



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:33 AM EDT

PDB ID : 2ACX / pdb_00002acx
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

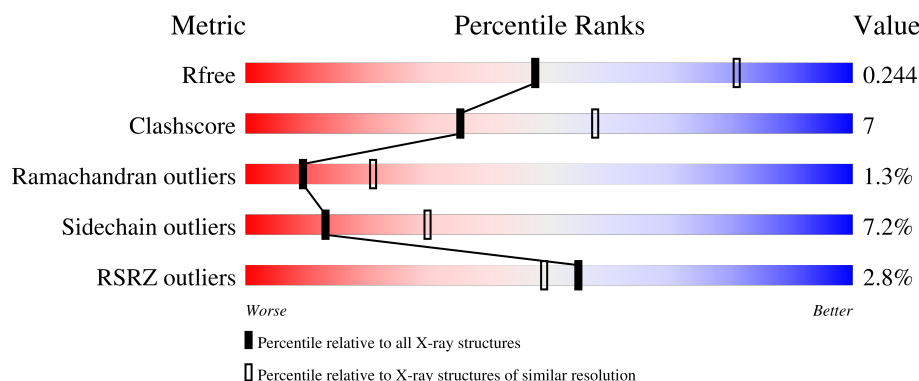
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

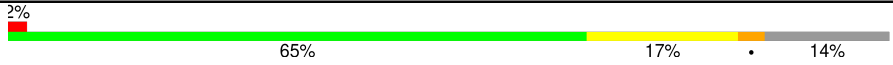
The reported resolution of this entry is 2.60 Å.

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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	
1	B	576	

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			

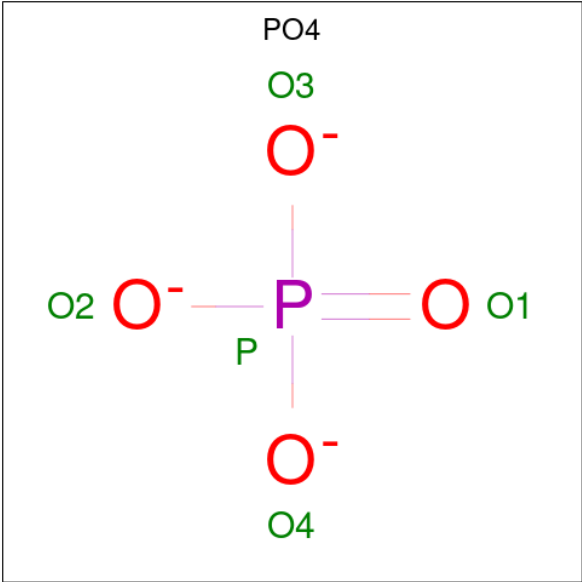
There are 10 discrepancies between the modelled and reference sequences:

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 (CCD ID: MG) (formula: Mg).

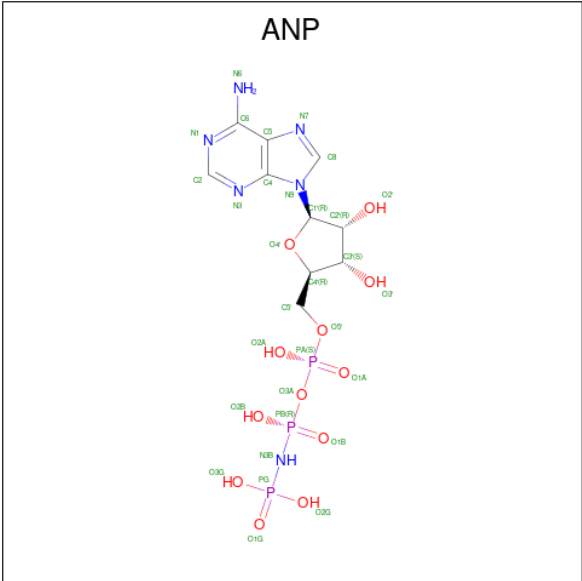
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: 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 (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

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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		

