



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:44 PM UTC

PDB ID : 9DRE / pdb_00009dre
Title : Crystal structure of ADP-ribose diphosphatase from *Klebsiella pneumoniae* (ADP bound, P21 form)
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2024-09-25
Resolution : 1.69 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

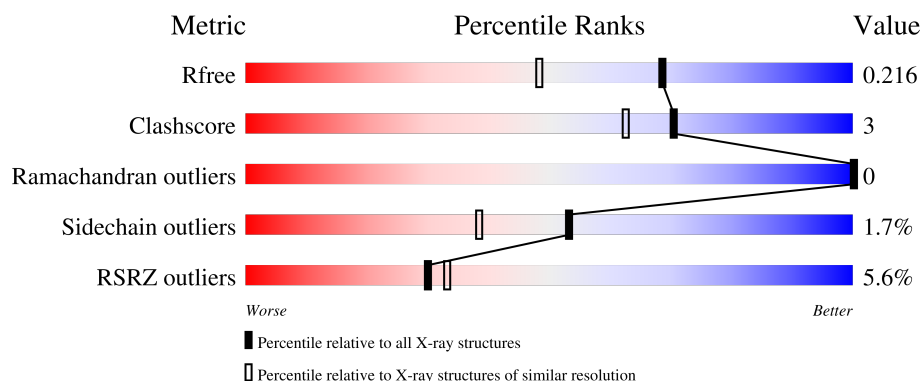
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

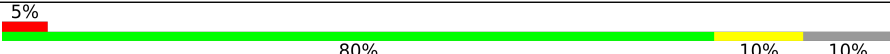
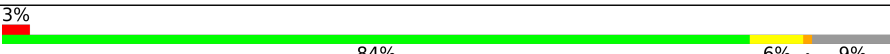
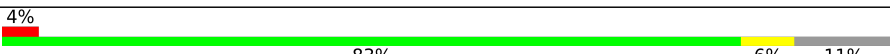
The reported resolution of this entry is 1.69 Å.

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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	218	
1	B	218	
1	C	218	
1	D	218	

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Mol	Chain	Length	Quality of chain
1	E	218	
1	F	218	
1	G	218	
1	H	218	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13700 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 ADP-ribose pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	5	0
			1608	1021	285	298	4			
1	B	197	Total	C	N	O	S	0	3	0
			1574	996	276	300	2			
1	C	199	Total	C	N	O	S	0	2	0
			1584	1004	277	300	3			
1	D	195	Total	C	N	O	S	0	1	0
			1559	985	275	296	3			
1	E	201	Total	C	N	O	S	0	3	0
			1621	1028	289	300	4			
1	F	193	Total	C	N	O	S	0	5	0
			1558	990	271	294	3			
1	G	193	Total	C	N	O	S	0	2	0
			1545	981	269	292	3			
1	H	192	Total	C	N	O	S	0	4	0
			1536	975	268	291	2			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP A0A0H3GVQ7
A	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
A	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
A	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
A	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
A	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
A	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
A	0	HIS	-	expression tag	UNP A0A0H3GVQ7
B	-7	MET	-	expression tag	UNP A0A0H3GVQ7
B	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
B	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
B	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
B	-3	HIS	-	expression tag	UNP A0A0H3GVQ7

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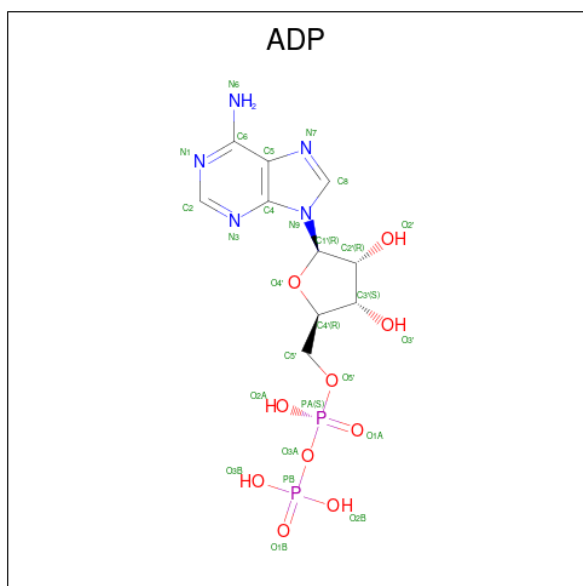
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
B	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
B	0	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-7	MET	-	expression tag	UNP A0A0H3GVQ7
C	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
C	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
C	0	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-7	MET	-	expression tag	UNP A0A0H3GVQ7
D	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
D	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
D	0	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-7	MET	-	expression tag	UNP A0A0H3GVQ7
E	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
E	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
E	0	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-7	MET	-	expression tag	UNP A0A0H3GVQ7
F	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
F	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
F	0	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-7	MET	-	expression tag	UNP A0A0H3GVQ7
G	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
G	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-1	HIS	-	expression tag	UNP A0A0H3GVQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-7	MET	-	expression tag	UNP A0A0H3GVQ7
H	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
H	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
H	0	HIS	-	expression tag	UNP A0A0H3GVQ7

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 54	C 20	N 10	O 20	P 4	0	1
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	D	1	Total 54	C 20	N 10	O 20	P 4	0	1
2	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	F	1	Total 54	C 20	N 10	O 20	P 4	0	1

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	2	Total	Mg	0	0
			2	2		
3	G	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

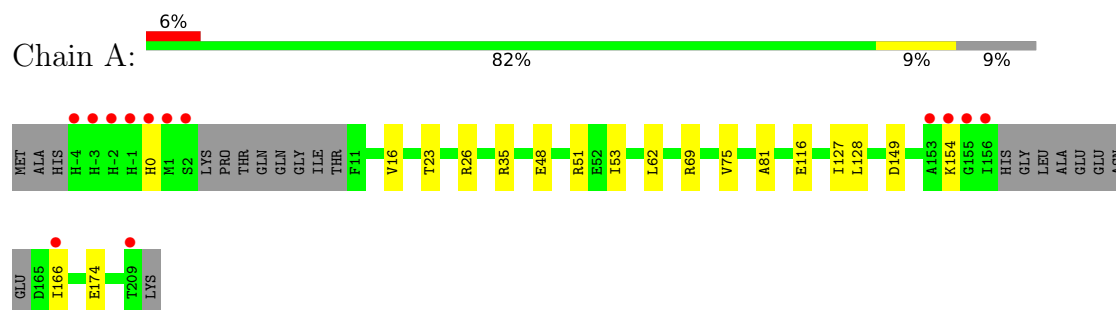
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	102	Total	O	0	0
			102	102		
4	B	123	Total	O	0	2
			123	123		
4	C	111	Total	O	0	0
			111	111		
4	D	71	Total	O	0	1
			71	71		
4	E	104	Total	O	0	0
			104	104		
4	F	100	Total	O	0	0
			100	100		
4	G	109	Total	O	0	0
			109	109		
4	H	91	Total	O	0	0
			91	91		

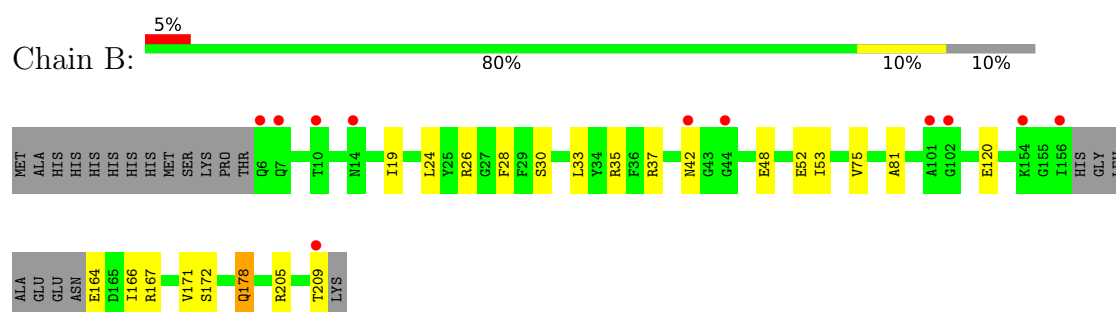
3 Residue-property plots [i](#)

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.

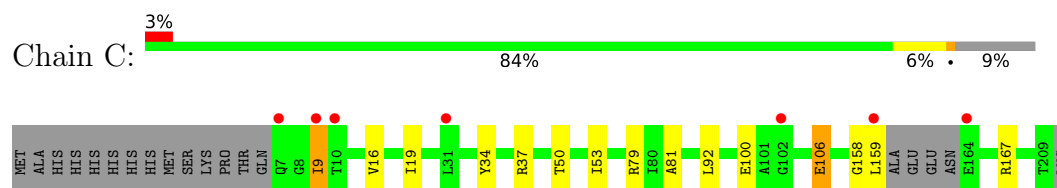
- Molecule 1: ADP-ribose pyrophosphatase



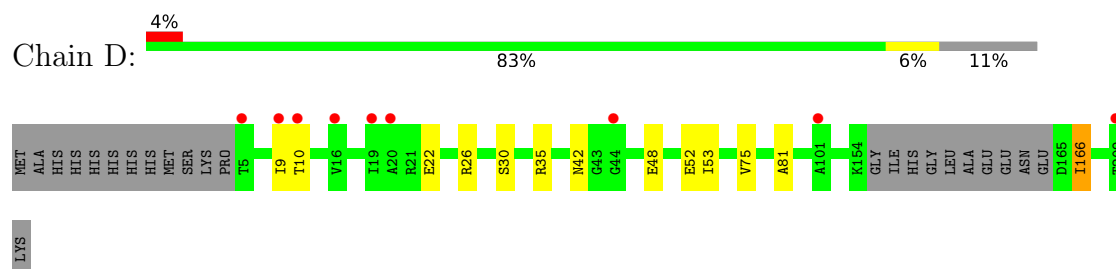
- Molecule 1: ADP-ribose pyrophosphatase



- Molecule 1: ADP-ribose pyrophosphatase

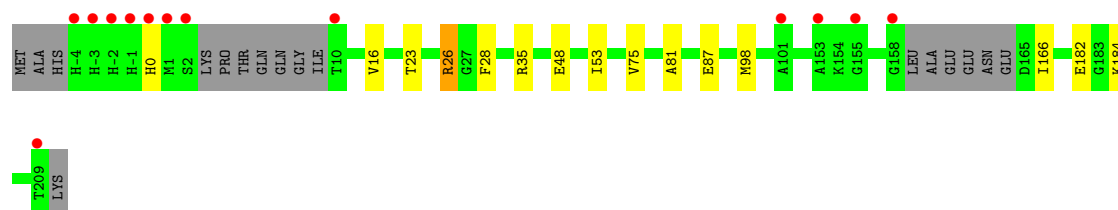


- Molecule 1: ADP-ribose pyrophosphatase



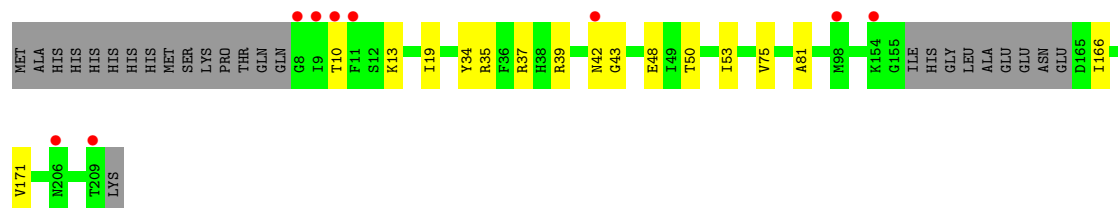
- Molecule 1: ADP-ribose pyrophosphatase

Chain E: 



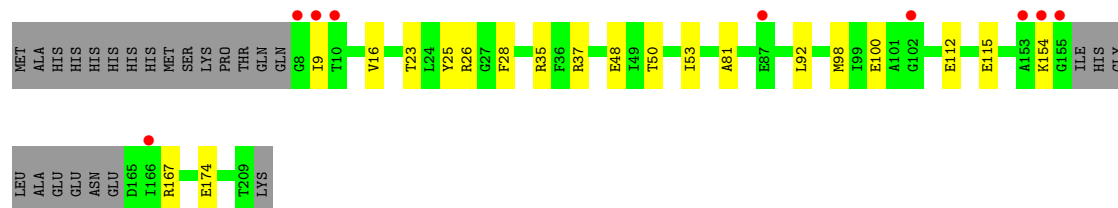
- Molecule 1: ADP-ribose pyrophosphatase

Chain F: 



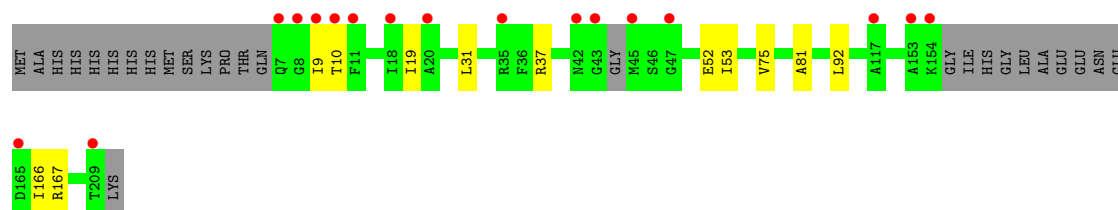
- Molecule 1: ADP-ribose pyrophosphatase

Chain G: 



- Molecule 1: ADP-ribose pyrophosphatase

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.87Å 80.11Å 115.83Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	49.19 – 1.69 49.19 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.19-1.69) 99.9 (49.19-1.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.69Å)	Xtriage
Refinement program	PHENIX (dev_5295: ???)	Depositor
R, R_{free}	0.175 , 0.210 0.185 , 0.216	Depositor DCC
R_{free} test set	9706 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13700	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6213e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	0/1653	0.58	0/2238
1	B	0.42	0/1612	0.60	0/2183
1	C	0.44	0/1620	0.59	0/2194
1	D	0.37	0/1591	0.55	0/2155
1	E	0.41	0/1664	0.60	0/2252
1	F	0.39	0/1602	0.56	0/2168
1	G	0.47	0/1580	0.63	0/2140
1	H	0.40	0/1576	0.57	0/2136
All	All	0.42	0/12898	0.59	0/17466

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1608	0	1579	13	0
1	B	1574	0	1536	19	0
1	C	1584	0	1552	12	0
1	D	1559	0	1525	11	0
1	E	1621	0	1590	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1558	0	1547	11	0
1	G	1545	0	1528	15	0
1	H	1536	0	1494	11	0
2	A	27	0	12	0	0
2	B	54	0	24	2	0
2	C	27	0	12	1	0
2	D	54	0	24	0	0
2	E	27	0	12	1	0
2	F	54	0	24	0	0
2	G	27	0	12	1	0
2	H	27	0	12	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	102	0	0	0	0
4	B	123	0	0	3	0
4	C	111	0	0	2	0
4	D	71	0	0	2	0
4	E	104	0	0	1	0
4	F	100	0	0	0	0
4	G	109	0	0	2	0
4	H	91	0	0	0	0
All	All	13700	0	12483	86	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 3.

