



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 04:13 pm GMT

PDB ID : 3F70
Title : Crystal structure of L3MBTL2-H4K20me1 complex
Authors : Guo, Y.; Qi, C.; Allali-Hassani, A.; Pan, P.; Zhu, H.; Dong, A.; Mackenzie, F.; Crombet, L.; Loppnau, P.; Kozieradzki, I.; Vedadi, M.; Edwards, A.M.; Weigelt, J.; Bountra, C.; Arrowsmith, C.H.; Botchkarev, A.; Read, R.; Min, J.; Structural Genomics Consortium (SGC)
Deposited on : 2008-11-07
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

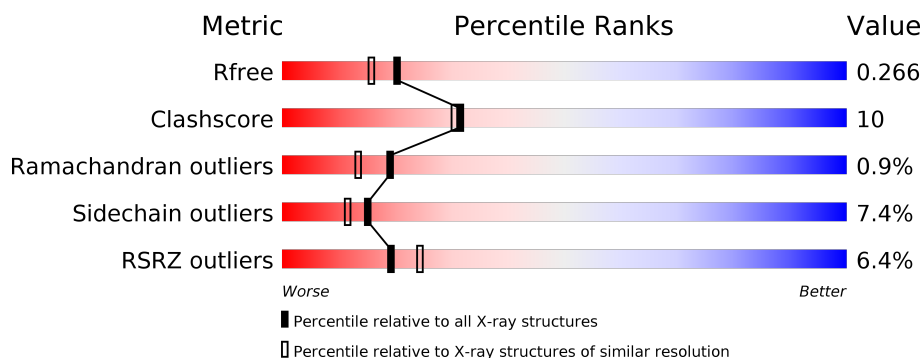
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (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. 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	456	<div> <div>8%</div> <div> <div></div> <div>67%</div> <div>16%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	456	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>18%</div> <div>•</div> <div>10%</div> </div> </div>

2 Entry composition [i](#)

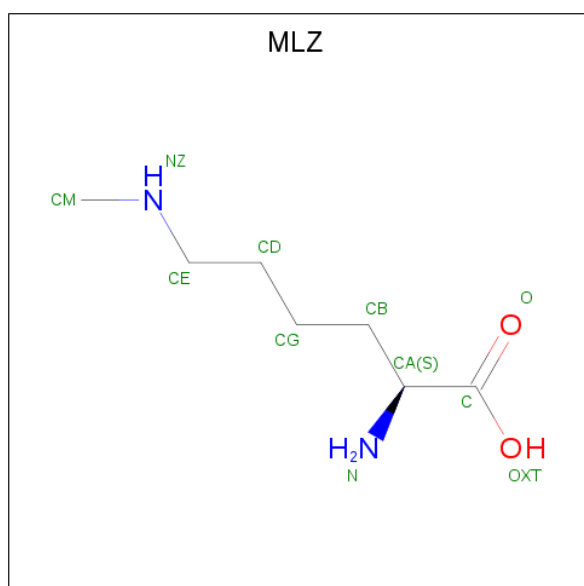
There are 3 unique types of molecules in this entry. The entry contains 6584 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	392	Total	C	N	O	S	0	0	0
			3077	1993	514	544	26			
1	B	410	Total	C	N	O	S	0	0	0
			3197	2080	530	559	28			

- Molecule 2 is N-METHYL-LYSINE (three-letter code: MLZ) (formula: $C_7H_{16}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	7	2	1		
2	B	1	Total	C	N	O	0	0
			10	7	2	1		

