



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:19 PM UTC

PDB ID : 5ORJ / pdb_00005orj
Title : The crystal structure of CK2alpha in complex with compound 3
Authors : Brear, P.; De Fusco, C.; Iegre, J.; Yoshida, M.; Mitchell, S.; Rossmann, M.; Carro, L.; Sore, H.; Hyvonen, M.; Spring, D.
Deposited on : 2017-08-16
Resolution : 1.99 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

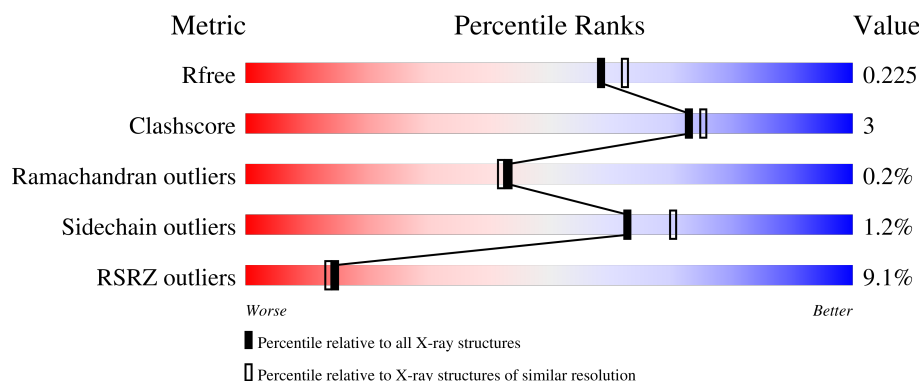
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	
1	B	352	

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
5	IHP	A	407	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5815 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	B	324	Total	C	N	O	S	0	2	0
			2757	1767	484	495	11			
1	A	325	Total	C	N	O	S	0	3	0
			2768	1773	486	498	11			

There are 50 discrepancies between the modelled and reference sequences:

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

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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

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

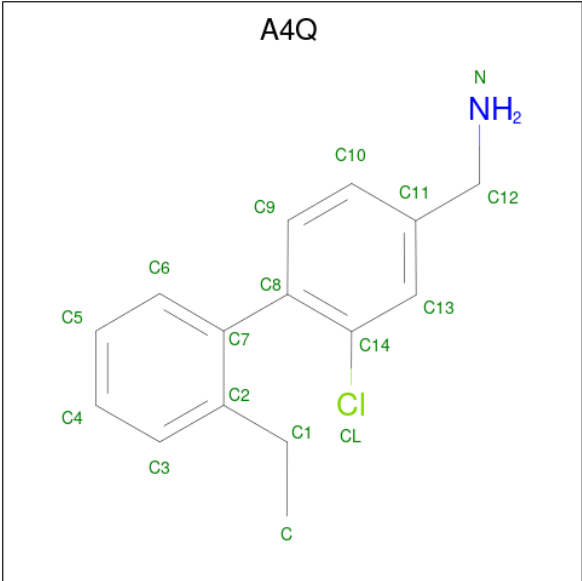
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mg 2 2	0	0
2	A	3	Total Mg 3 3	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is [3-chloranyl-4-(2-ethylphenyl)phenyl]methanamine (CCD ID: A4Q) (formula: C₁₅H₁₆ClN) (labeled as "Ligand of Interest" by depositor).



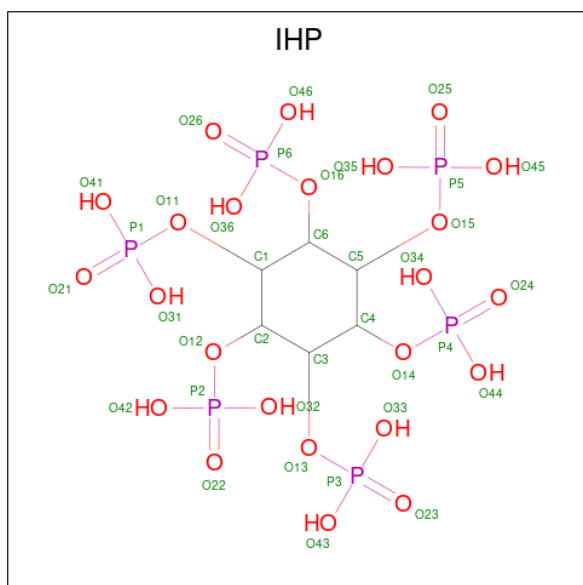
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	0	0
			17	15	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			17	15	1	1		
4	A	1	Total	C	Cl	N	0	0
			17	15	1	1		

- Molecule 5 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

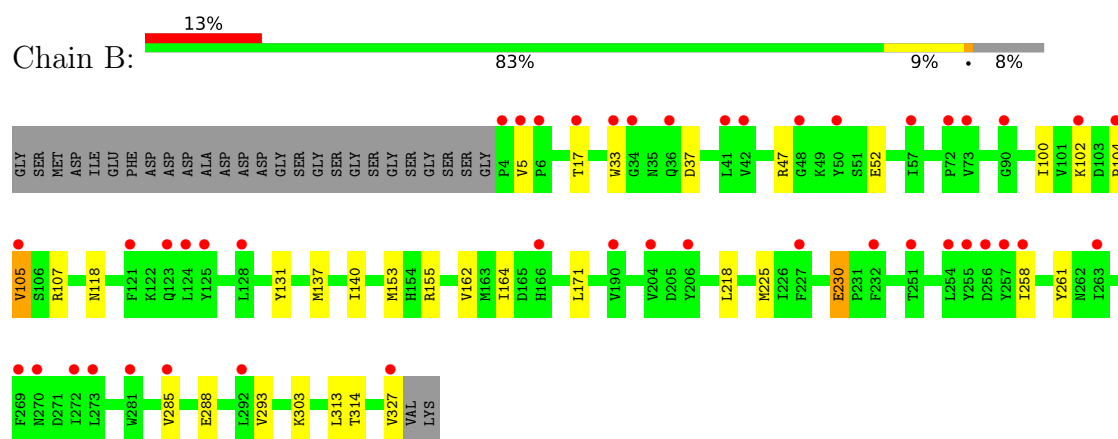
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	33	Total	O	0	0
			33	33		
6	A	111	Total	O	0	0
			111	111		

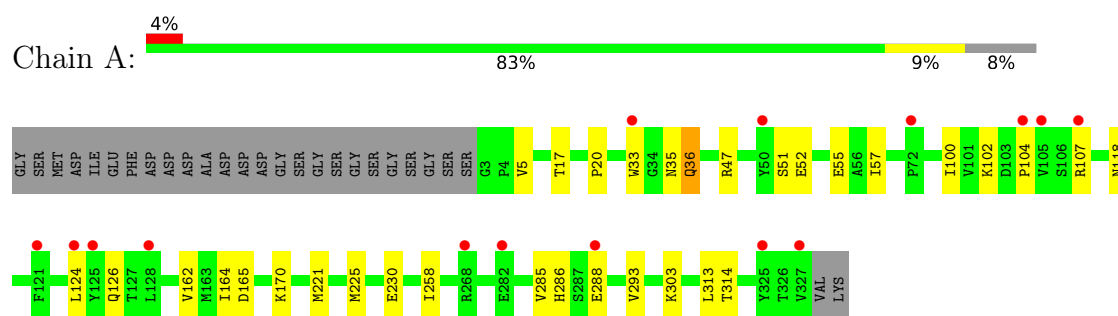
3 Residue-property plots [i](#)

