



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 07:02 PM BST

PDB ID : 6VZQ
Title : Engineered TTLL6 mutant bound to alpha-elongation analog
Authors : Mahalingan, K.K.; Keenen, E.K.; Strickland, E.K.; Li, Y.; Liu, Y.; Ball, H.L.;
Tanner, M.E.; Tjandra, N.; Roll-Mecak, A.
Deposited on : 2020-02-28
Resolution : 3.08 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

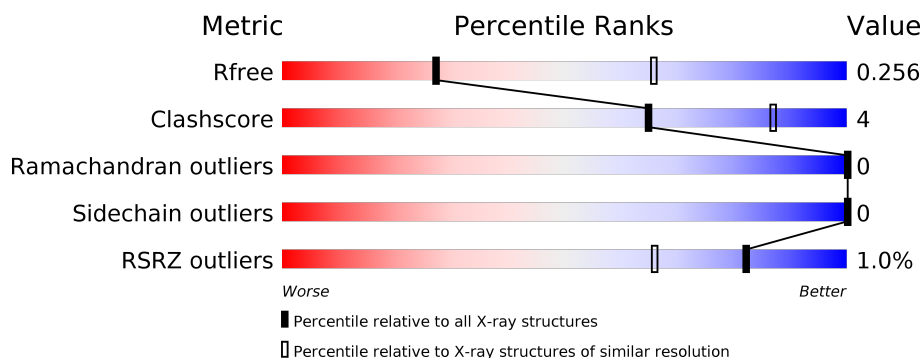
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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 on 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	453	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>12%</div> </div> </div>
1	B	453	<div> <div></div> <div>78%</div> <div>9%</div> <div>12%</div> </div>
1	C	453	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>11%</div> </div> </div>
1	D	453	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>11%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12466 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 Tubulin polyglutamylase TTL6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	1	0
			2969	1904	507	541	17			
1	B	398	Total	C	N	O	S	0	0	0
			3037	1945	520	553	19			
1	C	403	Total	C	N	O	S	0	1	0
			2960	1894	511	538	17			
1	D	404	Total	C	N	O	S	0	0	0
			3076	1970	529	558	19			

There are 12 discrepancies between the modelled and reference sequences:

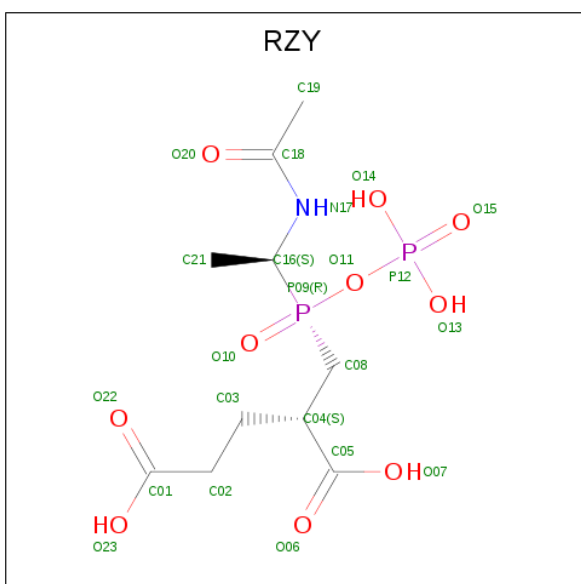
Chain	Residue	Modelled	Actual	Comment	Reference
A	179	ALA	CYS	engineered mutation	UNP A4Q9E8
A	180	ARG	GLN	engineered mutation	UNP A4Q9E8
A	362	ILE	HIS	engineered mutation	UNP A4Q9E8
B	179	ALA	CYS	engineered mutation	UNP A4Q9E8
B	180	ARG	GLN	engineered mutation	UNP A4Q9E8
B	362	ILE	HIS	engineered mutation	UNP A4Q9E8
C	179	ALA	CYS	engineered mutation	UNP A4Q9E8
C	180	ARG	GLN	engineered mutation	UNP A4Q9E8
C	362	ILE	HIS	engineered mutation	UNP A4Q9E8
D	179	ALA	CYS	engineered mutation	UNP A4Q9E8
D	180	ARG	GLN	engineered mutation	UNP A4Q9E8
D	362	ILE	HIS	engineered mutation	UNP A4Q9E8

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



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

- Molecule 3 is (2 {S})-2-[[[(1 {S})-1-acetamidoethyl]-phosphonooxy-phosphoryl]methyl]pentanedioic acid (three-letter code: RZY) (formula: $C_{10}H_{19}NO_{10}P_2$).

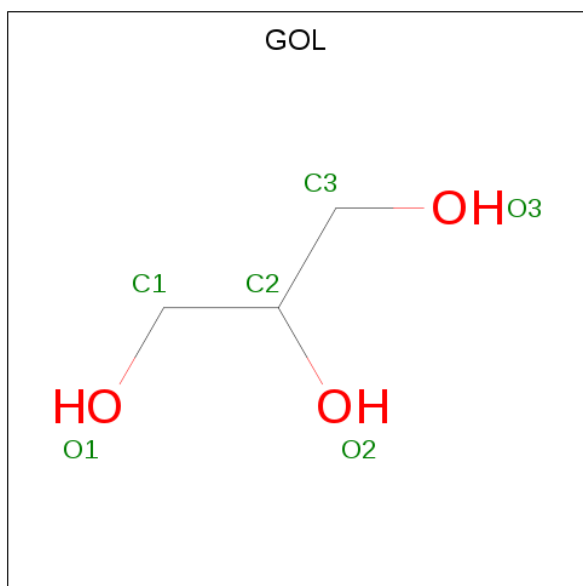


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	1	10	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



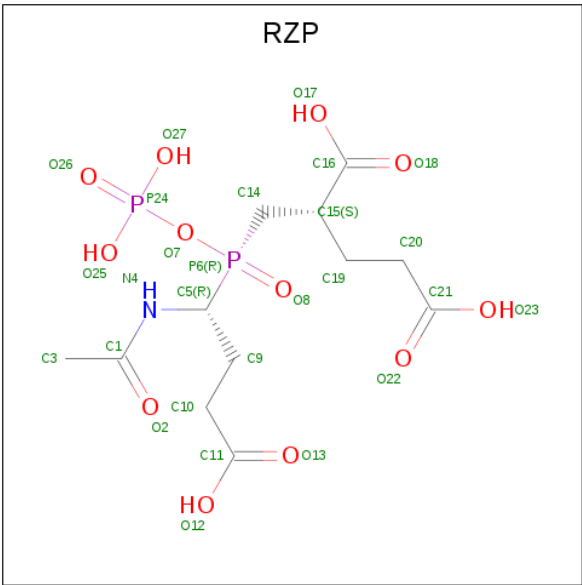
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is (2 {S})-2-[[[(1 {R})-1-acetamido-4-oxidanyl-4-oxidanylidene-butyl]-p
hosphonooxy-phosphoryl]methyl]pentanedioic acid (three-letter code: RZP) (formula:
C₁₂H₂₁NO₁₂P₂) (labeled as "Ligand of Interest" by author).



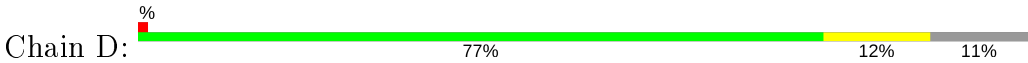
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	12	1	12	2		
6	C	1	Total	C	N	O	P	0	0
			27	12	1	12	2		
6	D	1	Total	C	N	O	P	0	0
			27	12	1	12	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total	O	0	0
			7	7		
7	B	34	Total	O	0	0
			34	34		
7	C	10	Total	O	0	0
			10	10		
7	D	45	Total	O	0	0
			45	45		

PHE
LEU
LYS
LYS
ALA
ARG
LYS
GLU

● Molecule 1: Tubulin polyglutamylase TTL6



GLY
LYS
LYS
LYS
ARG
LYS
K67
I62
M63
L64
R74
Q78
L81
R82
E83
D96
K112
I122
K125
R134
P140
H144
Q160
R164
T170
K174
R182
F185
R188
I200
P208
D212
V222
L223
P229
V234

T244
N251
N255
S266
K269
N273
M293
Y298
D299
V300
E301
R305
T314
S317
A318
S337
D350
L363
E359
S363
F366
S367
T368
K374
K377
L387
G393
L419
L430
P449
L453
F459
F460
GLN

ASP
ASN
SER
LEU
PHE
GLN
ASN
THR
VAL
ALA
SER
ARG
ALA
ARG
GLU
LEU
TYR
ALA
ARG
GLN
ILE
GLN
GLU
LEU
ARG
GLN
LYS
GLN
GLU
LYS
LYS
VAL
PHE
LEU
LYS
LYS
ALA
ARG
LYS
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.04Å 109.49Å 171.70Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	46.16 – 3.08 46.16 – 3.08	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.16-3.08) 99.8 (46.16-3.08)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.226 , 0.259 0.224 , 0.256	Depositor DCC
R_{free} test set	2623 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.440 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12466	wwPDB-VP
Average B, all atoms (Å ²)	68.0	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 43.11 % 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 1.8490e-04. 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: GOL, MG, RZY, ADP, RZP

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	0.24	0/3046	0.39	0/4151
1	B	0.24	0/3110	0.40	0/4226
1	C	0.23	0/3036	0.38	0/4142
1	D	0.24	0/3152	0.40	0/4285
All	All	0.24	0/12344	0.40	0/16804

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	2969	0	2592	22	0
1	B	3037	0	2781	27	0
1	C	2960	0	2560	20	0
1	D	3076	0	2810	32	0
2	A	27	0	12	1	0
2	B	27	0	12	1	0
2	C	27	0	12	0	0
2	D	27	0	12	1	0
3	A	23	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	B	42	0	56	0	0
5	C	6	0	8	0	0
5	D	60	0	80	2	0
6	B	27	0	0	1	0
6	C	27	0	0	1	0
6	D	27	0	0	0	0
7	A	7	0	0	0	0
7	B	34	0	0	0	0
7	C	10	0	0	0	0
7	D	45	0	0	0	0
All	All	12466	0	10935	96	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 4.

