



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:43 AM EDT

PDB ID : 5FBS / pdb_00005fbs
Title : Crystal structure of rifampin phosphotransferase RPH-Lm from *Listeria monocytogenes* in complex with ADP and magnesium
Authors : Stogios, P.J.; Wawrzak, Z.; Skarina, T.; Yim, V.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2015-12-14
Resolution : 2.59 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

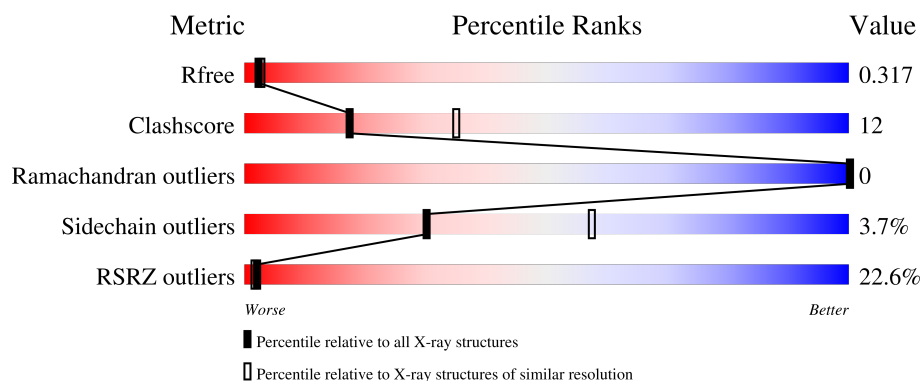
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	867	21% 65% 23% 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6238 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.

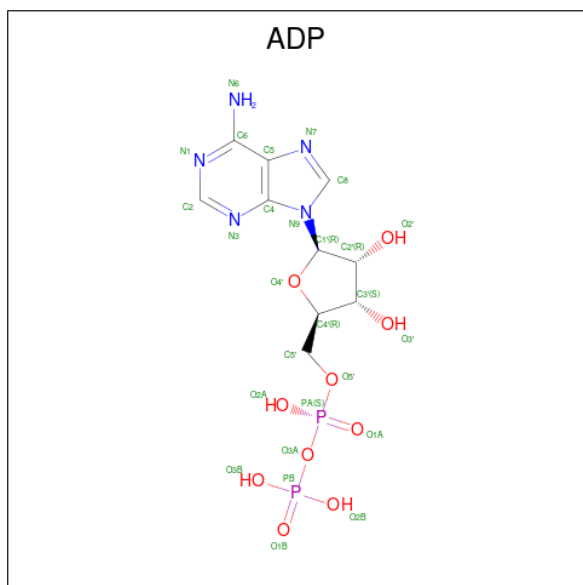
- Molecule 1 is a protein called Phosphoenolpyruvate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	787	Total	C	N	O	S	0	0	0
			6161	3916	1031	1186	28			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

