



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 05:21 AM EDT

PDB ID : 4R23
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

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>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

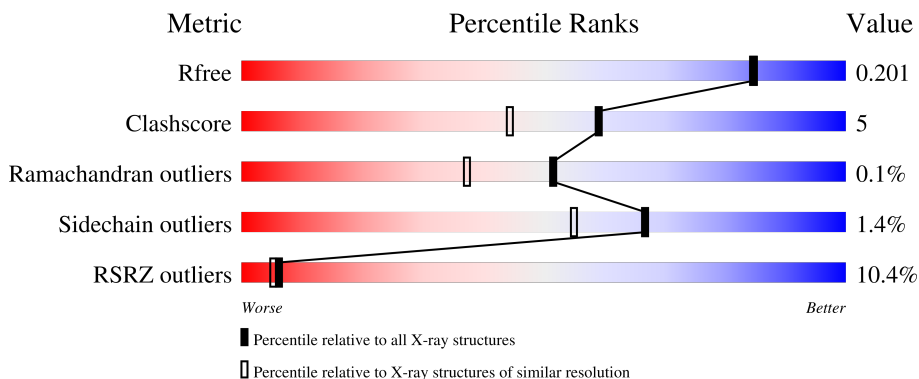
1 Overall quality at a glance

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}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 $\leq 5\%$. 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 i

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
			Total	C	N	O	S	Se			
1	A	416	3000	1864	510	611	2	13	0	1	0
1	B	411	2956	1837	501	603	2	13	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

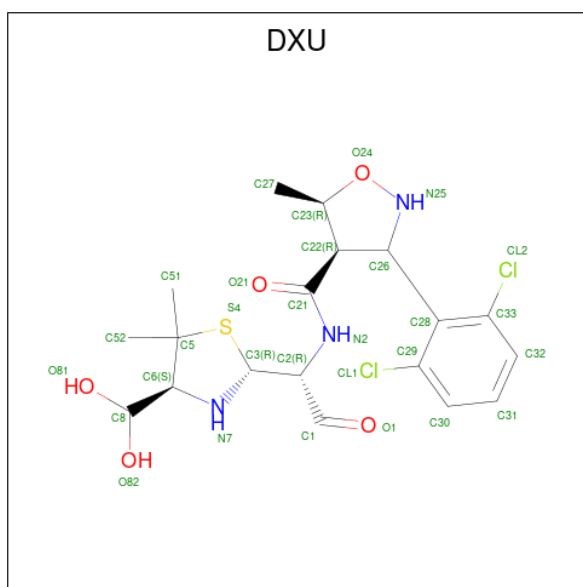
Chain	Residue	Modelled	Actual	Comment	Reference
A	473	MSE	-	expression tag	UNP C8W8H7
A	474	HIS	-	expression tag	UNP C8W8H7
A	475	HIS	-	expression tag	UNP C8W8H7
A	476	HIS	-	expression tag	UNP C8W8H7
A	477	HIS	-	expression tag	UNP C8W8H7
A	478	HIS	-	expression tag	UNP C8W8H7
A	479	HIS	-	expression tag	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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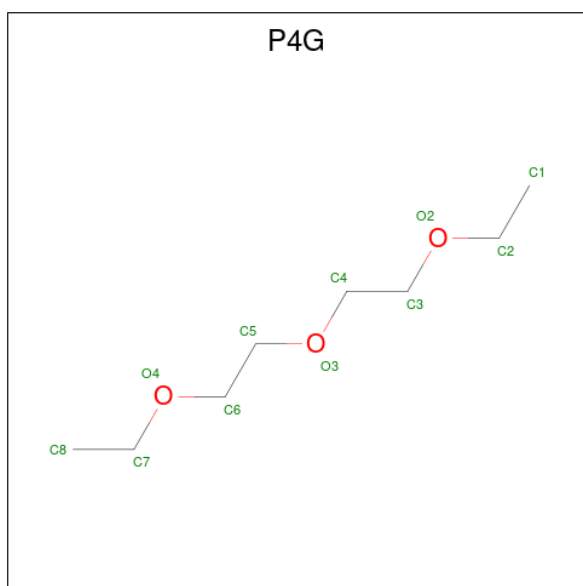
Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	expression tag	UNP C8W8H7
A	499	TYR	-	expression tag	UNP C8W8H7
A	500	PHE	-	expression tag	UNP C8W8H7
A	501	GLN	-	expression tag	UNP C8W8H7
A	502	SER	-	expression tag	UNP C8W8H7
A	503	ASN	-	expression tag	UNP C8W8H7
A	504	ALA	-	expression tag	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 (3R,4R,5R)-3-(2,6-dichlorophenyl)-N-{(1R)-1-[(2R,4S)-4-(dihydroxymethyl)-5,5-dimethyl-1,3-thiazolidin-2-yl]-2-oxoethyl} -5-methyl-1,2-oxazolidine-4-carboxamide (three-letter code: DXU) (formula: C₁₉H₂₅Cl₂N₃O₅S).



