

Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 11:32 pm BST

PDB ID	:	4A29
Title	:	Structure of the engineered retro-aldolase RA95.0
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Deposited on		
Resolution	:	1.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

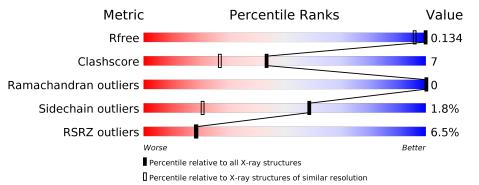
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R_{free}	130704	1619(1.14-1.06)
Clashscore	141614	1671(1.14-1.06)
Ramachandran outliers	138981	1615(1.14-1.06)
Sidechain outliers	138945	1613(1.14-1.06)
RSRZ outliers	127900	1588 (1.14-1.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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		
			6%		
1	A	258	80%	16%	·



2 Entry composition (i)

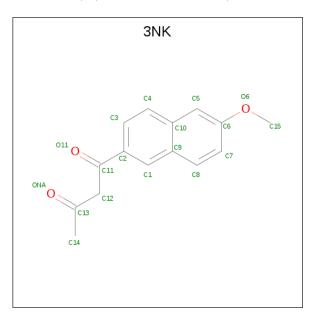
There are 4 unique types of molecules in this entry. The entry contains 5158 atoms, of which 2449 are hydrogens and 0 are deuteriums.

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 ENGINEERED RETRO-ALDOL ENZYME RA95.0.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	А	247	Total 4745	C 1470	Н 2431	N 398	O 436	S 10	0	44	0

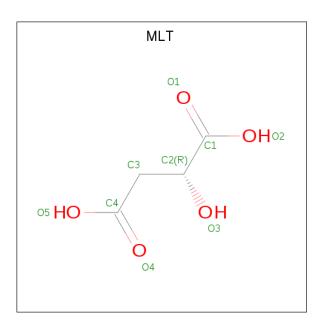
• Molecule 2 is 1-(6-METHOXYNAPHTHALEN-2-YL)BUTANE-1,3-DIONE (three-letter code: 3NK) (formula: C₁₅H₁₄O₃).



Mo	1 Cl	nain	Residues	Atoms				ZeroOcc	AltConf
2		Δ	1	Total	С	Η	Ο	0	0
		Л	I	31	15	14	2	0	0

• Molecule 3 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	А	1	Total 13	С 4	Н 4	O 5	0	0

• Molecule 4 is water.

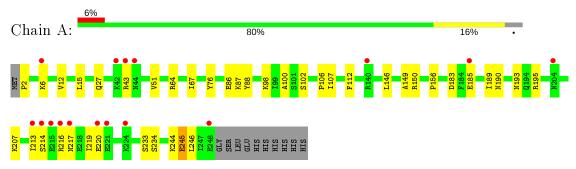
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	369	Total O 369 369	0	0



3 Residue-property plots (i)

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

• Molecule 1: ENGINEERED RETRO-ALDOL ENZYME RA95.0





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	53.94Å 62.59 Å 79.81 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.98 - 1.10	Depositor
Resolution (A)	7.98 - 1.10	EDS
% Data completeness	91.8 (7.98-1.10)	Depositor
(in resolution range)	91.8 (7.98-1.10)	EDS
R _{merge}	0.02	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.59 (at 1.10 \text{\AA})$	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
D D.	0.120 , 0.137	Depositor
R, R_{free}	0.119 , 0.134	DCC
R_{free} test set	2030 reflections $(2.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	12.6	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.61,82.9	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5158	wwPDB-VP
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.26% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: 3NK, MLT

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.44	0/2369	0.68	2/3184~(0.1%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	64	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	А	43	ARG	CG-CD-NE	5.49	123.33	111.80

