



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:51 AM GMT

PDB ID : 3CEY  
Title : Crystal structure of L3MBTL2  
Authors : Nady, N.; Guo, Y.; Pan, P.; Allali-Hassani, A.; Qi, C.; Zhu, H.; Dong, A.; Mackenzie, F.; Crombet, L.; Loppnau, P.; Kozieradzki, I.; Vedadi, M.; Edwards, A.M.; Weigelt, J.; Bountra, C.; Arrowsmith, C.H.; Bochkarev, A.; Read, R.; Min, J.; Structural Genomics Consortium (SGC)  
Deposited on : 2008-02-29  
Resolution : 2.20 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

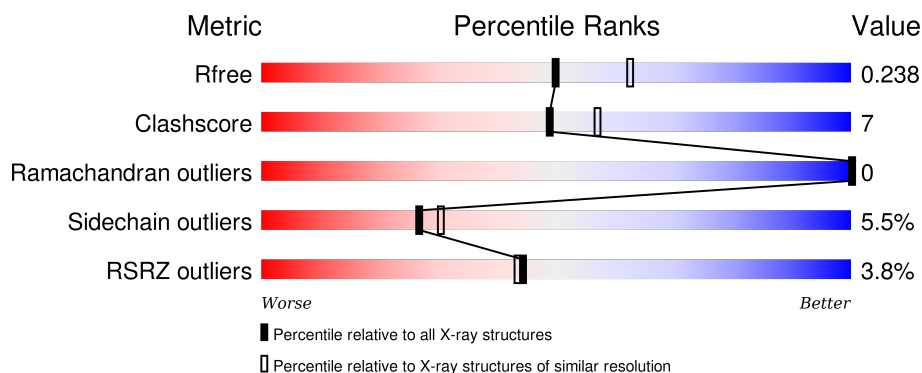
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	474	 4% 67% 14% • 18%
1	B	474	 2% 67% 14% •• 16%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6346 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 Lethal(3)malignant brain tumor-like 2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3068	2003	507	532	26			
1	B	396	Total	C	N	O	S	0	0	0
			3113	2027	519	541	26			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	MET	-	EXPRESSION TAG	UNP Q969R5
A	153	HIS	-	EXPRESSION TAG	UNP Q969R5
A	154	HIS	-	EXPRESSION TAG	UNP Q969R5
A	155	HIS	-	EXPRESSION TAG	UNP Q969R5
A	156	HIS	-	EXPRESSION TAG	UNP Q969R5
A	157	HIS	-	EXPRESSION TAG	UNP Q969R5
A	158	HIS	-	EXPRESSION TAG	UNP Q969R5
A	159	SER	-	EXPRESSION TAG	UNP Q969R5
A	160	SER	-	EXPRESSION TAG	UNP Q969R5
A	161	GLY	-	EXPRESSION TAG	UNP Q969R5
A	162	ARG	-	EXPRESSION TAG	UNP Q969R5
A	163	GLU	-	EXPRESSION TAG	UNP Q969R5
A	164	ASN	-	EXPRESSION TAG	UNP Q969R5
A	165	LEU	-	EXPRESSION TAG	UNP Q969R5
A	166	TYR	-	EXPRESSION TAG	UNP Q969R5
A	167	PHE	-	EXPRESSION TAG	UNP Q969R5
A	168	GLN	-	EXPRESSION TAG	UNP Q969R5
A	169	GLY	-	EXPRESSION TAG	UNP Q969R5
B	152	MET	-	EXPRESSION TAG	UNP Q969R5
B	153	HIS	-	EXPRESSION TAG	UNP Q969R5
B	154	HIS	-	EXPRESSION TAG	UNP Q969R5
B	155	HIS	-	EXPRESSION TAG	UNP Q969R5
B	156	HIS	-	EXPRESSION TAG	UNP Q969R5
B	157	HIS	-	EXPRESSION TAG	UNP Q969R5
B	158	HIS	-	EXPRESSION TAG	UNP Q969R5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	159	SER	-	EXPRESSION TAG	UNP Q969R5
B	160	SER	-	EXPRESSION TAG	UNP Q969R5
B	161	GLY	-	EXPRESSION TAG	UNP Q969R5
B	162	ARG	-	EXPRESSION TAG	UNP Q969R5
B	163	GLU	-	EXPRESSION TAG	UNP Q969R5
B	164	ASN	-	EXPRESSION TAG	UNP Q969R5
B	165	LEU	-	EXPRESSION TAG	UNP Q969R5
B	166	TYR	-	EXPRESSION TAG	UNP Q969R5
B	167	PHE	-	EXPRESSION TAG	UNP Q969R5
B	168	GLN	-	EXPRESSION TAG	UNP Q969R5
B	169	GLY	-	EXPRESSION TAG	UNP Q969R5

