



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:54 AM UTC

PDB ID : 5LU4 / pdb_00005lu4
Title : C4-type pyruvate phosphate dikinase: conformational intermediate of central domain in the swiveling mechanism
Authors : Minges, A.; Hoepfner, A.; Groth, G.
Deposited on : 2016-09-08
Resolution : 2.90 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

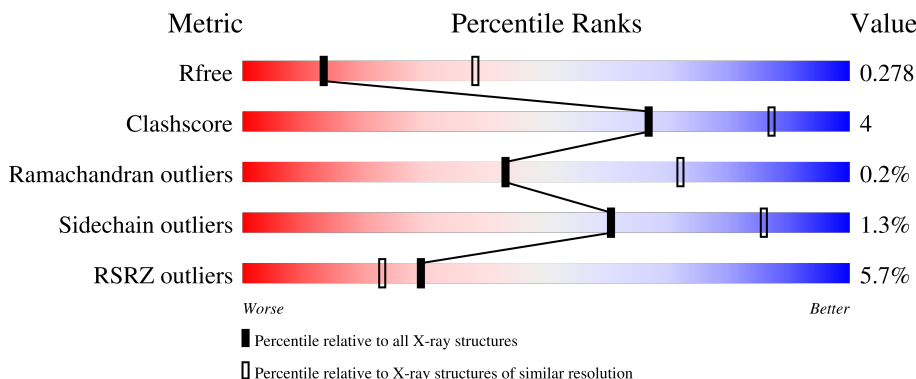
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	874	6% 86% 10% ...
1	B	874	5% 89% 7% ...

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12020 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 Pyruvate, phosphate dikinase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	850	Total	C	N	O	S	0	0	0
			6091	3819	1060	1172	40			
1	B	847	Total	C	N	O	S	0	0	0
			5863	3680	1024	1119	40			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

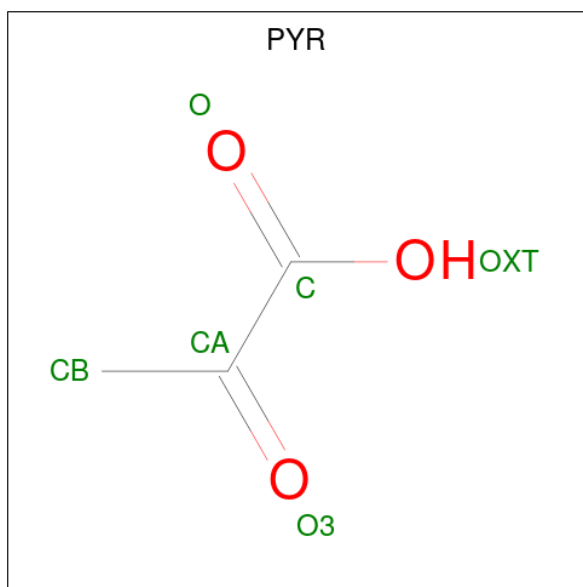


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		

- Molecule 4 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



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

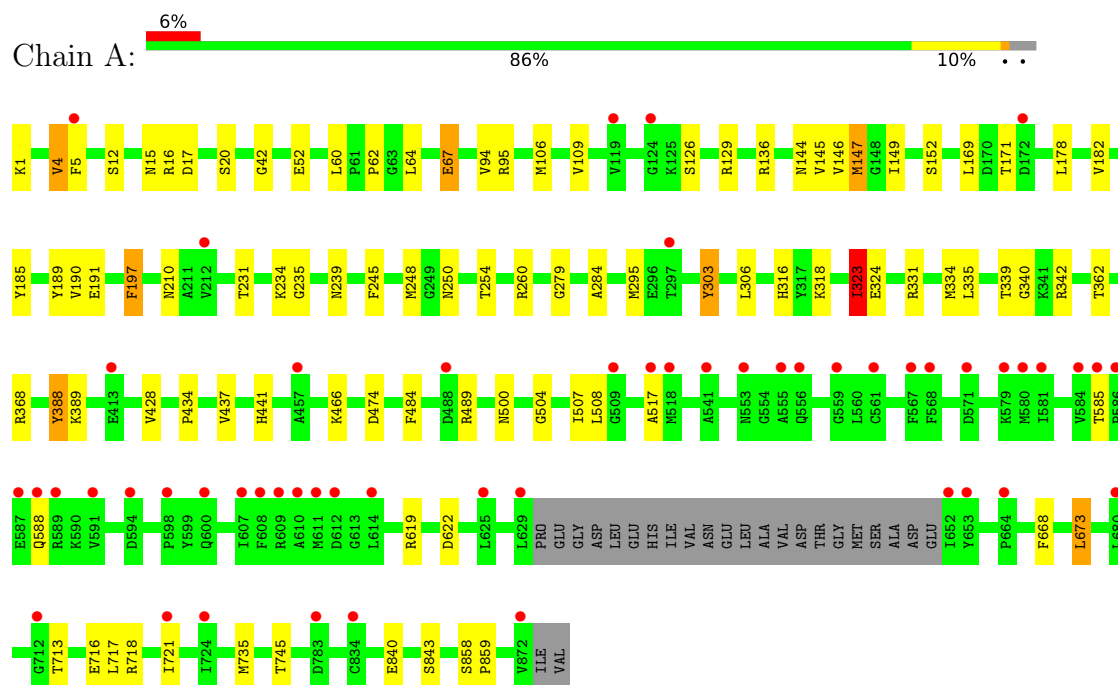
- Molecule 5 is water.

