

wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2022 - 04:41 pm BST

PDB ID	:	8B25
Title	:	Dihydroprecondylocarpine acetate synthase 2 from Tabernanthe iboga -
		stemmadenine acetate bound structure
Authors	:	Langley, C.; Basquin, J.; Caputi, L.; O'Connor, S.E.
Deposited on		
Resolution	:	2.24 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:

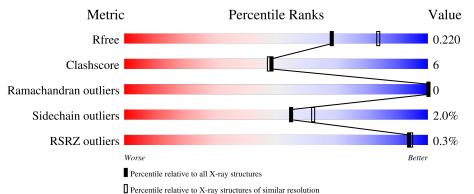
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.24 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	$2391 \ (2.26-2.22)$
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	А	365	% 85%	12%	•••
1	В	365	86%	12%	••

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	EDO	А	505	-	Х	-	-
3	EDO	В	502	-	Х	Х	-



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5554 atoms, of which 24 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.

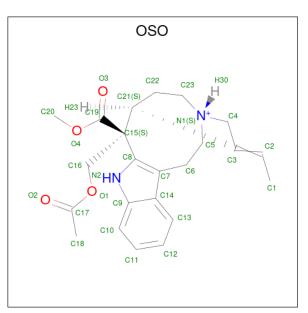
• Molecule 1 is a protein called Dihydroprecondylocarpine acetate synthase 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	358	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	A	200	2636	1692	440	493	11	0	0	0
1	В	359	Total	С	Ν	0	S	0	0	0
	D	009	2636	1691	438	496	11	0	U	U

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	HIS	GLN	conflict	UNP A0A5B8X8Z0
В	188	HIS	GLN	conflict	UNP A0A5B8X8Z0

• Molecule 2 is stemmadenine acetate (three-letter code: OSO) (formula: $C_{23}H_{29}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



[Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
	2	А	1	Total 29	C 23	N 2	0 4	0	0

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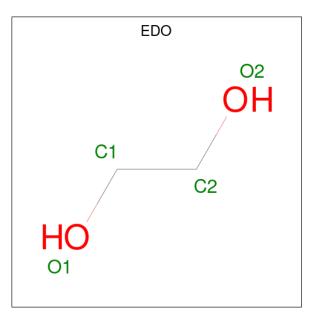




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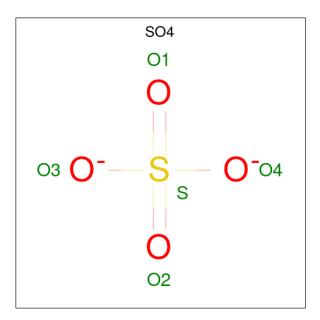
Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
2	В	1	Total 29	C 23	N 2	0 4	0	0

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	А	1	Total C H O 10 2 6 2	0	0
3	А	1	Total C H O 10 2 6 2	0	0
3	А	1	Total C H O 10 2 6 2	0	0
3	В	1	Total C H O 10 2 6 2	0	0





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Zn 1 1	0	0
5	В	1	Total Zn 1 1	0	0

• Molecule 6 is water.

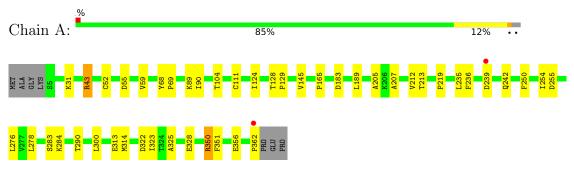
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	89	Total O 89 89	0	0
6	В	79	Total O 79 79	0	0



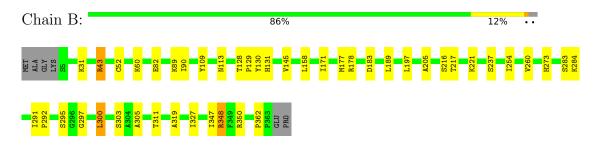
3 Residue-property plots (i)

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: Dihydroprecondylocarpine acetate synthase 2