GLY	GLN	PRO	ALA	PRO	LYS	GLY	LEU	GLN	ARG	LEU	PHE	SER	ARG	GLN	ASP	SER	SER	GLY	ASN	SER	SER	ASP	SER	GLU	GLU	LEU	PRO	THR	ARG	LEU
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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) 97.2 (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 (4.91%)	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)	0.31 , 76.5	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	0.94	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: ANP, PO4, 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	1.26	4/4101 (0.1%)	1.17	11/5521 (0.2%)
1	B	0.90	0/4074	1.02	2/5488 (0.0%)
All	All	1.10	4/8175 (0.0%)	1.10	13/11009 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	427	ASP	N-CA	5.63	1.52	1.46
1	A	362	TYR	CA-CB	5.57	1.63	1.53
1	A	308	VAL	CA-CB	-5.53	1.47	1.54
1	A	347	GLY	C-O	-5.16	1.18	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	SER	CB-CA-C	-7.70	106.63	115.79
1	A	168	ASN	N-CA-C	-7.31	103.25	111.07
1	A	404	VAL	CA-C-O	6.60	123.60	119.51
1	A	355	GLU	CB-CA-C	-6.48	99.99	110.74
1	A	349	VAL	N-CA-C	6.05	116.71	110.36
1	A	384	PRO	N-CA-C	5.83	121.14	113.86
1	A	336	VAL	CB-CA-C	-5.64	104.70	111.18
1	A	257	ASP	N-CA-C	5.55	120.05	113.28
1	B	404	VAL	N-CA-C	5.43	114.07	107.61
1	A	449	LYS	CB-CA-C	-5.28	99.91	110.42
1	A	397	VAL	CB-CA-C	-5.21	105.11	112.14
1	A	404	VAL	N-CA-C	5.05	113.62	107.61
1	B	258	ALA	N-CA-C	5.03	115.95	108.60

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	67	0
1	B	3984	0	3974	57	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	1	0
5	A	30	0	0	2	0
5	B	7	0	0	0	0
All	All	8106	0	8008	119	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 7.

All (119) 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
1:B:319:LEU:HD22	1:B:325:ILE:HG22	1.58	0.84
1:A:325:ILE:C	1:A:325:ILE:HD12	2.11	0.76
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:A:511:TRP:CZ2	1:A:515:MET:HE3	2.25	0.72
1:B:106:THR:HG22	1:B:110:LEU:HD12	1.72	0.71
1:B:352:MET:HE2	1:B:357:VAL:HG12	1.73	0.69
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:B:325:ILE:HD12	1:B:325:ILE:C	2.21	0.65
1:A:314:PRO:HG3	1:A:374:LEU:HD13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD22	1:A:325:ILE:HG22	1.78	0.64
1:B:278:MET:HA	1:B:278:MET:HE2	1.80	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:473:TYR:HD2	1:A:473:TYR:N	2.00	0.59
1:B:511:TRP:CZ2	1:B:515:MET:HE3	2.37	0.59
1:B:210:LYS:NZ	1:B:517:GLU:OE1	2.33	0.58
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:B:320:ASP:OD1	1:B:320:ASP:C	2.48	0.56
1:A:278:MET:HE3	1:A:278:MET:HA	1.86	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:45:LEU:O	1:A:46:ARG:C	2.49	0.55
1:B:266:MET:HE2	1:B:326:ARG:HB2	1.88	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:527:PHE:C	1:A:527:PHE:CD1	2.87	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: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:B:313:LYS:HB2	1:B:314:PRO:HD2	1.94	0.50
1:A:502:PHE:CD2	1:A:502:PHE:C	2.90	0.50
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
1:A:409:SER:C	1:A:411:ARG:H	2.21	0.48
4:B:577:ANP:O3A	4:B:577:ANP:O2G	2.31	0.48
1:A:40:SER:OG	1:B:163:ASP:OD2	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:33:MET:HE3	1:A:207:ALA:HA	1.95	0.48
1:A:244:ARG:HD2	1:A:457:GLY:O	2.13	0.48
1:B:230:MET:HE3	1:B:230:MET:C	2.39	0.48
1:B:352:MET:CE	1:B:357:VAL:HG12	2.41	0.48
1:B:60:ASN:HB3	1:B:512:GLN:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LYS:NZ	1:B:234:GLU:OE2	2.44	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:285:GLU:O	1:A:286:ALA:C	2.56	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:27:SER:HB3	1:A:33:MET:HE1	1.96	0.46
1:A:86:GLY:HA3	1:A:105:LEU:HD21	1.97	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:B:230:MET:HE3	1:B:230:MET:O	2.17	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:30:TRP:HA	1:A:33:MET:HE3	1.98	0.44
1:A:208:THR:HB	1:A:518:THR:HG21	2.00	0.44
1:B:311:ASP:OD2	1:B:316:ASN:ND2	2.50	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:A:345:ARG:HG2	1:A:356:VAL:O	2.18	0.43
1:A:30:TRP:HA	1:A:33:MET:HE2	2.01	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: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:A:325:ILE:C	1:A:325:ILE:CD1	2.84	0.42
1:B:518:THR:O	1:B:519:GLU:HB2	2.18	0.42
1:A:352:MET:HE2	1:A:357:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ASN:N	1:B:168:ASN:HD22	2.17	0.42
1:B:527:PHE:C	1:B:527:PHE:CD2	2.97	0.42
1:B:195:GLY:O	1:B:197:PHE:N	2.53	0.42
1:B:285:GLU:O	1:B:286:ALA:C	2.63	0.42
1:B:502:PHE:CD2	1:B:502:PHE:C	2.98	0.42
1:B:45:LEU:O	1:B:46:ARG:C	2.60	0.41
1:B:312:LEU:HB3	1:B:370:ALA:CB	2.51	0.41
1:B:448:PHE:O	1:B:449:LYS:C	2.62	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:HZ1	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:144:GLU:OE1	1:A:144:GLU:HA	2.20	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 [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	489/576 (85%)	458 (94%)	24 (5%)	7 (1%)	9 19
1	B	482/576 (84%)	459 (95%)	17 (4%)	6 (1%)	10 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	971/1152 (84%)	917 (94%)	41 (4%)	13 (1%)	9	21

