



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:55 am BST

PDB ID : 3LQI
Title : Crystal structure of MLL1 PHD3-Bromo complexed with H3(1-9)K4me2 peptide
Authors : Wang, Z.; Patel, D.J.
Deposited on : 2010-02-09
Resolution : 1.92 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

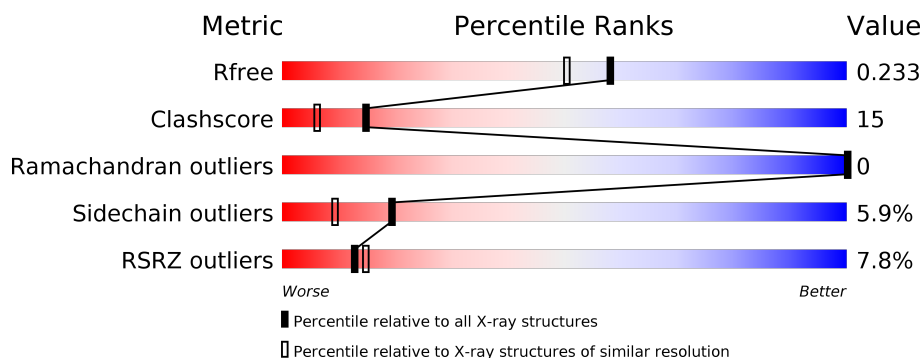
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	183	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	183	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• •</div> </div> </div>
1	C	183	<div> <div>9%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>• •</div> </div> </div>
2	R	9	<div> <div></div> <div> <div></div> <div>67%</div> <div>33%</div> </div> </div>
2	S	9	<div> <div>22%</div> <div> <div>44%</div> <div>33%</div> <div>22%</div> </div> </div>
2	T	9	<div> <div>33%</div> <div> <div></div> <div>67%</div> <div>33%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4901 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 MLL1 PHD3-Bromo.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1435	901	247	273	14			
1	B	177	Total	C	N	O	S	0	0	0
			1442	906	248	274	14			
1	C	181	Total	C	N	O	S	0	0	0
			1468	921	251	282	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1565	SER	-	EXPRESSION TAG	UNP Q03164
B	1565	SER	-	EXPRESSION TAG	UNP Q03164
C	1565	SER	-	EXPRESSION TAG	UNP Q03164

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	R	6	Total	C	N	O	0	0	0
			50	30	11	9			
2	S	7	Total	C	N	O	0	0	0
			55	33	12	10			
2	T	9	Total	C	N	O	0	0	0
			76	45	18	13			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Zn	0	0
			2	2		

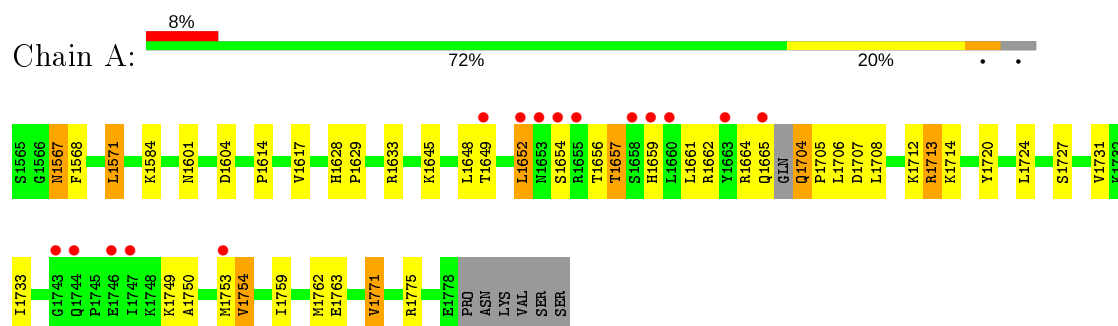
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total	O	0	0
			100	100		
4	B	124	Total	O	0	0
			124	124		
4	C	136	Total	O	0	0
			136	136		
4	R	1	Total	O	0	0
			1	1		
4	S	4	Total	O	0	0
			4	4		
4	T	4	Total	O	0	0
			4	4		

