



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2026 – 12:08 PM EDT

PDB ID : 9ZO1 / pdb\_00009zo1  
Title : Crystal structure of deoxypodophyllotoxin synthase (DPS) complexed with vanadyl(IV)-oxo, succinate and (-)-hydroxy-yatein  
Authors : Michael, C.; Zheng, Y.-C.; Chang, W.-c.  
Deposited on : 2025-12-15  
Resolution : 2.00 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

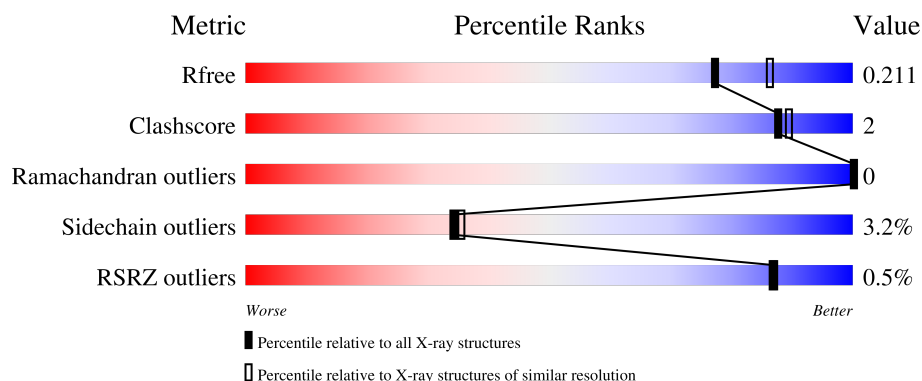
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	318	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>..</div> </div> </div>
1	B	318	<div> <div></div> <div>91%</div> <div>7% ..</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5811 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.

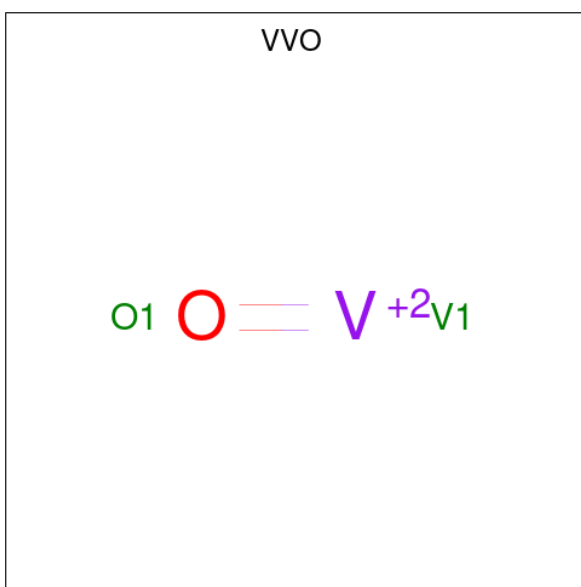
- Molecule 1 is a protein called Deoxypodophyllotoxin synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	3	0
			2538	1611	432	477	18			
1	B	314	Total	C	N	O	S	0	3	0
			2531	1607	431	476	17			

There are 16 discrepancies between the modelled and reference sequences:

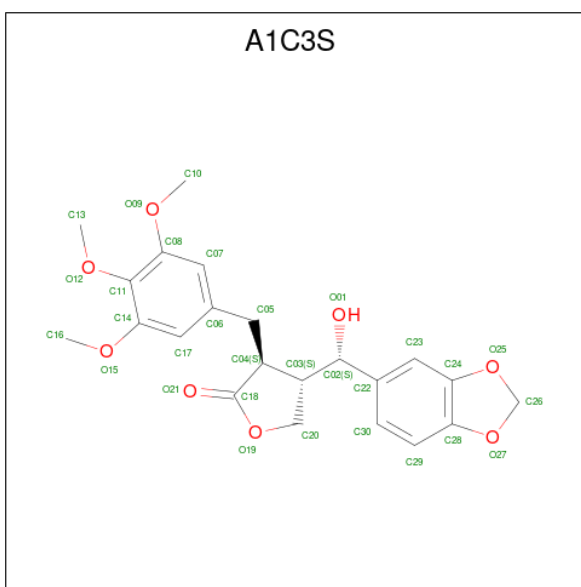
Chain	Residue	Modelled	Actual	Comment	Reference
A	311	LEU	-	expression tag	UNP A0A0N9HQ36
A	312	GLU	-	expression tag	UNP A0A0N9HQ36
A	313	HIS	-	expression tag	UNP A0A0N9HQ36
A	314	HIS	-	expression tag	UNP A0A0N9HQ36
A	315	HIS	-	expression tag	UNP A0A0N9HQ36
A	316	HIS	-	expression tag	UNP A0A0N9HQ36
A	317	HIS	-	expression tag	UNP A0A0N9HQ36
A	318	HIS	-	expression tag	UNP A0A0N9HQ36
B	311	LEU	-	expression tag	UNP A0A0N9HQ36
B	312	GLU	-	expression tag	UNP A0A0N9HQ36
B	313	HIS	-	expression tag	UNP A0A0N9HQ36
B	314	HIS	-	expression tag	UNP A0A0N9HQ36
B	315	HIS	-	expression tag	UNP A0A0N9HQ36
B	316	HIS	-	expression tag	UNP A0A0N9HQ36
B	317	HIS	-	expression tag	UNP A0A0N9HQ36
B	318	HIS	-	expression tag	UNP A0A0N9HQ36

- Molecule 2 is oxovanadium(2+) (CCD ID: VVO) (formula: OV) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	V	0	0
			2	1	1		
2	B	1	Total	O	V	0	0
			2	1	1		

- Molecule 3 is (3S,4S)-4-[(S)-(2H-1,3-benzodioxol-5-yl)(hydroxy)methyl]-3-[(3,4,5-trimethoxyphenyl)methyl]oxolan-2-one (CCD ID: A1C3S) (formula: C<sub>22</sub>H<sub>24</sub>O<sub>8</sub>) (labeled as "Ligand of Interest" by depositor).



