Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 10:03 PM EDT

PDB ID	:	6MM7
Title	:	Catalytic subunit of cAMP-dependent protein kinase A in complex with RyR2 K2879A, S2813D phosphomimetic (2699-2904) crystal form 1
Authors	:	van Petegem, F.; Haji-Ghassemi, O.
Deposited on	:	2018-09-29
Resolution	:	1.85 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:

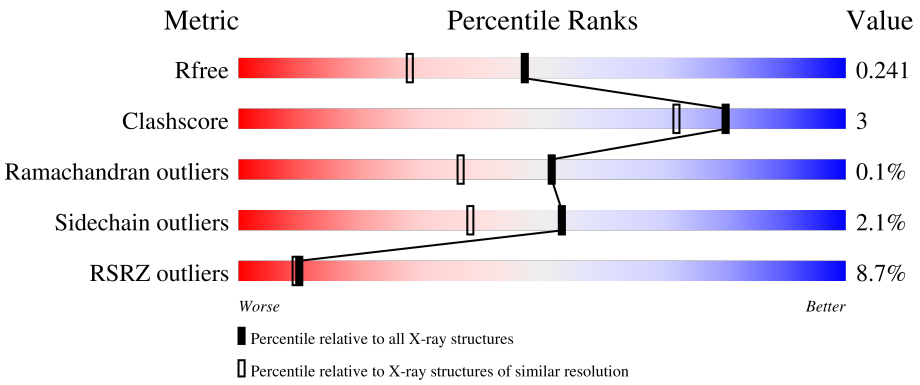
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	A	339	3% 91% • • •
1	D	339	4% 90% 5% •
2	C	209	21% 91% 7% ••
2	E	209	12% 92% 6% ••

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
4	ACY	A	403	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9661 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	A	327	2714	1758	456	488	2	10	0	5	0
1	D	324	2683	1746	451	475	2	9	0	3	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	-	expression tag	UNP P05132
A	13	ASN	-	expression tag	UNP P05132
A	14	ALA	-	expression tag	UNP P05132
D	12	SER	-	expression tag	UNP P05132
D	13	ASN	-	expression tag	UNP P05132
D	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	C	206	1664	1056	293	307	8	0	1	0
2	E	206	1650	1047	287	308	8	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2696	SER	-	expression tag	UNP E9Q401
C	2697	ASN	-	expression tag	UNP E9Q401
C	2698	ALA	-	expression tag	UNP E9Q401
C	2813	ASP	SER	engineered mutation	UNP E9Q401
C	2879	ALA	LYS	engineered mutation	UNP E9Q401
E	2696	SER	-	expression tag	UNP E9Q401

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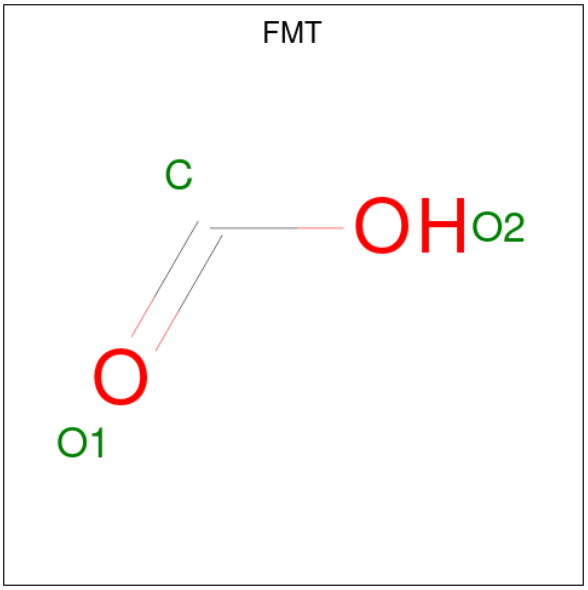
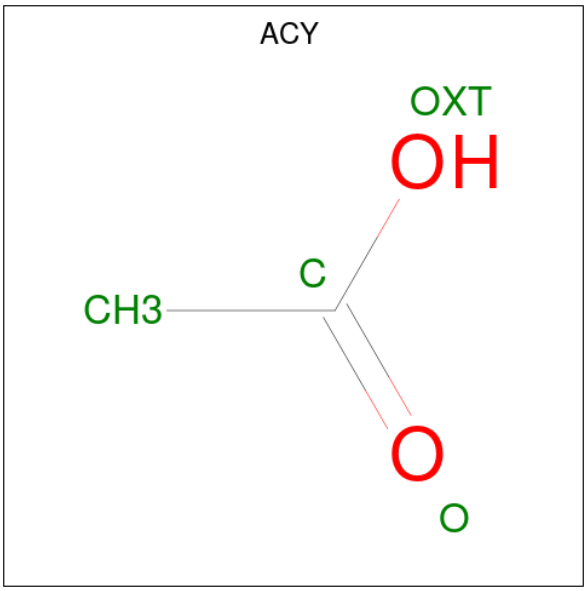
Chain	Residue	Modelled	Actual	Comment	Reference
E	2697	ASN	-	expression tag	UNP E9Q401
E	2698	ALA	-	expression tag	UNP E9Q401
E	2813	ASP	SER	engineered mutation	UNP E9Q401
E	2879	ALA	LYS	engineered mutation	UNP E9Q401

