



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 02:10 AM EDT

PDB ID : 3UDZ  
Title : Inositol 1,3,4,5,6-pentakisphosphate 2-kinase from *A. thaliana* in complex with ADP and IP6.  
Authors : Gosein, V.; Leung, T.-F.; Krajden, O.; Miller, G.J.  
Deposited on : 2011-10-28  
Resolution : 2.50 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	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

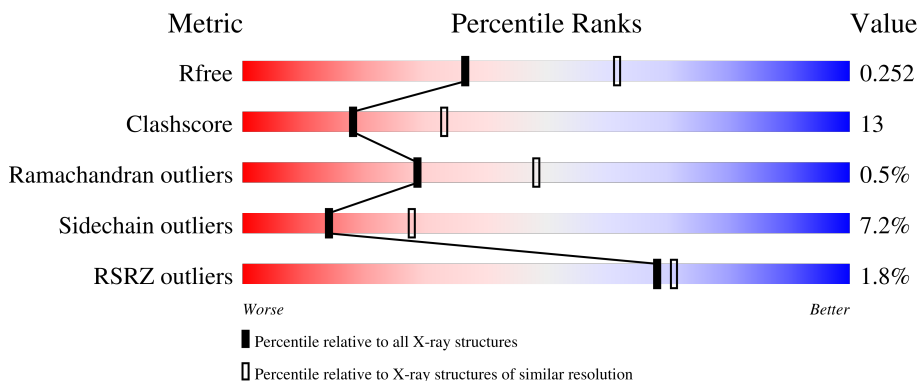
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	493	
1	B	493	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6760 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
1	A	379	Total	C	N	O	S	Se	0	0	0
			3028	1935	509	572	7	5			
1	B	393	Total	C	N	O	S	Se	0	0	0
			3140	2008	529	592	7	4			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MSE	-	expression tag	UNP Q93YN9
A	-32	GLY	-	expression tag	UNP Q93YN9
A	-31	SER	-	expression tag	UNP Q93YN9
A	-30	SER	-	expression tag	UNP Q93YN9
A	-29	HIS	-	expression tag	UNP Q93YN9
A	-28	HIS	-	expression tag	UNP Q93YN9
A	-27	HIS	-	expression tag	UNP Q93YN9
A	-26	HIS	-	expression tag	UNP Q93YN9
A	-25	HIS	-	expression tag	UNP Q93YN9
A	-24	HIS	-	expression tag	UNP Q93YN9
A	-23	SER	-	expression tag	UNP Q93YN9
A	-22	SER	-	expression tag	UNP Q93YN9
A	-21	GLY	-	expression tag	UNP Q93YN9
A	-20	LEU	-	expression tag	UNP Q93YN9
A	-19	VAL	-	expression tag	UNP Q93YN9
A	-18	PRO	-	expression tag	UNP Q93YN9
A	-17	ARG	-	expression tag	UNP Q93YN9
A	-16	GLY	-	expression tag	UNP Q93YN9
A	-15	SER	-	expression tag	UNP Q93YN9
A	-14	HIS	-	expression tag	UNP Q93YN9
A	-13	MSE	-	expression tag	UNP Q93YN9
A	-12	ALA	-	expression tag	UNP Q93YN9
A	-11	SER	-	expression tag	UNP Q93YN9
A	-10	MSE	-	expression tag	UNP Q93YN9
A	-9	THR	-	expression tag	UNP Q93YN9

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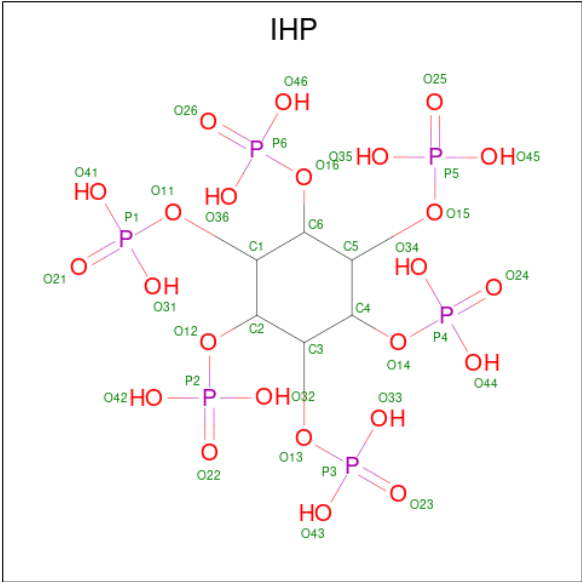
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP Q93YN9
A	-7	GLY	-	expression tag	UNP Q93YN9
A	-6	GLN	-	expression tag	UNP Q93YN9
A	-5	GLN	-	expression tag	UNP Q93YN9
A	-4	MSE	-	expression tag	UNP Q93YN9
A	-3	GLY	-	expression tag	UNP Q93YN9
A	-2	ARG	-	expression tag	UNP Q93YN9
A	-1	ILE	-	expression tag	UNP Q93YN9
A	0	LEU	-	expression tag	UNP Q93YN9
A	54	SER	ALA	conflict	UNP Q93YN9
A	90	GLN	LYS	conflict	UNP Q93YN9
A	157	THR	SER	conflict	UNP Q93YN9
A	185	ILE	MET	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
A	452	ASP	-	expression tag	UNP Q93YN9
A	453	TYR	-	expression tag	UNP Q93YN9
A	454	LYS	-	expression tag	UNP Q93YN9
A	455	ASP	-	expression tag	UNP Q93YN9
A	456	ASP	-	expression tag	UNP Q93YN9
A	457	ASP	-	expression tag	UNP Q93YN9
A	458	ASP	-	expression tag	UNP Q93YN9
A	459	LYS	-	expression tag	UNP Q93YN9
B	-33	MSE	-	expression tag	UNP Q93YN9
B	-32	GLY	-	expression tag	UNP Q93YN9
B	-31	SER	-	expression tag	UNP Q93YN9
B	-30	SER	-	expression tag	UNP Q93YN9
B	-29	HIS	-	expression tag	UNP Q93YN9
B	-28	HIS	-	expression tag	UNP Q93YN9
B	-27	HIS	-	expression tag	UNP Q93YN9
B	-26	HIS	-	expression tag	UNP Q93YN9
B	-25	HIS	-	expression tag	UNP Q93YN9
B	-24	HIS	-	expression tag	UNP Q93YN9
B	-23	SER	-	expression tag	UNP Q93YN9
B	-22	SER	-	expression tag	UNP Q93YN9
B	-21	GLY	-	expression tag	UNP Q93YN9
B	-20	LEU	-	expression tag	UNP Q93YN9
B	-19	VAL	-	expression tag	UNP Q93YN9
B	-18	PRO	-	expression tag	UNP Q93YN9