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	LEU
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%)	399 (92%)	33 (8%)	12	27
1	B	430/503 (86%)	401 (93%)	29 (7%)	15	33
All	All	862/1006 (86%)	800 (93%)	62 (7%)	13	30

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

Mol	Chain	Res	Type
1	A	27	SER
1	A	48	SER
1	A	60	ASN
1	A	78	SER
1	A	96	ASP

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Mol	Chain	Res	Type
1	A	104	ASN
1	A	106	THR
1	A	123	ARG
1	A	125	LEU
1	A	130	THR
1	A	135	GLN
1	A	138	CYS
1	A	169	ARG
1	A	199	GLU
1	A	255	THR
1	A	267	ASN
1	A	277	HIS
1	A	278	MET
1	A	280	GLN
1	A	357	VAL
1	A	359	ASN
1	A	374	LEU
1	A	382	GLN
1	A	390	LYS
1	A	396	GLU
1	A	411	ARG
1	A	435	ARG
1	A	472	ILE
1	A	473	TYR
1	A	474	CYS
1	A	494	THR
1	A	500	GLN
1	A	527	PHE
1	B	46	ARG
1	B	48	SER
1	B	60	ASN
1	B	89	GLU
1	B	98	ARG
1	B	107	GLN
1	B	121	VAL
1	B	125	LEU
1	B	134	GLU
1	B	146	THR
1	B	147	ARG
1	B	230	MET
1	B	257	ASP
1	B	278	MET

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Mol	Chain	Res	Type
1	B	317	ILE
1	B	319	LEU
1	B	342	ILE
1	B	345	ARG
1	B	346	VAL
1	B	355	GLU
1	B	374	LEU
1	B	394	ARG
1	B	395	GLU
1	B	407	GLU
1	B	421	SER
1	B	470	GLN
1	B	472	ILE
1	B	496	GLN
1	B	527	PHE

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	104	ASN
1	A	108	ASN
1	A	168	ASN
1	A	277	HIS
1	A	335	HIS
1	A	359	ASN
1	A	387	GLN
1	B	108	ASN
1	B	131	GLN
1	B	168	ASN
1	B	236	GLN
1	B	267	ASN
1	B	322	HIS
1	B	335	HIS
1	B	387	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	579	-	4,4,4	0.85	0	6,6,6	1.65	1 (16%)
4	ANP	A	577	2	33,33,33	2.25	9 (27%)	45,52,52	2.31	15 (33%)
3	PO4	B	579	-	4,4,4	0.74	0	6,6,6	1.56	1 (16%)
4	ANP	B	577	2	33,33,33	1.97	9 (27%)	45,52,52	2.22	15 (33%)