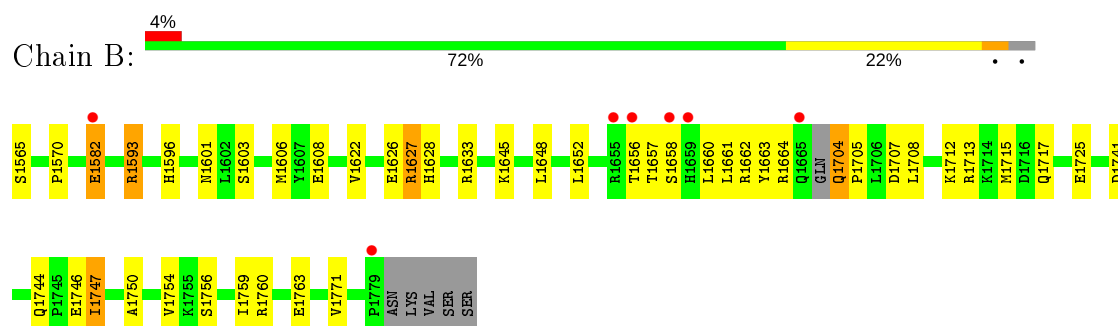
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

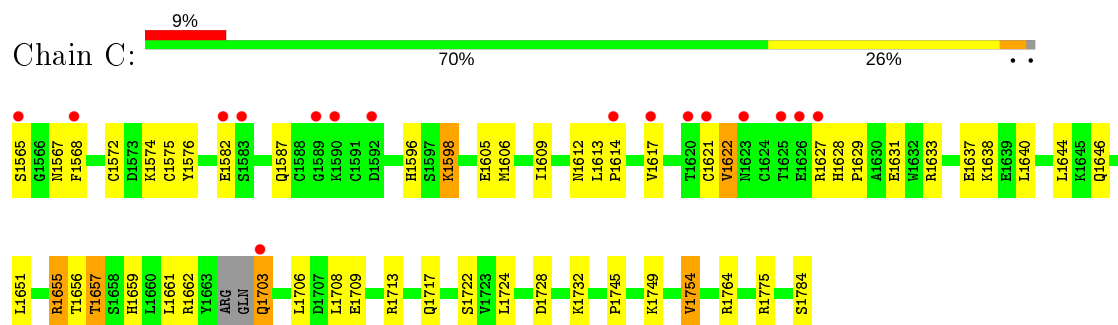
• Molecule 1: MLL1 PHD3-Bromo



• Molecule 1: MLL1 PHD3-Bromo

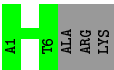


• Molecule 1: MLL1 PHD3-Bromo

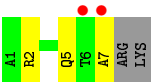


• Molecule 2: Histone H3





● Molecule 2: Histone H3



● Molecule 2: Histone H3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.74Å 90.58Å 125.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.92 45.42 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.92) 99.9 (45.42-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.241 0.205 , 0.233	Depositor DCC
R_{free} test set	2238 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4901	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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: ZN, MLY

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	0.32	0/1463	0.55	0/1968
1	B	0.39	1/1471 (0.1%)	0.55	0/1980
1	C	0.31	0/1497	0.54	0/2014
2	R	0.42	0/38	0.62	0/50
2	S	0.75	0/43	1.01	0/57
2	T	0.35	0/64	0.58	0/82
All	All	0.35	1/4576 (0.0%)	0.55	0/6151

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1596	HIS	C-O	-6.44	1.11	1.23

There are no bond angle outliers.

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	1435	0	1398	45	0
1	B	1442	0	1405	45	0
1	C	1468	0	1430	51	0
2	R	50	0	58	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	55	0	63	4	0
2	T	76	0	89	5	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	100	0	0	6	0
4	B	124	0	0	4	0
4	C	136	0	0	4	0
4	R	1	0	0	0	0
4	S	4	0	0	1	0
4	T	4	0	0	1	0
All	All	4901	0	4443	136	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 15.

