



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2024 – 11:57 am BST

PDB ID : 8PO7  
Title : Structure of Escherichia coli HrpA in complex with ADP and dinucleotide dCdC  
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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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

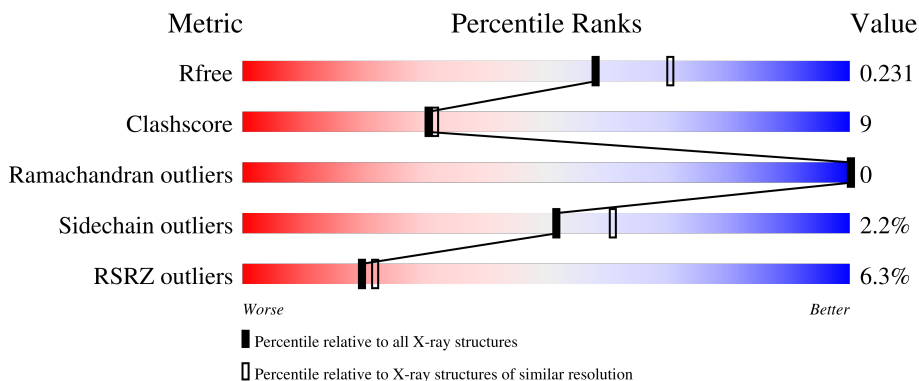
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


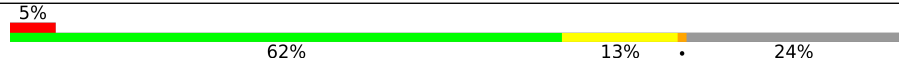
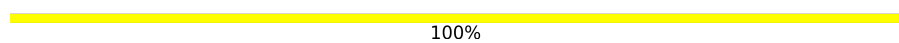
The reported resolution of this entry is 2.26 Å.

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))
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (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  $\geq 3$ , 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	
1	B	758	
2	C	2	

## 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
			Total	C	N	O	S			
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
			Total	C	N	O	P			
2	C	2	Total	C	N	O	P	0	0	0
			39	18	6	13	2			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

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

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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

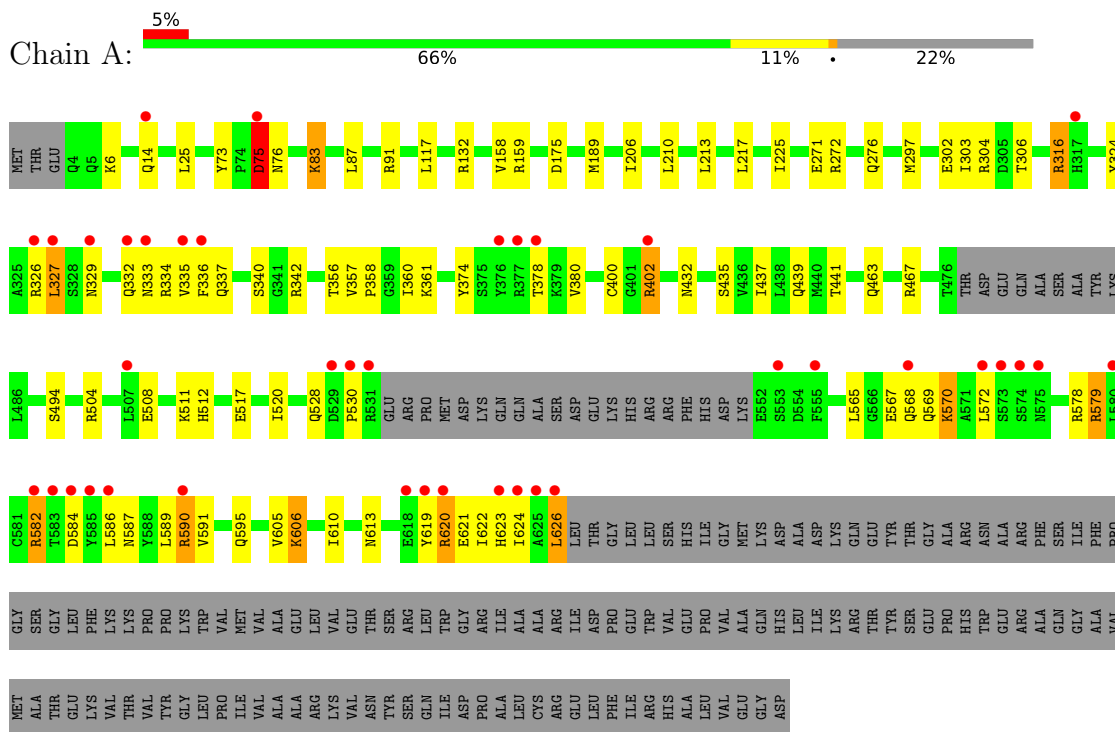
- Molecule 6 is water.

