



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2024 – 01:28 AM EDT

PDB ID : 2XAL
Title : Lead derivative of Inositol 1,3,4,5,6-pentakisphosphate 2-kinase from *A. thaliana* in complex with ADP and IP6.
Authors : Gonzalez, B.; Banos-Sanz, J.I.; Villate, M.; Brearley, C.A.; Sanz-Aparicio, J.
Deposited on : 2010-03-31
Resolution : 3.20 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

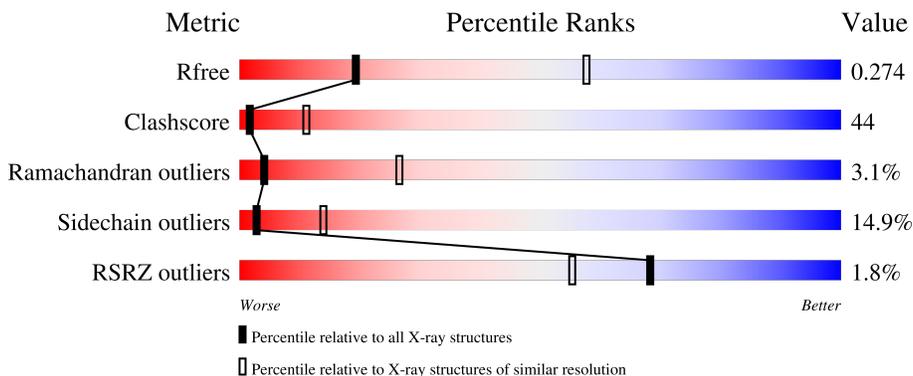
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	451	
1	B	451	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6851 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.

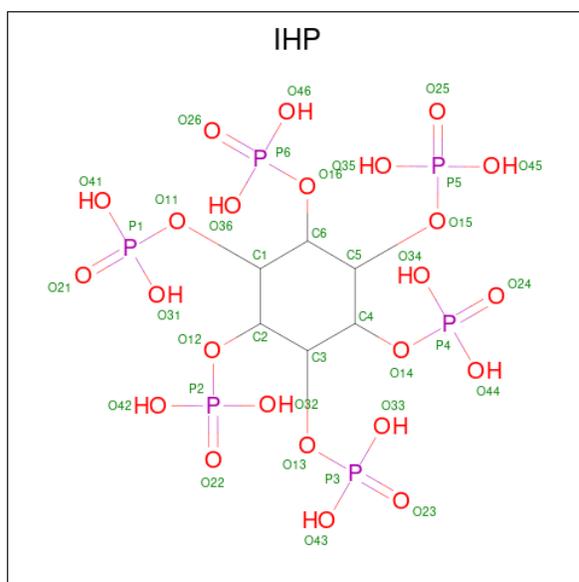
- Molecule 1 is a protein called INOSITOL-PENTAKISPHOSPHATE 2-KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	420	3338	2120	565	640	13	0	0	0
1	B	425	3381	2148	574	645	14	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	SER	ALA	conflict	UNP Q93YN9
A	90	GLN	LYS	conflict	UNP Q93YN9
A	157	THR	SER	conflict	UNP Q93YN9
A	204	ILE	ASN	conflict	UNP Q93YN9
A	224	ARG	SER	conflict	UNP Q93YN9
A	321	CYS	SER	conflict	UNP Q93YN9
A	325	ILE	LEU	conflict	UNP Q93YN9
A	337	ARG	LYS	conflict	UNP Q93YN9
B	54	SER	ALA	conflict	UNP Q93YN9
B	90	GLN	LYS	conflict	UNP Q93YN9
B	157	THR	SER	conflict	UNP Q93YN9
B	204	ILE	ASN	conflict	UNP Q93YN9
B	224	ARG	SER	conflict	UNP Q93YN9
B	321	CYS	SER	conflict	UNP Q93YN9
B	325	ILE	LEU	conflict	UNP Q93YN9
B	337	ARG	LYS	conflict	UNP Q93YN9

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).

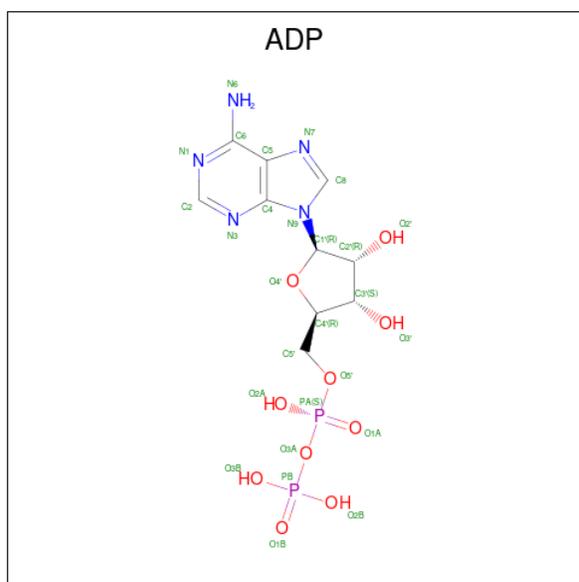


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			P
2	A	1	36	6	24	6	0	0
2	B	1	36	6	24	6	0	0