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

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



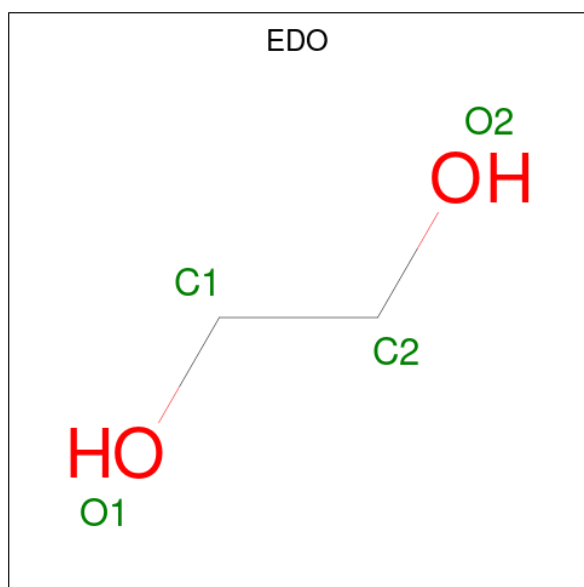
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	7	4	3	0	0

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is water.

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

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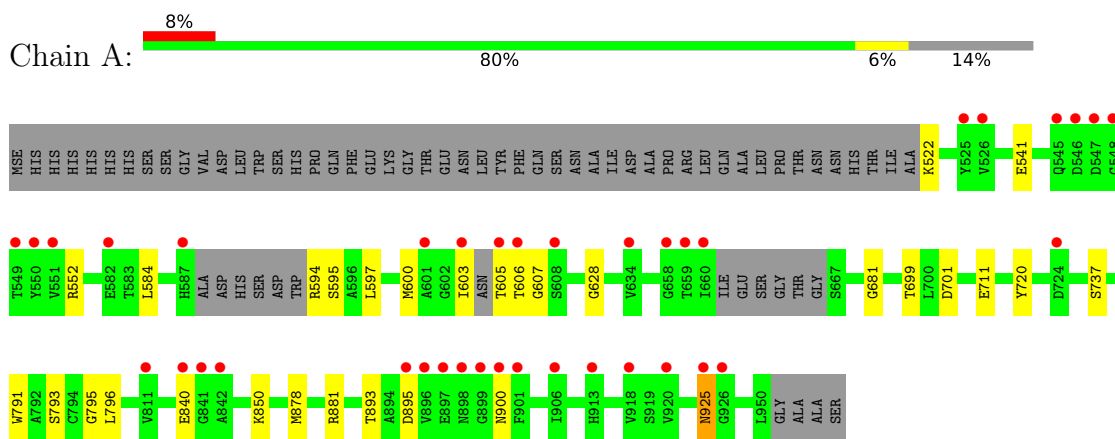
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	214	Total 216	O 216	0	2

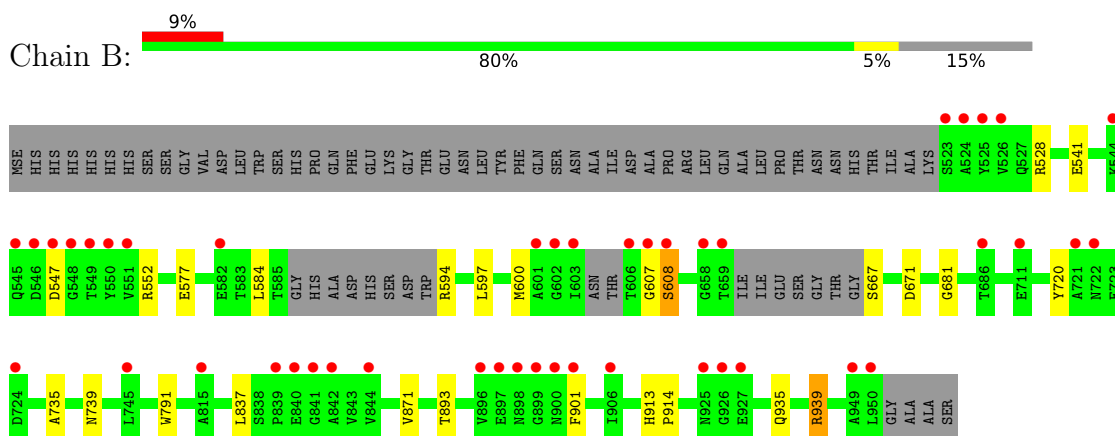
3 Residue-property plots [i](#)

