



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:34 AM UTC

PDB ID : 3NYO / pdb_00003nyo
Title : Crystal Structure of G Protein-Coupled Receptor Kinase 6 in Complex with AMP
Authors : Tesmer, J.J.G.; Singh, P.
Deposited on : 2010-07-15
Resolution : 2.92 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

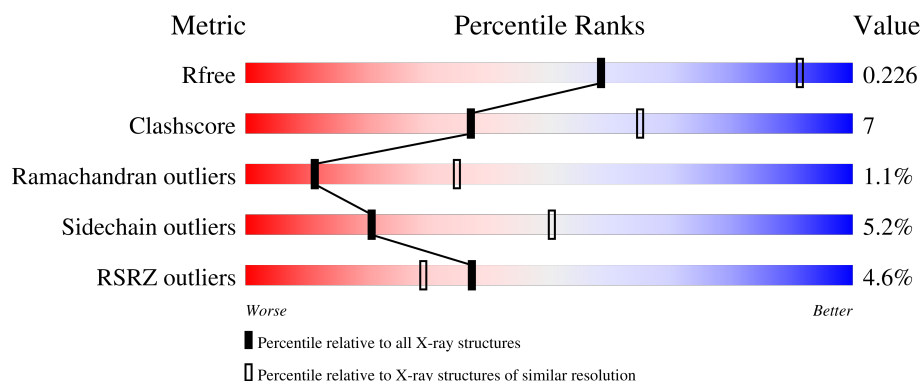
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	5% 76% 19% • •
1	B	576	4% 74% 21% • •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9039 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.

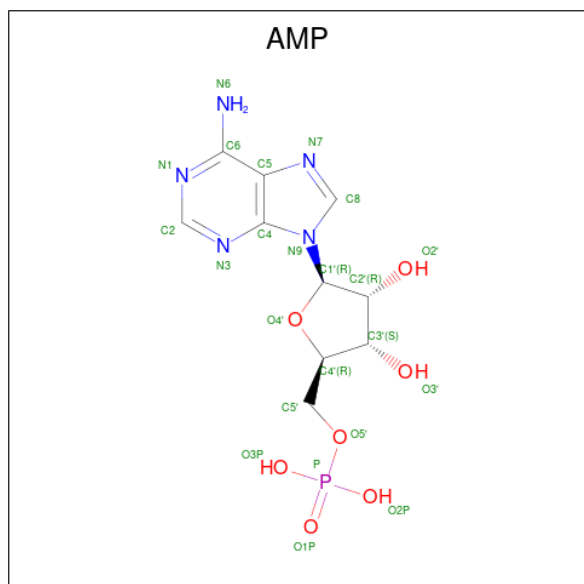
- Molecule 1 is a protein called G protein-coupled receptor kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4454	2834	785	807	28			
1	B	554	Total	C	N	O	S	0	0	0
			4454	2834	785	807	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ACE	-	acetylation	UNP P43250
B	1	ACE	-	acetylation	UNP P43250

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



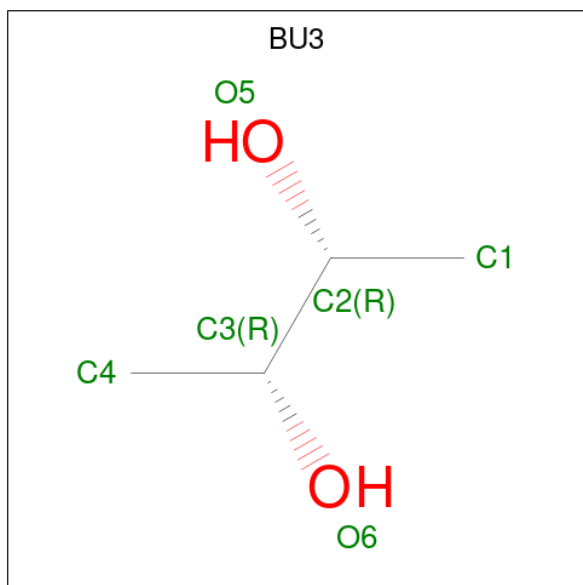
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is (R,R)-2,3-BUTANEDIOL (CCD ID: BU3) (formula: C₄H₁₀O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	2	Total	O	0	0
			2	2		

D538		A545 P546	S557	ARG	GLN	ASP	CYS	CYS	GLY	ASN	CYS	SER	ASP	SER	GLU	GLU	GLU	LEU	PRO	THR	ARG	LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	154.57Å 154.57Å 208.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.92 30.00 – 2.92	Depositor EDS
% Data completeness (in resolution range)	56.2 (30.00-2.92) 56.3 (30.00-2.92)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.14 (at 2.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.222 , 0.253 0.222 , 0.226	Depositor DCC
R_{free} test set	1797 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å ²)	70.3	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9039	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, AMP, BU3, SO4

