



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:59 AM EDT

PDB ID : 4QFG / pdb_00004qfg
Title : Structure of AMPK in complex with STAUROSPORINE inhibitor and in the absence of a synthetic activator
Authors : Calabrese, M.F.; Kurumbail, R.G.
Deposited on : 2014-05-20
Resolution : 3.46 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

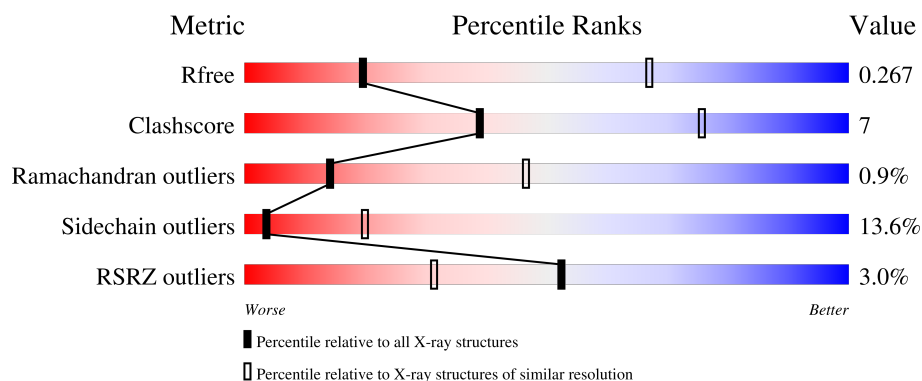
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	503	
2	B	204	
3	C	330	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6593 atoms, of which 26 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 5'-AMP-activated protein kinase catalytic subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	366	2970	1905	518	528	1	18	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P54645
A	517	ALA	-	SEE REMARK 999	UNP P54645
A	518	SER	-	SEE REMARK 999	UNP P54645
A	519	GLY	-	SEE REMARK 999	UNP P54645
A	520	GLY	-	SEE REMARK 999	UNP P54645
A	521	PRO	-	SEE REMARK 999	UNP P54645
A	522	GLY	-	SEE REMARK 999	UNP P54645
A	523	GLY	-	SEE REMARK 999	UNP P54645
A	524	SER	-	SEE REMARK 999	UNP P54645

- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	161	1271	828	215	225	3	0	0	0

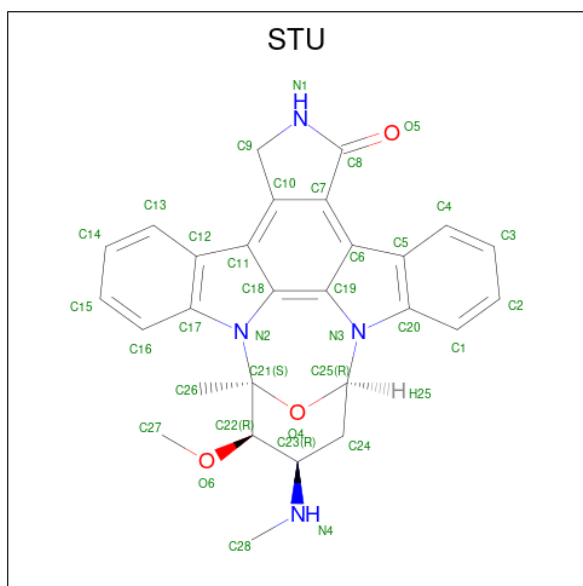
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MET	-	expression tag	UNP P80386
B	108	ASP	SER	engineered mutation	UNP P80386

- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	0	0	0
			2250	1463	376	404	7			

- Molecule 4 is STAUROSPORINE (CCD ID: STU) (formula: $C_{28}H_{26}N_4O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			61	28	26	4	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

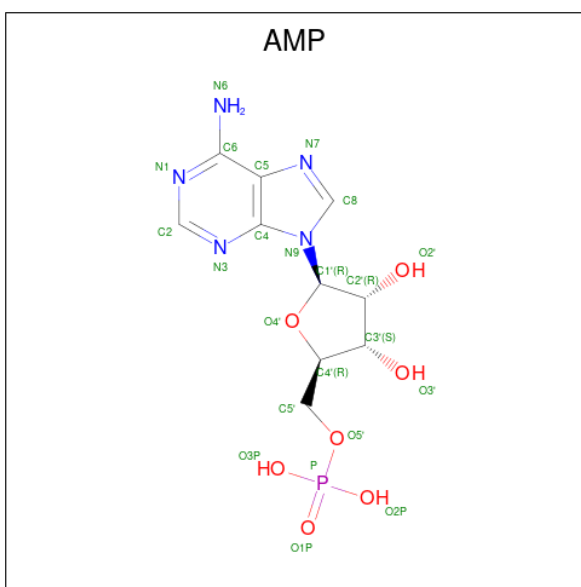
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Cl	0	0
			3 3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

