



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 08:29 AM EDT

PDB ID : 2QCS
Title : A complex structure between the Catalytic and Regulatory subunit of Protein Kinase A that represents the inhibited state
Authors : Kim, C.; Cheng, C.Y.; Saldanha, A.S.; Taylor, S.S.
Deposited on : 2007-06-19
Resolution : 2.20 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

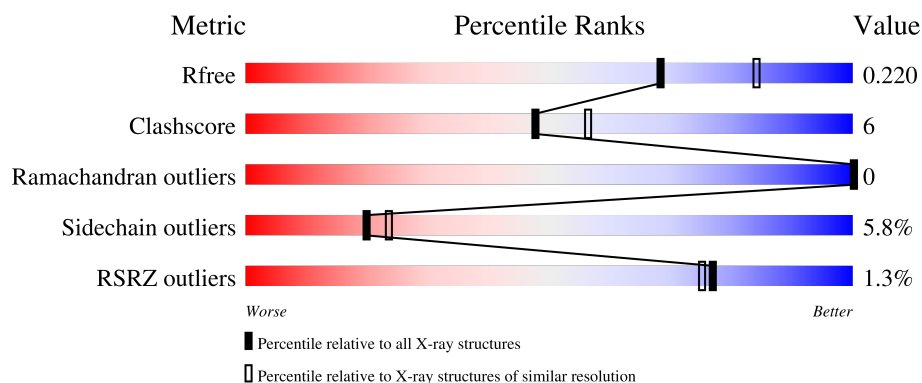
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	350	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>..</div> </div> </div>
2	B	291	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>.</div> </div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5459 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, alpha-catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	P	S	32	3	0
			2778	1795	465	507	3	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	SEP	SER	modified residue	UNP P05132
A	197	TPO	THR	modified residue	UNP P05132
A	338	SEP	SER	modified residue	UNP P05132

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	24	0	0
			2296	1453	397	438	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	333	LYS	ARG	engineered mutation	UNP P00514
B	380	ALA	-	expression tag	UNP P00514

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



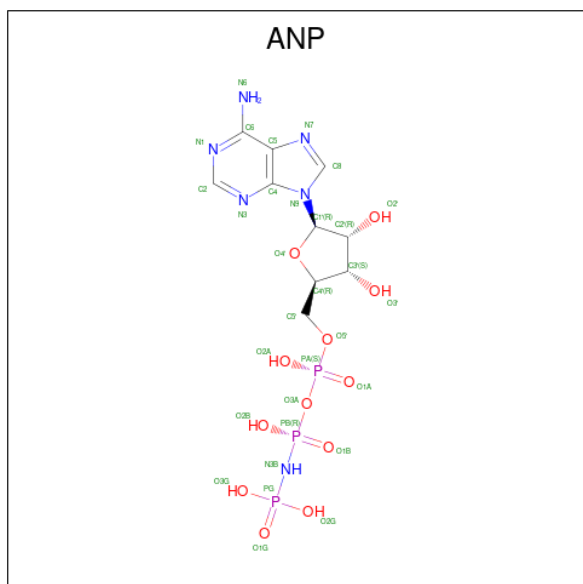
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



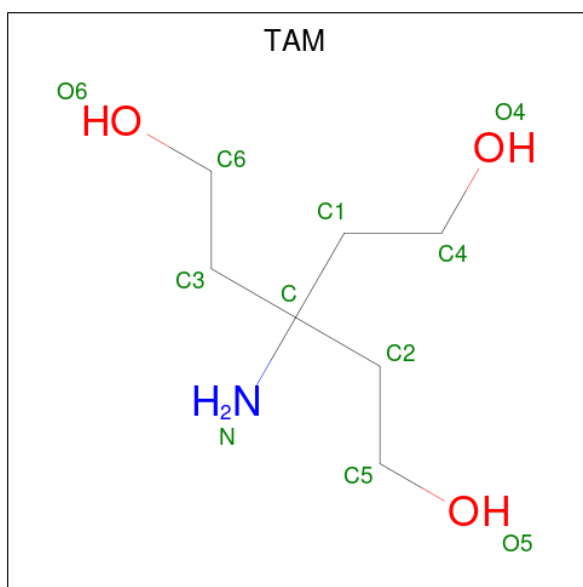
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O		0	0
			4	2	2			

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 7 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

