



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2017 – 02:13 PM EST

PDB ID : 1KD7  
Title : Crystal structure of an extracellular domain fragment of human BAFF  
Authors : Karpusas, M.; Cachero, T.G.; Qian, F.; Boriack-Sjodin, A.; Mullen, C.;  
Strauch, K.; Hsu, Y.-M.; Kalled, S.L.  
Deposited on : 2001-11-12  
Resolution : 2.80 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

<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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442



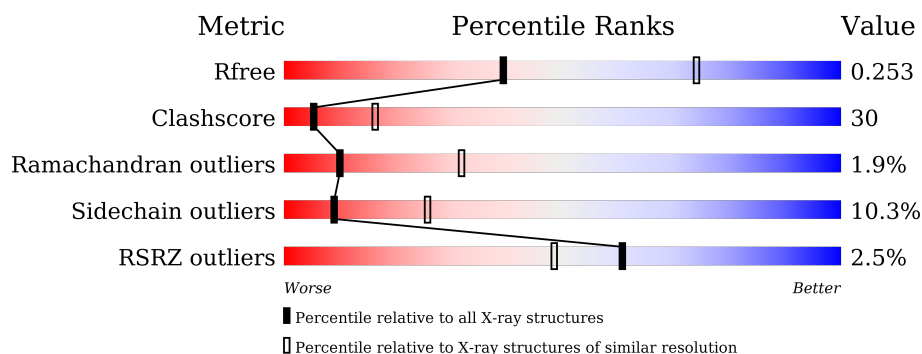
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	164	<div> <div>2%</div> <div> <div>45%</div> <div>39%</div> <div>• • 12%</div> </div> </div>
1	B	164	<div> <div>44%</div> <div>40%</div> <div>• • 12%</div> </div>
1	C	164	<div> <div>3%</div> <div> <div>42%</div> <div>40%</div> <div>• • 12%</div> </div> </div>
1	K	164	<div> <div>0%</div> <div> <div>41%</div> <div>42%</div> <div>• • 12%</div> </div> </div>
1	L	164	<div> <div>2%</div> <div> <div>46%</div> <div>37%</div> <div>• • 12%</div> </div> </div>
1	M	164	<div> <div>5%</div> <div> <div>43%</div> <div>41%</div> <div>• • 12%</div> </div> </div>



## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6858 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 TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	B	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	C	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	K	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	L	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	M	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLN	-	SEE REMARK 999	UNP Q9Y275
A	124	LYS	-	SEE REMARK 999	UNP Q9Y275
A	125	LEU	-	SEE REMARK 999	UNP Q9Y275
A	126	ILE	-	SEE REMARK 999	UNP Q9Y275
A	127	SER	-	SEE REMARK 999	UNP Q9Y275
A	128	GLU	-	SEE REMARK 999	UNP Q9Y275
A	129	GLU	-	SEE REMARK 999	UNP Q9Y275
A	130	ASP	-	SEE REMARK 999	UNP Q9Y275
A	131	LEU	-	SEE REMARK 999	UNP Q9Y275
A	132	ASN	-	SEE REMARK 999	UNP Q9Y275
A	133	LYS	-	SEE REMARK 999	UNP Q9Y275
A	134	GLU	-	SEE REMARK 999	UNP Q9Y275
A	135	LEU	-	SEE REMARK 999	UNP Q9Y275
B	123	GLN	-	SEE REMARK 999	UNP Q9Y275
B	124	LYS	-	SEE REMARK 999	UNP Q9Y275
B	125	LEU	-	SEE REMARK 999	UNP Q9Y275

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	126	ILE	-	SEE REMARK 999	UNP Q9Y275
B	127	SER	-	SEE REMARK 999	UNP Q9Y275
B	128	GLU	-	SEE REMARK 999	UNP Q9Y275
B	129	GLU	-	SEE REMARK 999	UNP Q9Y275
B	130	ASP	-	SEE REMARK 999	UNP Q9Y275
B	131	LEU	-	SEE REMARK 999	UNP Q9Y275
B	132	ASN	-	SEE REMARK 999	UNP Q9Y275
B	133	LYS	-	SEE REMARK 999	UNP Q9Y275
B	134	GLU	-	SEE REMARK 999	UNP Q9Y275
B	135	LEU	-	SEE REMARK 999	UNP Q9Y275
C	123	GLN	-	SEE REMARK 999	UNP Q9Y275
C	124	LYS	-	SEE REMARK 999	UNP Q9Y275
C	125	LEU	-	SEE REMARK 999	UNP Q9Y275
C	126	ILE	-	SEE REMARK 999	UNP Q9Y275
C	127	SER	-	SEE REMARK 999	UNP Q9Y275
C	128	GLU	-	SEE REMARK 999	UNP Q9Y275
C	129	GLU	-	SEE REMARK 999	UNP Q9Y275
C	130	ASP	-	SEE REMARK 999	UNP Q9Y275
C	131	LEU	-	SEE REMARK 999	UNP Q9Y275
C	132	ASN	-	SEE REMARK 999	UNP Q9Y275
C	133	LYS	-	SEE REMARK 999	UNP Q9Y275
C	134	GLU	-	SEE REMARK 999	UNP Q9Y275
C	135	LEU	-	SEE REMARK 999	UNP Q9Y275
K	123	GLN	-	SEE REMARK 999	UNP Q9Y275
K	124	LYS	-	SEE REMARK 999	UNP Q9Y275
K	125	LEU	-	SEE REMARK 999	UNP Q9Y275
K	126	ILE	-	SEE REMARK 999	UNP Q9Y275
K	127	SER	-	SEE REMARK 999	UNP Q9Y275
K	128	GLU	-	SEE REMARK 999	UNP Q9Y275
K	129	GLU	-	SEE REMARK 999	UNP Q9Y275
K	130	ASP	-	SEE REMARK 999	UNP Q9Y275
K	131	LEU	-	SEE REMARK 999	UNP Q9Y275
K	132	ASN	-	SEE REMARK 999	UNP Q9Y275
K	133	LYS	-	SEE REMARK 999	UNP Q9Y275
K	134	GLU	-	SEE REMARK 999	UNP Q9Y275
K	135	LEU	-	SEE REMARK 999	UNP Q9Y275
L	123	GLN	-	SEE REMARK 999	UNP Q9Y275
L	124	LYS	-	SEE REMARK 999	UNP Q9Y275
L	125	LEU	-	SEE REMARK 999	UNP Q9Y275
L	126	ILE	-	SEE REMARK 999	UNP Q9Y275
L	127	SER	-	SEE REMARK 999	UNP Q9Y275
L	128	GLU	-	SEE REMARK 999	UNP Q9Y275