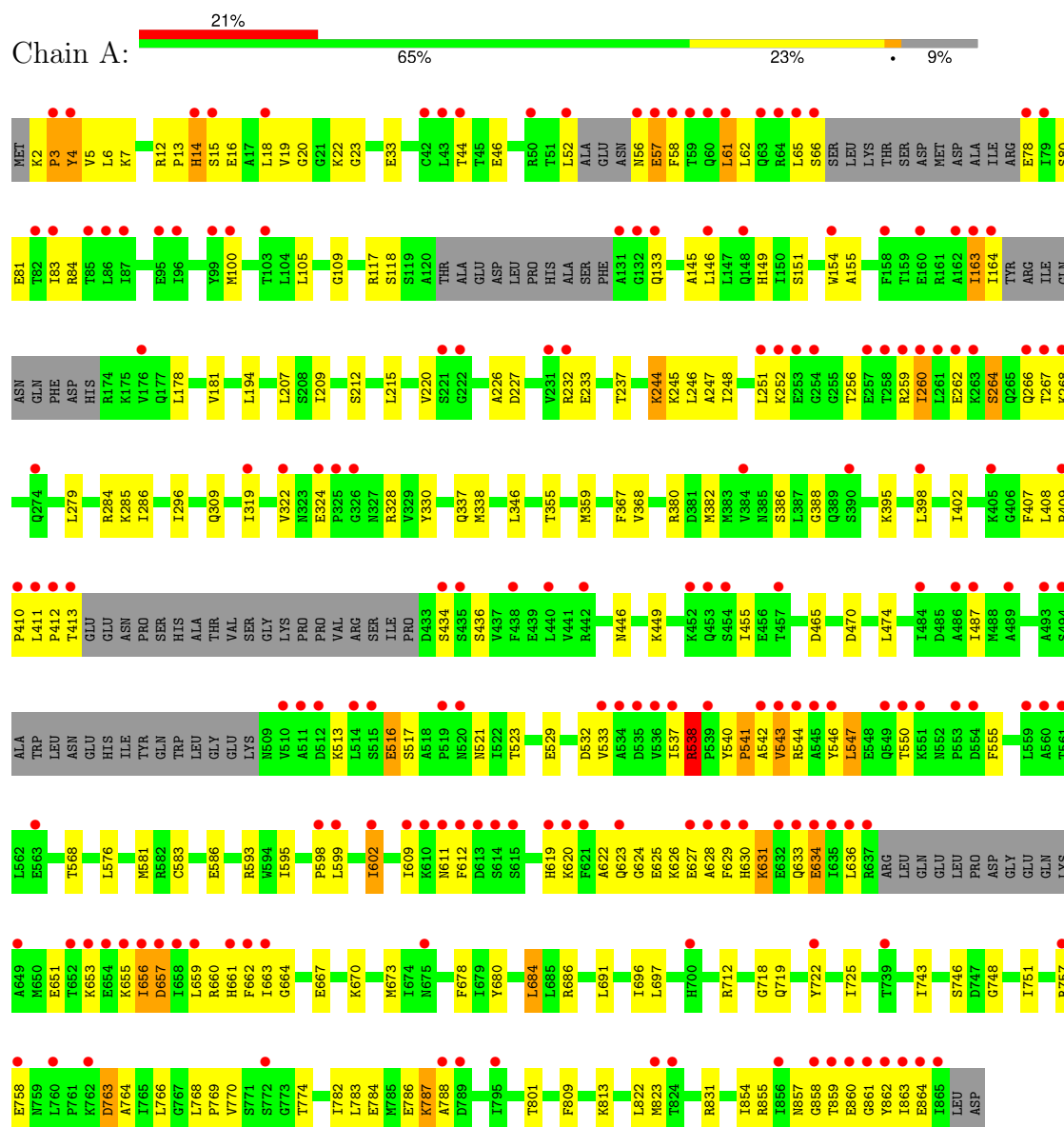
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total 49	O 49	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: Phosphoenolpyruvate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	58.51Å 58.51Å 601.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.54 – 2.59 50.54 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.54-2.59) 96.8 (50.54-2.59)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.260 , 0.318 0.264 , 0.317	Depositor DCC
R_{free} test set	1722 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 74.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6238	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: MG, ADP

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	0.47	1/6262 (0.0%)	0.94	30/8462 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	VAL	CA-C	5.53	1.59	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	612	PHE	N-CA-C	12.20	127.95	109.41
1	A	538	ARG	N-CA-C	10.49	128.06	113.16
1	A	264	SER	N-CA-C	-8.35	101.95	114.64
1	A	410	PRO	CA-N-CD	-7.71	101.21	112.00
1	A	409	PRO	O-C-N	7.70	124.85	121.31
1	A	653	LYS	N-CA-C	7.25	119.19	111.28
1	A	655	LYS	N-CA-C	-7.15	103.49	111.28
1	A	3	PRO	N-CA-C	6.70	126.27	112.47
1	A	787	LYS	N-CA-C	-6.49	104.94	112.92
1	A	163	ILE	N-CA-C	6.28	116.91	110.82
1	A	861	GLY	N-CA-C	-6.14	98.62	113.18
1	A	541	PRO	CA-C-O	6.00	128.17	119.34
1	A	634	GLU	N-CA-C	-5.97	104.77	111.28
1	A	611	ASN	N-CA-C	5.95	121.89	113.02
1	A	547	LEU	N-CA-C	5.89	119.56	112.38
1	A	657	ASP	N-CA-C	5.81	117.42	111.14
1	A	12	ARG	CA-C-N	-5.66	113.71	119.83
1	A	12	ARG	C-N-CA	-5.66	113.71	119.83
1	A	538	ARG	CA-C-N	-5.59	112.84	119.05
1	A	538	ARG	C-N-CA	-5.59	112.84	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	GLU	CA-C-N	5.58	125.28	119.64
1	A	324	GLU	C-N-CA	5.58	125.28	119.64
1	A	4	TYR	CA-C-N	-5.52	115.31	122.99
1	A	4	TYR	C-N-CA	-5.52	115.31	122.99
1	A	14	HIS	CB-CA-C	-5.51	102.13	110.06
1	A	541	PRO	N-CA-C	-5.47	106.40	113.57
1	A	859	THR	N-CA-C	5.41	119.58	111.96
1	A	57	GLU	N-CA-C	5.24	117.08	111.36
1	A	651	GLU	N-CA-C	-5.24	105.65	111.36
1	A	602	ILE	CB-CA-C	-5.00	108.95	113.70

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	6161	0	6230	155	0
2	A	1	0	0	0	0
3	A	27	0	12	1	0
4	A	49	0	0	3	0
All	All	6238	0	6242	155	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 12.

