:THR:HG22	2:H:214:VAL:HG23	2.00	0.42
1:L:180:MET:HG2	1:L:181:SER:N	2.35	0.41
1:L:52:LEU:HA	1:L:63:VAL:HG21	2.02	0.41
2:H:84:GLN:HG3	2:H:86:ASN:HD21	1.85	0.41
1:L:63:VAL:HA	1:L:64:PRO:HD3	1.93	0.41
1:L:112:LYS:O	1:L:113:ARG:HB2	2.20	0.41
1:L:144:PHE:O	1:L:177:THR:HB	2.20	0.41
1:L:141:LEU:HD11	1:L:151:VAL:HG22	2.02	0.41
1:L:187:THR:O	1:L:188:LYS:C	2.64	0.41
1:L:198:THR:OG1	1:L:213:SER:OG	2.24	0.41
2:H:6:GLU:OE2	2:H:114:GLY:HA2	2.19	0.41
2:H:32:ASN:HD21	2:H:100:ARG:NH1	2.17	0.40
1:L:152:LYS:HE3	1:L:160:ARG:NH1	2.31	0.40
2:H:40:ALA:O	2:H:41:PRO:C	2.64	0.40
2:H:207:HIS:ND1	2:H:210:SER:OG	2.52	0.40
1:L:120:VAL:HA	1:L:140:PHE:O	2.21	0.40
2:H:1:GLU:HA	2:H:110:TYR:CE2	2.56	0.40
2:H:196:TRP:CD1	2:H:201:VAL:HG23	2.57	0.40
2:H:131:PRO:HD3	2:H:216:LYS:HD2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:188:LYS:NZ	2:H:104:GLY:O[1_465]	2.18	0.02

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	217/219 (99%)	183 (84%)	29 (13%)	5 (2%)	5	2
2	H	217/219 (99%)	166 (76%)	30 (14%)	21 (10%)	0	0
All	All	434/438 (99%)	349 (80%)	59 (14%)	26 (6%)	1	0

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	174	LYS
2	H	2	VAL
2	H	25	SER
2	H	43	LYS
2	H	107	TRP
2	H	157	SER
2	H	169	SER
2	H	180	SER
1	L	36	THR
2	H	32	ASN
2	H	77	SER
2	H	168	SER
2	H	198	SER
2	H	27	PHE
2	H	52	ARG
2	H	91	GLU
2	H	210	SER
1	L	143	ASN
1	L	156	ASP
2	H	58	TYR
2	H	211	SER
2	H	170	SER
1	L	73	GLY
2	H	166	SER
2	H	41	PRO

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Mol	Chain	Res	Type
2	H	197	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	197/197 (100%)	148 (75%)	49 (25%)	0	0
2	H	186/186 (100%)	137 (74%)	49 (26%)	0	0
All	All	383/383 (100%)	285 (74%)	98 (26%)	0	0

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	VAL
1	L	4	MET
1	L	9	LEU
1	L	10	SER
1	L	13	VAL
1	L	14	SER
1	L	17	ASP
1	L	18	GLN
1	L	20	SER
1	L	25	SER
1	L	26	SER
1	L	31	HIS
1	L	35	ASN
1	L	38	LEU
1	L	39	HIS
1	L	42	LEU
1	L	48	SER
1	L	52	LEU
1	L	59	ARG
1	L	66	ARG
1	L	68	SER
1	L	74	THR

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Mol	Chain	Res	Type
1	L	80	ILE
1	L	82	ARG
1	L	88	LEU
1	L	94	SER
1	L	95	GLN
1	L	110	GLU
1	L	111	LEU
1	L	113	ARG
1	L	127	SER
1	L	128	GLU
1	L	131	THR
1	L	138	VAL
1	L	139	CYS
1	L	148	ASP
1	L	150	ASN
1	L	152	LYS
1	L	174	LYS
1	L	175	ASP
1	L	185	THR
1	L	193	ARG
1	L	196	SER
1	L	198	THR
1	L	207	THR
1	L	210	ILE
1	L	213	SER
1	L	215	ASN
1	L	219	CYS
2	H	5	VAL
2	H	15	LYS
2	H	18	LEU
2	H	19	LYS
2	H	20	LEU
2	H	25	SER
2	H	31	THR
2	H	51	ILE
2	H	52	ARG
2	H	54	LYS
2	H	55	SER
2	H	57	ASN
2	H	60	THR
2	H	71	THR
2	H	73	SER

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Mol	Chain	Res	Type
2	H	74	ARG
2	H	83	LEU
2	H	87	ASN
2	H	88	LEU
2	H	90	THR
2	H	91	GLU
2	H	98	CYS
2	H	99	VAL
2	H	103	THR
2	H	107	TRP
2	H	110	TYR
2	H	115	THR
2	H	118	THR
2	H	123	LYS
2	H	140	THR
2	H	142	SER
2	H	148	CYS
2	H	155	PRO
2	H	158	VAL
2	H	167	LEU
2	H	179	GLN
2	H	182	LEU
2	H	189	VAL
2	H	191	VAL
2	H	195	THR
2	H	200	THR
2	H	201	VAL
2	H	202	THR
2	H	203	CYS
2	H	204	SER
2	H	208	PRO
2	H	214	VAL
2	H	217	LYS
2	H	219	GLU

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	18	GLN
1	L	95	GLN
1	L	98	HIS
1	L	166	ASN

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Mol	Chain	Res	Type
2	H	32	ASN
2	H	35	ASN
2	H	79	ASN
2	H	86	ASN
2	H	179	GLN

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.