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, α , β , γ	67.61Å 69.88Å 114.25Å 90.00° 96.87° 90.00°	Depositor
Resolution (Å)	30.00 – 1.84 30.05 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-1.84) 98.2 (30.05-1.84)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 1.84Å)	Xtrriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.155 , 0.192 0.166 , 0.201	Depositor DCC
R_{free} test set	4501 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6490	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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.

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, DXU, P4G

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	0.71	1/3037 (0.0%)	0.81	1/4118 (0.0%)
1	B	0.69	0/2992	0.78	1/4058 (0.0%)
All	All	0.70	1/6029 (0.0%)	0.80	2/8176 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	793	SER	CB-OG	-5.88	1.34	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	895	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	671	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3000	0	2931	31	0
1	B	2956	0	2886	23	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	56	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 (56) 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:A:850:LYS:NZ	5:A:1223:HOH:O	2.54	0.40

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.

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%)	47	33
All	All	812/964 (84%)	793 (98%)	18 (2%)	1 (0%)	51	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	547	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/356 (89%)	311 (98%)	6 (2%)	57	42
1	B	312/356 (88%)	309 (99%)	3 (1%)	76	68
All	All	629/712 (88%)	620 (99%)	9 (1%)	67	55

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	737	SER
1	A	796	LEU
1	A	840	GLU
1	A	925	ASN
1	B	608	SER
1	B	901	PHE
1	B	939	ARG

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	EDO	A	1005	-	3,3,3	0.36	0	2,2,2	0.59	0
3	P4G	A	1003	-	6,6,10	0.28	0	5,5,9	0.83	0
4	EDO	A	1006	-	3,3,3	0.41	0	2,2,2	0.68	0
2	DXU	B	1001	1	25,32,32	2.40	6 (24%)	31,48,48	4.35	19 (61%)
3	P4G	A	1002	-	6,6,10	0.49	0	5,5,9	1.11	0
3	P4G	A	1004	-	6,6,10	0.26	0	5,5,9	0.87	0
3	P4G	B	1002	-	3,3,10	0.36	0	2,2,9	0.13	0
4	EDO	B	1003	-	3,3,3	0.48	0	2,2,2	0.60	0
4	EDO	B	1004	-	3,3,3	0.41	0	2,2,2	0.49	0
4	EDO	A	1007	-	3,3,3	0.44	0	2,2,2	0.64	0
2	DXU	A	1001	1	25,32,32	2.34	9 (36%)	31,48,48	4.22	16 (51%)