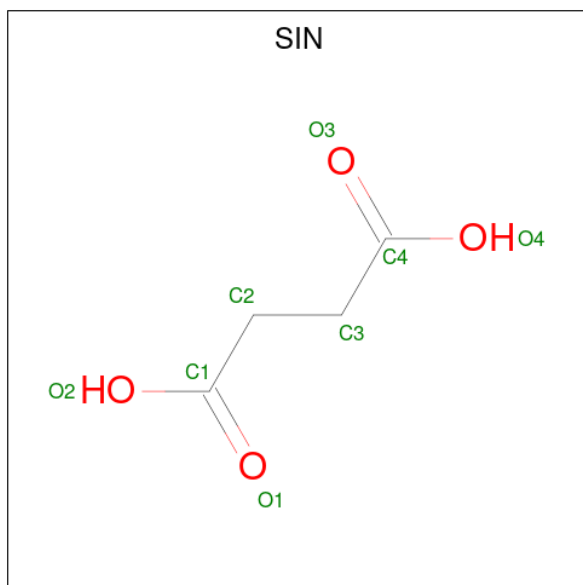
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			30	22	8		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			30	22	8		

- Molecule 4 is SUCCINIC ACID (CCD ID: SIN) (formula:  $C_4H_6O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	4	4		
4	B	1	Total	C	O	0	0
			8	4	4		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Cl 1	0	0
7	B	1	Total 1	Cl 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	340	Total 340	O 340	0	0
8	B	298	Total 298	O 298	0	0

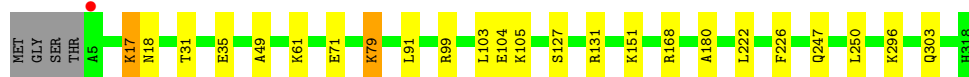
### 3 Residue-property plots [i](#)

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: Deoxypodophyllotoxin synthase



- Molecule 1: Deoxypodophyllotoxin synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.93Å 87.64Å 100.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.99 – 2.00 17.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (17.99-2.00) 92.3 (17.99-2.00)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.161 , 0.212 0.162 , 0.211	Depositor DCC
$R_{free}$ test set	2456 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5811	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, A1C3S, EDO, SIN, VVO

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	0.74	0/2601	0.75	0/3518
1	B	0.73	0/2597	0.75	0/3513
All	All	0.73	0/5198	0.75	0/7031

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	2538	0	2472	7	0
1	B	2531	0	2470	12	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	30	0	0	0	0
3	B	30	0	0	1	0
4	A	8	0	4	0	0
4	B	8	0	4	0	0
5	A	4	0	6	0	0
6	A	6	0	8	1	0
6	B	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	340	0	0	2	1
8	B	298	0	0	3	1
All	All	5811	0	4980	20	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 (20) 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:B:296:LYS:HG3	1:B:303:GLN:HB3	1.81	0.63
1:B:31:THR:O	1:B:35:GLU:HG2	2.02	0.58
1:A:171:GLN:NE2	8:A:501:HOH:O	2.24	0.56
1:A:293:GLU:CD	1:A:293:GLU:H	2.15	0.55
1:B:127:SER:OG	1:B:131[A]:ARG:NH1	2.40	0.55
1:A:104:GLU:HG2	1:A:105:LYS:N	2.24	0.53
1:B:99:ARG:HD3	1:B:105:LYS:HE2	1.91	0.52
1:A:130:LYS:NZ	8:A:513:HOH:O	2.48	0.47
1:B:17:LYS:HE2	1:B:18:ASN:ND2	2.29	0.47
1:A:151:LYS:HA	1:A:151:LYS:HD3	1.62	0.44
1:B:91:LEU:HD11	1:B:180:ALA:HA	1.98	0.44
1:B:49:ALA:O	1:B:131[B]:ARG:HG2	2.17	0.44
1:B:79:LYS:NZ	8:B:509:HOH:O	2.50	0.44
1:B:151:LYS:HG2	8:B:625:HOH:O	2.18	0.44
1:B:168:ARG:HB2	1:B:250:LEU:HD12	2.00	0.43
1:A:302:LYS:HE3	6:A:405:GOL:H32	2.00	0.43
1:A:185:LYS:HG3	1:A:238:LEU:HD23	2.00	0.43
3:B:401:A1C3S:C13	6:B:404:GOL:H11	2.49	0.42
1:B:103:LEU:HD12	1:B:103:LEU:O	2.21	0.41
1:B:61:LYS:NZ	8:B:512:HOH:O	2.51	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	Interatomic distance (Å)	Clash overlap (Å)
8:A:600:HOH:O	8:B:738:HOH:O[1_545]	1.98	0.22

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	315/318 (99%)	305 (97%)	10 (3%)	0	100	100
1	B	315/318 (99%)	305 (97%)	10 (3%)	0	100	100
All	All	630/636 (99%)	610 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	281/281 (100%)	270 (96%)	11 (4%)	28	28
1	B	281/281 (100%)	274 (98%)	7 (2%)	42	45
All	All	562/562 (100%)	544 (97%)	18 (3%)	34	35

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	17	LYS
1	A	24	THR
1	A	104	GLU
1	A	151	LYS
1	A	155	SER
1	A	221	LEU
1	A	226	PHE

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Mol	Chain	Res	Type
1	A	247	GLN
1	A	293	GLU
1	A	296	LYS
1	B	17	LYS
1	B	71	GLU
1	B	79	LYS
1	B	104	GLU
1	B	222	LEU
1	B	226	PHE
1	B	247	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	171	GLN
1	B	32	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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$
4	SIN	A	403	2	7,7,7	1.21	1 (14%)	8,8,8	2.60	3 (37%)
4	SIN	B	402	2	7,7,7	0.95	0	8,8,8	2.76	5 (62%)
2	VVO	A	401	4,8,1	0,1,1	-	-	-	-	-
6	GOL	B	404	-	5,5,5	1.02	1 (20%)	5,5,5	1.44	1 (20%)
6	GOL	B	405	-	5,5,5	1.09	0	5,5,5	0.79	0
6	GOL	A	405	-	5,5,5	0.93	0	5,5,5	1.37	0
3	A1C3S	A	402	-	33,33,33	6.16	21 (63%)	46,47,47	3.50	16 (34%)
5	EDO	A	404	-	3,3,3	0.62	0	2,2,2	0.34	0
3	A1C3S	B	401	-	33,33,33	5.72	19 (57%)	46,47,47	3.40	17 (36%)
2	VVO	B	403	4,8,1	0,1,1	-	-	-	-	-

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
4	SIN	A	403	2	-	2/5/5/5	-
4	SIN	B	402	2	-	0/5/5/5	-
6	GOL	B	404	-	-	2/4/4/4	-
6	GOL	B	405	-	-	4/4/4/4	-
6	GOL	A	405	-	-	2/4/4/4	-
5	EDO	A	404	-	-	1/1/1/1	-
3	A1C3S	A	402	-	-	3/18/37/37	0/4/4/4
3	A1C3S	B	401	-	-	2/18/37/37	0/4/4/4

