



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 11:17 am BST

PDB ID : 6NO7
Title : Crystal Structure of the full-length wild-type PKA RIa Holoenzyme
Authors : Lu, T.; Wu, J.; Taylor, S.S.
Deposited on : 2019-01-15
Resolution : 3.55 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 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 : 2.11
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) : 2.11

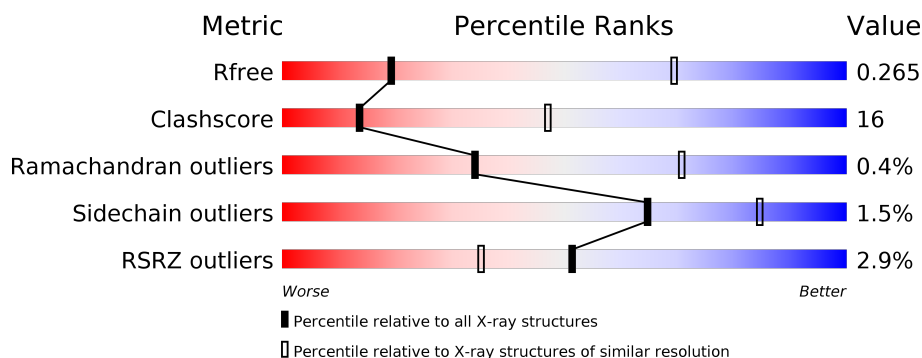
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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 on 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	350	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>.</div> </div> </div>
1	C	350	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>34%</div> <div>.</div> </div> </div>
1	E	350	<div> <div>5%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div>.</div> </div> </div>
1	G	350	<div> <div>6%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div>.</div> </div> </div>
2	B	380	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>23%</div> <div>.</div> <div>25%</div> </div> </div>
2	D	380	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>20%</div> <div>.</div> <div>25%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	380	
2	H	380	

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
1	SEP	C	338	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20128 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 cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	P	S	0	0	0
			2746	1778	460	497	3	8			
1	C	340	Total	C	N	O	P	S	0	0	0
			2775	1794	465	505	3	8			
1	E	339	Total	C	N	O	P	S	0	0	0
			2766	1789	464	502	3	8			
1	G	337	Total	C	N	O	P	S	0	0	0
			2752	1781	461	499	3	8			

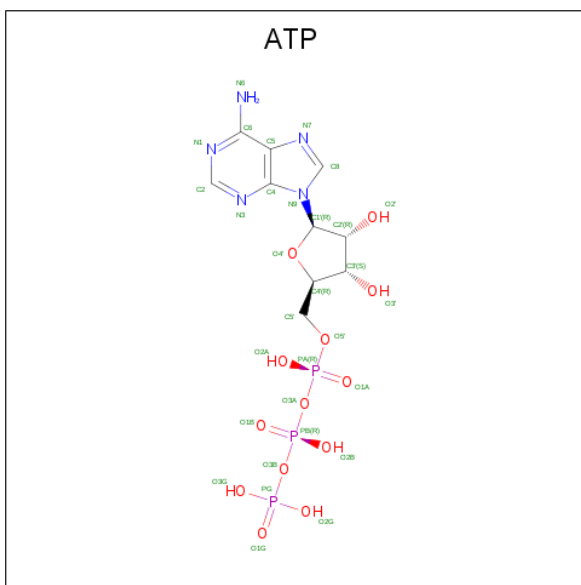
- Molecule 2 is a protein called cAMP-dependent protein kinase type I-alpha regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	285	Total	C	N	O	S	0	0	0
			2259	1428	392	431	8			
2	D	286	Total	C	N	O	S	0	0	0
			2268	1432	395	433	8			
2	F	284	Total	C	N	O	S	0	0	0
			2248	1422	388	430	8			
2	H	284	Total	C	N	O	S	0	0	0
			2248	1422	388	430	8			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

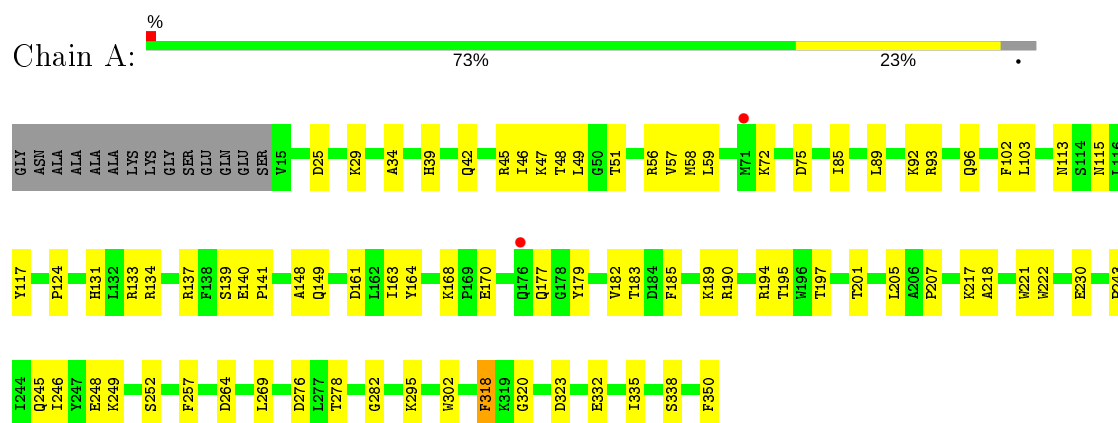


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	G	1	Total 31	C 10	N 5	O 13	P 3	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

