



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:32 PM UTC

PDB ID : 9S8I / pdb_00009s8i
Title : Crystal Structure of UDP-N-acetylmuramate-L-alanine ligase (MurC) from Pseudomonas aeruginosa in complex with compound OSA_001176 (WYH78)
Authors : Diaz-Saez, L.; Lloyd, A.J.; Wang, Y.; Todd, M.H.; Dowson, C.G.
Deposited on : 2025-08-05
Resolution : 2.30 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 : 4-5-2 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

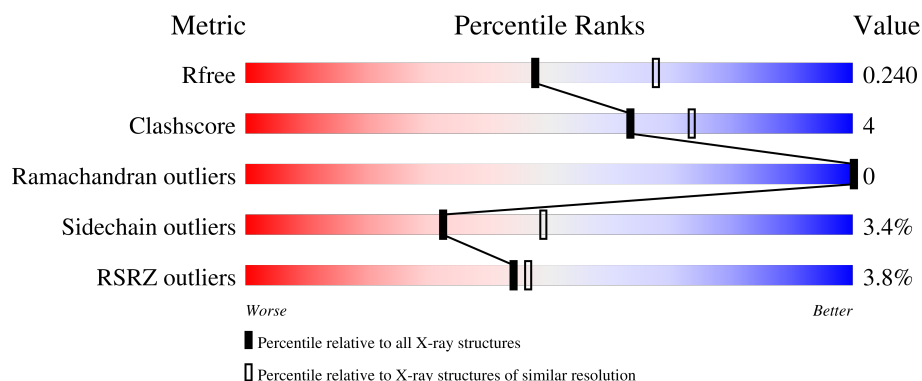
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	487	
1	B	487	

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	WIR	B	501	X	-	-	-
5	EDO	B	508	-	-	-	X
7	DMS	A	514	-	-	X	-
7	DMS	A	516	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7679 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.

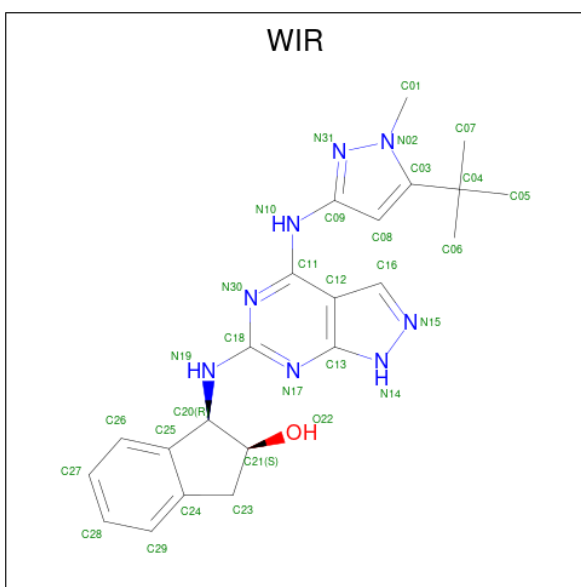
- Molecule 1 is a protein called UDP-N-acetylmuramate--L-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	23	0
			3621	2304	646	655	16			
1	B	452	Total	C	N	O	S	0	9	0
			3529	2234	636	644	15			

There are 14 discrepancies between the modelled and reference sequences:

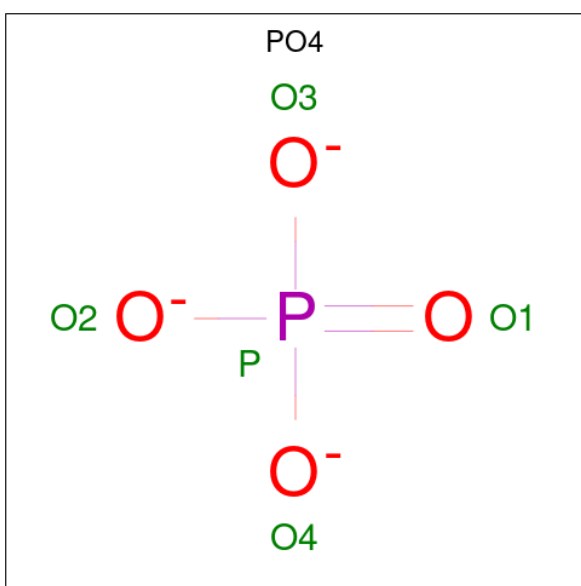
Chain	Residue	Modelled	Actual	Comment	Reference
A	481	ALA	-	expression tag	UNP Q9HW02
A	482	GLU	-	expression tag	UNP Q9HW02
A	483	ASN	-	expression tag	UNP Q9HW02
A	484	LEU	-	expression tag	UNP Q9HW02
A	485	TYR	-	expression tag	UNP Q9HW02
A	486	PHE	-	expression tag	UNP Q9HW02
A	487	GLN	-	expression tag	UNP Q9HW02
B	481	ALA	-	expression tag	UNP Q9HW02
B	482	GLU	-	expression tag	UNP Q9HW02
B	483	ASN	-	expression tag	UNP Q9HW02
B	484	LEU	-	expression tag	UNP Q9HW02
B	485	TYR	-	expression tag	UNP Q9HW02
B	486	PHE	-	expression tag	UNP Q9HW02
B	487	GLN	-	expression tag	UNP Q9HW02

- Molecule 2 is (1R,2S)-1-({4-[(5-tert-butyl-1-methyl-1H-pyrazol-3-yl)amino]-1H-pyrazolo[3,4-d]pyrimidin-6-yl}amino)-2,3-dihydro-1H-inden-2-ol (CCD ID: WIR) (formula: C₂₂H₂₆N₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	22	8	1		
2	B	1	Total	C	N	O	0	0
			31	22	8	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