*Continued on next page...*



*Continued from previous page...*

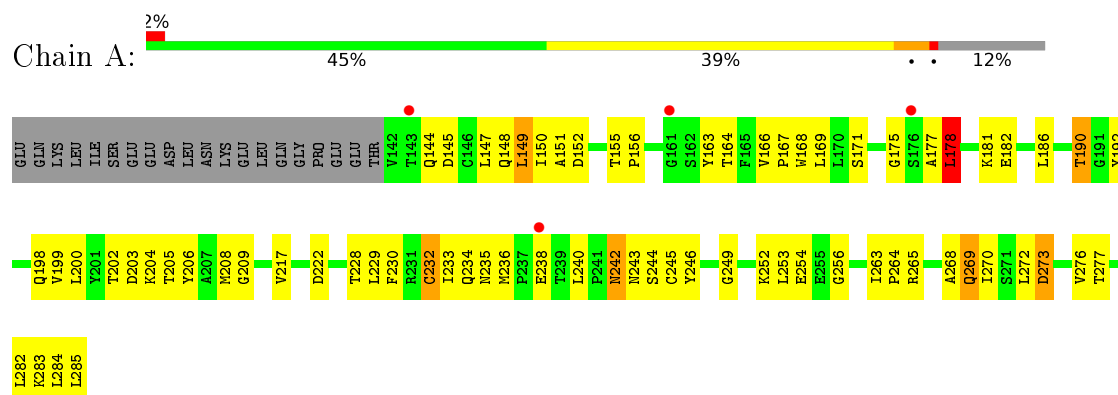
Chain	Residue	Modelled	Actual	Comment	Reference
L	129	GLU	-	SEE REMARK 999	UNP Q9Y275
L	130	ASP	-	SEE REMARK 999	UNP Q9Y275
L	131	LEU	-	SEE REMARK 999	UNP Q9Y275
L	132	ASN	-	SEE REMARK 999	UNP Q9Y275
L	133	LYS	-	SEE REMARK 999	UNP Q9Y275
L	134	GLU	-	SEE REMARK 999	UNP Q9Y275
L	135	LEU	-	SEE REMARK 999	UNP Q9Y275
M	123	GLN	-	SEE REMARK 999	UNP Q9Y275
M	124	LYS	-	SEE REMARK 999	UNP Q9Y275
M	125	LEU	-	SEE REMARK 999	UNP Q9Y275
M	126	ILE	-	SEE REMARK 999	UNP Q9Y275
M	127	SER	-	SEE REMARK 999	UNP Q9Y275
M	128	GLU	-	SEE REMARK 999	UNP Q9Y275
M	129	GLU	-	SEE REMARK 999	UNP Q9Y275
M	130	ASP	-	SEE REMARK 999	UNP Q9Y275
M	131	LEU	-	SEE REMARK 999	UNP Q9Y275
M	132	ASN	-	SEE REMARK 999	UNP Q9Y275
M	133	LYS	-	SEE REMARK 999	UNP Q9Y275
M	134	GLU	-	SEE REMARK 999	UNP Q9Y275
M	135	LEU	-	SEE REMARK 999	UNP Q9Y275



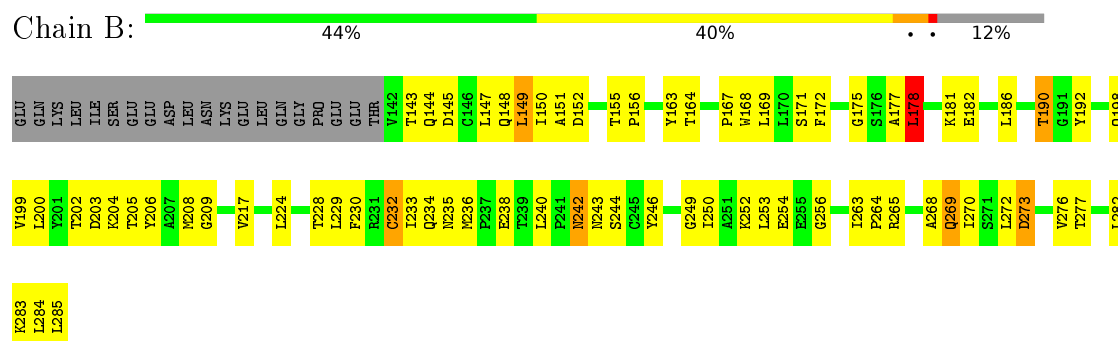
### 3 Residue-property plots [i](#)

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

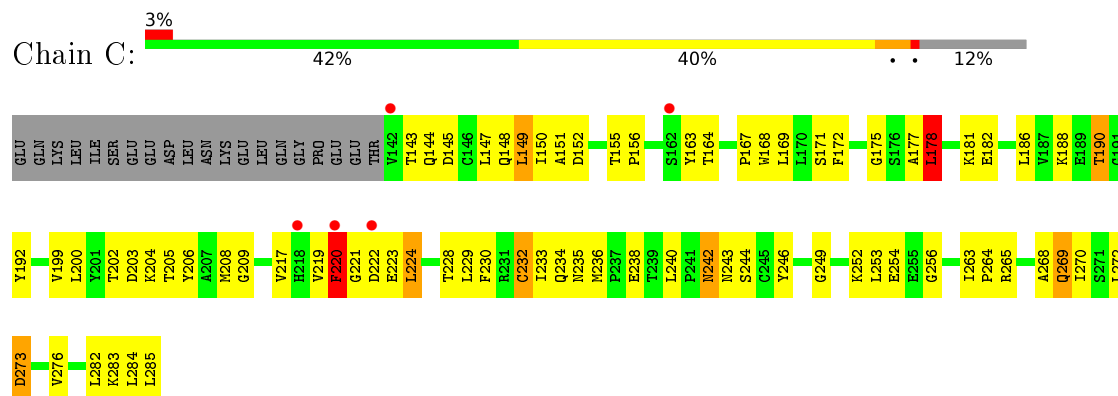
- Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B



- Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B

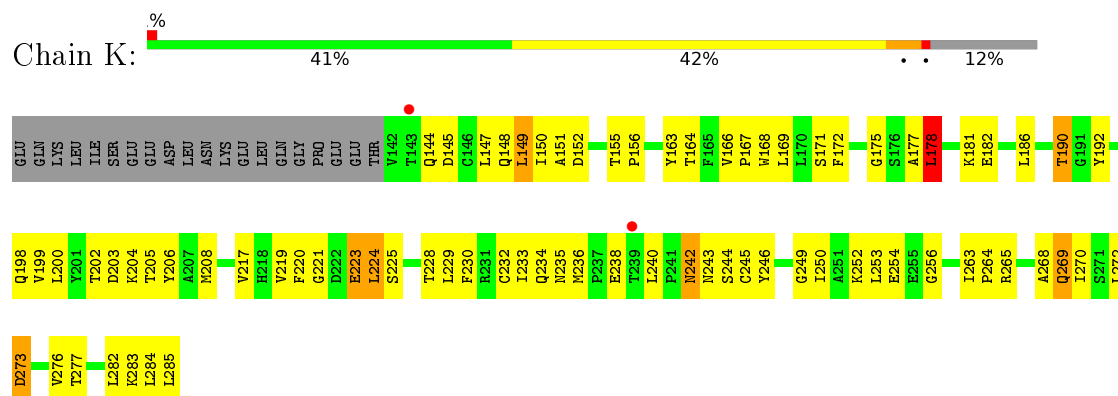


- Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B

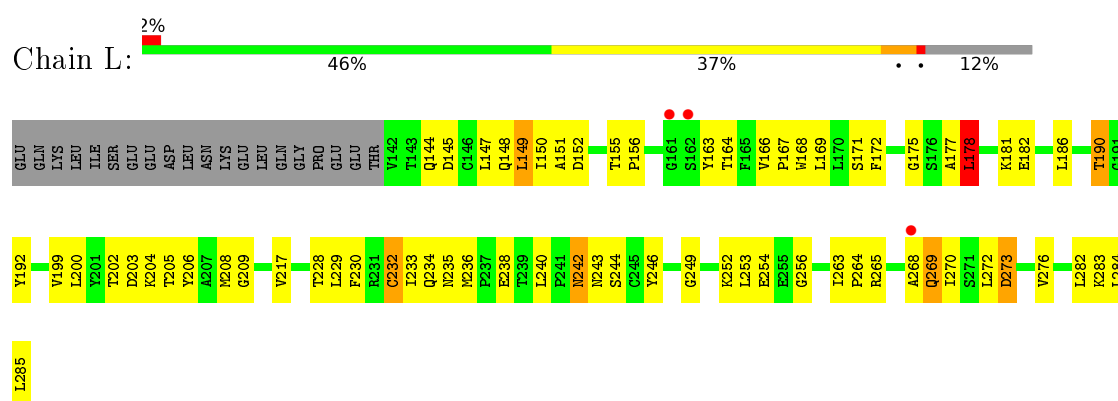




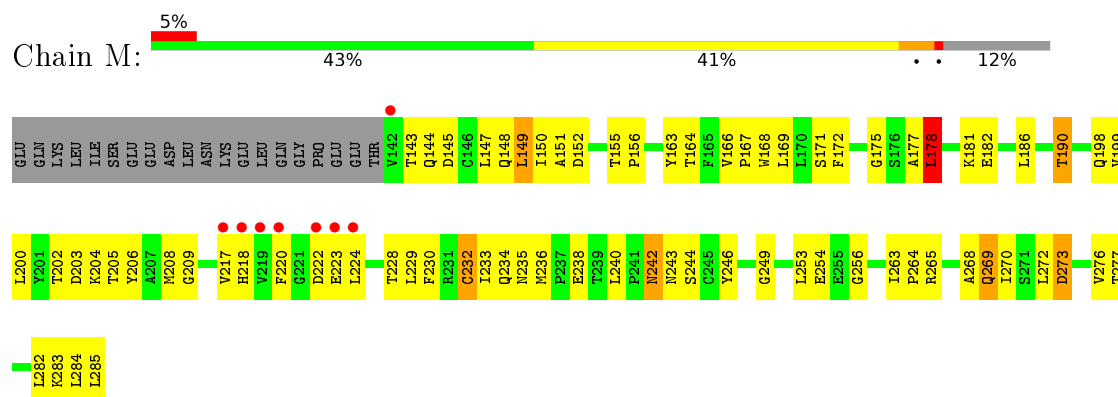
## ● Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B



## ● Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B



## ● Molecule 1: TUMOR NECROSIS FACTOR LIGAND SUPERFAMILY MEMBER 13B





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.72Å 121.72Å 160.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.80 26.45 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 97.3 (26.45-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.72 (at 2.89Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.217 , 0.250 0.221 , 0.253	Depositor DCC
$R_{free}$ test set	2876 reflections (9.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.5	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6858	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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

### 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	A	0.42	0/1165	0.67	0/1574
1	B	0.43	0/1165	0.66	0/1574
1	C	0.41	0/1165	0.66	0/1574
1	K	0.42	0/1165	0.67	0/1574
1	L	0.41	0/1165	0.67	0/1574
1	M	0.43	0/1165	0.67	0/1574
All	All	0.42	0/6990	0.67	0/9444

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	A	1143	0	1145	77	0
1	B	1143	0	1145	78	0
1	C	1143	0	1145	90	0
1	K	1143	0	1145	83	0
1	L	1143	0	1145	80	0
1	M	1143	0	1145	86	0
All	All	6858	0	6870	414	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 30.



All (414) 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)
1:A:164:THR:HG21	1:A:268:ALA:HB2	1.40	1.04
1:K:164:THR:HG21	1:K:268:ALA:HB2	1.42	1.02
1:L:242:ASN:H	1:M:235:ASN:HD21	1.09	1.01
1:L:243:ASN:HD21	1:M:235:ASN:H	1.05	1.01
1:B:164:THR:HG21	1:B:268:ALA:HB2	1.43	1.00
1:C:224:LEU:H	1:C:224:LEU:HD12	1.21	1.00
1:L:164:THR:HG21	1:L:268:ALA:HB2	1.42	1.00
1:C:164:THR:HG21	1:C:268:ALA:HB2	1.44	0.99
1:M:164:THR:HG21	1:M:268:ALA:HB2	1.41	0.99
1:K:235:ASN:HD21	1:M:242:ASN:H	1.00	0.97
1:B:242:ASN:H	1:C:235:ASN:HD21	1.09	0.94
1:A:235:ASN:HD21	1:C:242:ASN:H	0.98	0.92
1:A:243:ASN:HD21	1:B:235:ASN:H	1.17	0.92
1:K:235:ASN:H	1:M:243:ASN:HD21	1.14	0.92
1:A:242:ASN:H	1:B:235:ASN:HD21	1.18	0.89
1:B:243:ASN:HD21	1:C:235:ASN:H	1.16	0.88
1:K:243:ASN:HD21	1:L:235:ASN:H	1.17	0.88
1:K:235:ASN:H	1:M:243:ASN:ND2	1.72	0.88
1:A:235:ASN:H	1:C:243:ASN:HD21	1.22	0.87
1:L:243:ASN:ND2	1:M:235:ASN:H	1.71	0.87
1:K:242:ASN:H	1:L:235:ASN:HD21	1.18	0.87
1:A:164:THR:HG23	1:A:263:ILE:HB	1.59	0.84
1:M:181:LYS:HG3	1:M:182:GLU:HG3	1.61	0.83
1:B:181:LYS:HG3	1:B:182:GLU:HG3	1.61	0.83
1:K:181:LYS:HG3	1:K:182:GLU:HG3	1.62	0.82
1:L:164:THR:HG23	1:L:263:ILE:HB	1.59	0.82
1:A:181:LYS:HG3	1:A:182:GLU:HG3	1.61	0.82
1:B:164:THR:HG23	1:B:263:ILE:HB	1.59	0.82
1:C:164:THR:HG23	1:C:263:ILE:HB	1.60	0.82
1:M:164:THR:HG23	1:M:263:ILE:HB	1.62	0.81
1:C:181:LYS:HG3	1:C:182:GLU:HG3	1.62	0.81
1:C:190:THR:HB	1:C:254:GLU:HA	1.64	0.80
1:L:181:LYS:HG3	1:L:182:GLU:HG3	1.62	0.80
1:K:164:THR:HG23	1:K:263:ILE:HB	1.61	0.80
1:K:203:ASP:HB2	1:K:269:GLN:HB3	1.64	0.80
1:A:235:ASN:H	1:C:243:ASN:ND2	1.79	0.79
1:K:243:ASN:ND2	1:L:235:ASN:H	1.82	0.78
1:M:203:ASP:HB2	1:M:269:GLN:HB3	1.65	0.78
1:K:190:THR:HB	1:K:254:GLU:HA	1.65	0.78
1:A:190:THR:HB	1:A:254:GLU:HA	1.64	0.78

