



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 12:17 PM EDT

PDB ID : 9O3U / pdb_00009o3u
Title : Crystal Structure of K109A Variant of D-Dopachrome Tautomerase (D-DT)
Authors : Pilien, A.V.R.; Argueta, C.; Parkins, A.; Pantouris, G.
Deposited on : 2025-04-07
Resolution : 1.49 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

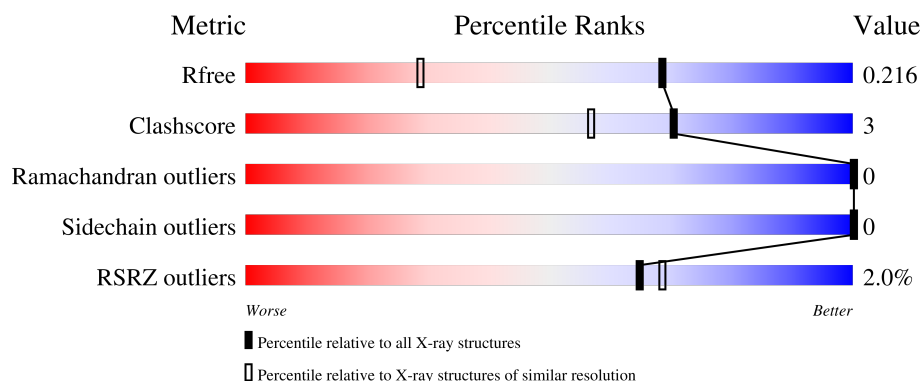
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.49 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.




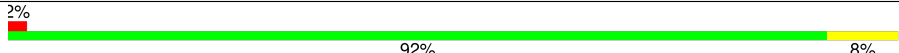
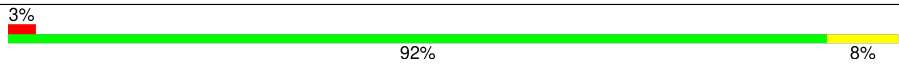
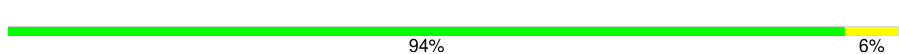

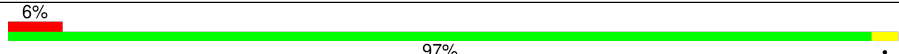
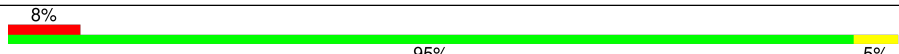
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	AAA	117	<div> <div>96%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	BBB	117	<div> <div>93%</div> <div>7%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	CCC	117	<div> <div>95%</div> <div>5%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	DDD	117	<div> <div>95%</div> <div>5%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	EEE	117	<div> <div>91%</div> <div>9%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	FFF	117	 92% 8%
1	GGG	117	 92% 8%
1	HHH	117	 92% 8%
1	III	117	 94% 6%
1	JJJ	117	 91% 9%
1	KKK	117	 97% .
1	LLL	117	 95% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12168 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 D-dopachrome decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	117	Total	C	N	O	S	0	0	0
			874	558	149	163	4			
1	BBB	117	Total	C	N	O	S	0	4	0
			890	568	151	167	4			
1	CCC	117	Total	C	N	O	S	0	4	0
			894	570	153	167	4			
1	DDD	117	Total	C	N	O	S	0	1	0
			876	560	149	163	4			
1	EEE	117	Total	C	N	O	S	0	4	0
			899	578	152	164	5			
1	FFF	117	Total	C	N	O	S	0	4	0
			894	573	150	167	4			
1	GGG	117	Total	C	N	O	S	0	2	0
			885	566	151	164	4			
1	HHH	117	Total	C	N	O	S	0	3	0
			875	560	146	163	6			
1	III	117	Total	C	N	O	S	0	4	0
			888	568	152	163	5			
1	JJJ	117	Total	C	N	O	S	0	2	0
			883	563	152	163	5			
1	KKK	117	Total	C	N	O	S	0	3	0
			866	554	144	162	6			
1	LLL	117	Total	C	N	O	S	0	2	0
			873	557	149	163	4			

