



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2025 – 12:19 AM JST

PDB ID : 9IR6 / pdb\_00009ir6  
Title : Crystal structure of UDP-N-acetylmuramic Acid L-alanine ligase (MurC) from Roseburia faecis in complex with UNAM  
Authors : Wang, Y.X.; Du, Y.H.  
Deposited on : 2024-07-14  
Resolution : 2.43 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 Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

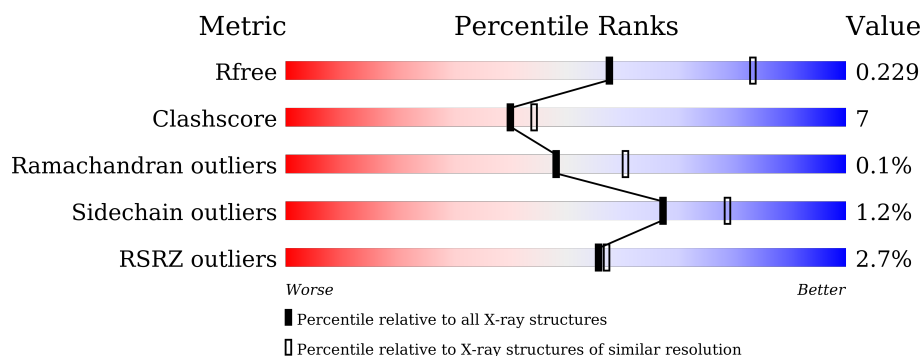
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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))
$R_{free}$	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

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	460	<div> <div>3%</div> <div>85%</div> <div>14%</div> </div>
1	B	460	<div> <div>3%</div> <div>81%</div> <div>18%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7438 atoms, of which 6 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.

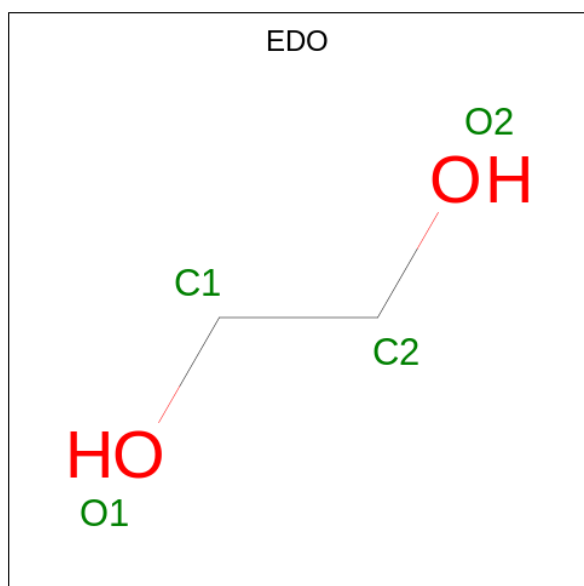
- Molecule 1 is a protein called UDP-N-acetylmuramate--L-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3529	2235	599	677	18			
1	B	459	Total	C	N	O	S	0	1	0
			3538	2241	601	678	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A0M6X1Q9
B	0	SER	-	expression tag	UNP A0A0M6X1Q9

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



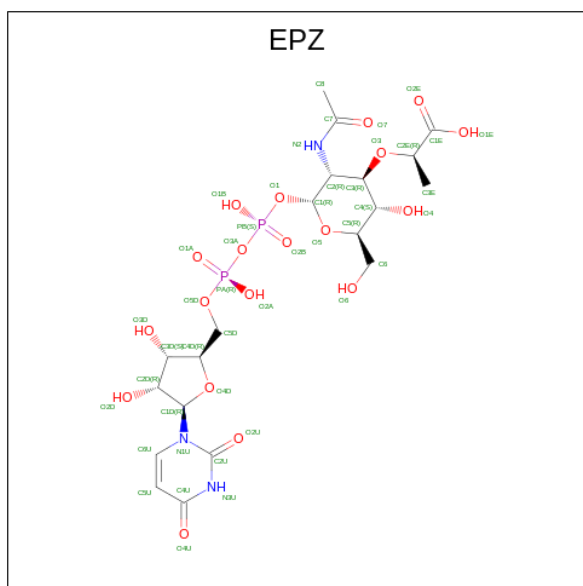
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	H	O	0
			10	2	6	2	
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is (2R)-2-[[[(2R,3R,4R,5S,6R)-3-(acetylamino)-2-[[[(S)-[[[(R)-[[[(2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methoxy}(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]oxy}-5-hydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-4-yl]oxy}propanoic acid (CCD ID: EPZ) (formula: C<sub>20</sub>H<sub>31</sub>N<sub>3</sub>O<sub>19</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	B	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