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ASN:ND2	1:C:235:ASN:H	1.81	0.78
1:A:203:ASP:HB2	1:A:269:GLN:HB3	1.66	0.77
1:L:190:THR:HB	1:L:254:GLU:HA	1.66	0.77
1:C:203:ASP:HB2	1:C:269:GLN:HB3	1.66	0.77
1:B:190:THR:HB	1:B:254:GLU:HA	1.66	0.77
1:M:190:THR:HB	1:M:254:GLU:HA	1.66	0.77
1:A:235:ASN:ND2	1:C:242:ASN:H	1.81	0.76
1:C:208:MET:O	1:C:233:ILE:HD12	1.86	0.76
1:L:203:ASP:HB2	1:L:269:GLN:HB3	1.66	0.76
1:L:203:ASP:OD2	1:L:205:THR:HG23	1.86	0.76
1:K:235:ASN:ND2	1:M:242:ASN:H	1.83	0.76
1:B:203:ASP:HB2	1:B:269:GLN:HB3	1.66	0.76
1:A:243:ASN:ND2	1:B:235:ASN:H	1.84	0.76
1:M:164:THR:CG2	1:M:268:ALA:HB2	2.16	0.75
1:M:208:MET:O	1:M:233:ILE:HD12	1.86	0.75
1:A:203:ASP:OD2	1:A:205:THR:HG23	1.88	0.74
1:K:203:ASP:OD2	1:K:205:THR:HG23	1.87	0.74
1:A:164:THR:CG2	1:A:268:ALA:HB2	2.17	0.74
1:C:203:ASP:OD2	1:C:205:THR:HG23	1.88	0.74
1:K:224:LEU:HD12	1:K:224:LEU:N	2.03	0.74
1:L:164:THR:CG2	1:L:268:ALA:HB2	2.18	0.73
1:B:208:MET:O	1:B:233:ILE:HD12	1.89	0.72
1:K:164:THR:CG2	1:K:268:ALA:HB2	2.18	0.72
1:L:208:MET:O	1:L:233:ILE:HD12	1.89	0.72
1:M:203:ASP:OD2	1:M:205:THR:HG23	1.91	0.71
1:A:208:MET:O	1:A:233:ILE:HD12	1.90	0.71
1:B:164:THR:CG2	1:B:268:ALA:HB2	2.20	0.71
1:K:224:LEU:H	1:K:224:LEU:HD12	1.54	0.70
1:B:203:ASP:OD2	1:B:205:THR:HG23	1.91	0.69
1:C:164:THR:CG2	1:C:268:ALA:HB2	2.19	0.69
1:K:155:THR:HG23	1:K:156:PRO:HD2	1.75	0.68
1:C:224:LEU:H	1:C:224:LEU:CD1	2.01	0.68
1:K:208:MET:O	1:K:233:ILE:HD12	1.94	0.67
1:L:144:GLN:NE2	1:M:285:LEU:H	1.93	0.66
1:A:155:THR:HG23	1:A:156:PRO:HD2	1.79	0.65
1:C:155:THR:HG23	1:C:156:PRO:HD2	1.79	0.65
1:B:144:GLN:NE2	1:C:285:LEU:H	1.95	0.64
1:L:150:ILE:HG23	1:L:171:SER:HB2	1.78	0.64
1:M:205:THR:HG21	1:M:265:ARG:CZ	2.27	0.64
1:B:155:THR:HG23	1:B:156:PRO:HD2	1.80	0.64
1:A:235:ASN:O	1:A:236:MET:HE2	1.98	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:THR:HG21	1:A:265:ARG:CZ	2.27	0.64
1:B:205:THR:HG21	1:B:265:ARG:CZ	2.28	0.64
1:K:150:ILE:HG23	1:K:171:SER:HB2	1.80	0.63
1:C:150:ILE:HG23	1:C:171:SER:HB2	1.80	0.63
1:C:220:PHE:HB2	1:C:223:GLU:CD	2.18	0.63
1:L:155:THR:HG23	1:L:156:PRO:HD2	1.80	0.63
1:L:282:LEU:HD11	1:M:284:LEU:CD2	2.29	0.62
1:K:268:ALA:O	1:K:269:GLN:CB	2.47	0.62
1:B:150:ILE:HG23	1:B:171:SER:HB2	1.81	0.62
1:C:205:THR:HG21	1:C:265:ARG:CZ	2.29	0.62
1:C:224:LEU:HD12	1:C:224:LEU:N	2.05	0.62
1:K:205:THR:HG21	1:K:265:ARG:CZ	2.29	0.62
1:M:155:THR:HG23	1:M:156:PRO:HD2	1.81	0.62
1:L:244:SER:HB3	1:M:233:ILE:HG22	1.81	0.61
1:M:150:ILE:HG23	1:M:171:SER:HB2	1.83	0.61
1:M:268:ALA:O	1:M:269:GLN:CB	2.48	0.61
1:A:164:THR:HG21	1:A:268:ALA:CB	2.25	0.60
1:L:242:ASN:H	1:M:235:ASN:ND2	1.91	0.60
1:L:205:THR:HG21	1:L:265:ARG:CZ	2.31	0.60
1:M:164:THR:HG21	1:M:268:ALA:CB	2.25	0.60
1:C:268:ALA:O	1:C:269:GLN:CB	2.48	0.60
1:B:268:ALA:O	1:B:269:GLN:CB	2.51	0.59
1:L:268:ALA:O	1:L:269:GLN:CB	2.50	0.59
1:A:268:ALA:O	1:A:269:GLN:CB	2.50	0.59
1:K:164:THR:HG21	1:K:268:ALA:CB	2.26	0.59
1:B:282:LEU:HD11	1:C:284:LEU:CD2	2.33	0.59
1:C:147:LEU:HD21	1:C:149:LEU:HD13	1.85	0.59
1:K:147:LEU:HD21	1:K:149:LEU:HD13	1.85	0.58
1:A:150:ILE:HG23	1:A:171:SER:HB2	1.84	0.58
1:L:282:LEU:HD11	1:M:284:LEU:HD22	1.85	0.58
1:K:285:LEU:H	1:M:144:GLN:NE2	2.02	0.58
1:C:167:PRO:HD2	1:C:272:LEU:HD11	1.85	0.58
1:C:220:PHE:HB2	1:C:223:GLU:HG3	1.86	0.58
1:K:285:LEU:OXT	1:M:143:THR:O	2.22	0.58
1:M:167:PRO:HD2	1:M:272:LEU:HD11	1.86	0.57
1:B:164:THR:HG21	1:B:268:ALA:CB	2.27	0.57
1:B:147:LEU:HD21	1:B:149:LEU:HD13	1.87	0.57
1:C:220:PHE:HB2	1:C:223:GLU:CG	2.35	0.57
1:L:167:PRO:HD2	1:L:272:LEU:HD11	1.86	0.57
1:K:268:ALA:O	1:K:269:GLN:HB2	2.05	0.56
1:A:147:LEU:HD21	1:A:149:LEU:HD13	1.87	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:PRO:HD2	1:B:272:LEU:HD11	1.87	0.56
1:K:284:LEU:CD2	1:M:282:LEU:HD11	2.35	0.56
1:M:164:THR:HG22	1:M:265:ARG:O	2.06	0.56
1:C:220:PHE:CB	1:C:223:GLU:HG3	2.35	0.56
1:L:243:ASN:HD22	1:M:234:GLN:HA	1.70	0.56
1:A:167:PRO:HD2	1:A:272:LEU:HD11	1.86	0.56
1:C:164:THR:HG22	1:C:265:ARG:O	2.05	0.56
1:C:164:THR:HG21	1:C:268:ALA:CB	2.28	0.55
1:L:144:GLN:HE22	1:M:285:LEU:H	1.53	0.55
1:L:147:LEU:HD21	1:L:149:LEU:HD13	1.86	0.55
1:M:203:ASP:OD2	1:M:204:LYS:N	2.39	0.55
1:C:273:ASP:HB3	1:C:276:VAL:HG12	1.88	0.55
1:B:203:ASP:OD2	1:B:204:LYS:N	2.39	0.55
