



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:08 PM UTC

PDB ID : 3F70 / pdb_00003f70
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

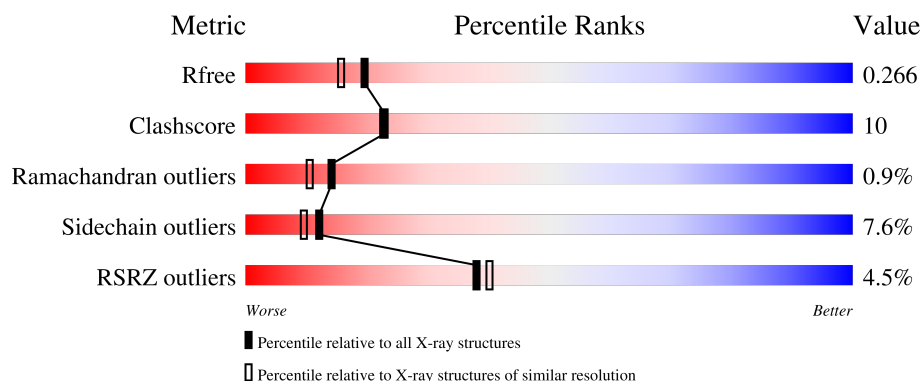
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	6% 64% 19% •• 14%
1	B	456	2% 65% 19% 6% 10%

2 Entry composition [i](#)

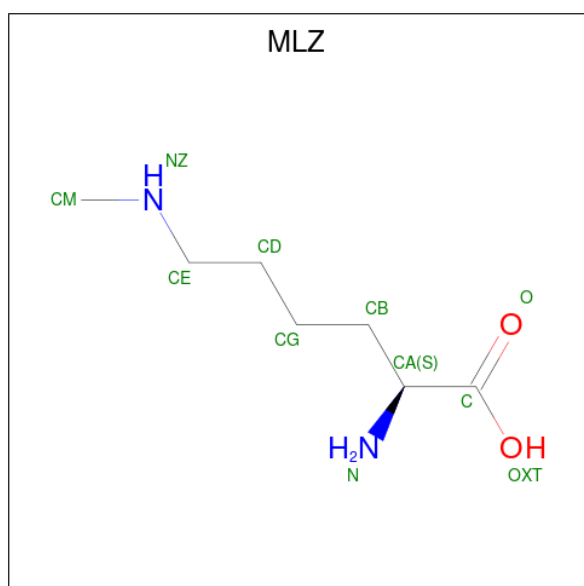
There are 3 unique types of molecules in this entry. The entry contains 6584 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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		

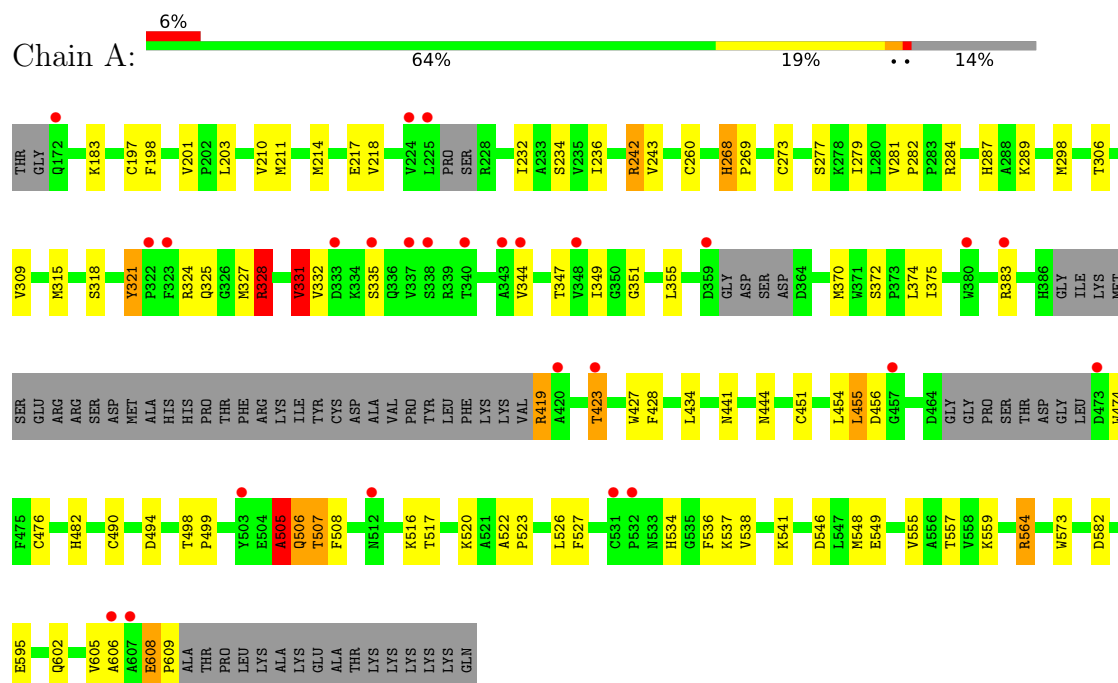
- Molecule 3 is water.

