



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 21, 2024 – 05:24 AM EST

PDB ID : 4NH0
Title : Cytoplasmic domain of the Thermomonospora curvata Type VII Secretion ATPase EccC
Authors : Rosenberg, O.S.; Cox, J.S.; Stroud, R.M.; Strauli, N.; Dovala, D.
Deposited on : 2013-11-03
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

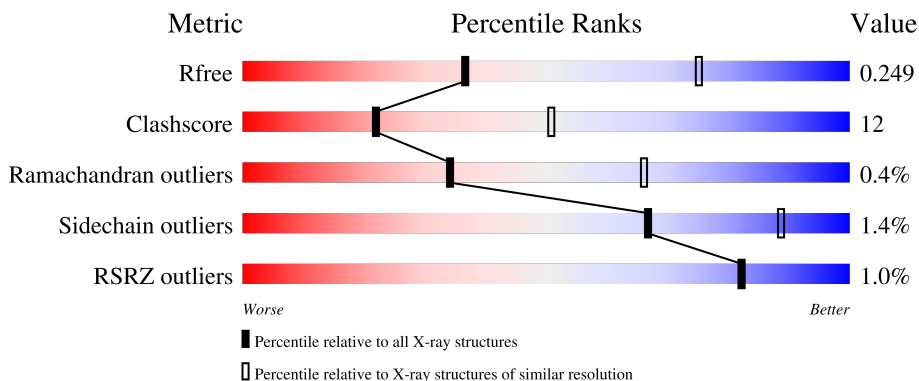
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


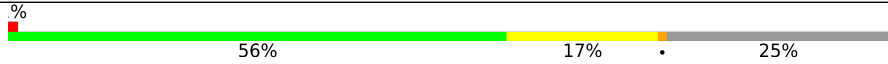
The reported resolution of this entry is 2.90 Å.

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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	1147	
1	B	1147	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13435 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 Cell divisionFtsK/SpoIIIE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	861	6663	4212	1181	1249	21	0	0	0
1	B	859	6626	4186	1175	1244	21	0	0	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	MET	-	expression tag	UNP D1A4G7
A	170	HIS	-	expression tag	UNP D1A4G7
A	171	HIS	-	expression tag	UNP D1A4G7
A	172	HIS	-	expression tag	UNP D1A4G7
A	173	HIS	-	expression tag	UNP D1A4G7
A	174	HIS	-	expression tag	UNP D1A4G7
A	175	HIS	-	expression tag	UNP D1A4G7
A	176	HIS	-	expression tag	UNP D1A4G7
A	177	HIS	-	expression tag	UNP D1A4G7
A	178	GLY	-	expression tag	UNP D1A4G7
A	179	GLY	-	expression tag	UNP D1A4G7
A	180	SER	-	expression tag	UNP D1A4G7
A	181	GLU	-	expression tag	UNP D1A4G7
A	182	PHE	-	expression tag	UNP D1A4G7
A	183	SER	-	expression tag	UNP D1A4G7
A	184	ILE	-	expression tag	UNP D1A4G7
A	185	ASP	-	expression tag	UNP D1A4G7
A	186	GLY	-	expression tag	UNP D1A4G7
A	187	GLY	-	expression tag	UNP D1A4G7
A	188	SER	-	expression tag	UNP D1A4G7
A	189	LEU	-	expression tag	UNP D1A4G7
A	190	GLU	-	expression tag	UNP D1A4G7
A	191	VAL	-	expression tag	UNP D1A4G7
A	192	LEU	-	expression tag	UNP D1A4G7
A	193	PHE	-	expression tag	UNP D1A4G7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	194	GLN	-	expression tag	UNP D1A4G7
A	195	GLY	-	expression tag	UNP D1A4G7
A	196	PRO	-	expression tag	UNP D1A4G7
A	197	SER	-	expression tag	UNP D1A4G7
A	198	SER	-	expression tag	UNP D1A4G7
A	199	PRO	-	expression tag	UNP D1A4G7
B	169	MET	-	expression tag	UNP D1A4G7
B	170	HIS	-	expression tag	UNP D1A4G7
B	171	HIS	-	expression tag	UNP D1A4G7
B	172	HIS	-	expression tag	UNP D1A4G7
B	173	HIS	-	expression tag	UNP D1A4G7
B	174	HIS	-	expression tag	UNP D1A4G7
B	175	HIS	-	expression tag	UNP D1A4G7
B	176	HIS	-	expression tag	UNP D1A4G7
B	177	HIS	-	expression tag	UNP D1A4G7
B	178	GLY	-	expression tag	UNP D1A4G7
B	179	GLY	-	expression tag	UNP D1A4G7
B	180	SER	-	expression tag	UNP D1A4G7
B	181	GLU	-	expression tag	UNP D1A4G7
B	182	PHE	-	expression tag	UNP D1A4G7
B	183	SER	-	expression tag	UNP D1A4G7
B	184	ILE	-	expression tag	UNP D1A4G7
B	185	ASP	-	expression tag	UNP D1A4G7
B	186	GLY	-	expression tag	UNP D1A4G7
B	187	GLY	-	expression tag	UNP D1A4G7
B	188	SER	-	expression tag	UNP D1A4G7
B	189	LEU	-	expression tag	UNP D1A4G7
B	190	GLU	-	expression tag	UNP D1A4G7
B	191	VAL	-	expression tag	UNP D1A4G7
B	192	LEU	-	expression tag	UNP D1A4G7
B	193	PHE	-	expression tag	UNP D1A4G7
B	194	GLN	-	expression tag	UNP D1A4G7
B	195	GLY	-	expression tag	UNP D1A4G7
B	196	PRO	-	expression tag	UNP D1A4G7
B	197	SER	-	expression tag	UNP D1A4G7
B	198	SER	-	expression tag	UNP D1A4G7
B	199	PRO	-	expression tag	UNP D1A4G7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: 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 ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