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	A	577	2	-	3/18/38/38	0/3/3/3
4	ANP	B	577	2	-	3/18/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	577	ANP	PB-O3A	5.87	1.66	1.59
4	A	577	ANP	PG-O1G	4.59	1.53	1.46
4	A	577	ANP	PG-N3B	4.59	1.75	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	577	ANP	PG-N3B	4.58	1.75	1.63
4	B	577	ANP	PB-N3B	4.19	1.74	1.63
4	A	577	ANP	PB-O1B	4.19	1.52	1.46
4	A	577	ANP	PB-N3B	4.15	1.74	1.63
4	A	577	ANP	PA-O3A	4.05	1.63	1.59
4	B	577	ANP	C5-C4	3.98	1.46	1.39
4	B	577	ANP	PG-O1G	3.78	1.51	1.46
4	B	577	ANP	PB-O1B	2.98	1.50	1.46
4	B	577	ANP	C5-C6	2.93	1.49	1.41
4	A	577	ANP	C5-C4	2.88	1.44	1.39
4	B	577	ANP	PB-O3A	2.69	1.62	1.59
4	B	577	ANP	C5-N7	-2.38	1.34	1.39
4	A	577	ANP	C4-N9	-2.23	1.33	1.37
4	A	577	ANP	C5-N7	-2.12	1.35	1.39
4	B	577	ANP	PB-O2B	-2.08	1.51	1.56

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	577	ANP	C5-C4-N3	-6.42	117.87	126.72
4	A	577	ANP	N3-C2-N1	-5.55	120.18	128.58
4	B	577	ANP	N3-C4-N9	5.30	136.18	127.17
4	A	577	ANP	C5-C4-N3	-5.01	119.82	126.72
4	A	577	ANP	O1B-PB-N3B	-4.77	104.75	111.77
4	A	577	ANP	N3-C4-N9	4.64	135.06	127.17
4	B	577	ANP	C2-N3-C4	4.54	122.91	111.83
4	B	577	ANP	O1G-PG-N3B	-4.43	105.24	111.77
4	A	577	ANP	C4-N9-C8	4.21	110.16	105.74
4	A	577	ANP	C2-N3-C4	4.19	122.05	111.83
4	B	577	ANP	N3-C2-N1	-3.98	122.55	128.58
4	A	577	ANP	O2G-PG-O3G	3.91	118.11	107.59
4	B	577	ANP	O2B-PB-O1B	3.58	117.56	109.87
4	B	577	ANP	C4-C5-N7	-3.39	106.70	110.58
4	A	577	ANP	N9-C8-N7	-3.38	109.14	113.94
4	A	577	ANP	C5-N7-C8	3.07	108.27	103.45
4	B	577	ANP	C5-N7-C8	2.91	108.02	103.45
4	A	577	ANP	C4-C5-N7	-2.82	107.36	110.58
4	A	577	ANP	C2-N1-C6	2.78	123.29	118.73
4	B	577	ANP	O2G-PG-O3G	2.77	115.03	107.59
4	B	577	ANP	O1B-PB-N3B	-2.75	107.72	111.77
4	A	577	ANP	C6-C5-N7	2.66	137.22	132.09
3	A	579	PO4	O4-P-O2	2.65	116.17	107.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	577	ANP	C4-N9-C8	2.65	108.52	105.74
4	A	577	ANP	O3'-C3'-C2'	-2.38	104.18	111.82
4	B	577	ANP	C6-C5-N7	2.26	136.44	132.09
4	B	577	ANP	N9-C8-N7	-2.21	110.81	113.94
4	B	577	ANP	O2A-PA-O1A	2.19	122.65	112.44
4	A	577	ANP	O2'-C2'-C3'	-2.17	104.87	111.82
4	B	577	ANP	O4'-C1'-N9	2.11	112.15	108.09
4	A	577	ANP	O2A-PA-O5'	-2.11	98.01	107.57
3	B	579	PO4	O3-P-O2	2.08	114.40	107.91

There are no chirality outliers.