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

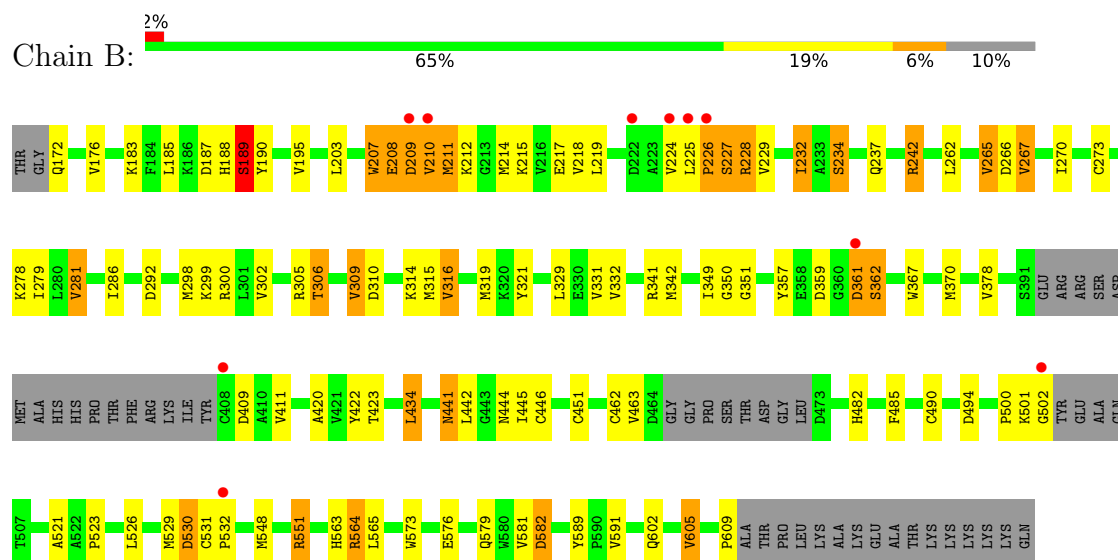
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 45.79 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.3 (45.79-2.10) 88.2 (45.79-2.10)	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 , 53.1	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	1.44	9/3169 (0.3%)	1.38	35/4317 (0.8%)
1	B	1.53	19/3294 (0.6%)	1.39	30/4492 (0.7%)
All	All	1.49	28/6463 (0.4%)	1.38	65/8809 (0.7%)

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 (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	581	VAL	CA-CB	7.21	1.67	1.55
1	A	476	CYS	CA-C	6.35	1.60	1.52
1	A	546	ASP	C-O	-6.23	1.15	1.23
1	B	226	PRO	CA-C	6.17	1.58	1.52
1	B	265	VAL	CA-CB	6.07	1.62	1.54
1	A	287	HIS	N-CA	5.87	1.53	1.46
1	B	434	LEU	C-O	5.83	1.29	1.24
1	A	281	VAL	CA-C	5.76	1.56	1.52
1	B	292	ASP	CA-CB	5.62	1.60	1.52
1	B	232	ILE	CG1-CD1	-5.58	1.29	1.51
1	A	328	ARG	CZ-NH1	5.51	1.40	1.32
1	B	195	VAL	N-CA	5.49	1.53	1.46
1	A	260	CYS	N-CA	-5.48	1.39	1.46
1	A	527	PHE	CA-C	5.44	1.59	1.52
1	B	306	THR	N-CA	-5.41	1.38	1.46
1	B	591	VAL	CA-CB	5.30	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	501	LYS	CA-C	5.29	1.59	1.52
1	A	555	VAL	CA-C	5.27	1.58	1.52
1	B	316	VAL	CA-CB	5.27	1.61	1.54
1	B	286	ILE	N-CA	5.19	1.51	1.46
1	A	243	VAL	CA-CB	-5.16	1.48	1.54
1	B	234	SER	N-CA	-5.12	1.39	1.46
1	B	266	ASP	CB-CG	5.11	1.64	1.52
1	B	281	VAL	CA-C	-5.10	1.47	1.52
1	B	576	GLU	N-CA	5.10	1.52	1.46
1	B	359	ASP	N-CA	5.05	1.52	1.46
1	B	521	ALA	CA-C	5.03	1.59	1.52
1	B	267	VAL	N-CA	5.02	1.52	1.46