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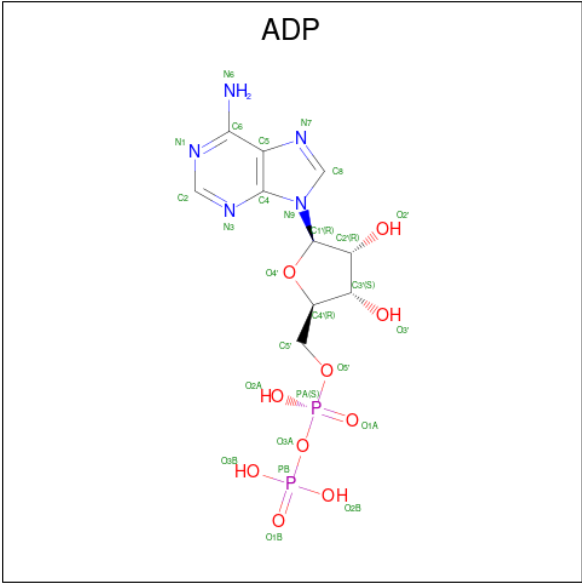
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	ARG	-	expression tag	UNP Q93YN9
B	-16	GLY	-	expression tag	UNP Q93YN9
B	-15	SER	-	expression tag	UNP Q93YN9
B	-14	HIS	-	expression tag	UNP Q93YN9
B	-13	MSE	-	expression tag	UNP Q93YN9
B	-12	ALA	-	expression tag	UNP Q93YN9
B	-11	SER	-	expression tag	UNP Q93YN9
B	-10	MSE	-	expression tag	UNP Q93YN9
B	-9	THR	-	expression tag	UNP Q93YN9
B	-8	GLY	-	expression tag	UNP Q93YN9
B	-7	GLY	-	expression tag	UNP Q93YN9
B	-6	GLN	-	expression tag	UNP Q93YN9
B	-5	GLN	-	expression tag	UNP Q93YN9
B	-4	MSE	-	expression tag	UNP Q93YN9
B	-3	GLY	-	expression tag	UNP Q93YN9
B	-2	ARG	-	expression tag	UNP Q93YN9
B	-1	ILE	-	expression tag	UNP Q93YN9
B	0	LEU	-	expression tag	UNP Q93YN9
B	54	SER	ALA	conflict	UNP Q93YN9
B	90	GLN	LYS	conflict	UNP Q93YN9
B	157	THR	SER	conflict	UNP Q93YN9
B	185	ILE	MET	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
B	452	ASP	-	expression tag	UNP Q93YN9
B	453	TYR	-	expression tag	UNP Q93YN9
B	454	LYS	-	expression tag	UNP Q93YN9
B	455	ASP	-	expression tag	UNP Q93YN9
B	456	ASP	-	expression tag	UNP Q93YN9
B	457	ASP	-	expression tag	UNP Q93YN9
B	458	ASP	-	expression tag	UNP Q93YN9
B	459	LYS	-	expression tag	UNP Q93YN9

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C<sub>6</sub>H<sub>18</sub>O<sub>24</sub>P<sub>6</sub>).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

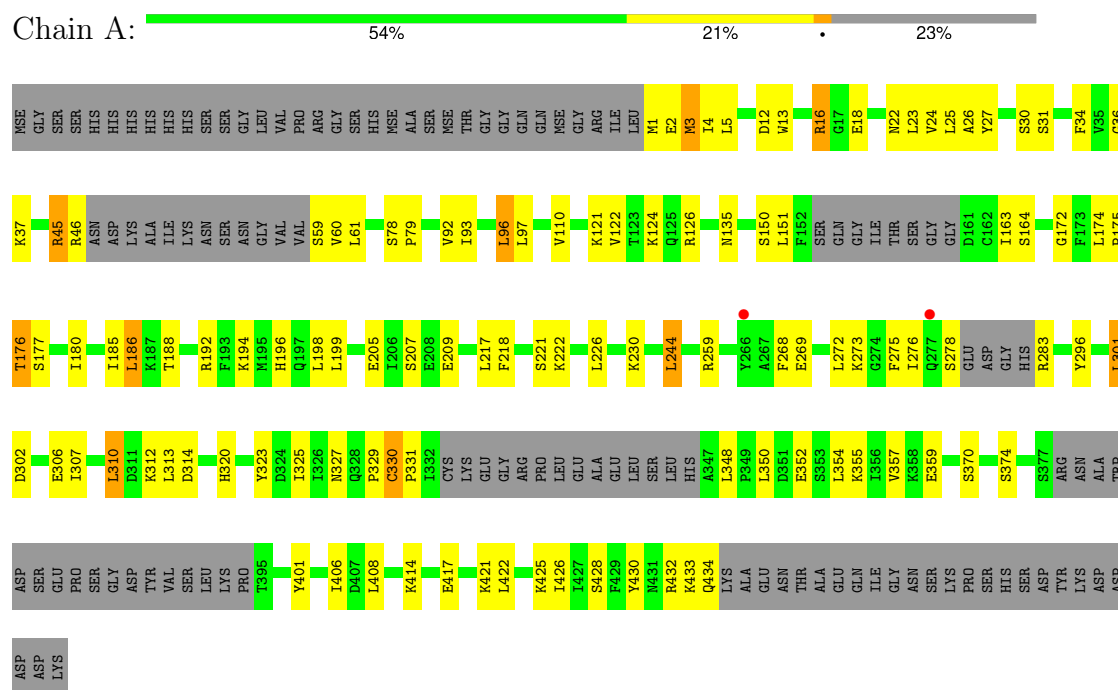
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	235	Total	O	0	0
			235	235		
6	B	226	Total	O	0	0
			226	226		

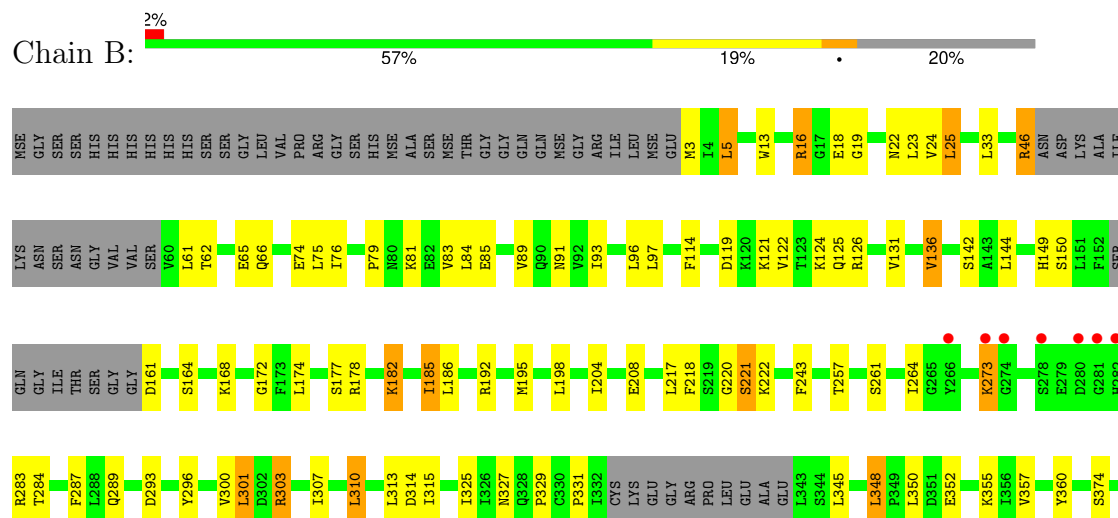
### 3 Residue-property plots

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.

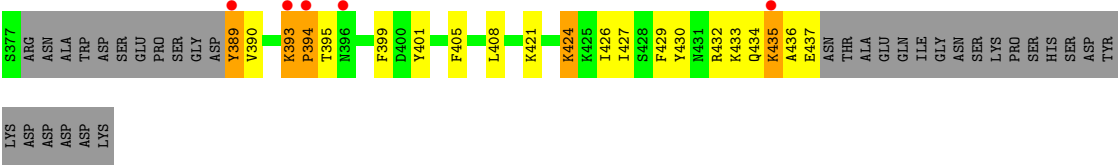
#### • Molecule 1: Inositol pentakisphosphate 2-kinase



#### • Molecule 1: Inositol pentakisphosphate 2-kinase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.06Å 59.39Å 82.75Å 89.84° 82.58° 63.36°	Depositor
Resolution (Å)	41.44 – 2.50 41.44 – 2.09	Depositor EDS
% Data completeness (in resolution range)	94.5 (41.44-2.50) 90.8 (41.44-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.49 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.6.3_473	Depositor
R, $R_{free}$	0.189 , 0.260 0.182 , 0.252	Depositor DCC
$R_{free}$ test set	2669 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6760	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

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

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	0.46	1/3076 (0.0%)	0.60	1/4136 (0.0%)
1	B	0.40	0/3194	0.56	0/4300
All	All	0.43	1/6270 (0.0%)	0.58	1/8436 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	330	CYS	CB-SG	10.34	1.99	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	CYS	CA-CB-SG	9.70	131.46	114.00

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	3028	0	3065	84	0
1	B	3140	0	3174	90	0
2	A	36	0	6	0	0
2	B	36	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	12	1	0
3	B	27	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	B	1	0	0	0	0
6	A	235	0	0	10	0
6	B	226	0	0	4	0
All	All	6760	0	6275	168	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 13.