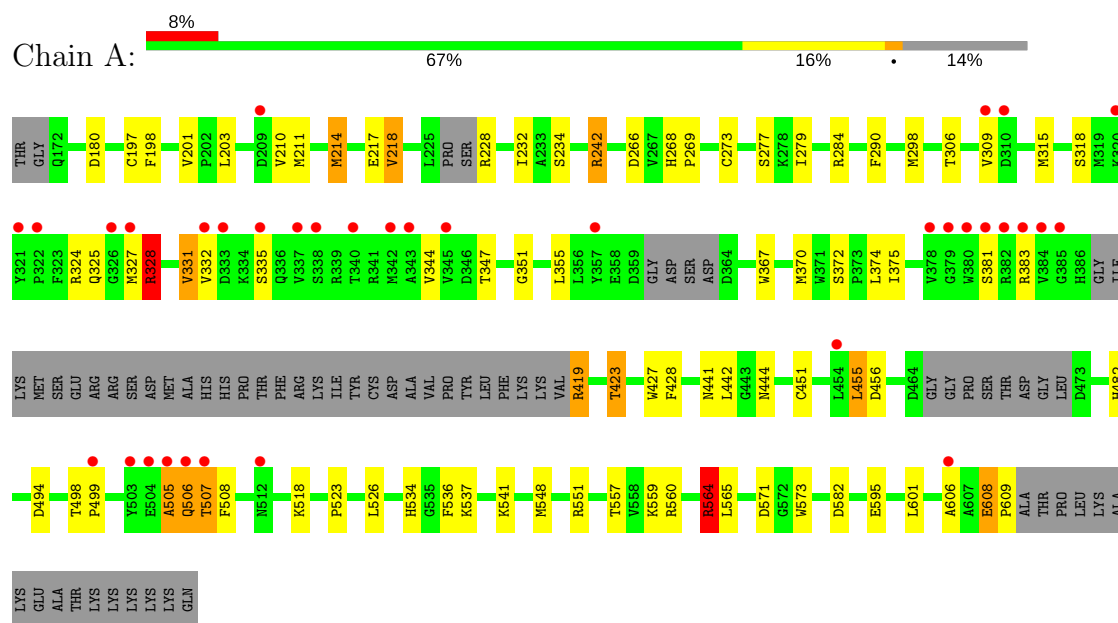
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total 119	O 119	0	0
3	B	171	Total 171	O 171	0	0

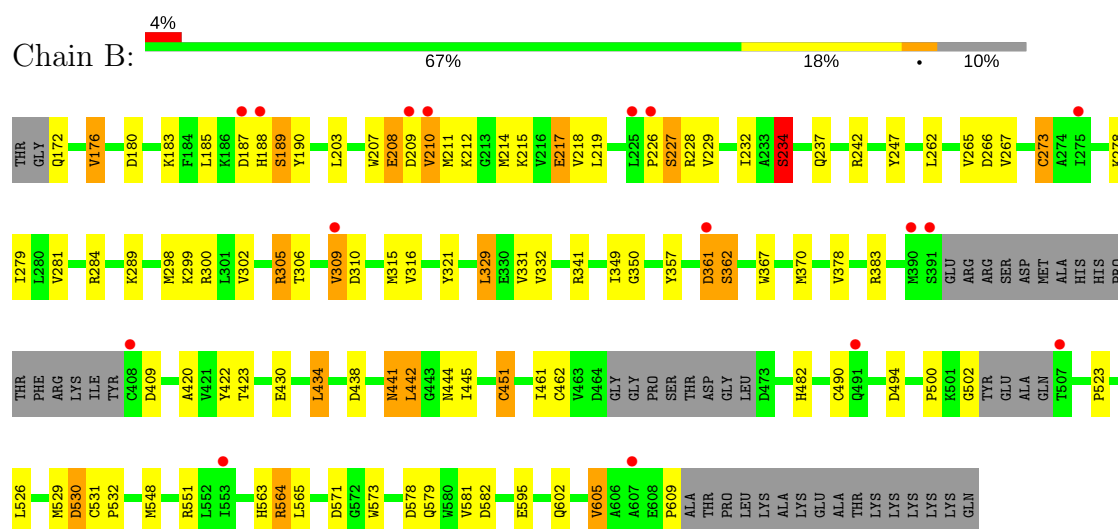
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 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, α , β , γ	55.59Å 55.49Å 324.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.79 – 2.10 45.78 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.3 (45.79-2.10) 88.3 (45.78-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.268 0.198 , 0.266	Depositor DCC
R_{free} test set	2662 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6584	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ

