



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2025 – 01:24 pm BST

PDB ID : 9FMP / pdb_00009fmp
Title : Crystal structure of phosphorylated C. merolae LAMMER-like dual specificity kinase (CmLIK) kinase domain in complex with adenosine
Authors : Dimos-Roehl, B.; Haltenhof, T.; Kotte, A.; Heyd, F.; Loll, B.
Deposited on : 2024-06-06
Resolution : 2.69 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 Phenix2.0rc1
Mogul : 1.8.4, 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 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

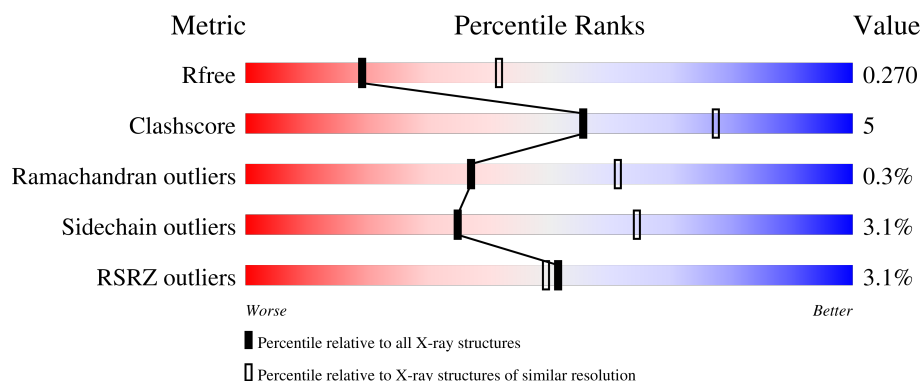
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


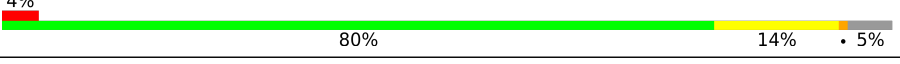
The reported resolution of this entry is 2.69 Å.

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	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	376	 2% 82% 14% •
2	B	376	 4% 80% 14% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6036 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 LAMMER-like dual specificity kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	361	2920	1857	539	509	15	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	GLY	-	expression tag	UNP M1UWB5
A	441	PRO	-	expression tag	UNP M1UWB5
A	442	LEU	-	expression tag	UNP M1UWB5
A	443	GLY	-	expression tag	UNP M1UWB5
A	444	SER	-	expression tag	UNP M1UWB5
A	445	PRO	-	expression tag	UNP M1UWB5
A	446	GLU	-	expression tag	UNP M1UWB5
A	447	PHE	-	expression tag	UNP M1UWB5

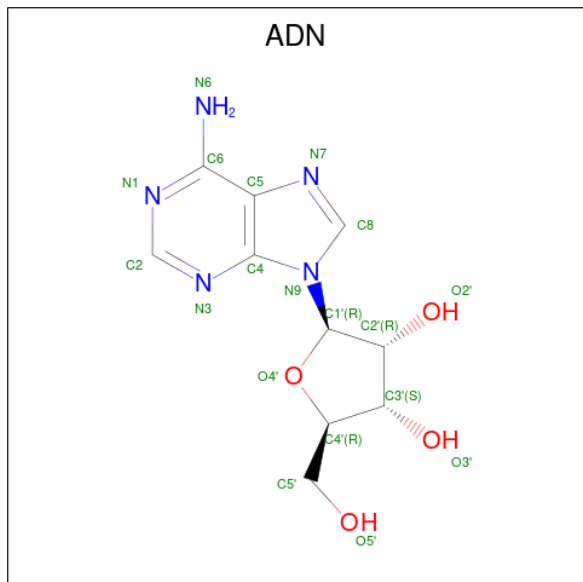
- Molecule 2 is a protein called LAMMER-like dual specificity kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	B	357	2878	1828	531	503	1	15	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

