Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 04:11 AM EDT

PDB ID	:	6MM6
Title	:	Catalytic subunit of cAMP-dependent protein kinase A in complex with RyR2 phosphorylation domain (2699-2904)
Authors	:	van Petegem, F.; Haji-Ghassemi, O.
Deposited on	:	2018-09-29
Resolution	:	2.39 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 (i) 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 (i)) were used in the production of this report:

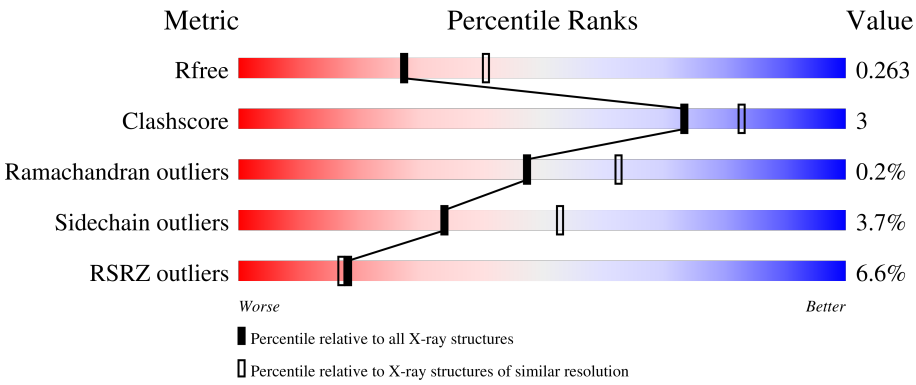
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	C	339	.% 86% 9% 5%
1	E	339	2% 88% 6% • 6%
2	D	209	14% 87% 9% • •
2	F	209	13% 82% 11% • 5%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9029 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
			Total	C	N	O	P	S			
1	C	322	2653	1719	448	476	2	8	0	0	0
1	E	320	2620	1698	444	468	2	8	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	12	SER	-	expression tag	UNP P05132
C	13	ASN	-	expression tag	UNP P05132
C	14	ALA	-	expression tag	UNP P05132
E	12	SER	-	expression tag	UNP P05132
E	13	ASN	-	expression tag	UNP P05132
E	14	ALA	-	expression tag	UNP P05132

- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	198	1611	1027	278	298	8	0	1	0
2	D	201	1635	1040	281	306	8	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

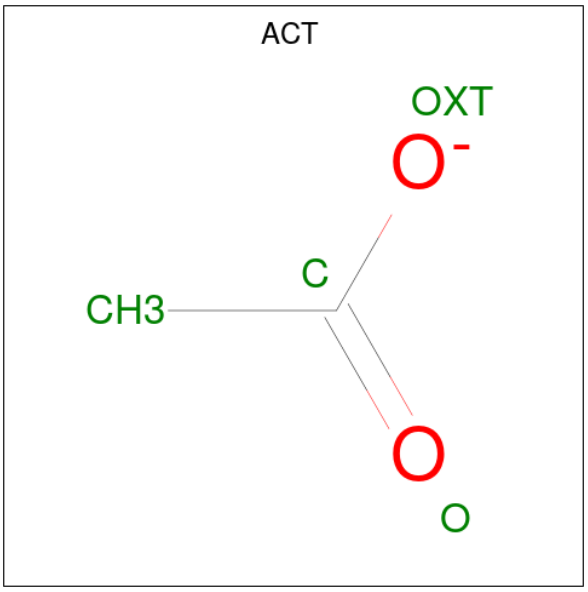
Chain	Residue	Modelled	Actual	Comment	Reference
F	2696	SER	-	expression tag	UNP E9Q401
F	2697	ASN	-	expression tag	UNP E9Q401
F	2698	ALA	-	expression tag	UNP E9Q401
F	2879	ALA	LYS	engineered mutation	UNP E9Q401
D	2696	SER	-	expression tag	UNP E9Q401
D	2697	ASN	-	expression tag	UNP E9Q401

Continued on next page...

Continued from previous page...

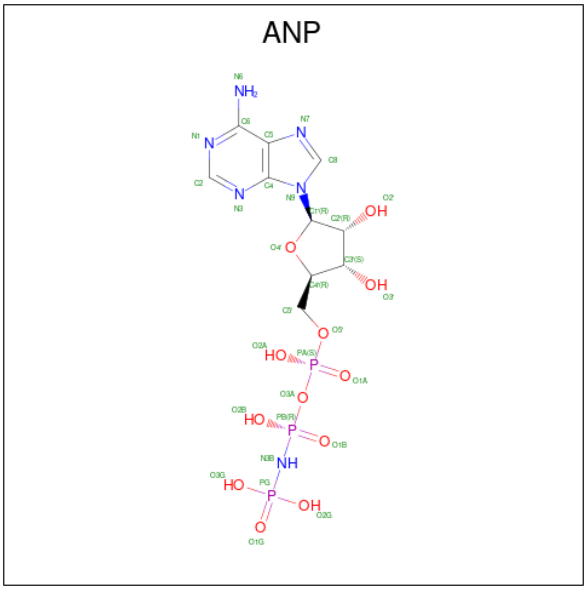
Chain	Residue	Modelled	Actual	Comment	Reference
D	2698	ALA	-	expression tag	UNP E9Q401
D	2879	ALA	LYS	engineered mutation	UNP E9Q401

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



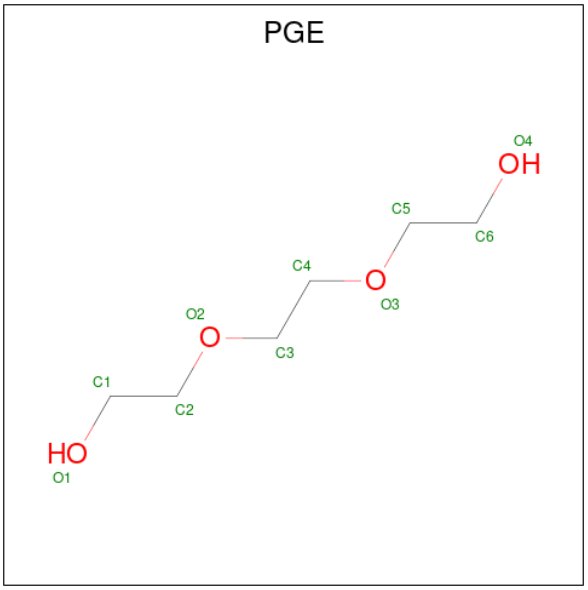
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	C	1	4	2	2	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	C	1	62	20	12	24	6	0	1
4	E	1	62	20	12	24	6	0	1