- Molecule 3 is LEAD (II) ION (three-letter code: PB) (formula: Pb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Pb		
3	A	2	2	2	0	0
3	B	2	2	2	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

ASN	Q376	L310	F218	L151
SER	S377	L311	F152	F152
LYS	R378	K312	SER	SER
PRO	M379	L313	GLN	GLN
SER	A380	D314	GLY	GLY
HIS	TRP	I315	ILE	ILE
SER	ASP	E316	THR	THR
	S383	G317	SER	SER
	E384	A318	GLY	GLY
	D388	I319	GLY	D161
	Y389	H320		
	V390	C321		V165
	S391	Y322		
	L392	Y323		
	K393	D324		K168
	P394	I325		P169
	T395	I326		K170
	N396			C171
	Q397	C330		G172
	T398	P331		F173
	F399	I332		L174
	D400	C333		P175
	Y401	K334		T176
	K402	E335		
	V403	G336		F179
	H404	R337		L180
	F405	P338		G181
	I406	L339		K182
	D407	E340		E183
	I408	A341		M184
	S409	E342		M185
		L343		L186
		S344		K187
		L345		T188
		H346		S189
		K414		V190
		R415		S191
				R192
				F193
				K194
				M195
				H196
				Q197
				L198
				L199
				K200
				E202
				Y203
				L204
				S207
				E208
				Y212
				Y213
				P214
				L215
				D216
				L217
				F219
				S219
				G220
				S221
				K222
				E223
				R224
				Y225
				L226
				L232
				P236
				Q237
				N238
				F240
				R241
				L244
				I249
				G252
				E255
				S256
				T257
				E269
				D270
				K273
				G274
				F275
				I276
				Q277
				S278
				E279
				D280
				G281
				H282
				R283
				T284
				E285
				C286
				F287
				L288
				S282
				V285
				Y296
				V300
				L301
				D302
				R303
				I307
				C330
				P331
				I332
				C333
				K334
				E335
				G336
				R337
				P338
				L339
				E340
				A341
				E342
				L343
				S344
				L345
				H346
				K414
				R415
				L422
				D423
				K424
				K425
				I426
				I427
				S428
				F429
				Y430
				K433
				O434
				K435
				A436
				E437
				N438
				THR
				ALA
				GLU
				GLN
				ILE
				GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.06Å 110.97Å 138.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.71 – 3.20 86.65 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (86.71-3.20) 99.9 (86.65-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 3.19Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.210 , 0.268 0.214 , 0.274	Depositor DCC
R_{free} test set	768 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtrriage
Anisotropy	0.201	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6851	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.27% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.56	0/3400	0.66	0/4584
1	B	0.56	0/3441	0.65	0/4637
All	All	0.56	0/6841	0.66	0/9221

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	3338	0	3344	263	3
1	B	3381	0	3406	358	4
2	A	36	0	6	1	0
2	B	36	0	6	5	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	27	0	12	4	0
4	B	27	0	12	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	6851	0	6786	604	4

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 44.

The worst 5 of 604 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:46:ARG:HH12	1:B:182:LYS:CG	1.14	1.58
1:B:52:LYS:HA	1:B:57:VAL:O	1.20	1.38
1:B:280:ASP:HB2	1:B:282:HIS:CD2	1.56	1.38
1:A:46:ARG:NH1	1:B:182:LYS:CG	1.86	1.37
1:A:46:ARG:NH1	1:B:182:LYS:HG3	1.36	1.37

All (4) 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:A:312:LYS:NZ	1:B:202:GLU:CG[1_455]	1.84	0.36
1:B:124:LYS:NZ	1:B:273:LYS:O[4_556]	1.87	0.33
1:A:312:LYS:NZ	1:B:202:GLU:CD[1_455]	2.04	0.16
1:A:381:TRP:CE3	1:B:223:GLU:OE1[3_655]	2.15	0.05

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	414/451 (92%)	366 (88%)	34 (8%)	14 (3%)	3	24
1	B	417/451 (92%)	374 (90%)	31 (7%)	12 (3%)	4	28
All	All	831/902 (92%)	740 (89%)	65 (8%)	26 (3%)	4	26