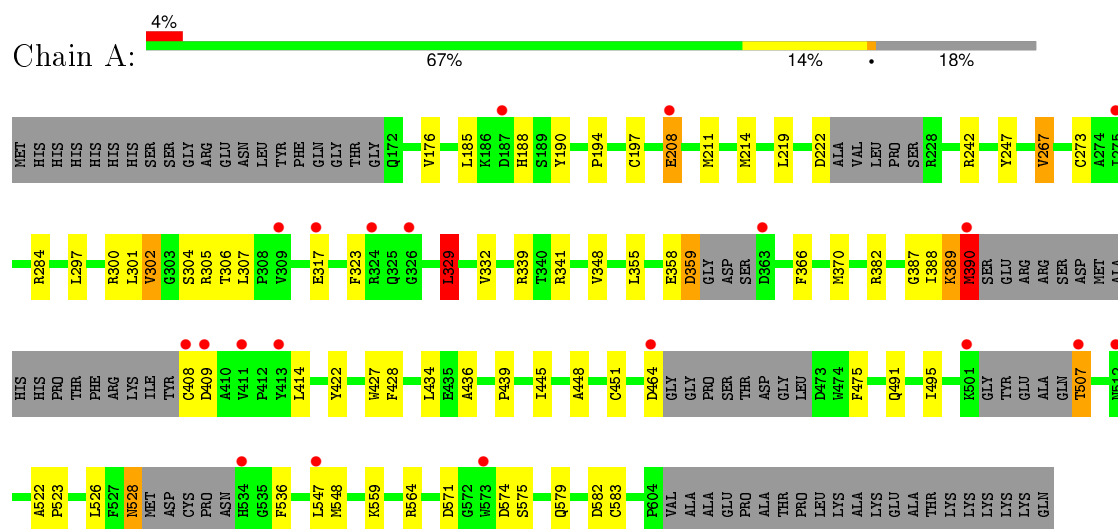
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	76	Total O 76 76	0	0
2	B	89	Total O 89 89	0	0

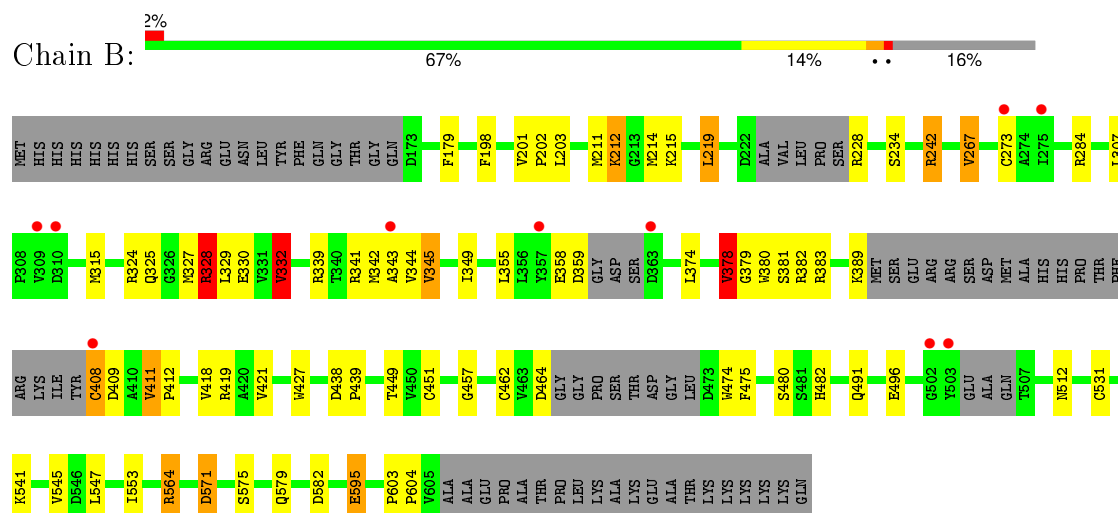
### 3 Residue-property plots [i](#)

