



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2025 – 10:05 AM EDT

PDB ID : 4R23 / pdb\_00004r23  
Title : Structure of a putative peptidoglycan glycosyltransferase from *Atopobium parvulum* in complex with dicloxacillin  
Authors : Filippova, E.V.; Minasov, G.; Kiryukhina, O.; Clancy, S.; Joachimiak, A.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2014-08-08  
Resolution : 1.84 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	:	2022.3.0, CSD as543be (2022)
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

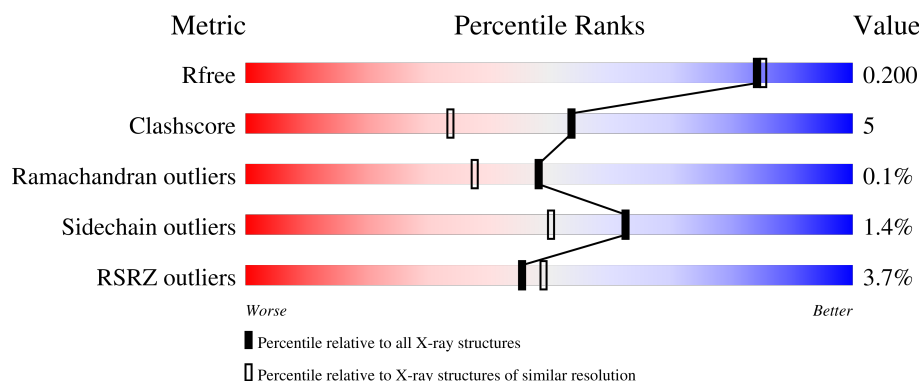
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

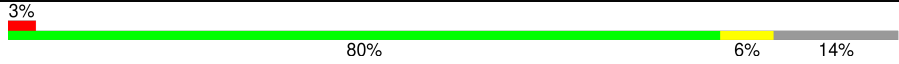

The reported resolution of this entry is 1.84 Å.

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	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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	482	
1	B	482	

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
2	DXU	A	1001	X	-	X	-
2	DXU	B	1001	X	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6490 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 Peptidoglycan glycosyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	Se	0	1	0
			3000	1864	510	611	2	13			
1	B	411	Total	C	N	O	S	Se	0	0	0
			2956	1837	501	603	2	13			

There are 64 discrepancies between the modelled and reference sequences:

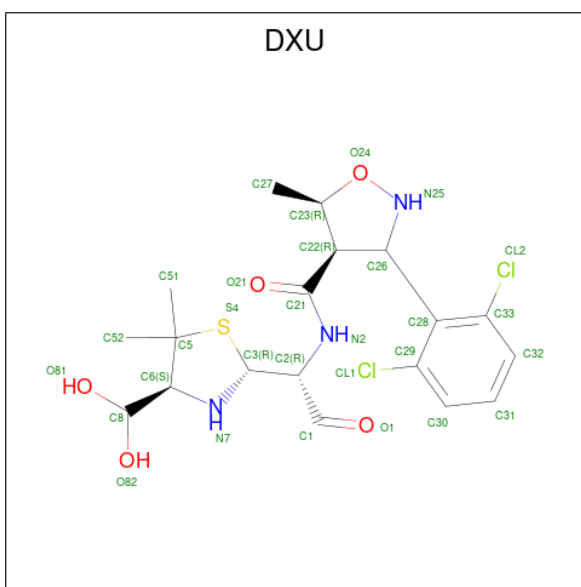
Chain	Residue	Modelled	Actual	Comment	Reference
A	473	MSE	-	expression tag	UNP C8W8H7
A	474	HIS	-	expression tag	UNP C8W8H7
A	475	HIS	-	expression tag	UNP C8W8H7
A	476	HIS	-	expression tag	UNP C8W8H7
A	477	HIS	-	expression tag	UNP C8W8H7
A	478	HIS	-	expression tag	UNP C8W8H7
A	479	HIS	-	expression tag	UNP C8W8H7
A	480	SER	-	expression tag	UNP C8W8H7
A	481	SER	-	expression tag	UNP C8W8H7
A	482	GLY	-	expression tag	UNP C8W8H7
A	483	VAL	-	expression tag	UNP C8W8H7
A	484	ASP	-	expression tag	UNP C8W8H7
A	485	LEU	-	expression tag	UNP C8W8H7
A	486	TRP	-	expression tag	UNP C8W8H7
A	487	SER	-	expression tag	UNP C8W8H7
A	488	HIS	-	expression tag	UNP C8W8H7
A	489	PRO	-	expression tag	UNP C8W8H7
A	490	GLN	-	expression tag	UNP C8W8H7
A	491	PHE	-	expression tag	UNP C8W8H7
A	492	GLU	-	expression tag	UNP C8W8H7
A	493	LYS	-	expression tag	UNP C8W8H7
A	494	GLY	-	expression tag	UNP C8W8H7
A	495	THR	-	expression tag	UNP C8W8H7
A	496	GLU	-	expression tag	UNP C8W8H7
A	497	ASN	-	expression tag	UNP C8W8H7

