



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:10 pm BST

PDB ID : 4A5Y  
Title : Intermediate state of human kinesin Eg5 in complex with Ispinesib  
Authors : Kaan, H.Y.K.; Kozielski, F.  
Deposited on : 2011-10-29  
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

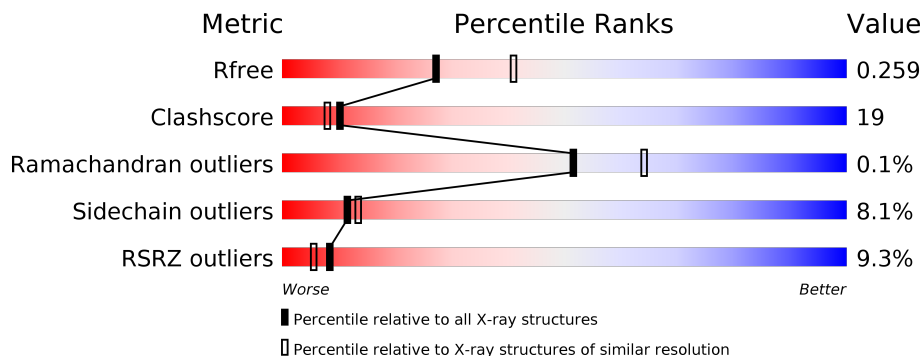
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	368	<p>9% 59% 28% • 9%</p>
1	B	368	<p>13% 45% 32% 5% 18%</p>
1	C	368	<p>3% 74% 17% • 8%</p>

## 2 Entry composition [i](#)

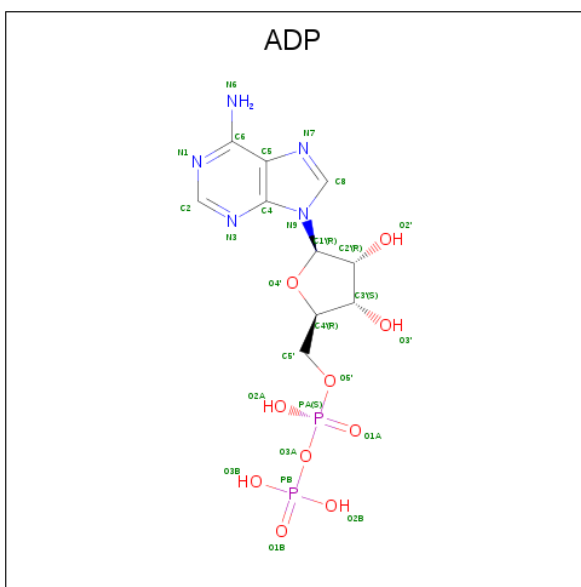
There are 7 unique types of molecules in this entry. The entry contains 8127 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	Total 2598	C 1631	N 448	O 509	S 10	0	4	0
1	B	302	Total 2364	C 1489	N 404	O 461	S 10	0	0	0
1	C	339	Total 2618	C 1643	N 458	O 507	S 10	0	1	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

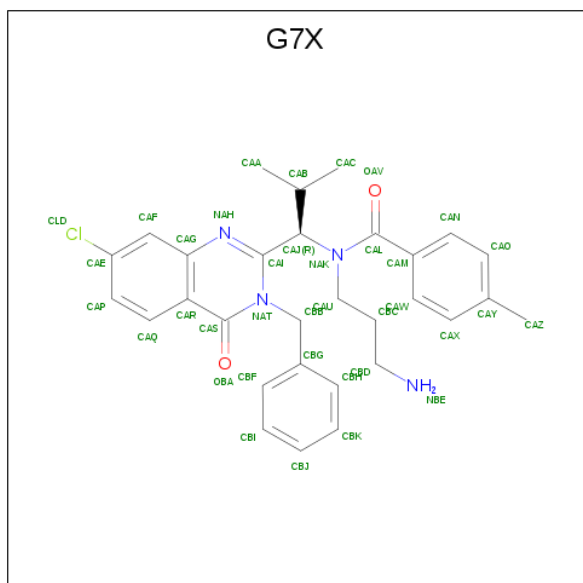


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

- Molecule 4 is ISPINESIB MESILATE (three-letter code: G7X) (formula: C<sub>30</sub>H<sub>33</sub>ClN<sub>4</sub>O<sub>2</sub>).

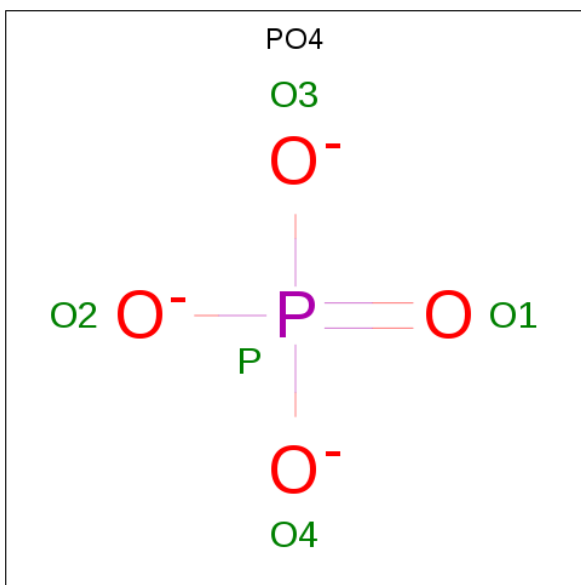


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl N O 37 30 1 4 2	0	0
4	B	1	Total C Cl N O 37 30 1 4 2	0	0
4	C	1	Total C Cl N O 37 30 1 4 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Mg 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

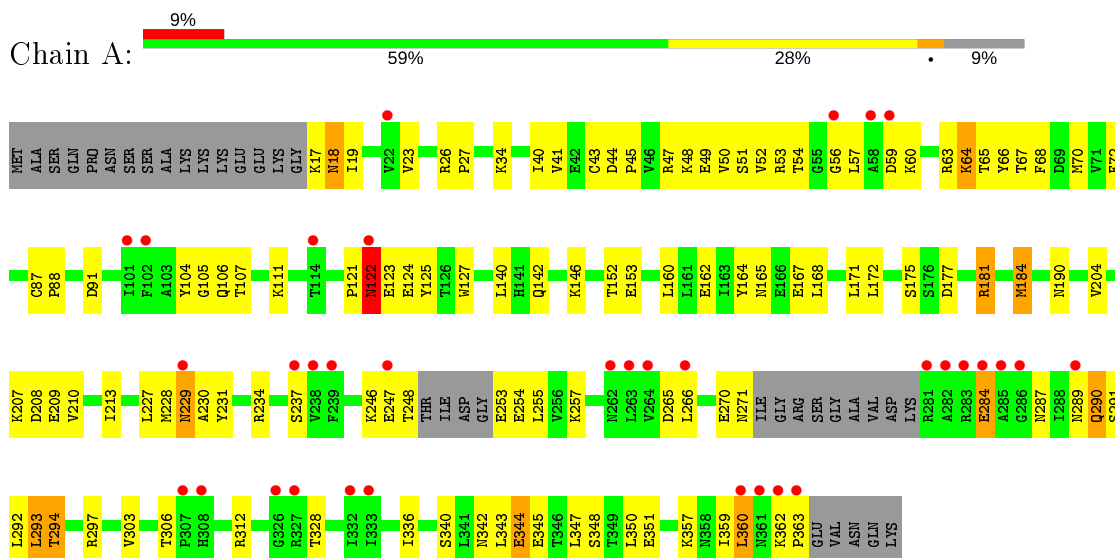
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	93	Total O 93 93	0	0
7	B	81	Total O 81 81	0	0
7	C	168	Total O 168 168	0	0

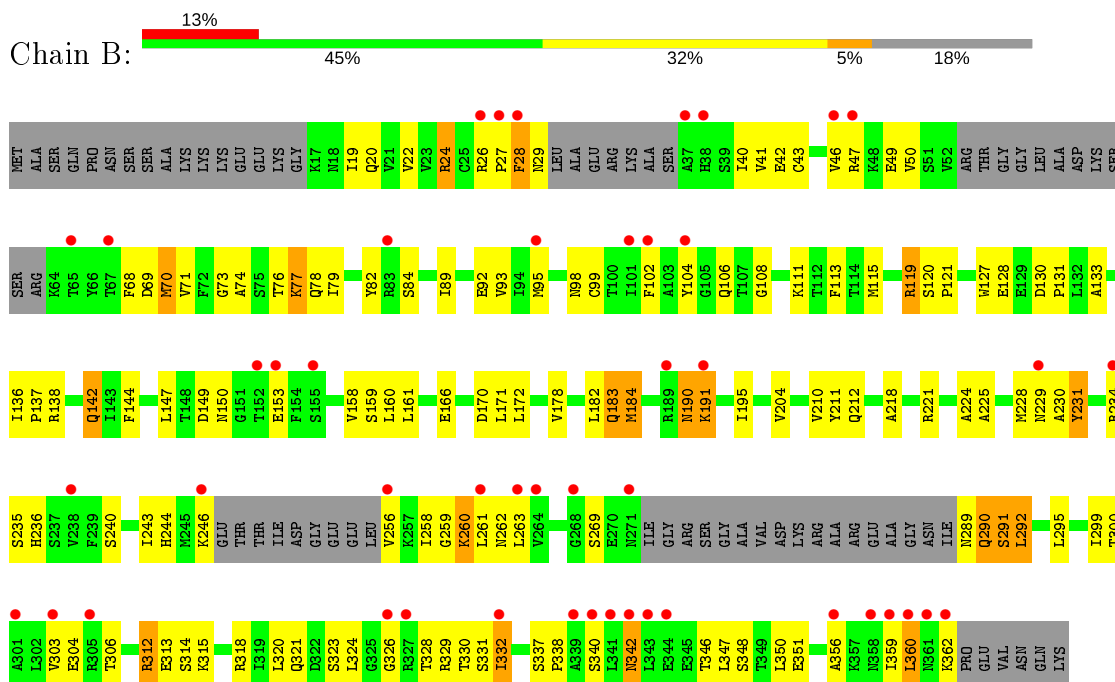
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

