



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 02:14 PM EDT

PDB ID : 2ACX
Title : Crystal Structure of G protein coupled receptor kinase 6 bound to AMPPNP
Authors : Lodowski, D.T.; Tesmer, V.M.; Benovic, J.L.; Tesmer, J.J.
Deposited on : 2005-07-19
Resolution : 2.60 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

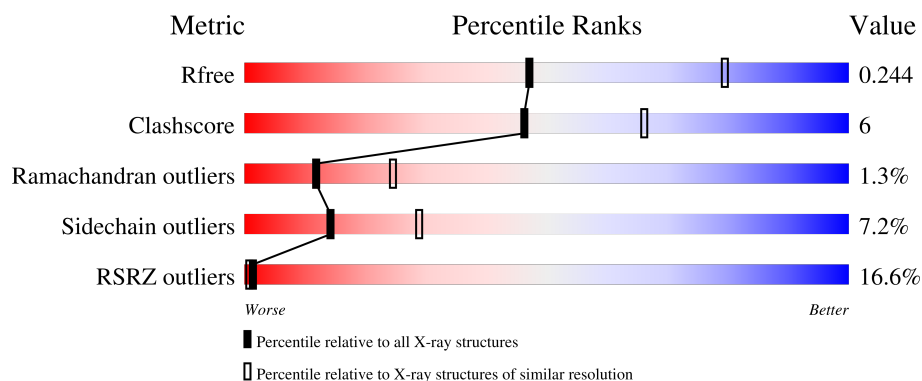
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	576	<div> <div>8%</div> <div>66%</div> <div>16%</div> <div>•</div> <div>14%</div> </div>
1	B	576	<div> <div>20%</div> <div>69%</div> <div>14%</div> <div>•</div> <div>15%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8106 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 G protein-coupled receptor kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			4011	2548	714	721	28			
1	B	492	Total	C	N	O	S	0	0	0
			3984	2535	705	717	27			

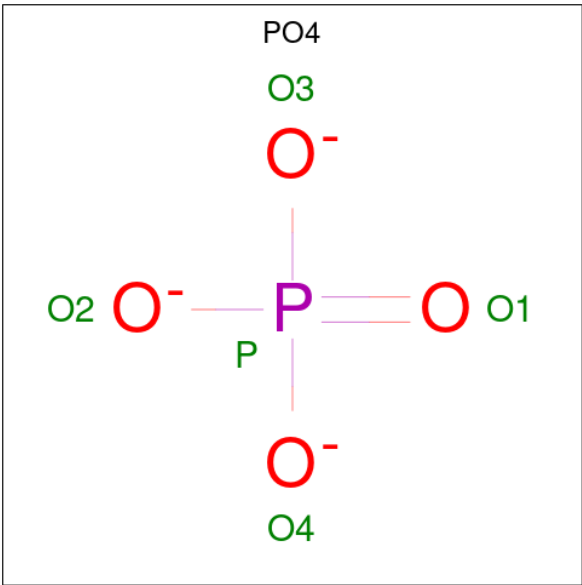
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASN	GLN	SEE REMARK 999	UNP P43250
A	104	ASN	GLN	SEE REMARK 999	UNP P43250
A	561	SER	CYS	engineered mutation	UNP P43250
A	562	SER	CYS	engineered mutation	UNP P43250
A	565	SER	CYS	engineered mutation	UNP P43250
B	60	ASN	GLN	SEE REMARK 999	UNP P43250
B	104	ASN	GLN	SEE REMARK 999	UNP P43250
B	561	SER	CYS	engineered mutation	UNP P43250
B	562	SER	CYS	engineered mutation	UNP P43250
B	565	SER	CYS	engineered mutation	UNP P43250

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

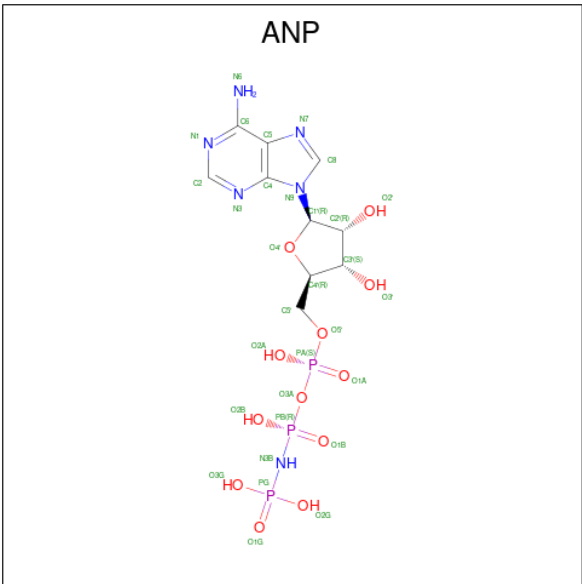
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