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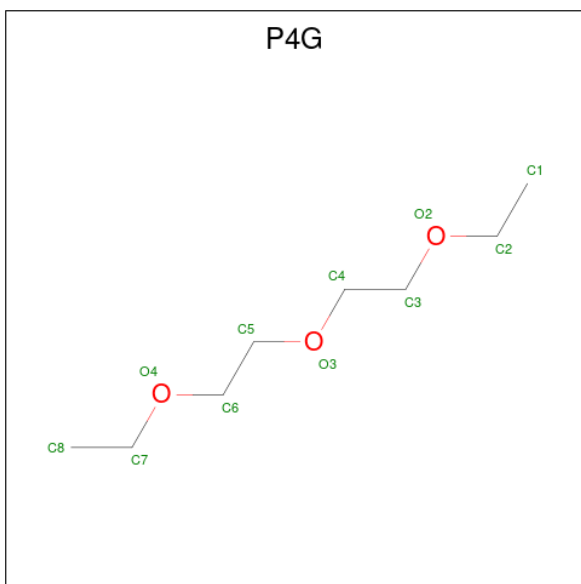
Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	expression tag	UNP C8W8H7
A	499	TYR	-	expression tag	UNP C8W8H7
A	500	PHE	-	expression tag	UNP C8W8H7
A	501	GLN	-	expression tag	UNP C8W8H7
A	502	SER	-	expression tag	UNP C8W8H7
A	503	ASN	-	expression tag	UNP C8W8H7
A	504	ALA	-	expression tag	UNP C8W8H7
B	473	MSE	-	expression tag	UNP C8W8H7
B	474	HIS	-	expression tag	UNP C8W8H7
B	475	HIS	-	expression tag	UNP C8W8H7
B	476	HIS	-	expression tag	UNP C8W8H7
B	477	HIS	-	expression tag	UNP C8W8H7
B	478	HIS	-	expression tag	UNP C8W8H7
B	479	HIS	-	expression tag	UNP C8W8H7
B	480	SER	-	expression tag	UNP C8W8H7
B	481	SER	-	expression tag	UNP C8W8H7
B	482	GLY	-	expression tag	UNP C8W8H7
B	483	VAL	-	expression tag	UNP C8W8H7
B	484	ASP	-	expression tag	UNP C8W8H7
B	485	LEU	-	expression tag	UNP C8W8H7
B	486	TRP	-	expression tag	UNP C8W8H7
B	487	SER	-	expression tag	UNP C8W8H7
B	488	HIS	-	expression tag	UNP C8W8H7
B	489	PRO	-	expression tag	UNP C8W8H7
B	490	GLN	-	expression tag	UNP C8W8H7
B	491	PHE	-	expression tag	UNP C8W8H7
B	492	GLU	-	expression tag	UNP C8W8H7
B	493	LYS	-	expression tag	UNP C8W8H7
B	494	GLY	-	expression tag	UNP C8W8H7
B	495	THR	-	expression tag	UNP C8W8H7
B	496	GLU	-	expression tag	UNP C8W8H7
B	497	ASN	-	expression tag	UNP C8W8H7
B	498	LEU	-	expression tag	UNP C8W8H7
B	499	TYR	-	expression tag	UNP C8W8H7
B	500	PHE	-	expression tag	UNP C8W8H7
B	501	GLN	-	expression tag	UNP C8W8H7
B	502	SER	-	expression tag	UNP C8W8H7
B	503	ASN	-	expression tag	UNP C8W8H7
B	504	ALA	-	expression tag	UNP C8W8H7

- Molecule 2 is Dicloxacillin, open form (CCD ID: DXU) (formula: C<sub>19</sub>H<sub>25</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			30	19	2	3	5	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			30	19	2	3	5	1		

- Molecule 3 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (CCD ID: P4G) (formula:  $C_8H_{18}O_3$ ).



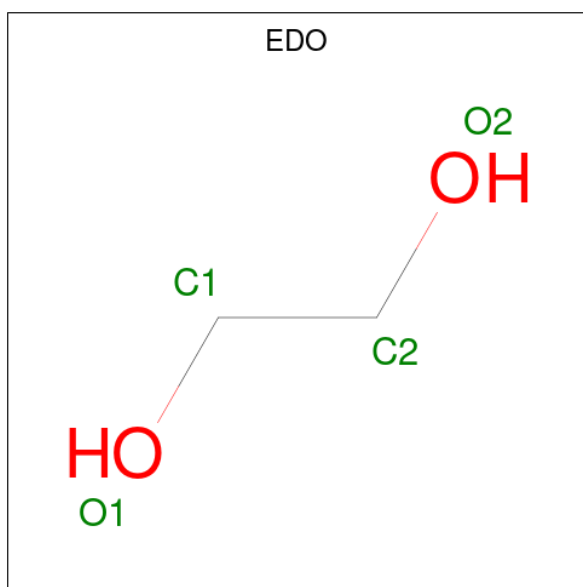
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	212	Total	O	0	1
			213	213		