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



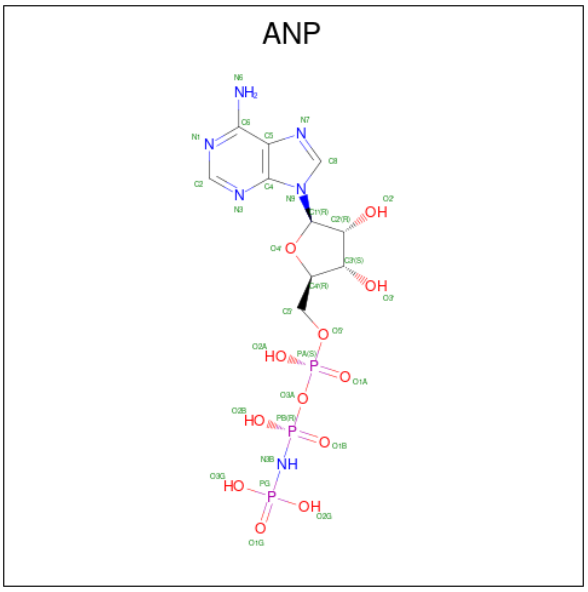
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	A	1	3	1	2		0	0
			Total	C	O			
3	A	1	3	1	2		0	0
			Total	C	O			
3	A	1	3	1	2		0	0
			Total	C	O			
3	A	1	3	1	2		0	0
			Total	C	O			
3	D	1	3	1	2		0	0
			Total	C	O			
3	D	1	3	1	2		0	0
			Total	C	O			
3	D	1	3	1	2		0	0
			Total	C	O			
3	D	1	3	1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

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



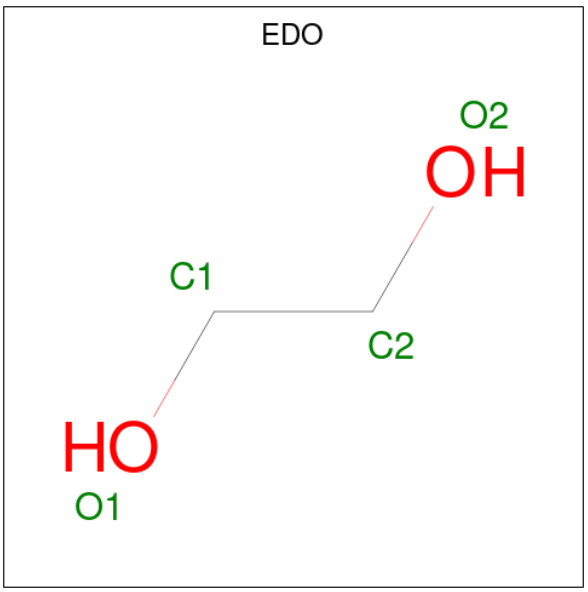
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0

- Molecule 5 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		
5	A	1	31	10	6	12	3	0	1
			Total	C	N	O	P		
5	D	1	31	10	6	12	3	0	1

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
6	C	1	4	2	2	0	0
6	D	1	4	2	2	0	0
6	D	1	4	2	2	0	0
6	D	1	4	2	2	0	0
6	D	1	4	2	2	0	0
6	E	1	4	2	2	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	D	1	1	1	0	0
7	E	1	1	1	0	0

- Molecule 8 is water.

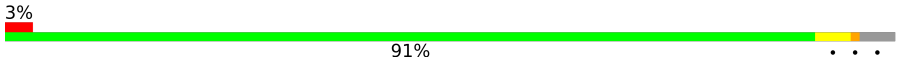
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	273	273	273	0	0
			Total	O		
8	C	112	112	112	0	0
			Total	O		
8	D	298	298	298	0	0
			Total	O		
8	E	147	147	147	0	0

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.

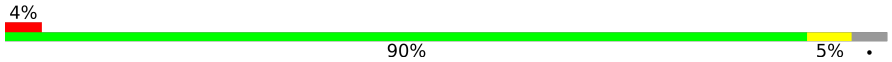
• Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

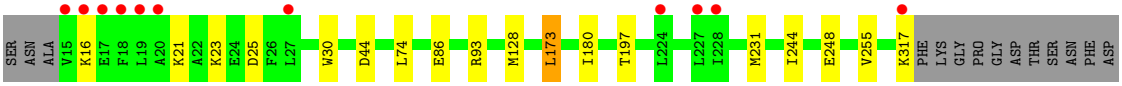
Chain A:

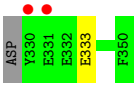


• Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain D:

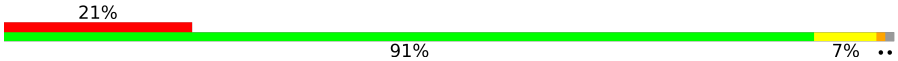


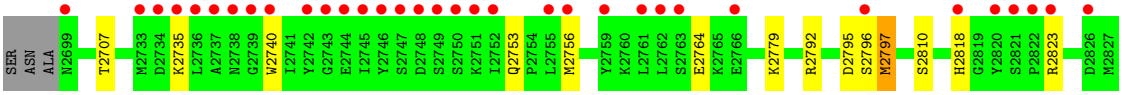


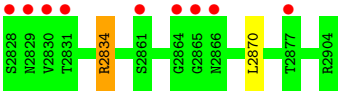


• Molecule 2: Ryanodine receptor 2

Chain C:

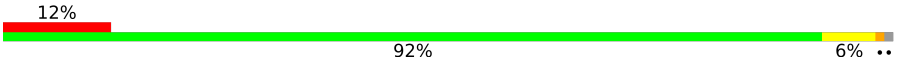


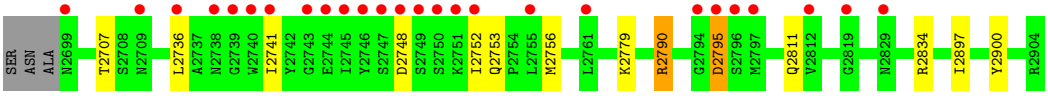




• Molecule 2: Ryanodine receptor 2

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	58.34Å 67.56Å 176.85Å 90.00° 90.73° 90.00°	Depositor
Resolution (Å)	33.80 – 1.85 33.78 – 1.85	Depositor EDS
% Data completeness (in resolution range)	94.1 (33.80-1.85) 94.1 (33.78-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.212 , 0.238 0.218 , 0.241	Depositor DCC
R_{free} test set	5824 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9661	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0008e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: SEP, ANP, FMT, CL, ACY, EDO, TPO

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	0.64	0/2772	0.75	0/3731
1	D	0.65	0/2736	0.76	0/3683
2	C	0.68	0/1706	0.75	0/2305
2	E	0.67	0/1691	0.75	0/2290
All	All	0.66	0/8905	0.75	0/12009

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	A	2714	0	2699	15	0
1	D	2683	0	2689	10	0
2	C	1664	0	1603	14	0
2	E	1650	0	1576	8	0
3	A	12	0	4	0	0
3	D	12	0	4	0	0
4	A	4	0	3	3	0
5	A	31	0	13	0	0
5	D	31	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	4	0	6	0	0
6	C	4	0	6	0	0
6	D	16	0	24	0	0
6	E	4	0	6	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	A	273	0	0	2	0
8	C	112	0	0	2	0
8	D	298	0	0	2	0
8	E	147	0	0	1	0
All	All	9661	0	8646	47	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 (47) 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:E:2790:ARG:HH11	2:E:2790:ARG:HG3	1.49	0.78
1:A:300:THR:HG23	4:A:403:ACY:H2	1.73	0.71
2:C:2735:LYS:HB3	2:C:2756:MET:HE1	1.74	0.68
2:E:2795:ASP:HB3	2:E:2897:ILE:O	1.96	0.66
1:A:242:GLN:HA	1:A:242:GLN:HE21	1.61	0.65
1:A:173:LEU:C	1:A:173:LEU:HD12	2.16	0.65
1:A:300:THR:CG2	4:A:403:ACY:H2	2.29	0.63
1:D:173:LEU:C	1:D:173:LEU:HD12	2.19	0.62
2:C:2735:LYS:HB3	2:C:2756:MET:CE	2.30	0.61
2:C:2792:ARG:HH12	2:C:2795:ASP:CG	2.04	0.60
1:A:125:GLY:HA3	1:A:174:ILE:O	2.02	0.60
2:E:2790:ARG:HG3	2:E:2790:ARG:NH1	2.20	0.54
1:A:255:VAL:HG12	8:A:684:HOH:O	2.07	0.53
2:E:2790:ARG:HG2	2:E:2900:TYR:CE2	2.43	0.53
1:D:30:TRP:O	1:D:93:ARG:NH1	2.38	0.53
1:D:86[A]:GLU:HG2	8:D:659:HOH:O	2.10	0.51
1:D:128[B]:MET:CE	1:D:180:ILE:HD11	2.41	0.51
1:A:144:ARG:HG2	4:A:403:ACY:H3	1.94	0.49
2:C:2740:TRP:HB3	2:C:2756:MET:CE	2.43	0.49
1:A:30:TRP:O	1:A:93[A]:ARG:NH1	2.42	0.49
1:A:53:SER:O	1:A:78:LYS:HE2	2.12	0.48
2:C:2740:TRP:HB3	2:C:2756:MET:HE3	1.97	0.46
2:C:2818[B]:HIS:ND1	2:C:2818[B]:HIS:C	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:VAL:HG12	8:D:691:HOH:O	2.14	0.46
1:A:241:ASP:HB2	2:C:2823:ARG:HH22	1.81	0.46
1:A:345[A]:LYS:HG3	8:A:655:HOH:O	2.16	0.45
2:C:2834:ARG:NH2	8:C:3108:HOH:O	2.49	0.45
1:A:74:LEU:HD12	1:A:74:LEU:N	2.32	0.45
2:E:2811:GLN:NE2	8:E:3108:HOH:O	2.49	0.44
2:C:2740:TRP:CB	2:C:2756:MET:HE1	2.47	0.44
1:D:74:LEU:HD12	1:D:74:LEU:N	2.33	0.44
2:E:2707:THR:HB	2:E:2779:LYS:HB3	1.99	0.44
1:D:244:ILE:O	1:D:248:GLU:HG2	2.17	0.44
2:C:2797:MET:CE	2:C:2797:MET:H	2.32	0.43
1:A:146:TYR:HB3	1:A:180:ILE:HD11	1.99	0.43
1:D:173:LEU:HD12	1:D:173:LEU:O	2.19	0.43
5:D:405[B]:ANP:H8	5:D:405[B]:ANP:O5'	2.19	0.43
2:C:2740:TRP:HB2	2:C:2756:MET:HE1	2.01	0.42
2:E:2741:ILE:CD1	2:E:2752:ILE:HG13	2.50	0.41
2:C:2870:LEU:HD23	2:C:2870:LEU:HA	1.91	0.41
1:D:128[A]:MET:HE3	1:D:231:MET:HG2	2.02	0.41
1:A:173:LEU:HD12	1:A:173:LEU:O	2.20	0.41
2:C:2707:THR:HB	2:C:2779:LYS:HB3	2.03	0.41
2:E:2736:LEU:HG	2:E:2756:MET:CE	2.51	0.41
1:A:173:LEU:C	1:A:173:LEU:CD1	2.87	0.41
2:C:2810:SER:HA	8:C:3190:HOH:O	2.21	0.41
1:D:21:LYS:HE2	1:D:25:ASP:OD1	2.20	0.41

