wwPDB X-ray Structure Validation Summary Report (i)

Sep 16, 2023 – 07:51 PM EDT

PDB ID	:	4R7W
Title	:	Crystal structure of 5-methylcytosine deaminase from Klebsiella pneumoniae liganded with phosphonocytosine
Authors	:	Fedorov, A.A.; Fedorov, E.V.; Hitchcock, D.S.; Raushel, F.M.; Almo, S.C.
Deposited on	:	2014-08-28
Resolution	:	1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

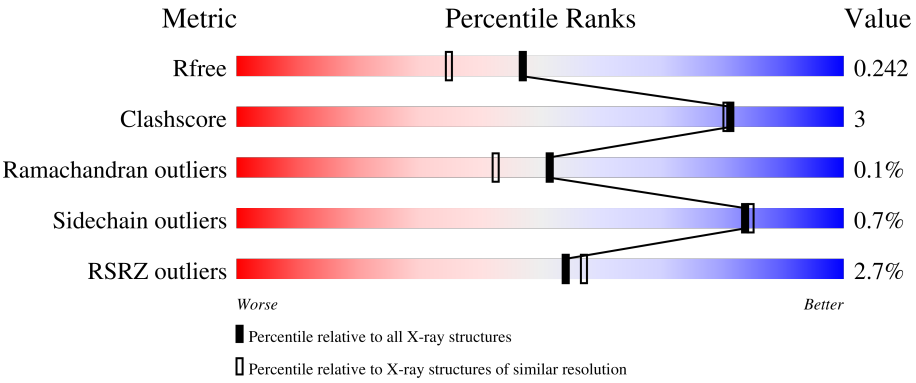
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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	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	431	89% 6% 5%
1	B	431	3% 91% 5%
1	C	431	3% 86% 9% 5%
1	D	431	3% 89% 6%
1	E	431	88% 7% 5%

