



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:35 AM UTC

PDB ID : 9I22 / pdb\_00009i22  
Title : Structure of Human helicase RecQ1- Myc G-quadruplex - ADP complex  
Authors : Song, Z.Y.; Liu, N.N.; Ai, X.; Rety, S.; Xi, X.G.  
Deposited on : 2025-01-17  
Resolution : 2.42 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 : 4-5-2 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

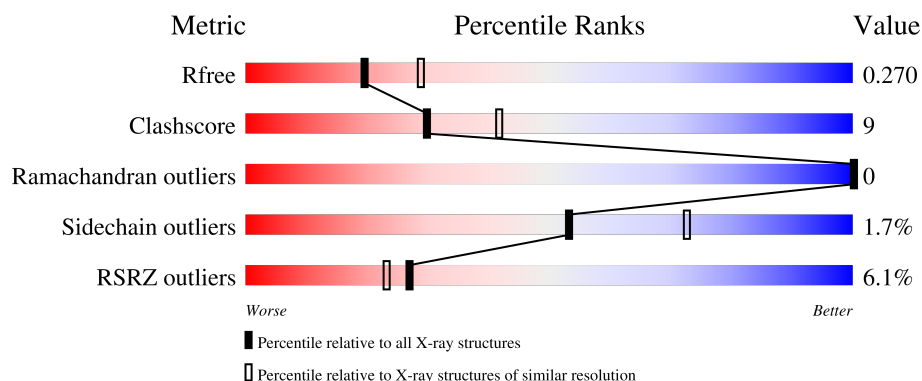
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	531	<div> <div>4%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	B	531	<div> <div>8%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
2	C	24	<div> <div>4%</div> <div>54%</div> <div>17%</div> <div>29%</div> </div>
2	D	24	<div> <div>4%</div> <div>50%</div> <div>25%</div> <div>25%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9282 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 DNA helicase Q1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	0	0
			4228	2690	721	782	35			
1	B	531	Total	C	N	O	S	0	0	0
			4228	2690	721	782	35			

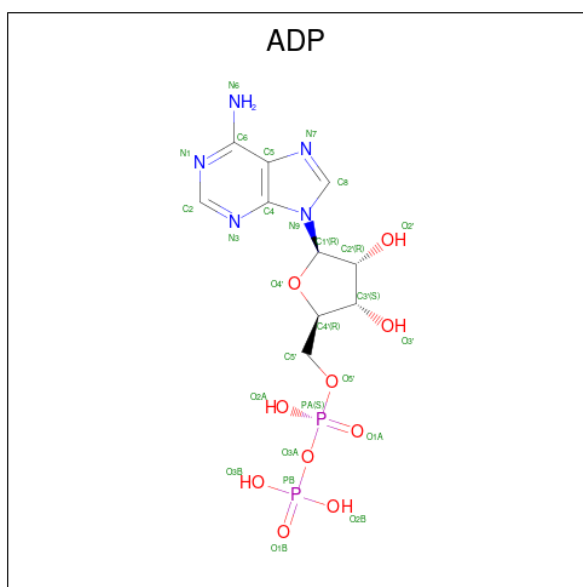
- Molecule 2 is a DNA chain called DNA (5'-D(P\*GP\*GP\*GP\*TP\*GP\*GP\*GP\*TP\*AP\*GP\*GP\*GP\*TP\*GP\*GP\*GP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	P	0	0	0
			364	169	73	105	17			
2	D	18	Total	C	N	O	P	0	0	0
			386	180	78	110	18			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

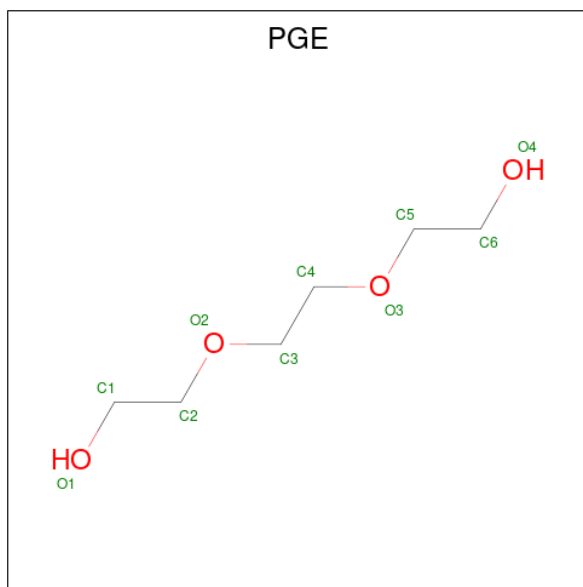
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

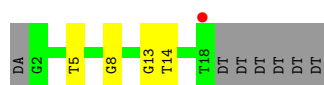
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	K	0	0
			1	1		
6	B	2	Total	K	0	0
			2	2		
6	C	3	Total	K	0	0
			3	3		
6	D	2	Total	K	0	0
			2	2		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).

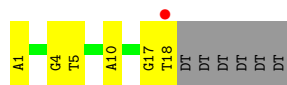


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		





● Molecule 2: DNA (5'-D(P\*GP\*GP\*GP\*TP\*GP\*GP\*GP\*TP\*AP\*GP\*GP\*GP\*TP\*GP\*GP\*GP\*T)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.19Å 155.19Å 126.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.60 – 2.42 77.60 – 2.42	Depositor EDS
% Data completeness (in resolution range)	68.6 (77.60-2.42) 68.7 (77.60-2.42)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.218 , 0.268 0.221 , 0.270	Depositor DCC
$R_{free}$ test set	1984 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9282	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	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.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, ZN, K, ADP, MG

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	0.30	1/4313 (0.0%)	0.67	10/5818 (0.2%)
1	B	0.34	1/4313 (0.0%)	0.90	28/5818 (0.5%)
2	C	0.29	0/409	0.44	0/632
2	D	0.27	0/435	0.39	0/674
All	All	0.32	2/9470 (0.0%)	0.77	38/12942 (0.3%)

