



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:37 am BST

PDB ID : 4MXV  
Title : Structure of Lymphotoxin alpha bound to anti-LTa Fab  
Authors : Yin, J.P.; Hymowitz, S.G.  
Deposited on : 2013-09-26  
Resolution : 3.20 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](mailto: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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

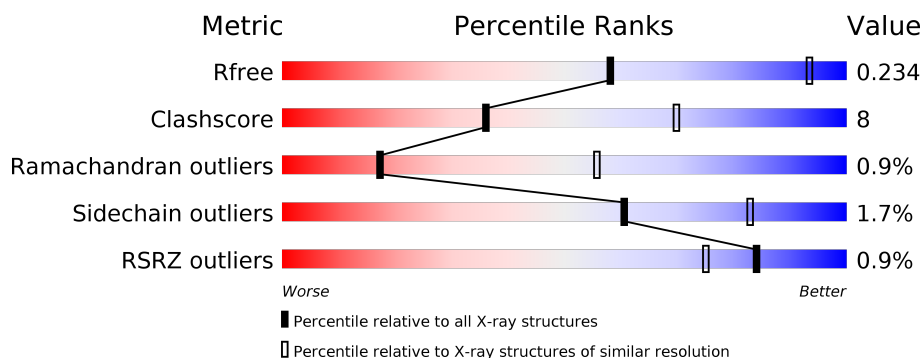
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	157	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>22%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	157	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>23%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	157	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>19%</div> <div>•</div> <div>16%</div> </div> </div>
2	E	211	<div> <div></div> <div>84%</div> <div>15%</div> </div>
2	L	211	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>19%</div> <div>•</div> </div> </div>
2	X	211	<div> <div></div> <div>83%</div> <div>16%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	213	 90% 9%
3	H	213	 3% 85% 15%
3	Y	213	 82% 17%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12881 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 Lymphotoxin-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1075	700	177	196	2			
1	B	137	Total	C	N	O	S	0	0	0
			1072	697	177	196	2			
1	D	132	Total	C	N	O	S	0	0	0
			1029	669	171	187	2			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ALA	-	EXPRESSION TAG	UNP P01374
A	16	ASP	-	EXPRESSION TAG	UNP P01374
A	17	LEU	-	EXPRESSION TAG	UNP P01374
A	18	GLY	-	EXPRESSION TAG	UNP P01374
A	19	SER	-	EXPRESSION TAG	UNP P01374
A	20	ASP	-	EXPRESSION TAG	UNP P01374
A	21	TYR	-	EXPRESSION TAG	UNP P01374
A	22	LYS	-	EXPRESSION TAG	UNP P01374
A	23	ASP	-	EXPRESSION TAG	UNP P01374
A	24	ASP	-	EXPRESSION TAG	UNP P01374
A	25	ASP	-	EXPRESSION TAG	UNP P01374
A	26	ASP	-	EXPRESSION TAG	UNP P01374
A	27	LYS	-	EXPRESSION TAG	UNP P01374
B	15	ALA	-	EXPRESSION TAG	UNP P01374
B	16	ASP	-	EXPRESSION TAG	UNP P01374
B	17	LEU	-	EXPRESSION TAG	UNP P01374
B	18	GLY	-	EXPRESSION TAG	UNP P01374
B	19	SER	-	EXPRESSION TAG	UNP P01374
B	20	ASP	-	EXPRESSION TAG	UNP P01374
B	21	TYR	-	EXPRESSION TAG	UNP P01374
B	22	LYS	-	EXPRESSION TAG	UNP P01374
B	23	ASP	-	EXPRESSION TAG	UNP P01374
B	24	ASP	-	EXPRESSION TAG	UNP P01374

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Chain	Residue	Modelled	Actual	Comment	Reference
B	25	ASP	-	EXPRESSION TAG	UNP P01374
B	26	ASP	-	EXPRESSION TAG	UNP P01374
B	27	LYS	-	EXPRESSION TAG	UNP P01374
D	15	ALA	-	EXPRESSION TAG	UNP P01374
D	16	ASP	-	EXPRESSION TAG	UNP P01374
D	17	LEU	-	EXPRESSION TAG	UNP P01374
D	18	GLY	-	EXPRESSION TAG	UNP P01374
D	19	SER	-	EXPRESSION TAG	UNP P01374
D	20	ASP	-	EXPRESSION TAG	UNP P01374
D	21	TYR	-	EXPRESSION TAG	UNP P01374
D	22	LYS	-	EXPRESSION TAG	UNP P01374
D	23	ASP	-	EXPRESSION TAG	UNP P01374
D	24	ASP	-	EXPRESSION TAG	UNP P01374
D	25	ASP	-	EXPRESSION TAG	UNP P01374
D	26	ASP	-	EXPRESSION TAG	UNP P01374
D	27	LYS	-	EXPRESSION TAG	UNP P01374

