



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:01 AM BST

PDB ID : 4GN1  
Title : Crystal Structure of the RA and PH domains of Lamellipodin  
Authors : Chang, Y.C.E.; Wu, J.  
Deposited on : 2012-08-16  
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

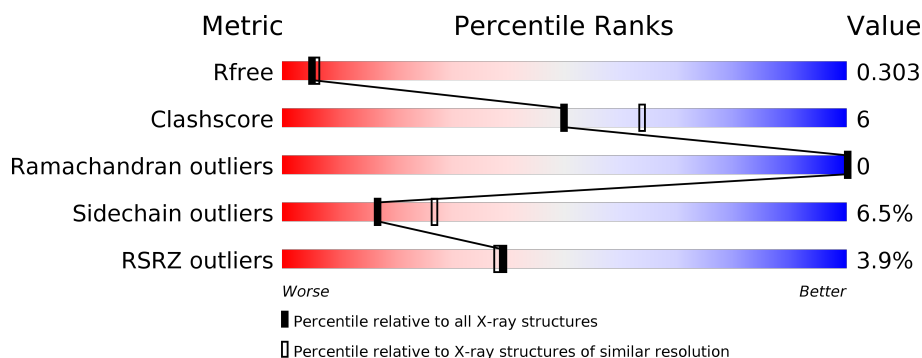
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	255	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>••</div> </div> </div>
1	B	255	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>••</div> </div> </div>
1	C	255	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>• 6%</div> </div> </div>
1	D	255	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 6%</div> </div> </div>

## 2 Entry composition [i](#)

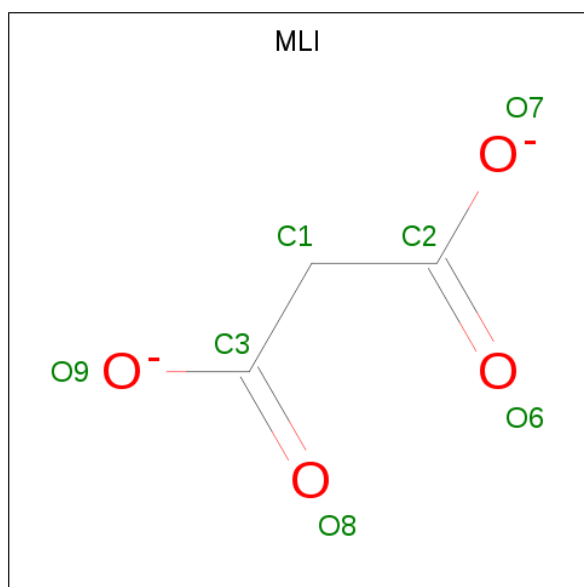
There are 3 unique types of molecules in this entry. The entry contains 8481 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ras-associated and pleckstrin homology domains-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	1	0
			2091	1334	359	382	16			
1	B	250	Total	C	N	O	S	0	4	0
			2099	1341	358	382	18			
1	C	240	Total	C	N	O	S	0	1	0
			2011	1284	342	369	16			
1	D	240	Total	C	N	O	S	0	0	0
			2003	1279	341	368	15			

- Molecule 2 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



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

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

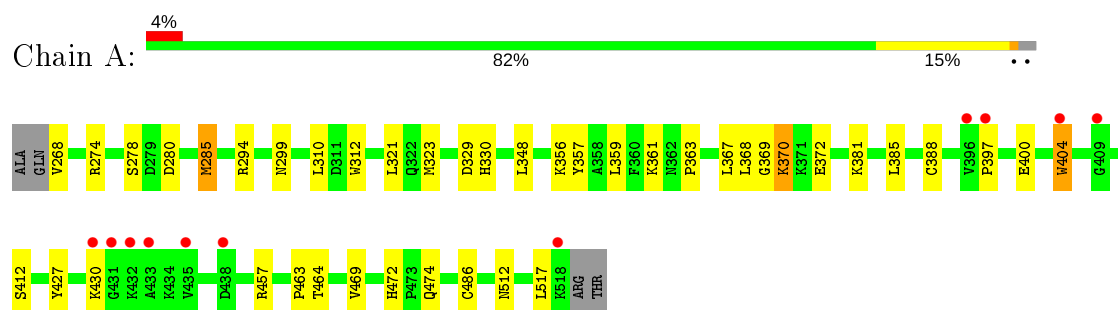
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	59	Total	O	0	0
			59	59		
3	C	68	Total	O	0	0
			68	68		
3	D	60	Total	O	0	0
			60	60		