All (96) 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:D:229:PRO:HG3	1:D:430:LEU:HD12	1.66	0.76
1:D:188:ARG:HG3	1:D:255:LEU:HD11	1.70	0.73
1:D:368:THR:HB	1:D:374:LYS:HG3	1.78	0.66
1:B:190:VAL:HG13	1:B:193:ILE:HD12	1.78	0.66
1:B:194:LYS:HG2	5:D:611:GOL:H32	1.79	0.64
1:B:266:SER:HA	1:B:269:LYS:HE3	1.81	0.63
1:A:366:PHE:HA	1:A:377:LYS:HD3	1.82	0.61
1:B:377:LYS:NZ	6:B:604:RZP:O22	2.28	0.60
1:D:112:LYS:NZ	1:D:337:SER:O	2.35	0.59
1:D:222:VAL:HG22	1:D:234:VAL:HG22	1.85	0.57
1:B:208:PRO:HA	1:B:350:ASP:HA	1.84	0.57
1:A:140:PRO:O	1:A:144:HIS:NE2	2.34	0.56
1:C:208:PRO:HA	1:C:350:ASP:HA	1.86	0.56
1:A:244:THR:HB	1:A:273:ASN:HB2	1.86	0.56
1:D:244:THR:HB	1:D:273:ASN:HB2	1.86	0.56
1:C:366:PHE:HA	1:C:377:LYS:HD3	1.87	0.56
1:B:140:PRO:O	1:B:144:HIS:NE2	2.34	0.56
1:D:266:SER:HA	1:D:269:LYS:HE2	1.88	0.55
1:B:244:THR:HB	1:B:273:ASN:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:LEU:HD13	1:B:441:CYS:HA	1.90	0.54
1:B:159:LEU:HG	1:B:190:VAL:HG11	1.90	0.54
1:C:181:GLY:HA2	1:C:184:ILE:HD12	1.90	0.54
1:D:223:LEU:HD23	1:D:387:LEU:HD23	1.89	0.54
1:A:223:LEU:HD23	1:A:387:LEU:HD23	1.89	0.54
1:C:244:THR:HB	1:C:273:ASN:HB2	1.89	0.53
1:A:387:LEU:HD13	1:A:441:CYS:HA	1.92	0.52
1:A:219:ARG:NH2	3:A:602:RZY:O10	2.39	0.52
1:D:170:THR:OG1	1:D:188:ARG:NH1	2.42	0.52
1:B:223:LEU:HD23	1:B:387:LEU:HD23	1.92	0.52
1:A:208:PRO:HA	1:A:350:ASP:HA	1.91	0.52
1:B:294:LYS:HG3	1:B:300:VAL:HG21	1.92	0.52
1:A:179:ALA:HB2	1:C:194:LYS:HE3	1.92	0.52
1:D:449:PRO:HB2	1:D:453:LEU:HD22	1.92	0.51
1:C:387:LEU:HD13	1:C:441:CYS:HA	1.93	0.50
1:D:208:PRO:HA	1:D:350:ASP:HA	1.94	0.50
1:A:298:TYR:HD1	1:A:353:LEU:HD11	1.75	0.50
1:C:190:VAL:HG23	1:C:193:ILE:HD12	1.93	0.50
1:B:222:VAL:HG22	1:B:234:VAL:HG22	1.93	0.50
1:C:241:ARG:NH1	6:C:602:RZP:O17	2.45	0.49
1:C:140:PRO:O	1:C:144:HIS:NE2	2.39	0.48
1:D:62:ILE:HB	1:D:81:LEU:HD13	1.95	0.48
1:D:64:LEU:HD12	1:D:83:GLU:HG2	1.96	0.47
1:B:298:TYR:CD1	1:B:353:LEU:HD11	2.49	0.47
1:B:74:ARG:O	1:B:78:GLN:HG3	2.14	0.47
1:B:301:GLU:O	1:B:305:ARG:HG2	2.14	0.47
1:D:125:LYS:NZ	2:D:601:ADP:O1A	2.47	0.47
1:D:140:PRO:O	1:D:144:HIS:NE2	2.41	0.46
1:A:298:TYR:CD1	1:A:353:LEU:HD11	2.51	0.46
1:A:181:GLY:HA2	1:A:184:ILE:HD12	1.99	0.45
1:D:314:THR:O	1:D:317:SER:OG	2.33	0.45
1:D:301:GLU:O	1:D:305:ARG:HG2	2.16	0.45
1:C:298:TYR:HD1	1:C:353:LEU:HD11	1.82	0.45
1:B:239:LEU:HD22	1:B:283:LYS:HD3	1.98	0.45
1:B:90:TRP:CZ3	1:B:93:TYR:HB2	2.52	0.45
1:D:212:ASP:N	5:D:609:GOL:H12	2.32	0.45
1:B:314:THR:O	1:B:317:SER:OG	2.34	0.44
1:B:125:LYS:NZ	2:B:601:ADP:O1B	2.40	0.44
1:C:74:ARG:NH1	1:C:378:ASP:OD1	2.49	0.44
1:C:113:ILE:HG23	1:C:115:HIS:H	1.82	0.44
1:D:366:PHE:HA	1:D:377:LYS:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:PRO:HB3	1:D:134:ARG:CZ	2.48	0.44
1:C:212:ASP:OD2	1:C:284:ARG:NH2	2.40	0.44
1:B:122:ILE:HG23	1:B:318:ALA:HB2	1.99	0.44
1:A:286:LEU:HD13	1:A:304:TRP:CH2	2.53	0.44
1:B:182:ARG:HD3	1:D:185:PHE:CE2	2.53	0.43
1:A:122:ILE:HG23	1:A:318:ALA:HB2	2.01	0.43
1:A:185:PHE:CG	1:C:182:ARG:HB3	2.54	0.43
1:B:99:VAL:HG11	1:B:113:ILE:HD11	1.99	0.43
1:A:314:THR:O	1:A:317:SER:OG	2.36	0.43
1:D:298:TYR:CD1	1:D:353:LEU:HD11	2.53	0.42
1:A:64:LEU:HD13	1:A:73:ARG:HG3	2.01	0.42
1:D:122:ILE:HG23	1:D:318:ALA:HB2	2.01	0.42
1:B:298:TYR:HD1	1:B:353:LEU:HD11	1.84	0.42
1:D:125:LYS:HD3	1:D:359:GLU:HG3	2.01	0.42
1:A:116:PHE:CE1	1:A:339:CYS:HB2	2.54	0.42
1:C:293:MET:HB2	1:C:300:VAL:HG22	2.01	0.42
1:A:125:LYS:HE3	2:A:601:ADP:O2A	2.20	0.42
1:B:181:GLY:HA2	1:B:184:ILE:HD12	2.02	0.42
1:D:174:LYS:HD2	1:D:200:ILE:HD11	2.01	0.42
1:A:108:LYS:O	1:A:333:HIS:NE2	2.53	0.42
1:C:348:LEU:HB2	1:C:358:LEU:HD11	2.01	0.42
1:D:251:ASN:O	1:D:255:LEU:HG	2.20	0.42
1:A:333:HIS:CG	1:A:338:ALA:HB2	2.55	0.42
1:A:74:ARG:O	1:A:78:GLN:HG3	2.20	0.42
1:D:298:TYR:HD1	1:D:353:LEU:HD11	1.85	0.42
1:C:448:TYR:HA	1:C:449:PRO:HA	1.89	0.41
1:D:96:ASP:O	1:D:363:SER:OG	2.33	0.41
1:D:74:ARG:O	1:D:78:GLN:HG3	2.20	0.41
1:A:359:GLU:HG2	1:A:360:VAL:N	2.36	0.41
1:B:185:PHE:CD1	1:D:182:ARG:HB3	2.55	0.41
1:B:239:LEU:HD11	1:B:377:LYS:HE2	2.03	0.41
1:C:298:TYR:CD1	1:C:353:LEU:HD11	2.57	0.40
1:B:359:GLU:HG2	1:B:360:VAL:N	2.35	0.40
1:C:90:TRP:CZ3	1:C:93:TYR:HB2	2.57	0.40
1:D:160:GLN:O	1:D:164:ARG:HG3	2.21	0.40
1:D:293:MET:HB2	1:D:300:VAL:HG22	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	397/453 (88%)	383 (96%)	14 (4%)	0	100	100
1	B	394/453 (87%)	385 (98%)	9 (2%)	0	100	100
1	C	400/453 (88%)	389 (97%)	11 (3%)	0	100	100
1	D	402/453 (89%)	389 (97%)	13 (3%)	0	100	100
All	All	1593/1812 (88%)	1546 (97%)	47 (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	268/415 (65%)	268 (100%)	0	100	100
1	B	298/415 (72%)	298 (100%)	0	100	100
1	C	262/415 (63%)	262 (100%)	0	100	100
1	D	300/415 (72%)	300 (100%)	0	100	100
All	All	1128/1660 (68%)	1128 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 8 are monoatomic - leaving 26 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$
5	GOL	D	607	-	5,5,5	0.86	0	5,5,5	1.14	0
3	RZY	A	602	4	10,22,22	2.61	2 (20%)	13,32,32	1.11	1 (7%)
5	GOL	B	609	-	5,5,5	0.89	0	5,5,5	0.98	0
5	GOL	C	605	-	5,5,5	0.90	0	5,5,5	1.01	0
5	GOL	D	611	-	5,5,5	0.85	0	5,5,5	1.18	1 (20%)
2	ADP	D	601	4	24,29,29	0.92	1 (4%)	29,45,45	1.42	5 (17%)
5	GOL	D	606	-	5,5,5	0.90	0	5,5,5	0.99	0
5	GOL	B	610	-	5,5,5	0.94	0	5,5,5	0.97	0
5	GOL	B	602	-	5,5,5	0.88	0	5,5,5	1.13	0
5	GOL	B	607	-	5,5,5	0.86	0	5,5,5	1.11	1 (20%)
6	RZP	D	602	4	12,26,26	0.76	0	18,37,37	1.28	3 (16%)
5	GOL	D	609	-	5,5,5	0.89	0	5,5,5	1.04	0
6	RZP	B	604	4	12,26,26	0.78	0	18,37,37	1.26	4 (22%)
5	GOL	D	608	-	5,5,5	0.92	0	5,5,5	0.99	0
5	GOL	B	608	-	5,5,5	0.87	0	5,5,5	1.20	1 (20%)
5	GOL	D	613	-	5,5,5	0.92	0	5,5,5	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	C	601	4	24,29,29	0.94	1 (4%)	29,45,45	1.49	4 (13%)
5	GOL	D	614	-	5,5,5	1.02	0	5,5,5	0.65	0
5	GOL	D	610	-	5,5,5	0.87	0	5,5,5	1.10	0
2	ADP	A	601	4	24,29,29	0.94	1 (4%)	29,45,45	1.51	4 (13%)
5	GOL	B	603	-	5,5,5	0.92	0	5,5,5	0.98	0
5	GOL	D	612	-	5,5,5	0.87	0	5,5,5	1.16	0
5	GOL	B	611	-	5,5,5	0.90	0	5,5,5	0.99	0
6	RZP	C	602	4	12,26,26	0.78	1 (8%)	18,37,37	1.25	2 (11%)
2	ADP	B	601	4	24,29,29	1.06	2 (8%)	29,45,45	1.53	5 (17%)
5	GOL	D	605	-	5,5,5	0.87	0	5,5,5	1.16	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
5	GOL	D	607	-	-	0/4/4/4	-
3	RZY	A	602	4	-	10/18/30/30	-
5	GOL	B	609	-	-	0/4/4/4	-
5	GOL	C	605	-	-	0/4/4/4	-
5	GOL	D	611	-	-	0/4/4/4	-
2	ADP	D	601	4	-	1/12/32/32	0/3/3/3
5	GOL	D	606	-	-	0/4/4/4	-
5	GOL	B	610	-	-	0/4/4/4	-
5	GOL	B	602	-	-	0/4/4/4	-
5	GOL	B	607	-	-	0/4/4/4	-
6	RZP	D	602	4	-	2/21/35/35	-
5	GOL	D	609	-	-	0/4/4/4	-
6	RZP	B	604	4	-	5/21/35/35	-
5	GOL	D	608	-	-	1/4/4/4	-
5	GOL	B	608	-	-	0/4/4/4	-
5	GOL	D	613	-	-	0/4/4/4	-
2	ADP	C	601	4	-	0/12/32/32	0/3/3/3
5	GOL	D	614	-	-	0/4/4/4	-
5	GOL	D	610	-	-	0/4/4/4	-
2	ADP	A	601	4	-	0/12/32/32	0/3/3/3
5	GOL	B	603	-	-	0/4/4/4	-
5	GOL	D	612	-	-	0/4/4/4	-
5	GOL	B	611	-	-	0/4/4/4	-
6	RZP	C	602	4	-	7/21/35/35	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	601	4	-	1/12/32/32	0/3/3/3
5	GOL	D	605	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	RZY	P09-C08	7.07	1.86	1.79
3	A	602	RZY	C18-N17	3.36	1.45	1.34
2	B	601	ADP	C5-C4	2.81	1.48	1.40
2	C	601	ADP	C5-C4	2.46	1.47	1.40
2	A	601	ADP	C5-C4	2.45	1.47	1.40
2	D	601	ADP	C5-C4	2.45	1.47	1.40
2	B	601	ADP	C2-N3	2.15	1.35	1.32
6	C	602	RZP	P6-C14	2.10	1.81	1.79

