



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:10 PM UTC

PDB ID : 8USO / pdb_00008uso
Title : Full-length human CaMKII delta holoenzyme
Authors : Ozden, C.; Abromson, N.L.; Tomchick, D.R.; Stratton, M.M.; Garman, S.C.
Deposited on : 2023-10-28
Resolution : 2.30 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

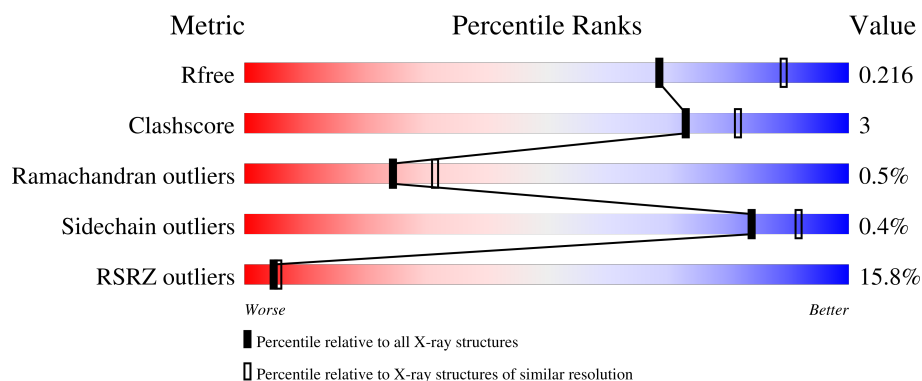
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	450	19% 91% 6% .
1	B	450	10% 90% 6% ..
1	C	450	17% 86% 10% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21153 atoms, of which 10372 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 calcium/calmodulin-dependent protein kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	438	Total	C	H	N	O	S	0	0	0
			6982	2233	3475	616	638	20			
1	B	436	Total	C	H	N	O	S	0	0	0
			6945	2222	3453	614	635	21			
1	C	433	Total	C	H	N	O	S	0	0	0
			6903	2204	3444	609	626	20			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP D6R938
A	?	-	ALA	deletion	UNP D6R938
A	?	-	LYS	deletion	UNP D6R938
A	?	-	SER	deletion	UNP D6R938
A	?	-	LEU	deletion	UNP D6R938
A	?	-	LEU	deletion	UNP D6R938
A	?	-	LYS	deletion	UNP D6R938
A	?	-	LYS	deletion	UNP D6R938
A	?	-	PRO	deletion	UNP D6R938
A	?	-	ASP	deletion	UNP D6R938
A	?	-	GLY	deletion	UNP D6R938
A	?	-	VAL	deletion	UNP D6R938
A	?	-	LYS	deletion	UNP D6R938
A	?	-	GLU	deletion	UNP D6R938
A	?	-	SER	deletion	UNP D6R938
A	?	-	THR	deletion	UNP D6R938
A	?	-	GLU	deletion	UNP D6R938
A	?	-	SER	deletion	UNP D6R938
A	?	-	SER	deletion	UNP D6R938
A	?	-	ASN	deletion	UNP D6R938
A	?	-	THR	deletion	UNP D6R938
A	?	-	THR	deletion	UNP D6R938
A	?	-	ILE	deletion	UNP D6R938