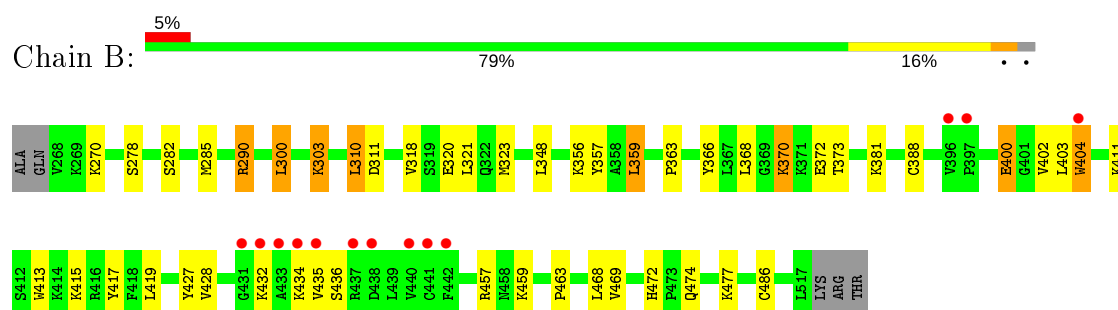
### 3 Residue-property plots

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.

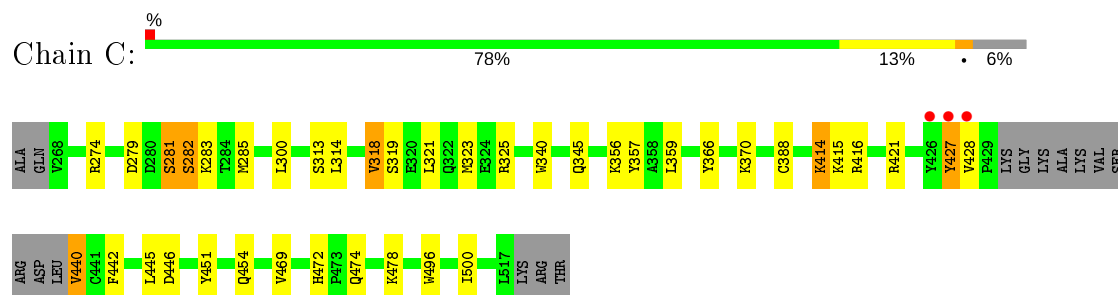
- Molecule 1: Ras-associated and pleckstrin homology domains-containing protein 1



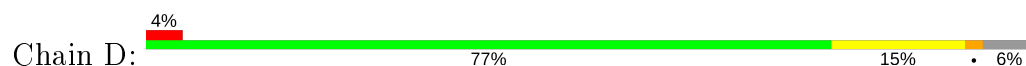
- Molecule 1: Ras-associated and pleckstrin homology domains-containing protein 1

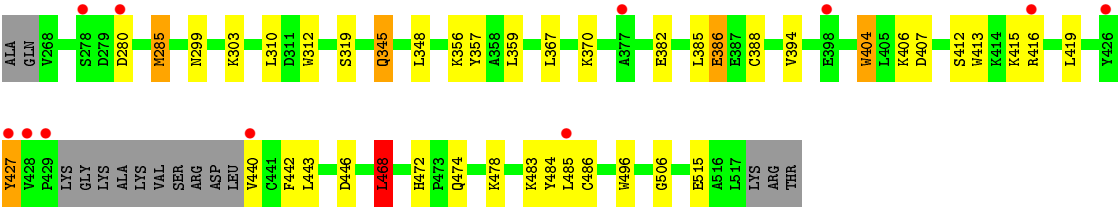


- Molecule 1: Ras-associated and pleckstrin homology domains-containing protein 1