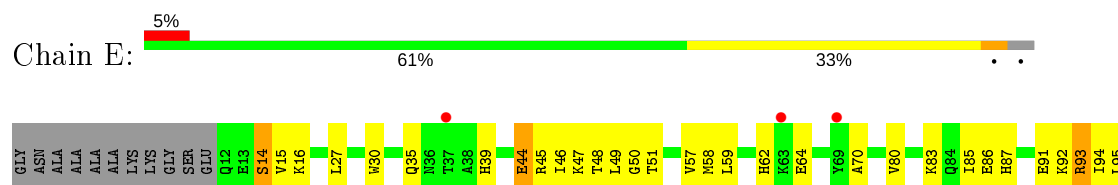
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

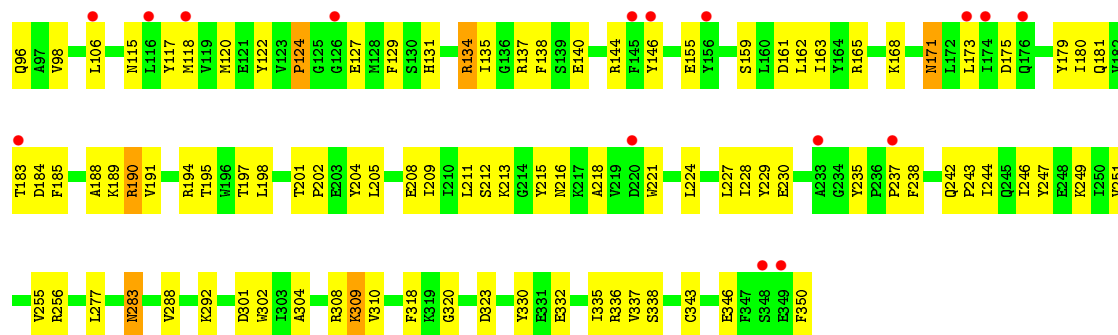


- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

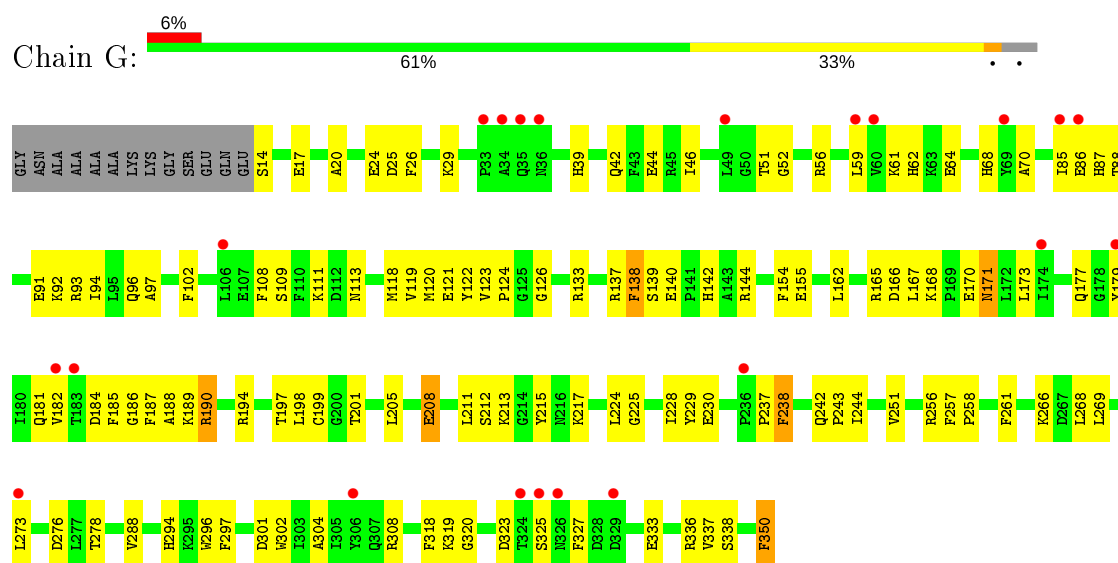


- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