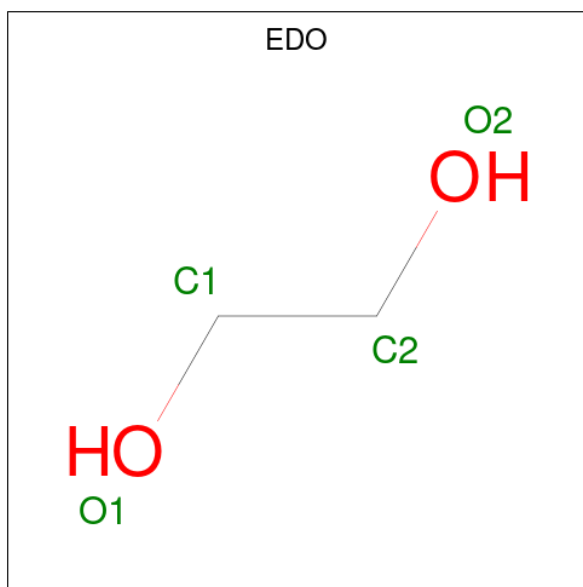
Chain	Residue	Modelled	Actual	Comment	Reference
B	440	GLY	-	expression tag	UNP M1UWB5
B	441	PRO	-	expression tag	UNP M1UWB5
B	442	LEU	-	expression tag	UNP M1UWB5
B	443	GLY	-	expression tag	UNP M1UWB5
B	444	SER	-	expression tag	UNP M1UWB5
B	445	PRO	-	expression tag	UNP M1UWB5
B	446	GLU	-	expression tag	UNP M1UWB5
B	447	PHE	-	expression tag	UNP M1UWB5

- Molecule 3 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	5	4		
3	B	1	Total	C	N	O	0	0
			19	10	5	4		

- 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 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	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	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	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	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
4	B	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
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

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

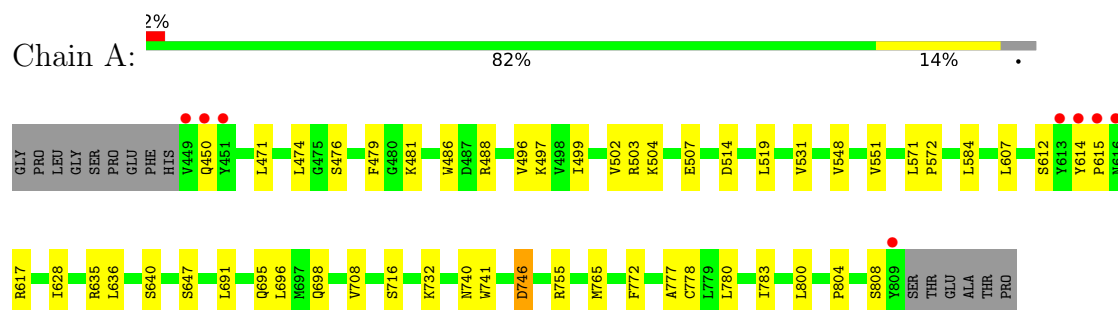
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	42	Total O 42 42	0	0
5	B	50	Total O 50 50	0	0

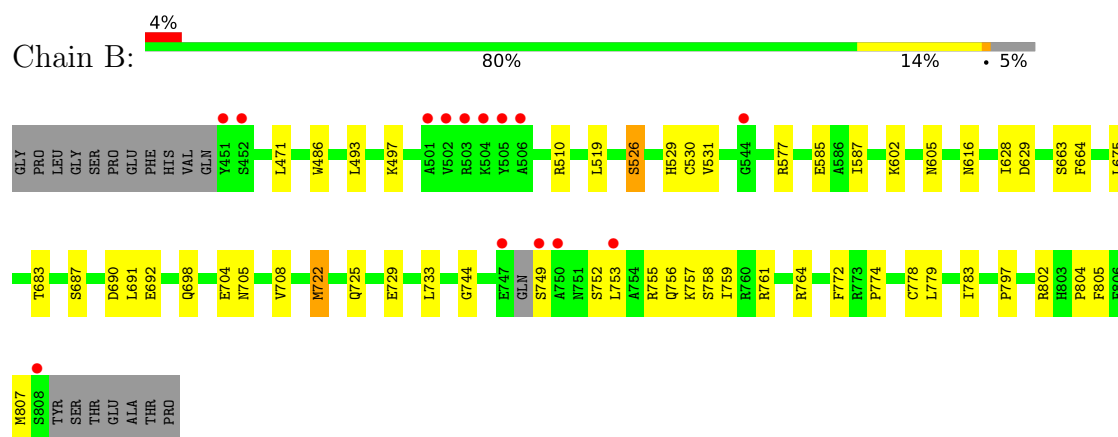
3 Residue-property plots

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: LAMMER-like dual specificity kinase



- Molecule 2: LAMMER-like dual specificity kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.13Å 100.89Å 109.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.18 – 2.69 48.18 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.18-2.69) 99.2 (48.18-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.203 , 0.268 0.205 , 0.270	Depositor DCC
R_{free} test set	1292 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.2	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	0.92	EDS
Total number of atoms	6036	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% 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: TPO, ADN, 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	0.13	0/2995	0.32	0/4063
2	B	0.13	0/2939	0.32	0/3983
All	All	0.13	0/5934	0.32	0/8046