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	1.21	5/3169 (0.2%)	1.13	15/4317 (0.3%)
1	B	1.29	15/3294 (0.5%)	1.15	19/4492 (0.4%)
All	All	1.25	20/6463 (0.3%)	1.14	34/8809 (0.4%)

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	B	0	2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	217	GLU	CB-CG	6.45	1.64	1.52
1	B	430	GLU	CB-CG	6.33	1.64	1.52
1	B	266	ASP	CB-CG	6.23	1.64	1.51
1	A	218	VAL	CB-CG1	-6.18	1.39	1.52
1	B	430	GLU	CD-OE2	6.12	1.32	1.25
1	B	210	VAL	CB-CG1	-6.01	1.40	1.52
1	B	595	GLU	CG-CD	5.97	1.60	1.51
1	B	581	VAL	CA-CB	5.95	1.67	1.54
1	B	176	VAL	CB-CG2	5.90	1.65	1.52
1	A	234	SER	CB-OG	-5.78	1.34	1.42
1	A	328	ARG	CZ-NH1	5.70	1.40	1.33
1	B	451	CYS	CB-SG	5.69	1.92	1.82
1	B	234	SER	CB-OG	-5.57	1.35	1.42
1	B	289	LYS	CE-NZ	5.47	1.62	1.49
1	B	284	ARG	CG-CD	5.40	1.65	1.51
1	A	367	TRP	CB-CG	-5.23	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	PHE	CD1-CE1	5.20	1.49	1.39
1	B	273	CYS	CB-SG	-5.15	1.73	1.81
1	B	441	ASN	CB-CG	5.12	1.62	1.51
1	B	247	TYR	CD2-CE2	5.06	1.47	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ARG	NE-CZ-NH2	-16.49	112.05	120.30
1	A	242	ARG	NE-CZ-NH1	14.15	127.38	120.30
1	B	242	ARG	NE-CZ-NH2	-14.04	113.28	120.30
1	A	564	ARG	NE-CZ-NH2	-13.05	113.77	120.30
1	B	242	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	A	564	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	B	578	ASP	CB-CG-OD1	7.24	124.81	118.30
1	A	564	ARG	CB-CA-C	-6.78	96.85	110.40
1	B	180	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	328	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	B	267	VAL	CG1-CB-CG2	6.50	121.31	110.90
1	B	383	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	A	180	ASP	CB-CG-OD1	6.39	124.06	118.30
1	B	284	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	242	ARG	CD-NE-CZ	6.31	132.44	123.60
1	B	564	ARG	CB-CA-C	-6.21	97.99	110.40
1	A	451	CYS	CA-CB-SG	-6.18	102.88	114.00
1	B	434	LEU	CA-CB-CG	6.07	129.25	115.30
1	A	309	VAL	CB-CA-C	-5.96	100.07	111.40
1	B	350	GLY	C-N-CA	-5.92	109.87	122.30
1	B	329	LEU	CB-CG-CD2	5.92	121.06	111.00
1	A	242	ARG	CD-NE-CZ	5.84	131.77	123.60
1	A	214	MET	CG-SD-CE	-5.59	91.25	100.20
1	B	383	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	266	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	560	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	438	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	442	LEU	CA-CB-CG	-5.26	103.20	115.30
1	B	305	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	605	VAL	CB-CA-C	-5.18	101.55	111.40
1	A	565	LEU	CA-CB-CG	5.18	127.20	115.30
1	B	461	ILE	CG1-CB-CG2	-5.15	100.07	111.40
1	B	267	VAL	CA-CB-CG2	5.04	118.47	110.90
1	A	601	LEU	CB-CG-CD2	-5.01	102.48	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	187	ASP	Peptide
1	B	208	GLU	Peptide

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	3077	0	2902	56	0
1	B	3197	0	3037	65	0
2	A	10	0	15	2	0
2	B	10	0	15	2	0
3	A	119	0	0	10	0
3	B	171	0	0	11	0
All	All	6584	0	5969	119	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 10.