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C3'-C2'-C1'	4.19	107.29	100.98
2	A	601	ADP	PA-O3A-PB	-3.32	121.45	132.83
2	B	601	ADP	N3-C2-N1	-3.28	123.55	128.68
2	C	601	ADP	C4-C5-N7	-3.27	105.99	109.40
2	D	601	ADP	N3-C2-N1	-3.21	123.67	128.68
2	C	601	ADP	N3-C2-N1	-3.21	123.67	128.68
2	A	601	ADP	C4-C5-N7	-3.20	106.06	109.40
2	A	601	ADP	N3-C2-N1	-3.19	123.70	128.68
2	C	601	ADP	C3'-C2'-C1'	3.09	105.63	100.98
2	C	601	ADP	PA-O3A-PB	-3.04	122.40	132.83
2	D	601	ADP	C3'-C2'-C1'	2.97	105.45	100.98
2	D	601	ADP	C4-C5-N7	-2.96	106.31	109.40
2	A	601	ADP	C3'-C2'-C1'	2.90	105.34	100.98
6	C	602	RZP	O7-P6-C5	2.87	110.69	103.40
6	D	602	RZP	O7-P6-C5	2.76	110.39	103.40
2	D	601	ADP	PA-O3A-PB	-2.51	124.23	132.83
2	B	601	ADP	PA-O3A-PB	-2.34	124.79	132.83
6	B	604	RZP	O7-P6-C5	2.33	109.30	103.40
2	B	601	ADP	C1'-N9-C4	2.32	130.72	126.64
6	D	602	RZP	C19-C20-C21	-2.32	108.61	113.59
6	B	604	RZP	O27-P24-O7	2.14	111.83	104.64
6	D	602	RZP	P6-C14-C15	-2.14	108.12	114.10
6	B	604	RZP	C19-C20-C21	-2.11	109.06	113.59
5	B	608	GOL	C3-C2-C1	-2.10	103.56	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	602	RZP	C19-C20-C21	-2.09	109.09	113.59
6	B	604	RZP	P6-C14-C15	-2.09	108.26	114.10
3	A	602	RZY	C19-C18-N17	2.08	119.62	116.10
5	B	607	GOL	C3-C2-C1	-2.07	103.65	111.70
2	D	601	ADP	C2-N1-C6	2.03	122.23	118.75
5	D	611	GOL	C3-C2-C1	-2.03	103.82	111.70
2	B	601	ADP	O2A-PA-O1A	2.02	122.20	112.24

There are no chirality outliers.

All (27) torsion outliers are listed below:

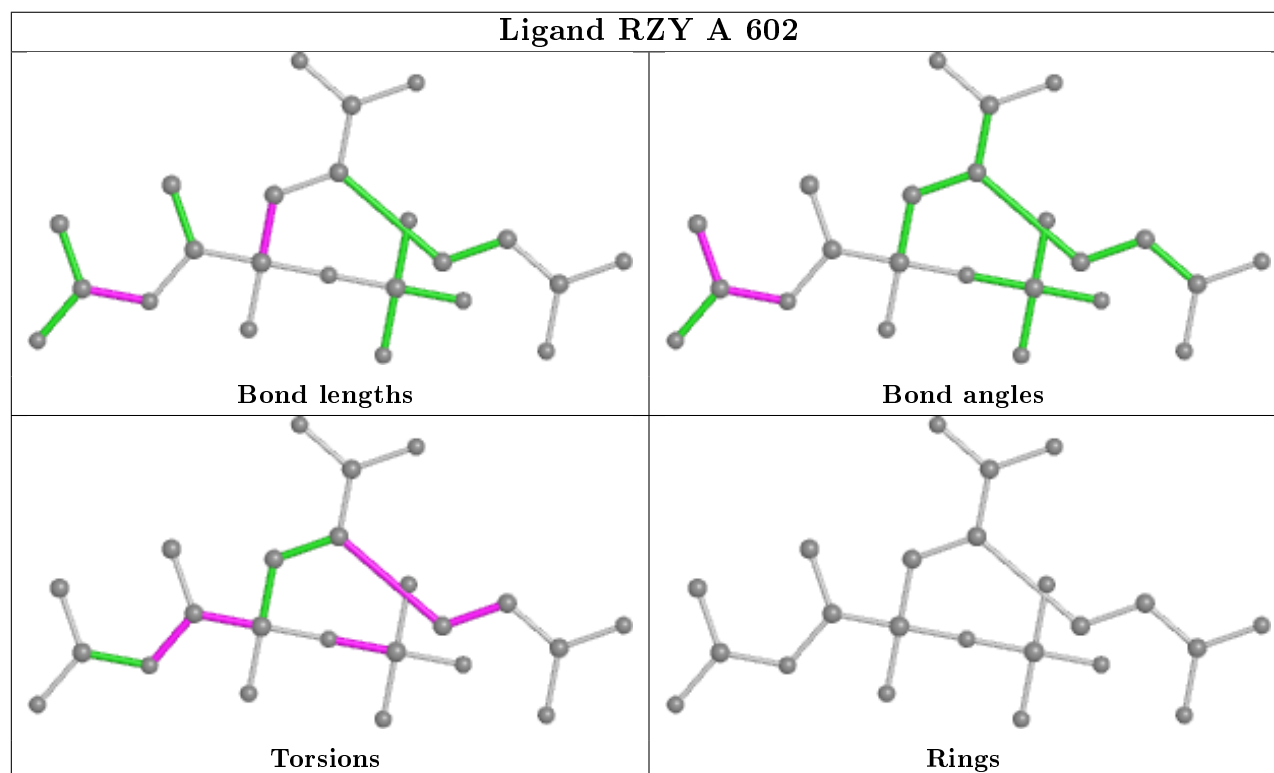
Mol	Chain	Res	Type	Atoms
3	A	602	RZY	P09-C16-N17-C18
3	A	602	RZY	C21-C16-P09-O10
3	A	602	RZY	C21-C16-P09-O11
3	A	602	RZY	N17-C16-P09-O10
3	A	602	RZY	N17-C16-P09-O11
3	A	602	RZY	P09-O11-P12-O14
3	A	602	RZY	P09-O11-P12-O13
6	D	602	RZP	P6-C14-C15-C19
3	A	602	RZY	C01-C02-C03-C04
3	A	602	RZY	C02-C03-C04-C05
6	B	604	RZP	C16-C15-C19-C20
6	C	602	RZP	C9-C5-P6-O7
3	A	602	RZY	C21-C16-N17-C18
6	B	604	RZP	C3-C1-N4-C5
6	D	602	RZP	P6-C14-C15-C16
6	B	604	RZP	P6-C14-C15-C16
6	C	602	RZP	C3-C1-N4-C5
6	B	604	RZP	P6-C14-C15-C19
6	C	602	RZP	N4-C5-P6-O7
6	B	604	RZP	O2-C1-N4-C5
6	C	602	RZP	N4-C5-P6-O8
6	C	602	RZP	O2-C1-N4-C5
2	B	601	ADP	PB-O3A-PA-O2A
2	D	601	ADP	PB-O3A-PA-O2A
5	D	608	GOL	C1-C2-C3-O3
6	C	602	RZP	P6-C14-C15-C16
6	C	602	RZP	C9-C5-P6-O8

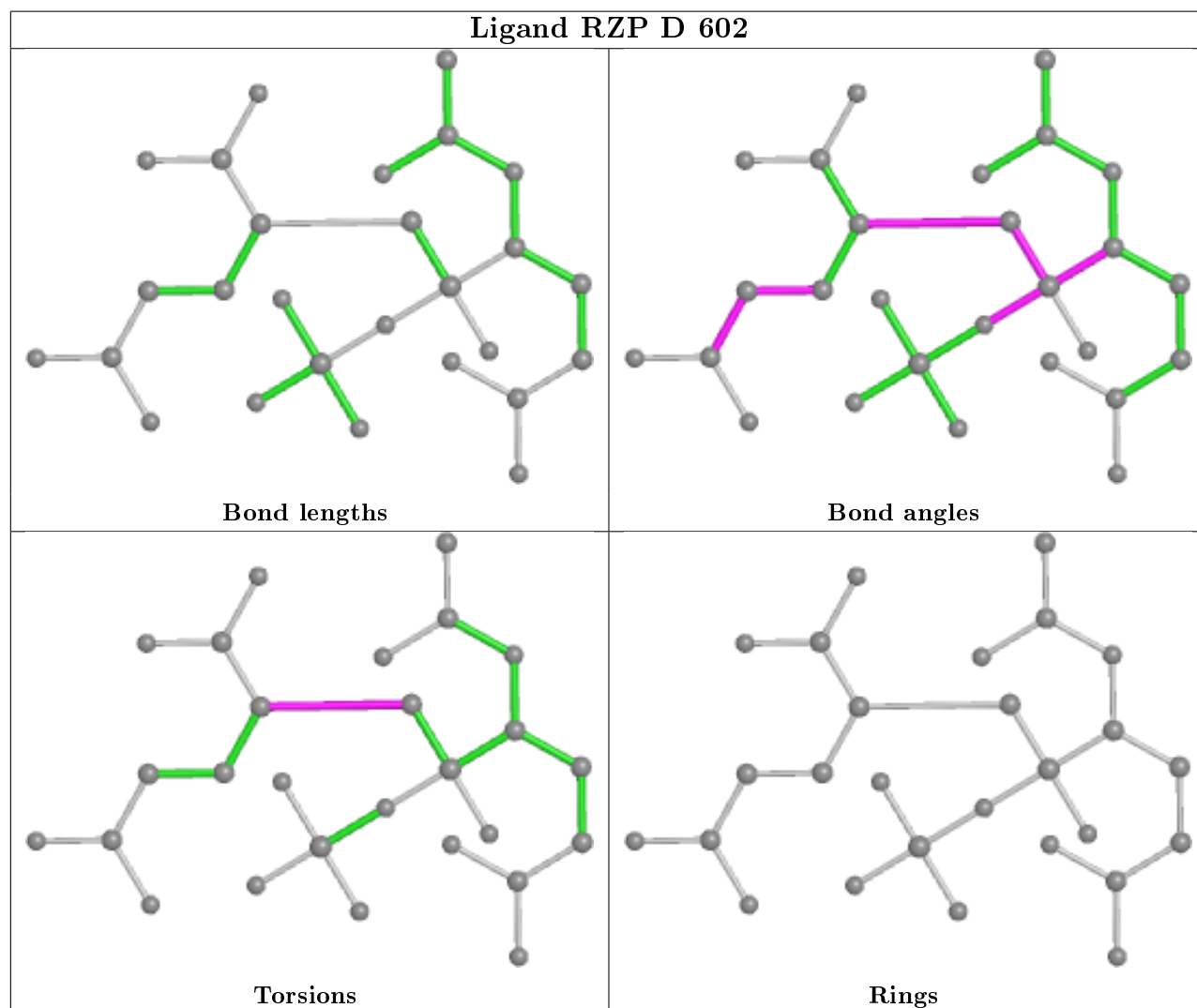
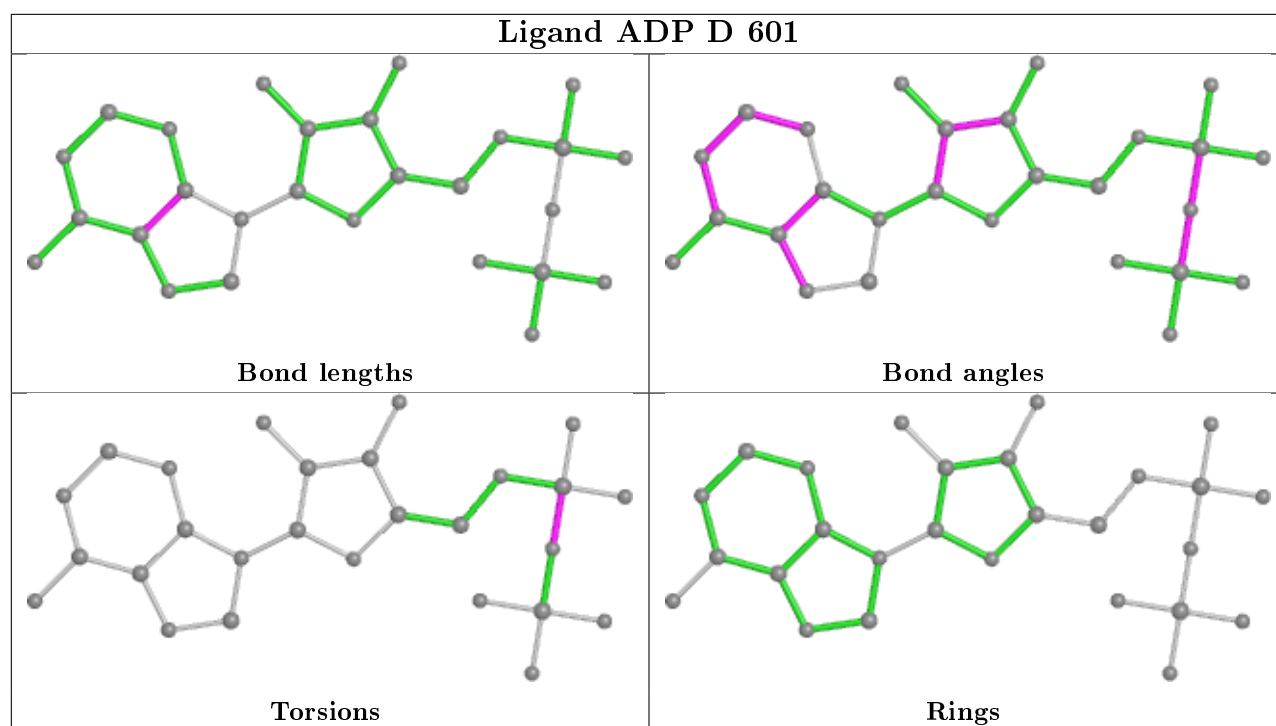
There are no ring outliers.

