



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 08:30 AM UTC

PDB ID : 4BXN / pdb_00004bxn
Title : Eg5(WT) complex
Authors : Talapatra, S.K.; Anthony, N.G.; Mackay, S.P.; Kozielski, F.
Deposited on : 2013-07-15
Resolution : 2.79 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

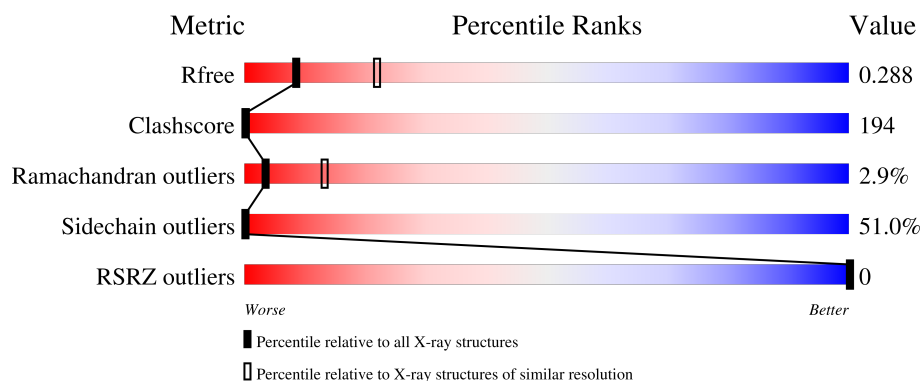
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	368	
1	B	368	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	B	601	-	-	X	-
3	CD	A	1365	-	-	X	-
3	CD	B	1367	-	-	X	-
4	CL	A	1376	-	-	X	-
4	CL	A	1377	-	-	X	-
4	CL	A	1378	-	-	X	-
4	CL	A	1381	-	-	X	-
4	CL	B	1377	-	-	X	-
5	6LX	A	1375	-	-	X	-

2 Entry composition [i](#)

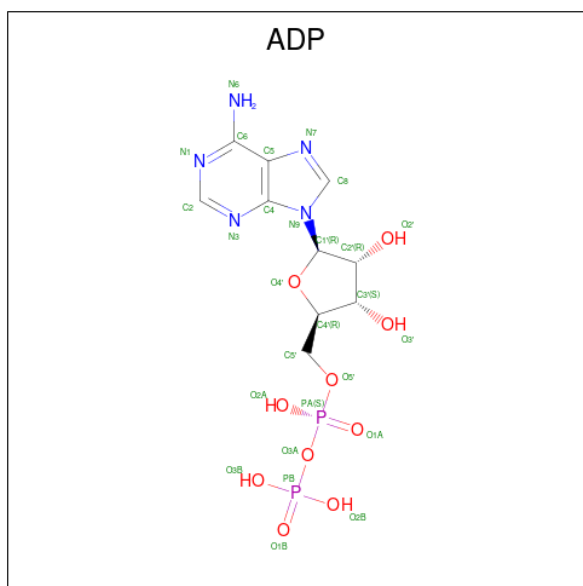
There are 6 unique types of molecules in this entry. The entry contains 5521 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	347	Total	C	N	O	S	2	0	0
			2663	1669	460	524	10			
1	B	345	Total	C	N	O	S	1	0	0
			2642	1657	455	520	10			

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



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		

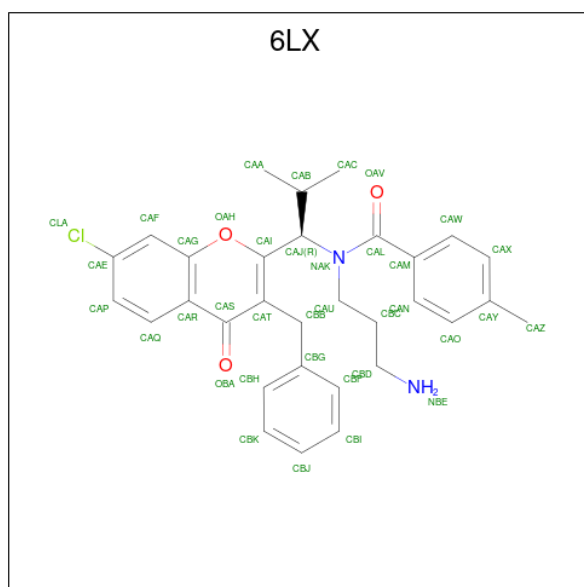
- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total Cd 9 9	0	0
3	B	13	Total Cd 13 13	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total Cl 5 5	0	0
4	B	3	Total Cl 3 3	0	0

- Molecule 5 is N-(3-aminopropyl)-N-[(1R)-1-(3-benzyl-7-chloro-4-oxo-4H-chromen-2-yl)-2-methylpropyl]-4-methylbenzamide (CCD ID: 6LX) (formula: C₃₁H₃₃ClN₂O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C Cl N O 37 31 1 2 3	0	0
5	B	1	Total C Cl N O 37 31 1 2 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	32	Total O 32 32	0	0

Continued on next page...