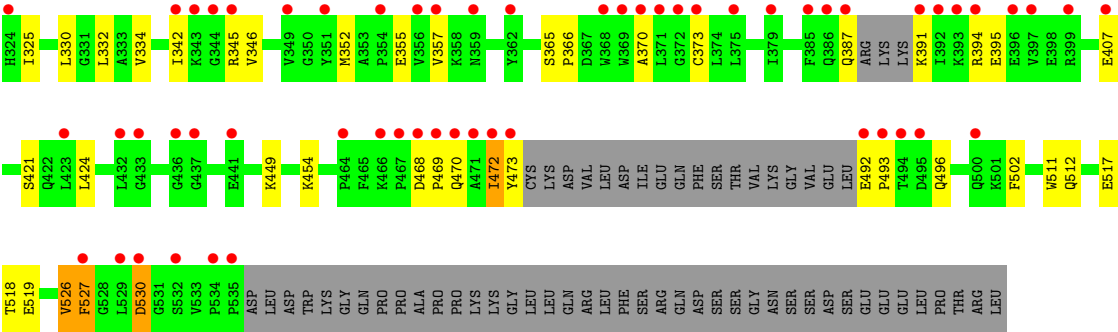


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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total	O	0	0
			30	30		
5	B	7	Total	O	0	0
			7	7		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.16Å 59.27Å 221.09Å 90.00° 102.58° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.60) 97.3 (30.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.202 , 0.243 0.208 , 0.244	Depositor DCC
R_{free} test set	2317 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 81.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8106	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: PO4, ANP, MG