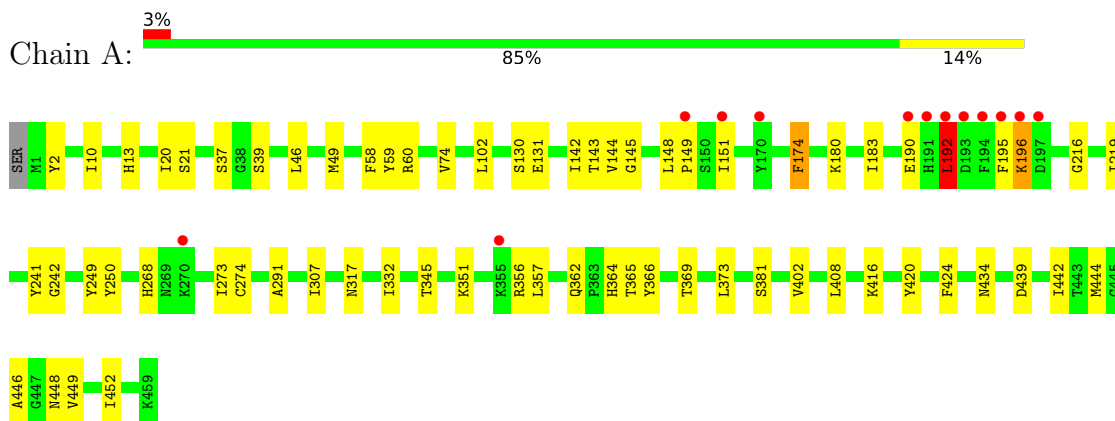
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total	O	0	0
			140	140		
4	B	121	Total	O	0	0
			121	121		

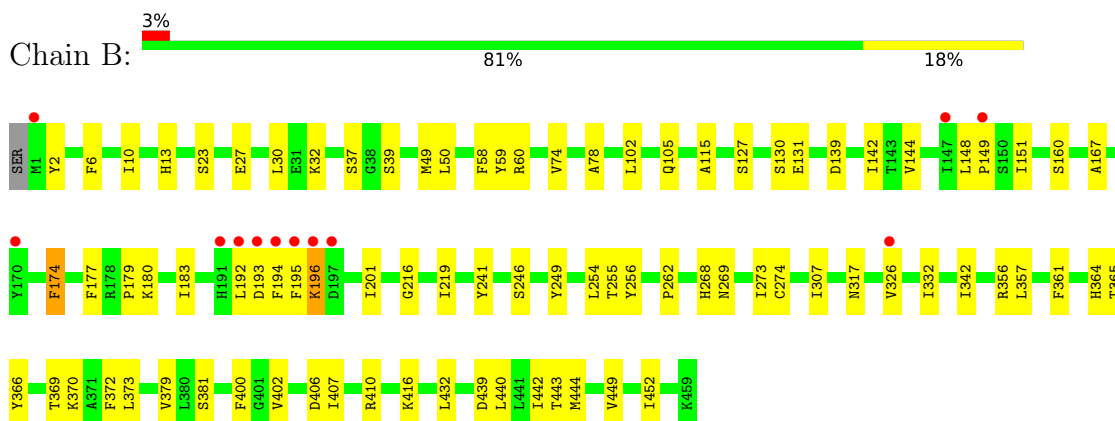
### 3 Residue-property plots

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: UDP-N-acetylmuramate--L-alanine ligase