There are 12 discrepancies between the modelled and reference sequences:

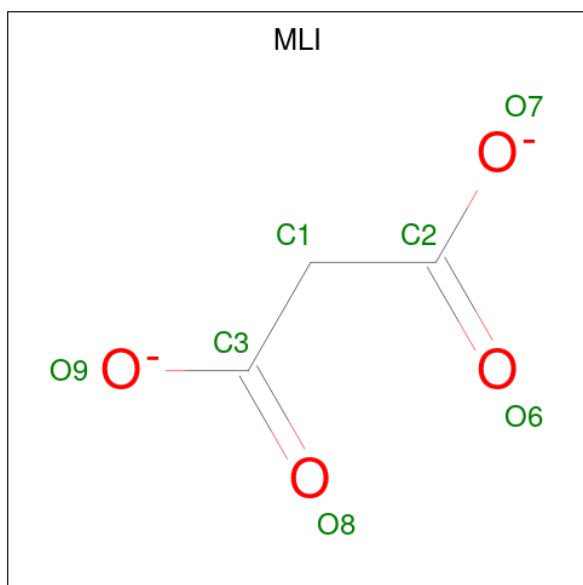
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	109	ALA	LYS	variant	UNP P30046
BBB	109	ALA	LYS	variant	UNP P30046
CCC	109	ALA	LYS	variant	UNP P30046
DDD	109	ALA	LYS	variant	UNP P30046
EEE	109	ALA	LYS	variant	UNP P30046

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Chain	Residue	Modelled	Actual	Comment	Reference
FFF	109	ALA	LYS	variant	UNP P30046
GGG	109	ALA	LYS	variant	UNP P30046
HHH	109	ALA	LYS	variant	UNP P30046
III	109	ALA	LYS	variant	UNP P30046
JJJ	109	ALA	LYS	variant	UNP P30046
KKK	109	ALA	LYS	variant	UNP P30046
LLL	109	ALA	LYS	variant	UNP P30046

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			7	3	4		
2	BBB	1	Total	C	O	0	0
			7	3	4		
2	CCC	1	Total	C	O	0	1
			14	6	8		
2	DDD	1	Total	C	O	0	0
			7	3	4		
2	DDD	1	Total	C	O	0	0
			7	3	4		
2	EEE	1	Total	C	O	0	0
			7	3	4		
2	FFF	1	Total	C	O	0	0
			7	3	4		
2	GGG	1	Total	C	O	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	HHH	1	Total	C	O	0	0
			7	3	4		
2	III	1	Total	C	O	0	0
			7	3	4		
2	JJJ	1	Total	C	O	0	0
			7	3	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	135	Total	O	0	0
			135	135		
3	BBB	160	Total	O	0	0
			160	160		
3	CCC	164	Total	O	0	0
			164	164		
3	DDD	138	Total	O	0	0
			138	138		
3	EEE	141	Total	O	0	0
			141	141		
3	FFF	134	Total	O	0	0
			134	134		
3	GGG	128	Total	O	0	0
			128	128		
3	HHH	109	Total	O	0	0
			109	109		
3	III	118	Total	O	0	0
			118	118		
3	JJJ	88	Total	O	0	0
			88	88		
3	KKK	80	Total	O	0	0
			80	80		
3	LLL	92	Total	O	0	0
			92	92		

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: D-dopachrome decarboxylase

Chain AAA:  96%



- Molecule 1: D-dopachrome decarboxylase

Chain BBB:  93% 7%



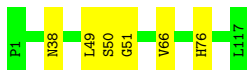
- Molecule 1: D-dopachrome decarboxylase

Chain CCC:  95% 5%



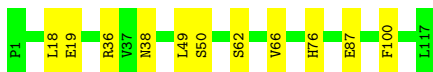
- Molecule 1: D-dopachrome decarboxylase