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

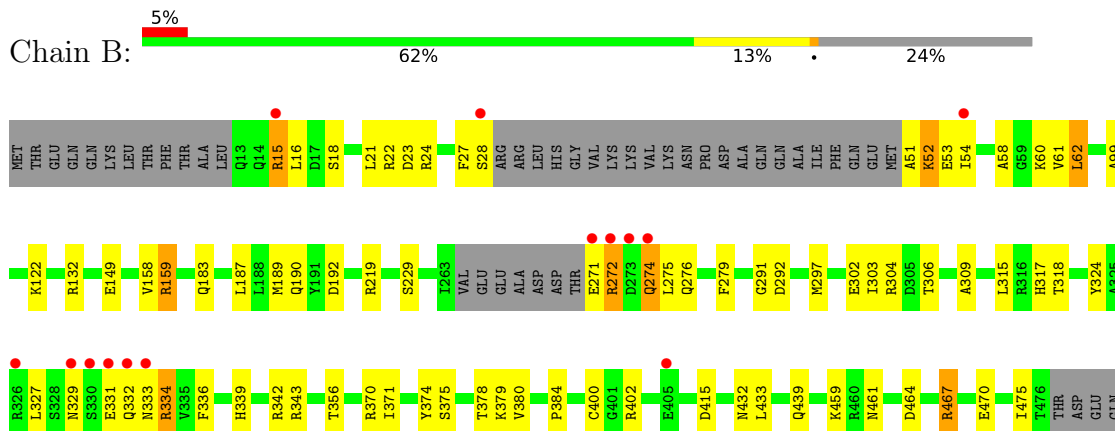
### 3 Residue-property plots i

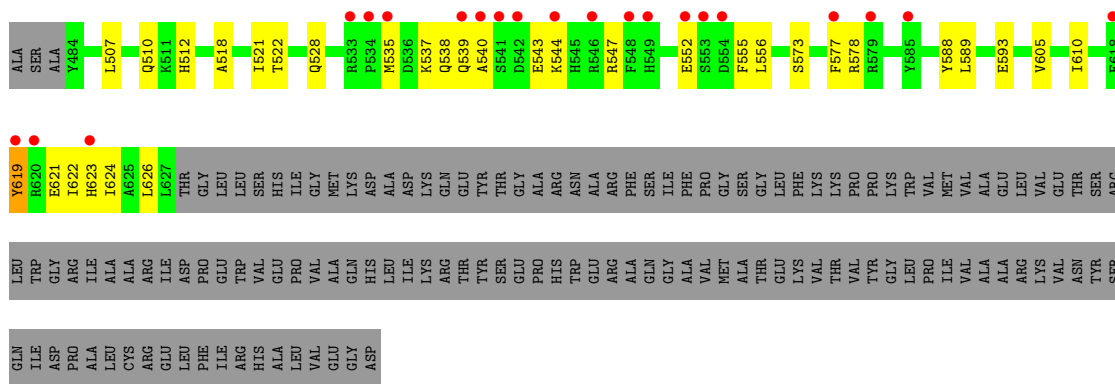
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ATP-dependent RNA helicase HrpA



- Molecule 1: ATP-dependent RNA helicase HrpA





- Molecule 2: DNA (5'-D(P\*CP\*C)-3')

Chain C:

100%

C1  
C2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.47Å 106.12Å 178.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.14 – 2.26 91.19 – 1.87	Depositor EDS
% Data completeness (in resolution range)	96.6 (89.14-2.26) 68.7 (91.19-1.87)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 1.87Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.190 , 0.232 0.187 , 0.231	Depositor DCC
$R_{free}$ test set	3466 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtrriage
Anisotropy	0.006	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, PO4, 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	0.44	2/4815 (0.0%)	0.66	8/6508 (0.1%)
1	B	0.42	1/4714 (0.0%)	0.71	9/6366 (0.1%)
2	C	1.71	1/42 (2.4%)	1.01	0/60
All	All	0.44	4/9571 (0.0%)	0.69	17/12934 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	DC	OP3-P	-10.36	1.48	1.61
1	B	400	CYS	CB-SG	-5.57	1.72	1.81
1	A	402	ARG	CB-CG	-5.39	1.38	1.52
1	A	528	GLN	CD-OE1	5.31	1.35	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	ARG	NE-CZ-NH2	-11.85	114.38	120.30
1	B	467	ARG	NE-CZ-NH1	10.64	125.62	120.30
1	A	402	ARG	CB-CA-C	-10.17	90.06	110.40
1	A	316	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	B	467	ARG	CA-CB-CG	7.90	130.79	113.40
1	B	467	ARG	CB-CA-C	5.95	122.30	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ASP	CB-CA-C	-5.88	98.63	110.40
1	A	327	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	584	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	A	402	ARG	N-CA-CB	5.67	120.81	110.60
1	B	62	LEU	CA-CB-CG	-5.65	102.31	115.30
1	A	494	SER	CB-CA-C	-5.59	99.47	110.10
1	B	274	GLN	CB-CG-CD	-5.58	97.10	111.60
1	B	467	ARG	CG-CD-NE	-5.25	100.77	111.80
1	B	272	ARG	N-CA-CB	5.23	120.02	110.60
1	B	274	GLN	CA-CB-CG	5.03	124.47	113.40
1	A	528	GLN	CA-CB-CG	5.03	124.46	113.40