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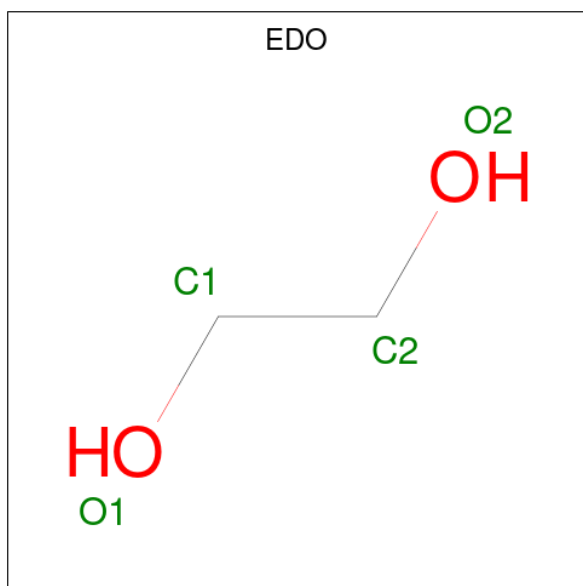
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	X	0	0
			1	1		
4	B	1	Total	X	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



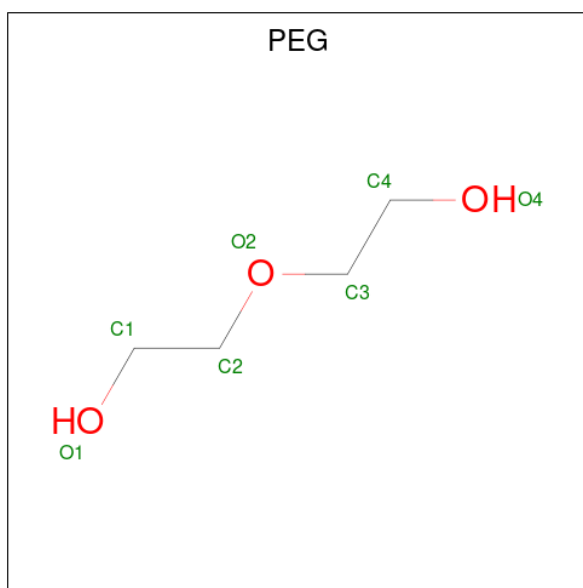
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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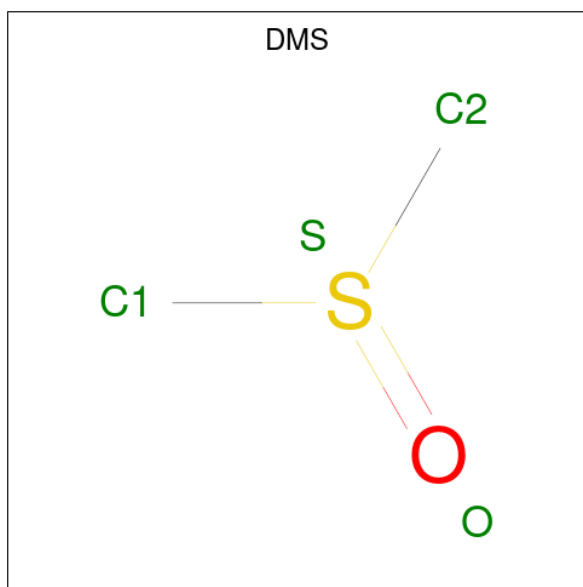
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

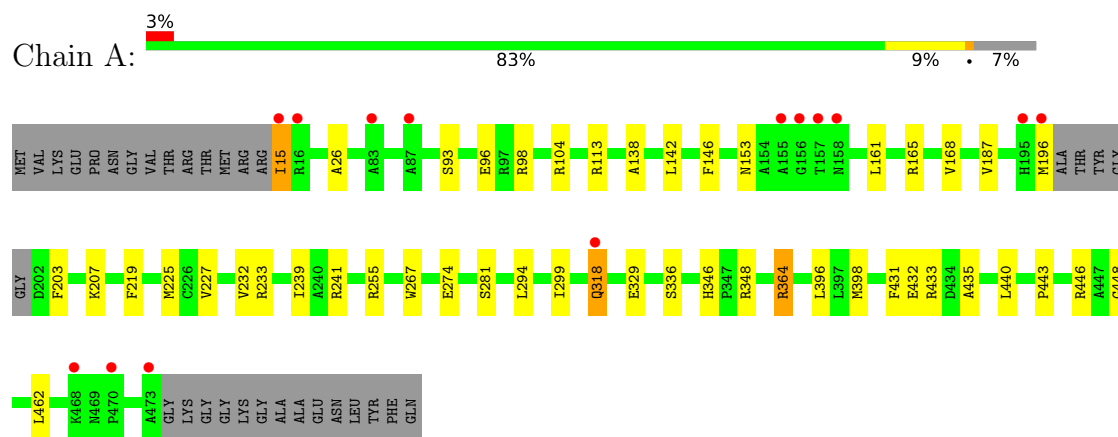
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	204	Total O 204 204	0	0
8	B	149	Total O 149 149	0	0

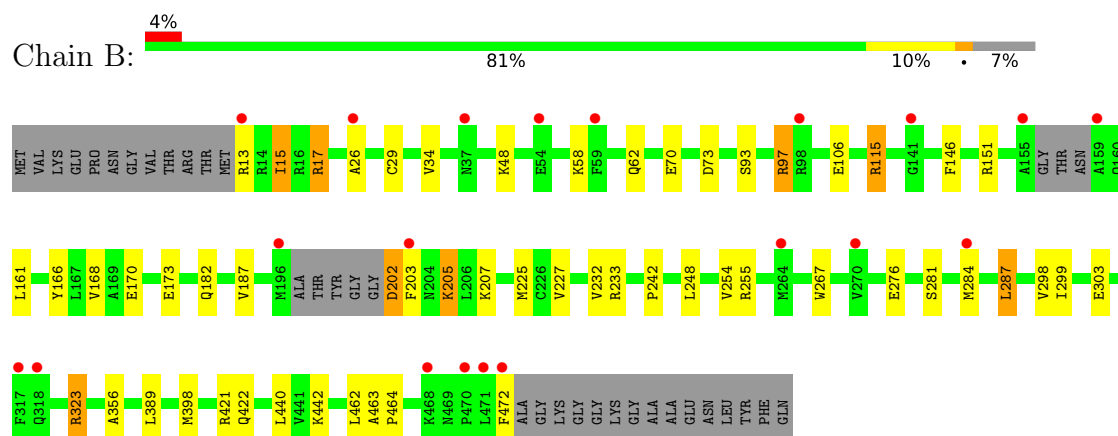
3 Residue-property plots [i](#)