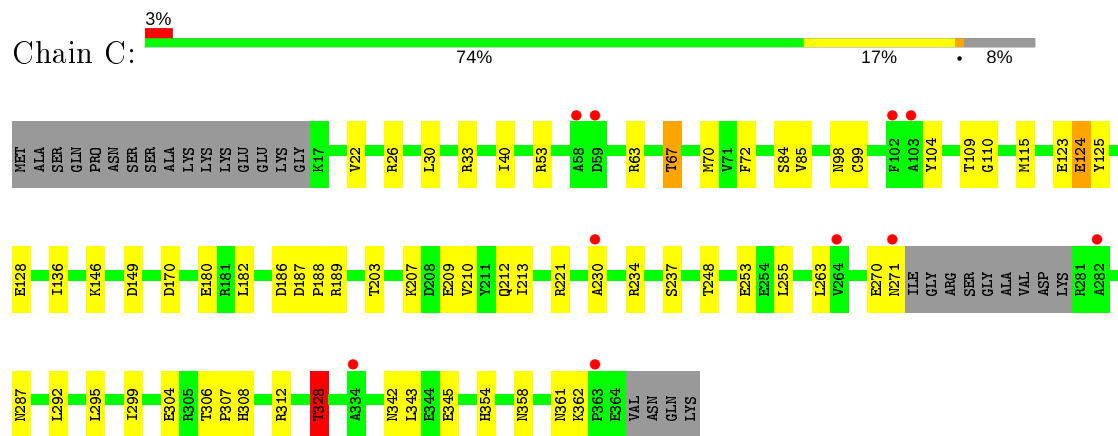
- Molecule 1: KINESIN-LIKE PROTEIN KIF11



- Molecule 1: KINESIN-LIKE PROTEIN KIF11



- Molecule 1: KINESIN-LIKE PROTEIN KIF11



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.63Å 91.93Å 163.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 2.45 29.60 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.60-2.45) 99.6 (29.60-2.45)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.74 (at 2.45Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.201 , 0.268 0.195 , 0.259	Depositor DCC
$R_{free}$ test set	2429 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtrriage
Anisotropy	0.112	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 59.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8127	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.27 % 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 2.7156e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: G7X, MG, PO4, ADP, CL

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	0.67	0/2648	0.81	0/3586
1	B	0.58	0/2399	0.71	1/3245 (0.0%)
1	C	0.78	0/2661	0.81	2/3603 (0.1%)
All	All	0.68	0/7708	0.78	3/10434 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	328	THR	CB-CA-C	-5.59	96.50	111.60
1	C	110	GLY	N-CA-C	5.50	126.84	113.10
1	B	326	GLY	N-CA-C	-5.03	100.52	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	PRO	Peptide
1	A	122	ASN	Peptide

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2598	0	2588	102	0
1	B	2364	0	2363	125	0
1	C	2618	0	2612	59	0
2	A	27	0	12	2	0
2	B	27	0	12	2	0
2	C	27	0	12	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	37	0	33	2	0
4	B	37	0	33	8	0
4	C	37	0	33	3	0
5	C	1	0	0	0	0
6	C	10	0	0	0	0
7	A	93	0	0	5	0
7	B	81	0	0	9	0
7	C	168	0	0	8	0
All	All	8127	0	7698	291	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 19.

