

# Full wwPDB X-ray Structure Validation Report (i)

#### May 26, 2020 - 02:31 am BST

PDB ID	:	1MLB
$\operatorname{Title}$	:	MONOCLONAL ANTIBODY FAB D44.1 RAISED AGAINST CHICKEN
		EGG-WHITE LYSOZYME
Authors	:	Braden, B.C.; Souchon, H.; Eisele, JL.; Bentley, G.A.; Bhat, T.N.; Navaza,
		J.; Poljak, R.J.
Deposited on	:	1995-03-08
Resolution	:	2.10  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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : $4.02b-467$	
Xtriage (Phenix) : <b>NOT EXECUTED</b>	
EDS : NOT EXECUTED	
$ \begin{tabular}{lllllllllllllllllllllllllllllllllll$	25 th 2019
Ideal geometry (proteins) : Engh & Huber (2001)	
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)	
Validation Pipeline (wwPDB-VP) : 2.11	

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647(2.10-2.10)
Sidechain outliers	138945	5648(2.10-2.10)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality o	f chain		
1	А	214	56%	34%	9%	·
2	В	218	50%	40%	9%	·



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3424 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 IGG1-KAPPA D44.1 FAB (LIGHT CHAIN).

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	214	Total 1670	C 1029	N 289	0 345	${ m S} 7$	0	2	0

• Molecule 2 is a protein called IGG1-KAPPA D44.1 FAB (HEAVY CHAIN).

Mol	Chain	Residues		Ate	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
2	В	218	Total 1639	C 1033	N 269	O 329	S 8	0	2	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	5	GLN	VAL	CONFLICT	PIR PC4202
В	11	VAL	LEU	CONFLICT	PIR PC4202
В	26	GLY	ASP	CONFLICT	PIR PC4202
В	28	THR	ARG	CONFLICT	PIR PC4202
В	31	THR	SER	CONFLICT	PIR PC4202
В	50	GLU	ASP	CONFLICT	PIR PC4202
В	57	SER	ASN	CONFLICT	PIR PC4202
В	59	TYR	ASN	CONFLICT	PIR PC4202
В	63	LYS	ARG	CONFLICT	PIR PC4202
В	98	ARG	ILE	CONFLICT	PIR PC4202
В	99	GLY	PRO	CONFLICT	PIR PC4202
В	101	GLY	-	INSERTION	PIR PC4202
В	102	ASN	-	INSERTION	PIR PC4202
В	103	TYR	-	INSERTION	PIR PC4202
В	104	GLY	-	INSERTION	PIR PC4202
В	118	SER	LYS	CONFLICT	PIR PC4202
В	125	PHE	TYR	CONFLICT	PIR PC4202

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	71	Total         O           71         71	0	0
3	В	44	Total         O           44         44	0	0

![](_page_3_Picture_4.jpeg)

## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

- Chain A:
   56%
   34%
   9%

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- Molecule 1: IGG1-KAPPA D44.1 FAB (LIGHT CHAIN)

![](_page_4_Picture_8.jpeg)

## 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	79.70Å 136.20Å 43.00Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	7.00 - 2.10	Depositor	
% Data completeness	(Not available) $(7.00-2.10)$	Depositor	
(in resolution range)	(100 available) (1.00 2.10)		
$R_{merge}$	0.10	Depositor	
R <sub>sym</sub>	(Not available)	Depositor	
Refinement program	PROLSQ	Depositor	
$R, R_{free}$	0.181 , $0.274$	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	3424	wwPDB-VP	
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP	

![](_page_5_Picture_6.jpeg)

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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).

Mal	Chain	Bo	nd lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	1.00	1/1717~(0.1%)	1.99	39/2326~(1.7%)	
2	В	1.00	0/1695	1.76	27/2315~(1.2%)	
All	All	1.00	1/3412~(0.0%)	1.88	66/4641~(1.4%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	195	GLU	CD-OE2	-5.43	1.19	1.25

