

Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 04:40 AM EDT

PDB ID : 5W3K

Title : Crystal structure of Staphylococcus aureus ketol-acid reductoisomerase in com-

plex NADPH, Mg2+ and CPD

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Deposited on : 2017-06-08

Resolution : 1.59 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 (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

 $EDS \quad : \quad 2.35.1$

buster-report : 1.1.7 (2018)

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)

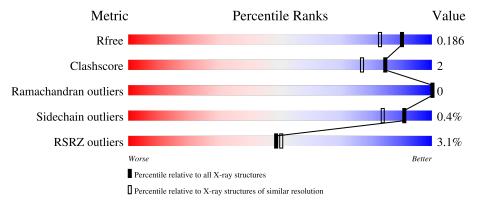
Validation Pipeline (wwPDB-VP) : 2.35.1

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 1.59 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	340	92%	·	-
1	В	340	91%	5%	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6070 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 (NADP(+)).

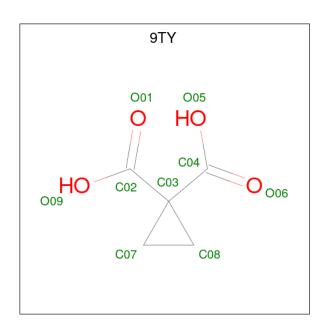
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	326	Total	С	N	О	S	0	10	0
1	A	320	2609	1658	444	499	8	0	10	U
1	D	326	Total	С	N	О	S	0	12	0
1	Ъ	320	2622	1670	441	503	8	0	10	U

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	HIS	-	expression tag	UNP A0A145BYP4
A	336	HIS	-	expression tag	UNP A0A145BYP4
A	337	HIS	-	expression tag	UNP A0A145BYP4
A	338	HIS	-	expression tag	UNP A0A145BYP4
A	339	HIS	-	expression tag	UNP A0A145BYP4
A	340	HIS	-	expression tag	UNP A0A145BYP4
В	335	HIS	-	expression tag	UNP A0A145BYP4
В	336	HIS	-	expression tag	UNP A0A145BYP4
В	337	HIS	-	expression tag	UNP A0A145BYP4
В	338	HIS	-	expression tag	UNP A0A145BYP4
В	339	HIS	-	expression tag	UNP A0A145BYP4
В	340	HIS	-	expression tag	UNP A0A145BYP4

• Molecule 2 is cyclopropane-1,1-dicarboxylic acid (three-letter code: 9TY) (formula: $C_5H_6O_4$) (labeled as "Ligand of Interest" by depositor).





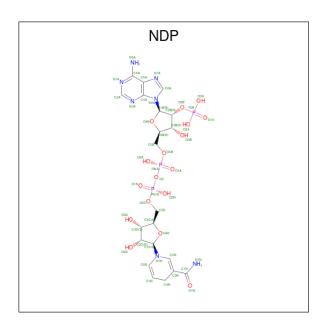
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 5 4	0	0
2	В	1	Total C O 9 5 4	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Mg 4 4	0	0
3	В	2	Total Mg 2 2	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		
1	٨	1	Total	С	N	О	Р	0	1	
4	A	1	96	42	14	34	6	0	1	
1	D	1	Total	С	N	О	Р	0	0	
4	Б	1	48	21	7	17	3	0	U	

• Molecule 5 is water.

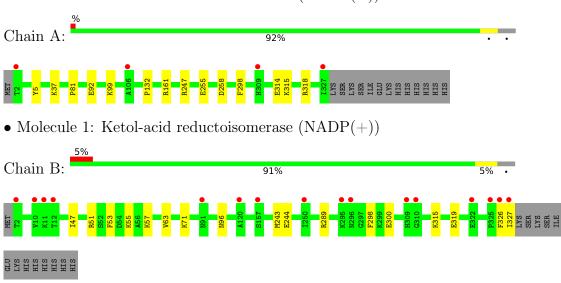
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	344	Total O 344 344	0	0
5	В	327	Total O 327 327	0	0



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 (NADP(+))





