



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:09 AM UTC

PDB ID : 8PO7 / pdb_00008po7
Title : Structure of Escherichia coli HrpA in complex with ADP and dinucleotide dCdC
Authors : Xin, B.G.; Yuan, L.G.; Zhang, L.L.; Xie, S.M.; Liu, N.N.; Ai, X.; Li, H.H.; Rety, S.; Xi, X.G.
Deposited on : 2023-07-03
Resolution : 2.26 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

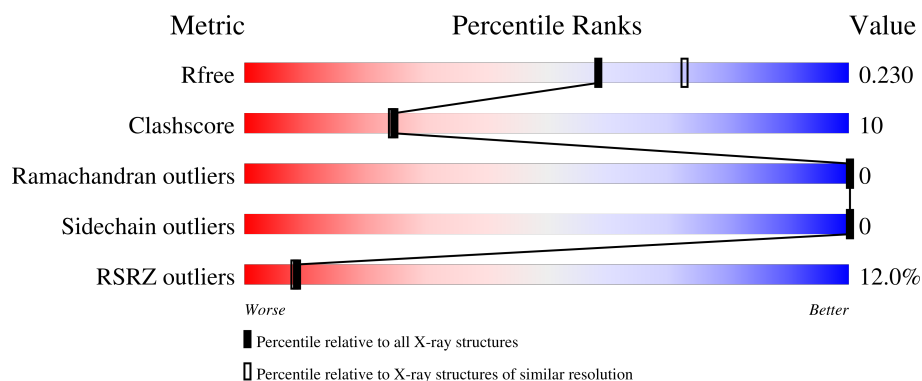
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	758	 9% 67% 11% 22%
1	B	758	 10% 62% 14% 24%
2	C	2	 50% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10066 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 ATP-dependent RNA helicase HrpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	0	0
			4742	2974	864	888	16			
1	B	579	Total	C	N	O	S	0	0	0
			4641	2909	850	866	16			

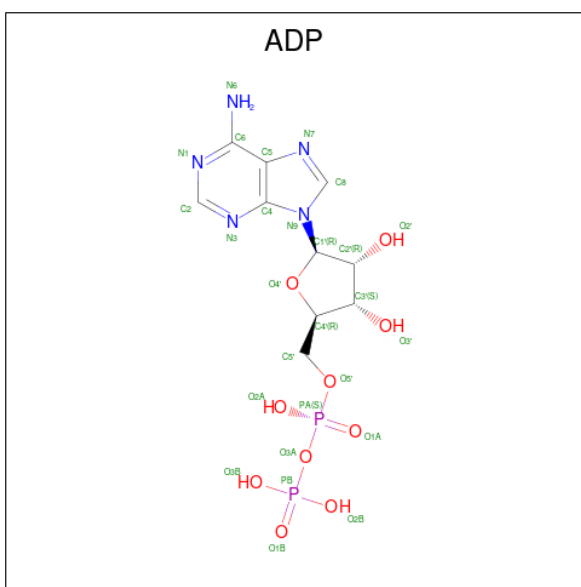
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	ASN	ASP	conflict	UNP P43329
A	290	PRO	HIS	conflict	UNP P43329
B	162	ASN	ASP	conflict	UNP P43329
B	290	PRO	HIS	conflict	UNP P43329

- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	P	0	0	0
			39	18	6	13	2			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



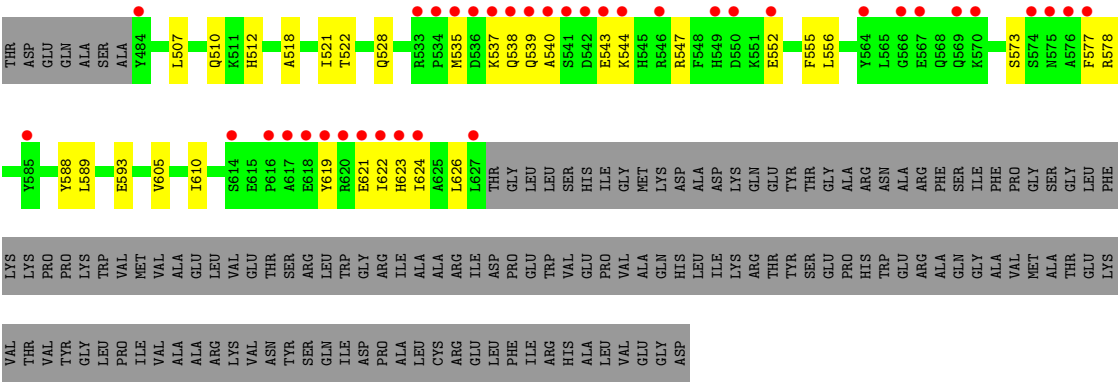
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	300	Total	O	0	0
			300	300		
6	B	282	Total	O	0	0
			282	282		
6	C	1	Total	O	0	0
			1	1		

- Molecule 1: ATP-dependent RNA helicase HrpA





● Molecule 2: DNA (5'-D(P*CP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.47Å 106.12Å 178.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.14 – 2.26 89.14 – 2.26	Depositor EDS
% Data completeness (in resolution range)	96.6 (89.14-2.26) 96.6 (89.14-2.26)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.190 , 0.232 0.188 , 0.230	Depositor DCC
R_{free} test set	3466 reflections (2.73%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.1	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	0.93	EDS
Total number of atoms	10066	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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, 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	0.42	1/4815 (0.0%)	0.66	6/6508 (0.1%)
1	B	0.37	0/4714	0.70	10/6366 (0.2%)
2	C	0.22	0/42	0.55	0/60
All	All	0.39	1/9571 (0.0%)	0.68	16/12934 (0.1%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	528	GLN	CD-OE1	6.36	1.35	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	ARG	CB-CA-C	-9.96	90.06	110.38
1	B	274	GLN	CB-CG-CD	-9.12	97.10	112.60
1	B	467	ARG	CA-CB-CG	8.34	130.79	114.10
1	A	75	ASP	CB-CA-C	-7.32	98.63	110.79
1	B	467	ARG	CB-CA-C	7.18	122.30	110.81
1	A	402	ARG	N-CA-CB	6.83	120.81	110.30
1	B	272	ARG	N-CA-CB	6.31	120.02	110.30
1	A	337	GLN	N-CA-CB	-5.42	101.80	110.63
1	B	274	GLN	N-CA-CB	-5.41	102.23	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	ARG	NE-CZ-NH2	-5.36	114.38	119.20
1	B	274	GLN	CA-CB-CG	5.18	124.47	114.10
1	A	528	GLN	CA-CB-CG	5.18	124.46	114.10
1	B	467	ARG	N-CA-CB	-5.18	102.22	109.94
1	A	494	SER	CB-CA-C	-5.14	99.47	110.32
1	B	467	ARG	CG-CD-NE	-5.11	100.77	112.00
1	B	274	GLN	CB-CA-C	5.06	118.90	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	569	GLN	Peptide
1	A	620	ARG	Peptide

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	4742	0	4831	95	0
1	B	4641	0	4722	91	1
2	C	39	0	23	1	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	5	0	0	1	0
6	A	300	0	0	7	1
6	B	282	0	0	5	0
6	C	1	0	0	1	0
All	All	10066	0	9600	187	1

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 10.

