



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:54 PM UTC

PDB ID : 3L6R / pdb_00003l6r
Title : The structure of mammalian serine racemase: Evidence for conformational changes upon inhibitor binding
Authors : Smith, M.A.; Mack, V.; Ebner, A.; Cesura, A.; Felicetti, B.; Barker, J.
Deposited on : 2009-12-24
Resolution : 1.70 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

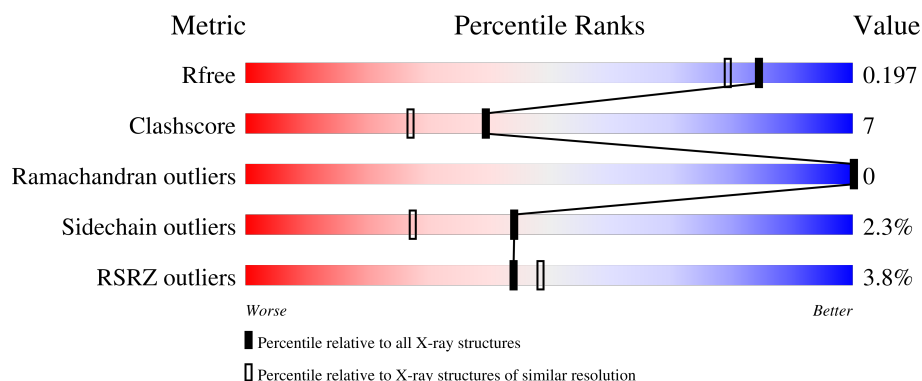
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

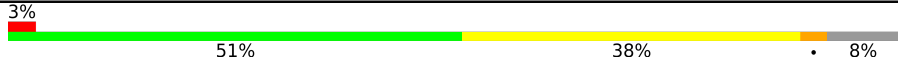
The reported resolution of this entry is 1.70 Å.

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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	346	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3080 atoms, of which 229 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.

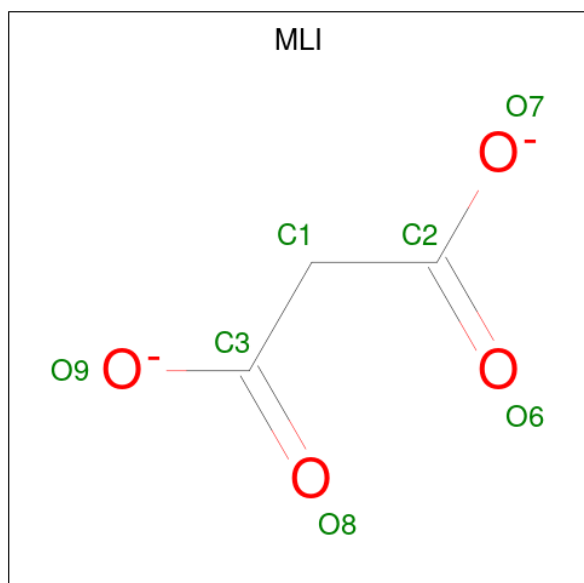
- Molecule 1 is a protein called Serine racemase.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P	S	Se			
1	A	320	2719	1595	229	414	470	1	6	4	0	13	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	CYS	engineered mutation	UNP Q9GZT4
A	6	ASP	CYS	engineered mutation	UNP Q9GZT4
A	341	HIS	-	expression tag	UNP Q9GZT4
A	342	HIS	-	expression tag	UNP Q9GZT4
A	343	HIS	-	expression tag	UNP Q9GZT4
A	344	HIS	-	expression tag	UNP Q9GZT4
A	345	HIS	-	expression tag	UNP Q9GZT4
A	346	HIS	-	expression tag	UNP Q9GZT4

- 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		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