All (168) 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:NH1	1:B:182:LYS:HD3	1.76	1.00
1:A:46:ARG:HH21	1:A:135:ASN:HB3	1.27	0.99
1:B:195:MSE:HE1	1:B:427:ILE:HA	1.43	0.97
1:A:46:ARG:NH2	1:A:135:ASN:HB3	1.81	0.95
1:A:320:HIS:ND1	1:A:330:CYS:SG	2.45	0.88
1:B:74:GLU:HG3	1:B:91:ASN:OD1	1.75	0.86
1:A:2:GLU:O	1:A:3:MSE:HB2	1.79	0.82
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.44	0.81
1:B:435:LYS:O	1:B:437:GLU:HG2	1.82	0.80
1:B:195:MSE:HE3	1:B:430:TYR:CB	2.12	0.79
1:A:275:PHE:HD1	1:A:276:ILE:HD12	1.48	0.78
1:A:46:ARG:HH21	1:A:135:ASN:CB	1.99	0.75
1:A:46:ARG:HH11	1:B:182:LYS:HD3	1.51	0.74
1:B:178:ARG:HH11	1:B:178:ARG:HG3	1.55	0.71
1:A:45:ARG:HH11	1:A:45:ARG:CG	2.05	0.69
1:B:16:ARG:NH2	1:B:150:SER:OG	2.25	0.69
1:B:222:LYS:HD3	1:B:296:TYR:CD2	2.28	0.69
1:B:46:ARG:NH2	1:B:131:VAL:O	2.26	0.68
1:B:195:MSE:HE2	1:B:426:ILE:HG22	1.74	0.68
1:A:18:GLU:OE1	1:A:126:ARG:HD2	1.95	0.67
1:B:195:MSE:CE	1:B:427:ILE:HA	2.23	0.67
1:B:18:GLU:OE1	1:B:126:ARG:HD2	1.95	0.67
1:B:97:LEU:O	1:B:303:ARG:NH1	2.19	0.66
1:A:226:LEU:HD11	1:A:230:LYS:HE3	1.76	0.65
1:B:220:GLY:O	1:B:296:TYR:HE1	1.81	0.63
1:B:195:MSE:HE3	1:B:430:TYR:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:HG3	1:A:296:TYR:CE2	2.35	0.62
1:B:25:LEU:HD22	1:B:25:LEU:N	2.14	0.61
1:A:198:LEU:HD12	1:A:430:TYR:CD1	2.36	0.61
1:B:195:MSE:HE3	1:B:430:TYR:HB2	1.83	0.61
1:B:5:LEU:HD23	1:B:114:PHE:CZ	2.36	0.61
1:A:16:ARG:NH1	1:A:26:ALA:HB2	2.15	0.60
1:A:97:LEU:HG	1:A:307:ILE:HD12	1.83	0.60
1:A:302:ASP:O	1:A:306:GLU:HG3	2.01	0.60
1:B:315:ILE:HB	1:B:360:TYR:OH	2.01	0.60
1:B:222:LYS:NZ	1:B:293:ASP:OD1	2.30	0.59
1:A:172:GLY:HA3	1:A:218:PHE:CD2	2.37	0.59
1:A:5:LEU:HB2	1:A:110:VAL:HG12	1.84	0.59
1:A:97:LEU:HG	1:A:307:ILE:CD1	2.34	0.58
1:B:74:GLU:HG2	1:B:75:LEU:N	2.18	0.58
1:B:393:LYS:HD3	1:B:393:LYS:H	1.67	0.58
1:A:269:GLU:OE2	1:A:283:ARG:HB2	2.05	0.57
1:A:93:ILE:HG21	1:A:408:LEU:HD13	1.85	0.57
1:B:172:GLY:HA3	1:B:218:PHE:CD2	2.40	0.57
1:B:25:LEU:N	1:B:25:LEU:CD2	2.67	0.56
1:B:204:ILE:HG22	1:B:204:ILE:O	2.05	0.56
1:B:352:GLU:OE2	1:B:355:LYS:HE3	2.04	0.56
1:B:79:PRO:HD2	1:B:83:VAL:HG11	1.87	0.56
1:B:97:LEU:HG	1:B:307:ILE:HD12	1.86	0.56
1:B:289:GLN:HG2	1:B:393:LYS:NZ	2.21	0.56
1:A:329:PRO:O	1:A:331:PRO:HD3	2.05	0.56
1:B:25:LEU:HD11	1:B:122:VAL:HG11	1.88	0.55
1:B:149:HIS:O	1:B:374:SER:OG	2.23	0.55
1:A:46:ARG:HH11	1:B:182:LYS:HB2	1.72	0.54
1:B:13:TRP:O	1:B:121:LYS:HE2	2.08	0.54
1:A:186:LEU:HB2	6:A:524:HOH:O	2.07	0.53
1:B:119:ASP:OD1	1:B:136:VAL:HG13	2.09	0.53
1:B:217:LEU:HG	1:B:301:LEU:HD21	1.90	0.53
1:A:12:ASP:HB3	1:A:27:TYR:CE1	2.43	0.53
1:A:45:ARG:N	1:A:45:ARG:HD2	2.23	0.53
1:B:393:LYS:N	1:B:394:PRO:HD2	2.23	0.53
1:A:422:LEU:O	1:A:426:ILE:HG12	2.08	0.53
1:B:307:ILE:O	1:B:310:LEU:HB2	2.09	0.52
1:A:46:ARG:HH11	1:B:182:LYS:CD	2.21	0.52
1:B:164:SER:OG	1:B:243:PHE:HB2	2.09	0.52
1:B:261:SER:OG	1:B:264:ILE:HG12	2.10	0.52
1:B:300:VAL:HG22	1:B:405:PHE:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ASN:N	3:A:600:ADP:O3B	2.42	0.52
1:A:192:ARG:HB2	6:A:581:HOH:O	2.10	0.51
1:A:275:PHE:HD1	1:A:276:ILE:CD1	2.19	0.51
1:B:25:LEU:CD1	1:B:122:VAL:HG11	2.41	0.51
1:A:92:VAL:O	1:A:96:LEU:HD22	2.10	0.51
1:A:370:SER:HB2	1:A:406:ILE:HG13	1.93	0.51
1:A:325:ILE:HD12	1:A:357:VAL:HG21	1.91	0.51
1:A:275:PHE:CD1	1:A:276:ILE:HD12	2.37	0.51
1:A:222:LYS:HE3	1:A:296:TYR:CE2	2.46	0.51
1:B:204:ILE:HD12	1:B:204:ILE:N	2.26	0.50
1:A:185:ILE:O	1:A:188:THR:HB	2.12	0.50
1:B:325:ILE:HD12	1:B:357:VAL:HG21	1.93	0.50
1:B:345:LEU:HA	1:B:348:LEU:HD22	1.94	0.50
1:B:62:THR:OG1	1:B:65:GLU:HG3	2.12	0.50
1:B:424:LYS:HD2	6:B:579:HOH:O	2.10	0.50
1:A:1:MSE:HB2	6:A:660:HOH:O	2.12	0.49
1:A:176:THR:HB	6:A:537:HOH:O	2.13	0.49
1:B:3:MSE:HE1	1:B:33:LEU:CD1	2.42	0.49
1:A:199:LEU:HD21	1:A:425:LYS:HE2	1.94	0.49
1:B:23:LEU:HD11	1:B:126:ARG:HD3	1.95	0.48
1:A:222:LYS:HG3	1:A:296:TYR:CZ	2.49	0.48
1:A:177:SER:HA	6:A:684:HOH:O	2.13	0.48
1:B:93:ILE:HG21	1:B:408:LEU:HD13	1.97	0.47
1:B:390:VAL:HG23	1:B:401:TYR:CD2	2.49	0.47
1:B:16:ARG:HB3	1:B:24:VAL:O	2.14	0.47
1:A:313:LEU:O	1:A:314:ASP:HB3	2.14	0.47
1:A:217:LEU:HG	1:A:301:LEU:HD21	1.95	0.47
1:B:429:PHE:CZ	1:B:433:LYS:HD3	2.50	0.47
1:A:124:LYS:HD3	1:A:124:LYS:HA	1.73	0.47
1:A:374:SER:O	1:A:401:TYR:HA	2.15	0.46
1:B:178:ARG:HH11	1:B:178:ARG:CG	2.24	0.46
1:A:323:TYR:CD2	1:A:331:PRO:HD2	2.50	0.46
1:A:428:SER:O	1:A:432:ARG:HG3	2.16	0.46
1:A:205:GLU:HG2	1:B:178:ARG:CZ	2.46	0.46
1:B:185:ILE:HD12	1:B:185:ILE:HA	1.67	0.46
1:A:36:GLY:HA2	1:A:151:LEU:HD12	1.97	0.45
1:A:45:ARG:CG	1:A:45:ARG:NH1	2.72	0.45
1:A:417:GLU:O	1:A:421:LYS:HG3	2.17	0.45
1:B:327:ASN:HB2	6:B:472:HOH:O	2.16	0.45
1:A:354:LEU:HB3	6:A:596:HOH:O	2.17	0.45
1:A:355:LYS:O	1:A:359:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLN:NE2	6:B:523:HOH:O	2.50	0.45
1:B:389:TYR:HA	1:B:399:PHE:O	2.17	0.45
1:A:27:TYR:OH	1:A:31:SER:HB3	2.17	0.45
1:B:222:LYS:HD3	1:B:296:TYR:CG	2.52	0.45
1:B:85:GLU:O	1:B:89:VAL:HG23	2.16	0.44
1:A:13:TRP:O	1:A:121:LYS:HE3	2.18	0.44
1:B:325:ILE:CD1	1:B:357:VAL:HG21	2.47	0.44
1:B:329:PRO:O	1:B:331:PRO:HD3	2.17	0.44
1:A:2:GLU:O	1:A:3:MSE:CB	2.55	0.44
1:A:268:PHE:CE2	1:A:272:LEU:HD11	2.53	0.44
1:A:23:LEU:HD21	1:A:122:VAL:HG21	2.00	0.44
1:A:13:TRP:CZ3	1:A:27:TYR:HB2	2.52	0.44
1:A:307:ILE:O	1:A:310:LEU:HB2	2.17	0.44
1:B:168:LYS:HE3	2:B:500:IHP:O22	2.18	0.44
1:B:433:LYS:O	1:B:436:ALA:HB3	2.18	0.44
1:B:393:LYS:HG2	1:B:394:PRO:HD3	2.00	0.43
1:A:25:LEU:HD21	1:A:122:VAL:HG11	2.00	0.43
1:B:437:GLU:HA	1:B:437:GLU:OE1	2.18	0.43
1:A:59:SER:HA	1:A:60:VAL:HA	1.64	0.43
1:A:327:ASN:ND2	6:A:523:HOH:O	2.26	0.43
1:A:25:LEU:CD2	1:A:122:VAL:HG11	2.48	0.43
1:B:310:LEU:HD12	1:B:310:LEU:HA	1.76	0.43
1:A:273:LYS:O	1:A:273:LYS:HG3	2.18	0.43
1:B:429:PHE:O	1:B:433:LYS:HG2	2.19	0.43
1:A:78:SER:HA	1:A:79:PRO:HD2	1.78	0.42
1:B:221:SER:N	6:B:520:HOH:O	2.51	0.42
1:A:150:SER:HA	1:A:164:SER:OG	2.19	0.42
1:A:194:LYS:NZ	6:A:669:HOH:O	2.52	0.42
1:A:16:ARG:HB3	1:A:24:VAL:O	2.20	0.42
1:A:34:PHE:HA	1:A:37:LYS:HG3	2.01	0.42
1:B:198:LEU:HD12	1:B:430:TYR:CD1	2.54	0.42
1:B:74:GLU:CG	1:B:75:LEU:N	2.81	0.42
1:B:394:PRO:HG2	1:B:395:THR:H	1.85	0.42
1:A:194:LYS:HE2	1:A:209:GLU:OE2	2.20	0.42
1:A:3:MSE:N	6:A:592:HOH:O	2.52	0.41
1:B:18:GLU:OE1	1:B:126:ARG:CD	2.66	0.41
1:B:273:LYS:HA	1:B:283:ARG:CZ	2.50	0.41
1:A:45:ARG:HD2	1:A:45:ARG:H	1.82	0.41
1:B:61:LEU:CD1	1:B:76:ILE:HG22	2.49	0.41
1:A:3:MSE:HE3	6:A:642:HOH:O	2.20	0.41
1:A:312:LYS:HB2	1:A:312:LYS:HE2	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LEU:HD21	1:B:122:VAL:HG21	2.02	0.41
1:A:46:ARG:HH11	1:B:182:LYS:CB	2.33	0.41
1:B:284:THR:O	1:B:287:PHE:HB3	2.20	0.41
1:B:393:LYS:CD	1:B:394:PRO:HD3	2.51	0.41
1:B:3:MSE:HE1	1:B:33:LEU:HD13	2.01	0.41
1:B:124:LYS:HE2	1:B:124:LYS:HB2	1.86	0.41
1:B:313:LEU:O	1:B:314:ASP:HB3	2.20	0.41
1:A:163:ILE:HD11	1:A:244:LEU:HG	2.02	0.41
1:A:176:THR:O	1:A:176:THR:HG23	2.20	0.41
1:B:429:PHE:O	1:B:432:ARG:HB3	2.21	0.41
1:A:188:THR:O	1:A:188:THR:HG22	2.21	0.41
1:A:430:TYR:O	1:A:434:GLN:HG2	2.20	0.41
1:B:19:GLY:HA3	2:B:500:IHP:O32	2.21	0.41
1:B:74:GLU:OE1	1:B:74:GLU:N	2.46	0.41
1:A:175:PRO:HB2	1:A:180:ILE:HD11	2.04	0.40
1:B:18:GLU:HB2	1:B:22:ASN:O	2.21	0.40
1:B:24:VAL:C	1:B:25:LEU:HD22	2.41	0.40
1:A:60:VAL:HG23	1:A:61:LEU:N	2.36	0.40
1:B:81:LYS:O	1:B:84:LEU:HB3	2.21	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	367/493 (74%)	349 (95%)	15 (4%)	3 (1%)	19	35
1	B	383/493 (78%)	367 (96%)	15 (4%)	1 (0%)	41	61
All	All	750/986 (76%)	716 (96%)	30 (4%)	4 (0%)	29	48