Chain DDD:  95% 5%



- Molecule 1: D-dopachrome decarboxylase

Chain EEE:  91% 9%



- Molecule 1: D-dopachrome decarboxylase

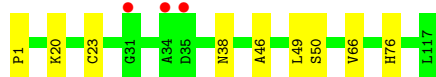
Chain FFF:  92% 8%



- Molecule 1: D-dopachrome decarboxylase



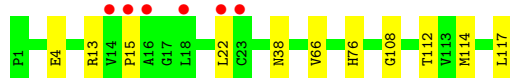
- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



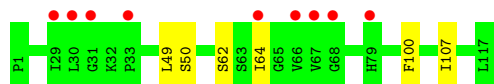
- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



- Molecule 1: D-dopachrome decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.72Å 94.45Å 95.25Å 90.00° 105.34° 90.00°	Depositor
Resolution (Å)	72.16 – 1.49 72.16 – 1.49	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.16-1.49) 100.0 (72.16-1.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.49Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.185 , 0.216 0.185 , 0.216	Depositor DCC
R_{free} test set	10237 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.9	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	0.96	EDS
Total number of atoms	12168	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: 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	AAA	1.10	0/891	1.16	0/1209
1	BBB	1.13	0/916	1.10	0/1242
1	CCC	1.12	0/923	1.19	0/1252
1	DDD	1.17	0/896	1.20	0/1216
1	EEE	1.11	0/928	1.14	0/1257
1	FFF	1.04	0/923	1.19	0/1251
1	GGG	1.10	0/908	1.18	0/1231
1	HHH	1.10	0/901	1.26	0/1224
1	III	1.13	0/917	1.23	0/1244
1	JJJ	1.13	0/906	1.32	0/1228
1	KKK	1.16	0/892	1.40	0/1214
1	LLL	1.23	0/896	1.34	0/1216
All	All	1.13	0/10897	1.23	0/14784