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	A1C3S	O25-C26	-16.16	1.11	1.43
3	B	401	A1C3S	O25-C26	-15.02	1.13	1.43
3	B	401	A1C3S	O27-C28	14.65	1.62	1.38
3	A	402	A1C3S	O27-C28	14.47	1.62	1.38
3	A	402	A1C3S	C30-C22	13.78	1.60	1.39
3	B	401	A1C3S	C30-C22	12.59	1.58	1.39
3	A	402	A1C3S	O19-C18	8.77	1.53	1.35
3	A	402	A1C3S	C17-C06	8.33	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	A1C3S	C07-C08	8.29	1.52	1.38
3	A	402	A1C3S	O27-C26	-8.25	1.26	1.43
3	B	401	A1C3S	O19-C18	7.87	1.51	1.35
3	B	401	A1C3S	C17-C06	7.45	1.51	1.39
3	A	402	A1C3S	O25-C24	-7.28	1.26	1.38
3	B	401	A1C3S	O27-C26	-6.87	1.29	1.43
3	B	401	A1C3S	O25-C24	-6.86	1.26	1.38
3	B	401	A1C3S	C23-C24	6.63	1.50	1.38
3	B	401	A1C3S	C07-C08	6.63	1.50	1.38
3	A	402	A1C3S	C23-C24	6.41	1.49	1.38
3	A	402	A1C3S	O19-C20	6.39	1.58	1.45
3	B	401	A1C3S	O19-C20	5.58	1.57	1.45
3	A	402	A1C3S	C29-C28	5.43	1.50	1.39
3	A	402	A1C3S	C14-C11	5.16	1.51	1.41
3	B	401	A1C3S	C05-C04	4.68	1.61	1.54
3	B	401	A1C3S	C14-C11	4.60	1.50	1.41
3	B	401	A1C3S	C08-C11	-4.58	1.31	1.41
3	B	401	A1C3S	C29-C28	4.46	1.48	1.39
3	A	402	A1C3S	C08-C11	-4.40	1.31	1.41
3	A	402	A1C3S	C28-C24	4.27	1.49	1.39
3	A	402	A1C3S	C05-C04	4.05	1.60	1.54
3	B	401	A1C3S	C17-C14	-3.87	1.32	1.38
3	B	401	A1C3S	C28-C24	3.69	1.48	1.39
3	A	402	A1C3S	C07-C06	-3.48	1.33	1.39
3	B	401	A1C3S	C07-C06	-3.42	1.33	1.39
3	A	402	A1C3S	C04-C03	-3.07	1.47	1.54
4	A	403	SIN	O3-C4	3.02	1.32	1.22
3	A	402	A1C3S	O12-C11	2.93	1.43	1.38
3	A	402	A1C3S	C17-C14	-2.72	1.34	1.38
3	B	401	A1C3S	O01-C02	-2.37	1.38	1.42
3	B	401	A1C3S	C04-C03	-2.30	1.49	1.54
3	A	402	A1C3S	O01-C02	-2.25	1.38	1.42
3	A	402	A1C3S	O15-C14	2.14	1.40	1.37
6	B	404	GOL	C1-C2	2.09	1.59	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	A1C3S	C26-O25-C24	10.59	119.50	105.32
3	B	401	A1C3S	C26-O25-C24	9.58	118.14	105.32
3	B	401	A1C3S	O25-C24-C23	8.87	139.65	127.86
3	A	402	A1C3S	O27-C28-C24	-8.45	99.56	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	A1C3S	O25-C24-C23	8.24	138.81	127.86
3	B	401	A1C3S	O27-C26-O25	8.02	120.68	108.09
3	A	402	A1C3S	O27-C26-O25	7.87	120.45	108.09
3	B	401	A1C3S	O27-C28-C24	-7.36	100.88	109.79
3	B	401	A1C3S	C26-O27-C28	-6.62	96.45	105.32
3	A	402	A1C3S	O25-C24-C28	-6.31	102.14	109.79
3	A	402	A1C3S	C26-O27-C28	-5.97	97.32	105.32
3	B	401	A1C3S	C20-C03-C04	5.85	109.38	101.69
3	A	402	A1C3S	O27-C28-C29	5.79	138.88	127.72
4	A	403	SIN	C3-C2-C1	-5.69	98.57	113.67
3	A	402	A1C3S	C20-O19-C18	-5.42	104.92	110.31
3	B	401	A1C3S	O25-C24-C28	-5.41	103.24	109.79
3	B	401	A1C3S	O27-C28-C29	5.11	137.57	127.72
3	A	402	A1C3S	C20-C03-C04	4.57	107.70	101.69
3	B	401	A1C3S	C23-C24-C28	-3.93	117.11	122.03
3	A	402	A1C3S	C22-C02-C03	-3.88	107.71	112.66
4	B	402	SIN	C3-C2-C1	-3.86	103.42	113.67
3	A	402	A1C3S	C05-C04-C18	-3.86	105.62	112.35
4	B	402	SIN	O3-C4-C3	-3.81	111.01	123.09
3	B	401	A1C3S	C10-O09-C08	3.52	122.67	117.51
4	B	402	SIN	O4-C4-C3	3.22	124.17	114.00
3	B	401	A1C3S	C22-C02-C03	-2.99	108.85	112.66
4	B	402	SIN	C2-C3-C4	-2.95	105.83	113.67
3	A	402	A1C3S	C03-C04-C18	2.81	106.39	102.53
4	B	402	SIN	O1-C1-C2	-2.73	114.44	123.09
3	B	401	A1C3S	C29-C30-C22	-2.69	118.50	121.18
3	A	402	A1C3S	C30-C22-C23	2.61	121.76	118.74
4	A	403	SIN	O1-C1-C2	-2.52	115.10	123.09
3	A	402	A1C3S	C16-O15-C14	-2.50	113.85	117.51
3	B	401	A1C3S	O01-C02-C22	-2.44	105.90	111.20
4	A	403	SIN	O2-C1-C2	2.44	121.71	114.00
3	A	402	A1C3S	C23-C24-C28	-2.38	119.05	122.03
6	B	404	GOL	C3-C2-C1	-2.35	103.19	111.80
3	B	401	A1C3S	O09-C08-C11	2.33	119.13	115.14
3	B	401	A1C3S	C20-O19-C18	-2.33	108.00	110.31
3	B	401	A1C3S	O19-C20-C03	-2.31	101.20	104.70
3	B	401	A1C3S	C03-C04-C18	2.21	105.56	102.53
3	A	402	A1C3S	C04-C03-C02	2.17	117.66	114.50

There are no chirality outliers.