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 [i](#)

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	85	0
1	B	4641	0	4722	90	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	6	0
6	C	1	0	0	1	0
All	All	10066	0	9600	176	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 9.

All (176) 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:297:MET:HE1	1:A:302:GLU:HG2	1.25	1.12
1:B:464:ASP:OD1	1:B:467:ARG:NH1	1.89	1.05
1:A:579:ARG:O	1:A:582:ARG:NH2	1.96	0.98
1:A:606:LYS:NZ	6:A:2102:HOH:O	1.91	0.96
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:A:356:THR:OG1	6:A:2101:HOH:O	1.88	0.91
1:B:297:MET:HE1	1:B:302:GLU:HG2	1.52	0.91
1:A:567:GLU:O	6:A:2103:HOH:O	1.91	0.88
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:A:297:MET:HE1	1:A:302:GLU:CG	2.10	0.77
1:B:132:ARG:HB2	1:B:159:ARG:NH2	2.01	0.75
1:B:297:MET:CE	1:B:302:GLU:HG2	2.16	0.74
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:HA	1:A:582:ARG:HE	1.54	0.73
1:A:435:SER:O	1:A:439:GLN:HG3	1.89	0.72
1:A:324:TYR:H	1:A:327:LEU:HD21	1.57	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:579:ARG:C	1:A:582:ARG:HH21	1.95	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:317:HIS:ND1	6:B:2106:HOH:O	2.27	0.66
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:B:552:GLU:CD	1:B:623:HIS:HD1	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:THR:CG2	1:B:402:ARG:NH2	2.63	0.61
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: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: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:A:297:MET:CE	1:A:306:THR:OG1	2.54	0.55
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: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:B:297:MET:CE	1:B:306:THR:OG1	2.56	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:297:MET:CE	1:A:302:GLU:CG	2.81	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:620:ARG:C	1:A:622:ILE:N	2.65	0.50
1:B:58:ALA:O	1:B:62:LEU:HD13	2.12	0.50
1:B:297:MET:HE1	1:B:306:THR:OG1	2.11	0.49
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:297:MET:HE1	1:B:302:GLU:CG	2.37	0.45
1:B:538:GLN:O	1:B:538:GLN:HG3	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: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:B:537:LYS:C	1:B:539:GLN:N	2.70	0.44
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:B:304:ARG:HE	1:B:304:ARG:HB3	1.71	0.43
1:B:52:LYS:C	1:B:54:ILE:H	2.22	0.43
1:B:22:ARG:NH2	1:B:190:GLN:HB2	2.34	0.42
1:A:25:LEU:HD22	1:A:189:MET:HE3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:507:LEU:O	1:B:510:GLN:HB3	2.20	0.41
1:B:537:LYS:C	1:B:539:GLN:H	2.23	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:21:LEU:HB3	1:B:189:MET:HE3	2.03	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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	519/657 (79%)	504 (97%)	15 (3%)	42	51
1	B	508/657 (77%)	500 (98%)	8 (2%)	62	73
All	All	1027/1314 (78%)	1004 (98%)	23 (2%)	52	61

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ASP
1	A	83	LYS
1	A	159	ARG
1	A	175	ASP
1	A	304	ARG
1	A	316	ARG
1	A	326	ARG
1	A	340	SER
1	A	342	ARG
1	A	570	LYS
1	A	579	ARG
1	A	582	ARG
1	A	590	ARG
1	A	606	LYS
1	A	626	LEU
1	B	15	ARG
1	B	52	LYS
1	B	159	ARG
1	B	183	GLN
1	B	274	GLN
1	B	334	ARG
1	B	459	LYS
1	B	619	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	528	GLN
1	A	575	ASN
1	B	332	GLN