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: 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.58Å 99.11Å 192.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.28 – 2.30 88.28 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (88.28-2.30) 100.0 (88.28-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.188 , 0.239 0.197 , 0.240	Depositor DCC
R_{free} test set	2705 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7679	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, PEG, WIR, EDO, DMS, UNX

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	0.50	0/3759	0.87	0/5097
1	B	0.50	0/3621	0.88	2/4910 (0.0%)
All	All	0.50	0/7380	0.87	2/10007 (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	A	0	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	GLU	CB-CA-C	-5.29	101.18	109.70
1	B	202	ASP	CA-CB-CG	5.07	117.67	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	348	ARG	Sidechain
1	A	364	ARG	Sidechain
1	A	98	ARG	Sidechain
1	B	115	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	13	ARG	Sidechain

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	3621	0	3703	29	0
1	B	3529	0	3574	34	0
2	A	31	0	0	0	0
2	B	31	0	0	1	0
3	A	15	0	0	1	0
3	B	15	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	32	0	48	0	0
5	B	28	0	42	2	0
6	A	14	0	20	0	0
7	A	8	0	12	4	0
8	A	204	0	0	0	0
8	B	149	0	0	4	0
All	All	7679	0	7399	59	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 4.

All (59) 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:26:ALA:O	7:A:514:DMS:H23	1.86	0.75
1:A:364:ARG:HD2	1:A:448:GLY:O	1.88	0.73
1:B:29:CYS:HB2	8:B:714:HOH:O	1.89	0.71
1:B:187:VAL:CG2	1:B:299:ILE:HD11	2.22	0.69
1:A:329:GLU:HG3	1:A:336:SER:HB2	1.74	0.67
1:A:196:MET:HE3	1:A:346[A]:HIS:HE2	1.59	0.66
1:B:173:GLU:OE1	8:B:601:HOH:O	2.13	0.66
1:A:26:ALA:O	7:A:514:DMS:C2	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:MET:HE3	1:A:232:VAL:HG13	1.82	0.61
1:B:323[A]:ARG:HH21	1:B:323[A]:ARG:HG3	1.66	0.61
1:B:151:ARG:HG2	1:B:151:ARG:HH11	1.65	0.61
1:A:398[B]:MET:HE1	1:A:462:LEU:HD11	1.82	0.60
1:B:398:MET:HE1	1:B:462:LEU:HD11	1.83	0.59
1:A:225:MET:HE2	1:A:239[B]:ILE:HD11	1.84	0.59
1:A:26:ALA:O	7:A:514:DMS:O	2.20	0.58
1:B:93:SER:OG	1:B:97:ARG:NH1	2.36	0.58
1:A:318:GLN:H	1:A:318:GLN:CD	2.12	0.57
1:B:187:VAL:HG22	1:B:299:ILE:HD11	1.86	0.57
1:B:421:ARG:HH12	5:B:508:EDO:C2	2.20	0.55
1:B:442:LYS:HG3	1:B:472:PHE:CE1	2.42	0.54
1:B:422[A]:GLN:OE1	8:B:602:HOH:O	2.18	0.53
1:B:146:PHE:HA	1:B:168:VAL:O	2.09	0.53
1:A:113:ARG:NH2	1:B:182:GLN:OE1	2.43	0.52
1:A:146:PHE:HA	1:A:168:VAL:O	2.09	0.52
1:A:255[B]:ARG:HG2	1:A:255[B]:ARG:HH11	1.76	0.51
1:B:225:MET:HE3	1:B:232:VAL:HG13	1.92	0.51
1:A:187:VAL:CG2	1:A:299:ILE:HD11	2.41	0.50
1:A:138:ALA:HA	1:A:142:LEU:O	2.12	0.49
1:A:443:PRO:O	1:A:446[B]:ARG:NH1	2.45	0.49
1:A:398[B]:MET:HE2	1:A:431:PHE:CZ	2.48	0.49
1:B:26:ALA:O	3:B:504:PO4:O3	2.31	0.48
1:B:255:ARG:HH11	1:B:255:ARG:HG2	1.78	0.48
1:B:203:PHE:CZ	1:B:207:LYS:HD2	2.50	0.47
1:A:26:ALA:O	7:A:514:DMS:S	2.73	0.47
1:A:15:ILE:HD11	1:B:242:PRO:HG3	1.96	0.47
1:A:93:SER:O	1:A:96[A]:GLU:HG2	2.15	0.47
1:B:323[A]:ARG:HH21	1:B:323[A]:ARG:CG	2.27	0.46
1:B:248:LEU:HD11	1:B:287:LEU:HD21	1.97	0.46
1:B:421:ARG:HH12	5:B:508:EDO:H22	1.80	0.46
1:A:227[A]:VAL:HG22	1:A:233:ARG:CZ	2.47	0.45
1:A:203:PHE:CE2	1:A:207:LYS:HE3	2.52	0.45
1:A:398[A]:MET:HE2	1:A:433:ARG:HA	1.99	0.44
1:B:17[B]:ARG:NH1	1:B:62:GLN:OE1	2.51	0.43
1:B:166:TYR:OH	1:B:303:GLU:OE2	2.33	0.43
1:B:267:TRP:CE3	1:B:281:SER:HB3	2.54	0.43
1:A:104:ARG:HD3	3:A:503:PO4:O2	2.18	0.43
1:B:202:ASP:HB2	1:B:205:LYS:HG2	2.00	0.42
1:A:267:TRP:CE3	1:A:281:SER:HB3	2.54	0.42
1:B:227:VAL:HG22	1:B:233:ARG:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17[A]:ARG:NH1	1:B:73:ASP:O	2.52	0.42
1:A:219:PHE:HE1	1:B:15:ILE:HD11	1.85	0.42
1:B:97:ARG:O	1:B:97:ARG:HG3	2.19	0.42
1:A:241:ARG:NH1	1:B:106:GLU:OE1	2.48	0.41
1:A:113:ARG:NH2	8:B:612:HOH:O	2.54	0.41
1:A:432[B]:GLU:HG2	1:A:435:ALA:HB2	2.02	0.41
1:B:151:ARG:HG2	1:B:151:ARG:NH1	2.33	0.40
1:B:254:VAL:HG21	1:B:298:VAL:HG22	2.04	0.40
1:B:356:ALA:HA	2:B:501:WIR:C29	2.51	0.40
1:B:463:ALA:N	1:B:464:PRO:CD	2.85	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	473/487 (97%)	465 (98%)	8 (2%)	0	100	100
1	B	455/487 (93%)	446 (98%)	9 (2%)	0	100	100
All	All	928/974 (95%)	911 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	387/387 (100%)	376 (97%)	11 (3%)	38	56
1	B	373/387 (96%)	354 (95%)	19 (5%)	21	32
All	All	760/774 (98%)	730 (96%)	30 (4%)	32	43