1:C:203:ASP:OD2	1:C:204:LYS:N	2.40	0.55
1:C:234:GLN:HG2	1:C:243:ASN:HB3	1.89	0.54
1:B:282:LEU:HD11	1:C:284:LEU:HD22	1.90	0.54
1:L:282:LEU:HD23	1:L:283:LYS:N	2.22	0.54
1:K:145:ASP:OD1	1:K:175:GLY:HA3	2.07	0.54
1:K:203:ASP:OD2	1:K:204:LYS:N	2.40	0.54
1:L:243:ASN:ND2	1:M:235:ASN:N	2.51	0.54
1:M:151:ALA:HB1	1:M:272:LEU:HA	1.90	0.54
1:M:268:ALA:O	1:M:269:GLN:HB2	2.06	0.54
1:K:235:ASN:O	1:K:236:MET:HE2	2.07	0.54
1:B:164:THR:HG22	1:B:265:ARG:O	2.08	0.54
1:K:167:PRO:HD2	1:K:272:LEU:HD11	1.89	0.54
1:C:268:ALA:O	1:C:269:GLN:HB2	2.07	0.54
1:C:220:PHE:HB2	1:C:223:GLU:OE1	2.07	0.54
1:K:164:THR:HG22	1:K:265:ARG:O	2.07	0.54
1:L:164:THR:HG22	1:L:265:ARG:O	2.07	0.54
1:L:234:GLN:OE1	1:M:234:GLN:OE1	2.25	0.54
1:A:282:LEU:HD23	1:A:283:LYS:N	2.23	0.53
1:K:224:LEU:CD1	1:K:224:LEU:H	2.21	0.53
1:K:151:ALA:HB1	1:K:272:LEU:HA	1.89	0.53
1:C:177:ALA:O	1:C:178:LEU:HB2	2.08	0.53
1:M:147:LEU:HD21	1:M:149:LEU:HD13	1.89	0.53
1:A:151:ALA:HB1	1:A:272:LEU:HA	1.90	0.53
1:B:234:GLN:HG2	1:B:243:ASN:HB3	1.90	0.53
1:C:219:VAL:O	1:C:219:VAL:HG13	2.09	0.53
1:C:282:LEU:HD23	1:C:283:LYS:N	2.24	0.53
1:L:203:ASP:OD2	1:L:204:LYS:N	2.41	0.53
1:A:235:ASN:HD21	1:C:242:ASN:N	1.84	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:LEU:HD23	1:B:283:LYS:N	2.24	0.53
1:M:200:LEU:HD11	1:M:242:ASN:HD22	1.74	0.53
1:M:234:GLN:HG2	1:M:243:ASN:HB3	1.91	0.53
1:A:203:ASP:OD2	1:A:204:LYS:N	2.41	0.53
1:B:151:ALA:HB1	1:B:272:LEU:HA	1.90	0.53
1:C:221:GLY:H	1:C:223:GLU:HG3	1.74	0.53
1:L:145:ASP:OD1	1:L:175:GLY:HA3	2.09	0.53
1:L:273:ASP:HB3	1:L:276:VAL:HG12	1.91	0.53
1:B:268:ALA:O	1:B:269:GLN:HB2	2.09	0.52
1:C:151:ALA:HB1	1:C:272:LEU:HA	1.91	0.52
1:A:200:LEU:HD13	1:B:233:ILE:HG21	1.92	0.52
1:L:268:ALA:O	1:L:269:GLN:HB2	2.08	0.52
1:L:202:THR:HG22	1:L:269:GLN:O	2.08	0.52
1:K:233:ILE:HG22	1:M:244:SER:HB3	1.90	0.52
1:K:202:THR:HG22	1:K:269:GLN:O	2.10	0.52
1:K:282:LEU:HD11	1:L:284:LEU:HD22	1.91	0.52
1:C:145:ASP:OD1	1:C:175:GLY:HA3	2.09	0.52
1:B:235:ASN:O	1:B:236:MET:HE2	2.10	0.52
1:K:234:GLN:HA	1:M:243:ASN:HD22	1.75	0.52
1:L:164:THR:HG21	1:L:268:ALA:CB	2.27	0.52
1:L:234:GLN:HG2	1:L:243:ASN:HB3	1.91	0.52
1:A:202:THR:HG22	1:A:269:GLN:O	2.09	0.52
1:B:202:THR:HG22	1:B:269:GLN:O	2.10	0.52
1:A:147:LEU:C	1:A:147:LEU:HD23	2.31	0.52
1:A:282:LEU:HD11	1:B:284:LEU:HD22	1.91	0.52
1:A:200:LEU:HD11	1:A:242:ASN:HD22	1.75	0.51
1:C:240:LEU:HD22	1:C:240:LEU:N	2.25	0.51
1:K:273:ASP:HB3	1:K:276:VAL:HG12	1.92	0.51
1:K:282:LEU:HD23	1:K:283:LYS:N	2.25	0.51
1:K:243:ASN:HD22	1:L:234:GLN:HA	1.75	0.51
1:A:234:GLN:HG2	1:A:243:ASN:HB3	1.91	0.51
1:B:147:LEU:HD23	1:B:147:LEU:C	2.31	0.51
1:A:164:THR:HG22	1:A:265:ARG:O	2.10	0.51
1:M:177:ALA:O	1:M:178:LEU:HB2	2.09	0.51
1:A:268:ALA:O	1:A:269:GLN:HB2	2.09	0.51
1:K:234:GLN:HG2	1:K:243:ASN:HB3	1.92	0.51
1:A:285:LEU:OXT	1:C:143:THR:O	2.28	0.51
1:B:273:ASP:HB3	1:B:276:VAL:HG12	1.92	0.51
1:K:177:ALA:O	1:K:178:LEU:HB2	2.10	0.51
1:B:145:ASP:OD1	1:B:175:GLY:HA3	2.11	0.51
1:M:147:LEU:HD23	1:M:147:LEU:C	2.31	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LEU:C	1:C:147:LEU:HD23	2.31	0.50
1:C:202:THR:HG22	1:C:269:GLN:O	2.10	0.50
1:A:240:LEU:N	1:A:240:LEU:HD22	2.26	0.50
1:A:273:ASP:HB3	1:A:276:VAL:HG12	1.93	0.50
1:M:282:LEU:HD23	1:M:283:LYS:N	2.26	0.50
1:A:177:ALA:O	1:A:178:LEU:HB2	2.11	0.50
1:A:244:SER:HB3	1:B:233:ILE:HG22	1.93	0.50
1:K:200:LEU:HD11	1:K:242:ASN:HD22	1.76	0.50
1:L:177:ALA:O	1:L:178:LEU:HB2	2.10	0.50
1:B:177:ALA:O	1:B:178:LEU:HB2	2.12	0.50
1:M:202:THR:HG22	1:M:269:GLN:O	2.11	0.50
1:K:147:LEU:C	1:K:147:LEU:HD23	2.31	0.50
1:C:217:VAL:HG11	1:C:256:GLY:HA3	1.94	0.50
1:B:205:THR:O	1:B:236:MET:HB2	2.11	0.49
1:L:200:LEU:HD11	1:L:242:ASN:HD22	1.77	0.49
1:K:284:LEU:HD22	1:M:282:LEU:HD11	1.92	0.49
1:L:144:GLN:NE2	1:M:285:LEU:N	2.60	0.49
1:A:217:VAL:HG11	1:A:256:GLY:HA3	1.93	0.49
1:M:240:LEU:HD22	1:M:240:LEU:N	2.28	0.49
1:A:242:ASN:H	1:B:235:ASN:ND2	2.00	0.49
1:B:240:LEU:HD22	1:B:240:LEU:N	2.28	0.49
1:K:155:THR:CG2	1:K:156:PRO:HD2	2.39	0.49
1:L:217:VAL:HG11	1:L:256:GLY:HA3	1.94	0.49
1:M:145:ASP:OD1	1:M:175:GLY:HA3	2.11	0.49
1:M:273:ASP:HB3	1:M:276:VAL:HG12	1.94	0.49
1:A:282:LEU:HD11	1:B:284:LEU:CD2	2.42	0.49
1:B:144:GLN:HE22	1:C:285:LEU:H	1.59	0.49
1:K:282:LEU:HD11	1:L:284:LEU:CD2	2.42	0.49