### 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 monosaccharides 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	B	2001	4	24,29,29	0.88	1 (4%)	29,45,45	1.32	4 (13%)
5	PO4	B	2003	-	4,4,4	0.87	0	6,6,6	0.46	0
3	ADP	A	2001	4	24,29,29	0.91	1 (4%)	29,45,45	1.48	4 (13%)

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	B	2001	4	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	2001	4	-	1/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	ADP	C5-C4	2.36	1.47	1.40
3	A	2001	ADP	C5-C4	2.34	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	ADP	C3'-C2'-C1'	3.86	106.78	100.98
3	A	2001	ADP	N3-C2-N1	-3.61	123.04	128.68
3	B	2001	ADP	N3-C2-N1	-3.41	123.34	128.68
3	B	2001	ADP	C3'-C2'-C1'	2.60	104.89	100.98
3	A	2001	ADP	C2-N1-C6	2.26	122.62	118.75
3	A	2001	ADP	C4-C5-N7	-2.22	107.09	109.40
3	B	2001	ADP	C2-N1-C6	2.13	122.40	118.75
3	B	2001	ADP	C4-C5-N7	-2.05	107.27	109.40

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

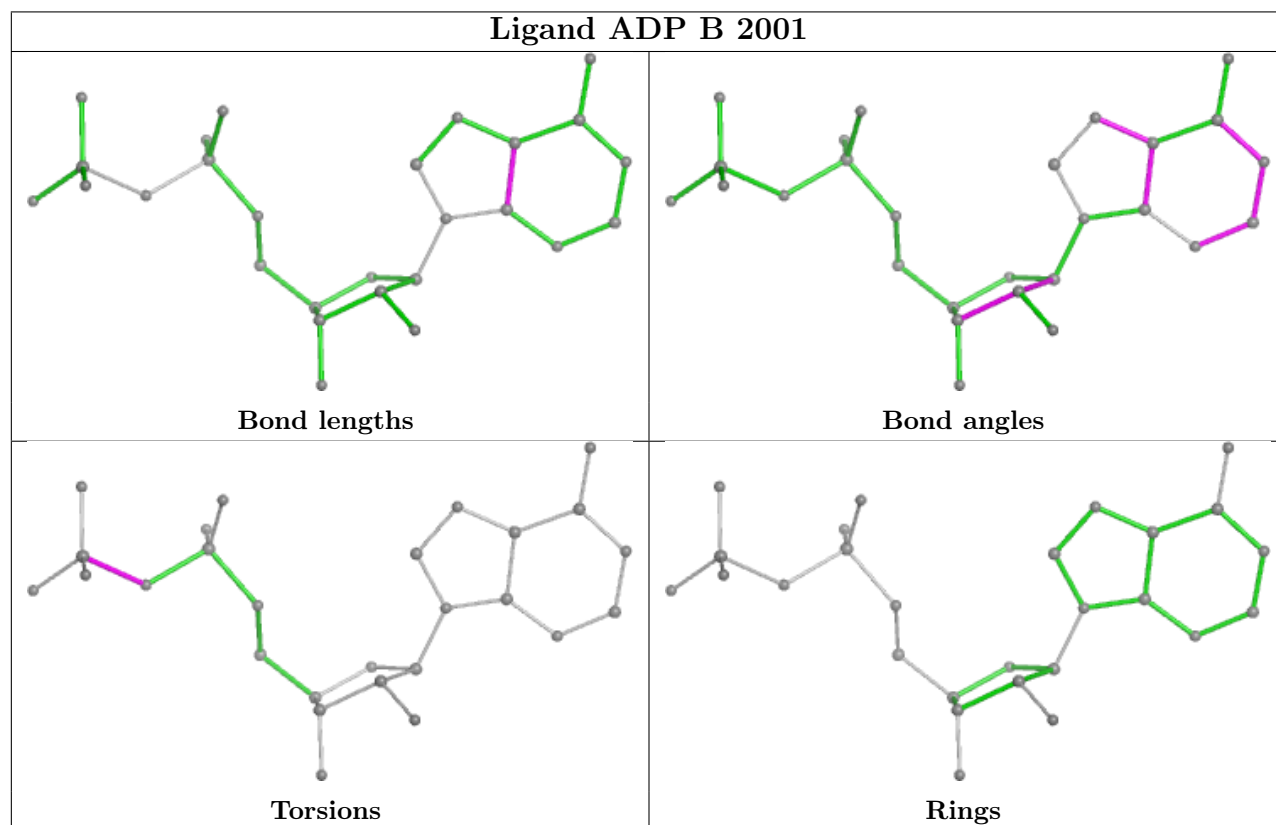
There are no ring outliers.