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2920	0	2931	25	0
2	B	2878	0	2888	31	0
3	A	19	0	13	0	0
3	B	19	0	13	0	0
4	A	60	0	90	2	0
4	B	48	0	72	8	0
5	A	42	0	0	0	0
5	B	50	0	0	0	0
All	All	6036	0	6007	55	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 (55) 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:746:ASP:O	1:A:755:ARG:NH2	2.32	0.62
2:B:497:LYS:HD2	4:B:907:EDO:H21	1.80	0.62
2:B:531:VAL:HB	2:B:628:ILE:HG22	1.84	0.60
1:A:531:VAL:HB	1:A:628:ILE:HG22	1.84	0.59
2:B:744:GLY:HA3	4:B:912:EDO:H11	1.88	0.56
2:B:529:HIS:NE2	2:B:585:GLU:OE1	2.31	0.55
1:A:571:LEU:HD12	1:A:572:PRO:HD2	1.87	0.55
1:A:479:PHE:CD1	1:A:497:LYS:HE3	2.41	0.55
2:B:628:ILE:HD12	4:B:907:EDO:H11	1.89	0.55
2:B:749:SER:O	2:B:755:ARG:NH2	2.40	0.54
2:B:761:ARG:O	2:B:764:ARG:HG3	2.08	0.54
2:B:526:SER:OG	2:B:530:CYS:O	2.28	0.52
1:A:732:LYS:HA	4:A:907:EDO:H21	1.92	0.52
2:B:471:LEU:HD11	2:B:486:TRP:HB2	1.92	0.52
1:A:503:ARG:O	1:A:507:GLU:HG2	2.10	0.52
1:A:804:PRO:O	1:A:808:SER:HB3	2.10	0.51
1:A:695:GLN:HG2	1:A:741:TRP:CD2	2.46	0.51
1:A:698:GLN:HE22	1:A:708:VAL:HG13	1.76	0.51
2:B:772:PHE:CZ	2:B:783:ILE:HD12	2.46	0.51
2:B:804:PRO:HB3	2:B:807:MET:HE2	1.93	0.51
1:A:514:ASP:OD2	1:A:635:ARG:NH1	2.38	0.50
1:A:636:LEU:HB3	1:A:640:SER:HA	1.94	0.48
1:A:471:LEU:HD11	1:A:486:TRP:HB2	1.95	0.47
1:A:772:PHE:CZ	1:A:783:ILE:HD12	2.49	0.47
1:A:496:VAL:HG22	1:A:551:VAL:HG22	1.96	0.47
1:A:488:ARG:HD2	4:A:911:EDO:H21	1.95	0.47
1:A:615:PRO:O	1:A:617:ARG:NH1	2.48	0.47
2:B:687:SER:OG	2:B:692:GLU:OE1	2.30	0.47
2:B:725:GLN:O	2:B:729:GLU:HG2	2.13	0.47
2:B:772:PHE:HZ	2:B:783:ILE:HD12	1.80	0.47
1:A:504:LYS:HD2	1:A:504:LYS:H	1.79	0.46
2:B:587:ILE:HG22	2:B:797:PRO:HG3	1.96	0.46
2:B:756:GLN:HA	2:B:759:ILE:HD12	1.97	0.46
2:B:629:ASP:HA	4:B:907:EDO:H22	1.98	0.45
2:B:691:LEU:HB2	2:B:733:LEU:HD22	1.99	0.44
2:B:722:MET:HE3	2:B:722:MET:HB2	1.93	0.44
1:A:696:LEU:HB3	1:A:765:MET:HE3	1.99	0.44
2:B:663:SER:OG	2:B:664:PHE:N	2.51	0.44
1:A:584:LEU:HD21	1:A:800:LEU:HB3	1.99	0.43
2:B:752:SER:OG	2:B:755:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:LEU:HD21	1:A:740:ASN:O	2.20	0.42
2:B:690:ASP:OD1	4:B:905:EDO:H11	2.20	0.42
2:B:802:ARG:HA	4:B:911:EDO:H12	2.01	0.42
1:A:499:ILE:HG12	1:A:548:VAL:O	2.19	0.42
1:A:777:ALA:O	1:A:780:LEU:HB3	2.20	0.42
2:B:602:LYS:HE2	2:B:605:ASN:ND2	2.35	0.41
2:B:757:LYS:O	2:B:761:ARG:HG3	2.20	0.41
2:B:675:LEU:HD23	2:B:675:LEU:HA	1.85	0.41
1:A:481:LYS:HD3	2:B:774:PRO:HG3	2.03	0.41
1:A:607:LEU:HD11	1:A:628:ILE:HD13	2.02	0.41
2:B:733:LEU:HD23	4:B:912:EDO:H22	2.03	0.41
1:A:474:LEU:HD23	1:A:474:LEU:HA	1.92	0.41
2:B:779:LEU:HD13	2:B:805:PHE:CZ	2.56	0.41
2:B:753:LEU:HG	2:B:757:LYS:HD2	2.03	0.40
2:B:577:ARG:HH22	4:B:910:EDO:H12	1.85	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	360/376 (96%)	345 (96%)	14 (4%)	1 (0%)	37	61
2	B	352/376 (94%)	336 (96%)	15 (4%)	1 (0%)	37	61
All	All	712/752 (95%)	681 (96%)	29 (4%)	2 (0%)	37	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	647	SER
2	B	616	ASN