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

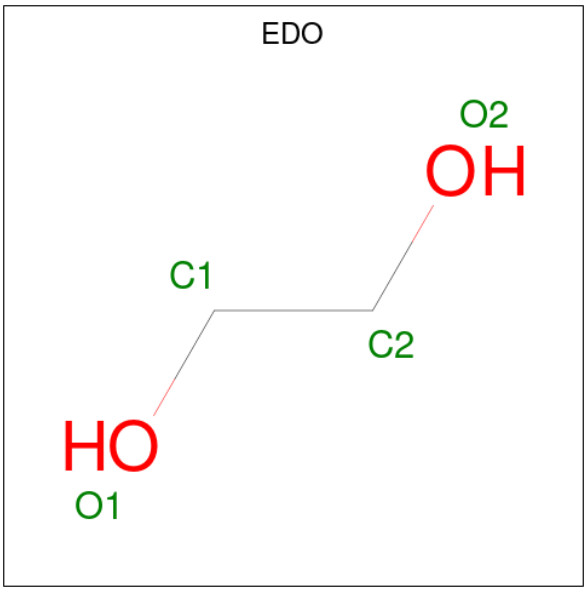


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	C	1	10	6	4	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
6	C	1	1	1	0	0
6	E	1	1	1	0	0
6	F	1	1	1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	E	1	4	2	2	0	0

- Molecule 8 is water.

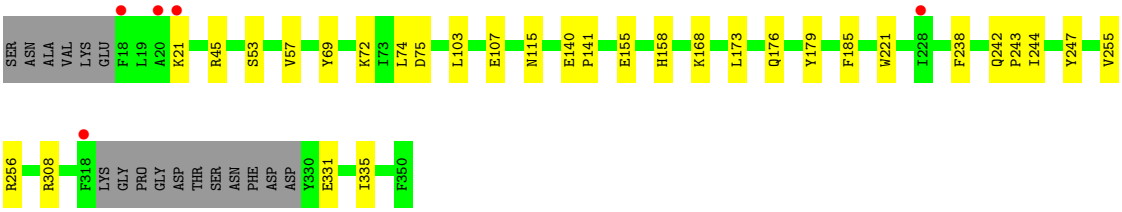
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	C	149	149	149	0	0
			Total	O		
8	E	124	124	124	0	0
			Total	O		
8	F	48	48	48	0	0
			Total	O		
8	D	44	44	44	0	0

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.

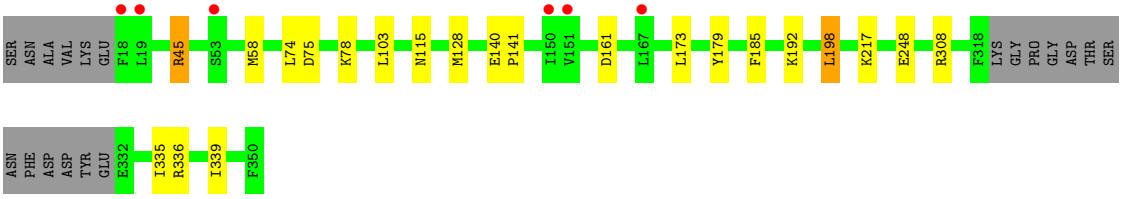
• Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain C:



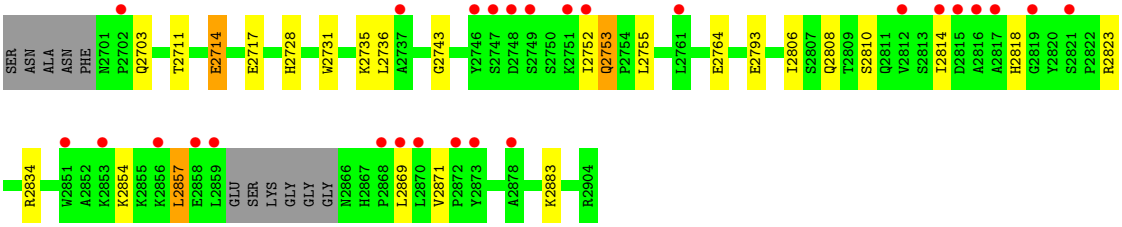
• Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain E:



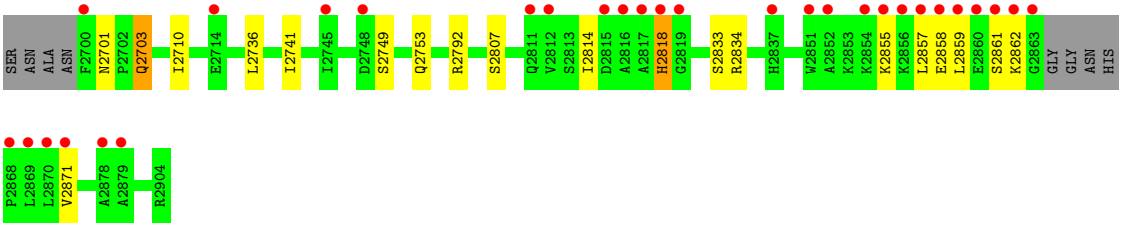
• Molecule 2: Ryanodine receptor 2

Chain F:



• Molecule 2: Ryanodine receptor 2

Chain D:


SER
ASN
ALA
ASN
F2700
N2701
P2702
Q2703
I2710
E2714
L2736
I2741
I2745
D2748
S2749
Q2753
R2792
S2807
Q2811
V2812
S2813
I2814
D2815
A2816
A2817
H2818
G2819
S2833
R2834
H2837
W2851
A2852
K2853
K2854
K2855
K2856
L2857
E2858
L2859
E2860
S2861
K2862
G2863
GLY
GLY
ASN
HIS

P2868
L2869
L2870
V2871
A2878
A2879
R2904

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.45Å 74.94Å 88.69Å 105.51° 90.14° 94.39°	Depositor
Resolution (Å)	34.87 – 2.39 34.85 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.3 (34.87-2.39) 98.3 (34.85-2.39)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.224 , 0.261 0.226 , 0.263	Depositor DCC
R_{free} test set	2830 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 30.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9029	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ANP, SEP, EDO, CL, TPO, ACT, PGE

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	C	0.65	0/2695	0.79	0/3628
1	E	0.66	0/2662	0.80	0/3587
2	D	0.68	0/1674	0.79	0/2258
2	F	0.68	0/1654	0.79	0/2237
All	All	0.66	0/8685	0.79	0/11710