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	326/339 (96%)	317 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	321/339 (95%)	314 (98%)	6 (2%)	1 (0%)	41	26
2	C	205/209 (98%)	199 (97%)	6 (3%)	0	100	100
2	E	204/209 (98%)	198 (97%)	6 (3%)	0	100	100
All	All	1056/1096 (96%)	1028 (97%)	27 (3%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	16	LYS

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	286/297 (96%)	282 (99%)	4 (1%)	67	55
1	D	283/297 (95%)	278 (98%)	5 (2%)	59	45
2	C	171/184 (93%)	166 (97%)	5 (3%)	42	26
2	E	169/184 (92%)	164 (97%)	5 (3%)	41	24
All	All	909/962 (94%)	890 (98%)	19 (2%)	53	38

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	173	LEU
1	A	207	PRO
1	A	242	GLN
2	C	2753	GLN
2	C	2764	GLU
2	C	2796	SER
2	C	2797	MET
2	C	2834	ARG
1	D	23	LYS

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Mol	Chain	Res	Type
1	D	44	ASP
1	D	173	LEU
1	D	317	LYS
1	D	333	GLU
2	E	2748	ASP
2	E	2753	GLN
2	E	2790	ARG
2	E	2795	ASP
2	E	2834	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	242	GLN
1	A	340	ASN
2	E	2811	GLN
2	E	2846	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	TPO	A	197	1	8,10,11	0.87	0	10,14,16	0.86	0
1	TPO	D	197	1	8,10,11	0.69	0	10,14,16	0.98	1 (10%)
1	SEP	D	338	1	8,9,10	0.75	0	8,12,14	0.96	0
1	SEP	A	338	1	8,9,10	0.64	0	8,12,14	0.93	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	TPO	A	197	1	-	0/9/11/13	-
1	TPO	D	197	1	-	1/9/11/13	-
1	SEP	D	338	1	-	4/5/8/10	-
1	SEP	A	338	1	-	5/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	197	TPO	P-OG1-CB	-2.08	116.92	123.21