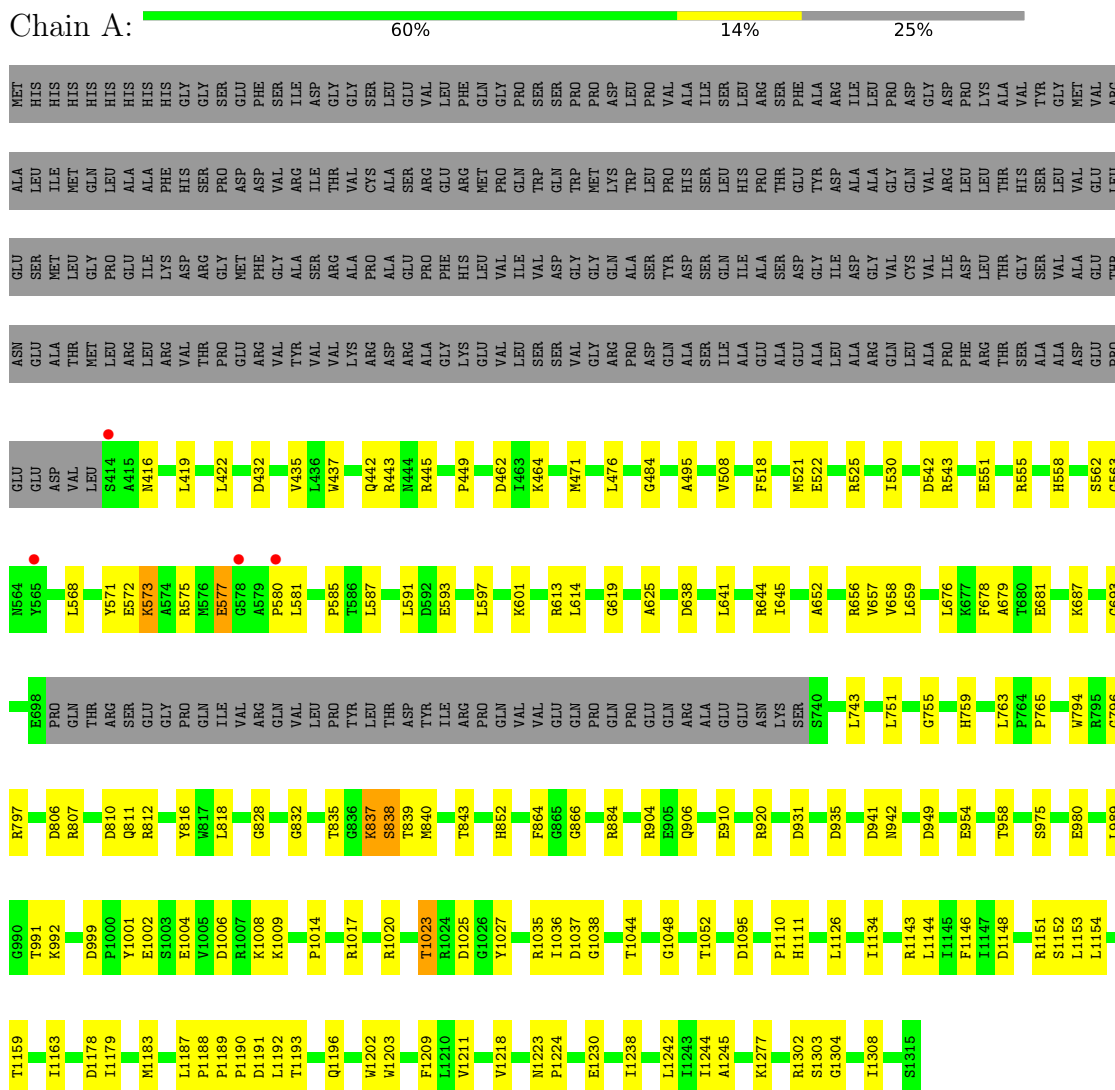
- Molecule 5 is water.