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

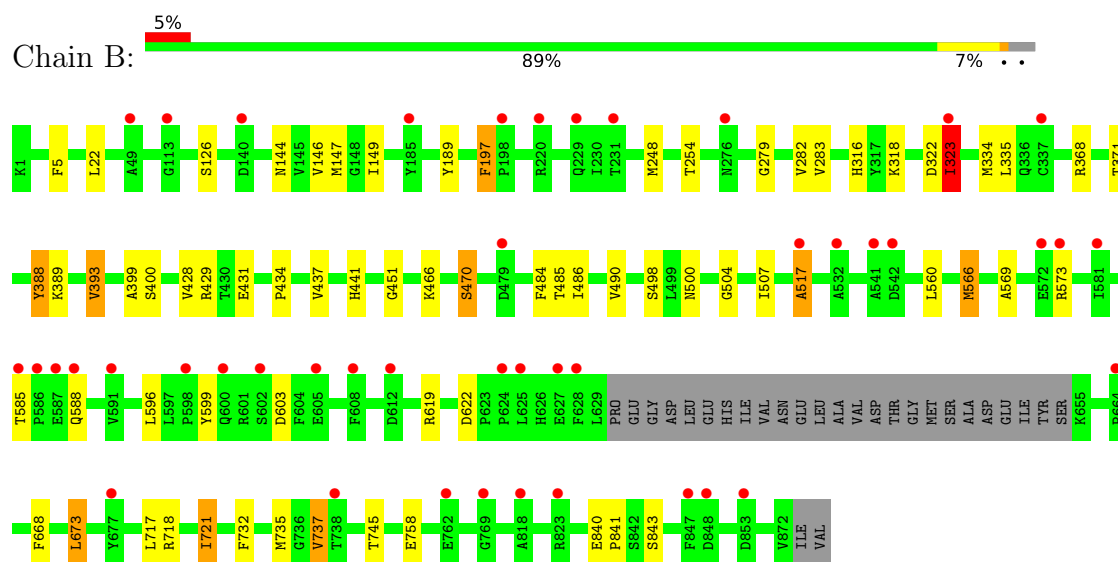
3 Residue-property plots [i](#)

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: Pyruvate, phosphate dikinase, chloroplastic



- Molecule 1: Pyruvate, phosphate dikinase, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.16Å 126.52Å 219.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.79 – 2.90 109.55 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (109.79-2.90) 99.6 (109.55-2.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0155, PHENIX dev_2499	Depositor
R, R_{free}	0.247 , 0.286 0.244 , 0.278	Depositor DCC
R_{free} test set	2229 reflections (3.79%)	wwPDB-VP
Wilson B-factor (Å ²)	83.0	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 88.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12020	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: ADP, MG, PYR