All (16) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	A	402	A1C3S	C03-C04-C05-C06
3	A	402	A1C3S	C18-C04-C05-C06
3	B	401	A1C3S	C03-C04-C05-C06
3	B	401	A1C3S	C18-C04-C05-C06
6	A	405	GOL	C1-C2-C3-O3
6	A	405	GOL	O2-C2-C3-O3
6	B	405	GOL	O1-C1-C2-O2
6	B	405	GOL	O1-C1-C2-C3
6	B	405	GOL	C1-C2-C3-O3
6	B	404	GOL	C1-C2-C3-O3
6	B	404	GOL	O2-C2-C3-O3
6	B	405	GOL	O2-C2-C3-O3
5	A	404	EDO	O1-C1-C2-O2
4	A	403	SIN	C2-C3-C4-O4
4	A	403	SIN	C2-C3-C4-O3
3	A	402	A1C3S	C03-C02-C22-C30

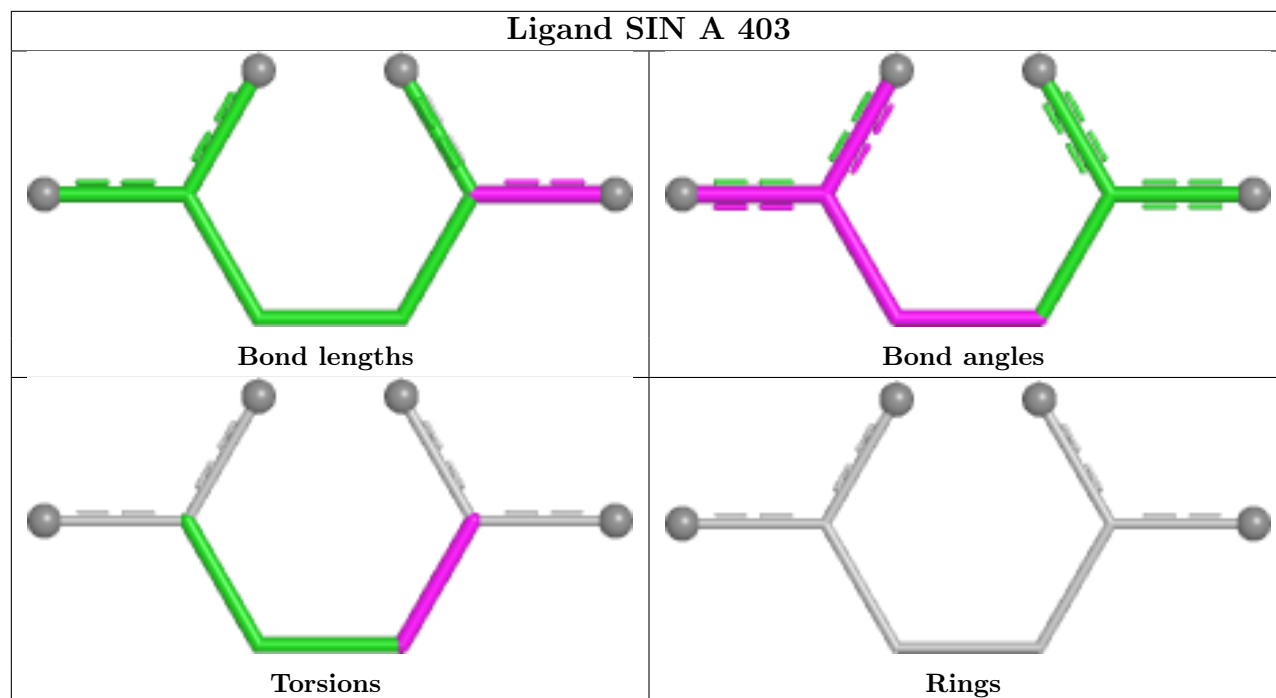
There are no ring outliers.

3 monomers are involved in 2 short contacts:

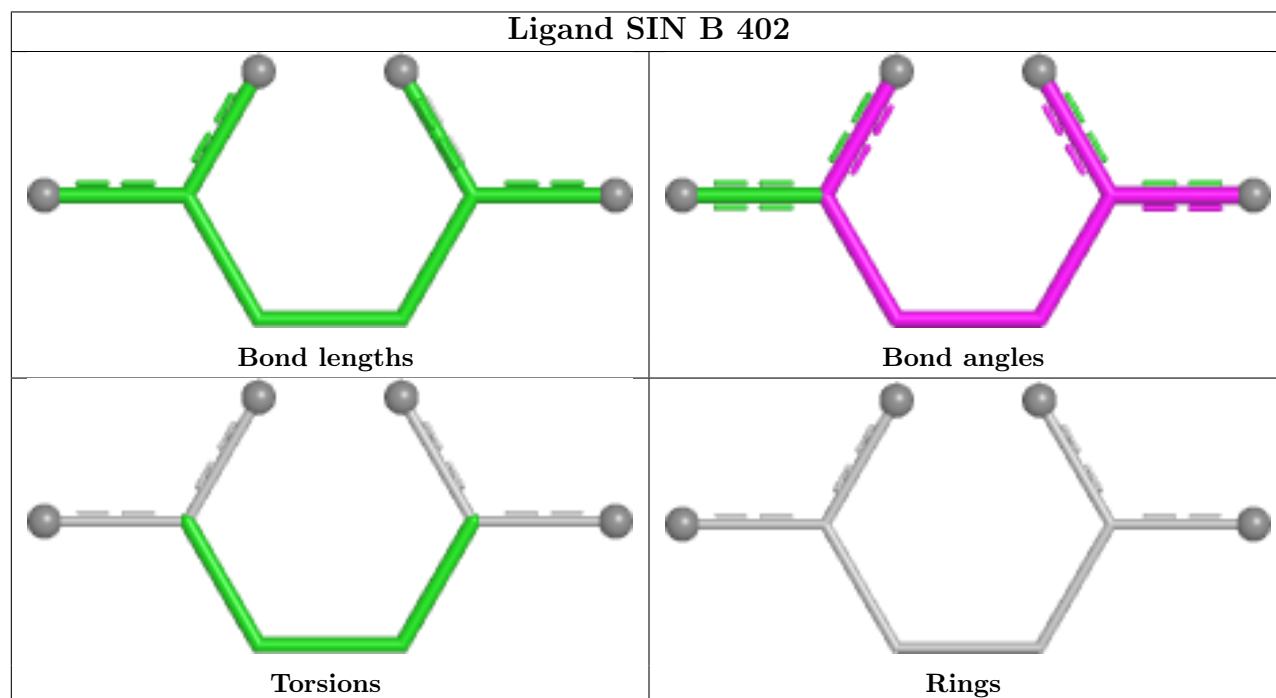
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	404	GOL	1	0
6	A	405	GOL	1	0
3	B	401	A1C3S	1	0