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	3	MSE
1	B	394	PRO
1	A	4	ILE
1	A	259	ARG

### 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	340/425 (80%)	321 (94%)	19 (6%)	21	40
1	B	352/425 (83%)	321 (91%)	31 (9%)	10	19
All	All	692/850 (81%)	642 (93%)	50 (7%)	14	28

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	30	SER
1	A	45	ARG
1	A	96	LEU
1	A	174	LEU
1	A	176	THR
1	A	186	LEU
1	A	196	HIS
1	A	207	SER
1	A	221	SER
1	A	244	LEU
1	A	278	SER
1	A	301	LEU
1	A	310	LEU
1	A	348	LEU
1	A	350	LEU
1	A	352	GLU
1	A	414	LYS
1	A	433	LYS
1	B	5	LEU

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Mol	Chain	Res	Type
1	B	16	ARG
1	B	25	LEU
1	B	46	ARG
1	B	96	LEU
1	B	125	GLN
1	B	136	VAL
1	B	142	SER
1	B	144	LEU
1	B	161	ASP
1	B	174	LEU
1	B	177	SER
1	B	182	LYS
1	B	185	ILE
1	B	186	LEU
1	B	192	ARG
1	B	208	GLU
1	B	221	SER
1	B	257	THR
1	B	273	LYS
1	B	301	LEU
1	B	303	ARG
1	B	310	LEU
1	B	348	LEU
1	B	350	LEU
1	B	389	TYR
1	B	393	LYS
1	B	421	LYS
1	B	424	LYS
1	B	434	GLN
1	B	435	LYS

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

Mol	Chain	Res	Type
1	A	147	ASN
1	B	66	GLN
1	B	125	GLN
1	B	289	GLN

### 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 9 ligands modelled in this entry, 5 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	4	36,36,36	1.02	0	60,60,60	1.37	9 (15%)
2	IHP	B	500	4	36,36,36	1.09	3 (8%)	60,60,60	1.12	5 (8%)
3	ADP	B	600	4	24,29,29	0.96	2 (8%)	29,45,45	1.10	3 (10%)
3	ADP	A	600	4	24,29,29	1.01	2 (8%)	29,45,45	1.14	2 (6%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	ADP	PA-O3A	2.89	1.62	1.59
3	B	600	ADP	O4'-C1'	2.51	1.44	1.40
3	A	600	ADP	O4'-C1'	2.29	1.43	1.40
2	B	500	IHP	O15-C5	-2.17	1.36	1.44
3	B	600	ADP	PA-O3A	2.14	1.61	1.59
2	B	500	IHP	O14-C4	-2.01	1.37	1.44
2	B	500	IHP	O12-C2	-2.00	1.37	1.44

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	IHP	P5-O15-C5	4.29	134.88	123.43
3	A	600	ADP	N3-C2-N1	-4.10	123.11	128.67
3	B	600	ADP	N3-C2-N1	-3.81	123.50	128.67
2	A	500	IHP	C5-C4-C3	3.69	118.52	110.43
2	B	500	IHP	C6-C1-C2	-3.45	102.86	110.43
2	B	500	IHP	C4-C3-C2	-3.35	103.08	110.43
2	A	500	IHP	C5-C6-C1	3.32	117.72	110.43
2	B	500	IHP	O12-C2-C1	2.72	114.56	108.76
2	A	500	IHP	C6-C5-C4	2.63	116.21	110.43
2	B	500	IHP	O11-C1-C2	2.60	114.30	108.76
3	A	600	ADP	C4-C5-N7	-2.42	106.78	109.34
2	B	500	IHP	C3-C2-C1	-2.41	105.14	110.43
2	A	500	IHP	O13-C3-C4	2.36	113.78	108.76
2	A	500	IHP	O45-P5-O15	2.36	115.04	105.85
2	A	500	IHP	O16-C6-C5	2.30	113.65	108.76
2	A	500	IHP	O15-P5-O25	-2.22	101.41	109.33
3	B	600	ADP	C4-C5-N7	-2.18	107.03	109.34
3	B	600	ADP	O3B-PB-O2B	2.10	115.68	107.80
2	A	500	IHP	O13-P3-O23	2.02	116.52	109.33

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	600	ADP	C5'-O5'-PA-O1A
2	A	500	IHP	C5-O15-P5-O45
2	A	500	IHP	C2-O12-P2-O22
2	B	500	IHP	C3-O13-P3-O23
2	A	500	IHP	C1-O11-P1-O41
2	A	500	IHP	C2-O12-P2-O42

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Mol	Chain	Res	Type	Atoms
2	B	500	IHP	C4-O14-P4-O24

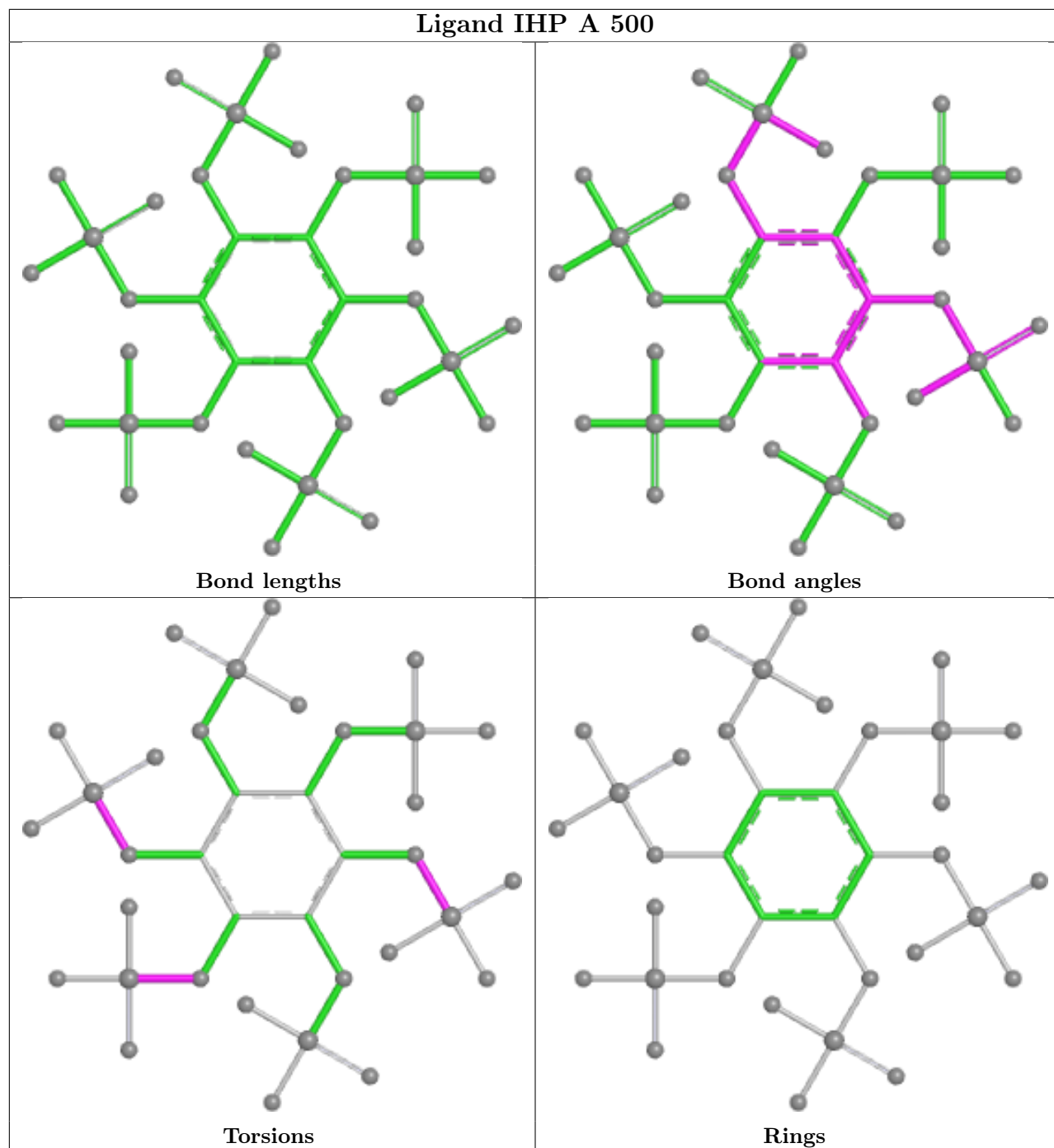
There are no ring outliers.