- Molecule 2 is a protein called anti-Lymphotoxin alpha antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	211	Total	C	N	O	S	0	0	0
			1622	1015	273	329	5			
2	L	211	Total	C	N	O	S	0	0	0
			1622	1015	273	329	5			
2	X	211	Total	C	N	O	S	0	0	0
			1622	1015	273	329	5			

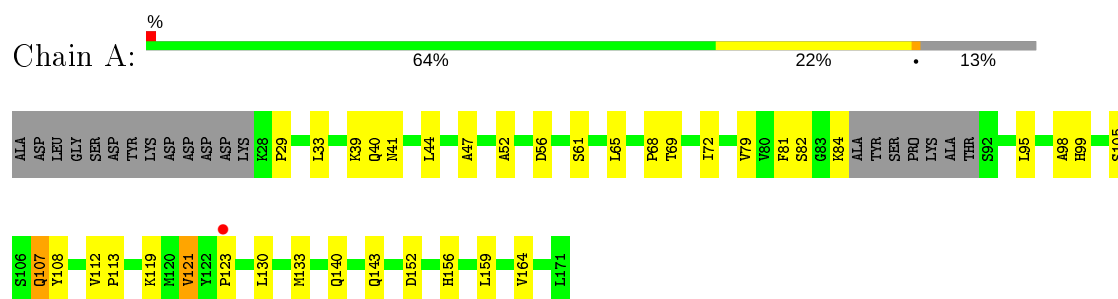
- Molecule 3 is a protein called anti-Lymphotoxin alpha antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	213	Total	C	N	O	S	0	0	0
			1613	1028	269	310	6			
3	H	213	Total	C	N	O	S	0	0	0
			1613	1028	269	310	6			
3	Y	213	Total	C	N	O	S	0	0	0
			1613	1028	269	310	6			

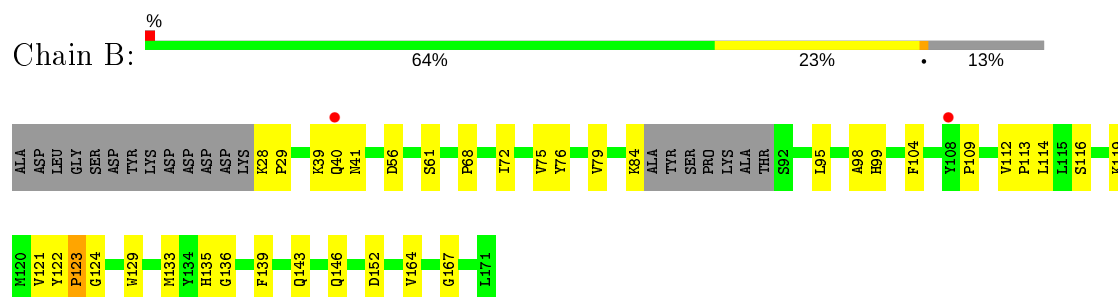
### 3 Residue-property plots [i](#)

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 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.