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	C	2653	0	2648	24	0
1	E	2620	0	2601	15	0
2	D	1635	0	1603	13	0
2	F	1611	0	1566	12	0
3	C	4	0	3	0	0
4	C	62	0	26	0	0
4	E	62	0	26	1	0
5	C	10	0	14	5	0
6	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	E	4	0	6	0	0
8	C	149	0	0	0	0
8	D	44	0	0	2	0
8	E	124	0	0	2	0
8	F	48	0	0	0	0
All	All	9029	0	8493	57	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 (57) 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:D:2818:HIS:HB3	8:D:3035:HOH:O	1.66	0.93
1:C:247:TYR:CE2	2:D:2814:ILE:HD13	2.08	0.89
1:C:247:TYR:CD2	2:D:2814:ILE:HG21	2.17	0.79
2:D:2855:LYS:O	2:D:2859:LEU:HB2	1.87	0.74
1:C:247:TYR:CZ	2:D:2814:ILE:HD13	2.32	0.64
1:E:103:LEU:HD22	1:E:185:PHE:HZ	1.64	0.63
1:C:103:LEU:HD22	1:C:185:PHE:HZ	1.66	0.61
2:D:2814:ILE:HG22	2:D:2814:ILE:O	2.00	0.60
1:C:168:LYS:NZ	2:D:2807:SER:OG	2.35	0.59
1:E:198:LEU:HD13	2:F:2810:SER:HB3	1.86	0.58
1:E:45:ARG:HB3	1:E:58:MET:HE3	1.87	0.57
1:E:74:LEU:HD12	1:E:74:LEU:N	2.22	0.55
8:E:583:HOH:O	2:F:2793:GLU:HG2	2.07	0.54
1:C:155:GLU:HG3	5:C:403:PGE:H42	1.90	0.53
1:C:221:TRP:HE1	5:C:403:PGE:H6	1.73	0.52
1:E:103:LEU:HD22	1:E:185:PHE:CZ	2.44	0.52
2:F:2743:GLY:HA3	2:F:2752:ILE:CG2	2.39	0.52
2:D:2834:ARG:HD3	2:D:2834:ARG:C	2.31	0.51
1:C:103:LEU:HD22	1:C:185:PHE:CZ	2.47	0.49
2:F:2834:ARG:HD3	2:F:2834:ARG:C	2.33	0.49
2:F:2854:LYS:O	2:F:2857:LEU:HD22	2.13	0.49
1:E:45:ARG:NE	1:E:335:ILE:HD12	2.28	0.49
1:C:158:HIS:HB2	5:C:403:PGE:H5	1.96	0.48
1:E:45:ARG:HB3	1:E:58:MET:CE	2.43	0.48
1:C:247:TYR:CD2	2:D:2814:ILE:CG2	2.95	0.48
1:C:74:LEU:HD12	1:C:74:LEU:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2728:HIS:HE1	2:F:2755:LEU:O	1.98	0.47
1:E:198:LEU:HD21	2:F:2814:ILE:HD11	1.97	0.47
1:C:75:ASP:HA	1:C:115:ASN:HD22	1.80	0.46
1:E:173:LEU:HD12	1:E:173:LEU:C	2.36	0.46
2:D:2701:ASN:HD21	2:D:2703:GLN:HE22	1.64	0.46
2:D:2857:LEU:O	2:D:2861:SER:OG	2.33	0.46
1:E:248:GLU:OE2	2:F:2818:HIS:NE2	2.48	0.45
1:C:173:LEU:C	1:C:173:LEU:HD12	2.36	0.44
1:E:140:GLU:N	1:E:141:PRO:CD	2.81	0.44
1:E:45:ARG:HD3	8:E:502:HOH:O	2.18	0.44
1:E:179:TYR:CZ	1:E:308:ARG:HA	2.53	0.43
1:C:244:ILE:HD11	8:D:3035:HOH:O	2.17	0.43
2:D:2710:ILE:HD12	2:D:2710:ILE:N	2.33	0.43
1:E:75:ASP:HA	1:E:115:ASN:HD22	1.82	0.43
1:C:140:GLU:N	1:C:141:PRO:CD	2.81	0.42
1:C:179:TYR:CZ	1:C:308:ARG:HA	2.54	0.42
1:C:331:GLU:HG3	1:C:331:GLU:O	2.19	0.42
2:D:2701:ASN:ND2	2:D:2703:GLN:HE22	2.17	0.42
1:C:69:TYR:CE1	1:C:107:GLU:HG3	2.54	0.42
1:C:57:VAL:HG22	1:C:72:LYS:HG2	2.02	0.41
1:C:238:PHE:CZ	1:C:255:VAL:HG22	2.56	0.41
1:C:242:GLN:HE21	1:C:243:PRO:HD2	1.85	0.41
2:F:2753:GLN:OE1	2:F:2755:LEU:HB2	2.20	0.41
4:E:401[C]:ANP:H5'1	4:E:401[C]:ANP:H8	2.03	0.41
2:F:2728:HIS:CE1	2:F:2755:LEU:O	2.74	0.41
1:E:161:ASP:OD2	1:E:192:LYS:HE2	2.20	0.41
1:C:221:TRP:NE1	5:C:403:PGE:H6	2.36	0.40
2:F:2714:GLU:O	2:F:2717:GLU:HG2	2.22	0.40
1:C:45:ARG:HD3	1:C:335:ILE:HD12	2.03	0.40
1:C:155:GLU:HG3	5:C:403:PGE:C4	2.50	0.40
2:F:2731:TRP:O	2:F:2735:LYS:HG2	2.22	0.40

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	C	316/339 (93%)	302 (96%)	14 (4%)	0	100	100
1	E	314/339 (93%)	304 (97%)	10 (3%)	0	100	100
2	D	197/209 (94%)	192 (98%)	3 (2%)	2 (1%)	15	23
2	F	195/209 (93%)	188 (96%)	7 (4%)	0	100	100
All	All	1022/1096 (93%)	986 (96%)	34 (3%)	2 (0%)	47	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	2862	LYS
2	D	2833	SER

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	C	280/297 (94%)	276 (99%)	4 (1%)	67	82
1	E	274/297 (92%)	267 (97%)	7 (3%)	46	66
2	D	174/184 (95%)	165 (95%)	9 (5%)	23	38
2	F	169/184 (92%)	156 (92%)	13 (8%)	13	20
All	All	897/962 (93%)	864 (96%)	33 (4%)	34	53

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	21	LYS
1	C	53	SER
1	C	176	GLN
1	C	256	ARG
1	E	45	ARG
1	E	78	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	128	MET
1	E	198	LEU
1	E	217	LYS
1	E	336	ARG
1	E	339	ILE
2	F	2703	GLN
2	F	2711	THR
2	F	2714	GLU
2	F	2736	LEU
2	F	2753	GLN
2	F	2764	GLU
2	F	2806	ILE
2	F	2808	GLN
2	F	2823	ARG
2	F	2857	LEU
2	F	2869	LEU
2	F	2871	VAL
2	F	2883	LYS
2	D	2703	GLN
2	D	2736	LEU
2	D	2741	ILE
2	D	2749	SER
2	D	2753	GLN
2	D	2792	ARG
2	D	2818	HIS
2	D	2858	GLU
2	D	2871	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	67	ASN
1	C	113	ASN
1	C	115	ASN
1	C	242	GLN
1	C	340	ASN
1	E	67	ASN
1	E	77	GLN
1	E	90	ASN
1	E	113	ASN
1	E	115	ASN
2	F	2726	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	2808	GLN
2	D	2701	ASN
2	D	2829	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)