All (155) 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:782:ILE:HG23	1:A:787:LYS:HG3	1.34	1.08
1:A:380:ARG:HH21	1:A:411:LEU:HD11	1.28	0.97
1:A:380:ARG:NH2	1:A:411:LEU:HD11	1.79	0.97
1:A:757:ARG:HB2	1:A:766:LEU:HD21	1.60	0.83
1:A:633:GLN:HG2	1:A:636:LEU:HD22	1.60	0.82
1:A:61:LEU:HG	1:A:83:ILE:CG2	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:PHE:O	1:A:630:HIS:ND1	2.14	0.80
1:A:412:PRO:O	1:A:413:THR:O	2.00	0.80
1:A:44:THR:HG22	1:A:46:GLU:H	1.46	0.78
1:A:61:LEU:HG	1:A:83:ILE:HG22	1.65	0.77
1:A:338:MET:HE2	1:A:801:THR:H	1.53	0.74
1:A:768:LEU:HD12	1:A:769:PRO:HD2	1.70	0.72
1:A:857:ASN:HB3	1:A:860:GLU:O	1.91	0.70
1:A:581:MET:SD	1:A:581:MET:N	2.66	0.69
1:A:631:LYS:HE3	1:A:634:GLU:OE1	1.93	0.69
1:A:763:ASP:N	1:A:763:ASP:OD1	2.24	0.69
1:A:626:LYS:HA	1:A:629:PHE:HB3	1.73	0.69
1:A:764:ALA:HA	1:A:862:TYR:HB2	1.77	0.67
1:A:455:ILE:O	1:A:686:ARG:NH2	2.28	0.66
1:A:434:SER:HA	1:A:662:PHE:HZ	1.63	0.64
1:A:782:ILE:HD13	1:A:788:ALA:HA	1.79	0.63
1:A:337:GLN:NE2	4:A:1003:HOH:O	2.31	0.63
1:A:657:ASP:HA	1:A:660:ARG:HB2	1.79	0.63
1:A:380:ARG:HD3	1:A:402:ILE:HD13	1.79	0.63
1:A:398:LEU:O	1:A:402:ILE:HG13	2.00	0.61
1:A:13:PRO:O	1:A:14:HIS:HB2	2.00	0.61
1:A:65:LEU:O	1:A:65:LEU:HG	2.00	0.61
1:A:232:ARG:HG3	1:A:237:THR:HG21	1.83	0.61
1:A:163:ILE:HG13	1:A:164:ILE:N	2.16	0.60
1:A:163:ILE:HG13	1:A:164:ILE:HG13	1.84	0.60
1:A:355:THR:HG21	1:A:359:MET:HE3	1.83	0.60
1:A:412:PRO:O	1:A:413:THR:C	2.43	0.60
1:A:56:ASN:OD1	1:A:57:GLU:N	2.35	0.60
1:A:757:ARG:O	1:A:758:GLU:HG2	2.01	0.59
1:A:523:THR:OG1	1:A:667:GLU:OE1	2.21	0.59
1:A:670:LYS:NZ	4:A:1003:HOH:O	2.35	0.59
1:A:388:GLY:HA2	1:A:395:LYS:HB2	1.84	0.59
1:A:857:ASN:OD1	1:A:858:GLY:N	2.35	0.59
1:A:7:LYS:HD2	1:A:7:LYS:H	1.68	0.59
1:A:633:GLN:HB3	1:A:636:LEU:HB3	1.85	0.59
1:A:546:TYR:O	1:A:550:THR:OG1	2.21	0.58
1:A:80:SER:HA	1:A:83:ILE:HG12	1.84	0.58
1:A:3:PRO:O	1:A:4:TYR:HB2	2.02	0.57
1:A:245:LYS:HB2	1:A:246:LEU:HD12	1.85	0.57
1:A:538:ARG:NH2	1:A:609:ILE:HA	2.19	0.57
1:A:474:LEU:HD21	1:A:673:MET:HG3	1.87	0.57
1:A:625:GLU:HA	1:A:628:ALA:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ASN:HD22	1:A:664:GLY:HA2	1.70	0.57
1:A:145:ALA:O	1:A:149:HIS:ND1	2.32	0.57
1:A:380:ARG:NH1	1:A:402:ILE:HG23	2.20	0.57
1:A:541:PRO:HD2	1:A:542:ALA:H	1.70	0.56
1:A:81:GLU:N	1:A:81:GLU:OE1	2.38	0.56
1:A:251:LEU:HD22	1:A:252:LYS:HG2	1.87	0.56
1:A:380:ARG:HH21	1:A:411:LEU:CD1	2.09	0.56
1:A:822:LEU:O	1:A:831:ARG:NH2	2.24	0.56
1:A:757:ARG:HB2	1:A:766:LEU:CD2	2.32	0.56
1:A:207:LEU:HB2	1:A:284:ARG:HH12	1.71	0.55
1:A:470:ASP:OD2	1:A:680:TYR:OH	2.21	0.55
1:A:2:LYS:N	1:A:3:PRO:HD3	2.22	0.55
1:A:16:GLU:O	1:A:20:GLY:N	2.32	0.55
1:A:541:PRO:CD	1:A:542:ALA:H	2.16	0.55
1:A:769:PRO:HB3	1:A:858:GLY:O	2.06	0.55
1:A:163:ILE:HG13	1:A:164:ILE:H	1.72	0.55
1:A:619:HIS:O	1:A:623:GLN:N	2.37	0.54
1:A:782:ILE:HG23	1:A:787:LYS:CG	2.23	0.54
1:A:84:ARG:HG2	1:A:155:ALA:HB1	1.90	0.54
1:A:105:LEU:HA	1:A:109:GLY:HA2	1.90	0.54
1:A:544:ARG:HA	1:A:547:LEU:HD12	1.90	0.54
1:A:267:THR:HG23	1:A:268:LYS:HG2	1.89	0.53
1:A:33:GLU:O	1:A:285:LYS:NZ	2.28	0.53
1:A:209:ILE:HD13	1:A:279:LEU:HD23	1.91	0.53
1:A:100:MET:HE3	1:A:146:LEU:HD23	1.91	0.52
1:A:576:LEU:HD23	1:A:595:ILE:HG13	1.91	0.52
1:A:629:PHE:O	1:A:629:PHE:CG	2.62	0.52
1:A:784:GLU:H	1:A:787:LYS:HE3	1.74	0.52
1:A:259:ARG:HB2	1:A:259:ARG:NH1	2.25	0.52
1:A:118:SER:HB2	1:A:178:LEU:HD21	1.92	0.52
1:A:434:SER:HA	1:A:662:PHE:CZ	2.44	0.51
1:A:622:ALA:O	1:A:626:LYS:HG2	2.10	0.51