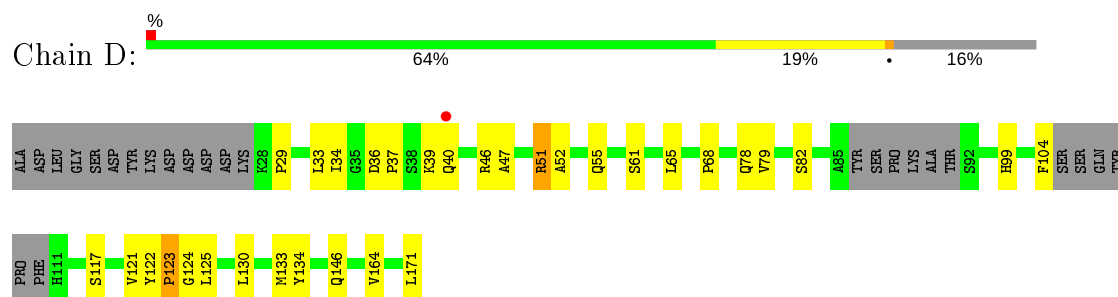
#### • Molecule 1: Lymphotoxin-alpha



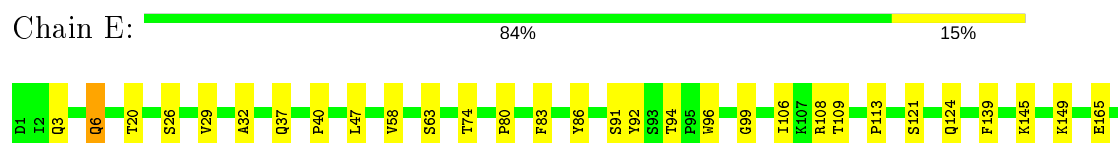
#### • Molecule 1: Lymphotoxin-alpha



#### • Molecule 1: Lymphotoxin-alpha

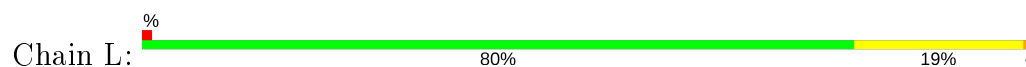


#### • Molecule 2: anti-Lymphotoxin alpha antibody light chain

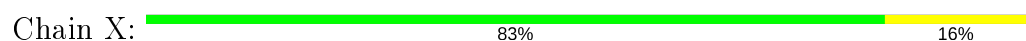




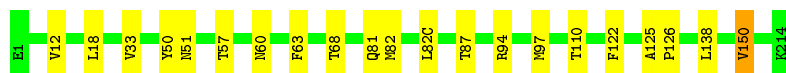
- Molecule 2: anti-Lymphotoxin alpha antibody light chain



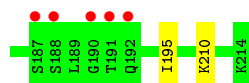
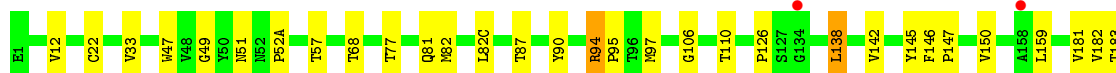
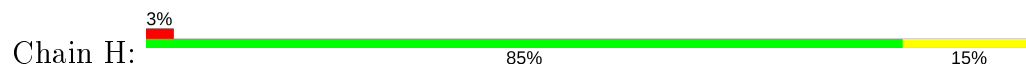
- Molecule 2: anti-Lymphotoxin alpha antibody light chain



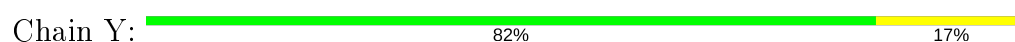
- Molecule 3: anti-Lymphotoxin alpha antibody heavy chain



- Molecule 3: anti-Lymphotoxin alpha antibody heavy chain



- Molecule 3: anti-Lymphotoxin alpha antibody heavy chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.85Å 209.85Å 130.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 3.20 29.80 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.80-3.20) 96.8 (29.80-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.177 , 0.235 0.177 , 0.234	Depositor DCC
$R_{free}$ test set	2796 reflections (5.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.1	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12881	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.46	0/1110	0.65	0/1512
1	B	0.45	0/1106	0.67	0/1505
1	D	0.50	0/1060	0.65	0/1442
2	E	0.45	0/1659	0.61	0/2255
2	L	0.42	0/1659	0.57	0/2255
2	X	0.48	0/1659	0.63	0/2255
3	F	0.43	0/1657	0.63	0/2261
3	H	0.39	0/1657	0.58	0/2261
3	Y	0.47	0/1657	0.66	1/2261 (0.0%)
All	All	0.45	0/13224	0.62	1/18007 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	178	LEU	CA-CB-CG	5.37	127.65	115.30