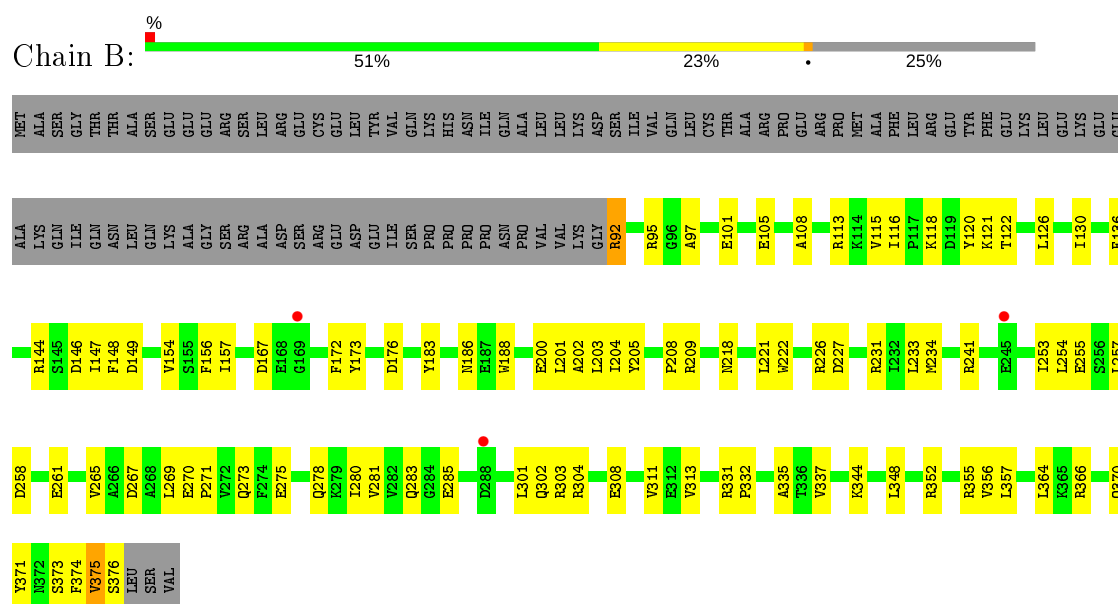




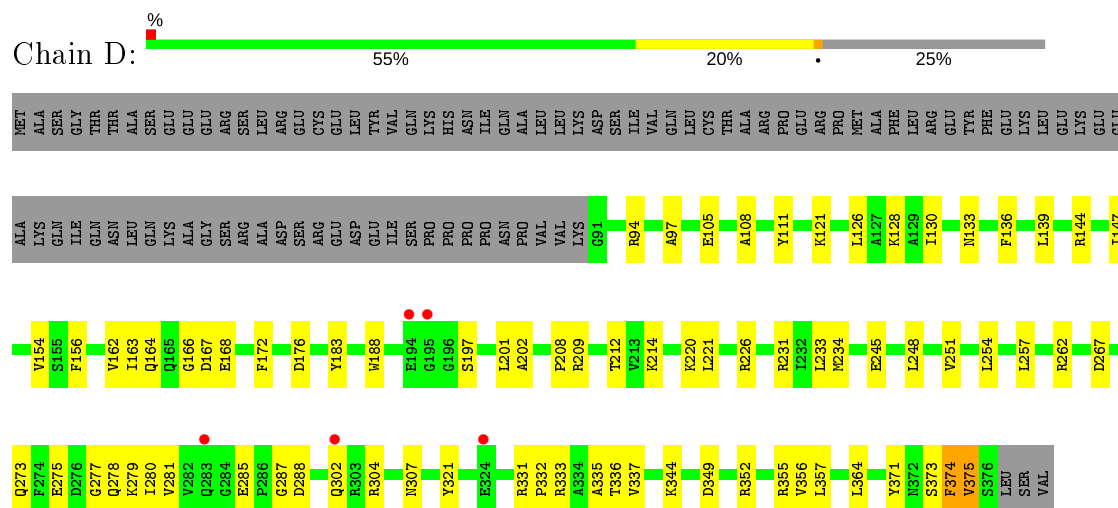
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha



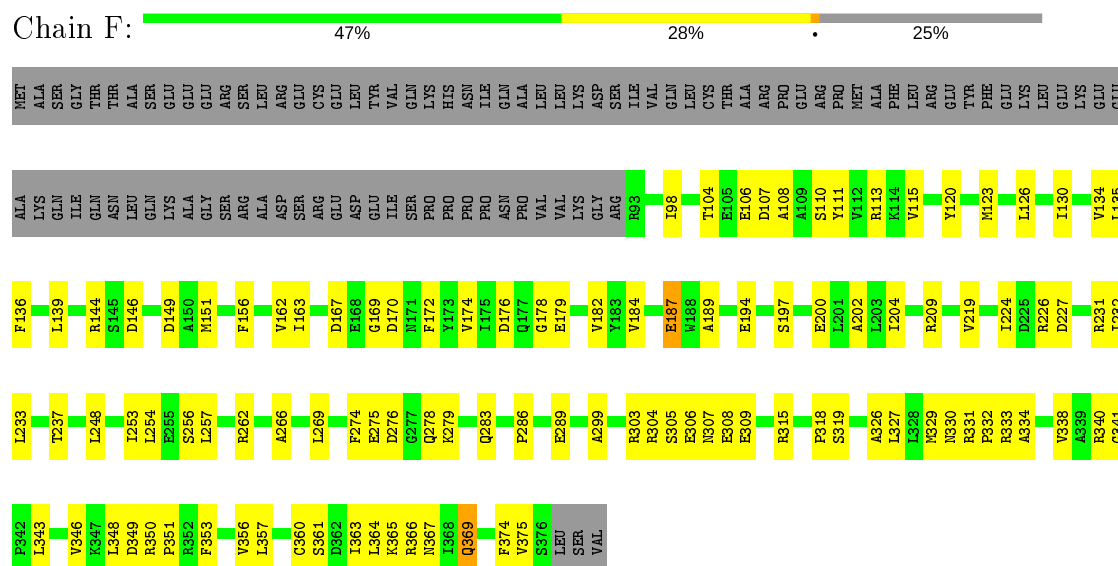
- Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit



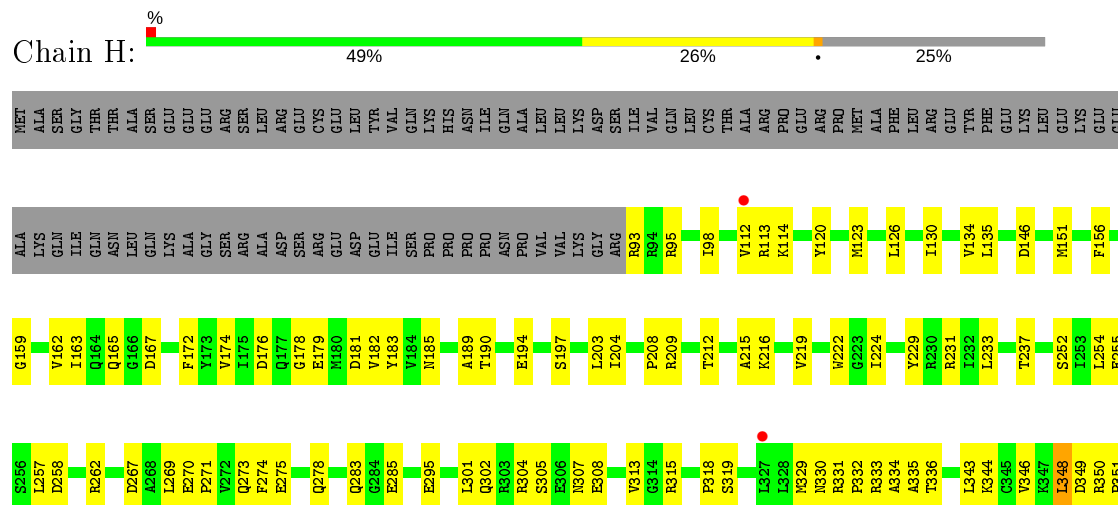
- Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit



- Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit



- Molecule 2: cAMP-dependent protein kinase type I-alpha regulatory subunit



R352	
R355	
V256	
L357	
C360	
S361	
D362	
I363	
L364	
K365	
Q369	
Q370	
S376	
LEU	
SER	
VAL	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.78Å 184.81Å 183.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.63 – 3.55 47.63 – 3.55	Depositor EDS
% Data completeness (in resolution range)	87.0 (47.63-3.55) 84.8 (47.63-3.55)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.256 , 0.269 0.255 , 0.265	Depositor DCC
R_{free} test set	2540 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	110.6	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.158 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20128	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% 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: TPO, MG, ATP, SEP

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	0.30	0/2784	0.57	1/3756 (0.0%)
1	C	0.30	0/2813	0.60	1/3795 (0.0%)
1	E	0.31	0/2804	0.68	1/3783 (0.0%)
1	G	0.33	0/2790	0.68	1/3764 (0.0%)
2	B	0.30	0/2299	0.60	0/3101
2	D	0.30	0/2308	0.58	0/3112
2	F	0.32	0/2288	0.67	0/3087
2	H	0.33	0/2288	0.69	0/3087
All	All	0.31	0/20374	0.64	4/27485 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	PRO	N-CA-CB	5.53	109.94	103.30
1	G	124	PRO	N-CA-CB	5.41	109.79	103.30
1	C	124	PRO	N-CA-CB	5.29	109.64	103.30
1	E	124	PRO	N-CA-CB	5.28	109.64	103.30

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	2746	0	2680	60	0
1	C	2775	0	2702	89	0
1	E	2766	0	2694	99	0
1	G	2752	0	2684	99	0
2	B	2259	0	2238	84	0
2	D	2268	0	2252	64	0
2	F	2248	0	2225	100	0
2	H	2248	0	2225	89	0
3	E	2	0	0	0	0
3	G	2	0	0	0	0
4	E	31	0	12	4	0
4	G	31	0	12	6	0
All	All	20128	0	19724	633	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 16.