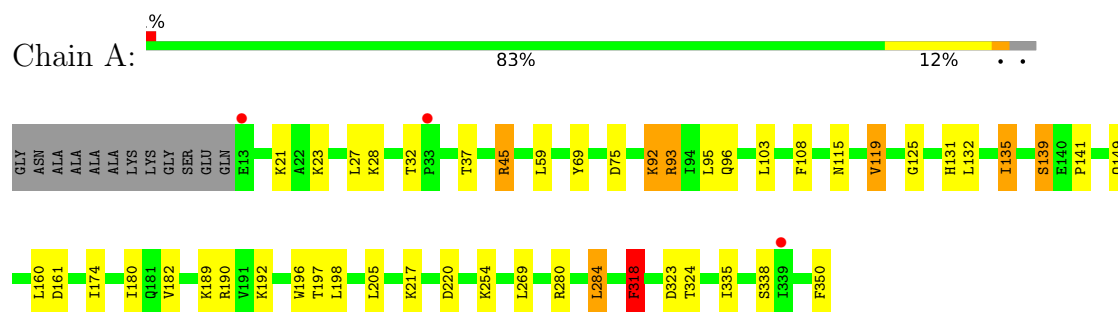
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	153	Total 153	O 153	0	0
9	B	136	Total 136	O 136	0	0

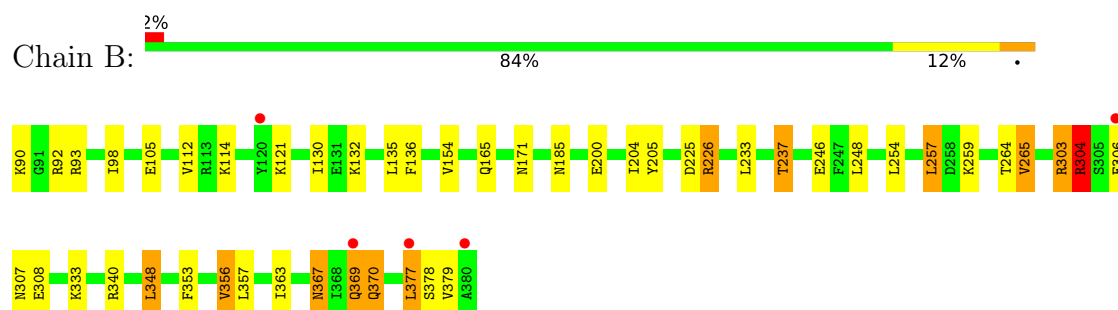
3 Residue-property plots [i](#)

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, alpha-catalytic subunit



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.81Å 125.81Å 140.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.20 43.14 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.9 (50.00-2.20) 94.9 (43.14-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.225 0.192 , 0.220	Depositor DCC
R_{free} test set	3160 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5459	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, TAM, SO4, ACT, ANP, TPO, MN, GOL

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	0.89	2/2815 (0.1%)	0.92	12/3796 (0.3%)
2	B	0.62	0/2336	0.84	11/3150 (0.3%)
All	All	0.78	2/5151 (0.0%)	0.89	23/6946 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254[A]	LYS	CB-CG	-24.00	0.87	1.52
1	A	254[B]	LYS	CB-CG	-24.00	0.87	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	PHE	CB-CG-CD2	-20.95	106.13	120.80
1	A	318	PHE	CB-CG-CD1	17.86	133.31	120.80
1	A	93	ARG	CD-NE-CZ	11.84	140.18	123.60
1	A	93	ARG	NE-CZ-NH1	-10.48	115.06	120.30
2	B	304	ARG	CG-CD-NE	10.42	133.67	111.80
1	A	318	PHE	CA-CB-CG	9.82	137.47	113.90
2	B	307	ASN	CB-CA-C	-9.60	91.20	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	LYS	CG-CD-CE	9.24	139.61	111.90
1	A	192	LYS	CD-CE-NZ	8.26	130.69	111.70
1	A	254[A]	LYS	CA-CB-CG	8.16	131.35	113.40
1	A	254[B]	LYS	CA-CB-CG	8.16	131.35	113.40
2	B	304	ARG	CD-NE-CZ	7.41	133.97	123.60
1	A	21	LYS	CD-CE-NZ	7.21	128.28	111.70
2	B	114	LYS	CB-CG-CD	6.92	129.59	111.60
2	B	340	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	A	93	ARG	NE-CZ-NH2	6.59	123.59	120.30
2	B	93	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	B	93	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	B	340	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	B	121	LYS	CB-CG-CD	-5.31	97.79	111.60
1	A	220	ASP	CB-CG-OD2	5.29	123.06	118.30
2	B	304	ARG	CB-CG-CD	-5.05	98.46	111.60
2	B	226	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	PHE	Sidechain
1	A	93	ARG	Sidechain
2	B	304	ARG	Sidechain