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	ILE

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Mol	Chain	Res	Type
1	A	161	ASP
1	A	343	LEU
1	A	386	SER
1	A	393	LYS

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	374/399 (94%)	322 (86%)	52 (14%)	3 16
1	B	379/399 (95%)	319 (84%)	60 (16%)	2 12
All	All	753/798 (94%)	641 (85%)	112 (15%)	3 14

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	LYS
1	B	437	GLU
1	B	97	LEU
1	B	428	SER
1	B	348	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	91	ASN
1	B	282	HIS
1	B	397	GLN
1	B	376	GLN
1	B	196	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 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	IHP	A	500	3	36,36,36	0.73	0	60,60,60	1.36	10 (16%)
4	ADP	B	600	3	24,29,29	1.03	1 (4%)	29,45,45	1.64	6 (20%)
4	ADP	A	600	3	24,29,29	1.22	2 (8%)	29,45,45	1.43	4 (13%)
2	IHP	B	500	3	36,36,36	0.84	0	60,60,60	1.50	16 (26%)

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	IHP	A	500	3	-	7/30/54/54	0/1/1/1
4	ADP	B	600	3	-	4/12/32/32	0/3/3/3
4	ADP	A	600	3	-	0/12/32/32	0/3/3/3
2	IHP	B	500	3	-	10/30/54/54	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	ADP	PA-O3A	4.09	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	ADP	PA-O3A	2.90	1.62	1.59
4	A	600	ADP	C1'-N9	-2.01	1.45	1.49

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	ADP	O4'-C1'-N9	-4.30	103.05	108.75
4	A	600	ADP	N3-C2-N1	-3.94	123.33	128.67
4	B	600	ADP	N3-C2-N1	-3.47	123.97	128.67
2	B	500	IHP	P2-O12-C2	-3.26	114.73	123.43
4	A	600	ADP	C1'-N9-C4	-2.97	121.43	126.64

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	IHP	C5-O15-P5-O25
2	A	500	IHP	C3-O13-P3-O23
2	B	500	IHP	C3-O13-P3-O23
4	B	600	ADP	C5'-O5'-PA-O1A
4	B	600	ADP	C5'-O5'-PA-O2A

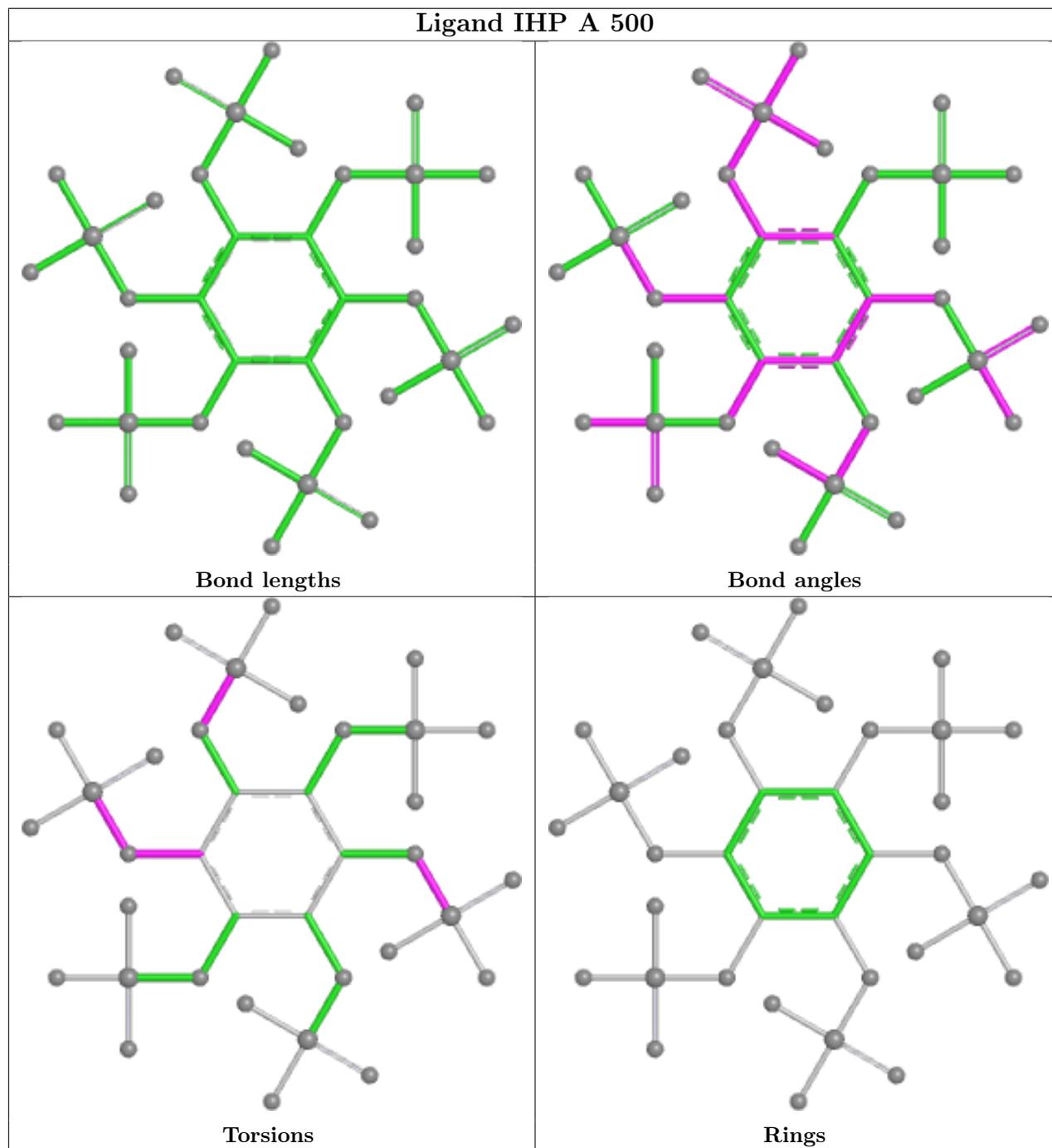
There are no ring outliers.