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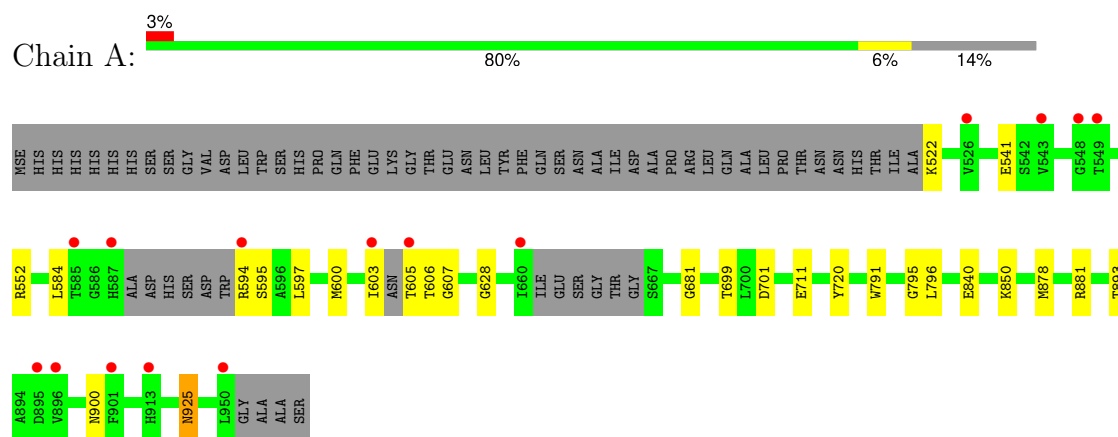
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	214	Total 216	O 216	0	2



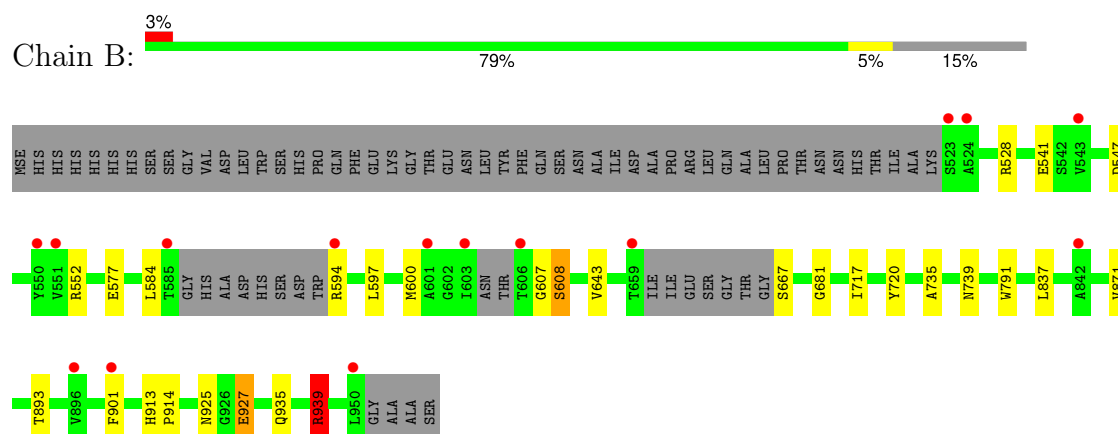
### 3 Residue-property plots [i](#)

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: Peptidoglycan glycosyltransferase



#### • Molecule 1: Peptidoglycan glycosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.61Å 69.88Å 114.25Å 90.00° 96.87° 90.00°	Depositor
Resolution (Å)	30.00 – 1.84 30.00 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-1.84) 98.2 (30.00-1.84)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.155 , 0.192 0.166 , 0.200	Depositor DCC
$R_{free}$ test set	4501 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: P4G, DXU, 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	0.96	0/3037	0.97	0/4118
1	B	0.94	1/2992 (0.0%)	0.94	2/4058 (0.0%)
All	All	0.95	1/6029 (0.0%)	0.96	2/8176 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	643	VAL	C-O	5.02	1.29	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	717	ILE	CB-CA-C	-5.06	103.08	110.62
1	B	939	ARG	CB-CG-CD	5.04	122.88	111.30

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	3000	0	2931	31	0
1	B	2956	0	2886	24	0
2	A	30	0	23	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	30	0	23	13	0
3	A	21	0	24	6	0
3	B	4	0	4	0	0
4	A	12	0	18	0	0
4	B	8	0	12	0	0
5	A	213	0	0	2	0
5	B	216	0	0	1	0
All	All	6490	0	5921	57	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 5.