1:A:533:VAL:O	1:A:537:ILE:HG13	2.10	0.51
1:A:529:GLU:HA	1:A:532:ASP:HB2	1.91	0.51
1:A:446:ASN:HA	1:A:449:LYS:HG2	1.93	0.50
1:A:407:PHE:HD2	1:A:408:LEU:HD12	1.77	0.50
1:A:52:LEU:HD13	1:A:58:PHE:CD2	2.47	0.50
1:A:251:LEU:HD23	1:A:252:LYS:H	1.75	0.50
1:A:854:ILE:HG22	1:A:863:ILE:HG22	1.94	0.50
1:A:855:ARG:NH1	1:A:864:GLU:OE2	2.45	0.49
1:A:151:SER:HA	1:A:154:TRP:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:CYS:HB3	1:A:593:ARG:HA	1.95	0.49
1:A:691:LEU:HB3	1:A:697:LEU:HD13	1.95	0.49
1:A:813:LYS:NZ	4:A:1007:HOH:O	2.44	0.49
1:A:22:LYS:NZ	3:A:902:ADP:O3B	2.36	0.48
1:A:227:ASP:OD1	1:A:244:LYS:NZ	2.47	0.48
1:A:743:ILE:HB	1:A:751:ILE:HB	1.96	0.48
1:A:61:LEU:CG	1:A:83:ILE:HG22	2.39	0.48
1:A:117:ARG:HB2	1:A:181:VAL:HB	1.96	0.47
1:A:465:ASP:OD1	1:A:712:ARG:NH2	2.46	0.47
1:A:722:TYR:HA	1:A:725:ILE:HG12	1.95	0.47
1:A:657:ASP:OD1	1:A:661:HIS:HB2	2.14	0.47
1:A:3:PRO:HD3	1:A:18:LEU:HD21	1.97	0.46
1:A:215:LEU:HD12	1:A:248:ILE:HG22	1.98	0.46
1:A:487:ILE:HD12	1:A:487:ILE:HA	1.82	0.46
1:A:656:ILE:O	1:A:659:LEU:HB3	2.15	0.46
1:A:117:ARG:HH22	1:A:309:GLN:HB2	1.80	0.46
1:A:625:GLU:O	1:A:629:PHE:HB2	2.15	0.46
1:A:763:ASP:HB2	1:A:862:TYR:CZ	2.51	0.46
1:A:782:ILE:CG2	1:A:787:LYS:HG3	2.24	0.46
1:A:61:LEU:HG	1:A:83:ILE:HG21	1.97	0.46
1:A:538:ARG:HH22	1:A:609:ILE:HA	1.81	0.46
1:A:593:ARG:HG3	1:A:678:PHE:CD1	2.51	0.45
1:A:633:GLN:CG	1:A:636:LEU:HD22	2.40	0.45
1:A:774:THR:HG23	1:A:774:THR:O	2.14	0.45
1:A:328:ARG:HB2	1:A:746:SER:HB3	1.98	0.45
1:A:3:PRO:HG2	1:A:6:LEU:HG	1.99	0.45
1:A:541:PRO:C	1:A:543:VAL:N	2.74	0.45
1:A:246:LEU:HG	1:A:259:ARG:HH21	1.82	0.45
1:A:382:MET:O	1:A:386:SER:OG	2.26	0.44
1:A:581:MET:O	1:A:593:ARG:HD2	2.17	0.44
1:A:19:VAL:HG12	1:A:23:GLY:HA3	1.99	0.44
1:A:801:THR:HG21	1:A:809:PHE:HZ	1.83	0.44
1:A:62:LEU:O	1:A:66:SER:HB3	2.17	0.44
1:A:286:ILE:HD12	1:A:296:ILE:HD13	1.99	0.44
1:A:626:LYS:HA	1:A:629:PHE:CB	2.46	0.44
1:A:319:ILE:HD11	1:A:748:GLY:N	2.33	0.44
1:A:537:ILE:HA	1:A:568:THR:HG22	1.98	0.44
1:A:619:HIS:HA	1:A:622:ALA:HB3	1.98	0.44
1:A:212:SER:HB3	1:A:226:ALA:HB2	2.00	0.44
1:A:251:LEU:HD12	1:A:256:THR:HB	1.99	0.44
1:A:346:LEU:HD21	1:A:684:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ARG:NH2	1:A:411:LEU:CD1	2.66	0.44
1:A:696:ILE:HD13	1:A:718:GLY:HA2	1.99	0.44
1:A:18:LEU:HG	1:A:44:THR:HG23	1.98	0.44
1:A:330:TYR:HB3	1:A:367:PHE:HB3	2.00	0.44
1:A:555:PHE:CE1	1:A:598:PRO:HB2	2.53	0.43
1:A:783:LEU:H	1:A:787:LYS:HD2	1.83	0.43
1:A:541:PRO:O	1:A:543:VAL:N	2.52	0.43
1:A:194:LEU:HD13	1:A:209:ILE:HG12	1.99	0.43
1:A:657:ASP:O	1:A:661:HIS:N	2.34	0.43
1:A:555:PHE:HE1	1:A:598:PRO:HB2	1.83	0.43
1:A:3:PRO:O	1:A:5:VAL:N	2.51	0.43
1:A:247:ALA:HB2	1:A:260:ILE:HD11	1.99	0.43
1:A:359:MET:HG2	1:A:368:VAL:HG22	2.01	0.43
1:A:801:THR:HG21	1:A:809:PHE:CZ	2.53	0.42
1:A:516:GLU:O	1:A:660:ARG:NH1	2.42	0.42
1:A:599:LEU:HD12	1:A:602:ILE:HG13	2.01	0.42
1:A:540:TYR:O	1:A:543:VAL:HG12	2.19	0.42
1:A:260:ILE:HG22	1:A:264:SER:HB3	2.02	0.42
1:A:81:GLU:HG3	1:A:84:ARG:HH22	1.84	0.41
1:A:434:SER:C	1:A:436:SER:H	2.27	0.41
1:A:583:CYS:H	1:A:586:GLU:HG2	1.86	0.41
1:A:2:LYS:HB2	1:A:2:LYS:HE2	1.84	0.41
1:A:626:LYS:C	1:A:629:PHE:H	2.29	0.41
1:A:517:SER:OG	1:A:624:GLY:HA3	2.21	0.40
1:A:533:VAL:HG12	1:A:537:ILE:HD11	2.04	0.40
1:A:6:LEU:HD23	1:A:6:LEU:HA	1.83	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	771/867 (89%)	724 (94%)	47 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	675/746 (90%)	650 (96%)	25 (4%)	30	57