All (291) 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:244:HIS:HD2	1:B:258:ILE:HG12	1.21	1.04
1:B:153:GLU:HG3	1:B:246:LYS:HB3	1.39	1.01
1:A:227:LEU:HG	1:A:228:MET:HG3	1.48	0.96
1:A:344:GLU:H	1:A:344:GLU:CD	1.68	0.93
1:B:304:GLU:HG3	1:B:306:THR:HG23	1.48	0.92
1:A:142:GLN:HE21	1:A:146:LYS:HD2	1.35	0.91
1:C:115:MET:HE1	1:C:263:LEU:HB3	1.54	0.90
1:B:106:GLN:HE21	1:B:342:ASN:ND2	1.69	0.89
1:B:244:HIS:CD2	1:B:258:ILE:HG12	2.07	0.89
1:A:57:LEU:HA	1:A:60:LYS:HB2	1.58	0.85
1:A:107:THR:OG1	1:A:270:GLU:OE2	1.96	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:TYR:HE2	1:B:142:GLN:HE21	1.23	0.82
1:A:294:THR:HA	1:A:297:ARG:HG3	1.62	0.81
1:A:190:ASN:HB2	7:A:2066:HOH:O	1.79	0.81
1:C:115:MET:CE	1:C:263:LEU:HB3	2.09	0.80
1:C:98:ASN:O	1:C:328:THR:CG2	2.29	0.80
1:B:289:ASN:OD1	1:B:290:GLN:N	2.13	0.80
1:C:287:ASN:ND2	7:C:2144:HOH:O	2.15	0.79
1:A:167:GLU:OE2	1:A:181:ARG:HD3	1.83	0.79
1:A:122:ASN:HB3	1:A:124:GLU:H	1.47	0.78
1:B:342:ASN:OD1	1:B:346:THR:OG1	1.99	0.77
1:A:270:GLU:O	1:A:271:ASN:ND2	2.18	0.77
1:A:142:GLN:HE21	1:A:146:LYS:CD	1.97	0.77
1:B:166:GLU:O	1:B:315:LYS:NZ	2.17	0.77
1:B:106:GLN:NE2	1:B:342:ASN:ND2	2.32	0.77
4:C:1369:G7X:OAV	4:C:1369:G7X:HBD2	1.86	0.76
1:A:248:THR:HA	1:A:253:GLU:O	1.85	0.74
1:B:291:SER:OG	7:B:2039:HOH:O	2.05	0.74
1:A:340:SER:HA	1:A:343:LEU:CD1	2.17	0.74
1:B:289:ASN:CG	1:B:290:GLN:H	1.91	0.73
1:B:76:THR:O	7:B:2004:HOH:O	2.05	0.73
1:A:140:LEU:HD13	1:A:210:VAL:HG11	1.71	0.73
1:B:40:ILE:CD1	1:B:340:SER:HA	2.20	0.72
1:B:28:PHE:O	1:B:29:ASN:HB2	1.89	0.71
1:B:150:ASN:OD1	1:C:308[B]:HIS:CD2	2.44	0.70
1:C:307:PRO:HG2	1:C:308[A]:HIS:CD2	2.27	0.69
1:A:152:THR:HG21	1:A:246:LYS:O	1.92	0.69
1:A:227:LEU:HG	1:A:228:MET:N	2.06	0.69
1:B:359:ILE:O	7:B:2002:HOH:O	2.10	0.69
1:C:221:ARG:HD2	7:C:2119:HOH:O	1.94	0.68
1:B:92:GLU:HG2	1:B:329:ARG:HD2	1.74	0.68
1:A:19:ILE:HD12	1:A:303:VAL:HG23	1.76	0.68
1:A:359:ILE:HG12	1:A:360:LEU:H	1.58	0.68
1:B:360:LEU:HD12	1:B:360:LEU:H	1.57	0.68
1:A:122:ASN:HB3	1:A:124:GLU:N	2.08	0.68
1:A:56:GLY:O	1:A:57:LEU:HB2	1.94	0.67
1:C:67:THR:HG21	1:C:361:ASN:HA	1.77	0.67
1:A:152:THR:CG2	1:A:153:GLU:H	2.07	0.67
1:B:28:PHE:H	1:B:28:PHE:HD1	1.42	0.66
1:C:123:GLU:O	1:C:124:GLU:HG2	1.93	0.66
1:B:98:ASN:ND2	1:B:260:LYS:HG2	2.10	0.66
1:A:43:CYS:O	1:A:45:PRO:HD3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:SER:O	1:B:318:ARG:HG3	1.96	0.66
1:A:340:SER:O	1:A:343:LEU:HD13	1.97	0.65
1:C:307:PRO:HG2	1:C:308[A]:HIS:HD2	1.62	0.65
1:A:53:ARG:O	7:A:2014:HOH:O	2.15	0.65
1:A:140:LEU:HD13	1:A:210:VAL:CG1	2.27	0.65
1:B:24:ARG:NH2	2:B:601:ADP:N6	2.45	0.64
1:B:41:VAL:HG12	1:B:42:GLU:H	1.63	0.64
1:A:142:GLN:NE2	1:A:146:LYS:HD2	2.11	0.63
7:A:2043:HOH:O	1:C:180:GLU:OE2	2.16	0.63
1:C:98:ASN:O	1:C:328:THR:HG23	1.98	0.63
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.80	0.63
1:B:115:MET:CE	1:B:263:LEU:HB3	2.30	0.62
1:C:98:ASN:O	1:C:328:THR:HG22	1.99	0.62
1:A:344:GLU:N	1:A:344:GLU:CD	2.49	0.62
1:C:123:GLU:O	1:C:124:GLU:CG	2.47	0.62
1:C:187:ASP:OD1	1:C:189:ARG:HD3	2.00	0.62
1:A:152:THR:CG2	1:A:153:GLU:N	2.62	0.62
1:B:41:VAL:HG12	1:B:42:GLU:N	2.14	0.62
1:A:51:SER:HA	1:A:64:LYS:O	1.99	0.61
1:C:128:GLU:OE2	1:C:207:LYS:HE2	2.01	0.61
1:A:40:ILE:CD1	1:A:343:LEU:HG	2.30	0.61
1:A:290:GLN:O	1:A:294:THR:HG23	2.01	0.61
1:B:178:VAL:CG2	1:B:224:ALA:HB2	2.30	0.61
1:A:17:LYS:HD2	1:A:17:LYS:N	2.14	0.61
1:A:231:TYR:O	1:A:234:ARG:N	2.32	0.61
1:B:218:ALA:HB2	4:B:1363:G7X:HAF	1.82	0.61
1:C:67:THR:CG2	1:C:361:ASN:HA	2.31	0.60
1:B:40:ILE:HD12	1:B:340:SER:HA	1.83	0.60
1:A:227:LEU:CG	1:A:228:MET:HG3	2.28	0.60
1:A:340:SER:HA	1:A:343:LEU:HD12	1.83	0.60
1:A:175:SER:HB2	1:C:203:THR:HB	1.82	0.60
1:C:124:GLU:HG2	1:C:125:TYR:H	1.66	0.60
1:B:136:ILE:N	1:B:137:PRO:HD2	2.15	0.60
1:B:28:PHE:N	1:B:28:PHE:CD1	2.70	0.60
1:C:312:ARG:NH2	7:C:2154:HOH:O	2.34	0.60
1:C:124:GLU:CG	1:C:125:TYR:H	2.15	0.59
1:C:186:ASP:O	1:C:188:PRO:HD3	2.02	0.59
1:A:344:GLU:HG2	1:A:345:GLU:OE1	2.02	0.59
1:C:328:THR:HG21	7:C:2045:HOH:O	2.01	0.59
1:B:150:ASN:OD1	1:C:308[B]:HIS:CG	2.56	0.59
1:B:289:ASN:CG	1:B:290:GLN:N	2.54	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLN:HG3	1:A:146:LYS:HD2	1.85	0.58
1:C:230:ALA:HB3	1:C:234:ARG:HD3	1.84	0.58
1:A:340:SER:O	1:A:343:LEU:CD1	2.50	0.58
1:B:130:ASP:OD1	1:B:131:PRO:HD2	2.04	0.58
1:A:152:THR:HG22	1:A:153:GLU:N	2.19	0.58
1:B:191:LYS:HD2	1:B:191:LYS:N	2.19	0.57
1:B:40:ILE:O	1:B:40:ILE:HG22	2.04	0.57
1:A:53:ARG:HH11	1:A:63:ARG:HG3	1.70	0.57
1:B:98:ASN:O	1:B:328:THR:OG1	2.20	0.57
1:C:271:ASN:HB2	7:C:2140:HOH:O	2.05	0.57
1:A:287:ASN:O	1:A:290:GLN:HB3	2.04	0.57
1:C:123:GLU:O	1:C:124:GLU:OE1	2.22	0.57
1:B:98:ASN:HD21	1:B:260:LYS:HG2	1.70	0.56
1:A:164:TYR:HE2	1:A:228:MET:HB3	1.70	0.56
1:B:40:ILE:HD11	1:B:340:SER:HA	1.87	0.56
1:B:133:ALA:O	1:B:138:ARG:NE	2.39	0.56
1:B:41:VAL:CG2	1:B:338:PRO:HA	2.36	0.56
1:A:127:TRP:HB2	4:A:1365:G7X:HAZ3	1.88	0.56
1:B:337:SER:HB3	1:B:342:ASN:ND2	2.21	0.55
1:A:254:GLU:O	1:A:255:LEU:HD22	2.06	0.55
1:B:225:ALA:HA	1:B:231:TYR:CD1	2.42	0.55
1:B:115:MET:HE1	1:B:263:LEU:HB3	1.89	0.55
1:A:152:THR:HG23	1:A:153:GLU:H	1.72	0.55
1:A:177:ASP:HA	7:A:2057:HOH:O	2.07	0.55
1:B:229:ASN:O	1:B:230:ALA:C	2.43	0.55
1:A:142:GLN:NE2	1:A:146:LYS:HG3	2.22	0.55
1:A:181:ARG:HH21	1:A:228:MET:HE1	1.72	0.54
1:B:70:MET:HE3	1:B:84:SER:HB2	1.90	0.54
1:C:295:LEU:O	1:C:299:ILE:HG12	2.07	0.54
1:B:147:LEU:HD11	1:B:243:ILE:HG21	1.89	0.54
1:B:231:TYR:C	1:B:231:TYR:CD1	2.80	0.54
1:B:43:CYS:HB3	1:B:71:VAL:CG1	2.38	0.54
1:B:20:GLN:OE1	1:B:69:ASP:HB3	2.07	0.54
1:A:290:GLN:O	1:A:294:THR:CG2	2.56	0.54
1:B:229:ASN:OD1	1:B:234:ARG:NE	2.40	0.54
1:B:70:MET:CE	1:B:84:SER:HB2	2.37	0.54
1:B:159:SER:HA	1:B:172:LEU:HD12	1.89	0.53
1:A:165[B]:ASN:OD1	1:A:284:GLU:HB3	2.09	0.53
4:B:1363:G7X:CAL	4:B:1363:G7X:HBD1	2.38	0.53
1:B:43:CYS:HB3	1:B:71:VAL:HG12	1.91	0.53
1:A:26:ARG:HB2	1:A:27:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:O	1:A:359:ILE:CG2	2.57	0.52
1:A:40:ILE:HD13	1:A:343:LEU:HG	1.89	0.52
1:A:53:ARG:NH1	1:A:63:ARG:HG3	2.25	0.52
1:A:87:CYS:HB2	1:A:88:PRO:HD3	1.90	0.52
1:A:23:VAL:HG21	1:A:68:PHE:CE2	2.44	0.52
1:B:144:PHE:HZ	1:B:204:VAL:HG22	1.75	0.52
1:B:98:ASN:OD1	1:B:323:SER:HB2	2.09	0.52
1:B:89:ILE:HD11	1:B:331:SER:OG	2.10	0.52
1:C:354:HIS:NE2	1:C:358:ASN:OD1	2.43	0.52
1:A:44:ASP:OD2	1:A:47:ARG:HD3	2.10	0.52
1:B:171:LEU:HD13	1:B:221:ARG:HB2	1.91	0.52
1:A:67:THR:O	1:A:359:ILE:HG21	2.10	0.52
1:B:204:VAL:HG21	1:B:210:VAL:HG23	1.92	0.52
1:C:67:THR:HG21	7:C:2019:HOH:O	2.09	0.52
1:A:26:ARG:HD3	2:A:601:ADP:C8	2.45	0.51
1:A:342:ASN:ND2	7:A:2010:HOH:O	2.11	0.51
1:B:41:VAL:HG23	1:B:338:PRO:HA	1.92	0.51
1:C:40:ILE:HD12	1:C:343:LEU:HD13	1.93	0.51
1:B:178:VAL:HG21	1:B:224:ALA:HB2	1.93	0.51
1:B:28:PHE:O	1:B:29:ASN:CB	2.57	0.51
1:A:359:ILE:HG12	1:A:360:LEU:N	2.26	0.51
1:B:144:PHE:HZ	1:B:204:VAL:CG2	2.24	0.51
1:B:26:ARG:NH1	1:B:27:PRO:O	2.43	0.51
1:B:77:LYS:HA	7:B:2005:HOH:O	2.10	0.51
1:B:73:GLY:HA3	7:B:2003:HOH:O	2.10	0.50
1:C:345:GLU:HG2	7:C:2163:HOH:O	2.10	0.50
1:A:340:SER:HA	1:A:343:LEU:HD11	1.92	0.50
1:B:131:PRO:HA	7:B:2026:HOH:O	2.10	0.50
1:A:160:LEU:HB3	1:A:172:LEU:HG	1.94	0.50
1:B:102:PHE:HB2	1:B:332:ILE:HB	1.94	0.50
1:B:93:VAL:O	1:B:259:GLY:HA3	2.12	0.50
1:C:115:MET:HE2	1:C:263:LEU:HB3	1.92	0.49
1:A:64:LYS:HD3	1:A:65:THR:H	1.77	0.49
1:C:99:CYS:HA	1:C:328:THR:HG22	1.94	0.49
1:A:209:GLU:O	1:A:213:ILE:HD12	2.13	0.49
1:B:22:VAL:CG1	1:B:70:MET:HB2	2.43	0.49
4:C:1369:G7X:CAL	4:C:1369:G7X:HBD2	2.42	0.49
1:C:67:THR:CG2	1:C:361:ASN:OD1	2.61	0.49
1:A:91:ASP:OD1	1:A:146:LYS:NZ	2.42	0.48
1:B:191:LYS:HZ3	1:B:191:LYS:HA	1.77	0.48
1:B:191:LYS:HA	1:B:191:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:GLU:OE2	1:C:255:LEU:HD11	2.13	0.48
1:B:347:LEU:O	1:B:351:GLU:HG2	2.13	0.48
1:B:47:ARG:O	1:B:49:GLU:HG3	2.13	0.48
1:C:170:ASP:HB2	1:C:182:LEU:HD11	1.96	0.48
1:A:237:SER:HB3	1:A:265:ASP:HB3	1.96	0.48
1:B:256:VAL:O	1:B:256:VAL:HG12	2.13	0.48
1:B:144:PHE:CZ	1:B:204:VAL:CG2	2.96	0.48
1:B:312:ARG:HG2	7:B:2071:HOH:O	2.13	0.47
1:B:160:LEU:HD21	4:B:1363:G7X:CLD	2.51	0.47
1:A:66:TYR:OH	1:A:351:GLU:OE2	2.28	0.47
1:A:303:VAL:HG21	1:A:357:LYS:HB2	1.94	0.47
1:A:18:ASN:HB2	1:A:328:THR:O	2.15	0.47
1:A:70:MET:HE3	1:A:72:PHE:HZ	1.78	0.47
1:B:128:GLU:OE2	7:B:2024:HOH:O	2.20	0.47
4:B:1363:G7X:NAH	4:B:1363:G7X:HBC1	2.28	0.47
1:B:342:ASN:OD1	1:B:342:ASN:C	2.53	0.47
1:C:306:THR:HG23	1:C:307:PRO:HD2	1.96	0.47
1:A:247:GLU:OE1	1:A:257:LYS:HG2	2.14	0.47
1:B:104:TYR:OH	1:B:269:SER:HB2	2.15	0.47
1:A:41:VAL:HG22	1:A:52:VAL:HG12	1.97	0.46
1:B:68:PHE:CZ	1:B:350:LEU:CD2	2.99	0.46
1:A:289:ASN:O	1:A:293:LEU:HB2	2.15	0.46
1:A:44:ASP:N	1:A:49:GLU:O	2.36	0.46
1:B:183:GLN:HA	1:B:183:GLN:OE1	2.14	0.46
1:B:228:MET:O	1:B:231:TYR:HB3	2.16	0.46
1:A:254:GLU:N	1:A:254:GLU:OE1	2.49	0.46
1:B:225:ALA:HB2	1:B:231:TYR:CE1	2.50	0.46
1:B:41:VAL:O	1:B:42:GLU:HB2	2.15	0.46
1:C:70:MET:CE	1:C:85:VAL:HG22	2.46	0.46
1:A:168:LEU:HD11	1:A:184:MET:HE2	1.97	0.46
1:C:115:MET:O	1:C:136:ILE:HG13	2.16	0.46
1:B:184:MET:HA	1:B:195:ILE:O	2.16	0.45
1:B:106:GLN:NE2	1:B:342:ASN:HD22	2.10	0.45
1:A:162:GLU:CG	1:A:171:LEU:HD11	2.46	0.45
1:A:204:VAL:CG1	1:A:213:ILE:CD1	2.95	0.45
1:A:164:TYR:CE2	1:A:228:MET:HB3	2.51	0.45
1:C:209:GLU:O	1:C:213:ILE:HD13	2.17	0.45
1:A:19:ILE:O	1:A:357:LYS:NZ	2.43	0.45
1:A:70:MET:HE3	1:A:72:PHE:CZ	2.51	0.45
1:C:124:GLU:HG3	1:C:125:TYR:CD2	2.52	0.45
1:A:104:TYR:HB2	1:A:266:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1369:G7X:OAV	4:C:1369:G7X:CBD	2.59	0.45
1:C:312:ARG:NH1	7:C:2105:HOH:O	2.45	0.45
1:B:119:ARG:NH2	1:B:211:TYR:OH	2.50	0.45
1:C:362:LYS:HE2	1:C:362:LYS:HB2	1.75	0.45
1:C:70:MET:HB2	1:C:70:MET:HE3	1.65	0.45
2:A:601:ADP:O2A	2:A:601:ADP:H3'	2.16	0.45
1:B:360:LEU:HD12	1:B:360:LEU:N	2.29	0.45
1:A:229:ASN:O	1:A:230:ALA:HB3	2.17	0.44
1:B:300:THR:O	1:B:304:GLU:HG2	2.17	0.44
1:C:270:GLU:O	1:C:271:ASN:HB2	2.16	0.44
1:B:299:ILE:HG21	1:B:356:ALA:HB1	1.99	0.44
1:B:149:ASP:HB3	1:C:308[B]:HIS:CD2	2.53	0.44
1:B:26:ARG:O	1:B:338:PRO:CG	2.65	0.44
1:B:190:ASN:C	1:B:191:LYS:HD2	2.38	0.44
1:A:344:GLU:N	1:A:344:GLU:OE1	2.50	0.44
1:B:24:ARG:NH2	2:B:601:ADP:HN61	2.13	0.44
1:C:67:THR:HG23	1:C:361:ASN:OD1	2.18	0.44
1:A:50:VAL:HG13	1:A:66:TYR:HB2	2.00	0.44
1:A:142:GLN:NE2	1:A:146:LYS:CG	2.82	0.43
1:B:224:ALA:HB3	1:B:231:TYR:OH	2.18	0.43
1:A:270:GLU:O	1:A:271:ASN:CB	2.66	0.43
1:B:19:ILE:HA	1:B:330:THR:O	2.17	0.43
1:B:295:LEU:O	1:B:299:ILE:HG12	2.18	0.43
1:A:105:GLY:O	1:A:111:LYS:NZ	2.34	0.43
1:C:70:MET:HE2	1:C:85:VAL:HG22	2.01	0.43
1:B:27:PRO:HG3	1:B:74:ALA:O	2.19	0.43
1:B:160:LEU:CD2	4:B:1363:G7X:CLD	3.03	0.43
1:B:243:ILE:O	1:B:258:ILE:HA	2.19	0.43
1:B:236:HIS:HE1	1:B:292:LEU:HD13	1.83	0.43
4:B:1363:G7X:HBD1	4:B:1363:G7X:OAV	2.19	0.43
1:B:78:GLN:HB2	1:B:138:ARG:HH21	1.84	0.42
1:B:24:ARG:HD2	1:B:76:THR:HG21	2.01	0.42
1:B:120:SER:HA	1:B:121:PRO:HD3	1.90	0.42
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.85	0.42
1:C:124:GLU:HG2	1:C:125:TYR:N	2.33	0.42
1:B:41:VAL:HG21	1:B:338:PRO:HA	2.01	0.42
1:B:92:GLU:HG2	1:B:329:ARG:CD	2.44	0.42
1:B:299:ILE:O	1:B:303:VAL:HG23	2.20	0.42
1:C:53:ARG:HH11	1:C:63:ARG:CG	2.32	0.42
1:B:144:PHE:CZ	1:B:204:VAL:HG22	2.55	0.42
1:B:127:TRP:HB2	4:B:1363:G7X:HAZ3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:HA	1:B:240:SER:O	2.20	0.42
1:C:26:ARG:HE	1:C:109:THR:HA	1.84	0.42
1:C:40:ILE:CD1	1:C:343:LEU:HD13	2.49	0.42
1:B:24:ARG:HH22	1:B:113:PHE:HE2	1.66	0.41
1:C:306:THR:CG2	1:C:307:PRO:HD2	2.49	0.41
1:A:106:GLN:NE2	1:A:345:GLU:HG2	2.35	0.41
1:A:44:ASP:O	1:A:48:LYS:N	2.53	0.41
1:B:136:ILE:N	1:B:137:PRO:CD	2.82	0.41
1:B:244:HIS:HD2	1:B:258:ILE:CG1	2.11	0.41
1:B:99:CYS:O	1:B:261:LEU:HA	2.19	0.41
4:A:1365:G7X:HBB2	4:A:1365:G7X:CAW	2.51	0.41
1:A:142:GLN:HE21	1:A:146:LYS:CG	2.33	0.41
1:A:293:LEU:HA	1:A:293:LEU:HD12	1.81	0.41
1:A:362:LYS:CB	1:A:363:PRO:HD2	2.49	0.41
1:B:320:LEU:O	1:B:321:GLN:C	2.59	0.41
1:C:70:MET:HE1	1:C:72:PHE:HZ	1.85	0.41
4:B:1363:G7X:HBB2	4:B:1363:G7X:CAW	2.50	0.41
1:A:59:ASP:O	1:A:60:LYS:HB3	2.21	0.41
1:A:64:LYS:HA	1:A:64:LYS:HD3	1.64	0.41
1:C:124:GLU:CG	1:C:125:TYR:N	2.82	0.41
1:A:40:ILE:HD13	1:A:343:LEU:CG	2.49	0.41
1:A:50:VAL:CG1	1:A:68:PHE:HE2	2.34	0.41
1:B:184:MET:HB2	1:B:184:MET:HE2	1.90	0.41
1:B:342:ASN:O	1:B:342:ASN:OD1	2.40	0.41
1:A:336:ILE:HD13	1:A:350:LEU:HD21	2.03	0.40
1:A:162:GLU:OE2	1:A:171:LEU:HD11	2.21	0.40
1:B:191:LYS:HD3	7:B:2052:HOH:O	2.21	0.40
1:B:50:VAL:HG22	1:B:71:VAL:HG11	2.03	0.40
1:A:362:LYS:O	1:A:363:PRO:C	2.59	0.40
1:C:104:TYR:CD1	1:C:104:TYR:C	2.94	0.40
1:C:342:ASN:O	1:C:343:LEU:C	2.60	0.40
1:B:26:ARG:NE	1:B:108:GLY:O	2.54	0.40
1:B:22:VAL:HG12	1:B:70:MET:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/368 (90%)	319 (96%)	12 (4%)	1 (0%)	41	49
1	B	292/368 (79%)	280 (96%)	12 (4%)	0	100	100
1	C	336/368 (91%)	332 (99%)	4 (1%)	0	100	100
All	All	960/1104 (87%)	931 (97%)	28 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	287/322 (89%)	264 (92%)	23 (8%)	12	14
1	B	266/322 (83%)	236 (89%)	30 (11%)	6	5
1	C	287/322 (89%)	272 (95%)	15 (5%)	23	30
All	All	840/966 (87%)	772 (92%)	68 (8%)	11	13