All (57) 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:878:MSE:HE3	1:A:881:ARG:HH21	1.30	0.94
1:B:791:TRP:CZ3	2:B:1001:DXU:H1	2.07	0.89
1:B:791:TRP:HZ3	2:B:1001:DXU:H1	1.40	0.84
1:A:791:TRP:CZ3	2:A:1001:DXU:H1	2.14	0.82
1:B:791:TRP:CZ3	2:B:1001:DXU:C30	2.65	0.78
1:A:791:TRP:HZ3	2:A:1001:DXU:H1	1.46	0.78
1:A:791:TRP:CZ3	2:A:1001:DXU:C30	2.67	0.77
1:A:699:THR:OG1	3:A:1002:P4G:H32	1.83	0.77
1:A:791:TRP:HZ3	2:A:1001:DXU:C30	1.96	0.77
1:B:791:TRP:HZ3	2:B:1001:DXU:C30	1.97	0.77
1:A:878:MSE:HE3	1:A:881:ARG:NH2	2.07	0.69
1:A:603:ILE:O	1:A:605:THR:OG1	2.17	0.63
1:A:628:GLY:H	3:A:1004:P4G:C3	2.11	0.63
1:A:791:TRP:HZ3	2:A:1001:DXU:C31	2.13	0.62
1:A:701:ASP:HB2	3:A:1002:P4G:C4	2.31	0.61
1:B:541:GLU:O	1:B:552:ARG:HD2	2.01	0.60
1:A:791:TRP:CZ3	2:A:1001:DXU:C31	2.85	0.59
1:B:935:GLN:O	1:B:939:ARG:HG2	2.02	0.59
1:A:701:ASP:HB2	3:A:1002:P4G:H41	1.88	0.55
1:A:522:LYS:CE	1:A:595:SER:O	2.56	0.53
1:A:522:LYS:HE2	1:A:595:SER:O	2.09	0.53
1:B:791:TRP:CZ3	2:B:1001:DXU:C31	2.92	0.53
1:B:584:LEU:O	1:B:607:GLY:HA3	2.09	0.52
1:B:791:TRP:HZ3	2:B:1001:DXU:C31	2.23	0.51
1:A:893:THR:O	2:A:1001:DXU:CL2	2.66	0.51
3:A:1003:P4G:H41	5:A:1307:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:THR:HG22	1:A:607:GLY:O	2.12	0.49
1:A:720:TYR:HD1	2:A:1001:DXU:H9	1.78	0.48
1:A:720:TYR:HB2	2:A:1001:DXU:S4	2.53	0.48
1:B:720:TYR:CD1	2:B:1001:DXU:H9	2.48	0.48
1:B:720:TYR:HD1	2:B:1001:DXU:H9	1.79	0.48
1:A:584:LEU:O	1:A:607:GLY:HA3	2.13	0.47
1:B:893:THR:O	2:B:1001:DXU:H10	2.15	0.47
1:A:791:TRP:CZ3	2:A:1001:DXU:H2	2.51	0.45
1:A:791:TRP:HZ3	2:A:1001:DXU:H2	1.82	0.45
1:B:681:GLY:HA2	2:B:1001:DXU:CL2	2.53	0.45
1:B:913:HIS:N	1:B:914:PRO:HD3	2.32	0.44
1:A:900:ASN:ND2	1:A:925:ASN:HA	2.33	0.44
1:B:720:TYR:HB2	2:B:1001:DXU:S4	2.58	0.43
1:B:597:LEU:HD12	1:B:597:LEU:N	2.33	0.43
1:A:597:LEU:HB2	1:A:600:MSE:HE2	2.00	0.43
1:A:603:ILE:O	1:A:603:ILE:HG22	2.19	0.43
1:B:667:SER:N	5:B:1138:HOH:O	2.50	0.43
1:A:701:ASP:HB2	3:A:1002:P4G:H42	2.01	0.43
1:B:739:ASN:ND2	2:B:1001:DXU:C30	2.83	0.42
1:B:608:SER:HB2	1:B:837:LEU:O	2.20	0.42
1:B:528:ARG:NH1	1:B:577:GLU:O	2.53	0.41
1:A:681:GLY:O	1:A:795:GLY:HA3	2.20	0.41
1:B:597:LEU:HB2	1:B:600:MSE:HE2	2.03	0.41
1:B:594:ARG:HA	1:B:600:MSE:CE	2.51	0.41
2:B:1001:DXU:H15	2:B:1001:DXU:H23	1.95	0.41
1:A:541:GLU:O	1:A:552:ARG:HD2	2.20	0.41
1:B:735:ALA:HA	1:B:871:VAL:HG22	2.03	0.41
1:A:720:TYR:CD1	2:A:1001:DXU:H9	2.56	0.40
1:A:522:LYS:HE3	1:A:595:SER:O	2.21	0.40
1:B:925:ASN:C	1:B:927:GLU:H	2.29	0.40
1:A:850:LYS:NZ	5:A:1223:HOH:O	2.54	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	409/482 (85%)	398 (97%)	11 (3%)	0	100	100
1	B	403/482 (84%)	395 (98%)	7 (2%)	1 (0%)	44	33
All	All	812/964 (84%)	793 (98%)	18 (2%)	1 (0%)	48	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	547	ASP

### 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	317/356 (89%)	312 (98%)	5 (2%)	58	44
1	B	312/356 (88%)	308 (99%)	4 (1%)	65	53
All	All	629/712 (88%)	620 (99%)	9 (1%)	62	50

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

Mol	Chain	Res	Type
1	A	594	ARG
1	A	711	GLU
1	A	796	LEU
1	A	840	GLU
1	A	925	ASN
1	B	608	SER
1	B	901	PHE
1	B	927	GLU
1	B	939	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	545	GLN
1	A	935	GLN
1	B	739	ASN
1	B	863	GLN
1	B	925	ASN
1	B	943	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](#)