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	63.94Å 80.77Å 66.75Å	Donositon
a, b, c, α , β , γ	90.00° 92.49° 90.00°	Depositor
Resolution (Å)	34.55 - 1.59	Depositor
rtesolution (A)	34.55 - 1.59	EDS
% Data completeness	98.7 (34.55-1.59)	Depositor
(in resolution range)	98.7 (34.55-1.59)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.60 (at 1.59Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.160 , 0.187	Depositor
it, itfree	0.160 , 0.186	DCC
R_{free} test set	1987 reflections (2.21%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 52.4	EDS
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
	0.000 for $l,k,-h$	
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
	0.017 for l,-k,h	
F_o, F_c correlation	0.97	EDS
Total number of atoms	6070	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.30% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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, 9TY, 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	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.43	0/2682	0.58	1/3620 (0.0%)	
1	В	0.42	0/2704	0.58	0/3650	
All	All	0.42	0/5386	0.58	1/7270 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	A	258	ASP	CB-CG-OD1	5.41	123.17	118.30

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	2609	0	2572	12	0
1	В	2622	0	2594	13	0
2	A	9	0	0	0	0
2	В	9	0	0	1	0
3	A	4	0	0	0	0
3	В	2	0	0	0	0
4	A	96	0	52	4	0
4	В	48	0	26	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	344	0	0	2	1
5	В	327	0	0	0	1
All	All	6070	0	5244	24	1

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 (24) 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:A:81:PRO:HD3	4:A:406[A]:NDP:H51A	1.74	0.68
1:A:5:TYR:OH	1:A:161[A]:ARG:NH2	2.35	0.59
1:B:51[A]:ARG:HE	1:B:55[A]:LYS:HE2	1.71	0.55
1:B:289:ARG:NH2	1:B:300:GLU:OE2	2.26	0.54
1:A:132:PRO:HA	4:A:406[B]:NDP:O7N	2.08	0.54
1:B:51[A]:ARG:HE	1:B:55[A]:LYS:HG3	1.73	0.53
1:A:314:GLU:OE2	1:B:243:MET:HB2	2.09	0.52
1:A:92[B]:GLU:OE1	5:A:501:HOH:O	2.20	0.50
1:B:51[A]:ARG:NE	1:B:55[A]:LYS:HG3	2.28	0.48
1:A:37:LYS:NZ	5:A:511:HOH:O	2.48	0.47
1:A:247:ARG:HG2	1:A:255:GLU:HG3	1.97	0.46
1:A:315[B]:LYS:HG2	1:A:318:ARG:NH2	2.30	0.46
1:A:315[B]:LYS:HG2	1:A:318:ARG:HH21	1.81	0.45
1:A:99:LYS:HB2	1:A:99:LYS:HE2	1.81	0.44
1:B:326:PHE:CD2	1:B:327:ILE:HG12	2.53	0.44
1:B:327:ILE:HD13	1:B:327:ILE:HA	1.85	0.43
1:B:71:LYS:HE2	1:B:96:ASN:OD1	2.18	0.43
1:B:51[A]:ARG:HA	1:B:51[A]:ARG:HD2	1.79	0.42
1:B:53:PHE:CE1	1:B:57:LYS:HD2	2.53	0.42
1:B:315:LYS:O	1:B:319:GLU:HG3	2.21	0.41
4:A:406[B]:NDP:H41N	2:B:401:9TY:C02	2.51	0.41
1:B:47:ILE:HG22	1:B:63:VAL:HG13	2.02	0.41
1:A:314:GLU:OE1	1:B:244[A]:GLU:OE2	2.38	0.41
1:A:132:PRO:HA	4:A:406[A]:NDP:O7N	2.22	0.40

All (1) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
5:A:681:HOH:O	5:B:665:HOH:O[2_545]	2.18	0.02



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	Outliers Percentile	
1	A	334/340 (98%)	328 (98%)	6 (2%)	0	100	100
1	В	337/340~(99%)	329 (98%)	8 (2%)	0	100	100
All	All	671/680 (99%)	657 (98%)	14 (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.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	A	279/283 (99%)	278 (100%)	1 (0%)	91	84	
1	В	282/283 (100%)	281 (100%)	1 (0%)	91	84	
All	All	561/566 (99%)	559 (100%)	2 (0%)	91	84	