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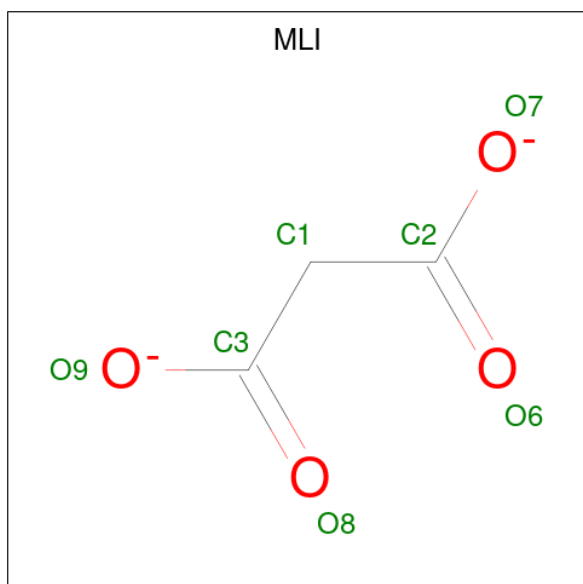
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP D6R938
A	?	-	ASP	deletion	UNP D6R938
A	?	-	GLU	deletion	UNP D6R938
A	?	-	ASP	deletion	UNP D6R938
A	?	-	VAL	deletion	UNP D6R938
A	?	-	LYS	deletion	UNP D6R938
A	364	CYS	ASP	engineered mutation	UNP D6R938
B	0	SER	-	expression tag	UNP D6R938
B	?	-	ALA	deletion	UNP D6R938
B	?	-	LYS	deletion	UNP D6R938
B	?	-	SER	deletion	UNP D6R938
B	?	-	LEU	deletion	UNP D6R938
B	?	-	LEU	deletion	UNP D6R938
B	?	-	LYS	deletion	UNP D6R938
B	?	-	LYS	deletion	UNP D6R938
B	?	-	PRO	deletion	UNP D6R938
B	?	-	ASP	deletion	UNP D6R938
B	?	-	GLY	deletion	UNP D6R938
B	?	-	VAL	deletion	UNP D6R938
B	?	-	LYS	deletion	UNP D6R938
B	?	-	GLU	deletion	UNP D6R938
B	?	-	SER	deletion	UNP D6R938
B	?	-	THR	deletion	UNP D6R938
B	?	-	GLU	deletion	UNP D6R938
B	?	-	SER	deletion	UNP D6R938
B	?	-	SER	deletion	UNP D6R938
B	?	-	ASN	deletion	UNP D6R938
B	?	-	THR	deletion	UNP D6R938
B	?	-	THR	deletion	UNP D6R938
B	?	-	ILE	deletion	UNP D6R938
B	?	-	GLU	deletion	UNP D6R938
B	?	-	ASP	deletion	UNP D6R938
B	?	-	GLU	deletion	UNP D6R938
B	?	-	ASP	deletion	UNP D6R938
B	?	-	VAL	deletion	UNP D6R938
B	?	-	LYS	deletion	UNP D6R938
B	364	CYS	ASP	engineered mutation	UNP D6R938
C	0	SER	-	expression tag	UNP D6R938
C	?	-	ALA	deletion	UNP D6R938
C	?	-	LYS	deletion	UNP D6R938
C	?	-	SER	deletion	UNP D6R938
C	?	-	LEU	deletion	UNP D6R938

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP D6R938
C	?	-	LYS	deletion	UNP D6R938
C	?	-	LYS	deletion	UNP D6R938
C	?	-	PRO	deletion	UNP D6R938
C	?	-	ASP	deletion	UNP D6R938
C	?	-	GLY	deletion	UNP D6R938
C	?	-	VAL	deletion	UNP D6R938
C	?	-	LYS	deletion	UNP D6R938
C	?	-	GLU	deletion	UNP D6R938
C	?	-	SER	deletion	UNP D6R938
C	?	-	THR	deletion	UNP D6R938
C	?	-	GLU	deletion	UNP D6R938
C	?	-	SER	deletion	UNP D6R938
C	?	-	SER	deletion	UNP D6R938
C	?	-	ASN	deletion	UNP D6R938
C	?	-	THR	deletion	UNP D6R938
C	?	-	THR	deletion	UNP D6R938
C	?	-	ILE	deletion	UNP D6R938
C	?	-	GLU	deletion	UNP D6R938
C	?	-	ASP	deletion	UNP D6R938
C	?	-	GLU	deletion	UNP D6R938
C	?	-	ASP	deletion	UNP D6R938
C	?	-	VAL	deletion	UNP D6R938
C	?	-	LYS	deletion	UNP D6R938
C	364	CYS	ASP	engineered mutation	UNP D6R938

- Molecule 2 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 3 4	0	0
2	B	1	Total C O 7 3 4	0	0
2	C	1	Total C O 7 3 4	0	0