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

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: Cell divisionFtsK/SpoIIIE



- Molecule 1: Cell divisionFtsK/SpoIIIE



V1176	R1177	K1180	M1183	L1187	P1188	P1189	L1192	R1200	S1201	W1202	P1227	R1236	D1237	I1238	L1242	I1243	I1244	M1248	G1275	G1294	F1298	I1308	G1309	T1310	S1315																											
Y1001	E1002	D1006	K1009	V1013	R1020	G1021	F1029	L1030	L1033	P1034	R1035	I1036	D1037	G1038	D1039	T1040	T1044	G1048	T1051	T1052	V1053	K1054	E1058	A1059	W1060	A1065	P1066	L1071	P1072	D1095	E1096	D1117	C1120	G1121	K1122	D1148	S1152	L1153	A1166	L1175												
L850	L851	H852	T853	P854	F859	D863	F864	G867	L872	L875	V876	V877	T883	R884	R891	E905	Q906	E910	T910	R920	R923	F933	G934	D935	D941	M942	Y950	L953	S956	R963	S975	E980	L989	E994	L995	R996	L997															
ARG	ALA	GLU	GLU	ASN	SER	SER	E741	S742	L743	F744	D745	V746	V747	P756	E757	P758	P764	P765	L766	P769	L772	S782	A783	G796	R797	L798	H799	L804	V805	D806	R807	F809	D810	Q811	R812	R813	D819	G822	G823	A824	G828	G832	F833	Q834	K837							
S855	R856	V857	V858	L859	G860	V861	Y865	Y865	E866	L867	P868	Y875	R885	Y890	V891	S892	G893	P894	V895	D896	E897	PRO	GLN	THR	THR	GLU	GLY	PRO	GLN	ILE	VAL	ARG	GLN	E830	E831	G632	K633	L634	R635	G636	L637	D638	T639	H640	L641	S642	Y643	R644	L647	F650	M653	E654
L859	R860	H861	S862	S8414	G860	A415	N416	L419	L422	Y429	D432	P433	A434	V435	Q442	R445	L446	P449	D453	R457	D462	L463	K464	Q468	R471	G475	L476	S483	E487	T491	E503	L528	L534	V541	D542	Y645	R555															
GLU	GLU	ASP	VAL	LEU	LEU	PRO	LEU	VAL	THR	PRO	GLU	ARG	VAL	TYR	VAL	ARG	ASP	VAL	GLN	D453	L607	R613	L614	A625	G626	Q627	R628	L629	E630	E631	G632	K633	L634	R635	G636	L637	D638	T639	H640	L641	S642	Y643	R644	L647	F650	M653	E654					
ASN	GLU	ALA	THR	MET	LEU	ARG	LEU	ARG	VAL	TYR	VAL	ARG	VAL	VAL	VAL	VAL	GLY	VAL	VAL	ILE	THR	SER	SER	GLY	GLY	ASP	GLN	PRO	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA			
GLU	SER	MET	GLY	GLU	GLU	ASP	ASP	PHE	GLY	VAL	SER	VAL	GLY	ASP	ARG	VAL	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA		
ALA	LEU	ILE	MET	LEU	GLN	LEU	ALA	PHE	HIS	GLY	SER	PRO	SER	GLY	GLY	ASP	ASP	VAL	VAL	ILE	ALA	ARG	ILE	GLY	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
MET	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	251.82Å 116.32Å 174.11Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	48.93 – 2.90 48.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.93-2.90) 86.2 (48.93-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 2.91Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.226 , 0.246 0.229 , 0.249	Depositor DCC
R_{free} test set	1523 reflections (1.41%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtrriage
Anisotropy	0.189	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13435	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG, ATP

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	0.25	0/6813	0.41	1/9264 (0.0%)
1	B	0.27	0/6774	0.47	2/9215 (0.0%)
All	All	0.26	0/13587	0.44	3/18479 (0.0%)

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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	807	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	579	ALA	C-N-CD	6.66	142.39	128.40
1	A	563	GLY	N-CA-C	-5.68	98.91	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	807	ARG	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6663	0	6636	118	0
1	B	6626	0	6588	196	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	62	0	24	1	0
4	B	62	0	24	4	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	13435	0	13272	314	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 12.

The worst 5 of 314 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:629:LEU:HD21	1:B:633:LYS:CB	1.81	1.09
1:B:629:LEU:CD2	1:B:633:LYS:HB2	1.87	1.05
1:B:629:LEU:HD21	1:B:633:LYS:HB2	1.08	1.03
1:B:1122:LYS:NZ	4:B:1404:ATP:O2B	1.97	0.97
1:B:764:PRO:O	1:B:813:ARG:NH2	2.02	0.93

There are no symmetry-related clashes.

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	857/1147 (75%)	799 (93%)	56 (6%)	2 (0%)	47 78
1	B	855/1147 (74%)	793 (93%)	58 (7%)	4 (0%)	29 61
All	All	1712/2294 (75%)	1592 (93%)	114 (7%)	6 (0%)	34 66

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	808	PRO
1	A	577	GLU
1	B	823	GLY
1	B	1034	PRO
1	A	580	PRO

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	709/953 (74%)	704 (99%)	5 (1%)	84 95
1	B	703/953 (74%)	688 (98%)	15 (2%)	53 81
All	All	1412/1906 (74%)	1392 (99%)	20 (1%)	67 89

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	644	ARG
1	B	743	LEU
1	B	1020	ARG
1	B	807	ARG
1	B	560	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	416	ASN
1	B	561	HIS
1	B	640	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 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
4	ATP	B	1404	3	26,33,33	0.93	1 (3%)	31,52,52	1.54	5 (16%)
2	SO4	B	1401	-	4,4,4	0.14	0	6,6,6	0.06	0
4	ATP	B	1405	3	26,33,33	0.94	1 (3%)	31,52,52	1.59	5 (16%)
4	ATP	A	1404	3	26,33,33	0.93	1 (3%)	31,52,52	1.62	5 (16%)
2	SO4	A	1401	-	4,4,4	0.15	0	6,6,6	0.06	0
4	ATP	A	1405	3	26,33,33	0.93	1 (3%)	31,52,52	1.60	5 (16%)

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
4	ATP	B	1404	3	-	0/18/38/38	0/3/3/3
4	ATP	A	1404	3	-	0/18/38/38	0/3/3/3
4	ATP	A	1405	3	-	0/18/38/38	0/3/3/3
4	ATP	B	1405	3	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1405	ATP	C5-C4	2.50	1.47	1.40
4	A	1405	ATP	C5-C4	2.47	1.47	1.40
4	B	1404	ATP	C5-C4	2.45	1.47	1.40
4	A	1404	ATP	C5-C4	2.43	1.47	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1404	ATP	PA-O3A-PB	-3.89	119.48	132.83
4	B	1405	ATP	PA-O3A-PB	-3.82	119.71	132.83
4	A	1405	ATP	PB-O3B-PG	-3.77	119.88	132.83
4	A	1405	ATP	PA-O3A-PB	-3.75	119.97	132.83
4	B	1404	ATP	PA-O3A-PB	-3.68	120.20	132.83

There are no chirality outliers.