The worst 5 of 633 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)
2:B:269:LEU:HD23	2:B:348:LEU:HG	1.30	1.09
2:F:274:PHE:HB3	2:F:278:GLN:HE21	1.18	1.01
2:D:356:VAL:HG12	2:D:357:LEU:HD22	1.44	1.00
2:F:275:GLU:N	2:F:278:GLN:HE22	1.58	0.99
2:B:157:ILE:HG22	2:H:112:VAL:HG23	1.42	0.99

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	331/350 (95%)	322 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	335/350 (96%)	320 (96%)	13 (4%)	2 (1%)	25	64
1	E	334/350 (95%)	311 (93%)	21 (6%)	2 (1%)	25	64
1	G	332/350 (95%)	311 (94%)	20 (6%)	1 (0%)	41	74
2	B	283/380 (74%)	275 (97%)	7 (2%)	1 (0%)	34	71
2	D	284/380 (75%)	274 (96%)	8 (3%)	2 (1%)	22	62
2	F	282/380 (74%)	270 (96%)	11 (4%)	1 (0%)	34	71
2	H	282/380 (74%)	271 (96%)	11 (4%)	0	100	100
All	All	2463/2920 (84%)	2354 (96%)	100 (4%)	9 (0%)	34	71

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	375	VAL
1	E	15	VAL
1	G	325	SER
2	D	375	VAL
1	E	14	SER

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	284/302 (94%)	281 (99%)	3 (1%)	73	88
1	C	287/302 (95%)	285 (99%)	2 (1%)	84	93
1	E	286/302 (95%)	277 (97%)	9 (3%)	40	71
1	G	285/302 (94%)	276 (97%)	9 (3%)	39	70
2	B	239/325 (74%)	237 (99%)	2 (1%)	81	92
2	D	241/325 (74%)	241 (100%)	0	100	100
2	F	238/325 (73%)	236 (99%)	2 (1%)	81	92
2	H	238/325 (73%)	234 (98%)	4 (2%)	60	83
All	All	2098/2508 (84%)	2067 (98%)	31 (2%)	65	84

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	309	LYS
2	F	369	GLN
2	H	305	SER
1	E	323	ASP
1	G	39	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	12	GLN
1	C	96	GLN
1	G	115	ASN
2	B	370	GLN
1	G	96	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	TPO	A	197	1	8,10,11	1.51	1 (12%)	10,14,16	2.16	2 (20%)
1	SEP	C	338	1	8,9,10	1.53	1 (12%)	8,12,14	1.09	0
1	TPO	C	197	1	8,10,11	1.56	1 (12%)	10,14,16	2.28	2 (20%)
1	TPO	E	197	1	8,10,11	1.63	1 (12%)	10,14,16	2.22	2 (20%)
1	SEP	E	338	1	8,9,10	1.52	1 (12%)	8,12,14	1.63	2 (25%)
1	SEP	E	139	1	8,9,10	1.56	1 (12%)	8,12,14	2.10	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	C	139	1	8,9,10	1.57	1 (12%)	8,12,14	3.09	2 (25%)
1	SEP	A	139	1	8,9,10	1.56	1 (12%)	8,12,14	2.31	2 (25%)
1	TPO	G	197	1	8,10,11	1.55	1 (12%)	10,14,16	2.16	2 (20%)
1	SEP	G	338	1	8,9,10	1.55	1 (12%)	8,12,14	2.17	2 (25%)
1	SEP	G	139	1	8,9,10	1.54	1 (12%)	8,12,14	2.57	2 (25%)
1	SEP	A	338	1	8,9,10	1.61	1 (12%)	8,12,14	2.09	2 (25%)

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
1	TPO	A	197	1	-	1/9/11/13	-
1	SEP	C	338	1	-	2/5/8/10	-
1	TPO	C	197	1	-	1/9/11/13	-
1	TPO	E	197	1	-	0/9/11/13	-
1	SEP	E	338	1	-	4/5/8/10	-
1	SEP	E	139	1	-	1/5/8/10	-
1	SEP	C	139	1	-	4/5/8/10	-
1	SEP	A	139	1	-	4/5/8/10	-
1	TPO	G	197	1	-	0/9/11/13	-
1	SEP	G	338	1	-	4/5/8/10	-
1	SEP	G	139	1	-	2/5/8/10	-
1	SEP	A	338	1	-	2/5/8/10	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	139	SEP	P-O1P	3.39	1.61	1.50
1	C	139	SEP	P-O1P	3.38	1.61	1.50
1	C	338	SEP	P-O1P	3.36	1.61	1.50
1	A	338	SEP	P-O1P	3.36	1.61	1.50
1	G	338	SEP	P-O1P	3.36	1.61	1.50

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	SEP	OG-CB-CA	7.06	115.02	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	TPO	P-OG1-CB	-6.19	104.51	123.21
1	E	197	TPO	P-OG1-CB	-5.85	105.54	123.21
1	A	197	TPO	P-OG1-CB	-5.58	106.35	123.21
1	G	197	TPO	P-OG1-CB	-5.49	106.63	123.21

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	197	TPO	O-C-CA-CB
1	E	338	SEP	CB-OG-P-O1P
1	E	338	SEP	CB-OG-P-O2P
1	E	338	SEP	CB-OG-P-O3P
1	C	139	SEP	CB-OG-P-O1P