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	34	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	54	THR
1	A	64	LYS
1	A	122	ASN
1	A	125	TYR
1	A	181	ARG
1	A	184	MET
1	A	207	LYS
1	A	208	ASP
1	A	229	ASN
1	A	284	GLU
1	A	290	GLN
1	A	291	SER
1	A	292	LEU
1	A	293	LEU
1	A	294	THR
1	A	306	THR
1	A	312	ARG
1	A	344	GLU
1	A	347	LEU
1	A	348	SER
1	A	360	LEU
1	B	24	ARG
1	B	28	PHE
1	B	46	VAL
1	B	70	MET
1	B	77	LYS
1	B	79	ILE
1	B	95	MET
1	B	111	LYS
1	B	119	ARG
1	B	142	GLN
1	B	161	LEU
1	B	183	GLN
1	B	184	MET
1	B	190	ASN
1	B	191	LYS
1	B	212	GLN
1	B	231	TYR
1	B	235	SER
1	B	260	LYS
1	B	262	ASN
1	B	290	GLN

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Mol	Chain	Res	Type
1	B	291	SER
1	B	292	LEU
1	B	312	ARG
1	B	313	GLU
1	B	332	ILE
1	B	342	ASN
1	B	348	SER
1	B	360	LEU
1	B	362	LYS
1	C	22	VAL
1	C	30	LEU
1	C	33	ARG
1	C	67	THR
1	C	84	SER
1	C	124	GLU
1	C	146	LYS
1	C	149	ASP
1	C	210	VAL
1	C	212	GLN
1	C	237	SER
1	C	248	THR
1	C	292	LEU
1	C	304	GLU
1	C	328	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	142	GLN
1	B	98	ASN
1	B	106	GLN
1	B	244	HIS
1	B	262	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	G7X	A	1365	-	38,40,40	1.06	4 (10%)	45,56,56	1.55	5 (11%)
6	PO4	C	1367	-	4,4,4	0.90	0	6,6,6	0.61	0
2	ADP	B	601	-	24,29,29	1.04	2 (8%)	29,45,45	1.39	4 (13%)
4	G7X	B	1363	-	38,40,40	1.25	5 (13%)	45,56,56	1.19	3 (6%)
6	PO4	C	1366	-	4,4,4	0.75	0	6,6,6	1.35	1 (16%)
4	G7X	C	1369	-	38,40,40	1.28	4 (10%)	45,56,56	1.36	5 (11%)
2	ADP	A	601	-	24,29,29	1.24	4 (16%)	29,45,45	1.78	6 (20%)
2	ADP	C	601	5	24,29,29	0.94	0	29,45,45	1.36	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	G7X	A	1365	-	-	0/24/28/28	0/4/4/4
2	ADP	B	601	-	-	2/12/32/32	0/3/3/3
4	G7X	B	1363	-	-	2/24/28/28	0/4/4/4
4	G7X	C	1369	-	-	2/24/28/28	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	601	-	-	3/12/32/32	0/3/3/3
2	ADP	C	601	5	-	2/12/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1363	G7X	CAM-CAL	3.23	1.55	1.50
4	C	1369	G7X	CAF-CAE	3.10	1.42	1.36
4	B	1363	G7X	CAI-CAJ	3.05	1.55	1.50
2	A	601	ADP	C2'-C1'	-2.98	1.49	1.53
4	C	1369	G7X	CAI-CAJ	2.96	1.55	1.50
2	A	601	ADP	C2-N3	2.64	1.36	1.32
4	C	1369	G7X	CAM-CAL	2.62	1.54	1.50
2	B	601	ADP	C5-C4	2.61	1.47	1.40
4	B	1363	G7X	CAI-NAH	2.59	1.35	1.31
2	A	601	ADP	C5-C4	2.41	1.47	1.40
4	A	1365	G7X	CAF-CAG	-2.31	1.38	1.41
2	A	601	ADP	O4'-C1'	2.20	1.44	1.41
4	A	1365	G7X	CAS-NAT	2.16	1.41	1.38
4	A	1365	G7X	CAM-CAL	2.15	1.53	1.50
4	B	1363	G7X	CAI-NAT	2.10	1.41	1.36
4	C	1369	G7X	CAU-NAK	2.10	1.50	1.46
4	A	1365	G7X	CAS-CAR	-2.09	1.37	1.41
2	B	601	ADP	C2-N3	2.08	1.35	1.32
4	B	1363	G7X	CAG-NAH	-2.07	1.34	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1365	G7X	CAR-CAS-NAT	5.68	120.03	116.15
4	C	1369	G7X	CAR-CAG-NAH	-4.35	121.24	123.60
2	A	601	ADP	PA-O3A-PB	-4.34	117.92	132.83
4	B	1363	G7X	CAR-CAG-NAH	-4.02	121.42	123.60
2	A	601	ADP	O3B-PB-O2B	3.56	121.26	107.64
2	A	601	ADP	N3-C2-N1	-3.48	123.24	128.68
2	B	601	ADP	N3-C2-N1	-3.45	123.29	128.68
4	A	1365	G7X	CAQ-CAR-CAG	3.13	122.11	117.55
2	A	601	ADP	C3'-C2'-C1'	3.05	105.57	100.98
2	C	601	ADP	N3-C2-N1	-3.01	123.97	128.68
2	C	601	ADP	O3'-C3'-C2'	-2.97	102.20	111.82
2	B	601	ADP	C4-C5-N7	-2.84	106.44	109.40
2	C	601	ADP	O3'-C3'-C4'	-2.78	103.00	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ADP	O2'-C2'-C1'	-2.78	100.58	110.85
4	B	1363	G7X	CBF-CBG-CBH	2.76	122.50	118.17
4	A	1365	G7X	CAR-CAG-NAH	-2.67	122.15	123.60
4	C	1369	G7X	OAV-CAL-CAM	-2.51	115.35	120.23
2	B	601	ADP	PA-O3A-PB	-2.45	124.40	132.83
4	C	1369	G7X	CAC-CAB-CAJ	-2.44	107.45	110.72
2	C	601	ADP	C4-C5-N7	-2.36	106.94	109.40
4	B	1363	G7X	CBG-CBB-NAT	-2.32	109.03	112.63
4	C	1369	G7X	CBG-CBB-NAT	-2.25	109.14	112.63
4	A	1365	G7X	CAF-CAE-CLD	-2.24	116.84	119.64
6	C	1366	PO4	O2-P-O1	-2.21	102.81	110.89
2	A	601	ADP	C4-C5-N7	-2.19	107.12	109.40
2	B	601	ADP	C2-N1-C6	2.17	122.47	118.75
4	A	1365	G7X	CBB-NAT-CAS	2.05	120.26	117.79
4	C	1369	G7X	CAQ-CAR-CAG	2.01	120.47	117.55

