



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:45 PM UTC

PDB ID : 5MOE / pdb_00005moe
Title : Crystal Structure of CK2alpha with N-(3-(((2-chloro-[1,1'-biphenyl]-4-yl)met
hyl)amino)propyl)methanesulfonamide bound
Authors : Brear, P.; De Fusco, C.; Georgiou, K.; Iegre, J.; Sore, H.; Hyvonen, M.; Spring,
D.
Deposited on : 2016-12-14
Resolution : 1.89 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

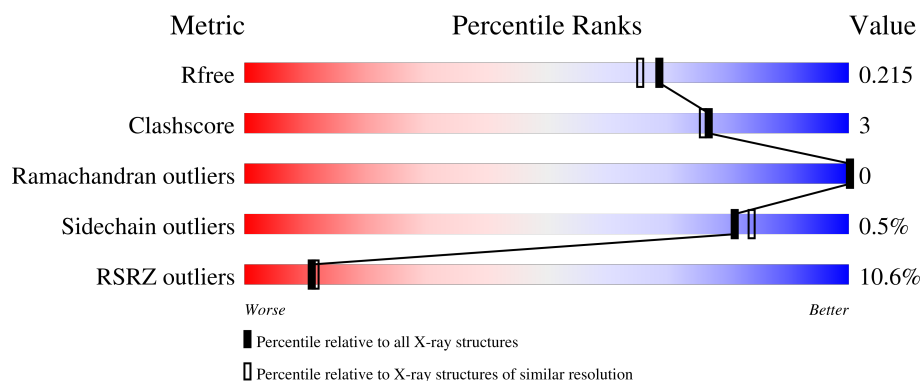
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	352	5% 85% 7% 8%
1	B	352	15% 86% 5% 8%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6006 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	7	0
			2796	1788	492	505	11			
1	B	323	Total	C	N	O	S	0	4	0
			2761	1768	483	498	12			

There are 50 discrepancies between the modelled and reference sequences:

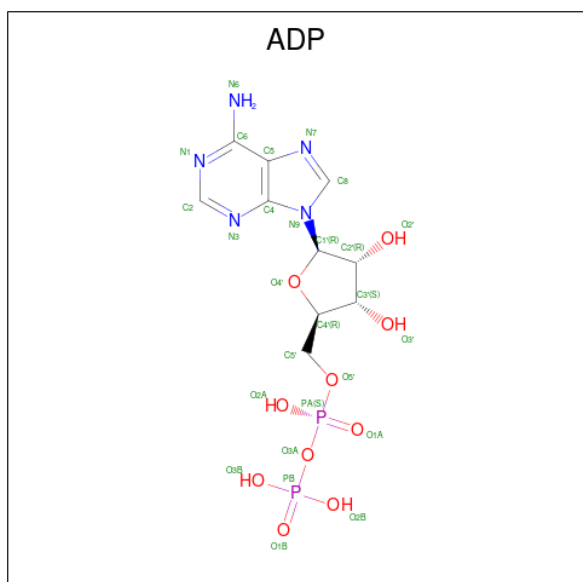
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	expression tag	UNP P68400
A	-21	SER	-	expression tag	UNP P68400
A	-20	MET	-	expression tag	UNP P68400
A	-19	ASP	-	expression tag	UNP P68400
A	-18	ILE	-	expression tag	UNP P68400
A	-17	GLU	-	expression tag	UNP P68400
A	-16	PHE	-	expression tag	UNP P68400
A	-15	ASP	-	expression tag	UNP P68400
A	-14	ASP	-	expression tag	UNP P68400
A	-13	ASP	-	expression tag	UNP P68400
A	-12	ALA	-	expression tag	UNP P68400
A	-11	ASP	-	expression tag	UNP P68400
A	-10	ASP	-	expression tag	UNP P68400
A	-9	ASP	-	expression tag	UNP P68400
A	-8	GLY	-	expression tag	UNP P68400
A	-7	SER	-	expression tag	UNP P68400
A	-6	GLY	-	expression tag	UNP P68400
A	-5	SER	-	expression tag	UNP P68400
A	-4	GLY	-	expression tag	UNP P68400
A	-3	SER	-	expression tag	UNP P68400
A	-2	GLY	-	expression tag	UNP P68400
A	-1	SER	-	expression tag	UNP P68400
A	0	GLY	-	expression tag	UNP P68400
A	1	SER	-	expression tag	UNP P68400
A	21	SER	ARG	engineered mutation	UNP P68400

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP P68400
B	-21	SER	-	expression tag	UNP P68400
B	-20	MET	-	expression tag	UNP P68400
B	-19	ASP	-	expression tag	UNP P68400
B	-18	ILE	-	expression tag	UNP P68400
B	-17	GLU	-	expression tag	UNP P68400
B	-16	PHE	-	expression tag	UNP P68400
B	-15	ASP	-	expression tag	UNP P68400
B	-14	ASP	-	expression tag	UNP P68400
B	-13	ASP	-	expression tag	UNP P68400
B	-12	ALA	-	expression tag	UNP P68400
B	-11	ASP	-	expression tag	UNP P68400
B	-10	ASP	-	expression tag	UNP P68400
B	-9	ASP	-	expression tag	UNP P68400
B	-8	GLY	-	expression tag	UNP P68400
B	-7	SER	-	expression tag	UNP P68400
B	-6	GLY	-	expression tag	UNP P68400
B	-5	SER	-	expression tag	UNP P68400
B	-4	GLY	-	expression tag	UNP P68400
B	-3	SER	-	expression tag	UNP P68400
B	-2	GLY	-	expression tag	UNP P68400
B	-1	SER	-	expression tag	UNP P68400
B	0	GLY	-	expression tag	UNP P68400
B	1	SER	-	expression tag	UNP P68400
B	21	SER	ARG	engineered mutation	UNP P68400

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

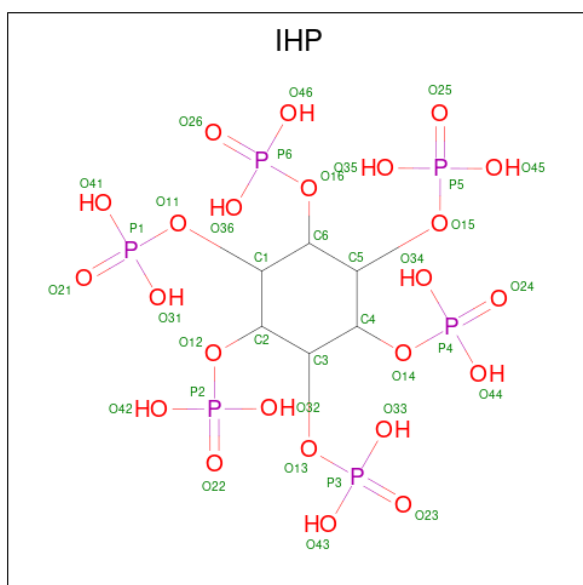


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	
			27	10	5	10	2	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