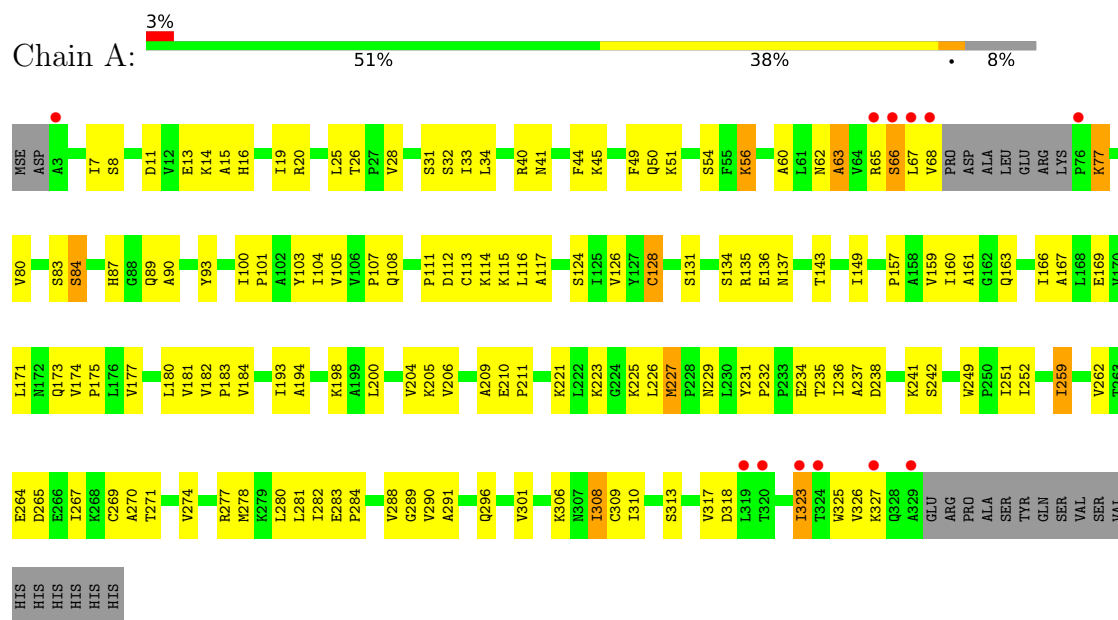
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	353	Total	O	0	0
			353	353		

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: Serine racemase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	54.54Å 84.21Å 70.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.78 – 1.70 45.78 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.1 (45.78-1.70) 97.0 (45.78-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.168 , 0.202 0.154 , 0.197	Depositor DCC
R_{free} test set	1955 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3080	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, MLI, MN

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	2.08	120/2537 (4.7%)	1.00	5/3446 (0.1%)