11 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	P4G	A	1002	-	6,6,10	0.50	0	5,5,9	1.10	0
3	P4G	A	1004	-	6,6,10	0.27	0	5,5,9	0.87	0
4	EDO	A	1006	-	3,3,3	0.38	0	2,2,2	0.70	0
4	EDO	A	1005	-	3,3,3	0.33	0	2,2,2	0.62	0
2	DXU	A	1001	1	26,32,32	2.59	10 (38%)	34,48,48	4.27	19 (55%)
4	EDO	B	1003	-	3,3,3	0.45	0	2,2,2	0.63	0
3	P4G	A	1003	-	6,6,10	0.29	0	5,5,9	0.82	0
4	EDO	A	1007	-	3,3,3	0.41	0	2,2,2	0.66	0
4	EDO	B	1004	-	3,3,3	0.38	0	2,2,2	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DXU	B	1001	1	26,32,32	2.63	8 (30%)	34,48,48	4.47	20 (58%)
3	P4G	B	1002	-	3,3,10	0.35	0	2,2,9	0.18	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	P4G	A	1002	-	-	2/4/4/8	-
3	P4G	A	1004	-	-	4/4/4/8	-
4	EDO	A	1006	-	-	1/1/1/1	-
4	EDO	A	1005	-	-	1/1/1/1	-
2	DXU	A	1001	1	1/1/9/13	5/14/50/50	0/3/3/3
4	EDO	B	1003	-	-	1/1/1/1	-
3	P4G	A	1003	-	-	2/4/4/8	-
4	EDO	A	1007	-	-	0/1/1/1	-
4	EDO	B	1004	-	-	1/1/1/1	-
2	DXU	B	1001	1	1/1/9/13	5/14/50/50	0/3/3/3
3	P4G	B	1002	-	-	1/1/1/8	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	DXU	C26-N25	-7.55	1.32	1.46
2	A	1001	DXU	C26-N25	-7.33	1.32	1.46
2	B	1001	DXU	C29-C28	5.52	1.47	1.39
2	A	1001	DXU	C29-C28	5.46	1.47	1.39
2	A	1001	DXU	C28-C26	-4.23	1.48	1.52
2	B	1001	DXU	C28-C26	-3.98	1.48	1.52
2	B	1001	DXU	C22-C26	-3.89	1.49	1.56
2	B	1001	DXU	C29-CL1	3.76	1.82	1.73
2	B	1001	DXU	C5-S4	-3.70	1.78	1.85
2	A	1001	DXU	C33-CL2	3.64	1.82	1.73
2	A	1001	DXU	C29-CL1	3.60	1.82	1.73
2	A	1001	DXU	C22-C26	-3.51	1.50	1.56
2	B	1001	DXU	C33-CL2	3.23	1.81	1.73
2	A	1001	DXU	C3-S4	-2.81	1.78	1.84
2	A	1001	DXU	C5-S4	-2.67	1.80	1.85
2	A	1001	DXU	O1-C1	2.26	1.28	1.20
2	A	1001	DXU	C22-C21	2.18	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	DXU	C3-S4	-2.02	1.80	1.84

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	DXU	C28-C26-N25	13.94	137.51	112.02
2	B	1001	DXU	C28-C26-N25	13.31	136.36	112.02
2	B	1001	DXU	C23-C22-C21	12.80	128.57	111.22
2	A	1001	DXU	C23-C22-C21	11.76	127.16	111.22
2	B	1001	DXU	C1-C2-N2	-8.01	97.17	109.80
2	B	1001	DXU	C29-C28-C26	-7.02	113.62	122.69
2	A	1001	DXU	C29-C28-C26	-6.66	114.08	122.69
2	A	1001	DXU	C1-C2-N2	-6.12	100.16	109.80
2	A	1001	DXU	C2-N2-C21	6.00	129.95	123.08
2	B	1001	DXU	C30-C29-C28	-5.71	114.81	122.38
2	A	1001	DXU	C30-C29-C28	-5.30	115.36	122.38
2	B	1001	DXU	C33-C28-C29	5.05	120.60	114.92
2	A	1001	DXU	C33-C28-C29	4.94	120.48	114.92
2	B	1001	DXU	C2-N2-C21	4.55	128.30	123.08
2	B	1001	DXU	C22-C26-N25	4.07	112.11	102.70
2	A	1001	DXU	O21-C21-C22	3.97	130.76	122.36
2	A	1001	DXU	C22-C26-N25	3.92	111.76	102.70
2	B	1001	DXU	C28-C33-CL2	3.88	125.17	120.54
2	B	1001	DXU	O21-C21-C22	3.79	130.39	122.36
2	B	1001	DXU	O24-C23-C27	3.57	116.92	108.74
2	A	1001	DXU	O24-C23-C27	3.56	116.88	108.74
2	A	1001	DXU	C3-C2-N2	3.48	117.29	109.93
2	B	1001	DXU	C3-C2-N2	3.39	117.12	109.93
2	B	1001	DXU	O1-C1-C2	-3.20	116.41	124.86
2	A	1001	DXU	O1-C1-C2	-3.02	116.88	124.86
2	B	1001	DXU	C22-C21-N2	-2.96	108.12	114.82
2	B	1001	DXU	C51-C5-S4	2.83	113.75	109.18
2	B	1001	DXU	C32-C33-CL2	-2.71	113.09	118.42
2	A	1001	DXU	C22-C21-N2	-2.61	108.90	114.82
2	B	1001	DXU	C31-C30-C29	2.50	123.18	119.42
2	A	1001	DXU	C30-C29-CL1	2.49	123.33	118.42
2	B	1001	DXU	C26-C22-C21	-2.40	108.98	113.21
2	B	1001	DXU	C27-C23-C22	2.32	117.99	115.05
2	A	1001	DXU	O81-C8-O82	2.27	115.17	111.26
2	A	1001	DXU	C31-C30-C29	2.20	122.73	119.42
2	B	1001	DXU	C30-C29-CL1	2.19	122.73	118.42
2	A	1001	DXU	C28-C26-C22	-2.18	110.09	115.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	DXU	C51-C5-C52	-2.17	107.16	110.70
2	A	1001	DXU	C28-C33-CL2	2.14	123.09	120.54