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	874	0	882	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BBB	890	0	902	9	0
1	CCC	894	0	911	7	0
1	DDD	876	0	884	8	0
1	EEE	899	0	931	13	0
1	FFF	894	0	918	11	0
1	GGG	885	0	901	8	0
1	HHH	875	0	881	10	0
1	III	888	0	902	8	0
1	JJJ	883	0	893	10	0
1	KKK	866	0	862	3	0
1	LLL	873	0	874	4	0
2	AAA	7	0	2	0	0
2	BBB	7	0	2	1	0
2	CCC	14	0	4	1	0
2	DDD	14	0	4	0	0
2	EEE	7	0	2	1	0
2	FFF	7	0	2	0	0
2	GGG	7	0	2	0	0
2	HHH	7	0	2	1	0
2	III	7	0	2	0	0
2	JJJ	7	0	2	0	0
3	AAA	135	0	0	1	0
3	BBB	160	0	0	1	0
3	CCC	164	0	0	1	0
3	DDD	138	0	0	1	0
3	EEE	141	0	0	1	0
3	FFF	134	0	0	0	0
3	GGG	128	0	0	1	0
3	HHH	109	0	0	0	0
3	III	118	0	0	1	0
3	JJJ	88	0	0	3	0
3	KKK	80	0	0	0	0
3	LLL	92	0	0	0	0
All	All	12168	0	10765	72	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (72) 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:HHH:46:ALA:HB1	1:III:19:GLU:OE2	1.79	0.83
1:FFF:82[A]:GLU:OE2	1:FFF:86:LYS:CE	2.30	0.80
1:FFF:82[A]:GLU:OE2	1:FFF:86:LYS:HE3	1.85	0.76
1:EEE:18[A]:LEU:HD13	1:EEE:87:GLU:HG2	1.70	0.73
1:BBB:38:ASN:HD22	1:FFF:49:LEU:HA	1.59	0.67
1:HHH:66:VAL:O	1:HHH:76:HIS:HE1	1.77	0.67
1:FFF:82[A]:GLU:OE2	1:FFF:86:LYS:HE2	1.94	0.66
1:EEE:18[A]:LEU:HD13	1:EEE:87:GLU:CG	2.25	0.66
1:GGG:66:VAL:O	1:GGG:76:HIS:HE1	1.79	0.64
1:FFF:66:VAL:O	1:FFF:76:HIS:HE1	1.80	0.64
1:DDD:66:VAL:O	1:DDD:76:HIS:HE1	1.82	0.63
1:GGG:76:HIS:HD2	3:GGG:347:HOH:O	1.82	0.61
1:DDD:50:SER:H	1:FFF:38:ASN:ND2	1.99	0.61
1:CCC:38:ASN:HD22	1:EEE:49:LEU:HA	1.68	0.59
1:LLL:64:ILE:HD11	1:LLL:107:ILE:HD12	1.84	0.59
1:AAA:50:SER:H	1:EEE:38:ASN:HD22	1.51	0.59
1:AAA:66:VAL:O	1:AAA:76:HIS:HE1	1.85	0.59
1:JJJ:76:HIS:HD2	3:JJJ:339:HOH:O	1.86	0.59
1:DDD:76:HIS:HD2	3:DDD:361:HOH:O	1.86	0.57
1:AAA:50:SER:H	1:EEE:38:ASN:ND2	2.03	0.57
1:AAA:38:ASN:ND2	1:CCC:50:SER:H	2.03	0.56
1:CCC:38:ASN:ND2	1:EEE:50:SER:H	2.03	0.56
1:EEE:18[A]:LEU:CD1	1:EEE:87:GLU:HG2	2.34	0.56
1:FFF:116:PHE:HB3	1:GGG:21:ARG:HG2	1.88	0.56
1:BBB:66:VAL:O	1:BBB:76:HIS:HE1	1.89	0.55
1:HHH:50:SER:H	1:III:38:ASN:ND2	2.04	0.55
1:BBB:38:ASN:ND2	1:FFF:50:SER:H	2.05	0.55
1:BBB:50:SER:H	1:DDD:38:ASN:ND2	2.05	0.54
1:CCC:66:VAL:O	1:CCC:76:HIS:HE1	1.90	0.53
1:JJJ:66:VAL:O	1:JJJ:76:HIS:HE1	1.92	0.53
1:BBB:76:HIS:HD2	3:BBB:345:HOH:O	1.90	0.53
1:EEE:66:VAL:O	1:EEE:76:HIS:HE1	1.91	0.53
1:EEE:36:ARG:NH1	2:EEE:201:MLI:O6	2.38	0.52
1:HHH:49:LEU:HA	1:III:38:ASN:HD22	1.75	0.52
1:JJJ:38:ASN:ND2	1:LLL:50:SER:H	2.07	0.52
1:AAA:76:HIS:HD2	3:AAA:340:HOH:O	1.92	0.52
1:HHH:1:PRO:H3	2:HHH:201:MLI:C3	2.23	0.51
1:KKK:107:ILE:HB	1:KKK:114[B]:MET:HG3	1.92	0.51
1:III:76:HIS:HD2	3:III:323:HOH:O	1.93	0.50
1:BBB:1:PRO:HD3	2:BBB:201:MLI:H11	1.92	0.50
1:CCC:76:HIS:HD2	3:CCC:344:HOH:O	1.95	0.49