8 monomers are involved in 8 short contacts:

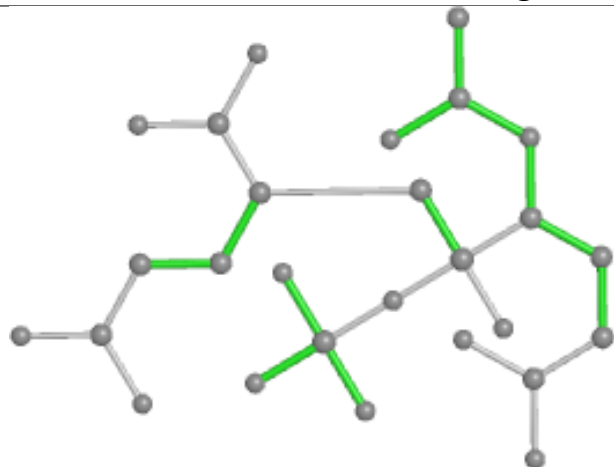
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	RZY	1	0
5	D	611	GOL	1	0
2	D	601	ADP	1	0
5	D	609	GOL	1	0
6	B	604	RZP	1	0
2	A	601	ADP	1	0
6	C	602	RZP	1	0
2	B	601	ADP	1	0

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

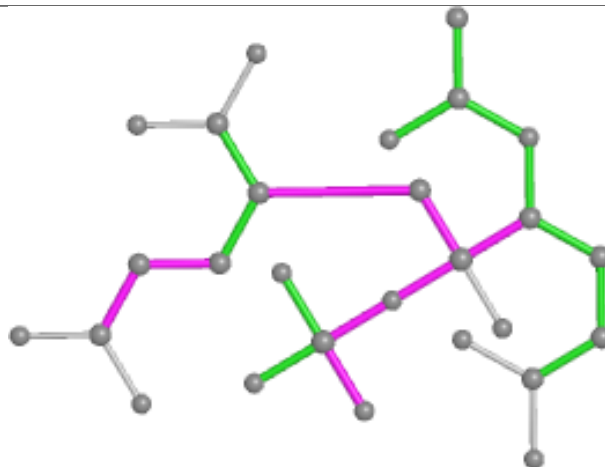




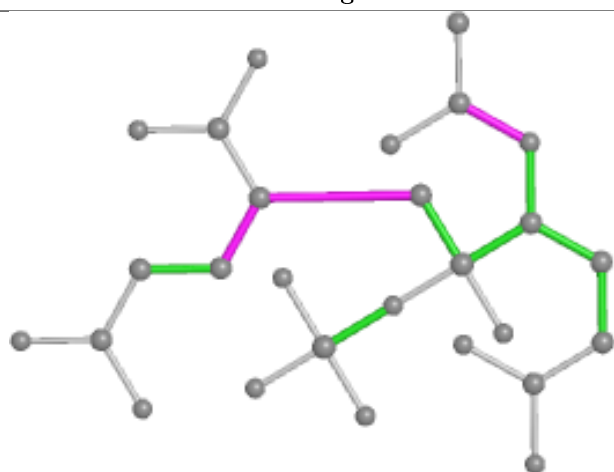
Ligand RZP B 604



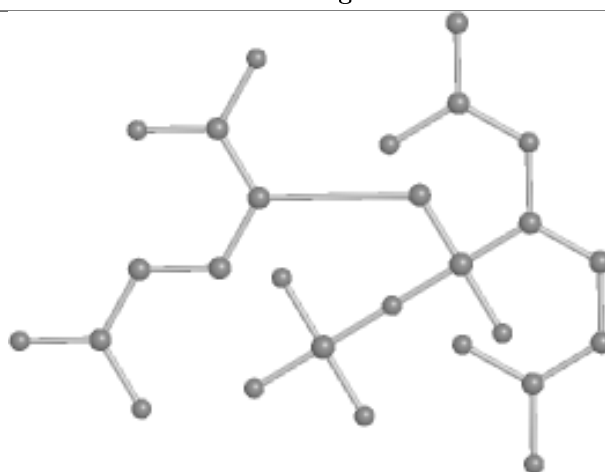
Bond lengths



Bond angles

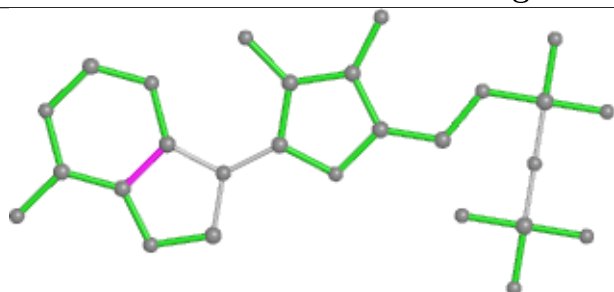


Torsions

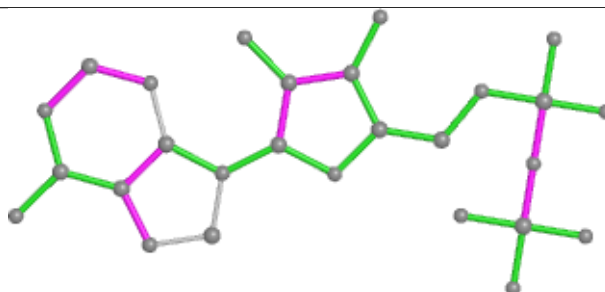


Rings

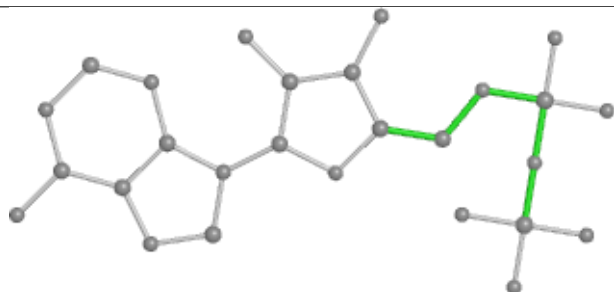
Ligand ADP C 601



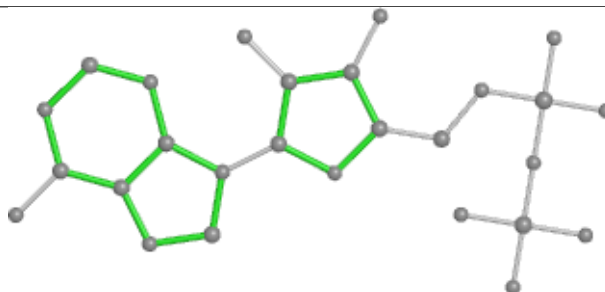
Bond lengths



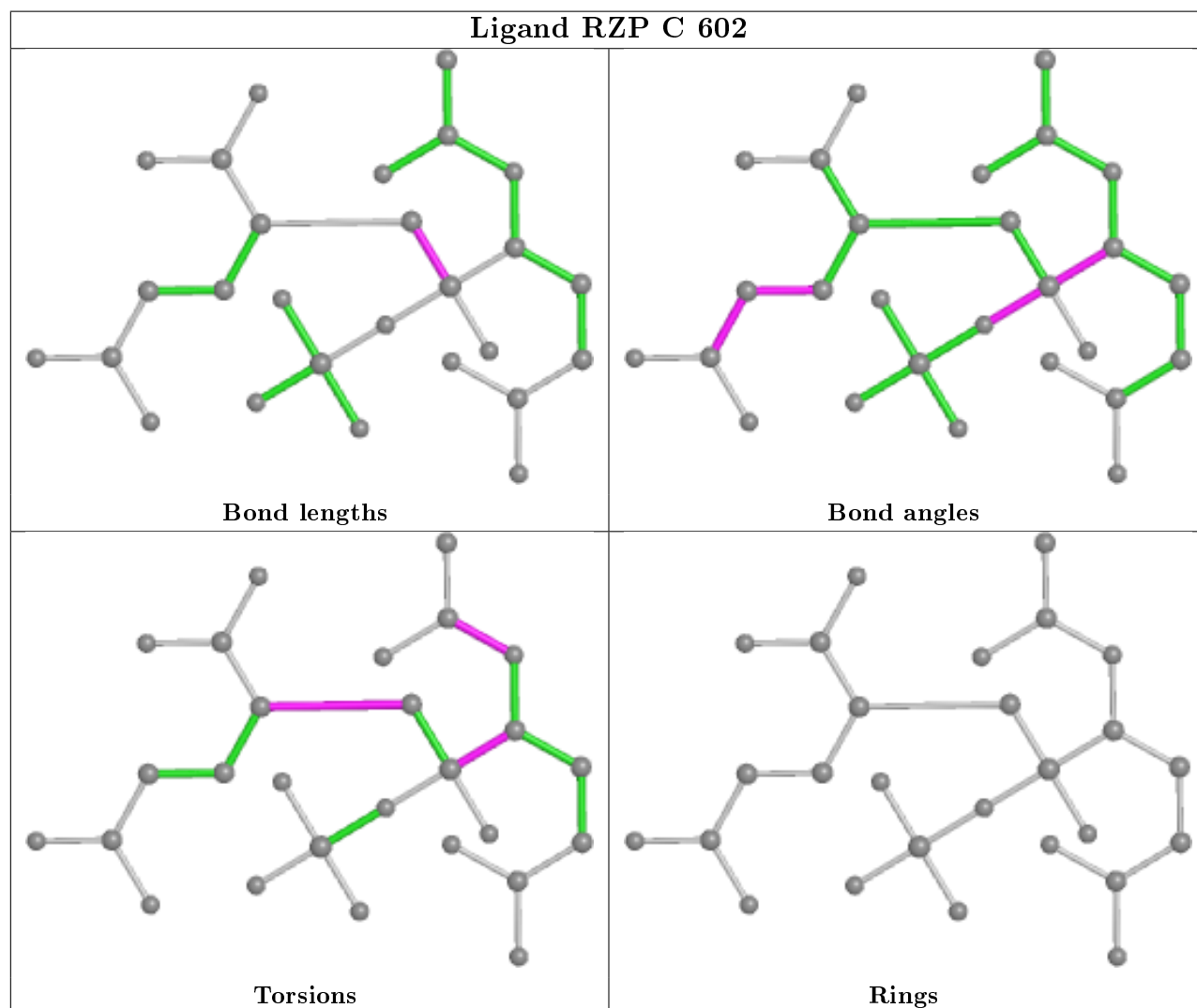
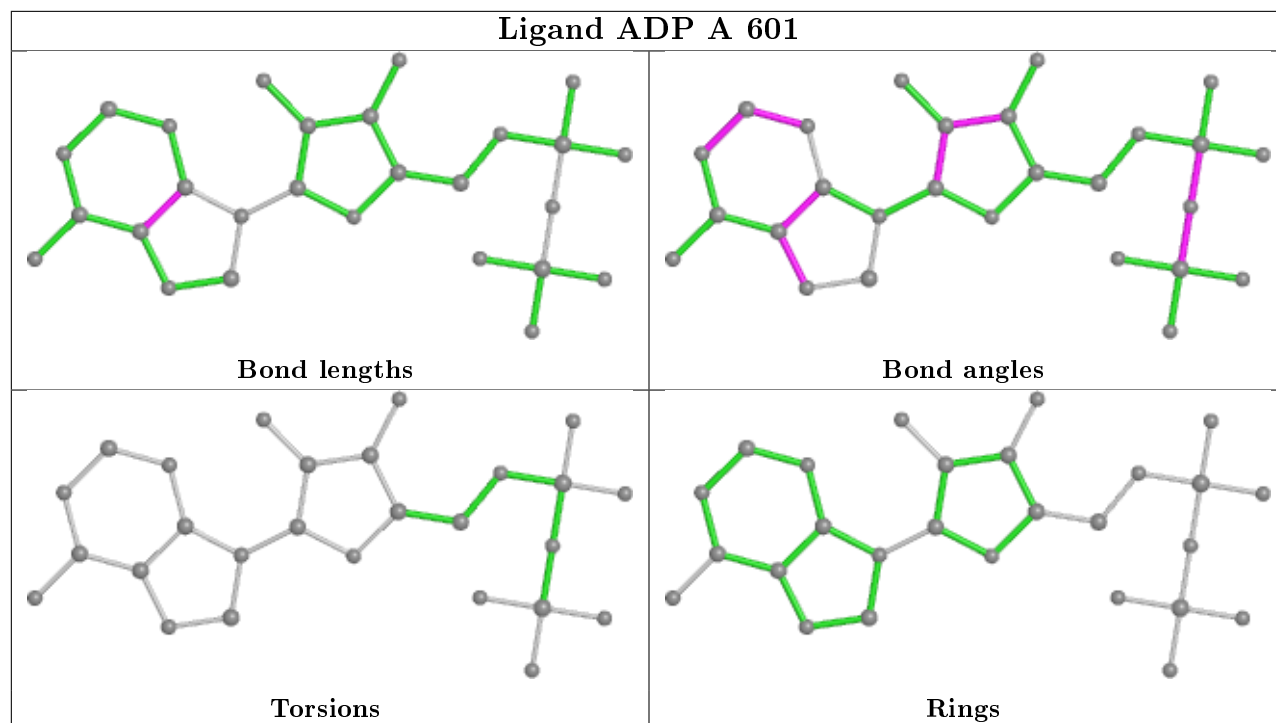
Bond angles