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	322/333 (97%)	313 (97%)	9 (3%)	38	68
2	B	316/332 (95%)	305 (96%)	11 (4%)	31	60
All	All	638/665 (96%)	618 (97%)	20 (3%)	35	64

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	A	476	SER
1	A	502	VAL
1	A	519	LEU
1	A	612	SER
1	A	614	TYR
1	A	716	SER
1	A	746	ASP
1	A	778	CYS
2	B	493	LEU
2	B	510	ARG
2	B	519	LEU
2	B	526	SER
2	B	698	GLN
2	B	704	GLU
2	B	705	ASN
2	B	708	VAL
2	B	722	MET
2	B	758	SER
2	B	778	CYS

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	547	HIS
1	A	688	HIS

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Mol	Chain	Res	Type
2	B	543	GLN
2	B	595	GLN
2	B	618	GLN
2	B	781	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	TPO	B	683	2	8,10,11	1.17	0	10,14,16	1.38	1 (10%)

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
2	TPO	B	683	2	-	5/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	683	TPO	P-OG1-CB	-3.74	111.90	123.21

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	683	TPO	N-CA-CB-CG2
2	B	683	TPO	N-CA-CB-OG1
2	B	683	TPO	C-CA-CB-CG2
2	B	683	TPO	CB-OG1-P-O1P
2	B	683	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

29 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	913	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	B	909	-	3,3,3	0.45	0	2,2,2	0.34	0
4	EDO	A	905	-	3,3,3	0.49	0	2,2,2	0.31	0
4	EDO	B	913	-	3,3,3	0.49	0	2,2,2	0.30	0
4	EDO	B	911	-	3,3,3	0.47	0	2,2,2	0.30	0
4	EDO	A	906	-	3,3,3	0.46	0	2,2,2	0.31	0
4	EDO	A	915	-	3,3,3	0.49	0	2,2,2	0.30	0
4	EDO	A	907	-	3,3,3	0.47	0	2,2,2	0.31	0
4	EDO	B	903	-	3,3,3	0.45	0	2,2,2	0.37	0
4	EDO	B	906	-	3,3,3	0.49	0	2,2,2	0.28	0
4	EDO	A	904	-	3,3,3	0.50	0	2,2,2	0.27	0
4	EDO	A	916	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	A	903	-	3,3,3	0.47	0	2,2,2	0.20	0
4	EDO	A	911	-	3,3,3	0.46	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADN	A	901	-	18,21,21	0.68	0	18,31,31	0.83	1 (5%)
3	ADN	B	902	-	18,21,21	0.65	0	18,31,31	0.78	1 (5%)
4	EDO	B	908	-	3,3,3	0.46	0	2,2,2	0.38	0
4	EDO	A	914	-	3,3,3	0.48	0	2,2,2	0.32	0
4	EDO	A	908	-	3,3,3	0.46	0	2,2,2	0.36	0
4	EDO	A	912	-	3,3,3	0.46	0	2,2,2	0.40	0
4	EDO	B	910	-	3,3,3	0.50	0	2,2,2	0.23	0
4	EDO	B	912	-	3,3,3	0.46	0	2,2,2	0.27	0
4	EDO	A	909	-	3,3,3	0.46	0	2,2,2	0.36	0
4	EDO	B	901	-	3,3,3	0.47	0	2,2,2	0.29	0
4	EDO	B	905	-	3,3,3	0.44	0	2,2,2	0.39	0
4	EDO	A	902	-	3,3,3	0.45	0	2,2,2	0.39	0
4	EDO	B	907	-	3,3,3	0.48	0	2,2,2	0.32	0
4	EDO	B	904	-	3,3,3	0.45	0	2,2,2	0.36	0
4	EDO	A	910	-	3,3,3	0.48	0	2,2,2	0.33	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
4	EDO	A	913	-	-	0/1/1/1	-
4	EDO	B	909	-	-	0/1/1/1	-
4	EDO	A	905	-	-	0/1/1/1	-
4	EDO	B	913	-	-	0/1/1/1	-
4	EDO	B	911	-	-	0/1/1/1	-
4	EDO	A	906	-	-	0/1/1/1	-
4	EDO	A	915	-	-	0/1/1/1	-
4	EDO	A	907	-	-	0/1/1/1	-
4	EDO	B	903	-	-	0/1/1/1	-
4	EDO	B	906	-	-	0/1/1/1	-
4	EDO	A	904	-	-	0/1/1/1	-
4	EDO	A	916	-	-	0/1/1/1	-
4	EDO	A	903	-	-	0/1/1/1	-
4	EDO	A	911	-	-	0/1/1/1	-
3	ADN	A	901	-	-	2/2/22/22	0/3/3/3
3	ADN	B	902	-	-	2/2/22/22	0/3/3/3
4	EDO	B	908	-	-	0/1/1/1	-
4	EDO	A	914	-	-	0/1/1/1	-
4	EDO	A	908	-	-	0/1/1/1	-
4	EDO	A	912	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	910	-	-	1/1/1/1	-
4	EDO	B	912	-	-	0/1/1/1	-
4	EDO	A	909	-	-	0/1/1/1	-
4	EDO	B	901	-	-	0/1/1/1	-
4	EDO	B	905	-	-	0/1/1/1	-
4	EDO	A	902	-	-	0/1/1/1	-
4	EDO	B	907	-	-	1/1/1/1	-
4	EDO	B	904	-	-	0/1/1/1	-
4	EDO	A	910	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	ADN	C5-C6-N6	2.29	123.83	120.35
3	A	901	ADN	C5-C6-N6	2.25	123.77	120.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