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: Lethal(3)malignant brain tumor-like 2 protein



- Molecule 1: Lethal(3)malignant brain tumor-like 2 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.64Å 55.94Å 329.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.91 – 2.20 35.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.7 (35.91-2.20) 87.7 (35.91-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.210 , 0.252 0.200 , 0.238	Depositor DCC
$R_{free}$ test set	2390 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.1	EDS
Estimated twinning fraction	0.048 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 46991 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6346	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.32	23/3159 (0.7%)	0.95	10/4301 (0.2%)
1	B	1.28	30/3206 (0.9%)	1.01	10/4367 (0.2%)
All	All	1.30	53/6365 (0.8%)	0.98	20/8668 (0.2%)

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
1	A	0	1
1	B	0	1
All	All	0	2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	ASP	C-O	27.71	1.76	1.23
1	A	390	MET	C-O	22.01	1.65	1.23
1	A	358	GLU	CD-OE1	21.35	1.49	1.25
1	B	212	LYS	CE-NZ	20.06	1.99	1.49
1	B	212	LYS	CD-CE	14.53	1.87	1.51
1	B	359	ASP	CG-OD1	14.28	1.58	1.25
1	A	389	LYS	CD-CE	13.58	1.85	1.51
1	B	328	ARG	CZ-NH1	12.62	1.49	1.33
1	B	380	TRP	CD2-CE2	11.06	1.54	1.41
1	A	358	GLU	CG-CD	10.58	1.67	1.51
1	A	408	CYS	CB-SG	8.78	1.97	1.82
1	B	324	ARG	CD-NE	8.71	1.61	1.46
1	A	305	ARG	CG-CD	8.29	1.72	1.51
1	A	389	LYS	CE-NZ	8.14	1.69	1.49
1	B	328	ARG	NE-CZ	7.99	1.43	1.33
1	B	344	VAL	CB-CG2	-7.75	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382	ARG	CB-CG	7.56	1.73	1.52
1	B	324	ARG	CG-CD	7.44	1.70	1.51
1	B	380	TRP	CE3-CZ3	7.36	1.50	1.38
1	A	304	SER	C-N	7.31	1.50	1.34
1	A	341	ARG	CZ-NH1	7.25	1.42	1.33
1	B	512	ASN	CG-OD1	7.20	1.39	1.24
1	A	358	GLU	CB-CG	7.03	1.65	1.52
1	B	378	VAL	C-O	6.97	1.36	1.23
1	B	327	MET	C-O	6.93	1.36	1.23
1	A	222	ASP	C-O	6.84	1.36	1.23
1	B	328	ARG	CD-NE	6.68	1.57	1.46
1	B	380	TRP	CD1-NE1	6.61	1.49	1.38
1	B	325	GLN	C-O	6.48	1.35	1.23
1	B	330	GLU	CD-OE2	6.47	1.32	1.25
1	B	381	SER	CB-OG	6.32	1.50	1.42
1	A	305	ARG	CZ-NH1	6.32	1.41	1.33
1	B	359	ASP	CG-OD2	6.28	1.39	1.25
1	A	390	MET	SD-CE	6.13	2.12	1.77
1	A	305	ARG	NE-CZ	6.10	1.41	1.33
1	B	595	GLU	CG-CD	5.99	1.60	1.51
1	A	247	TYR	CD2-CE2	5.74	1.48	1.39
1	A	382	ARG	CB-CG	5.68	1.67	1.52
1	A	409	ASP	CG-OD2	5.63	1.38	1.25
1	B	343	ALA	C-O	5.46	1.33	1.23
1	A	302	VAL	CA-CB	5.45	1.66	1.54
1	A	436	ALA	CA-CB	5.42	1.63	1.52
1	B	345	VAL	N-CA	5.40	1.57	1.46
1	B	380	TRP	CZ3-CH2	5.33	1.48	1.40
1	A	408	CYS	CA-CB	5.32	1.65	1.53
1	B	408	CYS	CB-SG	5.30	1.91	1.82
1	A	389	LYS	CG-CD	5.22	1.70	1.52
1	B	325	GLN	C-N	5.18	1.42	1.33
1	B	332	VAL	CB-CG1	-5.17	1.42	1.52
1	A	305	ARG	CD-NE	5.17	1.55	1.46
1	B	343	ALA	CA-CB	5.16	1.63	1.52
1	B	380	TRP	CG-CD1	5.10	1.43	1.36
1	B	379	GLY	C-O	-5.06	1.15	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	ARG	NE-CZ-NH2	-18.32	111.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ARG	NE-CZ-NH1	-18.07	111.27	120.30
1	B	359	ASP	CB-CG-OD2	-15.29	104.54	118.30
1	B	242	ARG	NE-CZ-NH1	11.01	125.81	120.30
1	B	564	ARG	NE-CZ-NH2	-10.77	114.91	120.30
1	B	242	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	A	305	ARG	NH1-CZ-NH2	8.98	129.28	119.40
1	A	242	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	359	ASP	CB-CG-OD1	6.93	124.53	118.30
1	B	564	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	B	324	ARG	CG-CD-NE	-6.48	98.20	111.80
1	A	359	ASP	CA-C-O	-6.06	107.37	120.10
1	A	389	LYS	CD-CE-NZ	-5.81	98.33	111.70
1	A	219	LEU	CB-CG-CD2	-5.81	101.13	111.00
1	B	328	ARG	CD-NE-CZ	-5.69	115.63	123.60
1	A	329	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	341	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	242	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	267	VAL	CB-CA-C	-5.13	101.64	111.40
1	B	267	VAL	CB-CA-C	-5.08	101.75	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	GLU	Peptide
1	B	328	ARG	Sidechain

