W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Sep 20, 2023 – 04:36 PM EDT

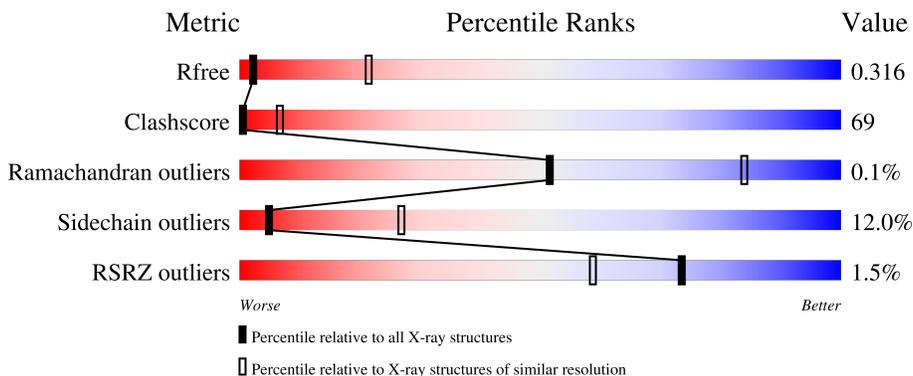|		
PDB ID	:	5JR7
Title	:	Crystal structure of an ACRDYS heterodimer [RIa(92-365):C] of PKA
Authors	:	Bruystens, J.G.H.; Wu, J.; Taylor, S.S.
Deposited on	:	2016-05-05
Resolution	:	3.56 Å(reported)

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 3.56 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	Percentile Ranks	Value
Rfree		0.316
Clashscore		69
Ramachandran outliers		0.1%
Sidechain outliers		12.0%
RSRZ outliers		1.5%

Worse ____ *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

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 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	350	42% · 47% · 7% ·
1	C	350	2% · 36% · 52% · 9% ·
2	B	275	% · 37% · 53% · 6% ·
2	D	275	3% · 32% · 52% · 13% ·

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
3	ADP	C	400	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9665 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	338	Total	C	N	O	P	S	6	0	0
			2734	1773	451	499	3	8			
1	C	338	Total	C	N	O	P	S	0	0	0
			2729	1767	451	500	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	267	Total	C	N	O	S	1	0	0
			2079	1321	354	397	7			
2	D	266	Total	C	N	O	S	1	0	0
			2069	1317	353	392	7			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

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

3 Residue-property plots ⓘ

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 C:

N271 L272 L273 F281 L284 K285 N286 G287 V288 N289 D290 I291 K292 N293 H294 K295 W296 F297 T300 D301 W302 I303 Q307 R308 K309 V310 E311 I315 K319 G320 P321 G322 D323 T324 F327 D328 D329 Y330 E331 E332 I335 R336 V337 S338 I339 N340 C343 T348 E349 F350

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

Chain B:

37%   53%   6%   •

GLY R92 R93 R94 R95 S99 V102 Y103 T104 E105 E106 D107 V115 I116 P117 K118 L126 I130 E131 K132 N133 F136 D141 N142 E143 R144 S145 D146 I147 F148 D149 A150 M151 F152 P153 V154 S155 F156 I157 E160 T161 Q164 Q165 G166 D167 N171 F172 Y173 Q177

G178 E179 M180 D181 V182 Y183 V184 N185 N186 E187 W188 A189 T190 S191 E194 G195 S197 F198 G199 E200 L201 A202 Y205 P208 R209 A210 A211 T212 V213 K214 A215 K216 V219 K220 L221 W222 G223 I224 D225 R226 D227 S228 Y229 R230 R231 I232 L233 S236 T237 L238 R239 K240 M243

Y244 E245 E246 F247 L248 S249 K250 V251 S252 I253 L254 E255 S256 L257 D258 K259 W260 E261 R262 L263 T264 V265 A266 D267 A268 L269 E270 P271 F274 E275 D276 I280 V281 V282 Q283 G287 D288 E289 F290 F291 I292 I293 L294 E295 G296 S297 A298 A299 V300 L301 Q302 R303 R304 S305 E308 E309

F310 V311 E312 V313 G314 R315 L316 G317 P318 S319 D320 Y321 F322 G323 A324 I325 A326 L327 L328 M329 N330 R331 P332 R333 A334 A335 T336 V337 V338 A339 R340 G341 P342 L343 L344 G345 V346 K347 L348 D349 P351 R352 E353 E354 R355 V356 L357 G358 PRO CYS SER ASP ILE LEU LYS