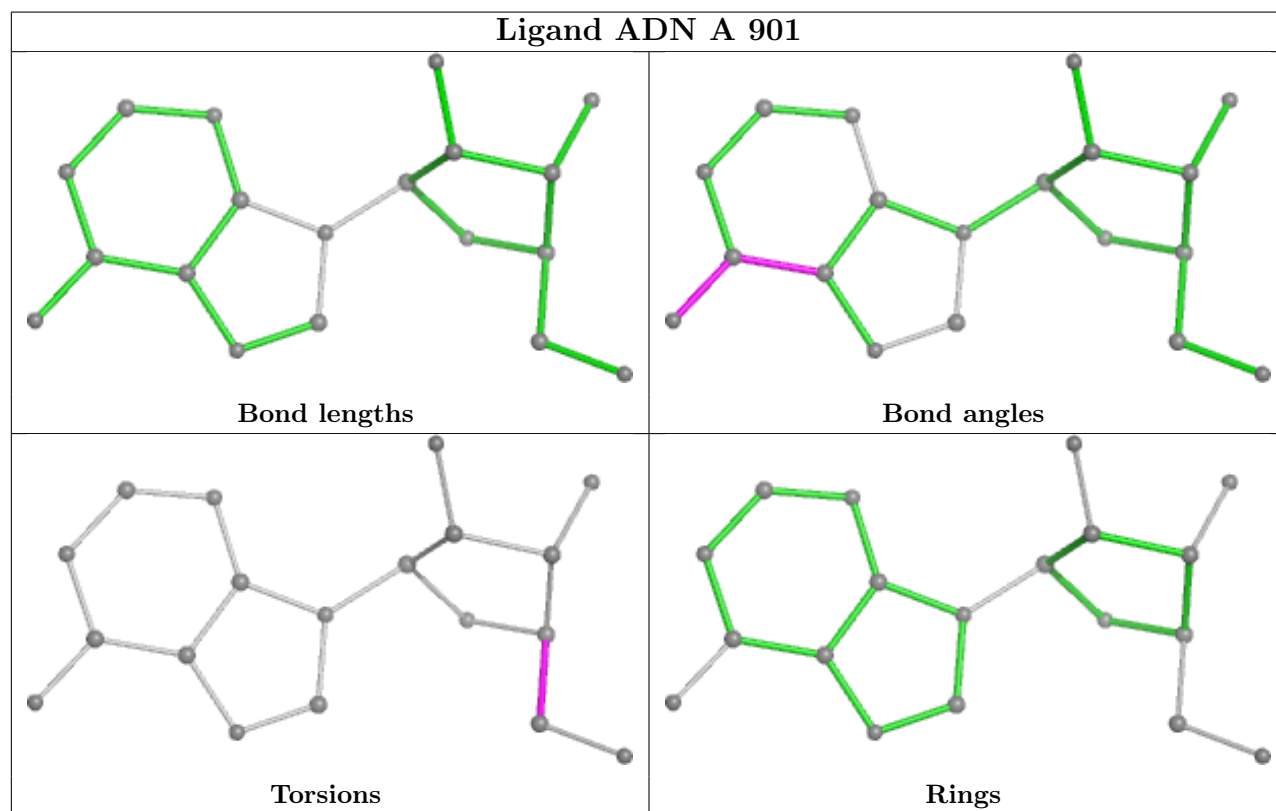
Mol	Chain	Res	Type	Atoms
3	B	902	ADN	C3'-C4'-C5'-O5'
3	B	902	ADN	O4'-C4'-C5'-O5'
4	B	907	EDO	O1-C1-C2-O2
4	B	910	EDO	O1-C1-C2-O2
3	A	901	ADN	O4'-C4'-C5'-O5'
4	A	910	EDO	O1-C1-C2-O2
3	A	901	ADN	C3'-C4'-C5'-O5'