All (136) 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:1567:ASN:HD22	1:A:1568:PHE:H	1.16	0.93
1:A:1664:ARG:O	1:A:1665:GLN:HB2	1.80	0.80
1:B:1741:ASP:HA	1:B:1747:ILE:HD11	1.66	0.78
1:B:1744:GLN:HB2	1:B:1747:ILE:HG23	1.66	0.77
1:C:1614:PRO:O	1:C:1617:VAL:HG22	1.85	0.76
1:C:1627:ARG:HH11	1:C:1627:ARG:HA	1.50	0.75
1:C:1627:ARG:NH1	1:C:1627:ARG:HA	2.03	0.74
1:B:1570:PRO:HD3	1:B:1593:ARG:HG2	1.72	0.70
1:C:1655:ARG:HD3	4:C:417:HOH:O	1.91	0.70
1:C:1724:LEU:HD22	2:S:7:ALA:HB3	1.76	0.68
1:B:1565:SER:HB3	1:C:1582:GLU:OE1	1.95	0.66
1:C:1775:ARG:HD3	2:S:5:GLN:CD	2.17	0.65
1:B:1627:ARG:HD3	1:B:1628:HIS:H	1.60	0.65
1:A:1645:LYS:O	1:A:1649:THR:HG23	1.96	0.65
1:C:1568:PHE:CE1	1:C:1575:CYS:HB3	2.32	0.64
1:C:1646:GLN:HE21	1:C:1764:ARG:HH21	1.45	0.64
1:C:1598:LYS:HG3	4:C:426:HOH:O	1.98	0.64
1:C:1775:ARG:HD3	2:S:5:GLN:OE1	1.98	0.64
1:B:1713:ARG:O	1:B:1717:GLN:HG2	1.99	0.63
1:C:1613:LEU:HB3	1:C:1617:VAL:HG21	1.79	0.63
1:C:1613:LEU:HB3	1:C:1617:VAL:CG2	2.29	0.62
1:A:1567:ASN:HD22	1:A:1568:PHE:N	1.91	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1750:ALA:O	1:B:1754:VAL:HG23	2.01	0.60
1:A:1713:ARG:HG3	1:A:1714:LYS:N	2.16	0.60
1:C:1617:VAL:O	1:C:1617:VAL:HG23	2.01	0.59
1:A:1614:PRO:HG2	1:A:1617:VAL:HG23	1.83	0.59
1:A:1633:ARG:HH11	1:B:1601:ASN:HD22	1.48	0.59
1:A:1662:ARG:HA	1:A:1708:LEU:HB2	1.85	0.59
1:A:1567:ASN:ND2	1:A:1568:PHE:H	1.94	0.59
1:A:1584:LYS:HE3	1:A:1604:ASP:OD1	2.02	0.59
1:A:1775:ARG:HD3	4:B:266:HOH:O	2.04	0.58
1:A:1601:ASN:HD22	1:B:1633:ARG:HH11	1.52	0.58
1:C:1622:VAL:HG13	1:C:1622:VAL:O	2.04	0.58
1:B:1662:ARG:HA	1:B:1708:LEU:HB2	1.86	0.57
1:C:1587:GLN:OE1	2:T:2:ARG:HD3	2.04	0.57
1:B:1656:THR:O	1:B:1660:LEU:HD13	2.05	0.56
1:A:1652:LEU:HG	1:A:1712:LYS:HD2	1.87	0.56
1:B:1704:GLN:N	1:B:1705:PRO:HD2	2.21	0.56
1:C:1657:THR:HG23	1:C:1708:LEU:HD12	1.88	0.56
1:A:1759:ILE:O	1:A:1763:GLU:HG3	2.06	0.56
1:A:1762:MET:HG3	1:A:1771:VAL:HG11	1.88	0.55
1:A:1714:LYS:HD3	1:A:1720:TYR:CZ	2.42	0.55
1:C:1656:THR:O	1:C:1754:VAL:HG13	2.07	0.54
2:T:9:LYS:HB3	4:T:465:HOH:O	2.07	0.54
1:B:1627:ARG:HD3	1:B:1628:HIS:N	2.22	0.54
1:A:1633:ARG:HH11	1:B:1601:ASN:ND2	2.06	0.54
1:B:1660:LEU:O	1:B:1661:LEU:HD23	2.08	0.54
1:B:1704:GLN:HB3	4:B:271:HOH:O	2.07	0.53
1:B:1656:THR:HG23	1:B:1657:THR:N	2.24	0.53