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	197	TPO	2	0
1	C	338	SEP	4	0
1	C	197	TPO	3	0
1	E	197	TPO	3	0
1	E	338	SEP	1	0
1	C	139	SEP	1	0
1	A	139	SEP	1	0
1	G	197	TPO	2	0
1	G	338	SEP	2	0
1	G	139	SEP	1	0
1	A	338	SEP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	E	403	3	26,33,33	0.95	1 (3%)	31,52,52	1.54	5 (16%)
4	ATP	G	403	3	26,33,33	0.88	1 (3%)	31,52,52	1.56	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	E	403	3	-	5/18/38/38	0/3/3/3
4	ATP	G	403	3	-	4/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	403	ATP	C5-C4	2.49	1.47	1.40
4	G	403	ATP	C5-C4	2.33	1.47	1.40

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	403	ATP	PA-O3A-PB	-3.82	119.71	132.83
4	E	403	ATP	C3'-C2'-C1'	3.63	106.44	100.98
4	G	403	ATP	PB-O3B-PG	-3.37	121.26	132.83
4	E	403	ATP	PB-O3B-PG	-3.16	121.97	132.83
4	E	403	ATP	PA-O3A-PB	-3.13	122.08	132.83

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	403	ATP	O4'-C4'-C5'-O5'
4	E	403	ATP	C3'-C4'-C5'-O5'
4	G	403	ATP	O4'-C4'-C5'-O5'
4	G	403	ATP	C3'-C4'-C5'-O5'

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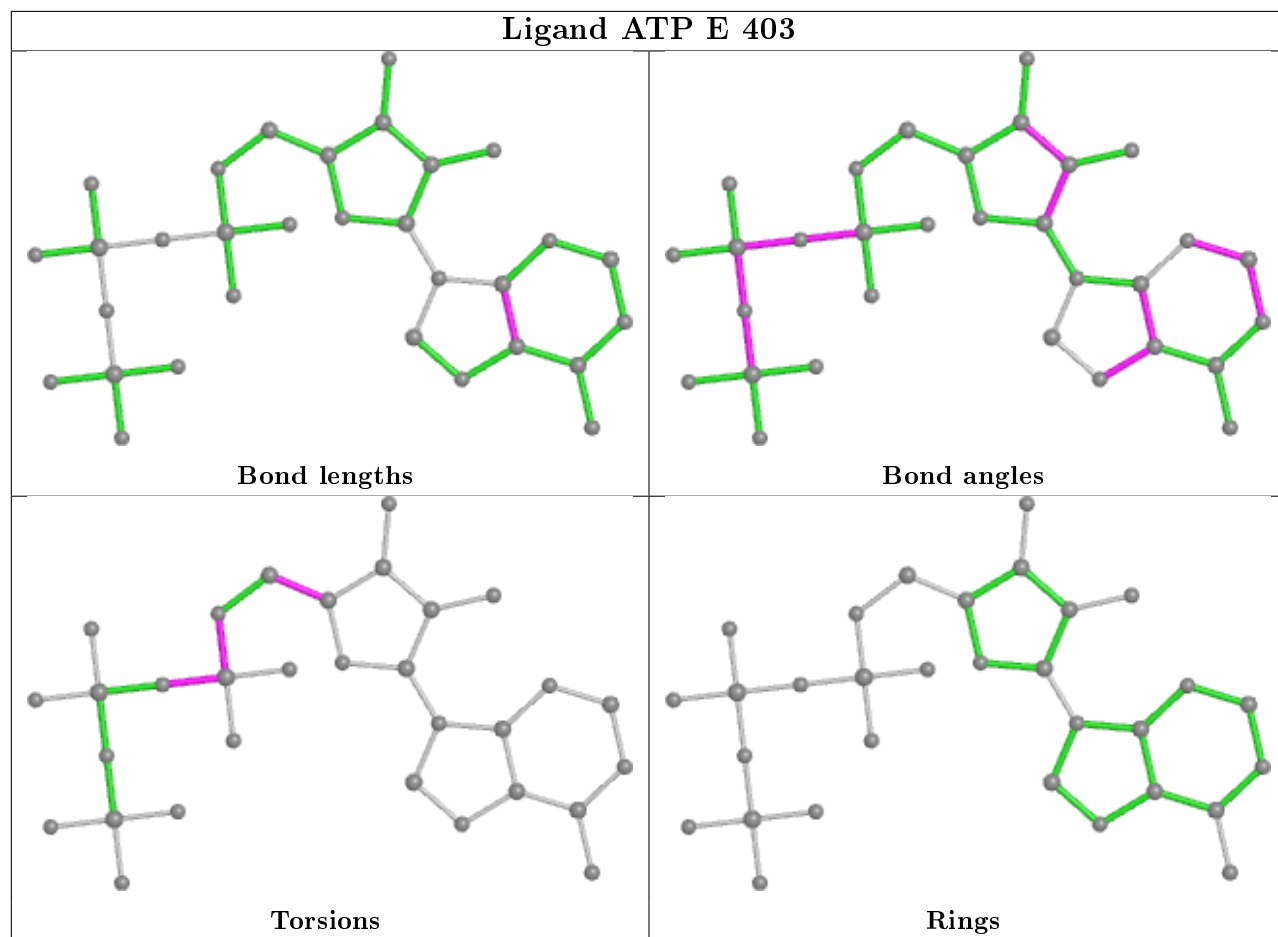
Mol	Chain	Res	Type	Atoms
4	E	403	ATP	PB-O3A-PA-O1A