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

Chain D:

3%   32%   52%   13%   •

GLY R92 R93 R94 R95 I98 V102 Y103 T104 E105 E106 D107 Y111 V112 R113 K114 V115 I116 P117 K118 D119 Y120 M123 A124 A125 L126 I130 N133 V134 L135 F136 S137 H138 L139 D140 R144 I147 F148 D149 A150 M151 F152 P153 V154 S155 F156 I157 A158 G159 E160 T161 V162

I163 Q164 Q165 G166 D167 E168 G169 D170 N171 F172 Y173 V174 I175 D176 Q177 G178 E179 M180 D181 V182 Y183 E187 W188 A189 T190 S191 V192 S197 F198 G199 E200 L201 A202 I204 T207 P208 R209 A210 A211 T212 V213 K214 A215 K216 T217 N218 V219 K220 L221 W222 G223 I224 D225 R226 R231

I232 L233 M234 G235 S236 T237 L238 R239 K240 R241 K242 M243 Y244 E245 E246 F247 L248 S249 K250 V251 S252 I253 L254 E255 S256 L257 D258 K259 W260 E261 R262 L263 T264 V265 A266 D267 A268 L269 V272 Q273 F274 E275 D276 Q277 Q278 K279 I280 V281 V282 Q283 G284 E285 P286 G287 D288 E289 F290 F291 I292

I293 L294 E295 V300 L301 Q302 R303 E309 F310 V311 E312 V313 L316 G317 P318 S319 D320 Y321 F322 G323 E324 L327 L328 M329 N330 R331 P332 R333 T336 V337 G341 P342 L343 K344 C345 V346 K347 L348 D349 R350 P351 R352 F353 E354 R355 V356 L357 GLY PRO CYS SER ASP ILE LEU

LYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.15Å 66.79Å 87.93Å 101.76° 89.37° 105.27°	Depositor
Resolution (Å)	49.11 – 3.56 49.10 – 3.51	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.11-3.56) 96.1 (49.10-3.51)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.11	Depositor
$<I/\sigma(I)>$ [1]	3.55 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.266 , 0.322 0.255 , 0.316	Depositor DCC
R_{free} test set	785 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	82.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 99.8	EDS
L-test for twinning[2]	$<|L|> = 0.51$, $<L^2> = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9665	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, ADP, 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	0.48	1/2771 (0.0%)	0.92	5/3745 (0.1%)
1	C	0.41	1/2765 (0.0%)	0.76	3/3736 (0.1%)
2	B	0.51	1/2116 (0.0%)	0.94	4/2857 (0.1%)
2	D	0.57	4/2106 (0.2%)	0.92	5/2845 (0.2%)
All	All	0.49	7/9758 (0.1%)	0.88	17/13183 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	333	ARG	NE-CZ	12.59	1.49	1.33
2	D	333	ARG	NE-CZ	12.46	1.49	1.33
2	D	181	ASP	CB-CG	-9.06	1.32	1.51
2	D	188	TRP	CZ3-CH2	-7.05	1.28	1.40
1	A	111	LYS	CE-NZ	-7.00	1.31	1.49

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	181	ASP	CB-CG-OD1	-23.64	97.02	118.30
2	D	181	ASP	CB-CG-OD2	18.74	135.17	118.30
1	C	61	LYS	CD-CE-NZ	-18.02	70.25	111.70
1	A	27	LEU	CB-CG-CD1	-17.41	81.41	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	227	LEU	CB-CG-CD1	-13.11	88.71	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	189	ALA	Mainchain

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	2734	0	2640	372	0
1	C	2729	0	2630	366	0
2	B	2079	0	2030	264	0
2	D	2069	0	2023	351	0
3	A	27	0	12	4	0
3	C	27	0	12	1	0
All	All	9665	0	9347	1314	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 69.