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	0.47	0/4553	0.81	3/6140 (0.0%)
1	B	0.44	0/4553	0.81	1/6140 (0.0%)
All	All	0.45	0/9106	0.81	4/12280 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	PRO	CA-C-N	5.85	125.86	119.89
1	A	534	PRO	C-N-CA	5.85	125.86	119.89
1	A	411	ARG	N-CA-C	-5.62	108.22	114.62
1	B	362	TYR	N-CA-C	5.01	116.69	109.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4454	0	4462	63	0
1	B	4454	0	4462	69	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
3	A	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	6	0	0	0	0
5	B	2	0	0	0	0
All	All	9039	0	8964	128	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 (128) 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:B:8:ALA:HB1	1:B:190:ARG:HB3	1.69	0.74
1:B:294:GLU:OE1	1:B:325:ILE:HG13	1.92	0.69
1:A:511:TRP:CZ2	1:A:515:MET:HE3	2.30	0.66
1:B:215:LYS:NZ	1:B:329:ASP:OD1	2.28	0.65
1:A:75:PRO:O	1:A:79:ARG:HG2	1.97	0.64
1:B:511:TRP:CE2	1:B:515:MET:HE3	2.33	0.63
1:B:511:TRP:CZ2	1:B:515:MET:HE3	2.33	0.63
1:A:365:SER:HA	1:A:434:CYS:SG	2.39	0.62
1:A:259:LEU:HB3	1:A:502:PHE:CE2	2.34	0.62
1:A:3:LEU:O	1:A:7:VAL:HG23	2.00	0.61
1:A:211:MET:HE3	1:A:211:MET:HA	1.84	0.60
1:B:293:ALA:O	1:B:296:CYS:HB3	2.01	0.60
1:B:509:ILE:HD12	1:B:509:ILE:H	1.66	0.60
1:B:251:TYR:HH	1:B:511:TRP:CD1	2.19	0.59
1:B:311:ASP:HB2	1:B:332:LEU:HD12	1.87	0.56
1:B:511:TRP:O	1:B:514:GLU:HB3	2.05	0.56
1:A:522:GLN:O	1:A:526:VAL:HG12	2.07	0.55
1:B:527:PHE:CD1	1:B:527:PHE:C	2.85	0.55
1:A:446:PRO:O	1:A:449:LYS:HG3	2.07	0.55
1:B:259:LEU:HB3	1:B:502:PHE:CE2	2.41	0.54
1:B:309:TYR:OH	1:B:328:SER:O	2.24	0.54
1:A:272:LYS:HD2	1:A:315:GLU:HG3	1.90	0.54
1:A:266:MET:HE2	1:A:326:ARG:HB2	1.91	0.54
1:A:38:HIS:HB3	1:B:163:ASP:CG	2.33	0.53
1:B:538:ASP:OD1	1:B:538:ASP:C	2.52	0.52
1:B:374:LEU:HD23	1:B:378:MET:HE2	1.91	0.52
1:A:313:LYS:HB2	1:A:314:PRO:CD	2.40	0.52
1:A:3:LEU:HG	1:A:4:GLU:N	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ILE:CG2	1:B:166:TYR:N	2.72	0.51
1:A:363:THR:OG1	1:A:364:PHE:N	2.40	0.51
1:A:355:GLU:OE2	1:A:355:GLU:N	2.33	0.51
1:B:419:LEU:HB2	1:B:445:HIS:CE1	2.46	0.51
1:A:294:GLU:OE1	1:A:325:ILE:HG13	2.09	0.51
1:A:509:ILE:HD12	1:A:509:ILE:H	1.76	0.51
1:B:184:ASN:O	1:B:206:ARG:HD3	2.10	0.50
1:A:62:ILE:HG13	1:A:512:GLN:HB3	1.94	0.50
1:B:507:VAL:O	1:B:510:PRO:HD2	2.12	0.50
1:A:8:ALA:HB1	1:A:190:ARG:HB3	1.94	0.49
1:B:2:GLU:HG3	1:B:6:ILE:HD11	1.94	0.49
1:B:38:HIS:HB2	1:B:41:GLN:HG3	1.93	0.49
1:A:161:TYR:CD2	1:A:161:TYR:C	2.91	0.49
1:B:190:ARG:NH1	1:B:191:VAL:O	2.46	0.48
1:B:60:GLN:O	1:B:63:GLY:N	2.46	0.48
1:B:309:TYR:CZ	1:B:327:ILE:HG23	2.48	0.48
1:B:76:GLU:HG2	1:B:77:LEU:N	2.28	0.48
1:B:64:ARG:O	1:B:68:ARG:HG3	2.14	0.48
1:A:2:GLU:O	1:A:3:LEU:C	2.57	0.48
1:A:6:ILE:H	1:A:6:ILE:HG13	1.32	0.48
1:B:437:GLY:O	1:B:440:ARG:HB2	2.13	0.48
1:B:299:LEU:HD22	1:B:367:ASP:HB3	1.95	0.47
1:B:375:LEU:HA	1:B:378:MET:HE3	1.94	0.47
1:A:60:GLN:O	1:A:63:GLY:N	2.48	0.47
1:A:190:ARG:NH1	1:A:191:VAL:O	2.48	0.47
1:B:53:TYR:CD1	1:B:154:SER:HA	2.50	0.47
1:B:74:ARG:HA	1:B:75:PRO:HD2	1.70	0.46
1:A:103:ARG:HH21	1:A:134:GLU:HG3	1.80	0.46
1:B:49:LEU:HD11	1:B:174:LYS:HG2	1.97	0.46
1:A:211:MET:HA	1:A:211:MET:CE	2.45	0.46
1:B:306:ARG:HH21	1:B:336:VAL:HG12	1.80	0.46
1:A:52:ASP:OD2	1:A:55:SER:HB2	2.16	0.46
1:B:292:ALA:HB2	1:B:375:LEU:HD13	1.98	0.46
1:B:312:LEU:HB3	1:B:370:ALA:HB1	1.98	0.45