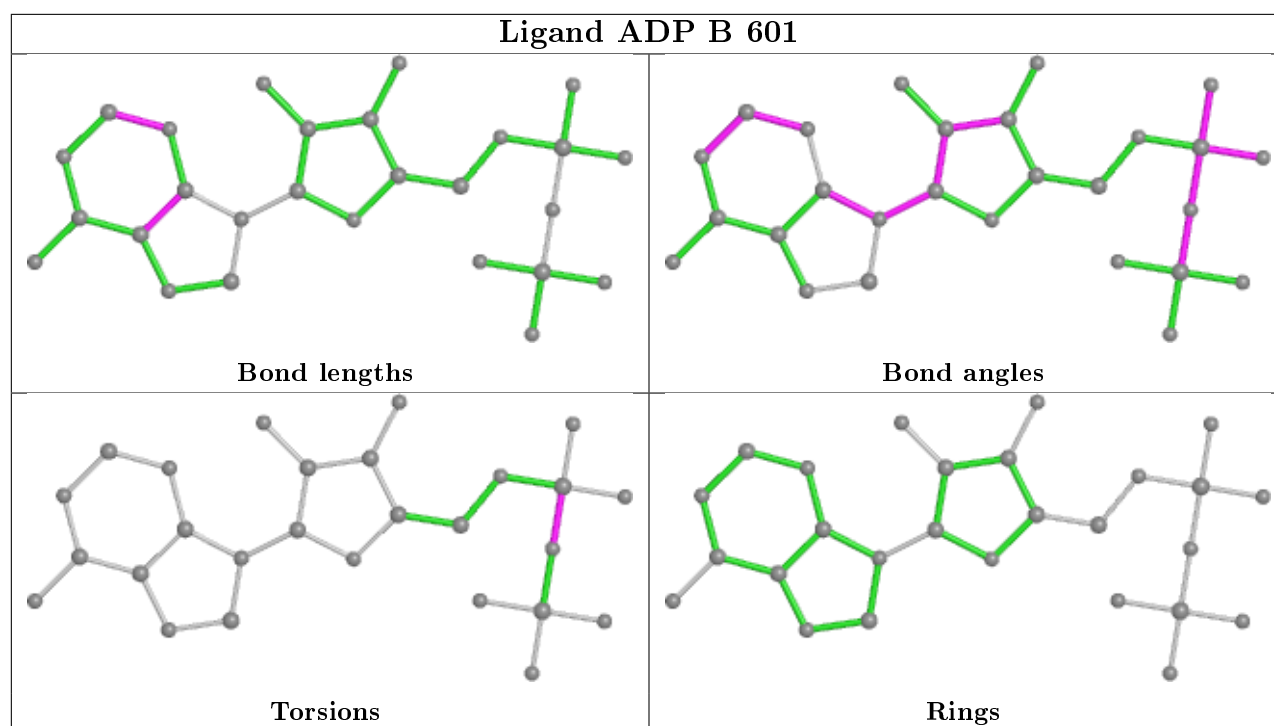


Torsions



Rings





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	400/453 (88%)	0.34	6 (1%) 73 53	59, 83, 126, 150	0
1	B	398/453 (87%)	0.12	1 (0%) 94 87	18, 50, 109, 162	0
1	C	403/453 (88%)	0.31	6 (1%) 73 53	55, 81, 120, 146	0
1	D	404/453 (89%)	0.13	3 (0%) 87 74	19, 50, 117, 170	0
All	All	1605/1812 (88%)	0.23	16 (0%) 82 66	18, 72, 122, 170	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	406	GLY	3.4
1	C	355	PRO	2.8
1	A	85	GLY	2.7
1	C	413	PRO	2.7
1	D	419	LEU	2.5
1	A	159	LEU	2.4
1	A	393	CYS	2.4
1	A	86	ASP	2.4
1	C	89	ASP	2.4
1	C	290	ASN	2.3
1	A	107	MET	2.3
1	D	393	CYS	2.2
1	A	75	ALA	2.2
1	C	459	PHE	2.0
1	D	459	PHE	2.0
1	C	393	CYS	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 ⓘ

There are no monosaccharides 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
5	GOL	D	605	6/6	0.69	0.27	73,77,82,83	0
5	GOL	D	614	6/6	0.83	0.23	59,66,72,79	0
5	GOL	D	606	6/6	0.84	0.30	69,82,95,97	0
5	GOL	B	608	6/6	0.86	0.27	59,73,81,81	0
5	GOL	B	603	6/6	0.87	0.19	33,47,56,56	0
5	GOL	D	610	6/6	0.87	0.27	48,58,62,70	0
5	GOL	B	610	6/6	0.88	0.30	60,73,86,91	0
5	GOL	B	609	6/6	0.89	0.34	56,67,73,73	0
5	GOL	D	612	6/6	0.90	0.22	42,65,75,78	0
5	GOL	C	605	6/6	0.91	0.26	71,82,84,84	0
5	GOL	B	607	6/6	0.91	0.32	50,63,77,78	0
5	GOL	B	602	6/6	0.93	0.23	49,70,72,72	0
5	GOL	D	613	6/6	0.94	0.32	37,68,73,74	0
4	MG	A	604	1/1	0.95	0.14	52,52,52,52	0
5	GOL	D	609	6/6	0.95	0.28	54,58,63,77	0
4	MG	A	603	1/1	0.95	0.19	43,43,43,43	0
6	RZP	B	604	27/27	0.95	0.29	17,44,73,173	0
4	MG	C	604	1/1	0.95	0.21	35,35,35,35	0
4	MG	B	606	1/1	0.95	0.25	26,26,26,26	0
2	ADP	A	601	27/27	0.96	0.25	48,58,78,89	0
4	MG	B	605	1/1	0.96	0.18	23,23,23,23	0
4	MG	C	603	1/1	0.96	0.12	88,88,88,88	0
5	GOL	B	611	6/6	0.96	0.42	39,54,62,64	0
6	RZP	C	602	27/27	0.96	0.25	50,64,88,89	0
5	GOL	D	608	6/6	0.96	0.29	43,66,90,92	0
5	GOL	D	607	6/6	0.97	0.42	38,64,70,82	0
3	RZY	A	602	23/23	0.97	0.24	44,64,84,85	0
2	ADP	C	601	27/27	0.97	0.21	47,62,76,84	0
2	ADP	D	601	27/27	0.98	0.23	4,23,43,67	0
4	MG	D	604	1/1	0.98	0.20	13,13,13,13	0
4	MG	D	603	1/1	0.98	0.20	20,20,20,20	0
2	ADP	B	601	27/27	0.98	0.23	5,26,46,80	0

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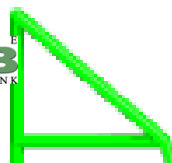
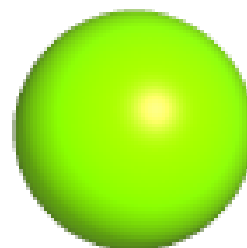
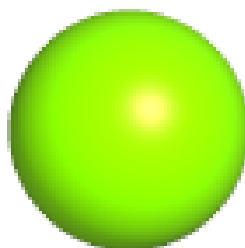
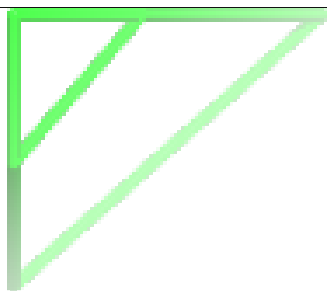
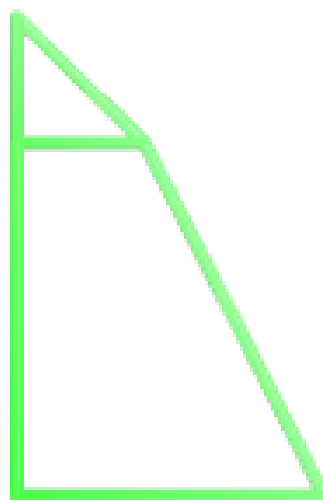
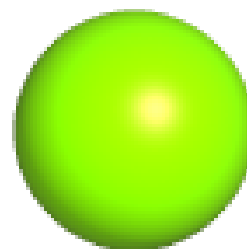
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	D	611	6/6	0.98	0.35	54,64,70,78	0
6	RZP	D	602	27/27	0.99	0.28	4,29,66,79	0

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.

