Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 08:25 AM EDT

PDB ID	:	5KDP
Title	:	E491A mutant of choline TMA-lyase
Authors	:	Funk, M.A.; Drennan, C.L.
Deposited on	:	2016-06-08
Resolution	:	1.90 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	Percentile Ranks	Value
Rfree		0.246
Clashscore		2
Ramachandran outliers		0.3%
Sidechain outliers		0.7%
RSRZ outliers		6.2%

Worse — *Better*

▌ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
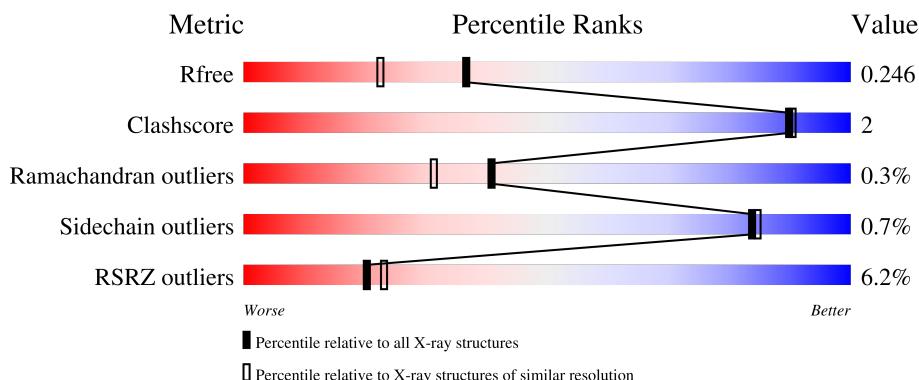
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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 <=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	815	4% / 94% / 5% •
1	C	815	8% / 94% / 5% •
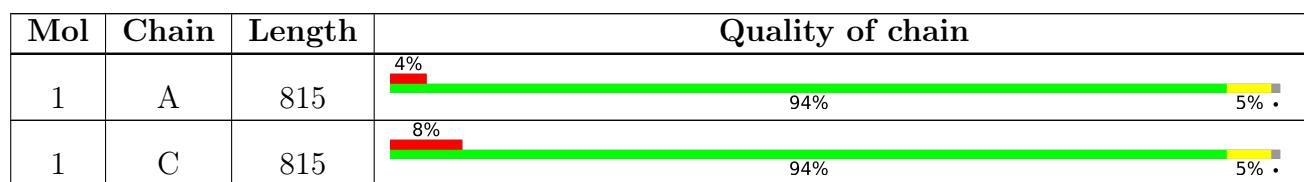
2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 26770 atoms, of which 12447 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 Choline trimethylamine-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	803	Total	C	H	N	O	S	0	6	0
			12561	4021	6214	1078	1202	46			
1	C	806	Total	C	H	N	O	S	0	0	0
			12567	4021	6221	1081	1198	46			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	MET	-	initiating methionine	UNP Q30W70
A	33	GLY	-	expression tag	UNP Q30W70
A	34	SER	-	expression tag	UNP Q30W70
A	35	SER	-	expression tag	UNP Q30W70
A	36	HIS	-	expression tag	UNP Q30W70
A	37	HIS	-	expression tag	UNP Q30W70
A	38	HIS	-	expression tag	UNP Q30W70
A	39	HIS	-	expression tag	UNP Q30W70
A	40	HIS	-	expression tag	UNP Q30W70
A	41	HIS	-	expression tag	UNP Q30W70
A	42	SER	-	expression tag	UNP Q30W70
A	43	SER	-	expression tag	UNP Q30W70
A	44	GLY	-	expression tag	UNP Q30W70
A	45	LEU	-	expression tag	UNP Q30W70
A	46	VAL	-	expression tag	UNP Q30W70
A	47	PRO	-	expression tag	UNP Q30W70
A	48	ARG	-	expression tag	UNP Q30W70
A	49	GLY	-	expression tag	UNP Q30W70
A	50	SER	-	expression tag	UNP Q30W70
A	51	HIS	-	expression tag	UNP Q30W70
A	52	MET	-	expression tag	UNP Q30W70
A	491	ALA	GLU	engineered mutation	UNP Q30W70
C	32	MET	-	initiating methionine	UNP Q30W70
C	33	GLY	-	expression tag	UNP Q30W70
C	34	SER	-	expression tag	UNP Q30W70