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	TRP	C-O	-8.38	1.16	1.24
1	A	206	VAL	C-O	-7.61	1.15	1.24
1	A	204	VAL	C-O	-7.48	1.16	1.24
1	A	232	PRO	C-O	-7.36	1.16	1.24
1	A	13	GLU	C-O	-7.10	1.15	1.24
1	A	211	PRO	C-O	-6.98	1.16	1.23
1	A	262	VAL	C-O	-6.95	1.17	1.24
1	A	231	TYR	C-O	-6.95	1.15	1.24
1	A	80	VAL	C-O	-6.94	1.17	1.24
1	A	288	VAL	C-O	-6.84	1.16	1.24
1	A	177	VAL	C-O	-6.81	1.16	1.24
1	A	182	VAL	C-O	-6.79	1.15	1.24
1	A	252	ILE	C-O	-6.79	1.16	1.24
1	A	242	SER	C-O	-6.67	1.15	1.23
1	A	100	ILE	C-O	-6.66	1.17	1.24
1	A	259	ILE	C-O	-6.58	1.17	1.24
1	A	317	VAL	C-O	-6.54	1.17	1.24
1	A	134	SER	C-O	-6.50	1.16	1.24
1	A	54	SER	C-O	-6.47	1.16	1.23
1	A	105	VAL	C-O	-6.47	1.17	1.24
1	A	157	PRO	C-O	-6.45	1.15	1.24
1	A	291	ALA	C-O	-6.43	1.16	1.24
1	A	87	HIS	C-O	-6.40	1.16	1.24
1	A	143	THR	C-O	-6.34	1.16	1.24
1	A	205[A]	LYS	C-O	-6.25	1.16	1.23
1	A	205[B]	LYS	C-O	-6.25	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	ILE	C-O	-6.22	1.17	1.24
1	A	237	ALA	C-O	-6.20	1.17	1.23
1	A	267	ILE	C-O	-6.18	1.17	1.24
1	A	264	GLU	C-O	-6.16	1.16	1.24
1	A	90	ALA	C-O	-6.15	1.17	1.24
1	A	131	SER	C-O	-6.14	1.16	1.23
1	A	235	THR	C-O	-6.02	1.16	1.23
1	A	163	GLN	C-O	-6.02	1.16	1.24
1	A	31	SER	C-O	-6.01	1.17	1.23
1	A	166	ILE	C-O	-6.01	1.17	1.24
1	A	180	LEU	C-O	-6.01	1.16	1.24
1	A	60	ALA	C-O	-6.00	1.16	1.24
1	A	15	ALA	C-O	-5.97	1.17	1.24
1	A	194	ALA	C-O	-5.96	1.17	1.24
1	A	234	GLU	C-O	-5.96	1.17	1.24
1	A	283	GLU	C-O	-5.95	1.16	1.23
1	A	169	GLU	C-O	-5.95	1.17	1.24
1	A	160	ILE	C-O	-5.93	1.17	1.24
1	A	229	ASN	C-O	-5.93	1.16	1.23
1	A	7	ILE	C-O	-5.92	1.17	1.23
1	A	181	VAL	C-O	-5.90	1.17	1.24
1	A	14	LYS	C-O	-5.87	1.17	1.24
1	A	19	ILE	C-O	-5.86	1.17	1.24
1	A	26	THR	C-O	-5.86	1.16	1.23
1	A	101	PRO	C-O	-5.85	1.17	1.23
1	A	93	TYR	C-O	-5.83	1.17	1.24
1	A	114	LYS	C-O	-5.82	1.17	1.24
1	A	51	LYS	C-O	-5.79	1.16	1.23
1	A	40	ARG	C-O	-5.76	1.16	1.23
1	A	282	ILE	C-O	-5.75	1.16	1.24
1	A	296	GLN	C-O	-5.74	1.17	1.24
1	A	135	ARG	C-O	-5.72	1.17	1.24
1	A	259	ILE	CG1-CD1	-5.72	1.29	1.51
1	A	137	ASN	C-O	-5.70	1.17	1.24
1	A	28	VAL	C-O	-5.70	1.18	1.24
1	A	225	LYS	C-O	-5.67	1.17	1.23
1	A	45	LYS	C-O	-5.66	1.17	1.24
1	A	161	ALA	C-O	-5.65	1.17	1.24