The worst 5 of 1314 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:HA	1:A:84:GLN:NE2	1.38	1.36
1:A:116:LEU:HD12	1:A:117:TYR:N	1.48	1.27
1:C:150:ILE:HG22	1:C:154:PHE:CE2	1.71	1.24
1:A:48:THR:HG21	1:A:330:TYR:HB2	1.20	1.16
1:A:175:ASP:HB3	1:A:181:GLN:NE2	1.60	1.15

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	333/350 (95%)	323 (97%)	10 (3%)	0	100	100
1	C	333/350 (95%)	296 (89%)	36 (11%)	1 (0%)	41	74
2	B	265/275 (96%)	255 (96%)	10 (4%)	0	100	100
2	D	264/275 (96%)	234 (89%)	30 (11%)	0	100	100
All	All	1195/1250 (96%)	1108 (93%)	86 (7%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	229	TYR

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	278/302 (92%)	254 (91%)	24 (9%)	10	41
1	C	277/302 (92%)	240 (87%)	37 (13%)	4	23
2	B	212/230 (92%)	192 (91%)	20 (9%)	8	37
2	D	210/230 (91%)	174 (83%)	36 (17%)	2	13
All	All	977/1064 (92%)	860 (88%)	117 (12%)	5	27

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	120	MET
2	D	321	TYR
1	C	284	LEU
2	D	319	SER
2	D	239	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	87	HIS
2	D	273	GLN
2	D	283	GLN
1	A	158	HIS
1	A	181	GLN

5.3.3   RNA   ⓘ

There are no RNA molecules in this entry.

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

6 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	A	338	1	8,9,10	1.54	1 (12%)	8,12,14	1.74	2 (25%)
1	TPO	A	197	1	8,10,11	1.52	1 (12%)	10,14,16	2.12	1 (10%)
1	SEP	C	139	1	8,9,10	1.62	1 (12%)	8,12,14	1.56	2 (25%)
1	SEP	C	338	1	8,9,10	1.55	1 (12%)	8,12,14	1.77	2 (25%)
1	TPO	C	197	1	8,10,11	1.53	1 (12%)	10,14,16	2.17	1 (10%)
1	SEP	A	139	1	8,9,10	1.54	1 (12%)	8,12,14	2.29	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	SEP	A	338	1	-	5/5/8/10	-
1	TPO	A	197	1	-	0/9/11/13	-
1	SEP	C	139	1	-	0/5/8/10	-
1	SEP	C	338	1	-	5/5/8/10	-
1	TPO	C	197	1	-	0/9/11/13	-
1	SEP	A	139	1	-	4/5/8/10	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	139	SEP	P-O1P	3.52	1.61	1.50
1	C	338	SEP	P-O1P	3.39	1.61	1.50
1	A	197	TPO	P-O1P	3.37	1.61	1.50
1	A	139	SEP	P-O1P	3.37	1.61	1.50
1	C	197	TPO	P-O1P	3.33	1.61	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	TPO	P-OG1-CB	-6.41	103.86	123.21
1	A	197	TPO	P-OG1-CB	-6.25	104.32	123.21
1	A	139	SEP	P-OG-CB	-4.93	104.72	118.30
1	A	139	SEP	OG-CB-CA	3.88	111.92	108.14
1	C	338	SEP	OG-CB-CA	3.75	111.80	108.14

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	139	SEP	N-CA-CB-OG
1	A	139	SEP	CB-OG-P-O1P
1	A	139	SEP	CB-OG-P-O2P
1	A	139	SEP	CB-OG-P-O3P
1	A	338	SEP	CB-OG-P-O2P

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	338	SEP	2	0
1	A	197	TPO	5	0
1	C	139	SEP	2	0
1	C	197	TPO	2	0
1	A	139	SEP	1	0

5.5   Carbohydrates (i)

There are no monosaccharides in this entry.

5.6   Ligand geometry (i)

2 ligands 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	$\#|Z| > 2$
3	ADP	A	400	-	24,29,29	0.97	1 (4%)	29,45,45	1.34	4 (13%)
3	ADP	C	400	-	24,29,29	0.99	1 (4%)	29,45,45	1.31	4 (13%)

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
3	ADP	A	400	-	-	3/12/32/32	0/3/3/3
3	ADP	C	400	-	-	6/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	ADP	C5-C4	2.53	1.47	1.40
3	C	400	ADP	C5-C4	2.53	1.47	1.40

WORLDWIDE PDB
PROTEIN DATA BANK

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	400	ADP	C3'-C2'-C1'	3.19	105.78	100.98
3	A	400	ADP	N3-C2-N1	-3.09	123.85	128.68
3	C	400	ADP	N3-C2-N1	-3.08	123.87	128.68
3	C	400	ADP	C3'-C2'-C1'	2.98	105.46	100.98
3	A	400	ADP	C4-C5-N7	-2.71	106.57	109.40