All (119) 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:505:ALA:HA	1:A:507:THR:H	0.97	1.13
1:B:563:HIS:HB2	3:B:730:HOH:O	1.52	1.10
1:A:505:ALA:HA	1:A:507:THR:N	1.65	1.09
1:A:344:VAL:HB	3:A:707:HOH:O	1.56	1.06
1:A:419:ARG:HG3	1:A:419:ARG:HH11	1.18	1.03
1:B:219:LEU:HD11	1:B:228:ARG:HD3	1.47	0.95
1:A:505:ALA:HB2	1:A:508:PHE:CB	2.00	0.91
1:B:529:MET:O	1:B:530:ASP:O	1.89	0.90
1:B:441:ASN:HB2	3:B:715:HOH:O	1.76	0.85
1:B:361:ASP:HB3	1:B:362:SER:HA	1.58	0.84
1:A:351:GLY:O	1:A:370:MET:HG2	1.83	0.78
1:B:378:VAL:HG21	1:B:409:ASP:OD2	1.85	0.77
1:A:419:ARG:HG3	1:A:419:ARG:NH1	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ALA:CA	1:A:507:THR:H	1.90	0.77
1:A:505:ALA:HB2	1:A:508:PHE:HB3	1.66	0.75
1:A:505:ALA:HB2	1:A:508:PHE:H	1.50	0.75
1:A:608:GLU:HG2	1:A:609:PRO:HD2	1.66	0.75
1:B:565:LEU:HD13	3:B:704:HOH:O	1.87	0.74
1:B:441:ASN:HA	1:B:548:MET:CE	2.19	0.72
1:A:608:GLU:HG2	1:A:609:PRO:CD	2.20	0.72
1:B:579:GLN:OE1	3:B:119:HOH:O	2.09	0.68
1:A:505:ALA:HB2	1:A:508:PHE:N	2.08	0.68
1:A:541:LYS:NZ	1:A:557:THR:OG1	2.24	0.66
1:A:419:ARG:CG	1:A:419:ARG:HH11	2.03	0.65
1:B:563:HIS:CD2	3:B:731:HOH:O	2.49	0.65
1:B:441:ASN:HA	1:B:548:MET:HE3	1.78	0.64
1:A:573:TRP:CZ2	2:A:20:MLZ:HE3	2.33	0.63
1:A:505:ALA:CB	1:A:508:PHE:HB3	2.29	0.63
1:B:214:MET:HE2	1:B:306:THR:O	1.99	0.62
1:B:442:LEU:HB2	1:B:579:GLN:HG2	1.83	0.61
1:B:211:MET:HG3	1:B:305:ARG:HH22	1.66	0.60
1:A:242:ARG:HD2	1:A:595:GLU:OE1	2.02	0.60
1:B:210:VAL:O	1:B:211:MET:HB3	2.02	0.59
1:B:530:ASP:OD1	1:B:532:PRO:HD3	2.03	0.59
1:B:228:ARG:HB2	3:B:728:HOH:O	2.00	0.59
1:A:582:ASP:HB3	3:A:26:HOH:O	2.02	0.59
1:A:331:VAL:HG13	1:A:375:ILE:HG22	1.86	0.58
1:B:441:ASN:HA	1:B:548:MET:HE1	1.84	0.58
1:B:299:LYS:O	1:B:302:VAL:HG22	2.03	0.57
1:A:505:ALA:HB2	1:A:508:PHE:HB2	1.86	0.57
1:B:229:VAL:N	3:B:728:HOH:O	2.25	0.57
1:A:444:ASN:ND2	3:A:695:HOH:O	2.39	0.56