1	A	310[A]	ILE	C-O	-5.65	1.17	1.24
1	A	310[B]	ILE	C-O	-5.65	1.17	1.24
1	A	116	LEU	C-O	-5.65	1.17	1.24
1	A	278	MSE	C-O	-5.62	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	ALA	C-O	-5.61	1.17	1.24
1	A	103	TYR	C-O	-5.59	1.17	1.24
1	A	173	GLN	C-O	-5.57	1.17	1.24
1	A	104	ILE	C-O	-5.56	1.18	1.24
1	A	251	ILE	C-O	-5.56	1.17	1.24
1	A	115	LYS	C-O	-5.53	1.17	1.24
1	A	274	VAL	C-O	-5.52	1.17	1.24
1	A	20	ARG	C-O	-5.51	1.17	1.24
1	A	126	VAL	C-O	-5.49	1.18	1.24
1	A	326	VAL	C-O	-5.48	1.18	1.24
1	A	11	ASP	C-O	-5.47	1.17	1.24
1	A	193	ILE	C-O	-5.45	1.17	1.24
1	A	290	VAL	C-O	-5.45	1.18	1.24
1	A	241	LYS	C-O	-5.43	1.16	1.24
1	A	111	PRO	C-O	-5.40	1.17	1.23
1	A	63	ALA	C-O	-5.39	1.17	1.24
1	A	284	PRO	C-O	-5.39	1.17	1.24
1	A	183	PRO	C-O	-5.38	1.17	1.23
1	A	16	HIS	C-O	-5.37	1.18	1.24
1	A	159	VAL	C-O	-5.33	1.18	1.24
1	A	210	GLU	C-O	-5.33	1.17	1.24
1	A	44	PHE	C-O	-5.32	1.17	1.24
1	A	117	ALA	C-O	-5.29	1.18	1.24
1	A	149	ILE	C-O	-5.29	1.18	1.24
1	A	32	SER	C-O	-5.26	1.17	1.24
1	A	175	PRO	C-O	-5.26	1.17	1.24
1	A	184	VAL	C-O	-5.24	1.18	1.24
1	A	198	LYS	C-O	-5.24	1.17	1.24
1	A	107	PRO	C-O	-5.24	1.17	1.23
1	A	8	SER	C-O	-5.23	1.17	1.23
1	A	83	SER	C-O	-5.19	1.17	1.23
1	A	174	VAL	C-O	-5.19	1.17	1.24
1	A	289	GLY	C-O	-5.18	1.17	1.23
1	A	128	CYS	C-O	-5.15	1.17	1.23
1	A	89	GLN	C-O	-5.14	1.18	1.24
1	A	84	SER	C-O	-5.14	1.17	1.24
1	A	238	ASP	C-O	-5.14	1.17	1.24
1	A	271	THR	C-O	-5.13	1.18	1.24
1	A	124[A]	SER	N-CA	-5.12	1.39	1.46
1	A	124[B]	SER	N-CA	-5.12	1.39	1.46
1	A	49	PHE	C-O	-5.10	1.17	1.24
1	A	227	MSE	C-O	-5.10	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	GLN	C-O	-5.09	1.17	1.23
1	A	309	CYS	C-O	-5.09	1.17	1.24
1	A	280	LEU	C-O	-5.09	1.18	1.24
1	A	112	ASP	C-O	-5.07	1.18	1.24
1	A	265	ASP	C-O	-5.06	1.18	1.24
1	A	136	GLU	C-O	-5.05	1.18	1.24
1	A	301	VAL	C-O	-5.05	1.18	1.24
1	A	327	LYS	C-O	-5.04	1.17	1.24
1	A	209	ALA	C-O	-5.03	1.18	1.24
1	A	269	CYS	C-O	-5.02	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	LEU	N-CA-C	6.05	117.87	111.28
1	A	323	ILE	CB-CA-C	-5.93	102.97	112.16
1	A	308	ILE	CB-CA-C	-5.55	102.42	110.63
1	A	184	VAL	N-CA-C	5.50	115.81	108.11
1	A	313	SER	N-CA-C	5.14	117.78	111.82