- Molecule 1: Ras-associated and pleckstrin homology domains-containing protein 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.34Å 93.47Å 80.72Å 90.00° 104.91° 90.00°	Depositor
Resolution (Å)	46.73 – 2.40 46.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.73-2.40) 98.8 (46.73-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.61 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.253 , 0.303 0.253 , 0.303	Depositor DCC
$R_{free}$ test set	2158 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8481	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5340e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.63	2/2136 (0.1%)	0.72	0/2874
1	B	0.62	2/2150 (0.1%)	0.72	0/2893
1	C	0.64	2/2052 (0.1%)	0.68	0/2763
1	D	0.65	4/2044 (0.2%)	0.72	1/2753 (0.0%)
All	All	0.63	10/8382 (0.1%)	0.71	1/11283 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	TRP	CD2-CE2	5.75	1.48	1.41
1	B	413	TRP	CD2-CE2	5.67	1.48	1.41
1	C	496	TRP	CD2-CE2	5.58	1.48	1.41
1	D	312	TRP	CD2-CE2	5.57	1.48	1.41
1	D	496	TRP	CD2-CE2	5.30	1.47	1.41
1	D	413	TRP	CD2-CE2	5.25	1.47	1.41
1	B	404	TRP	CD2-CE2	5.24	1.47	1.41
1	C	340	TRP	CD2-CE2	5.23	1.47	1.41
1	D	404	TRP	CD2-CE2	5.19	1.47	1.41
1	A	312	TRP	CD2-CE2	5.14	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	468	LEU	CA-CB-CG	5.85	128.76	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2091	0	2105	24	0
1	B	2099	0	2118	31	0
1	C	2011	0	2005	21	0
1	D	2003	0	1997	23	0
2	A	7	0	2	0	0
2	B	7	0	2	0	0
2	C	7	0	2	1	0
2	D	7	0	2	0	0
3	A	62	0	0	2	0
3	B	59	0	0	0	0
3	C	68	0	0	0	0
3	D	60	0	0	1	0
All	All	8481	0	8233	96	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 6.