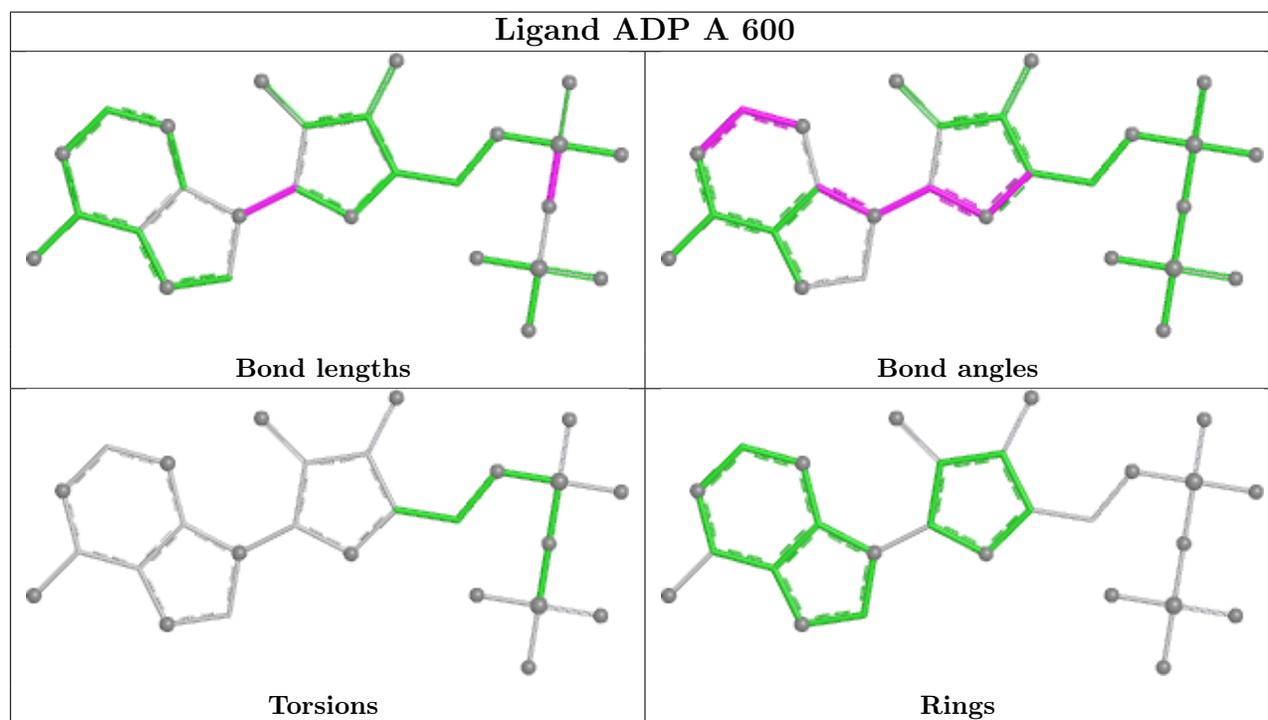
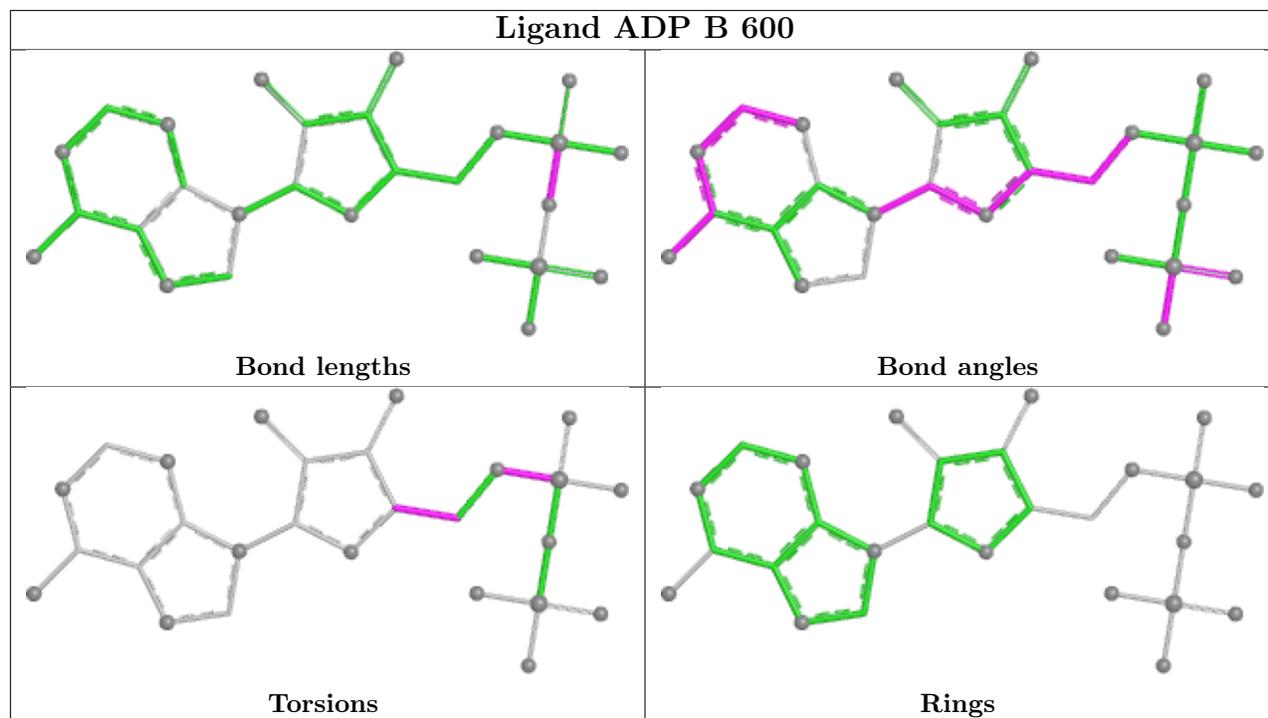
4 monomers are involved in 14 short contacts:

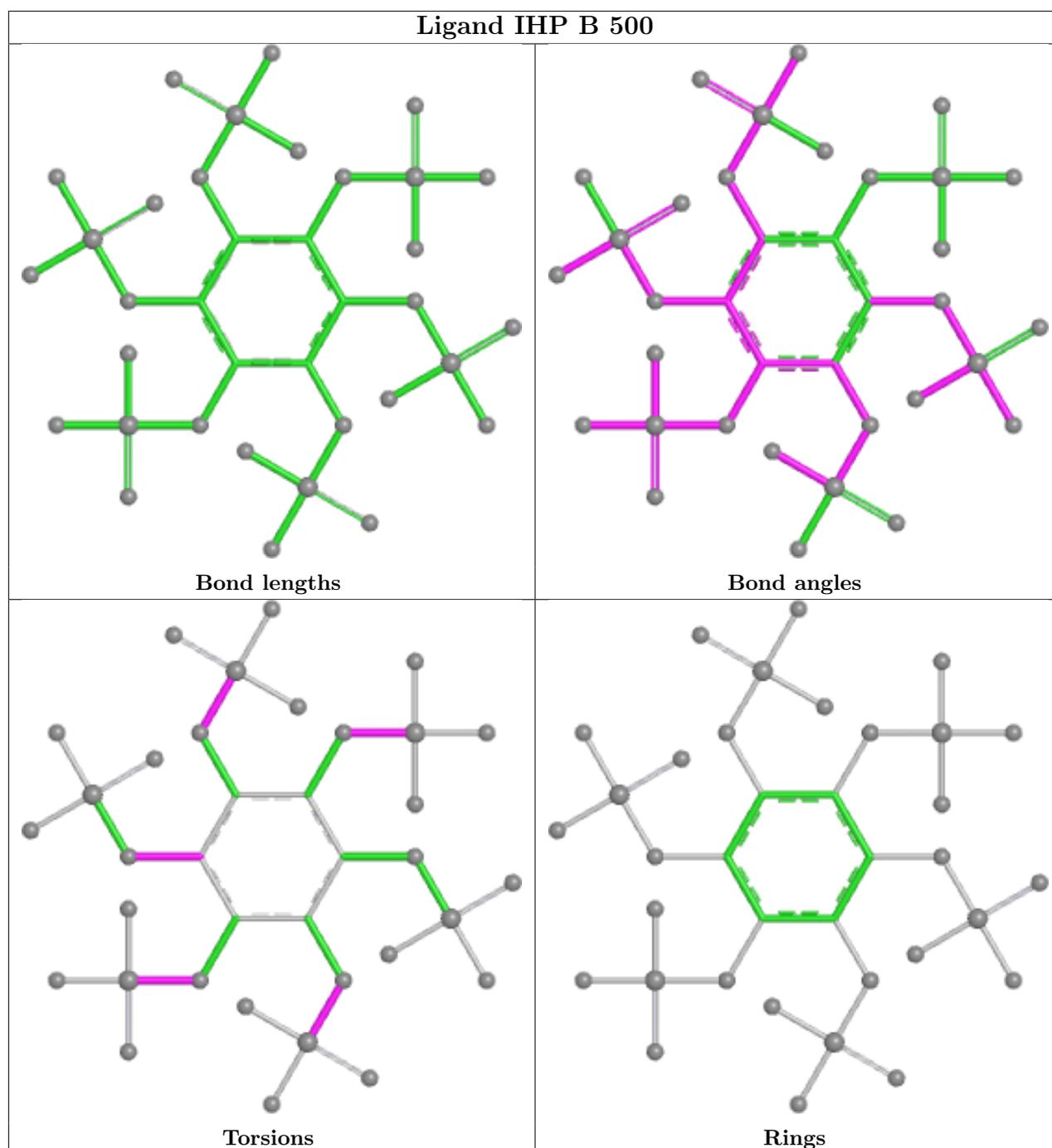
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	IHP	1	0
4	B	600	ADP	4	0
4	A	600	ADP	4	0
2	B	500	IHP	5	0