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Mol	Chain	Length	Quality of chain
1	F	431	5% 91% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	C	504	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20980 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 Cytosine deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	1	0
			3228	2012	596	602	18			
1	B	412	Total	C	N	O	S	0	0	0
			3222	2009	593	602	18			
1	C	411	Total	C	N	O	S	0	0	0
			3217	2006	592	601	18			
1	D	412	Total	C	N	O	S	0	2	0
			3242	2020	598	606	18			
1	E	410	Total	C	N	O	S	0	0	0
			3208	2001	591	598	18			
1	F	411	Total	C	N	O	S	0	0	0
			3217	2006	592	601	18			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	ASN	-	EXPRESSION TAG	UNP W8V4R8
A	414	SER	-	EXPRESSION TAG	UNP W8V4R8
A	415	SER	-	EXPRESSION TAG	UNP W8V4R8
A	416	SER	-	EXPRESSION TAG	UNP W8V4R8
A	417	VAL	-	EXPRESSION TAG	UNP W8V4R8
A	418	ASP	-	EXPRESSION TAG	UNP W8V4R8
A	419	LYS	-	EXPRESSION TAG	UNP W8V4R8
A	420	LEU	-	EXPRESSION TAG	UNP W8V4R8
A	421	ALA	-	EXPRESSION TAG	UNP W8V4R8
A	422	ALA	-	EXPRESSION TAG	UNP W8V4R8
A	423	ALA	-	EXPRESSION TAG	UNP W8V4R8
A	424	LEU	-	EXPRESSION TAG	UNP W8V4R8
A	425	GLU	-	EXPRESSION TAG	UNP W8V4R8
A	426	HIS	-	EXPRESSION TAG	UNP W8V4R8
A	427	HIS	-	EXPRESSION TAG	UNP W8V4R8
A	428	HIS	-	EXPRESSION TAG	UNP W8V4R8
A	429	HIS	-	EXPRESSION TAG	UNP W8V4R8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	430	HIS	-	EXPRESSION TAG	UNP W8V4R8
A	431	HIS	-	EXPRESSION TAG	UNP W8V4R8
B	413	ASN	-	EXPRESSION TAG	UNP W8V4R8
B	414	SER	-	EXPRESSION TAG	UNP W8V4R8
B	415	SER	-	EXPRESSION TAG	UNP W8V4R8
B	416	SER	-	EXPRESSION TAG	UNP W8V4R8
B	417	VAL	-	EXPRESSION TAG	UNP W8V4R8
B	418	ASP	-	EXPRESSION TAG	UNP W8V4R8
B	419	LYS	-	EXPRESSION TAG	UNP W8V4R8
B	420	LEU	-	EXPRESSION TAG	UNP W8V4R8
B	421	ALA	-	EXPRESSION TAG	UNP W8V4R8
B	422	ALA	-	EXPRESSION TAG	UNP W8V4R8
B	423	ALA	-	EXPRESSION TAG	UNP W8V4R8
B	424	LEU	-	EXPRESSION TAG	UNP W8V4R8
B	425	GLU	-	EXPRESSION TAG	UNP W8V4R8
B	426	HIS	-	EXPRESSION TAG	UNP W8V4R8
B	427	HIS	-	EXPRESSION TAG	UNP W8V4R8
B	428	HIS	-	EXPRESSION TAG	UNP W8V4R8
B	429	HIS	-	EXPRESSION TAG	UNP W8V4R8
B	430	HIS	-	EXPRESSION TAG	UNP W8V4R8
B	431	HIS	-	EXPRESSION TAG	UNP W8V4R8
C	413	ASN	-	EXPRESSION TAG	UNP W8V4R8
C	414	SER	-	EXPRESSION TAG	UNP W8V4R8
C	415	SER	-	EXPRESSION TAG	UNP W8V4R8
C	416	SER	-	EXPRESSION TAG	UNP W8V4R8
C	417	VAL	-	EXPRESSION TAG	UNP W8V4R8
C	418	ASP	-	EXPRESSION TAG	UNP W8V4R8
C	419	LYS	-	EXPRESSION TAG	UNP W8V4R8
C	420	LEU	-	EXPRESSION TAG	UNP W8V4R8
C	421	ALA	-	EXPRESSION TAG	UNP W8V4R8
C	422	ALA	-	EXPRESSION TAG	UNP W8V4R8
C	423	ALA	-	EXPRESSION TAG	UNP W8V4R8
C	424	LEU	-	EXPRESSION TAG	UNP W8V4R8
C	425	GLU	-	EXPRESSION TAG	UNP W8V4R8
C	426	HIS	-	EXPRESSION TAG	UNP W8V4R8
C	427	HIS	-	EXPRESSION TAG	UNP W8V4R8
C	428	HIS	-	EXPRESSION TAG	UNP W8V4R8
C	429	HIS	-	EXPRESSION TAG	UNP W8V4R8
C	430	HIS	-	EXPRESSION TAG	UNP W8V4R8
C	431	HIS	-	EXPRESSION TAG	UNP W8V4R8
D	413	ASN	-	EXPRESSION TAG	UNP W8V4R8
D	414	SER	-	EXPRESSION TAG	UNP W8V4R8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	415	SER	-	EXPRESSION TAG	UNP W8V4R8
D	416	SER	-	EXPRESSION TAG	UNP W8V4R8
D	417	VAL	-	EXPRESSION TAG	UNP W8V4R8
D	418	ASP	-	EXPRESSION TAG	UNP W8V4R8
D	419	LYS	-	EXPRESSION TAG	UNP W8V4R8
D	420	LEU	-	EXPRESSION TAG	UNP W8V4R8
D	421	ALA	-	EXPRESSION TAG	UNP W8V4R8
D	422	ALA	-	EXPRESSION TAG	UNP W8V4R8
D	423	ALA	-	EXPRESSION TAG	UNP W8V4R8
D	424	LEU	-	EXPRESSION TAG	UNP W8V4R8
D	425	GLU	-	EXPRESSION TAG	UNP W8V4R8
D	426	HIS	-	EXPRESSION TAG	UNP W8V4R8
D	427	HIS	-	EXPRESSION TAG	UNP W8V4R8
D	428	HIS	-	EXPRESSION TAG	UNP W8V4R8
D	429	HIS	-	EXPRESSION TAG	UNP W8V4R8
D	430	HIS	-	EXPRESSION TAG	UNP W8V4R8
D	431	HIS	-	EXPRESSION TAG	UNP W8V4R8
E	413	ASN	-	EXPRESSION TAG	UNP W8V4R8
E	414	SER	-	EXPRESSION TAG	UNP W8V4R8
E	415	SER	-	EXPRESSION TAG	UNP W8V4R8
E	416	SER	-	EXPRESSION TAG	UNP W8V4R8
E	417	VAL	-	EXPRESSION TAG	UNP W8V4R8
E	418	ASP	-	EXPRESSION TAG	UNP W8V4R8
E	419	LYS	-	EXPRESSION TAG	UNP W8V4R8
E	420	LEU	-	EXPRESSION TAG	UNP W8V4R8
E	421	ALA	-	EXPRESSION TAG	UNP W8V4R8
E	422	ALA	-	EXPRESSION TAG	UNP W8V4R8
E	423	ALA	-	EXPRESSION TAG	UNP W8V4R8
E	424	LEU	-	EXPRESSION TAG	UNP W8V4R8
E	425	GLU	-	EXPRESSION TAG	UNP W8V4R8
E	426	HIS	-	EXPRESSION TAG	UNP W8V4R8
E	427	HIS	-	EXPRESSION TAG	UNP W8V4R8
E	428	HIS	-	EXPRESSION TAG	UNP W8V4R8
E	429	HIS	-	EXPRESSION TAG	UNP W8V4R8
E	430	HIS	-	EXPRESSION TAG	UNP W8V4R8
E	431	HIS	-	EXPRESSION TAG	UNP W8V4R8
F	413	ASN	-	EXPRESSION TAG	UNP W8V4R8
F	414	SER	-	EXPRESSION TAG	UNP W8V4R8
F	415	SER	-	EXPRESSION TAG	UNP W8V4R8
F	416	SER	-	EXPRESSION TAG	UNP W8V4R8
F	417	VAL	-	EXPRESSION TAG	UNP W8V4R8
F	418	ASP	-	EXPRESSION TAG	UNP W8V4R8