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	400	ADP	PA-O3A-PB-O2B
3	C	400	ADP	PA-O3A-PB-O3B
3	C	400	ADP	C5'-O5'-PA-O2A
3	A	400	ADP	PA-O3A-PB-O3B
3	C	400	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	ADP	4	0
3	C	400	ADP	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 ADP A 400

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 400

Bond lengths

Bond angles

Torsions

Rings
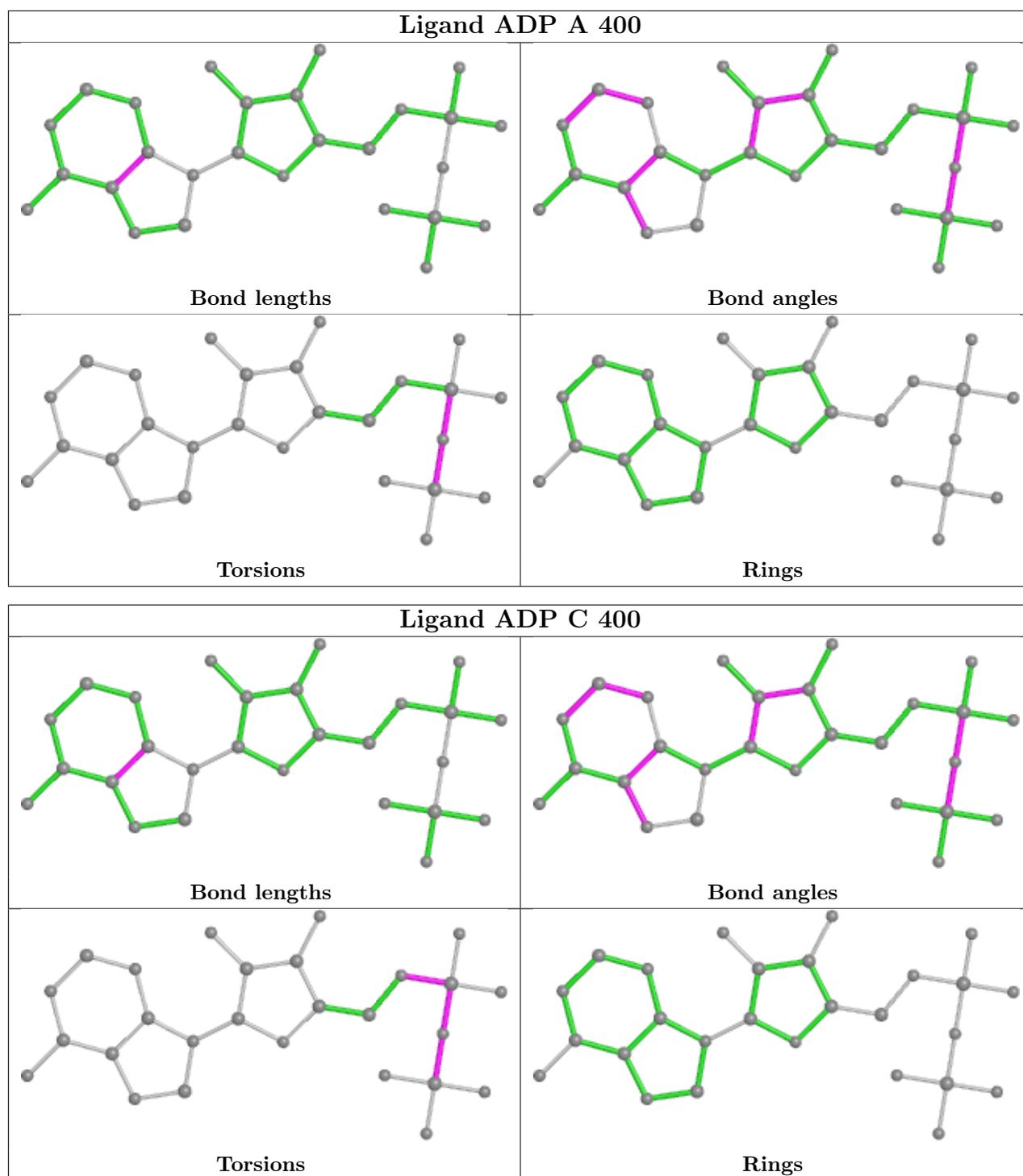
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	335/350 (95%)	-0.23	1 (0%)	94	88	33, 84, 183, 220	1 (0%)
1	C	335/350 (95%)	-0.11	6 (1%)	68	52	29, 101, 194, 292	0
2	B	267/275 (97%)	-0.02	4 (1%)	73	59	54, 100, 185, 222	1 (0%)
2	D	266/275 (96%)	0.08	7 (2%)	56	39	51, 119, 214, 254	2 (0%)
All	All	1203/1250 (96%)	-0.08	18 (1%)	73	59	29, 100, 196, 292	4 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	161	THR	7.7
1	C	64	GLU	3.9
1	C	34	SER	3.9
2	B	196	GLY	3.8
2	D	158	ALA	3.8