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: Casein kinase II subunit alpha



- 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	64.79Å 68.60Å 333.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.14 – 1.99 29.14 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.14-1.99) 99.8 (29.14-1.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.98Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.200 , 0.221 0.206 , 0.225	Depositor DCC
R_{free} test set	2637 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5815	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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: ADP, A4Q, MG, IHP

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	0.91	2/2843 (0.1%)	1.13	8/3847 (0.2%)
1	B	0.79	0/2832	1.11	2/3831 (0.1%)
All	All	0.85	2/5675 (0.0%)	1.12	10/7678 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	MET	SD-CE	-6.55	1.63	1.79
1	A	5	VAL	CA-C	5.02	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	GLU	CB-CG-CD	8.48	127.02	112.60
1	B	105	VAL	N-CA-C	6.84	117.60	110.62
1	A	124	LEU	CA-C-N	6.40	129.72	120.38
1	A	124	LEU	C-N-CA	6.40	129.72	120.38
1	A	35	ASN	CA-C-N	6.34	128.77	120.28
1	A	35	ASN	C-N-CA	6.34	128.77	120.28
1	A	55	GLU	N-CA-C	-5.39	101.68	110.20
1	A	51	SER	N-CA-C	5.39	116.47	108.60
1	B	314	THR	N-CA-C	-5.37	103.60	110.53
1	A	314	THR	N-CA-C	-5.04	104.03	110.53

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	2768	0	2706	17	1
1	B	2757	0	2698	19	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	34	0	0	3	0
4	B	17	0	0	3	0
5	A	36	0	6	1	56
6	A	111	0	0	2	0
6	B	33	0	0	1	0
All	All	5815	0	5434	36	57

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 (36) 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:230:GLU:HG2	1:B:230:GLU:O	1.89	0.71
1:A:36:GLN:CD	1:A:36:GLN:H	2.03	0.64
1:A:36:GLN:HG2	1:A:104:PRO:HD3	1.78	0.64
1:A:17[A]:THR:HG22	6:A:550:HOH:O	2.00	0.62
1:A:36:GLN:HG2	1:A:102:LYS:O	2.01	0.60
1:B:171:LEU:HD23	1:B:171:LEU:C	2.28	0.59
1:B:17:THR:HG22	6:B:515:HOH:O	2.07	0.54
1:B:137:MET:HE1	1:B:218:LEU:HG	1.89	0.53
1:A:225:MET:HG2	4:A:405:A4Q:C	2.39	0.53
1:B:225:MET:HG3	4:B:404:A4Q:C3	2.39	0.53
1:B:118:ASN:HD22	1:B:164:ILE:H	1.57	0.52
1:A:36:GLN:CG	1:A:102:LYS:O	2.57	0.52
1:B:33:TRP:CE3	1:B:102:LYS:HG3	2.44	0.52
1:B:225:MET:HG2	4:B:404:A4Q:C	2.41	0.51
1:A:225:MET:HG3	4:A:405:A4Q:C3	2.40	0.51
1:A:118:ASN:HD22	1:A:164:ILE:H	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TRP:CE3	1:A:100:ILE:HG22	2.47	0.50
1:A:102:LYS:HD3	1:A:107:ARG:HE	1.78	0.48
1:A:162:VAL:HG11	4:A:405:A4Q:CL	2.51	0.47
1:B:140:ILE:HG13	1:B:171:LEU:HD11	1.98	0.45
1:A:285:VAL:HG22	1:A:293:VAL:HG11	1.99	0.45
1:B:33:TRP:CE3	1:B:100:ILE:HG22	2.52	0.45
1:B:104:PRO:HA	1:B:107:ARG:HH21	1.82	0.44
1:B:153:MET:HE3	1:B:155:ARG:HD3	1.99	0.43
1:A:286:HIS:HE1	6:A:596:HOH:O	2.00	0.42
1:B:47:ARG:HG3	1:B:52:GLU:HG3	2.02	0.42
1:B:303:LYS:HB3	1:B:313:LEU:HG	2.02	0.42
1:A:303:LYS:HB3	1:A:313:LEU:HG	2.02	0.42
1:A:47:ARG:HG3	1:A:52:GLU:HG3	2.02	0.41
1:A:165:ASP:HB3	1:A:170:LYS:HB3	2.02	0.41
5:A:407:IHP:O15	5:A:407:IHP:P4	2.78	0.41
1:B:5:VAL:HB	1:B:261:TYR:HA	2.03	0.41
1:B:131:TYR:CE1	1:B:327:VAL:HG12	2.56	0.41
1:B:285:VAL:HG22	1:B:293:VAL:HG11	2.02	0.41
1:B:105:VAL:HG21	1:A:20:PRO:HD2	2.02	0.40
1:B:162:VAL:HG11	4:B:404:A4Q:CL	2.58	0.40