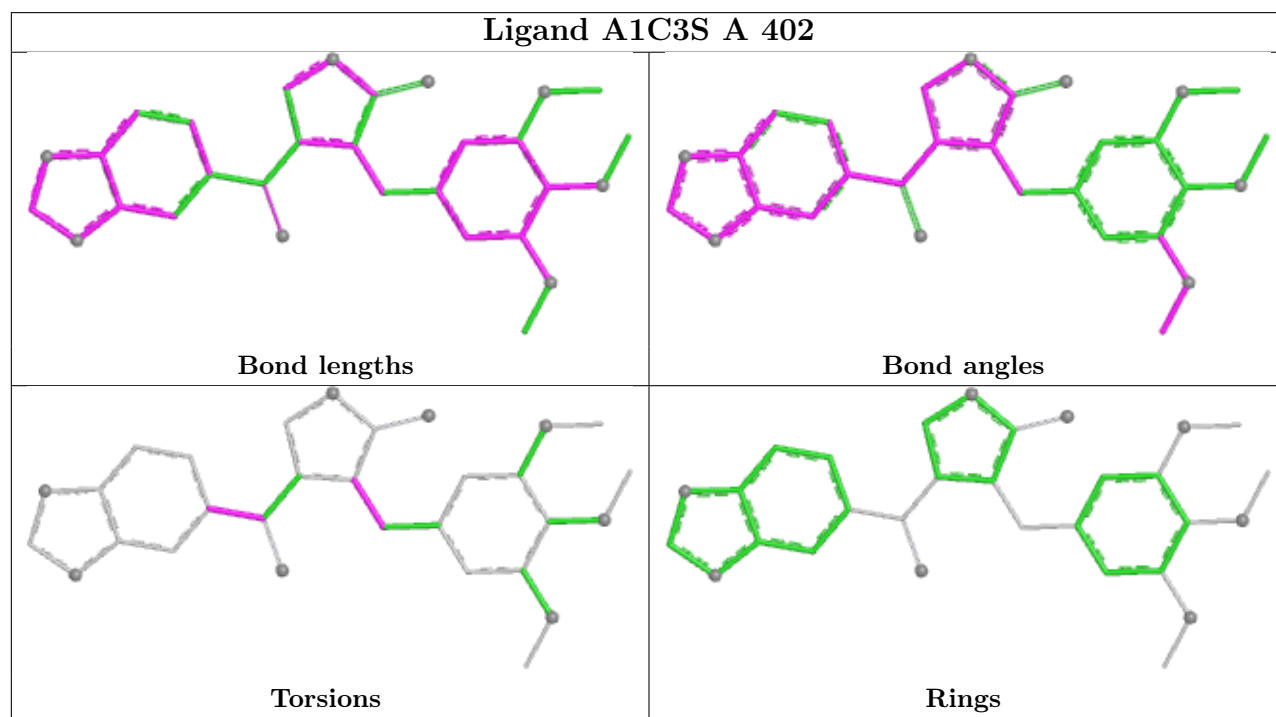
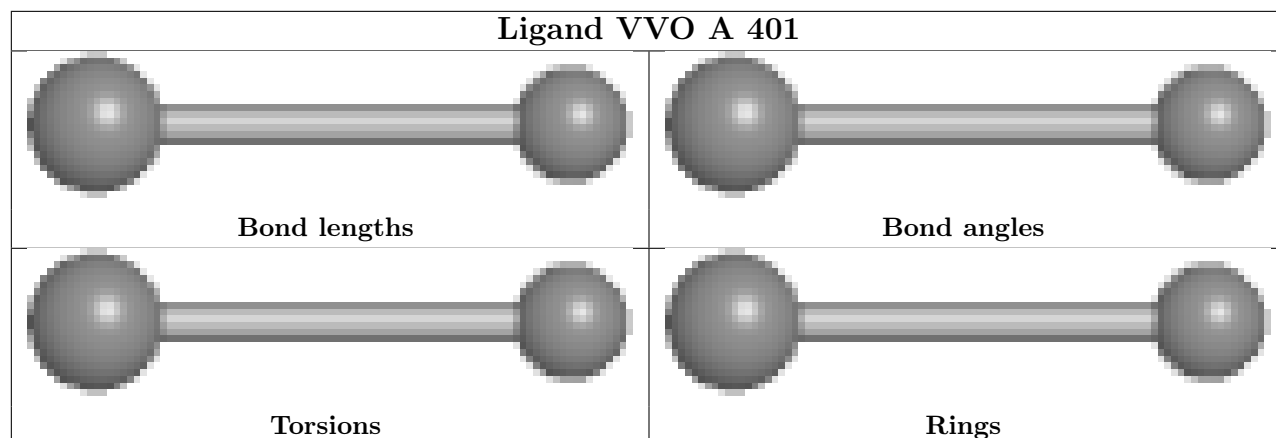
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