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	1.24	34/6201 (0.5%)	0.89	7/8435 (0.1%)
1	B	0.93	4/5973 (0.1%)	0.78	6/8155 (0.1%)
All	All	1.10	38/12174 (0.3%)	0.84	13/16590 (0.1%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	THR	C-O	-12.08	1.09	1.24
1	A	340	GLY	C-O	-10.62	1.12	1.23
1	A	210	ASN	CG-OD1	-10.14	1.04	1.23
1	A	342	ARG	CZ-NH2	9.07	1.45	1.33
1	A	16	ARG	CZ-NH1	8.49	1.44	1.32
1	A	106	MET	C-O	-7.91	1.14	1.23
1	A	17	ASP	CG-OD2	7.81	1.40	1.25
1	A	62	PRO	C-O	7.36	1.33	1.24
1	A	15	ASN	CG-OD1	-7.29	1.09	1.23
1	A	235	GLY	C-O	-7.24	1.13	1.24
1	A	109	VAL	C-O	-7.13	1.16	1.24
1	B	517	ALA	N-CA	6.98	1.55	1.46
1	A	231	THR	C-O	6.93	1.32	1.23
1	A	147	MET	C-O	6.91	1.33	1.23
1	A	52	GLU	CD-OE1	6.68	1.38	1.25
1	A	324	GLU	CD-OE1	6.66	1.38	1.25
1	A	331	ARG	C-O	-6.62	1.16	1.24
1	A	342	ARG	CZ-NH1	6.20	1.41	1.32
1	A	42	GLY	C-O	-6.15	1.17	1.23
1	A	67	GLU	CD-OE2	6.14	1.37	1.25
1	A	284	ALA	C-O	-6.11	1.16	1.24
1	A	303	TYR	CA-C	6.05	1.60	1.52
1	B	316	HIS	C-O	-6.04	1.17	1.24
1	A	12	SER	C-O	-6.03	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	ARG	C-O	-6.03	1.16	1.23
1	A	94	VAL	C-O	-5.95	1.17	1.24
1	A	145	VAL	CA-CB	5.94	1.62	1.54
1	A	191	GLU	C-O	-5.61	1.17	1.24
1	A	245	PHE	N-CA	-5.55	1.39	1.46
1	B	322	ASP	C-O	-5.50	1.17	1.24
1	A	316	HIS	C-O	-5.48	1.17	1.24
1	A	234	LYS	N-CA	5.44	1.52	1.46
1	A	1	LYS	N-CA	5.35	1.56	1.46
1	A	190	VAL	C-O	-5.22	1.18	1.24
1	B	451	GLY	C-O	-5.13	1.16	1.23
1	A	4	VAL	C-O	-5.08	1.18	1.24
1	A	323	ILE	CB-CG1	-5.07	1.43	1.53
1	A	362	THR	C-O	-5.01	1.17	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	566	MET	CA-CB-CG	8.10	130.30	114.10
1	B	737	VAL	N-CA-C	-6.12	106.46	111.91
1	A	342	ARG	NE-CZ-NH1	-5.91	115.59	121.50
1	A	342	ARG	NH1-CZ-NH2	5.82	126.87	119.30
1	A	340	GLY	N-CA-C	5.76	118.10	111.36
1	A	323	ILE	CG1-CB-CG2	-5.68	93.67	110.70
1	B	323	ILE	CG1-CB-CG2	-5.29	94.83	110.70
1	A	339	THR	CA-C-N	5.22	124.93	119.92
1	A	339	THR	C-N-CA	5.22	124.93	119.92
1	B	429	ARG	CA-CB-CG	5.20	124.49	114.10
1	A	20	SER	N-CA-C	5.17	117.66	111.71
1	B	737	VAL	N-CA-CB	-5.08	106.44	112.39
1	B	721	ILE	CB-CA-C	5.05	119.19	112.22