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	3
1	B	0	12
All	All	0	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	376	MET	CB-CG	5.63	1.69	1.52
1	A	481	ASP	CB-CG	5.50	1.65	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	ILE	CA-C-N	20.16	160.50	125.02
1	B	489	ILE	C-N-CA	20.16	160.50	125.02
1	A	480	LYS	N-CA-C	18.49	136.24	111.28
1	B	376	MET	CA-C-N	16.22	153.21	121.41
1	B	376	MET	C-N-CA	16.22	153.21	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	488	ASN	CA-C-N	-13.43	97.80	121.97
1	B	488	ASN	C-N-CA	-13.43	97.80	121.97
1	A	270	CYS	CA-C-N	12.85	139.46	120.69
1	A	270	CYS	C-N-CA	12.85	139.46	120.69
1	B	375	GLY	CA-C-N	11.32	146.60	125.66
1	B	375	GLY	C-N-CA	11.32	146.60	125.66
1	B	489	ILE	N-CA-C	10.65	131.50	109.34
1	A	478	CYS	CA-C-N	9.87	138.47	121.29
1	A	478	CYS	C-N-CA	9.87	138.47	121.29
1	A	480	LYS	O-C-N	-9.02	112.17	122.91
1	B	489	ILE	N-CA-CB	-8.68	96.91	111.23
1	B	371	THR	CA-C-N	-8.62	112.31	122.22
1	B	371	THR	C-N-CA	-8.62	112.31	122.22
1	B	490	THR	CA-C-N	8.01	131.33	120.44
1	B	490	THR	C-N-CA	8.01	131.33	120.44
1	B	490	THR	CB-CA-C	-7.68	95.67	110.65
1	A	271	ILE	N-CA-CB	-7.37	100.32	110.05
1	B	584	HIS	CA-C-N	7.28	132.92	121.72
1	B	584	HIS	C-N-CA	7.28	132.92	121.72
1	A	481	ASP	CB-CA-C	-7.05	98.61	109.89
1	B	464	GLU	N-CA-C	6.87	120.11	111.24
1	B	372	VAL	CA-C-N	6.76	132.32	121.98
1	B	372	VAL	C-N-CA	6.76	132.32	121.98
1	B	490	THR	N-CA-C	-6.73	103.49	113.72
1	A	270	CYS	CA-C-O	5.71	129.22	122.14
1	B	376	MET	CB-CA-C	-5.68	99.50	110.35
1	B	372	VAL	N-CA-C	-5.41	98.71	106.55
1	B	584	HIS	N-CA-CB	5.28	118.78	110.23
1	B	376	MET	CB-CG-SD	5.20	128.30	112.70
1	B	374	PHE	CA-C-N	5.19	131.58	121.41
1	B	374	PHE	C-N-CA	5.19	131.58	121.41
1	A	480	LYS	N-CA-CB	-5.18	103.55	111.74
1	B	490	THR	CA-CB-OG1	5.16	117.33	109.60

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	CYS	Peptide
1	A	375	GLY	Peptide
1	A	480	LYS	Mainchain
1	B	229	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	B	372	VAL	Peptide,Mainchain
1	B	373	ALA	Peptide
1	B	374	PHE	Peptide
1	B	375	GLY	Mainchain
1	B	376	MET	Peptide,Mainchain
1	B	489	ILE	Peptide
1	B	490	THR	Peptide,Mainchain
1	B	584	HIS	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	4228	0	4245	73	0
1	B	4228	0	4243	74	0
2	C	364	0	188	4	0
2	D	386	0	203	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	3	0	0	0	0
6	D	2	0	0	0	0
7	B	10	0	14	1	0
All	All	9282	0	8917	154	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 9.