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	PHE
1	В	298	PHE

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



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 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	Tuno	Chain	Res	Link	Во	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	9TY	A	401	3	9,9,9	1.13	0	13,14,14	1.12	1 (7%)	
2	9TY	В	401	3	9,9,9	0.92	0	13,14,14	1.71	4 (30%)	
4	NDP	A	406[A]	-	45,52,52	2.19	9 (20%)	53,80,80	1.45	8 (15%)	
4	NDP	В	404	-	45,52,52	1.68	2 (4%)	53,80,80	1.34	5 (9%)	
4	NDP	A	406[B]	-	45,52,52	2.22	7 (15%)	53,80,80	1.45	9 (16%)	

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	9TY	A	401	3	-	3/12/16/16	0/1/1/1
2	9TY	В	401	3	-	0/12/16/16	0/1/1/1
4	NDP	A	406[A]	-	-	9/30/77/77	0/5/5/5



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDP	В	404	-	-	4/30/77/77	0/5/5/5
4	NDP	A	406[B]	-	-	11/30/77/77	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
4	A	406[B]	NDP	P2B-O2B	12.12	1.82	1.59
4	A	406[A]	NDP	P2B-O2B	11.25	1.80	1.59
4	В	404	NDP	P2B-O2B	8.32	1.75	1.59
4	A	406[B]	NDP	PN-O5D	3.60	1.73	1.59
4	A	406[A]	NDP	C2A-N1A	3.13	1.39	1.33
4	A	406[A]	NDP	PN-O5D	3.00	1.71	1.59
4	A	406[A]	NDP	O4B-C1B	2.99	1.45	1.41
4	A	406[B]	NDP	O4B-C4B	-2.42	1.39	1.45
4	A	406[A]	NDP	O2B-C2B	-2.41	1.35	1.44
4	A	406[A]	NDP	C3D-C4D	2.39	1.59	1.53
4	A	406[B]	NDP	O2B-C2B	-2.38	1.35	1.44
4	A	406[A]	NDP	C3B-C4B	2.29	1.58	1.53
4	В	404	NDP	O4B-C1B	2.27	1.44	1.41
4	A	406[A]	NDP	O5B-C5B	-2.27	1.36	1.44
4	A	406[B]	NDP	C3D-C4D	2.27	1.58	1.53
4	A	406[B]	NDP	C7N-N7N	2.21	1.39	1.33
4	A	406[A]	NDP	C6N-N1N	2.16	1.42	1.37
4	A	406[B]	NDP	C2A-N1A	2.14	1.37	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	406[B]	NDP	PN-O3-PA	-4.96	115.82	132.83
4	A	406[A]	NDP	PN-O3-PA	-4.45	117.57	132.83
4	В	404	NDP	PN-O3-PA	-3.56	120.60	132.83
2	В	401	9TY	O06-C04-C03	-3.16	114.63	122.14
4	A	406[A]	NDP	O2B-P2B-O1X	-2.96	97.97	109.39
4	В	404	NDP	C3N-C2N-N1N	-2.96	118.88	123.10
4	A	406[A]	NDP	C3N-C2N-N1N	-2.83	119.06	123.10
4	В	404	NDP	C3B-C2B-C1B	-2.71	97.79	102.89
4	В	404	NDP	C3N-C7N-N7N	2.64	122.35	117.67
4	A	406[B]	NDP	PA-O5B-C5B	-2.61	106.36	121.68
2	В	401	9TY	C08-C03-C07	2.61	59.74	57.41
2	В	401	9TY	O05-C04-C03	2.60	121.98	114.91
2	A	401	9TY	C08-C03-C07	2.57	59.71	57.41
4	A	406[B]	NDP	O3X-P2B-O2X	2.47	117.09	107.64