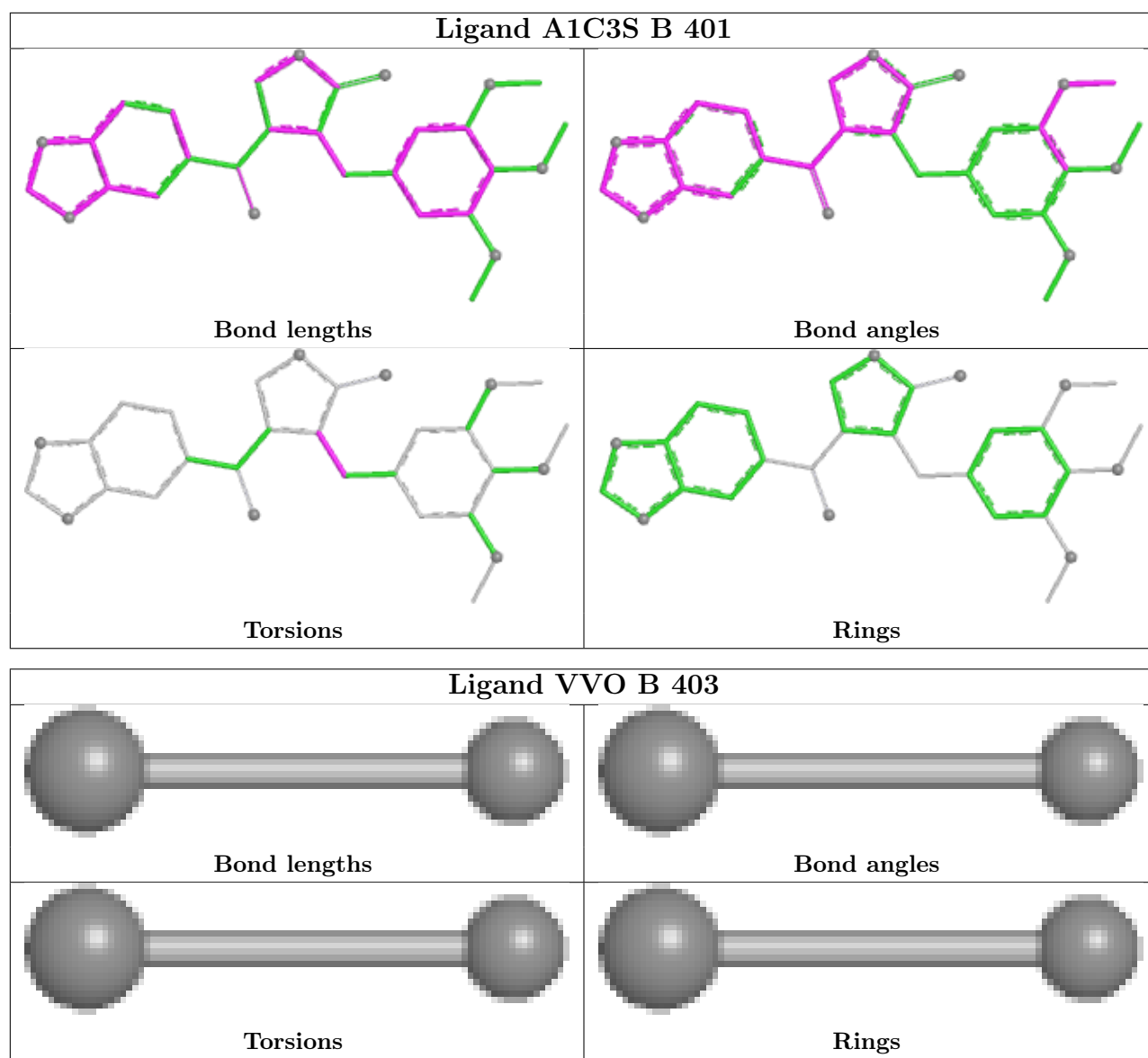
## Ligand SIN A 403



## Ligand SIN B 402







## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	314/318 (98%)	-0.70	2 (0%) 85 85	11, 24, 36, 50	3 (0%)
1	B	314/318 (98%)	-0.60	1 (0%) 90 89	12, 25, 40, 57	3 (0%)
All	All	628/636 (98%)	-0.65	3 (0%) 87 87	11, 24, 38, 57	6 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	PRO	3.4
1	A	5	ALA	2.9
1	B	5	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 oligosaccharides 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	CL	A	406	1/1	0.88	0.08	59,59,59,59	0
5	EDO	A	404	4/4	0.89	0.10	35,35,35,44	0

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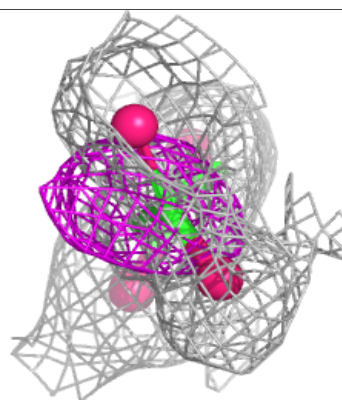
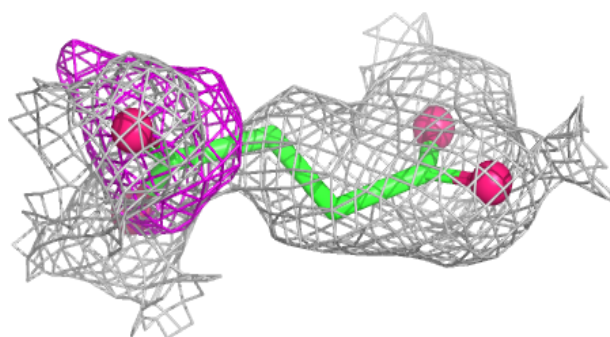
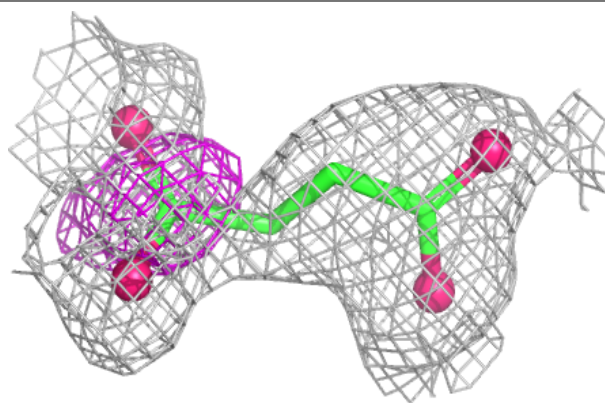
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SIN	A	403	8/8	0.89	0.13	22,30,36,44	0
6	GOL	B	405	6/6	0.90	0.10	37,39,46,47	0
4	SIN	B	402	8/8	0.90	0.11	18,27,31,38	0
7	CL	B	406	1/1	0.91	0.10	57,57,57,57	0
6	GOL	A	405	6/6	0.92	0.10	25,39,42,49	0
6	GOL	B	404	6/6	0.93	0.08	40,43,47,47	0
3	A1C3S	A	402	30/30	0.95	0.06	22,27,34,37	0
3	A1C3S	B	401	30/30	0.95	0.06	17,23,26,29	0
2	VVO	A	401	2/2	1.00	0.03	23,23,23,27	0
2	VVO	B	403	2/2	1.00	0.03	24,24,24,24	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.