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	420/451 (93%)	-0.13	8 (1%) 66 53	9, 21, 41, 54	0
1	B	425/451 (94%)	0.02	7 (1%) 72 59	9, 20, 41, 62	0
All	All	845/902 (93%)	-0.05	15 (1%) 68 55	9, 21, 41, 62	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	GLY	3.1
1	A	383	SER	3.0
1	A	437	GLU	2.9
1	A	379	ASN	2.8
1	B	396	ASN	2.5

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 monosaccharides in this entry.

6.4 Ligands [i](#)

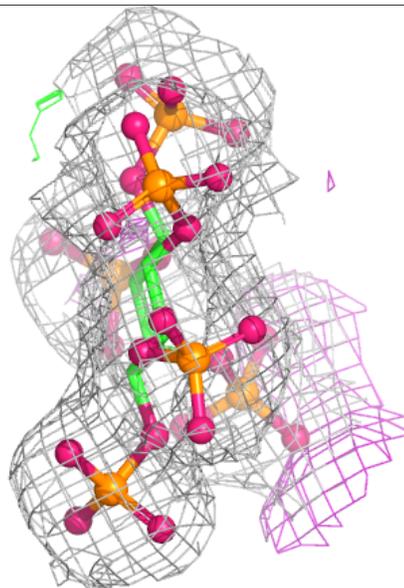
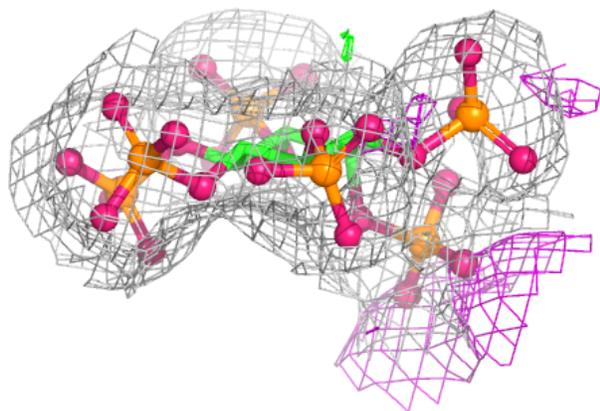
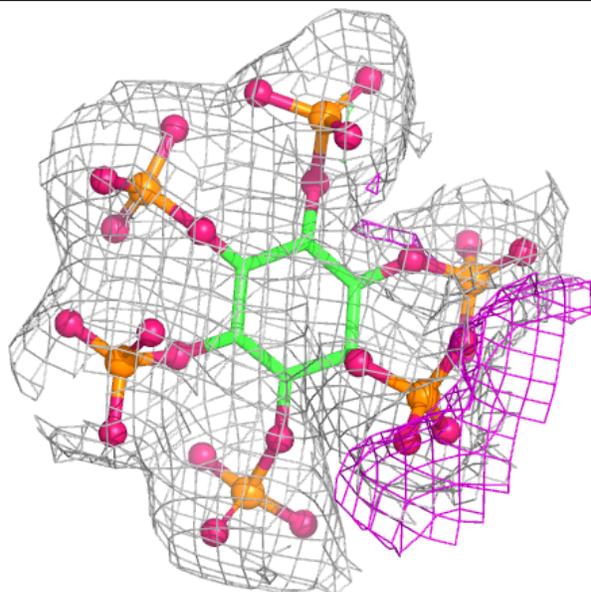
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