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	1.06	4/4101 (0.1%)	1.02	15/5521 (0.3%)
1	B	0.74	0/4074	0.87	7/5488 (0.1%)
All	All	0.92	4/8175 (0.0%)	0.95	22/11009 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	GLU	CD-OE2	6.82	1.33	1.25
1	A	517	GLU	CD-OE1	6.80	1.33	1.25
1	A	91	GLU	CD-OE2	5.24	1.31	1.25
1	A	240	LYS	CD-CE	5.14	1.64	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	A	96	ASP	CB-CG-OD2	9.15	126.54	118.30
1	B	96	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	394	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	270	ASP	CB-CG-OD2	6.62	124.26	118.30
1	B	52	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	52	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	431	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	523	GLU	OE1-CD-OE2	5.92	130.41	123.30
1	A	257	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	95	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	68	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	530	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	468	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	270	ASP	CB-CG-OD2	5.28	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	230	MET	CG-SD-CE	5.25	108.60	100.20
1	A	449	LYS	CB-CA-C	-5.25	99.91	110.40
1	A	355	GLU	CB-CA-C	-5.21	99.99	110.40
1	A	455	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	311	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	321	ASP	CB-CG-OD2	5.05	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4011	0	4008	59	0
1	B	3984	0	3974	47	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	31	0	13	0	0
4	B	31	0	13	2	0
5	A	30	0	0	2	0
5	B	7	0	0	0	0
All	All	8106	0	8008	102	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 (102) 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:132:ARG:NH2	1:A:138:CYS:SG	2.42	0.93
1:A:319:LEU:CD2	1:A:325:ILE:HG22	2.00	0.92
1:B:133:LEU:HB2	1:B:141:LEU:HD21	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:LEU:HD22	1:B:325:ILE:HG22	1.58	0.84
1:A:133:LEU:HB2	1:A:141:LEU:HD21	1.66	0.75
1:A:150:HIS:ND1	5:A:592:HOH:O	2.20	0.74
1:B:106:THR:HG22	1:B:110:LEU:HD12	1.72	0.71
1:A:325:ILE:C	1:A:325:ILE:HD12	2.11	0.71
1:A:255:THR:HG22	1:A:257:ASP:H	1.58	0.69
1:A:68:ARG:NH2	1:A:85:ASP:OD1	2.28	0.67
1:A:314:PRO:HG3	1:A:374:LEU:HD13	1.78	0.65
1:A:319:LEU:HD22	1:A:325:ILE:HG22	1.78	0.64
1:B:127:THR:HG22	1:B:131:GLN:HE22	1.64	0.62
1:B:334:VAL:HG11	1:B:342:ILE:HD13	1.81	0.61
1:A:319:LEU:HD23	1:A:325:ILE:HG22	1.81	0.60
1:A:530:ASP:HB3	1:B:72:ALA:CB	2.31	0.60
1:A:30:TRP:HA	1:A:33:MET:HE3	1.83	0.60
1:B:325:ILE:HD12	1:B:325:ILE:C	2.21	0.59
1:A:473:TYR:HD2	1:A:473:TYR:N	2.00	0.59
1:B:127:THR:CG2	1:B:131:GLN:HE22	2.17	0.57
1:A:473:TYR:N	1:A:473:TYR:CD2	2.72	0.57
1:A:155:VAL:HG12	1:A:156:ALA:N	2.20	0.56
1:A:132:ARG:CZ	1:A:138:CYS:SG	2.94	0.55
1:B:232:LEU:HD11	1:B:236:GLN:NE2	2.22	0.55
1:A:255:THR:HG22	1:A:257:ASP:N	2.21	0.55
1:A:197:PHE:CD2	1:A:222:ILE:HD13	2.43	0.54
1:B:387:GLN:O	1:B:391:LYS:NZ	2.36	0.53
1:A:30:TRP:HA	1:A:33:MET:CE	2.39	0.52
1:A:54:HIS:ND1	1:A:58:GLU:OE1	2.38	0.52
1:B:320:ASP:OD1	1:B:320:ASP:C	2.48	0.52
1:A:383:SER:OG	5:A:604:HOH:O	2.19	0.51
1:A:14:LYS:HG3	1:A:29:LYS:HE3	1.94	0.50
1:A:45:LEU:O	1:A:46:ARG:C	2.49	0.50
1:B:313:LYS:HB2	1:B:314:PRO:HD2	1.94	0.50
1:B:352:MET:CE	1:B:357:VAL:HG12	2.41	0.50
1:B:352:MET:HE2	1:B:357:VAL:HG12	1.93	0.49
1:B:526:VAL:HG22	1:B:527:PHE:H	1.77	0.49
1:B:98:ARG:HD2	1:B:137:PRO:O	2.13	0.49
1:A:365:SER:OG	1:A:366:PRO:HD3	2.12	0.48
4:B:577:ANP:O3A	4:B:577:ANP:O2G	2.31	0.48
1:A:418:SER:O	1:A:422:GLN:HG3	2.13	0.48
1:B:259:LEU:HB3	1:B:502:PHE:CE2	2.48	0.48
1:A:244:ARG:HD2	1:A:457:GLY:O	2.13	0.48
1:A:527:PHE:C	1:A:527:PHE:CD1	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ASN:HB3	1:B:512:GLN:OE1	2.14	0.48
1:A:168:ASN:ND2	1:B:168:ASN:OD1	2.47	0.47
1:A:492:GLU:N	1:A:493:PRO:CD	2.77	0.47
1:B:139:LYS:HD2	1:B:454:LYS:NZ	2.29	0.47
1:B:208:THR:HB	1:B:518:THR:HG21	1.97	0.47
1:A:197:PHE:CE2	1:A:222:ILE:HD13	2.49	0.47
1:A:355:GLU:CG	1:A:428:PRO:HG3	2.45	0.47
1:B:237:ILE:HG23	1:B:307:ILE:HD13	1.97	0.47
1:A:530:ASP:HB3	1:B:72:ALA:HB3	1.96	0.47
1:B:492:GLU:N	1:B:493:PRO:CD	2.77	0.47
1:A:86:GLY:HA3	1:A:105:LEU:HD21	1.97	0.46
1:B:215:LYS:NZ	1:B:234:GLU:OE2	2.44	0.46
1:A:509:ILE:HB	1:A:510:PRO:HD3	1.98	0.46
1:B:373:CYS:SG	1:B:424:LEU:HD21	2.56	0.46
1:A:45:LEU:O	1:A:46:ARG:O	2.34	0.45
1:B:29:LYS:O	1:B:33:MET:HG3	2.16	0.45
1:A:341:THR:OG1	1:A:361:ARG:HD3	2.16	0.45
1:A:502:PHE:CD2	1:A:502:PHE:C	2.90	0.45
1:A:72:ALA:HB1	1:B:530:ASP:HB3	1.99	0.45
1:B:177:GLU:HB2	1:B:511:TRP:CZ3	2.52	0.45
1:B:238:LEU:HD21	1:B:330:LEU:HD13	1.98	0.45
1:A:208:THR:HB	1:A:518:THR:HG21	2.00	0.44
1:A:409:SER:C	1:A:411:ARG:H	2.21	0.44
1:B:311:ASP:OD2	1:B:316:ASN:ND2	2.50	0.44
1:B:210:LYS:NZ	1:B:517:GLU:OE1	2.33	0.44
1:A:72:ALA:CB	1:B:530:ASP:HB3	2.48	0.43
1:A:355:GLU:HG3	1:A:428:PRO:HG3	2.00	0.43
1:B:526:VAL:HG22	1:B:527:PHE:N	2.33	0.43
1:B:109:PHE:O	1:B:110:LEU:HD23	2.18	0.43
1:B:334:VAL:HG11	1:B:342:ILE:CD1	2.47	0.43
1:B:215:LYS:NZ	4:B:577:ANP:O2B	2.52	0.43
1:A:345:ARG:HG2	1:A:356:VAL:O	2.18	0.43
1:A:365:SER:N	1:A:366:PRO:CD	2.82	0.43
1:A:313:LYS:HB2	1:A:314:PRO:CD	2.49	0.42
1:A:15:ALA:O	1:A:16:ARG:HG3	2.20	0.42
1:A:285:GLU:O	1:A:286:ALA:C	2.56	0.42
1:B:267:ASN:HD21	1:B:472:ILE:HD12	1.83	0.42
1:A:125:LEU:HD21	1:A:144:GLU:HG3	2.01	0.42
1:A:240:LYS:HE2	1:A:305:GLU:HB3	2.01	0.42
1:B:518:THR:O	1:B:519:GLU:HB2	2.18	0.42
1:B:168:ASN:N	1:B:168:ASN:HD22	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLU:HA	1:A:144:GLU:OE1	2.20	0.42
1:B:195:GLY:O	1:B:197:PHE:N	2.53	0.42
1:B:312:LEU:HB3	1:B:370:ALA:CB	2.51	0.41
1:A:95:ASP:OD1	1:A:98:ARG:NH2	2.53	0.41
1:A:325:ILE:HD12	1:A:325:ILE:O	2.21	0.41
1:A:93:THR:HB	1:A:98:ARG:HG3	2.03	0.41
1:A:396:GLU:HA	1:A:396:GLU:OE1	2.20	0.41
1:A:430:GLU:O	1:A:435:ARG:NH1	2.54	0.41
1:B:139:LYS:HD2	1:B:454:LYS:HZ2	1.84	0.41
1:B:176:LEU:HD23	1:B:176:LEU:HA	1.91	0.41
1:A:156:ALA:HB3	1:A:157:PRO:HD3	2.03	0.41
1:A:338:GLU:H	1:A:338:GLU:HG2	1.68	0.41
1:A:89:GLU:O	1:A:93:THR:OG1	2.38	0.40
1:B:311:ASP:HB2	1:B:332:LEU:HD12	2.04	0.40
1:A:232:LEU:HD11	1:A:236:GLN:NE2	2.37	0.40
1:B:330:LEU:HD12	1:B:330:LEU:N	2.36	0.40
1:B:365:SER:N	1:B:366:PRO:CD	2.84	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	489/576 (85%)	458 (94%)	24 (5%)	7 (1%)	11	22
1	B	482/576 (84%)	459 (95%)	17 (4%)	6 (1%)	13	27
All	All	971/1152 (84%)	917 (94%)	41 (4%)	13 (1%)	12	24