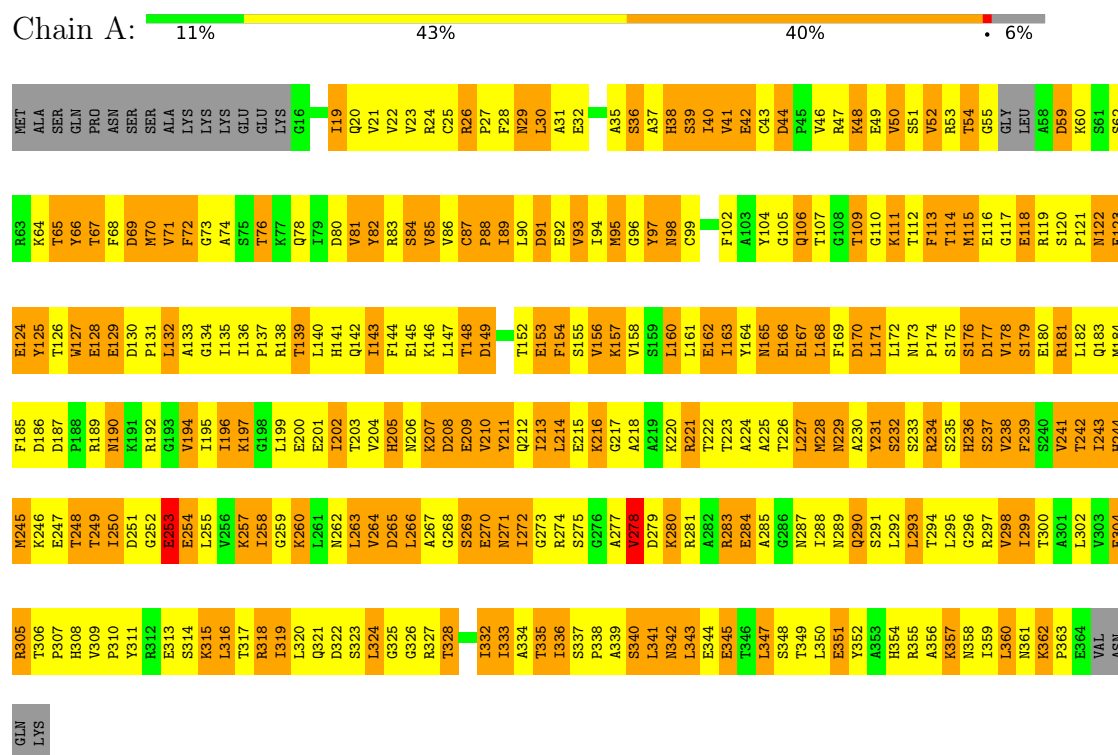
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	26	Total	O	0	0
			26	26		

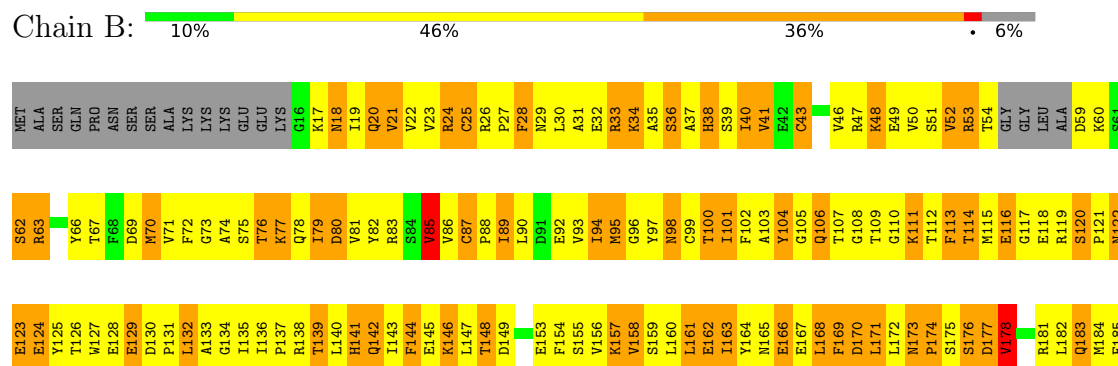
3 Residue-property plots

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: KINESIN-LIKE PROTEIN KIF11



• Molecule 1: KINESIN-LIKE PROTEIN KIF11



V309	P310	Y311	S314	K315	L316	T317	R318	I319	L320	Q321	D322	S323	L324	T328	R329	T330	S331	I332	I333	A334	T335	I336	S337	P338	A339	S340	L341	N342	L343	E344	E345	T346	L347	S348	T349	L350	E351	Y352	A353	H354	R355	A356	K357	N358	I359	L360	N361	K362	P363	E364	VAL	ASN	GLN	LYS				
D186	D187	P188	R189	N190	K191	R192	G193	V194	I195	I196	K197	G198	L199	E200	E201	I202	T203	V204	H205	N206	K207	D208	E209	V210	Y211	Q212	I213	L214	E215	K216	A219	K220	R221	T222	T223	A224	A225	T226	L227	M228	N229	A230	Y231	S232	S233	R234	S235	H236	S237	V238	F239	S240	V241	T242	E243	H244	M245	K246
E247	T248	T249	I250	D251	G252	E253	E254	L255	V256	K257	I258	G259	K260	L261	N262	L263	V264	D265	L266	A267	G268	S269	E270	N271	L272	G273	R274	S275	G276	A277	V278	D279	K280	R281	A282	R283	E284	N287	I288	S291	L292	L293	T294	L295	G296	R297	V298	I299	T300	A301	L302	V303	E304	R305	T306	H308		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	81.43Å 81.43Å 115.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.93 – 2.79 27.93 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.1 (27.93-2.79) 97.1 (27.93-2.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.230 , 0.274 0.279 , 0.288	Depositor DCC
R_{free} test set	1059 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 95.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.477 for -h,-k,l 0.075 for h,-h-k,-l 0.070 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
Outliers	0 of 20599 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5521	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CD, CL, ADP, 6LX