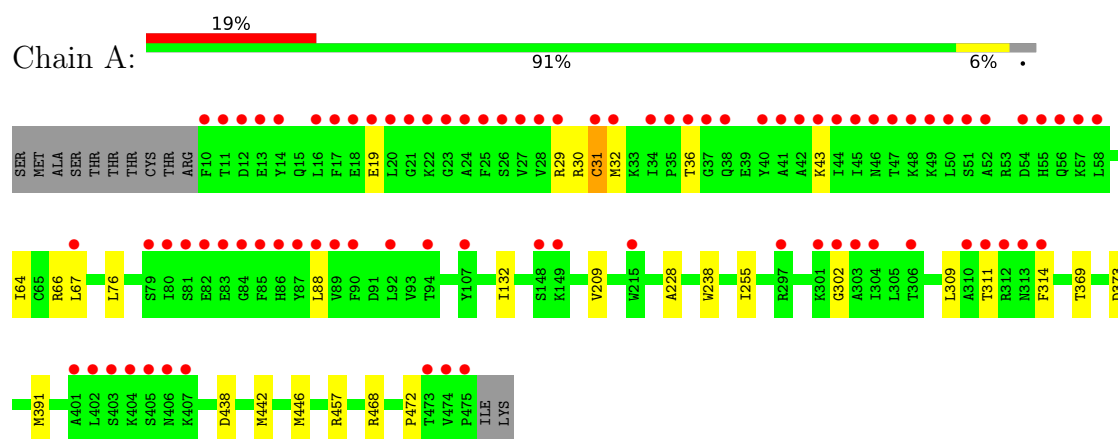
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	87	Total O 87 87	0	0
3	B	96	Total O 96 96	0	0
3	C	119	Total O 119 119	0	0

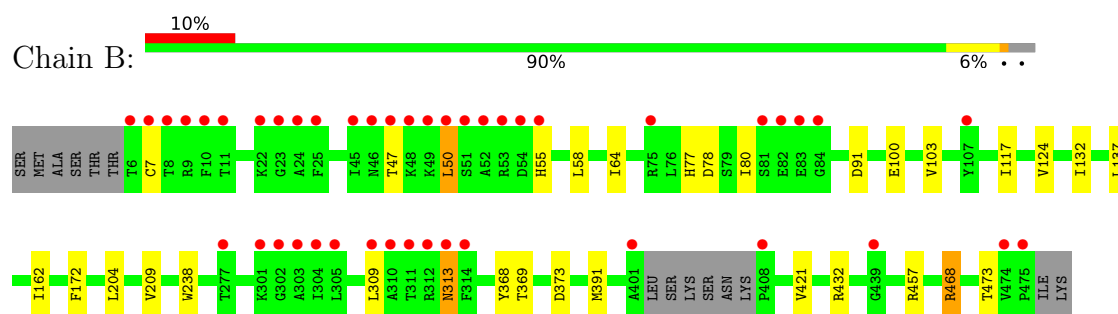
3 Residue-property plots [i](#)

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.

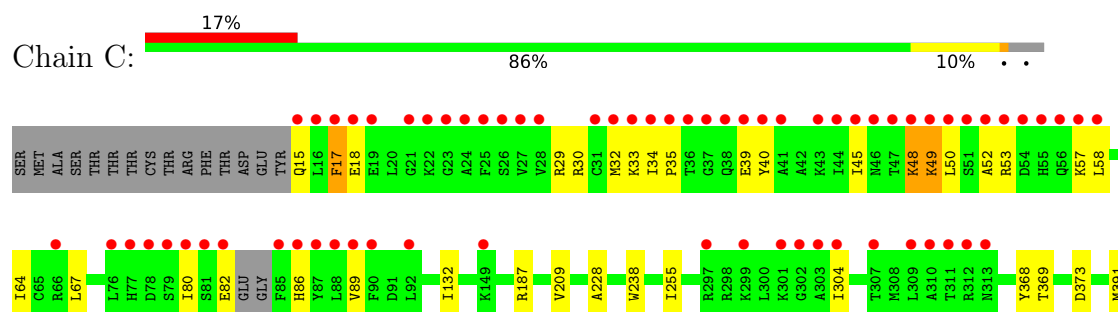
- Molecule 1: calcium/calmodulin-dependent protein kinase

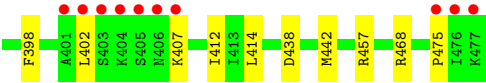


- Molecule 1: calcium/calmodulin-dependent protein kinase



- Molecule 1: calcium/calmodulin-dependent protein kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	174.98Å 174.98Å 140.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.53 – 2.30 48.53 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.8 (48.53-2.30) 89.8 (48.53-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.184 , 0.213 0.191 , 0.216	Depositor DCC
R_{free} test set	2000 reflections (2.07%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21153	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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: MLI