1:A:1654:SER:OG	1:A:1657:THR:HG23	2.08	0.53
2:T:8:ARG:O	2:T:9:LYS:HB2	2.09	0.53
1:A:1648:LEU:O	1:A:1652:LEU:HD22	2.08	0.53
1:C:1605:GLU:HG3	4:S:463:HOH:O	2.09	0.52
1:C:1713:ARG:O	1:C:1717:GLN:HG3	2.10	0.52
1:A:1771:VAL:HG22	4:A:123:HOH:O	2.09	0.52
1:A:1749:LYS:O	1:A:1753:MET:HG2	2.10	0.51
1:C:1657:THR:CG2	1:C:1708:LEU:HD12	2.40	0.51
1:B:1741:ASP:HA	1:B:1747:ILE:CD1	2.39	0.51
2:T:8:ARG:O	2:T:9:LYS:CB	2.59	0.50
1:A:1652:LEU:HD21	1:A:1712:LYS:HG2	1.94	0.50
1:C:1661:LEU:O	1:C:1709:GLU:HG3	2.12	0.50
1:B:1626:GLU:HB2	4:B:290:HOH:O	2.12	0.50
1:C:1596:HIS:HB3	1:C:1598:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1724:LEU:CD2	2:S:7:ALA:HB3	2.41	0.49
1:B:1627:ARG:NH1	4:B:289:HOH:O	2.45	0.49
1:A:1750:ALA:O	1:A:1754:VAL:HG13	2.12	0.49
1:A:1652:LEU:HD21	1:A:1712:LYS:CG	2.43	0.49
1:B:1627:ARG:CD	1:B:1628:HIS:N	2.76	0.49
1:A:1704:GLN:N	1:A:1705:PRO:CD	2.75	0.49
1:B:1627:ARG:CD	1:B:1628:HIS:H	2.26	0.49
1:A:1648:LEU:HG	1:A:1652:LEU:HD22	1.94	0.48
1:C:1596:HIS:HB3	1:C:1598:LYS:CD	2.42	0.48
1:C:1651:LEU:O	1:C:1657:THR:HG21	2.14	0.48
1:C:1657:THR:O	1:C:1657:THR:CG2	2.61	0.48
1:C:1631:GLU:HG3	4:C:434:HOH:O	2.12	0.48
1:A:1571:LEU:CD1	4:A:187:HOH:O	2.62	0.48
1:A:1571:LEU:HD11	4:A:187:HOH:O	2.14	0.48
1:B:1662:ARG:HG2	1:B:1663:TYR:CE2	2.49	0.48
1:A:1661:LEU:HD22	1:A:1733:ILE:HG22	1.95	0.47
1:A:1628:HIS:HE1	4:A:174:HOH:O	1.97	0.47
1:C:1646:GLN:NE2	1:C:1764:ARG:HH21	2.11	0.47
1:A:1652:LEU:CG	1:A:1712:LYS:HD2	2.45	0.47
1:A:1727:SER:O	1:A:1731:VAL:HG23	2.14	0.47
1:C:1659:HIS:HD1	1:C:1659:HIS:H	1.63	0.46
1:B:1741:ASP:HB2	1:B:1747:ILE:HG12	1.96	0.46
1:A:1633:ARG:HB3	1:B:1601:ASN:HD21	1.81	0.46
1:C:1703:GLN:HA	1:C:1703:GLN:HE21	1.81	0.46
1:B:1645:LYS:HB2	1:B:1715:MET:HE3	1.96	0.46
1:C:1614:PRO:HG2	1:C:1617:VAL:HG13	1.98	0.45
1:B:1603:SER:OG	1:B:1606:MET:HG2	2.16	0.45
1:C:1606:MET:CE	1:C:1609:ILE:HD12	2.47	0.45
1:C:1613:LEU:HB3	1:C:1614:PRO:HD2	1.99	0.45
1:A:1656:THR:O	1:A:1659:HIS:HB2	2.17	0.45
1:A:1601:ASN:ND2	1:B:1633:ARG:HH11	2.14	0.45
1:B:1756:SER:HB3	1:B:1760:ARG:NH1	2.32	0.45
1:B:1662:ARG:O	1:B:1707:ASP:HB2	2.17	0.44
1:C:1628:HIS:HA	1:C:1629:PRO:C	2.36	0.44
1:B:1756:SER:HB3	1:B:1760:ARG:HH12	1.82	0.44
1:C:1656:THR:O	1:C:1754:VAL:CG1	2.65	0.44
1:A:1661:LEU:O	1:A:1707:ASP:HB2	2.18	0.44