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	EDO	A	1005	-	-	1/1/1/1	-
3	P4G	A	1003	-	-	2/4/4/8	-
4	EDO	A	1006	-	-	1/1/1/1	-
2	DXU	B	1001	1	1/1/9/13	6/14/50/50	0/3/3/3
3	P4G	A	1002	-	-	2/4/4/8	-
3	P4G	A	1004	-	-	4/4/4/8	-
3	P4G	B	1002	-	-	1/1/1/8	-
4	EDO	B	1003	-	-	1/1/1/1	-
4	EDO	B	1004	-	-	1/1/1/1	-
4	EDO	A	1007	-	-	0/1/1/1	-
2	DXU	A	1001	1	1/1/9/13	6/14/50/50	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	DXU	C26-N25	-6.57	1.32	1.46
2	A	1001	DXU	C26-N25	-6.38	1.32	1.46
2	B	1001	DXU	C29-C28	5.34	1.47	1.39
2	A	1001	DXU	C29-C28	5.29	1.47	1.39
2	B	1001	DXU	C22-C26	-3.77	1.49	1.56
2	B	1001	DXU	C29-CL1	3.74	1.82	1.73
2	A	1001	DXU	C33-CL2	3.62	1.82	1.73
2	A	1001	DXU	C29-CL1	3.58	1.82	1.73
2	B	1001	DXU	C5-S4	-3.56	1.78	1.85
2	A	1001	DXU	C22-C26	-3.40	1.50	1.56
2	B	1001	DXU	C33-CL2	3.21	1.81	1.73
2	A	1001	DXU	C3-S4	-2.65	1.78	1.84
2	A	1001	DXU	C5-S4	-2.57	1.80	1.85
2	A	1001	DXU	O1-C1	2.17	1.28	1.19
2	A	1001	DXU	C22-C21	2.11	1.55	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	DXU	C28-C26-N25	14.47	137.51	111.85
2	B	1001	DXU	C28-C26-N25	13.82	136.36	111.85
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	A	1001	DXU	C2-N2-C21	6.25	129.95	123.12
2	B	1001	DXU	C30-C29-C28	-6.05	114.81	122.39
2	A	1001	DXU	C30-C29-C28	-5.62	115.36	122.39
2	B	1001	DXU	C33-C28-C29	4.94	120.60	114.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	DXU	C28-C33-CL2	4.84	125.17	120.49
2	A	1001	DXU	C33-C28-C29	4.83	120.48	114.91
2	B	1001	DXU	C2-N2-C21	4.74	128.30	123.12
2	B	1001	DXU	C29-C28-C26	-4.15	113.62	122.60
2	A	1001	DXU	C29-C28-C26	-3.94	114.08	122.60
2	A	1001	DXU	O21-C21-C22	3.86	130.76	122.37
2	B	1001	DXU	O21-C21-C22	3.69	130.39	122.37
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	3.36	117.29	109.98
2	B	1001	DXU	C3-C2-N2	3.27	117.12	109.98
2	B	1001	DXU	O1-C1-C2	-3.02	116.41	124.83
2	A	1001	DXU	O1-C1-C2	-2.85	116.88	124.83
2	B	1001	DXU	C22-C21-N2	-2.81	108.12	114.63
2	B	1001	DXU	C51-C5-S4	2.71	113.75	109.21
2	A	1001	DXU	C28-C33-CL2	2.69	123.09	120.49
2	B	1001	DXU	C32-C33-CL2	-2.65	113.09	118.41
2	B	1001	DXU	C26-C22-C21	-2.56	108.98	113.45
2	B	1001	DXU	C31-C30-C29	2.50	123.18	119.39
2	A	1001	DXU	C22-C21-N2	-2.47	108.90	114.63
2	B	1001	DXU	C27-C23-C22	2.46	117.99	114.96
2	A	1001	DXU	C30-C29-CL1	2.46	123.33	118.41
2	A	1001	DXU	C51-C5-C52	-2.22	107.16	110.78
2	A	1001	DXU	O81-C8-O82	2.22	115.17	111.27
2	A	1001	DXU	C31-C30-C29	2.21	122.73	119.39
2	B	1001	DXU	C30-C29-CL1	2.16	122.73	118.41
2	B	1001	DXU	C28-C29-CL1	2.01	122.44	120.49

All (2) chirality outliers are listed below:

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

All (25) 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	N25-C26-C28-C29
2	B	1001	DXU	N7-C6-C8-O82

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Mol	Chain	Res	Type	Atoms
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	A	1001	DXU	C3-C2-N2-C21
2	B	1001	DXU	C1-C2-N2-C21
3	A	1004	P4G	C6-C5-O3-C4
4	B	1003	EDO	O1-C1-C2-O2
3	A	1003	P4G	C6-C5-O3-C4
3	A	1004	P4G	C3-C4-O3-C5
4	A	1005	EDO	O1-C1-C2-O2
3	A	1004	P4G	O3-C5-C6-O4
2	A	1001	DXU	N25-C26-C28-C33
2	B	1001	DXU	N25-C26-C28-C33
2	B	1001	DXU	C3-C2-N2-C21