4 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	SEP	E	338	1	8,9,10	0.67	0	8,12,14	0.84	0
1	TPO	E	197	1	8,10,11	0.62	0	10,14,16	0.95	0
1	TPO	C	197	1	8,10,11	0.67	0	10,14,16	0.98	0
1	SEP	C	338	1	8,9,10	0.68	0	8,12,14	1.06	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
1	SEP	E	338	1	-	5/5/8/10	-
1	TPO	E	197	1	-	1/9/11/13	-
1	TPO	C	197	1	-	0/9/11/13	-
1	SEP	C	338	1	-	2/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	338	SEP	N-CA-CB-OG
1	E	197	TPO	CB-OG1-P-O3P
1	E	338	SEP	N-CA-CB-OG
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	E	338	SEP	CA-CB-OG-P
1	C	338	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
3	ACT	C	401	-	3,3,3	0.98	0	3,3,3	0.74	0
5	PGE	C	403	-	9,9,9	0.28	0	8,8,8	0.24	0
4	ANP	C	402[B]	-	29,33,33	1.26	4 (13%)	31,52,52	1.12	3 (9%)
4	ANP	E	401[B]	-	29,33,33	1.22	5 (17%)	31,52,52	1.11	3 (9%)
4	ANP	E	401[C]	-	29,33,33	1.21	4 (13%)	31,52,52	1.17	3 (9%)
4	ANP	C	402[C]	-	29,33,33	1.24	5 (17%)	31,52,52	1.10	2 (6%)
7	EDO	E	402	-	3,3,3	0.10	0	2,2,2	0.32	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	PGE	C	403	-	-	0/7/7/7	-
4	ANP	C	402[B]	-	-	3/14/38/38	0/3/3/3
4	ANP	E	401[B]	-	-	3/14/38/38	0/3/3/3
4	ANP	E	401[C]	-	-	5/14/38/38	0/3/3/3
4	ANP	C	402[C]	-	-	9/14/38/38	0/3/3/3
7	EDO	E	402	-	-	1/1/1/1	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402[B]	ANP	PG-O1G	3.52	1.51	1.46
4	C	402[C]	ANP	PG-O1G	3.40	1.51	1.46
4	E	401[B]	ANP	PG-O1G	3.25	1.51	1.46
4	E	401[C]	ANP	PG-O1G	3.16	1.51	1.46
4	E	401[C]	ANP	PB-O1B	3.01	1.50	1.46
4	E	401[B]	ANP	PB-O1B	2.98	1.50	1.46
4	C	402[B]	ANP	PB-O1B	2.97	1.50	1.46
4	C	402[C]	ANP	PB-O1B	2.97	1.50	1.46
4	E	401[B]	ANP	PB-O2B	-2.22	1.50	1.56
4	C	402[B]	ANP	PB-O2B	-2.22	1.50	1.56
4	E	401[C]	ANP	PB-O2B	-2.15	1.51	1.56
4	C	402[C]	ANP	PG-O2G	-2.15	1.51	1.56
4	C	402[C]	ANP	PB-O2B	-2.11	1.51	1.56
4	E	401[C]	ANP	PG-O3G	-2.06	1.51	1.56
4	E	401[B]	ANP	PG-O3G	-2.03	1.51	1.56
4	E	401[B]	ANP	PG-O2G	-2.03	1.51	1.56
4	C	402[C]	ANP	PG-O3G	-2.01	1.51	1.56
4	C	402[B]	ANP	PG-O3G	-2.01	1.51	1.56

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	402[C]	ANP	O2B-PB-O1B	4.19	118.71	109.92
4	E	401[C]	ANP	O2B-PB-O1B	4.05	118.42	109.92
4	C	402[B]	ANP	O2B-PB-O1B	4.05	118.41	109.92
4	E	401[B]	ANP	O2B-PB-O1B	4.00	118.31	109.92
4	C	402[B]	ANP	O3G-PG-O1G	-2.43	107.33	113.45
4	E	401[B]	ANP	C5-C6-N6	2.36	123.93	120.35
4	C	402[C]	ANP	C5-C6-N6	2.34	123.91	120.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	401[C]	ANP	C5-C6-N6	2.34	123.91	120.35
4	C	402[B]	ANP	C5-C6-N6	2.31	123.86	120.35
4	E	401[B]	ANP	O2G-PG-O1G	-2.22	107.87	113.45
4	E	401[C]	ANP	O2G-PG-O1G	-2.16	108.03	113.45

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	402[B]	ANP	PB-N3B-PG-O1G
4	C	402[B]	ANP	PG-N3B-PB-O1B
4	C	402[C]	ANP	PG-N3B-PB-O1B
4	C	402[C]	ANP	PA-O3A-PB-O1B
4	C	402[C]	ANP	PA-O3A-PB-O2B
4	C	402[C]	ANP	C5'-O5'-PA-O1A
4	C	402[C]	ANP	C5'-O5'-PA-O2A
4	E	401[B]	ANP	PB-N3B-PG-O1G
4	E	401[B]	ANP	PA-O3A-PB-O1B
4	E	401[B]	ANP	PA-O3A-PB-O2B
4	E	401[C]	ANP	PB-N3B-PG-O1G
4	E	401[C]	ANP	PG-N3B-PB-O1B
4	E	401[C]	ANP	PA-O3A-PB-O1B
4	E	401[C]	ANP	O4'-C4'-C5'-O5'
4	C	402[C]	ANP	O4'-C4'-C5'-O5'
4	C	402[C]	ANP	C3'-C4'-C5'-O5'
4	E	401[C]	ANP	C3'-C4'-C5'-O5'
7	E	402	EDO	O1-C1-C2-O2
4	C	402[C]	ANP	PB-O3A-PA-O5'
4	C	402[B]	ANP	C4'-C5'-O5'-PA
4	C	402[C]	ANP	C5'-O5'-PA-O3A

There are no ring outliers.