All (154) 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:480:LYS:HG2	1:A:480:LYS:O	1.66	0.92
1:A:345:HIS:HD2	1:A:347:ASN:HB3	1.54	0.73
1:A:81:ASP:OD1	1:A:85:ASN:ND2	2.21	0.72
1:B:223:CYS:SG	1:B:230:ASP:HB3	2.31	0.71
1:A:480:LYS:O	1:A:480:LYS:CG	2.40	0.69
1:A:520:MET:HB2	1:A:522:LYS:HD3	1.72	0.69
2:D:4:DG:H4'	2:D:5:DT:H5'	1.73	0.69
1:B:486:ARG:HH21	1:B:589:GLN:HB2	1.59	0.67
1:B:119:LYS:HD2	1:B:253:LEU:HB3	1.78	0.66
1:A:283:ARG:NH1	1:A:403:GLY:O	2.30	0.65
1:B:545:ILE:HA	1:B:588:MET:HE1	1.79	0.64
1:B:489:ILE:CG2	1:B:492:TYR:HB2	2.27	0.63
1:A:266:GLN:HG3	1:A:271:ILE:HG22	1.80	0.63
1:A:227:TRP:HE1	1:B:227:TRP:HZ2	1.46	0.62
1:A:449:ASN:HD21	1:A:452:LYS:HD3	1.64	0.61
1:A:431:VAL:O	1:B:243:ARG:NH2	2.34	0.61
1:B:386:VAL:HG23	1:B:405:ALA:HB2	1.82	0.61
1:A:475:CYS:SG	1:A:478:CYS:HB2	2.42	0.60
1:A:90:GLU:HG2	1:A:91:LYS:HG3	1.82	0.59
1:A:282:ASN:ND2	1:A:469:GLU:OE1	2.32	0.59
1:A:322:PHE:HZ	1:A:429:MET:HG3	1.66	0.59
1:B:173:VAL:HG12	1:B:177:MET:HE3	1.84	0.59
1:B:168:GLU:OE1	1:B:168:GLU:N	2.32	0.59
1:A:257:ALA:HB1	1:A:262:LEU:HD21	1.83	0.59
1:B:199:MET:HE2	2:C:8:DG:H2'	1.83	0.59
1:B:477:ASN:HA	1:B:480:LYS:HE3	1.86	0.58
1:A:526:LYS:H	1:A:526:LYS:HD3	1.70	0.57
1:A:500:LEU:HD23	1:A:510:LEU:HD12	1.86	0.56
1:B:294:PRO:HG2	1:B:300:PHE:HA	1.88	0.56
1:A:266:GLN:NE2	1:A:272:GLU:O	2.39	0.56
1:A:463:ASP:OD1	1:A:463:ASP:N	2.39	0.55
1:B:489:ILE:O	1:B:491:GLU:CD	2.50	0.55
2:D:10:DA:C8	2:D:10:DA:H5''	2.42	0.54
1:A:141:ILE:HA	1:A:144:MET:HE3	1.88	0.54
1:A:376:MET:HG3	1:A:404:ARG:HH21	1.71	0.54
1:A:179:ASN:HB3	1:A:182:SER:HB2	1.90	0.54
1:A:398:TYR:CE1	1:A:416:LEU:HD12	2.43	0.54
1:A:134:THR:HG23	1:A:215:ARG:HG3	1.90	0.53
1:B:90:GLU:HG2	1:B:91:LYS:HG3	1.90	0.53
2:D:1:DA:H2'	2:D:17:DG:H4'	1.90	0.53
2:D:10:DA:N3	2:D:10:DA:H2'	2.24	0.53
2:C:5:DT:H2'	2:C:5:DT:O2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HD11	1:A:113:MET:HE3	1.91	0.53
1:A:386:VAL:HG23	1:A:405:ALA:HB2	1.89	0.52
1:A:345:HIS:CD2	1:A:347:ASN:HB3	2.40	0.52
1:B:226:GLN:HA	1:B:231:PHE:CD1	2.44	0.52
1:B:189:VAL:HG11	1:B:200:PHE:CZ	2.44	0.52
1:B:529:VAL:O	1:B:532:VAL:HG12	2.10	0.52
1:B:177:MET:HE1	1:B:200:PHE:CE1	2.46	0.51
1:A:383:VAL:HB	1:A:405:ALA:HA	1.93	0.51
1:B:266:GLN:HG3	1:B:271:ILE:HB	1.92	0.51
1:B:372:VAL:HG23	1:B:372:VAL:O	2.11	0.51
1:A:103:THR:HG22	1:A:215:ARG:NH1	2.25	0.51
1:A:378:ILE:O	1:A:404:ARG:NH1	2.44	0.50
2:C:13:DG:H2''	2:C:14:DT:OP2	2.11	0.50
1:A:522:LYS:O	1:A:528:ARG:NH1	2.44	0.50
1:B:584:HIS:CG	1:B:585:ALA:N	2.80	0.50
1:B:95:LEU:HD13	1:B:277:PHE:HB3	1.94	0.49
1:B:81:ASP:OD1	1:B:85:ASN:ND2	2.45	0.49
1:A:160:MET:HE2	1:A:162:ASN:HD22	1.77	0.49
1:B:107:LYS:HD2	1:B:273:LYS:NZ	2.27	0.49
1:B:167:LYS:HA	1:B:170:VAL:HB	1.93	0.49
1:B:215:ARG:NH1	1:B:249:SER:OG	2.45	0.49
1:B:239:GLY:O	1:B:243:ARG:HG3	2.12	0.49
1:B:435:VAL:HG13	1:B:439:LYS:HE2	1.94	0.49
1:A:102:VAL:HG13	1:A:107:LYS:HB2	1.95	0.49
1:B:484:PHE:N	1:B:592:LYS:HE2	2.28	0.49
1:B:319:ILE:HG12	1:B:387:ILE:HB	1.94	0.48
1:B:485:GLU:HB3	1:B:592:LYS:HD3	1.96	0.48
1:B:293:LYS:HE3	1:B:300:PHE:CE2	2.48	0.48
1:A:119:LYS:HD2	1:A:253:LEU:HB3	1.96	0.48
1:B:493:CYS:HB2	1:B:549:PHE:CZ	2.49	0.48
1:B:446:TYR:CZ	1:B:454:ARG:HD2	2.49	0.47
1:B:225:SER:HB3	1:B:261:VAL:HG13	1.96	0.47
1:A:160:MET:HE2	1:A:162:ASN:ND2	2.30	0.47
1:B:449:ASN:ND2	1:B:452:LYS:HB2	2.30	0.47
1:B:293:LYS:HE3	1:B:300:PHE:HE2	1.80	0.47
1:B:232:ARG:HB2	1:B:235:TYR:HB2	1.97	0.46
1:A:493:CYS:O	1:A:497:ILE:HG12	2.15	0.46
1:A:562:THR:OG1	1:A:565:ALA:O	2.27	0.46
1:A:239:GLY:O	1:A:243:ARG:HG3	2.14	0.46
1:B:584:HIS:CG	1:B:585:ALA:H	2.33	0.46
1:B:489:ILE:HG22	1:B:492:TYR:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:GLU:HG3	1:A:592:LYS:HD3	1.97	0.46
1:A:522:LYS:HZ2	1:A:539:ARG:HH12	1.62	0.46
1:B:429:MET:SD	7:B:601:PGE:H2	2.55	0.46
1:A:258:THR:O	1:A:262:LEU:HD22	2.16	0.46
1:B:107:LYS:HD2	1:B:273:LYS:HZ1	1.80	0.46
1:B:324:GLN:HG3	1:B:345:HIS:CG	2.51	0.46
1:A:134:THR:HB	1:A:186:LEU:HD23	1.97	0.46
1:B:102:VAL:HG13	1:B:107:LYS:HB2	1.98	0.45
1:B:330:VAL:HB	1:B:369:VAL:HG11	1.98	0.45
1:A:552:GLN:O	1:A:575:LYS:HD3	2.16	0.45
1:B:191:PRO:HB2	1:B:234:ASP:HB3	1.99	0.45
1:A:481:ASP:OD1	1:A:481:ASP:O	2.34	0.45
1:A:257:ALA:HB1	1:A:262:LEU:CD2	2.47	0.45
1:B:235:TYR:HA	1:B:238:LEU:HG	1.97	0.45
1:A:513:LEU:O	1:A:516:ILE:HG22	2.16	0.44
1:B:493:CYS:O	1:B:497:ILE:HG12	2.17	0.44
1:A:522:LYS:NZ	1:A:539:ARG:HH12	2.14	0.44
1:B:219:ASP:OD2	1:B:220:GLU:HG2	2.17	0.44
1:B:391:MET:HA	1:B:416:LEU:HD11	2.00	0.44
2:C:13:DG:H4'	2:C:14:DT:O5'	2.18	0.44
1:B:141:ILE:HA	1:B:144:MET:HE2	1.99	0.44
1:B:434:ASN:N	1:B:434:ASN:OD1	2.51	0.44
2:D:18:DT:O2	2:D:18:DT:H2'	2.17	0.44
1:A:125:LEU:HB3	1:A:126:PRO:HD3	1.99	0.44
1:B:317:GLY:HA3	1:B:385:PHE:CZ	2.53	0.44
1:B:348:LEU:O	1:B:353:LYS:HE3	2.18	0.44
1:B:320:TYR:HA	1:B:370:ALA:O	2.17	0.43
1:A:294:PRO:HG2	1:A:300:PHE:HB2	1.99	0.43
1:B:427:SER:OG	1:B:559:TYR:OH	2.34	0.43
1:A:301:ILE:HG21	1:A:333:SER:HB3	1.99	0.43
1:A:63:SER:HB3	1:A:275:PHE:HD1	1.83	0.43
1:B:477:ASN:O	1:B:480:LYS:HG2	2.17	0.43
1:A:325:LYS:HB2	1:A:325:LYS:HE3	1.77	0.43
1:A:519:TRP:NE1	1:A:535:PRO:HG3	2.34	0.43
1:A:407:ARG:HD3	1:A:407:ARG:HA	1.82	0.42
2:D:4:DG:H4'	2:D:5:DT:C5'	2.45	0.42
1:B:125:LEU:HB3	1:B:126:PRO:HD3	2.00	0.42
1:B:173:VAL:O	1:B:177:MET:HG3	2.19	0.42
1:B:206:LYS:HA	1:B:206:LYS:HD3	1.89	0.42
1:A:132:GLY:HA3	1:A:212:ARG:O	2.20	0.42
1:B:282:ASN:OD1	1:B:455:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ARG:HD2	1:B:417:TYR:CE1	2.55	0.42
1:A:324:GLN:HA	1:A:371:THR:HG21	2.01	0.42
1:A:522:LYS:HZ2	1:A:539:ARG:NH1	2.17	0.42
1:A:519:TRP:CE2	1:A:535:PRO:HG3	2.55	0.41
1:B:395:MET:HE1	1:B:446:TYR:CD2	2.55	0.41
1:A:231:PHE:HZ	1:A:236:LYS:HD2	1.84	0.41
1:A:553:GLN:HB3	1:A:574:PRO:HG2	2.02	0.41
1:B:286:LEU:O	1:B:455:ARG:NH2	2.53	0.41
1:B:337:LEU:HD13	1:B:337:LEU:HA	1.92	0.41
1:B:482:SER:HA	1:B:484:PHE:CZ	2.55	0.41
1:A:141:ILE:HG23	1:A:160:MET:HE1	2.02	0.41
1:A:161:LEU:HB2	1:A:189:VAL:HG12	2.02	0.41
1:A:264:ASP:O	1:A:268:ILE:HG12	2.21	0.41
1:B:288:TYR:CZ	1:B:458:MET:HE1	2.56	0.41
1:A:466:TRP:CD1	1:A:466:TRP:C	2.99	0.41
1:B:550:LEU:HD12	1:B:555:LEU:O	2.21	0.41
1:A:359:LYS:HB3	1:A:365:ILE:HG13	2.03	0.41
1:A:442:GLU:HB3	1:A:461:HIS:NE2	2.36	0.41
1:A:522:LYS:C	1:A:528:ARG:HH22	2.29	0.41
1:A:493:CYS:HB2	1:A:549:PHE:CZ	2.56	0.41
1:B:208:TYR:HB2	1:B:213:PHE:CE1	2.56	0.41
1:A:180:LYS:HD3	1:A:180:LYS:H	1.86	0.40
1:B:161:LEU:HD22	1:B:170:VAL:HG22	2.04	0.40
1:A:293:LYS:HE3	1:A:300:PHE:CE2	2.56	0.40
1:B:214:THR:O	1:B:214:THR:OG1	2.39	0.40
1:B:373:ALA:O	1:B:375:GLY:HA2	2.21	0.40
1:B:483:ALA:C	1:B:592:LYS:HE2	2.46	0.40
1:A:180:LYS:HE2	1:A:180:LYS:HB2	1.88	0.40
1:A:360:TRP:HD1	1:A:365:ILE:O	2.05	0.40
1:A:411:LYS:HG3	1:A:474:MET:HE1	2.03	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	529/531 (100%)	528 (100%)	1 (0%)	0	100	100
1	B	529/531 (100%)	528 (100%)	1 (0%)	0	100	100
All	All	1058/1062 (100%)	1056 (100%)	2 (0%)	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	466/466 (100%)	460 (99%)	6 (1%)	61	78
1	B	466/466 (100%)	456 (98%)	10 (2%)	47	67
All	All	932/932 (100%)	916 (98%)	16 (2%)	53	73