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	0.47	0/2702	0.90	1/3658 (0.0%)
1	B	0.45	0/2680	0.98	11/3630 (0.3%)
All	All	0.46	0/5382	0.94	12/7288 (0.2%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	ASN	C-N-CD	-11.05	79.70	125.00
1	B	251	ASP	N-CA-C	-8.31	102.22	111.28
1	B	276	GLY	N-CA-C	-8.30	103.72	115.43
1	B	278	VAL	N-CA-C	8.21	118.99	110.62
1	A	278	VAL	N-CA-C	-7.75	102.71	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2663	0	2620	1057	18
1	B	2642	0	2599	1024	25
2	A	27	0	12	3	0
2	B	27	0	12	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	9	0	0	3	1
3	B	13	0	0	3	2
4	A	5	0	0	10	1
4	B	3	0	0	3	0
5	A	37	0	33	91	0
5	B	37	0	33	9	0
6	A	32	0	0	12	0
6	B	26	0	0	4	0
All	All	5521	0	5309	2094	32

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 194.

The worst 5 of 2094 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PHE:CE2	1:A:81:VAL:HG22	1.21	1.63
1:A:28:PHE:CE1	1:A:339:ALA:CB	1.80	1.63
1:A:28:PHE:CZ	1:A:339:ALA:CB	1.77	1.62
1:A:211:TYR:CE1	5:A:1375:6LX:HAA1	1.34	1.60
1:B:113:PHE:CE2	1:B:118:GLU:HG3	1.26	1.60

The worst 5 of 32 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:NH2	1:B:253:GLU:CD[3_565]	0.48	1.72
1:A:59:ASP:OD2	1:A:287:ASN:ND2[3_565]	0.80	1.40
1:B:33:ARG:CZ	1:B:253:GLU:OE1[3_565]	0.90	1.30
1:A:344:GLU:OE2	3:B:1369:CD:CD[3_565]	1.04	1.16
1:B:33:ARG:NH2	1:B:253:GLU:CG[3_565]	1.07	1.13

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	343/368 (93%)	325 (95%)	9 (3%)	9 (3%)	4	15
1	B	341/368 (93%)	318 (93%)	12 (4%)	11 (3%)	3	11
All	All	684/736 (93%)	643 (94%)	21 (3%)	20 (3%)	3	13

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	179	SER
1	B	18	ASN
1	B	53	ARG
1	B	74	ALA

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	290/322 (90%)	132 (46%)	158 (54%)	0	0
1	B	287/322 (89%)	151 (53%)	136 (47%)	0	0
All	All	577/644 (90%)	283 (49%)	294 (51%)	0	0

5 of 294 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	213	ILE
1	B	347	LEU
1	B	232	SER
1	B	278	VAL
1	A	232	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	20	GLN
1	B	150	ASN
1	B	321	GLN
1	B	212	GLN
1	B	244	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 34 ligands modelled in this entry, 30 are monoatomic - leaving 4 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	B	601	-	28,29,29	1.42	4 (14%)	43,45,45	1.85	9 (20%)
5	6LX	B	1375	-	40,40,40	2.35	15 (37%)	47,56,56	1.62	8 (17%)
5	6LX	A	1375	-	40,40,40	2.64	18 (45%)	47,56,56	1.20	5 (10%)
2	ADP	A	601	-	28,29,29	1.50	6 (21%)	43,45,45	1.87	11 (25%)

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	B	601	-	-	5/16/32/32	0/3/3/3
5	6LX	B	1375	-	-	3/24/28/28	0/4/4/4
5	6LX	A	1375	-	-	8/24/28/28	0/4/4/4
2	ADP	A	601	-	-	3/16/32/32	0/3/3/3

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1375	6LX	OBA-CAS	7.57	1.39	1.23
5	A	1375	6LX	CAT-CAI	7.30	1.47	1.35
5	B	1375	6LX	OBA-CAS	7.24	1.38	1.23
5	B	1375	6LX	CAT-CAI	6.01	1.45	1.35
5	A	1375	6LX	CAL-NAK	5.98	1.48	1.34

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C5-C4-N3	-5.83	118.69	126.72
2	A	601	ADP	C5-C4-N3	-4.83	120.07	126.72
5	B	1375	6LX	CBG-CBB-CAT	-4.71	105.04	114.24
2	B	601	ADP	N3-C4-N9	4.59	134.97	127.17
2	A	601	ADP	C4-C5-N7	-3.89	106.14	110.58