All (57) 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)
5:A:407:IHP:P1	5:A:407:IHP:P2[4_597]	0.04	2.16
5:A:407:IHP:P3	5:A:407:IHP:P6[4_597]	0.06	2.14
5:A:407:IHP:O41	5:A:407:IHP:O22[4_597]	0.07	2.13
5:A:407:IHP:O21	5:A:407:IHP:O42[4_597]	0.08	2.12
5:A:407:IHP:O31	5:A:407:IHP:O32[4_597]	0.09	2.11
5:A:407:IHP:O11	5:A:407:IHP:O12[4_597]	0.11	2.09
5:A:407:IHP:C4	5:A:407:IHP:C5[4_597]	0.19	2.01
5:A:407:IHP:C1	5:A:407:IHP:C2[4_597]	0.27	1.93
5:A:407:IHP:O24	5:A:407:IHP:O44[4_597]	0.38	1.82
5:A:407:IHP:C3	5:A:407:IHP:C6[4_597]	0.62	1.58
5:A:407:IHP:O14	5:A:407:IHP:O15[4_597]	0.63	1.57
5:A:407:IHP:O43	5:A:407:IHP:O46[4_597]	0.68	1.52
5:A:407:IHP:O33	5:A:407:IHP:O36[4_597]	0.71	1.49
5:A:407:IHP:O23	5:A:407:IHP:O26[4_597]	0.91	1.29
5:A:407:IHP:O13	5:A:407:IHP:O16[4_597]	1.08	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:407:IHP:C6	5:A:407:IHP:O13[4_597]	1.11	1.09
5:A:407:IHP:C3	5:A:407:IHP:O16[4_597]	1.22	0.98
5:A:407:IHP:C4	5:A:407:IHP:O15[4_597]	1.25	0.95
5:A:407:IHP:C1	5:A:407:IHP:O12[4_597]	1.34	0.86
5:A:407:IHP:P4	5:A:407:IHP:O24[4_597]	1.36	0.84
5:A:407:IHP:C1	5:A:407:IHP:C1[4_597]	1.41	0.79
5:A:407:IHP:O23	5:A:407:IHP:P6[4_597]	1.43	0.77
5:A:407:IHP:C3	5:A:407:IHP:C5[4_597]	1.45	0.75
5:A:407:IHP:O41	5:A:407:IHP:P2[4_597]	1.45	0.75
5:A:407:IHP:P3	5:A:407:IHP:O36[4_597]	1.46	0.74
5:A:407:IHP:P3	5:A:407:IHP:O46[4_597]	1.46	0.74
5:A:407:IHP:P1	5:A:407:IHP:O42[4_597]	1.46	0.74
5:A:407:IHP:O31	5:A:407:IHP:P2[4_597]	1.48	0.72
5:A:407:IHP:C5	5:A:407:IHP:C5[4_597]	1.48	0.72
5:A:407:IHP:C2	5:A:407:IHP:O11[4_597]	1.48	0.72
5:A:407:IHP:P1	5:A:407:IHP:O32[4_597]	1.48	0.72
5:A:407:IHP:O21	5:A:407:IHP:P2[4_597]	1.49	0.71
5:A:407:IHP:O43	5:A:407:IHP:P6[4_597]	1.51	0.69
5:A:407:IHP:C1	5:A:407:IHP:C3[4_597]	1.51	0.69
5:A:407:IHP:P1	5:A:407:IHP:O22[4_597]	1.51	0.69
5:A:407:IHP:P3	5:A:407:IHP:O26[4_597]	1.53	0.67
5:A:407:IHP:P1	5:A:407:IHP:O12[4_597]	1.53	0.67
5:A:407:IHP:O33	5:A:407:IHP:P6[4_597]	1.53	0.67
5:A:407:IHP:C4	5:A:407:IHP:C6[4_597]	1.55	0.65
5:A:407:IHP:P4	5:A:407:IHP:P4[4_597]	1.56	0.64
5:A:407:IHP:C4	5:A:407:IHP:C4[4_597]	1.56	0.64
5:A:407:IHP:C5	5:A:407:IHP:O14[4_597]	1.59	0.61
5:A:407:IHP:P4	5:A:407:IHP:O44[4_597]	1.60	0.60
5:A:407:IHP:O11	5:A:407:IHP:P2[4_597]	1.60	0.60
5:A:407:IHP:O13	5:A:407:IHP:P6[4_597]	1.60	0.60
5:A:407:IHP:C2	5:A:407:IHP:C6[4_597]	1.62	0.58
5:A:407:IHP:P3	5:A:407:IHP:O16[4_597]	1.64	0.56
5:A:407:IHP:C2	5:A:407:IHP:C2[4_597]	1.65	0.55
5:A:407:IHP:P4	5:A:407:IHP:O15[4_597]	1.78	0.42
5:A:407:IHP:O23	5:A:407:IHP:O16[4_597]	1.88	0.32
5:A:407:IHP:O34	5:A:407:IHP:O45[4_597]	2.02	0.18
5:A:407:IHP:O13	5:A:407:IHP:O46[4_597]	2.04	0.16
5:A:407:IHP:O13	5:A:407:IHP:O36[4_597]	2.05	0.15
5:A:407:IHP:O14	5:A:407:IHP:O24[4_597]	2.10	0.10
5:A:407:IHP:O14	5:A:407:IHP:P5[4_597]	2.14	0.06
5:A:407:IHP:O43	5:A:407:IHP:O26[4_597]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17[B]:THR:CG2	1:A:57:ILE:CD1[5_555]	2.16	0.04

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	326/352 (93%)	318 (98%)	8 (2%)	0	100	100
1	B	324/352 (92%)	314 (97%)	9 (3%)	1 (0%)	36	35
All	All	650/704 (92%)	632 (97%)	17 (3%)	1 (0%)	43	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	ASP

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	302/319 (95%)	298 (99%)	4 (1%)	61	68
1	B	301/319 (94%)	298 (99%)	3 (1%)	68	75
All	All	603/638 (94%)	596 (99%)	7 (1%)	63	70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	230	GLU
1	B	258	ILE
1	B	288	GLU
1	A	36	GLN
1	A	126	GLN
1	A	258	ILE
1	A	288	GLU

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

Mol	Chain	Res	Type
1	B	118	ASN
1	B	262	ASN
1	A	36	GLN
1	A	118	ASN
1	A	168	HIS
1	A	262	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	IHP	A	407	-	36,36,36	1.10	0	60,60,60	1.65	10 (16%)
4	A4Q	A	405	-	18,18,18	0.09	0	24,24,24	0.24	0
3	ADP	A	404	2	28,29,29	0.60	0	43,45,45	0.70	1 (2%)
4	A4Q	A	406	-	18,18,18	0.19	0	24,24,24	0.25	0
4	A4Q	B	404	-	18,18,18	0.09	0	24,24,24	0.23	0
3	ADP	B	403	2	28,29,29	0.48	1 (3%)	43,45,45	0.52	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
5	IHP	A	407	-	-	5/30/54/54	0/1/1/1
4	A4Q	A	405	-	-	0/8/8/8	0/2/2/2
3	ADP	A	404	2	-	1/16/32/32	0/3/3/3
4	A4Q	A	406	-	-	0/8/8/8	0/2/2/2
4	A4Q	B	404	-	-	1/8/8/8	0/2/2/2
3	ADP	B	403	2	-	2/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	ADP	PB-O1B	2.06	1.56	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	407	IHP	C5-C6-C1	-4.82	99.85	110.43
5	A	407	IHP	O15-C5-C4	4.00	117.26	108.76
5	A	407	IHP	O12-C2-C1	-3.54	101.22	108.76
5	A	407	IHP	C3-C2-C1	3.41	117.91	110.43
5	A	407	IHP	C6-C5-C4	-3.10	103.62	110.43
5	A	407	IHP	O11-C1-C2	-2.83	102.73	108.76
5	A	407	IHP	O42-P2-O32	2.40	116.80	107.80
5	A	407	IHP	O16-C6-C5	2.34	113.73	108.76
3	A	404	ADP	O2B-PB-O3A	2.27	112.24	104.64
5	A	407	IHP	O14-C4-C5	2.05	113.12	108.76
5	A	407	IHP	P2-O12-C2	-2.01	118.08	123.43

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	407	IHP	C3-C4-O14-P4
5	A	407	IHP	C5-C4-O14-P4
3	A	404	ADP	C5'-O5'-PA-O1A
3	B	403	ADP	PB-O3A-PA-O2A
5	A	407	IHP	C1-O11-P1-O21
4	B	404	A4Q	C-C1-C2-C3
3	B	403	ADP	PB-O3A-PA-O1A
5	A	407	IHP	C4-O14-P4-O34
5	A	407	IHP	C2-O12-P2-O22

