

Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2023 - 06:52 PM EDT

PDB ID	:	4TSK
Title	:	Ketol-acid reductoisomerase from Alicyclobacillus acidocaldarius
Authors	:	Cahn, J.K.B.; Brinkmann-Chen, S.; Arnold, F.H.
Deposited on		
Resolution	:	2.50 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 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:

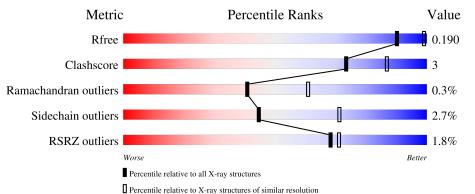
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	: : : : :	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.50 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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		
			2%		
1	А	350	84%	10%	• 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
3	TLA	А	404	-	Х	Х	-



4TSK

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2692 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 Ketol-acid reductoisomerase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	333	Total 2585	C 1641	N 453	O 480	S 11	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

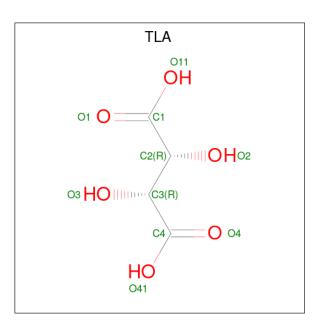
Chain	Residue	Modelled	Actual	Comment	Reference
А	345	HIS	-	expression tag	UNP C8WR67
А	346	HIS	-	expression tag	UNP C8WR67
А	347	HIS	-	expression tag	UNP C8WR67
A	348	HIS	-	expression tag	UNP C8WR67
А	349	HIS	-	expression tag	UNP C8WR67
А	350	HIS	-	expression tag	UNP C8WR67

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	3	Total Mg 3 3	0	0

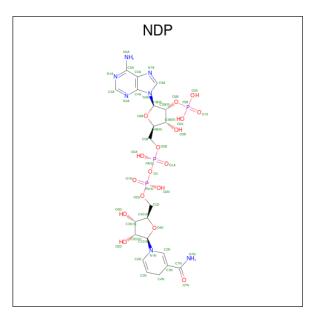
• Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 10	$\begin{array}{c} \mathrm{C} \\ 4 \end{array}$	O 6	0	0

• Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	А	1	Total 48	C 21	N 7	0 17	Р 3	0	0

• Molecule 5 is water.

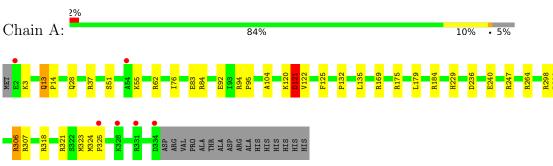


Mo	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	46	$\begin{array}{cc} \text{Total} & \text{O} \\ 46 & 46 \end{array}$	0	0



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: Ketol-acid reductoisomerase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants	124.10Å 124.10Å 124.10Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.10 - 2.50	Depositor
Itesolution (A)	39.24 - 2.07	EDS
% Data completeness	98.8(124.10-2.50)	Depositor
(in resolution range)	97.7(39.24-2.07)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	$1.08 (at 2.06 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.154 , 0.182	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.165 , 0.190	DCC
R_{free} test set	1916 reflections (5.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	37.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.41, 58.5	EDS
L-test for $twinning^2$	$< L > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.045 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2692	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.62% 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: NDP, TLA, MG

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		Bo	ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.96	2/2640~(0.1%)	1.06	17/3566~(0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	240	GLU	CD-OE2	5.86	1.32	1.25
1	А	92	GLU	CD-OE1	5.60	1.31	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	175	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	А	306	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	А	321	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	А	247	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	А	264	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	А	321	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	А	306	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	А	84	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	А	179	LEU	CB-CG-CD2	-5.60	101.48	111.00
1	А	318	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	А	236	ASP	CB-CG-OD1	5.52	123.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	135	LEU	CA-CB-CG	-5.51	102.62	115.30
1	А	62	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	А	37	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	А	318	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	А	121	ASP	N-CA-C	5.09	124.75	111.00
1	А	184	ARG	NE-CZ-NH1	5.05	122.83	120.30