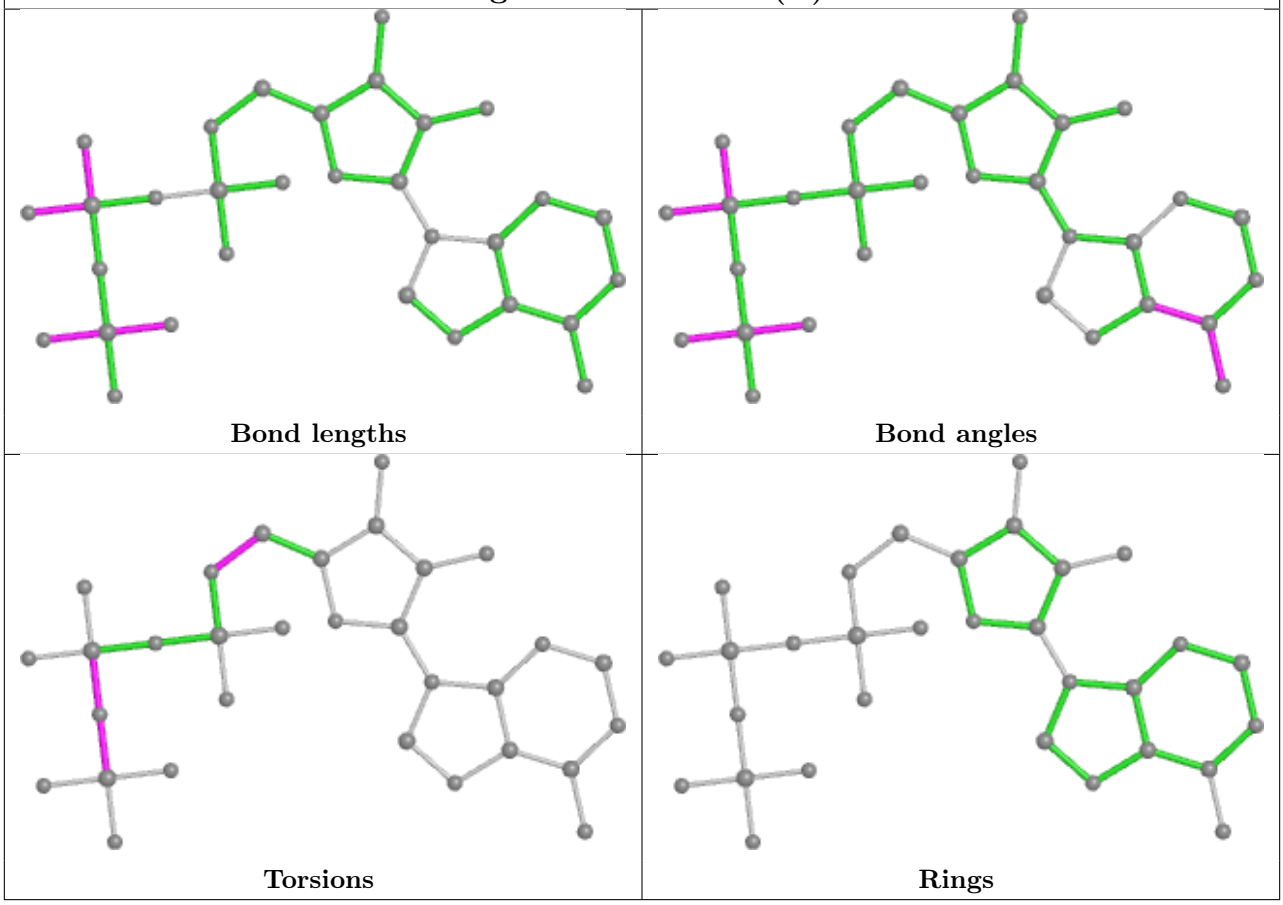
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	403	PGE	5	0
4	E	401[C]	ANP	1	0

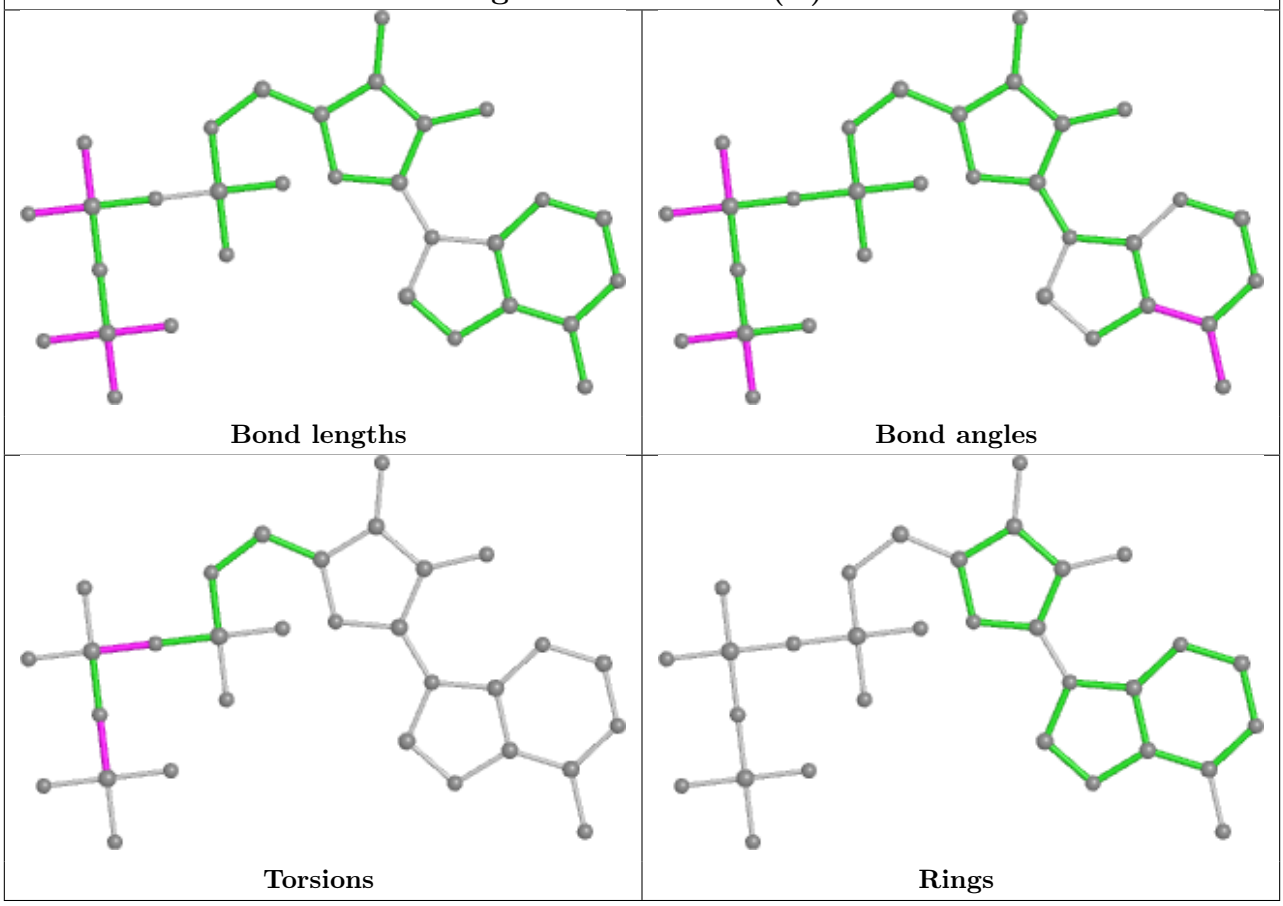
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