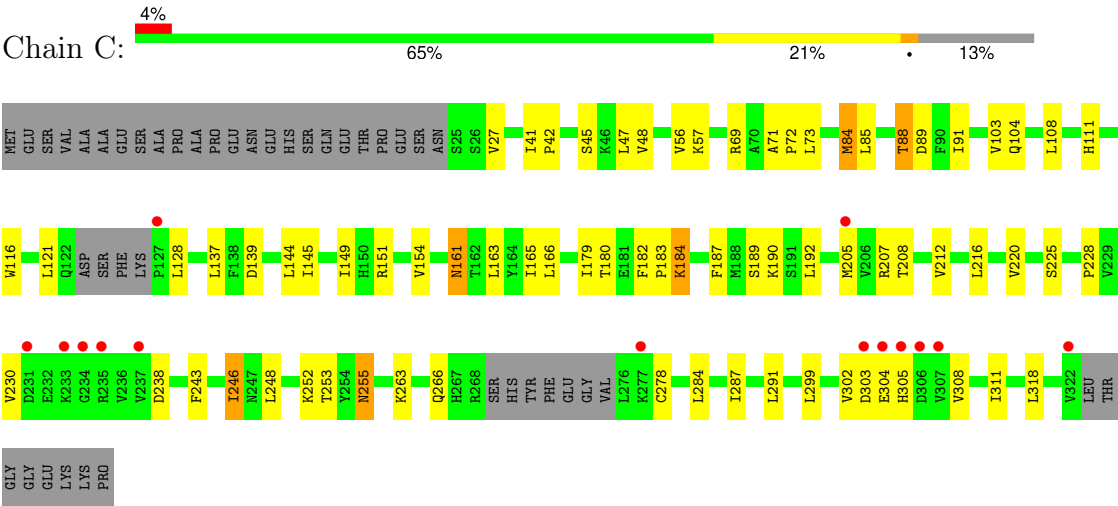


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.37 Å 124.37 Å 404.06 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.86 – 3.46 29.86 – 3.46	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.86-3.46) 96.1 (29.86-3.46)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.47 Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.5, BUSTER 2.11.5	Depositor
R, R_{free}	0.222 , 0.267 0.218 , 0.267	Depositor DCC
R_{free} test set	1210 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	79.2	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 98.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6593	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: STU, TPO, CL, SO4, AMP

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	0.84	0/3026	1.44	28/4081 (0.7%)
2	B	0.84	0/1306	1.29	3/1779 (0.2%)
3	C	0.85	0/2294	1.40	6/3119 (0.2%)
All	All	0.84	0/6626	1.40	37/8979 (0.4%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ALA	CA-C-N	-8.20	111.00	123.14
1	A	156	ALA	C-N-CA	-8.20	111.00	123.14
1	A	138	ARG	N-CA-C	-7.57	100.53	110.53
3	C	304	GLU	N-CA-C	-7.34	104.85	113.88
3	C	305	HIS	CA-C-N	6.86	129.48	120.28
3	C	305	HIS	C-N-CA	6.86	129.48	120.28
2	B	98	ASN	CA-CB-CG	6.49	119.09	112.60
1	A	67	ASN	CA-C-N	6.36	129.44	120.28
1	A	67	ASN	C-N-CA	6.36	129.44	120.28
1	A	57	VAL	N-CA-C	-5.77	105.22	113.07
1	A	82	VAL	CB-CA-C	5.69	116.90	110.41
2	B	121	GLY	N-CA-C	5.66	118.26	110.56
1	A	547	ALA	CA-C-N	5.57	131.73	121.70
1	A	547	ALA	C-N-CA	5.57	131.73	121.70
2	B	134	THR	CB-CA-C	-5.53	98.56	110.45
1	A	547	ALA	N-CA-C	5.52	117.23	108.67
1	A	62	ARG	CA-C-N	5.44	127.84	120.44
1	A	62	ARG	C-N-CA	5.44	127.84	120.44
1	A	77	ILE	CA-C-N	5.37	128.34	120.71
1	A	77	ILE	C-N-CA	5.37	128.34	120.71
1	A	456	SER	N-CA-C	-5.36	106.69	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ILE	N-CA-CB	5.33	116.92	110.95
1	A	546	LEU	CA-C-N	5.32	129.91	121.99
1	A	546	LEU	C-N-CA	5.32	129.91	121.99
1	A	101	LEU	N-CA-C	-5.30	105.67	111.82
3	C	183	PRO	CA-C-N	5.30	127.86	120.65
3	C	183	PRO	C-N-CA	5.30	127.86	120.65
1	A	110	ARG	N-CA-C	-5.20	102.78	110.48
1	A	428	ASN	N-CA-C	-5.20	104.16	110.13
1	A	71	PHE	CA-CB-CG	5.17	118.97	113.80
1	A	530	SER	N-CA-C	5.16	117.95	110.42
1	A	150	HIS	CA-C-N	5.16	131.38	121.54
1	A	150	HIS	C-N-CA	5.16	131.38	121.54
1	A	413	VAL	N-CA-CB	5.09	117.09	110.57
3	C	139	ASP	CA-CB-CG	5.08	117.69	112.60
1	A	268	PHE	CA-C-N	5.08	127.05	120.44
1	A	268	PHE	C-N-CA	5.08	127.05	120.44