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	ASP
1	A	262	LEU
1	A	271	ILE
1	A	307	LEU
1	A	480	LYS
1	A	522	LYS
1	B	167	LYS
1	B	214	THR
1	B	229	HIS
1	B	230	ASP
1	B	253	LEU
1	B	376	MET
1	B	407	ARG
1	B	465	VAL
1	B	491	GLU

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Mol	Chain	Res	Type
1	B	513	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	174	HIS
1	A	181	ASN
1	A	244	GLN
1	A	329	GLN
1	A	345	HIS
1	A	389	HIS
1	A	397	ASN
1	B	222	HIS

### 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 15 ligands modelled in this entry, 12 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	ADP	A	1002	5	28,29,29	1.48	4 (14%)	43,45,45	1.85	10 (23%)
4	ADP	B	603	5	28,29,29	1.42	4 (14%)	43,45,45	1.84	10 (23%)
7	PGE	B	601	-	9,9,9	0.36	0	8,8,8	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	1002	5	-	3/16/32/32	0/3/3/3
4	ADP	B	603	5	-	3/16/32/32	0/3/3/3
7	PGE	B	601	-	-	3/7/7/7	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	ADP	C5-C4	4.69	1.47	1.39
4	A	1002	ADP	C5-C4	4.65	1.47	1.39
4	A	1002	ADP	PA-O3A	3.23	1.63	1.59
4	A	1002	ADP	C5-C6	2.92	1.49	1.41
4	B	603	ADP	C5-C6	2.88	1.49	1.41
4	B	603	ADP	C8-N7	2.44	1.36	1.31
4	A	1002	ADP	C8-N7	2.28	1.36	1.31
4	B	603	ADP	PA-O3A	2.26	1.61	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	ADP	C5-C4-N3	-5.72	118.84	126.72
4	A	1002	ADP	C5-C4-N3	-5.71	118.86	126.72
4	A	1002	ADP	N3-C4-N9	4.51	134.84	127.17
4	B	603	ADP	N3-C4-N9	4.49	134.80	127.17
4	B	603	ADP	C2-N3-C4	3.76	121.01	111.83
4	A	1002	ADP	C2-N3-C4	3.69	120.85	111.83
4	A	1002	ADP	C4-C5-N7	-3.59	106.48	110.58
4	B	603	ADP	C4-C5-N7	-3.54	106.54	110.58
4	B	603	ADP	N3-C2-N1	-3.20	123.73	128.58
4	A	1002	ADP	N3-C2-N1	-3.11	123.88	128.58
4	A	1002	ADP	C4-N9-C8	2.88	108.77	105.74
4	B	603	ADP	C4-N9-C8	2.84	108.72	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	ADP	C5-N7-C8	2.63	107.59	103.45
4	B	603	ADP	C5-N7-C8	2.57	107.50	103.45
4	B	603	ADP	C6-C5-N7	2.31	136.54	132.09
4	A	1002	ADP	C6-C5-N7	2.29	136.50	132.09
4	A	1002	ADP	N9-C8-N7	-2.17	110.86	113.94
4	B	603	ADP	N9-C8-N7	-2.15	110.89	113.94
4	B	603	ADP	O4'-C1'-N9	2.09	112.10	108.09
4	A	1002	ADP	O4'-C1'-N9	2.06	112.05	108.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