- Molecule 1: UDP-N-acetylmuramate--L-alanine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.98Å 76.69Å 94.94Å 90.00° 97.46° 90.00°	Depositor
Resolution (Å)	47.07 – 2.43 47.07 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.07-2.43) 98.6 (47.07-2.43)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.188 , 0.228 0.188 , 0.229	Depositor DCC
$R_{free}$ test set	2121 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.760	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPZ, EDO

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	0.17	0/3597	0.35	2/4865 (0.0%)
1	B	0.17	0/3606	0.34	1/4876 (0.0%)
All	All	0.17	0/7203	0.35	3/9741 (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	B	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	192	LEU	N-CA-C	-5.86	106.11	113.20
1	B	174	PHE	CA-CB-CG	5.47	119.27	113.80
1	A	174	PHE	CA-CB-CG	5.46	119.26	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	196[A]	LYS	Mainchain
1	B	196[B]	LYS	Mainchain

## 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	3529	0	3492	40	0
1	B	3538	0	3504	52	0
2	A	8	0	12	0	0
2	B	8	6	12	1	0
3	A	44	0	28	2	0
3	B	44	0	28	1	0
4	A	140	0	0	3	0
4	B	121	0	0	3	0
All	All	7432	6	7076	93	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (93) 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:27:GLU:CD	1:B:49:MET:HE1	2.16	0.70
1:B:381:SER:HB2	1:B:416:LYS:HE3	1.74	0.69
1:A:183:ILE:HD13	1:A:219:ILE:HB	1.77	0.67
1:A:317:ASN:HB3	4:A:660:HOH:O	1.95	0.65
3:A:502:EPZ:H8A	4:A:614:HOH:O	1.98	0.63
1:B:142:ILE:HG22	1:B:144:VAL:HG23	1.81	0.62
1:B:317:ASN:HB3	4:B:660:HOH:O	1.98	0.62
1:B:268:HIS:HB2	1:B:273:ILE:HD11	1.81	0.61
1:A:130:SER:HB3	1:A:142:ILE:HD13	1.81	0.61
1:B:241:TYR:HA	1:B:249:TYR:O	2.02	0.60
1:A:345:THR:HG21	1:A:444:MET:HE2	1.84	0.60
1:B:449:VAL:HG23	1:B:452:ILE:HD12	1.82	0.60
1:A:369:THR:O	1:A:373:LEU:HG	2.02	0.59
1:B:269:ASN:HA	4:B:676:HOH:O	2.02	0.59
1:A:39:SER:HA	1:A:58:PHE:O	2.01	0.59
1:A:446:ALA:O	1:A:449:VAL:HG22	2.03	0.58
1:A:59:TYR:O	1:A:60:ARG:HB2	2.04	0.57
1:A:241:TYR:HA	1:A:249:TYR:O	2.04	0.57
1:B:192:LEU:HD23	1:B:326:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ILE:HD13	1:B:219:ILE:HB	1.87	0.56
1:B:370:LYS:HD2	1:B:400:PHE:HB3	1.86	0.56
1:A:424:PHE:HD1	1:A:452:ILE:HD11	1.71	0.56
1:B:74:VAL:HG21	1:B:102:LEU:HD22	1.88	0.55
1:A:131:GLU:HA	1:A:131:GLU:OE1	2.07	0.55
1:B:342:ILE:HG22	1:B:379:VAL:HG12	1.89	0.55
1:A:148:LEU:HD12	1:A:149:PRO:HD2	1.89	0.55
1:B:130:SER:HB3	1:B:142:ILE:HD13	1.89	0.54
1:A:21:SER:HB3	3:A:502:EPZ:H6	1.89	0.54
1:B:274:CYS:HB2	1:B:307:ILE:HD11	1.89	0.53
1:B:2:TYR:OH	1:B:10:ILE:HD13	2.09	0.53
1:B:39:SER:HA	1:B:58:PHE:O	2.08	0.53