All (187) 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:B:464:ASP:OD1	1:B:467:ARG:NH1	1.89	1.05
1:A:606:LYS:NZ	6:A:2102:HOH:O	1.91	1.04
1:A:579:ARG:O	1:A:582:ARG:NH2	1.96	0.98
1:B:132:ARG:HB2	1:B:159:ARG:HH22	1.29	0.96
1:A:297:MET:CE	1:A:302:GLU:HG2	1.95	0.95
1:B:297:MET:HE1	1:B:306:THR:OG1	1.67	0.92
1:A:356:THR:OG1	6:A:2101:HOH:O	1.88	0.91
1:A:567:GLU:O	6:A:2103:HOH:O	1.91	0.88
1:A:297:MET:HE2	1:A:302:GLU:HG2	1.55	0.87
1:A:297:MET:HE1	1:A:306:THR:OG1	1.76	0.85
1:B:512:HIS:HB3	1:B:621:GLU:HB2	1.60	0.84
1:A:579:ARG:O	1:A:582:ARG:CZ	2.26	0.83
1:A:271:GLU:HG3	1:A:589:LEU:HD21	1.62	0.81
1:A:402:ARG:NH1	6:A:2104:HOH:O	2.12	0.80
1:B:272:ARG:O	1:B:276:GLN:N	2.10	0.79
1:B:16:LEU:HD13	1:B:24:ARG:HG3	1.62	0.79
1:B:297:MET:CE	1:B:302:GLU:HG2	2.16	0.76
1:B:132:ARG:HB2	1:B:159:ARG:NH2	2.01	0.75
1:A:333:ASN:O	1:A:337:GLN:HG3	1.88	0.74
1:A:620:ARG:HB2	1:A:623:HIS:CG	2.23	0.73
1:A:579:ARG:C	1:A:582:ARG:HH21	1.95	0.73
1:A:579:ARG:HA	1:A:582:ARG:HE	1.54	0.73
1:B:297:MET:HE2	1:B:302:GLU:HG2	1.71	0.72
1:A:435:SER:O	1:A:439:GLN:HG3	1.89	0.72
1:A:297:MET:HE2	1:A:302:GLU:CG	2.20	0.71
1:A:324:TYR:H	1:A:327:LEU:HD21	1.57	0.70
1:B:552:GLU:CD	1:B:623:HIS:HD1	1.99	0.70
1:A:620:ARG:HA	1:A:623:HIS:H	1.57	0.69
1:B:271:GLU:OE2	1:B:578:ARG:HG2	1.91	0.69
2:C:2:DC:O3'	6:C:101:HOH:O	2.10	0.69
1:A:329:ASN:HA	1:A:332:GLN:HB3	1.76	0.68
1:A:324:TYR:O	1:A:327:LEU:HD23	1.93	0.68
1:A:333:ASN:OD1	1:A:337:GLN:NE2	2.23	0.68
1:B:556:LEU:HD11	1:B:623:HIS:NE2	2.11	0.66
1:B:439:GLN:OE1	6:B:2102:HOH:O	2.13	0.66
1:A:324:TYR:HB2	1:A:327:LEU:CD2	2.26	0.66
1:A:375:SER:OG	1:A:377:ARG:O	2.11	0.64
1:A:621:GLU:HA	1:A:624:ILE:HG22	1.78	0.63
1:B:556:LEU:HD11	1:B:623:HIS:CE1	2.34	0.63
1:B:528:GLN:NE2	5:B:2003:PO4:O3	2.32	0.62
1:B:356:THR:CG2	1:B:402:ARG:NH2	2.63	0.61
1:A:297:MET:HE2	1:A:302:GLU:CD	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:TYR:O	1:B:327:LEU:HG	1.99	0.61
1:A:357:VAL:O	6:A:2104:HOH:O	2.16	0.61
1:A:587:ASN:HB3	1:A:590:ARG:HE	1.66	0.61
1:A:579:ARG:O	1:A:582:ARG:NE	2.35	0.60
1:A:619:TYR:CE2	1:A:620:ARG:HG2	2.36	0.60
1:B:297:MET:HE1	1:B:306:THR:HG1	1.65	0.60
1:A:297:MET:HE1	1:A:302:GLU:HG2	1.84	0.59
1:B:329:ASN:HA	1:B:332:GLN:HG3	1.83	0.59
1:A:329:ASN:HA	1:A:332:GLN:CB	2.32	0.59
1:A:622:ILE:O	1:A:626:LEU:HD12	2.03	0.58
1:A:620:ARG:CA	1:A:623:HIS:H	2.16	0.58
1:B:292:ASP:OD2	1:B:339:HIS:NE2	2.36	0.58
1:B:61:VAL:HB	1:B:62:LEU:HD12	1.86	0.57
1:B:356:THR:OG1	6:B:2101:HOH:O	1.93	0.57
1:A:504:ARG:NH1	1:A:508:GLU:OE2	2.34	0.56
1:B:297:MET:HE2	1:B:302:GLU:CG	2.36	0.56
1:A:14:GLN:OE1	1:A:14:GLN:O	2.22	0.56
1:A:620:ARG:HA	1:A:623:HIS:N	2.20	0.56
1:A:437:ILE:O	1:A:441:THR:HG23	2.05	0.56
1:A:332:GLN:O	1:A:335:VAL:HG22	2.05	0.56
1:B:272:ARG:HG2	1:B:276:GLN:HB2	1.88	0.56
1:B:622:ILE:O	1:B:626:LEU:HG	2.06	0.56
1:B:539:GLN:HG3	1:B:540:ALA:N	2.21	0.56
1:B:132:ARG:HG3	1:B:158:VAL:HB	1.88	0.55
1:A:87:LEU:HG	1:A:117:LEU:HG	1.87	0.55
1:A:324:TYR:H	1:A:327:LEU:CD2	2.19	0.55
1:B:324:TYR:HD2	1:B:327:LEU:HD21	1.72	0.55
1:A:620:ARG:C	1:A:622:ILE:N	2.65	0.54
1:A:511:LYS:HE3	1:A:512:HIS:CE1	2.41	0.54
1:B:58:ALA:O	1:B:62:LEU:CD1	2.56	0.54
1:B:374:TYR:CD1	1:B:432:ASN:HB3	2.42	0.54
1:A:565:LEU:HD21	1:A:586:LEU:HD13	1.88	0.54
1:A:213:LEU:HD13	1:A:225:ILE:HD12	1.90	0.53
1:A:335:VAL:HG23	1:A:336:PHE:CD2	2.42	0.53
1:B:375:SER:HB3	1:B:378:THR:HG22	1.90	0.53
1:B:356:THR:CG2	1:B:402:ARG:HH22	2.21	0.53
1:A:297:MET:HE1	1:A:306:THR:HG1	1.74	0.53
1:A:582:ARG:HB2	1:A:582:ARG:NH1	2.23	0.53
1:A:605:VAL:HG13	1:A:610:ILE:HB	1.91	0.52
1:B:552:GLU:OE1	1:B:623:HIS:ND1	2.41	0.52
1:B:621:GLU:HA	1:B:624:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:O	1:A:337:GLN:HB2	2.10	0.52
1:A:132:ARG:HG3	1:A:158:VAL:HB	1.92	0.52
1:A:579:ARG:HD2	1:A:582:ARG:HH21	1.73	0.52
1:A:579:ARG:CA	1:A:582:ARG:HE	2.23	0.52
1:A:334:ARG:HA	1:A:337:GLN:CG	2.40	0.51
1:B:279:PHE:HZ	1:B:309:ALA:HB1	1.74	0.51
1:A:334:ARG:HA	1:A:337:GLN:HB2	1.92	0.51
1:B:27:PHE:CZ	1:B:53:GLU:O	2.63	0.51
1:B:16:LEU:HG	6:B:2248:HOH:O	2.09	0.51
1:B:21:LEU:HD11	1:B:192:ASP:HB3	1.92	0.51