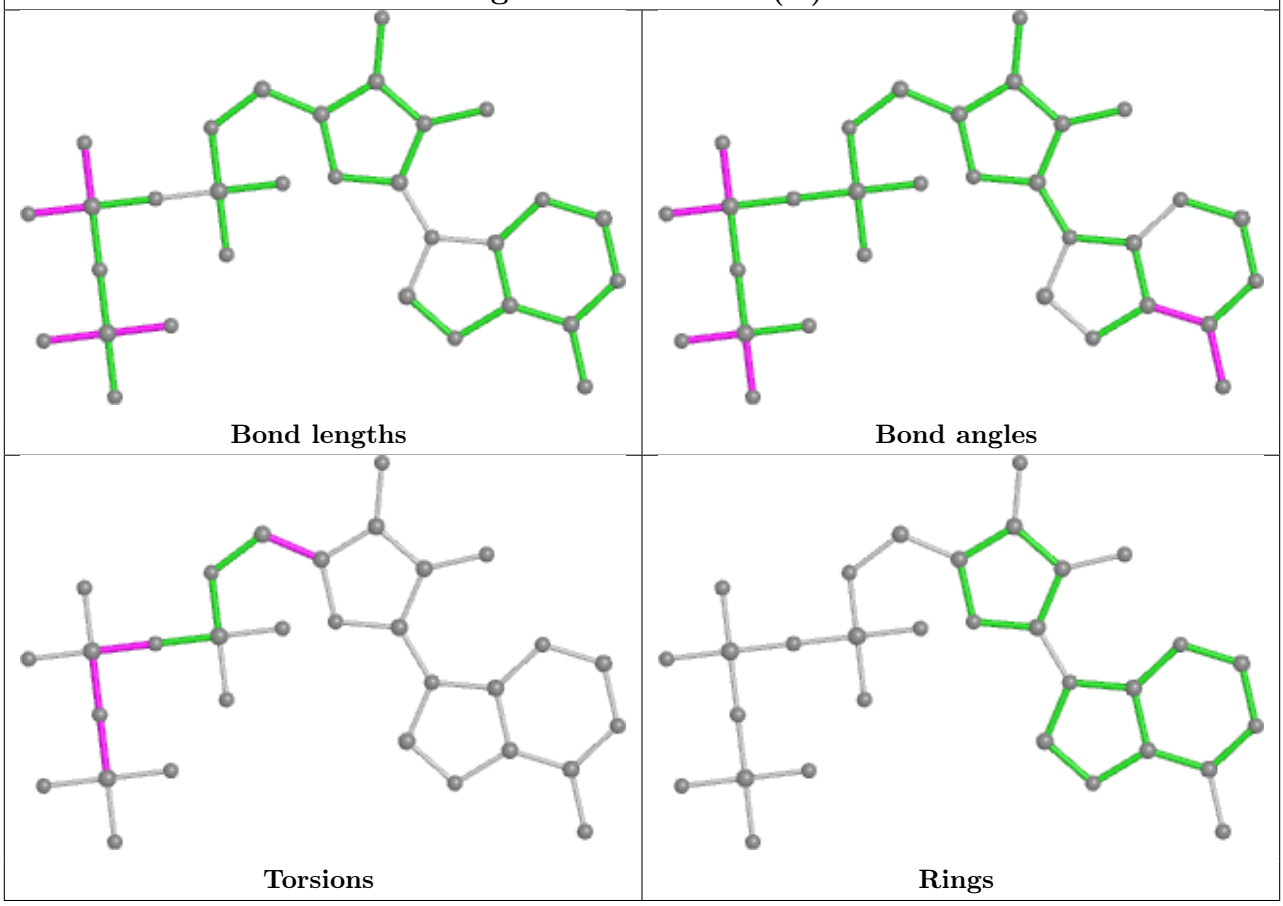
Ligand ANP C 402 (B)



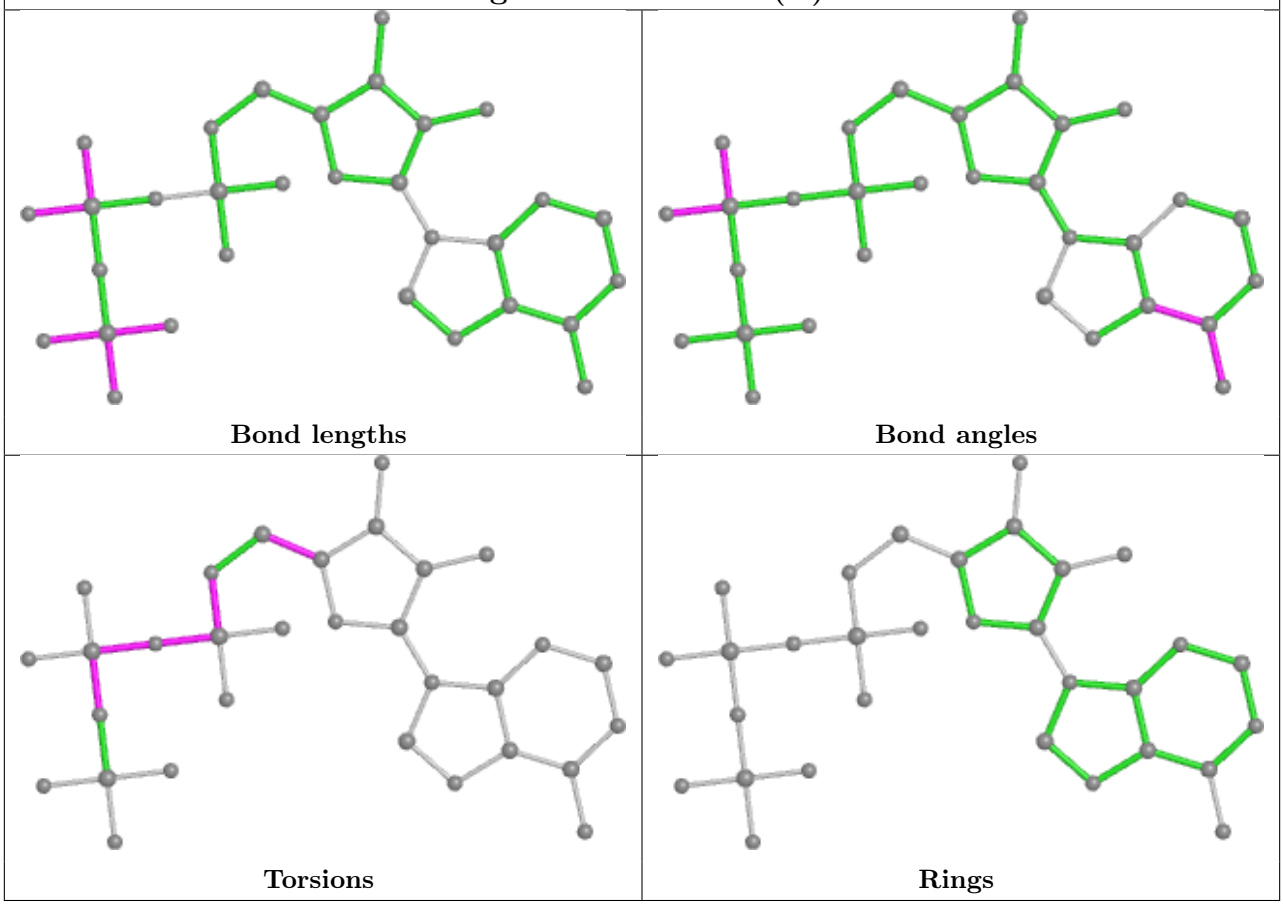
Ligand ANP E 401 (B)