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	A	1075	0	1040	21	0
1	B	1072	0	1033	24	0
1	D	1029	0	1001	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1622	0	1573	23	0
2	L	1622	0	1573	35	0
2	X	1622	0	1573	27	0
3	F	1613	0	1576	15	0
3	H	1613	0	1576	27	0
3	Y	1613	0	1576	29	0
All	All	12881	0	12521	203	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 8.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:195:ILE:HG12	3:H:210:LYS:HG2	1.39	1.04
2:X:135:LEU:HD22	3:Y:181:VAL:HG11	1.49	0.94
3:H:159:LEU:HD21	3:H:182:VAL:HG21	1.54	0.86
3:H:145:TYR:CE1	3:H:150:VAL:HG23	2.12	0.84
3:Y:126:PRO:HG3	3:Y:138:LEU:HB3	1.62	0.80
2:L:181:LEU:HD11	2:L:186:TYR:HB2	1.65	0.79
1:B:122:TYR:HB3	1:B:123:PRO:HD2	1.62	0.78
2:X:156:SER:OG	2:X:157:GLY:N	2.19	0.75
1:D:122:TYR:HB3	1:D:123:PRO:HD2	1.69	0.74
3:H:195:ILE:CG1	3:H:210:LYS:HG2	2.19	0.72
2:L:83:PHE:HB3	2:L:106:ILE:HD12	1.72	0.72
1:B:68:PRO:HB2	3:F:97:MET:HG3	1.74	0.68
3:H:126:PRO:HG3	3:H:138:LEU:HB3	1.74	0.68
1:A:79:VAL:HA	1:A:164:VAL:HG22	1.76	0.68
2:L:135:LEU:HD22	3:H:181:VAL:HG11	1.75	0.68
1:D:33:LEU:HD11	1:D:65:LEU:HD13	1.76	0.67
1:D:29:PRO:HG3	3:Y:97:MET:HE1	1.77	0.66
2:L:6:GLN:O	2:L:100:GLN:NE2	2.29	0.66
3:Y:33:VAL:CG1	3:Y:50:TYR:HB2	2.27	0.65
1:B:61:SER:HB2	2:E:94:THR:HG21	1.80	0.64
1:A:68:PRO:HB2	3:H:97:MET:HG3	1.81	0.63
1:B:84:LYS:HG3	1:B:129:TRP:HE1	1.62	0.63
1:A:95:LEU:HB3	1:A:121:VAL:HG13	1.81	0.63
3:H:145:TYR:CE1	3:H:150:VAL:CG2	2.82	0.63
2:L:29:VAL:O	2:L:29:VAL:HG12	1.98	0.62
1:B:61:SER:HA	2:E:94:THR:OG1	2.01	0.61
1:D:117:SER:HB2	1:D:133:MET:HE3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:135:LEU:HD22	3:Y:181:VAL:CG1	2.27	0.59
1:D:34:ILE:CG1	1:D:52:ALA:HB2	2.32	0.59
2:L:149:LYS:HB2	2:L:193:ALA:HB3	1.83	0.59
1:A:61:SER:HB2	2:L:94:THR:HG21	1.85	0.58
3:Y:51:ASN:HD22	3:Y:57:THR:HG22	1.69	0.58
1:A:72:ILE:CD1	1:A:140:GLN:HG3	2.34	0.58
2:L:181:LEU:CD1	2:L:186:TYR:HB2	2.33	0.58
3:F:82:MET:HE2	3:F:82(C):LEU:HD21	1.86	0.57
1:A:98:ALA:HB3	1:A:152:ASP:HB2	1.86	0.57
2:E:40:PRO:HG2	2:E:165:GLU:HG3	1.86	0.57
2:L:40:PRO:HG2	2:L:165:GLU:HG3	1.86	0.57
2:X:28:ALA:C	2:X:29:VAL:HG23	2.25	0.57
2:X:6:GLN:NE2	2:X:86:TYR:O	2.38	0.57
1:D:78:GLN:HB2	1:D:134:TYR:HD2	1.70	0.57
2:E:29:VAL:HG12	2:E:29:VAL:O	2.04	0.57
2:X:108:ARG:HD2	2:X:140:TYR:CG	2.40	0.56
2:E:149:LYS:NZ	2:E:195:GLU:OE1	2.35	0.56
3:Y:60:ASN:HB3	3:Y:63:PHE:HD2	1.70	0.56
1:B:99:HIS:HB3	1:B:133:MET:HE1	1.87	0.56
1:D:104:PHE:HB3	1:D:146:GLN:HB2	1.86	0.56
3:Y:59:TYR:HE2	3:Y:69:ILE:HG13	1.70	0.56
2:X:135:LEU:CD2	3:Y:181:VAL:HG11	2.29	0.56
3:F:87:THR:HG23	3:F:110:THR:HA	1.87	0.56
2:L:6:GLN:NE2	2:L:86:TYR:O	2.35	0.56
2:X:29:VAL:HG12	2:X:29:VAL:O	2.06	0.55
3:F:33:VAL:CG1	3:F:50:TYR:HB2	2.37	0.54
2:E:3:GLN:H	2:E:26:SER:HB3	1.71	0.54
1:D:123:PRO:O	1:D:125:LEU:N	2.40	0.54
3:Y:59:TYR:CE2	3:Y:69:ILE:HG13	2.43	0.54
2:L:135:LEU:CD2	3:H:181:VAL:HG11	2.38	0.54
1:B:98:ALA:HB3	1:B:152:ASP:HB2	1.90	0.54
3:H:87:THR:HG23	3:H:110:THR:HA	1.89	0.53
1:B:95:LEU:HB3	1:B:121:VAL:HG13	1.90	0.53
3:H:12:VAL:HG11	3:H:82(C):LEU:HD12	1.90	0.53
3:H:51:ASN:HB2	3:H:57:THR:HG22	1.90	0.53
1:A:47:ALA:HA	1:A:52:ALA:HB1	1.90	0.53
3:H:145:TYR:CZ	3:H:150:VAL:CG2	2.92	0.53
1:D:99:HIS:HB3	1:D:133:MET:HE2	1.90	0.53