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	0.09	0/3593	0.27	0/4862
1	B	0.09	0/3577	0.27	0/4840
1	C	0.38	2/3542 (0.1%)	0.72	6/4790 (0.1%)
All	All	0.23	2/10712 (0.0%)	0.47	6/14492 (0.0%)

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	1
1	C	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	49	LYS	C-N	-18.54	1.07	1.33
1	C	48	LYS	C-N	-11.64	1.18	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	48	LYS	CA-C-N	24.75	161.97	122.36
1	C	48	LYS	C-N-CA	24.75	161.97	122.36
1	C	48	LYS	O-C-N	-23.13	91.82	122.59
1	C	49	LYS	O-C-N	-12.05	107.78	122.96
1	C	49	LYS	CA-C-N	9.09	138.90	121.54
1	C	49	LYS	C-N-CA	9.09	138.90	121.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	468	ARG	Sidechain
1	C	48	LYS	Mainchain
1	C	49	LYS	Mainchain

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	3507	3475	3474	16	0
1	B	3492	3453	3453	21	0
1	C	3459	3444	3440	30	0
2	A	7	0	2	1	0
2	B	7	0	2	1	0
2	C	7	0	2	1	0
3	A	87	0	0	0	0
3	B	96	0	0	0	0
3	C	119	0	0	0	0
All	All	10781	10372	10373	67	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 3.