There are no chirality outliers.

All (11) torsion outliers are listed below:

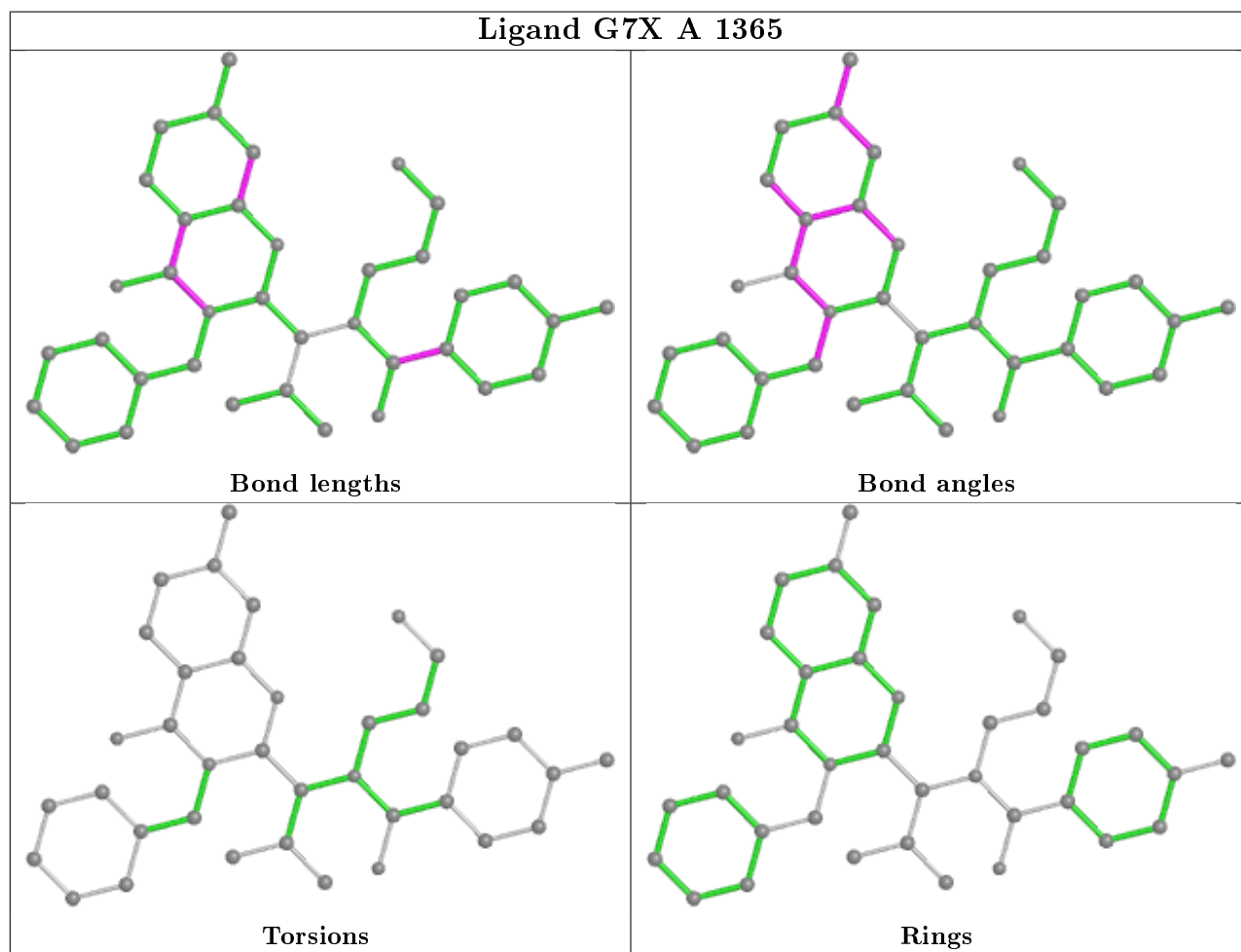
Mol	Chain	Res	Type	Atoms
2	A	601	ADP	C5'-O5'-PA-O3A
4	B	1363	G7X	NAK-CAU-CBC-CBD
4	B	1363	G7X	CAU-CBC-CBD-NBE
2	A	601	ADP	C4'-C5'-O5'-PA
2	A	601	ADP	C5'-O5'-PA-O2A
2	C	601	ADP	C4'-C5'-O5'-PA
4	C	1369	G7X	NAT-CBB-CBG-CBF
2	B	601	ADP	C5'-O5'-PA-O3A
4	C	1369	G7X	NAT-CBB-CBG-CBH
2	C	601	ADP	PB-O3A-PA-O1A
2	B	601	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

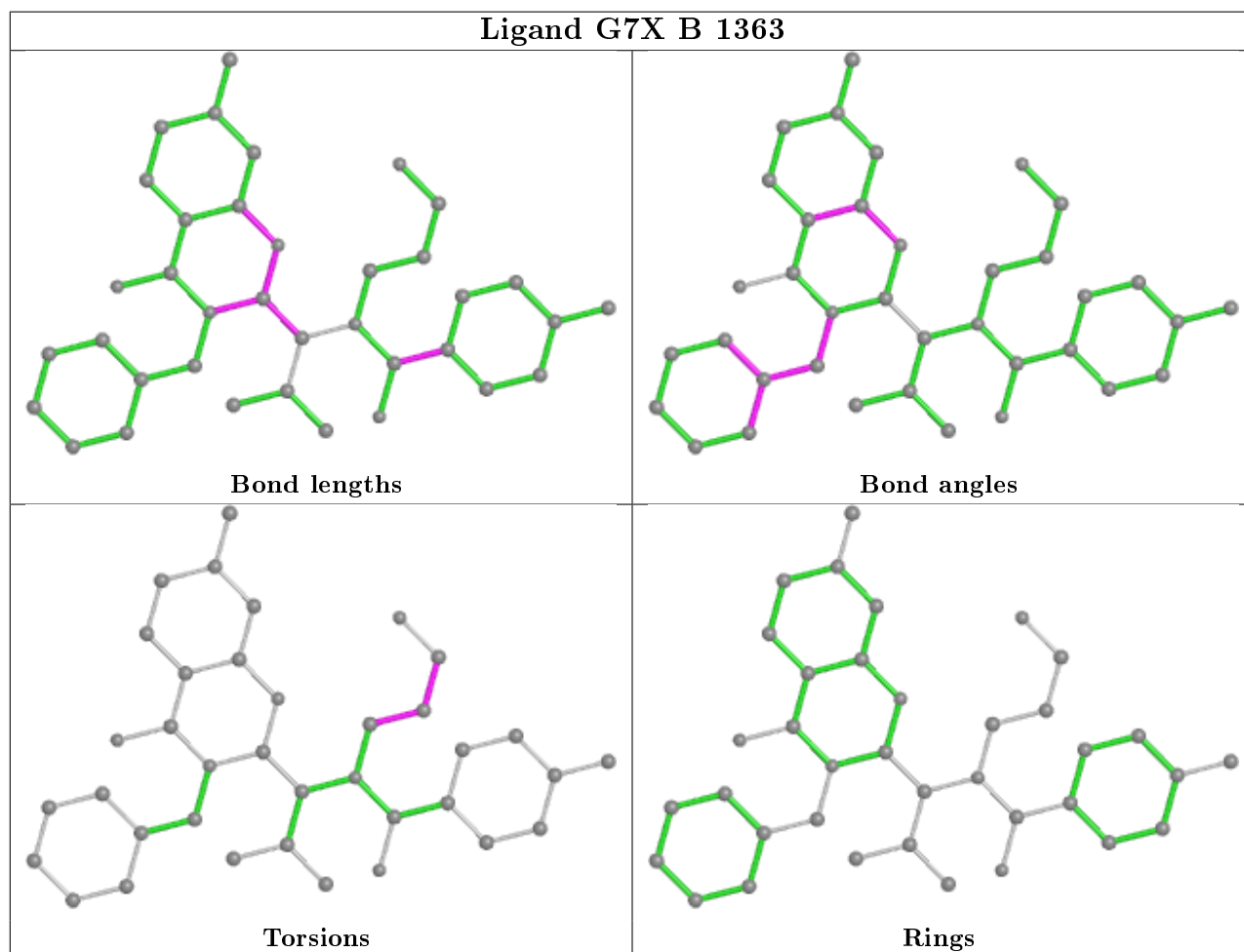
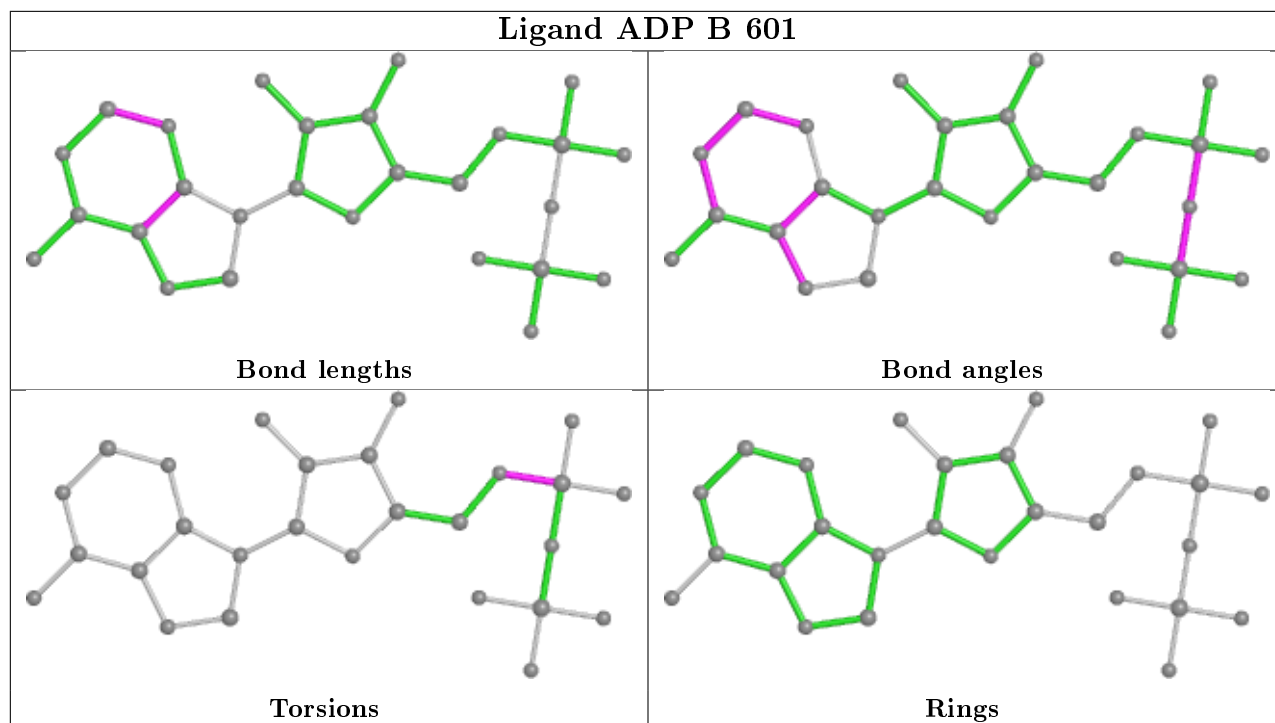
5 monomers are involved in 17 short contacts:

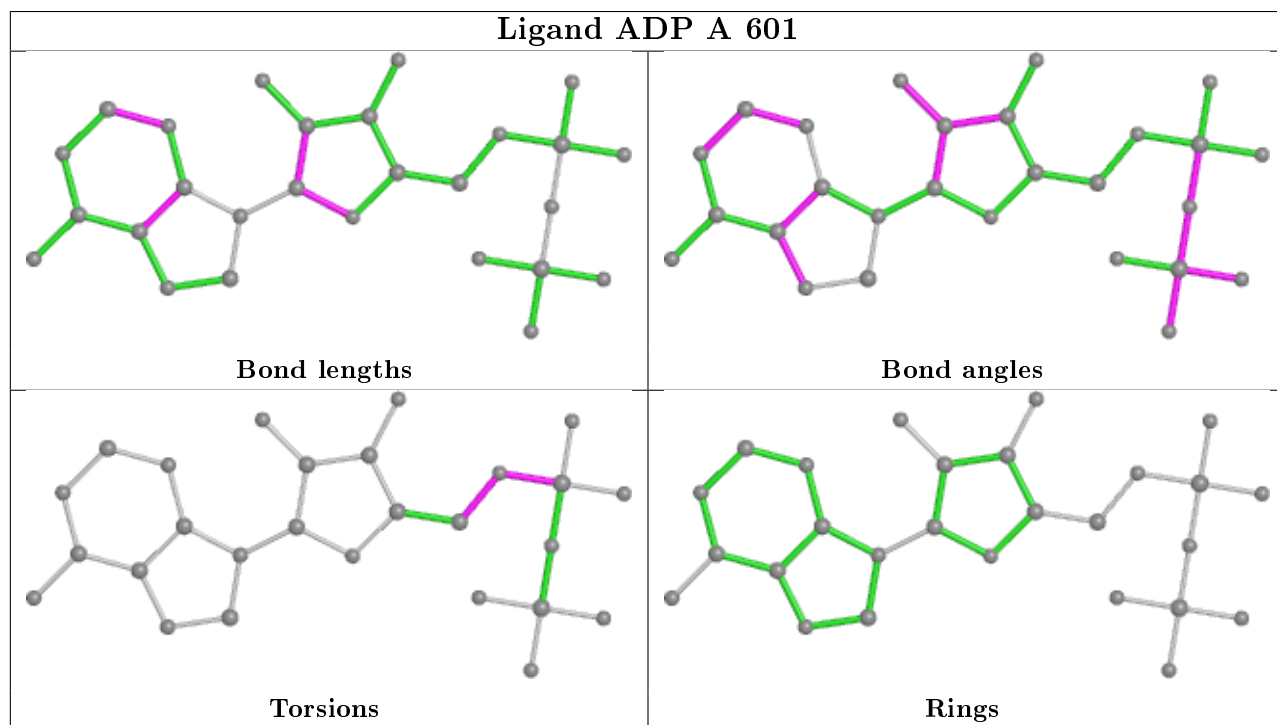
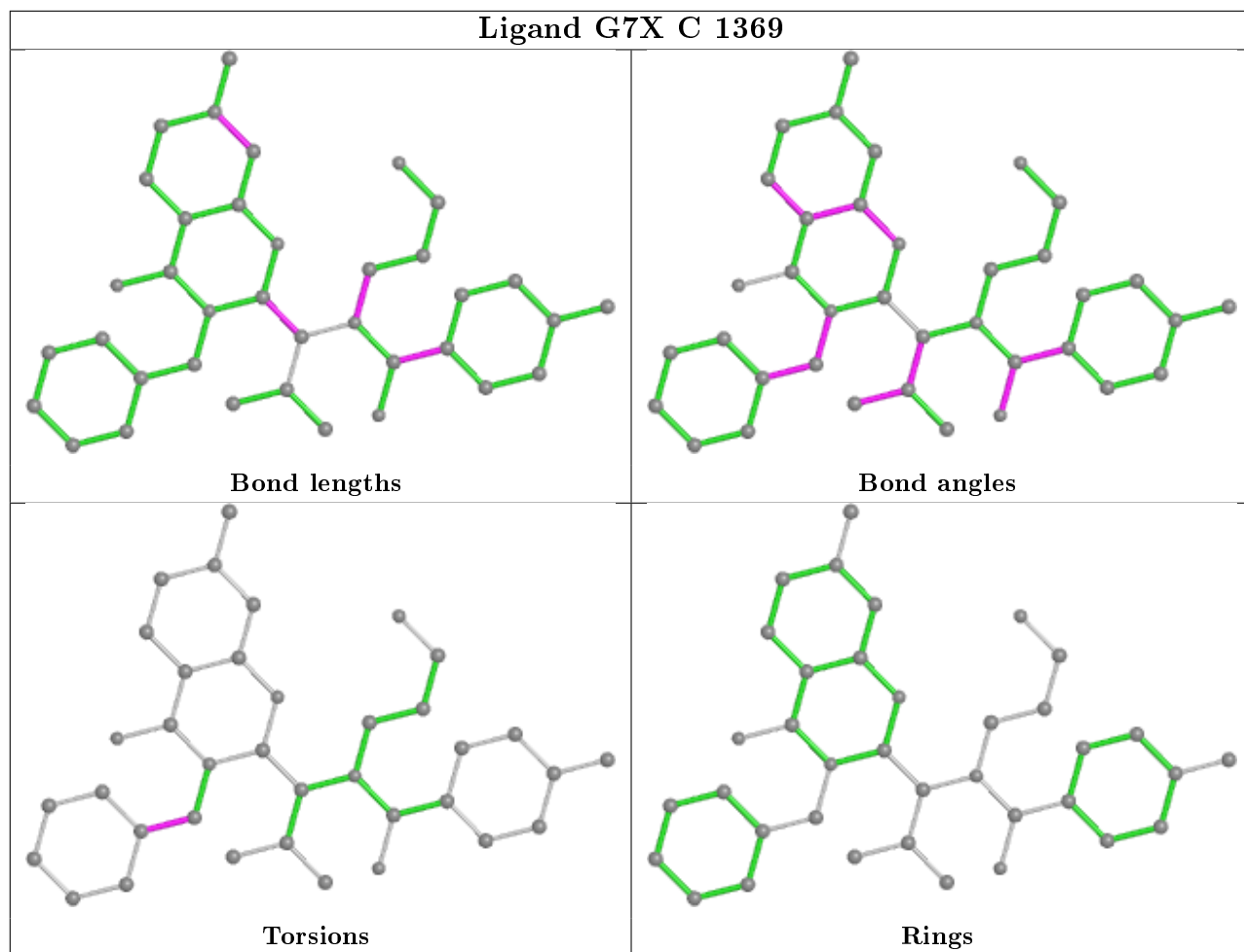
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1365	G7X	2	0
2	B	601	ADP	2	0
4	B	1363	G7X	8	0
4	C	1369	G7X	3	0
2	A	601	ADP	2	0