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.44	0.53
1:D:34:ILE:HG13	1:D:52:ALA:HB2	1.90	0.52
3:H:68:THR:HB	3:H:81:GLN:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:82:MET:HE2	3:Y:82(C):LEU:HD21	1.91	0.52
1:B:114:LEU:HB3	1:B:139:PHE:CZ	2.45	0.52
3:Y:87:THR:HG23	3:Y:110:THR:HA	1.90	0.52
1:B:76:TYR:CZ	1:B:167:GLY:HA3	2.45	0.52
2:L:28:ALA:C	2:L:29:VAL:HG23	2.30	0.51
2:X:37:GLN:HG3	2:X:86:TYR:CE2	2.45	0.51
1:B:122:TYR:HB3	1:B:123:PRO:CD	2.37	0.51
2:E:37:GLN:HG3	2:E:86:TYR:CE2	2.46	0.51
1:A:33:LEU:HD11	1:A:65:LEU:HD13	1.92	0.51
3:Y:33:VAL:HG12	3:Y:50:TYR:HB2	1.93	0.51
3:F:68:THR:HB	3:F:81:GLN:HB3	1.91	0.51
2:L:181:LEU:HD12	2:L:182:SER:O	2.11	0.50
3:Y:145:TYR:OH	3:Y:178:LEU:HD23	2.12	0.49
1:D:122:TYR:HB3	1:D:123:PRO:CD	2.40	0.49
3:Y:36:TRP:CD1	3:Y:69:ILE:HD13	2.47	0.49
2:X:92:TYR:HD2	2:X:93:SER:HG	1.59	0.49
2:L:80:PRO:HA	2:L:106:ILE:HD13	1.95	0.49
2:X:75:ILE:HG21	2:X:78:LEU:HD12	1.95	0.49
3:Y:121:VAL:O	3:Y:209:LYS:HE3	2.13	0.49
1:B:122:TYR:CB	1:B:123:PRO:HD2	2.40	0.48
2:X:31:SER:O	2:X:33:VAL:N	2.46	0.48
1:A:39:LYS:O	1:A:41:ASN:N	2.47	0.48
2:E:37:GLN:HB2	2:E:47:LEU:HD11	1.94	0.48
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.49	0.48
2:E:83:PHE:HB3	2:E:106:ILE:HD12	1.95	0.48
2:L:29:VAL:O	2:L:29:VAL:CG1	2.62	0.47
2:X:91:SER:HA	2:X:96:TRP:CD1	2.49	0.47
1:B:39:LYS:O	1:B:41:ASN:N	2.44	0.47
1:B:75:VAL:O	1:B:136:GLY:HA2	2.15	0.47
3:F:12:VAL:HG11	3:F:18:LEU:HB2	1.97	0.47
1:D:34:ILE:HG12	1:D:52:ALA:HB2	1.96	0.47
2:L:137:ASN:ND2	3:H:183:THR:HG21	2.29	0.47
3:F:60:ASN:HB3	3:F:63:PHE:HD2	1.80	0.47
1:D:33:LEU:O	1:D:34:ILE:HD13	2.15	0.47
2:E:91:SER:HA	2:E:96:TRP:CD1	2.50	0.46
3:H:82:MET:HE2	3:H:82(C):LEU:HD21	1.97	0.46
1:B:39:LYS:C	1:B:41:ASN:H	2.19	0.46
3:H:145:TYR:CZ	3:H:150:VAL:HG23	2.50	0.46
2:E:145:LYS:HB3	2:E:197:THR:HB	1.98	0.46
3:F:51:ASN:HB2	3:F:57:THR:HG22	1.98	0.46
2:X:28:ALA:C	2:X:29:VAL:CG2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLN:HB3	1:A:108:TYR:H	1.51	0.46
1:A:61:SER:HB2	2:L:94:THR:CG2	2.46	0.46
1:D:79:VAL:HA	1:D:164:VAL:HG22	1.96	0.46
2:L:161:GLU:HG2	2:L:175:LEU:HD21	1.98	0.46
3:Y:33:VAL:HG11	3:Y:50:TYR:CD2	2.51	0.46
1:A:119:LYS:HD2	1:A:119:LYS:HA	1.81	0.46
2:E:80:PRO:HA	2:E:106:ILE:HD13	1.98	0.46
2:X:3:GLN:H	2:X:26:SER:HB3	1.80	0.46
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.73	0.45
2:E:47:LEU:HA	2:E:58:VAL:HG21	1.97	0.45
3:H:142:VAL:HG11	3:H:150:VAL:HG11	1.97	0.45
3:Y:209:LYS:HB2	3:Y:209:LYS:HE2	1.76	0.45
3:Y:36:TRP:HD1	3:Y:69:ILE:HD13	1.81	0.45
2:L:181:LEU:HD11	2:L:186:TYR:CB	2.41	0.45
1:D:82:SER:HB3	1:D:130:LEU:HD12	1.98	0.45
2:E:63:SER:OG	2:E:74:THR:HB	2.17	0.45
2:E:32:ALA:HB3	2:E:92:TYR:HB2	1.99	0.45
3:F:150:VAL:HG12	3:F:150:VAL:O	2.14	0.45
2:L:24:ARG:NE	2:L:70:ASP:OD2	2.50	0.45
1:B:29:PRO:HA	1:B:56:ASP:HB3	1.99	0.45
1:B:61:SER:CB	2:E:94:THR:HG21	2.45	0.45
3:F:33:VAL:HG11	3:F:50:TYR:CD2	2.52	0.45
2:L:140:TYR:CG	2:L:141:PRO:HA	2.51	0.45
1:D:61:SER:HB2	2:X:94:THR:OG1	2.17	0.45
1:A:69:THR:HA	1:A:143:GLN:HB2	1.99	0.44
2:X:35:TRP:CZ3	2:X:88:CYS:HB3	2.52	0.44
3:Y:39:GLN:HB2	3:Y:45:LEU:HD23	1.97	0.44
3:Y:185:PRO:O	3:Y:188:SER:OG	2.30	0.44
1:A:159:LEU:HA	1:A:159:LEU:HD23	1.77	0.44
2:L:149:LYS:NZ	2:L:195:GLU:OE1	2.35	0.44
3:Y:180:SER:C	3:Y:181:VAL:HG23	2.38	0.44