1:A:357:LEU:HD11	1:A:442:ILE:HD12	1.90	0.52
1:B:6:PHE:CD2	1:B:32:LYS:HE2	2.44	0.52
1:A:268:HIS:HB2	1:A:273:ILE:HD11	1.92	0.52
1:A:13:HIS:HA	1:A:37:SER:O	2.10	0.51
1:A:345:THR:CG2	1:A:444:MET:HE2	2.40	0.51
1:B:105:GLN:HG2	4:B:629:HOH:O	2.11	0.51
1:A:74:VAL:HG21	1:A:102:LEU:HD22	1.93	0.50
1:B:131:GLU:HA	1:B:131:GLU:OE1	2.11	0.50
1:A:20:ILE:HD13	1:A:46:LEU:HD11	1.94	0.50
1:A:195:PHE:O	1:A:196:LYS:HB2	2.12	0.50
1:B:366:TYR:HB3	1:B:402:VAL:CG1	2.41	0.50
1:B:139:ASP:O	1:B:160:SER:OG	2.24	0.50
1:B:192:LEU:HD13	1:B:432:LEU:HD23	1.94	0.50
1:B:356:ARG:HB3	1:B:439:ASP:OD1	2.12	0.49
1:B:443:THR:HB	1:B:449:VAL:HG22	1.94	0.49
1:B:148:LEU:HD23	1:B:151:ILE:HG12	1.94	0.49
1:B:372:PHE:CE2	2:B:503:EDO:H21	2.48	0.49
1:B:59:TYR:O	1:B:60:ARG:HB2	2.12	0.49
1:B:406:ASP:O	1:B:410:ARG:HD3	2.14	0.48
1:A:356:ARG:HB3	1:A:439:ASP:OD1	2.13	0.48
1:A:434:ASN:HA	4:A:713:HOH:O	2.13	0.48
1:B:193:ASP:N	1:B:193:ASP:OD1	2.47	0.47
1:B:357:LEU:HD11	1:B:442:ILE:HD12	1.96	0.47
1:A:180:LYS:O	1:A:216:GLY:HA3	2.14	0.47
1:B:361:PHE:CD1	1:B:444:MET:HE3	2.50	0.47
1:B:254:LEU:HD21	1:B:256:TYR:CZ	2.50	0.47
1:B:13:HIS:HA	1:B:37:SER:O	2.15	0.46
1:A:2:TYR:OH	1:A:10:ILE:HD13	2.16	0.46
1:B:196[A]:LYS:HE3	1:B:201:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:TYR:HB3	1:A:402:VAL:CG1	2.45	0.45
1:B:78:ALA:HB2	3:B:502:EPZ:H2	1.98	0.45
1:A:408:LEU:HD22	1:A:420:TYR:HB3	1.99	0.45
1:A:144:VAL:HG22	1:A:145:GLY:N	2.33	0.44
1:B:148:LEU:HD12	1:B:149:PRO:HD2	1.97	0.44
1:B:23:SER:O	1:B:27:GLU:HG3	2.18	0.44
1:A:148:LEU:HD12	1:A:149:PRO:CD	2.47	0.44
1:A:242:GLY:O	1:A:250:TYR:HA	2.18	0.43
1:B:332:ILE:O	1:B:442:ILE:HA	2.17	0.43
1:B:195:PHE:HB3	1:B:196[B]:LYS:HE2	2.00	0.43
1:B:180:LYS:O	1:B:216:GLY:HA3	2.19	0.43
1:A:183:ILE:CD1	1:A:219:ILE:HB	2.45	0.43
1:B:142:ILE:HG22	1:B:144:VAL:CG2	2.47	0.43
1:A:362:GLN:OE1	1:A:448:ASN:HB2	2.19	0.43
1:A:332:ILE:O	1:A:442:ILE:HA	2.19	0.42
1:A:274:CYS:HB2	1:A:307:ILE:HD11	2.00	0.42
1:A:148:LEU:HB3	1:A:151:ILE:HG12	2.01	0.42
1:A:143:THR:O	1:A:143:THR:HG23	2.20	0.42
1:B:27:GLU:HG3	1:B:50:LEU:HD21	2.01	0.42
1:A:192:LEU:HD23	1:A:192:LEU:HA	1.91	0.41
1:B:332:ILE:HD12	1:B:440:LEU:HD11	2.02	0.41
1:B:373:LEU:HD23	1:B:410:ARG:CZ	2.51	0.41
1:B:364:HIS:C	1:B:365:THR:HG23	2.45	0.41
1:A:364:HIS:C	1:A:365:THR:HG23	2.46	0.41
1:B:369:THR:HG23	1:B:407:ILE:HD11	2.03	0.41
1:A:381:SER:HA	1:A:416:LYS:HE2	2.03	0.41
1:B:255:THR:O	1:B:262:PRO:HA	2.21	0.41
1:A:241:TYR:CZ	1:A:291:ALA:HB2	2.56	0.41
1:B:127:SER:O	1:B:131:GLU:HG2	2.21	0.41
1:B:361:PHE:HA	1:B:444:MET:O	2.21	0.41
1:A:183:ILE:CD1	1:A:219:ILE:HD12	2.51	0.40
1:B:115:ALA:HB3	1:B:179:PRO:HG3	2.02	0.40
1:B:167:ALA:HA	1:B:177:PHE:HE2	1.86	0.40