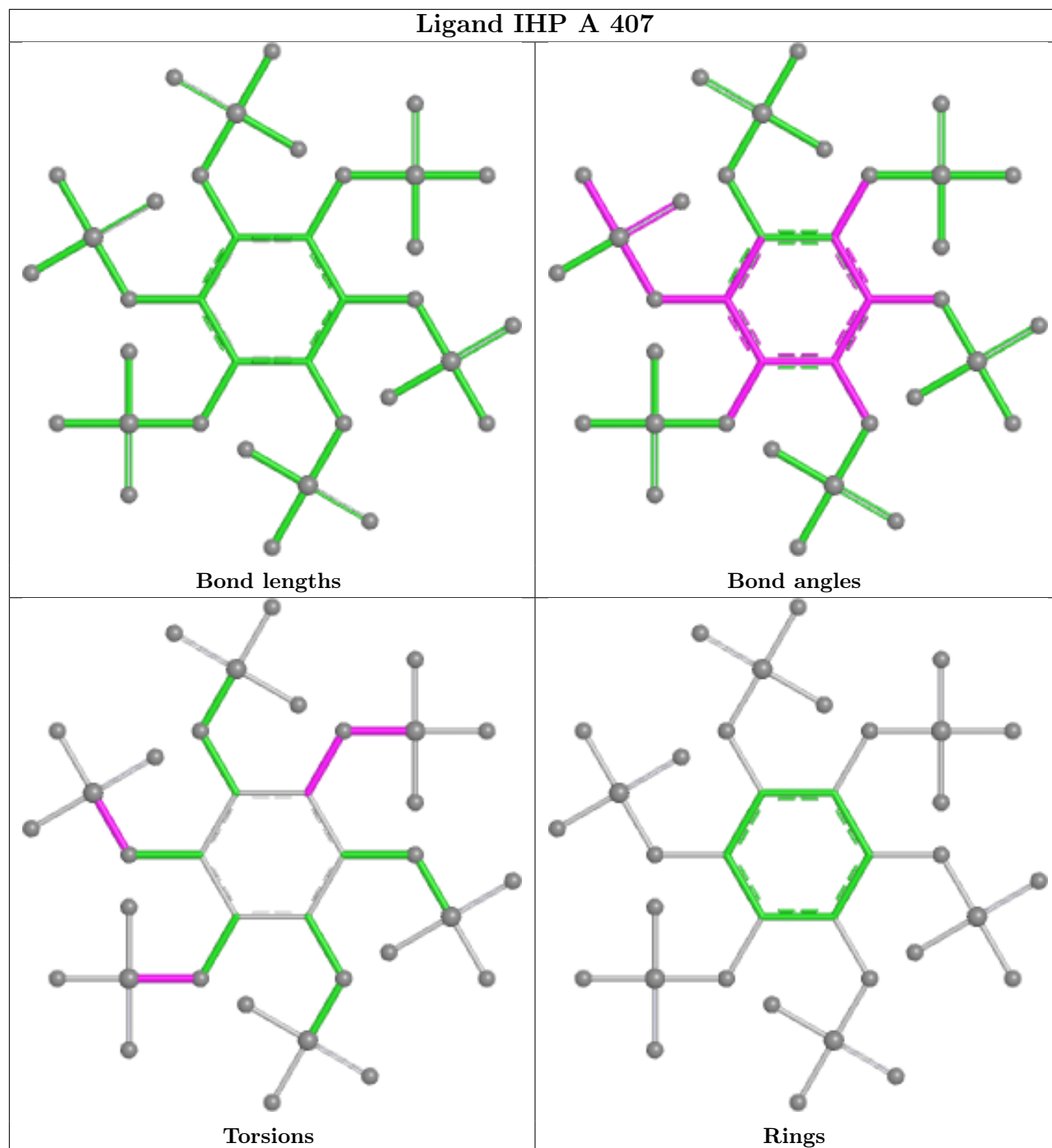
There are no ring outliers.

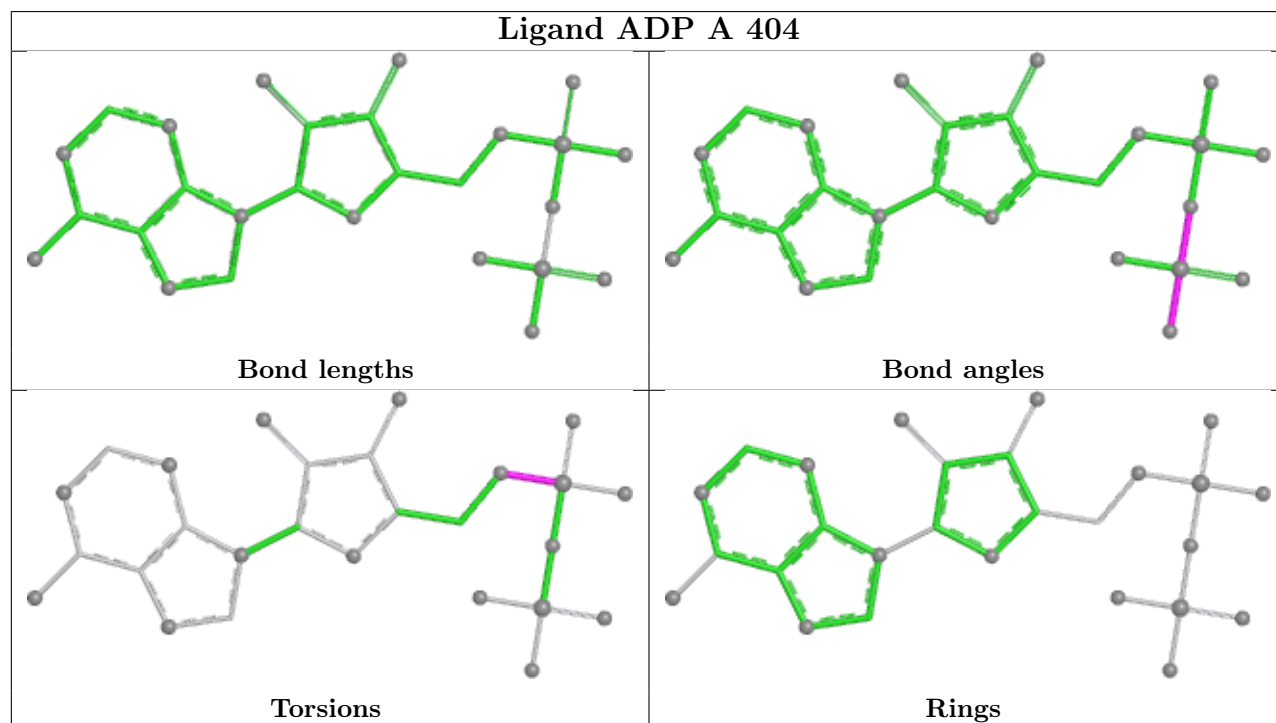
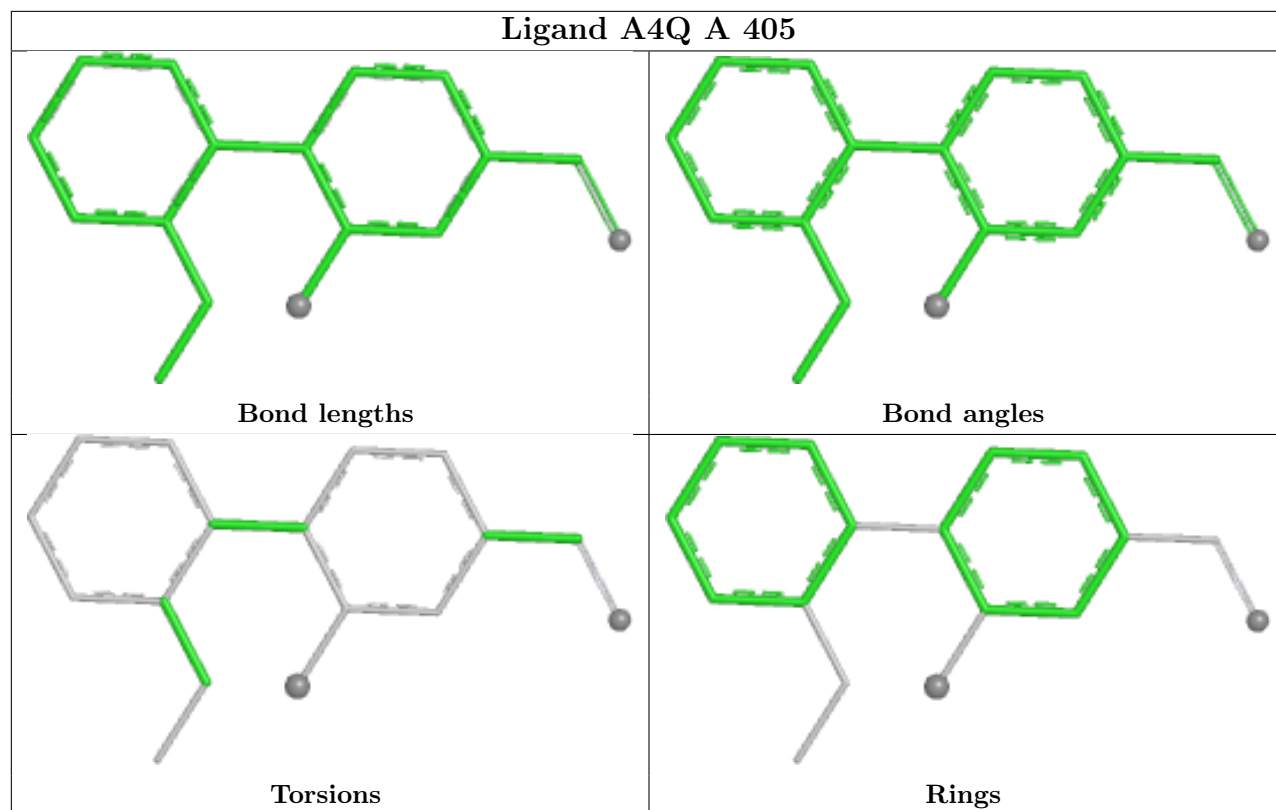
3 monomers are involved in 63 short contacts:

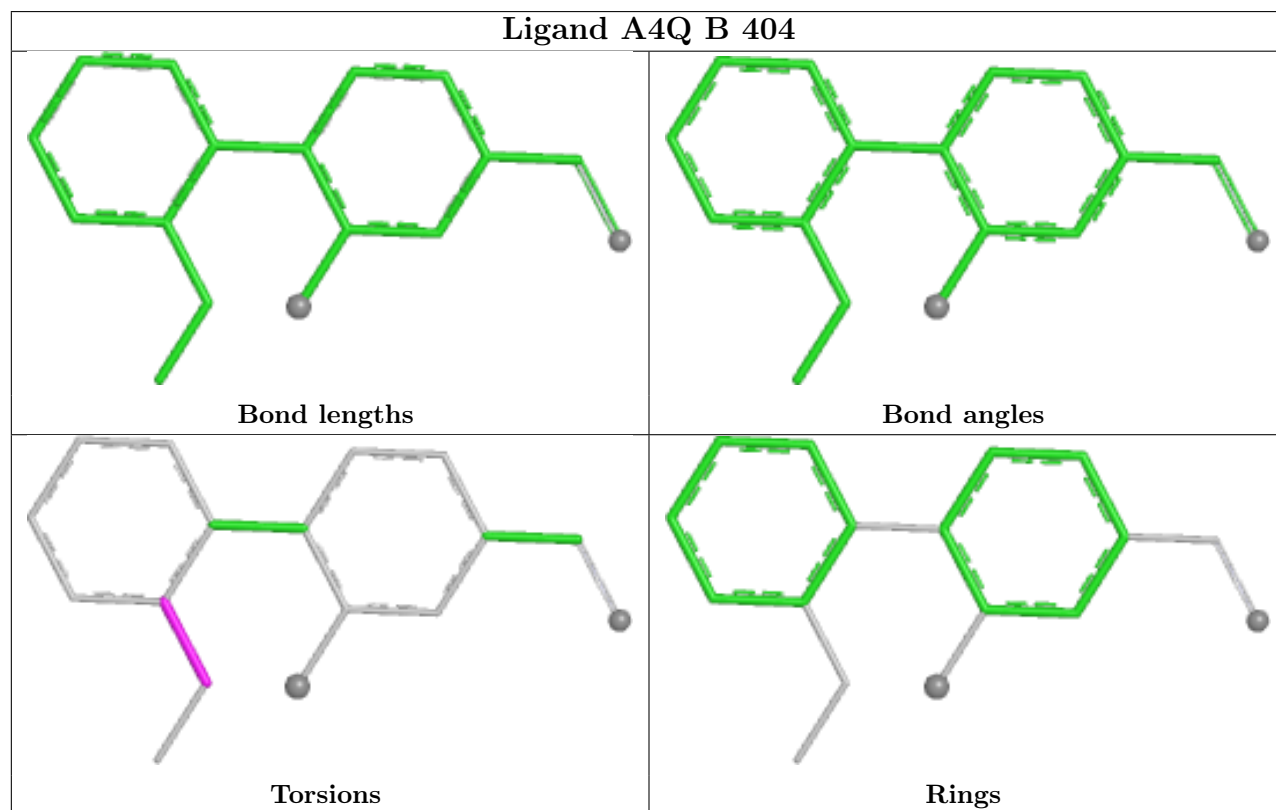
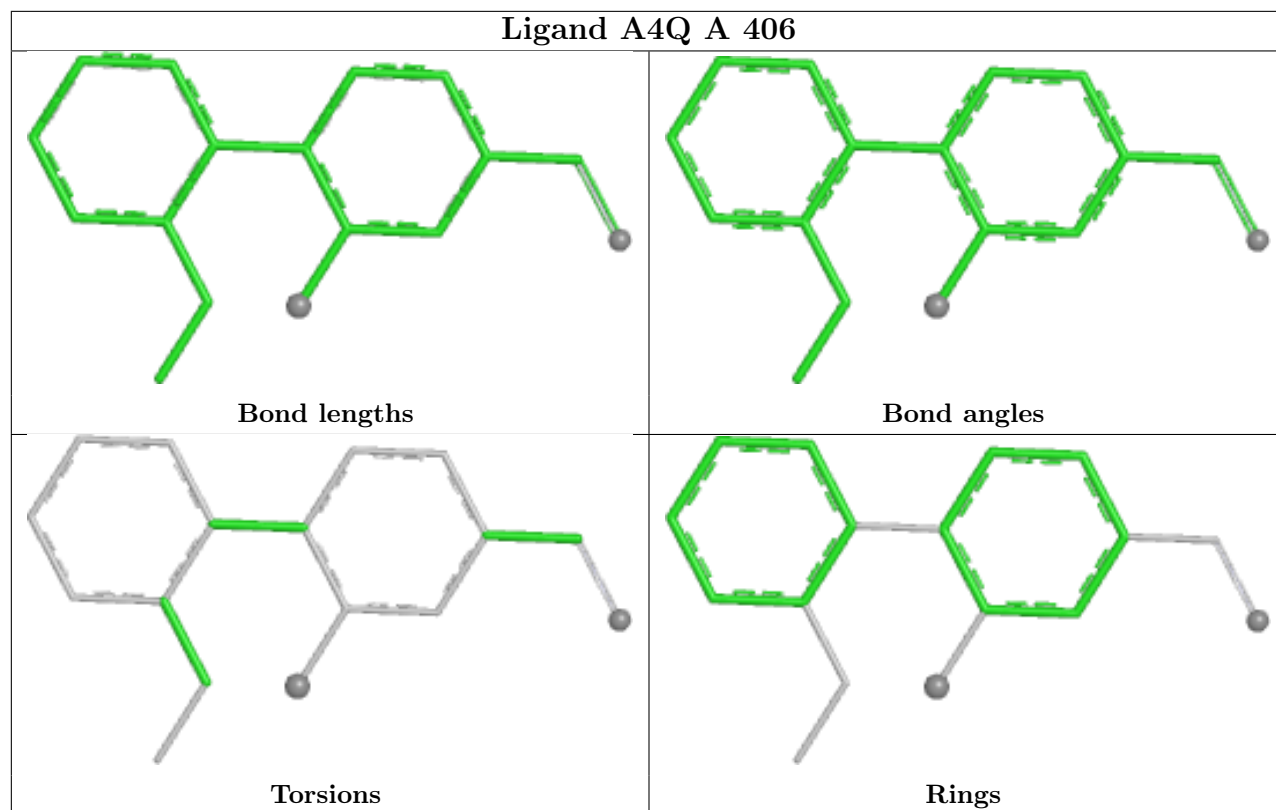
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	407	IHP	1	56
4	A	405	A4Q	3	0
4	B	404	A4Q	3	0