All (96) 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:400:GLU:HG3	1:B:417:TYR:OH	1.59	1.00
1:D:443:LEU:HD13	3:D:760:HOH:O	1.67	0.94
1:B:472:HIS:HD2	1:B:474:GLN:H	1.15	0.89
1:B:370:LYS:HE3	1:B:372:GLU:HB3	1.56	0.86
1:A:363:PRO:HD2	1:A:381:LYS:HG2	1.69	0.74
1:A:321:LEU:HB3	1:A:323:MET:HE2	1.69	0.73
1:D:468:LEU:HD13	1:D:485:LEU:HB2	1.71	0.72
1:B:472:HIS:CD2	1:B:474:GLN:H	2.04	0.71
1:A:356:LYS:HE3	1:A:357:TYR:CE2	2.27	0.69
1:A:367:LEU:O	1:A:397:PRO:HG2	1.91	0.69
1:C:279:ASP:OD1	1:C:281:SER:HB3	1.93	0.69
1:B:404:TRP:HB2	1:B:486:CYS:HB3	1.76	0.68
1:B:402:VAL:O	1:B:403:LEU:HD12	1.96	0.66
1:A:280:ASP:HB2	1:B:290:ARG:HH21	1.61	0.66
1:D:427:TYR:O	1:D:440:VAL:HB	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LEU:HB3	1:A:323:MET:CE	2.29	0.63
1:B:285[A]:MET:SD	1:B:300:LEU:HD13	2.39	0.62
1:A:280:ASP:HB2	1:B:290:ARG:NH2	2.15	0.61
1:A:404:TRP:HB2	1:A:486:CYS:HB3	1.82	0.61
1:B:356:LYS:HE3	1:B:357:TYR:CE2	2.36	0.60
1:D:416:ARG:HG2	1:D:427:TYR:HD1	1.65	0.60
1:D:472:HIS:HE1	1:D:474:GLN:OE1	1.85	0.60
1:B:323:MET:CE	1:B:469:VAL:HG11	2.32	0.59
1:A:330:HIS:HD2	1:A:512:ASN:HD21	1.50	0.58
1:C:323:MET:HE1	1:C:469:VAL:HG21	1.86	0.58
1:B:323:MET:HE1	1:B:469:VAL:HG11	1.84	0.58
1:B:404:TRP:CD2	1:B:463:PRO:HG2	2.40	0.57
1:A:330:HIS:CD2	1:A:512:ASN:HD21	2.23	0.57
1:C:323:MET:CE	1:C:469:VAL:HG11	2.35	0.57
1:C:472:HIS:HE1	1:C:474:GLN:OE1	1.88	0.56
1:C:319:SER:CB	1:C:345:GLN:HB2	2.36	0.56
1:D:299:ASN:HB3	1:D:303:LYS:HZ2	1.70	0.56
1:B:404:TRP:CG	1:B:463:PRO:HG2	2.41	0.54
1:C:415:LYS:O	1:C:416:ARG:HD3	2.07	0.54
1:D:382:GLU:O	1:D:386:GLU:HG2	2.08	0.53
1:A:363:PRO:HB3	1:A:385:LEU:HD21	1.91	0.53
1:C:274:ARG:NH1	1:C:282:SER:OG	2.43	0.52
1:C:323:MET:HE1	1:C:469:VAL:HG11	1.92	0.51
1:B:318[A]:VAL:HG12	1:B:323:MET:HG3	1.92	0.51
1:C:318:VAL:HG22	1:C:321:LEU:HB2	1.92	0.51
1:D:416:ARG:HG2	1:D:427:TYR:CD1	2.44	0.51
1:B:363:PRO:HD2	1:B:381:LYS:HG2	1.93	0.51
1:B:320:GLU:HG2	1:B:477:LYS:HA	1.93	0.51
1:A:369:GLY:HA2	1:A:370:LYS:C	2.31	0.50
1:C:319:SER:OG	1:C:345:GLN:HB2	2.11	0.50
1:B:428:VAL:HG11	1:B:435:VAL:HB	1.94	0.49
1:B:472:HIS:HD2	1:B:474:GLN:N	1.97	0.49
1:D:394:VAL:HG21	1:D:506:GLY:HA2	1.95	0.48
1:D:394:VAL:HG21	1:D:506:GLY:CA	2.43	0.48
1:C:427:TYR:CD2	1:C:442:PHE:HB2	2.49	0.48
1:A:404:TRP:CD2	1:A:463:PRO:HG3	2.49	0.48
1:C:359:LEU:HA	1:C:366:TYR:CD1	2.48	0.48
1:C:285[B]:MET:SD	1:C:300:LEU:HG	2.55	0.47
1:A:323:MET:HE1	1:A:469:VAL:HG11	1.96	0.47