There are no symmetry-related clashes.

## 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	457/460 (99%)	447 (98%)	9 (2%)	1 (0%)	44	53
1	B	458/460 (100%)	446 (97%)	12 (3%)	0	100	100
All	All	915/920 (100%)	893 (98%)	21 (2%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	LYS

### 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	375/376 (100%)	370 (99%)	5 (1%)	65	77
1	B	376/376 (100%)	372 (99%)	4 (1%)	70	80
All	All	751/752 (100%)	742 (99%)	9 (1%)	67	79

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	MET
1	A	174	PHE
1	A	190	GLU
1	A	192	LEU
1	A	351	LYS

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Mol	Chain	Res	Type
1	B	30	LEU
1	B	174	PHE
1	B	194	PHE
1	B	246	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	314	HIS
1	B	199	ASN
1	B	284	HIS
1	B	314	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EPZ	A	502	-	43,46,46	0.84	1 (2%)	60,69,69	1.10	5 (8%)
2	EDO	B	501	-	3,3,3	0.47	0	2,2,2	0.42	0
2	EDO	A	503	-	3,3,3	0.43	0	2,2,2	0.35	0
2	EDO	A	501	-	3,3,3	0.45	0	2,2,2	0.40	0
2	EDO	B	503	-	3,3,3	0.45	0	2,2,2	0.33	0
3	EPZ	B	502	-	43,46,46	0.79	0	60,69,69	0.80	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
3	EPZ	A	502	-	-	12/34/71/71	0/3/3/3
2	EDO	B	501	-	-	0/1/1/1	-
2	EDO	A	503	-	-	0/1/1/1	-
2	EDO	A	501	-	-	0/1/1/1	-
2	EDO	B	503	-	-	1/1/1/1	-
3	EPZ	B	502	-	-	10/34/71/71	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	EPZ	PB-O1	2.08	1.66	1.60

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	EPZ	C3-C2-N2	-3.11	105.75	110.91
3	A	502	EPZ	C3-C4-C5	2.81	115.64	109.66
3	A	502	EPZ	O5-C1-C2	-2.41	105.87	110.58
3	B	502	EPZ	O1B-PB-O2B	2.23	123.27	112.24
3	A	502	EPZ	O5-C5-C4	2.20	113.69	109.69
3	A	502	EPZ	O1B-PB-O2B	2.07	122.49	112.24