2 monomers are involved in 3 short contacts:

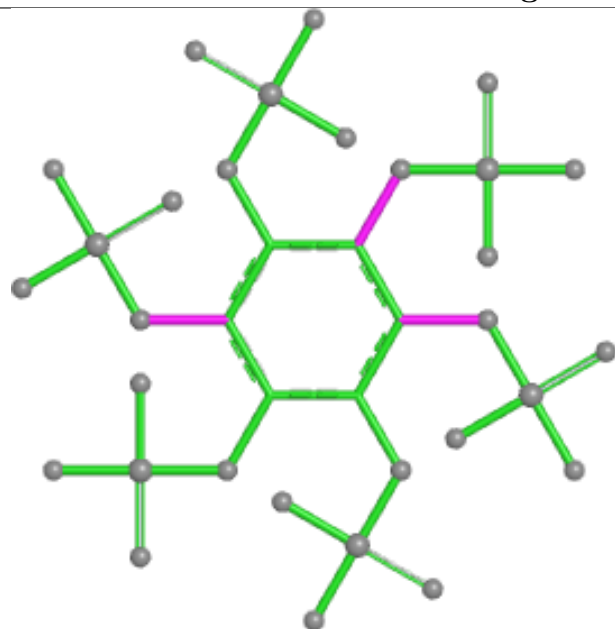
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	IHP	2	0
3	A	600	ADP	1	0

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.