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	2778	0	2716	29	0
2	B	2296	0	2284	33	0
3	A	2	0	0	0	0
4	A	5	0	0	0	0
4	B	25	0	0	0	0
5	A	4	0	3	0	0
6	A	31	0	13	0	0
7	A	11	0	17	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	12	0	16	0	0
8	B	6	0	8	1	0
9	A	153	0	0	1	0
9	B	136	0	0	3	0
All	All	5459	0	5057	61	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 6.

All (61) 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:149:GLN:HE22	1:A:180:ILE:H	1.17	0.89
2:B:356:VAL:HG12	2:B:357:LEU:HD22	1.67	0.76
1:A:32:THR:O	1:A:32:THR:HG23	1.86	0.74
2:B:92:ARG:NH2	9:B:531:HOH:O	2.20	0.74
1:A:198:LEU:HD13	2:B:204:ILE:HB	1.70	0.73
2:B:257:LEU:HD11	2:B:363:ILE:HD13	1.73	0.71
2:B:257:LEU:HD13	2:B:363:ILE:HG21	1.76	0.67
1:A:161:ASP:HA	1:A:217:LYS:HE2	1.76	0.66
2:B:356:VAL:CG1	2:B:357:LEU:HD22	2.28	0.64
1:A:28:LYS:O	1:A:32:THR:HG22	2.00	0.61
1:A:45:ARG:CD	1:A:335:ILE:HD12	2.31	0.60
2:B:233:LEU:O	2:B:237:THR:HG23	2.02	0.60
1:A:92:LYS:NZ	1:A:350:PHE:OXT	2.36	0.59
2:B:377:LEU:HD22	2:B:378:SER:N	2.19	0.57
2:B:264:THR:CG2	2:B:356:VAL:HG13	2.35	0.56
1:A:23:LYS:HA	1:A:160:LEU:HD21	1.87	0.56
1:A:149:GLN:HE22	1:A:180:ILE:N	1.97	0.56
1:A:45:ARG:HD3	1:A:335:ILE:HD12	1.88	0.55
1:A:131:HIS:O	1:A:135:ILE:HD12	2.06	0.55
2:B:254:LEU:HB3	2:B:257:LEU:HD22	1.88	0.55
2:B:135:LEU:HD12	2:B:200:GLU:HG2	1.89	0.54
2:B:264:THR:HG21	2:B:356:VAL:HG13	1.90	0.53
2:B:367:ASN:HD22	2:B:370:GLN:H	1.56	0.53
1:A:196:TRP:HD1	7:A:406:TAM:H22	1.74	0.53
1:A:132:LEU:O	1:A:135:ILE:HD13	2.08	0.53
2:B:233:LEU:O	2:B:237:THR:CG2	2.59	0.51
1:A:280:ARG:O	1:A:284:LEU:HD13	2.11	0.51
1:A:37:THR:HG23	1:A:108:PHE:HB3	1.93	0.51
1:A:189:LYS:NZ	7:A:406:TAM:H51	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:ILE:C	2:B:130:ILE:HD12	2.32	0.49
2:B:98:ILE:HD12	2:B:205:TYR:CZ	2.47	0.49
2:B:257:LEU:CD1	2:B:363:ILE:HD13	2.41	0.49
1:A:284:LEU:HB2	9:A:421:HOH:O	2.12	0.48
1:A:189:LYS:NZ	7:A:406:TAM:H41	2.29	0.48
2:B:165:GLN:HE22	2:B:185:ASN:ND2	2.12	0.47
2:B:98:ILE:HD12	2:B:205:TYR:CE1	2.49	0.47
2:B:248:LEU:HD11	2:B:265:VAL:HG22	1.96	0.47
1:A:75:ASP:HA	1:A:115:ASN:HD22	1.81	0.46
2:B:248:LEU:CD1	2:B:265:VAL:HG22	2.46	0.46
1:A:103:LEU:HD23	1:A:182:VAL:HB	1.98	0.46
2:B:348:LEU:HD13	2:B:353:PHE:HB2	1.99	0.45
2:B:112:VAL:HA	9:B:540:HOH:O	2.17	0.45
1:A:139:SEP:OG	1:A:141:PRO:HD2	2.19	0.43
2:B:369:GLN:HE21	2:B:369:GLN:HA	1.83	0.43
1:A:189:LYS:HZ1	7:A:406:TAM:H41	1.84	0.43
7:A:406:TAM:H31	2:B:105:GLU:HG3	2.00	0.43
2:B:303:ARG:HD3	2:B:308:GLU:O	2.18	0.43
2:B:333:LYS:NZ	9:B:417:HOH:O	2.50	0.43
1:A:125:GLY:O	1:A:131:HIS:CE1	2.72	0.43
1:A:23:LYS:HA	1:A:160:LEU:CD2	2.49	0.42
1:A:125:GLY:HA3	1:A:174:ILE:O	2.19	0.42
1:A:108:PHE:HB2	1:A:119:VAL:HG13	2.01	0.42
2:B:171:ASN:HD22	2:B:225:ASP:HA	1.84	0.42
1:A:59:LEU:HD22	1:A:324:THR:CG2	2.49	0.42
2:B:226:ARG:HH21	8:B:408:GOL:H2	1.85	0.41
2:B:303:ARG:HH21	2:B:303:ARG:HG2	1.85	0.41
1:A:149:GLN:NE2	1:A:180:ILE:H	2.00	0.41
2:B:98:ILE:CD1	2:B:205:TYR:CZ	3.03	0.41
1:A:69:TYR:HB3	1:A:119:VAL:HG23	2.04	0.40
2:B:130:ILE:HD13	2:B:136:PHE:HB3	2.02	0.40
2:B:264:THR:CG2	2:B:356:VAL:CG1	2.99	0.40