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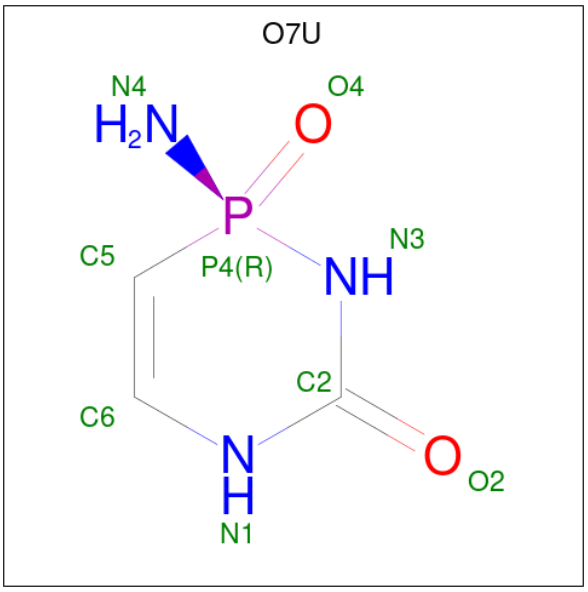
Chain	Residue	Modelled	Actual	Comment	Reference
F	419	LYS	-	EXPRESSION TAG	UNP W8V4R8
F	420	LEU	-	EXPRESSION TAG	UNP W8V4R8
F	421	ALA	-	EXPRESSION TAG	UNP W8V4R8
F	422	ALA	-	EXPRESSION TAG	UNP W8V4R8
F	423	ALA	-	EXPRESSION TAG	UNP W8V4R8
F	424	LEU	-	EXPRESSION TAG	UNP W8V4R8
F	425	GLU	-	EXPRESSION TAG	UNP W8V4R8
F	426	HIS	-	EXPRESSION TAG	UNP W8V4R8
F	427	HIS	-	EXPRESSION TAG	UNP W8V4R8
F	428	HIS	-	EXPRESSION TAG	UNP W8V4R8
F	429	HIS	-	EXPRESSION TAG	UNP W8V4R8
F	430	HIS	-	EXPRESSION TAG	UNP W8V4R8
F	431	HIS	-	EXPRESSION TAG	UNP W8V4R8