1:B:402:VAL:HG12	1:B:415:LYS:HD2	1.95	0.47
1:A:357:TYR:O	1:A:361:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:LEU:HD23	1:B:468:LEU:H	1.79	0.46
1:C:451:TYR:OH	2:C:601:MLI:O6	2.23	0.46
1:D:406:LYS:HG2	1:D:407:ASP:O	2.14	0.46
1:A:359:LEU:HB3	3:A:739:HOH:O	2.15	0.46
1:B:318[A]:VAL:HG13	1:B:318[A]:VAL:O	2.16	0.46
1:C:445:LEU:HD13	1:C:500:ILE:HG23	1.98	0.46
1:B:318[A]:VAL:HG13	1:B:321:LEU:HB2	1.98	0.45
1:D:319:SER:OG	1:D:345:GLN:HB2	2.17	0.45
1:B:359:LEU:HA	1:B:366:TYR:CD1	2.52	0.45
1:B:370:LYS:CE	1:B:372:GLU:HB3	2.38	0.45
1:D:442:PHE:CZ	1:D:483:LYS:HG2	2.50	0.45
1:D:404:TRP:CE3	1:D:415:LYS:HG3	2.52	0.45
1:A:323:MET:CE	1:A:469:VAL:HG11	2.46	0.45
1:D:310:LEU:H	1:D:310:LEU:HD23	1.80	0.45
1:B:411:LYS:HE2	1:B:459:LYS:O	2.17	0.44
1:D:356:LYS:HE3	1:D:357:TYR:CE2	2.53	0.44
1:D:406:LYS:HB3	1:D:484:TYR:HB2	1.99	0.44
1:C:414:LYS:HB3	1:C:414:LYS:HE3	1.59	0.43
1:D:359:LEU:HD12	1:D:359:LEU:C	2.39	0.43
1:B:472:HIS:CD2	1:B:474:GLN:HG3	2.53	0.43
1:A:363:PRO:CD	1:A:381:LYS:HG2	2.45	0.43
1:A:472:HIS:HE1	1:A:474:GLN:HG3	1.83	0.43
1:C:427:TYR:O	1:C:440:VAL:HG22	2.19	0.43
1:A:285:MET:HE1	1:A:299:ASN:HB3	2.00	0.43
1:A:310:LEU:HD13	1:A:517:LEU:HD13	2.02	0.42
1:C:356:LYS:HE3	1:C:357:TYR:CE2	2.54	0.42
1:C:314:LEU:HA	1:C:314:LEU:HD12	1.87	0.42
1:C:325:ARG:HB2	1:C:451:TYR:CD2	2.55	0.42
1:C:313:SER:OG	1:C:356:LYS:HE2	2.20	0.42
1:A:412:SER:HB2	1:D:515:GLU:HG2	2.01	0.42
1:B:303:LYS:HA	1:B:303:LYS:HD2	1.74	0.42
1:D:404:TRP:CZ3	1:D:415:LYS:HG3	2.55	0.42
1:D:367:LEU:HD11	1:D:385:LEU:HD23	2.02	0.41
1:B:310:LEU:HD13	1:B:311:ASP:OD1	2.20	0.41
1:B:434:LYS:HE3	1:B:434:LYS:HB2	1.96	0.41
1:A:274:ARG:HD2	3:A:757:HOH:O	2.22	0.40
1:D:404:TRP:HB2	1:D:486:CYS:HB3	2.03	0.40
1:A:294:ARG:HB2	1:A:329:ASP:HB3	2.03	0.40
1:D:285:MET:HE2	1:D:285:MET:HB2	1.93	0.40
1:B:472:HIS:NE2	1:B:474:GLN:HG3	2.36	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	250/255 (98%)	238 (95%)	12 (5%)	0	100	100
1	B	252/255 (99%)	239 (95%)	13 (5%)	0	100	100
1	C	237/255 (93%)	228 (96%)	9 (4%)	0	100	100
1	D	236/255 (92%)	227 (96%)	9 (4%)	0	100	100
All	All	975/1020 (96%)	932 (96%)	43 (4%)	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	234/236 (99%)	220 (94%)	14 (6%)	19	31
1	B	236/236 (100%)	216 (92%)	20 (8%)	10	16
1	C	225/236 (95%)	211 (94%)	14 (6%)	18	29
1	D	224/236 (95%)	211 (94%)	13 (6%)	20	32
All	All	919/944 (97%)	858 (93%)	61 (7%)	17	26