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	VAL	CB-CA-C	-9.13	100.07	112.04
1	A	242	ARG	NE-CZ-NH2	-7.94	112.05	119.20
1	B	350	GLY	CA-C-N	-7.76	109.87	122.20
1	B	350	GLY	C-N-CA	-7.76	109.87	122.20
1	B	209	ASP	N-CA-C	-7.62	103.24	112.54
1	A	321	TYR	CA-C-N	7.14	126.63	118.85
1	A	321	TYR	C-N-CA	7.14	126.63	118.85
1	B	207	TRP	N-CA-C	6.75	121.05	110.32
1	B	224	VAL	N-CA-C	6.72	120.76	113.43
1	B	242	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	A	564	ARG	CB-CA-C	-6.53	96.85	110.17
1	A	268	HIS	CA-C-N	6.45	126.21	119.76
1	A	268	HIS	C-N-CA	6.45	126.21	119.76
1	B	564	ARG	CB-CA-C	-6.38	97.99	110.11
1	B	286	ILE	CB-CA-C	-6.29	104.01	110.93
1	B	228	ARG	N-CA-C	6.27	118.81	110.53
1	A	516	LYS	N-CA-C	6.22	118.06	111.28
1	A	236	ILE	CB-CA-C	-6.15	102.98	111.65
1	A	564	ARG	NE-CZ-NH2	-6.03	113.77	119.20
1	B	446	CYS	N-CA-C	5.92	119.21	109.85
1	A	242	ARG	NE-CZ-NH1	5.88	127.38	121.50
1	B	270	ILE	CA-C-N	-5.80	117.15	123.30
1	B	270	ILE	C-N-CA	-5.80	117.15	123.30
1	B	189	SER	N-CA-C	5.79	123.12	110.80
1	B	242	ARG	CD-NE-CZ	5.74	132.44	124.40
1	A	282	PRO	CA-C-N	5.72	125.74	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	PRO	C-N-CA	5.72	125.74	119.90
1	B	605	VAL	CB-CA-C	-5.71	101.55	110.69
1	A	289	LYS	N-CA-C	5.69	117.48	111.28
1	A	331	VAL	N-CA-C	5.59	116.64	108.53
1	B	589	TYR	CA-C-N	-5.58	114.50	120.03
1	B	589	TYR	C-N-CA	-5.58	114.50	120.03
1	B	463	VAL	CA-C-N	-5.57	111.67	121.70
1	B	463	VAL	C-N-CA	-5.57	111.67	121.70
1	A	602	GLN	CA-C-N	-5.56	114.65	120.38
1	A	602	GLN	C-N-CA	-5.56	114.65	120.38
1	A	549	GLU	CA-C-N	5.50	126.23	120.12
1	A	549	GLU	C-N-CA	5.50	126.23	120.12
1	A	522	ALA	CA-C-N	-5.45	114.35	119.85
1	A	522	ALA	C-N-CA	-5.45	114.35	119.85
1	A	321	TYR	N-CA-C	5.43	116.67	109.93
1	A	555	VAL	N-CA-C	-5.42	102.58	109.58
1	A	331	VAL	CB-CA-C	-5.39	102.61	110.81
1	B	551	ARG	N-CA-C	-5.36	106.00	112.54
1	B	210	VAL	N-CA-C	5.31	116.23	108.58
1	A	517	THR	N-CA-C	-5.27	106.63	113.16
1	A	242	ARG	CD-NE-CZ	5.26	131.77	124.40
1	B	582	ASP	N-CA-CB	-5.25	102.25	109.97
1	B	226	PRO	CA-C-N	5.21	131.08	121.70
1	B	226	PRO	C-N-CA	5.21	131.08	121.70
1	A	234	SER	CA-CB-OG	-5.21	100.69	111.10
1	B	207	TRP	CA-C-N	5.20	129.72	122.08
1	B	207	TRP	C-N-CA	5.20	129.72	122.08
1	A	538	VAL	N-CA-C	-5.19	102.15	109.63
1	A	490	CYS	N-CA-C	5.17	116.60	110.97
1	A	505	ALA	CA-C-N	5.14	130.95	121.70
1	A	505	ALA	C-N-CA	5.14	130.95	121.70
1	A	520	LYS	N-CA-C	5.08	117.77	109.59
1	A	474	TRP	N-CA-C	-5.06	103.36	110.50
1	B	441	ASN	CB-CA-C	-5.05	105.08	111.70
1	A	534	HIS	N-CA-C	-5.04	107.18	113.38
1	B	441	ASN	N-CA-C	5.03	115.61	107.32
1	A	451	CYS	CA-CB-SG	-5.01	102.88	114.40
1	B	225	LEU	CA-C-N	-5.01	114.07	120.23
1	B	225	LEU	C-N-CA	-5.01	114.07	120.23