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Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	406[A]	NDP	C3B-C2B-C1B	-2.43	98.31	102.89
4	A	406[A]	NDP	PA-O5B-C5B	-2.40	107.59	121.68
4	A	406[B]	NDP	O2N-PN-O1N	2.40	124.08	112.24
4	A	406[A]	NDP	O3X-P2B-O2X	2.39	116.79	107.64
4	A	406[B]	NDP	C3N-C2N-N1N	-2.31	119.80	123.10
4	A	406[B]	NDP	O4B-C4B-C3B	2.30	109.66	105.11
2	В	401	9TY	O09-C02-C03	2.23	120.98	114.91
4	В	404	NDP	O3X-P2B-O2X	2.20	116.05	107.64
4	A	406[A]	NDP	O7N-C7N-N7N	-2.19	117.75	122.88
4	A	406[B]	NDP	O2B-P2B-O1X	-2.18	100.98	109.39
4	A	406[A]	NDP	C1D-N1N-C6N	-2.05	116.41	120.83
4	A	406[B]	NDP	O3X-P2B-O2B	-2.02	96.93	105.99
4	A	406[B]	NDP	C2A-N1A-C6A	-2.01	115.32	118.75

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	406[A]	NDP	C5B-O5B-PA-O1A
4	A	406[A]	NDP	C5B-O5B-PA-O2A
4	A	406[A]	NDP	C5B-O5B-PA-O3
4	A	406[B]	NDP	C5B-O5B-PA-O2A
4	A	406[A]	NDP	O4B-C4B-C5B-O5B
4	A	406[B]	NDP	O4B-C4B-C5B-O5B
4	A	406[B]	NDP	C3B-C4B-C5B-O5B
4	A	406[A]	NDP	C3B-C4B-C5B-O5B
4	В	404	NDP	C2D-C1D-N1N-C6N
4	A	406[A]	NDP	C2D-C1D-N1N-C6N
4	A	406[B]	NDP	C5B-O5B-PA-O3
4	A	406[B]	NDP	C5B-O5B-PA-O1A
2	A	401	9TY	O09-C02-C03-C07
4	A	406[A]	NDP	O4D-C1D-N1N-C6N
4	В	404	NDP	O4D-C1D-N1N-C6N
4	В	404	NDP	O4B-C4B-C5B-O5B
4	A	406[B]	NDP	O4D-C1D-N1N-C6N
4	A	406[B]	NDP	C2D-C1D-N1N-C6N
4	A	406[A]	NDP	C2B-O2B-P2B-O1X
4	A	406[B]	NDP	C2B-O2B-P2B-O1X
4	A	406[A]	NDP	C2B-O2B-P2B-O3X
4	A	406[B]	NDP	C2B-O2B-P2B-O2X
4	A	406[B]	NDP	PN-O3-PA-O1A
4	A	406[B]	NDP	PN-O3-PA-O2A



Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	В	404	NDP	PN-O3-PA-O2A
2	A	401	9TY	O01-C02-C03-C07
2	A	401	9TY	O09-C02-C03-C08

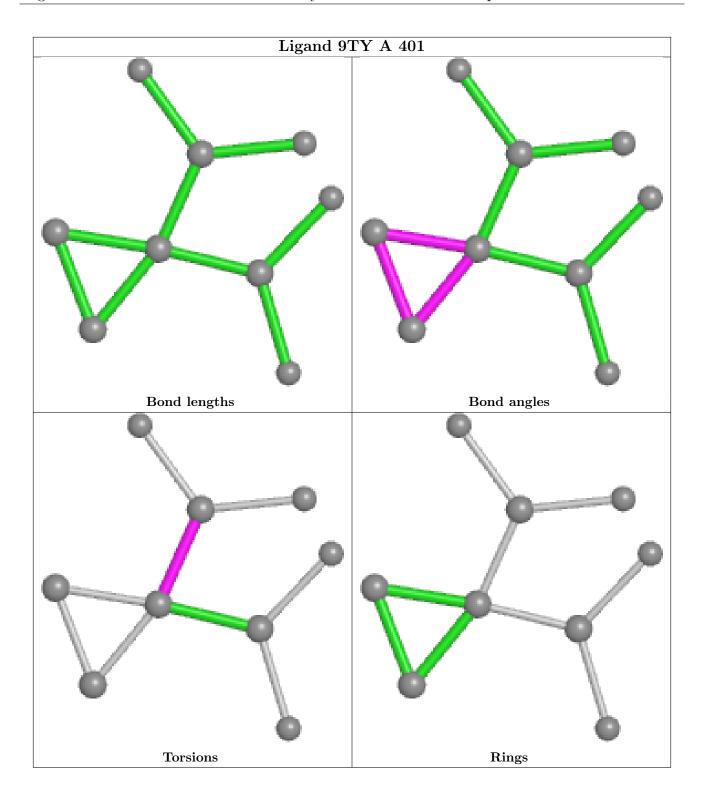
There are no ring outliers.