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	DXU	C26
2	B	1001	DXU	C26

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	DXU	N25-C26-C28-C29
2	A	1001	DXU	N7-C6-C8-O82
2	A	1001	DXU	N7-C6-C8-O81
2	B	1001	DXU	N7-C6-C8-O82
2	B	1001	DXU	N7-C6-C8-O81
3	A	1004	P4G	O2-C3-C4-O3
3	A	1002	P4G	O2-C3-C4-O3
3	A	1002	P4G	O3-C5-C6-O4
4	A	1006	EDO	O1-C1-C2-O2
4	B	1004	EDO	O1-C1-C2-O2
3	A	1003	P4G	O2-C3-C4-O3
3	B	1002	P4G	O2-C3-C4-O3
2	A	1001	DXU	C1-C2-N2-C21
2	B	1001	DXU	C1-C2-N2-C21
2	B	1001	DXU	N25-C26-C28-C29
2	A	1001	DXU	C3-C2-N2-C21
3	A	1004	P4G	C6-C5-O3-C4
3	A	1003	P4G	C6-C5-O3-C4
4	B	1003	EDO	O1-C1-C2-O2
4	A	1005	EDO	O1-C1-C2-O2
3	A	1004	P4G	C3-C4-O3-C5
3	A	1004	P4G	O3-C5-C6-O4
2	B	1001	DXU	C3-C2-N2-C21

There are no ring outliers.

5 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	P4G	4	0

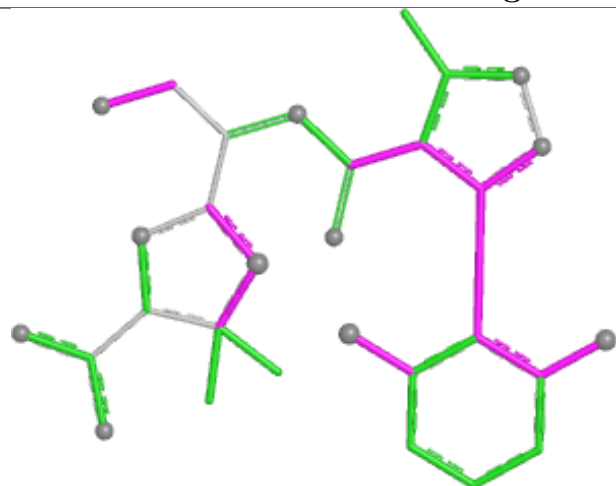
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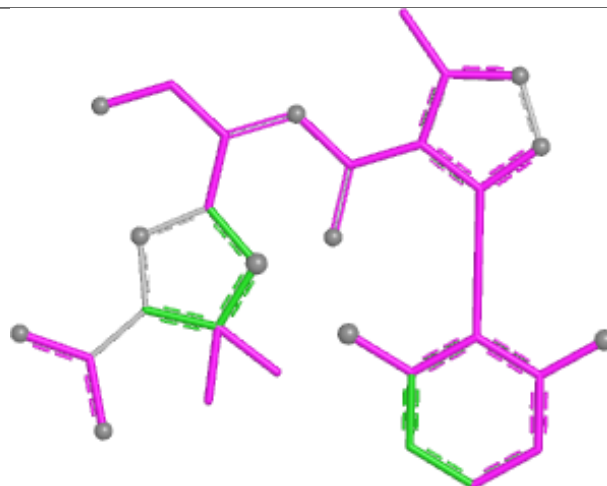
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1004	P4G	1	0
2	A	1001	DXU	12	0
3	A	1003	P4G	1	0
2	B	1001	DXU	13	0

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.