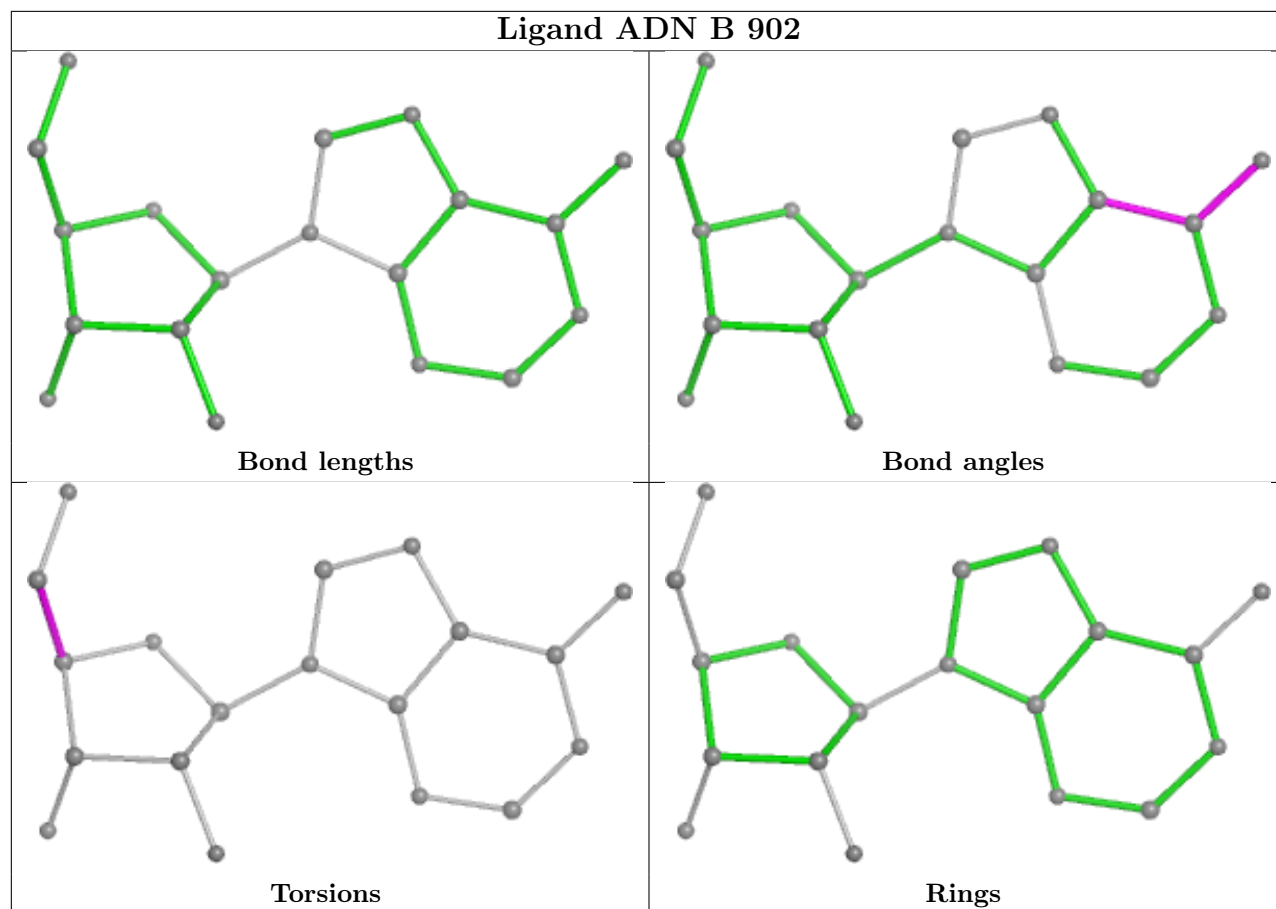
There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	911	EDO	1	0
4	A	907	EDO	1	0
4	A	911	EDO	1	0
4	B	910	EDO	1	0
4	B	912	EDO	2	0
4	B	905	EDO	1	0
4	B	907	EDO	3	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	361/376 (96%)	-0.00	8 (2%) 62 61	20, 38, 73, 110	1 (0%)
2	B	356/376 (94%)	-0.05	14 (3%) 44 42	24, 38, 83, 130	0
All	All	717/752 (95%)	-0.03	22 (3%) 51 49	20, 38, 81, 130	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	501	ALA	4.2
1	A	449	VAL	3.5
2	B	808	SER	3.3
1	A	615	PRO	3.3
2	B	451	TYR	3.3
1	A	451	TYR	3.2
1	A	450	GLN	2.8
2	B	503	ARG	2.8
1	A	616	ASN	2.7
1	A	614	TYR	2.6
2	B	452	SER	2.6
2	B	506	ALA	2.6
1	A	809	TYR	2.6
2	B	502	VAL	2.5
1	A	613	TYR	2.5
2	B	504	LYS	2.2
2	B	753	LEU	2.1
2	B	750	ALA	2.1
2	B	749	SER	2.1
2	B	505	TYR	2.1
2	B	747	GLU	2.0
2	B	544	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	TPO	B	683	11/12	0.87	0.17	33,43,53,66	3