3 monomers are involved in 4 short contacts:

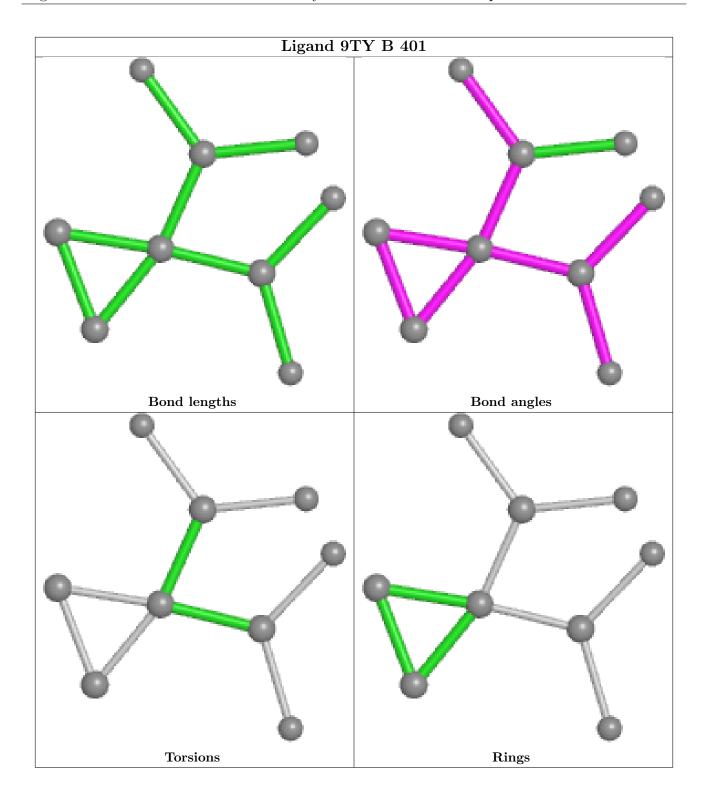
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	401	9TY	1	0
4	A	406[A]	NDP	2	0
4	A	406[B]	NDP	2	0

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 any 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.