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	2970	0	2997	50	0
2	B	1271	0	1268	20	0
3	C	2250	0	2283	25	0
4	A	35	26	26	6	0
5	A	3	0	0	0	0
6	A	5	0	0	0	0
6	C	10	0	0	0	0
7	C	23	0	12	0	0
All	All	6567	26	6586	89	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 (89) 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)
2:B:79:PRO:HB2	2:B:115:ILE:HG22	1.44	0.99
4:A:601:STU:H261	4:A:601:STU:H16	1.60	0.82
2:B:120:GLU:HA	2:B:155:VAL:HG22	1.72	0.70
1:A:51:LYS:O	1:A:54:SER:HB3	1.96	0.65
1:A:141:LYS:HG3	1:A:143:GLU:HB2	1.79	0.64
1:A:185:ILE:HD11	1:A:227:CYS:SG	2.38	0.62
1:A:77:ILE:HG21	4:A:601:STU:H91	1.81	0.62
1:A:401:ARG:O	1:A:548:GLN:HB3	2.00	0.62
3:C:69:ARG:HE	3:C:151:ARG:HH12	1.48	0.60
1:A:12:LYS:HB3	1:A:17:ILE:HA	1.85	0.59
2:B:145:GLN:H	2:B:145:GLN:CD	2.11	0.58
3:C:263:LYS:HA	3:C:266:GLN:HE21	1.69	0.57
1:A:540:ALA:HB2	2:B:251:LEU:HD11	1.87	0.56
1:A:160:LEU:HD13	1:A:174:CYS:HB2	1.88	0.56
2:B:232:ASN:HB3	2:B:235:MET:HE3	1.88	0.55
3:C:72:PRO:HB3	3:C:84:MET:HE2	1.89	0.55
3:C:104:GLN:HA	3:C:255:ASN:HD21	1.72	0.54
3:C:184:LYS:HE3	3:C:184:LYS:H	1.72	0.54
1:A:218:HIS:CE1	1:A:220:PRO:HD2	2.43	0.54
3:C:73:LEU:HD21	3:C:85:LEU:HB2	1.90	0.53
3:C:42:PRO:HG2	3:C:45:SER:HB3	1.91	0.53
1:A:49:ARG:HH21	1:A:86:PRO:HA	1.72	0.53
1:A:193:PRO:O	1:A:197:ILE:HG12	2.09	0.53
2:B:264:THR:HG23	3:C:47:LEU:HD23	1.91	0.53
1:A:398:LEU:HD22	2:B:210:LEU:HB3	1.91	0.52
1:A:12:LYS:HD3	1:A:17:ILE:HG22	1.92	0.51
1:A:171:ARG:HH22	2:B:204:PRO:HG3	1.75	0.51
3:C:248:LEU:HA	3:C:253:THR:HG23	1.92	0.51
3:C:243:PHE:O	3:C:246:ILE:HG13	2.10	0.51
3:C:179:ILE:HD11	3:C:184:LYS:HA	1.93	0.50
1:A:258:THR:H	1:A:261:ASP:HB2	1.76	0.50
1:A:127:VAL:CG2	1:A:140:LEU:HD21	2.42	0.50
4:A:601:STU:H272	4:A:601:STU:N4	2.26	0.50
1:A:273:PRO:HD2	1:A:276:LEU:HD12	1.93	0.49
1:A:447:MET:HE2	1:A:538:MET:HE2	1.95	0.49
1:A:237:LEU:HB3	1:A:242:ILE:HD11	1.94	0.49
1:A:247:HIS:CG	1:A:257:ALA:HB2	2.48	0.48
1:A:530:SER:HB2	3:C:161:ASN:HB3	1.96	0.48
3:C:212:VAL:O	3:C:216:LEU:HG	2.13	0.48
1:A:179:TYR:CD2	1:A:202:VAL:CG2	2.96	0.48
1:A:414:CYS:HA	1:A:417:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ARG:O	1:A:172:TPO:C	2.61	0.48
2:B:242:LEU:HB2	2:B:250:VAL:HB	1.96	0.48
3:C:302:VAL:HA	3:C:308:VAL:HA	1.96	0.48
1:A:77:ILE:HG12	1:A:154:LYS:HB3	1.95	0.47