All (86) 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:75:VAL:HG13	1:B:166:ILE:HG23	1.57	0.86
1:F:75:VAL:HG13	1:F:166:ILE:HG23	1.60	0.84
1:A:75[A]:VAL:HG13	1:A:166:ILE:HG23	1.62	0.81
1:G:167:ARG:NH2	1:H:10:THR:OG1	2.20	0.73
1:H:75:VAL:HG13	1:H:166:ILE:HG23	1.71	0.72
1:A:0:HIS:HB3	1:B:171:VAL:HG12	1.70	0.71
1:G:81:ALA:HB2	1:H:53:ILE:HD12	1.75	0.67
1:E:35:ARG:NH1	1:E:48:GLU:OE2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:VAL:HG13	1:D:166:ILE:HG23	1.80	0.64
1:B:75:VAL:HG13	1:B:166:ILE:CG2	2.26	0.64
1:E:75[A]:VAL:HG13	1:E:166:ILE:HG23	1.79	0.64
1:D:35:ARG:NH2	1:D:48:GLU:OE2	2.27	0.63
1:G:35:ARG:NH1	1:G:48:GLU:OE2	2.25	0.63
1:A:51:ARG:NH2	2:B:301[B]:ADP:O1B	2.33	0.61
1:A:81:ALA:HB2	1:B:53:ILE:HD12	1.81	0.61
1:G:35:ARG:HG2	1:G:50:THR:HG22	1.83	0.60
1:C:37:ARG:NH2	4:C:402:HOH:O	2.33	0.60
1:C:81:ALA:HB2	1:D:53:ILE:HD12	1.85	0.59
1:B:26[A]:ARG:NH2	4:B:401:HOH:O	2.36	0.59
1:C:19:ILE:HD11	1:C:37:ARG:HG3	1.85	0.58
1:F:75:VAL:HG13	1:F:166:ILE:CG2	2.34	0.58
1:H:75:VAL:HG13	1:H:166:ILE:CG2	2.34	0.57
1:E:98:MET:SD	4:E:494:HOH:O	2.58	0.56
1:F:42:ASN:OD1	1:F:43:GLY:N	2.39	0.56
1:B:205:ARG:O	1:B:209:THR:HG23	2.06	0.56
1:E:81:ALA:HB2	1:F:53:ILE:HD12	1.87	0.55
1:C:53:ILE:HD12	1:D:81:ALA:HB2	1.90	0.54
1:H:52:GLU:O	1:H:53:ILE:HD13	2.08	0.54
1:B:164:GLU:N	4:B:405:HOH:O	2.41	0.53
1:C:9:ILE:HD13	4:D:445:HOH:O	2.08	0.53
1:E:75[B]:VAL:HG23	1:E:166:ILE:HG23	1.91	0.53
1:G:53:ILE:HD12	1:H:81:ALA:HB2	1.91	0.53
1:A:23:THR:HG23	1:A:26:ARG:NH1	2.26	0.51
1:E:75[B]:VAL:CG2	1:E:166:ILE:HG23	2.41	0.51
1:A:116:GLU:HG2	1:A:166:ILE:HD13	1.93	0.50
1:B:35:ARG:HD3	1:B:48:GLU:OE2	2.12	0.49
1:A:75[A]:VAL:HG13	1:A:166:ILE:CG2	2.36	0.49
1:A:53:ILE:HD12	1:B:81:ALA:HB2	1.94	0.49
1:D:26:ARG:HD2	1:D:30:SER:OG	2.13	0.48
1:B:28:PHE:CZ	2:B:301[B]:ADP:H1'	2.49	0.48
1:E:53:ILE:HD12	1:F:81:ALA:HB2	1.95	0.48
1:B:26[A]:ARG:CZ	1:B:30:SER:OG	2.61	0.48
1:E:23:THR:HG23	1:E:26:ARG:HH11	1.79	0.47
1:H:19:ILE:HD11	1:H:37:ARG:HG3	1.96	0.47
1:A:0:HIS:CE1	1:B:172:SER:H	2.32	0.47
1:E:23:THR:HG23	1:E:26:ARG:NH1	2.29	0.47
1:G:9:ILE:HD11	1:H:92:LEU:HG	1.97	0.47
1:G:174:GLU:OE1	4:G:401:HOH:O	2.20	0.47
1:C:158:GLY:O	1:C:159:LEU:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LEU:HD11	1:B:33:LEU:HB2	1.97	0.46
1:B:26[A]:ARG:NE	1:B:30:SER:OG	2.48	0.46
1:E:87:GLU:O	1:F:13:LYS:HG3	2.15	0.46
1:D:52:GLU:O	1:D:53:ILE:HD13	2.16	0.46
1:A:35:ARG:HD3	1:A:48[A]:GLU:CD	2.42	0.45
1:C:79:ARG:NH1	2:C:301:ADP:O2A	2.48	0.45
1:C:92:LEU:HG	1:D:9:ILE:HD11	1.97	0.45
1:G:25:TYR:CE2	1:H:31:LEU:CD2	3.00	0.45
1:G:37:ARG:NH2	4:G:406:HOH:O	2.49	0.45
1:G:35:ARG:HD3	1:G:48:GLU:OE2	2.17	0.45
1:B:19:ILE:HD11	1:B:37:ARG:HG3	2.00	0.44
1:E:0:HIS:HB2	1:F:171:VAL:HG12	2.00	0.44
1:A:69:ARG:NH1	1:A:149:ASP:OD1	2.45	0.44
1:G:23:THR:HG23	1:G:26:ARG:NH1	2.32	0.44
1:B:52:GLU:O	1:B:53:ILE:HD13	2.18	0.43
1:D:75:VAL:HG13	1:D:166:ILE:CG2	2.47	0.43
1:E:182:GLU:OE1	1:E:184:LYS:NZ	2.51	0.43
1:A:127:ILE:O	1:A:128[A]:LEU:HD23	2.18	0.43
1:E:75[B]:VAL:HG23	1:E:166:ILE:CG2	2.48	0.43
1:B:164:GLU:HB2	4:B:455:HOH:O	2.18	0.43
1:B:178[A]:GLN:NE2	1:B:178[A]:GLN:HA	2.34	0.43
1:G:28:PHE:CE2	2:G:301:ADP:C4	3.06	0.43
1:F:19:ILE:HD11	1:F:37:ARG:HG3	2.01	0.42
1:D:42:ASN:C	1:D:42:ASN:OD1	2.61	0.42
1:C:34:TYR:O	1:C:50:THR:HA	2.20	0.42
1:C:167:ARG:NH2	1:D:10:THR:OG1	2.49	0.42
1:F:35:ARG:HD3	1:F:48:GLU:OE2	2.19	0.42
1:G:25:TYR:CD2	1:H:31:LEU:HD22	2.54	0.42
1:C:106:GLU:CD	1:C:106:GLU:H	2.26	0.42
1:E:28:PHE:CZ	2:E:301:ADP:H1'	2.53	0.42
1:G:92:LEU:HG	1:H:9:ILE:HD11	2.01	0.42
1:F:39:ARG:NH2	1:F:43:GLY:O	2.53	0.41
1:G:112:GLU:HA	1:G:115:GLU:HG2	2.01	0.41
1:C:9:ILE:CD1	4:D:445:HOH:O	2.67	0.41
1:F:34:TYR:O	1:F:50:THR:HA	2.21	0.41
4:C:457:HOH:O	1:D:9:ILE:HD13	2.21	0.41
1:A:0:HIS:ND1	1:B:171:VAL:HA	2.36	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	197/218 (90%)	190 (96%)	7 (4%)	0	100	100
1	B	196/218 (90%)	188 (96%)	8 (4%)	0	100	100
1	C	197/218 (90%)	191 (97%)	6 (3%)	0	100	100
1	D	192/218 (88%)	187 (97%)	5 (3%)	0	100	100
1	E	198/218 (91%)	193 (98%)	5 (2%)	0	100	100
1	F	194/218 (89%)	187 (96%)	7 (4%)	0	100	100
1	G	191/218 (88%)	185 (97%)	6 (3%)	0	100	100
1	H	190/218 (87%)	182 (96%)	8 (4%)	0	100	100
All	All	1555/1744 (89%)	1503 (97%)	52 (3%)	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	170/183 (93%)	165 (97%)	5 (3%)	37	20
1	B	163/183 (89%)	158 (97%)	5 (3%)	35	18
1	C	165/183 (90%)	161 (98%)	4 (2%)	43	26
1	D	163/183 (89%)	161 (99%)	2 (1%)	63	51
1	E	171/183 (93%)	168 (98%)	3 (2%)	51	36
1	F	165/183 (90%)	164 (99%)	1 (1%)	78	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	163/183 (89%)	159 (98%)	4 (2%)	42	24
1	H	159/183 (87%)	158 (99%)	1 (1%)	78	72
All	All	1319/1464 (90%)	1294 (98%)	25 (2%)	53	34

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

Mol	Chain	Res	Type
1	A	16[A]	VAL
1	A	16[B]	VAL
1	A	62	LEU
1	A	154	LYS
1	A	174	GLU
1	B	42	ASN
1	B	120	GLU
1	B	167	ARG
1	B	178[A]	GLN
1	B	178[B]	GLN
1	C	9	ILE
1	C	16	VAL
1	C	100	GLU
1	C	106	GLU
1	D	22	GLU
1	D	166	ILE
1	E	16[A]	VAL
1	E	16[B]	VAL
1	E	26	ARG
1	F	10	THR
1	G	16	VAL
1	G	98	MET
1	G	100	GLU
1	G	154	LYS
1	H	167	ARG

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

Mol	Chain	Res	Type
1	B	200	HIS
1	C	77	GLN
1	C	187	ASN
1	D	200	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 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$
2	ADP	H	301	-	28,29,29	1.42	4 (14%)	43,45,45	1.78	9 (20%)
2	ADP	E	301	-	28,29,29	1.36	5 (17%)	43,45,45	1.88	8 (18%)
2	ADP	A	301	-	28,29,29	1.30	4 (14%)	43,45,45	2.02	12 (27%)
2	ADP	G	301	3	28,29,29	1.35	4 (14%)	43,45,45	2.07	11 (25%)
2	ADP	F	301[B]	-	28,29,29	1.33	4 (14%)	43,45,45	1.88	10 (23%)
2	ADP	F	301[A]	-	28,29,29	1.38	5 (17%)	43,45,45	1.93	9 (20%)
2	ADP	D	301[B]	-	28,29,29	1.36	4 (14%)	43,45,45	1.89	10 (23%)
2	ADP	D	301[A]	-	28,29,29	1.37	4 (14%)	43,45,45	1.86	8 (18%)
2	ADP	C	301	-	28,29,29	1.38	5 (17%)	43,45,45	1.95	8 (18%)
2	ADP	B	301[B]	-	28,29,29	1.43	4 (14%)	43,45,45	1.84	8 (18%)
2	ADP	B	301[A]	3	28,29,29	1.31	5 (17%)	43,45,45	1.90	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
2	ADP	H	301	-	-	5/16/32/32	0/3/3/3
2	ADP	E	301	-	-	5/16/32/32	0/3/3/3
2	ADP	A	301	-	-	5/16/32/32	0/3/3/3
2	ADP	G	301	3	-	4/16/32/32	0/3/3/3
2	ADP	F	301[B]	-	-	5/16/32/32	0/3/3/3
2	ADP	F	301[A]	-	-	8/16/32/32	0/3/3/3
2	ADP	D	301[B]	-	-	6/16/32/32	0/3/3/3
2	ADP	D	301[A]	-	-	7/16/32/32	0/3/3/3
2	ADP	C	301	-	-	6/16/32/32	0/3/3/3
2	ADP	B	301[B]	-	-	5/16/32/32	0/3/3/3
2	ADP	B	301[A]	3	-	6/16/32/32	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301[B]	ADP	C5-C4	4.58	1.47	1.39
2	E	301	ADP	C5-C4	4.55	1.47	1.39
2	D	301[A]	ADP	C5-C4	4.54	1.47	1.39
2	C	301	ADP	C5-C4	4.41	1.47	1.39
2	F	301[A]	ADP	C5-C4	4.32	1.46	1.39
2	G	301	ADP	C5-C4	4.30	1.46	1.39
2	F	301[B]	ADP	C5-C4	4.27	1.46	1.39
2	H	301	ADP	C5-C4	4.23	1.46	1.39
2	B	301[A]	ADP	C5-C4	4.19	1.46	1.39
2	B	301[B]	ADP	C5-C4	4.11	1.46	1.39
2	A	301	ADP	C5-C4	4.02	1.46	1.39
2	B	301[B]	ADP	PA-O3A	3.80	1.63	1.59
2	H	301	ADP	PA-O3A	2.98	1.62	1.59
2	H	301	ADP	C8-N7	2.98	1.37	1.31
2	C	301	ADP	PA-O3A	2.84	1.62	1.59
2	G	301	ADP	PA-O3A	2.76	1.62	1.59
2	F	301[A]	ADP	PA-O3A	2.70	1.62	1.59
2	D	301[B]	ADP	C8-N7	2.57	1.36	1.31
2	A	301	ADP	C5-N7	-2.55	1.34	1.39
2	E	301	ADP	C8-N7	2.54	1.36	1.31
2	F	301[A]	ADP	C5-N7	-2.51	1.34	1.39
2	F	301[B]	ADP	C8-N7	2.49	1.36	1.31
2	G	301	ADP	C5-N7	-2.47	1.34	1.39
2	D	301[A]	ADP	C8-N7	2.44	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	ADP	C5-N7	-2.44	1.34	1.39
2	D	301[B]	ADP	C5-C6	2.36	1.47	1.41
2	D	301[A]	ADP	C5-N7	-2.36	1.34	1.39
2	A	301	ADP	PA-O3A	2.36	1.62	1.59
2	B	301[B]	ADP	C8-N7	2.35	1.36	1.31
2	F	301[B]	ADP	C5-N7	-2.34	1.34	1.39
2	D	301[A]	ADP	C5-C6	2.31	1.47	1.41
2	C	301	ADP	C8-N7	2.29	1.36	1.31
2	F	301[A]	ADP	C8-N7	2.28	1.36	1.31
2	B	301[A]	ADP	C8-N7	2.27	1.36	1.31
2	E	301	ADP	C5-N7	-2.26	1.35	1.39
2	B	301[A]	ADP	C5-C6	2.21	1.47	1.41
2	E	301	ADP	C5-C6	2.21	1.47	1.41
2	E	301	ADP	PA-O3A	2.20	1.61	1.59
2	A	301	ADP	C8-N7	2.19	1.35	1.31
2	B	301[B]	ADP	C5-C6	2.19	1.47	1.41
2	H	301	ADP	C5-N7	-2.18	1.35	1.39
2	F	301[B]	ADP	C5-C6	2.15	1.47	1.41
2	B	301[A]	ADP	C5-N7	-2.14	1.35	1.39
2	G	301	ADP	C5-C6	2.13	1.46	1.41
2	D	301[B]	ADP	C5-N7	-2.11	1.35	1.39
2	C	301	ADP	C5-C6	2.08	1.46	1.41
2	F	301[A]	ADP	C5-C6	2.06	1.46	1.41
2	B	301[A]	ADP	PA-O3A	2.05	1.61	1.59