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

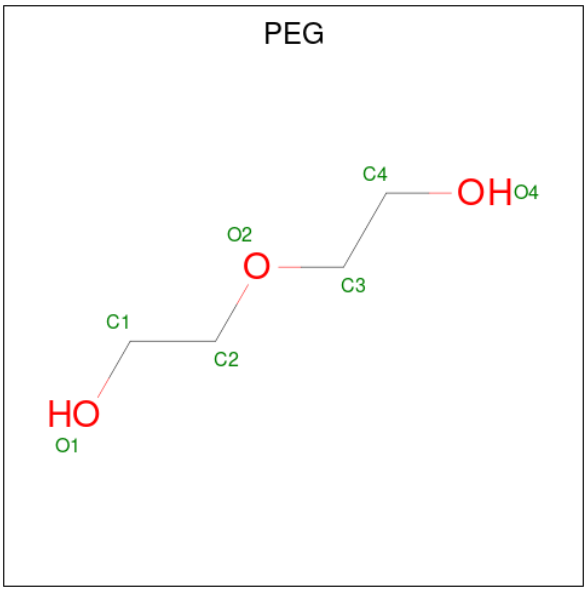
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0

- Molecule 3 is (2R)-2-amino-2,5-dihydro-1,5,2-diazaphosphinin-6(1H)-one 2-oxide (three-letter code: O7U) (formula: $C_3H_6N_3O_2P$).



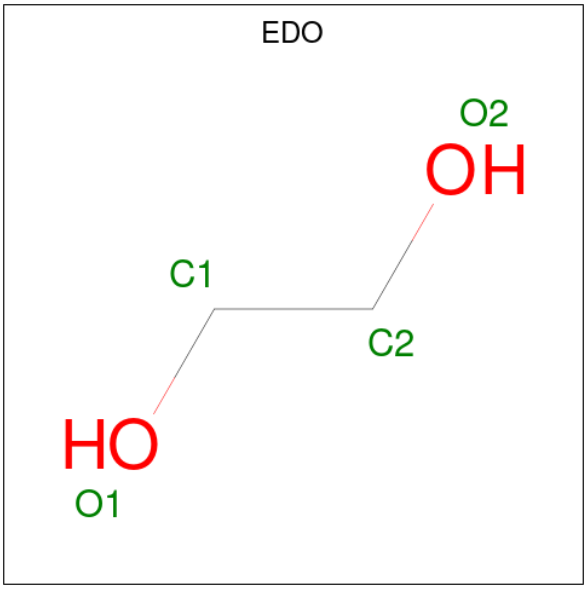
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			9	3	3	2	1		
3	B	1	Total	C	N	O	P	0	0
			9	3	3	2	1		
3	C	1	Total	C	N	O	P	0	0
			9	3	3	2	1		
3	D	1	Total	C	N	O	P	0	0
			9	3	3	2	1		
3	E	1	Total	C	N	O	P	0	0
			9	3	3	2	1		
3	F	1	Total	C	N	O	P	0	0
			9	3	3	2	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



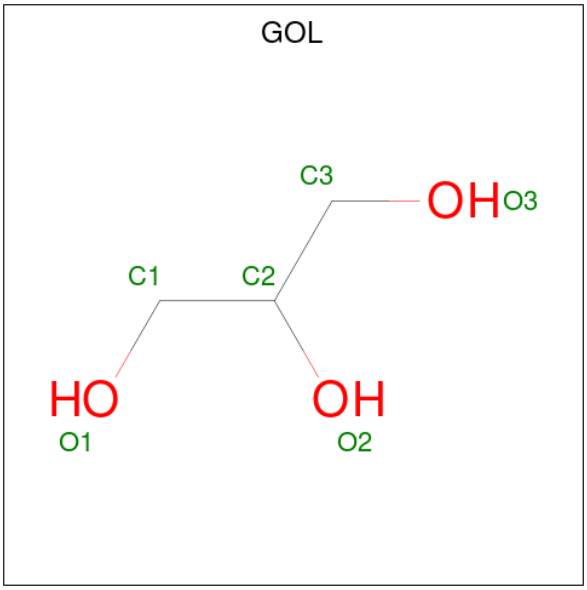
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	304	Total O 305 305	0	1
7	B	256	Total O 258 258	0	2
7	C	240	Total O 241 241	0	1