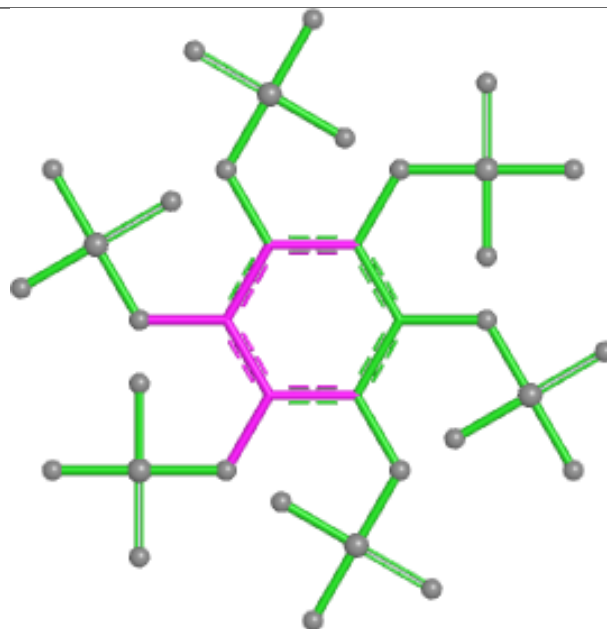
## Ligand IHP A 500



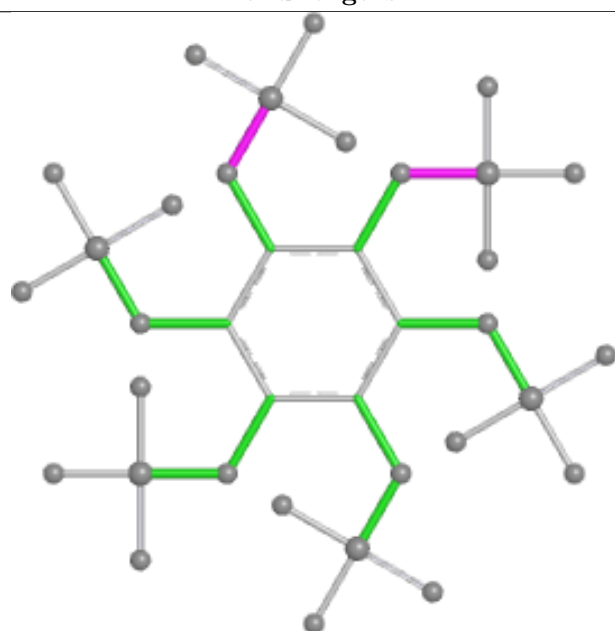
## Ligand IHP B 500



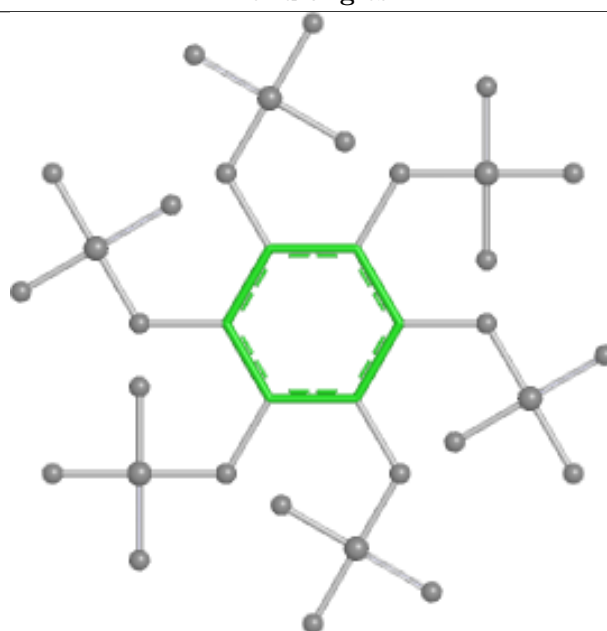
Bond lengths



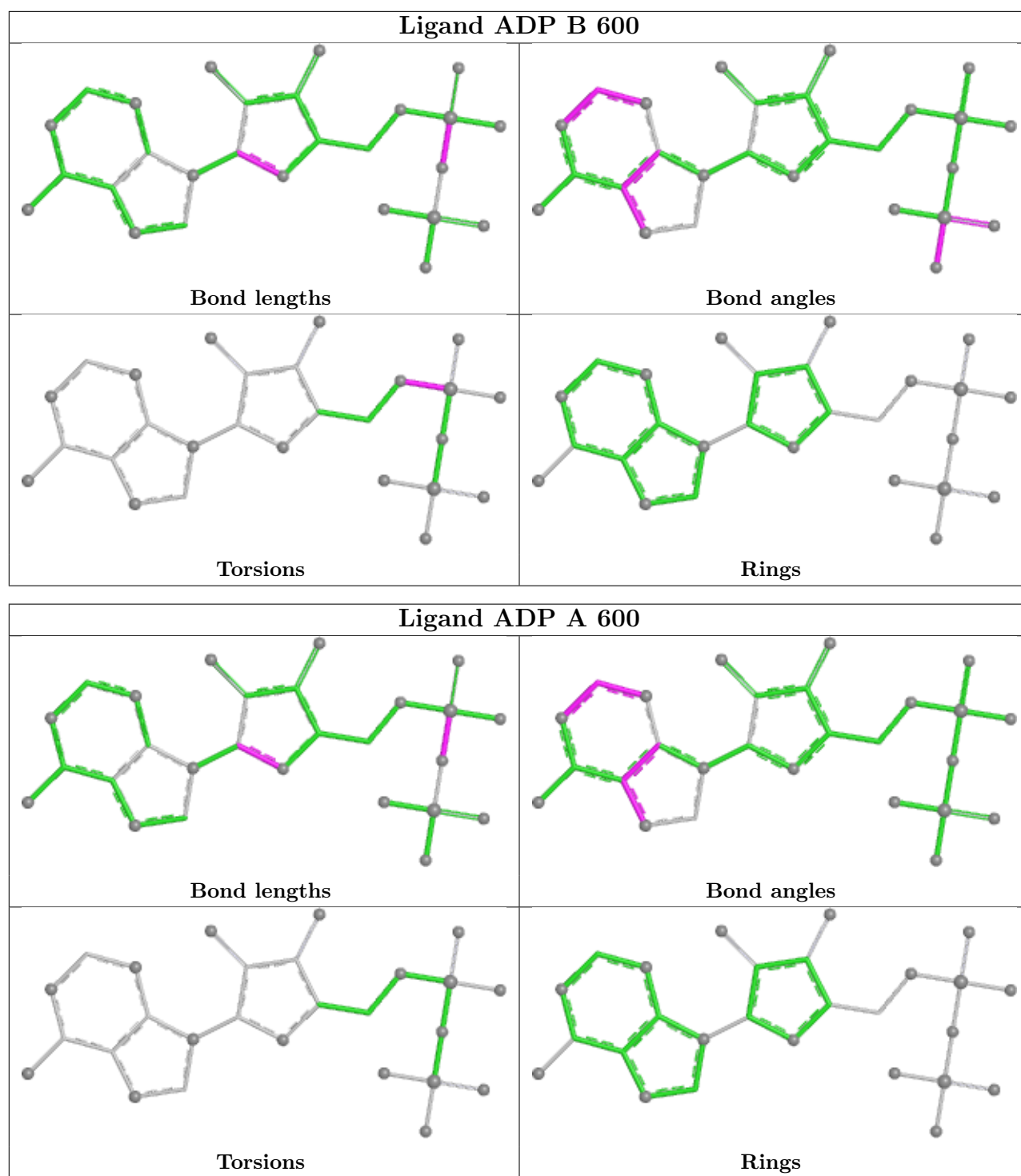
Bond angles



Torsions



Rings



## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 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	374/493 (75%)	-0.54	2 (0%) 91 91	15, 32, 51, 66	0
1	B	389/493 (78%)	-0.38	12 (3%) 49 52	17, 34, 63, 83	0
All	All	763/986 (77%)	-0.46	14 (1%) 68 71	15, 33, 58, 83	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	TYR	4.9
1	B	266	TYR	4.7
1	B	393	LYS	3.0
1	B	274	GLY	3.0
1	B	280	ASP	2.8
1	B	394	PRO	2.8
1	B	273	LYS	2.4
1	B	281	GLY	2.4
1	B	389	TYR	2.3
1	B	282	HIS	2.1
1	B	435	LYS	2.1
1	B	278	SER	2.1
1	A	277	GLN	2.0
1	B	396	ASN	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](#)