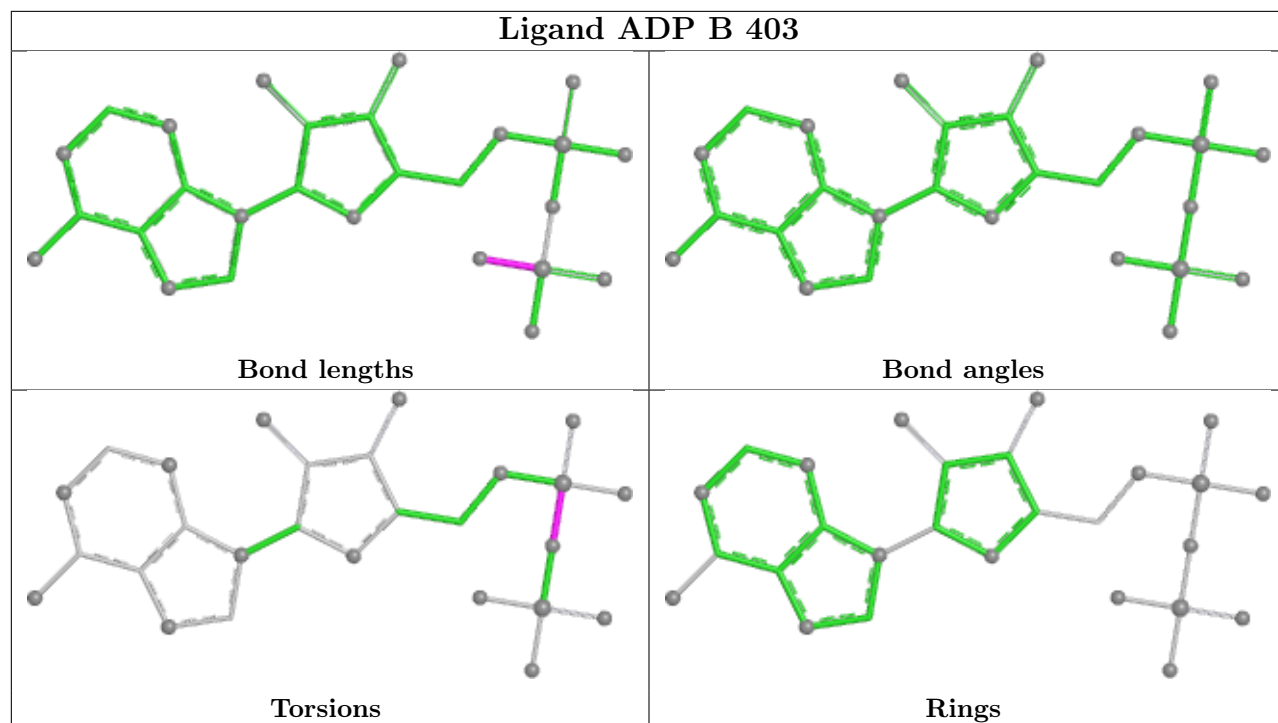
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand IHP A 407









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%)	0.34	15 (4%) 37 36	19, 44, 81, 116	3 (0%)
1	B	324/352 (92%)	1.06	44 (13%) 7 6	37, 71, 105, 125	2 (0%)
All	All	649/704 (92%)	0.70	59 (9%) 15 13	19, 58, 99, 125	5 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	PHE	5.2
1	B	50	TYR	5.2
1	A	125	TYR	5.1
1	A	50	TYR	4.8
1	A	33	TRP	4.6
1	B	124	LEU	4.5
1	A	124	LEU	4.5
1	B	33	TRP	4.2
1	B	105	VAL	3.8
1	A	327	VAL	3.7
1	A	72	PRO	3.5
1	B	255	TYR	3.4
1	B	327	VAL	3.4
1	B	272	ILE	3.3
1	B	125	TYR	3.3
1	B	104	PRO	3.3
1	B	273	LEU	3.1
1	A	325	TYR	3.1
1	B	258	ILE	3.1
1	A	105	VAL	3.0
1	B	263	ILE	3.0
1	B	17	THR	3.0
1	B	36	GLN	2.9
1	B	257	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	232	PHE	2.8
1	B	73	VAL	2.7
1	B	206	TYR	2.6
1	B	227	PHE	2.6
1	A	104	PRO	2.6
1	B	285	VAL	2.6
1	A	107	ARG	2.6
1	B	292	LEU	2.6
1	B	5	VAL	2.6
1	B	42	VAL	2.5
1	B	34	GLY	2.4
1	B	121	PHE	2.4
1	B	269	PHE	2.4
1	A	128	LEU	2.4
1	B	256	ASP	2.4
1	B	281	TRP	2.4
1	B	251	THR	2.4
1	A	268	ARG	2.4
1	B	190	VAL	2.4
1	B	204	VAL	2.3
1	B	57	ILE	2.3
1	B	254	LEU	2.3
1	B	6	PRO	2.3
1	B	4	PRO	2.2
1	B	102	LYS	2.2
1	B	128	LEU	2.2
1	B	166	HIS	2.2
1	B	123	GLN	2.2
1	B	72	PRO	2.2
1	B	41	LEU	2.1
1	B	48	GLY	2.1
1	A	282	GLU	2.1
1	B	270	ASN	2.1
1	B	90	GLY	2.0
1	A	288	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