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	336/350 (96%)	328 (98%)	8 (2%)	0	100	100
2	B	289/291 (99%)	282 (98%)	7 (2%)	0	100	100
All	All	625/641 (98%)	610 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	288/302 (95%)	275 (96%)	13 (4%)	27	34
2	B	243/245 (99%)	225 (93%)	18 (7%)	13	14
All	All	531/547 (97%)	500 (94%)	31 (6%)	20	23

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	45	ARG
1	A	92	LYS
1	A	95	LEU
1	A	96	GLN
1	A	119	VAL
1	A	135	ILE
1	A	190	ARG
1	A	205	LEU
1	A	269	LEU
1	A	284	LEU
1	A	318	PHE
1	A	323	ASP
2	B	90	LYS

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Mol	Chain	Res	Type
2	B	132	LYS
2	B	154	VAL
2	B	237	THR
2	B	246	GLU
2	B	257	LEU
2	B	259	LYS
2	B	265	VAL
2	B	303	ARG
2	B	304	ARG
2	B	306	GLU
2	B	348	LEU
2	B	356	VAL
2	B	367	ASN
2	B	369	GLN
2	B	370	GLN
2	B	377	LEU
2	B	379	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	67	ASN
1	A	90	ASN
1	A	96	GLN
1	A	99	ASN
1	A	115	ASN
1	A	142	HIS
1	A	149	GLN
1	A	181	GLN
1	A	242	GLN
1	A	286	ASN
1	A	307	GLN
2	B	171	ASN
2	B	185	ASN
2	B	367	ASN
2	B	369	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	0.80	0	10,14,16	1.14	1 (10%)
1	SEP	A	338	1	8,9,10	1.53	1 (12%)	8,12,14	2.30	2 (25%)
1	SEP	A	139	1	8,9,10	1.62	2 (25%)	8,12,14	4.29	4 (50%)