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	6091	0	5649	39	0
1	B	5863	0	5203	46	0
2	A	27	0	12	2	0
2	B	27	0	12	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	6	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	12020	0	10876	84	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 (84) 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:146:VAL:HG12	1:A:147:MET:HE2	1.52	0.92
1:B:732:PHE:CD2	1:B:737:VAL:HG13	2.07	0.89
1:B:146:VAL:HG12	1:B:147:MET:HE2	1.56	0.87
1:B:393:VAL:HG12	1:B:486:ILE:HD13	1.59	0.85
1:A:718:ARG:HA	1:A:721:ILE:HG12	1.66	0.76
1:B:189:TYR:CD2	1:B:197:PHE:HB2	2.22	0.74
1:B:393:VAL:HG12	1:B:486:ILE:CD1	2.19	0.72
1:A:189:TYR:CD2	1:A:197:PHE:HB2	2.26	0.70
1:B:146:VAL:HG12	1:B:147:MET:CE	2.20	0.70
1:A:146:VAL:HG12	1:A:147:MET:CE	2.23	0.69
1:B:393:VAL:CG1	1:B:486:ILE:HD12	2.24	0.68
1:B:393:VAL:CG1	1:B:486:ILE:CD1	2.71	0.67
1:B:596:LEU:HD12	1:B:599:TYR:CB	2.26	0.65
1:B:318:LYS:O	1:B:368:ARG:NH1	2.29	0.64
1:B:393:VAL:HG11	1:B:486:ILE:HD12	1.81	0.62
1:B:718:ARG:HA	1:B:721:ILE:HG13	1.80	0.61
1:A:713:THR:OG1	1:A:716:GLU:HG3	2.00	0.61
1:B:399:ALA:HB2	1:B:470:SER:HB3	1.83	0.61
1:B:732:PHE:CG	1:B:737:VAL:HG13	2.36	0.60
1:A:335:LEU:HD22	2:A:901:ADP:C4	2.36	0.59
1:A:250:ASN:ND2	1:B:431:GLU:OE1	2.32	0.59
1:A:318:LYS:O	1:A:368:ARG:NH1	2.30	0.58
1:A:254:THR:HG21	1:A:279:GLY:O	2.05	0.57
1:A:323:ILE:HG21	1:A:334:MET:HE1	1.87	0.57
1:B:282:VAL:HG23	1:B:283:VAL:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:TYR:CD2	1:B:507:ILE:HD13	2.41	0.55
1:B:254:THR:HG21	1:B:279:GLY:O	2.07	0.55
1:A:388:TYR:CD2	1:A:507:ILE:HD13	2.42	0.55
1:A:840:GLU:OE1	1:A:843:SER:N	2.39	0.55
1:B:189:TYR:CE2	1:B:197:PHE:HB2	2.43	0.52
1:B:323:ILE:HG21	1:B:334:MET:HE1	1.91	0.52
1:B:585:THR:O	1:B:588:GLN:N	2.43	0.52
1:A:585:THR:O	1:A:588:GLN:N	2.43	0.52
1:B:732:PHE:CD2	1:B:737:VAL:CG1	2.89	0.52
1:B:5:PHE:CD2	1:B:22:LEU:HD21	2.46	0.51
1:A:295:MET:HE3	1:A:303:TYR:HD1	1.76	0.50
1:A:189:TYR:CE2	1:A:197:PHE:HB2	2.47	0.50
1:A:619:ARG:NH2	1:A:622:ASP:OD2	2.45	0.50
1:B:840:GLU:OE1	1:B:843:SER:N	2.40	0.50
1:B:335:LEU:HD22	2:B:901:ADP:C4	2.47	0.49
1:B:619:ARG:NH2	1:B:622:ASP:OD2	2.46	0.48
1:B:717:LEU:HD13	1:B:745:THR:HG22	1.95	0.48
1:A:388:TYR:HD1	1:A:389:LYS:N	2.11	0.48
1:A:126:SER:HB3	1:A:248:MET:HE3	1.96	0.47
1:B:400:SER:OG	1:B:466:LYS:O	2.23	0.47
1:B:569:ALA:HB3	1:B:573:ARG:CB	2.45	0.47
1:A:441:HIS:O	1:A:466:LYS:NZ	2.48	0.47
1:A:717:LEU:HD13	1:A:745:THR:HG22	1.97	0.47
1:A:388:TYR:CD1	1:A:388:TYR:C	2.93	0.47
1:A:295:MET:HE1	1:A:306:LEU:HD22	1.98	0.46
1:B:126:SER:HB3	1:B:248:MET:HE3	1.98	0.46
1:B:388:TYR:HD1	1:B:389:LYS:N	2.14	0.45
1:A:129:ARG:HH22	1:A:171:THR:HA	1.80	0.45
1:B:732:PHE:HB3	1:B:737:VAL:HG22	1.99	0.45
1:A:388:TYR:HD1	1:A:388:TYR:C	2.25	0.45
1:A:428:VAL:HG11	1:A:484:PHE:CD2	2.52	0.45
1:A:60:LEU:HD22	1:A:64:LEU:HD23	1.99	0.45
1:B:668:PHE:CE2	1:B:673:LEU:HB2	2.51	0.45
1:A:434:PRO:HA	1:A:437:VAL:HG23	1.98	0.44
1:B:434:PRO:HA	1:B:437:VAL:HG23	1.99	0.44
1:A:144:ASN:HA	1:A:149:ILE:O	2.18	0.44
1:B:441:HIS:O	1:B:466:LYS:NZ	2.50	0.44
1:B:388:TYR:C	1:B:388:TYR:CD1	2.96	0.44
1:B:428:VAL:HG11	1:B:484:PHE:CD2	2.52	0.43
1:B:498:SER:HB2	1:B:507:ILE:HB	2.00	0.43
1:B:371:THR:HG21	1:B:841:PRO:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:THR:HG22	1:B:490:VAL:HG22	1.99	0.43
1:B:500:ASN:O	1:B:504:GLY:N	2.49	0.43
1:A:858:SER:OG	1:A:859:PRO:HD2	2.19	0.42
1:A:4:VAL:CG2	1:A:67:GLU:HG2	2.48	0.42
1:A:500:ASN:O	1:A:504:GLY:N	2.48	0.42
1:B:560:LEU:HD11	1:B:619:ARG:HD2	2.01	0.42
1:A:129:ARG:HG3	1:A:178:LEU:HD12	2.01	0.42
1:A:489:ARG:HH22	1:A:508:LEU:HD11	1.85	0.42
1:B:144:ASN:HA	1:B:149:ILE:O	2.20	0.42
1:A:136:ARG:HG3	1:A:185:TYR:CE2	2.55	0.41
1:A:474:ASP:OD1	1:A:474:ASP:N	2.52	0.41
1:B:732:PHE:CB	1:B:737:VAL:HG13	2.50	0.41
1:A:668:PHE:CE2	1:A:673:LEU:HB2	2.56	0.41
1:B:388:TYR:HD1	1:B:388:TYR:C	2.29	0.41
1:B:566:MET:HG2	1:B:603:ASP:OD2	2.21	0.41
1:A:5:PHE:CD1	1:A:5:PHE:N	2.89	0.41
1:A:95:ARG:HB2	1:A:239:ASN:HB2	2.03	0.41
1:A:279:GLY:HA2	2:A:901:ADP:O3'	2.21	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	846/874 (97%)	824 (97%)	20 (2%)	2 (0%)	43	72
1	B	843/874 (96%)	820 (97%)	21 (2%)	2 (0%)	43	72
All	All	1689/1748 (97%)	1644 (97%)	41 (2%)	4 (0%)	43	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	517	ALA
1	B	517	ALA
1	A	735	MET
1	B	735	MET