2:L:59:PRO:HG2	2:L:62:PHE:CD2	2.53	0.44
2:L:191:VAL:HG22	2:L:210:ASN:OD1	2.17	0.44
3:Y:125:ALA:HA	3:Y:126:PRO:HD3	1.78	0.44
3:F:33:VAL:HG12	3:F:50:TYR:HB2	2.00	0.44
3:H:22:CYS:O	3:H:77:THR:HA	2.18	0.44
2:X:59:PRO:HG2	2:X:62:PHE:CE2	2.53	0.44
2:L:137:ASN:HD21	3:H:183:THR:HG21	1.82	0.43
2:X:33:VAL:HG21	2:X:71:PHE:CE1	2.53	0.43
2:L:32:ALA:HB3	2:L:92:TYR:HB2	1.99	0.43
2:X:93:SER:O	2:X:96:TRP:CD1	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:PRO:O	1:B:143:GLN:HG3	2.18	0.43
3:H:90:TYR:O	3:H:106:GLY:HA2	2.19	0.43
2:L:181:LEU:HD12	2:L:181:LEU:C	2.38	0.43
1:B:112:VAL:HA	1:B:113:PRO:HD3	1.86	0.43
3:H:82:MET:HE2	3:H:82:MET:HB3	1.96	0.43
3:F:125:ALA:HA	3:F:126:PRO:HD3	1.81	0.43
1:B:79:VAL:HA	1:B:164:VAL:HG22	2.00	0.43
2:E:124:GLN:HG3	3:F:122:PHE:CE2	2.54	0.43
2:L:3:GLN:H	2:L:26:SER:HB3	1.83	0.43
1:B:28:LYS:HD2	1:D:171:LEU:OXT	2.19	0.42
3:H:94:ARG:HA	3:H:95:PRO:HD3	1.92	0.42
3:Y:200:HIS:CD2	3:Y:202:PRO:HD2	2.54	0.42
3:H:145:TYR:CZ	3:H:150:VAL:HG21	2.55	0.42
3:Y:52:ASN:HA	3:Y:52(A):PRO:HD3	1.82	0.42
3:F:12:VAL:HG21	3:F:82(C):LEU:HD13	2.00	0.42
1:D:36:ASP:HA	1:D:37:PRO:HD3	1.89	0.42
2:E:108:ARG:HG2	2:E:109:THR:N	2.35	0.42
1:A:72:ILE:HD11	1:D:55:GLN:NE2	2.34	0.41
2:X:29:VAL:HG13	2:X:92:TYR:CB	2.49	0.41
1:D:33:LEU:CD2	1:D:47:ALA:HB2	2.51	0.41
2:L:107:LYS:HE3	2:L:107:LYS:HB2	1.78	0.41
2:X:108:ARG:HH11	2:X:108:ARG:HD3	1.75	0.41
2:X:63:SER:O	2:X:73:LEU:HD12	2.20	0.41
1:A:112:VAL:HA	1:A:113:PRO:HD3	1.83	0.41
1:A:29:PRO:HA	1:A:56:ASP:HB3	2.02	0.41
1:A:81:PHE:HA	1:A:156:HIS:O	2.20	0.41
2:L:35:TRP:CD2	2:L:73:LEU:HB2	2.56	0.41
2:E:113:PRO:HB3	2:E:139:PHE:HB3	2.02	0.41
1:A:99:HIS:HB3	1:A:133:MET:HE1	2.02	0.41
1:B:119:LYS:HA	1:B:119:LYS:HD2	1.90	0.41
2:E:29:VAL:HG13	2:E:92:TYR:HB3	2.02	0.41
2:L:28:ALA:C	2:L:29:VAL:CG2	2.89	0.41
1:B:104:PHE:HB3	1:B:146:GLN:HB2	2.02	0.41
2:L:79:GLN:HB3	2:L:80:PRO:HD2	2.03	0.41
3:F:126:PRO:HG3	3:F:138:LEU:HB3	2.03	0.41
3:H:51:ASN:O	3:H:52(A):PRO:HD3	2.20	0.41
2:L:27:GLN:O	2:L:29:VAL:HG23	2.20	0.41
3:Y:67:PHE:N	3:Y:67:PHE:CD1	2.86	0.41
1:D:68:PRO:HB2	3:Y:97:MET:HE3	2.02	0.41
3:Y:66:ARG:HH11	3:Y:66:ARG:HD2	1.69	0.41
1:A:82:SER:HB3	1:A:130:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:LYS:HA	1:D:39:LYS:HD3	1.93	0.41
2:X:1:ASP:HB3	2:X:2:ILE:H	1.74	0.41
1:B:99:HIS:HB3	1:B:133:MET:CE	2.49	0.40
2:L:142:ARG:NH2	2:L:163:VAL:HB	2.36	0.40
2:E:121:SER:OG	2:E:124:GLN:HB2	2.21	0.40
2:X:59:PRO:HG2	2:X:62:PHE:CD2	2.57	0.40
2:E:29:VAL:HG13	2:E:92:TYR:CB	2.51	0.40
2:X:121:SER:OG	3:Y:122:PHE:HB3	2.22	0.40
1:D:51:ARG:HA	1:D:51:ARG:HD3	1.79	0.40
2:E:6:GLN:OE1	2:E:99:GLY:HA3	2.22	0.40
3:H:146:PHE:HA	3:H:147:PRO:HA	1.85	0.40
2:X:183:LYS:O	2:X:187:GLU:HG2	2.21	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	
1	A	133/157 (85%)	123 (92%)	6 (4%)	4 (3%)	4	28
1	B	133/157 (85%)	121 (91%)	8 (6%)	4 (3%)	4	28
1	D	126/157 (80%)	116 (92%)	6 (5%)	4 (3%)	4	26
2	E	209/211 (99%)	196 (94%)	13 (6%)	0	100	100
2	L	209/211 (99%)	196 (94%)	12 (6%)	1 (0%)	29	67
2	X	209/211 (99%)	197 (94%)	11 (5%)	1 (0%)	29	67
3	F	209/213 (98%)	197 (94%)	12 (6%)	0	100	100
3	H	209/213 (98%)	197 (94%)	12 (6%)	0	100	100
3	Y	209/213 (98%)	198 (95%)	11 (5%)	0	100	100
All	All	1646/1743 (94%)	1541 (94%)	91 (6%)	14 (1%)	17	56



