



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:16 AM UTC

PDB ID : 4GN1 / pdb_00004gn1
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

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

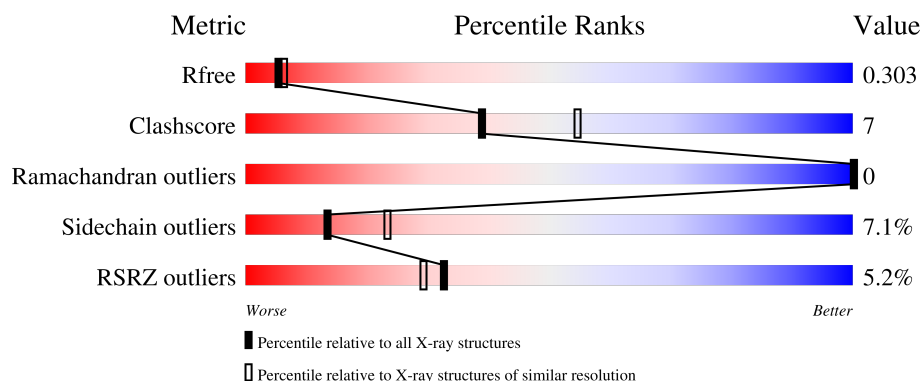
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	255	4% 82% 15% ..
1	B	255	7% 78% 17% ..
1	C	255	3% 78% 13% .. 6%
1	D	255	6% 75% 16% • 6%

2 Entry composition [i](#)

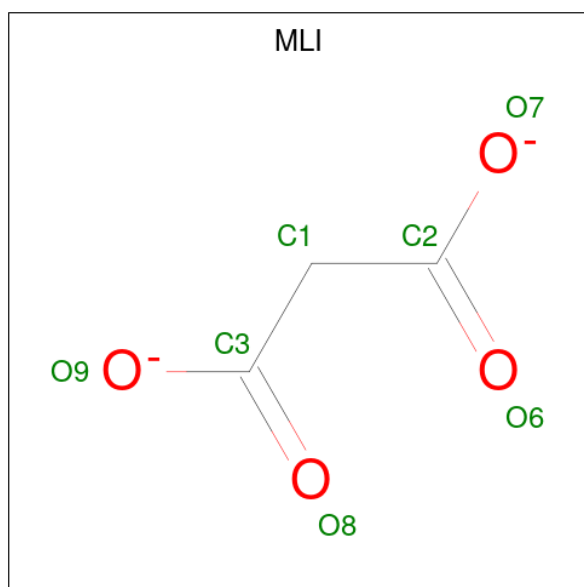
There are 3 unique types of molecules in this entry. The entry contains 8481 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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		

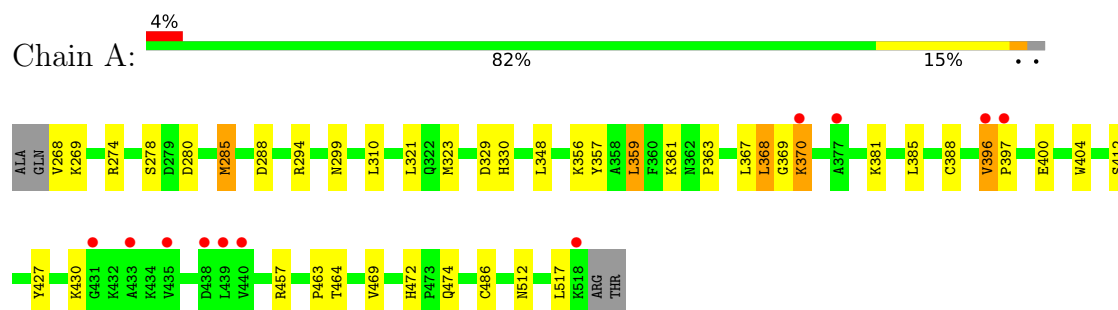
- Molecule 3 is water.