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	576/715 (81%)	569 (99%)	7 (1%)	63	86
1	B	510/715 (71%)	503 (99%)	7 (1%)	59	85
All	All	1086/1430 (76%)	1072 (99%)	14 (1%)	61	86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	SER
1	A	169	LEU
1	A	182	VAL
1	A	197	PHE
1	A	323	ILE
1	A	388	TYR
1	A	673	LEU
1	B	197	PHE
1	B	323	ILE
1	B	388	TYR
1	B	393	VAL
1	B	470	SER
1	B	673	LEU
1	B	758	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS

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Mol	Chain	Res	Type
1	A	500	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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$
4	PYR	A	903	3	5,5,5	1.53	1 (20%)	3,6,6	1.66	0
2	ADP	B	901	3	28,29,29	1.57	5 (17%)	43,45,45	1.90	13 (30%)
2	ADP	A	901	3	28,29,29	2.19	5 (17%)	43,45,45	2.03	12 (27%)

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	PYR	A	903	3	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	901	3	-	4/16/32/32	0/3/3/3
2	ADP	A	901	3	-	4/16/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	ADP	PA-O3A	7.60	1.67	1.59
2	A	901	ADP	C8-N7	5.14	1.41	1.31
2	B	901	ADP	PA-O3A	4.47	1.64	1.59
2	B	901	ADP	C5-C4	3.85	1.45	1.39
2	A	901	ADP	C5-N7	-3.43	1.32	1.39
2	A	901	ADP	C4-N9	-3.33	1.30	1.37
2	A	901	ADP	C4-N3	-3.01	1.28	1.34
2	B	901	ADP	C5-N7	-2.79	1.34	1.39
2	B	901	ADP	C4-N9	-2.63	1.32	1.37
2	B	901	ADP	C5-C6	2.26	1.47	1.41
4	A	903	PYR	O-C	2.08	1.27	1.22

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	ADP	C5-C4-N3	-6.09	118.33	126.72
2	B	901	ADP	C5-C4-N3	-5.18	119.58	126.72
2	A	901	ADP	C5-C4-N9	4.98	111.24	105.81
2	B	901	ADP	N3-C4-N9	4.03	134.02	127.17
2	B	901	ADP	C2-N3-C4	3.78	121.07	111.83
2	A	901	ADP	C2-N3-C4	3.60	120.62	111.83
2	B	901	ADP	N3-C2-N1	-3.51	123.28	128.58
2	A	901	ADP	C4-C5-N7	-3.35	106.75	110.58
2	B	901	ADP	O2A-PA-O1A	3.26	127.59	112.44
2	A	901	ADP	O2A-PA-O3A	-3.24	98.51	107.27
2	A	901	ADP	O2A-PA-O5'	-3.08	93.63	107.57
2	A	901	ADP	O4'-C4'-C3'	-2.93	99.33	105.15
2	A	901	ADP	N9-C8-N7	-2.92	109.79	113.94
2	B	901	ADP	C4-C5-N7	-2.79	107.39	110.58
2	A	901	ADP	O3A-PA-O1A	2.71	118.87	110.70
2	B	901	ADP	C4-N9-C8	2.63	108.50	105.74
2	B	901	ADP	N9-C8-N7	-2.48	110.42	113.94
2	B	901	ADP	C5-N7-C8	2.47	107.33	103.45
2	A	901	ADP	O2A-PA-O1A	2.39	123.54	112.44
2	B	901	ADP	O2A-PA-O3A	-2.34	100.96	107.27
2	A	901	ADP	O3B-PB-O3A	2.30	112.33	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	ADP	N3-C2-N1	-2.21	125.23	128.58
2	B	901	ADP	C5-C6-N6	-2.09	118.12	123.29
2	B	901	ADP	C6-C5-N7	2.08	136.10	132.09
2	B	901	ADP	N6-C6-N1	2.06	122.95	118.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