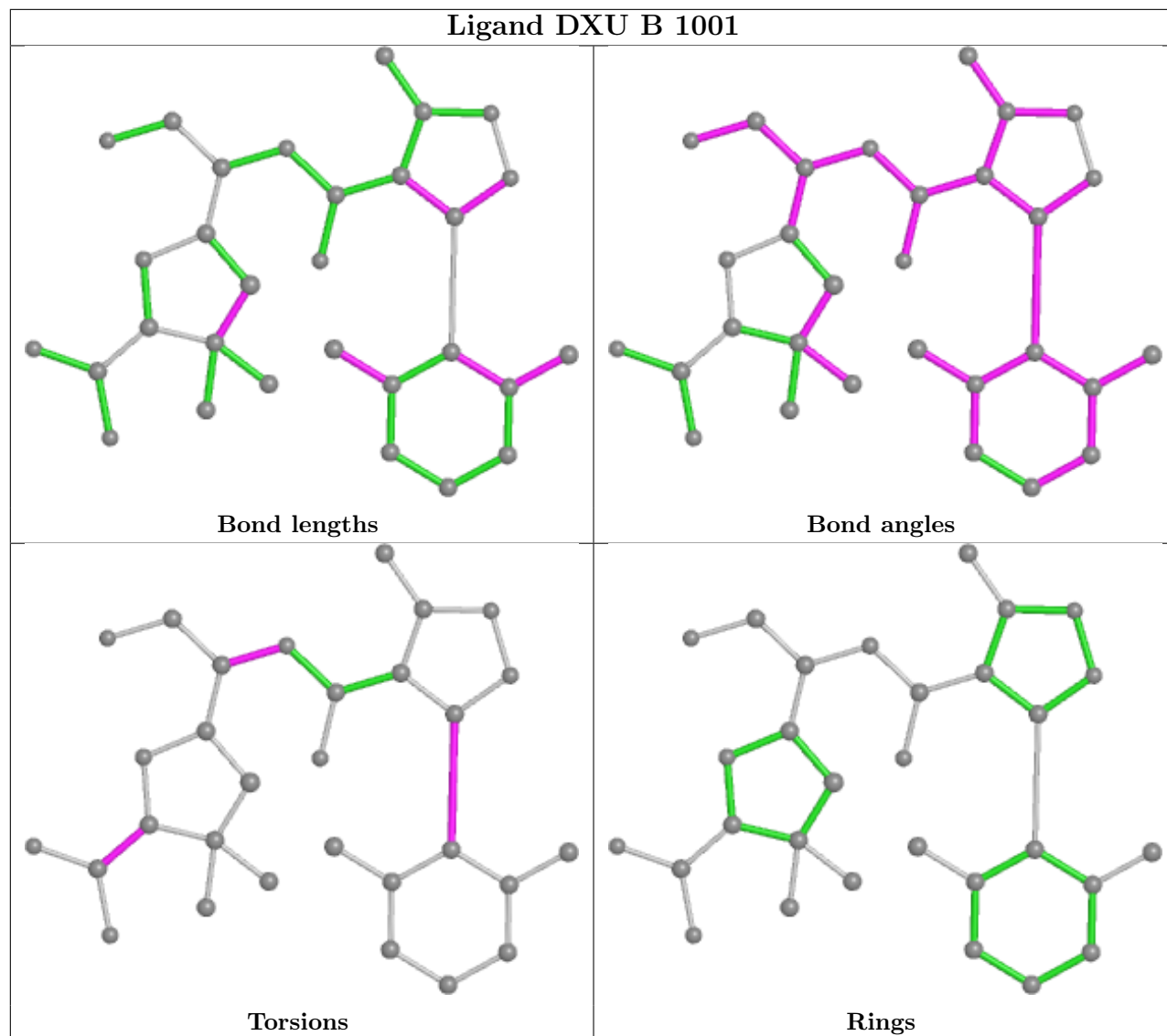
There are no ring outliers.