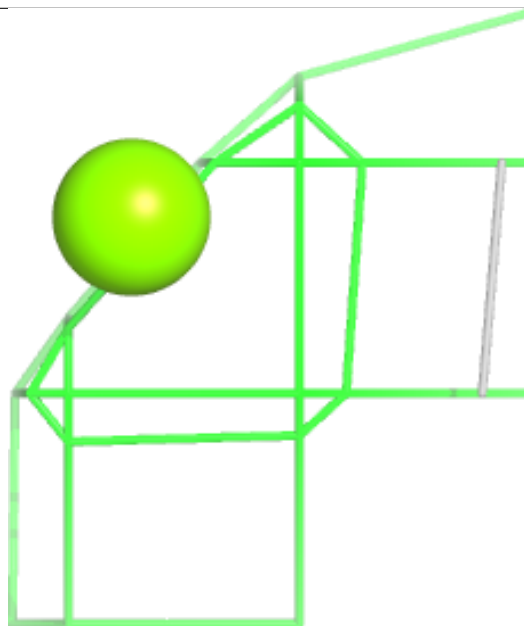
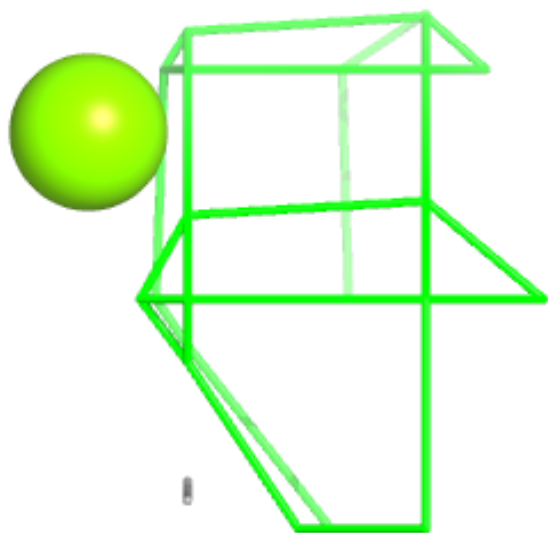
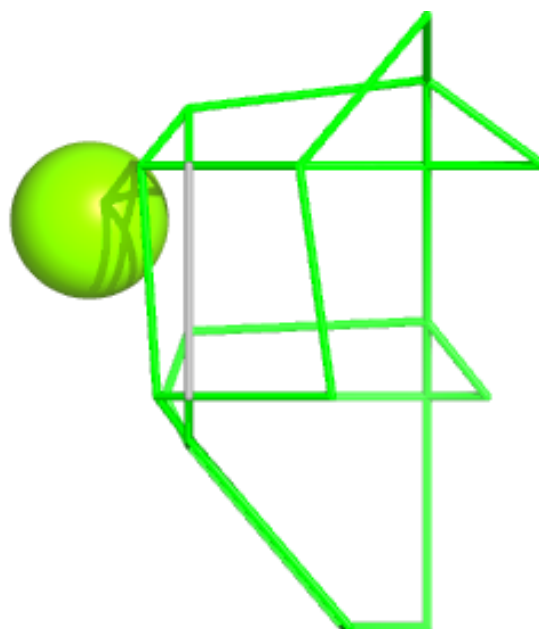
Electron density around MG A 604:

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



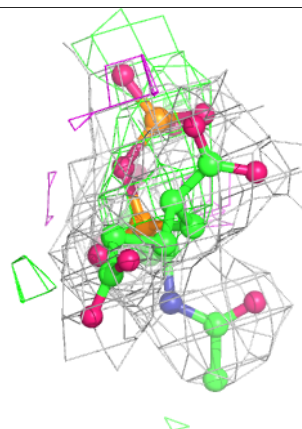
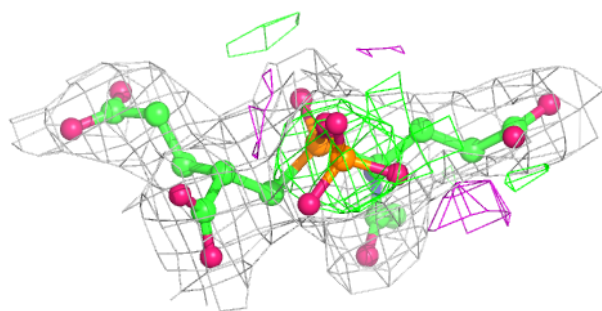
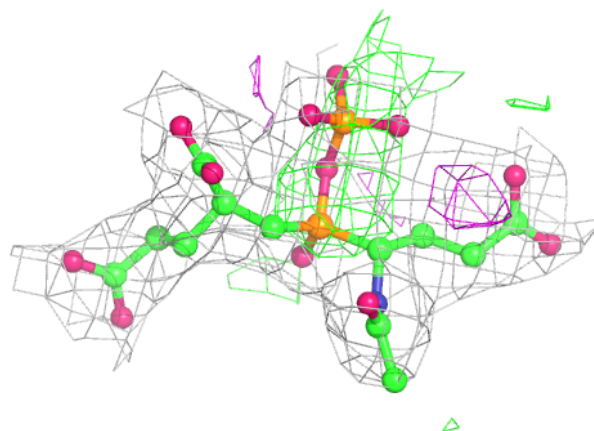
Electron density around MG A 603:

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



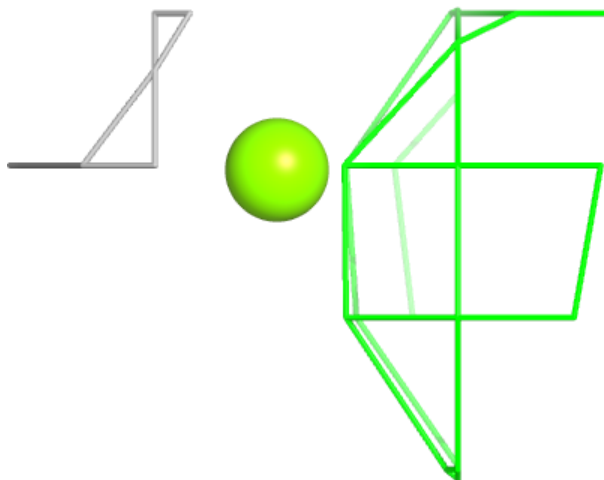
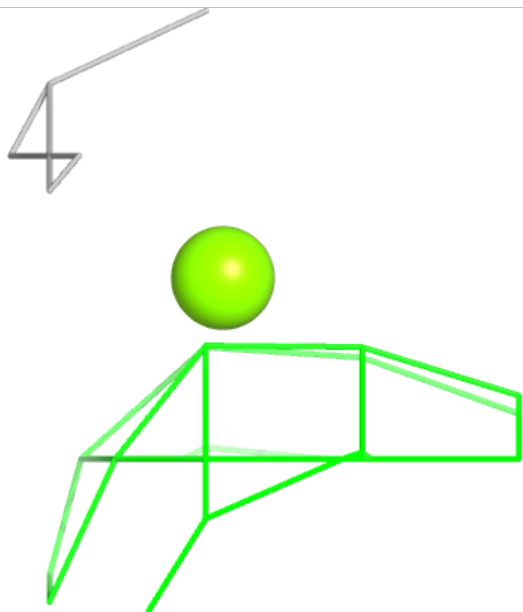
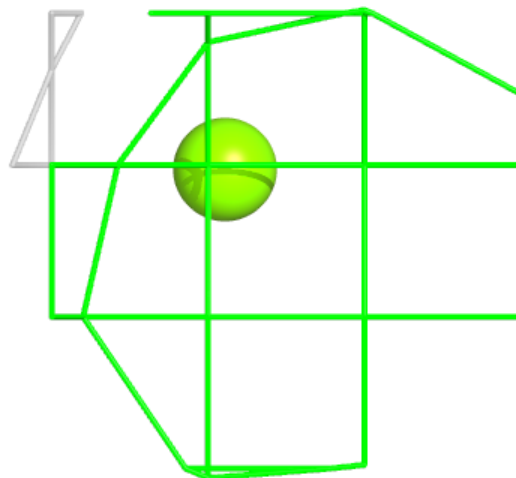
Electron density around RZP B 604:

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



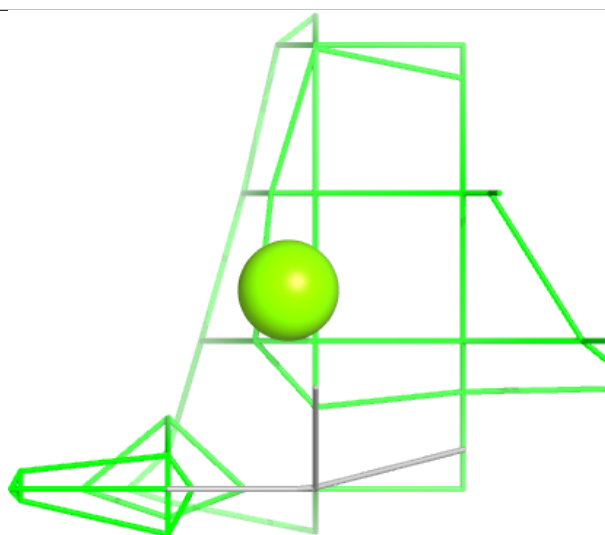
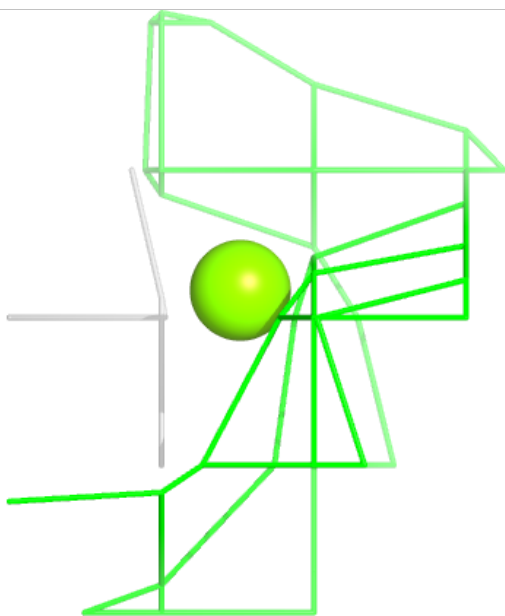
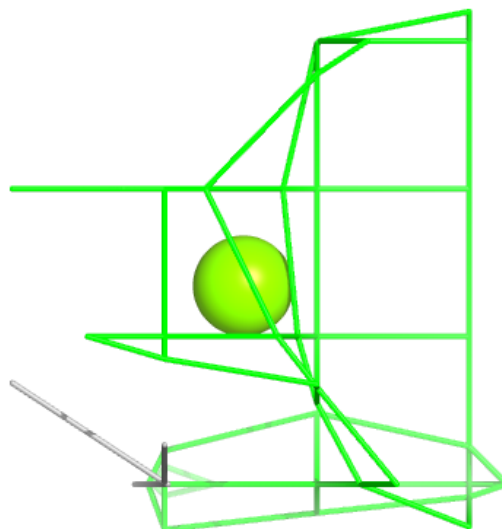
Electron density around MG C 604:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



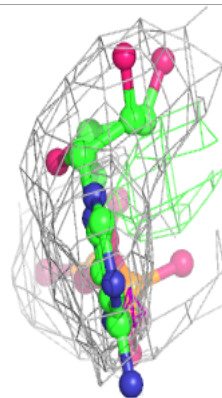
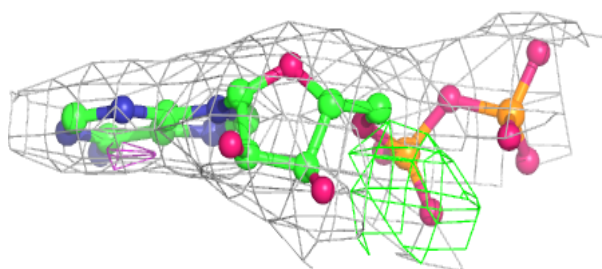
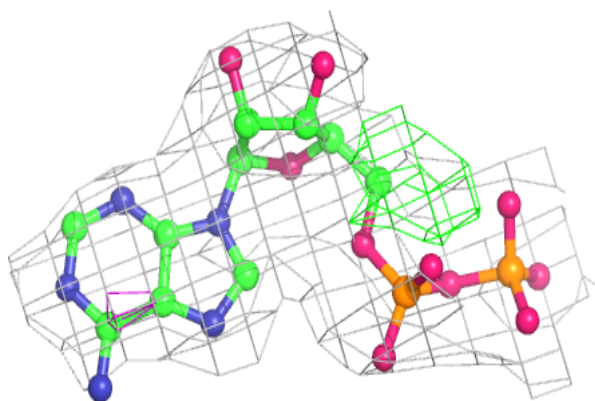
Electron density around MG B 606:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