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	VAL
1	A	278	SER

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Mol	Chain	Res	Type
1	A	285	MET
1	A	348	LEU
1	A	368	LEU
1	A	370	LYS
1	A	372	GLU
1	A	388[A]	CYS
1	A	388[B]	CYS
1	A	400	GLU
1	A	427	TYR
1	A	430	LYS
1	A	457	ARG
1	A	464	THR
1	B	270	LYS
1	B	278	SER
1	B	282	SER
1	B	290	ARG
1	B	300	LEU
1	B	303	LYS
1	B	310	LEU
1	B	348	LEU
1	B	359	LEU
1	B	368	LEU
1	B	370	LYS
1	B	373	THR
1	B	388[A]	CYS
1	B	388[B]	CYS
1	B	400	GLU
1	B	419	LEU
1	B	427	TYR
1	B	432	LYS
1	B	436	SER
1	B	457	ARG
1	C	281	SER
1	C	282	SER
1	C	283	LYS
1	C	318	VAL
1	C	370	LYS
1	C	388	CYS
1	C	414	LYS
1	C	421	ARG
1	C	427	TYR
1	C	428	VAL

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Mol	Chain	Res	Type
1	C	440	VAL
1	C	446	ASP
1	C	454	GLN
1	C	478	LYS
1	D	280	ASP
1	D	285	MET
1	D	345	GLN
1	D	348	LEU
1	D	370	LYS
1	D	386	GLU
1	D	388	CYS
1	D	412	SER
1	D	419	LEU
1	D	427	TYR
1	D	446	ASP
1	D	468	LEU
1	D	478	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	HIS
1	A	508	GLN
1	B	472	HIS
1	B	474	GLN
1	D	305	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

4 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	D	601	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	C	601	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	B	601	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	A	601	-	0,6,6	0.00	-	0,7,7	0.00	-

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	D	601	-	-	0/0/4/4	-
2	MLI	C	601	-	-	0/0/4/4	-
2	MLI	B	601	-	-	0/0/4/4	-
2	MLI	A	601	-	-	0/0/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	MLI	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	251/255 (98%)	0.18	11 (4%) 34 33	13, 33, 65, 78	0
1	B	250/255 (98%)	0.22	13 (5%) 27 26	14, 34, 64, 88	0
1	C	240/255 (94%)	0.08	3 (1%) 77 75	14, 32, 58, 86	1 (0%)
1	D	240/255 (94%)	0.26	11 (4%) 32 31	13, 37, 66, 94	0
All	All	981/1020 (96%)	0.19	38 (3%) 39 38	13, 34, 64, 94	1 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	433	ALA	7.4
1	C	428	VAL	7.0
1	B	438	ASP	4.9
1	A	438	ASP	4.6
1	B	440	VAL	3.9
1	D	485	LEU	3.9
1	A	433	ALA	3.7
1	D	428	VAL	3.6
1	B	432	LYS	3.6
1	A	518	LYS	3.5
1	B	434	LYS	3.4
1	A	396	VAL	3.4
1	B	397	PRO	3.2
1	D	398	GLU	2.9
1	B	431	GLY	2.9
1	A	397	PRO	2.9
1	C	427	TYR	2.8
1	A	409	GLY	2.8
1	B	404	TRP	2.8
1	B	441	CYS	2.8
1	C	426	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	426	TYR	2.6
1	B	437	ARG	2.5
1	D	440	VAL	2.4
1	D	427	TYR	2.4
1	D	416	ARG	2.4
1	D	377	ALA	2.3
1	A	435	VAL	2.3
1	B	435	VAL	2.3
1	A	431	GLY	2.2
1	B	396	VAL	2.2
1	D	278	SER	2.2
1	B	442	PHE	2.2
1	D	280	ASP	2.2
1	D	429	PRO	2.1
1	A	404	TRP	2.1
1	A	432	LYS	2.0
1	A	430	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MLI	C	601	7/7	0.93	0.16	29,31,34,35	0
2	MLI	B	601	7/7	0.94	0.19	21,23,26,29	0
2	MLI	D	601	7/7	0.96	0.18	28,30,30,31	0
2	MLI	A	601	7/7	0.97	0.15	19,21,23,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.