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(Å ²)	Q<0.9
4	EDO	B	910	4/4	0.35	0.26	52,54,56,62	0
4	EDO	A	906	4/4	0.54	0.25	56,58,60,60	0
4	EDO	A	910	4/4	0.65	0.17	52,55,58,63	0
4	EDO	A	916	4/4	0.69	0.13	56,56,58,63	0
4	EDO	B	913	4/4	0.71	0.19	43,43,53,54	0
4	EDO	B	908	4/4	0.72	0.15	44,54,54,55	0
4	EDO	B	911	4/4	0.73	0.17	50,55,55,61	0
4	EDO	A	908	4/4	0.73	0.17	55,62,63,70	0
4	EDO	A	907	4/4	0.75	0.13	50,50,56,62	0
4	EDO	A	904	4/4	0.77	0.16	43,46,50,51	0
4	EDO	A	913	4/4	0.78	0.19	35,37,41,46	0
4	EDO	A	905	4/4	0.80	0.16	46,48,53,56	0
4	EDO	B	907	4/4	0.80	0.17	43,45,45,47	0
4	EDO	A	909	4/4	0.80	0.13	36,36,43,55	0
4	EDO	B	901	4/4	0.81	0.15	49,55,57,65	0
3	ADN	B	902	19/19	0.81	0.15	31,43,52,57	19
4	EDO	B	903	4/4	0.82	0.13	43,44,54,54	0
4	EDO	A	912	4/4	0.82	0.16	44,44,44,45	0
4	EDO	B	905	4/4	0.83	0.16	37,40,41,50	0
4	EDO	A	915	4/4	0.84	0.15	43,50,53,56	0
4	EDO	B	904	4/4	0.84	0.14	43,47,53,58	0