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	61	LEU
1	A	78	GLU
1	A	133	GLN
1	A	220	VAL
1	A	233	GLU
1	A	244	LYS
1	A	260	ILE
1	A	262	GLU
1	A	266	GLN
1	A	322	VAL
1	A	513	LYS
1	A	516	GLU
1	A	538	ARG
1	A	620	LYS
1	A	627	GLU
1	A	631	LYS
1	A	656	ILE
1	A	663	ILE
1	A	684	LEU
1	A	719	GLN
1	A	763	ASP
1	A	770	VAL

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Mol	Chain	Res	Type
1	A	786	GLU
1	A	823	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	134	HIS
1	A	294	GLN
1	A	403	ASN

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
3	ADP	A	902	2	28,29,29	1.40	4 (14%)	43,45,45	1.80	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	902	2	-	3/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	ADP	C5-C4	4.76	1.47	1.39
3	A	902	ADP	C5-C6	2.68	1.48	1.41
3	A	902	ADP	C8-N7	2.38	1.36	1.31
3	A	902	ADP	C5-N7	-2.16	1.35	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	ADP	C5-C4-N3	-5.65	118.94	126.72
3	A	902	ADP	N3-C4-N9	4.58	134.96	127.17
3	A	902	ADP	C2-N3-C4	3.63	120.69	111.83
3	A	902	ADP	C4-C5-N7	-3.31	106.80	110.58
3	A	902	ADP	N3-C2-N1	-3.26	123.65	128.58
3	A	902	ADP	C4-N9-C8	2.86	108.74	105.74
3	A	902	ADP	C5-N7-C8	2.46	107.31	103.45
3	A	902	ADP	C3'-C2'-C1'	2.27	105.77	101.46
3	A	902	ADP	C6-C5-N7	2.06	136.06	132.09
3	A	902	ADP	N9-C8-N7	-2.04	111.05	113.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