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

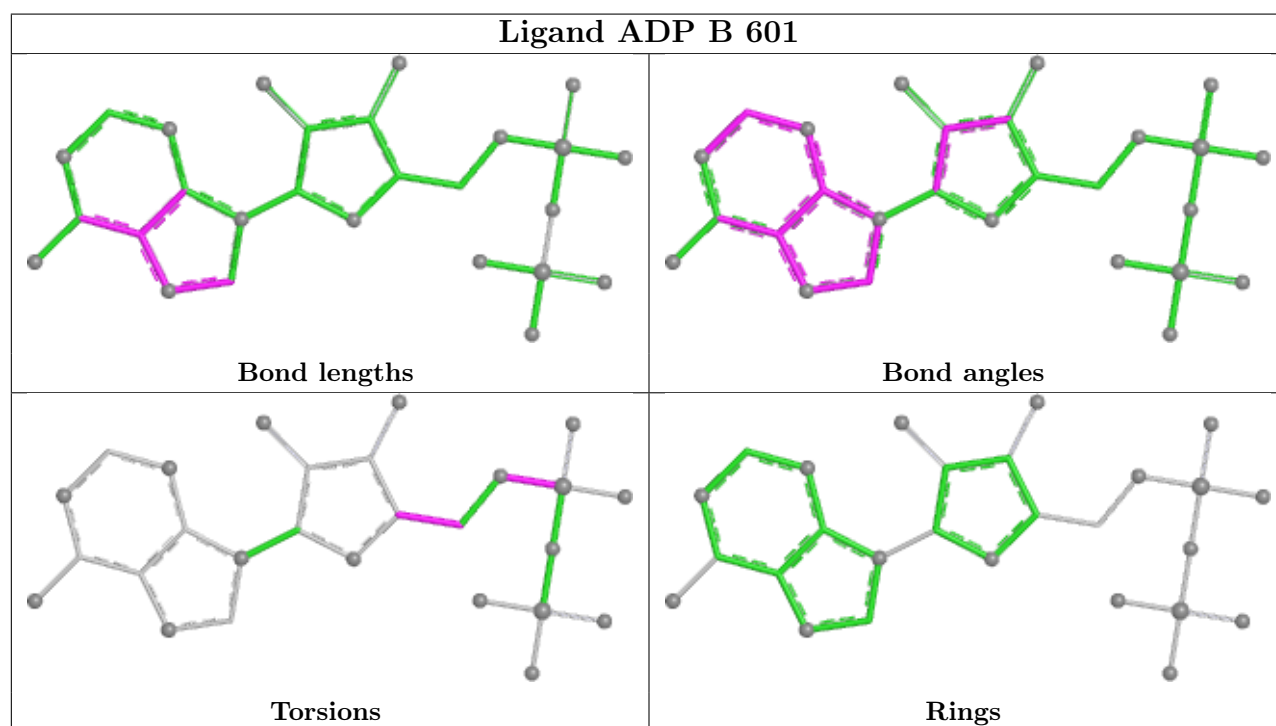
Mol	Chain	Res	Type	Atoms
2	A	601	ADP	C5'-O5'-PA-O3A
2	B	601	ADP	C5'-O5'-PA-O1A
2	B	601	ADP	C5'-O5'-PA-O2A
2	B	601	ADP	C5'-O5'-PA-O3A
5	A	1375	6LX	CAI-CAJ-NAK-CAU

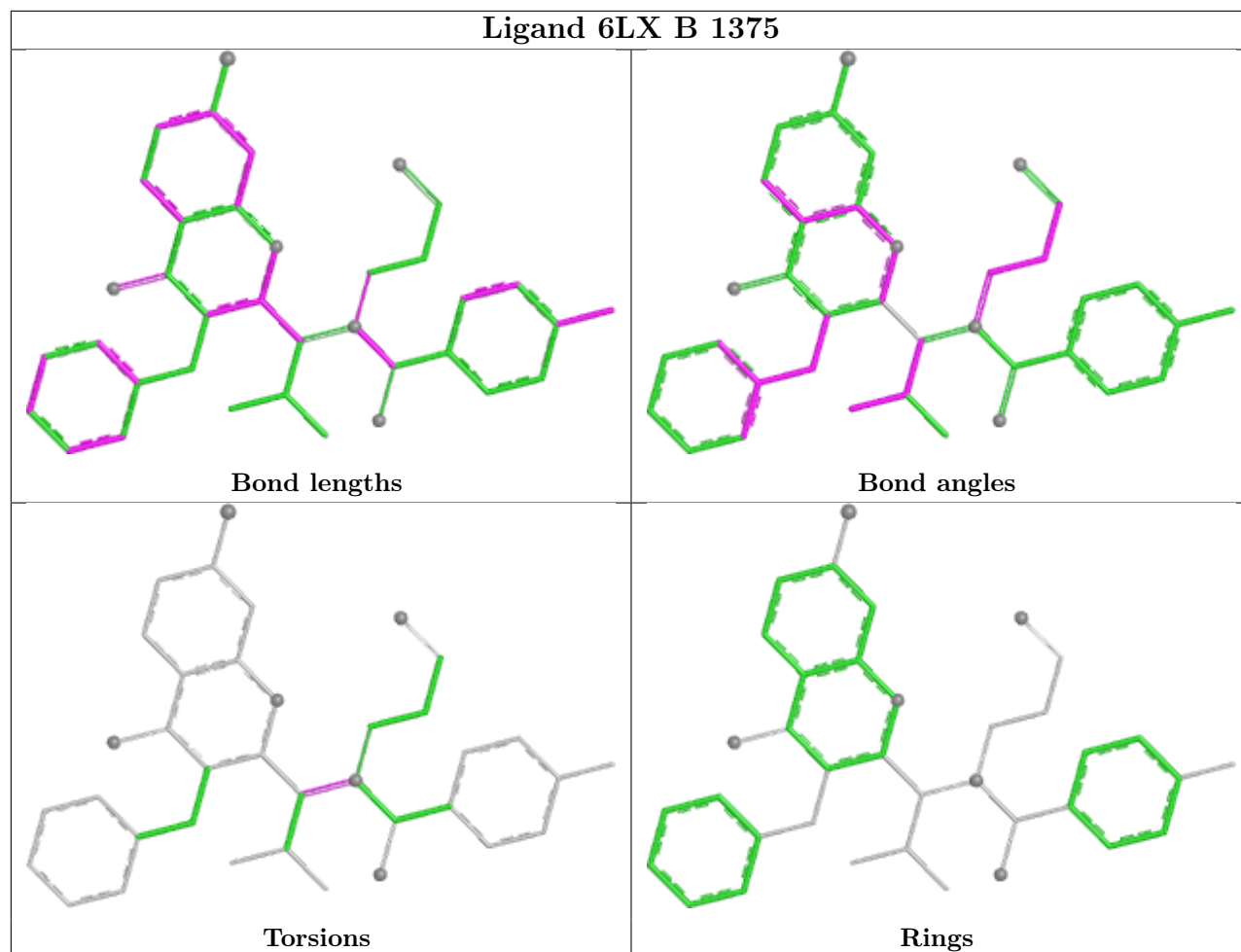
There are no ring outliers.