There are no torsion outliers.

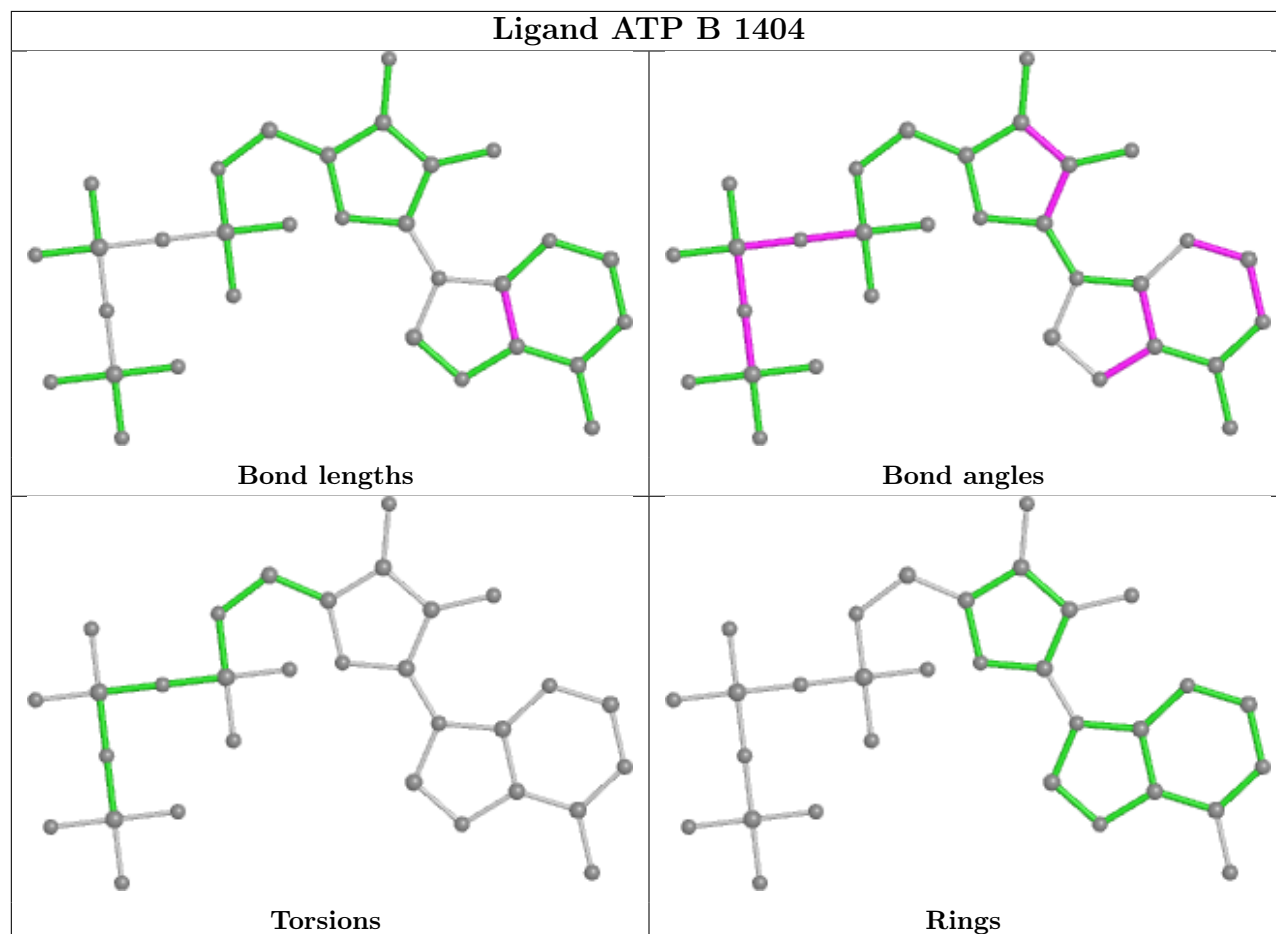
There are no ring outliers.