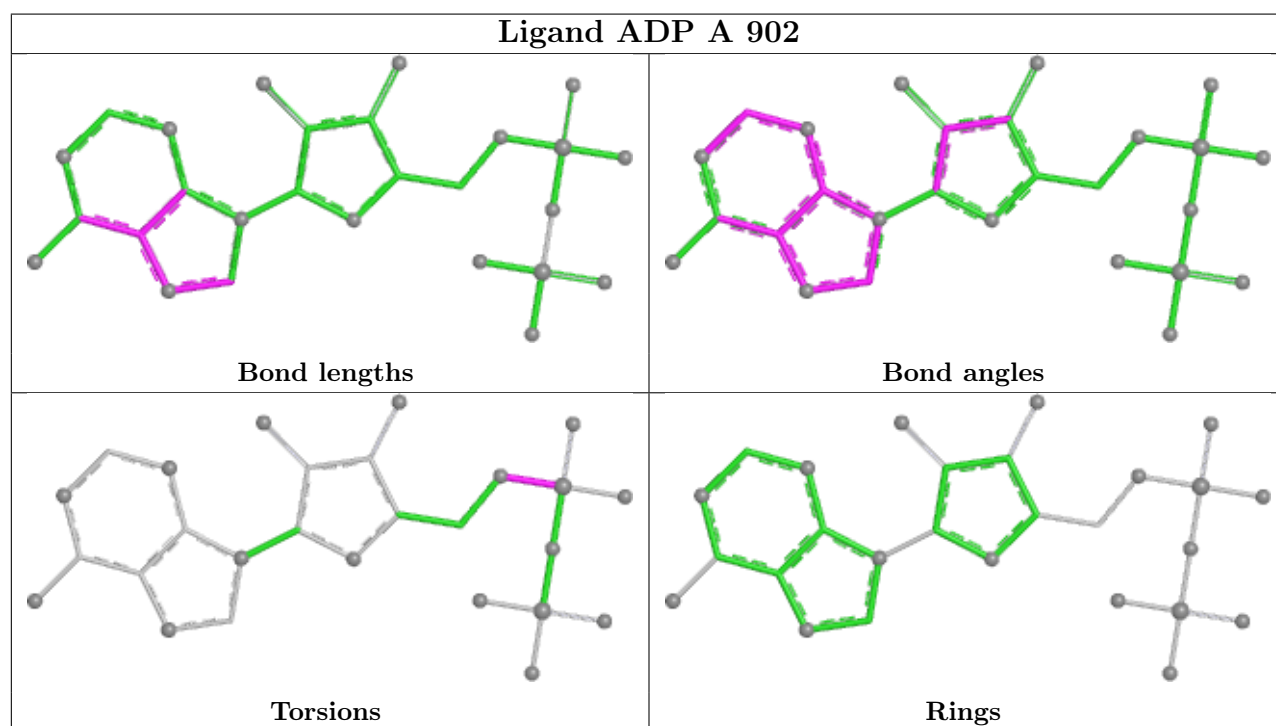
Mol	Chain	Res	Type	Atoms
3	A	902	ADP	C5'-O5'-PA-O1A
3	A	902	ADP	C5'-O5'-PA-O2A
3	A	902	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	ADP	1	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	787/867 (90%)	1.21	178 (22%) 2 2	36, 68, 135, 220	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	858	GLY	6.5
1	A	635	ILE	6.5
1	A	65	LEU	6.2
1	A	543	VAL	5.9
1	A	267	THR	5.6
1	A	859	THR	5.4
1	A	861	GLY	5.4
1	A	164	ILE	5.2
1	A	536	VAL	5.2
1	A	636	LEU	5.0
1	A	232	ARG	4.9
1	A	435	SER	4.7
1	A	788	ALA	4.7
1	A	862	TYR	4.7
1	A	860	GLU	4.7
1	A	629	PHE	4.5
1	A	262	GLU	4.4
1	A	649	ALA	4.3
1	A	627	GLU	4.3
1	A	259	ARG	4.3
1	A	612	PHE	4.2
1	A	56	ASN	4.2
1	A	63	GLN	4.2
1	A	266	GLN	4.0
1	A	656	ILE	3.9
1	A	257	GLU	3.9
1	A	632	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	662	PHE	3.8
1	A	3	PRO	3.8
1	A	252	LYS	3.7
1	A	154	TRP	3.7
1	A	510	VAL	3.6
1	A	772	SER	3.6
1	A	434	SER	3.6
1	A	546	TYR	3.6
1	A	15	SER	3.6
1	A	438	PHE	3.6
1	A	549	GLN	3.5
1	A	131	ALA	3.5
1	A	652	THR	3.5
1	A	511	ALA	3.5
1	A	52	LEU	3.5
1	A	325	PRO	3.5
1	A	412	PRO	3.5
1	A	760	LEU	3.5
1	A	44	THR	3.4
1	A	261	LEU	3.4
1	A	319	ILE	3.4
1	A	326	GLY	3.4
1	A	611	ASN	3.3
1	A	864	GLU	3.3
1	A	162	ALA	3.3
1	A	390	SER	3.3
1	A	657	ASP	3.3
1	A	628	ALA	3.3
1	A	253	GLU	3.2
1	A	544	ARG	3.2
1	A	863	ILE	3.2
1	A	487	ILE	3.2
1	A	79	ILE	3.1
1	A	95	GLU	3.1
1	A	534	ALA	3.0
1	A	324	GLU	3.0
1	A	762	LYS	3.0
1	A	4	TYR	3.0
1	A	554	ASP	3.0
1	A	66	SER	3.0
1	A	87	ILE	3.0
1	A	661	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	158	PHE	3.0
1	A	545	ALA	2.9
1	A	133	GLN	2.9
1	A	274	GLN	2.9
1	A	82	THR	2.9
1	A	659	LEU	2.9
1	A	512	ASP	2.8
1	A	675	ASN	2.8
1	A	865	ILE	2.8