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Chain	Residue	Modelled	Actual	Comment	Reference
C	35	SER	-	expression tag	UNP Q30W70
C	36	HIS	-	expression tag	UNP Q30W70
C	37	HIS	-	expression tag	UNP Q30W70
C	38	HIS	-	expression tag	UNP Q30W70
C	39	HIS	-	expression tag	UNP Q30W70
C	40	HIS	-	expression tag	UNP Q30W70
C	41	HIS	-	expression tag	UNP Q30W70
C	42	SER	-	expression tag	UNP Q30W70
C	43	SER	-	expression tag	UNP Q30W70
C	44	GLY	-	expression tag	UNP Q30W70
C	45	LEU	-	expression tag	UNP Q30W70
C	46	VAL	-	expression tag	UNP Q30W70
C	47	PRO	-	expression tag	UNP Q30W70
C	48	ARG	-	expression tag	UNP Q30W70
C	49	GLY	-	expression tag	UNP Q30W70
C	50	SER	-	expression tag	UNP Q30W70
C	51	HIS	-	expression tag	UNP Q30W70
C	52	MET	-	expression tag	UNP Q30W70
C	491	ALA	GLU	engineered mutation	UNP Q30W70

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Na 1	0	0
2	C	1	Total 1	Na 1	0	0

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).

MLI

O7

O⁻

C1   C2

C3

O9 O⁻

O6

O8
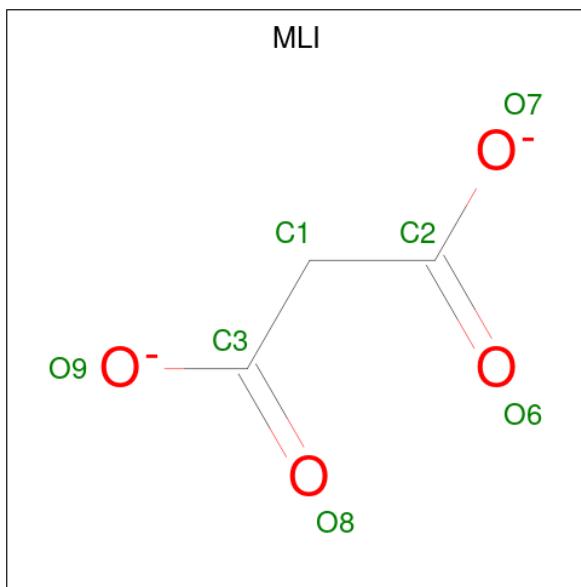
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 9	C 3	H 2	O 4	0	0
3	A	1	Total 9	C 3	H 2	O 4	0	0
3	A	1	Total 9	C 3	H 2	O 4	0	0
3	A	1	Total 9	C 3	H 2	O 4	0	0
3	C	1	Total 9	C 3	H 2	O 4	0	0
3	C	1	Total 9	C 3	H 2	O 4	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	826	Total 826	O 826	0	0
4	C	760	Total 760	O 760	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: Choline trimethylamine-lyase
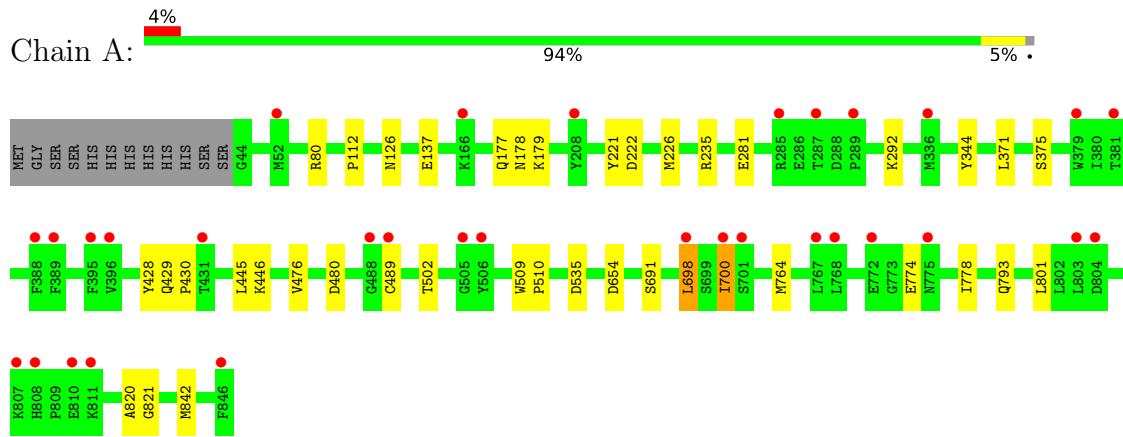
• Molecule 1: Choline trimethylamine-lyase
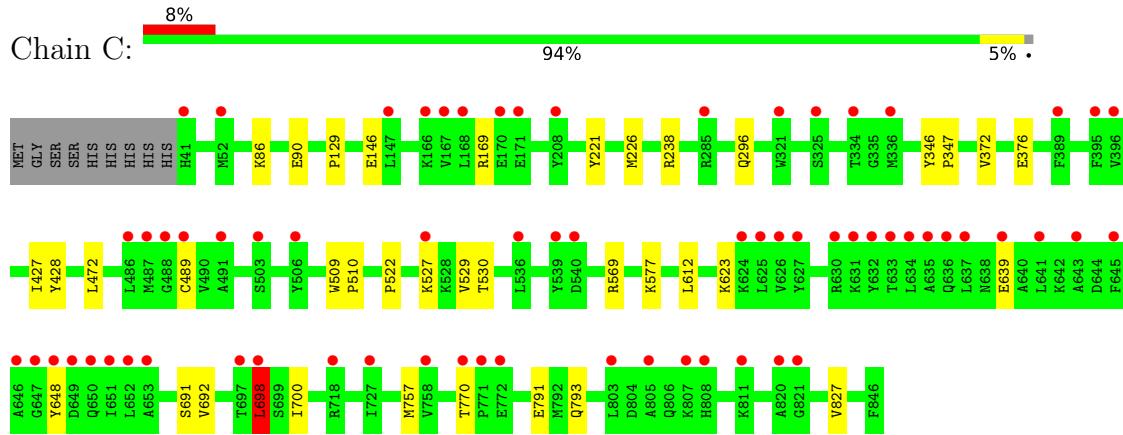
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	228.92Å 228.92Å 78.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 1.90 49.47 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.47-1.90) 99.0 (49.47-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.214 , 0.244 0.216 , 0.246	Depositor DCC
R_{free} test set	4917 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 43.6	EDS
L-test for twinning[2]	$< |L| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26770	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, NA