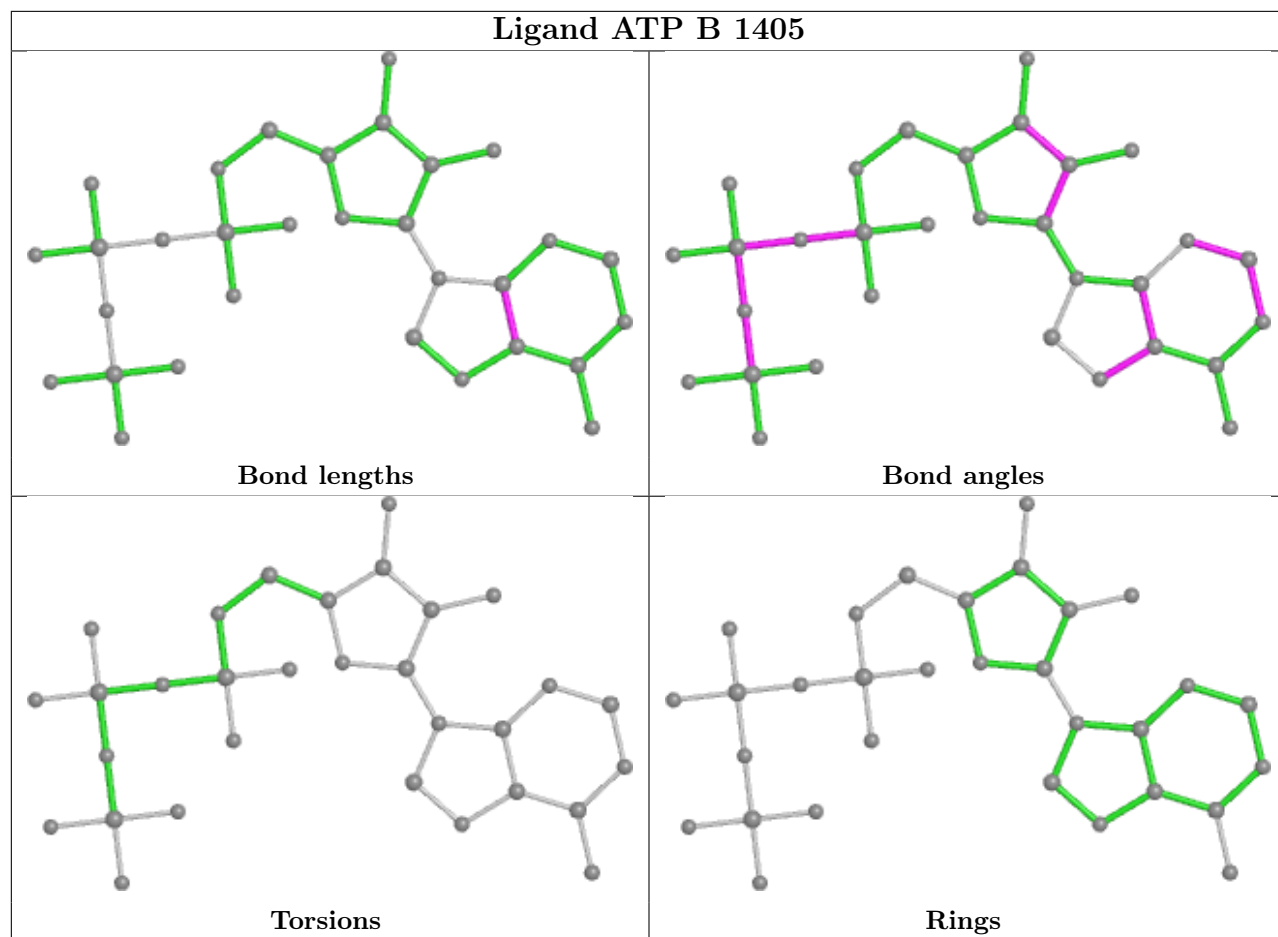
4 monomers are involved in 6 short contacts:

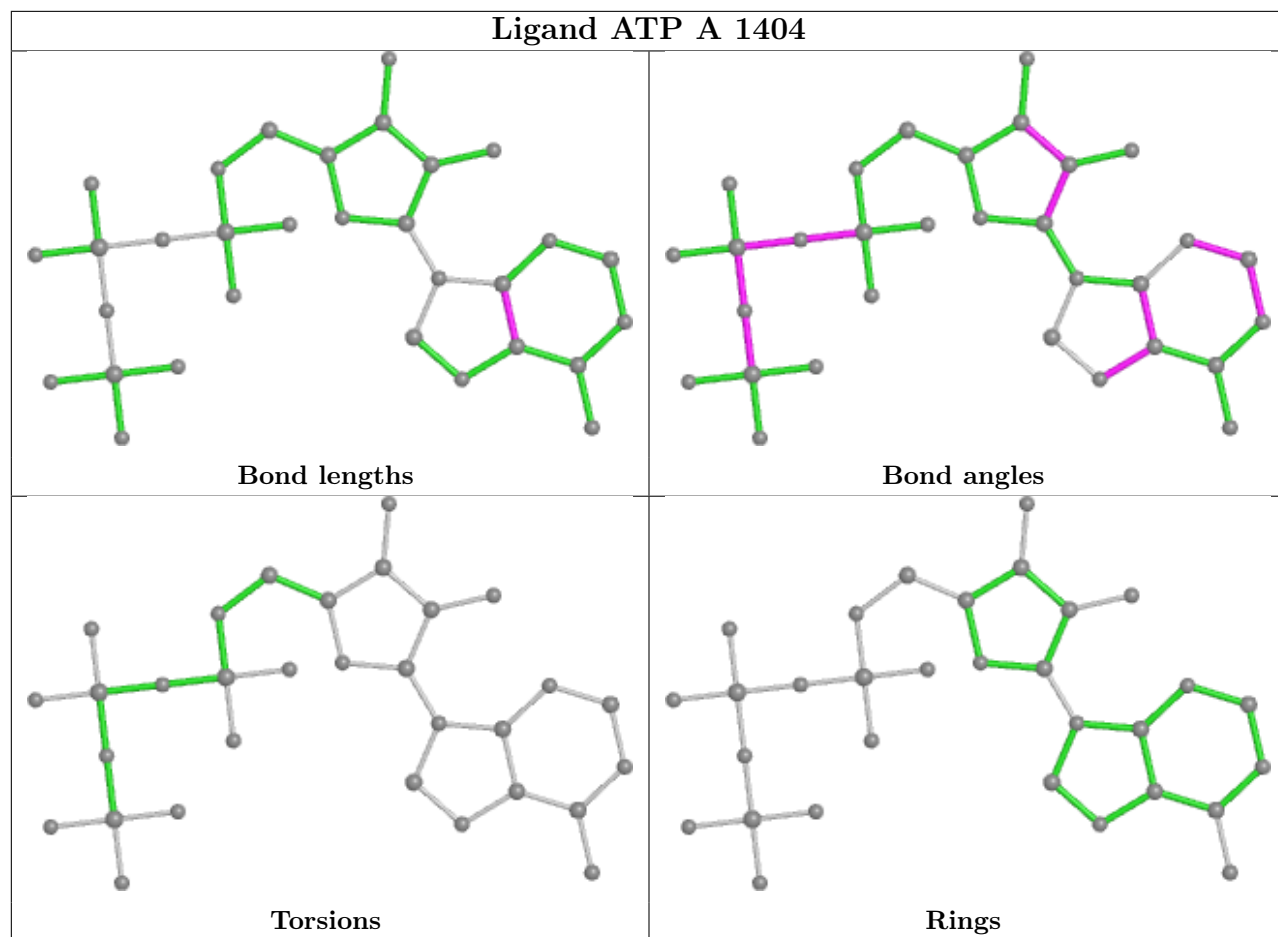
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1404	ATP	2	0
4	B	1405	ATP	2	0
2	A	1401	SO4	1	0
4	A	1405	ATP	1	0