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	153[A]	ASN
1	A	153[B]	ASN
1	A	161	LEU
1	A	165[A]	ARG
1	A	165[B]	ARG
1	A	274	GLU
1	A	294	LEU
1	A	318	GLN
1	A	396	LEU
1	A	440	LEU
1	B	15	ILE
1	B	17[A]	ARG
1	B	17[B]	ARG
1	B	34	VAL
1	B	48	LYS
1	B	58	LYS
1	B	70	GLU
1	B	97	ARG
1	B	115	ARG
1	B	161	LEU
1	B	205	LYS
1	B	276[A]	GLU
1	B	276[B]	GLU
1	B	284	MET
1	B	287	LEU
1	B	323[A]	ARG
1	B	323[B]	ARG
1	B	389	LEU
1	B	440	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	160	GLN
1	A	195	HIS
1	A	238	GLN
1	A	258	ASN
1	B	37	ASN
1	B	160	GLN
1	B	195	HIS
1	B	261	GLN
1	B	289	ASN
1	B	292	ASN
1	B	418	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](#)

Of 29 ligands modelled in this entry, 2 are unknown - leaving 27 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	$\# Z > 2$
5	EDO	A	509	-	3,3,3	0.08	0	2,2,2	0.19	0
5	EDO	B	511	-	3,3,3	0.05	0	2,2,2	0.17	0
6	PEG	A	507	-	6,6,6	0.21	0	5,5,5	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	B	503	-	4,4,4	0.78	0	6,6,6	0.46	0
3	PO4	A	503	-	4,4,4	0.61	0	6,6,6	0.49	0
5	EDO	A	508	-	3,3,3	0.13	0	2,2,2	0.21	0
3	PO4	A	504	-	4,4,4	0.85	0	6,6,6	0.43	0
5	EDO	A	512	-	3,3,3	0.13	0	2,2,2	0.16	0
3	PO4	B	504	-	4,4,4	0.98	0	6,6,6	0.45	0
2	WIR	A	501	-	35,35,35	3.46	14 (40%)	45,53,53	3.72	15 (33%)
5	EDO	B	507	-	3,3,3	0.07	0	2,2,2	0.14	0
5	EDO	A	511	-	3,3,3	0.13	0	2,2,2	0.09	0
5	EDO	A	506	-	3,3,3	0.12	0	2,2,2	0.38	0
5	EDO	B	509	-	3,3,3	0.07	0	2,2,2	0.14	0
7	DMS	A	516	-	3,3,3	0.19	0	3,3,3	0.16	0
5	EDO	B	512	-	3,3,3	0.13	0	2,2,2	0.13	0
5	EDO	B	510	-	3,3,3	0.15	0	2,2,2	0.10	0
5	EDO	A	510	-	3,3,3	0.09	0	2,2,2	0.02	0
5	EDO	A	515	-	3,3,3	0.04	0	2,2,2	0.10	0
5	EDO	A	513	-	3,3,3	0.17	0	2,2,2	0.11	0
5	EDO	B	508	-	3,3,3	0.06	0	2,2,2	0.12	0
2	WIR	B	501	-	35,35,35	3.28	14 (40%)	45,53,53	3.92	17 (37%)
3	PO4	A	502	-	4,4,4	0.85	0	6,6,6	0.52	0
6	PEG	A	517	-	6,6,6	0.15	0	5,5,5	0.10	0
3	PO4	B	502	-	4,4,4	0.72	0	6,6,6	0.47	0
7	DMS	A	514	-	3,3,3	0.26	0	3,3,3	0.27	0
5	EDO	B	506	-	3,3,3	0.17	0	2,2,2	0.05	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
5	EDO	A	509	-	-	1/1/1/1	-
5	EDO	B	511	-	-	1/1/1/1	-
6	PEG	A	507	-	-	1/4/4/4	-
5	EDO	A	508	-	-	0/1/1/1	-
5	EDO	A	512	-	-	1/1/1/1	-
2	WIR	A	501	-	-	0/14/32/32	0/5/5/5
5	EDO	B	507	-	-	1/1/1/1	-
5	EDO	A	511	-	-	1/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
5	EDO	B	509	-	-	0/1/1/1	-
5	EDO	B	512	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	510	-	-	0/1/1/1	-
5	EDO	A	510	-	-	1/1/1/1	-
5	EDO	A	515	-	-	1/1/1/1	-
5	EDO	A	513	-	-	1/1/1/1	-
5	EDO	B	508	-	-	0/1/1/1	-
2	WIR	B	501	-	1/1/3/7	3/14/32/32	0/5/5/5
6	PEG	A	517	-	-	0/4/4/4	-
5	EDO	B	506	-	-	0/1/1/1	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	WIR	C21-C20	-13.43	1.41	1.55