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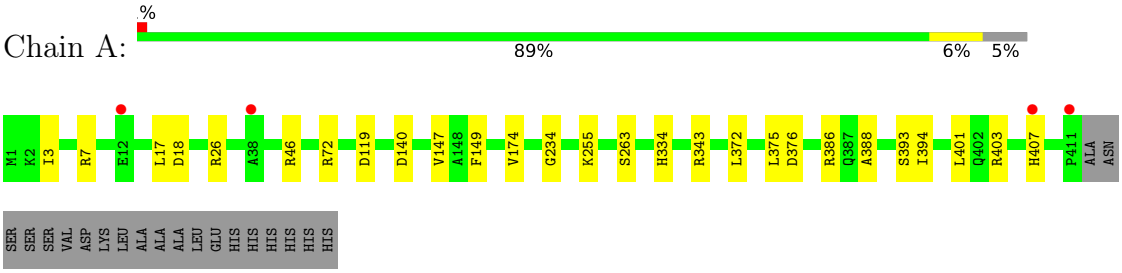
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	234	Total O 235 235	0	1
7	E	255	Total O 256 256	0	1
7	F	225	Total O 226 226	0	1

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.

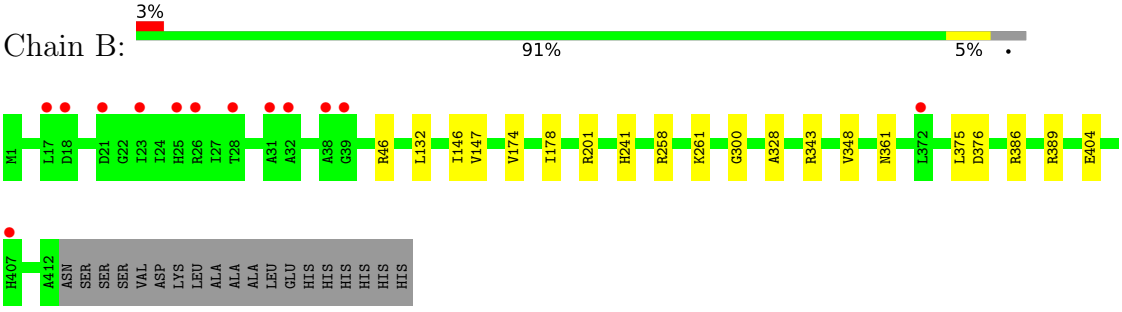
• Molecule 1: Cytosine deaminase

Chain A:



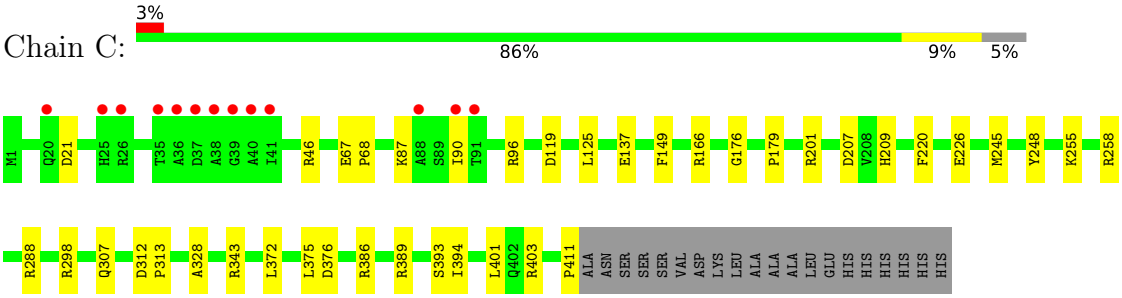
• Molecule 1: Cytosine deaminase

Chain B:



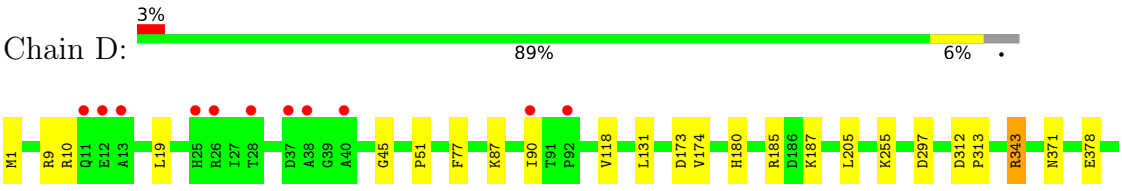
• Molecule 1: Cytosine deaminase

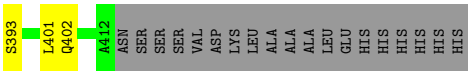
Chain C:



• Molecule 1: Cytosine deaminase

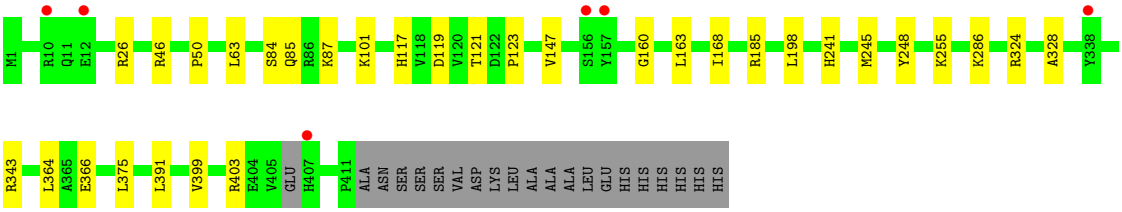
Chain D:





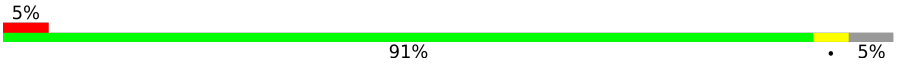
• Molecule 1: Cytosine deaminase

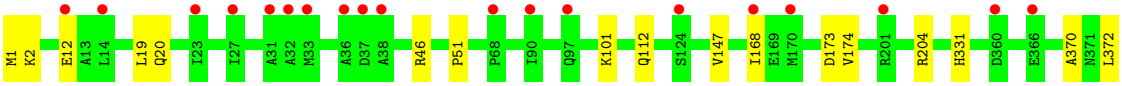
Chain E:

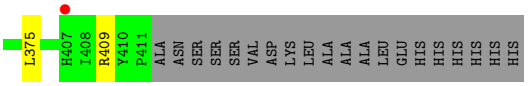


• Molecule 1: Cytosine deaminase

Chain F:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.17Å 147.81Å 185.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.78 – 1.90 49.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.78-1.90) 97.1 (49.78-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.198 , 0.242 0.199 , 0.242	Depositor DCC
R_{free} test set	6470 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20980	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 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, EDO, O7U, FE2, GOL

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	0.38	0/3286	0.55	0/4450
1	B	0.38	0/3280	0.53	0/4443
1	C	0.36	0/3275	0.53	0/4436
1	D	0.36	0/3300	0.52	0/4469
1	E	0.37	0/3265	0.53	0/4421
1	F	0.34	0/3275	0.51	0/4436
All	All	0.37	0/19681	0.53	0/26655

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

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	3228	0	3205	15	0
1	B	3222	0	3198	13	0
1	C	3217	0	3193	28	0
1	D	3242	0	3215	15	0
1	E	3208	0	3186	19	0
1	F	3217	0	3193	13	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	9	0	6	0	0
3	B	9	0	6	0	0
3	C	9	0	6	0	0
3	D	9	0	6	0	0
3	E	9	0	6	0	0
3	F	9	0	6	0	0
4	A	7	0	10	2	0
4	C	14	0	20	7	0
4	D	7	0	10	1	0
4	E	7	0	10	0	0
5	A	8	0	12	2	0
5	B	4	0	6	1	0
5	C	4	0	6	0	0
5	D	4	0	6	0	0
5	E	4	0	6	1	0
6	C	6	0	8	0	0
7	A	305	0	0	2	0
7	B	258	0	0	4	0
7	C	241	0	0	3	0
7	D	235	0	0	1	0
7	E	256	0	0	5	0
7	F	226	0	0	3	0
All	All	20980	0	19320	99	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.