## 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	3068	0	2911	48	0
1	B	3113	0	2951	40	0
2	A	76	0	0	2	0
2	B	89	0	0	4	0
All	All	6346	0	5862	87	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 7.

All (87) 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:389:LYS:CE	1:A:389:LYS:NZ	1.69	1.55
1:A:389:LYS:CD	1:A:389:LYS:CE	1.85	1.53
1:B:212:LYS:CD	1:B:212:LYS:CE	1.87	1.49
1:A:390:MET:CE	1:A:390:MET:SD	2.12	1.38
1:A:390:MET:O	1:A:390:MET:C	1.65	1.34
1:B:212:LYS:NZ	1:B:212:LYS:CE	1.99	1.25
1:A:359:ASP:C	1:A:359:ASP:O	1.76	1.24
1:A:389:LYS:O	1:A:390:MET:HB3	1.81	0.80
1:B:378:VAL:HG13	1:B:409:ASP:HB3	1.67	0.76
1:A:547:LEU:H	1:A:579:GLN:HE22	1.32	0.75
1:B:383:ARG:NH1	2:B:676:HOH:O	2.22	0.71
1:B:547:LEU:H	1:B:579:GLN:HE22	1.37	0.71
1:B:212:LYS:CG	1:B:212:LYS:CE	2.71	0.69
1:B:273:CYS:HB2	2:B:711:HOH:O	1.95	0.67
1:B:564:ARG:HD3	1:B:582:ASP:OD1	1.98	0.64
1:A:389:LYS:CG	1:A:389:LYS:CE	2.75	0.63
1:A:214:MET:HE2	1:A:307:LEU:HA	1.81	0.63
1:A:564:ARG:HD3	1:A:583:CYS:SG	2.40	0.62
1:A:339:ARG:HA	1:A:387:GLY:O	1.99	0.61
1:A:185:LEU:CD2	1:A:190:TYR:HB2	2.31	0.61
1:B:242:ARG:HD2	1:B:595:GLU:OE1	2.01	0.61
1:A:185:LEU:HD23	1:A:190:TYR:HB2	1.84	0.59
1:A:297:LEU:O	1:A:301:LEU:HG	2.03	0.58
1:A:389:LYS:CD	1:A:389:LYS:NZ	2.68	0.57
1:A:389:LYS:O	1:A:390:MET:CB	2.51	0.57
1:A:523:PRO:HD2	1:A:526:LEU:HD12	1.84	0.57
1:B:383:ARG:NH2	2:B:708:HOH:O	2.38	0.56
1:A:574:ASP:OD2	2:A:641:HOH:O	2.18	0.56
1:A:507:THR:O	1:A:507:THR:HG23	2.05	0.56
1:B:214:MET:HE2	1:B:307:LEU:HA	1.88	0.55
1:B:411:VAL:HG12	1:B:412:PRO:HD2	1.88	0.55
1:B:547:LEU:H	1:B:579:GLN:NE2	2.05	0.54
1:B:462:CYS:HB3	1:B:474:TRP:CD1	2.42	0.54
1:A:564:ARG:HD2	1:A:582:ASP:OD1	2.07	0.53
1:A:434:LEU:HD12	1:A:448:ALA:HB3	1.91	0.53
1:B:419:ARG:HD2	1:B:480:SER:HB2	1.91	0.52
1:B:449:THR:HB	1:B:462:CYS:SG	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:VAL:CG1	1:B:409:ASP:HB3	2.36	0.50
1:A:547:LEU:N	1:A:579:GLN:HE22	2.05	0.50
1:A:445:ILE:HD12	1:A:495:ILE:HG21	1.94	0.50
1:B:219:LEU:HD11	1:B:228:ARG:HB3	1.94	0.48
1:A:194:PRO:HD2	1:A:197:CYS:SG	2.53	0.48
1:A:273:CYS:HB2	2:A:628:HOH:O	2.13	0.48
1:A:197:CYS:HB3	1:A:536:PHE:CZ	2.49	0.47
1:A:388:ILE:HG12	1:A:390:MET:N	2.30	0.47