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	108	ARG	NE-CZ-NH1	23.13	131.87	120.30
1	А	211	ARG	NE-CZ-NH2	-17.58	111.51	120.30
1	А	211	ARG	NE-CZ-NH1	16.38	128.49	120.30
1	А	108	ARG	NE-CZ-NH2	-12.82	113.89	120.30
1	А	188[A]	ARG	NE-CZ-NH2	-10.73	114.93	120.30
1	А	188[B]	ARG	NE-CZ-NH2	-10.73	114.93	120.30
1	А	140	TYR	CB-CG-CD1	-10.36	114.78	121.00
1	А	140	TYR	CB-CG-CD2	10.21	127.12	121.00
2	В	94	TYR	CB-CG-CD1	-10.18	114.89	121.00
2	В	98	ARG	NE-CZ-NH2	-9.61	115.49	120.30
1	А	81	GLU	OE1-CD-OE2	8.96	134.05	123.30
1	А	188[A]	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	А	188[B]	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	А	61	ARG	NE-CZ-NH1	8.04	124.32	120.30
2	В	105	TYR	CB-CG-CD1	-7.93	116.24	121.00
2	В	216	ARG	NE-CZ-NH2	-7.93	116.34	120.30
2	В	46	GLU	OE1-CD-OE2	7.75	132.60	123.30
2	В	12	MET	CG-SD-CE	7.72	112.55	100.20
2	В	152	PRO	N-CA-CB	-7.33	94.51	103.30
1	А	82	ASP	CB-CG-OD2	7.28	124.86	118.30
1	A	82	ASP	CB-CG-OD1	-6.75	112.22	118.30

![](_page_6_Picture_12.jpeg)

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	46	LEU	CA-CB-CG	6.67	130.63	115.30
2	В	88	SER	O-C-N	6.54	133.16	122.70
1	А	79	GLU	CG-CD-OE1	6.53	131.35	118.30
1	А	96	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	А	85	MET	N-CA-CB	-6.47	98.96	110.60
2	В	79	ALA	CB-CA-C	6.45	119.77	110.10
2	В	176	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	А	80	THR	N-CA-CB	6.38	122.41	110.30
1	А	102	THR	O-C-N	6.37	132.89	122.70
2	В	98	ARG	NH1-CZ-NH2	6.30	126.33	119.40
1	А	45	ARG	CA-CB-CG	6.29	127.25	113.40
2	В	12	MET	O-C-N	6.29	132.76	122.70
1	А	61	ARG	NH1-CZ-NH2	-6.27	112.50	119.40
2	В	191[A]	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	В	191[B]	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	В	94	TYR	CB-CG-CD2	6.11	124.66	121.00
1	А	143	ASP	CB-CG-OD1	-6.11	112.81	118.30
2	В	141	LEU	CA-CB-CG	6.09	129.30	115.30
1	А	151	ASP	CB-CG-OD1	6.08	123.77	118.30
2	В	177	LEU	CB-CA-C	6.08	121.75	110.20
2	В	50	$\operatorname{GLU}$	CG-CD-OE2	5.96	130.21	118.30
1	А	176	SER	N-CA-CB	5.92	119.37	110.50
2	В	60	TYR	O-C-N	5.86	132.07	122.70
2	В	18	VAL	O-C-N	5.81	131.99	122.70
1	А	181	LEU	CA-CB-CG	5.67	128.34	115.30
1	А	61	ARG	NE-CZ-NH2	5.64	123.12	120.30
2	В	46	GLU	CG-CD-OE1	-5.64	107.03	118.30
1	А	21	LEU	CA-CB-CG	5.52	128.00	115.30
1	А	201	SER	N-CA-CB	5.50	118.75	110.50
1	A	144	ILE	O-C-N	5.50	131.50	122.70
2	В	141	LEU	CB-CA-C	5.46	120.57	110.20
1	A	41	HIS	CA-CB-CG	-5.41	104.41	113.60
2	В	114	VAL	O-C-N	5.37	131.29	122.70
1	A	77	SER	O-C-N	5.33	131.23	122.70
1	A	193	THR	O-C-N	5.25	131.10	122.70
2	В	10	GLU	CA-CB-CG	5.21	124.87	113.40
1	A	50	TYR	CB-CG-CD2	5.21	124.12	121.00
1	А	108	ARG	CB-CA-C	-5.20	100.01	110.40
2	В	86	LEU	CB-CA-C	5.19	120.06	110.20
1	А	89	GLN	CG-CD-OE1	5.12	131.83	121.60
2	В	105	TYR	CB-CG-CD2	5.10	124.06	121.00
2	В	143	CYS	O-C-N	5.10	130.85	122.70

![](_page_7_Picture_6.jpeg)

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	76	ASN	O-C-N	5.08	130.83	122.70
1	А	10	THR	O-C-N	5.04	130.76	122.70
1	А	10	THR	CA-CB-OG1	-5.02	98.47	109.00

Continued from previous page...