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	LEU

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Mol	Chain	Res	Type
1	A	449	LYS
1	A	526	VAL
1	B	141	LEU
1	B	196	GLY
1	B	449	LYS
1	A	46	ARG
1	B	46	ARG
1	B	526	VAL
1	A	471	ALA
1	A	196	GLY
1	A	469	PRO
1	B	469	PRO

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	432/503 (86%)	398 (92%)	34 (8%)	12	24
1	B	430/503 (86%)	402 (94%)	28 (6%)	17	34
All	All	862/1006 (86%)	800 (93%)	62 (7%)	14	29

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	27	SER
1	A	48	SER
1	A	60	ASN
1	A	78	SER
1	A	96	ASP
1	A	104	ASN
1	A	106	THR
1	A	112	HIS
1	A	123	ARG
1	A	130	THR

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Mol	Chain	Res	Type
1	A	135	GLN
1	A	138	CYS
1	A	169	ARG
1	A	248	SER
1	A	255	THR
1	A	277	HIS
1	A	278	MET
1	A	280	GLN
1	A	359	ASN
1	A	361	ARG
1	A	374	LEU
1	A	382	GLN
1	A	389	LYS
1	A	394	ARG
1	A	396	GLU
1	A	411	ARG
1	A	472	ILE
1	A	473	TYR
1	A	474	CYS
1	A	494	THR
1	A	496	GLN
1	A	500	GLN
1	A	527	PHE
1	B	46	ARG
1	B	48	SER
1	B	52	ASP
1	B	79	ARG
1	B	89	GLU
1	B	95	ASP
1	B	98	ARG
1	B	134	GLU
1	B	147	ARG
1	B	169	ARG
1	B	230	MET
1	B	257	ASP
1	B	278	MET
1	B	317	ILE
1	B	319	LEU
1	B	345	ARG
1	B	346	VAL
1	B	355	GLU
1	B	394	ARG

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Mol	Chain	Res	Type
1	B	395	GLU
1	B	407	GLU
1	B	421	SER
1	B	470	GLN
1	B	472	ILE
1	B	473	TYR
1	B	496	GLN
1	B	527	PHE
1	B	530	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	168	ASN
1	A	335	HIS
1	A	359	ASN
1	A	387	GLN
1	A	513	ASN
1	B	108	ASN
1	B	131	GLN
1	B	168	ASN
1	B	387	GLN
1	B	500	GLN
1	B	513	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	PO4	B	579	-	4,4,4	0.71	0	6,6,6	1.49	1 (16%)
4	ANP	B	577	2	29,33,33	1.83	6 (20%)	31,52,52	1.79	9 (29%)
3	PO4	A	579	-	4,4,4	0.80	0	6,6,6	1.59	1 (16%)
4	ANP	A	577	2	29,33,33	2.18	7 (24%)	31,52,52	1.96	8 (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
4	ANP	B	577	2	-	3/14/38/38	0/3/3/3
4	ANP	A	577	2	-	4/14/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	577	ANP	PB-O3A	5.80	1.66	1.59
4	A	577	ANP	PG-N3B	4.59	1.75	1.63
4	B	577	ANP	PG-N3B	4.58	1.75	1.63
4	A	577	ANP	PG-O1G	4.40	1.53	1.46
4	B	577	ANP	PB-N3B	4.19	1.74	1.63
4	A	577	ANP	PB-N3B	4.15	1.74	1.63
4	A	577	ANP	PB-O1B	4.01	1.52	1.46
4	B	577	ANP	PG-O1G	3.62	1.51	1.46
4	B	577	ANP	PB-O1B	2.86	1.50	1.46
4	B	577	ANP	PB-O3A	2.66	1.62	1.59
4	A	577	ANP	C2'-C1'	-2.36	1.50	1.53
4	A	577	ANP	O4'-C1'	2.25	1.44	1.41
4	B	577	ANP	PB-O2B	-2.03	1.51	1.56