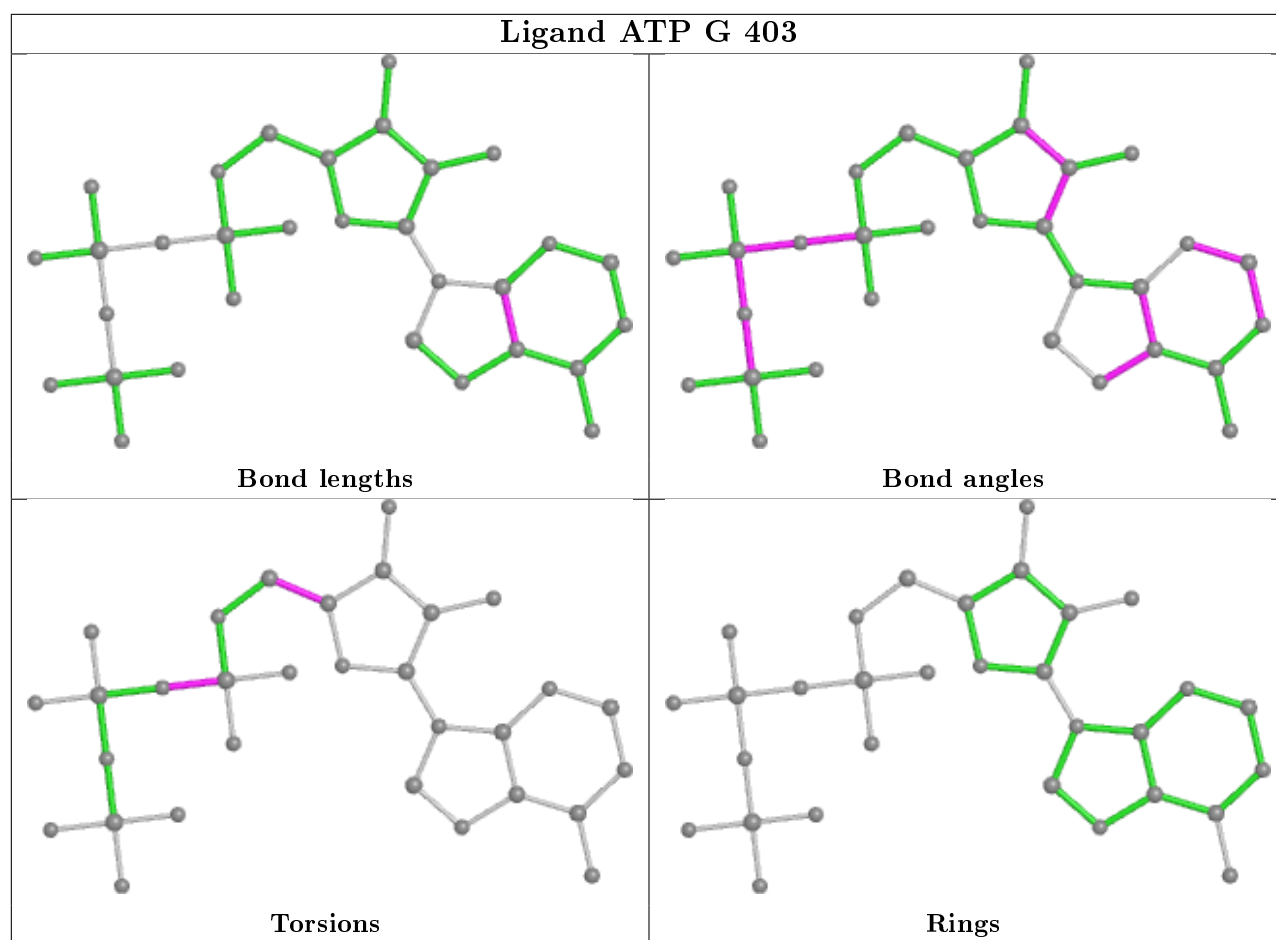
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	403	ATP	4	0
4	G	403	ATP	6	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	333/350 (95%)	0.16	2 (0%) 89 80	79, 133, 183, 214	0
1	C	337/350 (96%)	0.48	19 (5%) 24 15	102, 153, 242, 338	0
1	E	336/350 (96%)	0.29	19 (5%) 23 14	92, 169, 224, 256	0
1	G	334/350 (95%)	0.35	22 (6%) 18 11	98, 180, 247, 387	0
2	B	285/380 (75%)	0.13	3 (1%) 80 67	65, 118, 161, 195	0
2	D	286/380 (75%)	0.06	5 (1%) 70 55	79, 131, 182, 215	0
2	F	284/380 (74%)	0.09	0 100 100	76, 124, 173, 227	0
2	H	284/380 (74%)	0.13	2 (0%) 87 78	70, 130, 178, 207	0
All	All	2479/2920 (84%)	0.22	72 (2%) 51 35	65, 142, 217, 387	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	35	GLN	12.8
1	G	324	THR	11.5
1	C	34	ALA	11.2
1	C	33	PRO	8.4
1	G	36	ASN	6.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	G	139	10/11	0.79	0.19	177,191,214,244	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	SEP	C	139	10/11	0.85	0.16	142,153,176,212	0
1	TPO	C	197	11/12	0.85	0.19	120,136,158,184	0
1	SEP	E	139	10/11	0.86	0.12	161,175,186,215	0
1	SEP	A	338	10/11	0.90	0.14	134,136,142,147	0
1	SEP	A	139	10/11	0.91	0.14	105,128,150,187	0
1	TPO	A	197	11/12	0.91	0.27	79,92,126,210	0
1	SEP	E	338	10/11	0.91	0.10	152,155,171,181	0
1	SEP	G	338	10/11	0.92	0.16	162,173,186,195	0
1	SEP	C	338	10/11	0.93	0.10	173,178,194,208	0
1	TPO	G	197	11/12	0.94	0.18	108,111,127,128	0
1	TPO	E	197	11/12	0.95	0.20	105,108,115,122	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