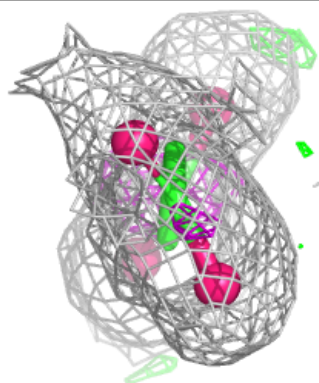
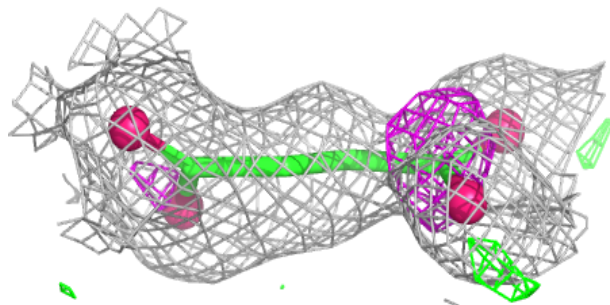
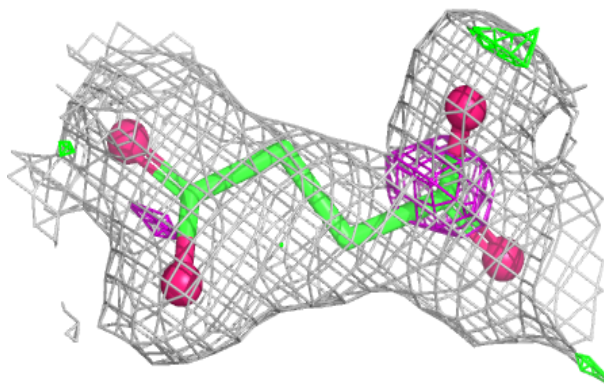
**Electron density around SIN A 403:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SIN B 402:**

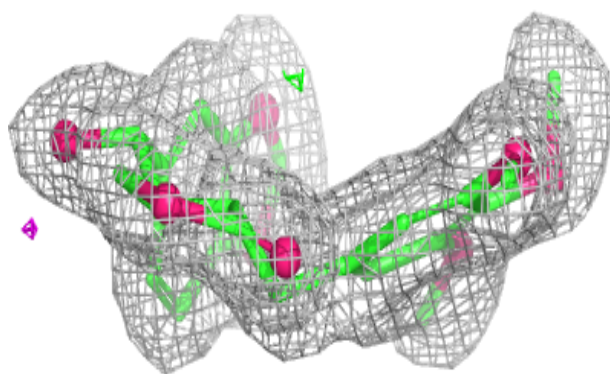
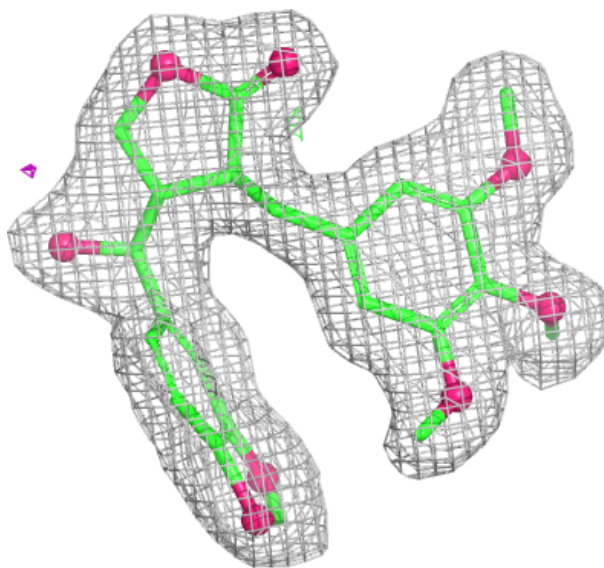
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around A1C3S A 402:**

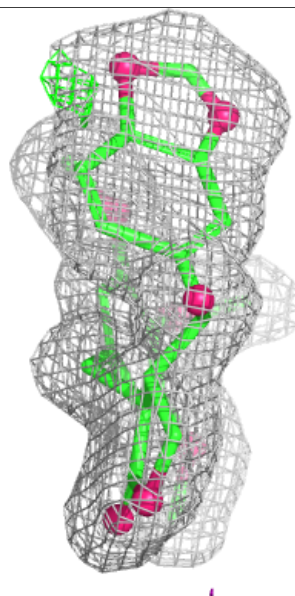
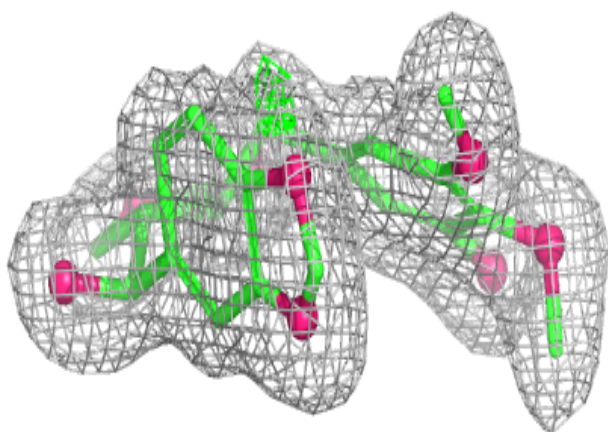
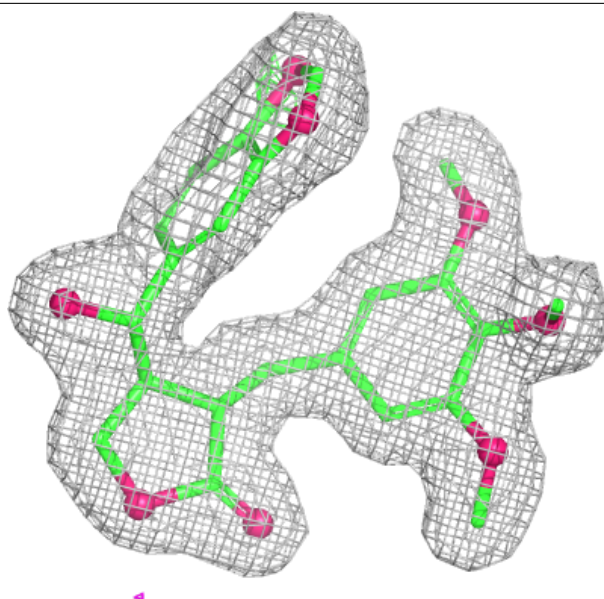
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