1:B:226:PRO:HA	1:B:227:SER:C	2.25	0.56
1:B:226:PRO:HA	1:B:228:ARG:N	2.22	0.54
1:B:442:LEU:H	1:B:548:MET:CE	2.19	0.54
1:B:188:HIS:HB3	1:B:190:TYR:CE2	2.42	0.54
1:B:309:VAL:O	1:B:310:ASP:CB	2.56	0.53
1:A:214:MET:HE2	1:A:306:THR:C	2.29	0.53
1:B:444:ASN:ND2	3:B:79:HOH:O	2.42	0.53
1:B:211:MET:HG2	1:B:305:ARG:HH12	1.73	0.53
1:A:427:TRP:CG	1:A:428:PHE:N	2.76	0.52
1:B:602:GLN:OE1	1:B:609:PRO:HB3	2.11	0.51
1:B:573:TRP:CZ2	2:B:20:MLZ:HE3	2.46	0.51
1:A:505:ALA:CB	1:A:508:PHE:H	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LEU:H	1:A:548:MET:HE1	1.75	0.51
1:A:498:THR:HG23	3:A:123:HOH:O	2.11	0.51
1:A:559:LYS:HA	3:A:719:HOH:O	2.11	0.51
1:B:321:TYR:HB3	1:B:370:MET:HE1	1.93	0.51
1:A:198:PHE:O	1:A:201:VAL:HG22	2.11	0.50
1:B:188:HIS:HB3	1:B:190:TYR:CZ	2.47	0.50
1:B:278:LYS:HE3	3:B:718:HOH:O	2.09	0.50
1:A:324:ARG:HH21	1:A:327:MET:HE2	1.78	0.49
1:B:273:CYS:HB2	3:B:72:HOH:O	2.11	0.49
1:A:203:LEU:HD21	1:A:315:MET:HB2	1.94	0.48
1:A:564:ARG:HD3	1:A:582:ASP:OD1	2.14	0.48
1:B:203:LEU:HG	1:B:315:MET:HG3	1.96	0.48
1:B:207:TRP:CG	1:B:208:GLU:N	2.82	0.48
1:B:212:LYS:O	1:B:305:ARG:NH2	2.47	0.48
1:A:441:ASN:HA	1:A:548:MET:CE	2.44	0.48
1:B:207:TRP:CD1	1:B:208:GLU:N	2.82	0.48
1:A:608:GLU:HG3	3:A:711:HOH:O	2.13	0.47
1:A:383:ARG:O	1:A:455:LEU:HD12	2.15	0.47
1:A:210:VAL:O	3:A:126:HOH:O	2.20	0.47
1:B:302:VAL:O	1:B:302:VAL:HG23	2.14	0.47
1:A:328:ARG:HD3	3:A:743:HOH:O	2.14	0.47
1:A:505:ALA:HB2	1:A:508:PHE:CA	2.45	0.47
1:B:482:HIS:CD2	1:B:564:ARG:CD	2.98	0.47
1:B:279:ILE:HG22	1:B:281:VAL:HG23	1.98	0.46
1:A:197:CYS:HB3	1:A:536:PHE:CZ	2.50	0.46
1:A:268:HIS:HB3	1:A:269:PRO:HD2	1.98	0.45
1:B:188:HIS:CB	1:B:190:TYR:CE2	3.00	0.45
1:A:372:SER:HB3	1:A:375:ILE:HG12	1.97	0.45
1:A:441:ASN:HA	1:A:548:MET:HE1	1.99	0.45
1:B:482:HIS:CD2	1:B:564:ARG:HD3	2.52	0.45
1:A:505:ALA:CB	1:A:508:PHE:CB	2.83	0.45
