



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:03 PM GMT

PDB ID : 1NBV
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

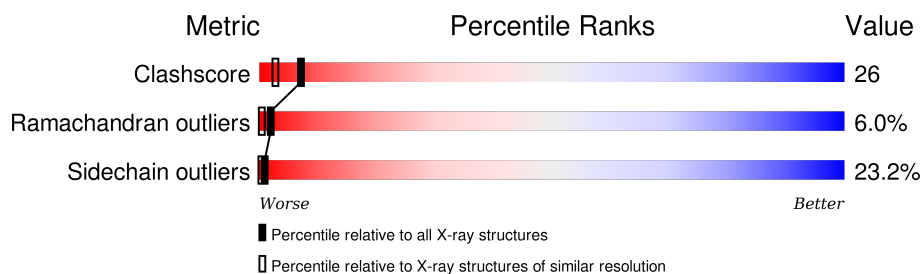
1 Overall quality at a glance

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	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).

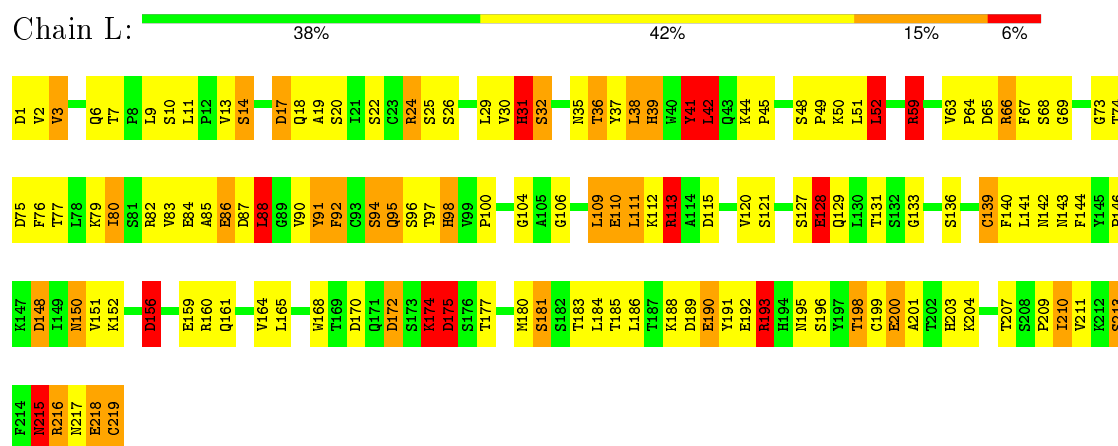
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1653	1038	275	330	10			

3 Residue-property plots

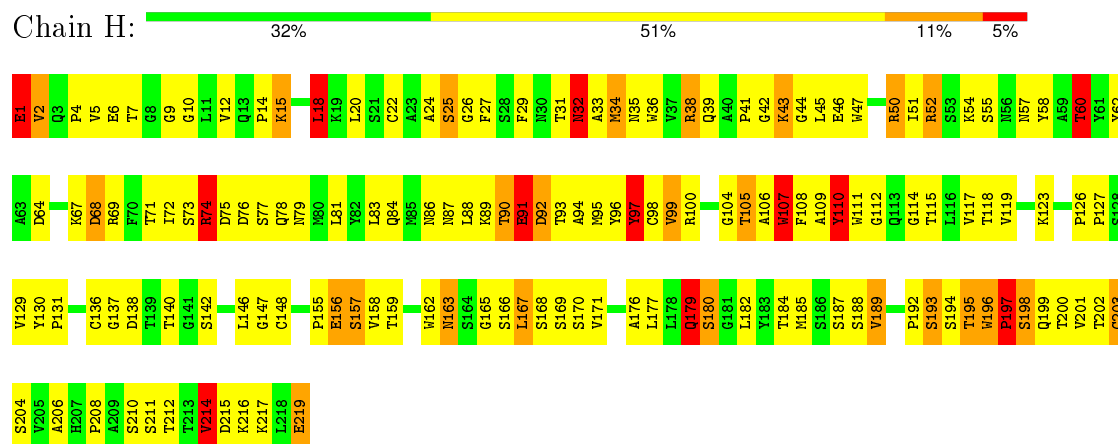
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: 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 will therefore be 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	1.24	7/1732 (0.4%)	1.79	51/2350 (2.2%)
2	H	1.20	6/1694 (0.4%)	1.77	30/2313 (1.3%)
All	All	1.22	13/3426 (0.4%)	1.78	81/4663 (1.7%)