All (6) torsion outliers are listed below:

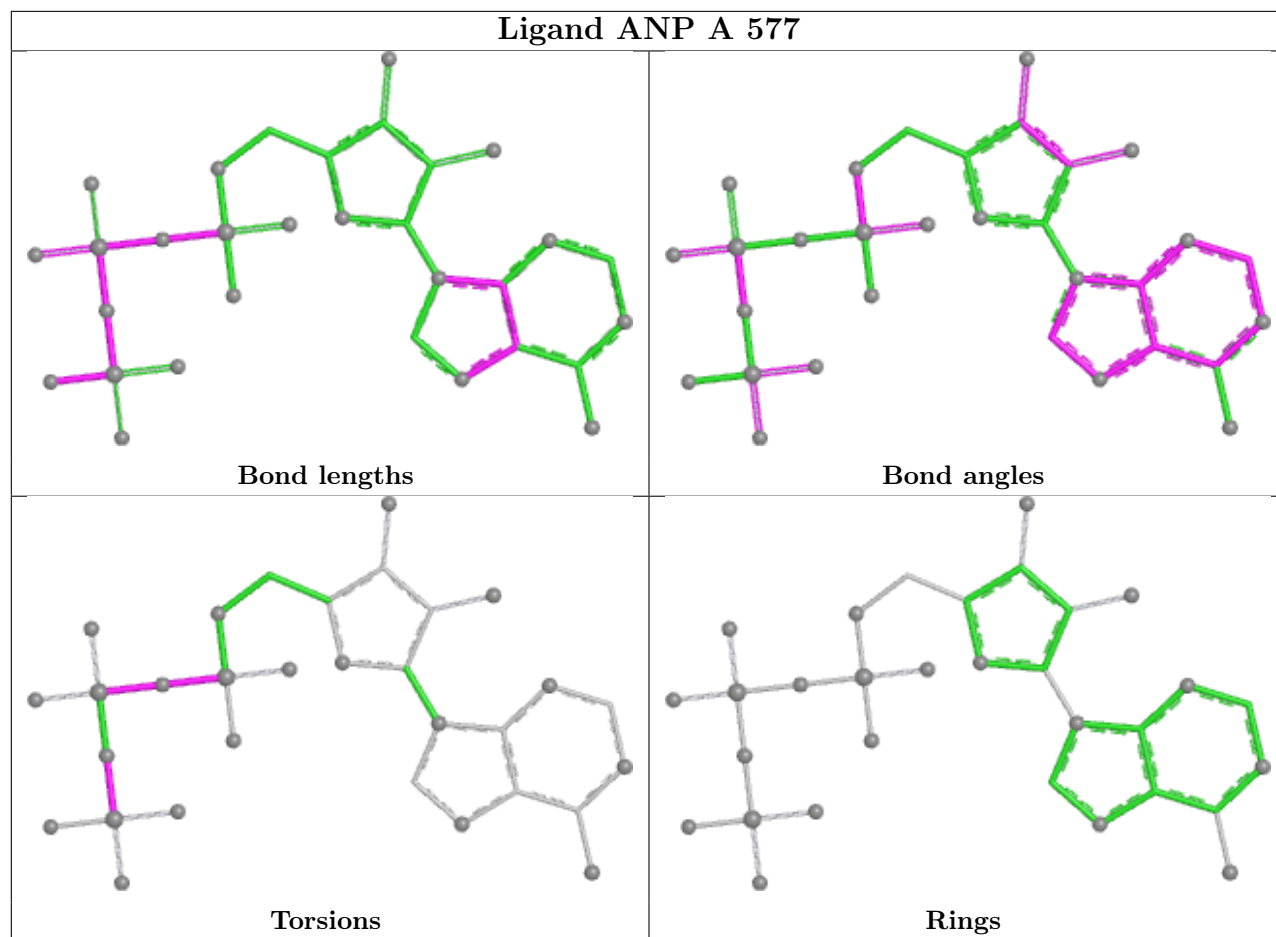
Mol	Chain	Res	Type	Atoms
4	A	577	ANP	PB-N3B-PG-O1G
4	A	577	ANP	PA-O3A-PB-O2B
4	B	577	ANP	PB-N3B-PG-O1G
4	B	577	ANP	C4'-C5'-O5'-PA
4	B	577	ANP	PG-N3B-PB-O1B
4	A	577	ANP	PB-O3A-PA-O1A