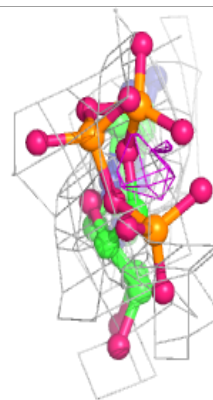
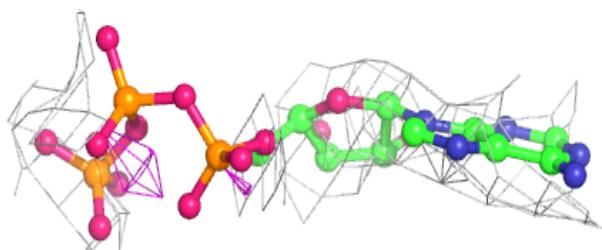
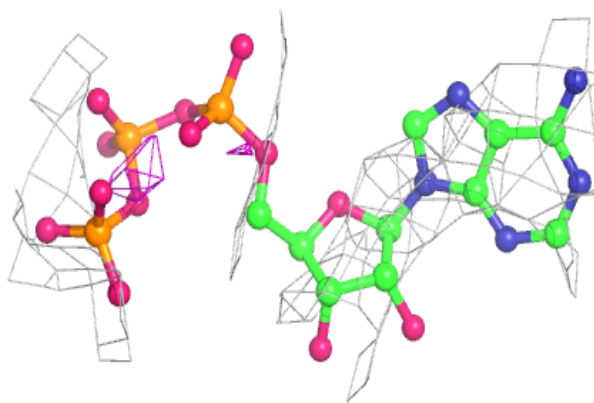
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	G	401	1/1	0.71	0.20	203,203,203,203	0
4	ATP	G	403	31/31	0.80	0.29	109,231,305,390	0
4	ATP	E	403	31/31	0.81	0.35	98,233,316,427	0
3	MG	G	402	1/1	0.90	0.12	212,212,212,212	0
3	MG	E	401	1/1	0.94	0.11	188,188,188,188	0
3	MG	E	402	1/1	0.97	0.13	202,202,202,202	0

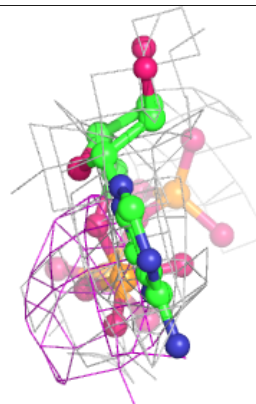
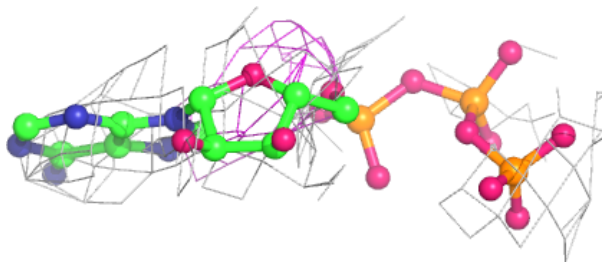
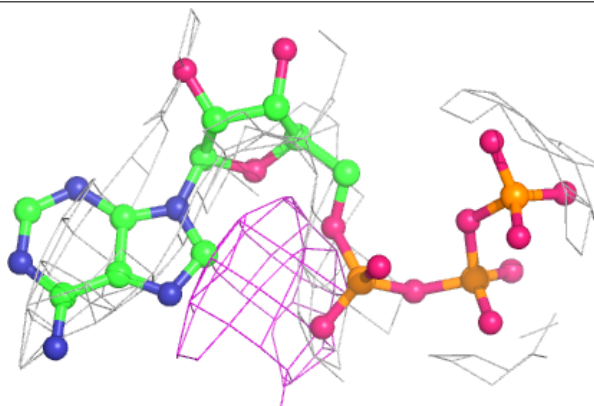
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP G 403:

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

**Electron density around ATP E 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.