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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	199	CYS	CB-SG	-9.35	1.66	1.82
1	L	128	GLU	CD-OE2	7.19	1.33	1.25
2	H	91	GLU	CD-OE1	6.76	1.33	1.25
1	L	110	GLU	CD-OE2	6.53	1.32	1.25
2	H	46	GLU	CD-OE2	6.46	1.32	1.25
2	H	1	GLU	CD-OE2	6.29	1.32	1.25
1	L	218	GLU	CD-OE1	6.21	1.32	1.25
2	H	156	GLU	CD-OE1	6.01	1.32	1.25
1	L	86	GLU	CD-OE2	5.99	1.32	1.25
2	H	219	GLU	CD-OE1	5.41	1.31	1.25
1	L	104	GLY	N-CA	5.40	1.54	1.46
1	L	190	GLU	CD-OE2	5.12	1.31	1.25
2	H	192	PRO	N-CD	5.01	1.54	1.47

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	75	ASP	CB-CG-OD1	10.50	127.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	156	GLU	CA-CB-CG	10.43	136.34	113.40
1	L	148	ASP	CB-CG-OD1	10.02	127.32	118.30
1	L	175	ASP	CB-CG-OD1	9.71	127.04	118.30
1	L	88	LEU	CA-CB-CG	9.55	137.27	115.30
1	L	175	ASP	CA-CB-CG	9.01	133.21	113.40
2	H	74	ARG	CD-NE-CZ	8.88	136.04	123.60
1	L	59	ARG	NE-CZ-NH1	-8.81	115.90	120.30
1	L	65	ASP	CB-CG-OD2	-8.69	110.48	118.30
2	H	38	ARG	NE-CZ-NH2	8.49	124.55	120.30
2	H	18	LEU	CA-CB-CG	8.46	134.77	115.30
1	L	216	ARG	CD-NE-CZ	8.43	135.40	123.60
1	L	79	LYS	CA-CB-CG	8.33	131.73	113.40
1	L	91	TYR	CB-CG-CD1	-8.21	116.08	121.00
2	H	110	TYR	CA-CB-CG	8.15	128.89	113.40
1	L	128	GLU	CA-CB-CG	8.08	131.19	113.40
2	H	68	ASP	CB-CG-OD2	7.66	125.20	118.30
2	H	197	PRO	N-CA-C	7.65	132.00	112.10
1	L	52	LEU	CA-CB-CG	7.46	132.46	115.30
1	L	216	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	L	109	LEU	CA-CB-CG	7.30	132.10	115.30
2	H	179	GLN	N-CA-CB	7.26	123.66	110.60
1	L	215	ASN	N-CA-CB	7.07	123.32	110.60
1	L	32	SER	CB-CA-C	7.00	123.41	110.10
2	H	137	GLY	N-CA-C	-6.78	96.15	113.10
2	H	34	MET	CB-CA-C	6.75	123.91	110.40
2	H	97	TYR	CA-CB-CG	6.67	126.06	113.40
1	L	113	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	L	215	ASN	CA-CB-CG	6.62	127.97	113.40
1	L	42	LEU	CA-CB-CG	6.58	130.44	115.30
1	L	113	ARG	CA-CB-CG	6.47	127.64	113.40
1	L	172	ASP	CB-CG-OD1	6.35	124.01	118.30
1	L	24	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	L	2	VAL	CB-CA-C	6.21	123.20	111.40
1	L	91	TYR	CB-CG-CD2	6.21	124.72	121.00
1	L	200	GLU	CA-CB-CG	6.21	127.05	113.40
1	L	31	HIS	CA-CB-CG	6.18	124.11	113.60
2	H	163	ASN	N-CA-CB	6.09	121.57	110.60
1	L	75	ASP	CB-CG-OD2	-6.04	112.86	118.30
2	H	50	ARG	NE-CZ-NH1	-5.99	117.30	120.30
1	L	159	GLU	CA-CB-CG	5.96	126.50	113.40
1	L	98	HIS	CA-CB-CG	5.93	123.68	113.60
2	H	1	GLU	C-N-CA	5.91	136.48	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	75	ASP	CB-CA-C	5.87	122.15	110.40
2	H	105	THR	N-CA-C	-5.84	95.22	111.00
2	H	38	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	L	3	VAL	CB-CA-C	5.78	122.38	111.40
1	L	193	ARG	CG-CD-NE	5.73	123.84	111.80
2	H	74	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	L	199	CYS	CA-CB-SG	5.69	124.24	114.00
2	H	215	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	L	79	LYS	N-CA-CB	5.67	120.81	110.60
2	H	193	SER	N-CA-CB	5.61	118.92	110.50
1	L	115	ASP	CB-CG-OD2	5.59	123.33	118.30
2	H	64	ASP	CB-CG-OD2	5.55	123.30	118.30
1	L	193	ARG	CD-NE-CZ	5.55	131.37	123.60
1	L	113	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	L	170	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	L	190	GLU	CG-CD-OE2	-5.49	107.32	118.30
1	L	113	ARG	CD-NE-CZ	5.45	131.23	123.60
1	L	204	LYS	CA-CB-CG	5.40	125.29	113.40
1	L	189	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	L	142	ASN	C-N-CA	5.34	135.04	121.70
1	L	113	ARG	CB-CA-C	5.32	121.05	110.40
2	H	214	VAL	CB-CA-C	5.29	121.45	111.40
2	H	138	ASP	C-N-CA	5.24	134.80	121.70
2	H	60	THR	N-CA-CB	-5.19	100.44	110.30
1	L	175	ASP	CB-CA-C	5.16	120.72	110.40
2	H	32	ASN	CA-CB-CG	5.16	124.75	113.40
2	H	163	ASN	O-C-N	5.15	130.94	122.70
1	L	156	ASP	CB-CG-OD1	5.14	122.92	118.30
2	H	193	SER	CA-CB-OG	5.14	125.07	111.20
1	L	90	VAL	CB-CA-C	5.13	121.16	111.40
2	H	92	ASP	N-CA-CB	5.13	119.84	110.60
1	L	199	CYS	N-CA-CB	5.13	119.83	110.60
1	L	41	TYR	CB-CG-CD2	5.05	124.03	121.00
1	L	193	ARG	CA-CB-CG	5.05	124.52	113.40
1	L	192	GLU	OE1-CD-OE2	5.03	129.33	123.30
2	H	76	ASP	CB-CG-OD1	5.03	122.82	118.30
1	L	215	ASN	O-C-N	5.00	130.71	122.70
2	H	10	GLY	N-CA-C	-5.00	100.59	113.10