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	EPZ	O5-C1-O1-PB

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Mol	Chain	Res	Type	Atoms
3	A	502	EPZ	C1-O1-PB-O3A
3	A	502	EPZ	C1-C2-N2-C7
3	A	502	EPZ	C2-C3-O3-C2E
3	B	502	EPZ	O5-C1-O1-PB
3	B	502	EPZ	O1E-C1E-C2E-O3
3	A	502	EPZ	C4-C5-C6-O6
3	A	502	EPZ	O5-C5-C6-O6
3	B	502	EPZ	C1-O1-PB-O3A
3	B	502	EPZ	O2E-C1E-C2E-O3
3	A	502	EPZ	PA-O3A-PB-O2B
2	B	503	EDO	O1-C1-C2-O2
3	A	502	EPZ	C1-O1-PB-O2B
3	B	502	EPZ	PB-O3A-PA-O2A
3	B	502	EPZ	O1E-C1E-C2E-C3E
3	B	502	EPZ	O2E-C1E-C2E-C3E
3	A	502	EPZ	PA-O3A-PB-O1B
3	B	502	EPZ	O4D-C4D-C5D-O5D
3	A	502	EPZ	C3-C2-N2-C7
3	A	502	EPZ	C5D-O5D-PA-O3A
3	A	502	EPZ	O4D-C4D-C5D-O5D
3	B	502	EPZ	C1-O1-PB-O1B
3	B	502	EPZ	C3E-C2E-O3-C3

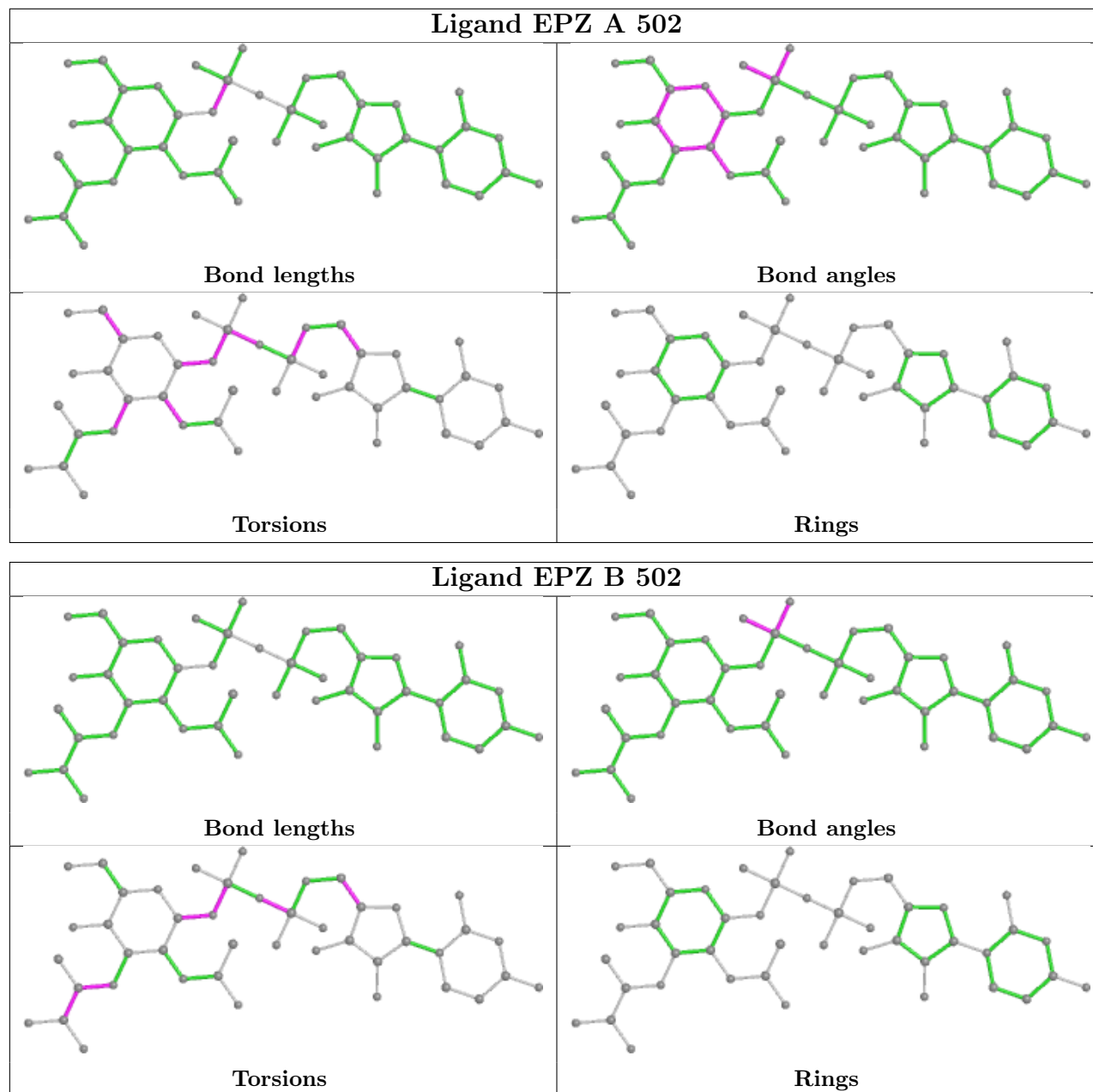
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	EPZ	2	0
2	B	503	EDO	1	0
3	B	502	EPZ	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.