1:B:419:ARG:NH2	1:B:482:HIS:HE1	2.12	0.47
1:A:422:TYR:CE2	1:B:421:VAL:HG13	2.49	0.47
1:A:370:MET:HB3	1:A:370:MET:HE2	1.63	0.46
1:A:439:PRO:HG3	1:A:475:PHE:CG	2.51	0.46
1:B:547:LEU:N	1:B:579:GLN:HE22	2.08	0.46
1:A:214:MET:HE2	1:A:306:THR:C	2.36	0.46
1:B:329:LEU:HD21	1:B:355:LEU:HD22	1.97	0.46
1:A:300:ARG:HB3	1:A:300:ARG:HE	1.53	0.46
1:B:339:ARG:HD2	1:B:389:LYS:HB2	1.98	0.45
1:A:388:ILE:HG12	1:A:390:MET:H	1.80	0.45
1:B:345:VAL:HA	1:B:355:LEU:HD23	1.99	0.45
1:A:390:MET:O	1:A:390:MET:HG2	2.17	0.44
1:B:427:TRP:CE3	1:B:427:TRP:HA	2.53	0.44
1:A:355:LEU:HD12	1:A:366:PHE:HD2	1.82	0.44
1:A:214:MET:HE2	1:A:307:LEU:CA	2.47	0.44
1:B:198:PHE:O	1:B:201:VAL:HG22	2.18	0.43
1:B:332:VAL:HG13	1:B:374:LEU:HB3	2.01	0.43
1:A:214:MET:CE	1:A:307:LEU:HA	2.48	0.43
1:A:523:PRO:HD2	1:A:526:LEU:CD1	2.48	0.43
1:B:457:GLY:HA2	2:B:683:HOH:O	2.19	0.43
1:A:559:LYS:NZ	1:A:575:SER:OG	2.51	0.43
1:A:390:MET:CE	1:A:390:MET:CG	2.95	0.42
1:B:341:ARG:HG3	1:B:389:LYS:HD2	2.01	0.42
1:B:179:PHE:HB2	1:B:603:PRO:HB3	2.01	0.42
1:B:215:LYS:HD3	1:B:234:SER:HB3	2.01	0.42
1:A:208:GLU:O	1:A:208:GLU:HG3	2.19	0.42
1:A:528:ASN:H	1:A:528:ASN:HD22	1.67	0.42
1:A:323:PHE:O	1:A:348:VAL:HG21	2.20	0.42
1:A:427:TRP:CG	1:A:428:PHE:N	2.88	0.42
1:B:438:ASP:HA	1:B:439:PRO:HD2	1.97	0.42
1:B:328:ARG:HG2	1:B:342:MET:CE	2.50	0.41
1:B:342:MET:HB3	1:B:358:GLU:HG3	2.00	0.41
1:A:547:LEU:H	1:A:579:GLN:NE2	2.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:PRO:HG3	1:B:475:PHE:CG	2.54	0.41
1:A:329:LEU:HD21	1:A:355:LEU:HD22	2.03	0.41
1:B:203:LEU:HD21	1:B:315:MET:HB2	2.02	0.41
1:A:522:ALA:HA	1:A:523:PRO:HD3	1.90	0.41
1:A:188:HIS:HB2	1:A:190:TYR:CE2	2.56	0.41
1:B:541:LYS:NZ	1:B:571:ASP:OD2	2.52	0.41
1:B:202:PRO:O	1:B:203:LEU:HB2	2.21	0.40
1:B:571:ASP:HB2	1:B:604:PRO:HB3	2.03	0.40
1:B:545:VAL:HG22	1:B:553:ILE:HG12	2.03	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	376/474 (79%)	366 (97%)	10 (3%)	0	100	100
1	B	384/474 (81%)	371 (97%)	13 (3%)	0	100	100
All	All	760/948 (80%)	737 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	315/413 (76%)	298 (95%)	17 (5%)	27	31
1	B	320/413 (78%)	302 (94%)	18 (6%)	26	29
All	All	635/826 (77%)	600 (94%)	35 (6%)	27	30