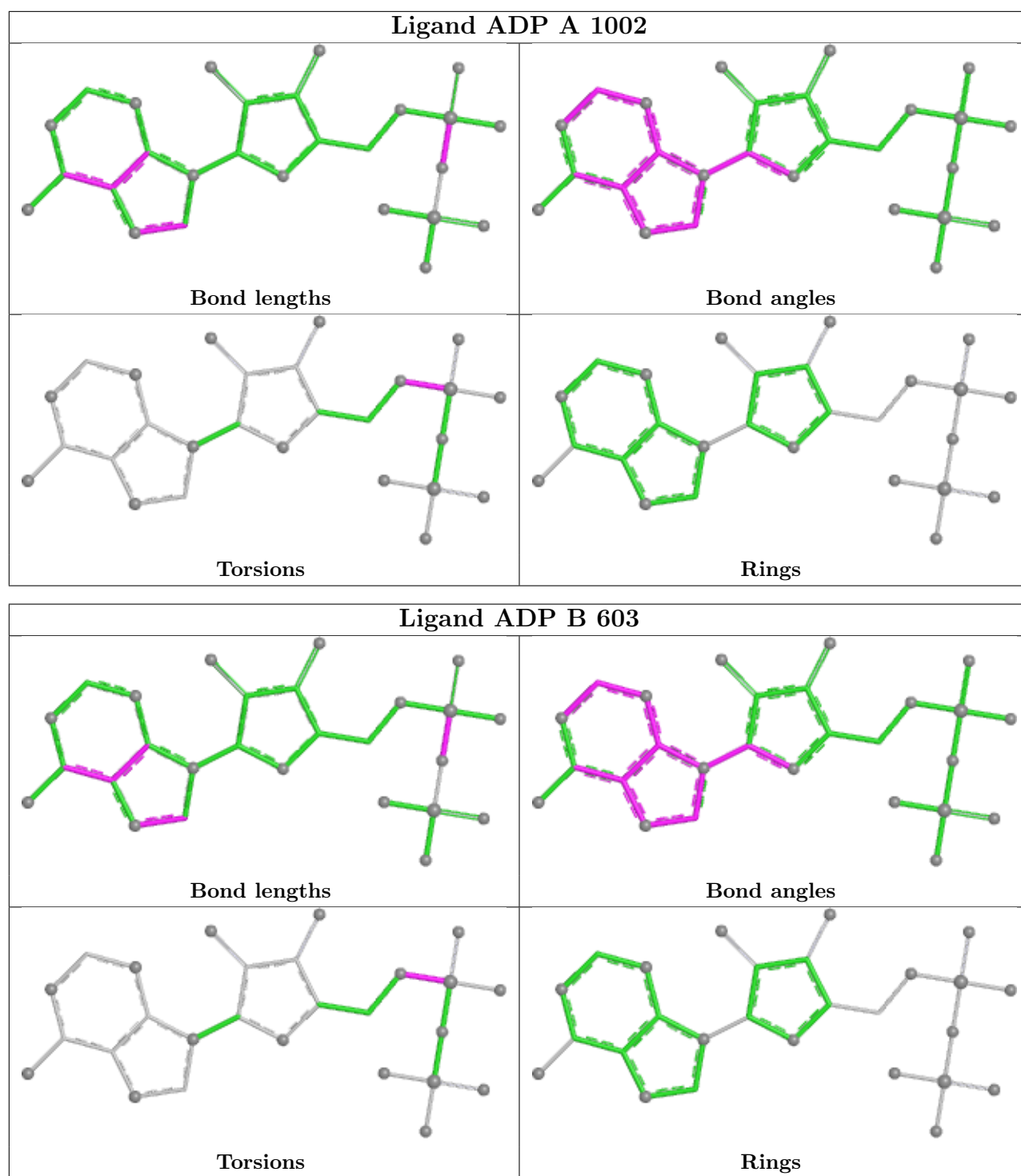
Mol	Chain	Res	Type	Atoms
4	A	1002	ADP	C5'-O5'-PA-O1A
4	A	1002	ADP	C5'-O5'-PA-O2A
4	A	1002	ADP	C5'-O5'-PA-O3A
4	B	603	ADP	C5'-O5'-PA-O1A
4	B	603	ADP	C5'-O5'-PA-O2A
4	B	603	ADP	C5'-O5'-PA-O3A
7	B	601	PGE	O2-C3-C4-O3
7	B	601	PGE	O3-C5-C6-O4
7	B	601	PGE	C3-C4-O3-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	601	PGE	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 ⓘ

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, 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	531/531 (100%)	0.32	23 (4%) 40 35	35, 62, 103, 160	0
1	B	531/531 (100%)	0.45	42 (7%) 18 15	40, 66, 109, 175	0
2	C	17/24 (70%)	0.38	1 (5%) 28 24	77, 91, 114, 138	0
2	D	18/24 (75%)	0.32	1 (5%) 30 26	70, 90, 155, 158	0
All	All	1097/1110 (98%)	0.39	67 (6%) 27 23	35, 65, 107, 175	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	ALA	7.3
1	B	465	VAL	5.0
1	B	375	GLY	4.9
1	A	564	TYR	4.8
1	A	372	VAL	4.6
1	A	376	MET	4.6
1	A	374	PHE	4.6
1	B	373	ALA	4.2
1	B	372	VAL	4.1
1	B	63	SER	3.9
1	A	467	ASN	3.6
1	B	62	ASP	3.5
1	A	227	TRP	3.5
1	A	62	ASP	3.4
1	B	466	TRP	3.4
1	B	374	PHE	3.2
1	B	227	TRP	3.2
1	A	509	LYS	3.2
1	B	273	LYS	3.1
1	A	346	ALA	3.0
1	B	585	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	63	SER	3.0
1	B	181	ASN	2.9
1	A	466	TRP	2.9
1	B	467	ASN	2.8
1	B	376	MET	2.8
1	B	163	ALA	2.7
1	B	564	TYR	2.7
1	B	156	ILE	2.5
1	B	178	VAL	2.5
1	B	168	GLU	2.5
1	A	375	GLY	2.5
1	B	346	ALA	2.5
1	B	482	SER	2.5
1	B	183	GLU	2.4
1	A	257	ALA	2.4
1	B	468	SER	2.4
1	B	206	LYS	2.4
2	C	18	DT	2.4
1	B	378	ILE	2.4
1	B	234	ASP	2.4
1	B	260	HIS	2.4
1	B	592	LYS	2.4
1	B	377	GLY	2.3
1	B	534	ALA	2.3
1	B	483	ALA	2.3
1	A	229	HIS	2.3
1	B	226	GLN	2.3
1	A	522	LYS	2.3
1	A	234	ASP	2.3
1	A	225	SER	2.2
1	B	379	ASP	2.2
1	B	167	LYS	2.2
1	A	256	THR	2.2
1	B	166	SER	2.2
1	B	231	PHE	2.2
1	B	533	VAL	2.1
1	A	226	GLN	2.1
1	B	347	ASN	2.1
2	D	18	DT	2.1
1	B	229	HIS	2.1
1	A	534	ALA	2.1
1	A	491	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	463	ASP	2.0
1	A	74	PRO	2.0
1	B	462	PHE	2.0
1	B	159	THR	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, 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.