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	577	ANP	N3-C2-N1	-5.44	120.18	128.68
4	A	577	ANP	O1B-PB-N3B	-4.77	104.75	111.77
4	B	577	ANP	O1G-PG-N3B	-4.43	105.24	111.77
4	A	577	ANP	O3G-PG-O2G	3.93	118.11	107.64
4	B	577	ANP	N3-C2-N1	-3.92	122.55	128.68
4	B	577	ANP	O2B-PB-O1B	3.64	117.56	109.92
4	B	577	ANP	O3G-PG-O2G	2.77	115.03	107.64
4	B	577	ANP	O1B-PB-N3B	-2.75	107.72	111.77
4	B	577	ANP	PA-O3A-PB	-2.73	122.98	132.62
4	A	577	ANP	C2-N1-C6	2.65	123.29	118.75
4	B	577	ANP	C3'-C2'-C1'	2.65	104.97	100.98
4	B	577	ANP	C4-C5-N7	-2.59	106.70	109.40
3	A	579	PO4	O4-P-O2	2.55	116.17	107.97
4	A	577	ANP	O3'-C3'-C2'	-2.36	104.18	111.82
4	A	577	ANP	O2'-C2'-C3'	-2.15	104.87	111.82
4	B	577	ANP	O2A-PA-O1A	2.11	122.65	112.24
4	A	577	ANP	O2A-PA-O5'	-2.10	98.01	107.75
4	A	577	ANP	C1'-N9-C4	-2.02	123.09	126.64
3	B	579	PO4	O3-P-O2	2.00	114.40	107.97

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	577	ANP	PB-N3B-PG-O1G
4	A	577	ANP	PA-O3A-PB-O1B
4	A	577	ANP	PA-O3A-PB-O2B
4	B	577	ANP	PB-N3B-PG-O1G
4	B	577	ANP	C4'-C5'-O5'-PA
4	B	577	ANP	PG-N3B-PB-O1B
4	A	577	ANP	PB-O3A-PA-O1A

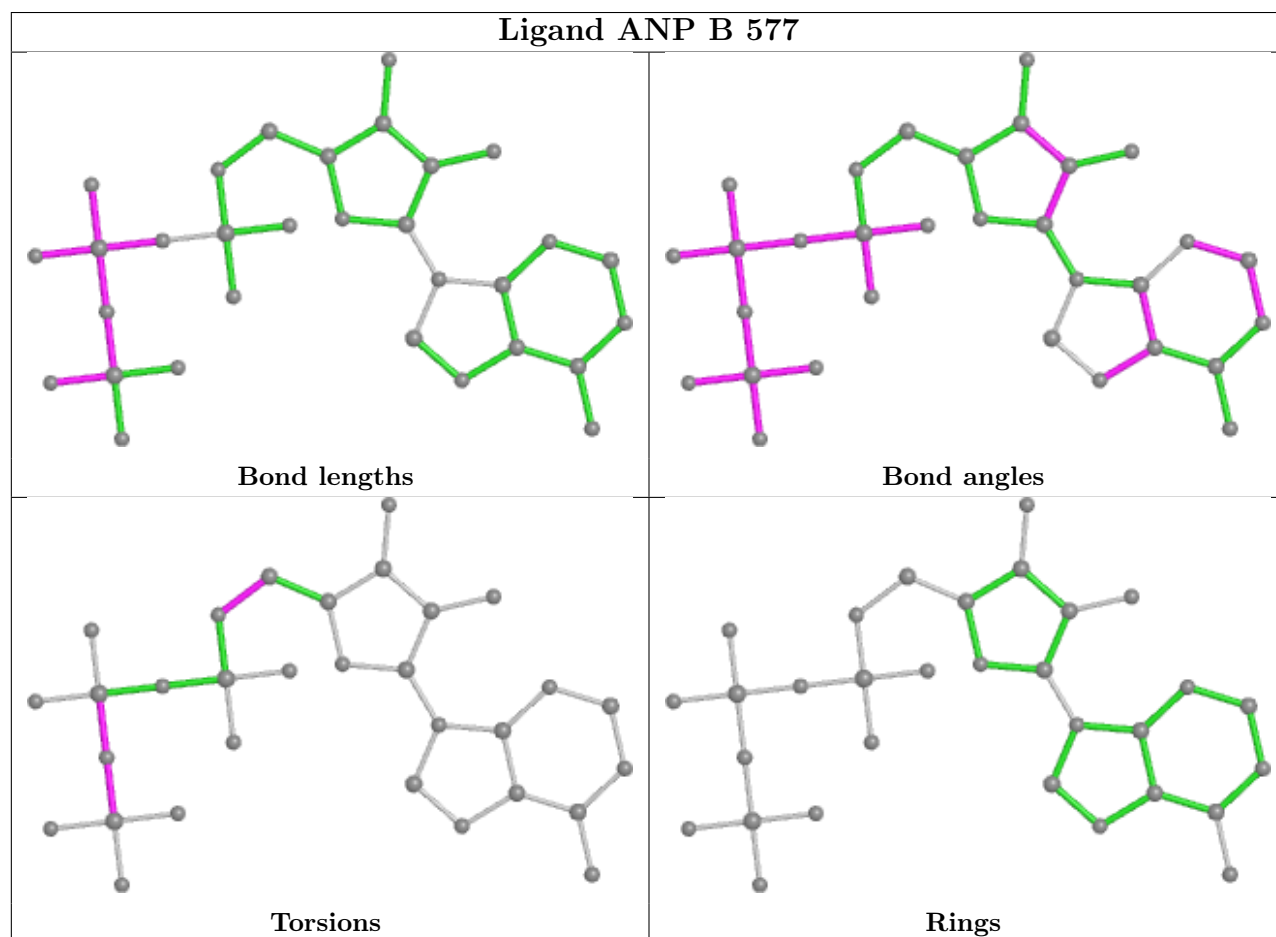
There are no ring outliers.