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	58	0
1	B	3197	0	3037	72	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	12	0
All	All	6584	0	5969	128	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 (128) 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:B:441:ASN:HA	1:B:548:MET:HE1	1.50	0.93
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:321:TYR:HB3	1:B:370:MET:HE1	1.55	0.89
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:B:485:PHE:HD2	1:B:529:MET:HE1	1.42	0.83
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:321:TYR:HB3	1:A:370:MET:HE1	1.66	0.76
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:A:441:ASN:HA	1:A:548:MET:HE1	1.70	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:214:MET:HE2	1:B:306:THR:O	1.91	0.70
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:HH11	1:A:419:ARG:CG	2.03	0.65
1:B:563:HIS:CD2	3:B:731:HOH:O	2.49	0.65
1:A:214:MET:HE2	1:A:306:THR:C	2.23	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:A:427:TRP:CG	1:A:428:PHE:H	2.17	0.62
1:B:226:PRO:HA	1:B:227:SER:C	2.25	0.61
1:B:442:LEU:HB2	1:B:579:GLN:HG2	1.83	0.61
1:B:441:ASN:CA	1:B:548:MET:HE1	2.29	0.60
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: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: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:B:207:TRP:CG	1:B:208:GLU:H	2.27	0.53
1:B:299:LYS:NZ	3:B:132:HOH:O	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:TRP:CG	1:A:428:PHE:N	2.76	0.52
1:A:324:ARG:HE	1:A:327:MET:HE3	1.75	0.52
1:B:315:MET:HE3	1:B:319:MET:SD	2.50	0.51
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
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:342:MET:HE1	1:B:378:VAL:HG12	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: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:B:207:TRP:CD1	1:B:208:GLU:H	2.30	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:212:LYS:O	1:B:305:ARG:NH2	2.47	0.48
1:B:530:ASP:OD1	1:B:530:ASP:C	2.57	0.48
1:B:207:TRP:CD1	1:B:208:GLU:N	2.82	0.48
1:B:207:TRP:CG	1:B:208:GLU:N	2.82	0.47
1:B:442:LEU:H	1:B:548:MET:HE2	1.79	0.47
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:214:MET:HE2	1:B:306:THR:C	2.39	0.46
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: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:A:419:ARG:NH1	1:B:422:TYR:HB3	2.31	0.45
1:A:582:ASP:CB	3:A:26:HOH:O	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:367:TRP:CD1	1:B:551:ARG:HB3	2.53	0.44
1:A:214:MET:HE2	1:A:306:THR:O	2.18	0.43
1:A:419:ARG:NH1	1:A:419:ARG:CG	2.72	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:O	1:B:332:VAL:HG13	2.17	0.43
1:B:207:TRP:C	1:B:209:ASP:H	2.25	0.43
1:A:441:ASN:HA	1:A:548:MET:CE	2.44	0.42
1:B:210:VAL:HG21	1:B:262:LEU:CD1	2.49	0.42
1:B:351:GLY:HA2	1:B:370:MET:HE3	2.00	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:217:GLU:HG2	1:B:232:ILE:CD1	2.51	0.41
1:B:573:TRP:CE2	2:B:20:MLZ:HE3	2.55	0.41
1:B:378:VAL:HG21	1:B:409:ASP:CG	2.45	0.41
1:A:332:VAL:HG21	1:A:374:LEU:HD22	2.01	0.41
1:A:482:HIS:CD2	1:A:564:ARG:HD2	2.54	0.41
1:A:498:THR:HA	1:A:499:PRO:HD3	1.81	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