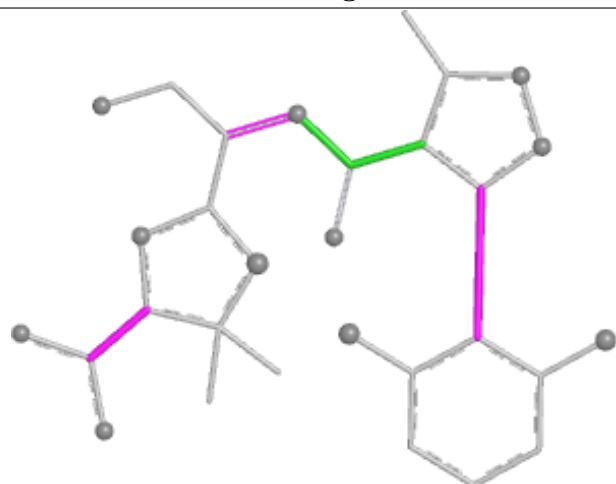
## Ligand DXU A 1001



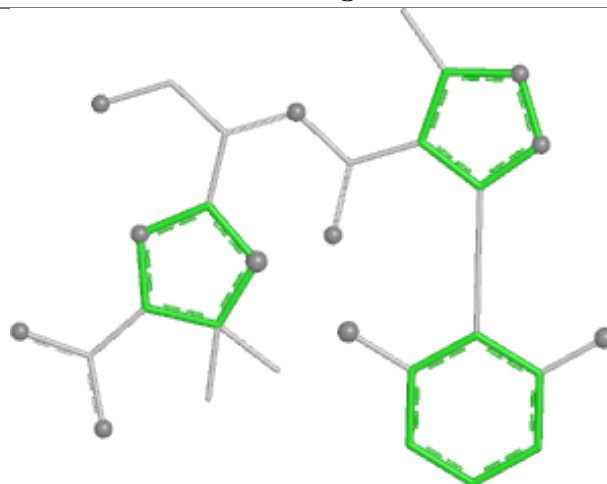
Bond lengths



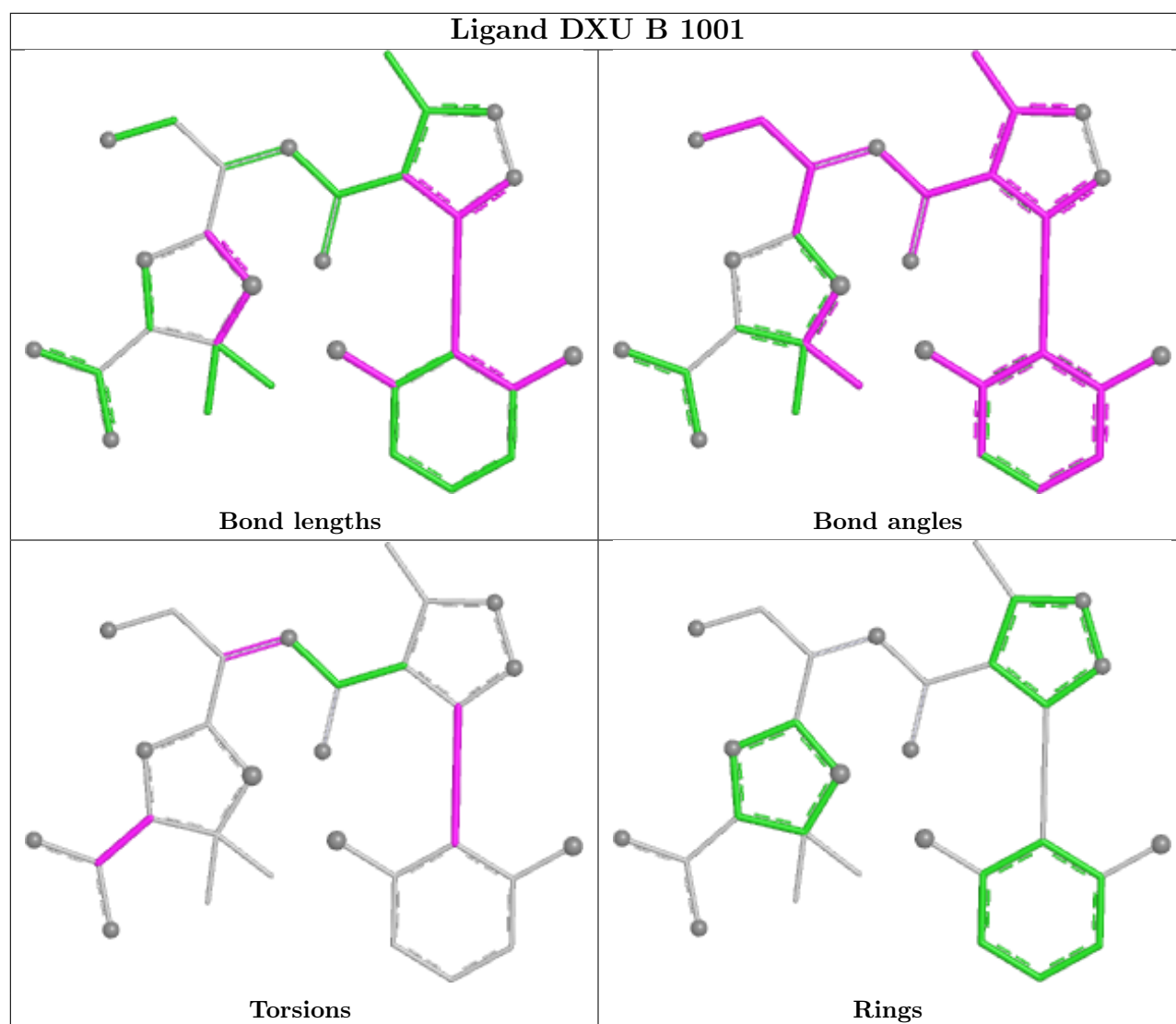
Bond angles



Torsions



Rings



## 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	403/482 (83%)	-0.07	15 (3%)	45 49	18, 34, 74, 113	1 (0%)
1	B	398/482 (82%)	-0.03	15 (3%)	44 48	24, 37, 78, 110	0
All	All	801/964 (83%)	-0.05	30 (3%)	45 49	18, 36, 76, 113	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	660	ILE	5.2
1	B	585	THR	3.7
1	B	950	LEU	3.5
1	A	594	ARG	3.3
1	A	605	THR	3.1
1	B	603	ILE	3.1
1	A	603	ILE	3.1
1	A	587	HIS	3.1
1	B	901	PHE	3.0
1	B	659	THR	3.0
1	A	950	LEU	2.8
1	B	543	VAL	2.8
1	A	585	THR	2.7
1	A	896	VAL	2.7
1	B	551	VAL	2.6
1	B	524	ALA	2.5
1	A	901	PHE	2.5
1	A	543	VAL	2.4
1	A	913	HIS	2.3
1	B	606	THR	2.3
1	A	549	THR	2.1
1	B	523	SER	2.1
1	A	548	GLY	2.1
1	A	895	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	550	TYR	2.1
1	B	594	ARG	2.1
1	B	896	VAL	2.0
1	B	601	ALA	2.0
1	A	526	VAL	2.0
1	B	842	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](#)