1:B:521:ILE:HD13	1:B:555:PHE:HB3	1.92	0.51
1:A:75:ASP:N	1:A:75:ASP:OD1	2.41	0.51
1:A:272:ARG:O	1:A:276:GLN:HG3	2.10	0.51
1:B:272:ARG:NH2	1:B:276:GLN:OE1	2.43	0.51
1:B:333:ASN:O	1:B:336:PHE:N	2.41	0.51
1:A:297:MET:SD	1:A:303:ILE:HA	2.51	0.50
1:B:356:THR:HG21	1:B:402:ARG:NH2	2.25	0.50
1:B:415:ASP:OD2	6:B:2103:HOH:O	2.19	0.50
1:B:187:LEU:HD21	1:B:219:ARG:NH2	2.25	0.50
1:A:91:ARG:HB2	1:A:117:LEU:HD21	1.94	0.50
1:B:15:ARG:HG2	6:B:2248:HOH:O	2.10	0.50
1:A:619:TYR:CD2	1:A:620:ARG:HG2	2.46	0.50
1:A:297:MET:CE	1:A:306:THR:OG1	2.54	0.50
1:B:58:ALA:O	1:B:62:LEU:HD13	2.12	0.50
1:A:25:LEU:HD22	1:A:189:MET:HE3	1.92	0.50
1:A:579:ARG:HD2	1:A:582:ARG:NH2	2.28	0.49
1:B:51:ALA:O	1:B:54:ILE:HB	2.11	0.49
1:B:271:GLU:O	1:B:275:LEU:N	2.41	0.49
1:B:297:MET:SD	1:B:303:ILE:HA	2.53	0.49
1:A:213:LEU:O	1:A:217:LEU:HG	2.13	0.49
1:B:573:SER:O	1:B:577:PHE:N	2.43	0.48
1:A:336:PHE:HA	1:A:358:PRO:HG3	1.96	0.48
1:B:378:THR:O	1:B:380:VAL:HG23	2.13	0.48
1:B:537:LYS:C	1:B:539:GLN:N	2.70	0.48
1:B:15:ARG:HD3	1:B:15:ARG:H	1.78	0.48
1:A:568:GLN:O	1:A:572:LEU:HD12	2.14	0.48
1:B:297:MET:HE2	1:B:302:GLU:CD	2.38	0.48
1:A:360:ILE:HB	6:A:2104:HOH:O	2.14	0.47
1:B:16:LEU:HD11	1:B:28:SER:OG	2.14	0.47
1:B:371:ILE:O	1:B:384:PRO:HD2	2.13	0.47
1:B:52:LYS:C	1:B:54:ILE:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ARG:NE	1:B:276:GLN:OE1	2.45	0.47
1:B:18:SER:HA	1:B:122:LYS:NZ	2.30	0.46
1:B:329:ASN:HA	1:B:332:GLN:CG	2.46	0.46
1:B:375:SER:CB	1:B:378:THR:HG22	2.45	0.46
1:A:620:ARG:HD3	1:A:623:HIS:ND1	2.31	0.46
1:B:605:VAL:HG13	1:B:610:ILE:HB	1.96	0.46
1:A:271:GLU:OE1	1:A:578:ARG:HD3	2.15	0.46
1:B:315:LEU:HB2	1:B:318:THR:HB	1.98	0.46
1:A:374:TYR:CD2	1:A:432:ASN:HB3	2.50	0.46
1:A:570:LYS:HD3	1:A:570:LYS:HA	1.60	0.46
1:B:539:GLN:O	1:B:543:GLU:HG3	2.15	0.46
1:B:537:LYS:C	1:B:539:GLN:H	2.23	0.46
1:B:544:LYS:HG3	1:B:547:ARG:HE	1.80	0.46
1:B:16:LEU:HD21	1:B:28:SER:OG	2.16	0.45
1:B:334:ARG:O	1:B:343:ARG:NH1	2.49	0.45
1:B:619:TYR:HE1	1:B:623:HIS:ND1	2.15	0.45
1:A:206:ILE:O	1:A:210:LEU:HG	2.17	0.45
1:A:378:THR:O	1:A:380:VAL:HG23	2.17	0.45
1:B:23:ASP:OD2	1:B:60:LYS:HE2	2.17	0.45
1:A:329:ASN:CA	1:A:332:GLN:HB3	2.45	0.45
1:B:589:LEU:HA	1:B:589:LEU:HD23	1.79	0.45
1:A:361:LYS:O	1:A:400:CYS:HB2	2.17	0.44
1:B:291:GLY:O	1:B:342:ARG:HD3	2.17	0.44
1:A:587:ASN:HB3	1:A:590:ARG:NE	2.31	0.44
1:A:619:TYR:OH	6:A:2105:HOH:O	2.20	0.44
1:B:538:GLN:O	1:B:538:GLN:HG3	2.16	0.44
1:A:356:THR:HG22	1:A:402:ARG:NH2	2.32	0.44
1:A:613:ASN:OD1	1:A:613:ASN:N	2.48	0.44
1:B:370:ARG:NE	1:B:593:GLU:HG3	2.33	0.44
1:A:329:ASN:C	1:A:332:GLN:HB3	2.42	0.43
1:B:275:LEU:HD21	1:B:279:PHE:CZ	2.53	0.43
1:B:331:GLU:HA	1:B:334:ARG:HG2	1.99	0.43
1:B:58:ALA:O	1:B:62:LEU:HD12	2.18	0.43
1:B:379:LYS:N	1:B:379:LYS:HD2	2.33	0.43
1:B:275:LEU:HD13	1:B:578:ARG:CZ	2.49	0.43
1:B:518:ALA:O	1:B:522:THR:HG23	2.19	0.43
1:B:470:GLU:HG3	1:B:475:ILE:HD11	2.00	0.43
1:A:504:ARG:HH12	1:A:508:GLU:CD	2.25	0.43
1:B:304:ARG:HE	1:B:304:ARG:HB3	1.71	0.43
1:B:22:ARG:NH2	1:B:190:GLN:HB2	2.34	0.42
1:B:535:MET:HE2	1:B:535:MET:HB3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLN:OE1	1:A:14:GLN:C	2.62	0.42
1:A:517:GLU:HA	1:A:520:ILE:HD12	2.00	0.42
1:A:579:ARG:CD	1:A:582:ARG:HH21	2.32	0.42
1:A:73:TYR:CE1	1:A:83:LYS:HD2	2.54	0.42
1:B:271:GLU:HG3	1:B:588:TYR:HB2	2.01	0.42
1:B:272:ARG:HG3	1:B:275:LEU:HB3	2.01	0.42
1:B:535:MET:HG2	1:B:535:MET:O	2.19	0.42
1:A:324:TYR:C	1:A:327:LEU:HD23	2.45	0.42
1:A:463:GLN:HB3	1:A:467:ARG:NH2	2.35	0.41
1:A:620:ARG:CA	1:A:622:ILE:H	2.33	0.41
1:A:75:ASP:OD1	1:A:76:ASN:N	2.54	0.41
1:B:99:ALA:HA	1:B:229:SER:O	2.20	0.41
1:B:433:LEU:HD13	1:B:461:ASN:HB2	2.03	0.41
1:A:508:GLU:CD	1:A:511:LYS:HE2	2.46	0.41
1:B:507:LEU:O	1:B:510:GLN:HB3	2.20	0.41
1:A:579:ARG:C	1:A:579:ARG:HD2	2.46	0.41
1:A:334:ARG:HA	1:A:337:GLN:CB	2.50	0.41
1:A:530:PRO:HA	1:A:590:ARG:HB3	2.02	0.41
1:A:6:LYS:HD2	1:A:6:LYS:HA	1.68	0.40
1:A:582:ARG:CZ	1:A:582:ARG:HB2	2.51	0.40
1:A:591:VAL:O	1:A:595:GLN:HG3	2.22	0.40
1:B:292:ASP:CG	1:B:343:ARG:HB3	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLU:OE1	6:A:2102:HOH:O[1_655]	2.03	0.17