1:A:205:THR:O	1:A:236:MET:HB2	2.12	0.49
1:L:147:LEU:HD23	1:L:147:LEU:C	2.32	0.49
1:L:151:ALA:HB1	1:L:272:LEU:HA	1.93	0.49
1:M:270:ILE:HG13	1:M:272:LEU:CD2	2.43	0.49
1:A:144:GLN:NE2	1:B:285:LEU:H	2.10	0.49
1:K:200:LEU:HD13	1:L:233:ILE:HG21	1.95	0.49
1:L:240:LEU:N	1:L:240:LEU:HD22	2.28	0.49
1:A:243:ASN:HD22	1:B:234:GLN:HA	1.78	0.48
1:K:240:LEU:N	1:K:240:LEU:HD22	2.28	0.48
1:K:244:SER:HB3	1:L:233:ILE:HG22	1.96	0.48
1:L:200:LEU:HD13	1:M:233:ILE:HG21	1.95	0.48
1:B:234:GLN:OE1	1:C:234:GLN:OE1	2.30	0.48
1:B:217:VAL:HG11	1:B:256:GLY:HA3	1.95	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:217:VAL:HG11	1:K:256:GLY:HA3	1.95	0.48
1:B:144:GLN:HG2	1:B:282:LEU:HD21	1.96	0.48
1:B:230:PHE:CE2	1:B:249:GLY:HA3	2.49	0.48
1:C:155:THR:CG2	1:C:156:PRO:HD2	2.44	0.48
1:A:270:ILE:HG13	1:A:272:LEU:CD2	2.44	0.47
1:B:200:LEU:HD11	1:B:242:ASN:HD22	1.79	0.47
1:M:181:LYS:HG3	1:M:182:GLU:N	2.29	0.47
1:M:224:LEU:N	1:M:224:LEU:HD22	2.29	0.47
1:C:270:ILE:HG13	1:C:272:LEU:CD2	2.44	0.47
1:L:205:THR:O	1:L:236:MET:HB2	2.15	0.47
1:K:205:THR:O	1:K:236:MET:HB2	2.14	0.47
1:L:243:ASN:ND2	1:M:234:GLN:HA	2.30	0.47
1:C:200:LEU:HD11	1:C:242:ASN:HD22	1.78	0.47
1:L:282:LEU:HD11	1:M:284:LEU:HD21	1.96	0.47
1:A:192:TYR:CZ	1:A:252:LYS:HD2	2.50	0.47
1:K:181:LYS:HG3	1:K:182:GLU:N	2.30	0.47
1:B:181:LYS:HG3	1:B:182:GLU:N	2.30	0.47
1:K:233:ILE:CG2	1:M:200:LEU:HD13	2.45	0.47
1:B:243:ASN:HD22	1:C:234:GLN:HA	1.79	0.47
1:A:181:LYS:HG3	1:A:182:GLU:N	2.30	0.46
1:A:181:LYS:HD3	1:A:186:LEU:HD22	1.97	0.46
1:A:145:ASP:OD1	1:A:175:GLY:HA3	2.15	0.46
1:B:270:ILE:HG13	1:B:272:LEU:CD2	2.46	0.46
1:C:205:THR:O	1:C:236:MET:HB2	2.15	0.46
1:L:270:ILE:HG13	1:L:272:LEU:CD2	2.45	0.46
1:M:205:THR:O	1:M:236:MET:HB2	2.16	0.46
1:A:155:THR:CG2	1:A:156:PRO:HD2	2.44	0.46
1:K:192:TYR:CZ	1:K:252:LYS:HD2	2.51	0.46
1:K:144:GLN:HG2	1:K:282:LEU:HD21	1.97	0.46
1:L:155:THR:CG2	1:L:156:PRO:HD2	2.46	0.46
1:M:144:GLN:HG2	1:M:282:LEU:HD21	1.97	0.46
1:L:181:LYS:HD3	1:L:186:LEU:HD22	1.97	0.46
1:K:148:GLN:O	1:K:171:SER:HB3	2.16	0.46
1:K:270:ILE:HG13	1:K:272:LEU:CD2	2.46	0.46
1:M:217:VAL:HG11	1:M:256:GLY:HA3	1.96	0.46
1:A:149:LEU:HG	1:A:168:TRP:HB3	1.98	0.46
1:K:233:ILE:HG21	1:M:200:LEU:HD13	1.98	0.46
1:L:148:GLN:O	1:L:171:SER:HB3	2.16	0.46
1:A:233:ILE:HG22	1:C:244:SER:HB3	1.98	0.46
1:L:144:GLN:HG2	1:L:282:LEU:HD21	1.98	0.46
1:C:144:GLN:HG2	1:C:282:LEU:HD21	1.97	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:TYR:CD1	1:C:264:PRO:HA	2.50	0.46
1:B:163:TYR:CD1	1:B:264:PRO:HA	2.51	0.45
1:K:152:ASP:HB3	1:K:167:PRO:HB2	1.99	0.45
1:L:181:LYS:HG3	1:L:182:GLU:N	2.30	0.45
1:M:246:TYR:CD2	1:M:246:TYR:C	2.90	0.45
1:C:181:LYS:HG3	1:C:182:GLU:N	2.30	0.45
1:B:242:ASN:H	1:C:235:ASN:ND2	1.93	0.45
1:C:230:PHE:CE2	1:C:249:GLY:HA3	2.52	0.45
1:B:152:ASP:HB3	1:B:167:PRO:HB2	1.99	0.45
1:B:282:LEU:HD11	1:C:284:LEU:HD21	1.98	0.45
1:L:235:ASN:O	1:L:236:MET:HE2	2.17	0.45
1:K:230:PHE:CE2	1:K:249:GLY:HA3	2.52	0.45
1:A:181:LYS:HB2	1:A:186:LEU:HB2	1.99	0.45
1:A:144:GLN:HG2	1:A:282:LEU:HD21	1.97	0.45
1:A:200:LEU:HD13	1:B:233:ILE:CG2	2.47	0.45
1:C:181:LYS:HD3	1:C:186:LEU:HD22	1.99	0.45
1:K:284:LEU:HD21	1:M:282:LEU:HD11	1.99	0.45
1:M:155:THR:CG2	1:M:156:PRO:HD2	2.45	0.45
1:B:198:GLN:O	1:B:277:THR:HA	2.17	0.45
1:B:144:GLN:NE2	1:C:285:LEU:N	2.64	0.44
1:K:149:LEU:HG	1:K:168:TRP:HB3	1.98	0.44
1:K:181:LYS:HD3	1:K:186:LEU:HD22	1.98	0.44
1:K:250:ILE:HD13	1:K:284:LEU:HD11	1.98	0.44
1:A:166:VAL:HA	1:A:167:PRO:HD3	1.83	0.44
1:K:220:PHE:O	1:K:223:GLU:HG2	2.18	0.44
1:L:149:LEU:HG	1:L:168:TRP:HB3	2.00	0.44
1:M:235:ASN:O	1:M:236:MET:HE2	2.18	0.44
1:M:230:PHE:CE2	1:M:249:GLY:HA3	2.52	0.44
1:B:149:LEU:HG	1:B:168:TRP:HB3	1.99	0.44
1:B:192:TYR:CZ	1:B:252:LYS:HD2	2.52	0.44
1:A:285:LEU:H	1:C:144:GLN:NE2	2.16	0.44
1:C:235:ASN:O	1:C:236:MET:HE2	2.18	0.44
1:K:200:LEU:HA	1:K:244:SER:HA	1.99	0.44
1:K:234:GLN:OE1	1:M:234:GLN:OE1	2.36	0.44
1:B:246:TYR:CD2	1:B:246:TYR:C	2.90	0.44
1:L:200:LEU:HA	1:L:244:SER:HA	2.00	0.44
1:B:155:THR:CG2	1:B:156:PRO:HD2	2.45	0.43
1:B:238:GLU:OE1	1:B:238:GLU:HA	2.18	0.43
1:B:244:SER:HB3	1:C:233:ILE:HG22	1.99	0.43
1:K:219:VAL:HG11	1:K:225:SER:HB3	1.99	0.43
1:L:181:LYS:HB2	1:L:186:LEU:HB2	1.99	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:230:PHE:CE2	1:L:249:GLY:HA3	2.53	0.43