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	SEP	A	338	1	-	2/5/8/10	-
1	SEP	A	139	1	-	4/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	SEP	P-O1P	3.06	1.60	1.50
1	A	139	SEP	P-O1P	3.05	1.60	1.50
1	A	139	SEP	OG-CB	-2.45	1.35	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	SEP	OG-CB-CA	8.93	116.83	108.14
1	A	338	SEP	OG-CB-CA	5.50	113.50	108.14
1	A	139	SEP	P-OG-CB	-5.05	104.39	118.30
1	A	139	SEP	OG-P-O1P	4.57	119.29	106.47
1	A	139	SEP	O3P-P-OG	-3.55	97.28	106.73
1	A	338	SEP	OG-P-O1P	3.11	115.20	106.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	TPO	O3P-P-O2P	2.32	116.50	107.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	139	SEP	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	$\# Z > 2$
6	ANP	A	400	3	29,33,33	1.73	9 (31%)	31,52,52	1.56	5 (16%)
4	SO4	B	400	-	4,4,4	0.25	0	6,6,6	0.45	0
7	TAM	A	406	-	7,10,10	0.42	0	9,12,12	1.05	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	B	408	-	5,5,5	0.44	0	5,5,5	0.84	0
4	SO4	B	403	-	4,4,4	0.21	0	6,6,6	0.36	0
4	SO4	B	401	-	4,4,4	0.15	0	6,6,6	0.34	0
4	SO4	B	404	-	4,4,4	0.15	0	6,6,6	0.22	0
8	GOL	A	410	-	5,5,5	0.41	0	5,5,5	0.65	0
4	SO4	A	403	-	4,4,4	0.18	0	6,6,6	0.43	0
4	SO4	B	405	-	4,4,4	0.29	0	6,6,6	0.60	0
5	ACT	A	412	-	1,3,3	1.93	0	0,3,3	-	-
8	GOL	A	407	-	5,5,5	0.29	0	5,5,5	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
6	ANP	A	400	3	-	1/14/38/38	0/3/3/3
7	TAM	A	406	-	-	4/12/12/12	-
8	GOL	B	408	-	-	4/4/4/4	-
8	GOL	A	410	-	-	4/4/4/4	-
8	GOL	A	407	-	-	1/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	400	ANP	PB-N3B	4.48	1.75	1.63
6	A	400	ANP	PG-N3B	3.72	1.73	1.63
6	A	400	ANP	PG-O1G	2.43	1.50	1.46
6	A	400	ANP	PB-O1B	2.43	1.50	1.46
6	A	400	ANP	PG-O2G	-2.39	1.50	1.56
6	A	400	ANP	C5-C4	2.23	1.46	1.40
6	A	400	ANP	PG-O3G	-2.11	1.51	1.56
6	A	400	ANP	PB-O2B	-2.05	1.51	1.56
6	A	400	ANP	C2-N3	2.01	1.35	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	400	ANP	O2B-PB-O1B	4.19	118.70	109.92
6	A	400	ANP	N3-C2-N1	-3.88	122.61	128.68
6	A	400	ANP	O1G-PG-N3B	-3.40	106.77	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	400	ANP	O3A-PB-N3B	-2.27	100.28	106.59
6	A	400	ANP	O2B-PB-O3A	2.18	111.92	104.64
7	A	406	TAM	C2-C-C1	-2.13	106.75	110.50

There are no chirality outliers.

All (14) torsion outliers are listed below:

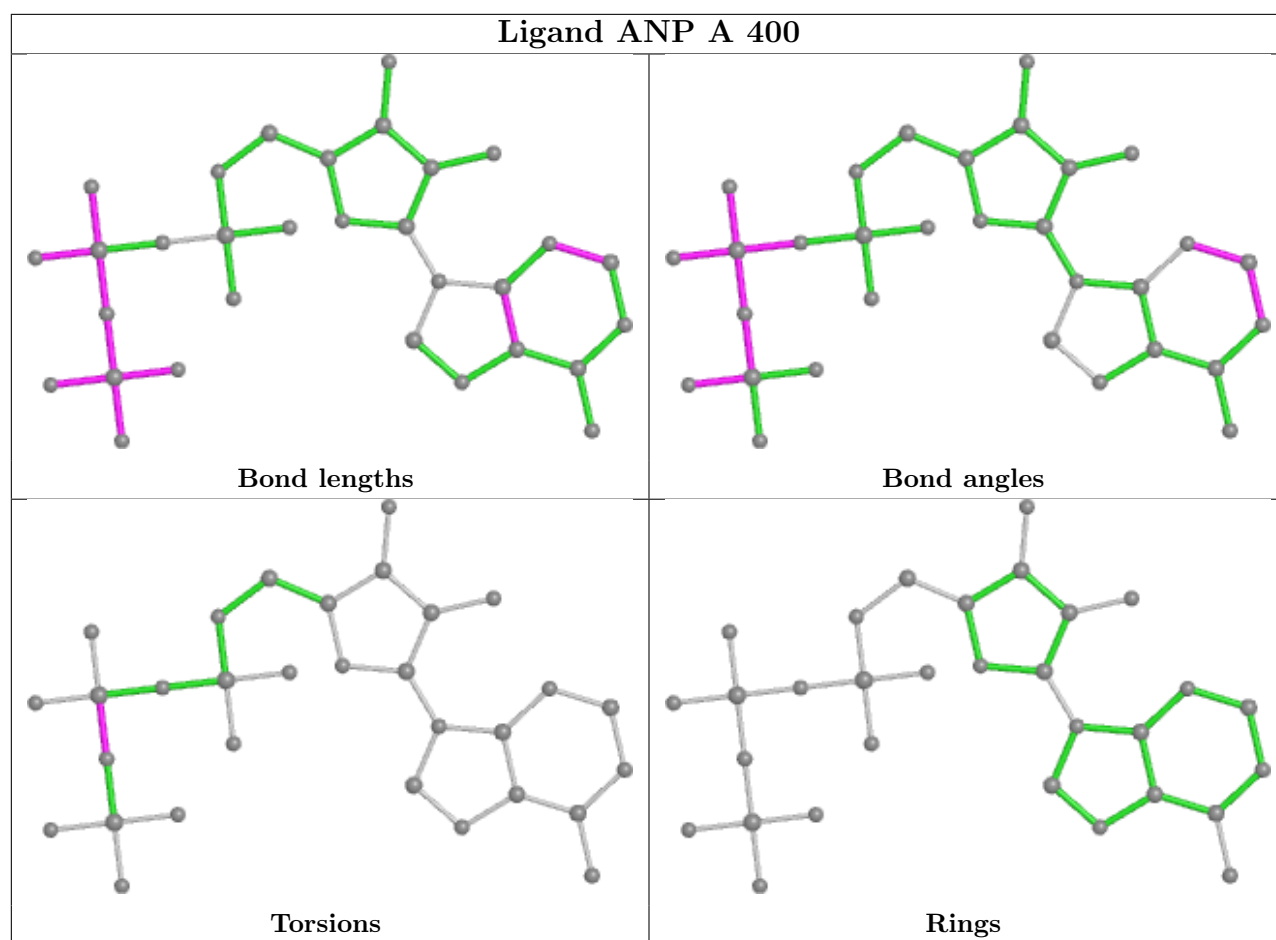
Mol	Chain	Res	Type	Atoms
6	A	400	ANP	PG-N3B-PB-O1B
7	A	406	TAM	C1-C-C2-C5
7	A	406	TAM	C3-C-C2-C5
7	A	406	TAM	N-C-C2-C5
7	A	406	TAM	C-C3-C6-O6
8	A	410	GOL	O1-C1-C2-C3
8	A	410	GOL	C1-C2-C3-O3
8	B	408	GOL	O1-C1-C2-C3
8	B	408	GOL	C1-C2-C3-O3
8	A	410	GOL	O1-C1-C2-O2
8	A	410	GOL	O2-C2-C3-O3
8	B	408	GOL	O1-C1-C2-O2
8	B	408	GOL	O2-C2-C3-O3
8	A	407	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	406	TAM	5	0
8	B	408	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/350 (95%)	-0.03	3 (0%) 84 83	28, 37, 52, 64	10 (2%)
2	B	291/291 (100%)	-0.21	5 (1%) 70 68	30, 40, 51, 60	11 (3%)
All	All	626/641 (97%)	-0.11	8 (1%) 77 75	28, 38, 51, 64	21 (3%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	380	ALA	6.3
1	A	339	ILE	4.3
2	B	306	GLU	3.6
1	A	33	PRO	3.6
1	A	13	GLU	3.2
2	B	120	TYR	3.1
2	B	369	GLN	2.3
2	B	377	LEU	2.1

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	139	10/11	0.95	0.10	30,31,35,37	0
1	SEP	A	338	10/11	0.95	0.20	41,43,43,44	0
1	TPO	A	197	11/12	0.99	0.15	29,30,32,34	0