1:A:463:PHE:HB2	2:B:239:LEU:HB3	1.96	0.47
1:A:465:SER:H	2:B:237:ASN:HB3	1.79	0.47
1:A:218:HIS:HD2	1:A:221:THR:HG23	1.79	0.47
1:A:143:GLU:HB3	4:A:601:STU:H281	1.96	0.47
1:A:254:MET:CG	2:B:208:PRO:HB2	2.45	0.47
3:C:216:LEU:O	3:C:220:VAL:HG23	2.15	0.46
2:B:84:TRP:HB3	2:B:112:PHE:HB2	1.97	0.46
3:C:187:PHE:HA	3:C:190:LYS:HD2	1.96	0.46
1:A:179:TYR:CD2	1:A:202:VAL:HG23	2.51	0.45
1:A:55:LEU:HB2	1:A:57:VAL:HG22	1.99	0.45
1:A:78:LYS:H	1:A:94:GLU:HG2	1.81	0.45
4:A:601:STU:H261	4:A:601:STU:C16	2.29	0.45
3:C:27:VAL:HG11	3:C:182:PHE:CZ	2.51	0.45
3:C:89:ASP:OD2	3:C:116:TRP:HZ3	1.99	0.45
3:C:278:CYS:HB3	3:C:299:LEU:HD13	1.99	0.45
2:B:145:GLN:H	2:B:145:GLN:NE2	2.14	0.45
1:A:433:ARG:HE	1:A:466:ILE:HD13	1.82	0.44
3:C:144:LEU:HD23	3:C:149:ILE:HG23	1.98	0.44
3:C:72:PRO:HD3	3:C:165:ILE:HD11	1.98	0.44
1:A:61:ILE:HD11	2:B:166:LEU:HD11	2.00	0.44
3:C:41:ILE:HD11	3:C:154:VAL:HG11	2.00	0.44
3:C:205:MET:HA	3:C:228:PRO:HD2	1.99	0.44
3:C:48:VAL:O	3:C:71:ALA:HB1	2.18	0.43
1:A:434:VAL:HG13	1:A:447:MET:HG3	2.01	0.43
4:A:601:STU:C16	4:A:601:STU:C26	2.95	0.43
2:B:166:LEU:HD12	2:B:166:LEU:HA	1.91	0.43
1:A:48:ASN:HA	1:A:88:ASP:OD2	2.19	0.42
1:A:132:ARG:HH21	1:A:278:PRO:HG2	1.84	0.42
1:A:136:VAL:HB	1:A:164:MET:HE2	2.01	0.42
2:B:110:ASN:ND2	2:B:110:ASN:H	2.17	0.42
1:A:179:TYR:HD2	1:A:202:VAL:CG2	2.31	0.42
3:C:88:THR:HA	3:C:91:ILE:HD12	2.02	0.42
1:A:35:HIS:CE1	1:A:37:LEU:HB2	2.55	0.42
1:A:132:ARG:NH2	1:A:278:PRO:HG2	2.35	0.42
1:A:49:ARG:O	1:A:53:ARG:HB3	2.20	0.41
1:A:71:PHE:CD1	1:A:129:TYR:HE1	2.38	0.41
1:A:179:TYR:HD2	1:A:202:VAL:HG23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLY:O	1:A:41:LYS:HA	2.21	0.41
2:B:93:LEU:HB2	2:B:105:LEU:HD21	2.02	0.41
1:A:539:CYS:HB3	2:B:239:LEU:HD22	2.03	0.41
1:A:127:VAL:HG22	1:A:140:LEU:HD21	2.02	0.41
1:A:138:ARG:O	1:A:139:ASP:HB3	2.21	0.41
2:B:79:PRO:HA	2:B:117:ASP:HA	2.03	0.41
1:A:137:HIS:HE1	1:A:139:ASP:O	2.04	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	359/503 (71%)	333 (93%)	22 (6%)	4 (1%)	11	42
2	B	155/204 (76%)	143 (92%)	10 (6%)	2 (1%)	9	39
3	C	281/330 (85%)	265 (94%)	15 (5%)	1 (0%)	30	62
All	All	795/1037 (77%)	741 (93%)	47 (6%)	7 (1%)	14	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	108	ASP
3	C	303	ASP
1	A	139	ASP
2	B	223	CYS
1	A	399	GLY
1	A	151	MET
1	A	427	VAL