2	B	501	WIR	C21-C20	-11.18	1.43	1.55
2	A	501	WIR	C23-C24	-7.21	1.38	1.50
2	A	501	WIR	C12-C16	-6.10	1.35	1.42
2	B	501	WIR	C12-C16	-6.05	1.35	1.42
2	B	501	WIR	C23-C24	-6.00	1.40	1.50
2	B	501	WIR	C26-C25	-5.84	1.32	1.39
2	B	501	WIR	C12-C13	-5.39	1.34	1.41
2	A	501	WIR	C12-C13	-5.18	1.34	1.41
2	A	501	WIR	C25-C20	-4.69	1.37	1.50
2	B	501	WIR	C29-C24	-4.62	1.32	1.39
2	B	501	WIR	C25-C20	-4.37	1.38	1.50
2	A	501	WIR	C12-C11	-3.75	1.37	1.42
2	B	501	WIR	C12-C11	-3.66	1.37	1.42
2	A	501	WIR	C26-C25	-3.57	1.35	1.39
2	B	501	WIR	C18-N19	-3.27	1.30	1.34
2	A	501	WIR	C29-C24	-3.23	1.34	1.39
2	B	501	WIR	C08-C09	-3.18	1.34	1.40
2	A	501	WIR	C08-C09	-2.87	1.35	1.40
2	B	501	WIR	N14-N15	-2.75	1.34	1.36
2	A	501	WIR	N14-N15	-2.73	1.34	1.36
2	A	501	WIR	C04-C03	2.66	1.57	1.52
2	A	501	WIR	C11-N10	-2.60	1.33	1.39
2	B	501	WIR	C24-C25	-2.51	1.35	1.39
2	A	501	WIR	C24-C25	-2.47	1.35	1.39
2	B	501	WIR	C04-C03	2.38	1.57	1.52
2	A	501	WIR	C16-N15	2.28	1.33	1.32
2	B	501	WIR	C16-N15	2.27	1.33	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	WIR	C13-N14-N15	-16.91	107.30	111.26
2	A	501	WIR	C13-N14-N15	-14.50	107.87	111.26
2	A	501	WIR	C25-C20-C21	10.42	110.09	102.48
2	B	501	WIR	C12-C13-N17	-9.09	119.43	127.10
2	A	501	WIR	C12-C13-N17	-8.83	119.65	127.10
2	B	501	WIR	C12-C13-N14	7.52	110.48	107.21
2	B	501	WIR	C25-C20-C21	7.01	107.60	102.48
2	A	501	WIR	C08-C09-N31	-6.95	107.37	112.34
2	A	501	WIR	N14-C13-N17	6.73	131.18	125.64
2	B	501	WIR	C08-C09-N31	-5.85	108.15	112.34
2	B	501	WIR	N14-C13-N17	5.40	130.08	125.64
2	B	501	WIR	C23-C21-C20	-4.97	99.02	103.70
2	B	501	WIR	N19-C18-N30	4.41	124.02	117.09
2	B	501	WIR	C03-N02-N31	-4.36	107.82	112.48
2	A	501	WIR	C12-C13-N14	4.31	109.08	107.21
2	A	501	WIR	C03-N02-N31	-3.99	108.21	112.48
2	B	501	WIR	C25-C20-N19	3.81	126.08	114.56
2	A	501	WIR	C25-C20-N19	3.75	125.90	114.56
2	A	501	WIR	N30-C18-N17	-3.70	120.20	126.26
2	B	501	WIR	C24-C25-C20	-3.27	105.30	110.12
2	B	501	WIR	N30-C18-N17	-3.05	121.27	126.26
2	A	501	WIR	C13-C12-C16	3.00	105.87	104.25
2	A	501	WIR	C12-C16-N15	-2.84	110.15	111.34
2	B	501	WIR	O22-C21-C20	-2.59	102.61	110.00
2	B	501	WIR	C24-C23-C21	-2.45	101.19	103.43
2	A	501	WIR	C01-N02-C03	2.18	132.07	128.80
2	B	501	WIR	C27-C28-C29	-2.15	117.59	120.24
2	B	501	WIR	C01-N02-C03	2.12	131.98	128.80
2	B	501	WIR	C26-C25-C20	2.11	132.70	129.17
2	A	501	WIR	C04-C03-N02	-2.06	123.42	125.72
2	A	501	WIR	C28-C27-C26	-2.03	117.74	120.24
2	A	501	WIR	C18-N30-C11	2.02	121.32	116.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	501	WIR	C20

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	WIR	N17-C18-N19-C20
2	B	501	WIR	N30-C18-N19-C20