1	A	757	ARG	2.8
1	A	160	GLU	2.8
1	A	610	LYS	2.8
1	A	493	ALA	2.7
1	A	630	HIS	2.7
1	A	99	TYR	2.7
1	A	824	THR	2.7
1	A	410	PRO	2.7
1	A	655	LYS	2.7
1	A	18	LEU	2.7
1	A	61	LEU	2.6
1	A	457	THR	2.6
1	A	633	GLN	2.6
1	A	163	ILE	2.6
1	A	494	SER	2.6
1	A	486	ALA	2.6
1	A	58	PHE	2.6
1	A	614	SER	2.6
1	A	620	LYS	2.6
1	A	789	ASP	2.5
1	A	619	HIS	2.5
1	A	700	HIS	2.5
1	A	83	ILE	2.5
1	A	654	GLU	2.5
1	A	563	GLU	2.5
1	A	146	LEU	2.5
1	A	268	LYS	2.5
1	A	519	PRO	2.5
1	A	602	ILE	2.5
1	A	86	LEU	2.5
1	A	60	GLN	2.5
1	A	258	THR	2.5
1	A	535	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	637	ARG	2.4
1	A	42	CYS	2.4
1	A	514	LEU	2.4
1	A	599	LEU	2.4
1	A	542	ALA	2.4
1	A	221	SER	2.4
1	A	653	LYS	2.4
1	A	856	ILE	2.4
1	A	43	LEU	2.4
1	A	148	GLN	2.4
1	A	251	LEU	2.4
1	A	57	GLU	2.4
1	A	409	PRO	2.4
1	A	453	GLN	2.3
1	A	452	LYS	2.3
1	A	489	ALA	2.3
1	A	615	SER	2.3
1	A	222	GLY	2.3
1	A	263	LYS	2.3
1	A	14	HIS	2.3
1	A	613	ASP	2.3
1	A	722	TYR	2.3
1	A	484	ILE	2.3
1	A	559	LEU	2.3
1	A	78	GLU	2.3
1	A	260	ILE	2.2
1	A	405	LYS	2.2
1	A	411	LEU	2.2
1	A	795	ILE	2.2
1	A	598	PRO	2.2
1	A	398	LEU	2.2
1	A	823	MET	2.2
1	A	96	ILE	2.2
1	A	176	VAL	2.2
1	A	553	PRO	2.2
1	A	413	THR	2.2
1	A	739	THR	2.2
1	A	609	ILE	2.2
1	A	533	VAL	2.2
1	A	551	LYS	2.2
1	A	560	ALA	2.2
1	A	537	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	454	SER	2.2
1	A	50	ARG	2.2
1	A	539	PRO	2.2
1	A	59	THR	2.1
1	A	132	GLY	2.1
1	A	550	THR	2.1
1	A	64	ARG	2.1
1	A	758	GLU	2.1
1	A	658	ILE	2.1
1	A	442	ARG	2.1
1	A	100	MET	2.1
1	A	621	PHE	2.1
1	A	623	GLN	2.1
1	A	561	THR	2.1
1	A	231	VAL	2.1
1	A	440	LEU	2.1
1	A	634	GLU	2.1
1	A	384	VAL	2.0
1	A	520	ASN	2.0
1	A	85	THR	2.0
1	A	103	THR	2.0
1	A	663	ILE	2.0
1	A	322	VAL	2.0
1	A	254	GLY	2.0
1	A	515	SER	2.0