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1670	0	1590	70	0
2	В	1639	0	1582	100	0
3	А	71	0	0	0	0
3	В	44	0	0	1	0
All	All	3424	0	3172	161	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 25.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:188[B]:ARG:CZ	1:A:188[B]:ARG:NE	1.82	1.42
1:A:24[B]:ARG:CG	1:A:24[B]:ARG:CD	2.02	1.38
2:B:51:ILE:HG13	2:B:58:THR:HG22	1.45	0.97
2:B:187:PRO:O	2:B:190:PRO:HD2	1.73	0.89
2:B:48:ILE:HG21	2:B:81[A]:MET:CE	2.02	0.89
2:B:173:LEU:HD13	2:B:178:TYR:CE1	2.09	0.88
2:B:212:LYS:NZ	2:B:212:LYS:HB2	1.91	0.85
2:B:35:GLU:HG3	2:B:103:TYR:CE1	2.12	0.83
2:B:189:SER:HB2	2:B:190:PRO:HD3	1.60	0.82
2:B:48:ILE:HG21	2:B:81[A]:MET:HE3	1.61	0.81
1:A:160:LEU:HD23	2:B:172:VAL:HG21	1.62	0.81
1:A:61:ARG:NH1	1:A:82:ASP:OD1	2.16	0.79
1:A:188[B]:ARG:NH2	1:A:188[B]:ARG:NE	2.30	0.78

![](_page_8_Picture_14.jpeg)

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	l puge	Interatomic Clash		
Atom-1	Atom-2	distance $(Å)$	overlan (Å)	
1:A:160:LEU:HD23	2:B:172:VAL:CG2	2.13	0.77	
1:A:147:LYS:HZ3	1:A:147:LYS:HB2	1.50	0.76	
2:B:187:PBO:HG2	2:B:190:PBO:HG2	1.60	0.76	
2:B:141:LEU:HD11	2:B:191[B]:ABG:NE	$\frac{1.01}{2.02}$	0.75	
2:B:3:GLN:HA	2:B:3:GLN:HE21	1 51	0.74	
1:A:155:ABG:NE	1:A:157:ASN:HD22	1.81	0.72	
2:B:47:TRP:HH2	2:B:59:TYB:HD2	1.36	0.72	
$1 \cdot A \cdot 2 \cdot ILE \cdot HD13$	$1 \cdot A \cdot 29 \cdot ILE \cdot HG22$	1.33	0.72	
2:B:212:LYS:CB	2:B:212:LYS:NZ	2.53	0.72	
2:B:190:PRO:HA	2:B:194:GLU:HG2	1 71	0.71	
$2 \cdot B \cdot 3 \cdot GLN \cdot HE 21$	2:B:3:GLN:CA	2.03	0.71	
$\frac{1 \cdot A \cdot 76 \cdot A SN \cdot O}{1 \cdot A \cdot 76 \cdot A SN \cdot O}$	1.A.77.SEB.HB2	1.90	0.71	
1 · A · 29 · ILE · HD11	1.A.33.LEU.HB2	1.20	0.69	
1:A:155:ABG:HE	1:A:157:ASN:HD22	1.39	0.69	
2·B·141·LEU·HD11	$2 \cdot B \cdot 191[B] \cdot ABG \cdot CD$	2.23	0.09	
2:B:47:TRP:HH2	$2 \cdot B \cdot 59 \cdot TYB \cdot CD2$	2.20	0.68	
1.A.155.ABG:NE	1 · A · 157 · A SN · ND2	2.10	0.68	
1.A.19.VAL.:HG23	1:A:21:LEU:CD1	2.12	0.68	
1.A.193.THB.OG1	1.A.208.SEB.HB3	1.94	0.00	
1:A:61:ABG:HH11	1:A:82:ASP:CG	1.01	0.07	
2·B·173·LEU·HD13	2·B·178·TYB·CD1	2.30	0.66	
2·B·203·PRO·HD2	3·B·454·HOH·O	1.94	0.66	
2:B:205:SEB:HB2	$2 \cdot B \cdot 207 \cdot THB \cdot OG1$	1.01	0.00	
1:A:29:ILE:CD1	1:A:33:LEU:HB2	$\frac{1.00}{2.27}$	0.65	
$2 \cdot B \cdot 202 \cdot HIS \cdot ND1$	$2 \cdot B \cdot 205 \cdot SEB \cdot OG$	2.21	0.64	
2:B:139:VAL:N	2:B:186:VAL:O	2.20	0.64	
1:A:19:VAL:HG13	1:A:78:VAL:HG21	1 78	0.64	
1.A.108.ABG.HD2	1.A.170.ASP.O	1.08	0.63	
1:A:19:VAL:HG13	1:A:78:VAL:CG2	2 29	0.62	
$2 \cdot B \cdot 48 \cdot ILE \cdot HD13$	$2 \cdot B \cdot 81 [A] \cdot MET \cdot CE$	2.29	0.61	
2:B:212:LYS:HZ2	2:B:212:LYS:HB2	1.64	0.61	
$2 \cdot B \cdot 52 \cdot L E U \cdot H D 12$	$2 \cdot B \cdot 53 \cdot PBO \cdot HD2$	1.83	0.61	
1:A:151:ASP:OD2	1:A:189:HIS:HB3	2.00	0.60	
2:B:68:ALA:HB1	2:B:81[A]:MET:HE2	1.83	0.60	
2:B:51:ILE:HG13	2:B:58:THB:CG2	2.26	0.60	
1:A:61:ARG:NH1	1:A:82:ASP:CG	2.54	0.59	
2:B:138:MET:HB3	2:B:185:THR:CG2	2.33	0.59	
1:A:188[B]:ARG:NH1	1:A:188[B]:ARG:NE	2.37	0.59	
1:A:47:LEU:O	1:A:48:ILE:HD13	2.02	0.59	
2:B:141:LEU:HD21	2:B:191[B]:ARG:HG3	1.84	0.59	
2:B:4:LEU:O	2:B:107:GLY:HA2	2.03	0.58	