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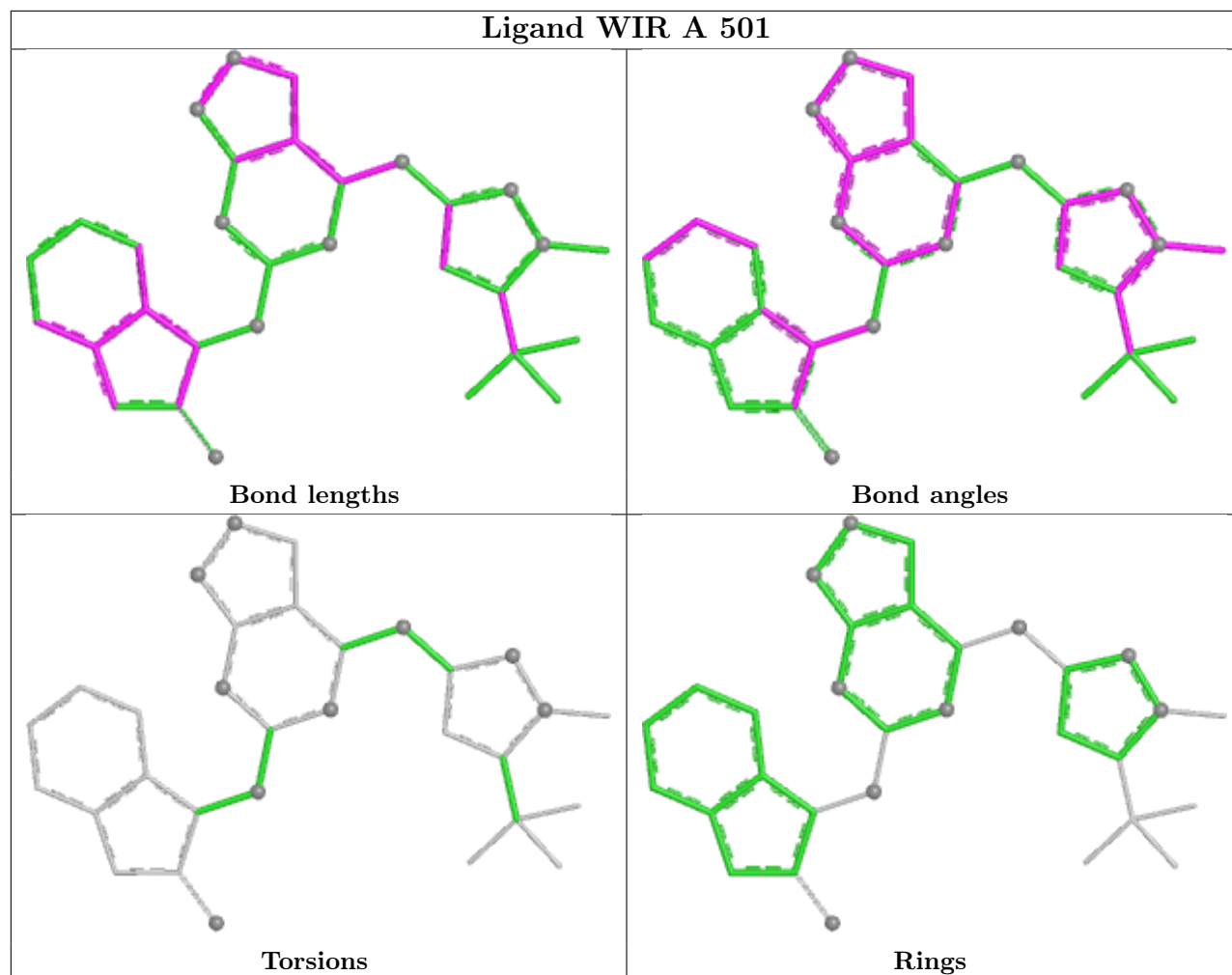
Mol	Chain	Res	Type	Atoms
6	A	507	PEG	O2-C3-C4-O4
5	A	509	EDO	O1-C1-C2-O2
5	A	510	EDO	O1-C1-C2-O2
5	A	515	EDO	O1-C1-C2-O2
5	A	511	EDO	O1-C1-C2-O2
5	A	513	EDO	O1-C1-C2-O2
2	B	501	WIR	C25-C20-N19-C18
5	A	512	EDO	O1-C1-C2-O2
5	B	507	EDO	O1-C1-C2-O2
5	B	511	EDO	O1-C1-C2-O2