1:A:507:VAL:O	1:A:510:PRO:HD2	2.16	0.45
1:B:509:ILE:HB	1:B:510:PRO:HD3	1.98	0.45
1:B:62:ILE:O	1:B:63:GLY:C	2.58	0.45
1:B:60:GLN:HA	1:B:61:PRO:HD2	1.84	0.45
1:A:27:SER:O	1:A:30:TRP:HD1	2.00	0.45
1:A:267:ASN:HB2	1:A:321:ASP:OD1	2.17	0.45
1:B:274:HIS:HB3	1:B:283:PHE:HZ	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:VAL:HG22	1:A:215:LYS:HA	1.99	0.45
1:A:511:TRP:O	1:A:514:GLU:HB3	2.16	0.44
1:B:273:PHE:CE1	1:B:474:CYS:HA	2.53	0.44
1:A:30:TRP:CD1	1:A:30:TRP:H	2.34	0.44
1:B:334:VAL:HG22	1:B:335:HIS:H	1.82	0.44
1:B:52:ASP:O	1:B:53:TYR:C	2.61	0.44
1:B:309:TYR:OH	1:B:316:ASN:HB3	2.17	0.44
1:A:294:GLU:HB3	1:A:325:ILE:HD11	2.00	0.44
1:B:6:ILE:H	1:B:6:ILE:HG13	1.37	0.43
1:B:169:ARG:HD2	1:B:172:GLN:OE1	2.17	0.43
1:A:37:PRO:HG3	1:A:175:TRP:CG	2.53	0.43
1:A:80:CYS:O	1:A:83:PHE:HB3	2.17	0.43
1:A:366:PRO:O	1:A:369:TRP:HB3	2.17	0.43
1:B:30:TRP:O	1:B:33:MET:N	2.52	0.43
1:A:509:ILE:HG22	1:A:513:ASN:HD21	1.83	0.43
1:B:192:LEU:HD11	1:B:202:ALA:HB2	2.00	0.43
1:A:311:ASP:CG	1:A:332:LEU:HD12	2.44	0.43
1:B:413:SER:HB2	1:B:414:PRO:HD2	2.01	0.43
1:B:509:ILE:HD12	1:B:509:ILE:N	2.33	0.43
1:A:165:ILE:HG23	1:A:166:TYR:N	2.34	0.43
1:B:43:GLU:OE1	1:B:43:GLU:HA	2.17	0.43
1:A:74:ARG:HA	1:A:75:PRO:HD2	1.91	0.43
1:A:106:THR:HA	1:A:110:LEU:HD12	2.00	0.43
1:A:413:SER:HB2	1:A:414:PRO:HD2	2.01	0.43
1:A:509:ILE:HB	1:A:510:PRO:HD3	2.00	0.42
1:B:212:TYR:HB3	1:B:262:VAL:CG1	2.49	0.42
1:A:60:GLN:HA	1:A:61:PRO:HD2	1.79	0.42
1:A:306:ARG:NH2	1:A:338:GLU:HA	2.35	0.42
1:B:165:ILE:HG22	1:B:166:TYR:N	2.34	0.42
1:B:68:ARG:NH2	1:B:85:ASP:OD2	2.52	0.42
1:A:433:GLY:N	1:A:441:GLU:OE1	2.47	0.42
1:A:527:PHE:HZ	1:B:169:ARG:HG2	1.85	0.42
1:B:446:PRO:O	1:B:449:LYS:HG3	2.20	0.42
1:A:23:ARG:O	1:A:25:GLY:N	2.53	0.42
1:B:508:PRO:HB2	1:B:509:ILE:HD12	2.02	0.42
1:B:213:ALA:HB2	1:B:265:LEU:HD12	2.00	0.42
1:A:151:GLU:O	1:A:155:VAL:HG23	2.20	0.42
1:A:177:GLU:HB3	1:A:511:TRP:CE3	2.54	0.42
1:A:285:GLU:O	1:A:286:ALA:C	2.63	0.42
1:A:37:PRO:HG3	1:A:175:TRP:CD2	2.55	0.41
1:A:517:GLU:C	1:A:519:GLU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LEU:HD11	1:B:529:LEU:HD11	2.02	0.41
1:B:291:TYR:O	1:B:292:ALA:C	2.62	0.41
1:A:4:GLU:O	1:A:7:VAL:HB	2.21	0.41
1:A:263:LEU:O	1:A:264:THR:C	2.63	0.41
1:B:445:HIS:HA	1:B:446:PRO:HD3	1.95	0.41
1:B:159:ALA:HA	1:B:162:LEU:HD12	2.01	0.41
1:A:77:LEU:O	1:A:78:SER:C	2.64	0.41
1:B:439:ALA:O	1:B:440:ARG:C	2.64	0.41
1:A:191:VAL:HA	1:A:201:CYS:HB3	2.03	0.41
1:B:37:PRO:HG3	1:B:175:TRP:CD2	2.56	0.41
1:A:156:ALA:HB3	1:A:157:PRO:HD3	2.03	0.41
1:B:545:ALA:HA	1:B:546:PRO:HA	1.96	0.41
1:A:251:TYR:HB2	1:A:262:VAL:CG2	2.51	0.40
1:B:171:LEU:HD23	1:B:171:LEU:HA	1.84	0.40
1:A:165:ILE:HD11	1:B:165:ILE:HG12	2.03	0.40
1:B:167:PHE:O	1:B:170:PHE:HB3	2.22	0.40
1:B:346:VAL:C	1:B:352:MET:HE3	2.45	0.40
1:A:125:LEU:HD22	1:A:144:GLU:HG2	2.04	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	550/576 (96%)	475 (86%)	66 (12%)	9 (2%)	7	25
1	B	550/576 (96%)	475 (86%)	72 (13%)	3 (0%)	24	53
All	All	1100/1152 (96%)	950 (86%)	138 (12%)	12 (1%)	11	35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	3	LEU
1	A	329	ASP
1	B	7	VAL
1	B	17	GLU
1	A	183	LYS
1	A	24	LYS
1	A	137	PRO
1	B	155	VAL
1	A	18	GLY
1	A	493	PRO
1	A	508	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	481/502 (96%)	459 (95%)	22 (5%)	24	56
1	B	481/502 (96%)	453 (94%)	28 (6%)	18	47
All	All	962/1004 (96%)	912 (95%)	50 (5%)	21	50