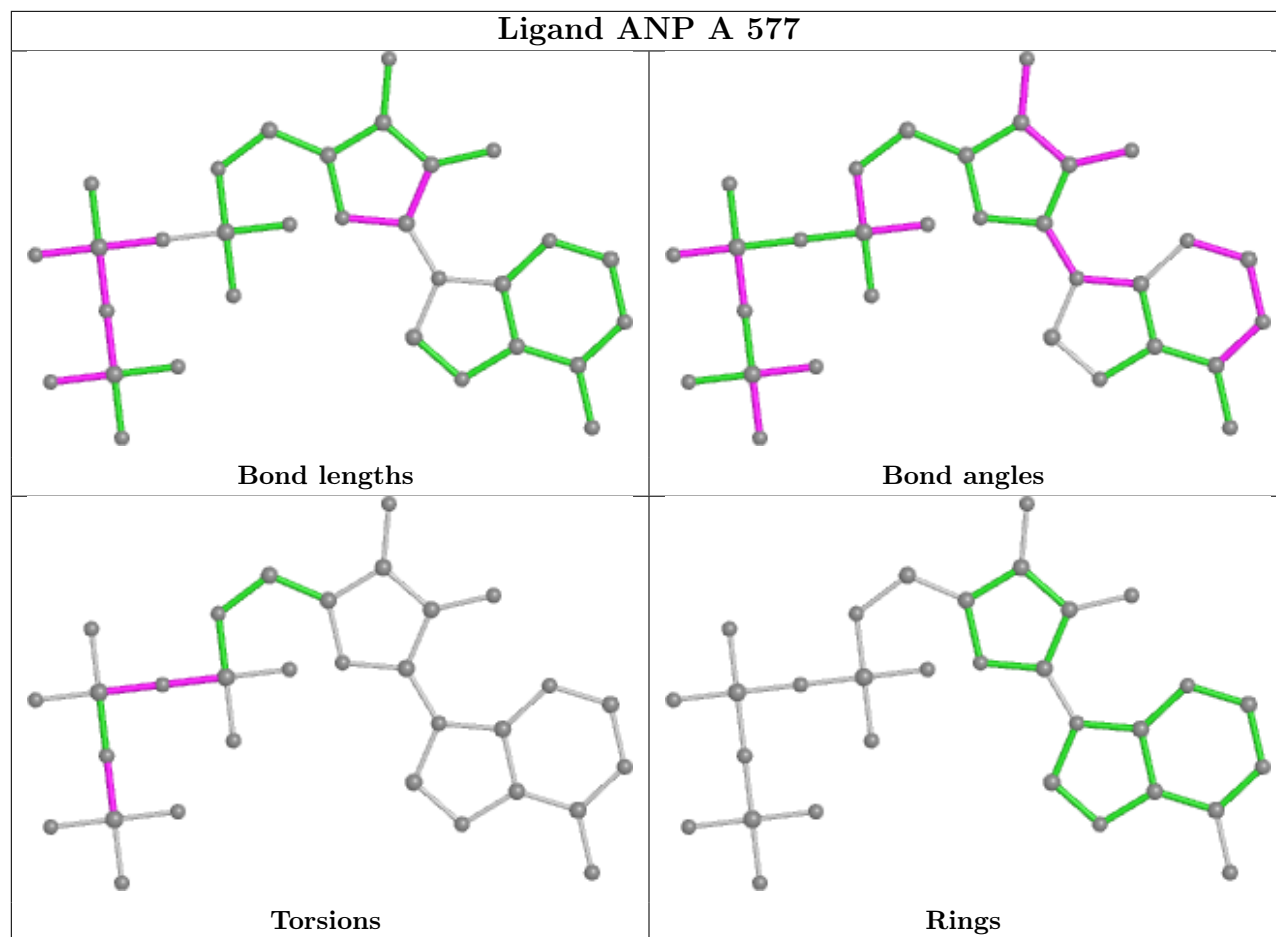
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	577	ANP	2	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	495/576 (85%)	0.83	47 (9%) 8 5	56, 67, 85, 106	0
1	B	492/576 (85%)	1.37	117 (23%) 0 0	58, 68, 84, 111	0
All	All	987/1152 (85%)	1.10	164 (16%) 1 1	56, 68, 85, 111	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	473	TYR	13.9
1	B	391	LYS	9.3
1	B	222	ILE	7.3
1	B	281	ALA	6.9
1	B	282	GLY	6.7
1	B	387	GLN	6.0
1	B	535	PRO	5.8
1	B	258	ALA	5.6
1	A	470	GLN	5.5
1	B	129	CYS	5.5
1	A	474	CYS	5.5
1	B	392	ILE	5.4
1	A	469	PRO	5.4
1	A	140	ASP	5.3
1	B	138	CYS	5.2
1	A	530	ASP	5.1
1	B	394	ARG	5.1
1	B	342	ILE	4.9
1	B	44	GLU	4.9
1	B	396	GLU	4.8
1	B	278	MET	4.8
1	B	349	VAL	4.8
1	B	500	GLN	4.7
1	B	436	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	28	LYS	4.7
1	B	494	THR	4.5
1	B	103	ARG	4.5
1	A	14	LYS	4.4
1	B	375	LEU	4.4
1	B	530	ASP	4.3
1	B	121	VAL	4.3
1	B	257	ASP	4.3
1	B	104	ASN	4.2
1	B	399	ARG	4.2
1	A	95	ASP	4.2
1	B	356	VAL	4.1
1	B	493	PRO	4.1
1	B	344	GLY	4.0
1	B	139	LYS	3.9
1	B	223	LYS	3.9
1	B	357	VAL	3.8
1	A	473	TYR	3.8
1	B	110	LEU	3.7
1	B	470	GLN	3.7
1	B	24	LYS	3.6
1	B	130	THR	3.6
1	A	373	CYS	3.6
1	B	86	GLY	3.6
1	A	135	GLN	3.6
1	B	165	ILE	3.6
1	A	494	THR	3.5
1	B	166	TYR	3.5
1	B	14	LYS	3.5
1	B	386	GLN	3.5
1	A	128	ASN	3.5
1	B	220	LYS	3.4
1	B	125	LEU	3.3
1	A	277	HIS	3.3
1	A	472	ILE	3.3
1	B	277	HIS	3.3
1	B	43	GLU	3.2
1	B	140	ASP	3.2
1	B	371	LEU	3.2
1	B	534	PRO	3.2
1	A	262	VAL	3.2
1	B	468	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	495	ASP	3.2
1	B	48	SER	3.2
1	B	385	PHE	3.2
1	B	317	ILE	3.2
1	B	471	ALA	3.2
1	B	227	GLY	3.2
1	B	492	GLU	3.1
1	B	30	TRP	3.1
1	B	111	SER	3.1
1	B	351	TYR	3.1
1	B	228	GLU	3.1
1	B	309	TYR	3.0
1	B	372	GLY	3.0
1	B	464	PRO	3.0
1	A	125	LEU	2.9
1	B	368	TRP	2.9
1	B	273	PHE	2.9
1	B	137	PRO	2.9
1	A	256	LYS	2.9
1	A	370	ALA	2.9
1	B	407	GLU	2.9
1	B	45	LEU	2.8
1	B	441	GLU	2.8
1	B	373	CYS	2.8
1	B	99	LYS	2.8
1	A	279	GLY	2.8
1	A	16	ARG	2.8
1	B	345	ARG	2.8
1	A	493	PRO	2.8
1	B	112	HIS	2.8
1	A	213	ALA	2.8
1	B	469	PRO	2.7
1	B	370	ALA	2.7
1	B	393	LYS	2.7
1	A	496	GLN	2.7
1	B	529	LEU	2.7
1	A	372	GLY	2.7
1	A	226	LYS	2.7
1	B	437	GLY	2.6
1	B	66	LEU	2.6
1	A	465	PHE	2.6
1	B	275	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	44	GLU	2.6
1	A	468	ASP	2.6
1	A	165	ILE	2.6
1	A	214	CYS	2.5
1	A	410	GLU	2.5
1	B	202	ALA	2.5
1	B	432	LEU	2.5
1	B	51	ARG	2.5
1	B	122	PRO	2.5
1	B	224	LYS	2.4
1	B	369	TRP	2.4
1	B	362	TYR	2.4
1	B	343	LYS	2.4
1	B	315	GLU	2.4
1	A	143	GLN	2.4
1	A	374	LEU	2.4
1	B	472	ILE	2.4
1	A	24	LYS	2.4
1	B	466	LYS	2.4
1	B	148	LEU	2.3
1	B	359	ASN	2.3
1	B	527	PHE	2.3
1	B	49	LEU	2.3
1	A	124	GLN	2.3
1	B	379	ILE	2.3
1	B	397	VAL	2.3
1	B	268	GLY	2.3
1	B	87	VAL	2.3
1	A	169	ARG	2.3
1	A	136	GLY	2.2
1	B	467	PRO	2.2
1	B	433	GLY	2.2
1	B	94	PRO	2.2
1	B	16	ARG	2.2
1	B	532	SER	2.2
1	B	423	LEU	2.2
1	A	368	TRP	2.2
1	A	497	ASP	2.2
1	B	15	ALA	2.2
1	B	190	ARG	2.2
1	B	295	ILE	2.2
1	B	324	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	127	THR	2.2
1	B	169	ARG	2.2
1	A	258	ALA	2.1
1	A	351	TYR	2.1
1	A	263	LEU	2.1
1	B	321	ASP	2.1
1	A	203	CYS	2.1
1	A	317	ILE	2.1
1	B	34	LEU	2.1
1	A	390	LYS	2.1
1	B	113	THR	2.1
1	B	100	ALA	2.1
1	A	495	ASP	2.1
1	B	354	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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.