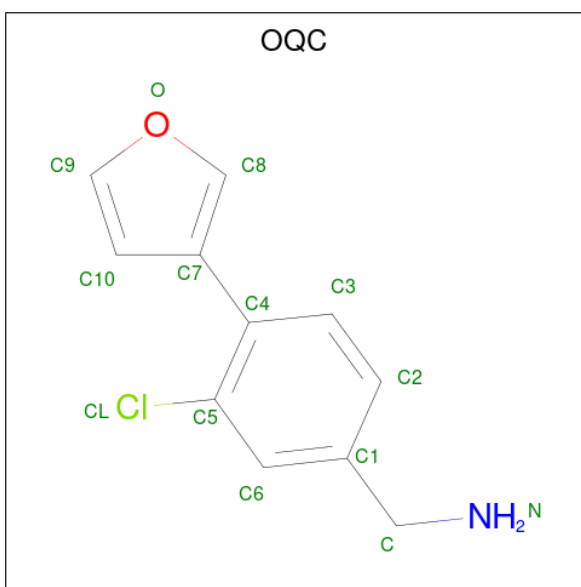
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P		
			36	6	24	6	0	0
4	B	1	Total	C	O	P		
			36	6	24	6	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



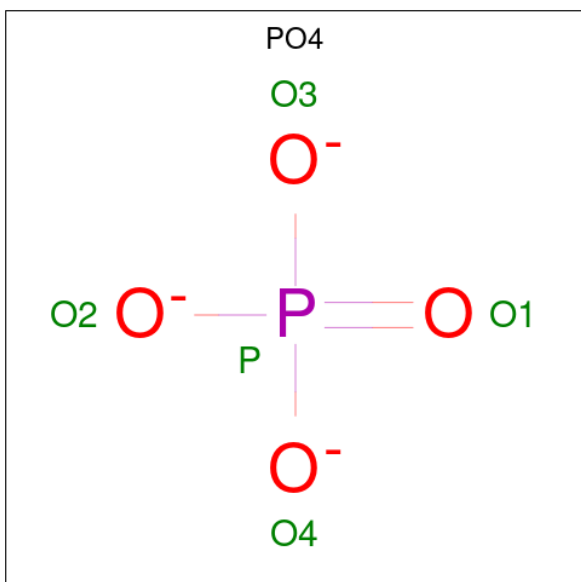
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is [3-chloranyl-4-(furan-3-yl)phenyl]methanamine (CCD ID: OQC) (formula: C₁₁H₁₀ClNO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	0	0
			14	11	1	1	1		
6	A	1	Total	C	Cl	N	O	0	0
			14	11	1	1	1		
6	A	1	Total	C	Cl	N	O	0	0
			14	11	1	1	1		
6	B	1	Total	C	Cl	N	O	0	0
			14	11	1	1	1		
6	B	1	Total	C	Cl	N	O	0	0
			14	11	1	1	1		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

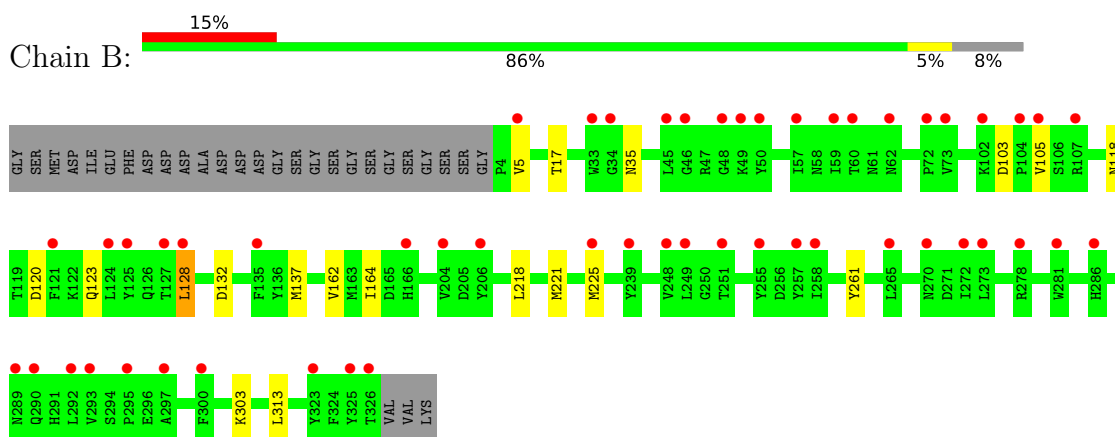
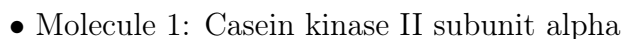


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	151	Total	O	0	0
			151	151		
8	B	65	Total	O	0	0
			65	65		

- Molecule 1: Casein kinase II subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	64.61Å 68.23Å 333.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	166.74 – 1.89 166.74 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.5 (166.74-1.89) 99.9 (166.74-1.89)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 1.88Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.197 , 0.208 0.200 , 0.215	Depositor DCC
R_{free} test set	3021 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6006	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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: OQC, PO4, ADP, MG, IHP, ACT

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	0.93	1/2871 (0.0%)	1.07	5/3884 (0.1%)
1	B	0.83	0/2836	1.06	1/3835 (0.0%)
All	All	0.88	1/5707 (0.0%)	1.07	6/7719 (0.1%)

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
1	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	MET	SD-CE	-5.92	1.64	1.79

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	GLU	CB-CG-CD	6.88	124.30	112.60
1	A	314	THR	N-CA-C	-6.63	101.98	110.53
1	A	282	GLU	CB-CG-CD	5.37	121.73	112.60
1	A	51	SER	N-CA-C	5.24	116.25	108.60
1	A	197	PHE	CA-CB-CG	-5.19	108.61	113.80
1	B	105	VAL	N-CA-C	5.15	115.26	110.42

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35[A]	ASN	Mainchain
1	A	35[B]	ASN	Mainchain
1	B	35[A]	ASN	Mainchain
1	B	35[B]	ASN	Mainchain

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	2796	0	2725	15	0
1	B	2761	0	2693	15	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	36	0	6	0	0
4	B	36	0	6	0	0
5	A	16	0	12	0	0
5	B	12	0	9	0	0
6	A	42	0	0	6	0
6	B	28	0	0	5	0
7	A	5	0	0	0	0
8	A	151	0	0	0	0
8	B	65	0	0	1	0
All	All	6006	0	5475	33	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 3.