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	6	ILE
1	A	10	THR
1	A	22	ASN
1	A	48	SER
1	A	96	ASP
1	A	107	GLN
1	A	130	THR
1	A	133	LEU
1	A	140	ASP
1	A	161	TYR
1	A	190	ARG

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Mol	Chain	Res	Type
1	A	192	LEU
1	A	211	MET
1	A	307	ILE
1	A	313	LYS
1	A	342	ILE
1	A	365	SER
1	A	506	SER
1	A	527	PHE
1	A	529	LEU
1	A	533	VAL
1	B	6	ILE
1	B	10	THR
1	B	12	LEU
1	B	35	GLN
1	B	92	VAL
1	B	98	ARG
1	B	130	THR
1	B	133	LEU
1	B	140	ASP
1	B	148	LEU
1	B	165	ILE
1	B	185	THR
1	B	190	ARG
1	B	211	MET
1	B	230	MET
1	B	232	LEU
1	B	260	CYS
1	B	274	HIS
1	B	346	VAL
1	B	349	VAL
1	B	357	VAL
1	B	363	THR
1	B	365	SER
1	B	374	LEU
1	B	434	CYS
1	B	524	LEU
1	B	527	PHE
1	B	533	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	35	GLN
1	A	54	HIS
1	A	108	ASN
1	A	274	HIS
1	A	324	HIS
1	A	422	GLN
1	A	496	GLN
1	A	513	ASN
1	A	542	GLN
1	B	35	GLN
1	B	108	ASN
1	B	168	ASN
1	B	179	GLN