The worst 5 of 99 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)
4:C:504:PEG:H32	1:E:328:ALA:HA	1.67	0.74
1:B:258:ARG:HH21	5:B:503:EDO:H11	1.57	0.69
1:C:328:ALA:HB2	4:C:504:PEG:H21	1.76	0.68
1:C:255:LYS:NZ	7:C:652:HOH:O	2.26	0.67
4:A:503:PEG:H31	1:B:328:ALA:HB2	1.77	0.67

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	410/431 (95%)	395 (96%)	15 (4%)	0	100 100
1	B	410/431 (95%)	396 (97%)	13 (3%)	1 (0%)	47 38
1	C	409/431 (95%)	394 (96%)	15 (4%)	0	100 100
1	D	412/431 (96%)	400 (97%)	12 (3%)	0	100 100
1	E	406/431 (94%)	395 (97%)	10 (2%)	1 (0%)	47 38
1	F	409/431 (95%)	392 (96%)	17 (4%)	0	100 100
All	All	2456/2586 (95%)	2372 (97%)	82 (3%)	2 (0%)	51 42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	241	HIS
1	E	241	HIS

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	340/355 (96%)	336 (99%)	4 (1%)	71 70
1	B	339/355 (96%)	338 (100%)	1 (0%)	92 93
1	C	339/355 (96%)	337 (99%)	2 (1%)	86 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	341/355 (96%)	338 (99%)	3 (1%)	78	79
1	E	338/355 (95%)	336 (99%)	2 (1%)	86	87
1	F	339/355 (96%)	337 (99%)	2 (1%)	86	87
All	All	2036/2130 (96%)	2022 (99%)	14 (1%)	84	84

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	173	ASP
1	D	185	ARG
1	F	101	LYS
1	E	343	ARG
1	F	1	MET

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

Mol	Chain	Res	Type
1	B	136	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
5	EDO	A	505	-	3,3,3	0.37	0	2,2,2	0.44	0
5	EDO	B	503	-	3,3,3	0.46	0	2,2,2	0.36	0
4	PEG	A	503	-	6,6,6	0.36	0	5,5,5	0.45	0
5	EDO	C	506	-	3,3,3	0.49	0	2,2,2	0.47	0
3	O7U	B	502	2	4,9,9	3.74	2 (50%)	2,13,13	2.25	1 (50%)
3	O7U	E	502	2	4,9,9	3.63	2 (50%)	2,13,13	2.00	1 (50%)
6	GOL	C	503	-	5,5,5	0.32	0	5,5,5	0.34	0
4	PEG	D	503	-	6,6,6	0.39	0	5,5,5	0.82	0
3	O7U	F	502	2	4,9,9	3.55	2 (50%)	2,13,13	1.78	1 (50%)
4	PEG	C	505	-	6,6,6	0.45	0	5,5,5	0.30	0
5	EDO	A	504	-	3,3,3	0.47	0	2,2,2	0.36	0
3	O7U	D	502	2	4,9,9	3.81	2 (50%)	2,13,13	2.05	1 (50%)
4	PEG	E	504	-	6,6,6	0.48	0	5,5,5	0.18	0
5	EDO	E	503	-	3,3,3	0.51	0	2,2,2	0.31	0
3	O7U	C	502	2	4,9,9	3.86	2 (50%)	2,13,13	1.31	0
4	PEG	C	504	-	6,6,6	0.55	0	5,5,5	0.81	0
3	O7U	A	502	2	4,9,9	4.05	2 (50%)	2,13,13	2.43	1 (50%)
5	EDO	D	504	-	3,3,3	0.47	0	2,2,2	0.35	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
5	EDO	A	505	-	-	1/1/1/1	-
5	EDO	B	503	-	-	1/1/1/1	-
4	PEG	A	503	-	-	2/4/4/4	-
5	EDO	C	506	-	-	1/1/1/1	-
3	O7U	B	502	2	-	-	0/0/1/1
6	GOL	C	503	-	-	2/4/4/4	-
3	O7U	E	502	2	-	-	0/0/1/1
4	PEG	D	503	-	-	2/4/4/4	-
5	EDO	A	504	-	-	1/1/1/1	-
4	PEG	C	505	-	-	2/4/4/4	-
5	EDO	E	503	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	O7U	D	502	2	-	-	0/0/1/1
4	PEG	E	504	-	-	3/4/4/4	-
3	O7U	F	502	2	-	-	0/0/1/1
3	O7U	C	502	2	-	-	0/0/1/1
4	PEG	C	504	-	-	3/4/4/4	-
3	O7U	A	502	2	-	-	0/0/1/1
5	EDO	D	504	-	-	0/1/1/1	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	O7U	C6-N1	7.31	1.47	1.36
3	D	502	O7U	C6-N1	7.14	1.47	1.36
3	B	502	O7U	C6-N1	6.94	1.46	1.36
3	A	502	O7U	C6-N1	6.83	1.46	1.36
3	E	502	O7U	C6-N1	6.74	1.46	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	O7U	O2-C2-N1	3.44	126.58	122.79
3	B	502	O7U	O2-C2-N1	2.90	125.99	122.79
3	E	502	O7U	O2-C2-N1	2.60	125.66	122.79
3	D	502	O7U	C6-N1-C2	2.24	123.77	122.40
3	F	502	O7U	C6-N1-C2	2.10	123.69	122.40