Ligand ANP E 401 (C)



Ligand ANP C 402 (C)



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	C	320/339 (94%)	0.18	5 (1%)	72	70	23, 33, 45, 60	0
1	E	318/339 (93%)	0.15	6 (1%)	66	64	24, 35, 49, 58	0
2	D	201/209 (96%)	0.85	30 (14%)	2	2	35, 49, 81, 104	0
2	F	198/209 (94%)	0.69	27 (13%)	3	2	35, 51, 89, 109	0
All	All	1037/1096 (94%)	0.40	68 (6%)	18	17	23, 39, 72, 109	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	2863	GLY	10.9
2	D	2869	LEU	6.9
2	D	2818	HIS	6.2
2	D	2817	ALA	6.0
2	D	2856	LYS	5.9
2	D	2870	LEU	5.9
2	D	2857	LEU	5.8
2	D	2861	SER	5.7
2	D	2819	GLY	5.4
2	D	2859	LEU	5.4
2	F	2748	ASP	4.3
2	F	2816	ALA	4.1
2	F	2870	LEU	4.1
2	D	2860	GLU	3.9
2	D	2816	ALA	3.8
2	F	2737	ALA	3.8
2	D	2700	PHE	3.6
1	E	19	LEU	3.4
2	D	2815	ASP	3.3
2	F	2856	LYS	3.3
1	E	53	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	2862	LYS	3.3
2	D	2878	ALA	3.2
1	C	18	PHE	3.0
1	E	18	PHE	3.0
2	D	2855	LYS	2.9
2	F	2858	GLU	2.9
2	F	2761	LEU	2.8
2	F	2749	SER	2.7
2	D	2811	GLN	2.7
2	F	2815	ASP	2.6
2	D	2858	GLU	2.6
2	D	2879	ALA	2.5
2	F	2752	ILE	2.5
1	C	21	LYS	2.5
1	C	228	ILE	2.5
2	F	2702	PRO	2.5
2	D	2748	ASP	2.5
2	F	2751	LYS	2.4
2	F	2859	LEU	2.4
1	C	318	PHE	2.4
1	E	151	VAL	2.4
2	F	2851	TRP	2.4
2	F	2878	ALA	2.4
2	F	2869	LEU	2.4
2	F	2819	GLY	2.3
2	D	2852	ALA	2.3
2	F	2821	SER	2.3
1	C	20	ALA	2.3
2	D	2812	VAL	2.3
2	D	2871	VAL	2.3
2	D	2837	HIS	2.3
2	D	2851	TRP	2.2
2	F	2817	ALA	2.2
1	E	150	ILE	2.2
2	F	2814	ILE	2.2
2	F	2853	LYS	2.2
1	E	167	LEU	2.2
2	F	2873	TYR	2.2
2	F	2868	PRO	2.1
2	D	2854	LYS	2.1
2	D	2745	ILE	2.1
2	D	2868	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	2812	VAL	2.1
2	F	2872	PRO	2.1
2	F	2747	SER	2.1
2	D	2714	GLU	2.0
2	F	2746	TYR	2.0

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	C	338	10/11	0.93	0.12	42,43,47,48	0
1	SEP	E	338	10/11	0.94	0.10	49,51,56,57	0
1	TPO	E	197	11/12	0.96	0.11	30,31,32,32	0
1	TPO	C	197	11/12	0.98	0.10	30,31,32,32	0

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(Å^2)	Q<0.9
5	PGE	C	403	10/10	0.81	0.25	39,47,53,54	0
7	EDO	E	402	4/4	0.83	0.19	51,52,52,53	0
4	ANP	E	401[B]	31/31	0.85	0.24	47,63,72,77	31
6	CL	C	404	1/1	0.85	0.11	57,57,57,57	0
4	ANP	E	401[C]	31/31	0.85	0.24	50,67,85,86	31
4	ANP	C	402[C]	31/31	0.87	0.21	43,57,76,76	31
4	ANP	C	402[B]	31/31	0.87	0.21	40,53,65,66	31
3	ACT	C	401	4/4	0.95	0.20	52,52,53,53	0
6	CL	E	403	1/1	0.96	0.09	31,31,31,31	0

Continued on next page...

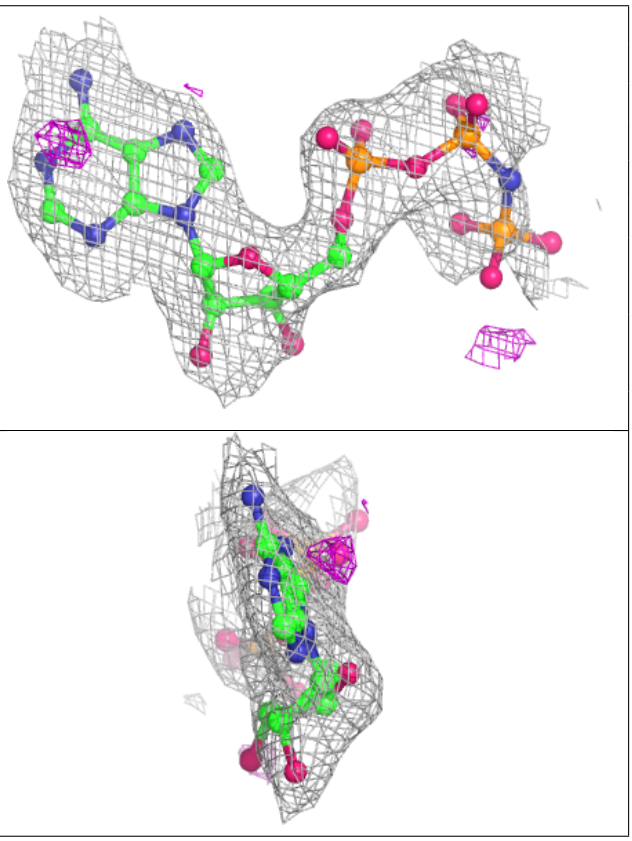
Continued from previous page...