5.3.3 RNA [i](#)

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](#)

17 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	SO4	B	584	-	4,4,4	0.23	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	578	-	4,4,4	0.24	0	6,6,6	0.19	0
3	SO4	B	581	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	A	581	-	4,4,4	0.22	0	6,6,6	0.13	0
3	SO4	A	585	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	A	586	-	4,4,4	0.27	0	6,6,6	0.17	0
3	SO4	B	579	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	A	584	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	B	580	-	4,4,4	0.23	0	6,6,6	0.12	0
2	AMP	A	577	-	25,25,25	1.45	5 (20%)	37,38,38	1.91	9 (24%)
4	BU3	B	583	-	4,5,5	5.20	4 (100%)	6,6,6	0.29	0
4	BU3	A	583	-	4,5,5	5.12	4 (100%)	6,6,6	0.34	0
2	AMP	B	577	-	25,25,25	1.44	4 (16%)	37,38,38	2.05	11 (29%)
3	SO4	A	582	-	4,4,4	0.28	0	6,6,6	0.19	0
3	SO4	B	578	-	4,4,4	0.22	0	6,6,6	0.24	0
3	SO4	A	580	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	A	579	-	4,4,4	0.24	0	6,6,6	0.09	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
2	AMP	A	577	-	-	0/10/26/26	0/3/3/3
4	BU3	A	583	-	-	0/4/4/4	-
2	AMP	B	577	-	-	3/10/26/26	0/3/3/3
4	BU3	B	583	-	-	0/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	583	BU3	C1-C2	-6.63	1.32	1.51
4	A	583	BU3	C4-C3	-6.53	1.33	1.51
4	B	583	BU3	C4-C3	-6.53	1.33	1.51
4	A	583	BU3	C1-C2	-6.52	1.33	1.51
2	A	577	AMP	C5-C4	4.66	1.47	1.39
2	B	577	AMP	C5-C4	4.60	1.47	1.39
4	B	583	BU3	O5-C2	-3.36	1.34	1.43
4	B	583	BU3	O6-C3	-3.24	1.34	1.43
4	A	583	BU3	O6-C3	-3.18	1.34	1.43
4	A	583	BU3	O5-C2	-3.12	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	577	AMP	C5-C6	2.84	1.48	1.41
2	B	577	AMP	C5-C6	2.78	1.48	1.41
2	B	577	AMP	C8-N7	2.57	1.36	1.31
2	A	577	AMP	C5-N7	-2.34	1.34	1.39
2	A	577	AMP	C8-N7	2.23	1.36	1.31
2	B	577	AMP	C5-N7	-2.13	1.35	1.39
2	A	577	AMP	C4-N9	-2.05	1.33	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	577	AMP	C5-C4-N3	-5.73	118.83	126.72
2	B	577	AMP	C5-C4-N3	-5.68	118.90	126.72
2	A	577	AMP	N3-C4-N9	4.43	134.70	127.17
2	B	577	AMP	N3-C4-N9	4.40	134.66	127.17
2	B	577	AMP	C2-N3-C4	3.92	121.42	111.83
2	A	577	AMP	C2-N3-C4	3.79	121.08	111.83
2	B	577	AMP	N3-C2-N1	-3.67	123.02	128.58
2	B	577	AMP	C4-C5-N7	-3.48	106.60	110.58
2	A	577	AMP	C4-C5-N7	-3.35	106.76	110.58
2	A	577	AMP	N3-C2-N1	-3.29	123.60	128.58
2	B	577	AMP	C2'-C1'-N9	-3.16	105.45	113.30
2	B	577	AMP	C4-N9-C8	2.79	108.66	105.74
2	B	577	AMP	C5-N7-C8	2.67	107.65	103.45
2	A	577	AMP	C2'-C1'-N9	-2.64	106.74	113.30
2	B	577	AMP	C6-C5-N7	2.60	137.10	132.09
2	A	577	AMP	C5-N7-C8	2.37	107.18	103.45
2	A	577	AMP	C4-N9-C8	2.35	108.21	105.74
2	B	577	AMP	N9-C8-N7	-2.33	110.63	113.94
2	A	577	AMP	C6-C5-N7	2.29	136.51	132.09
2	B	577	AMP	O4'-C1'-N9	2.22	112.36	108.09

There are no chirality outliers.