1:A:238:GLU:OE1	1:A:238:GLU:HA	2.18	0.43
1:M:148:GLN:O	1:M:171:SER:HB3	2.18	0.43
1:M:149:LEU:HG	1:M:168:TRP:HB3	2.00	0.43
1:A:163:TYR:CD1	1:A:264:PRO:HA	2.53	0.43
1:M:200:LEU:HA	1:M:244:SER:HA	2.01	0.43
1:C:167:PRO:HD2	1:C:272:LEU:CD1	2.49	0.43
1:K:144:GLN:NE2	1:L:285:LEU:H	2.16	0.43
1:K:243:ASN:ND2	1:L:234:GLN:HA	2.33	0.43
1:C:200:LEU:HA	1:C:244:SER:HA	2.01	0.43
1:K:200:LEU:HD13	1:L:233:ILE:CG2	2.48	0.43
1:B:200:LEU:HA	1:B:244:SER:HA	2.01	0.43
1:K:238:GLU:HA	1:K:238:GLU:OE1	2.19	0.43
1:K:246:TYR:C	1:K:246:TYR:CD2	2.92	0.43
1:M:238:GLU:HA	1:M:238:GLU:OE1	2.19	0.43
1:C:152:ASP:HB3	1:C:167:PRO:HB2	2.00	0.43
1:C:238:GLU:HA	1:C:238:GLU:OE1	2.18	0.43
1:K:172:PHE:CD1	1:K:172:PHE:C	2.92	0.43
1:L:172:PHE:CD1	1:L:172:PHE:C	2.91	0.43
1:L:163:TYR:CD1	1:L:264:PRO:HA	2.54	0.43
1:M:152:ASP:HB3	1:M:167:PRO:HB2	2.01	0.43
1:M:200:LEU:HD11	1:M:242:ASN:ND2	2.34	0.43
1:M:198:GLN:O	1:M:277:THR:HA	2.18	0.43
1:A:234:GLN:HA	1:C:243:ASN:HD22	1.83	0.43
1:A:284:LEU:CD2	1:C:282:LEU:HD11	2.48	0.43
1:M:181:LYS:HB2	1:M:186:LEU:HB2	2.01	0.43
1:K:198:GLN:O	1:K:277:THR:HA	2.19	0.42
1:L:152:ASP:HB3	1:L:167:PRO:HB2	2.00	0.42
1:L:238:GLU:HA	1:L:238:GLU:OE1	2.19	0.42
1:L:246:TYR:C	1:L:246:TYR:CD2	2.93	0.42
1:B:263:ILE:HA	1:B:264:PRO:HD3	1.85	0.42
1:C:181:LYS:HB2	1:C:186:LEU:HB2	2.01	0.42
1:C:246:TYR:C	1:C:246:TYR:CD2	2.92	0.42
1:K:163:TYR:CD1	1:K:264:PRO:HA	2.53	0.42
1:L:263:ILE:HA	1:L:264:PRO:HD3	1.86	0.42
1:A:166:VAL:HG22	1:A:168:TRP:CE2	2.54	0.42
1:A:209:GLY:HA3	1:A:232:CYS:O	2.19	0.42
1:C:148:GLN:O	1:C:171:SER:HB3	2.19	0.42
1:K:181:LYS:HB2	1:K:186:LEU:HB2	2.00	0.42
1:B:167:PRO:HD2	1:B:272:LEU:CD1	2.49	0.42
1:B:181:LYS:HD3	1:B:186:LEU:HD22	2.00	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:PHE:CD1	1:B:172:PHE:C	2.93	0.42
1:B:250:ILE:HD13	1:B:284:LEU:HD11	2.02	0.42
1:C:209:GLY:HA3	1:C:232:CYS:O	2.19	0.42
1:B:181:LYS:HB2	1:B:186:LEU:HB2	2.01	0.42
1:A:236:MET:HE1	1:A:243:ASN:HB2	2.02	0.42
1:L:192:TYR:CZ	1:L:252:LYS:HD2	2.54	0.42
1:L:200:LEU:HD13	1:M:233:ILE:CG2	2.49	0.42
1:A:284:LEU:HD22	1:C:282:LEU:HD11	2.01	0.42
1:A:198:GLN:O	1:A:277:THR:HA	2.20	0.41
1:A:246:TYR:CD2	1:A:246:TYR:C	2.93	0.41
1:A:230:PHE:CE2	1:A:249:GLY:HA3	2.54	0.41
1:C:149:LEU:HG	1:C:168:TRP:HB3	2.01	0.41
1:C:172:PHE:C	1:C:172:PHE:CD1	2.94	0.41
1:C:222:ASP:N	1:C:222:ASP:OD2	2.53	0.41
1:M:172:PHE:C	1:M:172:PHE:CD1	2.93	0.41
1:A:152:ASP:HB3	1:A:167:PRO:HB2	2.00	0.41
1:A:200:LEU:HD11	1:A:242:ASN:ND2	2.33	0.41
1:L:166:VAL:HG22	1:L:168:TRP:CE2	2.55	0.41
1:M:166:VAL:HA	1:M:167:PRO:HD3	1.86	0.41
1:A:200:LEU:HA	1:A:244:SER:HA	2.02	0.41
1:A:263:ILE:HA	1:A:264:PRO:HD3	1.86	0.41
1:B:148:GLN:O	1:B:171:SER:HB3	2.20	0.41
1:L:167:PRO:HD2	1:L:272:LEU:CD1	2.50	0.41
1:M:167:PRO:HD2	1:M:272:LEU:CD1	2.50	0.41
1:C:270:ILE:HG13	1:C:272:LEU:HD22	2.03	0.41
1:L:200:LEU:HD11	1:L:242:ASN:ND2	2.35	0.41
1:C:192:TYR:CZ	1:C:252:LYS:HD2	2.55	0.41
1:B:143:THR:O	1:C:285:LEU:OXT	2.39	0.41
1:K:200:LEU:HD11	1:K:242:ASN:ND2	2.36	0.41
1:K:198:GLN:HA	1:K:245:CYS:O	2.21	0.41
1:L:209:GLY:HA3	1:L:232:CYS:O	2.21	0.41
1:M:220:PHE:N	1:M:220:PHE:CD2	2.87	0.41
1:M:234:GLN:HB3	1:M:236:MET:HE1	2.02	0.41
1:B:209:GLY:HA3	1:B:232:CYS:O	2.21	0.41
1:C:147:LEU:HD21	1:C:149:LEU:CD1	2.51	0.41
1:K:167:PRO:HD2	1:K:272:LEU:CD1	2.51	0.41
1:M:163:TYR:CD1	1:M:264:PRO:HA	2.55	0.41
1:K:166:VAL:HA	1:K:167:PRO:HD3	1.85	0.41
1:M:181:LYS:HD3	1:M:186:LEU:HD22	2.03	0.40
1:A:233:ILE:CG2	1:C:200:LEU:HD13	2.51	0.40
1:C:177:ALA:HA	1:C:188:LYS:HB2	2.03	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ASN:ND2	1:C:234:GLN:HA	2.36	0.40
1:A:148:GLN:O	1:A:171:SER:HB3	2.21	0.40
1:A:198:GLN:HA	1:A:245:CYS:O	2.22	0.40
1:M:209:GLY:HA3	1:M:232:CYS:O	2.21	0.40
1:M:218:HIS:HB3	1:M:220:PHE:CE2	2.57	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	Percentiles	
1	A	142/164 (87%)	125 (88%)	15 (11%)	2 (1%)	14	42
1	B	142/164 (87%)	127 (89%)	13 (9%)	2 (1%)	14	42
1	C	142/164 (87%)	125 (88%)	14 (10%)	3 (2%)	9	29
1	K	142/164 (87%)	124 (87%)	14 (10%)	4 (3%)	6	21
1	L	142/164 (87%)	127 (89%)	13 (9%)	2 (1%)	14	42
1	M	142/164 (87%)	126 (89%)	13 (9%)	3 (2%)	9	29
All	All	852/984 (87%)	754 (88%)	82 (10%)	16 (2%)	10	32