All (33) 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:221:MET:HE1	6:B:409:OQC:CL	2.27	0.71
1:B:162:VAL:HG11	6:B:409:OQC:CL	2.36	0.62
1:A:221:MET:HE1	6:A:410:OQC:CL	2.36	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASP:HB2	6:A:411:OQC:C8	2.31	0.60
6:B:408:OQC:C10	6:B:408:OQC:CL	2.89	0.58
6:A:411:OQC:CL	6:A:411:OQC:C10	2.89	0.58
6:A:410:OQC:CL	6:A:410:OQC:C8	2.90	0.56
1:B:221:MET:CE	6:B:409:OQC:CL	2.92	0.54
1:A:15[B]:VAL:CG1	1:A:19:ARG:NH1	2.71	0.54
1:B:128:LEU:HD13	1:B:225[B]:MET:HE1	1.89	0.53
1:B:221:MET:HE2	1:B:225[A]:MET:HE1	1.91	0.53
1:B:225[B]:MET:CA	1:B:225[B]:MET:HE3	2.40	0.51
1:A:68:LYS:HE3	2:A:401:ADP:O1A	2.11	0.50
1:B:103:ASP:HB2	6:B:408:OQC:C8	2.43	0.49
1:B:303:LYS:HB3	1:B:313:LEU:HG	1.96	0.47
1:A:221:MET:CE	6:A:410:OQC:CL	3.01	0.46
1:B:118:ASN:HD22	1:B:164:ILE:H	1.62	0.46
1:B:128:LEU:HD23	1:B:132:ASP:HB3	1.97	0.46
1:A:110:ALA:HB2	6:A:411:OQC:C9	2.46	0.46
1:B:137:MET:HE1	1:B:218:LEU:HG	1.99	0.45
1:B:5:VAL:HB	1:B:261:TYR:HA	2.00	0.44
1:B:17:THR:HG22	8:B:521:HOH:O	2.18	0.43
1:A:128:LEU:HD13	1:A:225:MET:CE	2.49	0.43
1:A:118:ASN:HD22	1:A:164:ILE:H	1.67	0.42
1:B:221:MET:CE	1:B:225[A]:MET:HE1	2.49	0.42
1:A:5:VAL:HB	1:A:261:TYR:HA	2.01	0.42
1:A:128:LEU:HD13	1:A:225:MET:HE1	2.02	0.41
1:A:15[B]:VAL:HG13	1:A:19:ARG:NH1	2.35	0.41
1:A:128:LEU:HD23	1:A:132:ASP:HB3	2.02	0.41
1:A:33:TRP:CE3	1:A:100:ILE:HG22	2.56	0.41
1:A:134:ARG:HG2	1:A:323:TYR:CZ	2.55	0.41
1:A:73:VAL:HG11	1:A:77:LYS:CE	2.51	0.41
1:B:120:ASP:HB3	1:B:123:GLN:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/352 (94%)	319 (97%)	11 (3%)	0	100	100
1	B	325/352 (92%)	315 (97%)	10 (3%)	0	100	100
All	All	655/704 (93%)	634 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/319 (96%)	304 (99%)	2 (1%)	76	78
1	B	302/319 (95%)	301 (100%)	1 (0%)	86	88
All	All	608/638 (95%)	605 (100%)	3 (0%)	81	84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	327	VAL
1	B	128	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	186	GLN
1	A	207	GLN
1	A	262	ASN
1	B	118	ASN
1	B	168	HIS
1	B	186	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	ACT	A	405	-	3,3,3	1.29	0	3,3,3	0.88	0
6	OQC	A	409	-	14,15,15	0.07	0	18,20,20	0.32	0
5	ACT	A	407	-	3,3,3	1.14	0	3,3,3	1.22	0
4	IHP	A	404	-	36,36,36	0.73	0	60,60,60	1.05	1 (1%)
2	ADP	A	401	3	28,29,29	0.48	1 (3%)	43,45,45	1.02	5 (11%)
5	ACT	A	406	-	3,3,3	1.02	0	3,3,3	0.93	0
6	OQC	A	411	-	14,15,15	0.14	0	18,20,20	0.37	0
6	OQC	B	409	-	14,15,15	0.14	0	18,20,20	0.39	0
2	ADP	B	401	3	28,29,29	0.48	0	43,45,45	0.51	0
5	ACT	A	408	-	3,3,3	1.29	0	3,3,3	0.75	0
5	ACT	B	407	-	3,3,3	1.18	0	3,3,3	1.07	0
6	OQC	A	410	-	14,15,15	0.11	0	18,20,20	0.32	0
6	OQC	B	408	-	14,15,15	0.13	0	18,20,20	0.39	0
4	IHP	B	404	-	36,36,36	0.80	0	60,60,60	1.31	6 (10%)
5	ACT	B	406	-	3,3,3	1.14	0	3,3,3	0.96	0
7	PO4	A	412	-	4,4,4	2.57	3 (75%)	6,6,6	0.60	0
5	ACT	B	405	-	3,3,3	1.30	0	3,3,3	0.88	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OQC	A	409	-	-	3/6/6/6	0/2/2/2
4	IHP	A	404	-	-	3/30/54/54	0/1/1/1
2	ADP	A	401	3	-	4/16/32/32	0/3/3/3
6	OQC	A	411	-	-	4/6/6/6	0/2/2/2
6	OQC	B	409	-	-	4/6/6/6	0/2/2/2
2	ADP	B	401	3	-	3/16/32/32	0/3/3/3
6	OQC	A	410	-	-	4/6/6/6	0/2/2/2
6	OQC	B	408	-	-	4/6/6/6	0/2/2/2
4	IHP	B	404	-	-	2/30/54/54	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	412	PO4	P-O1	4.21	1.60	1.50
2	A	401	ADP	PB-O2B	-2.16	1.46	1.54
7	A	412	PO4	P-O4	2.06	1.60	1.54
7	A	412	PO4	P-O2	2.04	1.60	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ADP	O2B-PB-O3A	3.82	117.45	104.64
4	B	404	IHP	C5-C4-C3	3.66	118.45	110.43
4	B	404	IHP	C6-C5-C4	2.84	116.65	110.43
2	A	401	ADP	O3A-PB-O1B	-2.41	98.38	111.04
4	B	404	IHP	O14-C4-C3	2.34	113.74	108.76
4	B	404	IHP	C4-C3-C2	2.33	115.55	110.43
2	A	401	ADP	O3A-PA-O1A	-2.30	103.78	110.70
4	A	404	IHP	C3-C2-C1	2.28	115.42	110.43
2	A	401	ADP	O2A-PA-O3A	2.22	113.27	107.27
4	B	404	IHP	O12-C2-C3	2.17	113.37	108.76
2	A	401	ADP	O5'-PA-O1A	-2.06	100.77	108.94
4	B	404	IHP	C6-C1-C2	-2.02	106.00	110.43