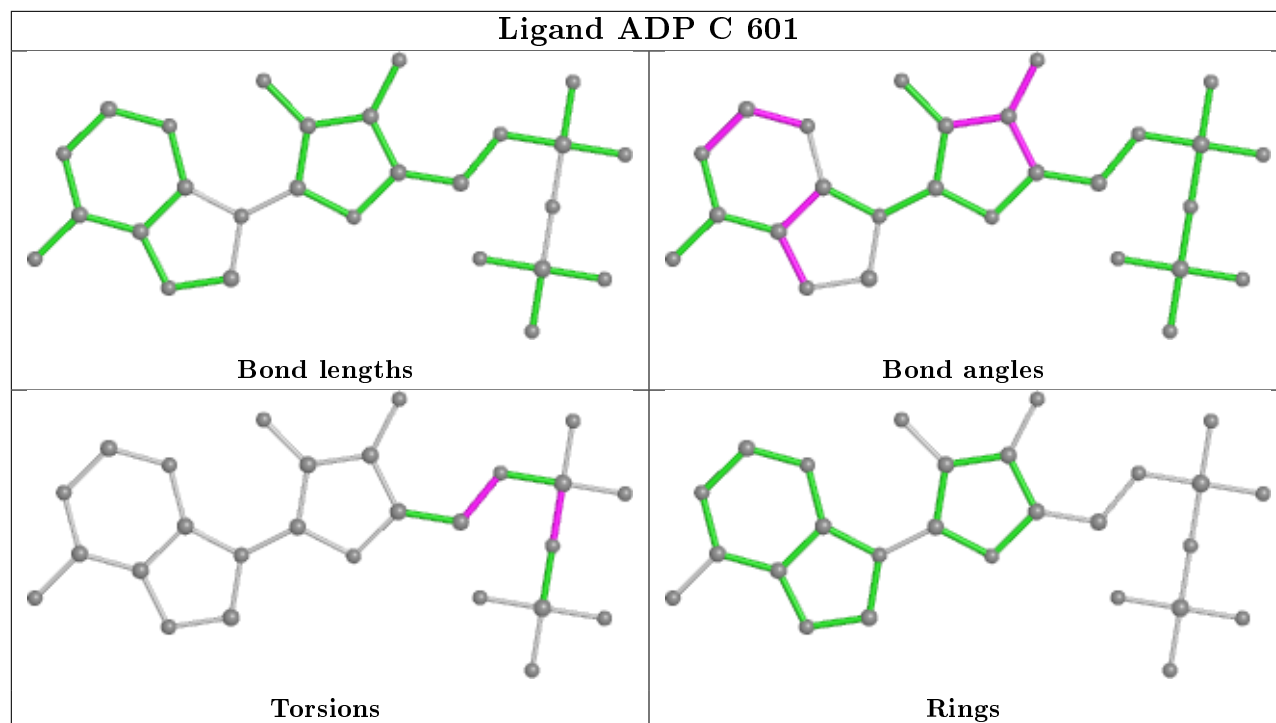
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	334/368 (90%)	0.35	34 (10%) <b>6</b> <b>4</b>	26, 49, 91, 110	0
1	B	302/368 (82%)	0.58	47 (15%) <b>2</b> <b>1</b>	37, 62, 98, 118	0
1	C	339/368 (92%)	-0.08	10 (2%) 51 47	18, 37, 65, 99	0
All	All	975/1104 (88%)	0.27	91 (9%) <b>8</b> <b>5</b>	18, 49, 91, 118	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	ALA	9.0
1	B	46	VAL	7.5
1	B	343	LEU	6.7
1	A	360	LEU	6.0
1	A	285	ALA	6.0
1	C	230	ALA	6.0
1	B	341	LEU	5.4
1	B	47	ARG	5.0
1	A	282	ALA	5.0
1	B	340	SER	4.7
1	B	38	HIS	4.5
1	A	307	PRO	4.2
1	B	342	ASN	4.2
1	B	95	MET	4.1
1	B	360	LEU	4.1
1	B	37	ALA	4.0
1	A	363	PRO	4.0
1	B	271	ASN	3.9
1	A	229	ASN	3.8
1	B	263	LEU	3.8
1	A	289	ASN	3.7
1	B	189	ARG	3.6
1	B	246	LYS	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	229	ASN	3.5
1	B	339	ALA	3.5
1	A	327	ARG	3.5
1	A	102	PHE	3.4
1	A	264	VAL	3.4
1	B	27	PRO	3.4
1	B	264	VAL	3.4
1	B	327	ARG	3.4
1	A	56	GLY	3.3
1	B	191	LYS	3.2
1	A	286	GLY	3.1
1	C	58	ALA	3.1
1	B	152	THR	3.1
1	A	101	ILE	3.0
1	B	305	ARG	3.0
1	B	326	GLY	2.9
1	B	28	PHE	2.9
1	B	83	ARG	2.9
1	A	308	HIS	2.8
1	B	65	THR	2.8
1	B	361	ASN	2.8
1	B	67	THR	2.7
1	B	359	ILE	2.7
1	A	247	GLU	2.7
1	C	59	ASP	2.7
1	A	263	LEU	2.7
1	B	256	VAL	2.6
1	A	284	GLU	2.6
1	B	301	ALA	2.6
1	B	102	PHE	2.6
1	B	358	ASN	2.5
1	A	59	ASP	2.5
1	A	239	PHE	2.5
1	A	281	ARG	2.5
1	B	153	GLU	2.5
1	C	363	PRO	2.5
1	A	326	GLY	2.5
1	A	266	LEU	2.4
1	A	283	ARG	2.4
1	A	122	ASN	2.4
1	B	234	ARG	2.4
1	B	238	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	332	ILE	2.4
1	B	362	LYS	2.3
1	B	261	LEU	2.3
1	B	104	TYR	2.3
1	A	332	ILE	2.3
1	A	333	ILE	2.3
1	B	101	ILE	2.2
1	C	103	ALA	2.2
1	A	238	VAL	2.2
1	B	155	SER	2.2
1	C	282	ALA	2.2
1	A	361	ASN	2.1
1	B	356	ALA	2.1
1	C	334	ALA	2.1
1	A	362	LYS	2.1
1	B	268	GLY	2.1
1	C	264	VAL	2.1
1	A	262	ASN	2.1
1	B	344	GLU	2.0
1	A	237	SER	2.0
1	C	102	PHE	2.0
1	A	114	THR	2.0
1	A	22	VAL	2.0
1	B	303	VAL	2.0
1	C	271	ASN	2.0
1	B	26	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

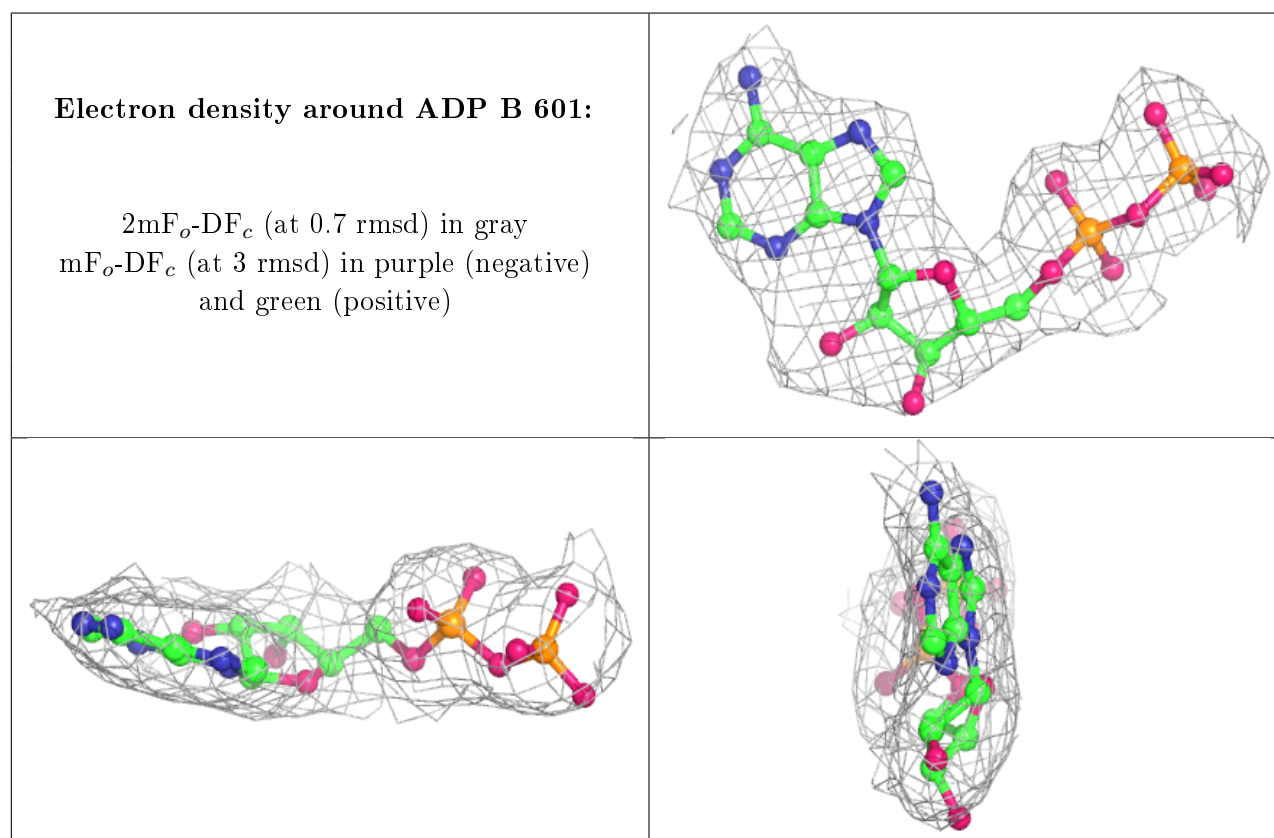
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

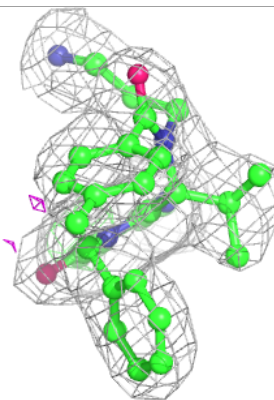
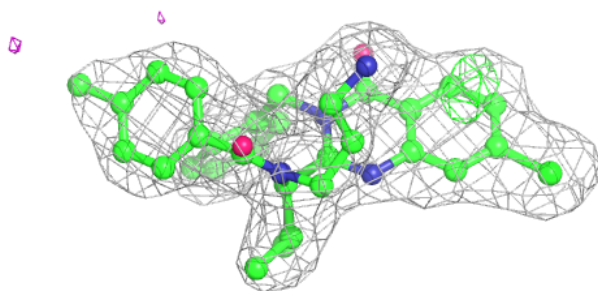
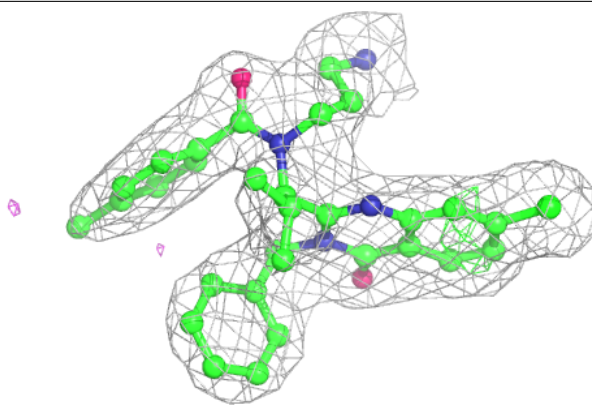
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	C	1365	1/1	0.91	0.13	48,48,48,48	0
2	ADP	B	601	27/27	0.92	0.11	69,76,84,88	0
4	G7X	A	1365	37/37	0.93	0.15	30,38,47,51	0
3	CL	A	1364	1/1	0.94	0.12	74,74,74,74	0
2	ADP	A	601	27/27	0.94	0.12	42,52,61,62	0
6	PO4	C	1366	5/5	0.95	0.11	53,54,57,60	0
6	PO4	C	1367	5/5	0.95	0.12	63,71,86,86	0
4	G7X	B	1363	37/37	0.95	0.13	36,45,53,56	0
4	G7X	C	1369	37/37	0.97	0.11	22,27,37,39	0
2	ADP	C	601	27/27	0.97	0.13	26,36,45,48	0
3	CL	C	1368	1/1	0.99	0.12	38,38,38,38	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.