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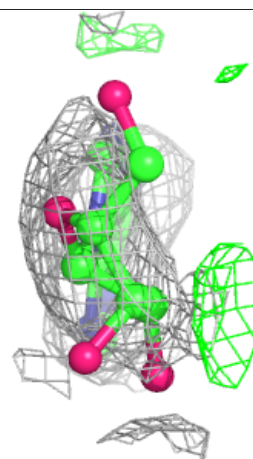
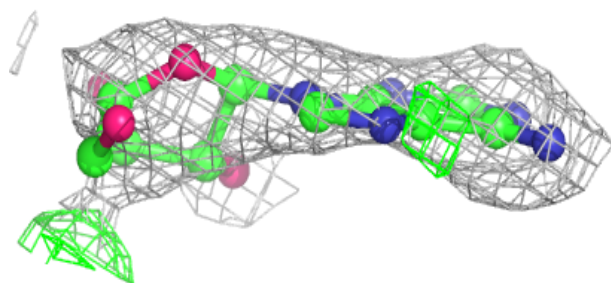
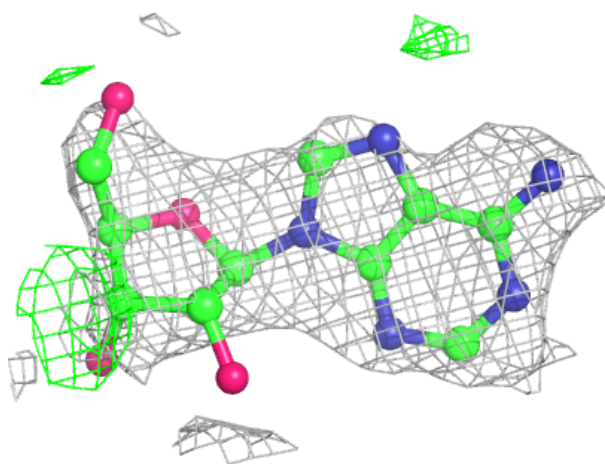
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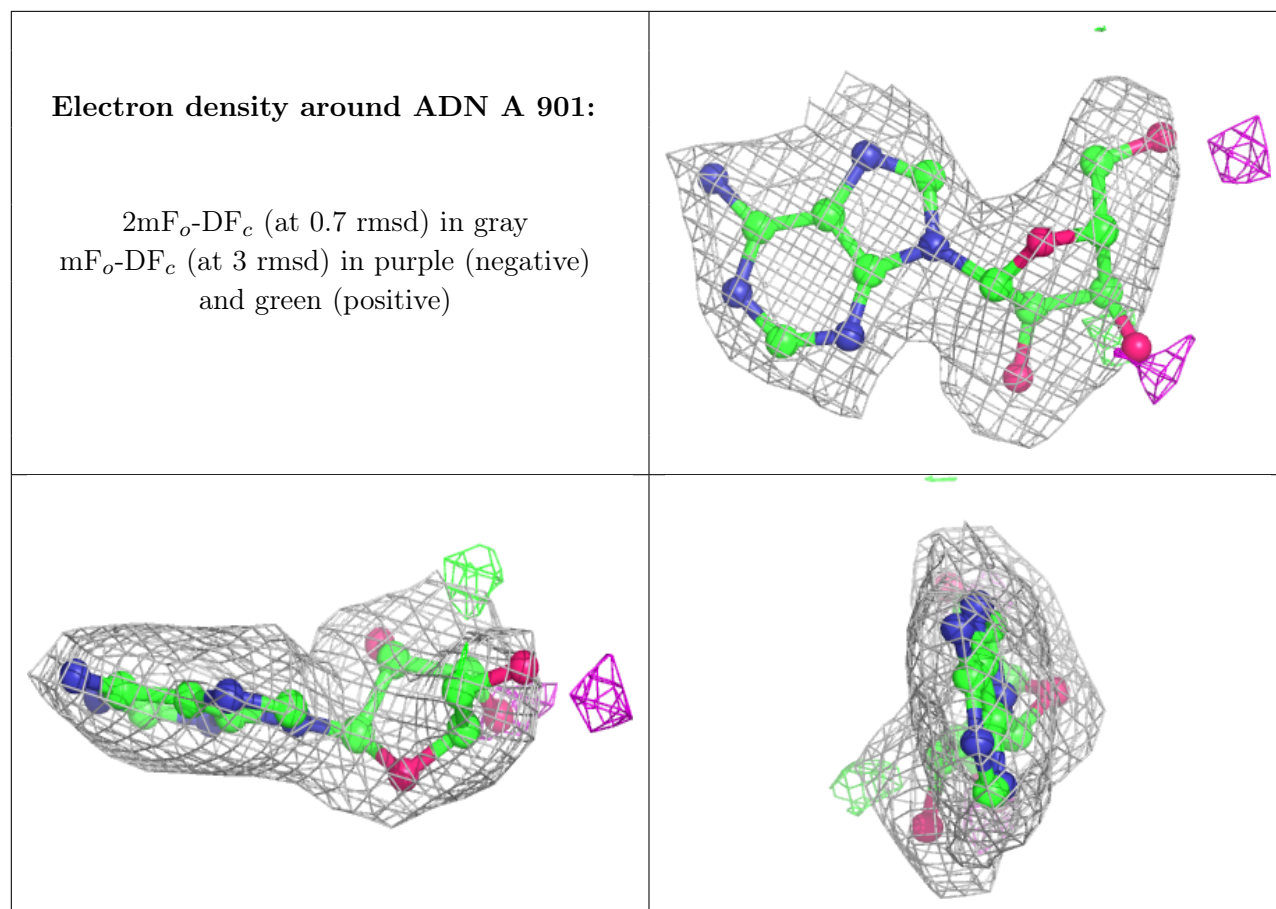
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	B	906	4/4	0.86	0.16	38,42,42,47	0
4	EDO	A	914	4/4	0.86	0.13	42,45,49,51	0
4	EDO	A	911	4/4	0.87	0.17	48,48,48,53	0
3	ADN	A	901	19/19	0.88	0.12	32,36,48,63	0
4	EDO	B	909	4/4	0.89	0.15	30,30,30,46	0
4	EDO	A	902	4/4	0.89	0.10	39,44,46,46	0
4	EDO	B	912	4/4	0.91	0.16	48,49,49,53	0
4	EDO	A	903	4/4	0.92	0.10	36,38,44,45	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 ADN B 902:

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.