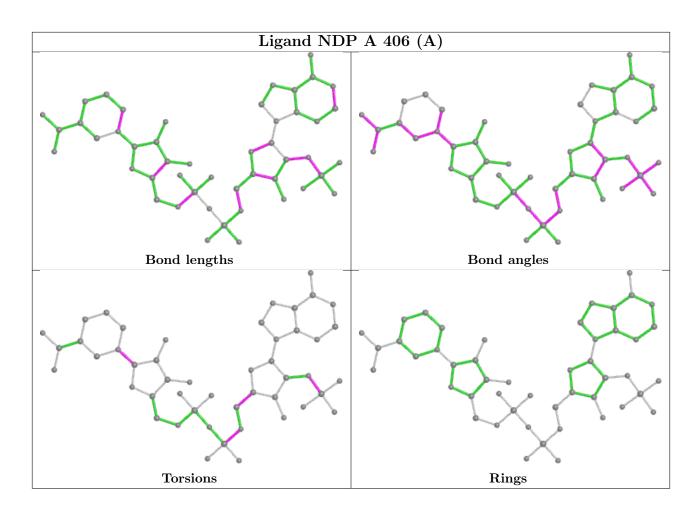




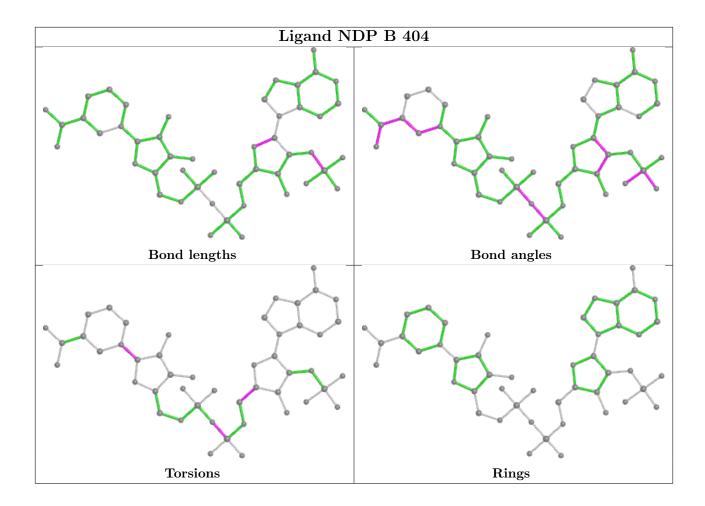




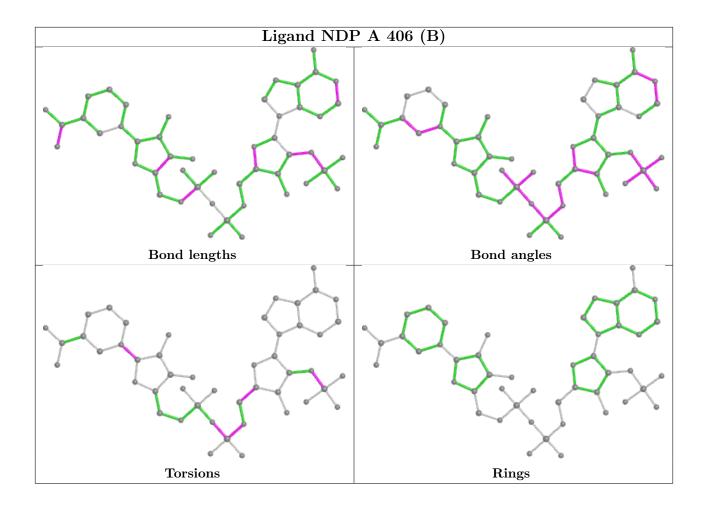












5.7 Other polymers (i)

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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	326/340~(95%)	0.12	4 (1%) 79 80	11, 18, 29, 37	0
1	В	326/340~(95%)	0.30	16 (4%) 29 29	10, 19, 32, 46	0
All	All	652/680 (95%)	0.21	20 (3%) 49 50	10, 18, 31, 46	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Res Type	
1	В	327	ILE	5.8
1	В	325	PRO	4.7
1	A	327	ILE	4.3
1	В	12	THR	3.7
1	В	11	LYS	3.2
1	В	10	VAL	2.9
1	A	309	HIS	2.8
1	В	2	THR	2.7
1	В	322	GLU	2.7
1	В	326	PHE	2.6
1	A	2	THR	2.4
1	В	296	ASN	2.3
1	В	309	HIS	2.2
1	В	295[A]	LYS	2.2
1	В	157	SER	2.2
1	В	120	ALA	2.1
1	В	310	GLY	2.1
1	В	91	ASN	2.1
1	В	250	ILE	2.0
1	A	106	ALA	2.0



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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
3	MG	A	404	1/1	0.93	0.12	25,25,25,25	0
3	MG	A	405	1/1	0.94	0.07	49,49,49,49	0
2	9TY	A	401	9/9	0.96	0.11	10,11,12,12	0
4	NDP	A	406[A]	48/48	0.96	0.11	11,13,19,21	48
4	NDP	A	406[B]	48/48	0.96	0.11	10,14,19,21	48
4	NDP	В	404	48/48	0.96	0.08	10,15,20,23	0
2	9TY	В	401	9/9	0.97	0.11	10,12,13,15	0
3	MG	A	403	1/1	0.99	0.09	12,12,12,12	0
3	MG	A	402	1/1	1.00	0.10	12,12,12,12	0
3	MG	В	402	1/1	1.00	0.07	13,13,13,13	0
3	MG	В	403	1/1	1.00	0.11	12,12,12,12	0

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.