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

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 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	ANP	A	406[B]	-	29,33,33	1.23	2 (6%)	31,52,52	1.31	5 (16%)
3	FMT	A	401	-	2,2,2	0.42	0	1,1,1	0.16	0
3	FMT	D	403	-	2,2,2	0.75	0	1,1,1	0.12	0
6	EDO	D	409	-	3,3,3	0.16	0	2,2,2	0.16	0
6	EDO	D	410	-	3,3,3	0.13	0	2,2,2	0.22	0
3	FMT	D	402	-	2,2,2	0.17	0	1,1,1	0.22	0
3	FMT	D	404	-	2,2,2	0.43	0	1,1,1	0.06	0
6	EDO	C	3001	-	3,3,3	0.12	0	2,2,2	0.28	0
6	EDO	A	407	-	3,3,3	0.09	0	2,2,2	0.15	0
6	EDO	D	408	-	3,3,3	0.08	0	2,2,2	0.30	0
3	FMT	A	402	-	2,2,2	0.45	0	1,1,1	0.04	0
6	EDO	E	3002	-	3,3,3	0.09	0	2,2,2	0.17	0
3	FMT	D	401	-	2,2,2	0.43	0	1,1,1	0.09	0
5	ANP	D	405[B]	-	29,33,33	1.31	2 (6%)	31,52,52	1.24	5 (16%)
4	ACY	A	403	-	3,3,3	1.03	0	3,3,3	0.64	0
3	FMT	A	405	-	2,2,2	0.30	0	1,1,1	0.22	0
6	EDO	D	407	-	3,3,3	0.17	0	2,2,2	0.08	0
3	FMT	A	404	-	2,2,2	0.29	0	1,1,1	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	D	410	-	-	1/1/1/1	-
6	EDO	D	409	-	-	0/1/1/1	-
6	EDO	C	3001	-	-	1/1/1/1	-
6	EDO	A	407	-	-	1/1/1/1	-
6	EDO	D	408	-	-	1/1/1/1	-
6	EDO	E	3002	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	D	405[B]	-	-	4/14/38/38	0/3/3/3
5	ANP	A	406[B]	-	-	5/14/38/38	0/3/3/3
6	EDO	D	407	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	405[B]	ANP	PG-O1G	4.34	1.53	1.46
5	A	406[B]	ANP	PG-O1G	3.63	1.51	1.46
5	A	406[B]	ANP	PB-O1B	3.20	1.51	1.46
5	D	405[B]	ANP	PB-O1B	3.04	1.51	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	405[B]	ANP	O2B-PB-O1B	4.24	118.80	109.92
5	A	406[B]	ANP	O2B-PB-O1B	4.01	118.33	109.92
5	A	406[B]	ANP	O1G-PG-N3B	-3.06	107.27	111.77
5	A	406[B]	ANP	O3A-PB-N3B	-2.51	99.63	106.59
5	D	405[B]	ANP	PB-O3A-PA	-2.40	124.16	132.62
5	A	406[B]	ANP	C5-C6-N6	2.32	123.88	120.35
5	D	405[B]	ANP	C5-C6-N6	2.30	123.85	120.35
5	D	405[B]	ANP	O2G-PG-O1G	-2.28	107.72	113.45
5	D	405[B]	ANP	O3G-PG-O1G	-2.09	108.20	113.45
5	A	406[B]	ANP	O2G-PG-O1G	-2.04	108.31	113.45

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	406[B]	ANP	PG-N3B-PB-O1B
5	A	406[B]	ANP	PA-O3A-PB-O1B
5	A	406[B]	ANP	PA-O3A-PB-O2B
5	D	405[B]	ANP	PB-N3B-PG-O1G
5	D	405[B]	ANP	PG-N3B-PB-O1B
6	C	3001	EDO	O1-C1-C2-O2
6	D	408	EDO	O1-C1-C2-O2
5	D	405[B]	ANP	C5'-O5'-PA-O3A
5	A	406[B]	ANP	O4'-C4'-C5'-O5'
5	A	406[B]	ANP	C4'-C5'-O5'-PA
6	D	410	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	D	405[B]	ANP	C5'-O5'-PA-O1A
6	A	407	EDO	O1-C1-C2-O2
6	D	407	EDO	O1-C1-C2-O2

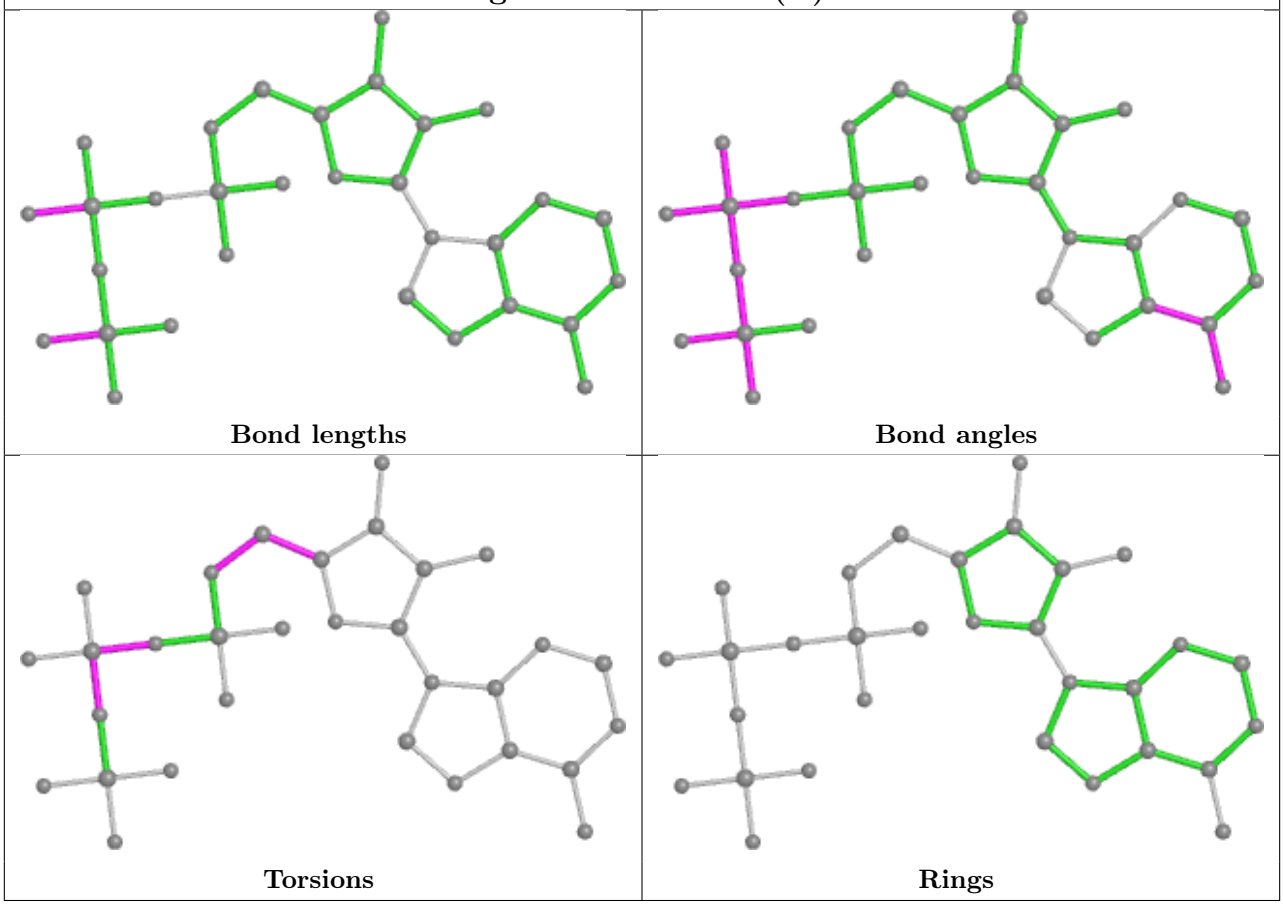
There are no ring outliers.