1:III:66:VAL:O	1:III:76:HIS:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:38:ASN:HD22	1:CCC:49:LEU:HA	1.76	0.49
1:BBB:49:LEU:HA	1:DDD:38:ASN:HD22	1.77	0.49
1:EEE:76:HIS:HD2	3:EEE:322:HOH:O	1.96	0.48
1:DDD:49:LEU:HA	1:FFF:38:ASN:HD22	1.79	0.48
1:GGG:50:SER:H	1:HHH:38:ASN:ND2	2.12	0.48
1:GGG:23:CYS:HA	1:GGG:37:VAL:HG11	1.97	0.46
1:GGG:49:LEU:HA	1:HHH:38:ASN:HD22	1.80	0.46
1:DDD:51:GLY:HA2	1:FFF:23:CYS:SG	2.57	0.45
1:JJJ:38:ASN:HD22	1:LLL:49:LEU:HA	1.81	0.45
1:KKK:66:VAL:O	1:KKK:76:HIS:HE1	1.99	0.45
1:JJJ:114[A]:MET:HE2	3:JJJ:375:HOH:O	2.16	0.45
1:CCC:36:ARG:NH1	2:CCC:201[B]:MLI:O7	2.44	0.45
1:HHH:20:LYS:O	1:HHH:23[A]:CYS:HB3	2.17	0.45
1:GGG:51:GLY:HA2	1:HHH:23[A]:CYS:SG	2.57	0.44
1:FFF:66:VAL:O	1:FFF:76:HIS:CE1	2.67	0.43
1:GGG:38:ASN:ND2	1:III:50:SER:H	2.16	0.43
1:KKK:114[B]:MET:HE3	1:KKK:114[B]:MET:HB3	1.77	0.43
1:EEE:62:SER:HA	1:EEE:100:PHE:O	2.18	0.43
1:AAA:46:ALA:HB1	1:EEE:19:GLU:OE2	2.19	0.42
1:JJJ:108:GLY:HA2	1:JJJ:112:THR:O	2.20	0.42
1:JJJ:114[B]:MET:SD	1:JJJ:117:LEU:HD12	2.59	0.42
1:LLL:62:SER:HA	1:LLL:100:PHE:O	2.21	0.41
1:JJJ:13:ARG:O	1:JJJ:15:PRO:HD3	2.20	0.41
1:JJJ:4[B]:GLU:OE1	3:JJJ:301:HOH:O	2.22	0.41
1:JJJ:22:LEU:O	1:JJJ:22:LEU:HD12	2.21	0.41
1:HHH:50:SER:H	1:III:38:ASN:HD22	1.69	0.40
1:III:62:SER:HA	1:III:100:PHE:O	2.21	0.40
1:BBB:50:SER:H	1:DDD:38:ASN:HD22	1.67	0.40
1:BBB:62[A]:SER:HA	1:BBB:100:PHE:O	2.21	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	AAA	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
1	BBB	119/117 (102%)	115 (97%)	4 (3%)	0	100	100
1	CCC	119/117 (102%)	116 (98%)	3 (2%)	0	100	100
1	DDD	116/117 (99%)	112 (97%)	4 (3%)	0	100	100
1	EEE	119/117 (102%)	116 (98%)	3 (2%)	0	100	100
1	FFF	119/117 (102%)	116 (98%)	3 (2%)	0	100	100
1	GGG	117/117 (100%)	113 (97%)	4 (3%)	0	100	100
1	HHH	118/117 (101%)	114 (97%)	4 (3%)	0	100	100
1	III	119/117 (102%)	116 (98%)	3 (2%)	0	100	100
1	JJJ	117/117 (100%)	113 (97%)	4 (3%)	0	100	100
1	KKK	118/117 (101%)	115 (98%)	3 (2%)	0	100	100
1	LLL	117/117 (100%)	113 (97%)	4 (3%)	0	100	100
All	All	1413/1404 (101%)	1371 (97%)	42 (3%)	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	AAA	92/94 (98%)	92 (100%)	0	100	100
1	BBB	95/94 (101%)	95 (100%)	0	100	100
1	CCC	96/94 (102%)	96 (100%)	0	100	100
1	DDD	92/94 (98%)	92 (100%)	0	100	100
1	EEE	97/94 (103%)	97 (100%)	0	100	100
1	FFF	97/94 (103%)	97 (100%)	0	100	100
1	GGG	94/94 (100%)	94 (100%)	0	100	100
1	HHH	93/94 (99%)	93 (100%)	0	100	100
1	III	94/94 (100%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JJJ	93/94 (99%)	93 (100%)	0	100	100
1	KKK	91/94 (97%)	91 (100%)	0	100	100
1	LLL	91/94 (97%)	91 (100%)	0	100	100
All	All	1125/1128 (100%)	1125 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