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	ADP	C5-C4-N3	-6.75	117.42	126.72
2	C	301	ADP	C5-C4-N3	-6.49	117.77	126.72
2	F	301[A]	ADP	C5-C4-N3	-6.17	118.22	126.72
2	A	301	ADP	C5-C4-N3	-6.10	118.32	126.72
2	B	301[A]	ADP	C5-C4-N3	-6.01	118.45	126.72
2	G	301	ADP	N3-C4-N9	5.94	137.26	127.17
2	E	301	ADP	C5-C4-N3	-5.87	118.63	126.72
2	F	301[B]	ADP	C5-C4-N3	-5.87	118.64	126.72
2	B	301[B]	ADP	C5-C4-N3	-5.86	118.65	126.72
2	D	301[B]	ADP	C5-C4-N3	-5.84	118.67	126.72
2	D	301[A]	ADP	C5-C4-N3	-5.84	118.67	126.72
2	C	301	ADP	N3-C4-N9	5.79	137.01	127.17
2	A	301	ADP	N3-C4-N9	5.46	136.45	127.17
2	F	301[A]	ADP	N3-C4-N9	5.44	136.42	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301[A]	ADP	N3-C4-N9	5.22	136.04	127.17
2	H	301	ADP	C5-C4-N3	-5.04	119.77	126.72
2	B	301[B]	ADP	N3-C4-N9	4.96	135.61	127.17
2	E	301	ADP	N3-C4-N9	4.96	135.61	127.17
2	D	301[A]	ADP	N3-C4-N9	4.94	135.56	127.17
2	D	301[B]	ADP	N3-C4-N9	4.90	135.49	127.17
2	F	301[B]	ADP	N3-C4-N9	4.89	135.49	127.17
2	H	301	ADP	N3-C4-N9	4.44	134.71	127.17
2	A	301	ADP	N3-C2-N1	-4.24	122.17	128.58
2	G	301	ADP	C2-N3-C4	4.22	122.13	111.83
2	A	301	ADP	C2-N3-C4	4.18	122.05	111.83
2	C	301	ADP	C2-N3-C4	4.11	121.87	111.83
2	E	301	ADP	C2-N3-C4	4.10	121.84	111.83
2	E	301	ADP	N3-C2-N1	-4.09	122.39	128.58
2	H	301	ADP	N3-C2-N1	-4.08	122.40	128.58
2	D	301[B]	ADP	C2-N3-C4	4.04	121.70	111.83
2	B	301[A]	ADP	C2-N3-C4	3.95	121.47	111.83
2	B	301[B]	ADP	C2-N3-C4	3.94	121.44	111.83
2	D	301[A]	ADP	C2-N3-C4	3.92	121.40	111.83
2	F	301[A]	ADP	C2-N3-C4	3.88	121.31	111.83
2	D	301[B]	ADP	N3-C2-N1	-3.74	122.92	128.58
2	F	301[B]	ADP	C2-N3-C4	3.72	120.91	111.83
2	D	301[A]	ADP	N3-C2-N1	-3.67	123.03	128.58
2	B	301[A]	ADP	N3-C2-N1	-3.66	123.04	128.58
2	C	301	ADP	N3-C2-N1	-3.66	123.05	128.58
2	B	301[B]	ADP	N3-C2-N1	-3.65	123.05	128.58
2	F	301[A]	ADP	N3-C2-N1	-3.63	123.09	128.58
2	G	301	ADP	N3-C2-N1	-3.61	123.11	128.58
2	F	301[B]	ADP	N3-C2-N1	-3.36	123.49	128.58
2	H	301	ADP	C2-N3-C4	3.29	119.88	111.83
2	F	301[B]	ADP	C2'-C1'-N9	-3.21	105.33	113.30
2	A	301	ADP	C4-N9-C8	3.14	109.04	105.74
2	G	301	ADP	C2'-C1'-N9	-3.13	105.53	113.30
2	A	301	ADP	C5-C6-N6	-3.00	115.85	123.29
2	C	301	ADP	C5-C6-N6	-2.97	115.92	123.29
2	A	301	ADP	N6-C6-N1	2.96	124.96	118.38
2	B	301[A]	ADP	C4-N9-C8	2.92	108.80	105.74
2	C	301	ADP	N6-C6-N1	2.89	124.81	118.38
2	D	301[B]	ADP	C4-N9-C8	2.84	108.72	105.74
2	F	301[A]	ADP	N6-C6-N1	2.78	124.57	118.38
2	H	301	ADP	C4-N9-C8	2.74	108.62	105.74
2	B	301[B]	ADP	C4-N9-C8	2.74	108.61	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301[A]	ADP	C4-N9-C8	2.72	108.60	105.74
2	F	301[A]	ADP	C4-N9-C8	2.71	108.58	105.74
2	D	301[B]	ADP	C4-C5-N7	-2.70	107.49	110.58
2	F	301[A]	ADP	C5-C6-N6	-2.69	116.63	123.29
2	F	301[B]	ADP	C4-N9-C8	2.67	108.54	105.74
2	H	301	ADP	N6-C6-N1	2.67	124.31	118.38
2	B	301[B]	ADP	C3'-C2'-C1'	2.63	106.44	101.46
2	H	301	ADP	C5-C6-N6	-2.63	116.77	123.29
2	G	301	ADP	C4-N9-C8	2.61	108.48	105.74
2	G	301	ADP	C5-C6-N6	-2.58	116.89	123.29
2	G	301	ADP	N6-C6-N1	2.58	124.13	118.38
2	C	301	ADP	C4-N9-C8	2.56	108.43	105.74
2	D	301[A]	ADP	C4-C5-N7	-2.55	107.67	110.58
2	B	301[A]	ADP	C2'-C1'-N9	-2.54	106.99	113.30
2	E	301	ADP	C4-N9-C8	2.54	108.40	105.74
2	A	301	ADP	C3'-C2'-C1'	2.52	106.23	101.46
2	D	301[B]	ADP	C3'-C2'-C1'	2.47	106.13	101.46
2	F	301[B]	ADP	C4-C5-N7	-2.43	107.81	110.58
2	G	301	ADP	C4-C5-N7	-2.43	107.81	110.58
2	B	301[A]	ADP	C4-C5-N7	-2.33	107.92	110.58
2	G	301	ADP	C5-N7-C8	2.31	107.08	103.45
2	F	301[A]	ADP	C3'-C2'-C1'	2.25	105.72	101.46
2	E	301	ADP	C4-C5-N7	-2.25	108.02	110.58
2	F	301[B]	ADP	N6-C6-N1	2.24	123.37	118.38
2	F	301[B]	ADP	C5-C6-N6	-2.24	117.74	123.29
2	H	301	ADP	C2-N1-C6	2.23	122.39	118.73
2	B	301[B]	ADP	C4-C5-N7	-2.22	108.04	110.58
2	F	301[B]	ADP	O4'-C1'-N9	2.20	112.32	108.09
2	D	301[B]	ADP	C5-N7-C8	2.18	106.88	103.45
2	B	301[B]	ADP	C5-C6-N6	-2.14	117.99	123.29
2	B	301[A]	ADP	C5-C6-N6	-2.12	118.03	123.29
2	E	301	ADP	C2'-C1'-N9	-2.11	108.05	113.30
2	A	301	ADP	C2'-C1'-N9	-2.11	108.05	113.30
2	A	301	ADP	N9-C8-N7	-2.11	110.94	113.94
2	H	301	ADP	C2'-C1'-N9	-2.11	108.06	113.30
2	D	301[A]	ADP	C5-N7-C8	2.11	106.76	103.45
2	A	301	ADP	C4-C5-N7	-2.10	108.18	110.58
2	F	301[A]	ADP	C4-C5-N7	-2.09	108.20	110.58
2	E	301	ADP	O3B-PB-O2B	2.07	115.57	107.80
2	B	301[A]	ADP	N6-C6-N1	2.07	122.99	118.38
2	C	301	ADP	C2'-C1'-N9	-2.05	108.21	113.30
2	D	301[A]	ADP	N6-C6-N1	2.04	122.92	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301[A]	ADP	C5-N7-C8	2.02	106.63	103.45
2	D	301[B]	ADP	N9-C8-N7	-2.02	111.07	113.94
2	A	301	ADP	C5-N7-C8	2.01	106.61	103.45
2	D	301[B]	ADP	C6-C5-N7	2.01	135.96	132.09
2	G	301	ADP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301[A]	ADP	PA-O3A-PB-O2B
2	B	301[A]	ADP	C5'-O5'-PA-O1A
2	B	301[A]	ADP	C5'-O5'-PA-O2A
2	B	301[B]	ADP	PA-O3A-PB-O2B
2	B	301[B]	ADP	C5'-O5'-PA-O2A
2	B	301[B]	ADP	C5'-O5'-PA-O3A
2	C	301	ADP	C5'-O5'-PA-O1A
2	C	301	ADP	C5'-O5'-PA-O2A
2	C	301	ADP	C5'-O5'-PA-O3A
2	D	301[A]	ADP	PA-O3A-PB-O3B
2	D	301[A]	ADP	C5'-O5'-PA-O2A
2	D	301[B]	ADP	PA-O3A-PB-O2B
2	D	301[B]	ADP	PB-O3A-PA-O5'
2	D	301[B]	ADP	C5'-O5'-PA-O1A
2	D	301[B]	ADP	C5'-O5'-PA-O2A
2	D	301[B]	ADP	C5'-O5'-PA-O3A
2	E	301	ADP	PA-O3A-PB-O2B
2	E	301	ADP	PA-O3A-PB-O3B
2	E	301	ADP	C5'-O5'-PA-O1A
2	E	301	ADP	C5'-O5'-PA-O3A
2	F	301[B]	ADP	C5'-O5'-PA-O2A
2	F	301[B]	ADP	C5'-O5'-PA-O3A
2	H	301	ADP	PA-O3A-PB-O2B
2	H	301	ADP	C5'-O5'-PA-O1A
2	H	301	ADP	C5'-O5'-PA-O2A
2	H	301	ADP	C5'-O5'-PA-O3A
2	C	301	ADP	O4'-C4'-C5'-O5'
2	C	301	ADP	C3'-C4'-C5'-O5'
2	D	301[A]	ADP	O4'-C4'-C5'-O5'
2	G	301	ADP	O4'-C4'-C5'-O5'
2	G	301	ADP	C3'-C4'-C5'-O5'
2	B	301[A]	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	F	301[A]	ADP	O4'-C4'-C5'-O5'
2	D	301[A]	ADP	C3'-C4'-C5'-O5'
2	H	301	ADP	PA-O3A-PB-O1B
2	F	301[A]	ADP	C3'-C4'-C5'-O5'
2	F	301[B]	ADP	PB-O3A-PA-O1A
2	F	301[A]	ADP	PA-O3A-PB-O1B
2	F	301[A]	ADP	PB-O3A-PA-O1A
2	A	301	ADP	C5'-O5'-PA-O1A
2	A	301	ADP	C5'-O5'-PA-O2A
2	A	301	ADP	C5'-O5'-PA-O3A
2	B	301[A]	ADP	C5'-O5'-PA-O3A
2	B	301[B]	ADP	C5'-O5'-PA-O1A
2	D	301[A]	ADP	C5'-O5'-PA-O1A
2	D	301[A]	ADP	C5'-O5'-PA-O3A
2	E	301	ADP	C5'-O5'-PA-O2A
2	F	301[A]	ADP	C5'-O5'-PA-O1A
2	F	301[A]	ADP	C5'-O5'-PA-O2A
2	F	301[A]	ADP	C5'-O5'-PA-O3A
2	F	301[B]	ADP	C5'-O5'-PA-O1A
2	C	301	ADP	PA-O3A-PB-O1B
2	A	301	ADP	PB-O3A-PA-O1A
2	A	301	ADP	PB-O3A-PA-O2A
2	F	301[B]	ADP	PB-O3A-PA-O2A
2	D	301[A]	ADP	C4'-C5'-O5'-PA
2	B	301[A]	ADP	PA-O3A-PB-O1B
2	D	301[B]	ADP	PA-O3A-PB-O1B
2	G	301	ADP	PA-O3A-PB-O1B
2	B	301[B]	ADP	PA-O3A-PB-O3B
2	F	301[A]	ADP	PB-O3A-PA-O2A
2	G	301	ADP	C4'-C5'-O5'-PA

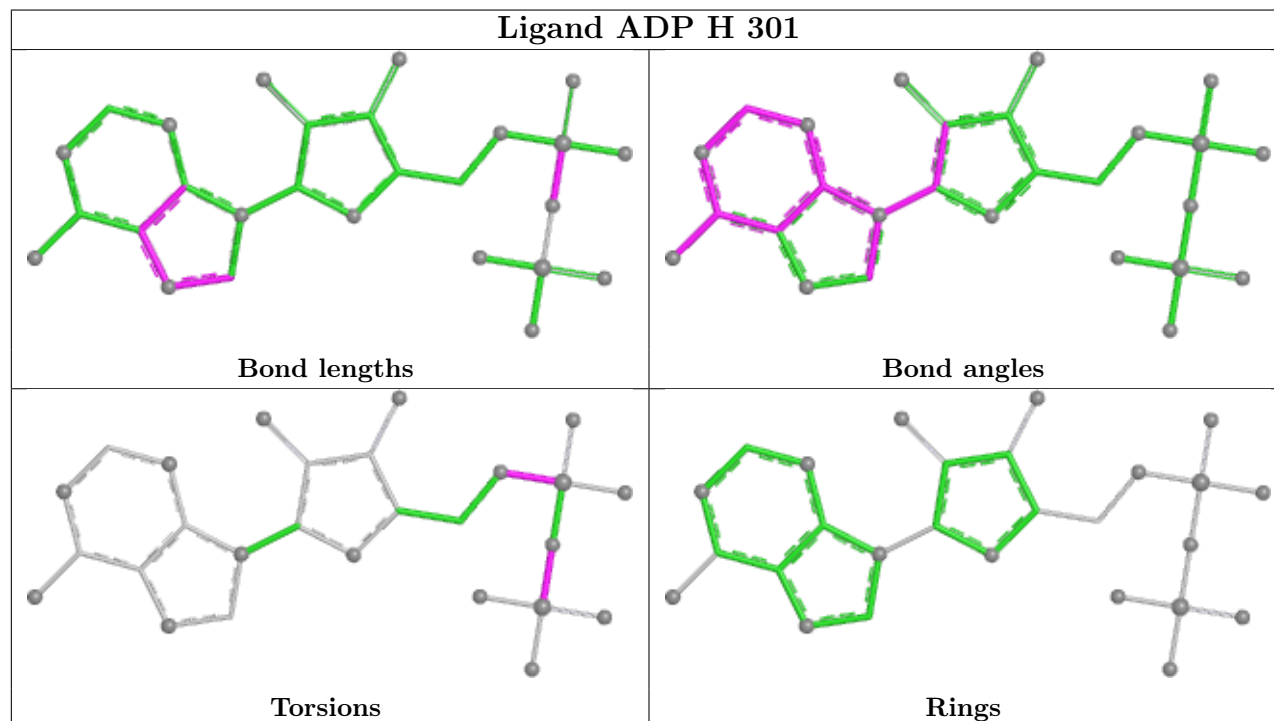
There are no ring outliers.

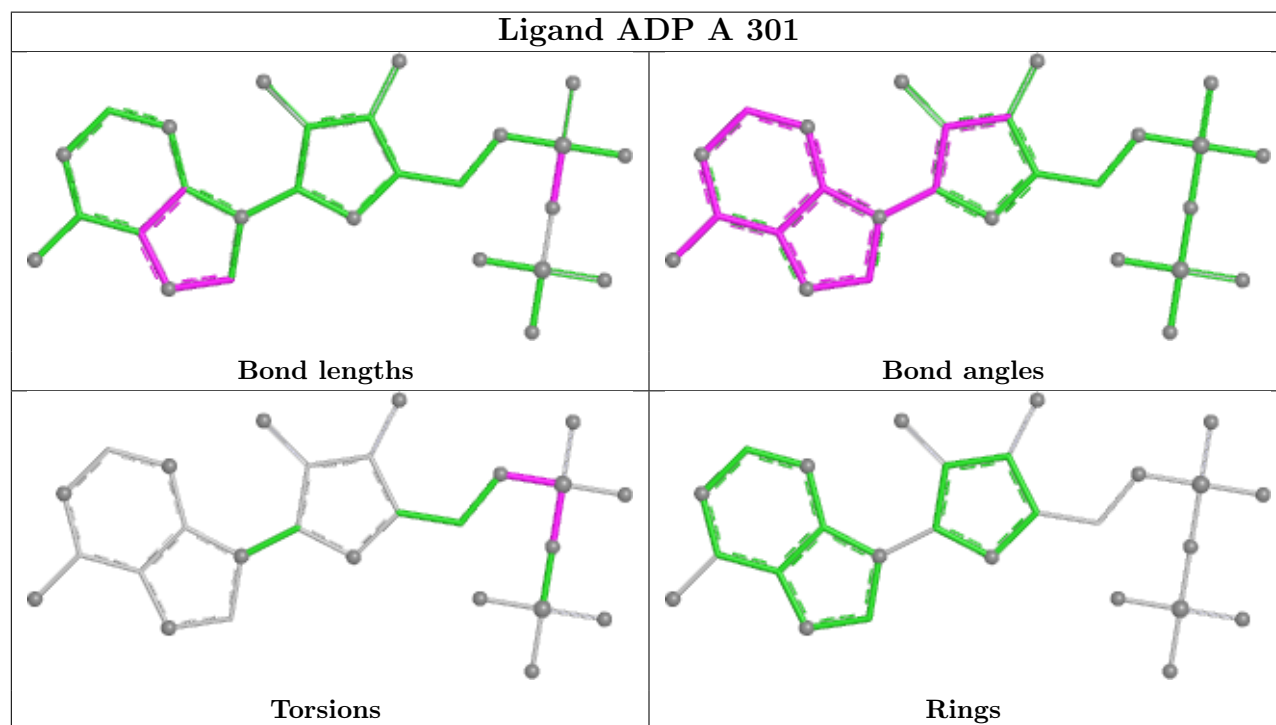
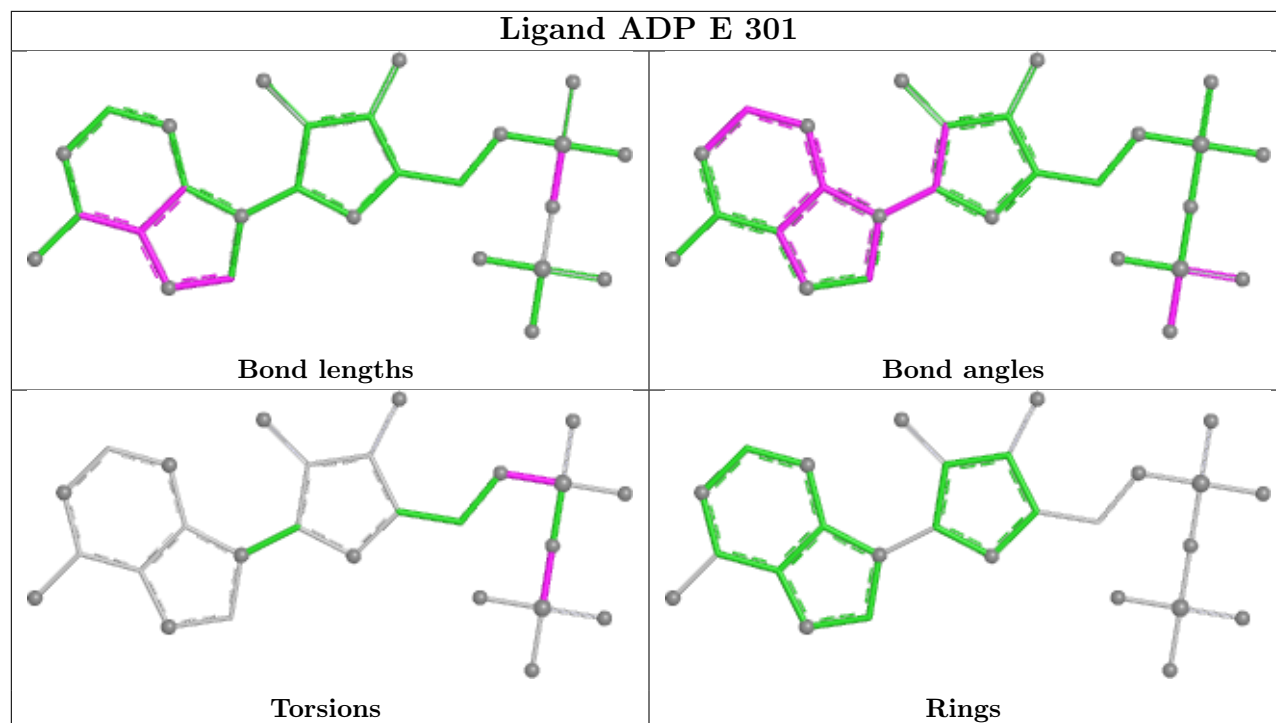
4 monomers are involved in 5 short contacts:

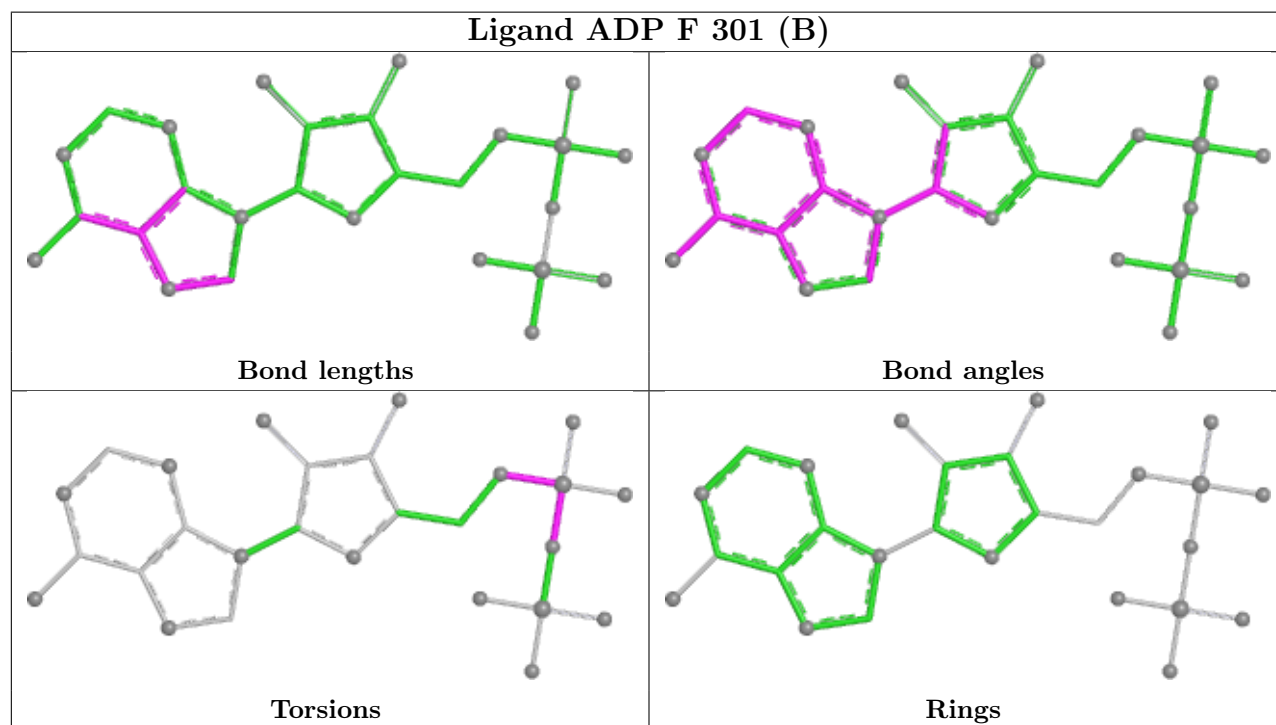
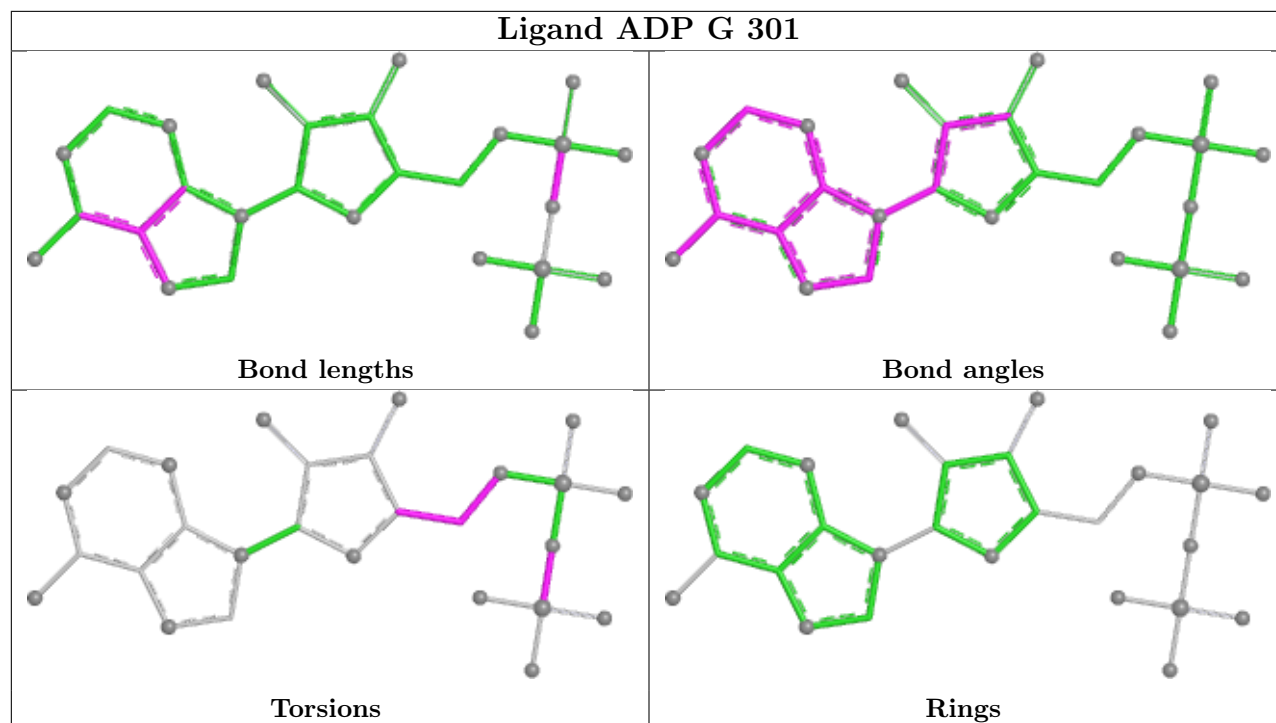
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	ADP	1	0
2	G	301	ADP	1	0
2	C	301	ADP	1	0
2	B	301[B]	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

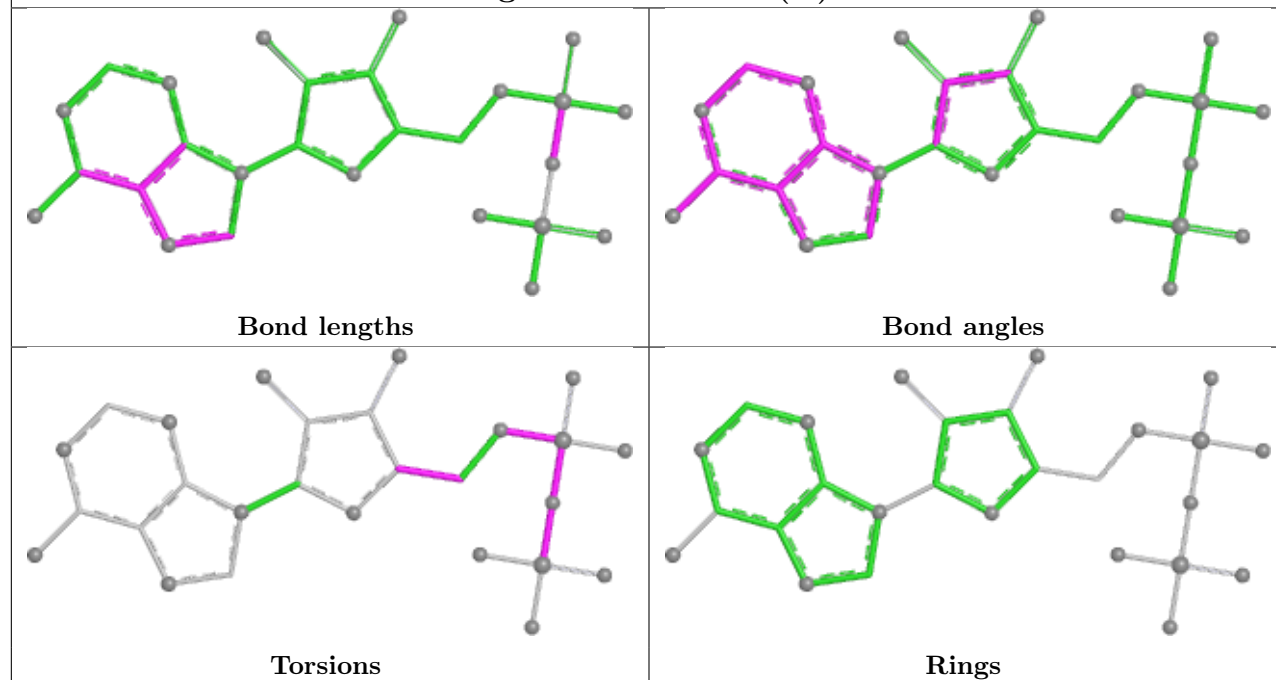
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



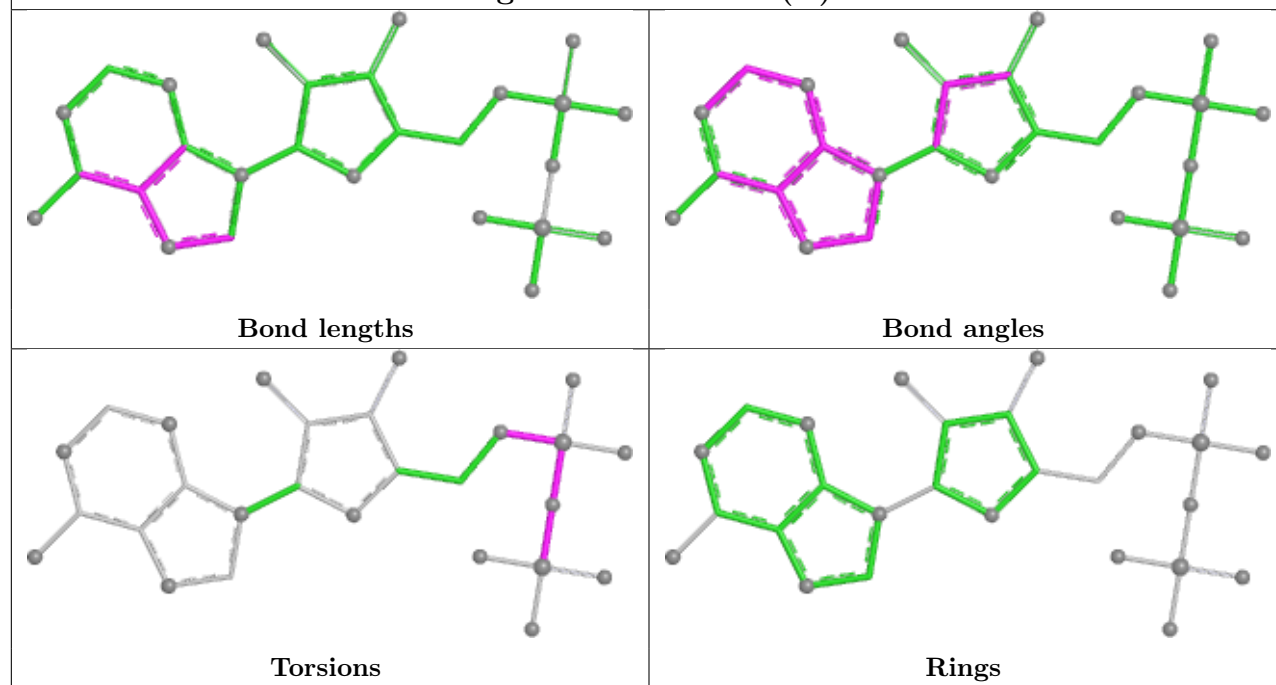




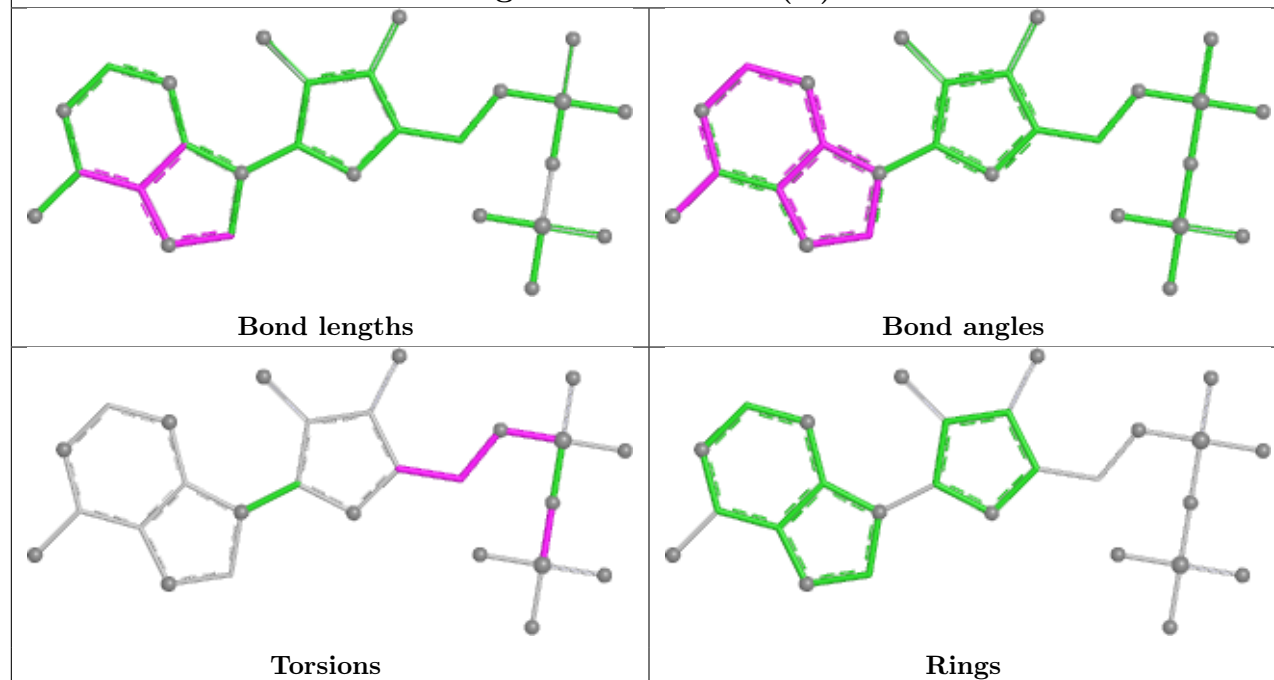
Ligand ADP F 301 (A)