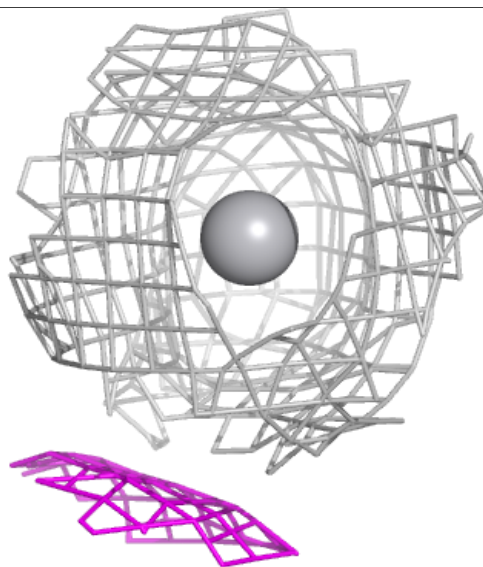
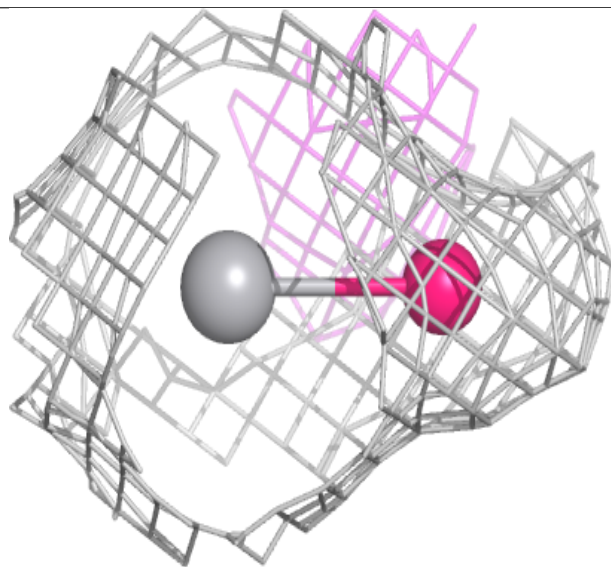
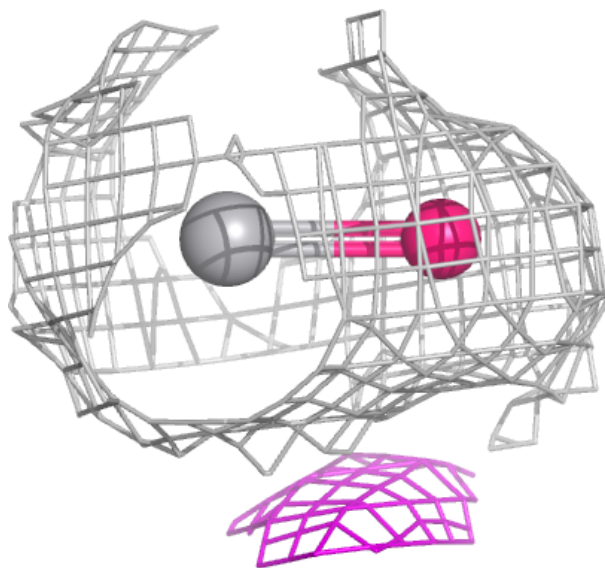
**Electron density around A1C3S B 401:**

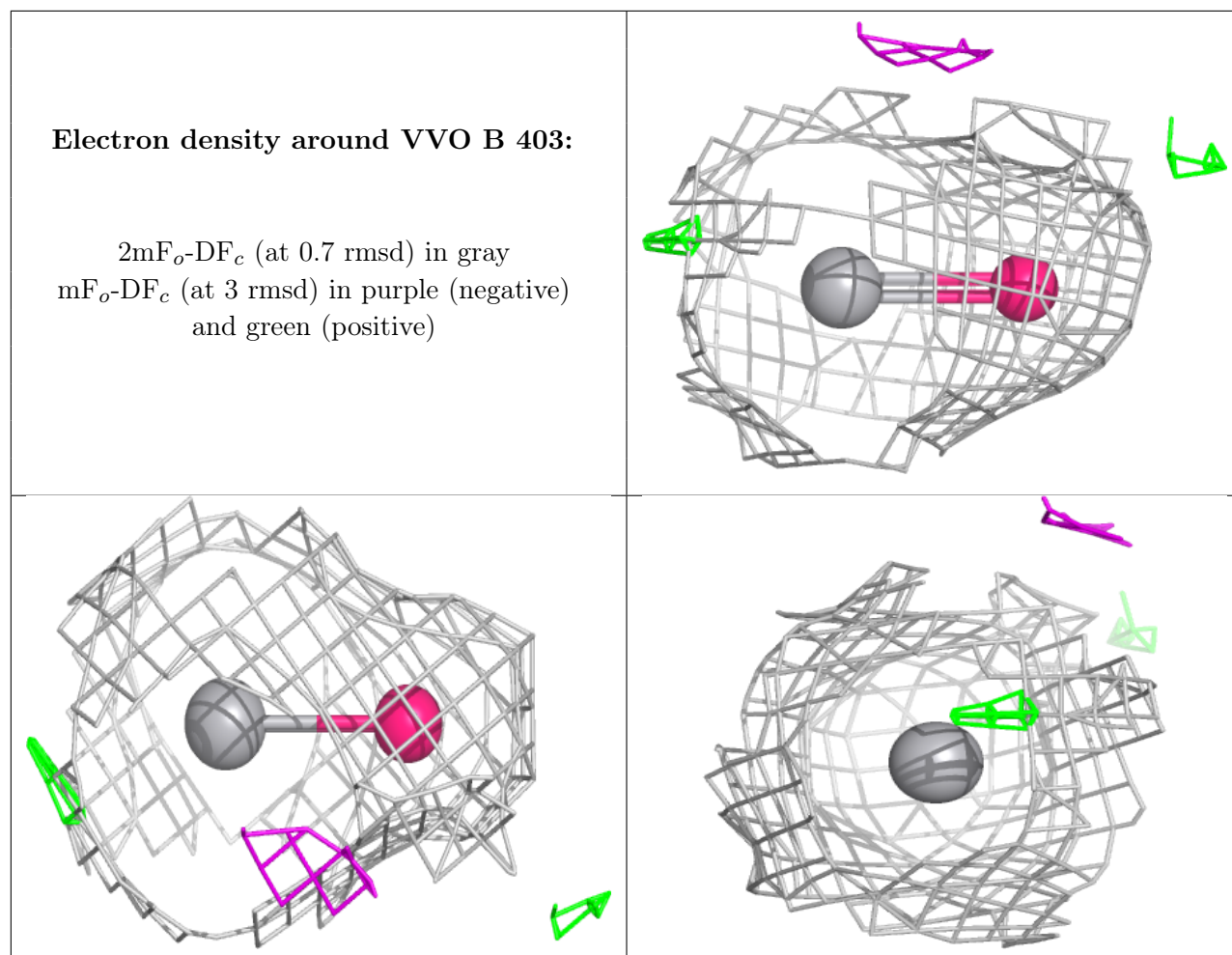
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around VVO 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.