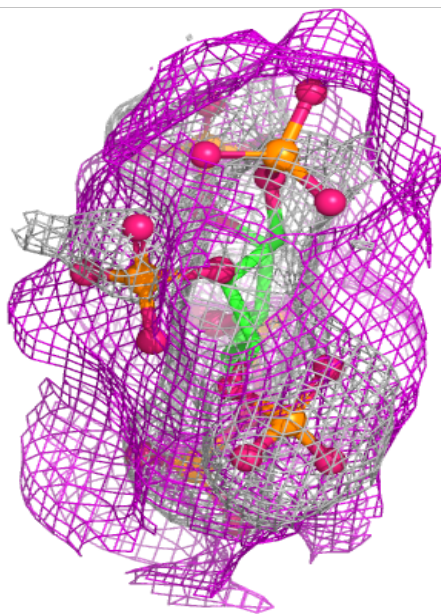
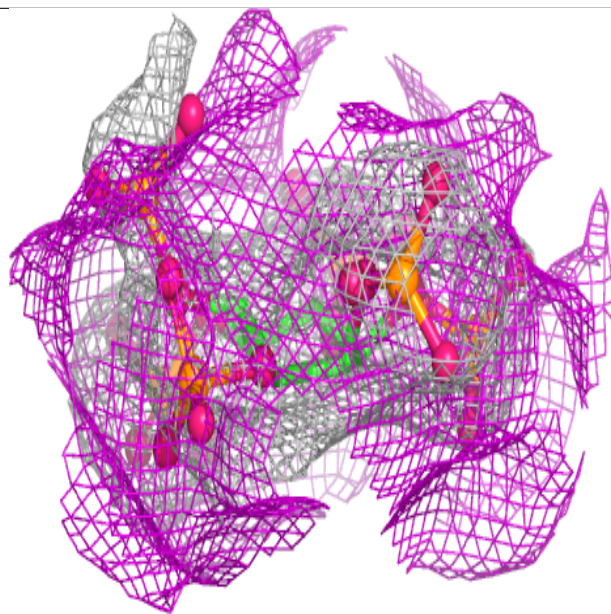
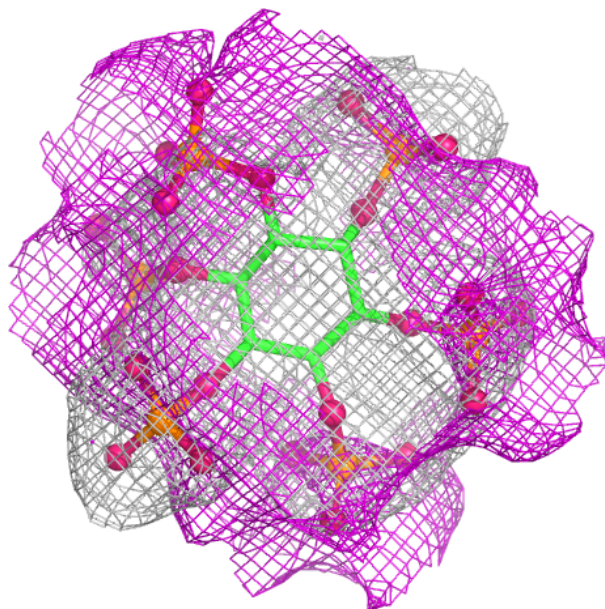
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	IHP	A	407	36/36	0.45	0.15	197,199,201,201	0
4	A4Q	A	405	17/17	0.71	0.19	48,54,63,71	0
4	A4Q	B	404	17/17	0.75	0.17	52,75,81,83	0
4	A4Q	A	406	17/17	0.82	0.14	66,72,78,81	0
2	MG	A	402	1/1	0.83	0.14	76,76,76,76	0
3	ADP	B	403	27/27	0.87	0.09	54,67,73,75	0
2	MG	A	403	1/1	0.89	0.08	37,37,37,37	0
2	MG	B	402	1/1	0.92	0.13	55,55,55,55	0
2	MG	B	401	1/1	0.93	0.06	55,55,55,55	0
3	ADP	A	404	27/27	0.94	0.07	38,46,56,57	0
2	MG	A	401	1/1	0.95	0.08	52,52,52,52	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.

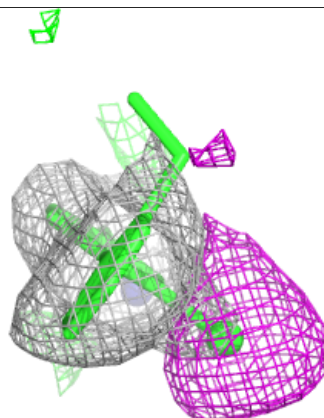
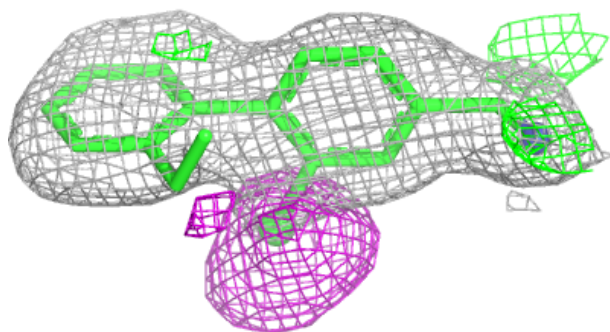
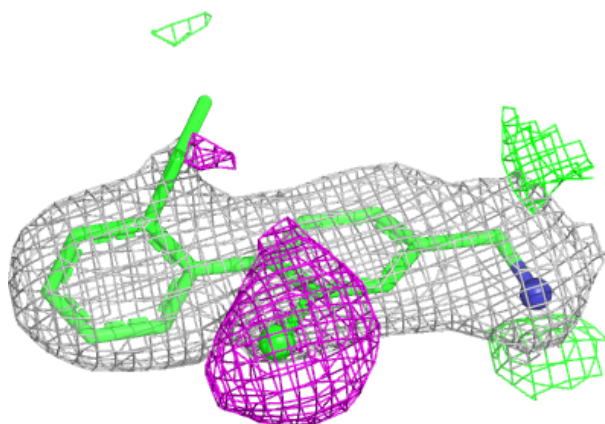
Electron density around IHP A 407:

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

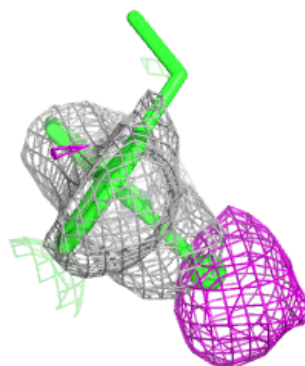
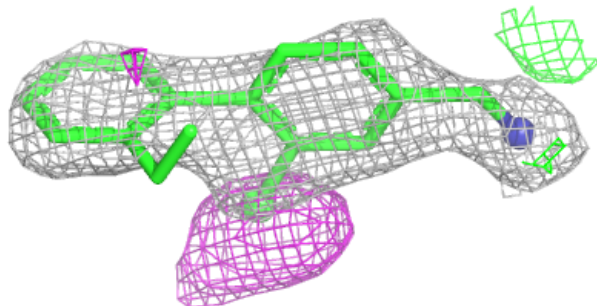
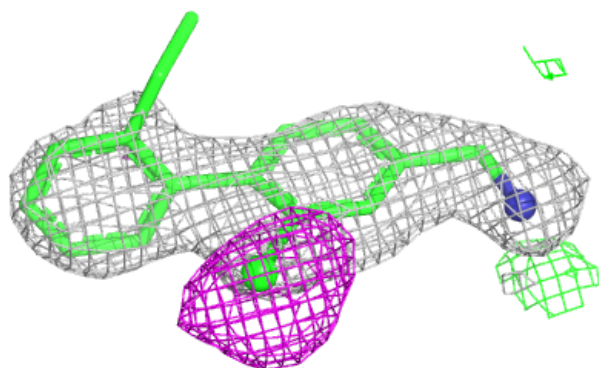