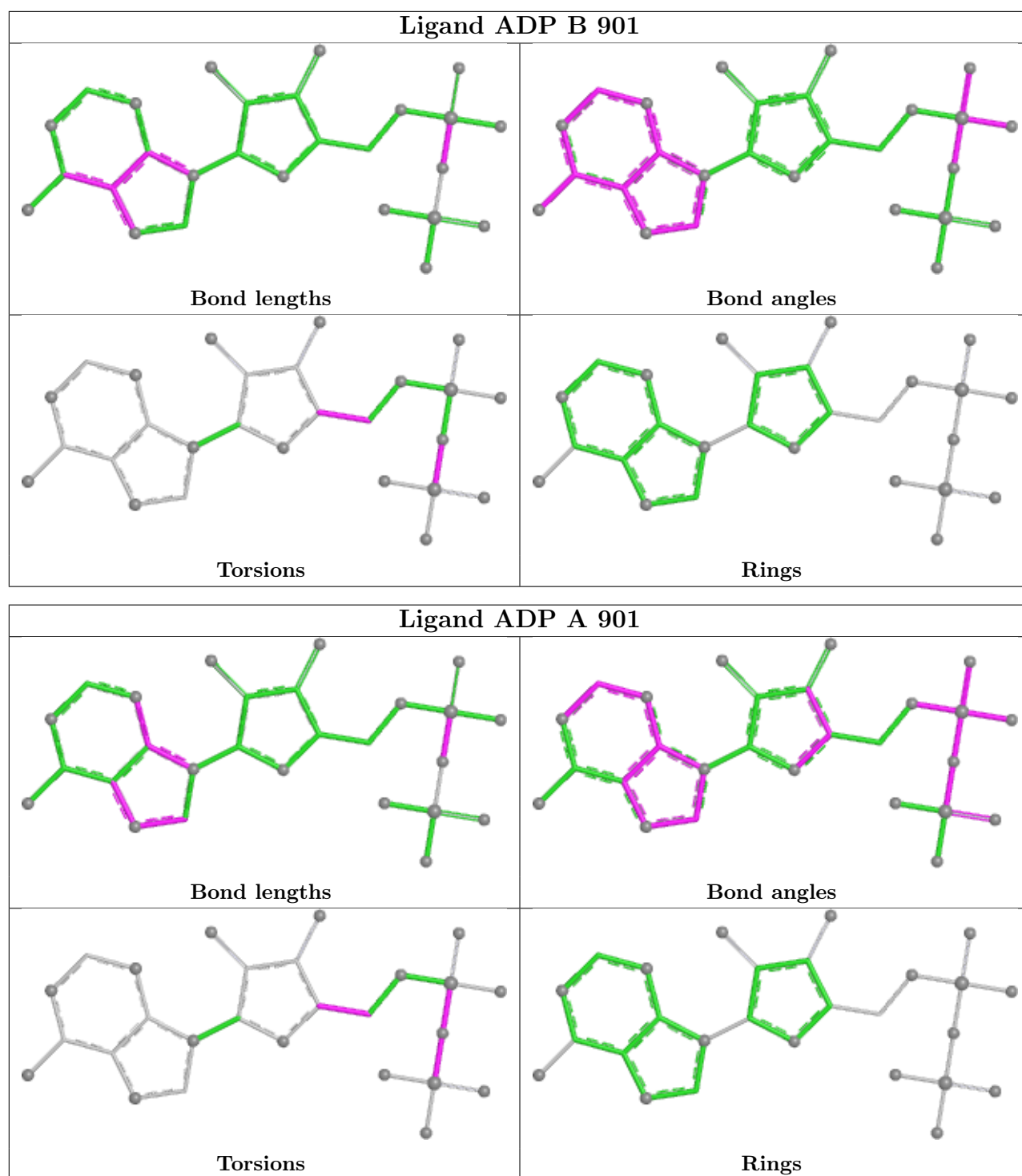
Mol	Chain	Res	Type	Atoms
2	A	901	ADP	PA-O3A-PB-O2B
2	A	901	ADP	O4'-C4'-C5'-O5'
2	B	901	ADP	PA-O3A-PB-O3B
4	A	903	PYR	OXT-C-CA-CB
2	A	901	ADP	C3'-C4'-C5'-O5'
2	B	901	ADP	O4'-C4'-C5'-O5'
2	B	901	ADP	C3'-C4'-C5'-O5'
4	A	903	PYR	O-C-CA-CB
2	B	901	ADP	PA-O3A-PB-O2B
2	A	901	ADP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	ADP	1	0
2	A	901	ADP	2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	850/874 (97%)	0.58	53 (6%)	26 21	46, 90, 181, 225	0
1	B	847/874 (96%)	0.59	44 (5%)	33 26	71, 99, 156, 202	0
All	All	1697/1748 (97%)	0.58	97 (5%)	29 23	46, 96, 165, 225	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	ALA	5.4
1	A	611	MET	4.1
1	A	571	ASP	3.7
1	B	323	ILE	3.7
1	A	607	ILE	3.6
1	A	586	PRO	3.4
1	B	532	ALA	3.3
1	A	172	ASP	3.2
1	A	587	GLU	3.2
1	A	580	MET	3.2
1	B	198	PRO	3.1
1	B	276	ASN	3.1
1	A	652	ILE	3.1
1	A	541	ALA	3.1
1	A	568	PHE	3.0
1	A	614	LEU	3.0
1	A	413	GLU	3.0
1	B	586	PRO	2.9
1	A	555	ALA	2.9
1	A	567	PHE	2.9
1	A	509	GLY	2.8
1	B	598	PRO	2.8
1	B	587	GLU	2.8
1	B	605	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	847	PHE	2.8
1	B	581	ILE	2.8
1	A	608	PHE	2.8
1	B	625	LEU	2.8
1	B	337	CYS	2.7
1	A	584	VAL	2.7
1	B	49	ALA	2.7
1	B	738	THR	2.7
1	A	588	GLN	2.7
1	B	600	GLN	2.7
1	A	664	PRO	2.6
1	B	113	GLY	2.6
1	A	585	THR	2.6
1	B	627	GLU	2.6
1	A	119	VAL	2.6
1	B	823	ARG	2.6
1	B	628	PHE	2.6
1	A	591	VAL	2.5
1	A	872	VAL	2.5
1	B	572	GLU	2.5
1	A	600	GLN	2.5
1	A	559	GLY	2.5
1	A	212	VAL	2.5
1	B	140	ASP	2.4
1	A	579	LYS	2.4
1	A	610	ALA	2.4
1	B	585	THR	2.4
1	B	602	SER	2.4
1	A	721	ILE	2.4
1	A	783	ASP	2.4
1	A	518	MET	2.4
1	B	185	TYR	2.4
1	A	724	ILE	2.4
1	B	624	PRO	2.4
1	A	609	ARG	2.3
1	B	229	GLN	2.3
1	A	5	PHE	2.3
1	A	556	GLN	2.3
1	B	853	ASP	2.3
1	A	581	ILE	2.3
1	A	297	THR	2.3
1	B	231	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	653	TYR	2.3
1	A	680	LEU	2.2
1	B	479	ASP	2.2
1	A	712	GLY	2.2
1	B	848	ASP	2.2
1	A	457	ALA	2.2
1	B	541	ALA	2.2
1	B	818	ALA	2.2
1	A	594	ASP	2.2
1	B	608	PHE	2.2
1	B	220	ARG	2.2
1	B	588	GLN	2.2
1	B	612	ASP	2.2
1	B	677	TYR	2.2
1	B	762	GLU	2.2
1	B	769	GLY	2.1
1	B	517	ALA	2.1
1	A	589	ARG	2.1
1	A	625	LEU	2.1
1	A	629	LEU	2.1
1	A	834	CYS	2.1
1	A	598	PRO	2.1
1	A	124	GLY	2.1
1	A	561	CYS	2.1
1	B	664	PRO	2.1
1	A	488	ASP	2.0
1	A	553	ASN	2.0
1	B	573	ARG	2.0
1	A	612	ASP	2.0
1	B	542	ASP	2.0
1	B	591	VAL	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](#)