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		

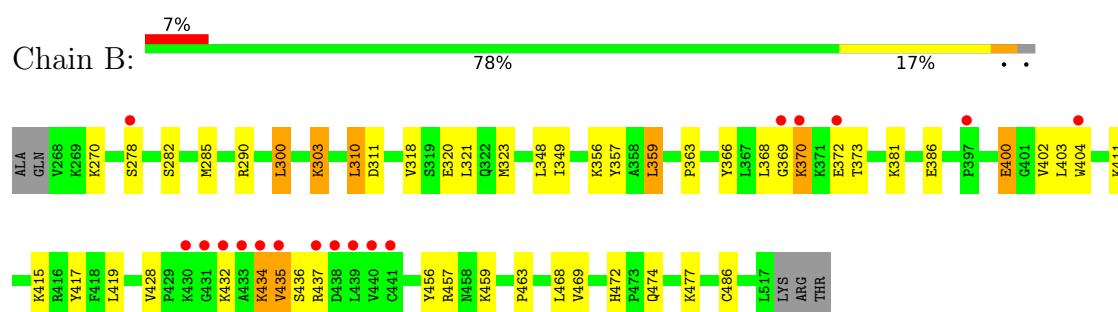
3 Residue-property plots [i](#)

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.

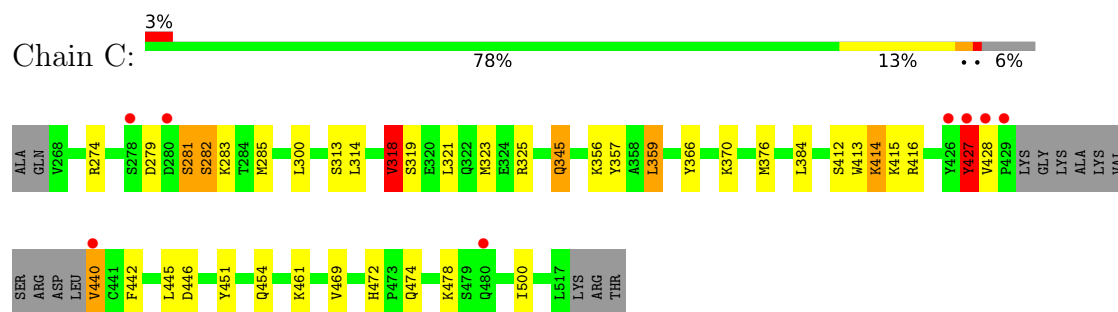
- Molecule 1: Ras-associated and pleckstrin homology domains-containing protein 1



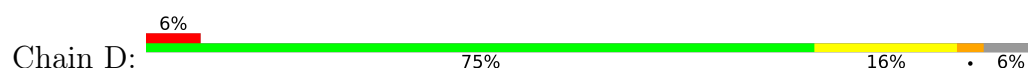
- Molecule 1: Ras-associated and pleckstrin homology domains-containing protein 1

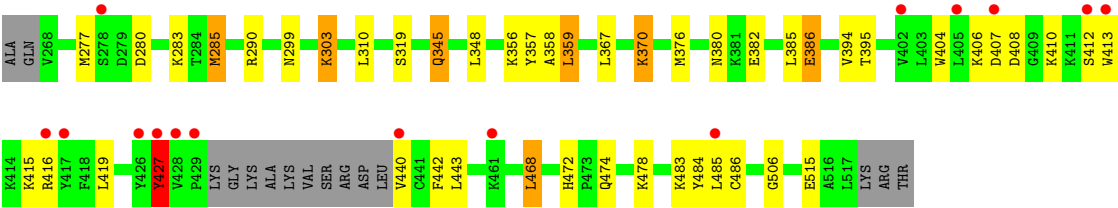


- Molecule 1: Ras-associated and pleckstrin homology domains-containing protein 1