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	588/758 (78%)	582 (99%)	6 (1%)	0	100	100
1	B	571/758 (75%)	567 (99%)	4 (1%)	0	100	100
All	All	1159/1516 (76%)	1149 (99%)	10 (1%)	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	519/657 (79%)	519 (100%)	0	100	100
1	B	508/657 (77%)	508 (100%)	0	100	100
All	All	1027/1314 (78%)	1027 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	162	ASN
1	A	163	HIS
1	A	311	ASN
1	A	461	ASN
1	A	528	GLN
1	A	575	ASN
1	A	600	GLN
1	B	163	HIS
1	B	240	HIS
1	B	332	GLN

5.3.3 RNA ⓘ

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 5 ligands modelled in this entry, 2 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	$\# Z > 2$
3	ADP	A	2001	4	28,29,29	1.38	5 (17%)	43,45,45	2.02	13 (30%)
5	PO4	B	2003	-	4,4,4	0.91	0	6,6,6	0.49	0
3	ADP	B	2001	4	28,29,29	1.36	5 (17%)	43,45,45	1.85	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	2001	4	-	1/16/32/32	0/3/3/3
3	ADP	B	2001	4	-	1/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	ADP	C5-C4	4.53	1.47	1.39
3	A	2001	ADP	C5-C4	4.51	1.47	1.39
3	B	2001	ADP	C5-C6	2.63	1.48	1.41
3	A	2001	ADP	C5-C6	2.53	1.48	1.41
3	B	2001	ADP	C4-N9	-2.34	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	ADP	C8-N7	2.34	1.36	1.31
3	A	2001	ADP	C5-N7	-2.25	1.35	1.39
3	B	2001	ADP	C5-N7	-2.16	1.35	1.39
3	A	2001	ADP	PA-O3A	2.14	1.61	1.59
3	B	2001	ADP	C8-N7	2.10	1.35	1.31