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	VAL
1	A	211	MET
1	A	267	VAL
1	A	284	ARG
1	A	302	VAL
1	A	317	GLU
1	A	329	LEU
1	A	332	VAL
1	A	390	MET
1	A	414	LEU
1	A	451	CYS
1	A	464	ASP
1	A	491	GLN
1	A	507	THR
1	A	528	ASN
1	A	548	MET
1	A	571	ASP
1	B	211	MET
1	B	219	LEU
1	B	267	VAL
1	B	284	ARG
1	B	328	ARG
1	B	332	VAL
1	B	349	ILE
1	B	378	VAL
1	B	408	CYS
1	B	411	VAL
1	B	418	VAL
1	B	451	CYS
1	B	464	ASP
1	B	491	GLN
1	B	496	GLU
1	B	531	CYS
1	B	571	ASP
1	B	575	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	A	444	ASN
1	A	528	ASN
1	A	579	GLN
1	B	206	GLN
1	B	444	ASN
1	B	482	HIS
1	B	512	ASN
1	B	579	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](#)

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	390/474 (82%)	0.16	20 (5%) 32 31	20, 36, 46, 56	0
1	B	396/474 (83%)	0.14	10 (2%) 61 60	17, 36, 52, 63	0
All	All	786/948 (82%)	0.15	30 (3%) 44 43	17, 36, 50, 63	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	CYS	6.2
1	A	413	TYR	4.1
1	A	275	ILE	3.8
1	B	408	CYS	3.7
1	B	502	GLY	3.4
1	A	501	LYS	3.2
1	A	363	ASP	3.2
1	B	363	ASP	3.1
1	A	507	THR	3.0
1	A	208	GLU	2.9
1	B	309	VAL	2.9
1	A	534	HIS	2.8
1	A	409	ASP	2.7
1	B	357	TYR	2.6
1	B	275	ILE	2.6
1	A	547	LEU	2.5
1	A	309	VAL	2.5
1	A	326	GLY	2.4
1	A	390	MET	2.4
1	B	273	CYS	2.4
1	A	187	ASP	2.3
1	A	411	VAL	2.3
1	A	512	ASN	2.3
1	B	310	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	343	ALA	2.1
1	A	573	TRP	2.1
1	A	317	GLU	2.1
1	A	464	ASP	2.1
1	A	324	ARG	2.0
1	B	503	TYR	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.