Electron density around A4Q A 405:

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

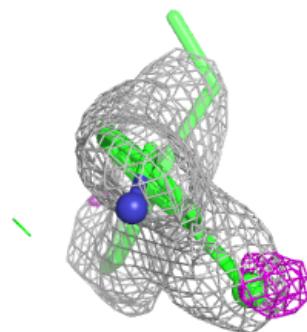
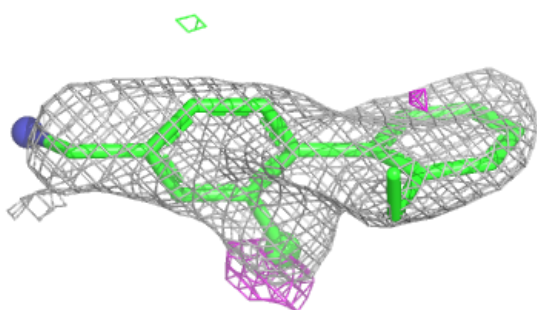
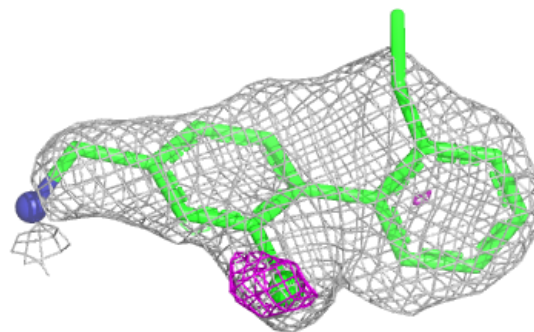
**Electron density around A4Q B 404:**

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

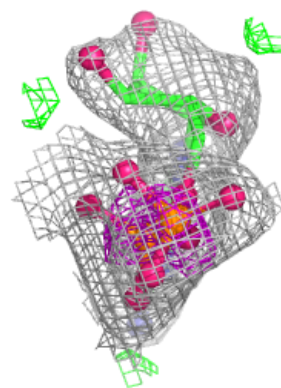
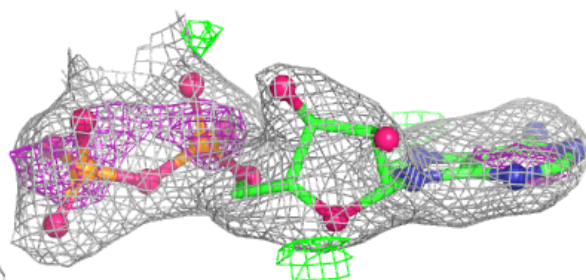
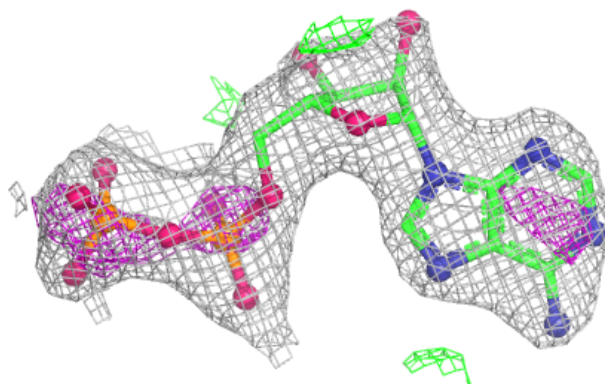


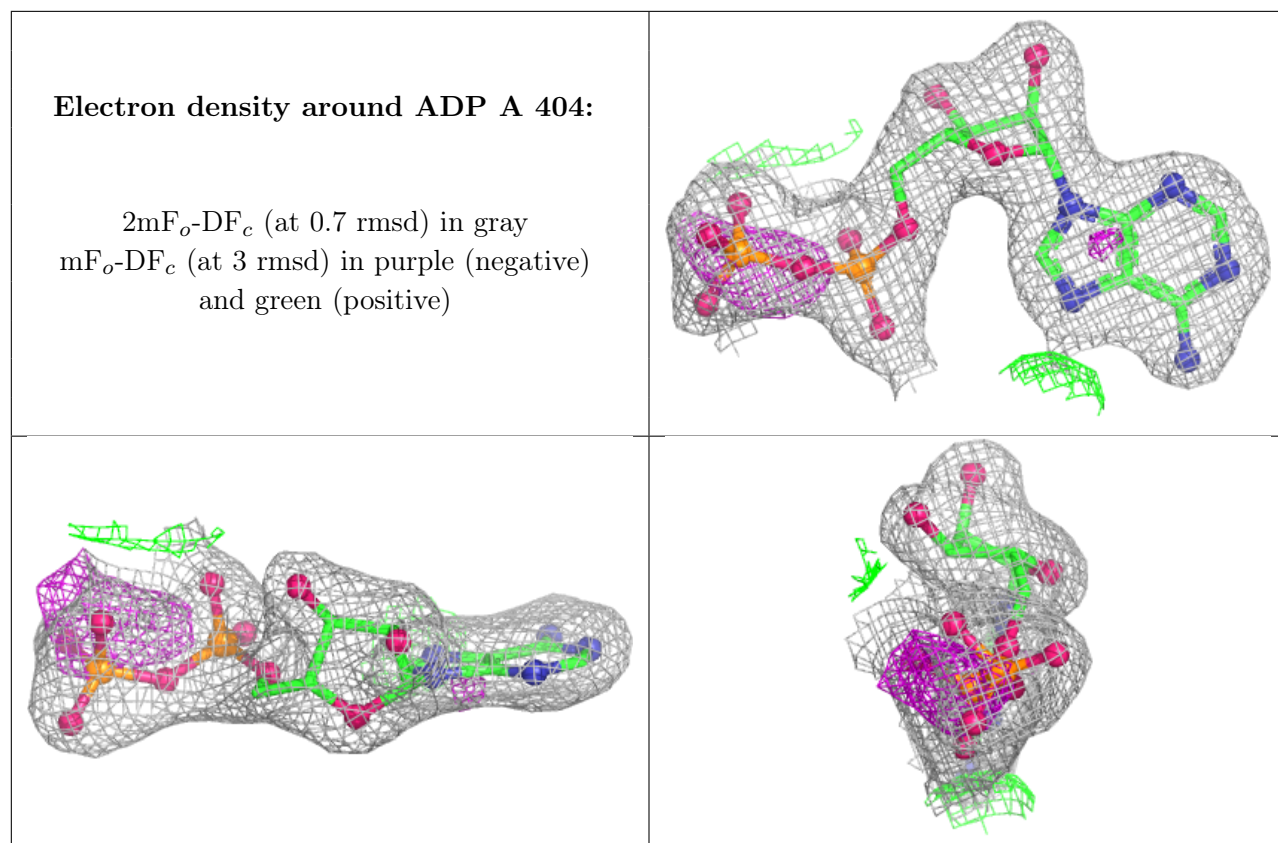
Electron density around A4Q A 406:

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

**Electron density around ADP B 403:**

$2mF_o-DF_c$ (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.