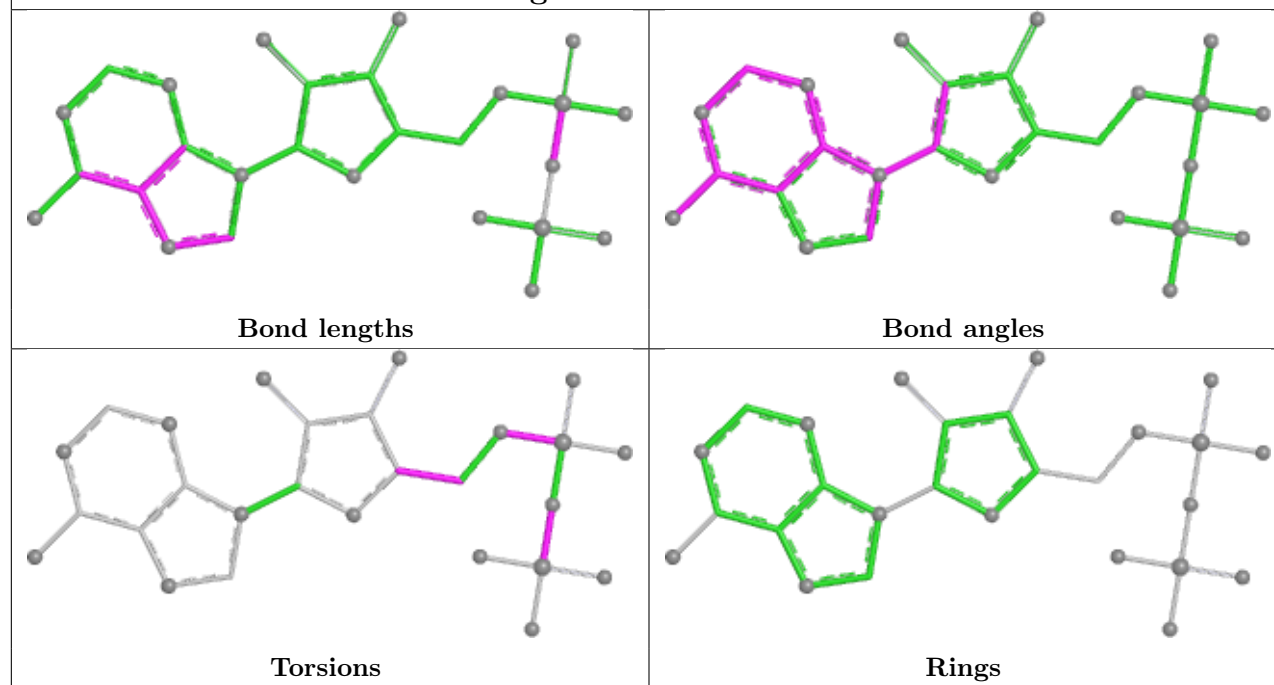
Ligand ADP D 301 (B)

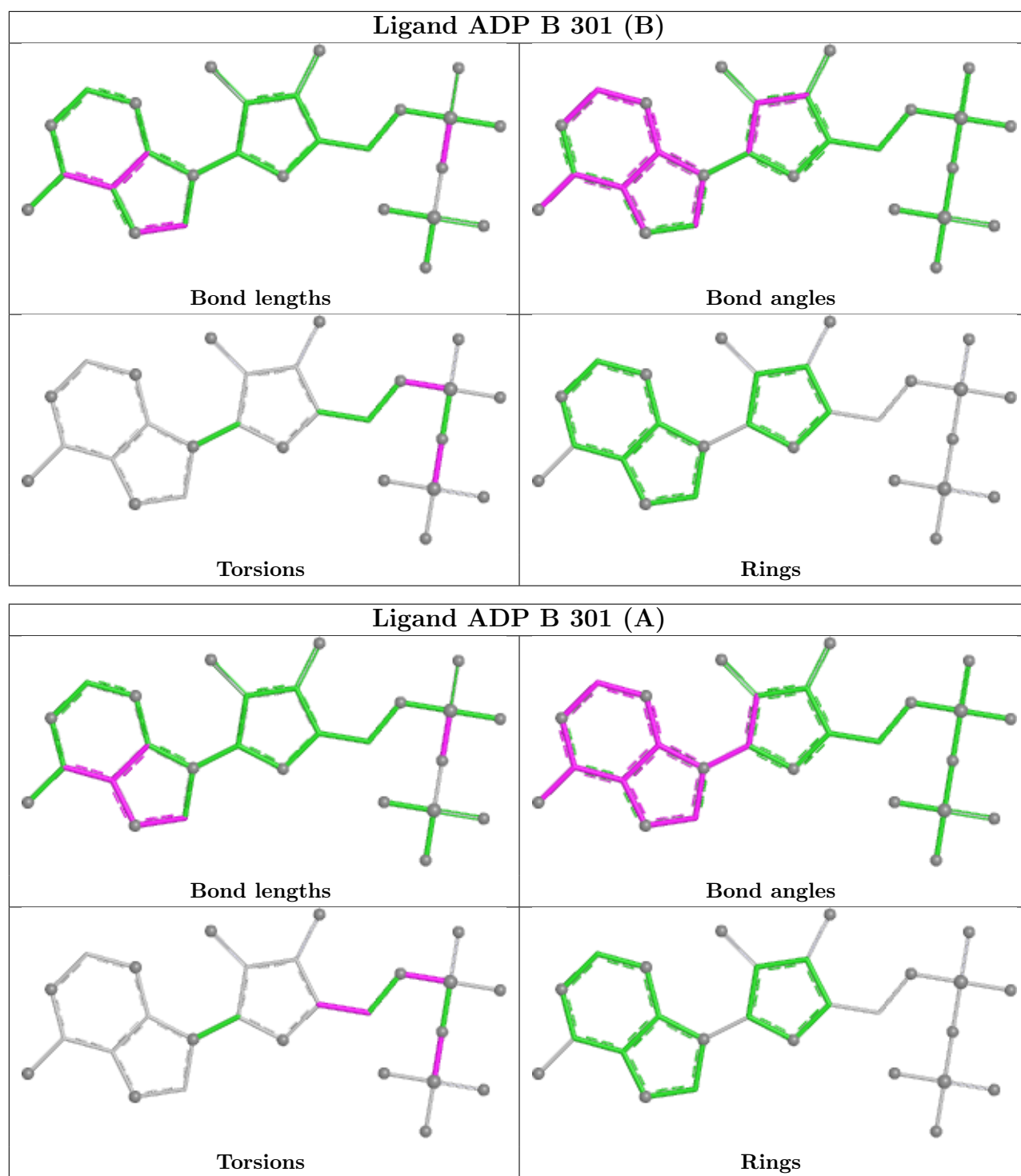


Ligand ADP D 301 (A)



Ligand ADP C 301





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	198/218 (90%)	0.33	13 (6%)	24 26	17, 35, 71, 103	5 (2%)
1	B	197/218 (90%)	0.31	11 (5%)	30 33	20, 33, 73, 89	3 (1%)
1	C	199/218 (91%)	0.20	7 (3%)	47 52	15, 34, 57, 84	2 (1%)
1	D	195/218 (89%)	0.47	9 (4%)	37 41	21, 43, 73, 95	1 (0%)
1	E	201/218 (92%)	0.37	13 (6%)	25 27	16, 37, 61, 83	3 (1%)
1	F	193/218 (88%)	0.31	9 (4%)	36 40	17, 35, 72, 90	5 (2%)
1	G	193/218 (88%)	0.10	9 (4%)	36 40	15, 31, 59, 85	2 (1%)
1	H	192/218 (88%)	0.39	17 (8%)	15 16	18, 35, 76, 93	4 (2%)
All	All	1568/1744 (89%)	0.31	88 (5%)	30 33	15, 35, 72, 103	25 (1%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	HIS	5.2
1	A	156	ILE	5.1
1	F	209	THR	5.1
1	B	156	ILE	5.1
1	E	0	HIS	4.7
1	H	209	THR	4.7
1	H	7	GLN	4.7
1	F	9	ILE	4.7
1	D	5	THR	4.6
1	G	155	GLY	4.6
1	D	209	THR	4.5
1	F	8	GLY	4.4
1	C	159	LEU	4.2
1	G	9	ILE	3.8
1	H	9	ILE	3.8
1	E	158	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	-2	HIS	3.7
1	A	-3	HIS	3.7
1	B	14	ASN	3.7
1	D	10	THR	3.5
1	A	-2	HIS	3.5
1	G	102	GLY	3.3
1	E	2	SER	3.3
1	E	10	THR	3.2
1	F	10	THR	3.2
1	H	47	GLY	3.2
1	A	1	MET	3.1
1	B	7	GLN	3.0
1	H	8	GLY	3.0
1	A	209	THR	3.0
1	E	-4	HIS	3.0
1	G	154	LYS	3.0
1	E	-1	HIS	2.9
1	D	20	ALA	2.9
1	H	43	GLY	2.9
1	B	209	THR	2.9
1	H	10	THR	2.9
1	A	-1	HIS	2.9
1	B	44	GLY	2.8
1	A	2	SER	2.8
1	A	155	GLY	2.8
1	E	155	GLY	2.8
1	H	20	ALA	2.8
1	C	7	GLN	2.7
1	A	166	ILE	2.7
1	H	18	ILE	2.7
1	H	153	ALA	2.7
1	E	209	THR	2.6
1	E	1	MET	2.6
1	C	10	THR	2.6
1	A	-4	HIS	2.6
1	F	42	ASN	2.5
1	G	10	THR	2.5
1	F	11	PHE	2.5
1	C	31	LEU	2.5
1	D	9	ILE	2.5
1	G	166	ILE	2.5
1	B	10	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	42	ASN	2.4
1	H	11	PHE	2.4
1	D	101	ALA	2.4
1	G	8	GLY	2.4
1	B	6	GLN	2.4
1	H	117	ALA	2.4
1	F	98	MET	2.4
1	B	42	ASN	2.3
1	B	101	ALA	2.3
1	D	19	ILE	2.3
1	A	153	ALA	2.2
1	B	154	LYS	2.2
1	H	165	ASP	2.2
1	B	102	GLY	2.2
1	C	9	ILE	2.2
1	F	154	LYS	2.2
1	C	164	GLU	2.1
1	A	154	LYS	2.1
1	D	16	VAL	2.1
1	G	87	GLU	2.1
1	H	35	ARG	2.1
1	C	102	GLY	2.1
1	G	153	ALA	2.1
1	E	101	ALA	2.0
1	H	45	MET	2.0
1	D	44	GLY	2.0
1	F	206	ASN	2.0
1	E	153	ALA	2.0
1	E	-3	HIS	2.0
1	H	154	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

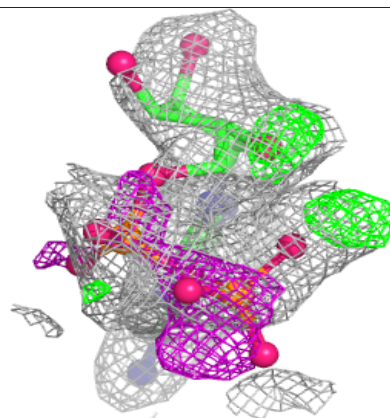
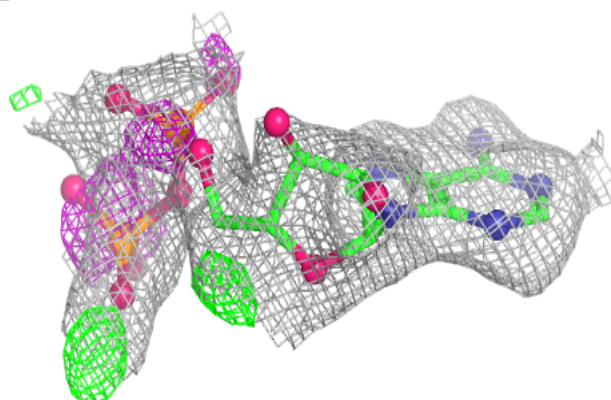
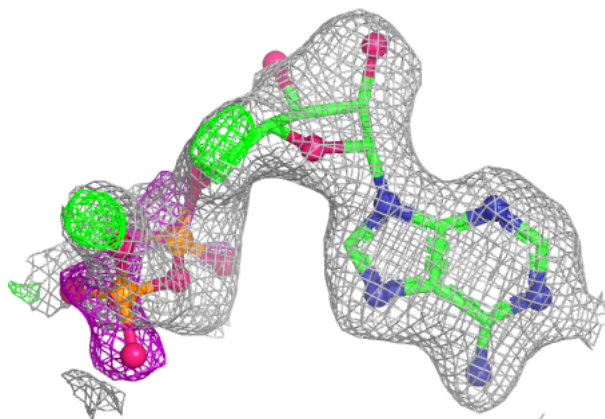
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	C	301	27/27	0.72	0.14	47,70,91,111	0
2	ADP	G	301	27/27	0.73	0.12	41,77,90,105	0
3	MG	B	302	1/1	0.73	0.19	64,64,64,64	0
3	MG	C	302	1/1	0.74	0.16	56,56,56,56	0
3	MG	E	302	1/1	0.75	0.16	60,60,60,60	0
2	ADP	A	301	27/27	0.78	0.12	38,68,94,108	0
2	ADP	E	301	27/27	0.79	0.13	41,66,86,101	0
3	MG	F	303	1/1	0.80	0.13	54,54,54,54	0
2	ADP	F	301[B]	27/27	0.82	0.13	26,42,50,55	27
2	ADP	F	301[A]	27/27	0.82	0.13	24,42,53,57	27
2	ADP	B	301[B]	27/27	0.83	0.12	27,44,51,60	27
2	ADP	B	301[A]	27/27	0.83	0.12	27,43,52,56	27
2	ADP	D	301[A]	27/27	0.85	0.11	31,47,55,57	27
2	ADP	D	301[B]	27/27	0.85	0.11	30,48,58,61	27
3	MG	G	302	1/1	0.89	0.09	53,53,53,53	0
3	MG	H	302	1/1	0.90	0.23	48,48,48,48	0
2	ADP	H	301	27/27	0.92	0.09	26,39,78,88	0
3	MG	F	302	1/1	0.94	0.18	45,45,45,45	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.