1:C:1622:VAL:CG1	1:C:1622:VAL:O	2.64	0.44
1:C:1657:THR:HG23	1:C:1708:LEU:CD1	2.48	0.44
1:C:1657:THR:CG2	1:C:1708:LEU:CD1	2.96	0.43
1:C:1612:ASN:HB2	4:C:425:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1627:ARG:HD3	1:B:1627:ARG:HA	1.88	0.43
1:B:1627:ARG:HD2	1:B:1628:HIS:O	2.19	0.43
1:B:1759:ILE:O	1:B:1763:GLU:HG3	2.19	0.43
1:C:1572:CYS:SG	1:C:1574:LYS:HB2	2.59	0.43
1:C:1605:GLU:OE1	1:C:1722:SER:HB2	2.18	0.43
1:C:1567:ASN:HB3	1:C:1576:TYR:CZ	2.53	0.42
1:B:1704:GLN:N	1:B:1705:PRO:CD	2.83	0.42
1:A:1629:PRO:HG3	1:B:1622:VAL:HG21	2.01	0.42
1:A:1662:ARG:NH2	1:A:1712:LYS:HE2	2.34	0.42
1:C:1633:ARG:O	1:C:1637:GLU:HG3	2.19	0.42
1:C:1728:ASP:O	1:C:1732:LYS:HG3	2.20	0.42
1:A:1724:LEU:HD23	1:C:1784:SER:HA	2.01	0.42
1:A:1571:LEU:HD11	4:A:119:HOH:O	2.19	0.42
1:A:1652:LEU:CD2	1:A:1712:LYS:HD2	2.50	0.42
1:B:1608:GLU:OE1	1:C:1775:ARG:HD2	2.19	0.42
2:T:8:ARG:O	2:T:9:LYS:HG3	2.20	0.42
1:A:1648:LEU:HG	1:A:1652:LEU:CD2	2.49	0.42
1:B:1744:GLN:HB2	1:B:1747:ILE:CG2	2.43	0.41
1:B:1645:LYS:HB2	1:B:1715:MET:CE	2.49	0.41
1:C:1617:VAL:O	1:C:1617:VAL:CG2	2.66	0.41
1:C:1640:LEU:O	1:C:1644:LEU:HG	2.21	0.41
1:C:1745:PRO:O	1:C:1749:LYS:HG3	2.20	0.41
1:B:1662:ARG:HG2	1:B:1663:TYR:CD2	2.55	0.41
1:A:1664:ARG:O	1:A:1665:GLN:CB	2.59	0.41
1:A:1654:SER:HA	4:A:176:HOH:O	2.21	0.41
1:B:1648:LEU:HD21	1:B:1712:LYS:HA	2.03	0.41
1:B:1717:GLN:H	1:B:1717:GLN:HG2	1.60	0.40
1:B:1746:GLU:HG2	1:B:1747:ILE:N	2.37	0.40
1:C:1764:ARG:HB3	1:C:1764:ARG:HE	1.52	0.40
1:B:1652:LEU:HD22	1:B:1662:ARG:HD2	2.04	0.40
1:A:1762:MET:HE2	1:A:1771:VAL:HG13	2.04	0.40
1:B:1582:GLU:OE1	1:B:1582:GLU:HA	2.22	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	172/183 (94%)	169 (98%)	3 (2%)	0	100	100
1	B	173/183 (94%)	172 (99%)	1 (1%)	0	100	100
1	C	177/183 (97%)	172 (97%)	5 (3%)	0	100	100
2	R	3/9 (33%)	3 (100%)	0	0	100	100
2	S	4/9 (44%)	4 (100%)	0	0	100	100
2	T	6/9 (67%)	6 (100%)	0	0	100	100
All	All	535/576 (93%)	526 (98%)	9 (2%)	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	163/170 (96%)	154 (94%)	9 (6%)	21	11
1	B	164/170 (96%)	155 (94%)	9 (6%)	21	11
1	C	168/170 (99%)	157 (94%)	11 (6%)	17	7
2	R	4/6 (67%)	4 (100%)	0	100	100
2	S	4/6 (67%)	3 (75%)	1 (25%)	0	0
2	T	6/6 (100%)	6 (100%)	0	100	100
All	All	509/528 (96%)	479 (94%)	30 (6%)	19	9