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

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.

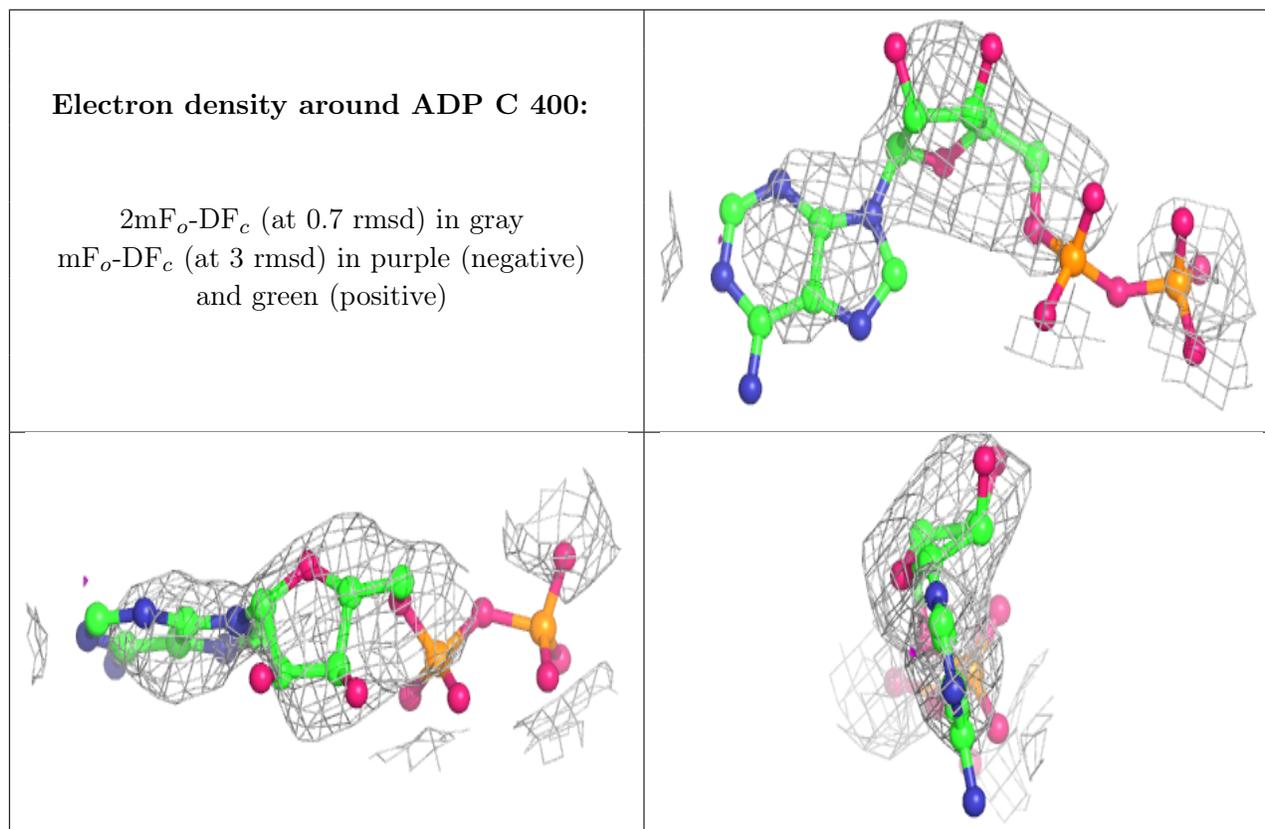| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	C	338	10/11	0.19	0.67	214,238,337,355	0
1	SEP	A	338	10/11	0.73	0.21	153,180,183,187	0
1	SEP	C	139	10/11	0.92	0.10	43,85,92,195	0
1	SEP	A	139	10/11	0.92	0.16	50,70,84,155	0
1	TPO	C	197	11/12	0.93	0.18	51,90,107,164	0
1	TPO	A	197	11/12	0.97	0.16	35,83,96,186	0