2 monomers are involved in 4 short contacts:

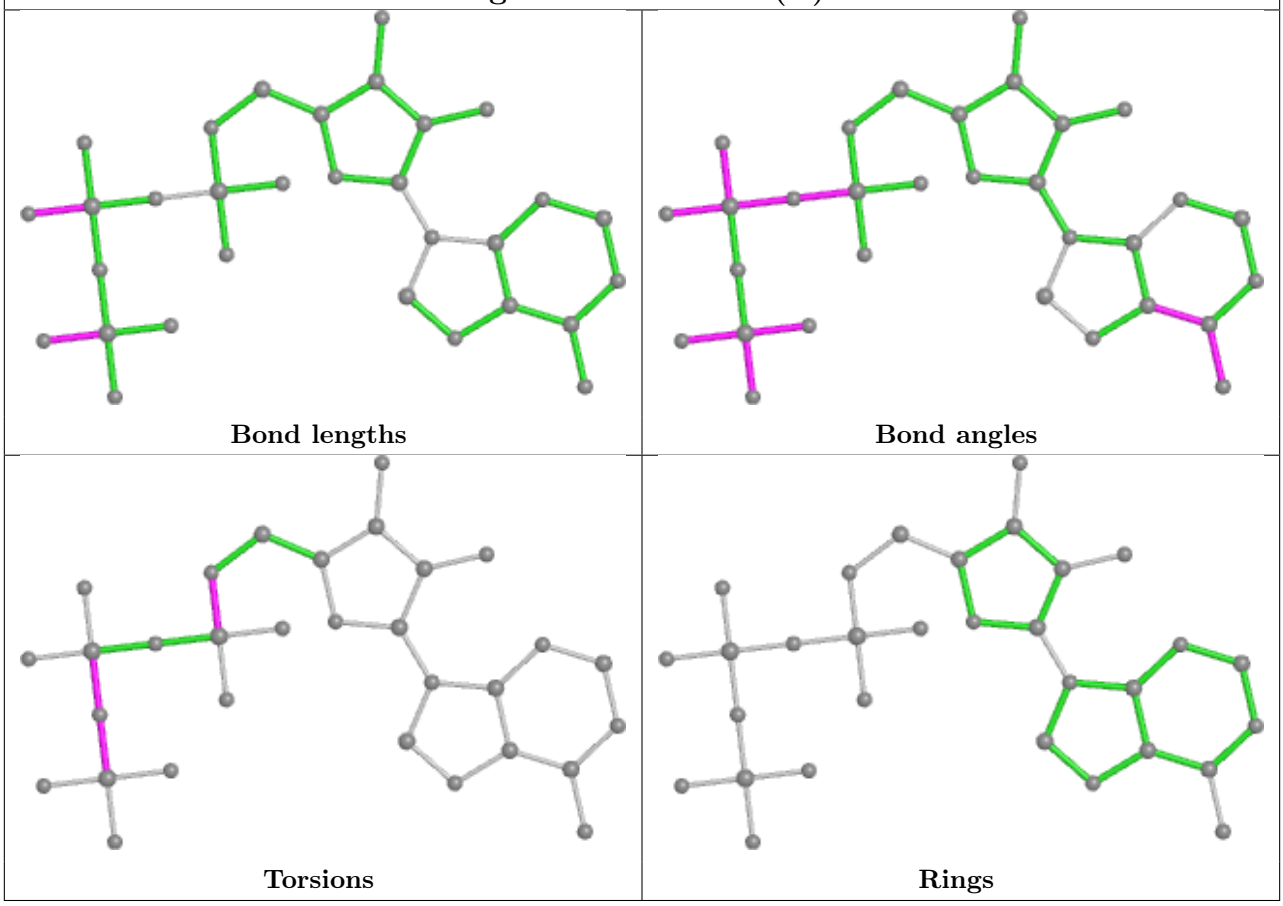
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	405[B]	ANP	1	0
4	A	403	ACY	3	0