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	328/448 (73%)	282 (86%)	46 (14%)	3	19
2	B	140/185 (76%)	120 (86%)	20 (14%)	3	18
3	C	247/299 (83%)	216 (87%)	31 (13%)	4	22
All	All	715/932 (77%)	618 (86%)	97 (14%)	3	20

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	20	ASP
1	A	22	LEU
1	A	29	LYS
1	A	32	VAL
1	A	52	ILE
1	A	53	ARG
1	A	61	ILE
1	A	70	LEU
1	A	78	LYS
1	A	85	THR
1	A	89	ILE
1	A	107	LYS
1	A	110	ARG
1	A	112	ASP
1	A	147	LEU
1	A	150	HIS
1	A	154	LYS
1	A	170	LEU
1	A	171	ARG
1	A	185	ILE
1	A	189	LEU
1	A	207	LEU
1	A	215	ASP
1	A	219	VAL
1	A	222	LEU

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Mol	Chain	Res	Type
1	A	224	LYS
1	A	226	ILE
1	A	233	THR
1	A	237	LEU
1	A	251	VAL
1	A	272	LEU
1	A	397	HIS
1	A	401	ARG
1	A	402	SER
1	A	403	GLN
1	A	405	ARG
1	A	418	LYS
1	A	432	LEU
1	A	434	VAL
1	A	457	ARG
1	A	458	THR
1	A	537	GLU
1	A	538	MET
1	A	545	ILE
1	A	548	GLN
2	B	90	GLU
2	B	94	SER
2	B	110	ASN
2	B	111	ASN
2	B	116	LEU
2	B	129	VAL
2	B	134	THR
2	B	142	VAL
2	B	145	GLN
2	B	153	ILE
2	B	155	VAL
2	B	158	THR
2	B	166	LEU
2	B	170	SER
2	B	205	ILE
2	B	230	GLU
2	B	234	VAL
2	B	262	VAL
2	B	263	THR
2	B	264	THR
3	C	56	VAL
3	C	57	LYS

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Mol	Chain	Res	Type
3	C	84	MET
3	C	88	THR
3	C	103	VAL
3	C	108	LEU
3	C	111	HIS
3	C	121	LEU
3	C	128	LEU
3	C	137	LEU
3	C	145	ILE
3	C	161	ASN
3	C	163	LEU
3	C	166	LEU
3	C	180	THR
3	C	184	LYS
3	C	189	SER
3	C	192	LEU
3	C	207	ARG
3	C	208	THR
3	C	225	SER
3	C	230	VAL
3	C	238	ASP
3	C	246	ILE
3	C	252	LYS
3	C	255	ASN
3	C	284	LEU
3	C	287	ILE
3	C	291	LEU
3	C	311	ILE
3	C	318	LEU

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	218	HIS
1	A	397	HIS
2	B	109	GLN
2	B	110	ASN
2	B	212	GLN
2	B	232	ASN
2	B	233	HIS
2	B	255	HIS
3	C	66	ASN

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Mol	Chain	Res	Type
3	C	221	GLN
3	C	255	ASN
3	C	266	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	172	1	8,10,11	1.46	3 (37%)	10,14,16	2.56	6 (60%)

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	172	1	-	3/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	TPO	P-O1P	2.15	1.57	1.50
1	A	172	TPO	P-OG1	-2.04	1.55	1.59
1	A	172	TPO	CG2-CB	2.04	1.56	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TPO	P-OG1-CB	-4.72	110.50	123.33
1	A	172	TPO	O3P-P-O2P	-3.44	94.91	107.80
1	A	172	TPO	O2P-P-OG1	2.96	117.40	105.85
1	A	172	TPO	CG2-CB-CA	2.86	118.83	113.26
1	A	172	TPO	OG1-P-O1P	-2.18	101.55	109.33
1	A	172	TPO	O3P-P-OG1	2.06	113.86	105.85

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	172	TPO	CB-OG1-P-O1P
1	A	172	TPO	CB-OG1-P-O2P
1	A	172	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	172	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	SO4	C	402	-	4,4,4	0.32	0	6,6,6	0.23	0
6	SO4	A	605	-	4,4,4	0.29	0	6,6,6	0.11	0
6	SO4	C	403	-	4,4,4	0.23	0	6,6,6	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	STU	A	601	-	39,42,42	2.53	14 (35%)	50,68,68	2.73	17 (34%)
7	AMP	C	401	-	25,25,25	0.37	0	37,38,38	0.54	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
7	AMP	C	401	-	-	3/10/26/26	0/3/3/3
4	STU	A	601	-	-	1/4/42/42	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	STU	C12-C17	5.21	1.49	1.41
4	A	601	STU	C9-C10	-5.11	1.46	1.50
4	A	601	STU	C5-C20	5.07	1.48	1.41
4	A	601	STU	C11-C10	4.85	1.49	1.40
4	A	601	STU	C6-C7	4.66	1.49	1.40
4	A	601	STU	C7-C10	4.35	1.47	1.39
4	A	601	STU	C19-C18	4.17	1.49	1.40
4	A	601	STU	C25-N3	3.72	1.48	1.45
4	A	601	STU	C11-C18	3.54	1.47	1.41
4	A	601	STU	C18-N2	-3.42	1.36	1.40
4	A	601	STU	C9-N1	3.34	1.49	1.45
4	A	601	STU	C6-C19	2.93	1.46	1.41
4	A	601	STU	C17-N2	-2.45	1.37	1.40
4	A	601	STU	O5-C8	2.40	1.28	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	STU	C11-C10-C7	-7.09	116.58	121.25
4	A	601	STU	C18-N2-C17	5.60	114.14	107.37
4	A	601	STU	C28-N4-C23	5.56	121.02	114.39
4	A	601	STU	C12-C17-N2	-5.42	105.38	108.94
4	A	601	STU	C6-C7-C10	5.36	124.50	120.76
4	A	601	STU	C9-C10-C11	5.24	132.71	128.73
4	A	601	STU	C16-C17-N2	4.99	137.70	130.22
4	A	601	STU	C10-C7-C8	-4.43	104.39	108.09
4	A	601	STU	C1-C20-C5	-4.25	116.61	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	STU	C16-C17-C12	-4.00	116.92	121.59
4	A	601	STU	C7-C8-N1	3.89	110.08	106.38
4	A	601	STU	C4-C5-C20	3.40	123.16	119.24
4	A	601	STU	C13-C12-C17	3.02	122.73	119.24
4	A	601	STU	C1-C20-N3	2.88	134.64	129.73
4	A	601	STU	C9-N1-C8	-2.70	111.40	113.86
4	A	601	STU	O5-C8-C7	-2.43	124.95	128.47
4	A	601	STU	C9-C10-C7	2.27	110.72	109.88