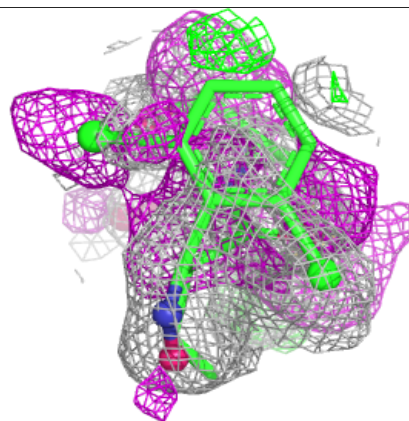
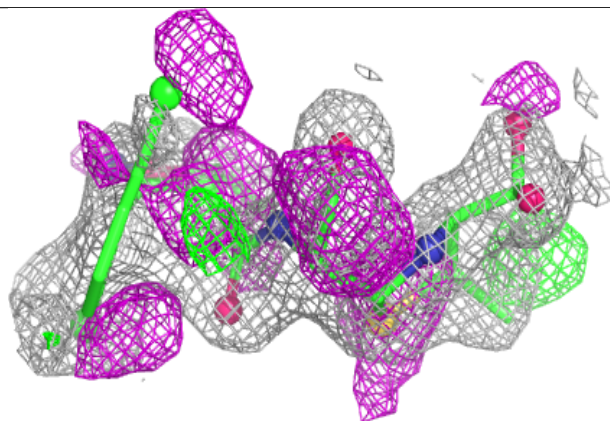
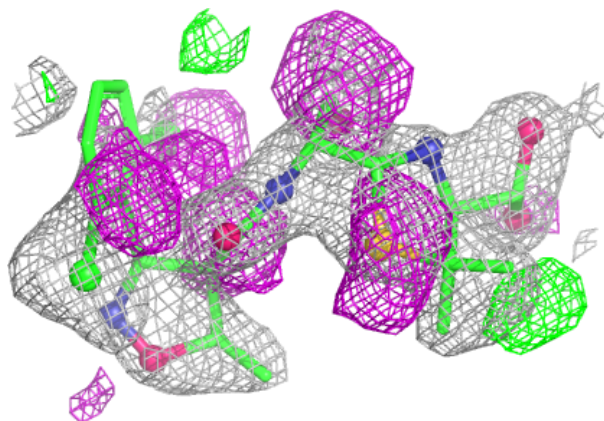
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	DXU	A	1001	30/30	0.79	0.17	35,63,104,108	0
4	EDO	A	1006	4/4	0.80	0.19	62,68,68,71	0
3	P4G	A	1004	7/11	0.81	0.14	60,63,68,73	0
2	DXU	B	1001	30/30	0.85	0.15	36,61,95,107	0
4	EDO	A	1005	4/4	0.86	0.13	69,70,70,76	0
4	EDO	A	1007	4/4	0.86	0.15	62,64,64,66	0
4	EDO	B	1003	4/4	0.87	0.14	67,69,72,73	0
3	P4G	A	1003	7/11	0.89	0.15	57,60,70,73	0
3	P4G	A	1002	7/11	0.89	0.11	35,43,49,50	0
4	EDO	B	1004	4/4	0.91	0.09	44,48,49,55	0
3	P4G	B	1002	4/11	0.92	0.13	46,51,53,60	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 DXU A 1001:**

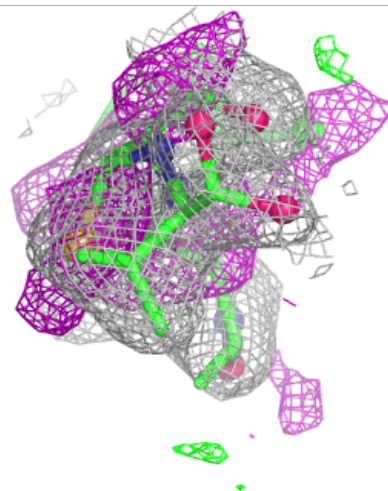
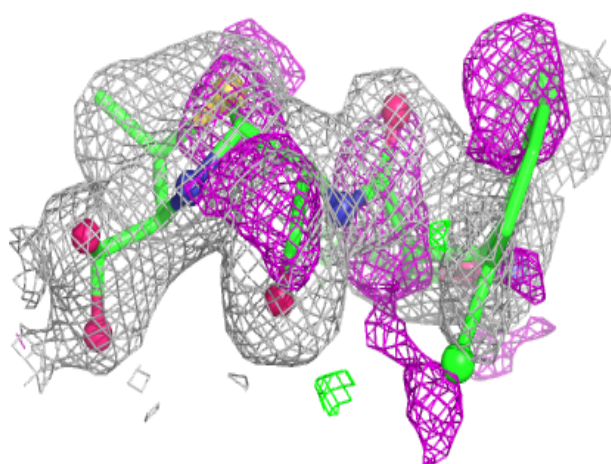
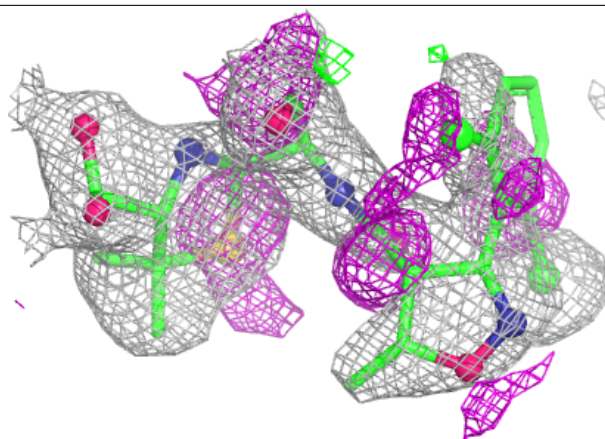
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around DXU B 1001:**

$2mF_o-DF_c$  (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.