6.3 Carbohydrates (i)
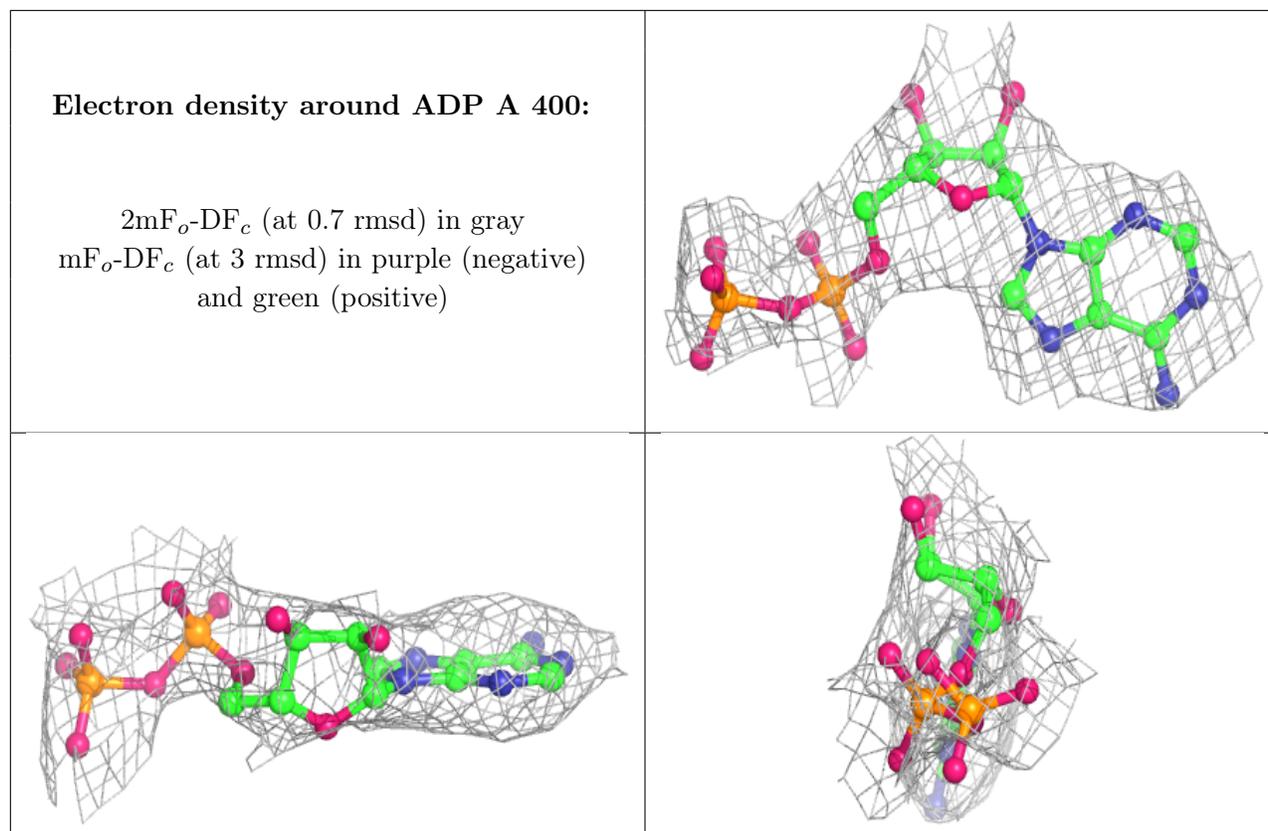
There are no monosaccharides in this entry.

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
3	ADP	C	400	27/27	0.72	0.51	101,118,305,311	0
3	ADP	A	400	27/27	0.87	0.24	57,103,213,304	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 ADP C 400:

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

Electron density around ADP A 400:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.