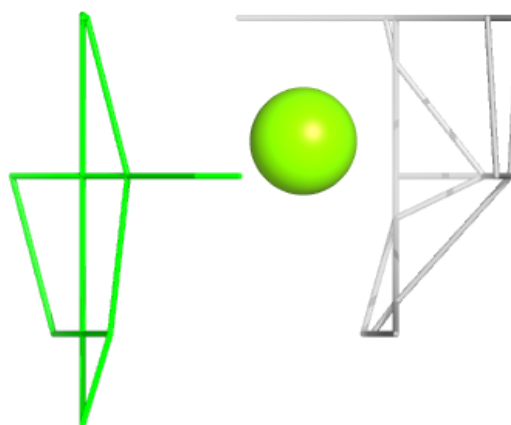
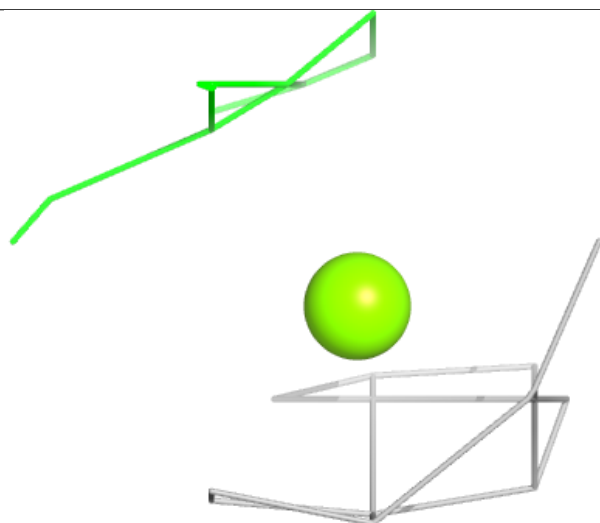
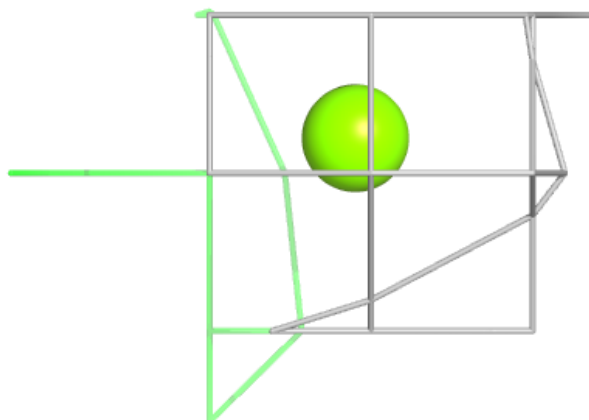
Electron density around ADP A 601:

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



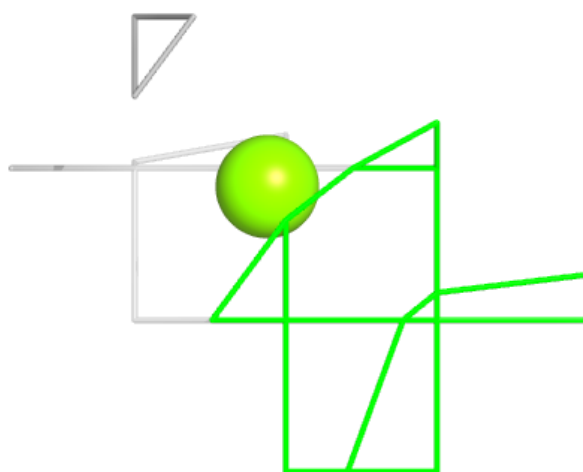
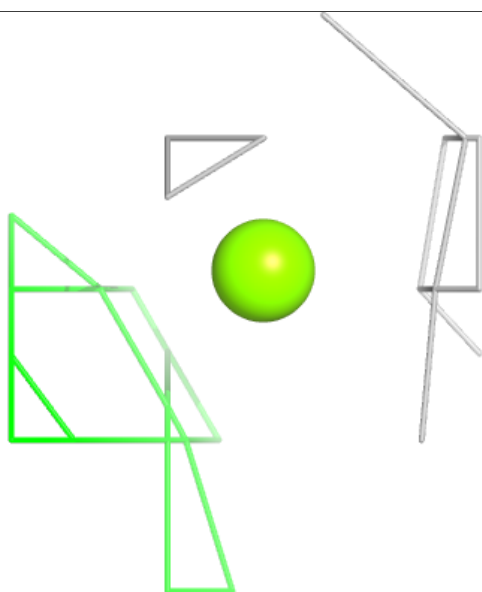
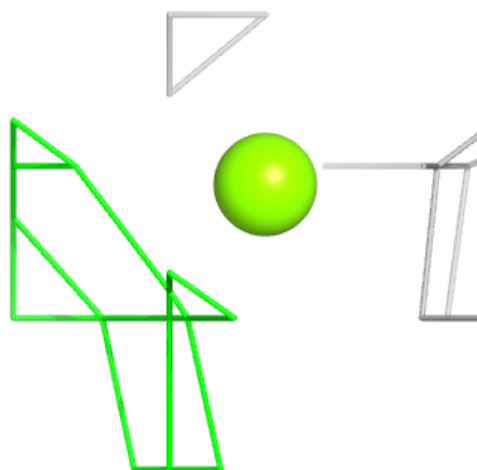
Electron density around MG B 605:

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



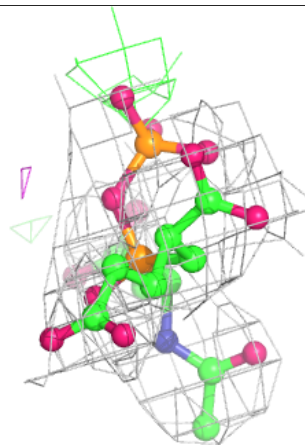
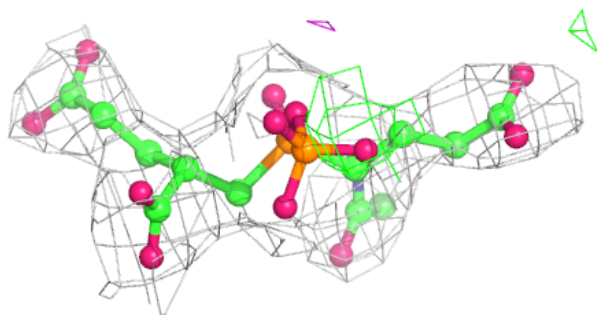
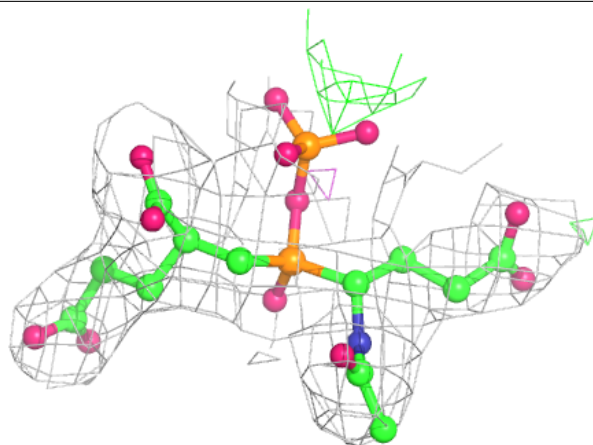
Electron density around MG C 603:

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and green (positive)



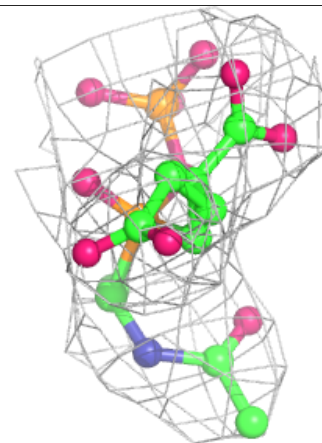
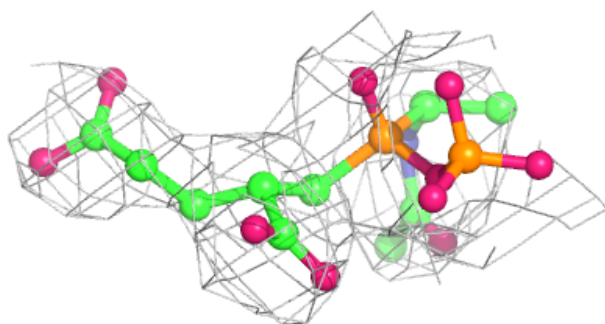
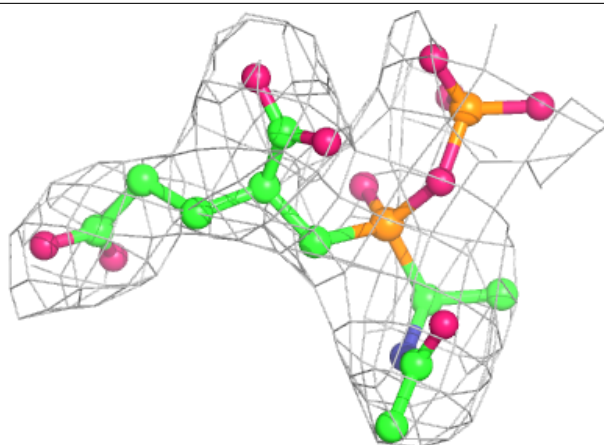
Electron density around RZP C 602:

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

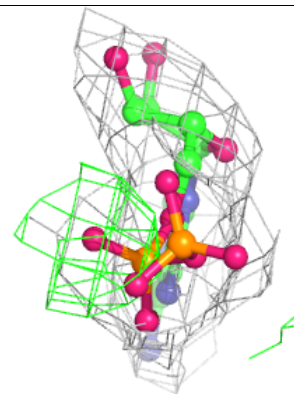
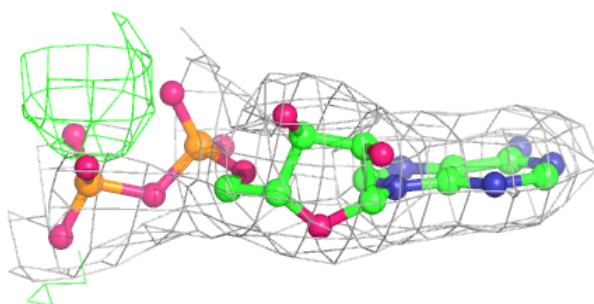
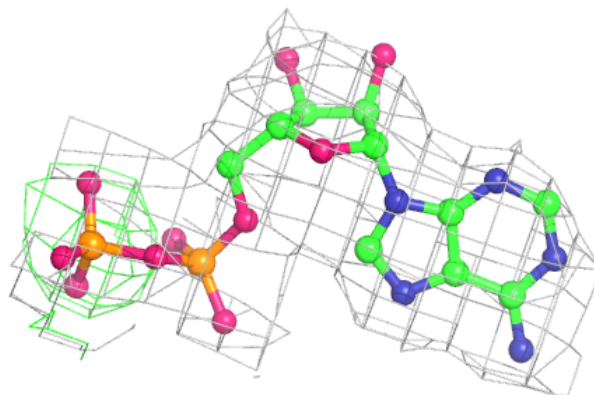


Electron density around RZY A 602:

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

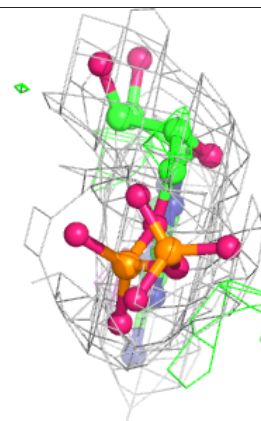
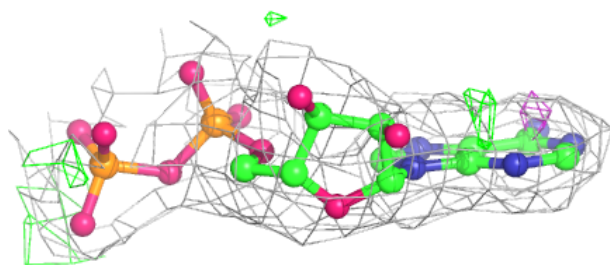
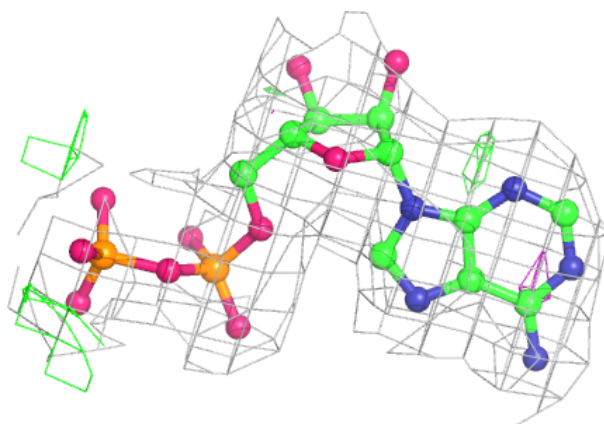
**Electron density around ADP C 601:**