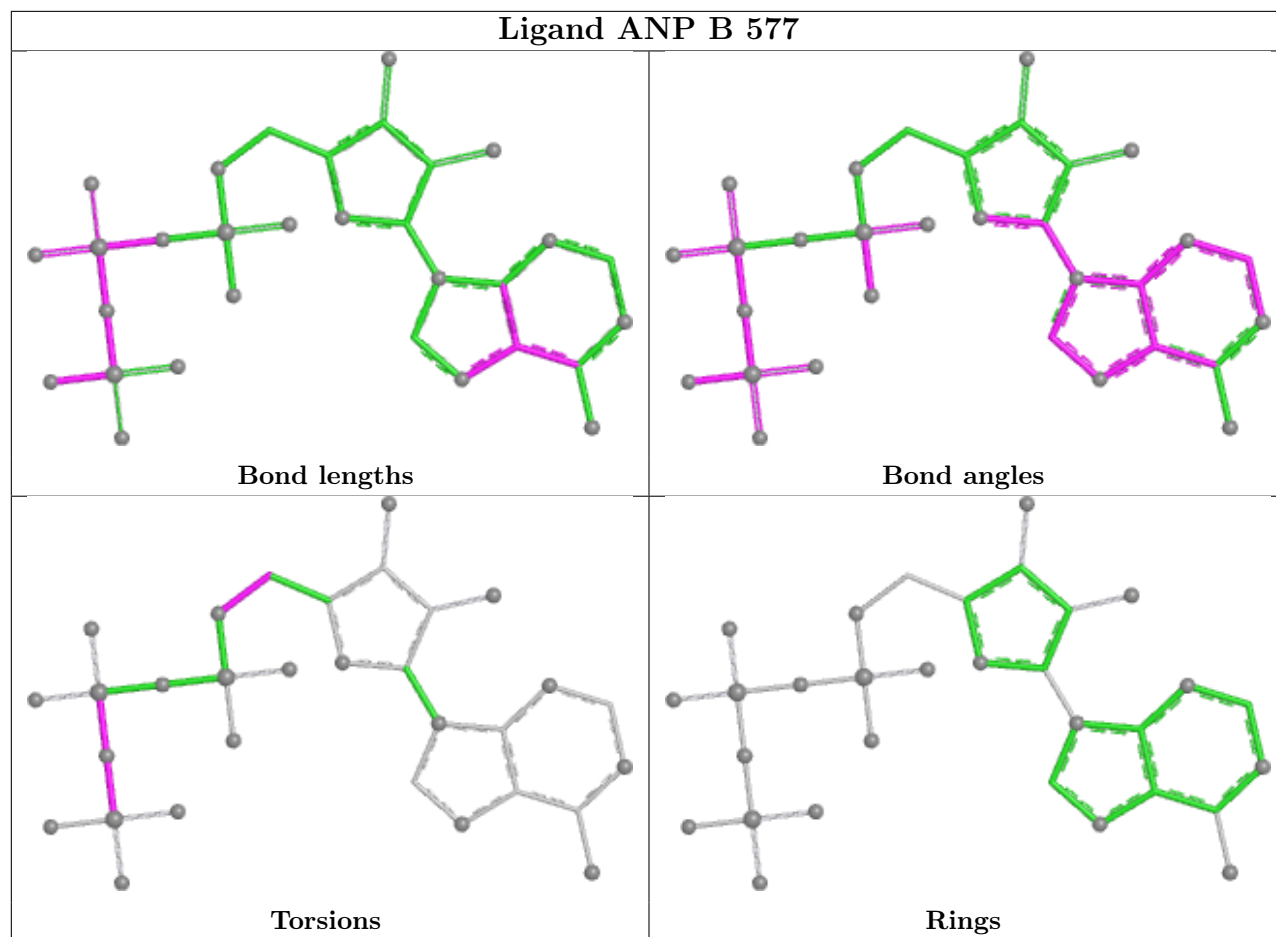
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	577	ANP	1	0