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	2188 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.5	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	0.95	EDS
Total number of atoms	8481	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.77	0/2136	0.92	2/2874 (0.1%)
1	B	0.76	0/2150	0.88	0/2893
1	C	0.80	0/2052	0.88	2/2763 (0.1%)
1	D	0.81	0/2044	0.93	2/2753 (0.1%)
All	All	0.78	0/8382	0.91	6/11283 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	VAL	CB-CA-C	-7.63	101.91	110.68
1	A	368	LEU	N-CA-C	-5.96	99.69	109.40
1	D	370	LYS	N-CA-C	5.55	117.90	110.35
1	C	318	VAL	CB-CA-C	5.20	118.42	111.19
1	C	427	TYR	N-CA-C	5.20	116.33	108.07
1	D	427	TYR	N-CA-C	5.13	115.99	107.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2091	0	2105	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2099	0	2118	37	0
1	C	2011	0	2005	23	0
1	D	2003	0	1997	28	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	112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (112) 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:321:LEU:HB3	1:A:323:MET:HE3	1.39	1.04
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:C:323:MET:HE1	1:C:469:VAL:HG11	1.57	0.84
1:B:321:LEU:HB3	1:B:323:MET:HE3	1.63	0.81
1:A:363:PRO:HD2	1:A:381:LYS:HG2	1.69	0.74
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:B:323:MET:HE1	1:B:469:VAL:HG11	1.72	0.70
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:A:321:LEU:CB	1:A:323:MET:HE3	2.20	0.67
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
1:D:277:MET:HE2	1:D:283:LYS:HD2	1.78	0.65
1:B:285[A]:MET:SD	1:B:300:LEU:HD13	2.39	0.62
1:D:376:MET:HE2	1:D:380:ASN:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:299:ASN:HB3	1:D:303:LYS:HZ1	1.65	0.60
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: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:321:LEU:HB3	1:C:323:MET:HE3	1.86	0.56
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:A:369:GLY:HA2	1:A:370:LYS:C	2.31	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:A:323:MET:HE1	1:A:469:VAL:HG11	1.88	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: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:C:451:TYR:OH	2:C:601:MLI:O6	2.23	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:C:319:SER:OG	1:C:345:GLN:HB2	2.11	0.50
1:C:323:MET:CE	1:C:469:VAL:HG11	2.35	0.50
1:C:376:MET:HE1	1:C:384:LEU:HD22	1.92	0.50
1:B:428:VAL:HG11	1:B:435:VAL:HB	1.94	0.49
1:B:323:MET:HE2	1:B:456:TYR:OH	2.12	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:359:LEU:C	1:D:359:LEU:HD12	2.39	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: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:H	1:B:468:LEU:HD23	1.79	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:A:285:MET:HE1	1:A:299:ASN:HB3	1.98	0.46
1:B:318[A]:VAL:O	1:B:318[A]:VAL:HG13	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:B:400:GLU:HG3	1:B:417:TYR:HH	1.74	0.45
1:D:310:LEU:H	1:D:310:LEU:HD23	1.80	0.45
1:A:321:LEU:HB3	1:A:323:MET:CE	2.29	0.44
1:B:411:LYS:HE2	1:B:459:LYS:O	2.17	0.44
1:B:285[A]:MET:HE3	1:B:285[A]:MET:HB2	1.85	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:285:MET:HE2	1:D:285:MET:HB2	1.75	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: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:B:359:LEU:HD12	1:B:359:LEU:C	2.44	0.42
1:C:314:LEU:HD12	1:C:314:LEU:HA	1.87	0.42
1:A:412:SER:HB2	1:D:515:GLU:HG2	2.01	0.42
1:C:313:SER:OG	1:C:356:LYS:HE2	2.20	0.42
1:C:325:ARG:HB2	1:C:451:TYR:CD2	2.55	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:D:408:ASP:C	1:D:410:LYS:H	2.29	0.41
1:B:310:LEU:HD13	1:B:311:ASP:OD1	2.20	0.41
1:D:357:TYR:O	1:D:358:ALA:C	2.62	0.41
1:B:369:GLY:HA2	1:B:370:LYS:C	2.45	0.41
1:B:434:LYS:HE3	1:B:434:LYS:HB2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:MET:HE2	1:A:285:MET:HB2	1.91	0.40
1:A:288:ASP:OD1	1:A:288:ASP:C	2.64	0.40
1:C:412:SER:C	1:C:413:TRP:CD1	2.99	0.40
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:412:SER:C	1:D:413:TRP:CD1	3.00	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 [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	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 [i](#)

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%)	218 (93%)	16 (7%)	14	25
1	B	236/236 (100%)	215 (91%)	21 (9%)	9	15
1	C	225/236 (95%)	210 (93%)	15 (7%)	15	26
1	D	224/236 (95%)	210 (94%)	14 (6%)	16	29
All	All	919/944 (97%)	853 (93%)	66 (7%)	13	23

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	VAL
1	A	269	LYS
1	A	278	SER
1	A	285	MET
1	A	348	LEU
1	A	359	LEU
1	A	368	LEU
1	A	370	LYS
1	A	388[A]	CYS
1	A	388[B]	CYS
1	A	396	VAL
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	300	LEU
1	B	303	LYS
1	B	310	LEU
1	B	348	LEU
1	B	349	ILE
1	B	359	LEU
1	B	368	LEU
1	B	370	LYS
1	B	373	THR
1	B	386	GLU
1	B	400	GLU
1	B	419	LEU
1	B	432	LYS
1	B	434	LYS