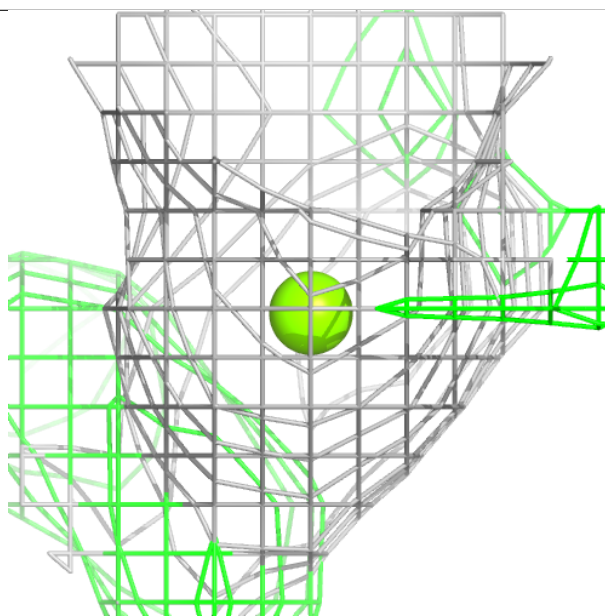
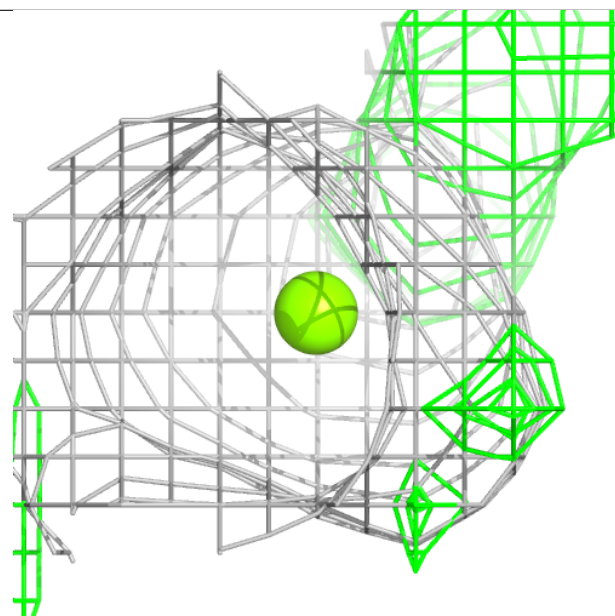
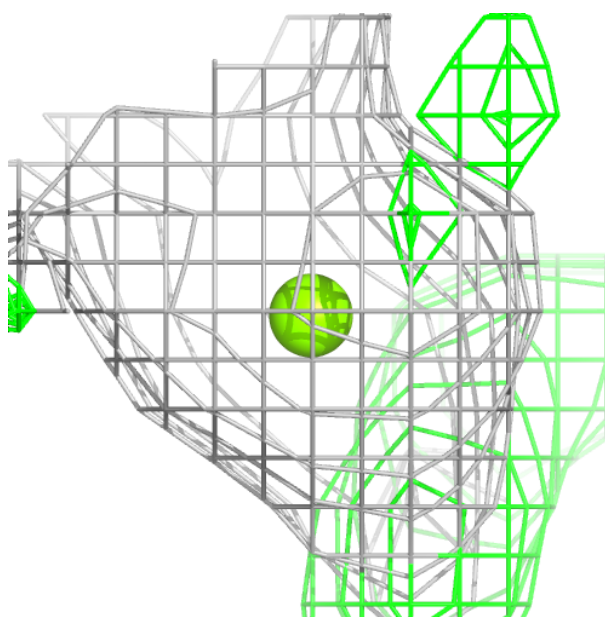
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	A	1003	1/1	0.75	0.19	68,68,68,68	0
5	MG	B	604	1/1	0.77	0.13	60,60,60,60	0
6	K	B	605	1/1	0.77	0.17	87,87,87,87	0
7	PGE	B	601	10/10	0.77	0.16	49,67,76,78	0
6	K	B	606	1/1	0.90	0.17	82,82,82,82	0
4	ADP	B	603	27/27	0.94	0.07	49,59,76,78	0
4	ADP	A	1002	27/27	0.94	0.08	45,54,63,77	0
6	K	C	102	1/1	0.95	0.07	77,77,77,77	0
6	K	A	1004	1/1	0.95	0.13	81,81,81,81	0
6	K	D	201	1/1	0.97	0.05	70,70,70,70	0
6	K	D	202	1/1	0.97	0.04	70,70,70,70	0
6	K	C	101	1/1	0.97	0.07	78,78,78,78	0
6	K	C	103	1/1	0.98	0.04	78,78,78,78	0
3	ZN	B	602	1/1	0.99	0.02	62,62,62,62	0
3	ZN	A	1001	1/1	0.99	0.03	55,55,55,55	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.