All (67) 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:B:369:THR:HG22	1:B:391:MET:HE2	1.58	0.85
1:C:369:THR:HG22	1:C:391:MET:HE2	1.67	0.77
1:C:64:ILE:HG23	1:C:132:ILE:HD13	1.74	0.70
1:A:369:THR:HG22	1:A:391:MET:HE2	1.76	0.68
1:C:442:MET:HE2	1:C:442:MET:HA	1.77	0.65
1:A:67:LEU:HD23	1:A:132:ILE:HD11	1.77	0.65
1:A:64:ILE:HG23	1:A:132:ILE:HD13	1.79	0.63
1:B:309:LEU:HD12	1:B:309:LEU:O	1.99	0.61
1:B:162:ILE:HD13	1:B:172:PHE:CG	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ASP:OD2	1:B:457:ARG:NH1	2.36	0.57
1:A:442:MET:HA	1:A:442:MET:HE2	1.85	0.57
1:B:50:LEU:HD22	1:B:55:HIS:HA	1.88	0.56
1:B:368:TYR:CE2	1:B:391:MET:HE1	2.41	0.55
1:C:15:GLN:HB2	1:C:32:MET:HB2	1.87	0.55
1:B:368:TYR:CD2	1:B:391:MET:HE1	2.41	0.55
1:C:18:GLU:CD	1:C:30:ARG:HE	2.15	0.54
1:B:468:ARG:NH2	2:B:501:MLI:O6	2.41	0.54
1:B:77:HIS:NE2	1:B:91:ASP:OD1	2.40	0.53
1:C:50:LEU:HD12	1:C:50:LEU:O	2.09	0.52
1:C:228:ALA:C	1:C:255:ILE:HD11	2.34	0.52
1:C:412:ILE:HG22	1:C:414:LEU:CD1	2.39	0.52
1:C:438:ASP:OD1	1:C:442:MET:N	2.43	0.52
1:C:398:PHE:HA	1:C:402:LEU:HD12	1.92	0.52
1:B:7:CYS:SG	1:B:80:ILE:HG23	2.50	0.51
1:A:43:LYS:HD3	1:A:88:LEU:HD12	1.92	0.51
1:C:32:MET:CG	1:C:39:GLU:HG2	2.41	0.51
1:C:373:ASP:OD2	1:C:457:ARG:NH1	2.42	0.51
1:C:45:ILE:HD12	1:C:58:LEU:HD21	1.91	0.51
1:A:373:ASP:OD1	1:A:457:ARG:NH1	2.41	0.50
1:C:67:LEU:HD23	1:C:132:ILE:HD11	1.94	0.50
1:C:368:TYR:CD2	1:C:391:MET:HE1	2.47	0.49
1:C:45:ILE:HB	1:C:86:HIS:HB3	1.93	0.49
1:C:34:ILE:CG2	1:C:35:PRO:HD3	2.42	0.48
1:C:33:LYS:HB2	1:C:40:TYR:HE2	1.77	0.48
1:A:228:ALA:C	1:A:255:ILE:HD11	2.38	0.48
1:B:100:GLU:O	1:B:103:VAL:HG22	2.13	0.47
1:A:311:THR:HG1	1:A:314:PHE:HZ	1.62	0.47
1:A:209:VAL:HG11	1:A:238:TRP:CE2	2.51	0.46
1:B:117:ILE:HG13	1:B:204:LEU:HD13	1.98	0.46
1:B:421:VAL:HG12	1:B:421:VAL:O	2.15	0.46
1:B:209:VAL:HG11	1:B:238:TRP:CE2	2.51	0.45
1:C:32:MET:HG2	1:C:39:GLU:HG2	1.99	0.45
1:C:89:VAL:O	1:C:89:VAL:HG13	2.17	0.45
1:A:446:MET:HE1	1:A:472:PRO:O	2.17	0.45
1:C:209:VAL:HG11	1:C:238:TRP:CE2	2.52	0.44
1:C:398:PHE:CG	1:C:402:LEU:HD12	2.52	0.44
1:C:468:ARG:NH2	2:C:501:MLI:O8	2.51	0.44
1:C:34:ILE:HG23	1:C:35:PRO:HD3	1.99	0.43
1:B:50:LEU:HD21	1:B:58:LEU:HD22	2.00	0.43
1:A:36:THR:HG22	1:A:36:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ARG:HE	1:C:57:LYS:HE3	1.83	0.43
1:A:66:ARG:HG3	1:A:76:LEU:HD23	2.00	0.43
1:C:304:ILE:N	1:C:304:ILE:HD12	2.34	0.42
1:A:31:CYS:SG	1:A:32:MET:N	2.92	0.42
1:A:438:ASP:OD1	1:A:442:MET:N	2.43	0.42
1:B:47:THR:HA	1:B:50:LEU:HD12	2.01	0.42
1:C:17:PHE:C	1:C:29:ARG:HE	2.28	0.42
1:B:432:ARG:NH1	1:B:473:THR:HG21	2.35	0.41
1:B:124:VAL:HG21	1:B:137:LEU:HD21	2.02	0.41
1:C:368:TYR:CE2	1:C:391:MET:HE1	2.55	0.41
1:B:64:ILE:HG23	1:B:132:ILE:HD13	2.02	0.41
1:B:313:ASN:O	1:B:313:ASN:ND2	2.53	0.41
1:C:187:ARG:HH12	1:C:255:ILE:HG23	1.85	0.41
1:B:78:ASP:CG	1:B:80:ILE:HD11	2.46	0.41
1:A:19:GLU:HA	1:A:29:ARG:HG2	2.02	0.41
1:C:80:ILE:CG2	1:C:82:GLU:HG3	2.51	0.40
1:A:468:ARG:NH2	2:A:501:MLI:O8	2.54	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	436/450 (97%)	416 (95%)	19 (4%)	1 (0%)	43	55
1	B	432/450 (96%)	413 (96%)	17 (4%)	2 (0%)	24	31
1	C	429/450 (95%)	401 (94%)	25 (6%)	3 (1%)	18	23
All	All	1297/1350 (96%)	1230 (95%)	61 (5%)	6 (0%)	24	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	GLY
1	B	50	LEU
1	B	313	ASN
1	C	17	PHE
1	C	52	ALA
1	C	475	PRO

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	376/387 (97%)	373 (99%)	3 (1%)	73	86
1	B	374/387 (97%)	374 (100%)	0	100	100
1	C	371/387 (96%)	370 (100%)	1 (0%)	86	93
All	All	1121/1161 (97%)	1117 (100%)	4 (0%)	84	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	31	CYS
1	A	309	LEU
1	C	407	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	220	HIS
1	A	415	ASN
1	A	462	GLN
1	B	224	GLN
1	B	250	ASN
1	C	126	HIS
1	C	347	GLN

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Mol	Chain	Res	Type
1	C	386	ASN
1	C	419	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](#)

3 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	MLI	B	501	-	6,6,6	1.58	1 (16%)	7,7,7	1.14	0
2	MLI	C	501	-	6,6,6	1.59	1 (16%)	7,7,7	1.23	1 (14%)
2	MLI	A	501	-	6,6,6	1.60	1 (16%)	7,7,7	1.01	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	MLI	B	501	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLI	C	501	-	-	4/4/4/4	-
2	MLI	A	501	-	-	4/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	MLI	C1-C3	2.47	1.54	1.51
2	C	501	MLI	C1-C3	2.38	1.54	1.51
2	B	501	MLI	C1-C3	2.26	1.54	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	MLI	O8-C3-C1	-2.12	116.07	122.11