All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	B	109	PRO
1	B	123	PRO
1	D	123	PRO
1	A	40	GLN
1	A	107	GLN
1	B	124	GLY
1	D	121	VAL
1	D	124	GLY
1	A	123	PRO
1	B	40	GLN
1	D	40	GLN
2	X	29	VAL
2	L	29	VAL

### 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	A	119/135 (88%)	117 (98%)	2 (2%)	60	83
1	B	118/135 (87%)	115 (98%)	3 (2%)	47	77
1	D	113/135 (84%)	111 (98%)	2 (2%)	59	82
2	E	185/185 (100%)	182 (98%)	3 (2%)	62	84
2	L	185/185 (100%)	183 (99%)	2 (1%)	73	88
2	X	185/185 (100%)	182 (98%)	3 (2%)	62	84
3	F	179/179 (100%)	177 (99%)	2 (1%)	73	88
3	H	179/179 (100%)	176 (98%)	3 (2%)	60	83
3	Y	179/179 (100%)	175 (98%)	4 (2%)	52	79
All	All	1442/1497 (96%)	1418 (98%)	24 (2%)	60	83

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	LYS
1	A	105	SER
1	B	72	ILE
1	B	116	SER
1	B	135	HIS
1	D	46	ARG
1	D	51	ARG
2	E	6	GLN
2	E	20	THR
2	E	187	GLU
3	F	94	ARG
3	F	150	VAL
2	L	26	SER
2	L	155	GLN
3	H	33	VAL
3	H	94	ARG
3	H	138	LEU
2	X	50	SER
2	X	108	ARG
2	X	211	ARG
3	Y	62	LYS
3	Y	94	ARG
3	Y	148	GLU
3	Y	197	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	135	HIS
3	F	82(A)	ASN
2	L	137	ASN
3	Y	171	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	1
3	Y	1
3	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	127:SER	C	134:GLY	N	12.37
1	F	127:SER	C	134:GLY	N	11.97
1	H	127:SER	C	134:GLY	N	11.96