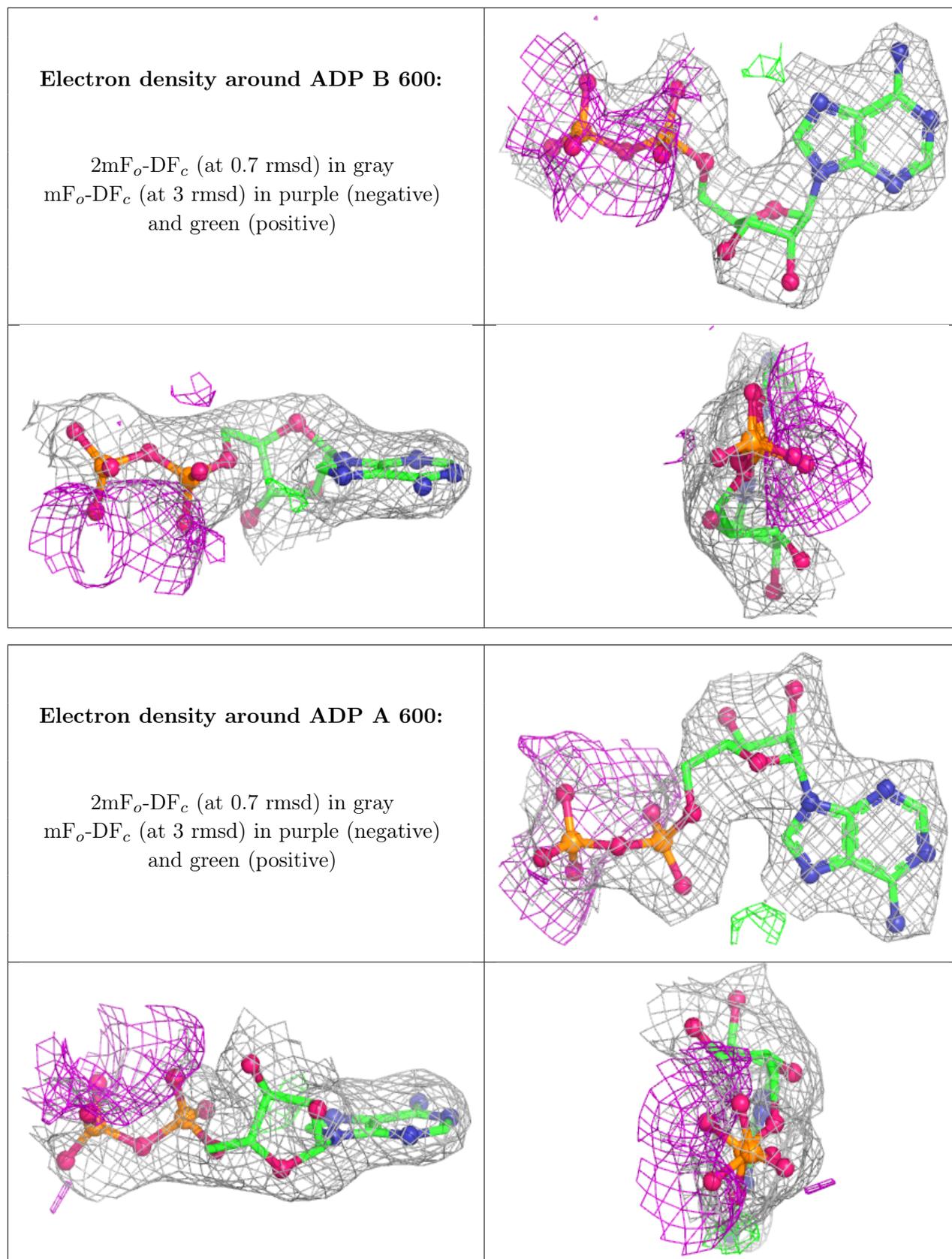
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	IHP	B	500	36/36	0.97	0.11	11,14,18,18	0
4	ADP	B	600	27/27	0.97	0.14	4,8,11,11	0
4	ADP	A	600	27/27	0.98	0.13	9,12,23,24	0
2	IHP	A	500	36/36	0.98	0.11	9,12,22,24	0
5	ZN	A	700	1/1	0.98	0.06	33,33,33,33	0
5	ZN	B	700	1/1	0.98	0.06	56,56,56,56	0
3	PB	A	502	1/1	0.99	0.02	20,20,20,20	0
3	PB	B	503	1/1	0.99	0.03	30,30,30,30	0
3	PB	A	501	1/1	0.99	0.04	27,27,27,27	0
3	PB	B	504	1/1	1.00	0.01	22,22,22,22	0