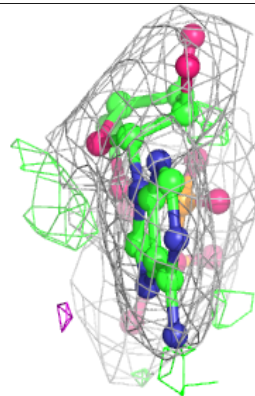
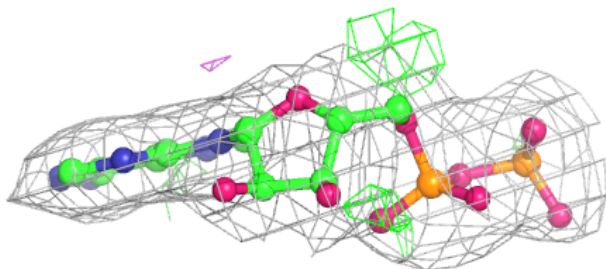
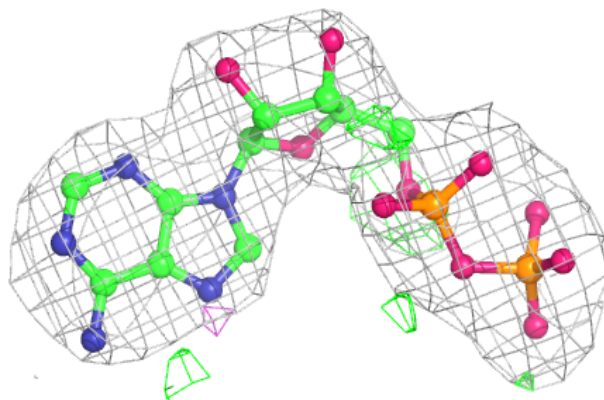


**Electron density around G7X A 1365:**

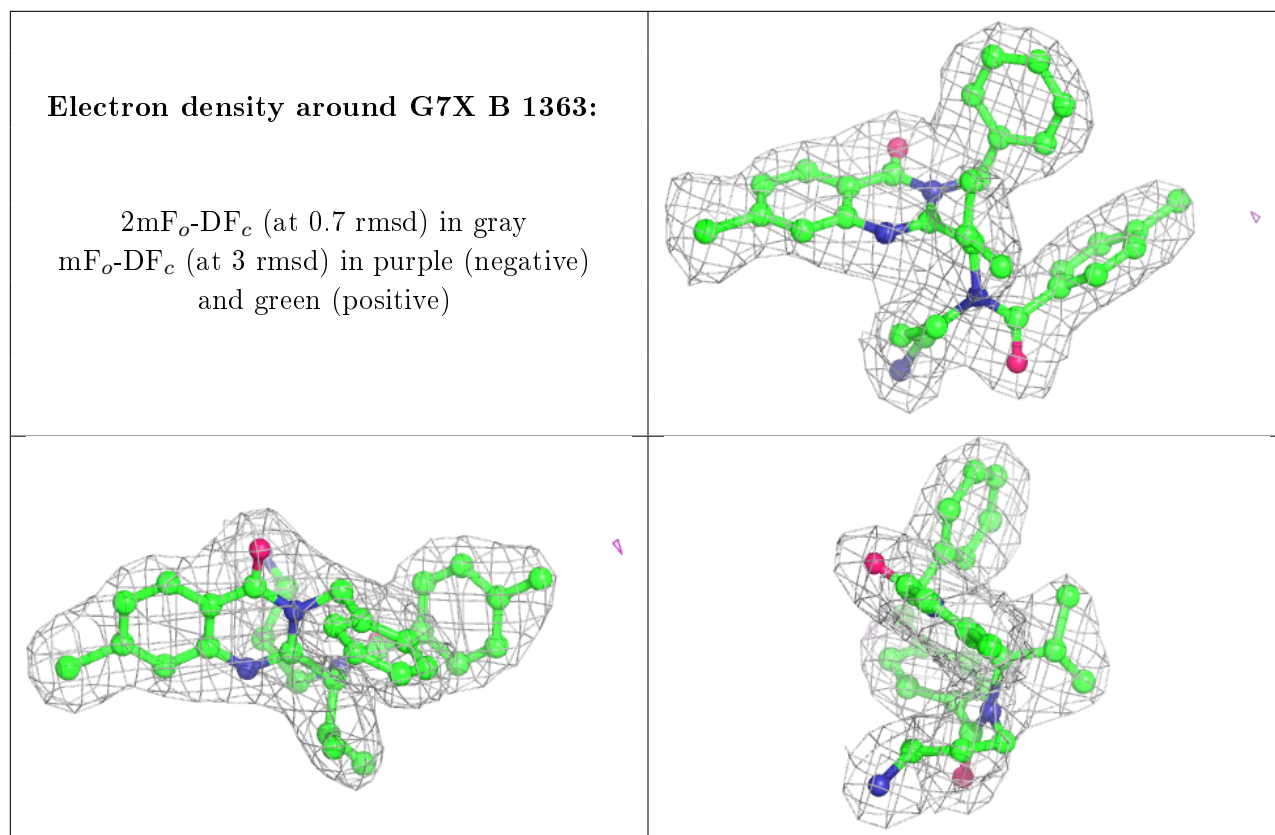
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP A 601:**

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

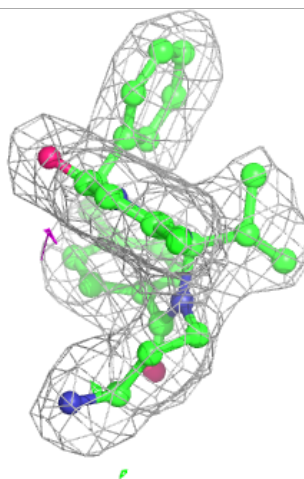
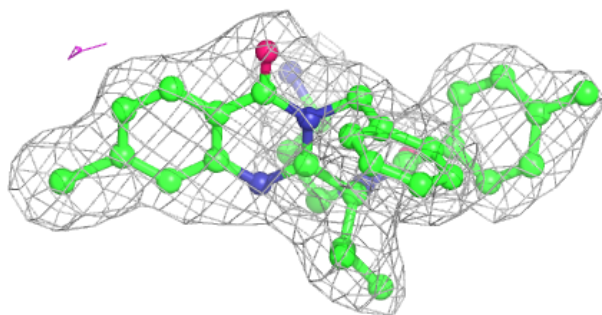
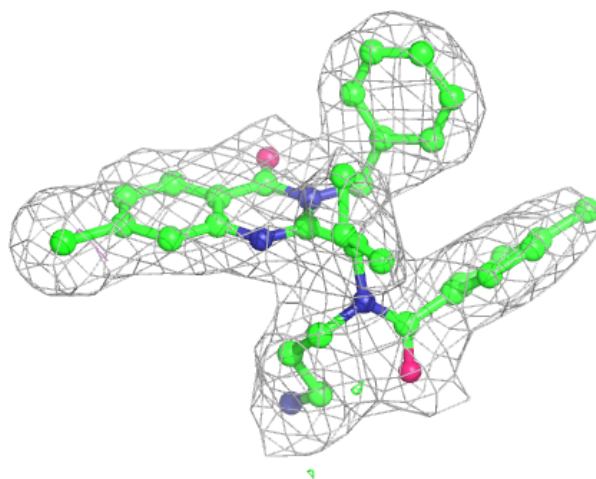


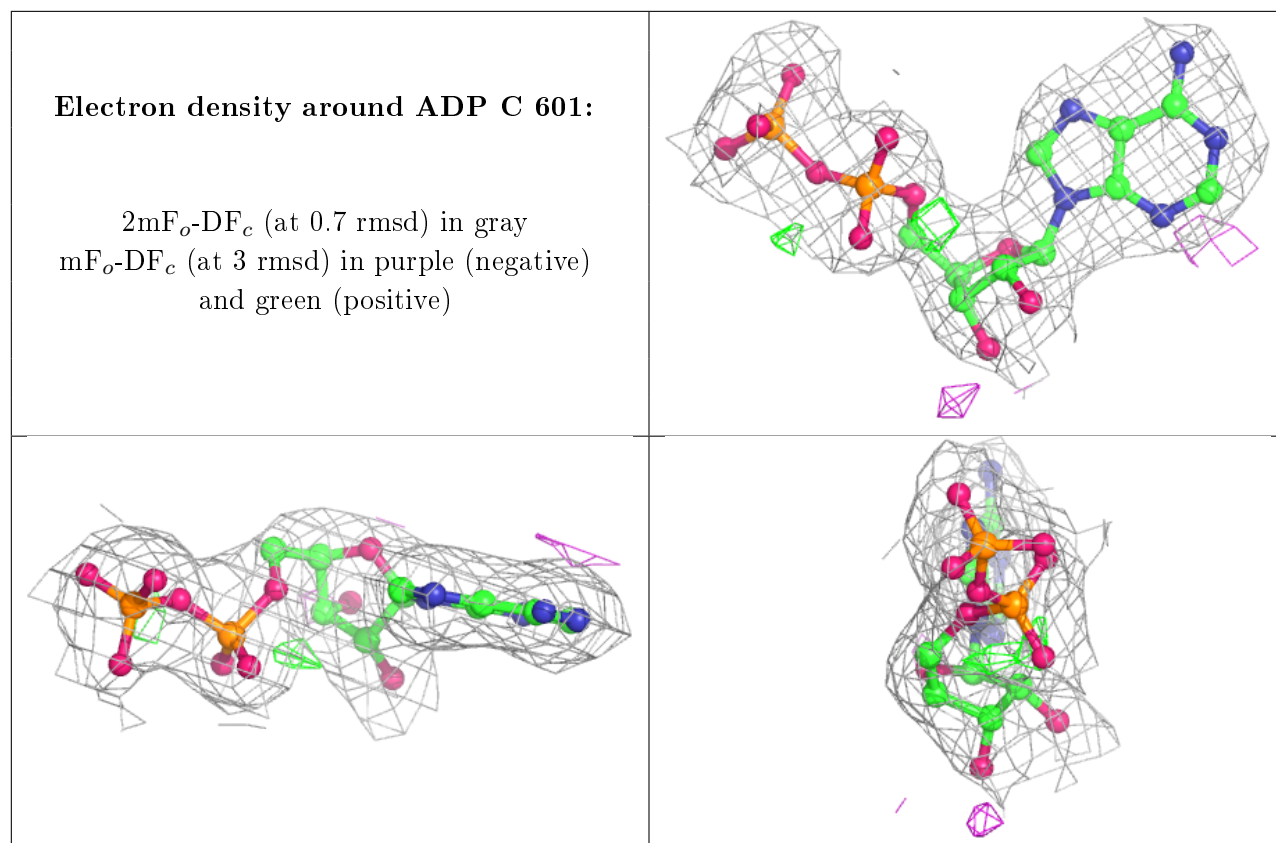




**Electron density around G7X C 1369:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.