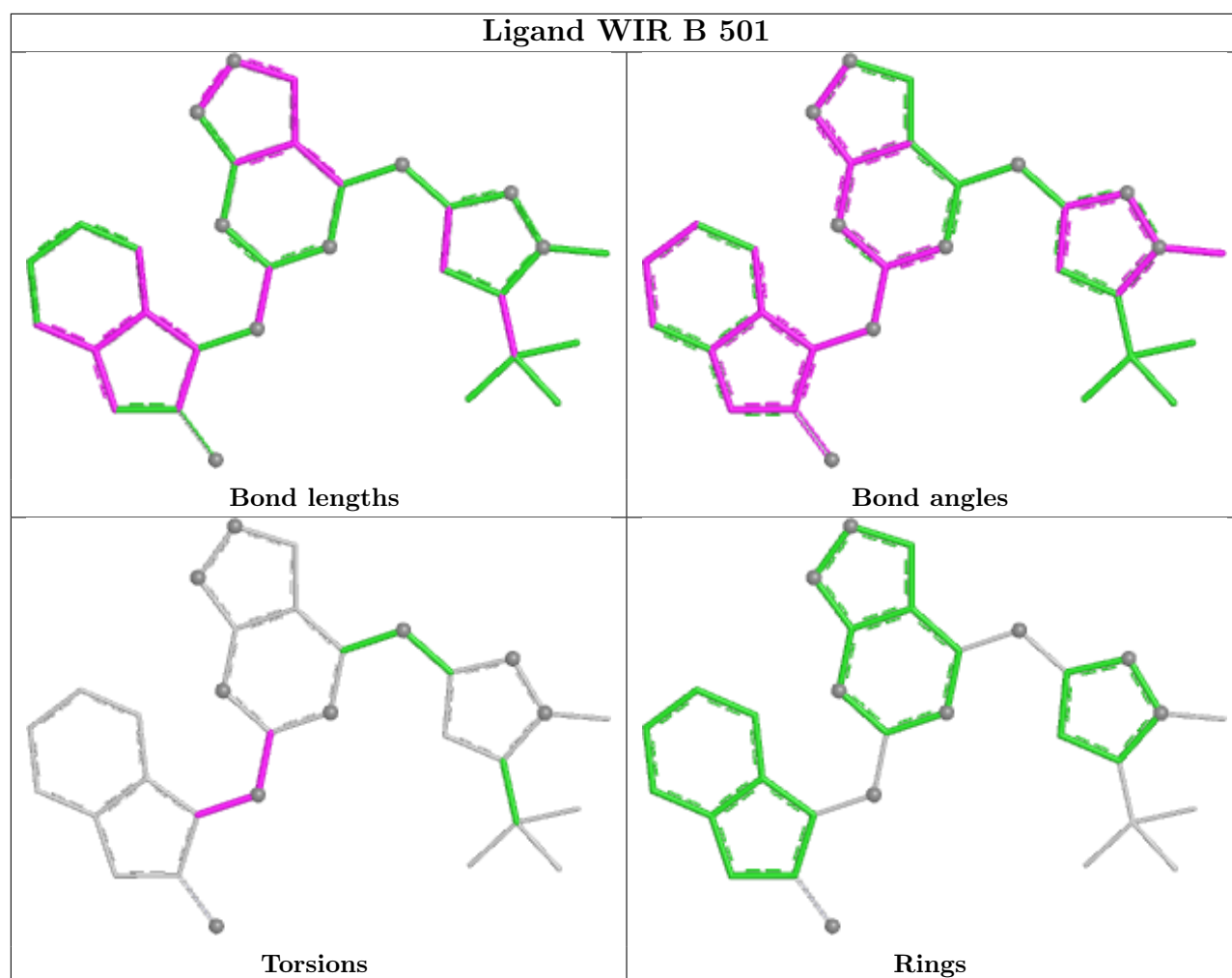
There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	PO4	1	0
3	B	504	PO4	1	0
5	B	508	EDO	2	0
2	B	501	WIR	1	0
7	A	514	DMS	4	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	454/487 (93%)	0.08	14 (3%)	51 53	19, 40, 69, 105	24 (5%)
1	B	452/487 (92%)	0.46	20 (4%)	39 41	21, 48, 81, 105	9 (1%)
All	All	906/974 (93%)	0.27	34 (3%)	44 46	19, 44, 76, 105	33 (3%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	155	ALA	5.4
1	B	159	ALA	4.5
1	A	155	ALA	3.8
1	A	196	MET	3.7
1	B	196	MET	3.5
1	B	203	PHE	3.5
1	A	473	ALA	3.3
1	B	472	PHE	3.3
1	A	156	GLY	3.2
1	B	13	ARG	3.1
1	B	470	PRO	3.0
1	A	16[A]	ARG	2.8
1	B	317	PHE	2.8
1	A	157	THR	2.7
1	A	158	ASN	2.7
1	B	141	GLY	2.5
1	B	284	MET	2.4
1	B	98	ARG	2.4
1	B	471	LEU	2.4
1	B	468[A]	LYS	2.4
1	B	318	GLN	2.4
1	A	468[A]	LYS	2.3
1	A	195	HIS	2.3
1	B	59	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	87	ALA	2.2
1	B	270	VAL	2.2
1	B	37	ASN	2.2
1	B	264	MET	2.2
1	B	26	ALA	2.2
1	B	54	GLU	2.1
1	A	15	ILE	2.1
1	A	470	PRO	2.1
1	A	83	ALA	2.0
1	A	318	GLN	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 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, 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(Å ²)	Q<0.9
5	EDO	A	510	4/4	0.66	0.21	77,80,80,90	0
7	DMS	A	516	4/4	0.71	0.40	48,52,57,60	4
7	DMS	A	514	4/4	0.74	0.32	28,32,34,51	4
5	EDO	B	508	4/4	0.77	0.41	40,44,45,50	4
6	PEG	A	517	7/7	0.80	0.20	74,82,91,96	0
5	EDO	B	507	4/4	0.81	0.18	66,66,70,70	0
3	PO4	A	504	5/5	0.82	0.11	65,73,79,86	0
5	EDO	A	513	4/4	0.84	0.16	51,54,56,58	0
6	PEG	A	507	7/7	0.85	0.20	59,75,83,84	0
5	EDO	A	509	4/4	0.87	0.19	71,74,74,79	0
3	PO4	B	503	5/5	0.88	0.16	37,40,45,52	5
3	PO4	B	504	5/5	0.89	0.14	41,42,45,49	5
5	EDO	A	515	4/4	0.90	0.18	61,61,66,78	0