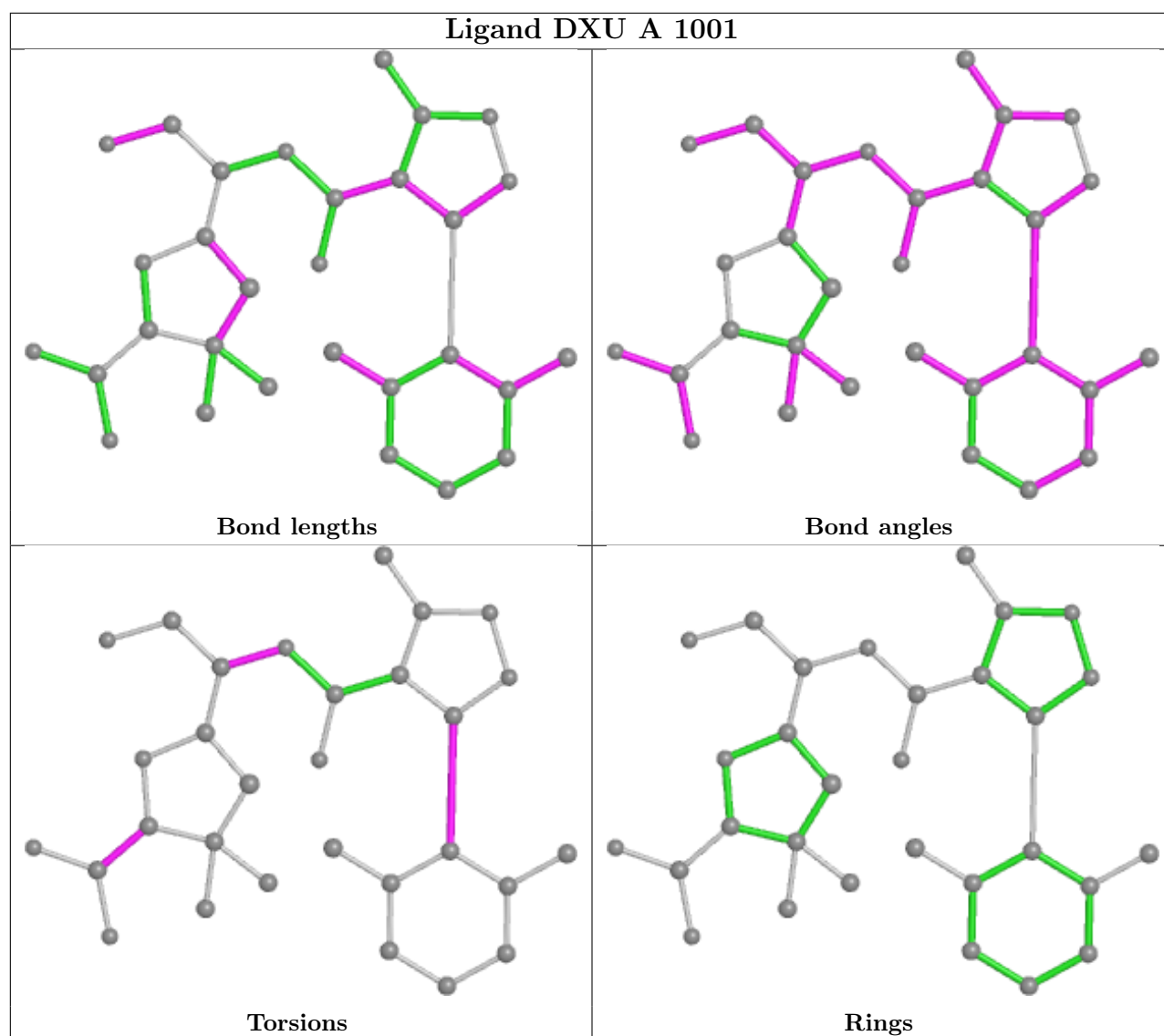
5 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	P4G	1	0
2	B	1001	DXU	13	0
3	A	1002	P4G	4	0
3	A	1004	P4G	1	0
2	A	1001	DXU	12	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, 95th 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 ²)	Q<0.9
1	A	403/482 (83%)	0.27	38 (9%) 8 7	24, 34, 74, 113	0
1	B	398/482 (82%)	0.32	45 (11%) 5 4	24, 37, 78, 110	0
All	All	801/964 (83%)	0.29	83 (10%) 6 5	24, 36, 76, 113	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	898	ASN	7.5
1	A	897	GLU	7.4
1	B	898	ASN	6.4
1	A	587	HIS	5.5
1	A	660	ILE	5.0
1	B	897	GLU	4.8
1	B	550	TYR	4.8
1	B	548	GLY	4.5
1	B	549	THR	4.3
1	B	840	GLU	4.3
1	B	925	ASN	4.0
1	A	548	GLY	3.9
1	B	546	ASP	3.8
1	B	545	GLN	3.8
1	A	546	ASP	3.7
1	A	901	PHE	3.6
1	B	551	VAL	3.6
1	B	525	TYR	3.6
1	A	896	VAL	3.5
1	B	842	ALA	3.5
1	B	658	GLY	3.5
1	A	550	TYR	3.5
1	B	602	GLY	3.4
1	A	551	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	523	SER	3.3
1	B	526	VAL	3.3
1	A	899	GLY	3.3
1	A	549	THR	3.3
1	A	926	GLY	3.3
1	B	841	GLY	3.3
1	A	526	VAL	3.3
1	B	608	SER	3.3
1	B	839	PRO	3.3
1	A	659	THR	3.2
1	A	545	GLN	3.2
1	B	949	ALA	3.2
1	B	900	ASN	3.1
1	A	606	THR	3.0
1	B	603	ILE	2.9
1	A	840	GLU	2.9
1	B	524	ALA	2.8
1	A	658	GLY	2.8
1	A	900	ASN	2.8
1	B	601	ALA	2.6
1	A	918	VAL	2.6
1	A	925	ASN	2.6
1	B	899	GLY	2.6
1	A	906	ILE	2.6
1	B	844	VAL	2.6
1	A	525	TYR	2.5
1	B	547	ASP	2.5
1	B	607	GLY	2.5
1	B	906	ILE	2.5
1	B	544	LYS	2.5
1	B	926	GLY	2.5
1	A	634	VAL	2.4
1	A	608	SER	2.4
1	A	913	HIS	2.4
1	A	601	ALA	2.4
1	B	659	THR	2.4
1	A	605	THR	2.3
1	B	815	ALA	2.3
1	A	920	VAL	2.3
1	A	547	ASP	2.3
1	B	745	LEU	2.3
1	A	895	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	896	VAL	2.3
1	B	606	THR	2.3
1	A	603	ILE	2.2
1	B	582	GLU	2.2
1	B	686	THR	2.2
1	B	711	GLU	2.1
1	B	724	ASP	2.1
1	A	811	VAL	2.1
1	B	721	ALA	2.1
1	B	927	GLU	2.1
1	B	901	PHE	2.1
1	A	841	GLY	2.1
1	B	722	ASN	2.0
1	A	842	ALA	2.0
1	A	724	ASP	2.0
1	B	950	LEU	2.0
1	A	582	GLU	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, 95th 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.