• Molecule 1: Dihydroprecondylocarpine acetate synthase 2





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	73.19Å 79.84Å 130.92Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	39.92 - 2.24	Depositor	
Resolution (A)	41.63 - 2.24	EDS	
% Data completeness	94.5 (39.92-2.24)	Depositor	
(in resolution range)	94.5 (41.63 - 2.24)	EDS	
R _{merge}	(Not available)	Depositor	
R _{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.44 (at 2.24 \text{\AA})$	Xtriage	
Refinement program	PHENIX 1.19rc6_4061	Depositor	
D D.	0.174 , 0.221	Depositor	
R, R_{free}	0.173 , 0.220	DCC	
R_{free} test set	1784 reflections $(5.00%)$	wwPDB-VP	
Wilson B-factor $(Å^2)$	44.7	Xtriage	
Anisotropy	0.503	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS	
L-test for twinning ²	$ L > = 0.50, < L^2 > = 0.33$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.96	EDS	
Total number of atoms	5554	wwPDB-VP	
Average B, all atoms $(Å^2)$	45.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 27.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0466e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: EDO, OSO, SO4, ZN $\,$

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		Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.73	2/2691~(0.1%)	0.76	1/3668~(0.0%)	
1	В	0.67	0/2691	0.78	1/3669~(0.0%)	
All	All	0.70	2/5382~(0.0%)	0.77	2/7337~(0.0%)	

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	В	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	А	351	PHE	CE2-CZ	6.96	1.50	1.37
1	А	313	GLU	CG-CD	5.27	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	В	300	LEU	CB-CG-CD1	-8.47	96.60	111.00
1	А	314	MET	CG-SD-CE	5.95	109.72	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	348	ARG	Sidechain



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	2636	0	2594	28	0
1	В	2636	0	2577	32	0
2	А	29	0	0	1	0
2	В	29	0	0	1	0
3	А	16	18	24	3	0
3	В	4	6	6	5	0
4	А	5	0	0	0	0
4	В	5	0	0	0	0
5	А	1	0	0	0	0
5	В	1	0	0	0	0
6	А	89	0	0	6	0
6	В	79	0	0	2	0
All	All	5530	24	5201	63	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 6.

The worst 5 of 63 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:31:LYS:HG2	1:A:362:PRO:HG2	1.51	0.93
1:B:89:LYS:HG2	1:B:90:ILE:HG12	1.55	0.88
1:A:189:LEU:HD11	1:A:254:ILE:HG13	1.63	0.80
1:A:43:ARG:HG2	1:A:145:VAL:HG22	1.64	0.78
1:A:276:LEU:HD23	1:A:300:LEU:HD21	1.69	0.74

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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	356/365~(98%)	343~(96%)	13~(4%)	0	100	100
1	В	357/365~(98%)	345~(97%)	12 (3%)	0	100	100
All	All	713/730~(98%)	688 (96%)	25~(4%)	0	100	100

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

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	А	271/298~(91%)	266~(98%)	5(2%)	59 66
1	В	267/298~(90%)	261~(98%)	6(2%)	52 59
All	All	538/596~(90%)	527~(98%)	11 (2%)	55 62

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	197	LEU
1	В	237	SER
1	В	295	SER
1	В	283	SER
1	А	350	ARG