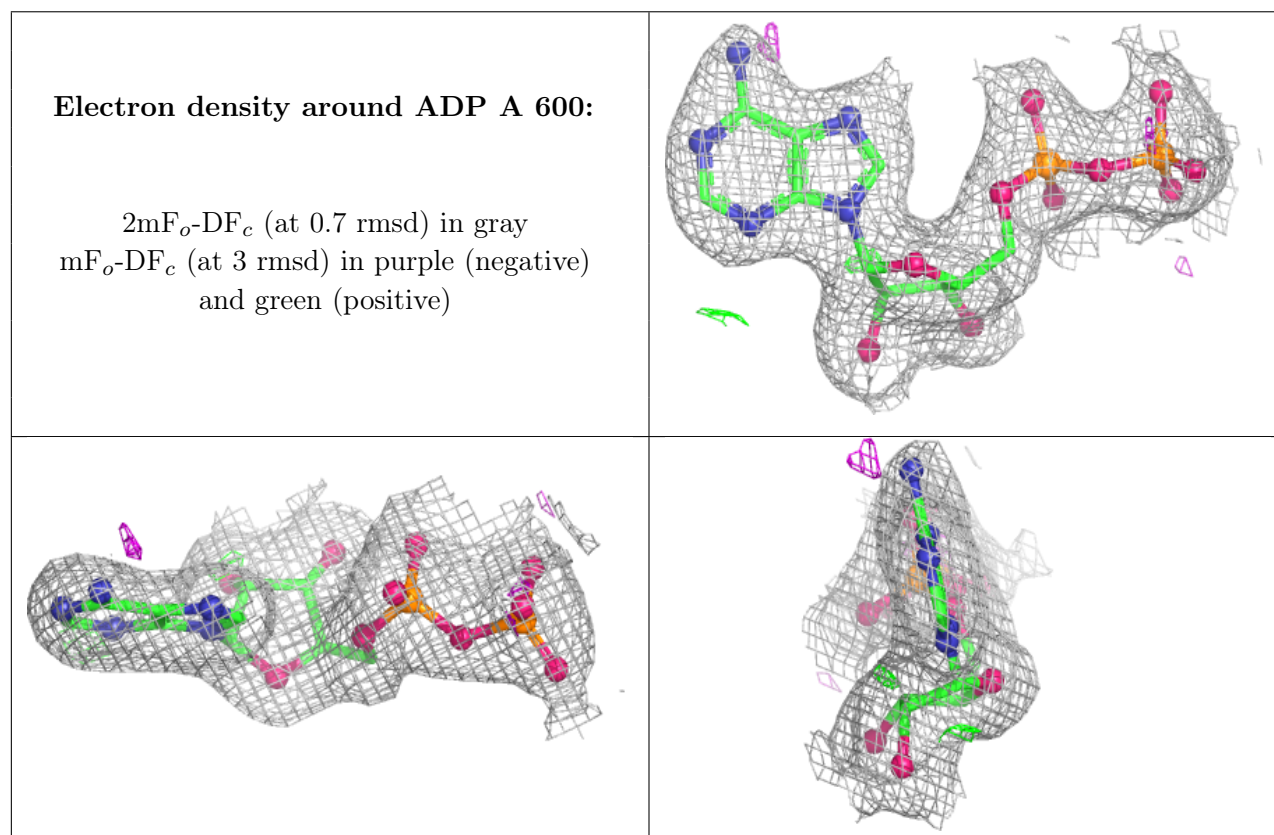
There are no monosaccharides in this entry.

## 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, 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.

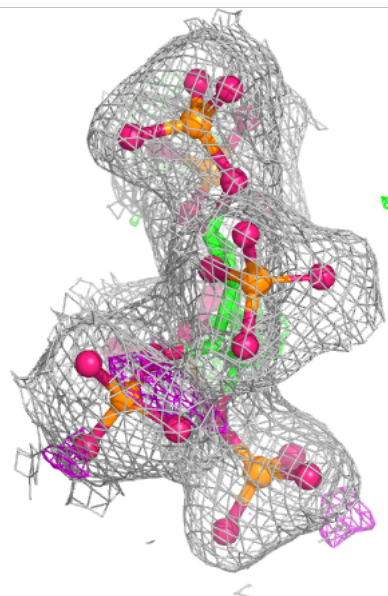
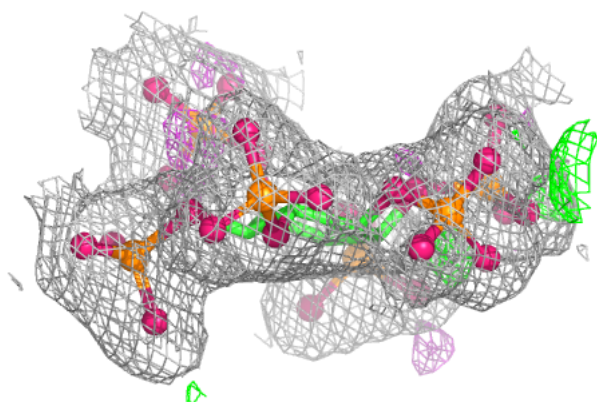
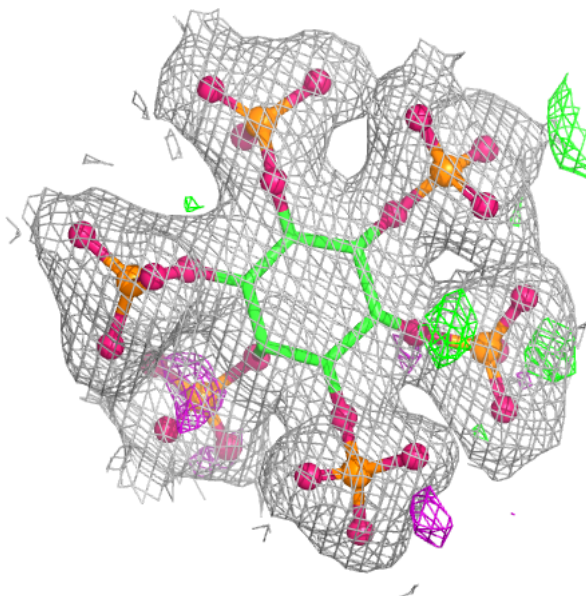
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	A	701	1/1	0.74	0.10	38,38,38,38	0
4	MG	B	701	1/1	0.90	0.12	41,41,41,41	0
3	ADP	A	600	27/27	0.96	0.13	23,28,32,32	0
2	IHP	A	500	36/36	0.97	0.16	14,23,31,38	0
4	MG	B	700	1/1	0.97	0.20	29,29,29,29	0
4	MG	A	700	1/1	0.97	0.08	32,32,32,32	0
2	IHP	B	500	36/36	0.98	0.13	16,25,33,45	0
3	ADP	B	600	27/27	0.98	0.12	27,31,35,39	0
5	ZN	B	800	1/1	1.00	0.06	33,33,33,33	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.