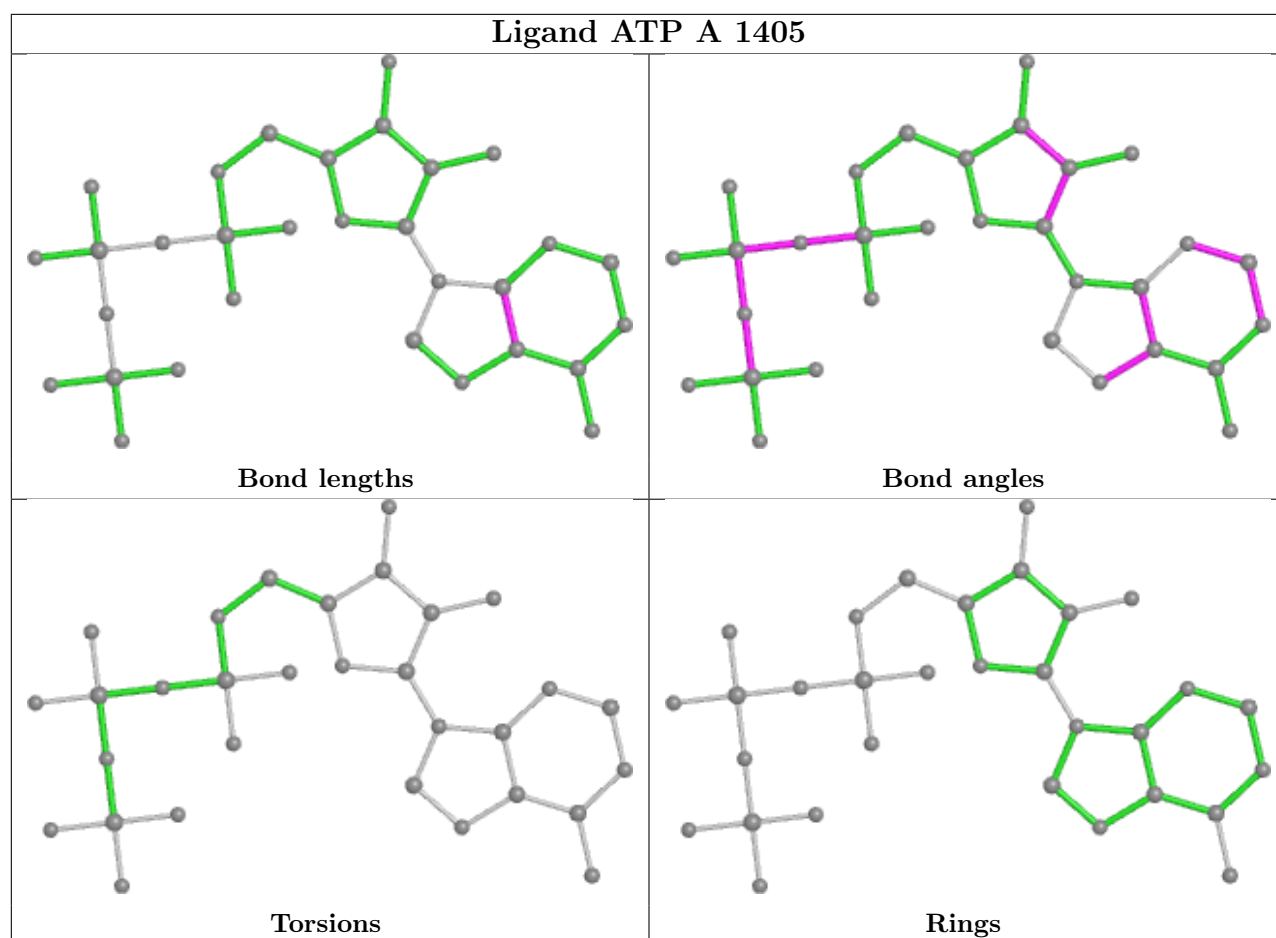
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	861/1147 (75%)	-0.19	4 (0%) 91 91	44, 80, 113, 151	0
1	B	859/1147 (74%)	-0.10	13 (1%) 73 73	35, 84, 128, 161	0
All	All	1720/2294 (74%)	-0.14	17 (0%) 82 82	35, 82, 125, 161	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	578	GLY	3.8
1	B	580	PRO	3.5
1	B	634	LEU	3.3
1	B	565	TYR	2.5
1	A	580	PRO	2.2