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	0.26	0/6511	0.44	0/8818
1	C	0.27	0/6494	0.45	1/8794 (0.0%)
All	All	0.26	0/13005	0.44	1/17612 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	698	LEU	CA-CB-CG	5.46	127.86	115.30

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	6347	6214	6191	23	0
1	C	6346	6221	6220	22	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	28	8	8	0	0
3	C	14	4	4	0	0
4	A	826	0	0	10	3
4	C	760	0	0	10	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14323	12447	12423	45	5

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 2.

All (45) 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:C:238:ARG:NH1	4:C:1001:HOH:O	2.01	0.93
1:A:535:ASP:OD1	4:A:1001:HOH:O	1.91	0.86
1:A:292:LYS:NZ	4:A:1003:HOH:O	2.12	0.82
1:C:146:GLU:OE1	4:C:1002:HOH:O	2.06	0.73
1:A:179:LYS:NZ	4:A:1005:HOH:O	2.17	0.71
1:A:281:GLU:OE1	4:A:1002:HOH:O	2.09	0.69
1:C:827:VAL:O	4:C:1003:HOH:O	2.09	0.69
1:C:472:LEU:O	4:C:1004:HOH:O	2.09	0.68
1:C:527:LYS:NZ	4:C:1009:HOH:O	2.27	0.66
1:A:654:ASP:OD1	4:A:1004:HOH:O	2.15	0.64
1:C:569:ARG:NH1	4:C:1005:HOH:O	2.22	0.57
1:A:80:ARG:NH2	1:A:137:GLU:OE2	2.36	0.57
1:A:177:GLN:NE2	4:A:1035:HOH:O	2.38	0.56
1:A:446:LYS:NZ	1:A:774:GLU:OE2	2.39	0.54
1:A:445:LEU:HB3	1:A:778:ILE:HD12	1.92	0.52
1:A:235:ARG:NH1	4:A:1053:HOH:O	2.43	0.51
1:C:529:VAL:HG13	1:C:530:THR:HG23	1.94	0.50
1:C:522:PRO:HD3	1:C:529:VAL:HG12	1.95	0.49
1:A:764:MET:HE2	1:A:842:MET:HG2	1.96	0.48
1:A:178:ASN:OD1	4:A:1006:HOH:O	2.20	0.48
1:A:502:THR:HG21	1:A:698:LEU:HD11	1.96	0.47
1:C:623:LYS:NZ	4:C:1054:HOH:O	2.48	0.47
1:C:698:LEU:H	1:C:698:LEU:HD13	1.81	0.46
1:C:791:GLU:OE2	1:C:793:GLN:NE2	2.45	0.45
1:C:296:GLN:NE2	4:C:1055:HOH:O	2.48	0.45
1:A:112:PRO:O	4:A:1008:HOH:O	2.21	0.44
1:C:372:VAL:HA	1:C:427:ILE:HD13	2.00	0.43
1:C:221:TYR:O	1:C:226:MET:HG2	2.18	0.43
1:A:793:GLN:HE22	1:A:821:GLY:H	1.65	0.42
1:A:371:LEU:HD22	1:A:430:PRO:HD2	2.01	0.42
1:C:639:GLU:OE2	1:C:648:TYR:OH	2.34	0.42
1:C:691:SER:OG	1:C:692:VAL:N	2.52	0.42
1:A:509:TRP:N	1:A:510:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ASN:OD1	4:A:1009:HOH:O	2.22	0.42
1:C:86:LYS:NZ	1:C:90:GLU:OE1	2.39	0.42
1:C:129:PRO:HB3	1:C:376:GLU:HG2	2.02	0.41
1:C:296:GLN:NE2	4:C:1087:HOH:O	2.53	0.41
1:A:476:VAL:HG13	1:A:480:ASP:HB2	2.03	0.41
1:C:346:TYR:N	1:C:347:PRO:HD2	2.35	0.41
1:A:221:TYR:O	1:A:226:MET:HG2	2.20	0.41
1:A:700:ILE:O	1:A:820:ALA:HB3	2.21	0.40
1:C:169:ARG:NH1	4:C:1021:HOH:O	2.38	0.40
1:A:375:SER:HA	1:A:429:GLN:HB2	2.03	0.40
1:C:509:TRP:N	1:C:510:PRO:CD	2.84	0.40
1:A:222:ASP:HB3	1:A:344:TYR:CD2	2.57	0.40