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	2490	229	2583	34	7
2	A	7	0	2	0	0
3	A	1	0	0	0	0
4	A	353	0	0	5	5
All	All	2851	229	2585	34	8

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 (34) 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:33:ILE:HD12	1:A:33:ILE:H	1.43	0.83
1:A:223:LYS:CE	1:A:227:MSE:HE2	2.13	0.78
1:A:41[B]:ASN:OD1	1:A:306:LYS:HE3	1.93	0.68
1:A:223:LYS:HE2	1:A:227:MSE:HE2	1.78	0.64
1:A:236[B]:ILE:HD11	1:A:325:TRP:NE1	2.15	0.62
1:A:167:ALA:O	1:A:171[A]:LEU:HD23	2.00	0.61
1:A:113:CYS:HB3	1:A:318:ASP:OD1	2.01	0.60
1:A:33:ILE:H	1:A:33:ILE:CD1	2.12	0.57
1:A:63:ALA:O	1:A:67:LEU:HD23	2.05	0.56
1:A:221:LYS:HG3	1:A:259:ILE:CD1	2.36	0.56
1:A:77:LYS:HG2	4:A:540:HOH:O	2.07	0.55
1:A:221:LYS:HG3	1:A:259:ILE:HD11	1.90	0.53
1:A:236[B]:ILE:HD11	1:A:325:TRP:CE2	2.44	0.53
1:A:108:GLN:HG3	1:A:128:CYS:O	2.10	0.52
1:A:223:LYS:NZ	4:A:506:HOH:O	2.38	0.51
1:A:34:LEU:HD12	1:A:34:LEU:N	2.26	0.50
1:A:223:LYS:HE2	1:A:227:MSE:HG3	1.92	0.50
1:A:62:ASN:O	1:A:66[A]:SER:HB3	2.12	0.49
1:A:113:CYS:CB	1:A:318:ASP:OD1	2.60	0.49
1:A:67:LEU:O	1:A:68:VAL:C	2.57	0.47
1:A:306:LYS:HG3	4:A:537:HOH:O	2.16	0.45
1:A:33:ILE:HD13	4:A:631:HOH:O	2.17	0.44
1:A:323:ILE:O	1:A:323:ILE:HG22	2.14	0.44
1:A:84:SER:HB2	4:A:558:HOH:O	2.18	0.43
1:A:33:ILE:HD12	1:A:33:ILE:N	2.22	0.43
1:A:56:LLP:O3	1:A:56:LLP:NZ	2.49	0.43
1:A:281[A]:LEU:HD23	1:A:281[A]:LEU:HA	1.70	0.43
1:A:323:ILE:O	1:A:323:ILE:CG2	2.65	0.41
1:A:221:LYS:HG3	1:A:259:ILE:HD12	2.02	0.41
1:A:41[B]:ASN:OD1	1:A:306:LYS:CE	2.65	0.40
1:A:77:LYS:HE3	1:A:77:LYS:HB2	1.62	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:OE1	4:A:522:HOH:O[4_554]	0.27	1.93
1:A:108:GLN:CD	4:A:522:HOH:O[4_554]	1.24	0.96
1:A:323:ILE:CG1	1:A:323:ILE:CD1[2_565]	1.65	0.55
4:A:373:HOH:O	4:A:655:HOH:O[4_554]	1.75	0.45
1:A:65[B]:ARG:HD3	4:A:620:HOH:O[4_555]	1.21	0.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ILE:CD1	1:A:323:ILE:CD1[2_565]	1.98	0.22
1:A:65[B]:ARG:CD	4:A:620:HOH:O[4_555]	2.07	0.13
1:A:65[B]:ARG:HH12	1:A:200:LEU:O[4_555]	1.50	0.10

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	327/346 (94%)	321 (98%)	6 (2%)	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	278/285 (98%)	271 (98%)	7 (2%)	42	24

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	66[A]	SER
1	A	66[B]	SER
1	A	77	LYS
1	A	226	LEU

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Mol	Chain	Res	Type
1	A	277	ARG
1	A	308	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	89	GLN
1	A	296	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	LLP	A	56	1	23,24,25	2.12	5 (21%)	25,32,34	1.79	5 (20%)

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
1	LLP	A	56	1	-	3/16/17/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	LLP	O3-C3	-7.20	1.20	1.36
1	A	56	LLP	P-OP2	-3.53	1.41	1.54
1	A	56	LLP	P-OP3	-3.52	1.41	1.54
1	A	56	LLP	P-OP1	-2.86	1.41	1.50
1	A	56	LLP	C3-C2	-2.05	1.38	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	LLP	OP4-C5'-C5	6.33	121.22	109.36
1	A	56	LLP	C4-C3-C2	-2.66	118.65	120.14
1	A	56	LLP	OP2-P-OP4	-2.42	100.36	106.67
1	A	56	LLP	OP3-P-OP4	-2.33	100.60	106.67
1	A	56	LLP	C4-C4'-NZ	-2.19	113.94	124.04

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	56	LLP	C4-C5-C5'-OP4
1	A	56	LLP	C4-C4'-NZ-CE
1	A	56	LLP	CG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	56	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	A	347	-	6,6,6	1.39	1 (16%)	7,7,7	1.12	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	A	347	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	347	MLI	C1-C2	2.03	1.54	1.51

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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	315/346 (91%)	-0.20	12 (3%)	44 48	7, 17, 45, 95	12 (3%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	VAL	7.5
1	A	323	ILE	6.5
1	A	67	LEU	5.9
1	A	329	ALA	5.3
1	A	65[A]	ARG	4.4
1	A	3	ALA	4.1
1	A	76	PRO	3.8
1	A	320	THR	2.8
1	A	66[A]	SER	2.4
1	A	324	THR	2.3
1	A	327	LYS	2.1
1	A	319	LEU	2.1

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
1	LLP	A	56	24/25	0.98	0.05	20,20,20,20	0

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	A	347	7/7	0.98	0.04	14,14,16,16	0
3	MN	A	348	1/1	1.00	0.01	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.