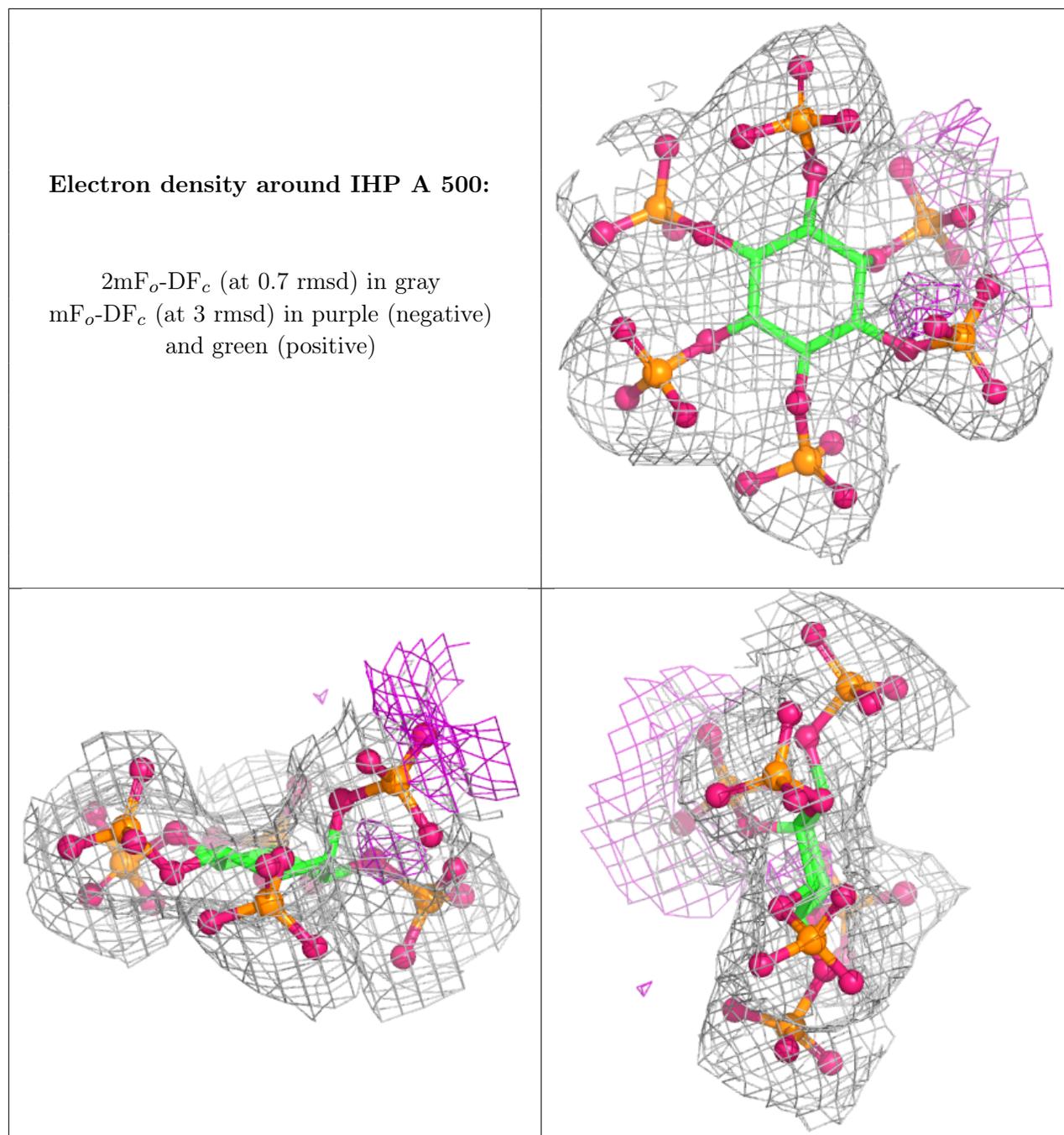
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IHP B 500:

$2mF_o-DF_c$ (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.