All (5) 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)
4:C:1005:HOH:O	4:C:1298:HOH:O[8_776]	1.80	0.40
4:A:1327:HOH:O	4:A:1371:HOH:O[1_554]	2.03	0.17
4:C:1457:HOH:O	4:C:1487:HOH:O[8_775]	2.05	0.15
4:A:1005:HOH:O	4:A:1289:HOH:O[8_776]	2.08	0.12
4:A:1636:HOH:O	4:A:1799:HOH:O[8_775]	2.10	0.10

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	807/815 (99%)	786 (97%)	18 (2%)	3 (0%)	34	24
1	C	804/815 (99%)	786 (98%)	16 (2%)	2 (0%)	47	38
All	All	1611/1630 (99%)	1572 (98%)	34 (2%)	5 (0%)	41	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	489	CYS
1	A	700	ILE
1	A	489	CYS
1	A	691	SER
1	C	700	ILE

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	678/686 (99%)	675 (100%)	3 (0%)	91	91
1	C	678/686 (99%)	672 (99%)	6 (1%)	78	79
All	All	1356/1372 (99%)	1347 (99%)	9 (1%)	84	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	428	TYR
1	A	698	LEU
1	A	801	LEU
1	C	428	TYR
1	C	577	LYS
1	C	612	LEU
1	C	698	LEU
1	C	757	MET
1	C	770	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
3	MLI	C	902	-	6,6,6	1.08	0	7,7,7	0.99	0
3	MLI	C	903	-	6,6,6	1.07	0	7,7,7	0.93	0
3	MLI	A	904	-	6,6,6	1.09	0	7,7,7	0.99	0
3	MLI	A	905	-	6,6,6	1.10	0	7,7,7	0.95	0
3	MLI	A	902	-	6,6,6	1.07	0	7,7,7	0.98	0
3	MLI	A	903	-	6,6,6	1.11	0	7,7,7	0.95	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
3	MLI	C	902	-	-	2/4/4/4	-
3	MLI	C	903	-	-	2/4/4/4	-
3	MLI	A	904	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLI	A	905	-	-	<mark>2/4/4/4</mark>	-
3	MLI	A	902	-	-	<mark>4/4/4/4</mark>	-
3	MLI	A	903	-	-	<mark>2/4/4/4</mark>	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	905	MLI	C3-C1-C2-O6
3	C	903	MLI	C3-C1-C2-O6
3	A	904	MLI	C3-C1-C2-O6
3	A	905	MLI	C3-C1-C2-O7
3	C	903	MLI	C3-C1-C2-O7
3	A	902	MLI	C2-C1-C3-O8
3	A	904	MLI	C3-C1-C2-O7
3	C	902	MLI	C3-C1-C2-O6
3	C	902	MLI	C3-C1-C2-O7
3	A	902	MLI	C3-C1-C2-O6
3	A	902	MLI	C2-C1-C3-O9
3	A	903	MLI	C2-C1-C3-O9
3	A	902	MLI	C3-C1-C2-O7
3	A	903	MLI	C2-C1-C3-O8