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 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 A 406 (B)



Ligand ANP D 405 (B)



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	325/339 (95%)	0.10	10 (3%)	49	47	23, 33, 52, 80	0
1	D	322/339 (94%)	0.17	13 (4%)	38	36	20, 29, 52, 80	0
2	C	206/209 (98%)	0.98	43 (20%)	1	0	27, 53, 96, 124	0
2	E	206/209 (98%)	0.47	26 (12%)	3	3	27, 44, 83, 98	0
All	All	1059/1096 (96%)	0.36	92 (8%)	10	9	20, 36, 74, 124	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	PHE	7.1
2	C	2749	SER	7.1
2	C	2755	LEU	6.8
2	C	2746	TYR	6.7
2	C	2739	GLY	6.6
2	E	2746	TYR	5.7
2	E	2745	ILE	5.6
1	A	19	LEU	5.3
2	C	2752	ILE	5.2
2	C	2865	GLY	5.0
2	C	2737	ALA	4.9
2	C	2743	GLY	4.9
2	C	2699	ASN	4.9
2	C	2866	ASN	4.8
2	C	2750	SER	4.8
2	E	2748	ASP	4.6
2	C	2864	GLY	4.5
2	C	2736	LEU	4.5
1	A	18	PHE	4.5
2	C	2748	ASP	4.4
1	D	15	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
2	C	2738	ASN	4.3
2	C	2761	LEU	4.3
2	C	2745	ILE	4.2
2	C	2740	TRP	4.1
1	D	18	PHE	3.9
2	E	2749	SER	3.9
1	D	330	TYR	3.8
2	C	2829	ASN	3.8
2	E	2699	ASN	3.7
2	C	2828	SER	3.7
2	E	2740	TRP	3.7
2	C	2744	GLU	3.6
1	D	19	LEU	3.6
2	C	2823	ARG	3.6
2	E	2752	ILE	3.4
2	E	2819	GLY	3.3
2	E	2795	ASP	3.3
1	D	16	LYS	3.3
2	E	2794	GLY	3.1
2	E	2738	ASN	3.1
2	C	2861	SER	3.1
2	E	2797	MET	3.0
2	E	2739	GLY	3.0
2	E	2743	GLY	3.0
2	E	2755	LEU	3.0
2	C	2820	TYR	3.0
2	C	2733	MET	3.0
1	A	124	ALA	2.9
2	E	2736	LEU	2.9
2	E	2750	SER	2.9
2	E	2812	VAL	2.9
2	C	2762	LEU	2.9
1	D	17	GLU	2.8
2	C	2734	ASP	2.8
2	E	2744	GLU	2.8
2	C	2818[A]	HIS	2.7
2	E	2741	ILE	2.7
2	C	2742	TYR	2.7
2	C	2747	SER	2.7
1	D	224	LEU	2.7
1	D	228	ILE	2.6
2	C	2826	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	2877	THR	2.6
2	E	2829	ASN	2.6
1	D	317	LYS	2.6
2	C	2796	SER	2.6
2	C	2830	VAL	2.5
2	C	2751	LYS	2.5
1	D	20	ALA	2.5
2	C	2756	MET	2.4
1	A	16	LYS	2.4
1	A	17	GLU	2.4
1	D	227	LEU	2.4
1	A	327	PHE	2.4
2	E	2709	ASN	2.4
1	A	328	ASP	2.3
1	D	331	GLU	2.3
2	C	2735	LYS	2.3
2	C	2759	TYR	2.3
1	A	227	LEU	2.2
2	C	2822	PRO	2.2
2	C	2821	SER	2.2
2	E	2751	LYS	2.1
2	C	2831	THR	2.1
2	E	2796	SER	2.1
1	D	27	LEU	2.1
2	C	2763	SER	2.0
1	A	150	ILE	2.0
2	C	2766	GLU	2.0
2	E	2761	LEU	2.0
2	E	2747	SER	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	A	338	10/11	0.95	0.09	37,39,43,45	0
1	TPO	A	197	11/12	0.97	0.08	33,34,35,36	0
1	SEP	D	338	10/11	0.97	0.08	32,34,38,39	0
1	TPO	D	197	11/12	0.98	0.08	34,37,38,40	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