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There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	120	LYS	Peptide

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	2585	0	2558	13	0
2	А	3	0	0	0	0
3	А	10	0	3	4	0
4	А	48	0	26	6	0
5	А	46	0	0	1	0
All	All	2692	0	2587	17	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 (17) 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)
3:A:404:TLA:H2	4:A:405:NDP:H41N	1.65	0.76
1:A:323:MET:O	1:A:325:PRO:HD3	1.88	0.73
1:A:229:HIS:HD2	5:A:501:HOH:O	1.82	0.61
3:A:404:TLA:C2	4:A:405:NDP:H41N	2.29	0.61
1:A:28:GLN:NE2	4:A:405:NDP:H42N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ILE:HD12	1:A:76:ILE:N	2.22	0.55
1:A:132:PRO:HA	4:A:405:NDP:O7N	2.08	0.53
3:A:404:TLA:H2	4:A:405:NDP:C4N	2.39	0.52
3:A:404:TLA:O41	3:A:404:TLA:C1	2.55	0.50
1:A:298:ARG:N	1:A:299:PRO:CD	2.77	0.47
1:A:83:GLU:OE2	1:A:298:ARG:NH2	2.46	0.47
1:A:94:ARG:N	1:A:95:PRO:CD	2.79	0.46
1:A:324:MET:O	1:A:325:PRO:C	2.55	0.45
1:A:104:ALA:HA	1:A:125:PHE:O	2.17	0.44
1:A:28:GLN:HE21	4:A:405:NDP:H42N	1.82	0.43
1:A:121:ASP:HB3	1:A:122:VAL:HG13	2.01	0.42
1:A:13:GLN:N	1:A:14:PRO:CD	2.83	0.41

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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	А	331/350~(95%)	314 (95%)	16(5%)	1 (0%)	41 61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	121	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	262/277~(95%)	255~(97%)	7 (3%)	44 71

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

Mol	Chain	Res	Type
1	А	3	LYS
1	А	13	GLN
1	А	51	SER
1	А	55	LYS
1	А	169	ARG
1	А	306	ARG
1	А	307	ARG

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

Mol	Chain	Res	Type
1	A	229	HIS

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 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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).

Mal	Mol Type	Chain	Chain	Chain	Chain	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
Moi Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2					
3	TLA	А	404	2	9,9,9	1.80	2 (22%)	12,12,12	2.16	4 (33%)				
4	NDP	А	405	-	45,52,52	1.43	4 (8%)	53,80,80	1.45	<u>6 (11%)</u>				

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	TLA	А	404	2	-	8/12/12/12	-
4	NDP	А	405	-	-	3/30/77/77	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
4	А	405	NDP	C6N-C5N	4.43	1.41	1.33
4	А	405	NDP	C4N-C5N	-4.18	1.38	1.48
4	А	405	NDP	C4N-C3N	-3.96	1.42	1.49
3	А	404	TLA	C3-C4	-3.61	1.47	1.52
3	А	404	TLA	O41-C4	-2.27	1.23	1.30
4	А	405	NDP	C2N-C3N	2.01	1.40	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	405	NDP	N3A-C2A-N1A	-4.90	121.02	128.68
3	А	404	TLA	C2-C3-C4	-3.92	101.12	109.87
3	А	404	TLA	O2-C2-C3	-3.83	102.62	110.23
4	А	405	NDP	C3N-C7N-N7N	3.79	124.40	117.67
3	А	404	TLA	O2-C2-C1	3.42	117.84	110.66
4	А	405	NDP	PN-O3-PA	-3.42	121.09	132.83
4	А	405	NDP	O7N-C7N-C3N	-3.33	114.62	120.90
4	А	405	NDP	O2X-P2B-O1X	2.58	120.78	110.68
4	А	405	NDP	C3N-C2N-N1N	-2.51	119.52	123.10
3	А	404	TLA	O11-C1-C2	2.45	119.90	113.27