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

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

6.3 Carbohydrates [i](#)

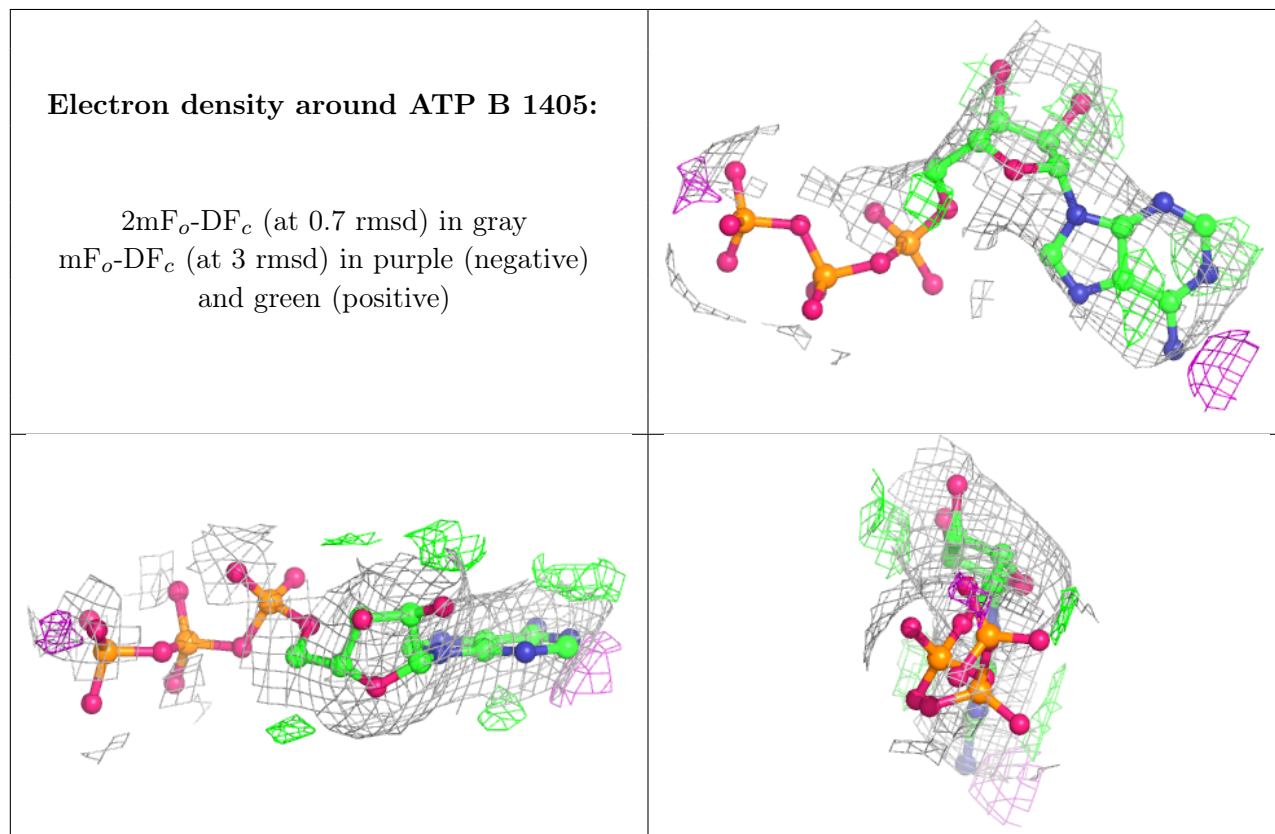
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

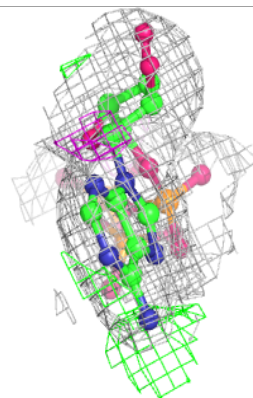
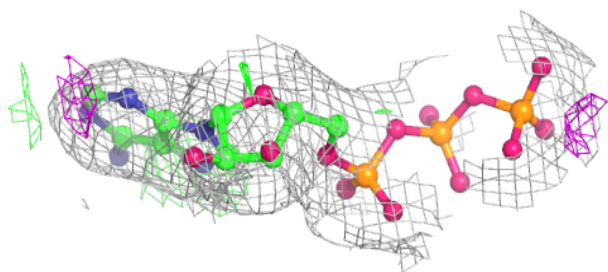
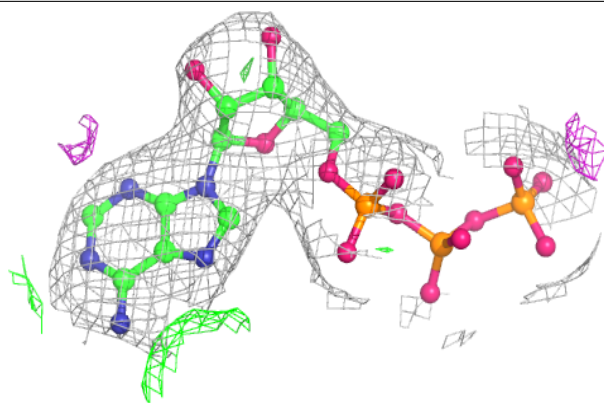
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	B	1401	5/5	0.92	0.11	97,105,124,150	0
2	SO4	A	1401	5/5	0.96	0.11	72,86,91,93	0
3	MG	A	1403	1/1	0.96	0.11	77,77,77,77	0
4	ATP	B	1405	31/31	0.96	0.14	69,117,135,141	0
3	MG	B	1402	1/1	0.97	0.11	59,59,59,59	0
3	MG	B	1403	1/1	0.97	0.06	86,86,86,86	0
4	ATP	A	1404	31/31	0.97	0.14	61,73,96,101	0
4	ATP	A	1405	31/31	0.97	0.14	65,92,108,113	0
4	ATP	B	1404	31/31	0.97	0.16	34,63,78,97	0
3	MG	A	1402	1/1	0.97	0.05	82,82,82,82	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.