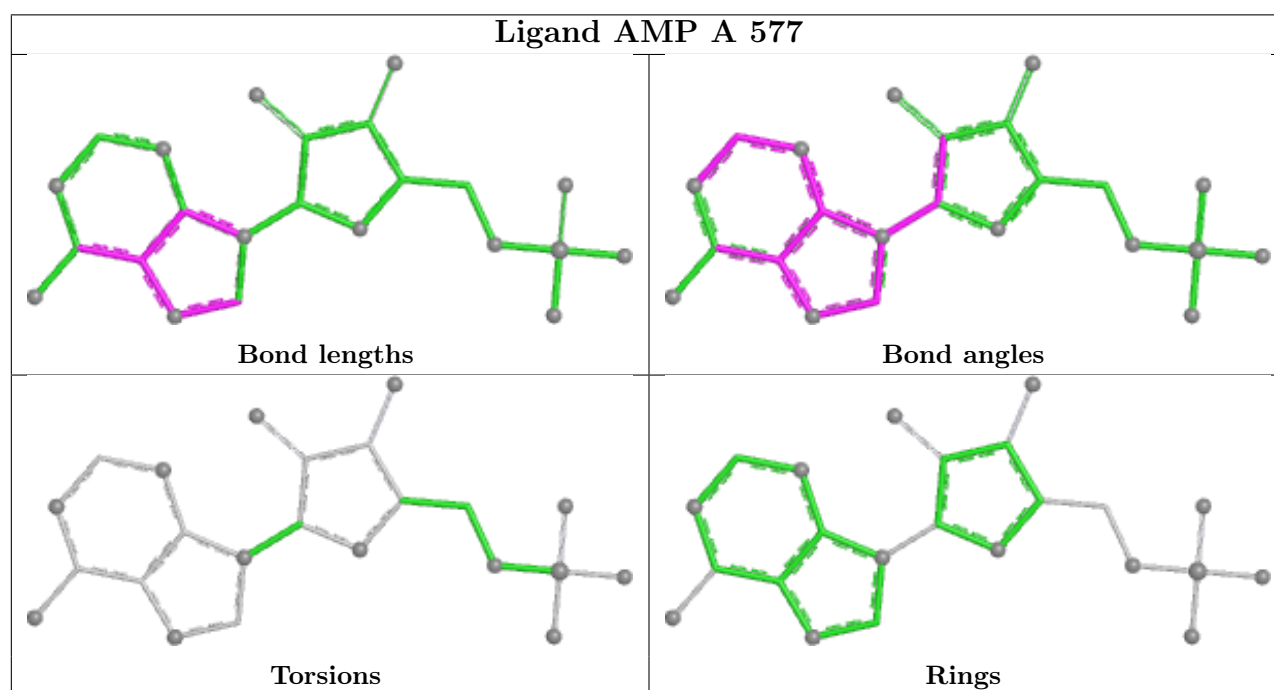
All (3) torsion outliers are listed below:

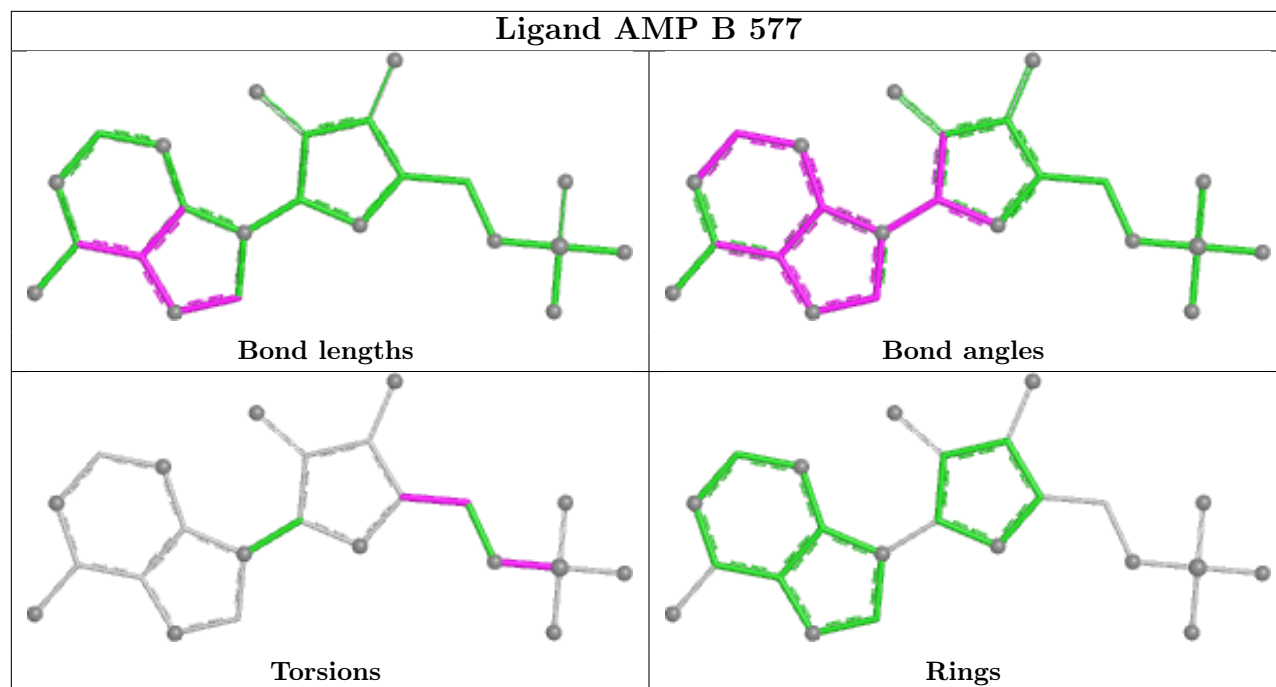
Mol	Chain	Res	Type	Atoms
2	B	577	AMP	O4'-C4'-C5'-O5'
2	B	577	AMP	C3'-C4'-C5'-O5'
2	B	577	AMP	C5'-O5'-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