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	137/157 (87%)	-0.31	1 (0%) 87 81	17, 36, 88, 127	0
1	B	137/157 (87%)	-0.24	2 (1%) 73 61	19, 43, 96, 137	0
1	D	132/157 (84%)	-0.27	1 (0%) 86 78	15, 36, 92, 115	0
2	E	211/211 (100%)	-0.37	0 100 100	23, 48, 77, 105	0
2	L	211/211 (100%)	-0.18	3 (1%) 75 63	29, 59, 87, 101	0
2	X	211/211 (100%)	-0.45	1 (0%) 91 86	17, 36, 71, 86	0
3	F	213/213 (100%)	-0.29	0 100 100	18, 42, 68, 100	0
3	H	213/213 (100%)	0.04	7 (3%) 46 30	28, 65, 108, 138	0
3	Y	213/213 (100%)	-0.43	0 100 100	12, 33, 71, 96	0
All	All	1678/1743 (96%)	-0.28	15 (0%) 84 75	12, 45, 87, 138	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	191	THR	4.0
3	H	187	SER	2.9
3	H	134	GLY	2.9
2	L	210	ASN	2.8
1	D	40	GLN	2.3
3	H	192	GLN	2.3
3	H	188	SER	2.3
1	B	40	GLN	2.2
2	L	202	SER	2.2
2	X	184	ALA	2.2
3	H	158	ALA	2.2
3	H	190	GLY	2.1
2	L	1	ASP	2.1
1	B	108	TYR	2.1
1	A	123	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.