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	89	1
2	H	1653	0	1600	98	1
All	All	3347	0	3238	173	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 26.

All (173) 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: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:34:MET:HG2	2:H:81:LEU:HD22	1.79	0.64
2:H:14:PRO:O	2:H:15:LYS:HB2	1.97	0.64
2:H:171:VAL:HG12	2:H:189:VAL:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:24:ALA:C	2:H:26:GLY:H	2.01	0.63
2:H:107:TRP:HE3	2:H:107:TRP:H	1.47	0.62
1:L:44:LYS:HE2	1:L:86:GLU:HG2	1.82	0.62
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
2:H:193:SER:O	2:H:194:SER:C	2.42	0.58
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
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:O	1:L:86:GLU:HG2	2.04	0.58
2:H:26:GLY:O	2:H:100:ARG:NH2	2.36	0.57
1:L:133:GLY:HA2	1:L:188:LYS:HB2	1.86	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:HG3	1:L:193:ARG:HH11	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
2:H:198:SER:O	2:H:199:GLN:HG2	2.04	0.56
2:H:35:ASN:HD22	2:H:47:TRP:HE1	1.53	0.56
2:H:7:THR:O	2:H:20:LEU:HD13	2.05	0.56
2:H:1:GLU:O	2:H:2:VAL:HG23	2.05	0.56
1:L:165:LEU:HD11	2:H:177:LEU:HB3	1.87	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
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
1:L:174:LYS:HD3	1:L:175:ASP:HB3	1.88	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
1:L:41:TYR:CE1	1:L:94:SER:HB3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:126:PRO:HB3	2:H:212:THR:OG1	2.08	0.54
1:L:164:VAL:HA	1:L:183:THR:O	2.08	0.54
1:L:44:LYS:HE2	1:L:86:GLU:O	2.06	0.54
1:L:49:PRO:HG3	2:H:45:LEU:HD11	1.90	0.54
1:L:219:CYS:C	2:H:136:CYS:HB2	2.27	0.53
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
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
1:L:29:LEU:O	1:L:36:THR:HA	2.11	0.51
2:H:62:TYR:OH	2:H:71:THR:HA	2.10	0.51
1:L:140:PHE:CD2	2:H:188:SER:HB3	2.46	0.51
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:90:THR:C	2:H:92:ASP:H	2.14	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
2:H:52:ARG:O	2:H:74:ARG:NH2	2.45	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:24:ALA:C	2:H:26:GLY:N	2.65	0.49
1:L:64:PRO:HD2	1:L:67:PHE:CE1	2.47	0.49
2:H:5:VAL:O	2:H:22:CYS:HA	2.13	0.48
1:L:150:ASN:O	1:L:201:ALA:HA	2.13	0.48
2:H:24:ALA:HB3	2:H:29:PHE:CD2	2.47	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:195:ASN:OD1	1:L:216:ARG:HB3	2.13	0.48
1:L:191:TYR:C	1:L:193:ARG:H	2.16	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:107:TRP:HE3	2:H:107:TRP:N	2.11	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: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
2:H:35:ASN:CG	2:H:50:ARG:HB3	2.36	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: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
2:H:38:ARG:NH1	2:H:96:TYR:OH	2.47	0.46
1:L:59:ARG:NH1	1:L:67:PHE:O	2.49	0.46
1:L:31:HIS:HB2	1:L:37:TYR:CE1	2.47	0.45
1:L:193:ARG:CG	1:L:193:ARG:HH11	2.29	0.45
1:L:146:PRO:HD2	1:L:203:HIS:CE1	2.52	0.45
2:H:197:PRO:C	2:H:199:GLN:H	2.19	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:SG	2:H:203:CYS:O	2.76	0.44