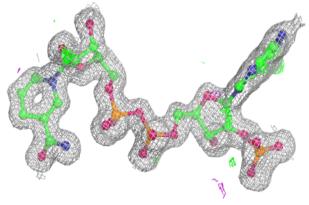


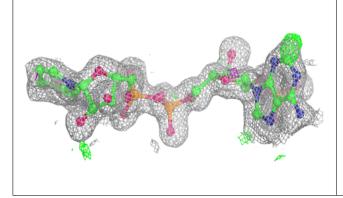
Electron density around 9TY A 401: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

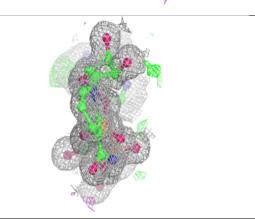


Electron density around NDP A 406 (A): $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c \ (\mathrm{at}\ 0.7\ \mathrm{rmsd}) \ \mathrm{in}\ \mathrm{gray}$

 ${
m mF}_o{
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

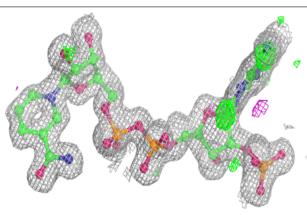


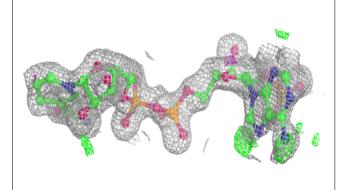


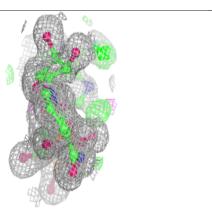


Electron density around NDP A 406 (B):

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



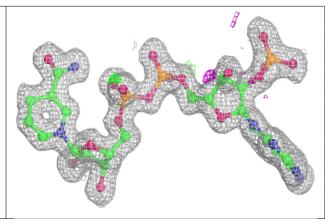


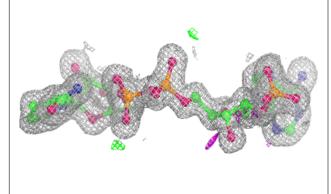


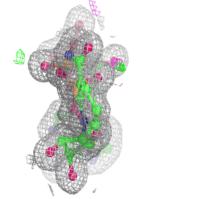


Electron density around NDP B 404:

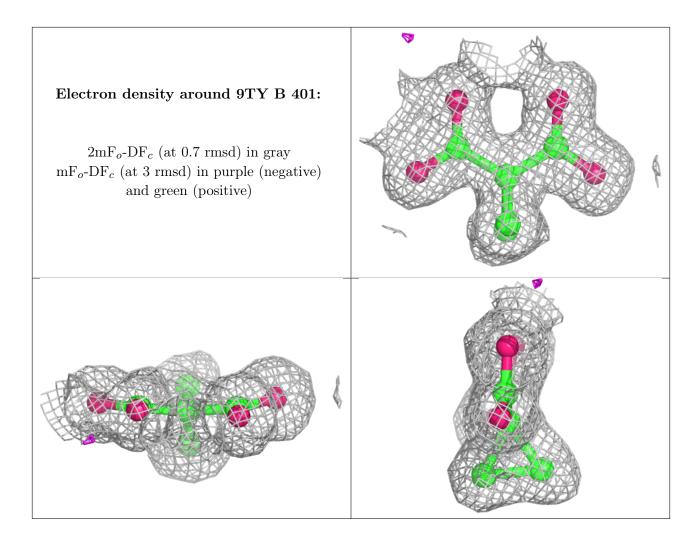
 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