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ADP	PA-O3A-PB-O2B
2	B	401	ADP	PA-O3A-PB-O3B
6	A	410	OQC	C5-C4-C7-C10
6	A	410	OQC	C5-C4-C7-C8
6	A	411	OQC	C5-C4-C7-C10
6	A	411	OQC	C3-C4-C7-C10
6	A	411	OQC	C5-C4-C7-C8
6	A	411	OQC	C3-C4-C7-C8
6	B	408	OQC	C5-C4-C7-C10
6	B	408	OQC	C3-C4-C7-C10
6	B	408	OQC	C5-C4-C7-C8
6	B	408	OQC	C3-C4-C7-C8
6	B	409	OQC	C5-C4-C7-C10
6	B	409	OQC	C3-C4-C7-C10
6	B	409	OQC	C5-C4-C7-C8
6	B	409	OQC	C3-C4-C7-C8
2	A	401	ADP	PA-O3A-PB-O1B
6	A	410	OQC	C3-C4-C7-C8
6	A	410	OQC	C3-C4-C7-C10
2	A	401	ADP	PB-O3A-PA-O1A
4	A	404	IHP	C3-O13-P3-O43
4	A	404	IHP	C6-O16-P6-O46
6	A	409	OQC	C3-C4-C7-C10
4	B	404	IHP	C3-O13-P3-O23
4	B	404	IHP	C5-O15-P5-O25
6	A	409	OQC	C5-C4-C7-C10
2	B	401	ADP	PA-O3A-PB-O2B
6	A	409	OQC	C5-C4-C7-C8
2	A	401	ADP	PB-O3A-PA-O2A
2	B	401	ADP	PA-O3A-PB-O1B
4	A	404	IHP	C6-O16-P6-O26

There are no ring outliers.

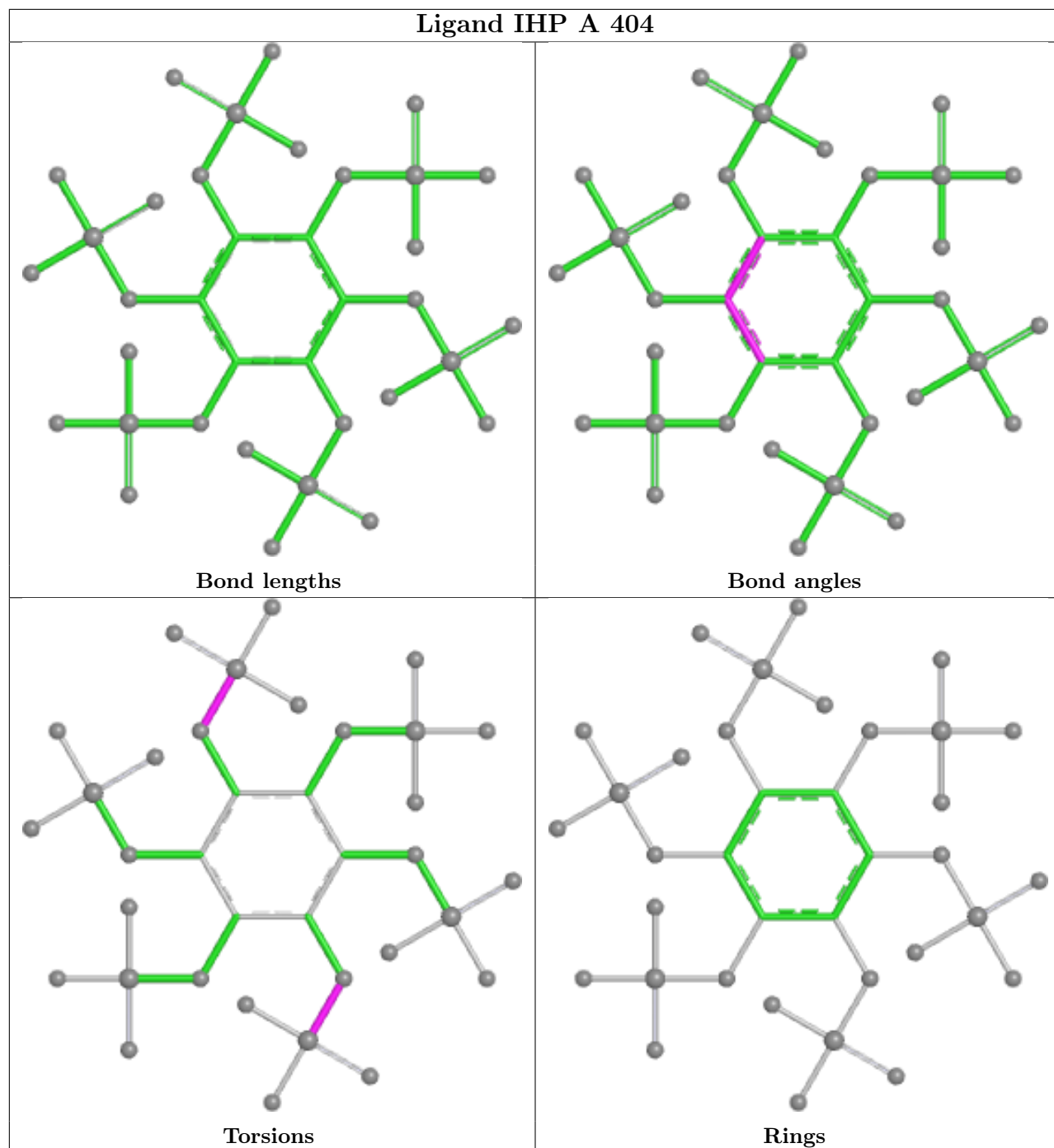
5 monomers are involved in 12 short contacts:

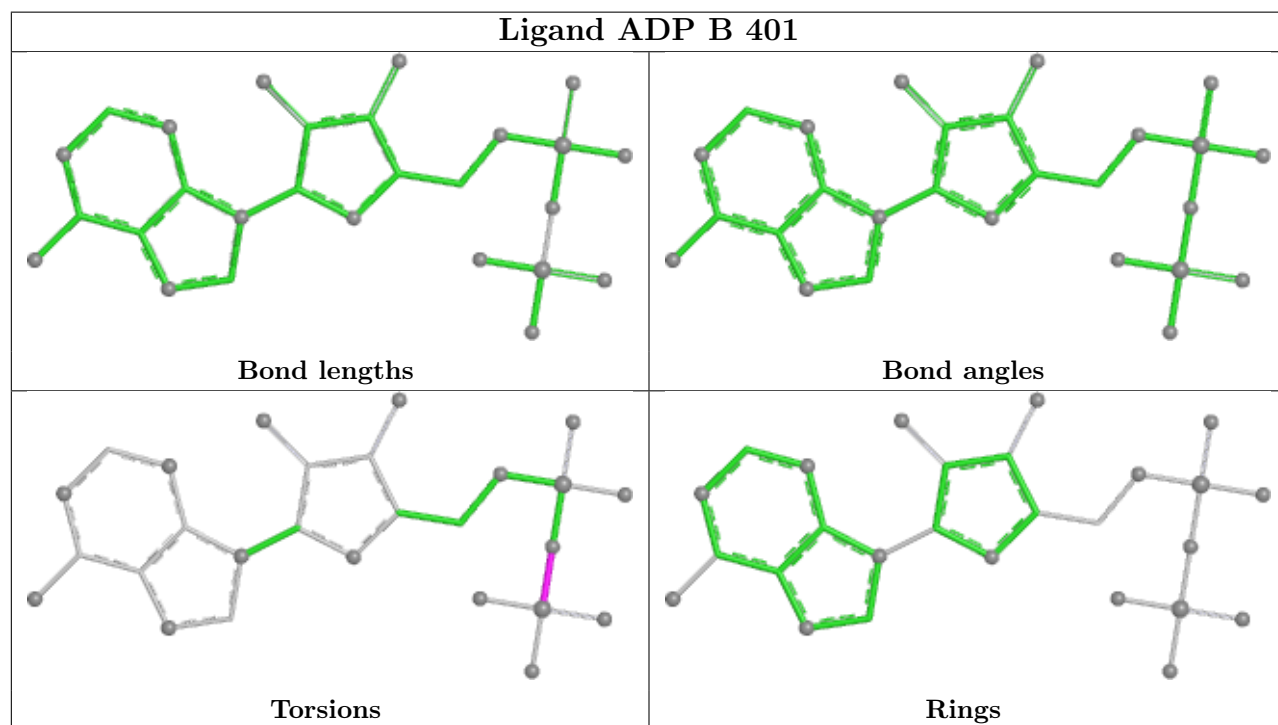
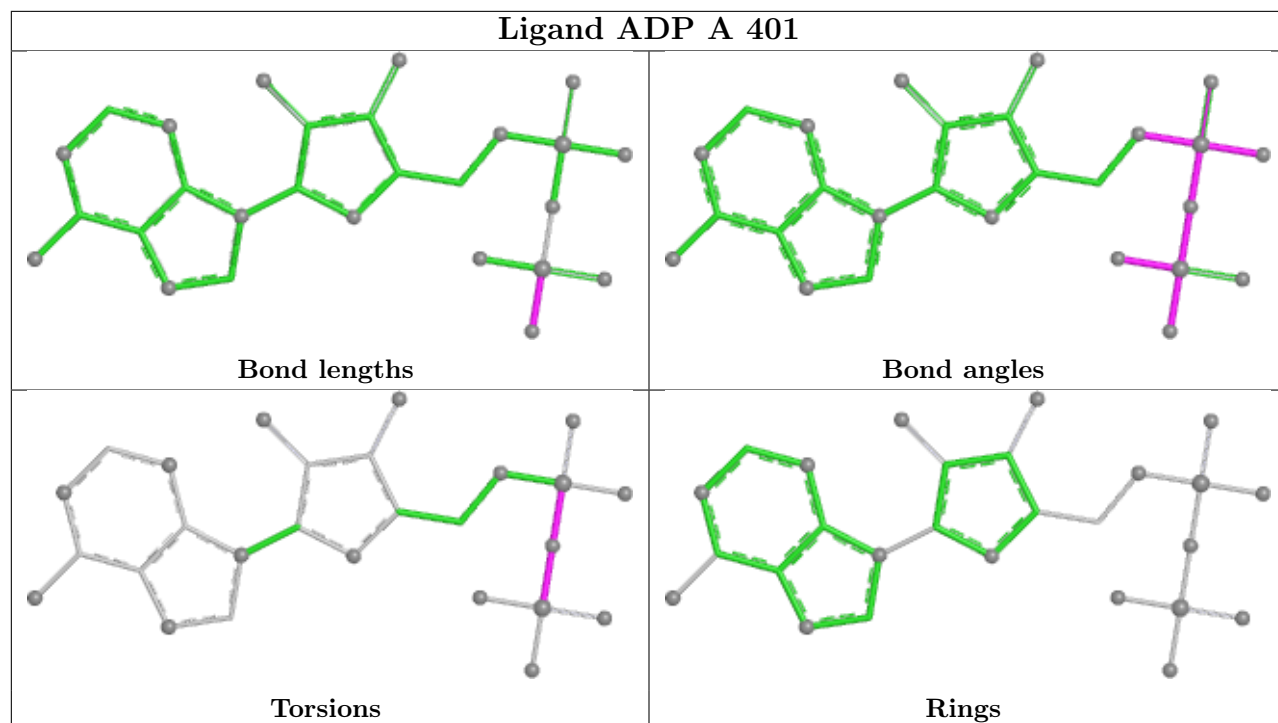
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ADP	1	0
6	A	411	OQC	3	0
6	B	409	OQC	3	0
6	A	410	OQC	3	0
6	B	408	OQC	2	0