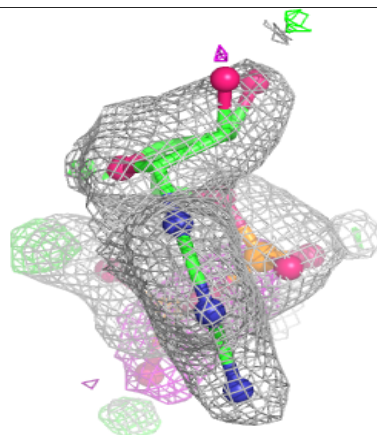
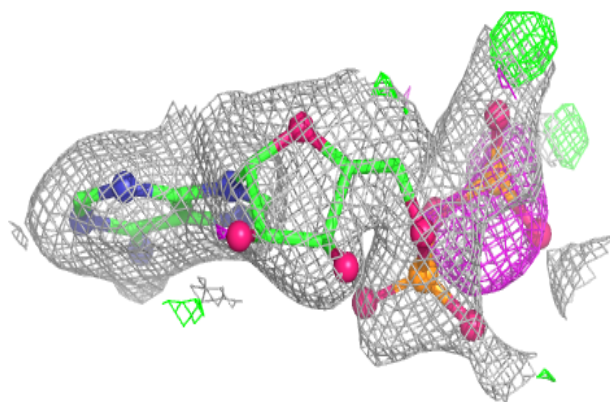
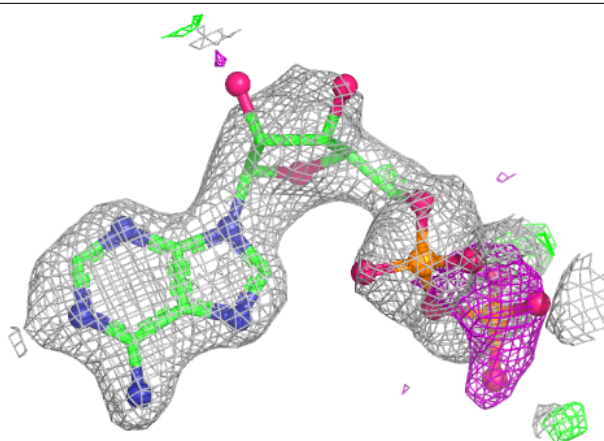
Electron density around ADP C 301:

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



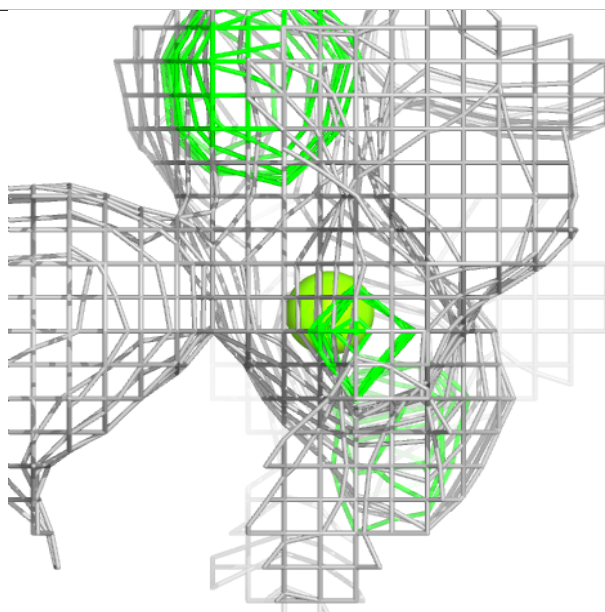
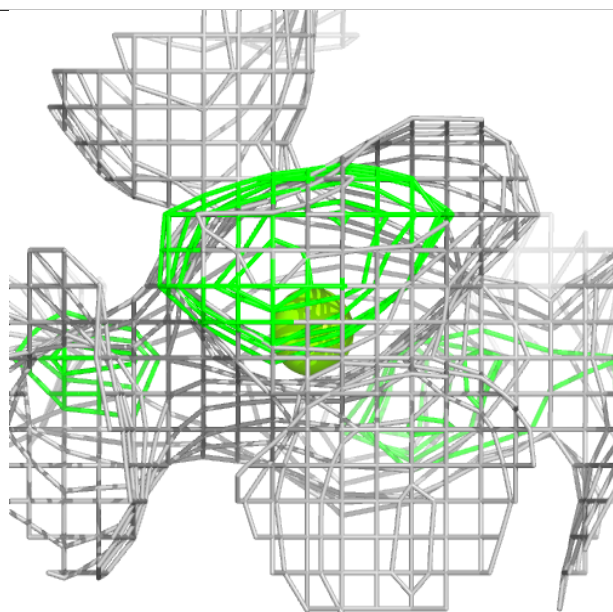
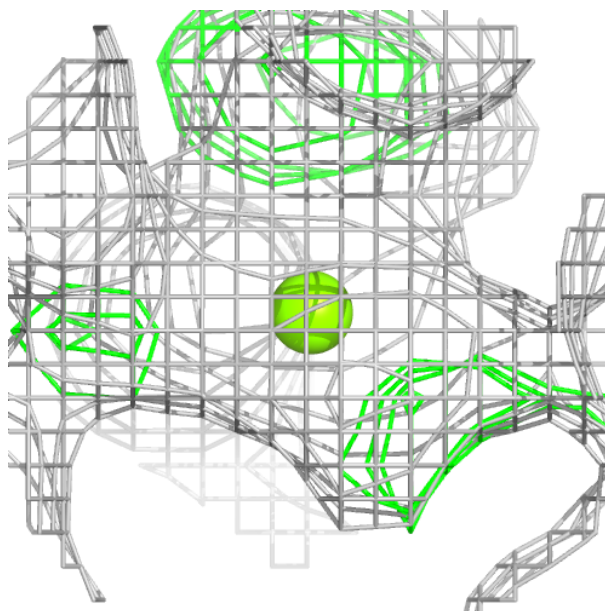
Electron density around ADP G 301:

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



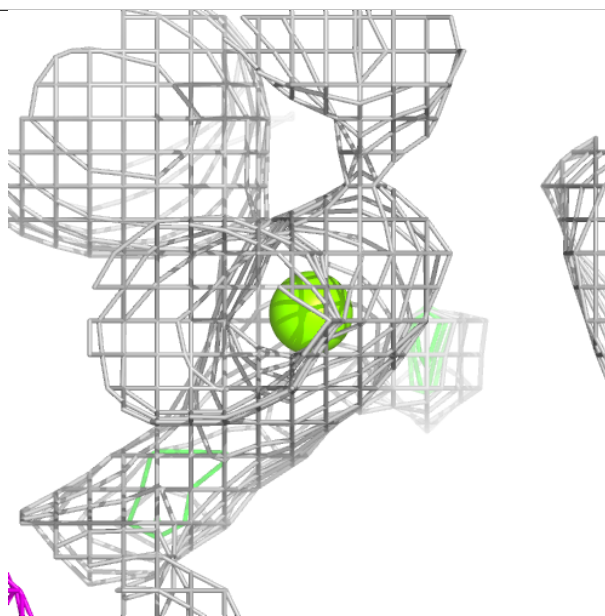
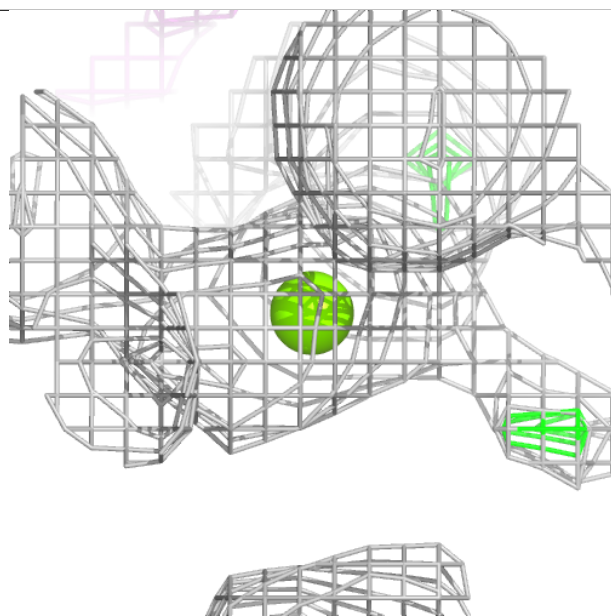
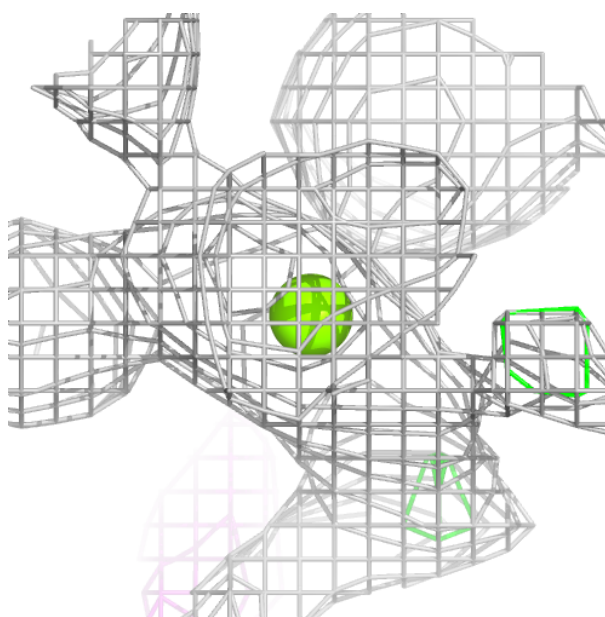
Electron density around MG B 302:

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



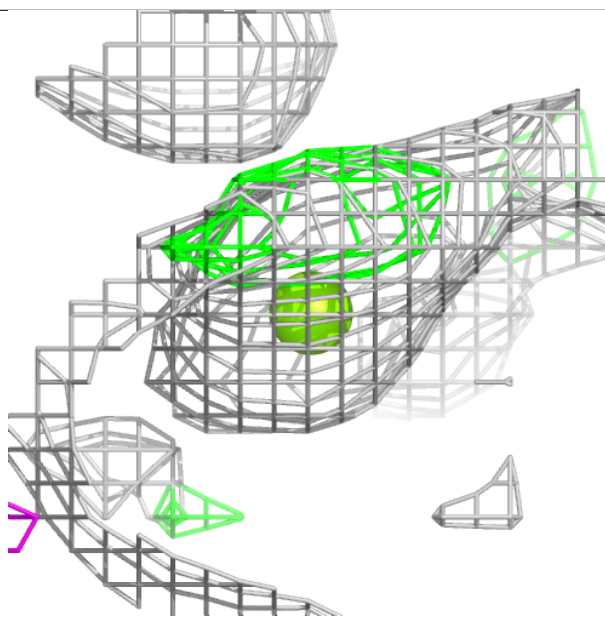
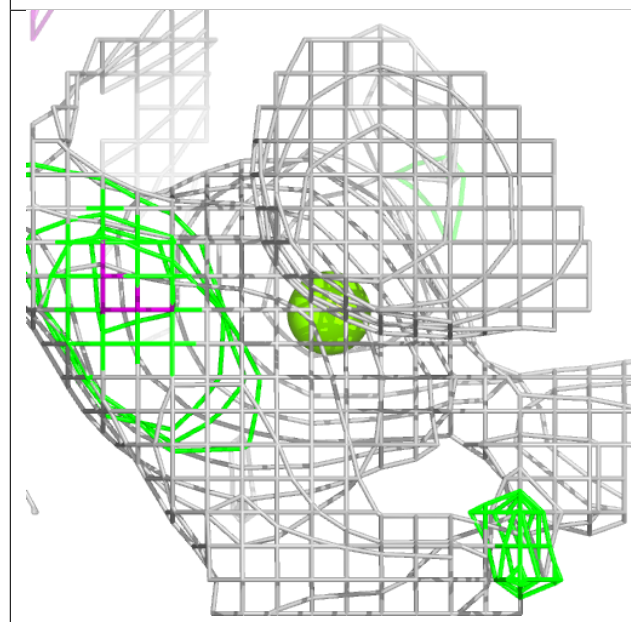
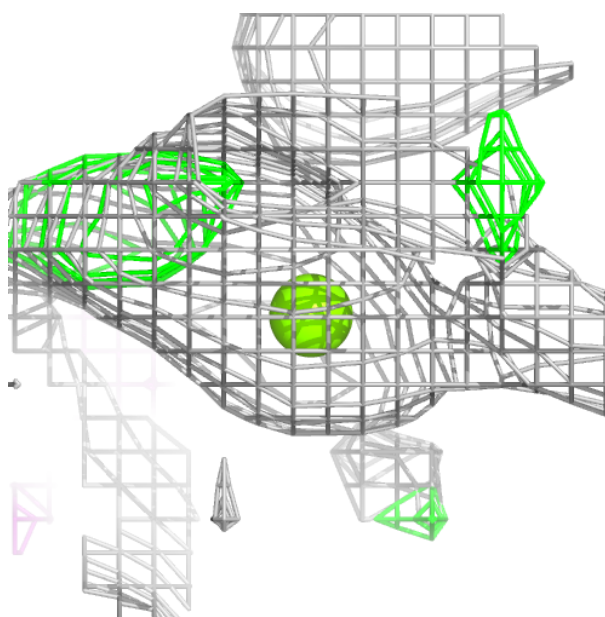
Electron density around MG C 302:

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



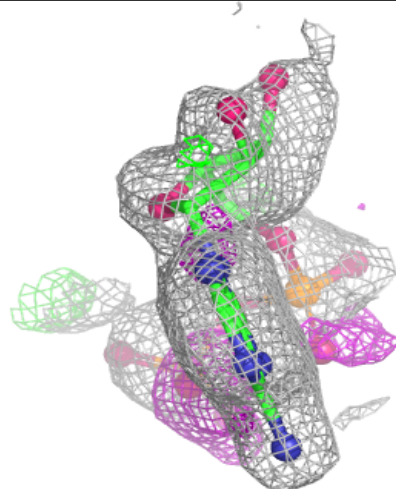
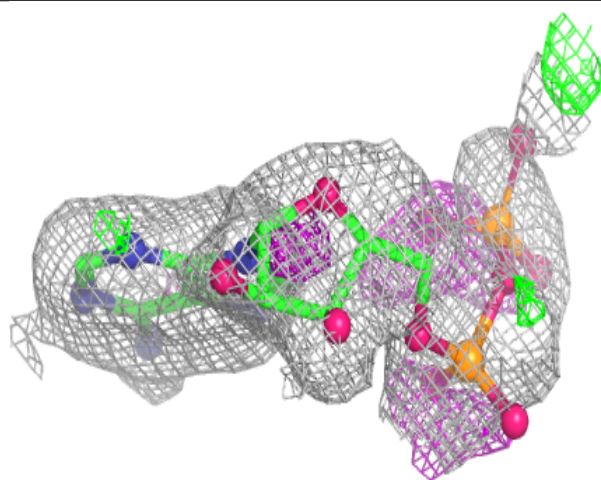
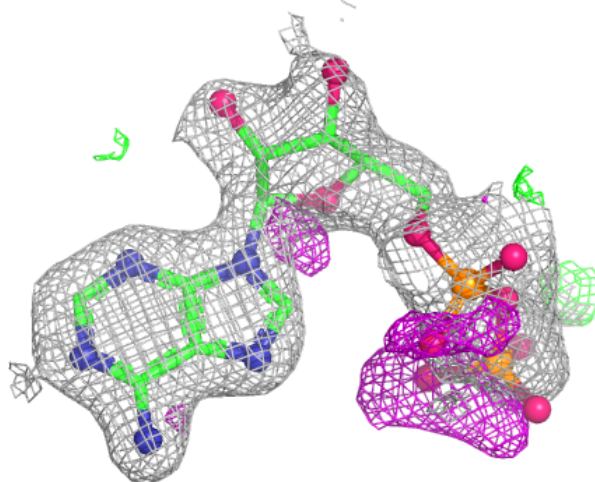
Electron density around MG E 302:

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



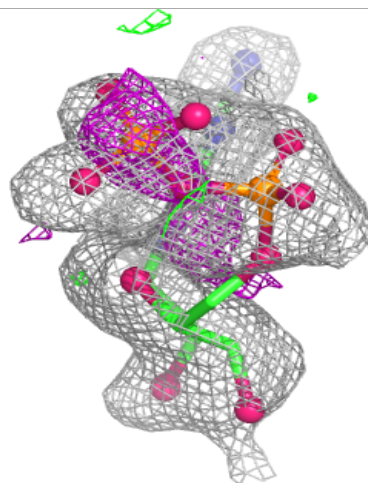
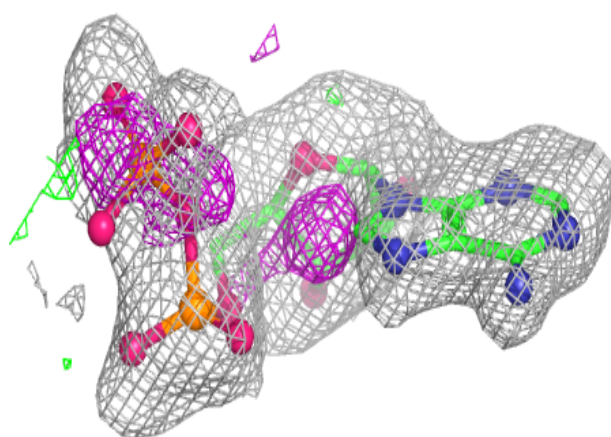
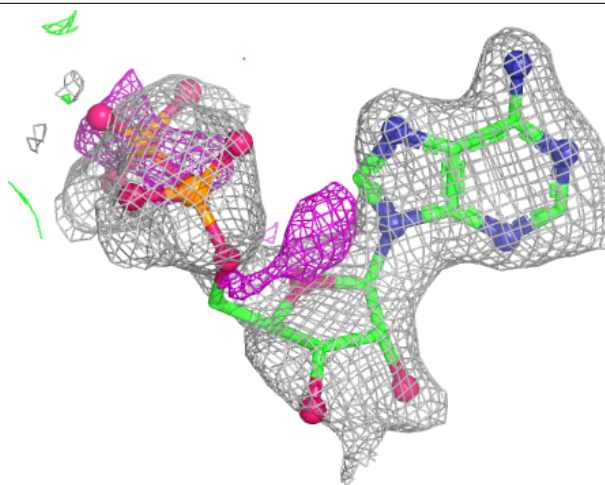
Electron density around ADP A 301:

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



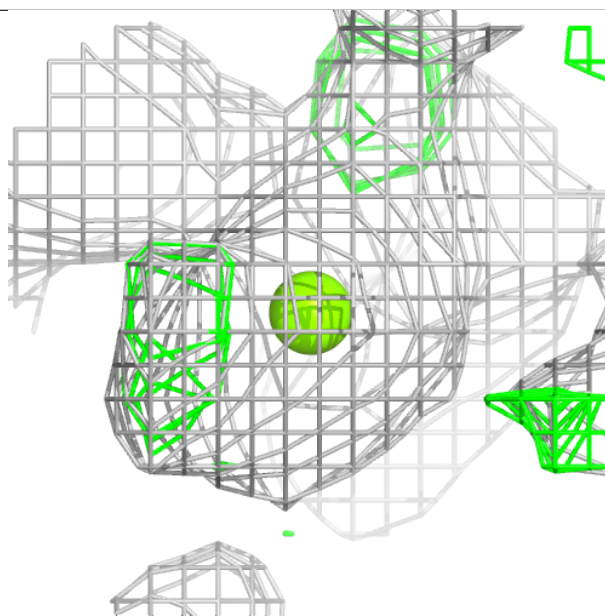
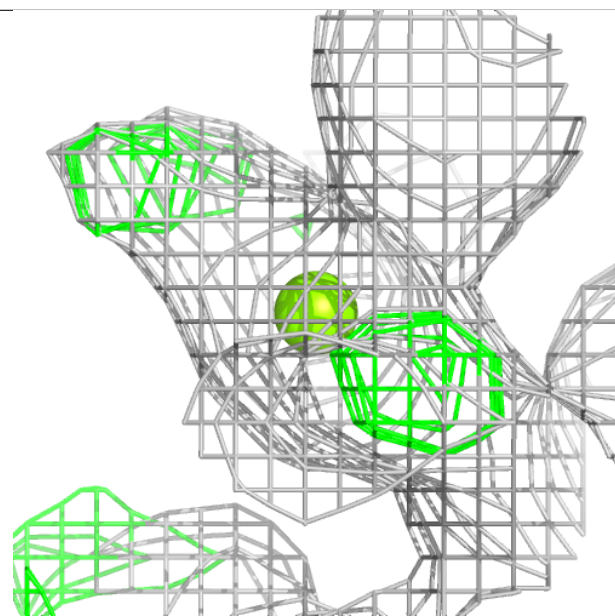
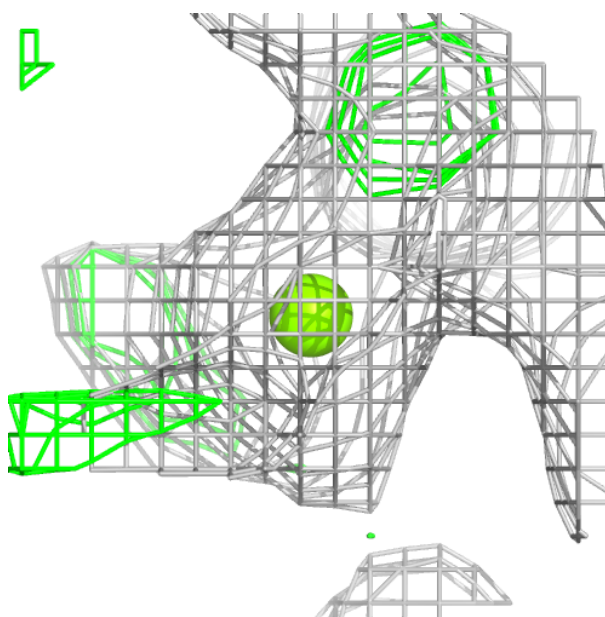
Electron density around ADP E 301:

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



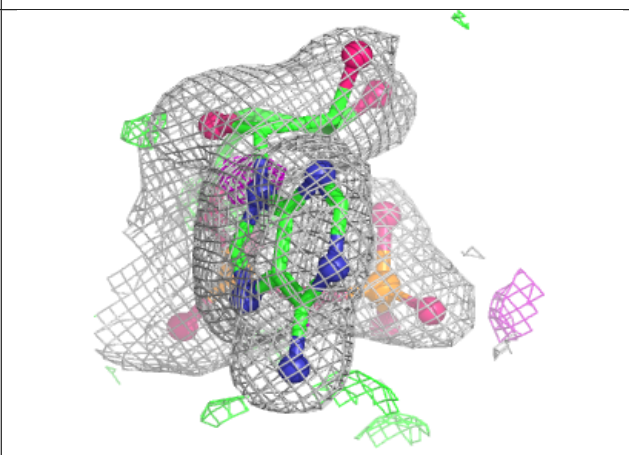
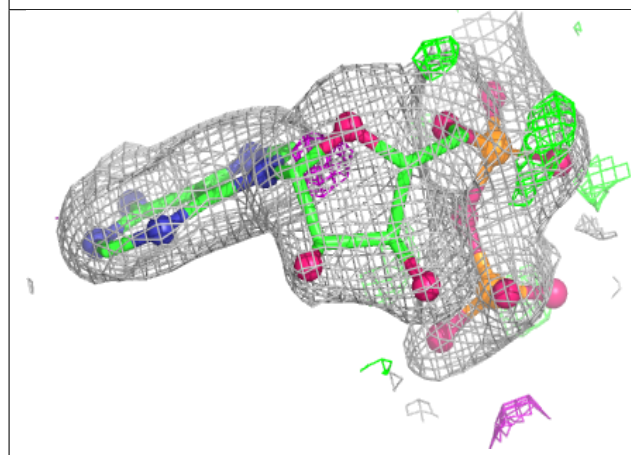
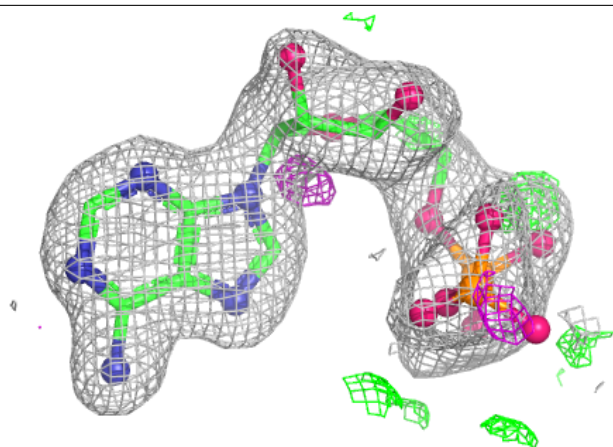
Electron density around MG F 303:

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



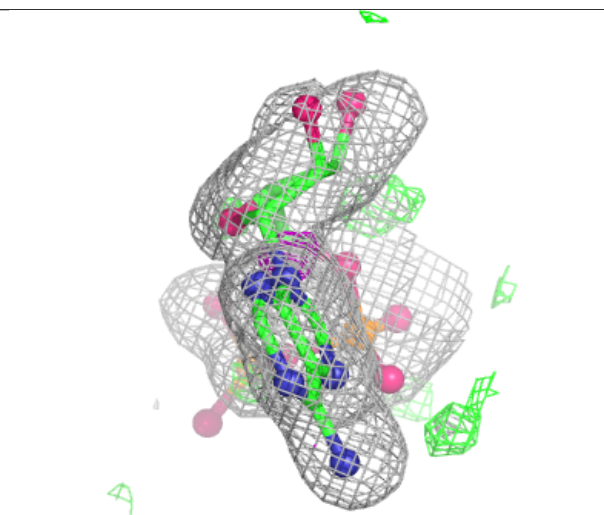
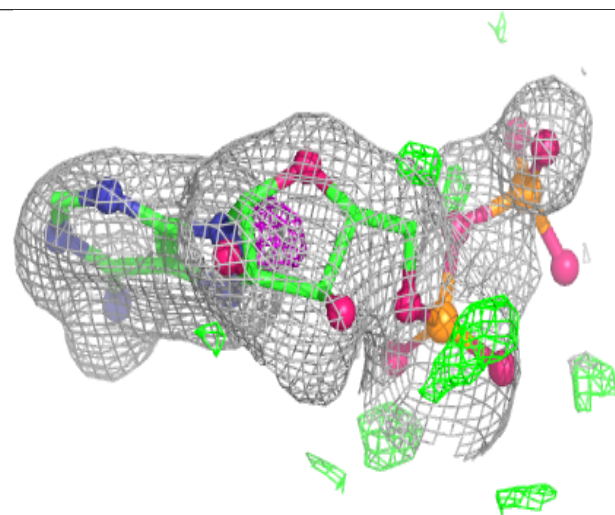
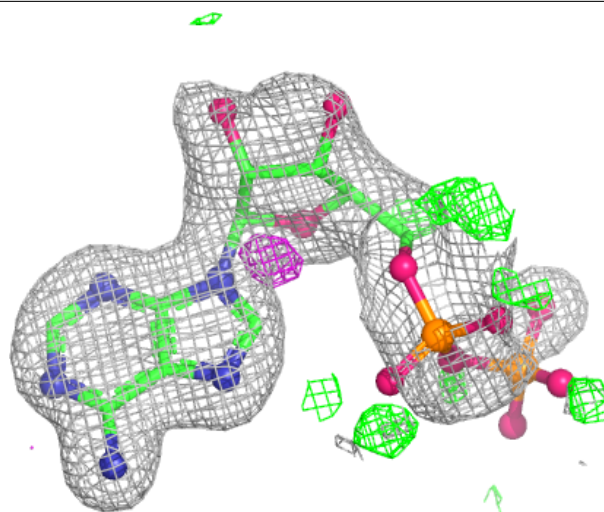
Electron density around ADP F 301 (B):

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



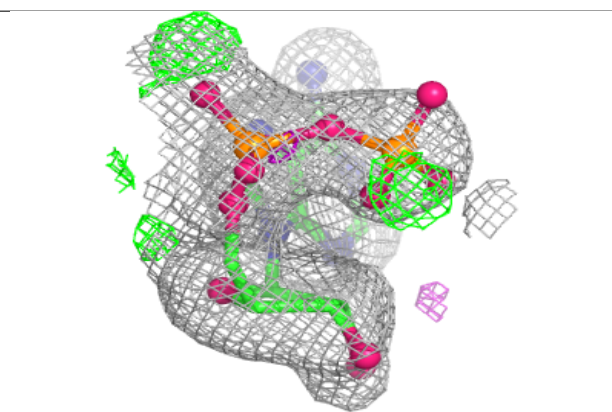
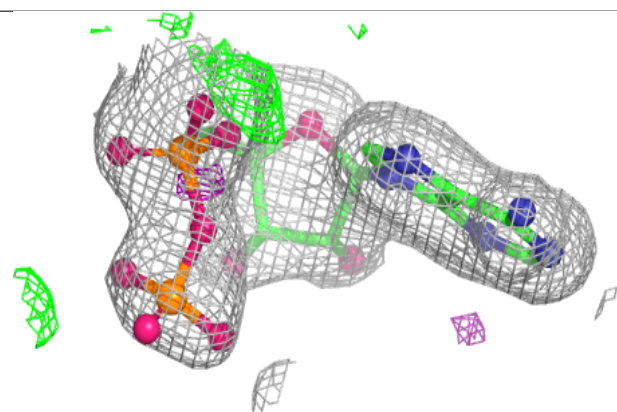
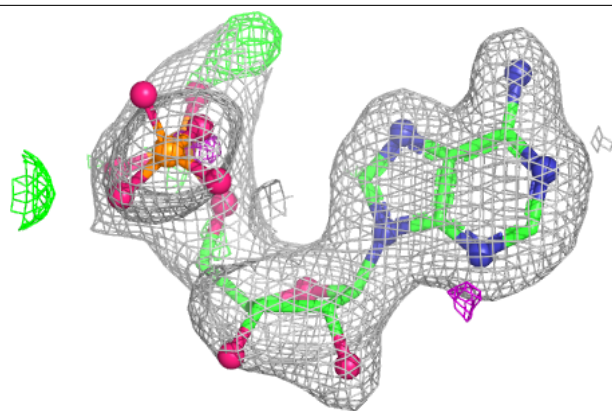
Electron density around ADP F 301 (A):

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

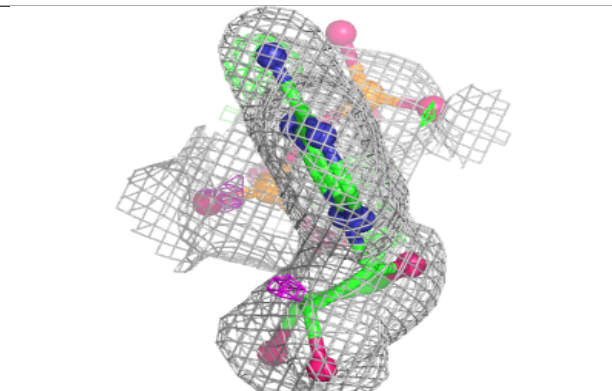
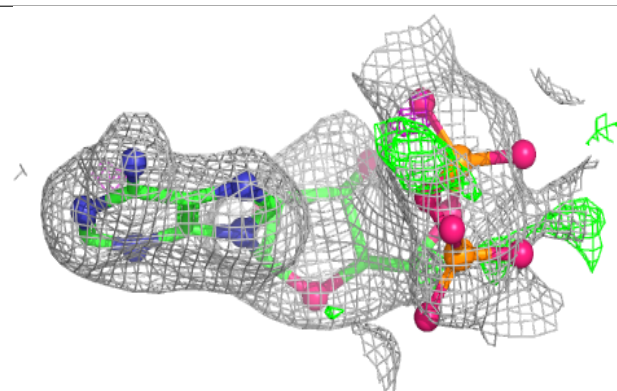
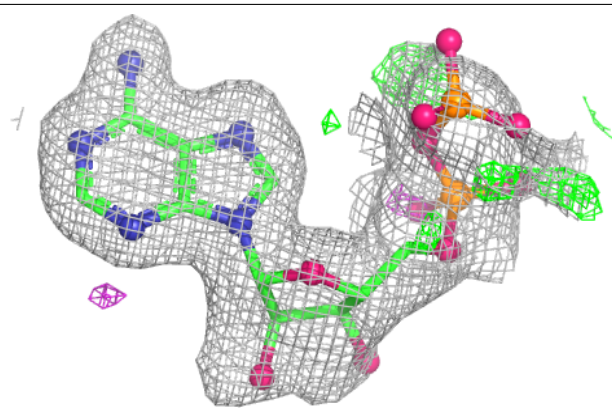


Electron density around ADP B 301 (B):

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

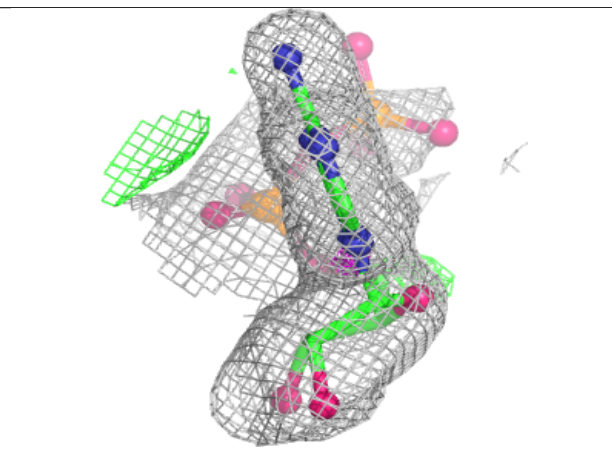
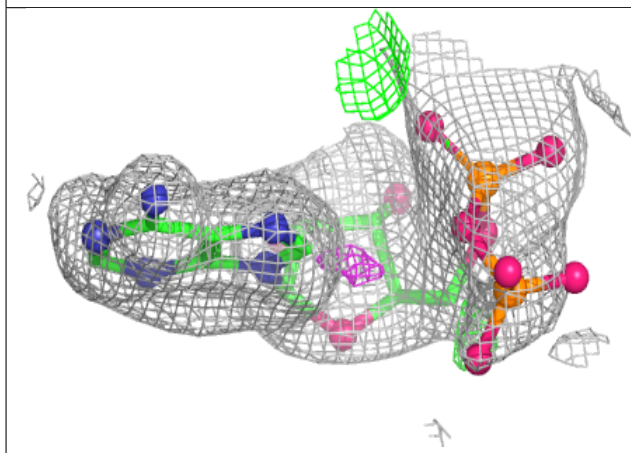
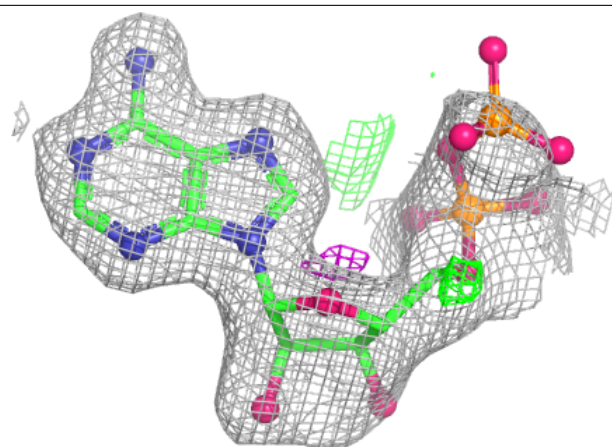
**Electron density around ADP B 301 (A):**