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1567	ASN
1	A	1571	LEU
1	A	1652	LEU

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Mol	Chain	Res	Type
1	A	1657	THR
1	A	1704	GLN
1	A	1706	LEU
1	A	1713	ARG
1	A	1754	VAL
1	A	1771	VAL
1	B	1582	GLU
1	B	1593	ARG
1	B	1627	ARG
1	B	1658	SER
1	B	1664	ARG
1	B	1704	GLN
1	B	1725	GLU
1	B	1747	ILE
1	B	1771	VAL
1	C	1565	SER
1	C	1598	LYS
1	C	1621	CYS
1	C	1622	VAL
1	C	1638	LYS
1	C	1655	ARG
1	C	1657	THR
1	C	1662	ARG
1	C	1703	GLN
1	C	1706	LEU
1	C	1754	VAL
2	S	2	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1567	ASN
1	A	1601	ASN
1	A	1623	ASN
1	A	1653	ASN
1	A	1659	HIS
1	A	1665	GLN
1	A	1704	GLN
1	A	1719	ASN
1	B	1601	ASN
1	B	1612	ASN
1	B	1628	HIS

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Mol	Chain	Res	Type
1	B	1719	ASN
1	C	1646	GLN
1	C	1703	GLN
1	C	1704	GLN
1	C	1719	ASN
1	C	1751	ASN
1	C	1780	ASN
2	R	5	GLN
2	S	5	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	MLY	S	4	2	9,10,11	0.54	0	6,11,13	0.75	0
2	MLY	R	4	2	9,10,11	0.46	0	6,11,13	0.65	0
2	MLY	T	4	2	9,10,11	0.48	0	6,11,13	0.81	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	MLY	S	4	2	-	0/8/9/11	-
2	MLY	R	4	2	-	0/8/9/11	-
2	MLY	T	4	2	-	0/8/9/11	-

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.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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, 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	176/183 (96%)	0.44	15 (8%) 10 12	12, 28, 55, 65	0
1	B	177/183 (96%)	0.24	7 (3%) 38 41	13, 25, 50, 58	0
1	C	181/183 (98%)	0.32	16 (8%) 10 11	13, 27, 54, 60	0
2	R	5/9 (55%)	0.37	0 100 100	18, 22, 44, 51	0
2	S	6/9 (66%)	1.27	2 (33%) 0 0	23, 31, 45, 57	0
2	T	8/9 (88%)	1.93	3 (37%) 0 0	34, 48, 58, 59	0
All	All	553/576 (96%)	0.37	43 (7%) 13 15	12, 27, 55, 65	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1659	HIS	5.4
2	T	9	LYS	4.6
1	C	1589	GLY	3.7
1	C	1617	VAL	3.7
1	A	1652	LEU	3.6
1	C	1623	ASN	3.5
1	B	1658	SER	3.5
1	A	1743	GLY	3.4
2	T	7	ALA	3.3
2	T	8	ARG	3.2
1	A	1658	SER	3.0
1	C	1703	GLN	2.9
1	A	1653	ASN	2.9
1	C	1568	PHE	2.8
1	A	1663	TYR	2.8
2	S	7	ALA	2.8
1	A	1744	GLN	2.7
1	B	1656	THR	2.7
1	C	1590	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	1565	SER	2.6
1	C	1627	ARG	2.6
1	B	1655	ARG	2.6
1	A	1660	LEU	2.5
1	A	1649	THR	2.5
1	B	1582	GLU	2.4
1	C	1626	GLU	2.4
1	C	1621	CYS	2.4
1	C	1592	ASP	2.3
1	C	1583	SER	2.3
1	C	1625	THR	2.3
1	B	1779	PRO	2.3
1	A	1654	SER	2.2
1	C	1582	GLU	2.2
1	A	1665	GLN	2.2
1	A	1753	MET	2.2
1	A	1655	ARG	2.1
1	A	1746	GLU	2.1
1	C	1614	PRO	2.1
1	C	1620	THR	2.1
1	A	1747	ILE	2.1
1	B	1659	HIS	2.1
2	S	6	THR	2.1
1	B	1665	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	MLY	T	4	11/12	0.79	0.19	36,38,42,43	0
2	MLY	S	4	11/12	0.91	0.12	23,24,28,28	0
2	MLY	R	4	11/12	0.96	0.12	19,21,28,28	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	C	6	1/1	0.96	0.08	52,52,52,52	0
3	ZN	C	5	1/1	0.98	0.04	31,31,31,31	0
3	ZN	B	3	1/1	0.99	0.05	26,26,26,26	0
3	ZN	B	4	1/1	0.99	0.06	38,38,38,38	0
3	ZN	A	1	1/1	1.00	0.05	24,24,24,24	0
3	ZN	A	2	1/1	1.00	0.06	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.