1:L:195:ASN:ND2	1:L:217:ASN:OD1	2.38	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:129:VAL:HG12	2:H:216:LYS:HG3	2.00	0.44
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:130:TYR:HA	2:H:131:PRO:HD2	1.69	0.43
1:L:11:LEU:HD23	1:L:109:LEU:CD2	2.49	0.43
2:H:42:GLY:O	2:H:43:LYS:O	2.37	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
2:H:163:ASN:C	2:H:163:ASN:OD1	2.57	0.42
1:L:39:HIS:HE1	2:H:106:ALA:CB	2.32	0.42
1:L:59:ARG:HD3	1:L:59:ARG:HH11	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:176:ALA:CB	2:H:185:MET:HB2	2.48	0.42
1:L:42:LEU:CD1	1:L:44:LYS:HE3	2.48	0.42
2:H:179:GLN:O	2:H:180:SER:CB	2.67	0.42
1:L:129:GLN:OE1	1:L:136:SER:HB2	2.19	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
2:H:212:THR:HG22	2:H:214:VAL:HG23	2.00	0.42
1:L:42:LEU:HD11	1:L:44:LYS:HE3	2.02	0.42
1:L:38:LEU:HD22	1:L:76:PHE:CG	2.55	0.42
1:L:180:MET:HG2	1:L:181:SER:N	2.35	0.41
1:L:216:ARG:C	1:L:218:GLU:H	2.22	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:112:LYS:O	1:L:113:ARG:HB2	2.20	0.41
1:L:63:VAL:HA	1:L:64:PRO:HD3	1.93	0.41
1:L:128:GLU:HG2	2:H:216:LYS:HZ2	1.80	0.41
1:L:144:PHE:O	1:L:177:THR:HB	2.20	0.41
1:L:128:GLU:HG2	2:H:216:LYS:HZ3	1.85	0.41
1:L:198:THR:OG1	1:L:213:SER:OG	2.24	0.41
1:L:141:LEU:HD11	1:L:151:VAL:HG22	2.02	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: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
1:L:120:VAL:HA	1:L:140:PHE:O	2.21	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%)	8	3
2	H	217/219 (99%)	166 (76%)	30 (14%)	21 (10%)	1	0
All	All	434/438 (99%)	349 (80%)	59 (14%)	26 (6%)	2	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%)	149 (76%)	48 (24%)	1	0
2	H	186/186 (100%)	145 (78%)	41 (22%)	1	0
All	All	383/383 (100%)	294 (77%)	89 (23%)	1	0

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	VAL
1	L	9	LEU
1	L	10	SER
1	L	14	SER
1	L	17	ASP
1	L	18	GLN
1	L	20	SER
1	L	24	ARG
1	L	25	SER
1	L	26	SER
1	L	31	HIS
1	L	38	LEU
1	L	39	HIS
1	L	41	TYR
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
1	L	80	ILE

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Mol	Chain	Res	Type
1	L	82	ARG
1	L	88	LEU
1	L	92	PHE
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	139	CYS
1	L	148	ASP
1	L	150	ASN
1	L	168	TRP
1	L	174	LYS
1	L	175	ASP
1	L	181	SER
1	L	185	THR
1	L	193	ARG
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	1	GLU
2	H	15	LYS
2	H	18	LEU
2	H	25	SER
2	H	31	THR
2	H	54	LYS
2	H	55	SER
2	H	57	ASN
2	H	60	THR
2	H	73	SER
2	H	74	ARG
2	H	83	LEU
2	H	87	ASN
2	H	88	LEU
2	H	90	THR
2	H	91	GLU

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Mol	Chain	Res	Type
2	H	97	TYR
2	H	98	CYS
2	H	99	VAL
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	195	THR
2	H	200	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) 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
2	H	32	ASN
2	H	86	ASN
2	H	179	GLN

5.3.3 RNA ⓘ

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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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