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	503	GOL	O1-C1-C2-C3
4	C	504	PEG	C1-C2-O2-C3
4	D	503	PEG	O1-C1-C2-O2
4	D	503	PEG	O2-C3-C4-O4
4	C	504	PEG	O2-C3-C4-O4

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	503	EDO	1	0
4	A	503	PEG	2	0
4	D	503	PEG	1	0
4	C	505	PEG	2	0
5	E	503	EDO	1	0
4	C	504	PEG	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	411/431 (95%)	-0.07	4 (0%)	82	84	8, 14, 30, 58	0
1	B	412/431 (95%)	0.04	13 (3%)	47	50	9, 17, 38, 66	0
1	C	411/431 (95%)	0.12	13 (3%)	47	50	9, 19, 39, 61	0
1	D	412/431 (95%)	0.09	11 (2%)	54	57	9, 17, 42, 68	0
1	E	410/431 (95%)	-0.05	6 (1%)	73	76	8, 16, 35, 66	0
1	F	411/431 (95%)	0.30	20 (4%)	29	33	10, 21, 45, 67	0
All	All	2467/2586 (95%)	0.07	67 (2%)	54	57	8, 17, 39, 68	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	10	ARG	6.9
1	C	38	ALA	6.6
1	F	38	ALA	6.6
1	D	38	ALA	5.3
1	C	39	GLY	4.7

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 (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, 95^{th} 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
5	EDO	B	503	4/4	0.76	0.38	41,42,43,46	0
4	PEG	C	505	7/7	0.83	0.25	9,14,22,23	7
5	EDO	E	503	4/4	0.84	0.17	17,20,25,33	0
5	EDO	D	504	4/4	0.85	0.18	36,37,39,41	0
4	PEG	A	503	7/7	0.85	0.20	20,23,27,35	0
5	EDO	C	506	4/4	0.86	0.17	25,27,31,34	0
6	GOL	C	503	6/6	0.86	0.16	21,26,35,41	0
4	PEG	C	504	7/7	0.87	0.21	20,26,35,39	0
4	PEG	E	504	7/7	0.88	0.12	30,35,37,38	0
4	PEG	D	503	7/7	0.88	0.19	25,29,30,31	0
5	EDO	A	505	4/4	0.94	0.21	28,32,35,37	0
5	EDO	A	504	4/4	0.94	0.24	14,21,27,28	0
3	O7U	A	502	9/9	0.96	0.09	7,8,10,10	0
3	O7U	C	502	9/9	0.97	0.10	10,13,17,18	0
3	O7U	D	502	9/9	0.97	0.10	9,12,16,18	0
3	O7U	F	502	9/9	0.97	0.11	11,14,16,18	0
3	O7U	E	502	9/9	0.98	0.08	9,12,15,18	0
3	O7U	B	502	9/9	0.98	0.09	8,10,13,15	0
2	FE2	D	501	1/1	0.99	0.07	22,22,22,22	0
2	FE2	F	501	1/1	0.99	0.04	16,16,16,16	1
2	FE2	A	501	1/1	0.99	0.03	15,15,15,15	0
2	FE2	B	501	1/1	0.99	0.04	18,18,18,18	0
2	FE2	C	501	1/1	0.99	0.06	21,21,21,21	0
2	FE2	E	501	1/1	1.00	0.04	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.