1:B:209:ASP:O	1:B:214:MET:HE1	2.16	0.45
1:A:582:ASP:CB	3:A:26:HOH:O	2.61	0.45
1:A:419:ARG:NH1	1:B:422:TYR:HB3	2.31	0.45
1:A:273:CYS:HB2	3:A:48:HOH:O	2.17	0.44
1:B:185:LEU:CD2	1:B:190:TYR:HB2	2.48	0.44
1:B:300:ARG:HE	1:B:300:ARG:HB3	1.56	0.44
1:A:523:PRO:HG2	1:A:526:LEU:HG	1.99	0.44
1:B:442:LEU:H	1:B:548:MET:HE1	1.83	0.44
1:B:367:TRP:CD1	1:B:551:ARG:HB3	2.53	0.44
1:A:419:ARG:CG	1:A:419:ARG:NH1	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:ASP:OD1	1:B:530:ASP:C	2.57	0.43
1:B:215:LYS:HD3	1:B:234:SER:HB2	2.01	0.43
1:B:185:LEU:HD23	1:B:190:TYR:HD2	1.84	0.43
1:B:298:MET:O	1:B:302:VAL:HG13	2.19	0.43
1:B:451:CYS:SG	1:B:462:CYS:SG	3.16	0.43
1:B:523:PRO:HD2	1:B:526:LEU:HD12	1.99	0.43
1:A:217:GLU:HG2	1:A:232:ILE:CD1	2.48	0.43
1:B:332:VAL:HG13	1:B:332:VAL:O	2.17	0.43
1:B:370:MET:HB3	1:B:370:MET:HE3	1.84	0.42
1:B:210:VAL:HG21	1:B:262:LEU:CD1	2.49	0.42
1:A:573:TRP:CE2	2:A:20:MLZ:HE3	2.54	0.42
1:B:445:ILE:HG21	1:B:490:CYS:SG	2.60	0.42
1:B:500:PRO:O	1:B:502:GLY:HA2	2.19	0.42
1:A:279:ILE:HD12	1:A:279:ILE:HG23	1.74	0.41
1:B:331:VAL:HG13	1:B:357:TYR:HE1	1.84	0.41
1:B:573:TRP:CE2	2:B:20:MLZ:HE3	2.55	0.41
1:B:217:GLU:HG2	1:B:232:ILE:CD1	2.51	0.41
1:A:332:VAL:HG21	1:A:374:LEU:HD22	2.01	0.41
1:A:498:THR:HA	1:A:499:PRO:HD3	1.81	0.41
1:A:482:HIS:CD2	1:A:564:ARG:HD2	2.54	0.41
1:A:423:THR:HG23	1:B:420:ALA:HB2	2.04	0.40
1:A:242:ARG:CD	1:A:595:GLU:OE1	2.69	0.40
1:B:183:LYS:HB2	3:B:745:HOH:O	2.20	0.40
1:B:321:TYR:HB3	1:B:370:MET:CE	2.51	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	382/456 (84%)	352 (92%)	27 (7%)	3 (1%)	21 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	402/456 (88%)	369 (92%)	29 (7%)	4 (1%)	17	12
All	All	784/912 (86%)	721 (92%)	56 (7%)	7 (1%)	19	13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	505	ALA
1	A	506	GLN
1	B	361	ASP
1	B	530	ASP
1	B	227	SER
1	A	606	ALA
1	B	189	SER