![](_page_9_Picture_6.jpeg)

1	MI D	
Т	MLD	

Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:A:94:TRP:HB3	2:B:59:TYR:CZ	2.37	0.58
I:A:24[B]:ARG:NE	I:A:24[B]:ARG:CD	2.66	0.58
2:B:173:LEU:HD12	2:B:177:LEU:O	2.03	0.58
2:B:48:ILE:HD13	2:B:81[A]:MET:HE3	1.85	0.58
2:B:47:TRP:CH2	2:B:59:TYR:CD2	2.92	0.57
1:A:19:VAL:HG23	1:A:21:LEU:HD12	1.87	0.57
2:B:191[B]:ARG:CD	2:B:191[B]:ARG:HB3	2.32	0.57
1:A:136:LEU:HD21	1:A:196:ALA:HB2	1.87	0.56
1:A:94:TRP:HB3	2:B:59:TYR:CE2	2.41	0.56
1:A:61:ARG:NH1	1:A:82:ASP:OD2	2.33	0.56
1:A:8:PRO:O	1:A:102:THR:HG23	2.06	0.56
2:B:67:LYS:NZ	2:B:90:ASP:OD2	2.38	0.56
2:B:187:PRO:HG2	2:B:190:PRO:CG	2.35	0.55
2:B:47:TRP:CH2	2:B:59:TYR:HD2	2.23	0.55
1:A:33:LEU:HD13	1:A:71:PHE:CD2	2.43	0.54
1:A:108:ARG:HG3	1:A:171:SER:HB2	1.90	0.54
2:B:212:LYS:HZ3	2:B:212:LYS:HB2	1.71	0.54
1:A:182:THR:OG1	1:A:185:GLU:HB2	2.08	0.53
2:B:129:PRO:HD3	2:B:141:LEU:HD12	1.91	0.53
2:B:3:GLN:HA	2:B:3:GLN:NE2	2.24	0.52
1:A:147:LYS:NZ	1:A:147:LYS:HB2	2.20	0.52
2:B:48:ILE:CG2	2:B:81[A]:MET:HE3	2.38	0.52
1:A:66:GLY:O	1:A:67:SER:HB2	2.09	0.52
2:B:33:TRP:O	2:B:99:GLY:N	2.36	0.52
2:B:122:PRO:HB3	2:B:148:TYR:HB3	1.93	0.51
2:B:67:LYS:HE2	2:B:84:SER:O	2.10	0.51
1:A:17:ASP:O	1:A:78:VAL:N	2.33	0.51
1:A:6:GLN:HA	1:A:22:SER:O	2.11	0.51
1:A:19:VAL:CG1	1:A:78:VAL:HG21	2.41	0.50
2:B:199:ASN:HA	2:B:209:VAL:O	2.11	0.50
2:B:2:VAL:HG13	2:B:27:TYR:CD1	2.46	0.50
2:B:29:PHE:O	2:B:53:PRO:HG2	2.12	0.50
1:A:24[A]:ARG:HH21	1:A:69:THR:HB	1.77	0.50
2:B:141:LEU:HD11	2:B:191[B]:ARG:HD2	1.92	0.50
2:B:91:SER:HA	2:B:112:LEU:O	2.12	0.50
1:A:2:ILE:HD13	1:A:29:ILE:CG2	2.41	0.49
1:A:34:HIS:ND1	2:B:102:ASN:HB3	2.27	0.49
2:B:137:SER:O	2:B:188:SER:OG	2.19	0.49
2:B:47:TRP:CZ3	2:B:59:TYR:HE2	2.30	0.49
1:A:192:TYR:O	1:A:208:SER:CB	2.61	0.49
2:B:67:LYS:HG3	2:B:67:LYS:O	2.12	0.49