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

Mol	Chain	Res	Type	
1	А	228	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	Turne	Chain	Res	Link	B	ond leng	gths	B	ond ang	gles
	Type	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	EDO	А	504	-	3,3,3	0.78	0	2,2,2	0.14	0
4	SO4	В	503	-	4,4,4	0.19	0	$6,\!6,\!6$	0.79	0
3	EDO	А	503	-	3,3,3	1.15	0	2,2,2	0.21	0
2	OSO	А	501	-	28,32,32	5.27	11 (39%)	$26,\!47,\!47$	<mark>3.58</mark>	11 (42%)
2	OSO	В	501	-	28,32,32	<mark>5.30</mark>	14 (50%)	26,47,47	3.25	11 (42%)
3	EDO	В	502	-	3,3,3	0.42	0	2,2,2	2.34	2 (100%)
4	SO4	А	506	-	4,4,4	0.32	0	6,6,6	0.66	0
3	EDO	А	505	-	3,3,3	0.25	0	2,2,2	3.10	2 (100%)
3	EDO	А	502	-	3,3,3	0.59	0	2,2,2	0.01	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	EDO	А	504	-	-	1/1/1/1	-
3	EDO	А	503	-	-	1/1/1/1	-
2	OSO	А	501	-	-	8/16/46/46	0/2/4/4
2	OSO	В	501	-	-	5/16/46/46	0/2/4/4
3	EDO	В	502	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	А	505	-	-	1/1/1/1	-
3	EDO	А	502	-	-	0/1/1/1	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	501	OSO	C2-C3	23.79	1.64	1.33
2	В	501	OSO	C2-C3	23.01	1.63	1.33
2	В	501	OSO	C7-C8	8.04	1.51	1.39
2	А	501	OSO	C7-C8	5.83	1.47	1.39
2	В	501	OSO	C4-N1	-5.78	1.41	1.46

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	501	OSO	C1-C2-C3	-11.01	106.00	127.22
2	В	501	OSO	C1-C2-C3	-8.76	110.35	127.22
2	А	501	OSO	O4-C19-C15	7.21	122.22	112.02
2	В	501	OSO	C21-C3-C2	-6.42	105.12	124.62
2	А	501	OSO	C21-C3-C2	-5.59	107.64	124.62

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
2	А	501	OSO	C1-C2-C3-C21
2	А	501	OSO	C16-C15-C19-O3
2	А	501	OSO	C16-C15-C19-O4
2	А	501	OSO	C21-C15-C19-O3
2	А	501	OSO	C21-C15-C19-O4

5 of 17 torsion outliers are listed below:

There are no ring outliers.

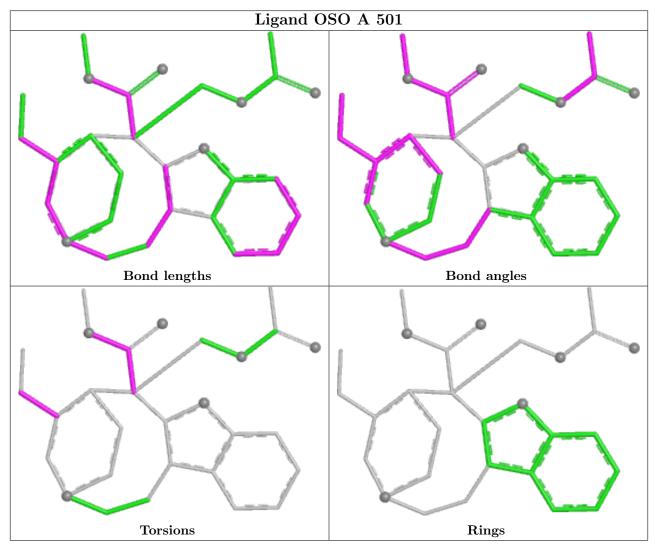
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	501	OSO	1	0
2	В	501	OSO	1	0
3	В	502	EDO	5	0
3	А	502	EDO	3	0

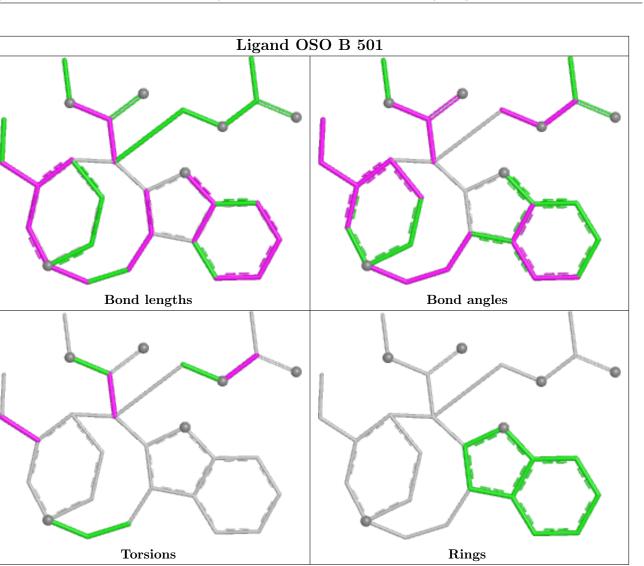
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,