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	ADP	C5-C4-N3	-5.38	119.31	126.72
3	B	2001	ADP	C5-C4-N3	-4.99	119.85	126.72
3	A	2001	ADP	N3-C4-N9	4.50	134.81	127.17
3	A	2001	ADP	C2'-C1'-N9	-4.37	102.45	113.30
3	B	2001	ADP	N3-C4-N9	4.31	134.50	127.17
3	A	2001	ADP	N3-C2-N1	-3.66	123.04	128.58
3	B	2001	ADP	C2'-C1'-N9	-3.62	104.31	113.30
3	A	2001	ADP	C2-N3-C4	3.56	120.53	111.83
3	B	2001	ADP	N3-C2-N1	-3.46	123.34	128.58
3	B	2001	ADP	C2-N3-C4	3.44	120.24	111.83
3	B	2001	ADP	C4-N9-C8	3.37	109.27	105.74
3	A	2001	ADP	O4'-C1'-N9	3.17	114.19	108.09
3	A	2001	ADP	C4-C5-N7	-3.05	107.09	110.58
3	A	2001	ADP	C4-N9-C8	3.02	108.91	105.74
3	B	2001	ADP	C4-C5-N7	-2.90	107.27	110.58
3	A	2001	ADP	C3'-C2'-C1'	2.81	106.78	101.46
3	A	2001	ADP	C5-N7-C8	2.49	107.36	103.45
3	A	2001	ADP	C2-N1-C6	2.37	122.62	118.73
3	A	2001	ADP	N9-C8-N7	-2.24	110.76	113.94
3	B	2001	ADP	C2-N1-C6	2.24	122.40	118.73
3	B	2001	ADP	C5-N7-C8	2.20	106.91	103.45
3	B	2001	ADP	N9-C8-N7	-2.15	110.89	113.94
3	A	2001	ADP	O2A-PA-O1A	2.06	122.04	112.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

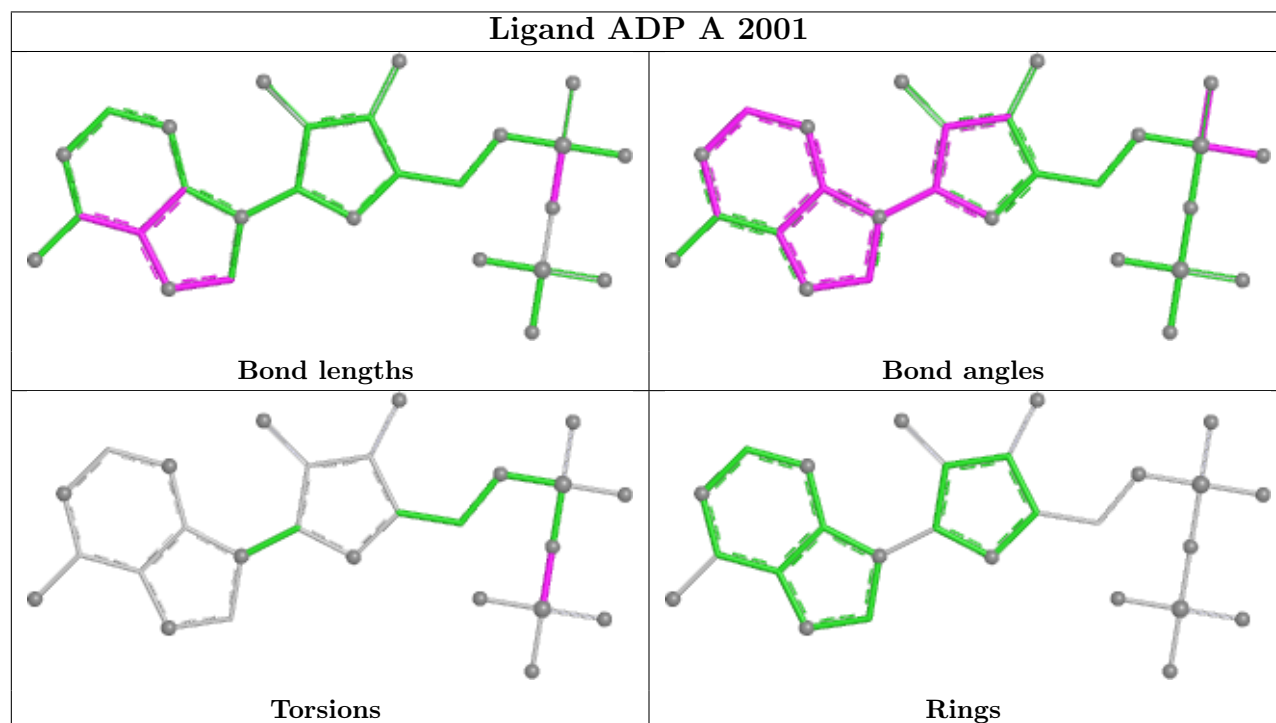
Mol	Chain	Res	Type	Atoms
3	B	2001	ADP	PA-O3A-PB-O2B
3	A	2001	ADP	PA-O3A-PB-O2B