![](_page_10_Picture_6.jpeg)

1MLB	

	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:B:51:ILE:HD13	2:B:72:ALA:HB2	1.94	0.48
2:B:118:SER:O	2:B:119:THR:C	2.50	0.48
2:B:32:TYR:N	2:B:32:TYR:CD1	2.82	0.48
1:A:23:CYS:HB2	1:A:35:TRP:CH2	2.49	0.47
1:A:19:VAL:CG2	1:A:21:LEU:HD11	2.45	0.47
2:B:47:TRP:HZ3	2:B:59:TYR:HE2	1.64	0.46
2:B:152:PRO:O	2:B:152:PRO:HG2	2.16	0.46
1:A:147:LYS:NZ	1:A:154:GLU:OE2	2.44	0.46
1:A:10:THR:HG22	1:A:11:LEU:N	2.31	0.46
1:A:195:GLU:HA	1:A:205:ILE:O	2.17	0.45
2:B:47:TRP:CZ3	2:B:59:TYR:CE2	3.04	0.45
1:A:110:ASP:HB3	1:A:200:THR:HG22	1.97	0.45
2:B:173:LEU:HA	2:B:173:LEU:HD12	1.90	0.45
2:B:190:PRO:HA	2:B:194:GLU:CG	2.43	0.45
2:B:60:TYR:CE1	2:B:70:PHE:CD2	3.05	0.45
1:A:163:TRP:O	2:B:170:PRO:HG2	2.17	0.45
2:B:25:THR:HG22	2:B:26:GLY:N	2.31	0.45
1:A:170:ASP:OD1	1:A:172:THR:OG1	2.21	0.45
2:B:189:SER:HB2	2:B:190:PRO:CD	2.39	0.45
2:B:212:LYS:HB3	2:B:212:LYS:HE2	1.66	0.45
2:B:128:ALA:HB1	2:B:129:PRO:HD2	1.98	0.44
1:A:125:LEU:CD1	1:A:130:ALA:HB2	2.48	0.44
2:B:141:LEU:CD1	2:B:191[B]:ARG:HD2	2.47	0.44
1:A:164:THR:HG23	2:B:169:PHE:CD1	2.53	0.44
2:B:31:THR:HG22	2:B:32:TYR:CE1	2.52	0.44
1:A:188[B]:ARG:HH21	1:A:188[B]:ARG:NE	2.12	0.44
2:B:38:LYS:HG3	2:B:94:TYR:CE1	2.53	0.44
1:A:145:ASN:HD22	1:A:145:ASN:HA	1.50	0.43
2:B:42:GLY:O	2:B:43:HIS:CG	2.71	0.43
1:A:159:VAL:HA	1:A:178:THR:O	2.18	0.43
1:A:169:LYS:HD3	1:A:169:LYS:HA	1.48	0.43
2:B:38:LYS:HB2	2:B:48:ILE:HD11	2.01	0.43
1:A:192:TYR:O	1:A:208:SER:HB3	2.19	0.43
2:B:3:GLN:O	2:B:4:LEU:HD23	2.18	0.43
2:B:27:TYR:CE2	2:B:98:ARG:HD2	2.54	0.43
1:A:114:THR:HG22	1:A:114:THR:O	2.18	0.42
2:B:194:GLU:OE1	2:B:194:GLU:HA	2.19	0.42
1:A:125:LEU:HA	1:A:125:LEU:HD12	1.76	0.42
2:B:191[A]:ARG:HH11	2:B:215:PRO:HD3	1.85	0.42
2:B:155:VAL:HG21	2:B:180:LEU:HD21	2.02	0.42
1:A:67:SER:HA	1:A:71:PHE:HE1	1.84	0.42

![](_page_11_Picture_6.jpeg)