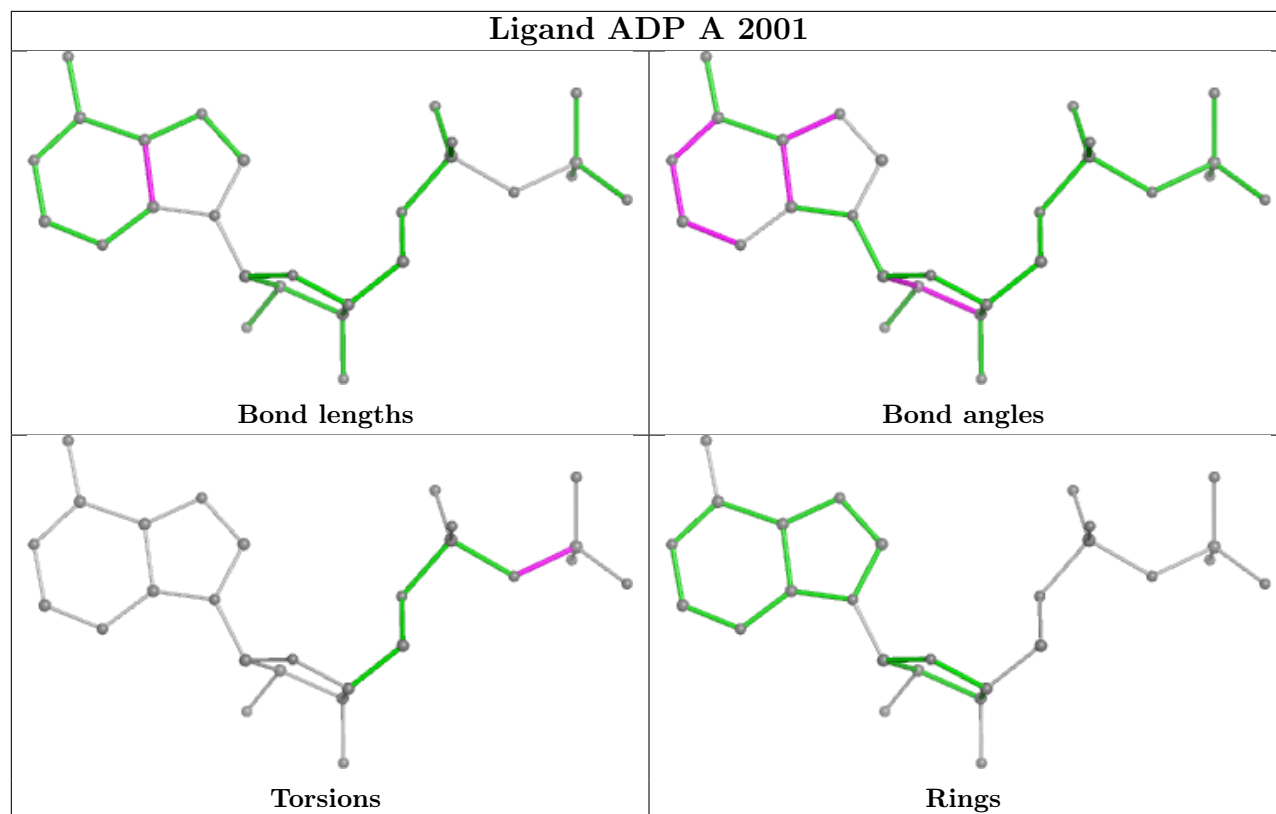
1 monomer is involved in 1 short contact:

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	594/758 (78%)	0.20	39 (6%) 18 20	16, 38, 103, 142	0
1	B	579/758 (76%)	0.23	35 (6%) 21 23	14, 39, 98, 149	0
2	C	2/2 (100%)	0.64	0 100 100	67, 67, 67, 75	0
All	All	1175/1518 (77%)	0.21	74 (6%) 20 22	14, 38, 101, 149	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	585	TYR	8.1
1	B	623	HIS	8.0
1	B	552	GLU	7.6
1	A	574	SER	6.3
1	B	274	GLN	6.1
1	A	531	ARG	5.9
1	A	530	PRO	5.9
1	B	619	TYR	5.2
1	B	273	ASP	5.2
1	A	329	ASN	5.1
1	B	332	GLN	5.1
1	A	402	ARG	5.1
1	B	28	SER	4.9
1	B	329	ASN	4.8
1	B	540	ALA	4.8
1	B	535	MET	4.4
1	A	333	ASN	4.3
1	B	620	ARG	4.0
1	B	539	GLN	3.7
1	A	332	GLN	3.6
1	A	573	SER	3.6
1	A	376	TYR	3.6
1	A	575	ASN	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	327	LEU	3.3
1	B	553	SER	3.3
1	A	529	ASP	3.3
1	A	317	HIS	3.2
1	A	620	ARG	3.1
1	B	333	ASN	3.1
1	B	544	LYS	3.1
1	B	331	GLU	3.1
1	A	625	ALA	3.0
1	A	553	SER	3.0
1	A	326	ARG	3.0
1	A	572	LEU	3.0
1	B	272	ARG	3.0
1	B	534	PRO	3.0
1	B	271	GLU	2.9
1	A	619	TYR	2.9
1	B	618	GLU	2.8
1	A	623	HIS	2.7
1	A	626	LEU	2.7
1	A	568	GLN	2.7
1	A	582	ARG	2.6
1	B	326	ARG	2.6
1	B	405	GLU	2.6
1	A	584	ASP	2.6
1	A	624	ILE	2.6
1	B	549	HIS	2.5
1	A	377	ARG	2.5
1	B	548	PHE	2.5
1	A	14	GLN	2.5
1	B	541	SER	2.5
1	B	533	ARG	2.4
1	A	507	LEU	2.4
1	A	378	THR	2.4
1	A	335	VAL	2.4
1	A	555	PHE	2.4
1	A	590	ARG	2.4
1	B	546	ARG	2.4
1	A	586	LEU	2.3
1	A	75	ASP	2.3
1	A	580	LEU	2.3
1	B	577	PHE	2.2
1	A	583	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	579	ARG	2.2
1	B	585	TYR	2.2
1	B	330	SER	2.2
1	B	554	ASP	2.1
1	B	15	ARG	2.1
1	A	618	GLU	2.0
1	A	336	PHE	2.0
1	B	542	ASP	2.0
1	B	54	ILE	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 monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

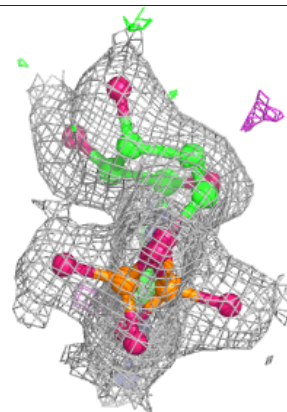
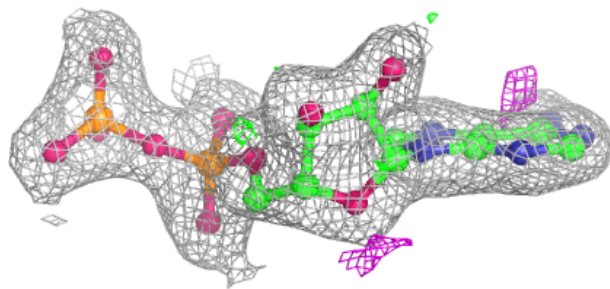
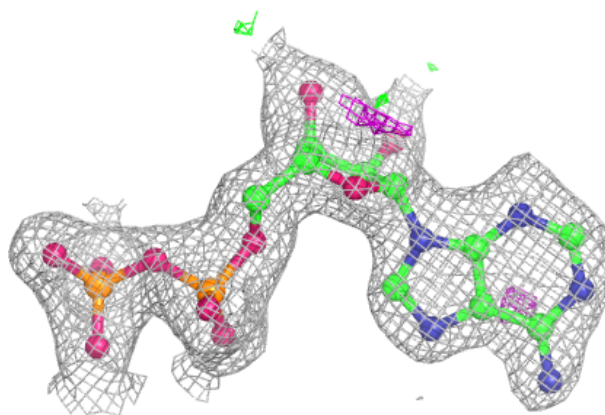
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	0.88	0.26	67,72,76,86	0
3	ADP	B	2001	27/27	0.97	0.15	14,32,43,49	0
4	MG	B	2002	1/1	0.97	0.06	20,20,20,20	0
3	ADP	A	2001	27/27	0.97	0.15	13,34,41,68	0
4	MG	A	2002	1/1	0.98	0.11	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 ADP B 2001:**