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Mol	Chain	Res	Type
1	B	435	VAL
1	B	436	SER
1	B	437	ARG
1	B	457	ARG
1	C	281	SER
1	C	282	SER
1	C	283	LYS
1	C	318	VAL
1	C	345	GLN
1	C	359	LEU
1	C	370	LYS
1	C	414	LYS
1	C	427	TYR
1	C	428	VAL
1	C	440	VAL
1	C	446	ASP
1	C	454	GLN
1	C	461	LYS
1	C	478	LYS
1	D	280	ASP
1	D	285	MET
1	D	290	ARG
1	D	303	LYS
1	D	345	GLN
1	D	348	LEU
1	D	359	LEU
1	D	370	LYS
1	D	386	GLU
1	D	395	THR
1	D	419	LEU
1	D	427	TYR
1	D	468	LEU
1	D	478	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	HIS
1	A	447	HIS
1	A	508	GLN
1	B	276	HIS
1	B	472	HIS

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Mol	Chain	Res	Type
1	B	474	GLN
1	B	508	GLN
1	C	276	HIS
1	C	305	HIS
1	D	305	HIS
1	D	454	GLN

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 oligosaccharides 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	-	6,6,6	1.09	0	7,7,7	1.35	1 (14%)
2	MLI	C	601	-	6,6,6	1.21	0	7,7,7	1.07	0
2	MLI	B	601	-	6,6,6	1.33	0	7,7,7	1.33	0
2	MLI	A	601	-	6,6,6	1.28	0	7,7,7	1.40	1 (14%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	MLI	O7-C2-C1	2.14	121.14	114.51
2	D	601	MLI	O9-C3-C1	2.11	121.05	114.51

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	MLI	C3-C1-C2-O7
2	B	601	MLI	C3-C1-C2-O6
2	A	601	MLI	C3-C1-C2-O6
2	C	601	MLI	C2-C1-C3-O9
2	A	601	MLI	C3-C1-C2-O7
2	C	601	MLI	C2-C1-C3-O8

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 [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	251/255 (98%)	0.25	11 (4%) 39 34	13, 33, 65, 78	1 (0%)
1	B	250/255 (98%)	0.28	17 (6%) 23 20	13, 33, 64, 88	4 (1%)
1	C	240/255 (94%)	0.12	8 (3%) 49 45	14, 32, 58, 86	2 (0%)
1	D	240/255 (94%)	0.44	15 (6%) 26 22	13, 37, 66, 94	0
All	All	981/1020 (96%)	0.27	51 (5%) 33 29	13, 34, 64, 94	7 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	428	VAL	8.4
1	D	428	VAL	6.5
1	B	431	GLY	5.8
1	B	433	ALA	4.6
1	A	433	ALA	4.4
1	D	429	PRO	4.3
1	B	435	VAL	4.1
1	C	429	PRO	3.8
1	D	440	VAL	3.8
1	C	280	ASP	3.8
1	A	431	GLY	3.6
1	B	397	PRO	3.5
1	A	435	VAL	3.3
1	B	440	VAL	3.3
1	D	426	TYR	3.2
1	D	278	SER	3.1
1	A	396	VAL	3.0
1	A	397	PRO	2.9
1	D	485	LEU	2.9
1	B	438	ASP	2.9
1	D	407	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	402	VAL	2.8
1	C	427	TYR	2.8
1	D	461	LYS	2.7
1	D	405	LEU	2.6
1	B	439	LEU	2.6
1	B	434	LYS	2.5
1	B	437	ARG	2.5
1	D	416	ARG	2.5
1	A	440	VAL	2.5
1	B	278	SER	2.5
1	D	427	TYR	2.5
1	B	370	LYS	2.5
1	B	369	GLY	2.4
1	C	440	VAL	2.4
1	B	430	LYS	2.4
1	D	413	TRP	2.3
1	B	441	CYS	2.3
1	C	426	TYR	2.3
1	B	432	LYS	2.2
1	C	480	GLN	2.2
1	A	518	LYS	2.2
1	A	370	LYS	2.2
1	D	417	TYR	2.1
1	A	377	ALA	2.1
1	A	439	LEU	2.1
1	A	438	ASP	2.1
1	B	372	GLU	2.1
1	D	412	SER	2.1
1	B	404	TRP	2.0
1	C	278	SER	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	MLI	C	601	7/7	0.91	0.11	29,31,34,35	0
2	MLI	B	601	7/7	0.93	0.11	21,23,26,29	0
2	MLI	D	601	7/7	0.94	0.09	28,30,30,31	0
2	MLI	A	601	7/7	0.96	0.07	19,21,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.