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	B	269	GLN
1	C	220	PHE
1	C	269	GLN
1	K	269	GLN
1	L	269	GLN
1	M	269	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	K	223	GLU
1	M	223	GLU
1	A	178	LEU
1	B	178	LEU
1	C	178	LEU
1	K	178	LEU
1	L	178	LEU
1	M	178	LEU
1	K	221	GLY

### 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	126/145 (87%)	113 (90%)	13 (10%)	9	26
1	B	126/145 (87%)	113 (90%)	13 (10%)	9	26
1	C	126/145 (87%)	112 (89%)	14 (11%)	8	23
1	K	126/145 (87%)	113 (90%)	13 (10%)	9	26
1	L	126/145 (87%)	114 (90%)	12 (10%)	11	30
1	M	126/145 (87%)	113 (90%)	13 (10%)	9	26
All	All	756/870 (87%)	678 (90%)	78 (10%)	9	26

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	LEU
1	A	169	LEU
1	A	178	LEU
1	A	190	THR
1	A	199	VAL
1	A	206	TYR
1	A	222	ASP
1	A	228	THR
1	A	229	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	232	CYS
1	A	242	ASN
1	A	253	LEU
1	A	273	ASP
1	B	149	LEU
1	B	169	LEU
1	B	178	LEU
1	B	190	THR
1	B	199	VAL
1	B	206	TYR
1	B	224	LEU
1	B	228	THR
1	B	229	LEU
1	B	232	CYS
1	B	242	ASN
1	B	253	LEU
1	B	273	ASP
1	C	149	LEU
1	C	169	LEU
1	C	178	LEU
1	C	190	THR
1	C	199	VAL
1	C	206	TYR
1	C	220	PHE
1	C	224	LEU
1	C	228	THR
1	C	229	LEU
1	C	232	CYS
1	C	242	ASN
1	C	253	LEU
1	C	273	ASP
1	K	149	LEU
1	K	169	LEU
1	K	178	LEU
1	K	190	THR
1	K	199	VAL
1	K	206	TYR
1	K	224	LEU
1	K	228	THR
1	K	229	LEU
1	K	232	CYS
1	K	242	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	K	253	LEU
1	K	273	ASP
1	L	149	LEU
1	L	169	LEU
1	L	178	LEU
1	L	190	THR
1	L	199	VAL
1	L	206	TYR
1	L	228	THR
1	L	229	LEU
1	L	232	CYS
1	L	242	ASN
1	L	253	LEU
1	L	273	ASP
1	M	149	LEU
1	M	169	LEU
1	M	178	LEU
1	M	190	THR
1	M	199	VAL
1	M	206	TYR
1	M	222	ASP
1	M	228	THR
1	M	229	LEU
1	M	232	CYS
1	M	242	ASN
1	M	253	LEU
1	M	273	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	159	GLN
1	A	235	ASN
1	A	242	ASN
1	A	243	ASN
1	A	260	GLN
1	B	144	GLN
1	B	159	GLN
1	B	234	GLN
1	B	235	ASN
1	B	242	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	243	ASN
1	B	260	GLN
1	C	144	GLN
1	C	159	GLN
1	C	235	ASN
1	C	242	ASN
1	C	243	ASN
1	C	260	GLN
1	K	144	GLN
1	K	159	GLN
1	K	235	ASN
1	K	242	ASN
1	K	243	ASN
1	K	260	GLN
1	L	144	GLN
1	L	159	GLN
1	L	234	GLN
1	L	235	ASN
1	L	242	ASN
1	L	243	ASN
1	L	260	GLN
1	M	144	GLN
1	M	159	GLN
1	M	235	ASN
1	M	242	ASN
1	M	243	ASN
1	M	260	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	144/164 (87%)	-0.05	4 (2%) 56 44	12, 34, 74, 113	0
1	B	144/164 (87%)	-0.10	0 100 100	14, 36, 67, 101	0
1	C	144/164 (87%)	-0.14	5 (3%) 48 35	14, 38, 85, 157	0
1	K	144/164 (87%)	-0.19	2 (1%) 78 69	13, 36, 68, 104	0
1	L	144/164 (87%)	-0.15	3 (2%) 67 56	12, 37, 75, 133	0
1	M	144/164 (87%)	-0.06	8 (5%) 28 18	8, 34, 77, 112	0
All	All	864/984 (87%)	-0.12	22 (2%) 61 48	8, 36, 77, 157	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	222	ASP	4.2
1	C	218	HIS	4.2
1	L	161	GLY	3.5
1	M	218	HIS	3.5
1	M	142	VAL	3.5
1	A	161	GLY	3.3
1	C	220	PHE	3.1
1	M	220	PHE	3.1
1	M	224	LEU	2.9
1	A	176	SER	2.9
1	M	223	GLU	2.7
1	L	268	ALA	2.7
1	K	143	THR	2.5
1	C	222	ASP	2.5
1	C	162	SER	2.2
1	M	217	VAL	2.2
1	M	219	VAL	2.2
1	C	142	VAL	2.2
1	K	239	THR	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	143	THR	2.1
1	A	238	GLU	2.1
1	L	162	SER	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.