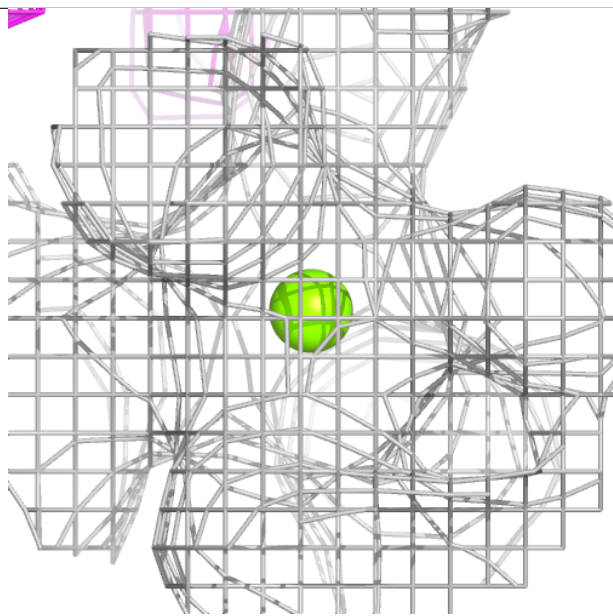
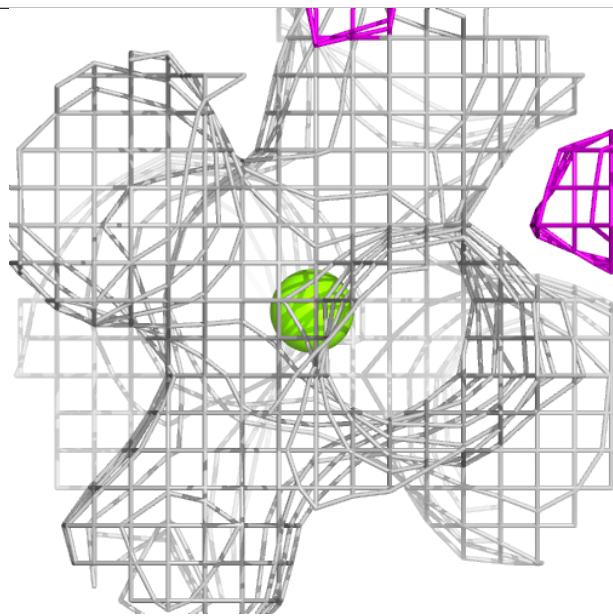
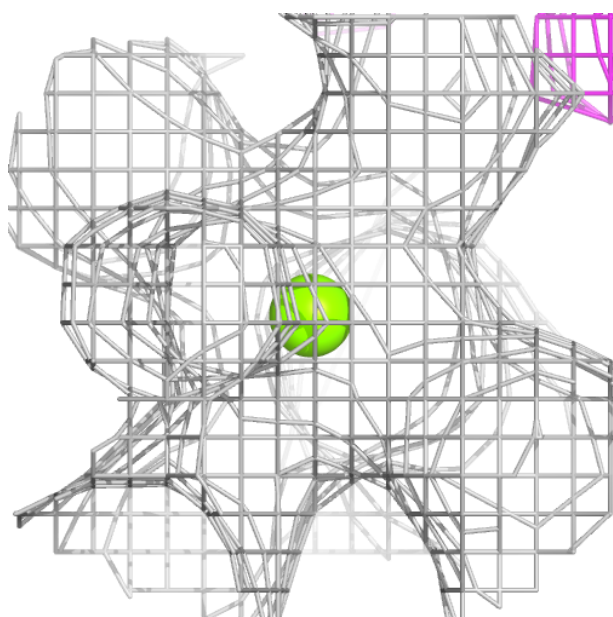
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





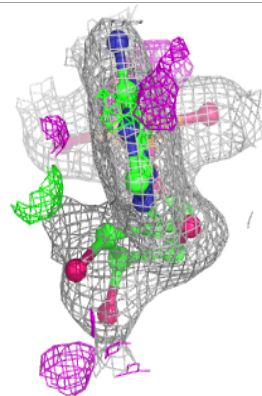
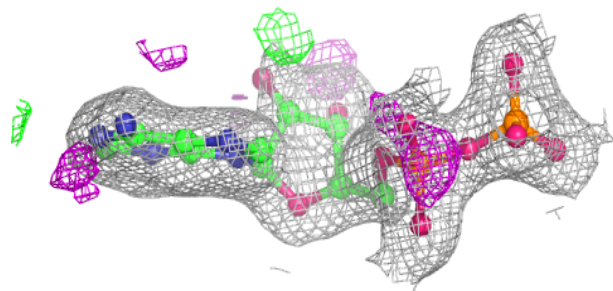
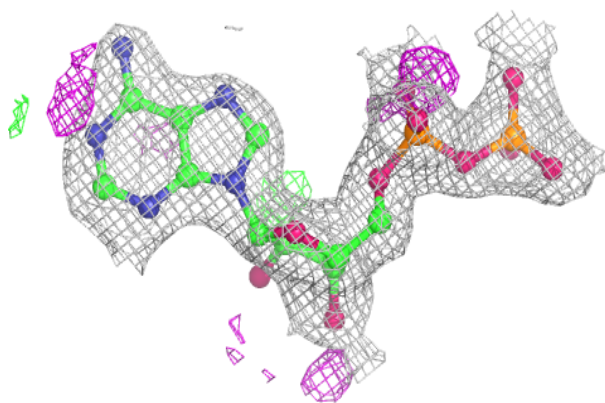
**Electron density around MG B 2002:**