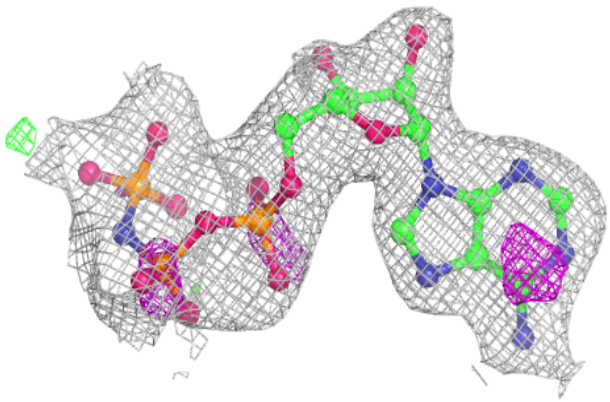
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

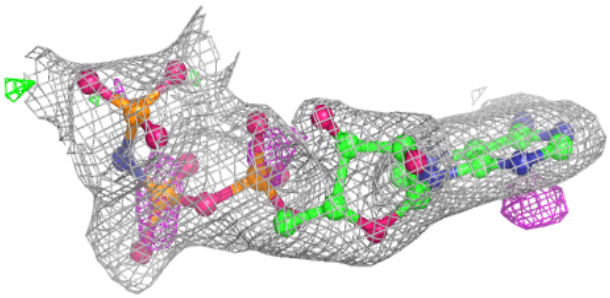
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	D	409	4/4	0.75	0.18	41,41,42,44	0
6	EDO	D	410	4/4	0.81	0.20	48,50,50,51	0
6	EDO	E	3002	4/4	0.82	0.29	42,48,49,51	0
6	EDO	A	407	4/4	0.85	0.21	38,41,41,41	0
6	EDO	C	3001	4/4	0.86	0.22	43,47,48,48	0
6	EDO	D	408	4/4	0.88	0.20	47,47,48,50	0
5	ANP	A	406[B]	31/31	0.88	0.14	38,48,64,65	0
5	ANP	D	405[B]	31/31	0.89	0.11	27,43,62,67	0
6	EDO	D	407	4/4	0.90	0.20	34,37,39,44	0
4	ACY	A	403	4/4	0.91	0.27	43,44,45,45	0
3	FMT	A	404	3/3	0.92	0.14	41,41,42,44	0
3	FMT	D	404	3/3	0.92	0.11	41,41,47,48	0
3	FMT	D	403	3/3	0.93	0.11	32,32,37,39	0
3	FMT	A	402	3/3	0.93	0.09	46,46,52,52	0
3	FMT	A	405	3/3	0.93	0.14	46,46,48,49	0
3	FMT	D	401	3/3	0.96	0.10	32,32,36,41	0
3	FMT	A	401	3/3	0.98	0.04	37,37,38,39	0
3	FMT	D	402	3/3	0.98	0.07	39,39,40,40	0
7	CL	D	406	1/1	0.99	0.12	26,26,26,26	0
7	CL	E	3001	1/1	0.99	0.12	28,28,28,28	0

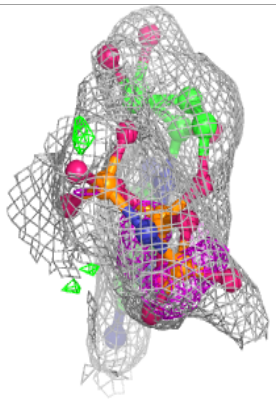
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 406 (B):

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

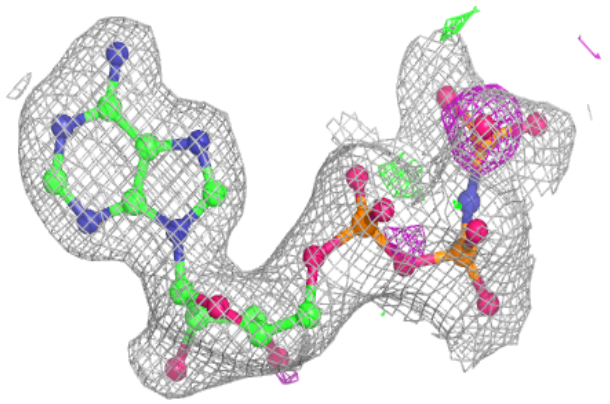


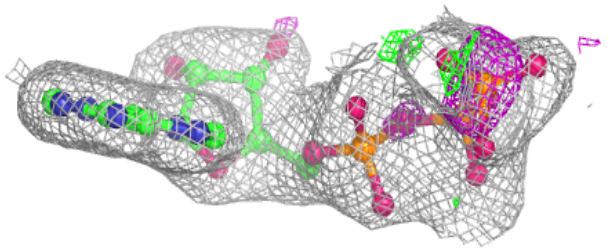


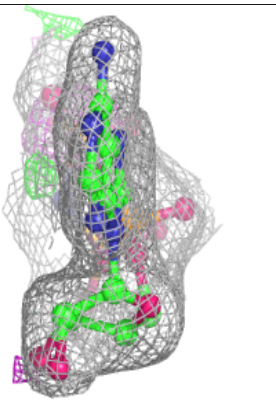


Electron density around ANP D 405 (B):

$2mF_o$-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.