Atom 1	Atom 2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
1:A:13:VAL:HG21	1:A:19:VAL:HG11	2.02	0.42
1:A:135:PHE:CE2	2:B:183:SER:HB3	2.54	0.42
2:B:29:PHE:HB3	2:B:77:ASN:ND2	2.35	0.42
2:B:60:TYR:CE1	2:B:70:PHE:CE2	3.07	0.42
2:B:10:GLU:HG3	2:B:18:VAL:HG21	2.01	0.41
2:B:187:PRO:HG2	2:B:190:PRO:CD	2.49	0.41
2:B:154:THR:O	2:B:200:VAL:HA	2.20	0.41
2:B:191[A]:ARG:NH1	2:B:215:PRO:HG3	2.35	0.41
2:B:128:ALA:HB2	2:B:213:ILE:HG22	2.01	0.41
1:A:161:ASN:ND2	1:A:177:SER:OG	2.53	0.41
1:A:34:HIS:CG	2:B:102:ASN:HB3	2.56	0.41
2:B:25:THR:CG2	2:B:26:GLY:N	2.83	0.41
1:A:13:VAL:HG11	1:A:78:VAL:HG21	2.03	0.41
2:B:153:VAL:HG12	2:B:202:HIS:CD2	2.55	0.41
2:B:192:PRO:HB3	2:B:215:PRO:HG3	2.03	0.41
1:A:34:HIS:CD2	1:A:34:HIS:N	2.88	0.40
2:B:146:LYS:HE2	2:B:174:GLN:OE1	2.21	0.40
2:B:211:LYS:HD3	2:B:211:LYS:HA	1.81	0.40
1:A:2:ILE:HG12	1:A:27:GLN:CG	2.51	0.40
2:B:175:SER:OG	2:B:175:SER:O	2.38	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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	Per	cer	ntil	es
1	А	214/214~(100%)	201 (94%)	10~(5%)	3 (1%)	1	l1	6	
2	В	218/218~(100%)	201~(92%)	12~(6%)	5(2%)	(	6	2	
All	All	432/432~(100%)	402 (93%)	22~(5%)	8 (2%)	8	8	3	

All (8) Ramachandran outliers are listed below:

![](_page_12_Picture_12.jpeg)

Mol	Chain	Res	Type
1	А	67	SER
1	А	110	ASP
2	В	190	PRO
2	В	42	GLY
1	А	77	SER
2	В	100	ASP
2	В	65	LYS
2	В	41	PRO

#### 5.3.2 Protein sidechains (i)

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	Perce	$\mathbf{ntiles}$
1	А	196/194~(101%)	175~(89%)	21 (11%)	6	3
2	В	186/184~(101%)	159~(86%)	27 (14%)	3	1
All	All	382/378~(101%)	334 (87%)	48 (13%)	4	2

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

Mol	Chain	$\mathbf{Res}$	Type
1	А	4	LEU
1	А	7	SER
1	А	12	SER
1	А	19	VAL
1	А	22	SER
1	А	43	SER
1	А	46	LEU
1	А	49	LYS
1	А	67	SER
1	А	77	SER
1	А	93	SER
1	А	105	GLU
1	А	116	SER
1	А	143	ASP
1	A	147	LYS
1	A	153	SER

![](_page_13_Picture_11.jpeg)

Mol	Chain	Res	Type
1	А	157	ASN
1	А	191	SER
1	А	197	THR
1	А	202	THR
1	А	208	SER
2	В	3	GLN
2	В	4	LEU
2	В	17	SER
2	В	30	SER
2	В	51	ILE
2	В	57	SER
2	В	67	LYS
2	В	87	THR
2	В	116	SER
2	В	134	GLN
2	В	141	LEU
2	В	143	CYS
2	В	152	PRO
2	В	154	THR
2	В	161	SER
2	В	163	SER
2	В	174	GLN
2	В	180	LEU
2	В	182	SER
2	В	191[A]	ARG
2	В	191[B]	ARG
2	В	194	GLU
2	В	195	THR
2	В	205	SER
2	В	212	LYS
2	В	214	VAL
2	В	215	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	41	HIS
1	А	76	ASN
1	А	145	ASN
1	А	156	GLN
1	А	157	ASN
1	А	161	ASN

![](_page_14_Picture_8.jpeg)

Continued from previous page...

Mol	Chain	Res	Type
1	А	198	HIS
2	В	3	GLN
2	В	82	GLN
2	В	102	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 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.

![](_page_15_Picture_17.jpeg)

## 6 Fit of model and data (i)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

![](_page_16_Picture_14.jpeg)