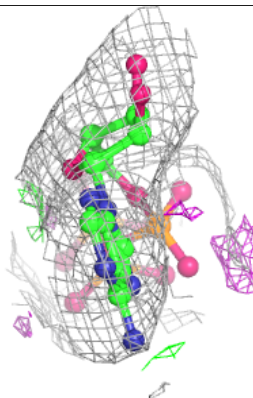
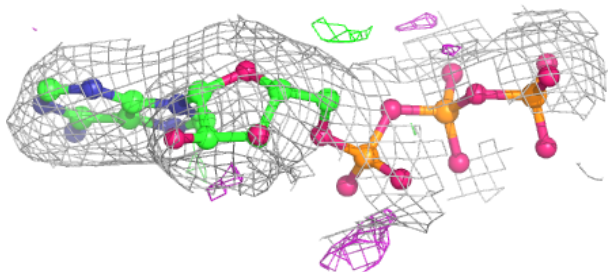
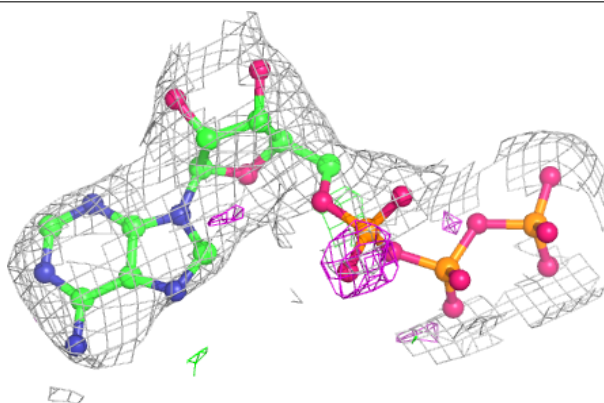


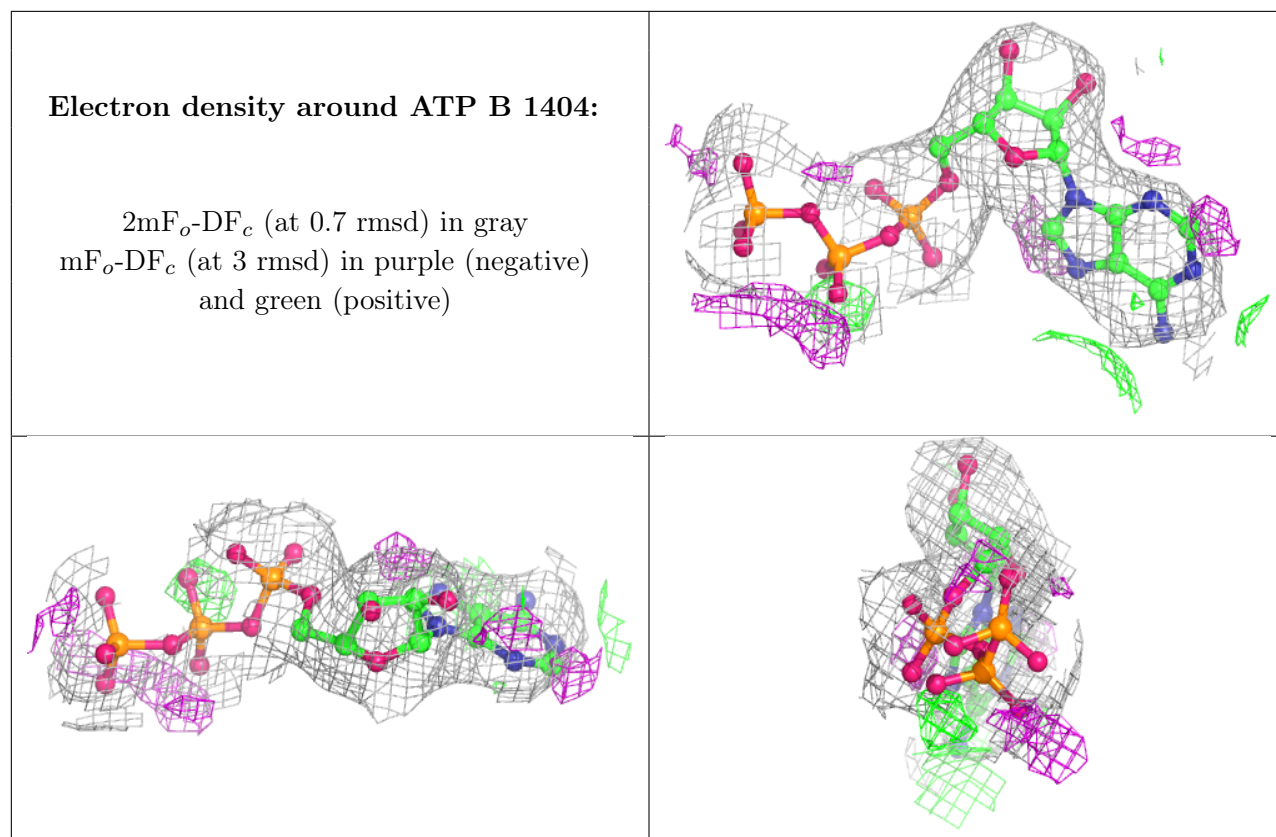
Electron density around ATP A 1404:

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

**Electron density around ATP A 1405:**

$2mF_o-DF_c$ (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.