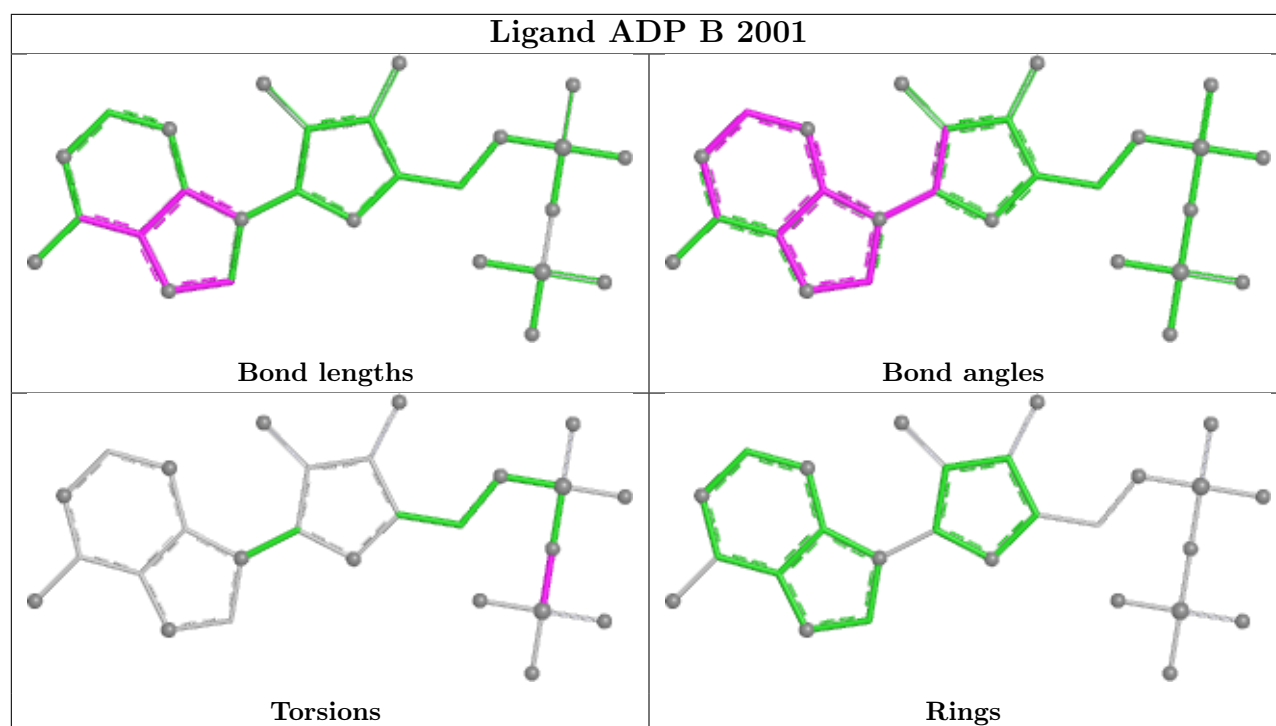
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2003	PO4	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	594/758 (78%)	0.32	65 (10%) 10 10	16, 38, 103, 142	0
1	B	579/758 (76%)	0.43	76 (13%) 7 6	14, 39, 98, 149	0
2	C	2/2 (100%)	1.04	0 100 100	67, 67, 67, 75	0
All	All	1175/1518 (77%)	0.37	141 (12%) 9 8	14, 38, 101, 149	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	585	TYR	6.7
1	A	576	ALA	6.6
1	B	263	ILE	6.2
1	B	619	TYR	5.6
1	B	28	SER	5.6
1	A	530	PRO	5.5
1	A	626	LEU	5.5
1	A	402	ARG	5.5
1	B	274	GLN	5.5
1	B	51	ALA	5.4
1	A	553	SER	5.1
1	B	272	ARG	5.1
1	A	476	THR	4.7
1	B	27	PHE	4.7
1	B	627	LEU	4.5
1	B	15	ARG	4.4
1	B	273	ASP	4.4
1	A	573	SER	4.4
1	A	619	TYR	4.3
1	B	535	MET	4.2
1	B	542	ASP	4.1
1	B	540	ALA	4.1
1	B	552	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	534	PRO	4.1
1	B	623	HIS	4.0
1	A	575	ASN	4.0
1	B	574	SER	4.0
1	A	583	THR	3.9
1	A	376	TYR	3.9
1	A	571	ALA	3.8
1	A	580	LEU	3.7
1	A	574	SER	3.7
1	B	405	GLU	3.7
1	A	332	GLN	3.6
1	A	577	PHE	3.6
1	A	572	LEU	3.6
1	A	555	PHE	3.5
1	A	582	ARG	3.5
1	B	577	PHE	3.4
1	A	570	LYS	3.4
1	B	52	LYS	3.4
1	B	544	LYS	3.4
1	B	271	GLU	3.3
1	A	625	ALA	3.3
1	B	484	TYR	3.3
1	B	476	THR	3.2
1	B	575	ASN	3.2
1	A	486	LEU	3.2
1	A	528	GLN	3.2
1	A	624	ILE	3.2
1	A	620	ARG	3.2
1	A	586	LEU	3.2
1	A	342	ARG	3.1
1	B	62	LEU	3.1
1	B	620	ARG	3.1
1	B	533	ARG	3.1
1	A	623	HIS	3.1
1	A	329	ASN	3.1
1	B	329	ASN	3.1
1	B	576	ALA	3.1
1	B	332	GLN	3.0
1	B	327	LEU	3.0
1	B	326	ARG	3.0
1	A	269	ASP	3.0
1	A	297	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	5	GLN	3.0
1	A	327	LEU	3.0
1	A	531	ARG	2.9
1	B	159	ARG	2.9
1	A	529	ASP	2.8
1	B	546	ARG	2.8
1	B	14	GLN	2.8
1	B	402	ARG	2.8
1	B	614	SER	2.7
1	A	556	LEU	2.7
1	B	160	PHE	2.7
1	B	621	GLU	2.7
1	B	331	GLU	2.7
1	A	340	SER	2.7
1	B	297	MET	2.7
1	B	567	GLU	2.6
1	A	164	VAL	2.6
1	A	326	ARG	2.6
1	B	539	GLN	2.6
1	B	325	ALA	2.6
1	B	19	LEU	2.6
1	A	614	SER	2.6
1	B	541	SER	2.6
1	B	622	ILE	2.6
1	B	538	GLN	2.5
1	A	377	ARG	2.5
1	B	537	LYS	2.5
1	B	421	PRO	2.5
1	A	569	GLN	2.5
1	B	13	GLN	2.5
1	B	340	SER	2.5
1	A	590	ARG	2.5
1	B	624	ILE	2.4
1	A	75	ASP	2.4
1	A	163	HIS	2.4
1	A	333	ASN	2.4
1	A	527	ILE	2.4
1	B	570	LYS	2.4
1	B	618	GLU	2.4
1	B	616	PRO	2.4
1	A	330	SER	2.4
1	B	312	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	4	GLN	2.4
1	A	355	LEU	2.4
1	B	17	ASP	2.3
1	B	564	TYR	2.3
1	B	26	ARG	2.3
1	A	183	GLN	2.3
1	B	569	GLN	2.3
1	A	316	ARG	2.3
1	B	18	SER	2.3
1	B	467	ARG	2.3
1	A	584	ASP	2.3
1	A	267	ALA	2.3
1	A	552	GLU	2.3
1	A	268	ASP	2.2
1	B	566	GLY	2.2
1	A	338	SER	2.2
1	B	55	ASP	2.2
1	A	14	GLN	2.2
1	B	550	ASP	2.2
1	B	543	GLU	2.2
1	B	549	HIS	2.2
1	A	579	ARG	2.1
1	B	536	ASP	2.1
1	A	439	GLN	2.1
1	A	159	ARG	2.1
1	A	621	GLU	2.1
1	B	313	LEU	2.1
1	B	617	ALA	2.0
1	B	333	ASN	2.0
1	B	585	TYR	2.0
1	B	132	ARG	2.0
1	A	266	GLU	2.0
1	A	162	ASN	2.0
1	B	447	ASP	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 [i](#)