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 ⓘ

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(Å²)	Q<0.9
1	A	803/815 (98%)	0.32	32 (3%)	38	41	18, 30, 47, 73	0
1	C	806/815 (98%)	0.48	67 (8%)	11	13	17, 30, 50, 75	0
All	All	1609/1630 (98%)	0.40	99 (6%)	20	23	17, 30, 49, 75	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	489	CYS	6.6
1	C	630	ARG	4.9
1	C	634	LEU	4.2
1	C	632	TYR	3.9
1	A	489	CYS	3.8
1	C	625	LEU	3.8
1	A	846	PHE	3.6
1	C	167	VAL	3.5
1	C	651	ILE	3.5
1	C	646	ALA	3.5
1	C	645	PHE	3.5
1	A	395	PHE	3.4
1	C	626	VAL	3.4
1	C	771	PRO	3.3
1	C	698	LEU	3.3
1	C	649	ASP	3.3
1	A	810	GLU	3.2
1	C	643	ALA	3.2
1	A	807	LYS	3.2
1	A	700	ILE	3.2
1	C	285	ARG	3.1
1	A	52	MET	3.1
1	A	379	TRP	3.1
1	C	166	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	648	TYR	3.1
1	C	697	THR	3.0
1	C	635	ALA	3.0
1	A	285	ARG	3.0
1	C	536	LEU	2.9
1	C	772	GLU	2.9
1	C	653	ALA	2.9
1	A	389	PHE	2.9
1	C	395	PHE	2.9
1	C	639	GLU	2.8
1	C	540	ASP	2.8
1	A	808	HIS	2.7
1	C	486	LEU	2.7
1	C	336	MET	2.6
1	C	811	LYS	2.6
1	A	506	TYR	2.6
1	C	803	LEU	2.6
1	A	811	LYS	2.6
1	C	631	LYS	2.6
1	C	637	LEU	2.6
1	C	727	ILE	2.6
1	A	388	PHE	2.5
1	C	820	ALA	2.5
1	A	208	TYR	2.5
1	C	491	ALA	2.5
1	C	641	LEU	2.5
1	C	652	LEU	2.5
1	A	488	GLY	2.4
1	C	389	PHE	2.4
1	A	166	LYS	2.4
1	A	336	MET	2.4
1	C	633	THR	2.4
1	C	334	THR	2.4
1	A	775	ASN	2.4
1	C	170	GLU	2.4
1	A	803	LEU	2.3
1	C	171	GLU	2.3
1	C	41	HIS	2.3
1	C	627	TYR	2.3
1	C	168	LEU	2.3
1	C	208	TYR	2.3
1	C	808	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	396	VAL	2.3
1	A	767	LEU	2.2
1	C	527	LYS	2.2
1	C	624	LYS	2.2
1	C	807	LYS	2.2
1	C	770	THR	2.2
1	A	804	ASP	2.2
1	C	488	GLY	2.2
1	C	821	GLY	2.2
1	A	698	LEU	2.2
1	A	768	LEU	2.2
1	C	718	ARG	2.2
1	A	701	SER	2.2
1	C	503	SER	2.2
1	A	431	THR	2.2
1	C	758	VAL	2.2
1	A	396	VAL	2.2
1	C	805	ALA	2.1
1	C	647	GLY	2.1
1	C	321	TRP	2.1
1	A	505	GLY	2.1
1	C	487	MET	2.1
1	A	381	THR	2.1
1	C	636	GLN	2.1
1	C	506	TYR	2.1
1	C	539	TYR	2.1
1	C	650	GLN	2.1
1	C	52	MET	2.1
1	A	289	PRO	2.1
1	A	287	THR	2.0
1	A	772	GLU	2.0
1	C	325	SER	2.0
1	C	147	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	MLI	A	902	7/7	0.73	0.26	41,44,53,53	0
3	MLI	C	903	7/7	0.73	0.34	49,52,62,62	0
3	MLI	A	905	7/7	0.74	0.28	46,49,59,59	0
3	MLI	A	904	7/7	0.79	0.18	50,51,61,61	0
3	MLI	A	903	7/7	0.84	0.23	44,47,57,57	0
3	MLI	C	902	7/7	0.86	0.23	35,36,44,44	0
2	NA	A	901	1/1	0.97	0.09	27,27,27,27	0
2	NA	C	901	1/1	0.99	0.13	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.