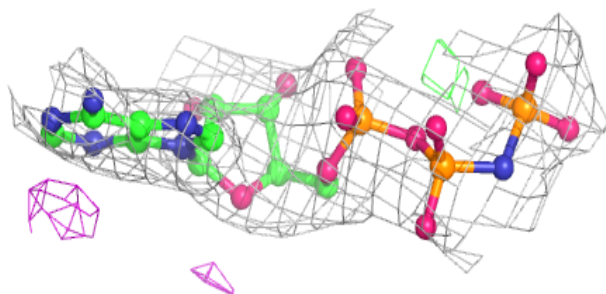
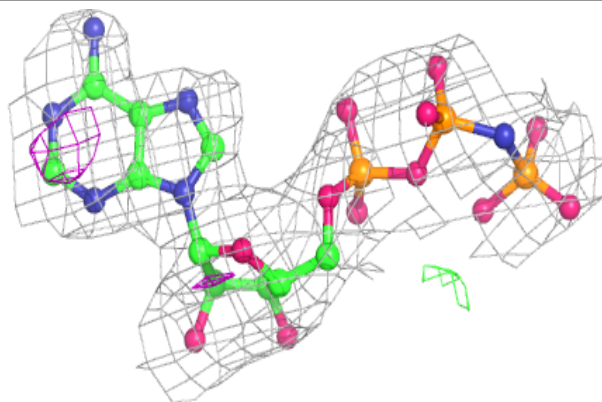
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	B	578	1/1	0.73	0.25	87,87,87,87	0
3	PO4	A	579	5/5	0.83	0.34	83,83,87,87	0
3	PO4	B	579	5/5	0.89	0.31	91,93,95,97	0
2	MG	A	578	1/1	0.90	0.16	92,92,92,92	0
4	ANP	B	577	31/31	0.90	0.16	60,63,92,93	0
4	ANP	A	577	31/31	0.91	0.19	60,65,103,105	0