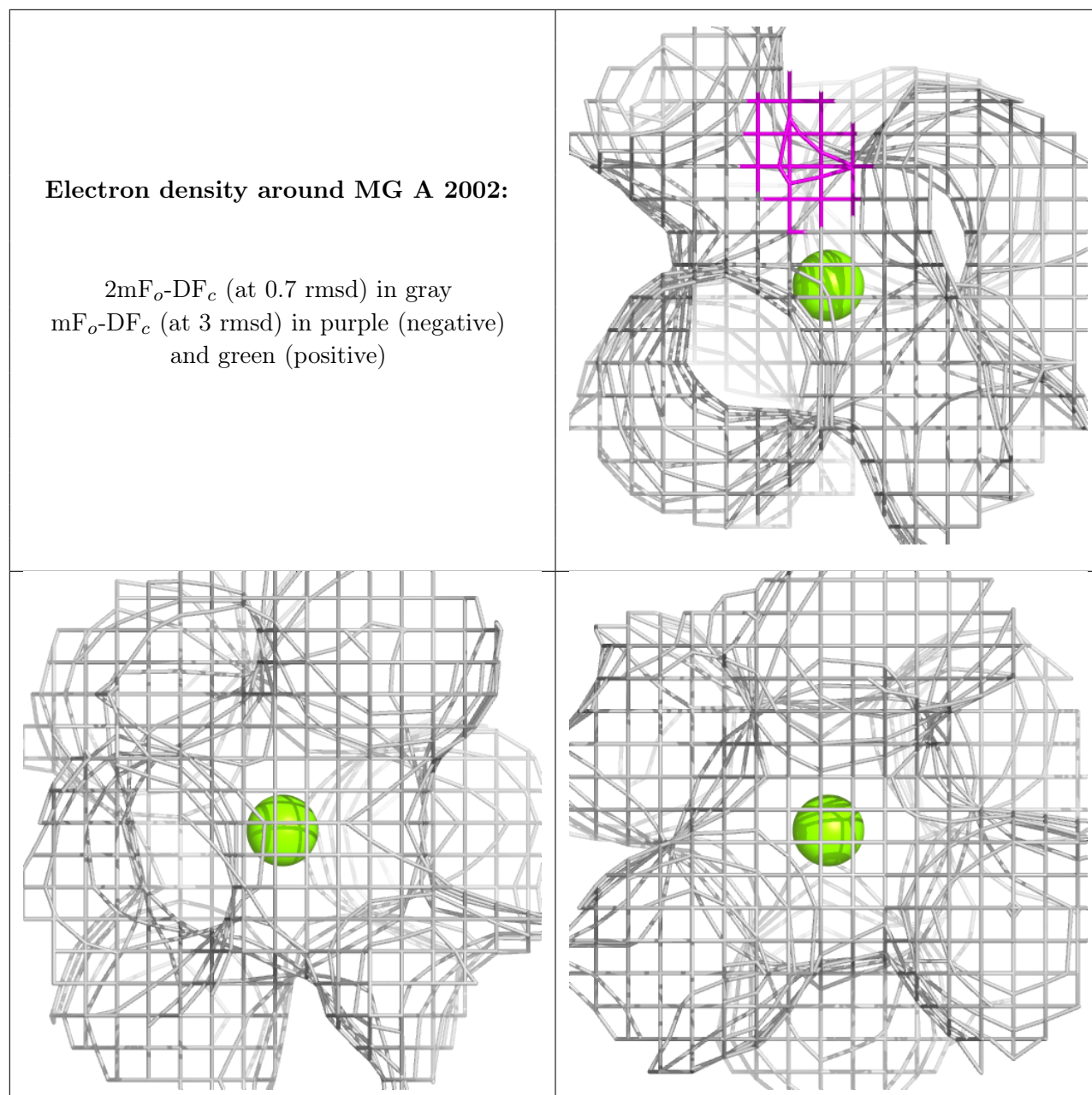
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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 [i](#)

There are no such residues in this entry.