6.3 Carbohydrates

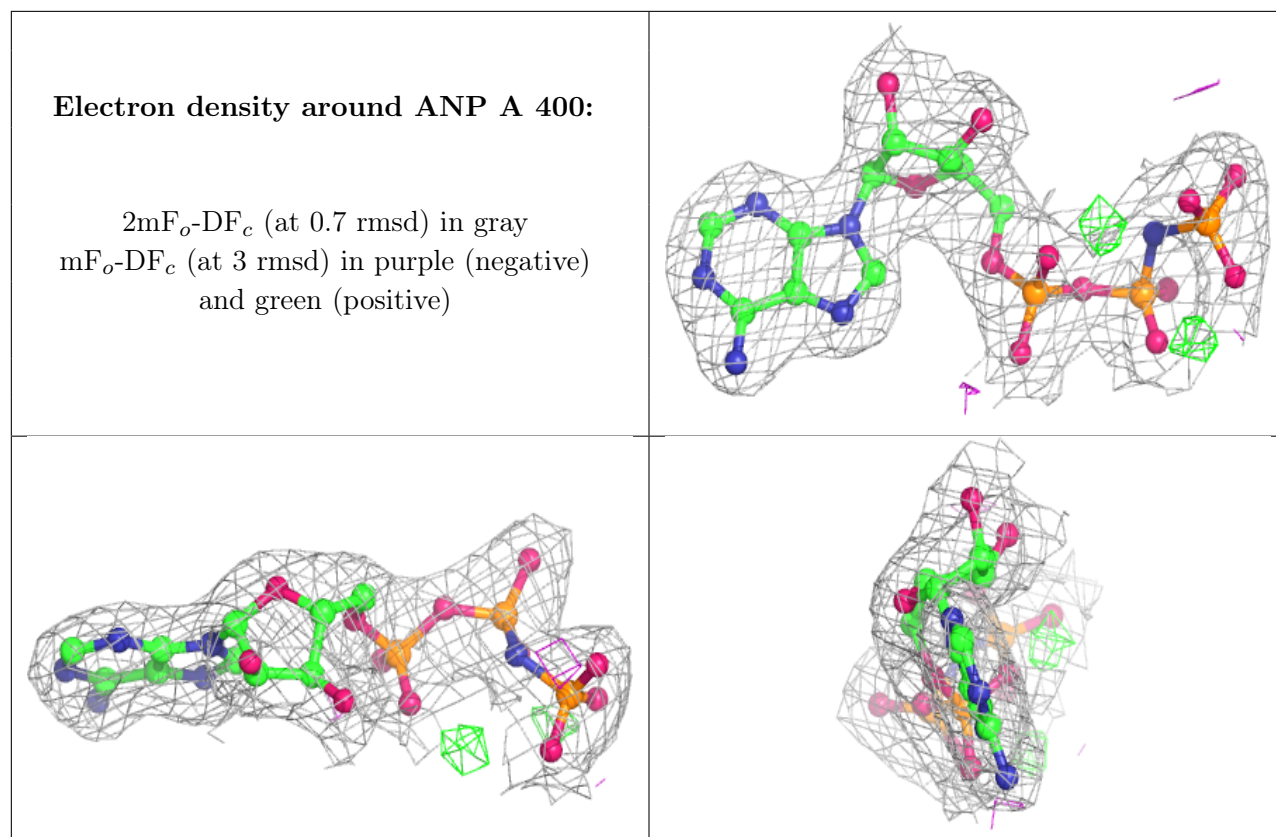
There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	GOL	B	408	6/6	0.59	0.28	56,59,59,63	0
7	TAM	A	406	11/11	0.73	0.27	49,52,53,54	0
4	SO4	B	404	5/5	0.83	0.18	90,90,91,92	0
8	GOL	A	410	6/6	0.85	0.14	58,60,61,62	0
5	ACT	A	412	4/4	0.86	0.31	70,70,70,70	0
8	GOL	A	407	6/6	0.88	0.27	65,66,66,66	0
4	SO4	A	403	5/5	0.94	0.19	65,67,67,67	0
4	SO4	B	403	5/5	0.96	0.22	55,58,58,60	0
4	SO4	B	401	5/5	0.96	0.17	58,58,60,61	0
4	SO4	B	405	5/5	0.98	0.07	32,33,35,36	0
6	ANP	A	400	31/31	0.98	0.17	25,29,30,33	0
3	MN	A	401	1/1	0.99	0.19	31,31,31,31	0
4	SO4	B	400	5/5	0.99	0.09	40,41,43,43	0
3	MN	A	402	1/1	0.99	0.18	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.