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

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	495/576 (85%)	0.07	9 (1%) 67 63	56, 67, 85, 106	0
1	B	492/576 (85%)	0.37	19 (3%) 43 38	58, 68, 84, 111	0
All	All	987/1152 (85%)	0.22	28 (2%) 55 49	56, 68, 85, 111	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	473	TYR	4.4
1	B	472	ILE	3.7
1	B	531	GLY	3.3
1	B	533	VAL	3.0
1	B	471	ALA	2.7
1	A	470	GLN	2.6
1	B	278	MET	2.5
1	B	289	VAL	2.4
1	A	277	HIS	2.4
1	A	14	LYS	2.4
1	B	414	PRO	2.4
1	A	529	LEU	2.3
1	B	277	HIS	2.3
1	A	16	ARG	2.3
1	A	531	GLY	2.3
1	A	15	ALA	2.3
1	B	269	GLY	2.3
1	A	469	PRO	2.2
1	B	528	GLY	2.2
1	B	350	GLY	2.2
1	B	224	LYS	2.1
1	B	331	GLY	2.1
1	B	385	PHE	2.1
1	B	535	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	281	ALA	2.1
1	B	469	PRO	2.0
1	B	15	ALA	2.0
1	B	16	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

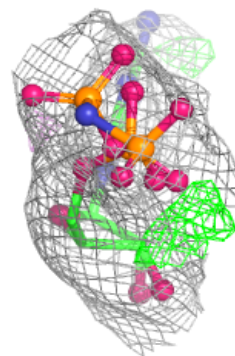
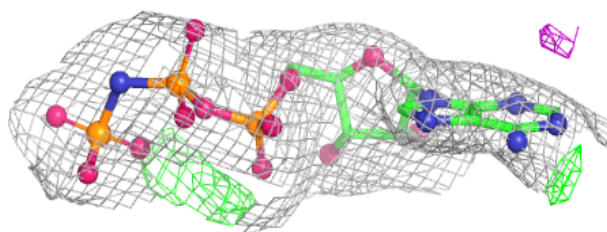
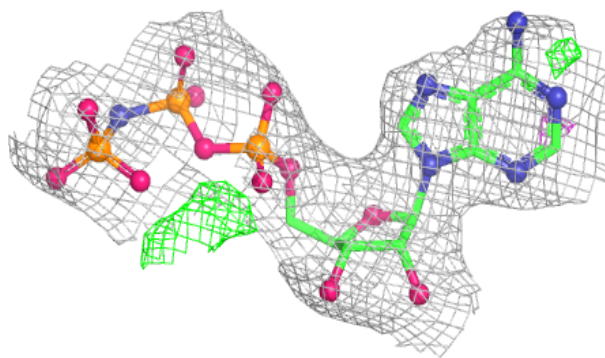
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	578	1/1	0.53	0.24	87,87,87,87	0
2	MG	A	578	1/1	0.87	0.10	92,92,92,92	0
3	PO4	B	579	5/5	0.89	0.17	91,93,95,97	0
3	PO4	A	579	5/5	0.90	0.19	83,83,87,87	0
4	ANP	B	577	31/31	0.93	0.08	60,63,92,93	0
4	ANP	A	577	31/31	0.95	0.07	60,65,103,105	0

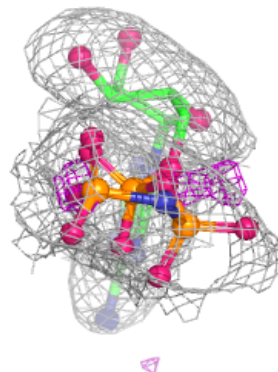
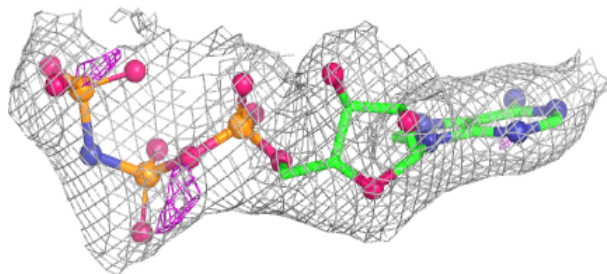
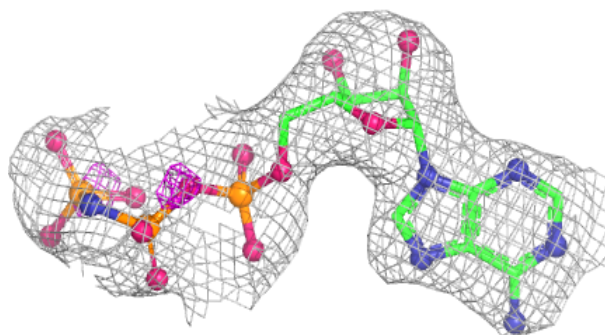
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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