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.

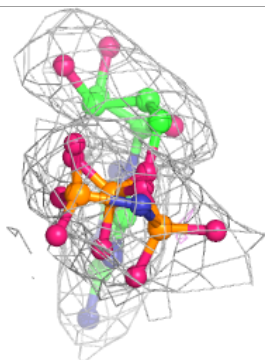
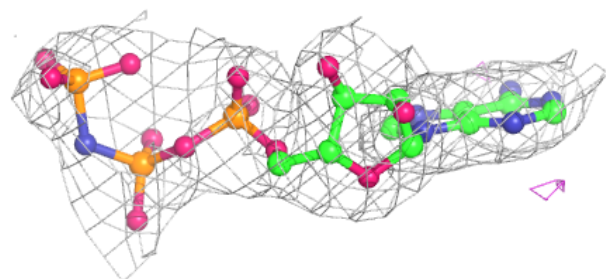
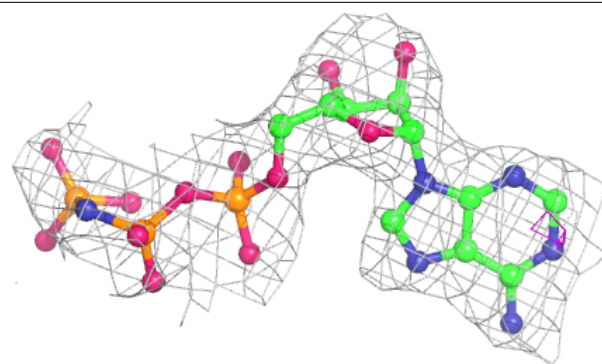
Electron density around ANP B 577:

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



Electron density around ANP A 577:

$2mF_o-DF_c$ (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.