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	382/456 (84%)	352 (92%)	27 (7%)	3 (1%)	16	12
1	B	402/456 (88%)	369 (92%)	29 (7%)	4 (1%)	12	9
All	All	784/912 (86%)	721 (92%)	56 (7%)	7 (1%)	14	10

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%)	290 (92%)	26 (8%)	10	8
1	B	329/397 (83%)	306 (93%)	23 (7%)	14	11
All	All	645/794 (81%)	596 (92%)	49 (8%)	12	9

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LYS
1	A	211	MET
1	A	218	VAL
1	A	277	SER
1	A	284	ARG
1	A	298	MET

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Mol	Chain	Res	Type
1	A	318	SER
1	A	325	GLN
1	A	328	ARG
1	A	331	VAL
1	A	335	SER
1	A	347	THR
1	A	349	ILE
1	A	355	LEU
1	A	419	ARG
1	A	423	THR
1	A	434	LEU
1	A	454	LEU
1	A	455	LEU
1	A	456	ASP
1	A	494	ASP
1	A	506	GLN
1	A	507	THR
1	A	537	LYS
1	A	605	VAL
1	A	608	GLU
1	B	172	GLN
1	B	176	VAL
1	B	189	SER
1	B	211	MET
1	B	218	VAL
1	B	237	GLN
1	B	242	ARG
1	B	265	VAL
1	B	267	VAL
1	B	309	VAL
1	B	314	LYS
1	B	316	VAL
1	B	329	LEU
1	B	341	ARG
1	B	349	ILE
1	B	362	SER
1	B	411	VAL
1	B	423	THR
1	B	434	LEU
1	B	494	ASP
1	B	531	CYS
1	B	582	ASP

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Mol	Chain	Res	Type
1	B	605	VAL

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

Mol	Chain	Res	Type
1	A	386	HIS
1	A	482	HIS
1	A	506	GLN
1	B	256	HIS
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 oligosaccharides 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	B	20	-	8,9,10	1.05	1 (12%)	4,9,11	1.48	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLZ	A	20	-	8,9,10	0.58	0	4,9,11	0.80	0

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	B	20	-	-	2/7/8/10	-
2	MLZ	A	20	-	-	2/7/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	20	MLZ	O-C	2.15	1.28	1.20

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	20	MLZ	CM-NZ-CE	2.68	119.47	112.01

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	20	MLZ	C-CA-CB-CG
2	B	20	MLZ	CG-CD-CE-NZ
2	A	20	MLZ	CA-CB-CG-CD
2	A	20	MLZ	CE-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	20	MLZ	2	0
2	A	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%)	0.33	26 (6%) 24 26	18, 32, 57, 64	0
1	B	410/456 (89%)	0.02	10 (2%) 59 62	16, 28, 52, 63	0
All	All	802/912 (87%)	0.18	36 (4%) 38 40	16, 30, 55, 64	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	226	PRO	4.2
1	A	225	LEU	3.9
1	B	210	VAL	3.8
1	A	323	PHE	3.7
1	A	343	ALA	3.7
1	A	607	ALA	3.7
1	A	359	ASP	3.5
1	A	531	CYS	3.3
1	B	532	PRO	3.2
1	A	172	GLN	3.1
1	B	225	LEU	3.0
1	B	361	ASP	2.8
1	A	333	ASP	2.8
1	A	337	VAL	2.8
1	A	380	TRP	2.8
1	A	606	ALA	2.7
1	A	224	VAL	2.6
1	B	209	ASP	2.5
1	A	340	THR	2.4
1	B	224	VAL	2.4
1	A	423	THR	2.3
1	A	503	TYR	2.3
1	A	348	VAL	2.3
1	B	222	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	408	CYS	2.2
1	A	473	ASP	2.2
1	A	532	PRO	2.2
1	A	512	ASN	2.2
1	A	344	VAL	2.1
1	A	457	GLY	2.1
1	A	420	ALA	2.1
1	B	502	GLY	2.1
1	A	383	ARG	2.1
1	A	338	SER	2.1
1	A	335	SER	2.1
1	A	322	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 oligosaccharides 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(Å ²)	Q<0.9
2	MLZ	A	20	10/11	0.82	0.13	35,62,68,70	0
2	MLZ	B	20	10/11	0.90	0.12	38,60,69,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.