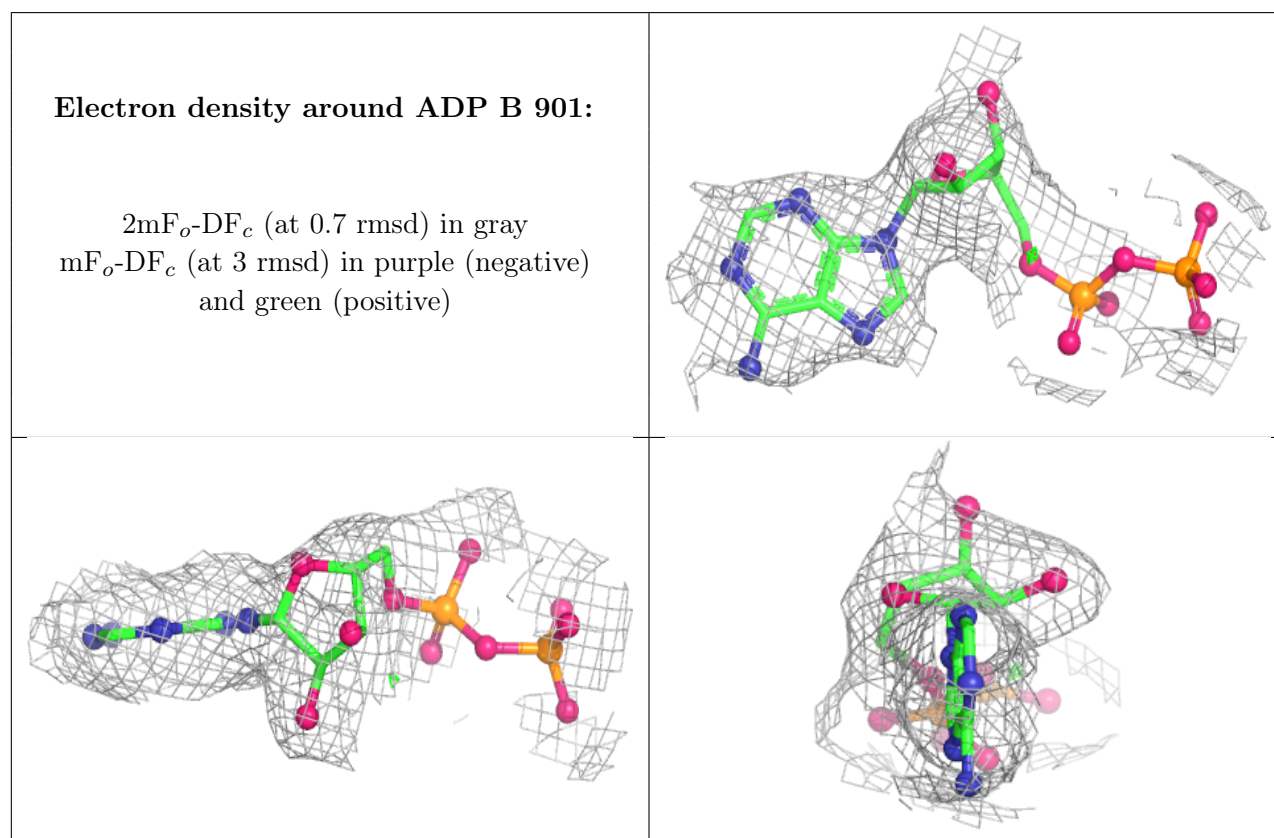
There are no oligosaccharides in this entry.