12 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	CCC	201[B]	-	6,6,6	1.26	0	7,7,7	1.04	0
2	MLI	HHH	201	-	6,6,6	1.30	0	7,7,7	1.04	0
2	MLI	FFF	201	-	6,6,6	1.70	1 (16%)	7,7,7	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLI	DDD	201	-	6,6,6	1.64	1 (16%)	7,7,7	0.80	0
2	MLI	CCC	201[A]	-	6,6,6	1.43	0	7,7,7	1.00	0
2	MLI	III	201	-	6,6,6	1.35	1 (16%)	7,7,7	0.96	0
2	MLI	JJJ	201	-	6,6,6	1.13	1 (16%)	7,7,7	1.13	0
2	MLI	AAA	201	-	6,6,6	1.26	1 (16%)	7,7,7	1.01	0
2	MLI	GGG	201	-	6,6,6	1.52	2 (33%)	7,7,7	1.12	0
2	MLI	EEE	201	-	6,6,6	1.17	0	7,7,7	1.31	0
2	MLI	DDD	202	-	6,6,6	1.36	0	7,7,7	1.48	2 (28%)
2	MLI	BBB	201	-	6,6,6	1.18	0	7,7,7	1.20	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	CCC	201[B]	-	-	3/4/4/4	-
2	MLI	HHH	201	-	-	2/4/4/4	-
2	MLI	FFF	201	-	-	4/4/4/4	-
2	MLI	DDD	201	-	-	0/4/4/4	-
2	MLI	CCC	201[A]	-	-	2/4/4/4	-
2	MLI	III	201	-	-	0/4/4/4	-
2	MLI	JJJ	201	-	-	2/4/4/4	-
2	MLI	AAA	201	-	-	0/4/4/4	-
2	MLI	GGG	201	-	-	0/4/4/4	-
2	MLI	EEE	201	-	-	3/4/4/4	-
2	MLI	DDD	202	-	-	2/4/4/4	-
2	MLI	BBB	201	-	-	1/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	FFF	201	MLI	O9-C3	-2.70	1.21	1.30
2	DDD	201	MLI	O8-C3	2.61	1.30	1.22
2	AAA	201	MLI	O9-C3	-2.22	1.23	1.30
2	GGG	201	MLI	O7-C2	-2.16	1.23	1.30
2	III	201	MLI	O7-C2	-2.08	1.23	1.30
2	GGG	201	MLI	O9-C3	-2.03	1.24	1.30
2	JJJ	201	MLI	O9-C3	-2.01	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	202	MLI	O6-C2-C1	-2.34	115.44	122.11
2	DDD	202	MLI	C3-C1-C2	-2.19	105.22	112.95