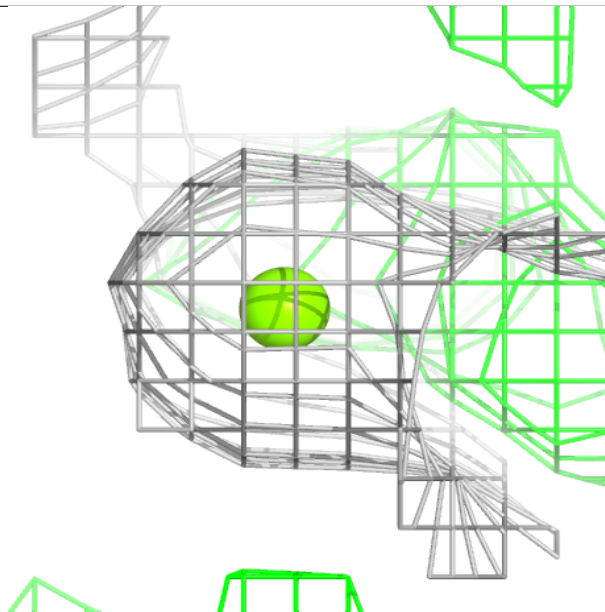
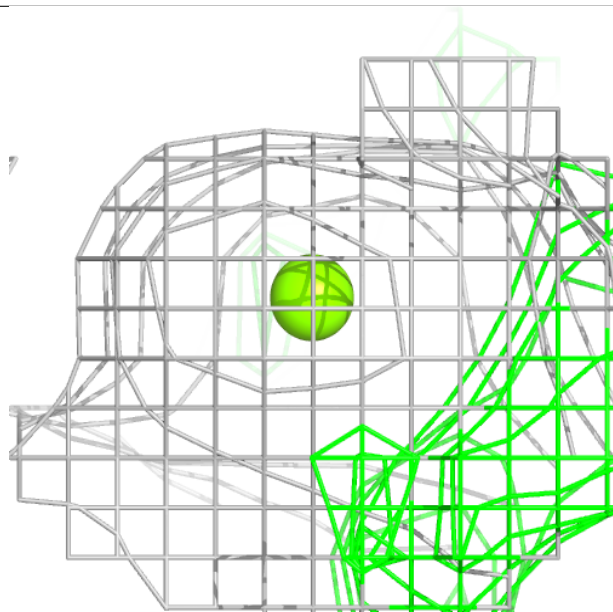
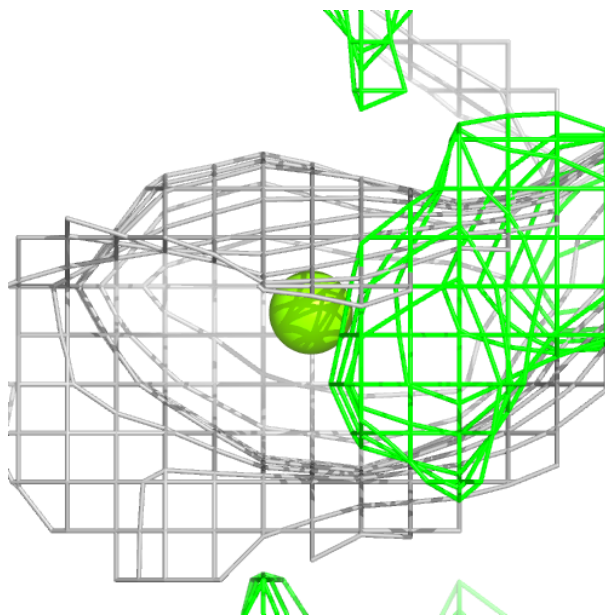
**Electron density around MG A 1003:**

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



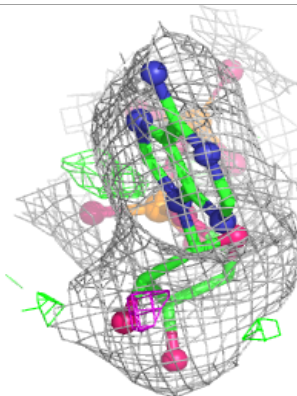
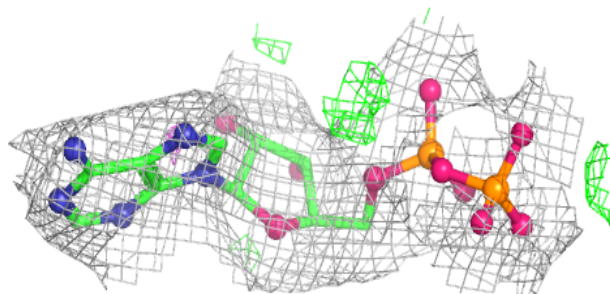
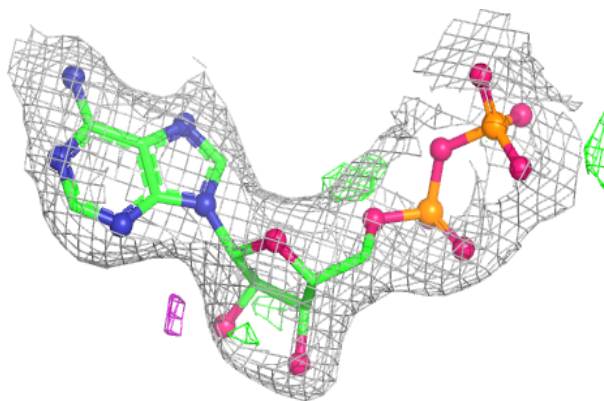
**Electron density around MG B 604:**

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

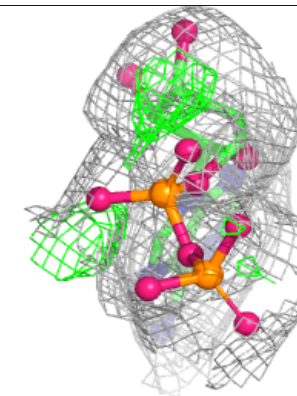
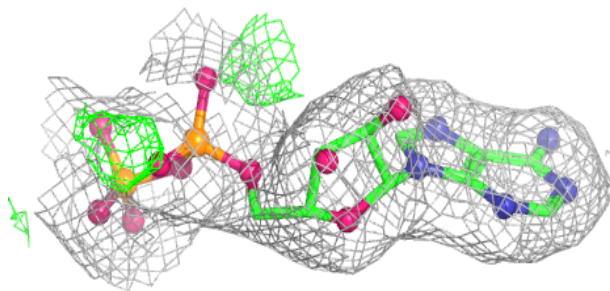
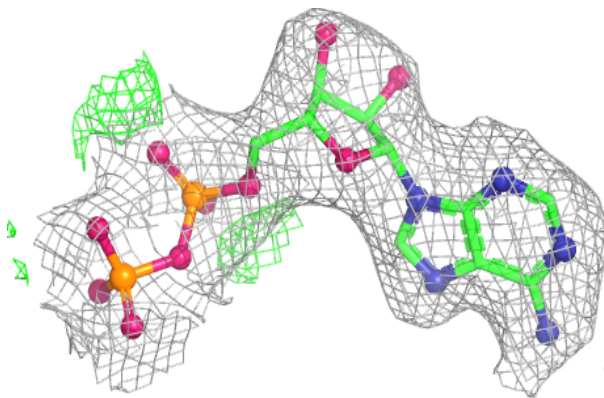