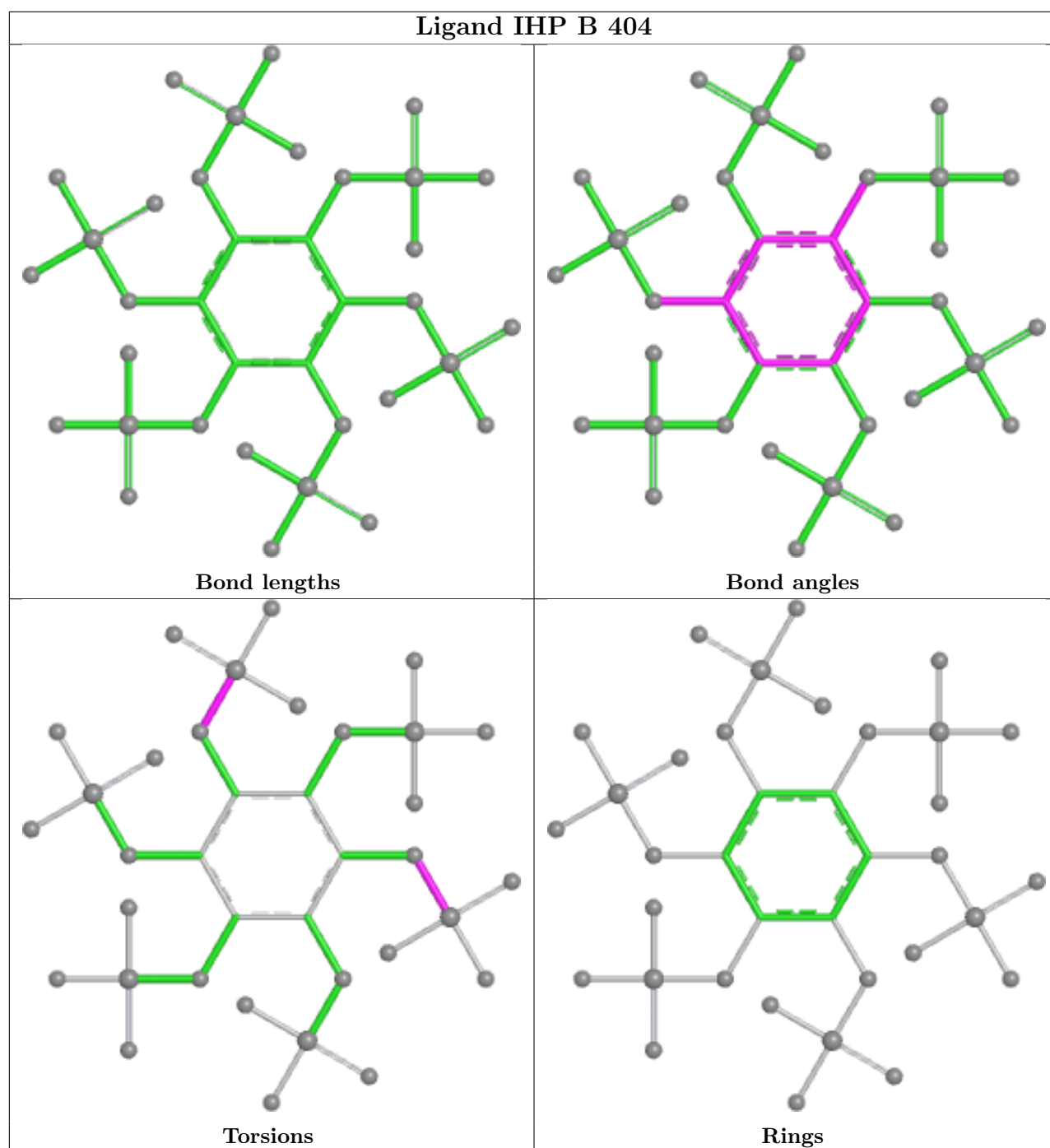
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

Ligand IHP A 404







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, 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	325/352 (92%)	0.20	17 (5%)	33 35	11, 34, 72, 118	7 (2%)
1	B	323/352 (91%)	1.06	52 (16%)	4 4	20, 63, 102, 131	4 (1%)
All	All	648/704 (92%)	0.63	69 (10%)	11 12	11, 49, 96, 131	11 (1%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	LEU	7.7
1	A	121	PHE	7.0
1	A	125	TYR	6.8
1	B	121	PHE	6.0
1	B	125	TYR	5.3
1	B	50	TYR	4.9
1	B	124	LEU	4.8
1	A	72	PRO	4.7
1	A	33	TRP	4.5
1	B	33	TRP	4.2
1	B	128	LEU	3.9
1	B	292	LEU	3.9
1	B	104	PRO	3.6
1	A	50	TYR	3.5
1	B	105	VAL	3.5
1	A	327	VAL	3.2
1	B	248	VAL	3.2
1	B	45	LEU	3.1
1	B	73	VAL	3.1
1	A	105	VAL	3.1
1	B	57	ILE	3.0
1	B	270	ASN	3.0
1	B	249	LEU	2.9
1	B	265	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	72	PRO	2.9
1	A	128	LEU	2.9
1	B	102	LYS	2.9
1	B	46	GLY	2.9
1	B	239	TYR	2.8
1	B	258	ILE	2.8
1	B	297	ALA	2.7
1	A	104	PRO	2.7
1	B	326	THR	2.7
1	B	255	TYR	2.6
1	B	166	HIS	2.6
1	B	48	GLY	2.6
1	B	49	LYS	2.6
1	B	127	THR	2.6
1	A	122	LYS	2.5
1	B	325	TYR	2.5
1	B	60	THR	2.5
1	B	293	VAL	2.5
1	B	281	TRP	2.5
1	B	59	ILE	2.4
1	B	34	GLY	2.4
1	B	289	ASN	2.3
1	A	73	VAL	2.3
1	B	225[A]	MET	2.3
1	B	206	TYR	2.2
1	B	290	GLN	2.2
1	B	135	PHE	2.2
1	A	57	ILE	2.2
1	B	251	THR	2.2
1	A	21	SER	2.2
1	B	286	HIS	2.1
1	B	62	ASN	2.1
1	B	323	TYR	2.1
1	A	127	THR	2.1
1	B	5	VAL	2.1
1	B	295	PRO	2.1
1	B	107	ARG	2.1
1	A	35[A]	ASN	2.1
1	B	300	PHE	2.1
1	B	278	ARG	2.1
1	B	204	VAL	2.1
1	B	273	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	272	ILE	2.0
1	B	257	TYR	2.0
1	A	268	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 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
6	OQC	B	409	14/14	0.28	0.25	20,20,20,20	14
4	IHP	B	404	36/36	0.54	0.16	216,217,218,218	36
5	ACT	B	406	4/4	0.62	0.26	66,69,70,70	0
5	ACT	A	407	4/4	0.65	0.19	58,58,59,62	0
4	IHP	A	404	36/36	0.69	0.13	78,88,93,94	36
6	OQC	A	410	14/14	0.70	0.21	43,58,60,74	0
5	ACT	A	408	4/4	0.70	0.16	65,67,67,70	0
5	ACT	B	405	4/4	0.76	0.21	69,70,70,72	0
2	ADP	B	401	27/27	0.77	0.13	57,78,94,95	0
6	OQC	A	411	14/14	0.78	0.16	54,58,62,62	0
6	OQC	B	408	14/14	0.79	0.16	62,66,72,74	0
5	ACT	A	405	4/4	0.80	0.19	55,62,64,67	0
6	OQC	A	409	14/14	0.82	0.14	66,67,71,71	0
5	ACT	B	407	4/4	0.83	0.14	72,74,75,78	0
7	PO4	A	412	5/5	0.83	0.13	72,75,76,78	0
2	ADP	A	401	27/27	0.87	0.11	36,50,69,70	0
3	MG	B	403	1/1	0.91	0.08	54,54,54,54	0
5	ACT	A	406	4/4	0.92	0.10	47,52,55,55	0
3	MG	A	402	1/1	0.95	0.07	33,33,33,33	0
3	MG	B	402	1/1	0.95	0.07	47,47,47,47	0