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	EEE	201	MLI	C3-C1-C2-O7
2	DDD	202	MLI	C3-C1-C2-O7
2	FFF	201	MLI	C3-C1-C2-O6
2	DDD	202	MLI	C3-C1-C2-O6
2	EEE	201	MLI	C3-C1-C2-O6
2	CCC	201[B]	MLI	C2-C1-C3-O8
2	CCC	201[A]	MLI	C2-C1-C3-O9
2	FFF	201	MLI	C2-C1-C3-O8
2	HHH	201	MLI	C2-C1-C3-O8
2	HHH	201	MLI	C2-C1-C3-O9
2	FFF	201	MLI	C3-C1-C2-O7
2	BBB	201	MLI	C2-C1-C3-O9
2	CCC	201[A]	MLI	C2-C1-C3-O8
2	FFF	201	MLI	C2-C1-C3-O9
2	CCC	201[B]	MLI	C2-C1-C3-O9
2	EEE	201	MLI	C2-C1-C3-O8
2	JJJ	201	MLI	C2-C1-C3-O8
2	CCC	201[B]	MLI	C3-C1-C2-O7
2	JJJ	201	MLI	C2-C1-C3-O9

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	201[B]	MLI	1	0
2	HHH	201	MLI	1	0
2	EEE	201	MLI	1	0
2	BBB	201	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, 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	AAA	117/117 (100%)	-0.37	0 100 100	10, 13, 21, 31	0
1	BBB	117/117 (100%)	-0.25	0 100 100	6, 14, 21, 27	4 (3%)
1	CCC	117/117 (100%)	-0.32	0 100 100	7, 14, 23, 30	4 (3%)
1	DDD	117/117 (100%)	-0.22	0 100 100	8, 14, 24, 31	1 (0%)
1	EEE	117/117 (100%)	-0.23	0 100 100	8, 15, 24, 35	4 (3%)
1	FFF	117/117 (100%)	-0.16	1 (0%) 81 84	8, 15, 23, 30	4 (3%)
1	GGG	117/117 (100%)	-0.04	2 (1%) 69 72	9, 17, 26, 33	2 (1%)
1	HHH	117/117 (100%)	0.16	3 (2%) 57 61	10, 20, 33, 43	3 (2%)
1	III	117/117 (100%)	0.07	0 100 100	10, 19, 27, 33	4 (3%)
1	JJJ	117/117 (100%)	0.64	6 (5%) 33 36	12, 24, 37, 43	2 (1%)
1	KKK	117/117 (100%)	0.74	7 (5%) 27 30	15, 24, 40, 46	3 (2%)
1	LLL	117/117 (100%)	0.72	9 (7%) 19 21	13, 22, 35, 44	2 (1%)
All	All	1404/1404 (100%)	0.06	28 (1%) 65 68	6, 17, 32, 46	33 (2%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	LLL	67	VAL	4.7
1	LLL	66	VAL	4.0
1	JJJ	14	VAL	3.7
1	JJJ	15	PRO	3.4
1	KKK	34	ALA	3.2
1	LLL	64	ILE	3.2
1	JJJ	23	CYS	3.0
1	JJJ	16	ALA	2.8
1	KKK	66	VAL	2.7
1	KKK	35	ASP	2.7
1	GGG	23	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	HHH	34	ALA	2.6
1	JJJ	22	LEU	2.6
1	LLL	31	GLY	2.5
1	FFF	12	ASN	2.4
1	LLL	79	HIS	2.3
1	HHH	31	GLY	2.2
1	JJJ	18	LEU	2.2
1	KKK	117	LEU	2.2
1	KKK	11	ALA	2.2
1	LLL	68	GLY	2.2
1	LLL	30	LEU	2.1
1	GGG	35	ASP	2.1
1	KKK	31	GLY	2.1
1	KKK	33	PRO	2.1
1	LLL	29	ILE	2.1
1	HHH	35	ASP	2.1
1	LLL	33	PRO	2.1

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	FFF	201	7/7	0.75	0.18	36,41,44,47	0
2	MLI	HHH	201	7/7	0.75	0.17	41,57,72,72	0
2	MLI	BBB	201	7/7	0.81	0.16	29,37,47,53	0
2	MLI	III	201	7/7	0.83	0.14	38,45,59,61	0
2	MLI	CCC	201[B]	7/7	0.85	0.14	26,27,28,28	7
2	MLI	CCC	201[A]	7/7	0.85	0.14	27,30,32,36	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MLI	JJJ	201	7/7	0.85	0.13	36,43,49,50	0
2	MLI	AAA	201	7/7	0.87	0.12	32,34,38,41	0
2	MLI	DDD	201	7/7	0.88	0.11	22,33,35,37	0
2	MLI	EEE	201	7/7	0.88	0.12	36,44,51,54	0
2	MLI	DDD	202	7/7	0.90	0.10	23,24,27,29	0
2	MLI	GGG	201	7/7	0.92	0.08	24,26,32,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.