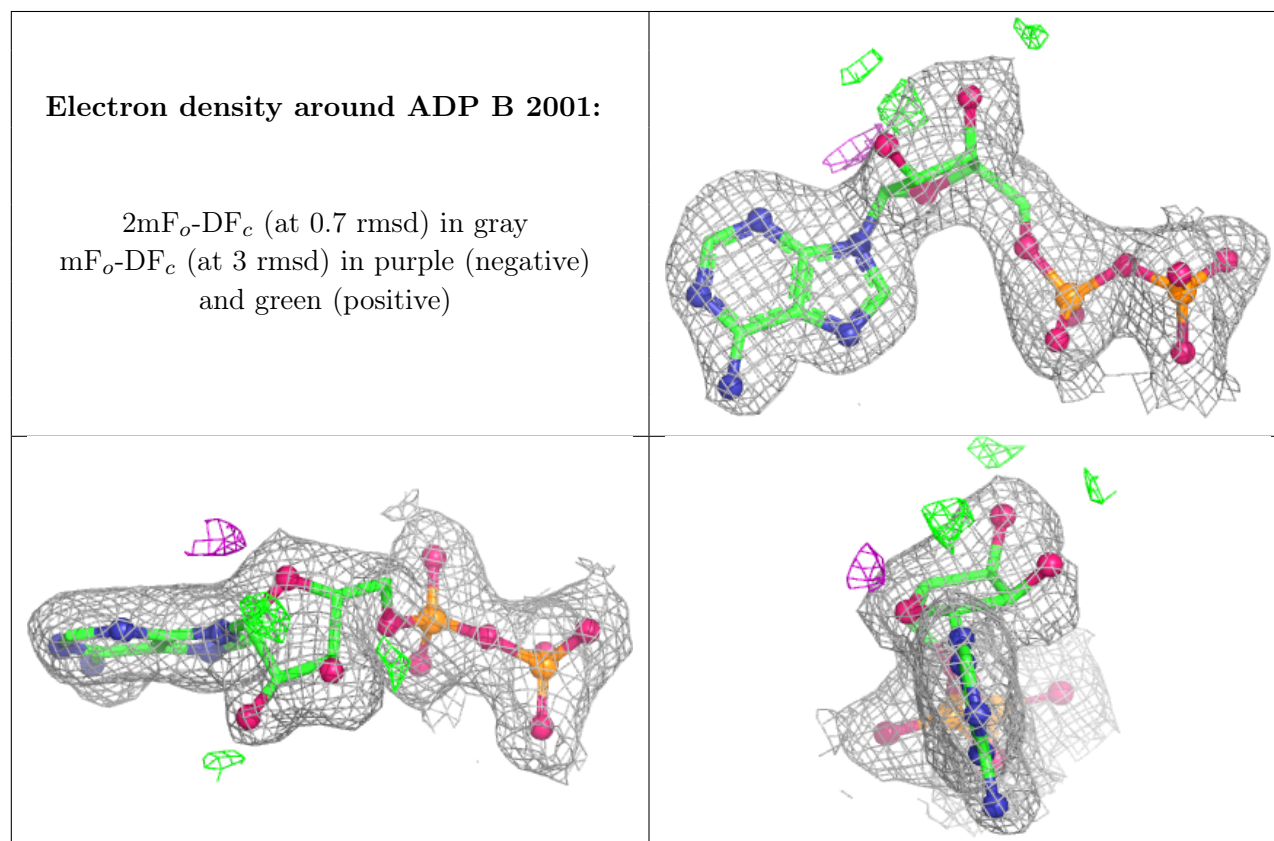
There are no oligosaccharides in this entry.

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.

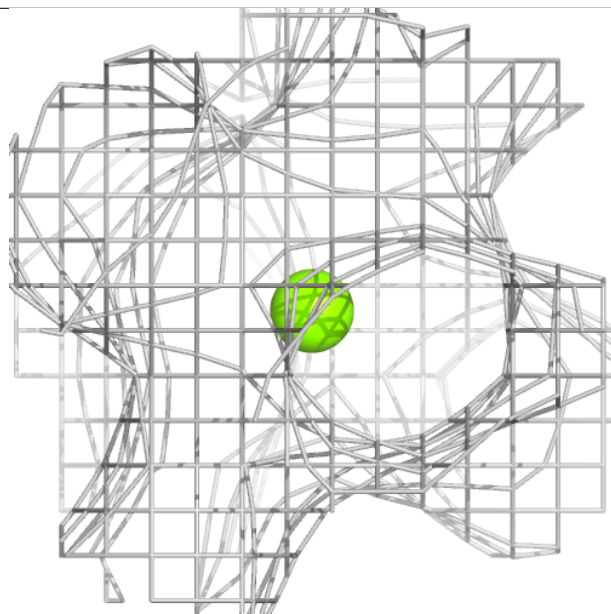
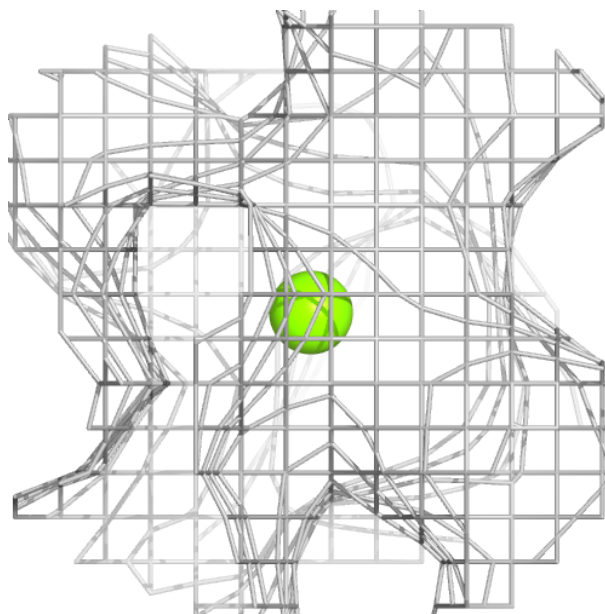
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	B	2003	5/5	0.84	0.15	67,72,76,86	0
3	ADP	B	2001	27/27	0.98	0.06	14,32,43,49	0
4	MG	B	2002	1/1	0.98	0.02	20,20,20,20	0
3	ADP	A	2001	27/27	0.98	0.07	13,34,41,68	0
4	MG	A	2002	1/1	0.99	0.03	18,18,18,18	0

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.