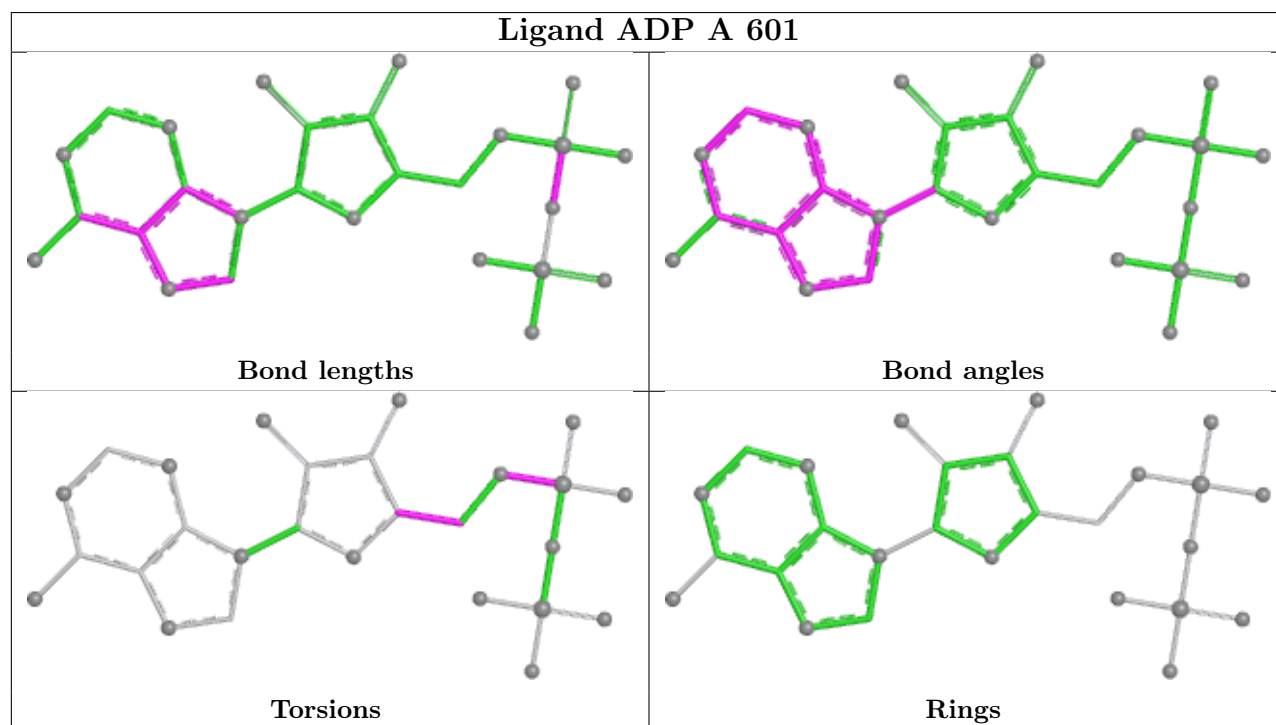
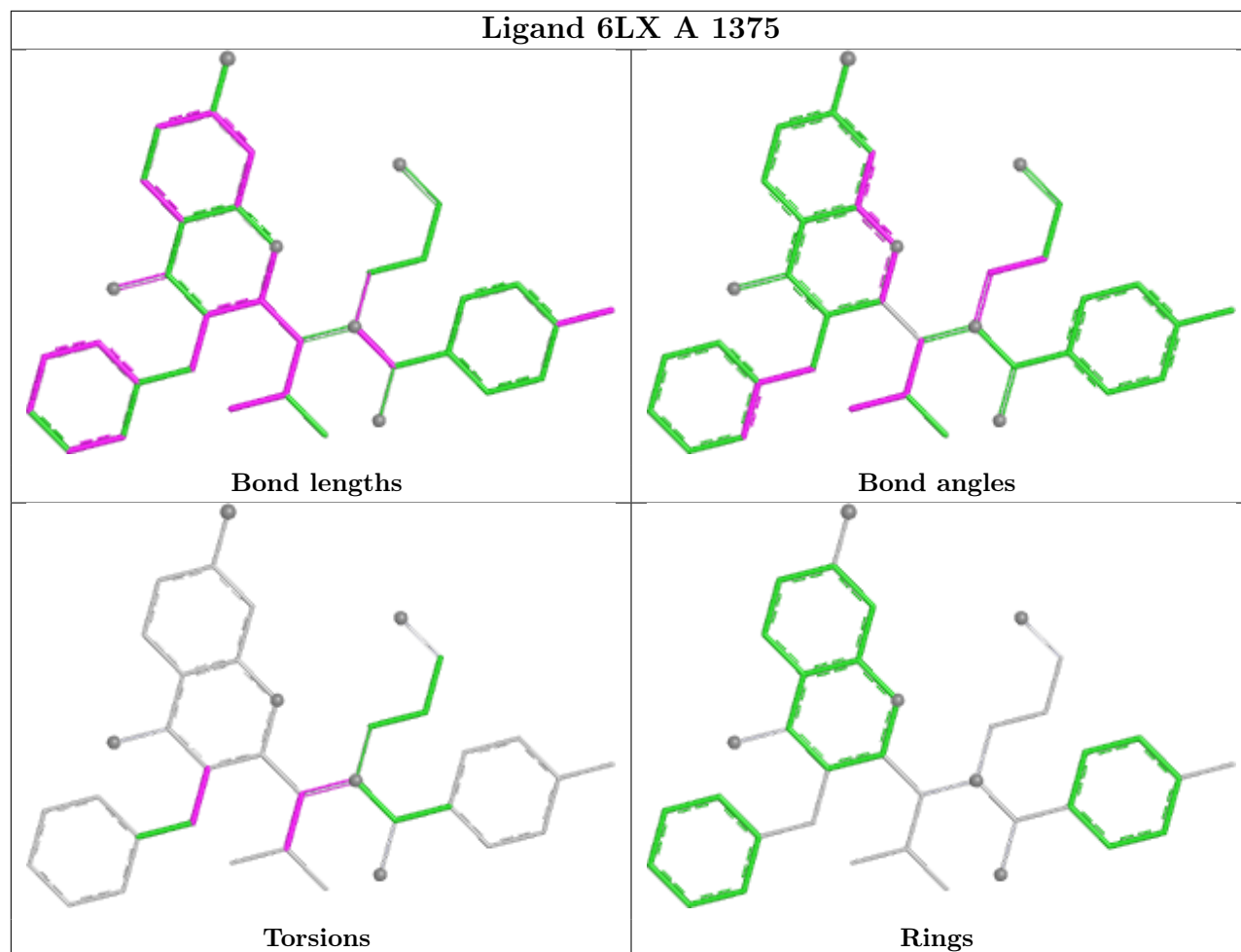
4 monomers are involved in 124 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	ADP	21	0
5	B	1375	6LX	9	0
5	A	1375	6LX	91	0
2	A	601	ADP	3	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 [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	347/368 (94%)	-1.48	0 100 100	48, 71, 88, 93	1 (0%)
1	B	345/368 (93%)	-1.47	0 100 100	48, 72, 87, 96	0
All	All	692/736 (94%)	-1.48	0 100 100	48, 72, 88, 96	1 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	CL	A	1381	1/1	0.95	0.04	80,80,80,80	0
2	ADP	B	601	27/27	0.99	0.03	60,67,69,73	0
3	CD	B	1374	1/1	0.99	0.02	115,115,115,115	0
3	CD	B	1378	1/1	0.99	0.03	106,106,106,106	0
3	CD	B	1379	1/1	0.99	0.03	120,120,120,120	0
2	ADP	A	601	27/27	0.99	0.03	61,66,74,79	0
4	CL	B	1377	1/1	0.99	0.02	67,67,67,67	0