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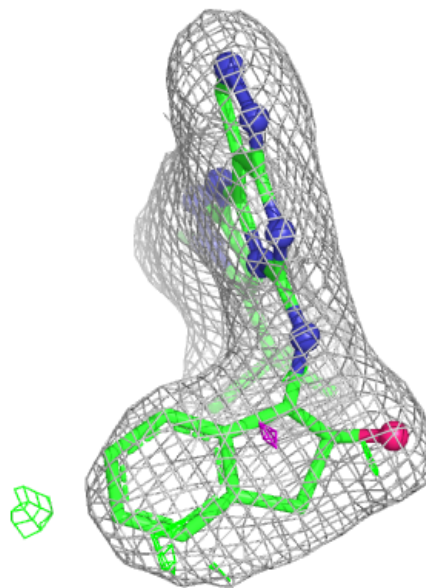
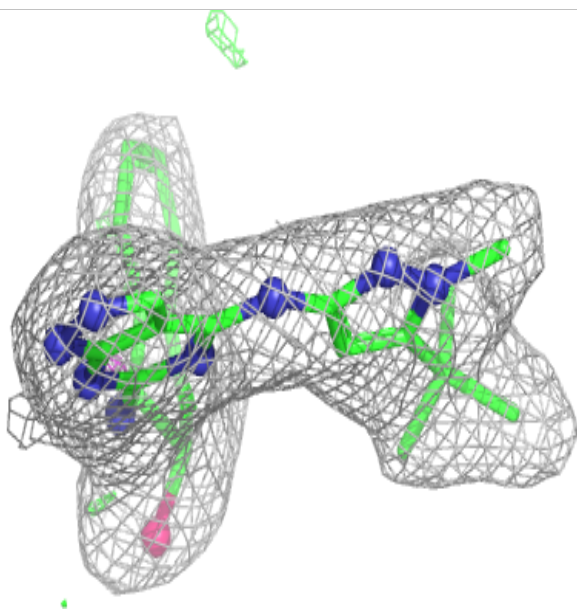
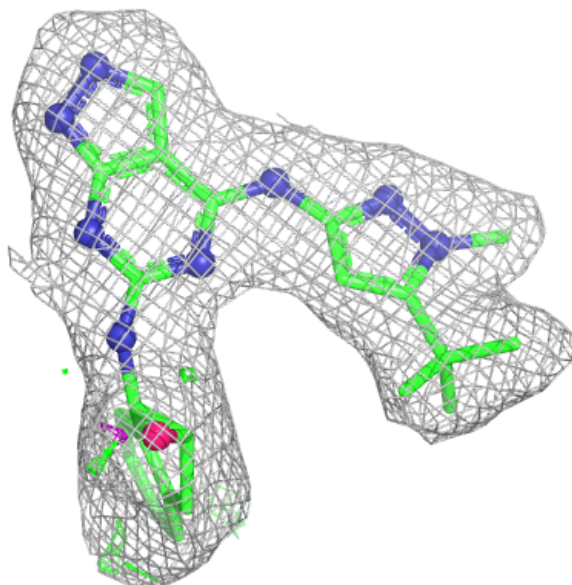
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	508	4/4	0.91	0.19	38,54,58,70	0
5	EDO	B	512	4/4	0.91	0.12	46,50,55,68	0
5	EDO	B	510	4/4	0.92	0.25	48,49,49,55	0
5	EDO	B	511	4/4	0.93	0.12	45,46,48,57	0
3	PO4	A	503	5/5	0.94	0.18	54,63,69,70	0
5	EDO	B	506	4/4	0.94	0.09	38,39,40,45	0
5	EDO	A	511	4/4	0.94	0.15	36,48,48,62	0
5	EDO	A	512	4/4	0.94	0.12	39,40,50,55	0
5	EDO	B	509	4/4	0.94	0.08	44,46,50,59	0
2	WIR	B	501	31/31	0.94	0.09	30,39,68,69	0
4	UNX	B	505	1/1	0.96	0.13	18,18,18,18	0
5	EDO	A	506	4/4	0.96	0.07	31,35,35,36	0
3	PO4	A	502	5/5	0.96	0.12	39,53,55,76	0
3	PO4	B	502	5/5	0.96	0.09	44,46,46,59	0
2	WIR	A	501	31/31	0.98	0.05	21,28,37,40	0
4	UNX	A	505	1/1	0.99	0.11	8,8,8,8	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.

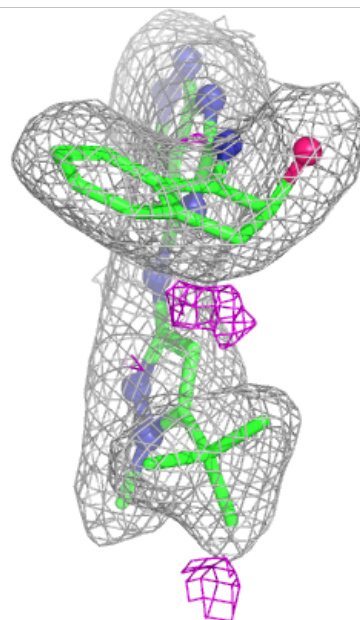
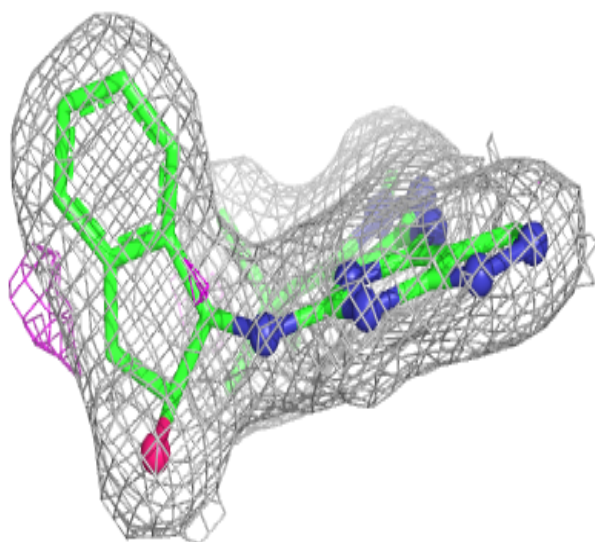
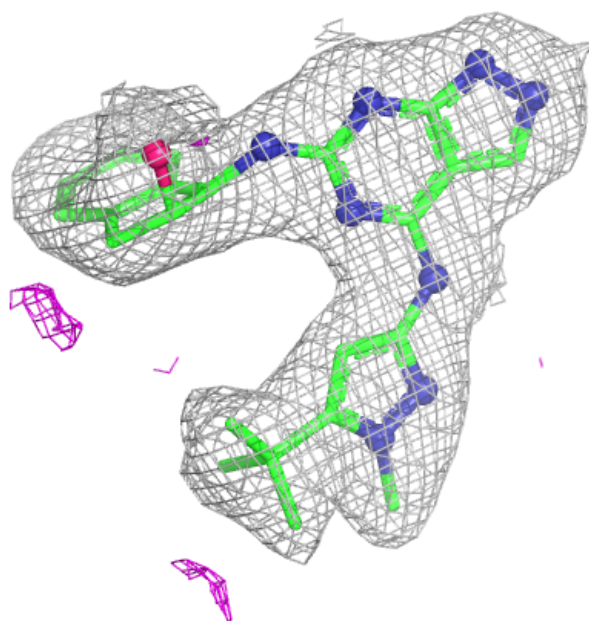
Electron density around WIR B 501:

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



Electron density around WIR A 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.