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	MLI	C3-C1-C2-O7
2	C	501	MLI	C3-C1-C2-O6
2	A	501	MLI	C2-C1-C3-O9
2	C	501	MLI	C2-C1-C3-O9
2	A	501	MLI	C2-C1-C3-O8
2	C	501	MLI	C2-C1-C3-O8
2	A	501	MLI	C3-C1-C2-O7
2	A	501	MLI	C3-C1-C2-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	MLI	1	0
2	C	501	MLI	1	0
2	A	501	MLI	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	48:LYS	C	49:LYS	N	1.18
1	C	49:LYS	C	50:LEU	N	1.07

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	438/450 (97%)	0.62	84 (19%) 3 3	18, 48, 132, 160	0
1	B	436/450 (96%)	0.26	44 (10%) 12 14	18, 45, 104, 156	0
1	C	433/450 (96%)	0.55	78 (18%) 3 4	16, 41, 142, 183	0
All	All	1307/1350 (96%)	0.47	206 (15%) 5 5	16, 45, 131, 183	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	303	ALA	9.9
1	C	85	PHE	9.5
1	B	50	LEU	9.0
1	A	302	GLY	8.9
1	C	24	ALA	8.8
1	A	311	THR	8.2
1	C	50	LEU	7.8
1	B	312	ARG	7.3
1	C	34	ILE	7.2
1	B	310	ALA	7.1
1	C	25	PHE	7.0
1	C	45	ILE	6.9
1	A	405	SER	6.5
1	A	303	ALA	6.3
1	C	44	ILE	6.1
1	C	310	ALA	6.1
1	C	23	GLY	6.0
1	B	311	THR	5.9
1	C	47	THR	5.9
1	C	87	TYR	5.8
1	B	309	LEU	5.8
1	C	28	VAL	5.6
1	A	52	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	25	PHE	5.5
1	B	475	PRO	5.5
1	C	302	GLY	5.4
1	C	27	VAL	5.4
1	C	88	LEU	5.4
1	B	48	LYS	5.4
1	C	476	ILE	5.3
1	A	310	ALA	5.3
1	A	474	VAL	5.3
1	A	85	PHE	5.3
1	C	46	ASN	5.3
1	C	311	THR	5.3
1	B	6	THR	5.1
1	B	474	VAL	5.1
1	A	10	PHE	5.1
1	C	312	ARG	5.1
1	A	313	ASN	5.0
1	B	49	LYS	5.0
1	A	406	ASN	5.0
1	C	402	LEU	4.9
1	C	82	GLU	4.9
1	C	43	LYS	4.9
1	C	16	LEU	4.9
1	C	86	HIS	4.9
1	C	35	PRO	4.8
1	A	23	GLY	4.8
1	C	22	LYS	4.8
1	A	27	VAL	4.8
1	B	46	ASN	4.7
1	C	313	ASN	4.7
1	A	16	LEU	4.7
1	C	80	ILE	4.7
1	A	149	LYS	4.6
1	C	301	LYS	4.6
1	A	12	ASP	4.6
1	A	312	ARG	4.6
1	C	36	THR	4.5
1	A	404	LYS	4.5
1	A	83	GLU	4.5
1	A	50	LEU	4.5
1	C	81	SER	4.5
1	C	54	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	17	PHE	4.4
1	B	52	ALA	4.4
1	B	25	PHE	4.4
1	C	403	SER	4.3
1	A	44	ILE	4.2
1	C	48	LYS	4.2
1	B	47	THR	4.2
1	A	304	ILE	4.2
1	A	87	TYR	4.2
1	A	401	ALA	4.2
1	B	305	LEU	4.2
1	A	34	ILE	4.1
1	A	51	SER	4.1
1	C	26	SER	4.1
1	A	11	THR	4.1
1	A	17	PHE	4.0
1	A	20	LEU	3.9
1	C	309	LEU	3.9
1	B	313	ASN	3.9
1	A	24	ALA	3.9
1	A	45	ILE	3.9
1	A	215	TRP	3.9