Continued on next page...

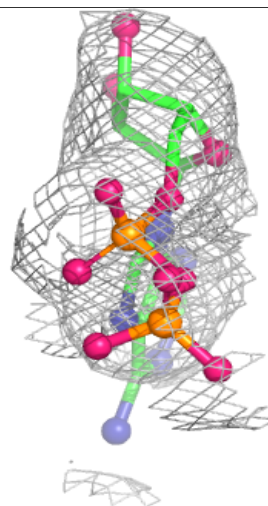
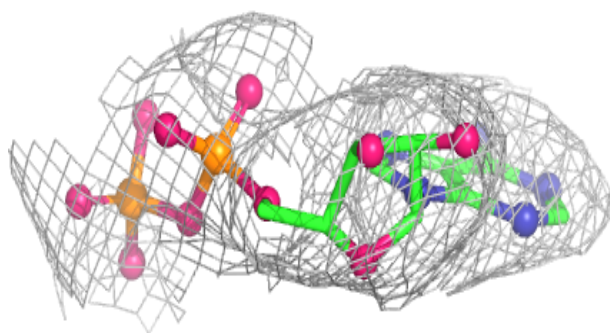
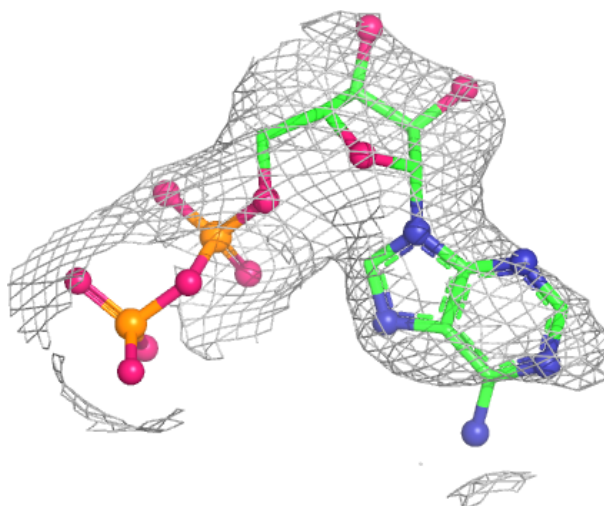
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	B	1385	1/1	0.99	0.04	83,83,83,83	0
4	CL	B	1386	1/1	0.99	0.02	66,66,66,66	0
5	6LX	A	1375	37/37	0.99	0.04	67,76,80,87	0
5	6LX	B	1375	37/37	0.99	0.04	67,76,80,87	0
3	CD	B	1365	1/1	1.00	0.02	82,82,82,82	0
3	CD	B	1366	1/1	1.00	0.01	90,90,90,90	0
3	CD	B	1367	1/1	1.00	0.02	78,78,78,78	0
3	CD	B	1368	1/1	1.00	0.01	51,51,51,51	0
3	CD	B	1369	1/1	1.00	0.01	80,80,80,80	0
3	CD	B	1370	1/1	1.00	0.01	60,60,60,60	0
3	CD	B	1371	1/1	1.00	0.02	100,100,100,100	0
3	CD	B	1372	1/1	1.00	0.01	115,115,115,115	0
3	CD	B	1373	1/1	1.00	0.01	107,107,107,107	0
3	CD	A	1365	1/1	1.00	0.01	66,66,66,66	0
3	CD	B	1376	1/1	1.00	0.04	30,30,30,30	0
3	CD	A	1366	1/1	1.00	0.02	86,86,86,86	0
3	CD	A	1367	1/1	1.00	0.01	59,59,59,59	0
4	CL	A	1374	1/1	1.00	0.01	54,54,54,54	0
4	CL	A	1376	1/1	1.00	0.02	85,85,85,85	0
4	CL	A	1377	1/1	1.00	0.02	74,74,74,74	0
4	CL	A	1378	1/1	1.00	0.02	84,84,84,84	0
3	CD	A	1368	1/1	1.00	0.01	91,91,91,91	0
3	CD	A	1369	1/1	1.00	0.01	100,100,100,100	0
3	CD	A	1370	1/1	1.00	0.01	69,69,69,69	0
3	CD	A	1371	1/1	1.00	0.03	100,100,100,100	0
3	CD	A	1372	1/1	1.00	0.01	104,104,104,104	0
3	CD	A	1373	1/1	1.00	0.02	112,112,112,112	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

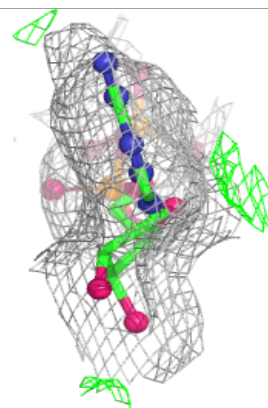
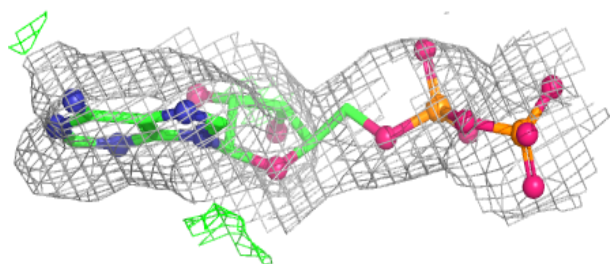
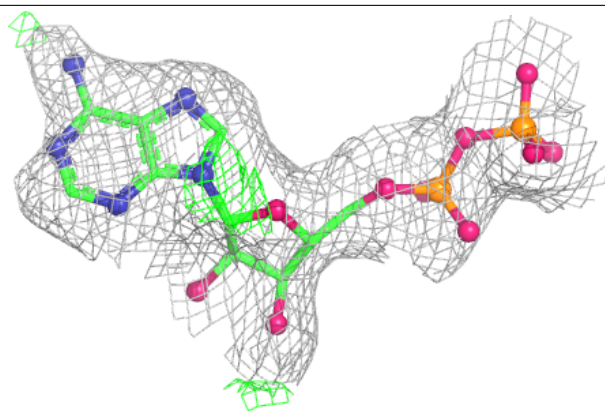
Electron density around ADP B 601:

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

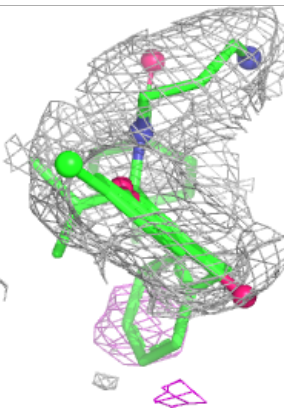
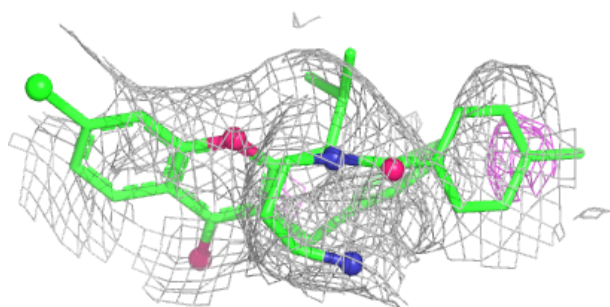
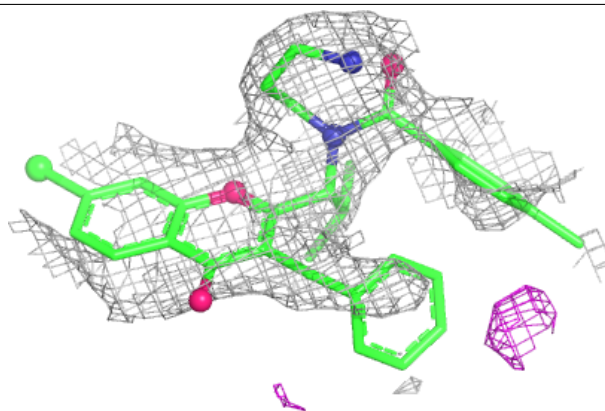


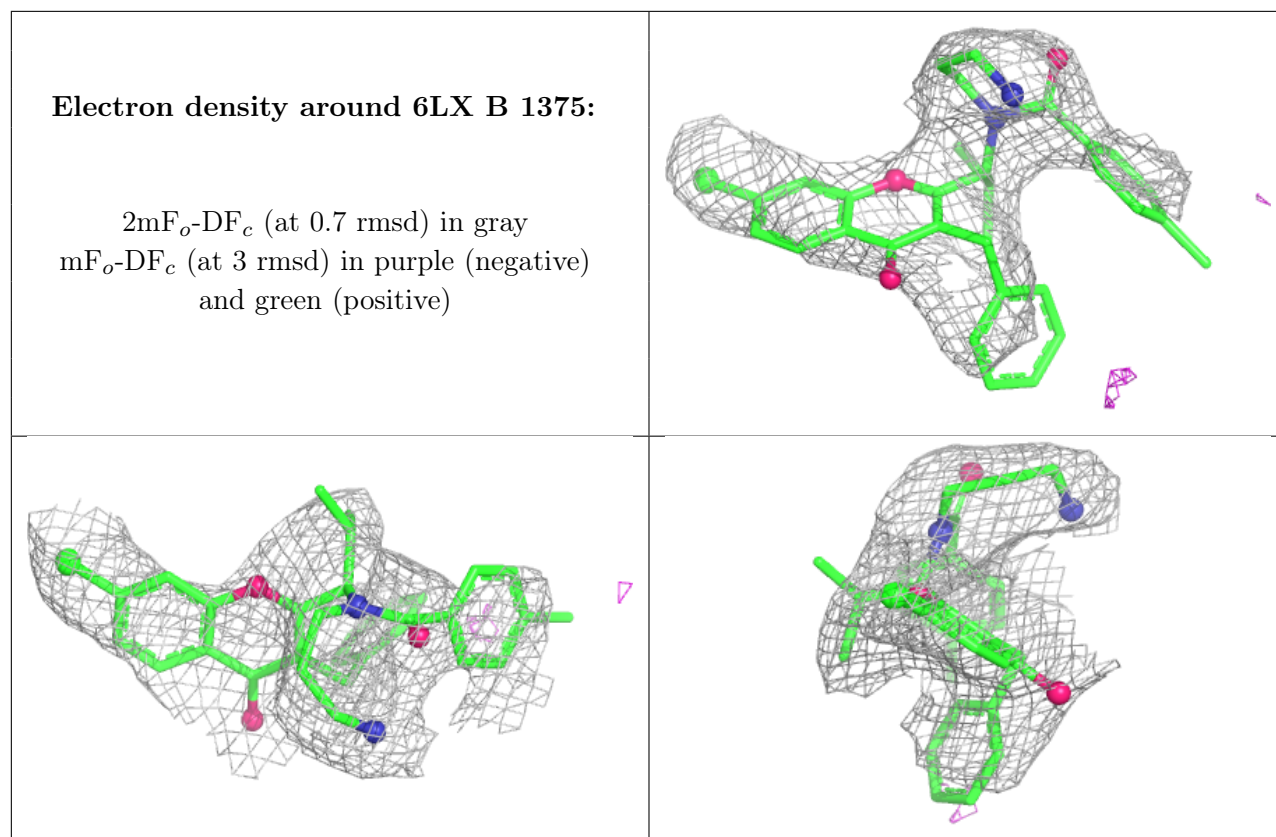
Electron density around ADP A 601:

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

**Electron density around 6LX A 1375:**

$2mF_o-DF_c$ (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.