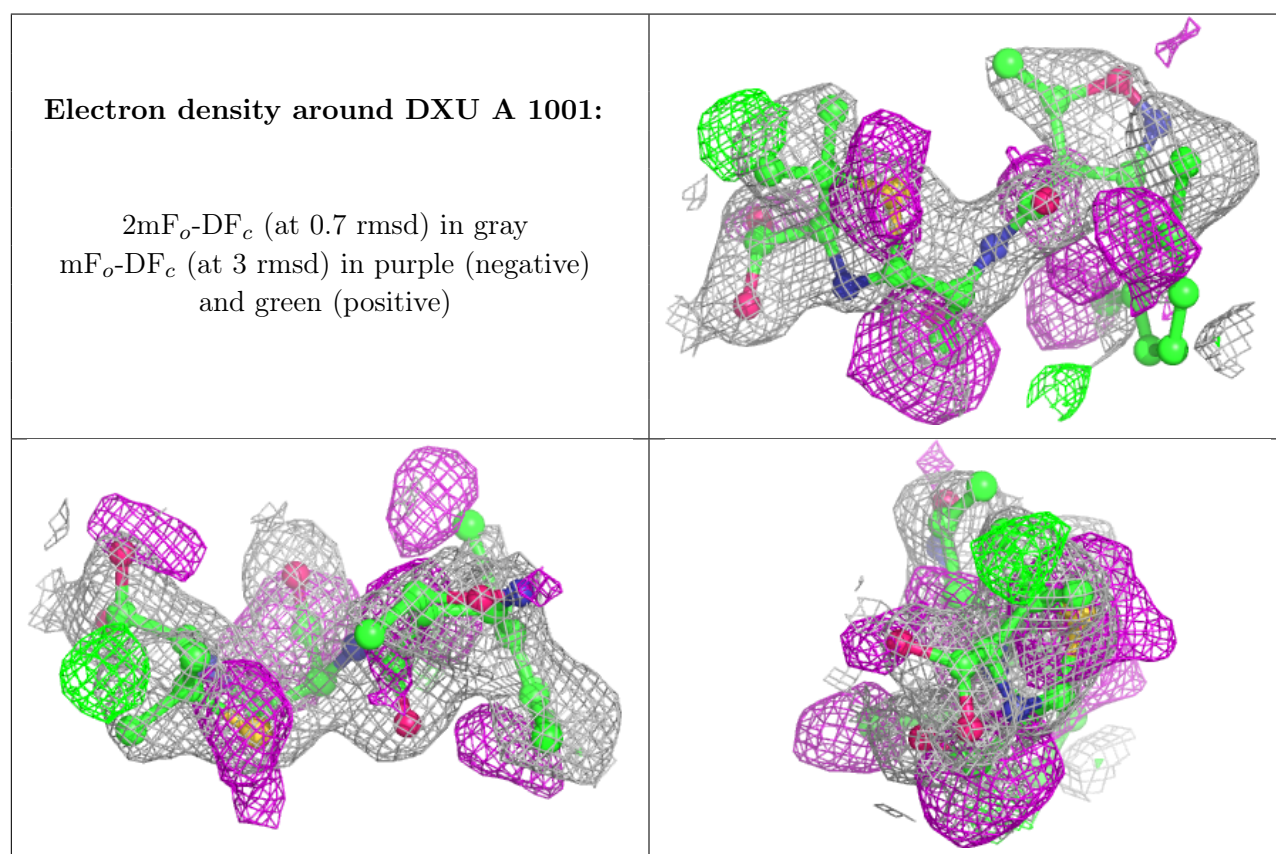
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	1007	4/4	0.77	0.14	62,64,64,66	0
4	EDO	A	1006	4/4	0.81	0.11	62,68,68,71	0
2	DXU	A	1001	30/30	0.83	0.27	35,63,104,108	0
2	DXU	B	1001	30/30	0.84	0.22	36,61,95,107	0
4	EDO	A	1005	4/4	0.86	0.09	69,70,70,76	0
3	P4G	A	1004	7/11	0.87	0.34	60,63,68,73	0