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
3	А	404	TLA	O1-C1-C2-O2
3	А	404	TLA	O3-C3-C4-O4
3	А	404	TLA	O3-C3-C4-O41
3	А	404	TLA	O1-C1-C2-C3
3	А	404	TLA	O11-C1-C2-C3
3	А	404	TLA	O11-C1-C2-O2
3	А	404	TLA	C1-C2-C3-C4
3	А	404	TLA	O2-C2-C3-O3
4	А	405	NDP	O4D-C1D-N1N-C6N
4	А	405	NDP	C2B-O2B-P2B-O2X
4	А	405	NDP	O4B-C4B-C5B-O5B

All (11) torsion outliers are listed below:

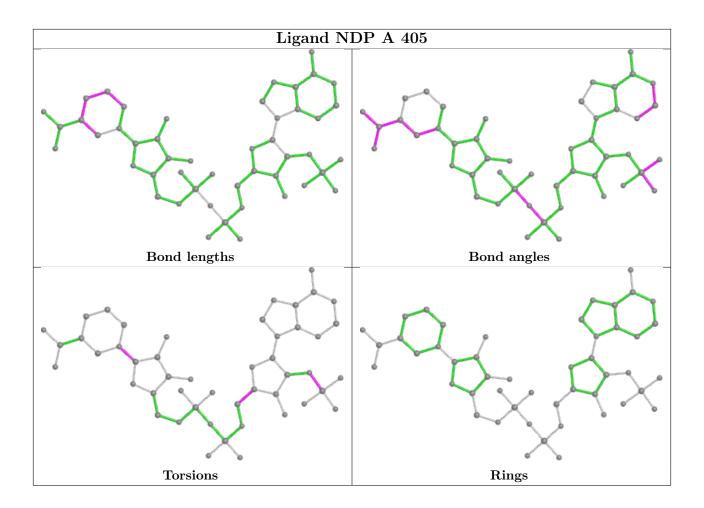
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	404	TLA	4	0
4	А	405	NDP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sup Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9	
1	А	333/350~(95%)	-0.68	6 (1%)	68	71	25, 37, 62, 96	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	2	GLU	4.6
1	А	334	ASP	4.4
1	А	328	LYS	3.7
1	А	331	ARG	2.8
1	А	325	PRO	2.6
1	А	54	ALA	2.4

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 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
4	NDP	А	405	48/48	0.96	0.08	$33,\!38,\!47,\!51$	0

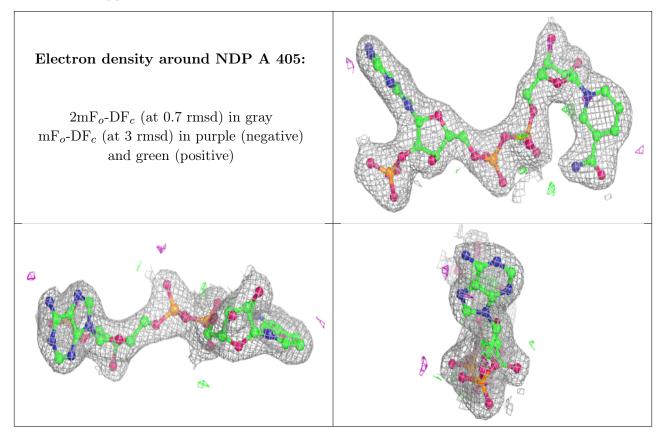
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q < 0.9				
3	TLA	А	404	10/10	0.97	0.14	33,51,74,86	0				
2	MG	А	401	1/1	0.97	0.10	18,18,18,18	0				
2	MG	А	402	1/1	0.98	0.04	33,33,33,33	0				
2	MG	А	403	1/1	0.98	0.07	34,34,34,34	0				

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The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers (i)

There are no such residues in this entry.