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	401	AMP	C5'-O5'-P-O3P
7	C	401	AMP	C5'-O5'-P-O1P
4	A	601	STU	C24-C23-N4-C28
7	C	401	AMP	C5'-O5'-P-O2P

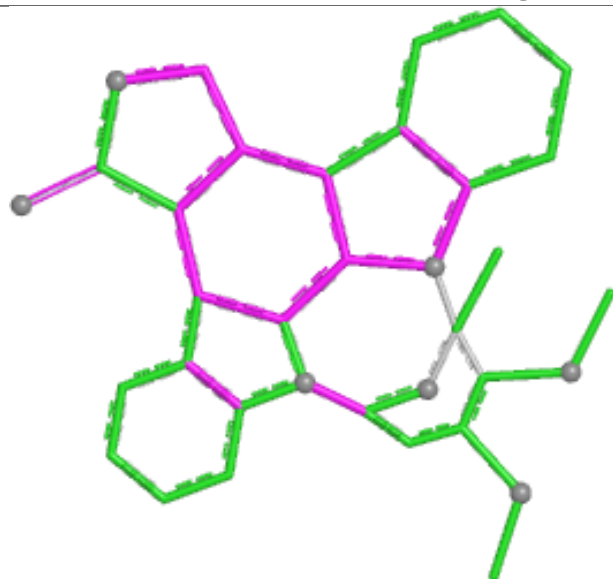
There are no ring outliers.

1 monomer is involved in 6 short contacts:

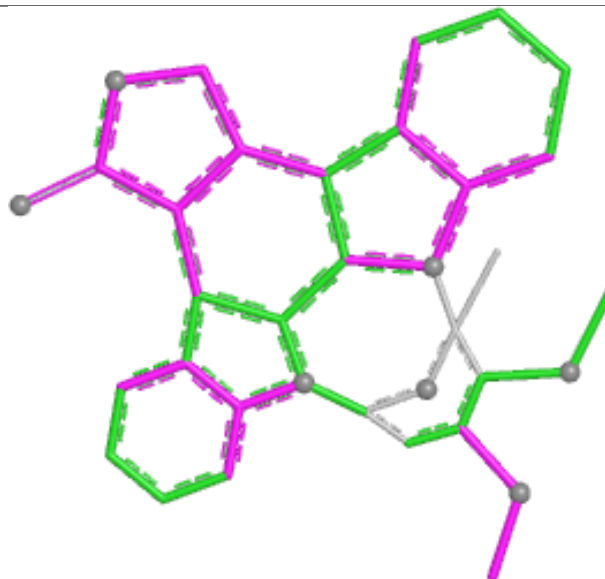
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	STU	6	0

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.