1	A	48	LYS	3.8
1	A	90	PHE	3.8
1	B	302	GLY	3.8
1	A	35	PRO	3.8
1	C	37	GLY	3.8
1	C	40	TYR	3.7
1	C	55	HIS	3.7
1	A	43	LYS	3.7
1	A	28	VAL	3.7
1	C	307	THR	3.7
1	B	401	ALA	3.6
1	C	52	ALA	3.6
1	A	84	GLY	3.6
1	A	475	PRO	3.6
1	C	51	SER	3.6
1	B	45	ILE	3.6
1	B	84	GLY	3.6
1	C	15	GLN	3.5
1	A	55	HIS	3.5
1	B	8	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	31	CYS	3.5
1	C	49	LYS	3.5
1	C	149	LYS	3.5
1	B	303	ALA	3.5
1	C	33	LYS	3.5
1	A	47	THR	3.4
1	A	22	LYS	3.4
1	C	405	SER	3.4
1	B	24	ALA	3.4
1	A	58	LEU	3.3
1	A	107	TYR	3.3
1	A	42	ALA	3.3
1	C	89	VAL	3.3
1	A	88	LEU	3.3
1	A	80	ILE	3.3
1	A	301	LYS	3.3
1	A	37	GLY	3.2
1	C	53	ARG	3.2
1	C	32	MET	3.2
1	A	13	GLU	3.2
1	A	403	SER	3.2
1	B	439	GLY	3.2
1	B	51	SER	3.1
1	B	314	PHE	3.1
1	B	408	PRO	3.1
1	B	7	CYS	3.1
1	A	81	SER	3.1
1	B	107	TYR	3.1
1	B	22	LYS	3.1
1	C	21	GLY	3.0
1	C	39	GLU	3.0
1	B	75	ARG	3.0
1	A	407	LYS	3.0
1	A	49	LYS	2.9
1	C	404	LYS	2.9
1	C	477	LYS	2.9
1	C	79	SER	2.9
1	B	304	ILE	2.9
1	A	14	TYR	2.8
1	A	31	CYS	2.8
1	C	406	ASN	2.8
1	A	26	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	76	LEU	2.8
1	C	57	LYS	2.8
1	C	38	GLN	2.8
1	A	18	GLU	2.8
1	B	82	GLU	2.8
1	A	92	LEU	2.7
1	A	56	GLN	2.7
1	A	46	ASN	2.7
1	C	41	ALA	2.7
1	A	36	THR	2.7
1	A	402	LEU	2.7
1	A	89	VAL	2.7
1	C	475	PRO	2.7
1	A	86	HIS	2.6
1	B	81	SER	2.6
1	A	19	GLU	2.6
1	C	90	PHE	2.6
1	A	54	ASP	2.6
1	B	23	GLY	2.6
1	B	277	THR	2.6
1	A	29	ARG	2.6
1	A	314	PHE	2.6
1	A	306	THR	2.5
1	B	53	ARG	2.5
1	C	78	ASP	2.5
1	A	79	SER	2.4
1	C	92	LEU	2.4
1	B	11	THR	2.4
1	C	407	LYS	2.4
1	A	297	ARG	2.4
1	C	304	ILE	2.4
1	A	40	TYR	2.4
1	A	41	ALA	2.4
1	C	401	ALA	2.4
1	A	473	THR	2.4
1	C	18	GLU	2.4
1	C	19	GLU	2.4
1	A	57	LYS	2.3
1	A	38	GLN	2.3
1	B	83	GLU	2.3
1	C	56	GLN	2.3
1	B	301	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	21	GLY	2.3
1	B	10	PHE	2.3
1	C	299	LYS	2.3
1	A	32	MET	2.2
1	B	9	ARG	2.2
1	A	148	SER	2.2
1	A	67	LEU	2.1
1	A	82	GLU	2.1
1	C	297	ARG	2.1
1	C	66	ARG	2.1
1	B	55	HIS	2.1
1	A	94	THR	2.0
1	B	54	ASP	2.0
1	C	77	HIS	2.0
1	C	58	LEU	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($\text{\AA}^2$)	Q<0.9
2	MLI	B	501	7/7	0.93	0.11	26,33,44,58	0
2	MLI	A	501	7/7	0.95	0.08	25,29,40,41	0
2	MLI	C	501	7/7	0.97	0.06	26,28,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.