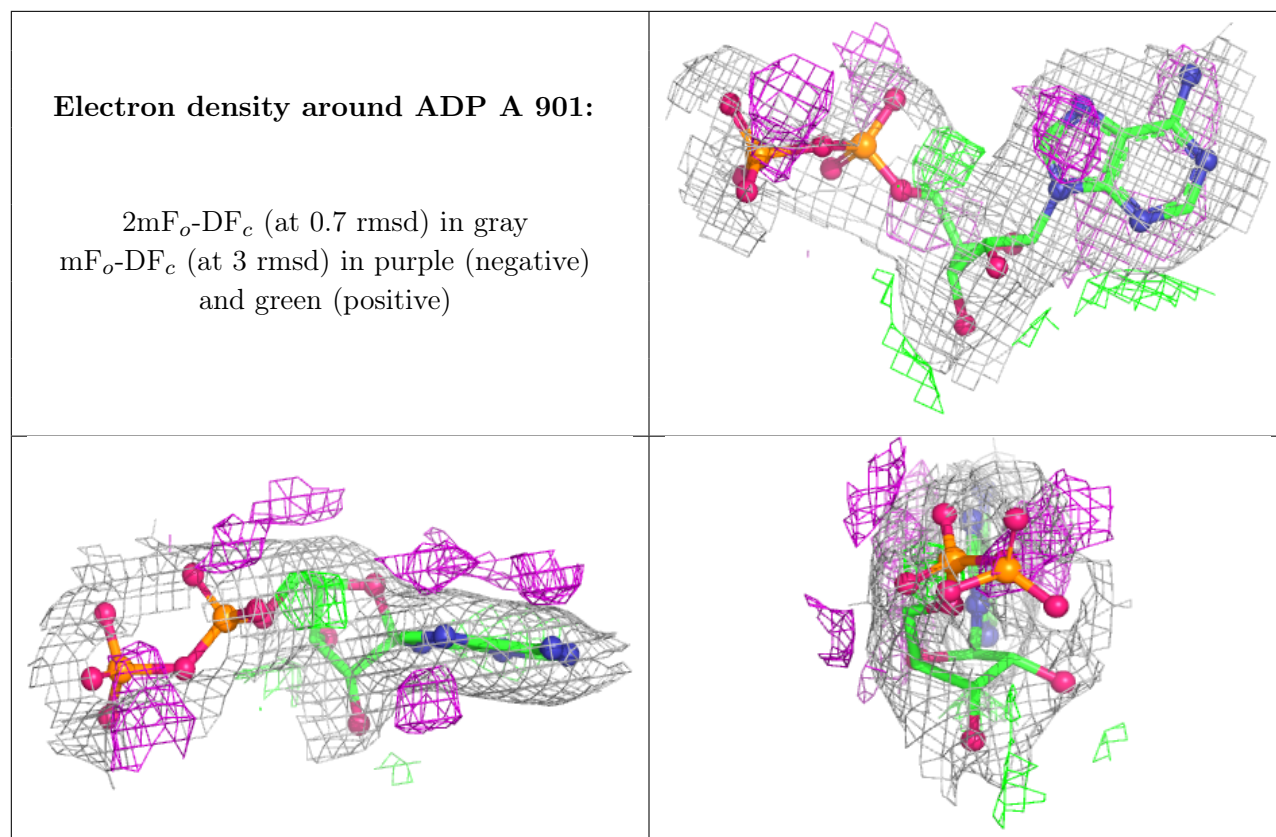
6.4 Ligands [i](#)

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
3	MG	B	903	1/1	0.84	0.09	78,78,78,78	0
4	PYR	A	903	6/6	0.84	0.13	84,99,107,112	0
2	ADP	B	901	27/27	0.92	0.09	57,74,97,121	0
3	MG	A	902	1/1	0.92	0.08	40,40,40,40	0
2	ADP	A	901	27/27	0.93	0.09	18,35,75,110	0
3	MG	A	904	1/1	0.93	0.12	87,87,87,87	0
3	MG	B	902	1/1	0.98	0.04	64,64,64,64	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.