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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{A}^2)$	Q < 0.9
1	А	358/365~(98%)	-0.08	2 (0%) 89 89	31, 44, 61, 81	0
1	В	359/365~(98%)	-0.16	0 100 100	30, 45, 61, 77	0
All	All	717/730~(98%)	-0.12	2 (0%) 94 94	30, 44, 61, 81	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	362	PRO	3.4
1	А	239	ASP	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 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
3	EDO	А	503	4/4	0.63	0.16	$56,\!67,\!69,\!70$	0
3	EDO	А	502	4/4	0.72	0.17	54,54,55,59	0
3	EDO	А	504	4/4	0.84	0.14	60,72,76,79	0

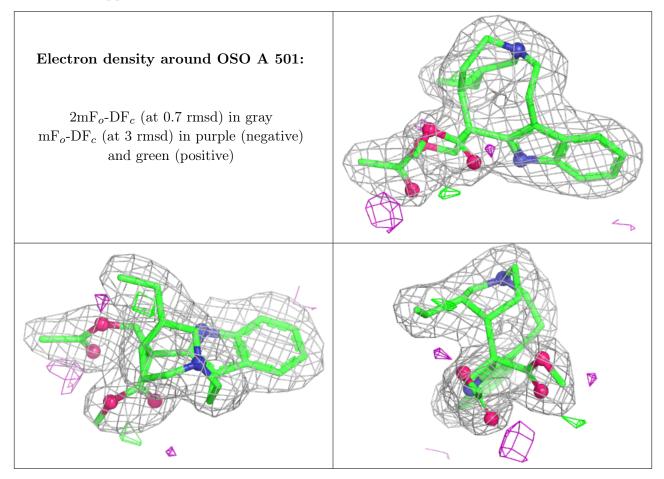
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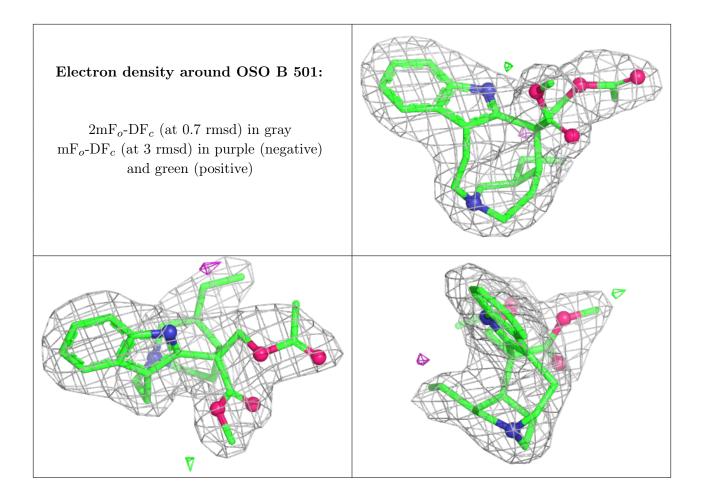
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
2	OSO	А	501	29/29	0.91	0.15	33,40,49,50	0
2	OSO	В	501	29/29	0.94	0.12	35,44,54,56	0
3	EDO	В	502	4/4	0.94	0.21	40,49,59,59	0
3	EDO	А	505	4/4	0.96	0.24	$39,\!48,\!58,\!58$	0
4	SO4	В	503	5/5	0.97	0.14	44,48,54,54	0
5	ZN	А	507	1/1	0.98	0.11	46,46,46,46	0
5	ZN	В	504	1/1	0.98	0.12	54,54,54,54	0
4	SO4	А	506	5/5	0.99	0.16	$35,\!41,\!56,\!56$	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.