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	553/576 (96%)	0.31	30 (5%) 31 24	63, 118, 224, 258	0
1	B	553/576 (96%)	0.19	21 (3%) 44 36	64, 126, 240, 265	0
All	All	1106/1152 (96%)	0.25	51 (4%) 37 29	63, 120, 230, 265	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	125	LEU	3.8
1	A	3	LEU	3.7
1	A	404	VAL	3.5
1	A	28	LYS	3.4
1	A	402	LYS	3.4
1	B	338	GLU	3.4
1	A	397	VAL	3.2
1	B	473	TYR	3.1
1	B	489	VAL	3.1
1	A	460	MET	3.0
1	A	473	TYR	2.9
1	B	6	ILE	2.9
1	A	9	ASN	2.8
1	A	472	ILE	2.8
1	B	472	ILE	2.8
1	A	11	VAL	2.8
1	A	403	GLU	2.8
1	B	436	GLY	2.7
1	A	400	LEU	2.7
1	A	291	TYR	2.6
1	A	126	VAL	2.6
1	B	15	ALA	2.6
1	A	405	PRO	2.5
1	A	125	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	404	VAL	2.5
1	A	408	TYR	2.4
1	A	12	LEU	2.4
1	A	409	SER	2.4
1	B	486	VAL	2.4
1	B	285	GLU	2.4
1	B	107	GLN	2.4
1	A	315	GLU	2.3
1	A	351	TYR	2.3
1	B	7	VAL	2.3
1	B	360	GLU	2.2
1	A	491	LEU	2.2
1	A	8	ALA	2.2
1	A	199	GLU	2.2
1	B	491	LEU	2.2
1	B	351	TYR	2.2
1	A	273	PHE	2.2
1	A	110	LEU	2.2
1	B	405	PRO	2.2
1	B	3	LEU	2.2
1	B	402	LYS	2.1
1	A	412	PHE	2.1
1	B	118	ILE	2.1
1	A	401	VAL	2.1
1	A	398	GLU	2.1
1	B	18	GLY	2.0
1	A	189	TYR	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,