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	316/397 (80%)	288 (91%)	28 (9%)	11	7
1	B	329/397 (83%)	309 (94%)	20 (6%)	20	17
All	All	645/794 (81%)	597 (93%)	48 (7%)	15	11

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

Mol	Chain	Res	Type
1	A	211	MET
1	A	218	VAL
1	A	228	ARG
1	A	277	SER
1	A	284	ARG
1	A	298	MET
1	A	318	SER
1	A	325	GLN
1	A	328	ARG

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Mol	Chain	Res	Type
1	A	331	VAL
1	A	335	SER
1	A	347	THR
1	A	355	LEU
1	A	381	SER
1	A	419	ARG
1	A	423	THR
1	A	455	LEU
1	A	456	ASP
1	A	494	ASP
1	A	506	GLN
1	A	507	THR
1	A	518	LYS
1	A	534	HIS
1	A	537	LYS
1	A	551	ARG
1	A	564	ARG
1	A	571	ASP
1	A	608	GLU
1	B	172	GLN
1	B	176	VAL
1	B	189	SER
1	B	218	VAL
1	B	234	SER
1	B	237	GLN
1	B	265	VAL
1	B	309	VAL
1	B	316	VAL
1	B	329	LEU
1	B	341	ARG
1	B	349	ILE
1	B	362	SER
1	B	423	THR
1	B	434	LEU
1	B	494	ASP
1	B	531	CYS
1	B	571	ASP
1	B	582	ASP
1	B	605	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	444	ASN
1	A	482	HIS
1	A	493	ASN
1	A	506	GLN
1	B	444	ASN
1	B	482	HIS
1	B	563	HIS

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MLZ	A	20	-	9,9,10	0.69	0	6,9,11	1.29	1 (16%)
2	MLZ	B	20	-	9,9,10	1.22	2 (22%)	6,9,11	1.77	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLZ	A	20	-	-	0/6/8/10	0/0/0/0
2	MLZ	B	20	-	-	0/6/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	20	MLZ	O-C	2.02	1.28	1.19
2	B	20	MLZ	CA-C	2.10	1.53	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	20	MLZ	O-C-CA	-2.62	117.77	124.96
2	B	20	MLZ	CM-NZ-CE	2.54	119.47	111.74
2	B	20	MLZ	CB-CA-C	2.98	117.54	111.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	20	MLZ	2	0
2	B	20	MLZ	2	0

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, 95th 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 ²)	Q<0.9
1	A	392/456 (85%)	0.32	35 (8%) 9 12	18, 32, 57, 64	0
1	B	410/456 (89%)	0.12	16 (3%) 39 46	16, 28, 52, 63	0
All	All	802/912 (87%)	0.22	51 (6%) 19 24	16, 30, 55, 64	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	507	THR	5.7
1	A	343	ALA	5.5
1	A	322	PRO	5.3
1	A	337	VAL	4.6
1	A	503	TYR	4.6
1	A	335	SER	4.6
1	A	380	TRP	4.3
1	B	209	ASP	4.1
1	A	378	VAL	4.0
1	A	512	ASN	3.9
1	A	506	GLN	3.7
1	A	342	MET	3.7
1	A	505	ALA	3.6
1	A	384	VAL	3.5
1	A	345	VAL	3.3
1	A	379	GLY	3.3
1	A	504	GLU	3.2
1	A	340	THR	3.2
1	A	327	MET	3.1
1	B	390	MET	3.0
1	B	361	ASP	2.9
1	A	333	ASP	2.9
1	B	408	CYS	2.9
1	B	275	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	382	ARG	2.8
1	B	491	GLN	2.7
1	B	210	VAL	2.7
1	A	454	LEU	2.7
1	B	309	VAL	2.6
1	B	226	PRO	2.6
1	A	606	ALA	2.6
1	B	391	SER	2.4
1	B	507	THR	2.4
1	A	309	VAL	2.4
1	A	320	LYS	2.4
1	A	357	TYR	2.4
1	A	381	SER	2.4
1	A	321	TYR	2.4
1	A	338	SER	2.4
1	B	607	ALA	2.3
1	A	385	GLY	2.3
1	B	188	HIS	2.3
1	A	332	VAL	2.3
1	B	225	LEU	2.2
1	A	209	ASP	2.2
1	A	310	ASP	2.1
1	B	553	ILE	2.1
1	A	499	PRO	2.1
1	A	383	ARG	2.1
1	B	187	ASP	2.0
1	A	326	GLY	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MLZ	B	20	10/11	0.86	0.13	38,60,69,71	0
2	MLZ	A	20	10/11	0.92	0.11	35,62,68,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.