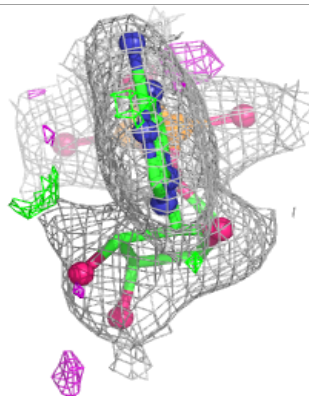
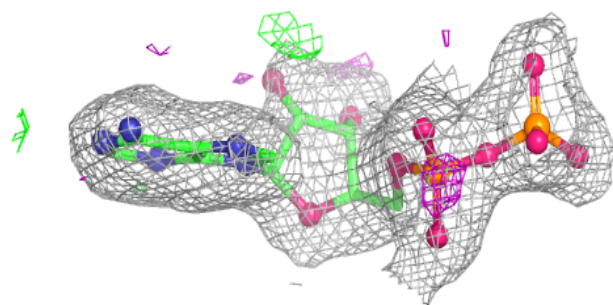
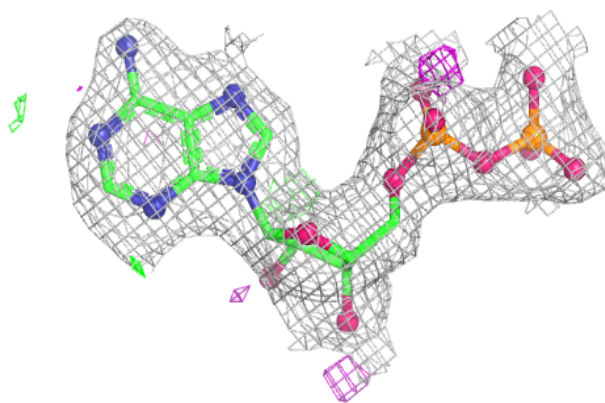
Electron density around MG B 2002:

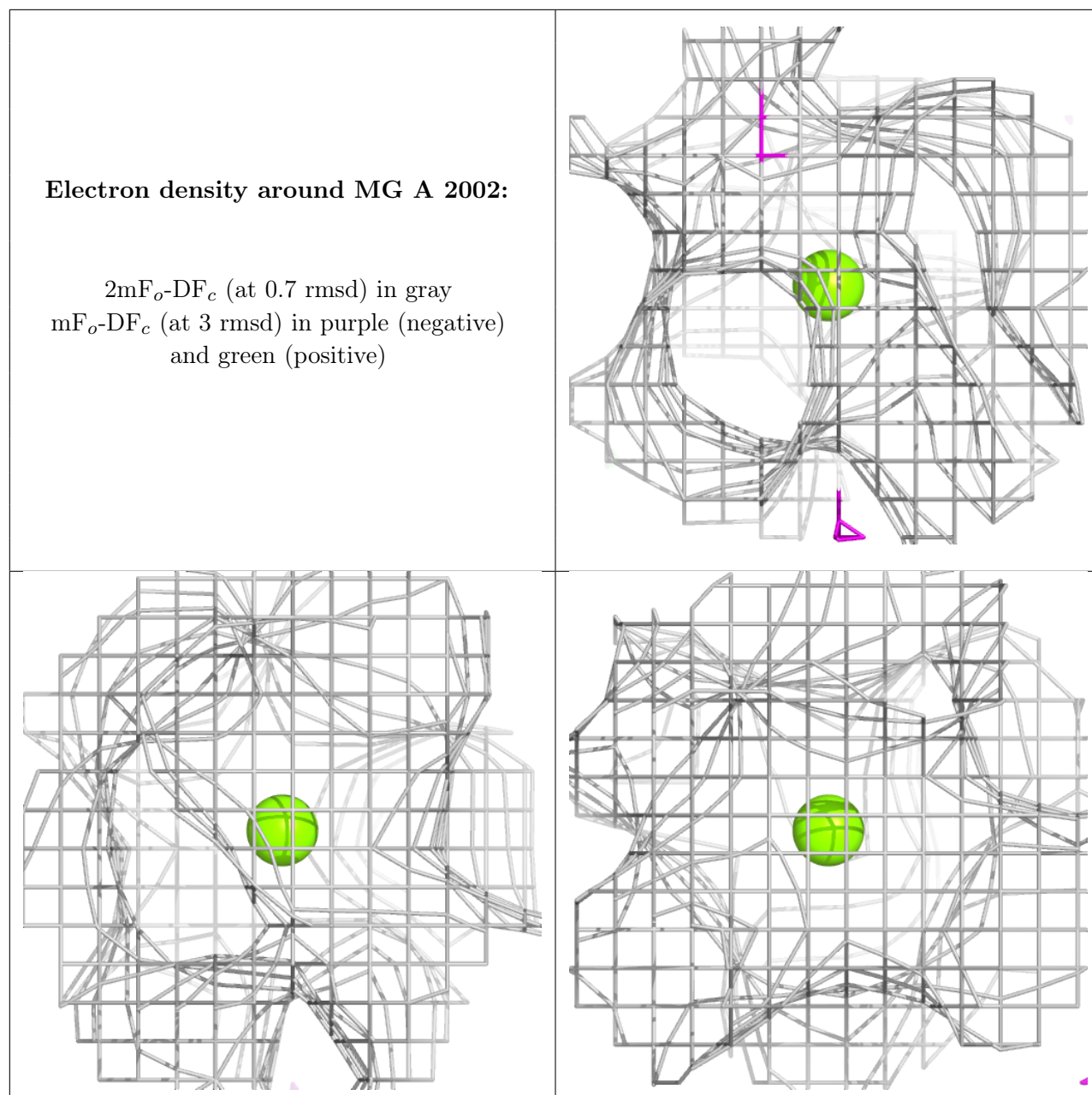
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP A 2001:

$2mF_o-DF_c$ (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.