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

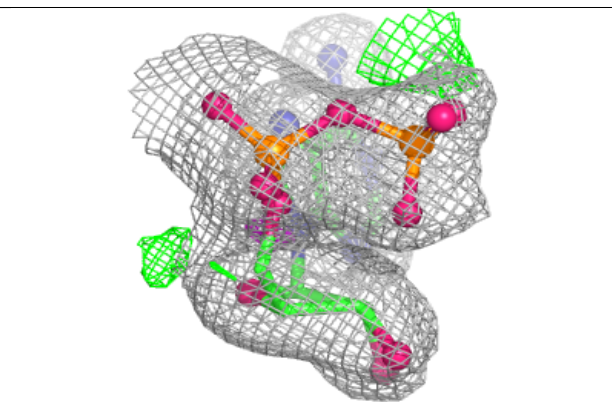
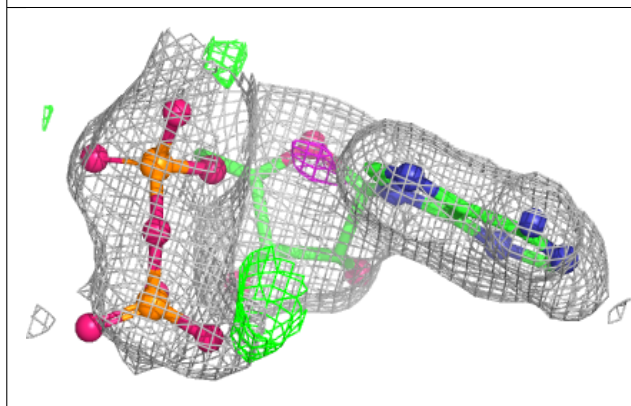
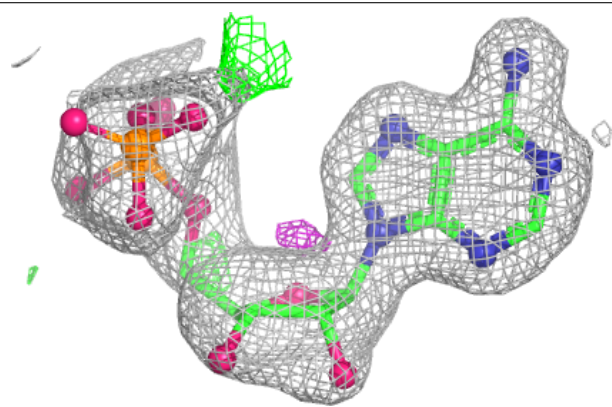


Electron density around ADP D 301 (A):

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

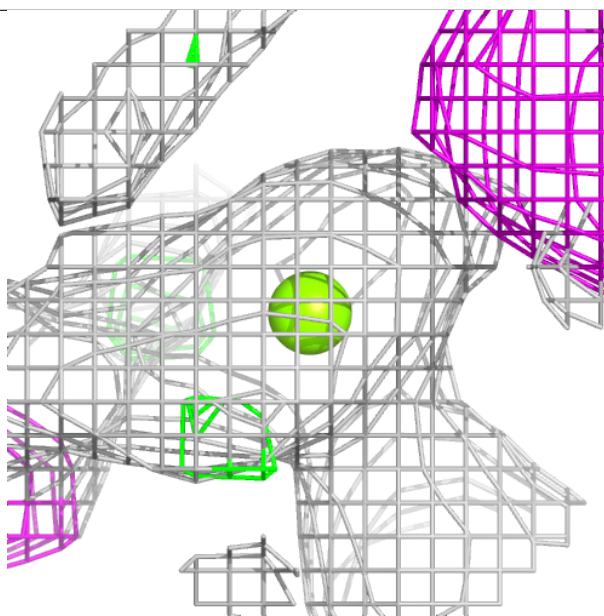
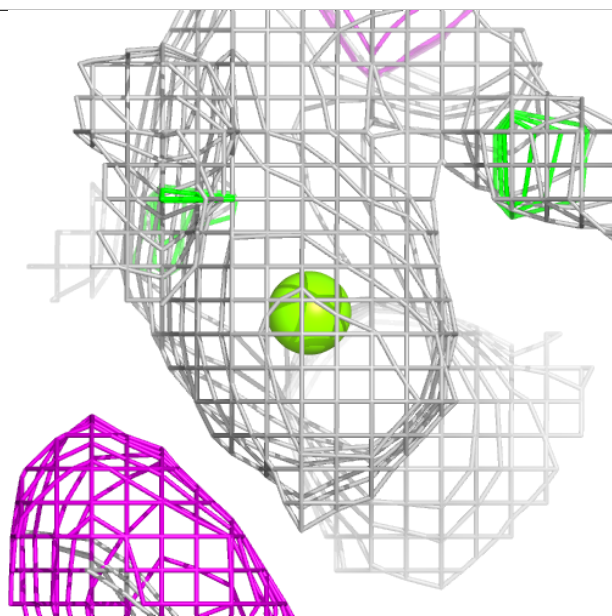
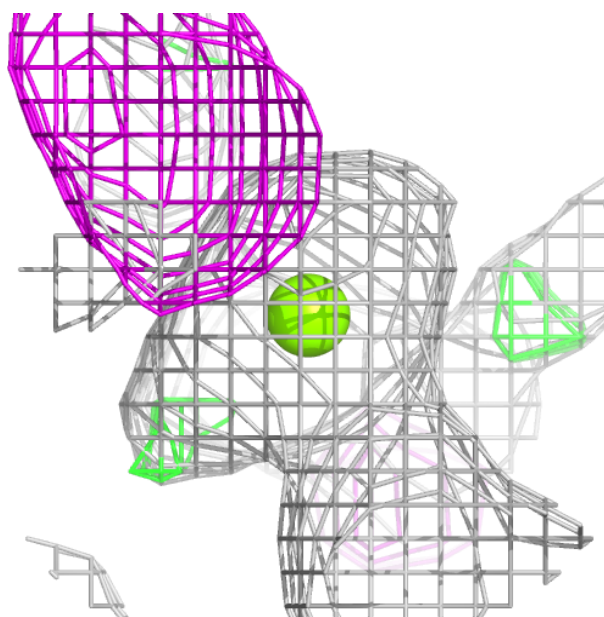
**Electron density around ADP D 301 (B):**

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



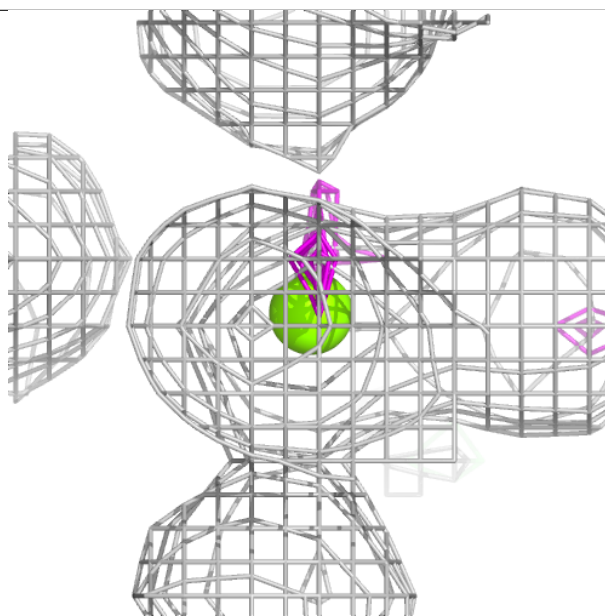
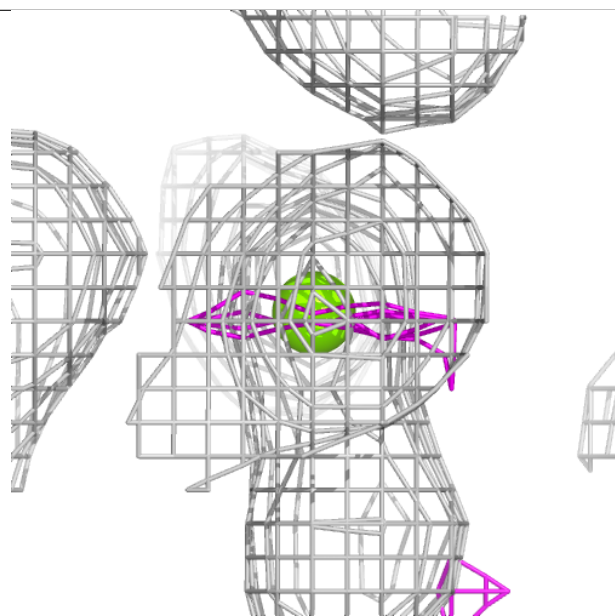
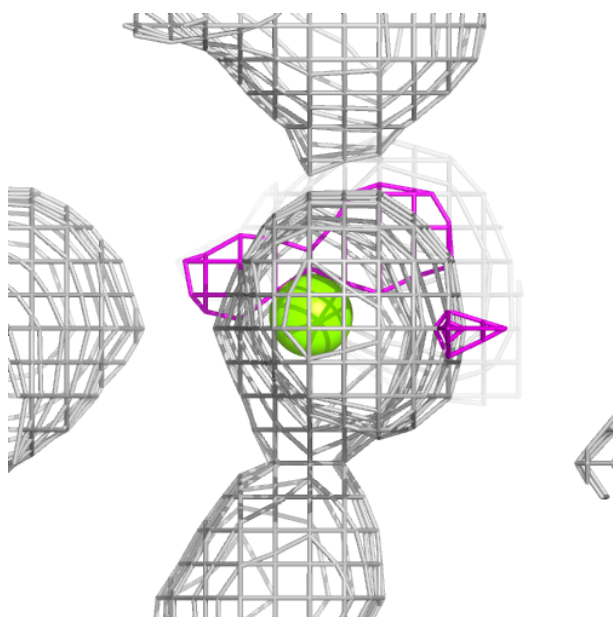
Electron density around MG G 302:

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



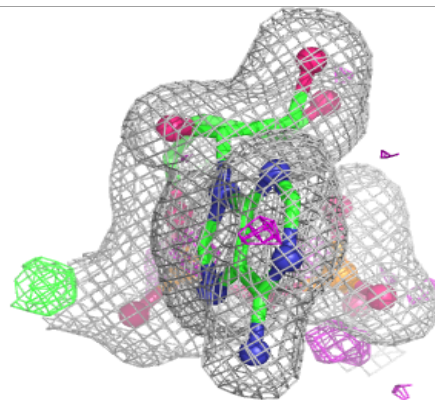
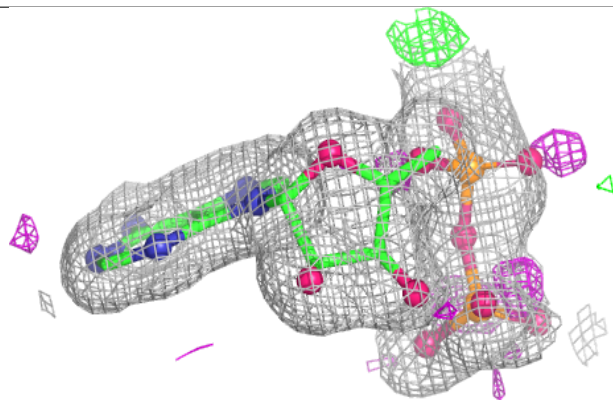
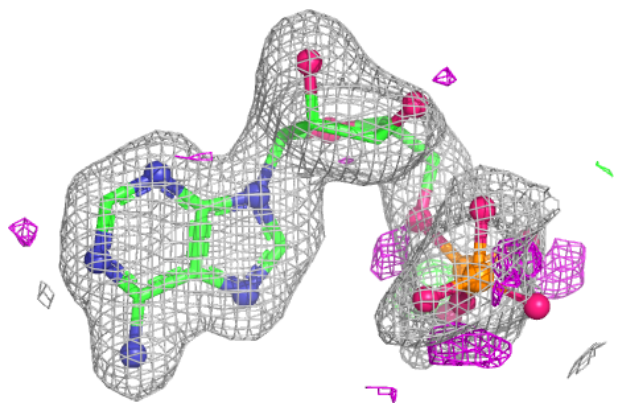
Electron density around MG H 302:

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



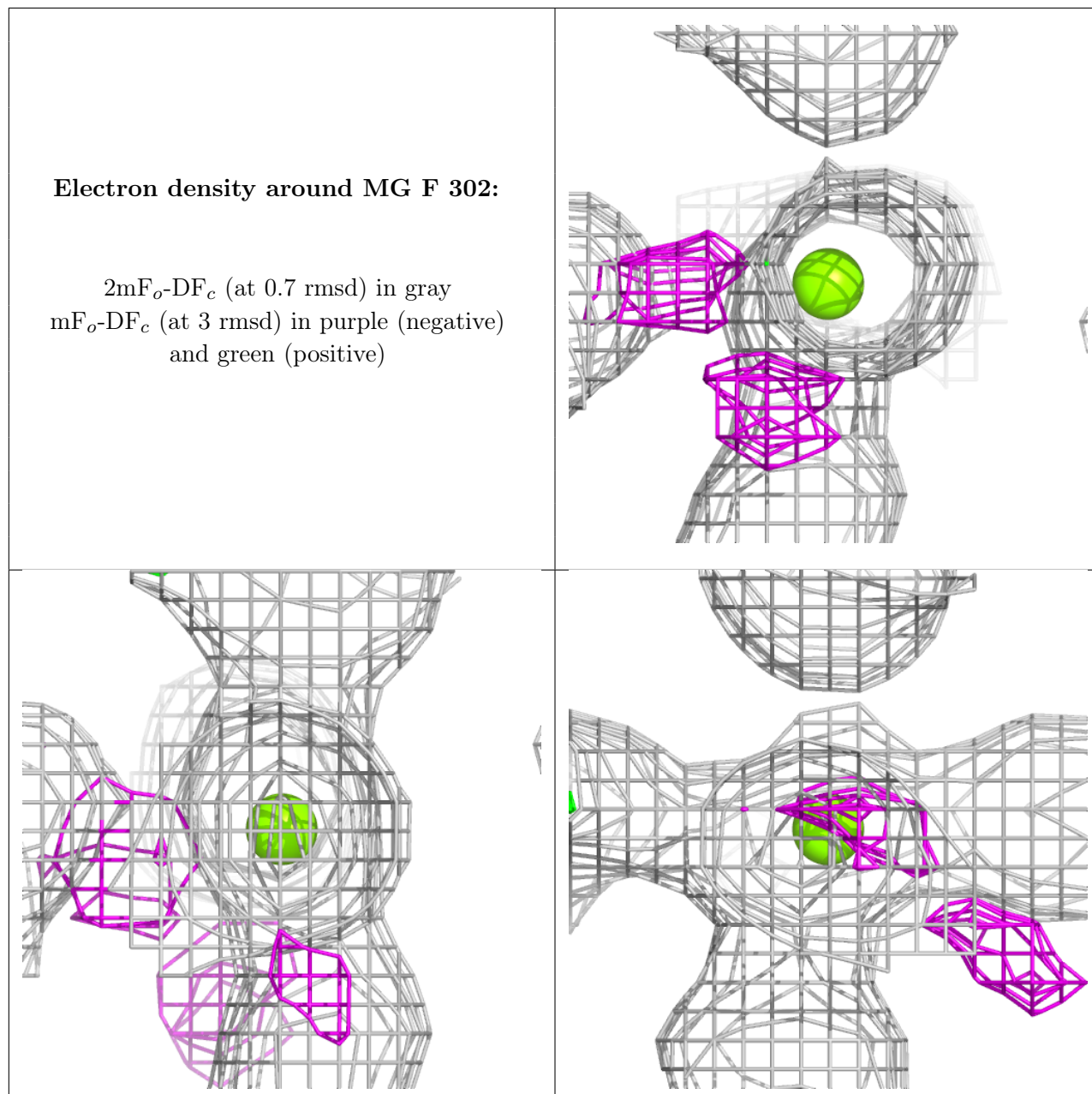
Electron density around ADP H 301:

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



Electron density around MG F 302:

$2mF_o-DF_c$ (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.