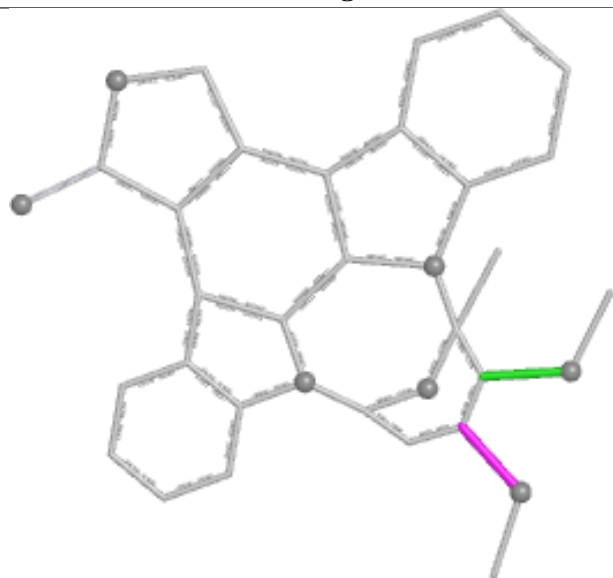
Ligand STU A 601



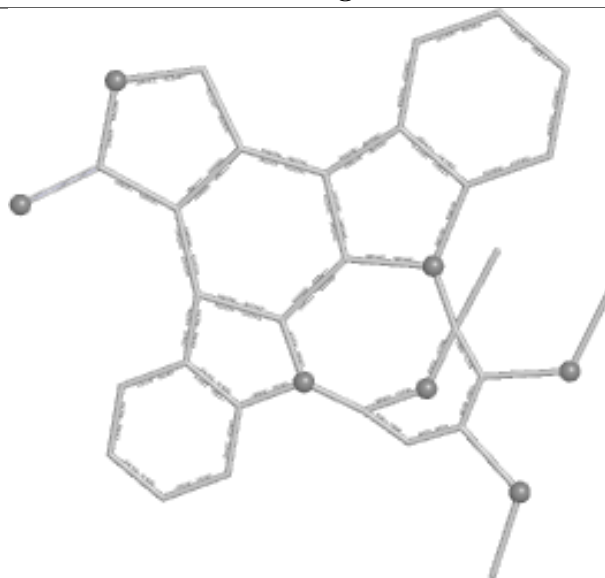
Bond lengths



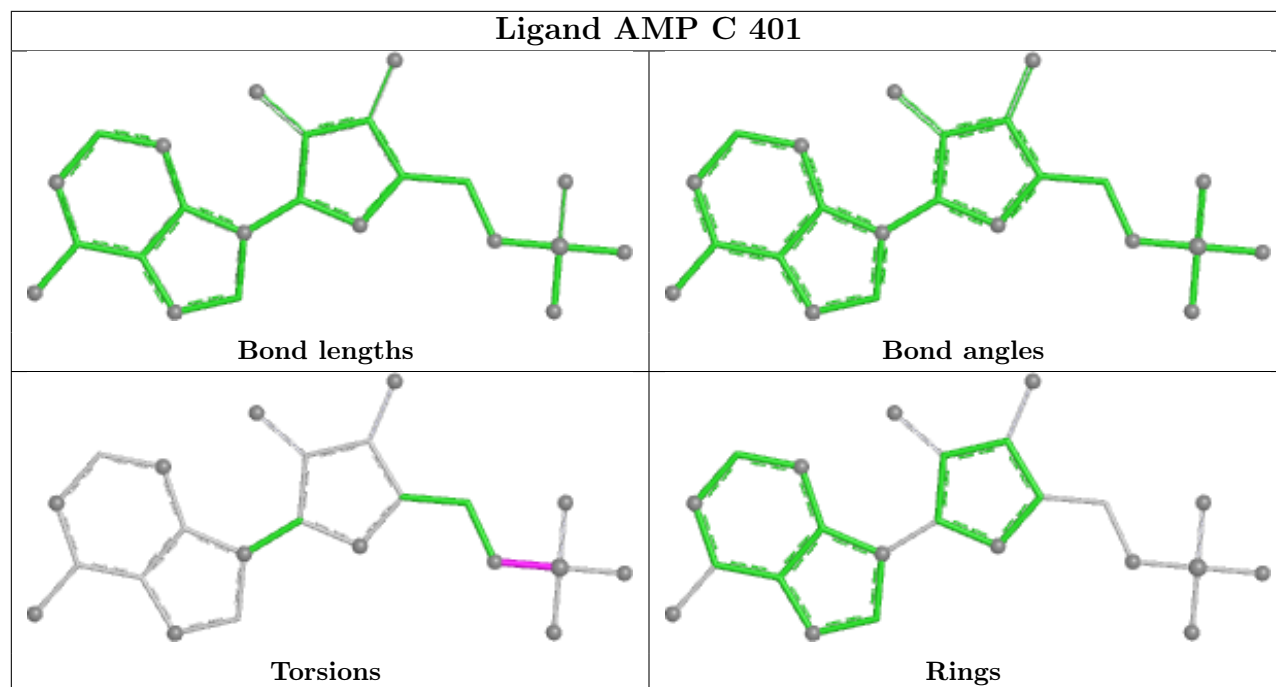
Bond angles



Torsions



Rings



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	365/503 (72%)	0.03	4 (1%)	78 54	38, 70, 125, 160	0
2	B	161/204 (78%)	0.15	6 (3%)	45 27	52, 80, 116, 144	0
3	C	287/330 (86%)	0.22	14 (4%)	35 21	65, 95, 126, 173	0
All	All	813/1037 (78%)	0.12	24 (2%)	52 31	38, 84, 125, 173	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	307	VAL	5.9
3	C	306	ASP	5.9
3	C	303	ASP	4.2
3	C	304	GLU	4.0
3	C	305	HIS	4.0
1	A	547	ALA	3.9
3	C	231	ASP	3.9
2	B	217	LYS	3.8
3	C	235	ARG	3.6
2	B	215	LEU	3.1
3	C	205	MET	2.7
3	C	234	GLY	2.7
1	A	278	PRO	2.6
1	A	70	LEU	2.5
3	C	127	PRO	2.5
3	C	322	VAL	2.4
2	B	214	ILE	2.4
3	C	237	VAL	2.4
3	C	233	LYS	2.3
3	C	277	LYS	2.3
2	B	167	MET	2.3
2	B	224	ASP	2.3
1	A	54	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	246	ASP	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	TPO	A	172	11/12	0.96	0.08	74,76,84,87	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