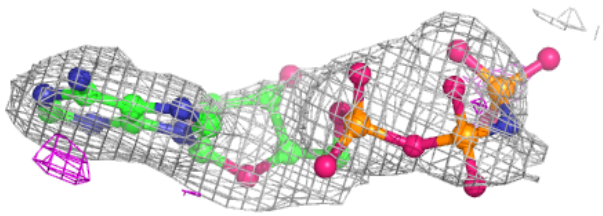
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CL	F	3001	1/1	0.97	0.08	34,34,34,34	0

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 ANP E 401 (B):

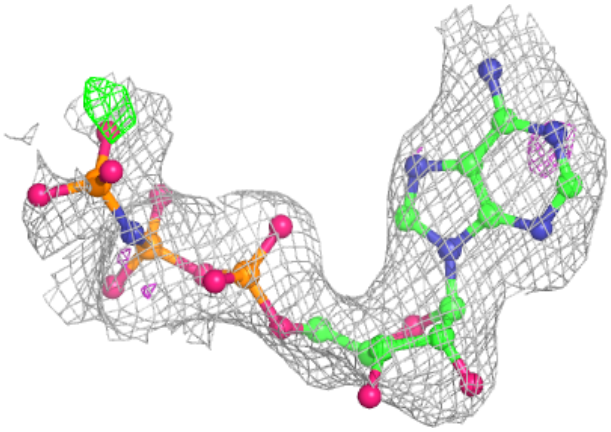
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

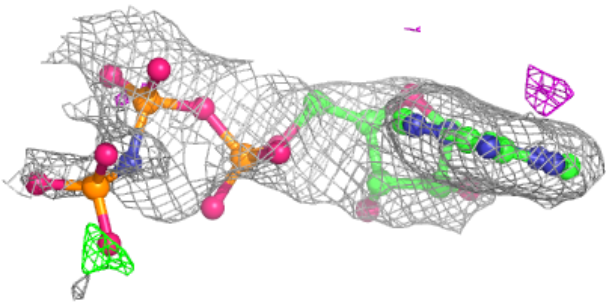


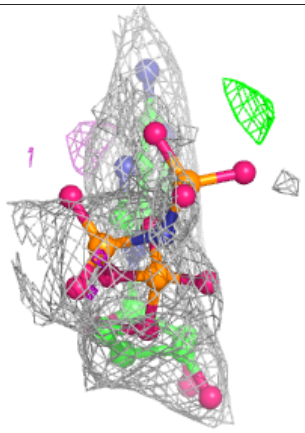


Electron density around ANP E 401 (C):

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

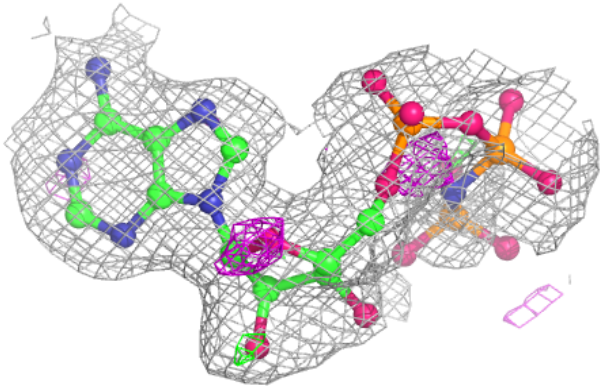


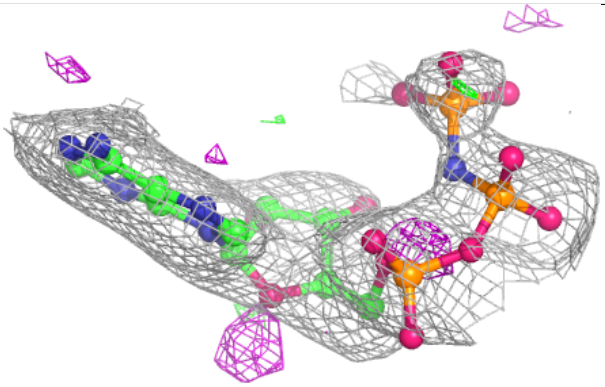


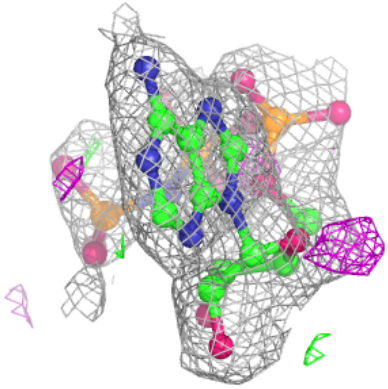


Electron density around ANP C 402 (C):

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

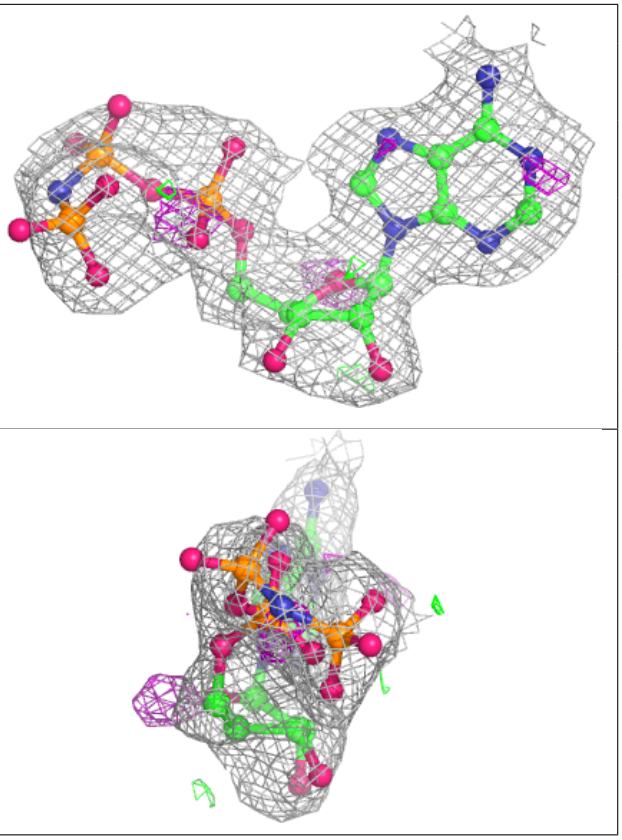


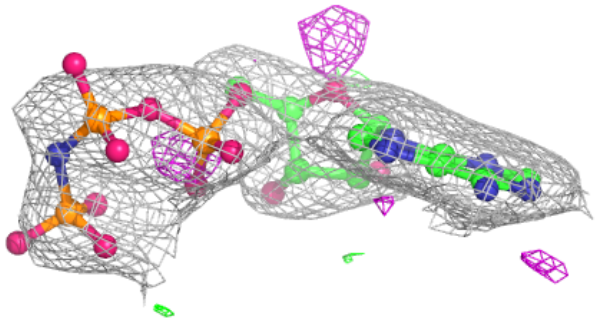




Electron density around ANP C 402 (B):

$2mF_o$-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.