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

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

6.3 Carbohydrates ⓘ

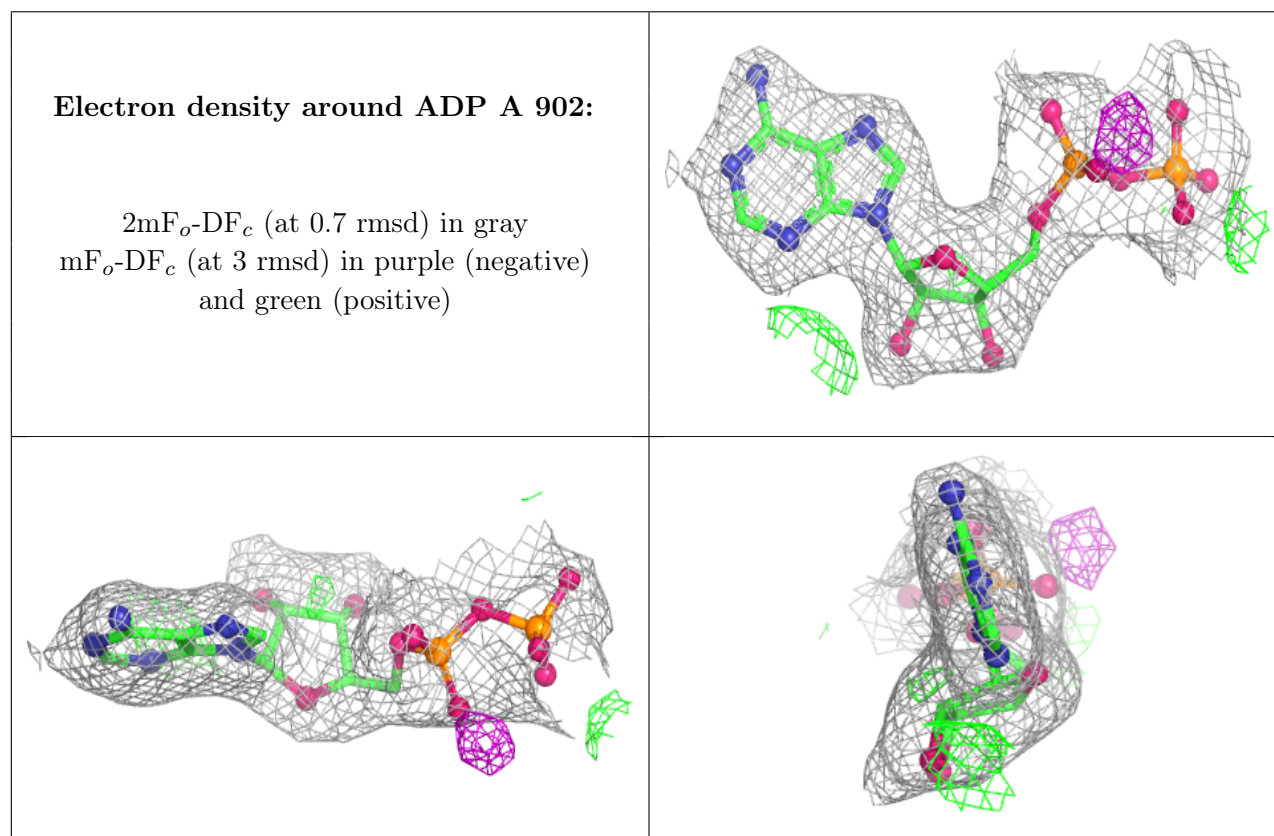
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
3	ADP	A	902	27/27	0.93	0.12	37,58,81,242	0
2	MG	A	901	1/1	0.97	0.11	36,36,36,36	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.