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	А	2314	2431	2394	31	0
2	А	17	14	14	1	0
3	А	9	4	4	0	0
4	А	369	0	0	14	0
All	All	2709	2449	2412	32	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 7.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:299:3NK:H143	4:A:2340:HOH:O	<u>1.61</u>	1.00
1:A:214:SER:OG	4:A:2344:HOH:O	1.80	0.98
1:A:190:ASN:ND2	1:A:193[B]:ASN:OD1	2.10	0.84
1:A:100:ALA:HA	1:A:107[A]:ILE:CD1	$\frac{2.10}{2.09}$	0.83
1:A:189[A]:ILE:HD11	4:A:2307:HOH:O	1.78	0.83
1:A:27:GLN:OE1	4:A:2097:HOH:O	2.04	0.76
1:A:245[A]:GLU:OE2	1:A:246:LEU:HD23	1.92	0.69
1:A:15[B]:LEU:HD11	1:A:87:LYS:HD3	1.77	0.67
1:A:100:ALA:HA	1:A:107[A]:ILE:HD11	1.82	0.61
1:A:86:GLU:HB3	4:A:2216:HOH:O	2.01	0.60
1:A:149:ALA:CB	1:A:156[B]:PRO:HG3	2.34	0.57
1:A:67[A]:ILE:HD12	1:A:102[A]:SER:OG	$\frac{2.04}{2.05}$	0.57
1:A:207[B]:LYS:NZ	4:A:2336:HOH:O	2.39	0.54
1:A:216:ARG:HB2	1:A:245[A]:GLU:OE2	2.08	0.53
1:A:2:PRO:HD3	4:A:2243:HOH:O	2.10	0.51
1:A:183[B]:ASP:OD2	4:A:2308:HOH:O	2.20	0.49
1:A:12[B]:VAL:HG11	1:A:112:PHE:CG	$\frac{2.20}{2.47}$	0.49
1:A:190:ASN:ND2	4:A:2308:HOH:O	2.45	0.49
1:A:146[A]:LEU:HD21	1:A:150:ARG:NH1	2.28	0.48
1:A:219:ILE:HG13	4:A:2344:HOH:O	2.14	0.48
1:A:216:ARG:O	1:A:220:GLU:HG3	2.14	0.47
1:A:15[B]:LEU:HD11	1:A:87:LYS:CD	2.45	0.47
1:A:183[B]:ASP:CG	4:A:2308:HOH:O	2.54	0.46
1:A:12[B]:VAL:HG22	1:A:88:TYR:CD2	2.52	0.44
1:A:98:LYS:HB2	1:A:98:LYS:HE2	1.78	0.43
1:A:183[A]:ASP:OD2	1:A:185:GLU:N	2.50	0.42
1:A:27:GLN:NE2	4:A:2099:HOH:O	2.52	0.42
1:A:51:VAL:HB	1:A:233[A]:SER:HA	2.01	0.41
1:A:195[B]:ARG:CZ	4:A:2323:HOH:O	2.67	0.41
1:A:76:TYR:CZ	1:A:244:LYS:HE2	2.56	0.41
1:A:213:ILE:HD13	1:A:234[B]:SER:OG	2.20	0.41
1:A:195[B]:ARG:NH2	4:A:2323:HOH:O	2.54	0.41

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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		
1	А	289/258~(112%)	283~(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.

M	Iol	Chain	Analysed	alysed Rotameric		Percentiles	
	1	А	267/233~(115%)	262~(98%)	5(2%)	57 18	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	6	LYS
1	А	106	PRO
1	А	217	ASN
1	А	245[A]	GLU
1	А	245[B]	GLU

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

Mol	Chain	Res	Type
1	А	217	ASN



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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	B	ond leng	gths	B	ond ang	les
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	MLT	А	300	-	$2,\!8,\!8$	0.50	0	3,10,10	1.12	0
2	3NK	А	299	1	18,18,19	4.13	12 (66%)	10,24,26	2.74	4 (40%)

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	MLT	А	300	-	-	1/2/8/8	-
2	3NK	А	299	1	-	2/8/31/32	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(\operatorname{\AA})$
2	А	299	3NK	C4-C10	-8.30	1.42	1.54

Continued on next page...



4	А	29

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	299	3NK	C7-C6	-8.27	1.40	1.49
2	А	299	3NK	C4-C3	-5.95	1.37	1.50
2	А	299	3NK	C7-C8	-5.42	1.35	1.52
2	А	299	3NK	C8-C9	-4.15	1.40	1.50
2	А	299	3NK	C1-C9	4.10	1.40	1.34
2	А	299	3NK	C10-C9	-3.56	1.40	1.52
2	А	299	3NK	C5-C6	3.55	1.38	1.32
2	А	299	3NK	C1-C2	-3.41	1.36	1.43
2	А	299	3NK	C10-C5	-3.36	1.44	1.50
2	А	299	3NK	C3-C2	3.04	1.42	1.34
2	А	299	3NK	C2-C11	2.41	1.49	1.46

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All (4) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	299	3NK	C10-C4-C3	5.67	121.12	112.48
2	А	299	3NK	C8-C7-C6	4.81	120.06	109.56
2	А	299	3NK	O6-C6-C7	3.08	117.23	110.87
2	А	299	3NK	C12-C11-C2	-2.38	114.40	119.06

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	299	3NK	C12-C11-C2-C3
3	А	300	MLT	O3-C2-C3-C4
2	А	299	3NK	O11-C11-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	299	3NK	1	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 (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, 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	А	247/258~(95%)	-0.22	16 (6%) 18 19	9, 15, 30, 40	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	213	ILE	7.5
1	А	217	ASN	6.4
1	А	248	GLU	5.3
1	А	216	ARG	3.6
1	А	224	LYS	3.6
1	А	185	GLU	3.5
1	А	42	LYS	3.3
1	А	220	GLU	3.1
1	А	221	GLU	2.8
1	А	6	LYS	2.5
1	А	140	ARG	2.4
1	А	44	ASN	2.3
1	А	43	ARG	2.2
1	А	214	SER	2.1
1	А	204	ASN	2.1
1	А	215	GLU	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 carbohydrates in this entry.



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	3NK	А	299	17/18	0.86	0.13	$12,\!15,\!20,\!21$	31
3	MLT	А	300	9/9	0.92	0.10	$14,\!19,\!23,\!27$	13

6.5 Other polymers (i)

There are no such residues in this entry.