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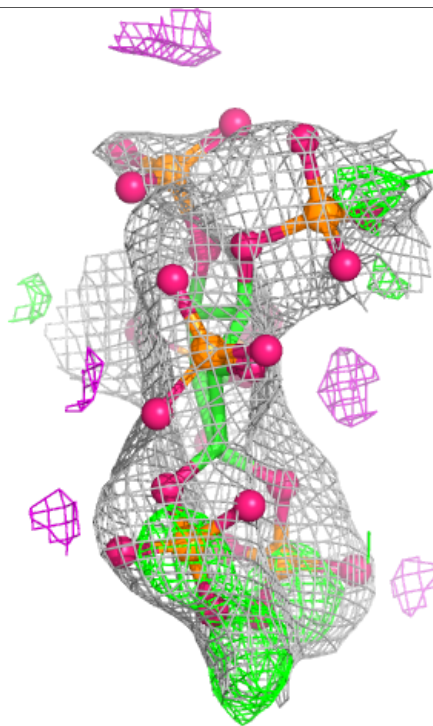
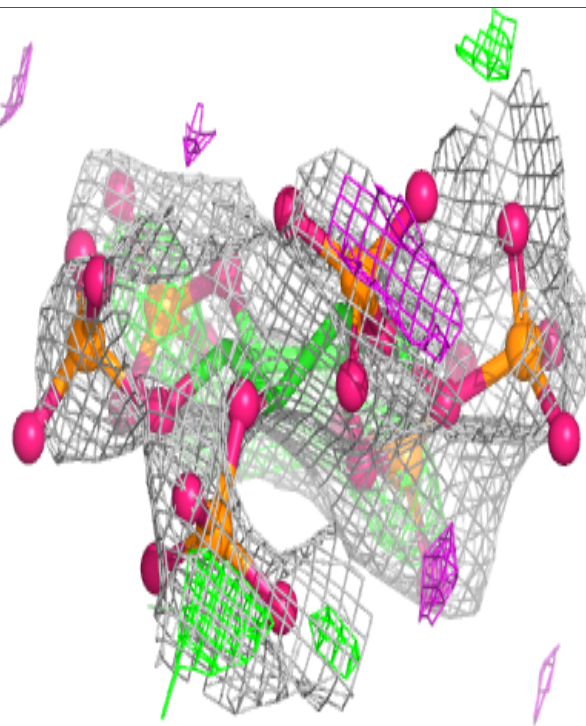
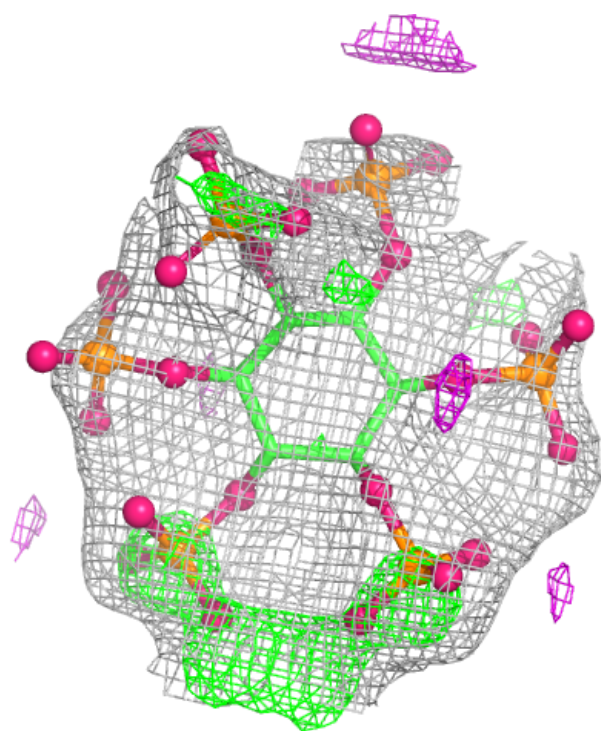
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	403	1/1	0.97	0.08	42,42,42,42	0

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.