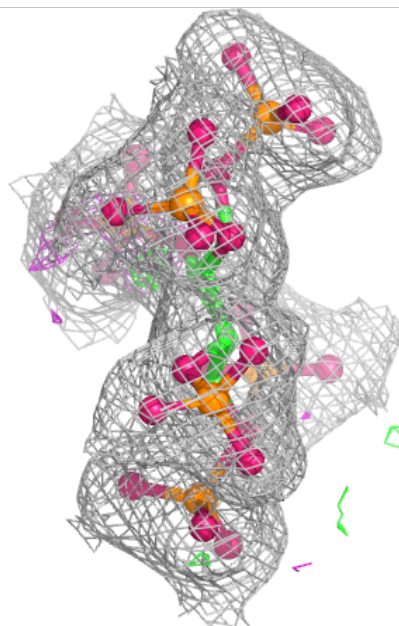
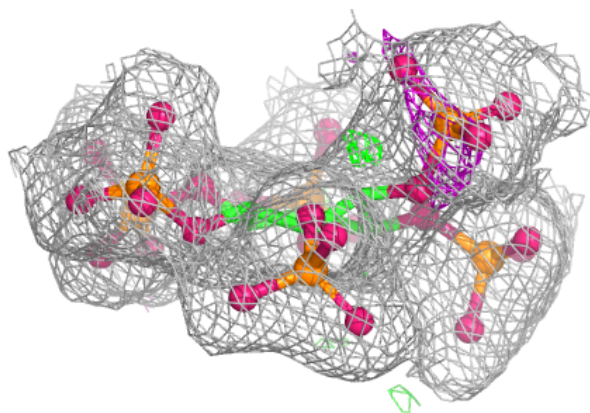
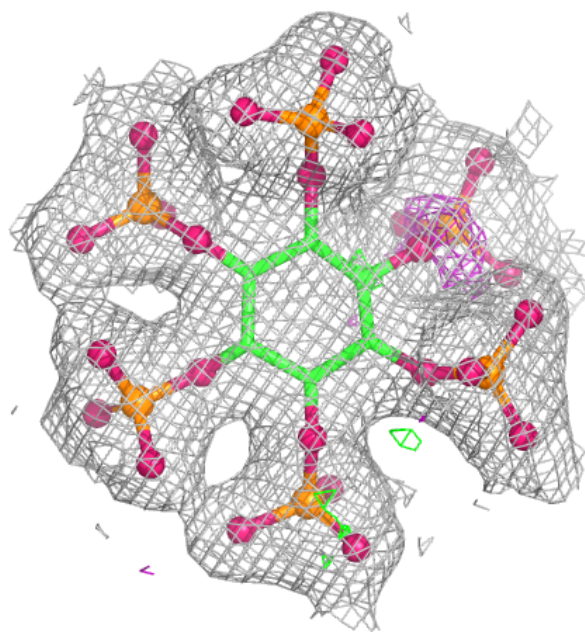
**Electron density around IHP A 500:**

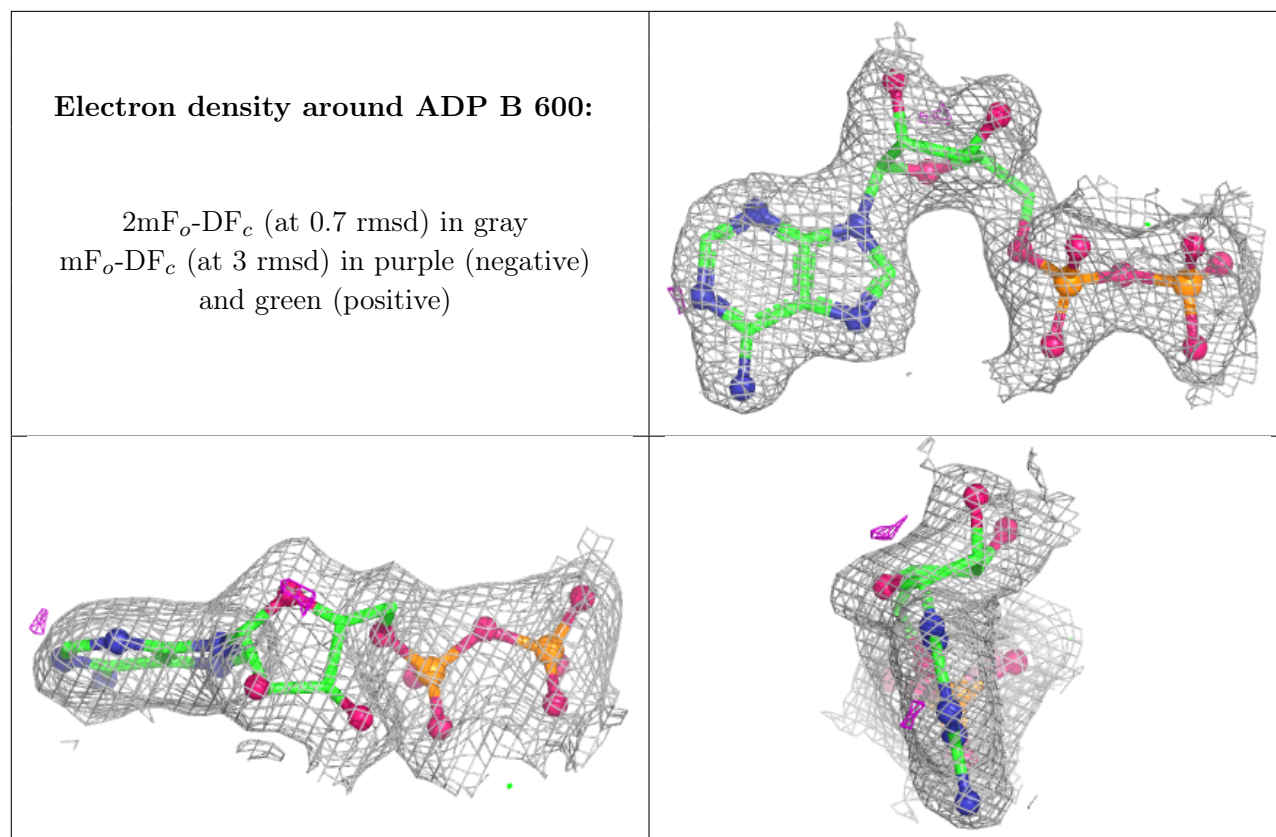
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 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.