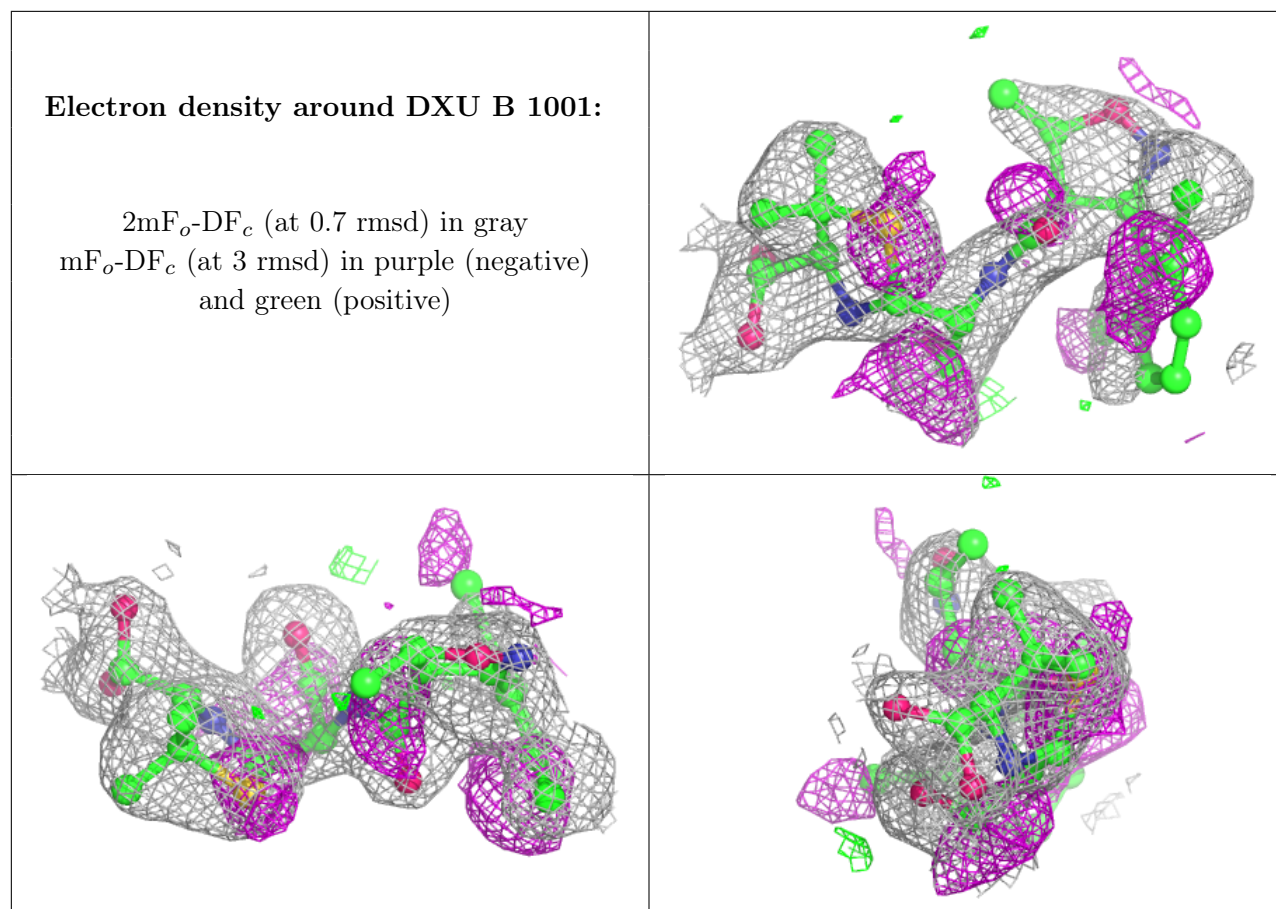
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	P4G	A	1002	7/11	0.87	0.31	35,43,49,50	0
3	P4G	A	1003	7/11	0.88	0.14	57,60,70,73	0
4	EDO	B	1003	4/4	0.90	0.14	67,69,72,73	0
3	P4G	B	1002	4/11	0.95	0.15	46,51,53,60	0
4	EDO	B	1004	4/4	0.95	0.13	44,48,49,55	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.