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



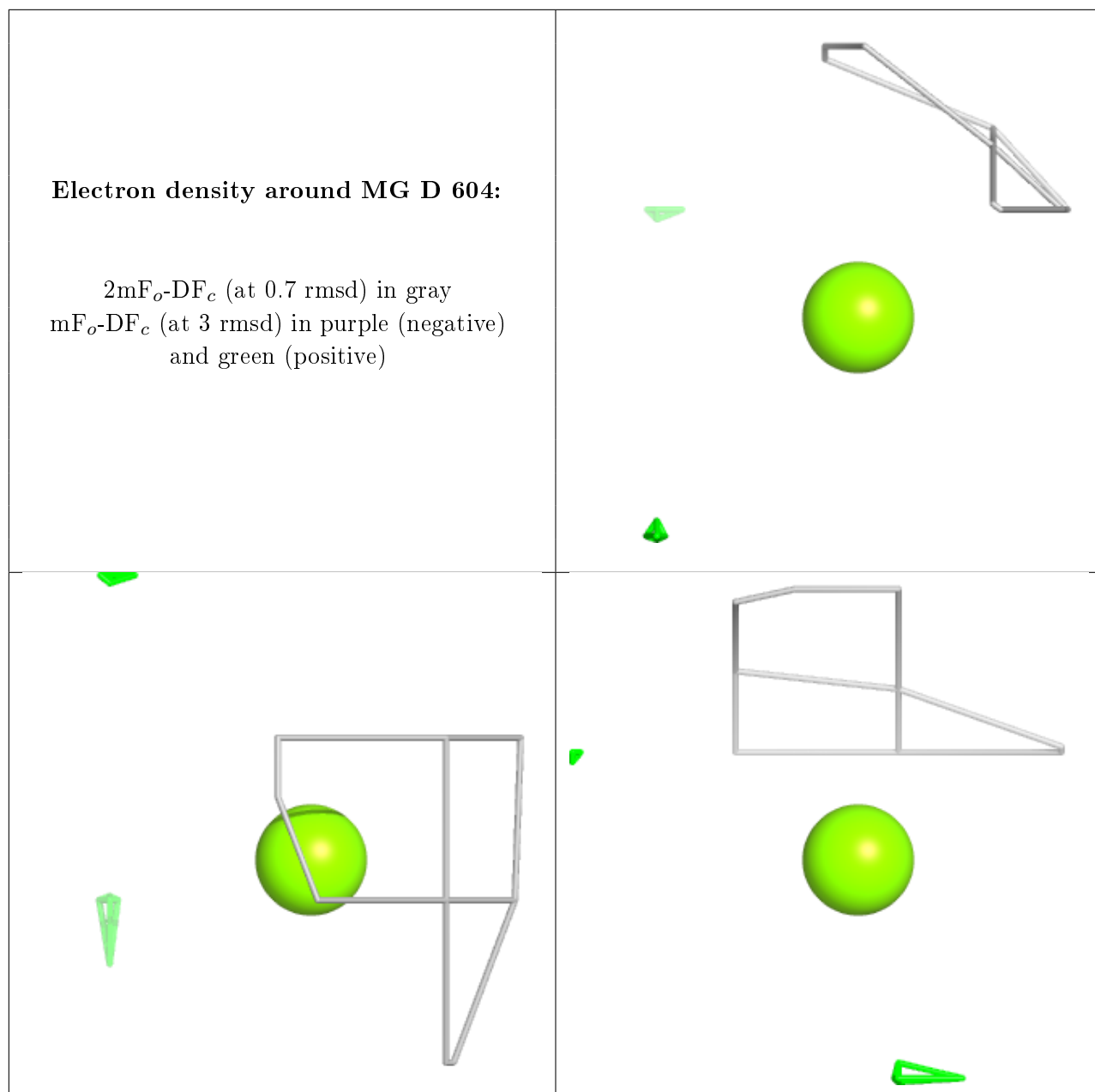
Electron density around ADP D 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



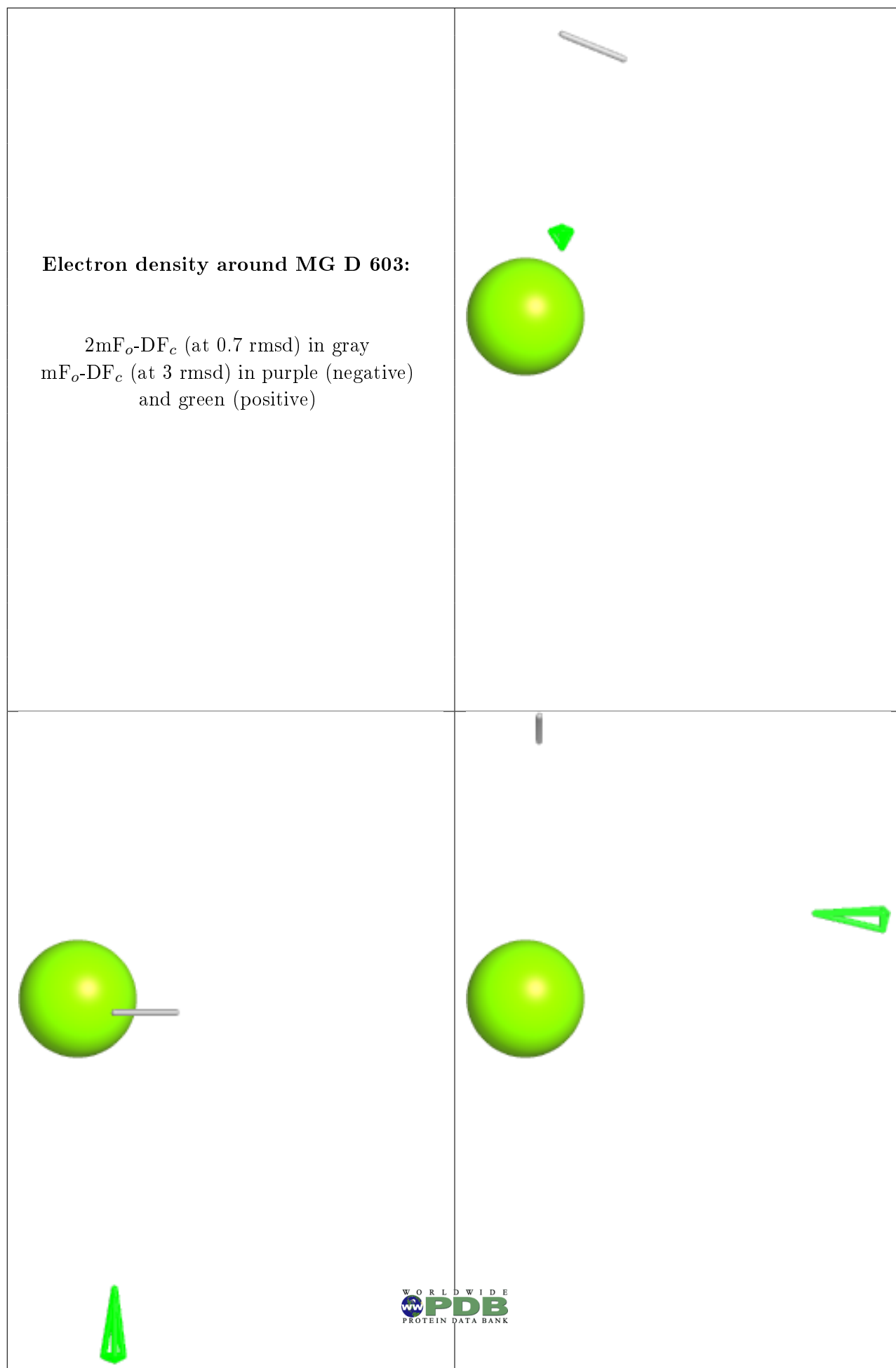
Electron density around MG D 604:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



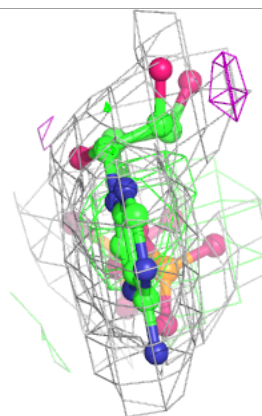
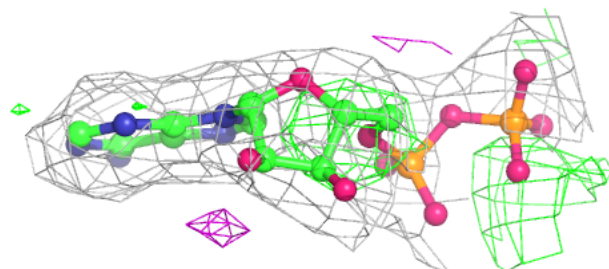
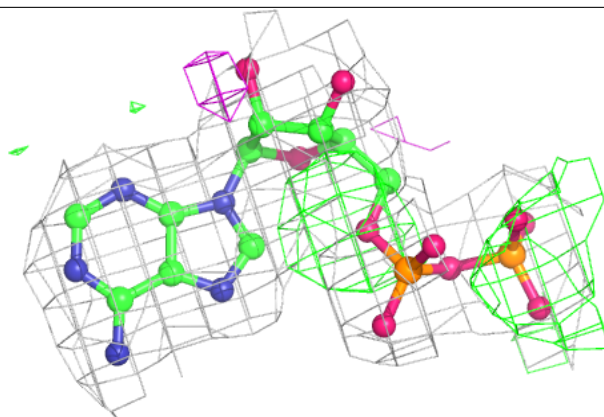
Electron density around MG D 603:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

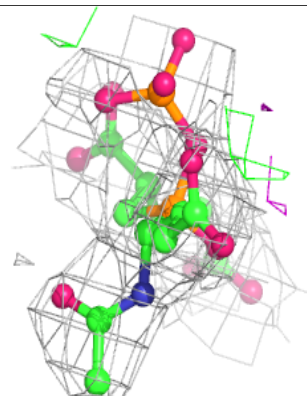
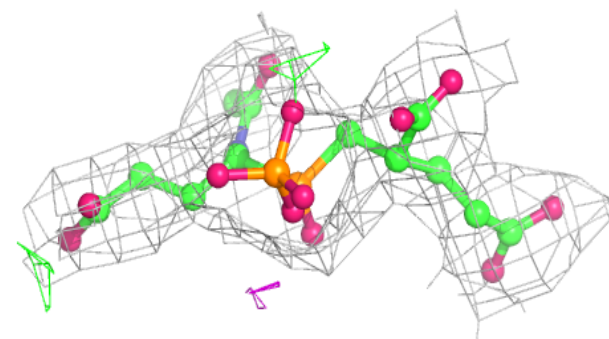
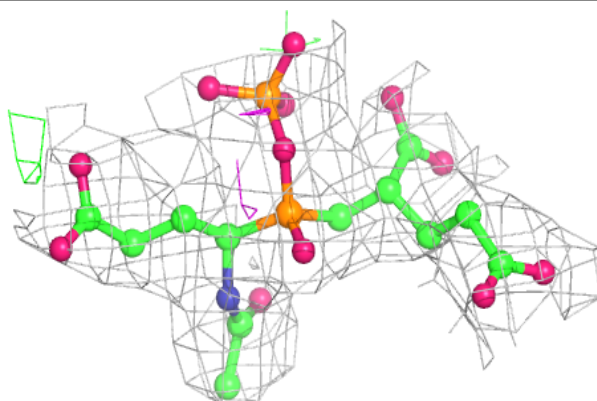


Electron density around ADP B 601:

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

**Electron density around RZP D 602:**

$2mF_o - DF_c$ (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.