**Electron density around ADP B 603:**

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

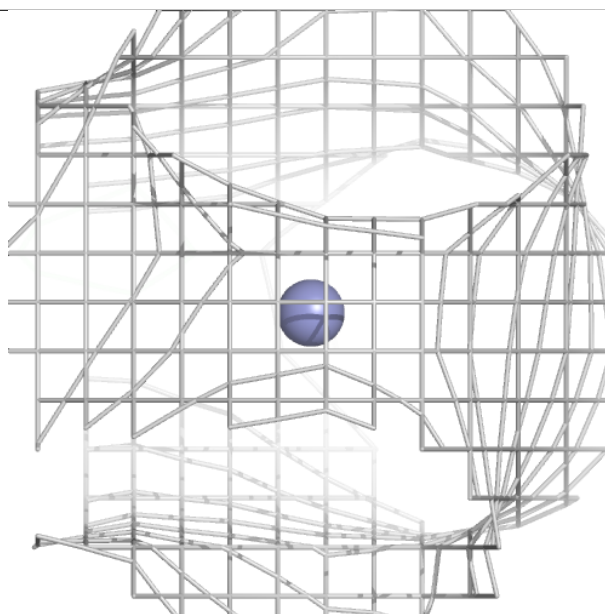
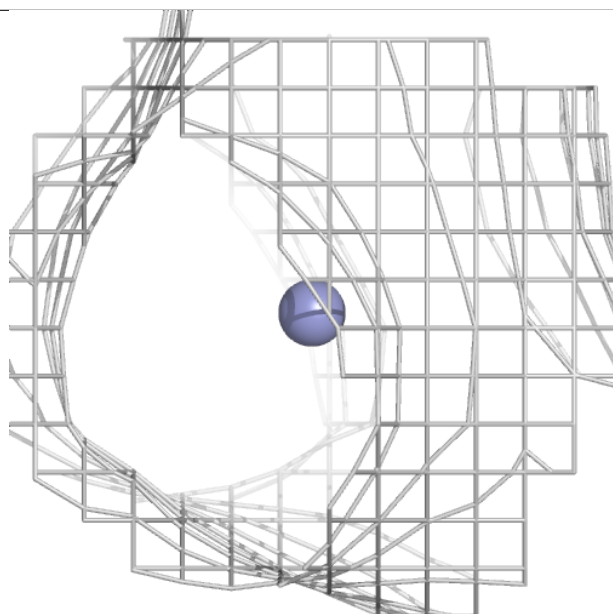
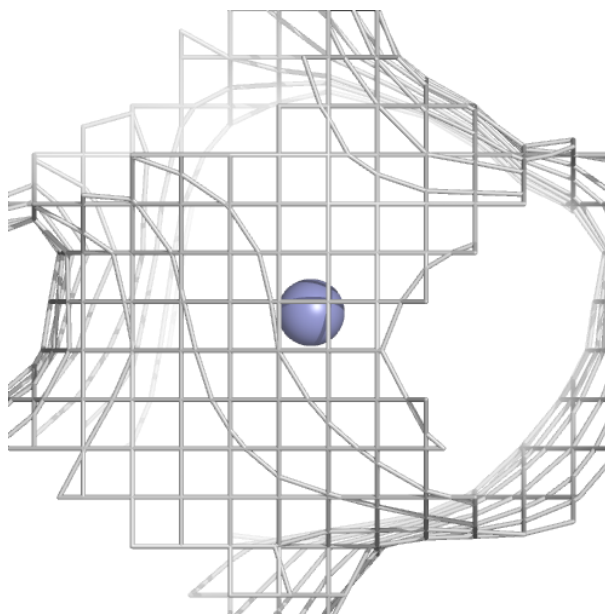
**Electron density around ADP A 1002:**

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



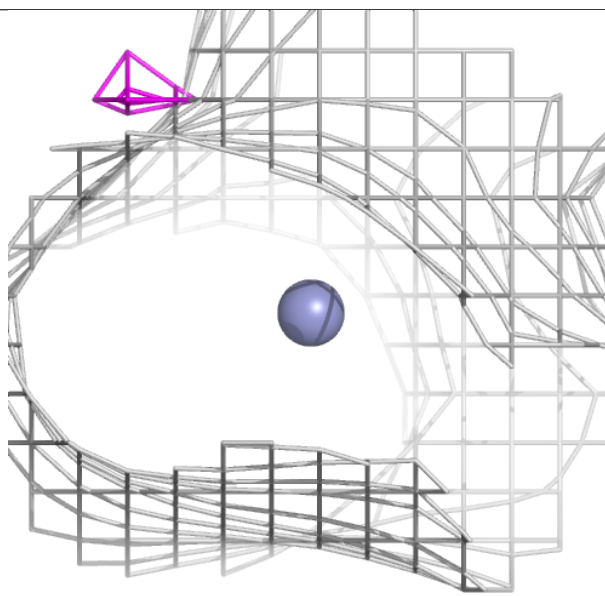
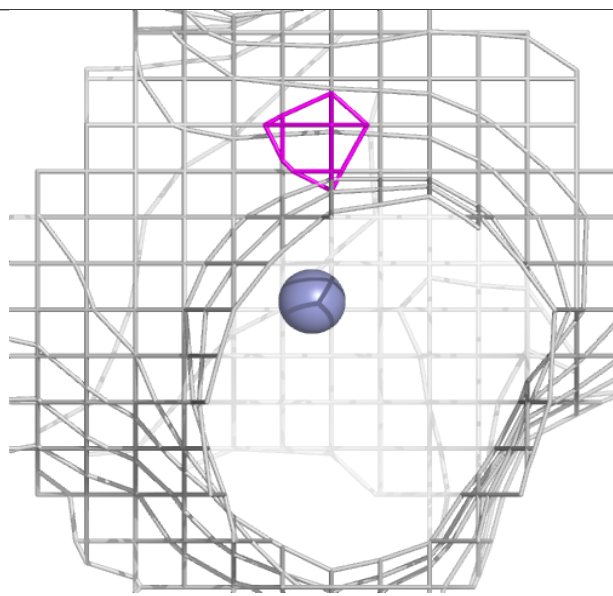
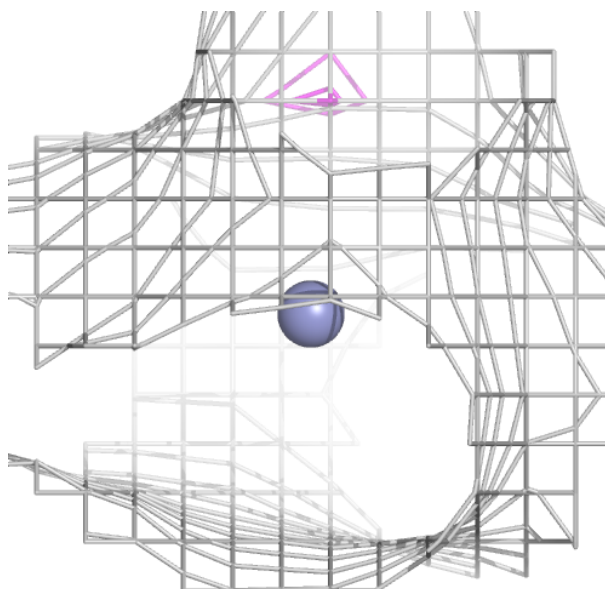
**Electron density around ZN B 602:**

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



**Electron density around ZN A 1001:**

$2mF_o-DF_c$  (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.