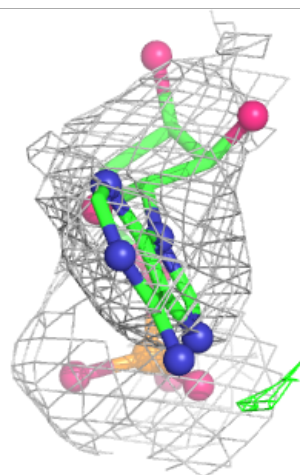
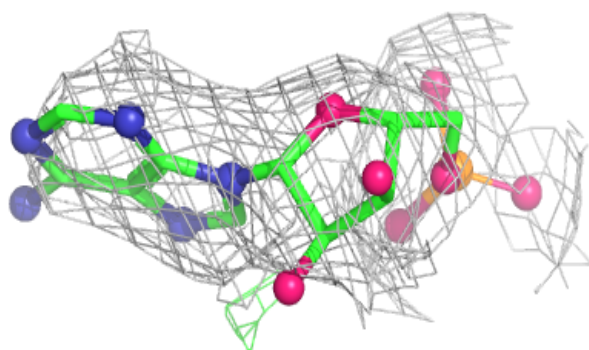
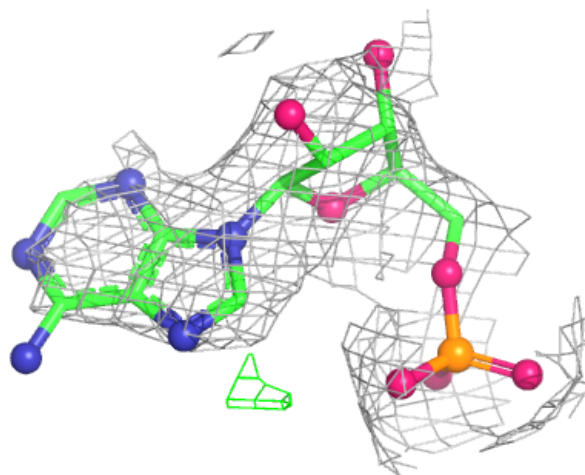
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	C	403	5/5	0.84	0.11	145,145,145,146	0
7	AMP	C	401	23/23	0.88	0.13	139,151,154,156	0
5	CL	A	603	1/1	0.89	0.10	95,95,95,95	0
6	SO4	C	402	5/5	0.89	0.10	144,145,145,146	0
6	SO4	A	605	5/5	0.96	0.06	76,78,79,79	0
4	STU	A	601	35/35	0.96	0.09	41,50,59,61	0
5	CL	A	602	1/1	0.98	0.07	65,65,65,65	0
5	CL	A	604	1/1	0.98	0.16	52,52,52,52	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.

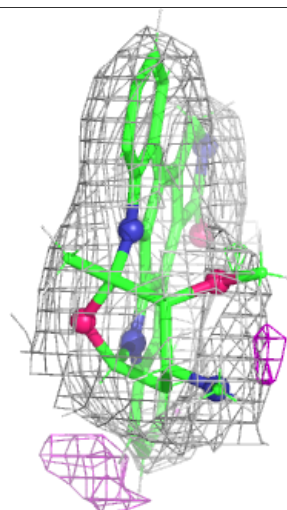
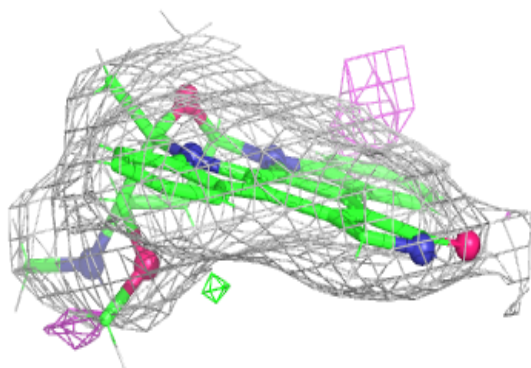
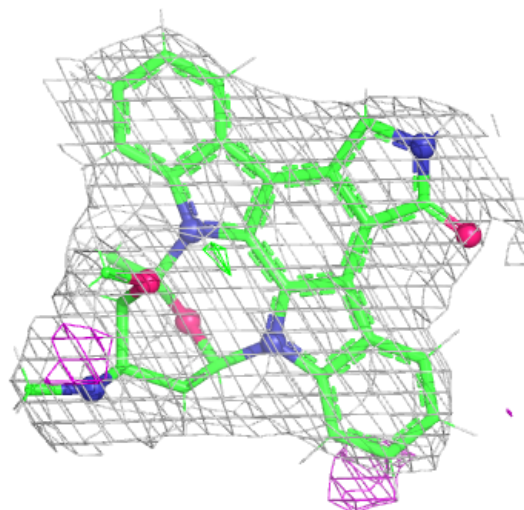
Electron density around AMP C 401:

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



Electron density around STU A 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.