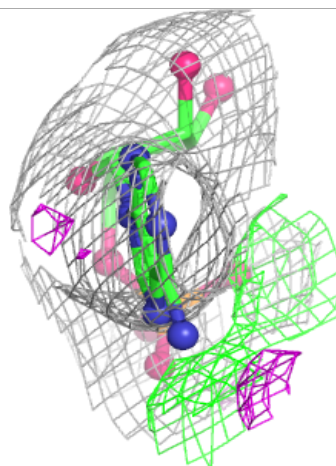
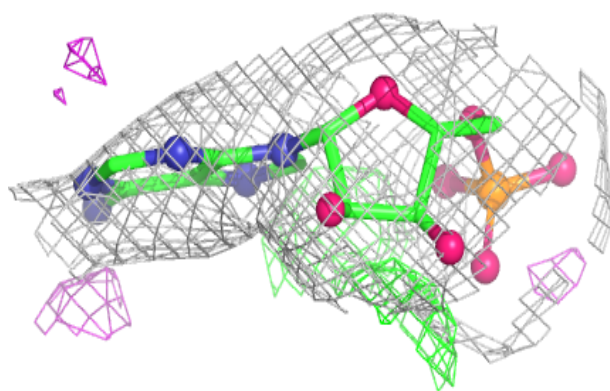
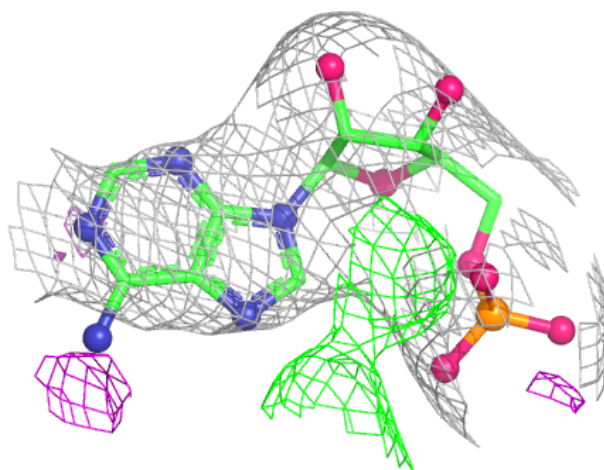
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	584	5/5	0.62	0.08	258,258,259,259	0
3	SO4	A	585	5/5	0.69	0.10	175,175,175,176	0
3	SO4	A	579	5/5	0.71	0.07	218,218,218,219	0
3	SO4	A	584	5/5	0.76	0.08	253,253,254,255	0
3	SO4	B	579	5/5	0.82	0.07	233,233,233,235	0
3	SO4	B	581	5/5	0.87	0.05	168,168,169,170	0
3	SO4	A	580	5/5	0.91	0.14	135,135,136,136	0
3	SO4	B	580	5/5	0.91	0.13	140,140,141,142	0
3	SO4	A	581	5/5	0.91	0.05	162,162,163,163	0
3	SO4	B	578	5/5	0.91	0.07	110,111,111,113	0
2	AMP	B	577	23/23	0.92	0.10	104,106,108,109	0
2	AMP	A	577	23/23	0.93	0.10	99,101,102,103	0
3	SO4	A	586	5/5	0.95	0.07	92,93,93,93	0
3	SO4	A	582	5/5	0.96	0.06	85,87,87,88	0
4	BU3	A	583	6/6	0.96	0.17	68,69,70,71	0
3	SO4	A	578	5/5	0.97	0.07	105,105,105,106	0
4	BU3	B	583	6/6	0.98	0.12	72,73,74,74	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.

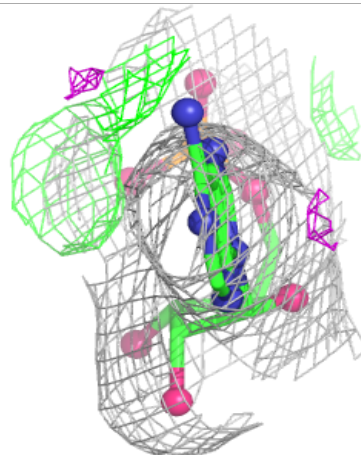
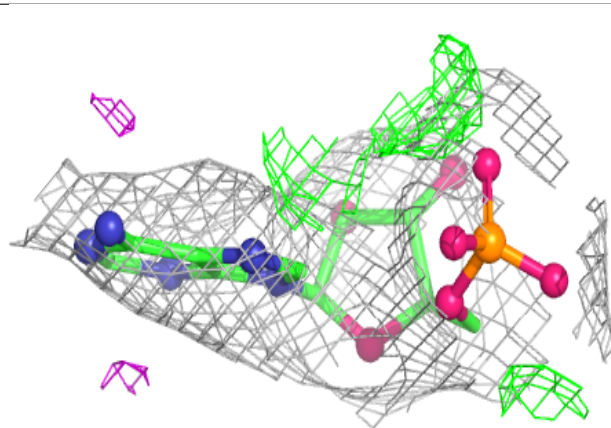
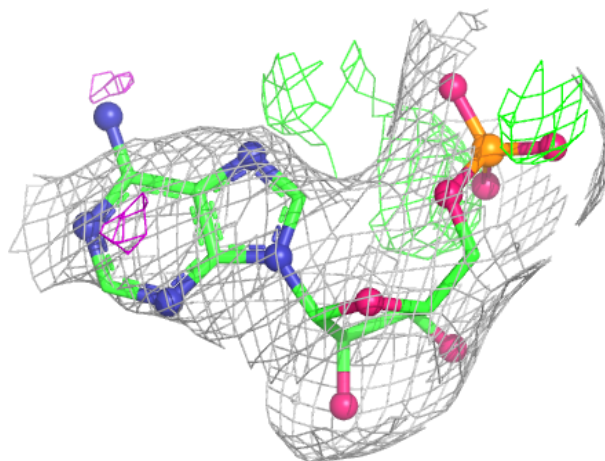
Electron density around AMP B 577:

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



Electron density around AMP 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.