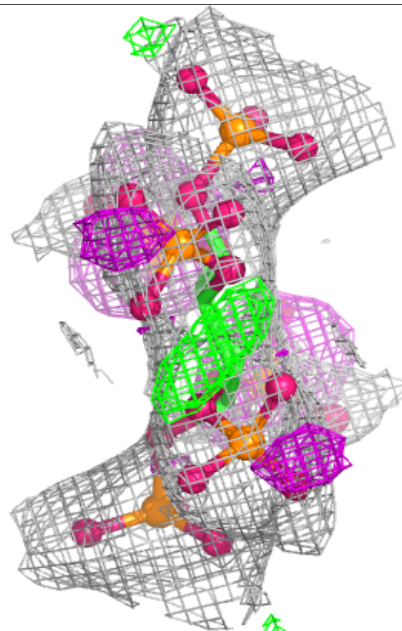
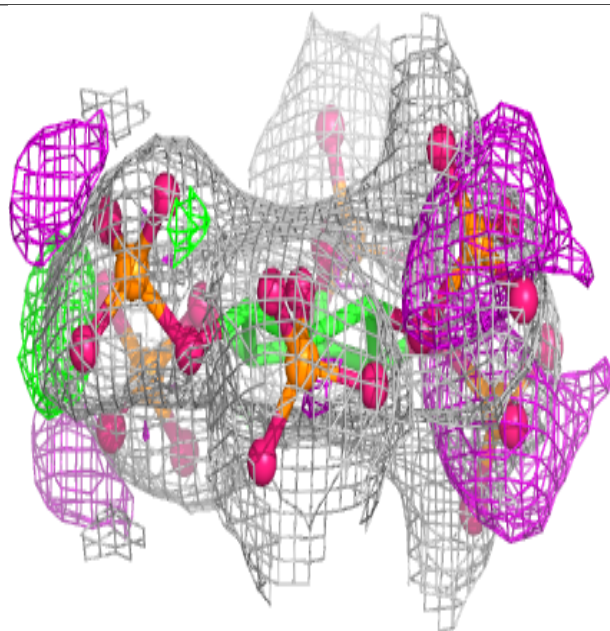
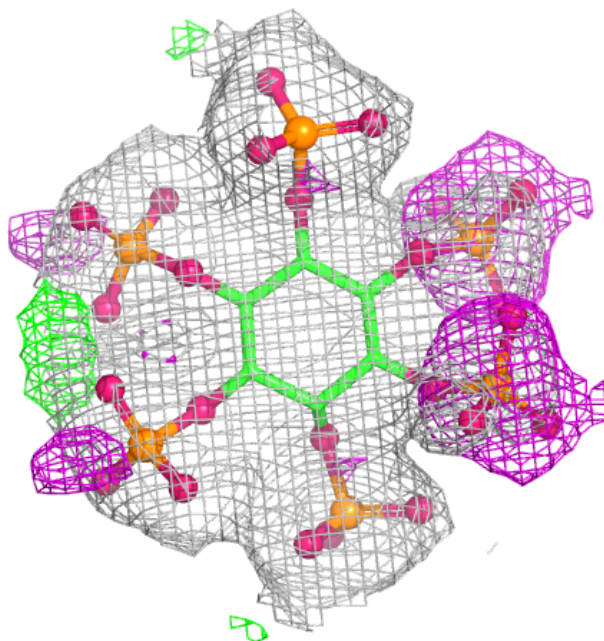
Electron density around IHP B 404:

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



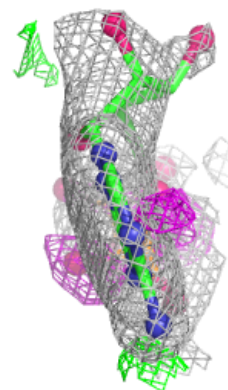
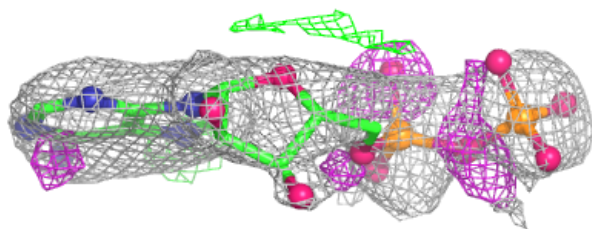
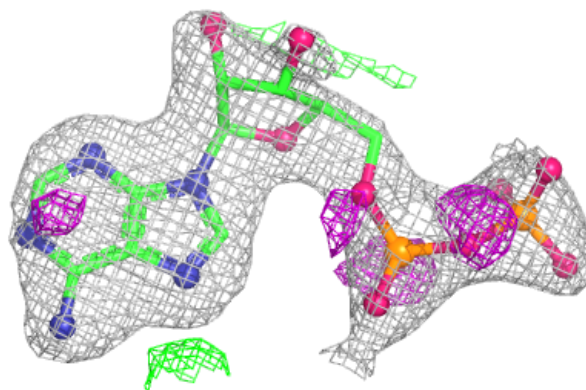
Electron density around IHP A 404:

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

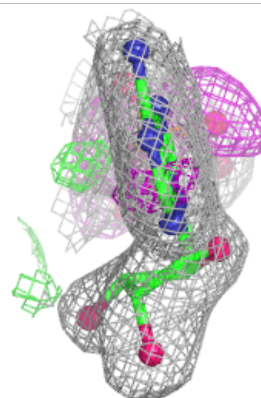
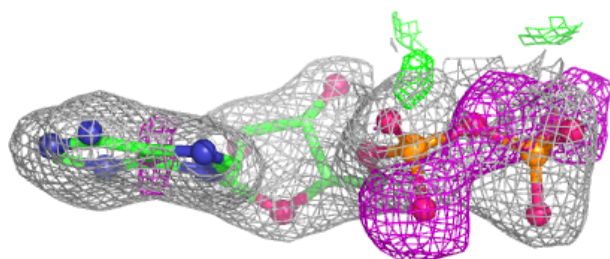
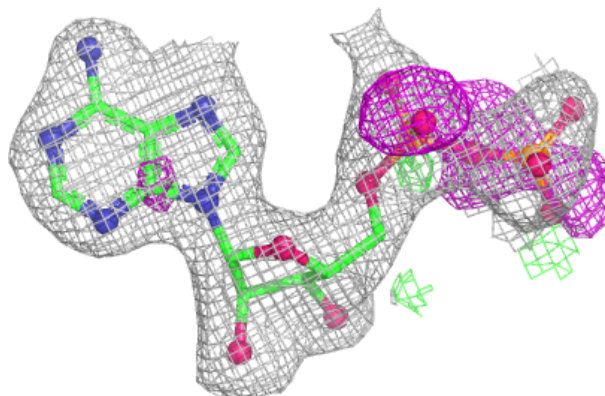


Electron density around ADP B 401:

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

**Electron density around ADP A 401:**

$2mF_o-DF_c$ (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.