## 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

### 6.1 Protein, DNA and RNA chains

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	459/460 (99%)	-0.13	13 (2%) 55 56	25, 36, 59, 122	0
1	B	459/460 (99%)	-0.12	12 (2%) 57 58	26, 36, 61, 117	1 (0%)
All	All	918/920 (99%)	-0.12	25 (2%) 56 57	25, 36, 60, 122	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	PHE	5.5
1	A	195	PHE	5.1
1	B	196[A]	LYS	4.9
1	B	194	PHE	4.8
1	A	194	PHE	4.6
1	B	197	ASP	3.6
1	B	170	TYR	3.5
1	B	192	LEU	3.4
1	A	191	HIS	3.3
1	A	197	ASP	3.2
1	A	149	PRO	3.2
1	A	192	LEU	3.1
1	B	193	ASP	3.1
1	A	270	LYS	3.1
1	A	196	LYS	3.0
1	A	190	GLU	3.0
1	A	170	TYR	2.9
1	B	326	VAL	2.7
1	B	191	HIS	2.6
1	A	193	ASP	2.5
1	A	355	LYS	2.2
1	A	151	ILE	2.2
1	B	1	MET	2.1
1	B	149	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	147	ILE	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](#)

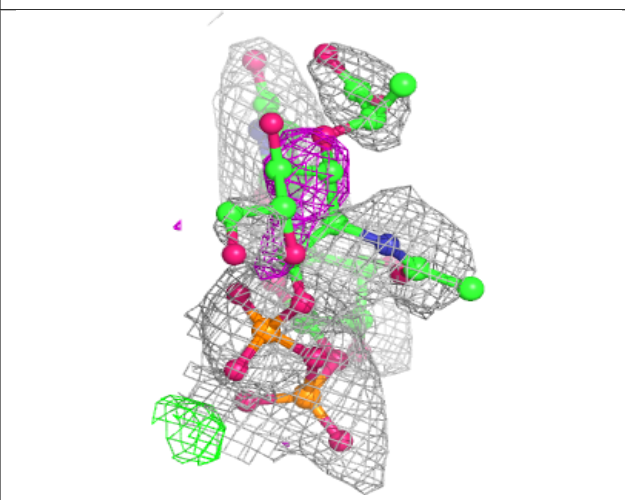
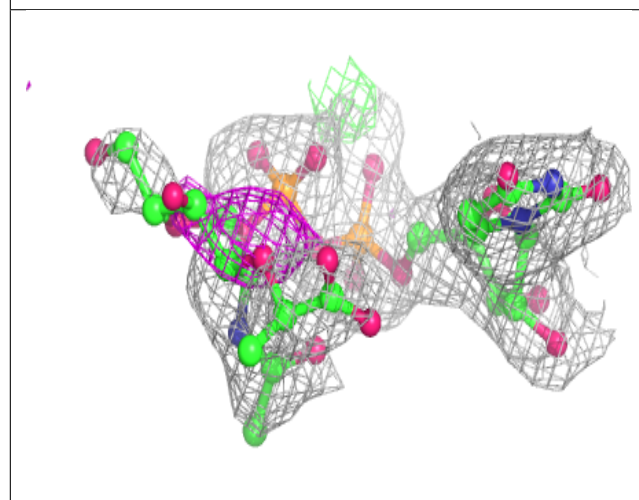
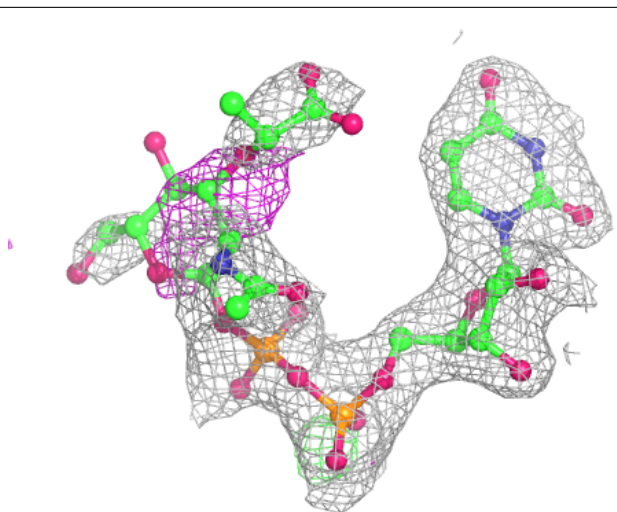
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	EDO	A	503	4/4	0.80	0.22	64,65,66,75	0
2	EDO	B	501	4/4	0.80	0.15	52,62,71,73	0
3	EPZ	B	502	44/44	0.86	0.15	34,58,84,91	0
3	EPZ	A	502	44/44	0.88	0.14	32,65,92,101	0
2	EDO	B	503	4/4	0.89	0.13	43,51,53,54	0
2	EDO	A	501	4/4	0.91	0.10	43,43,45,48	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.

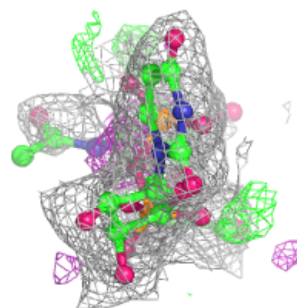
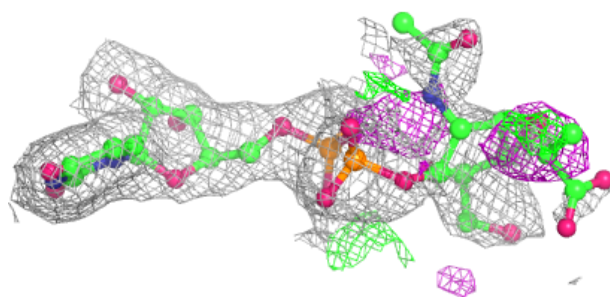
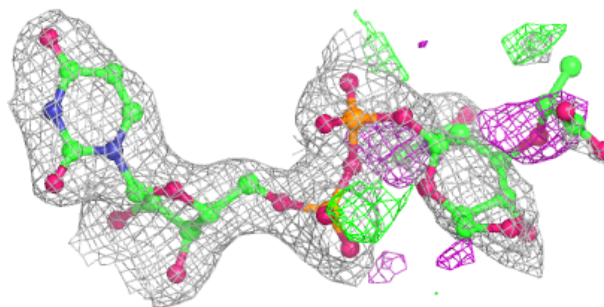
**Electron density around EPZ B 502:**

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



**Electron density around EPZ A 502:**

$2mF_o - DF_c$  (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.