



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:10 AM UTC

PDB ID : 7P7F / pdb_00007p7f
Title : Crystal structure of phosphorylated pT220 Casein Kinase I delta (CK1d), conformation 1
Authors : Chaikuad, A.; Zhubi, R.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2021-07-19
Resolution : 1.96 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

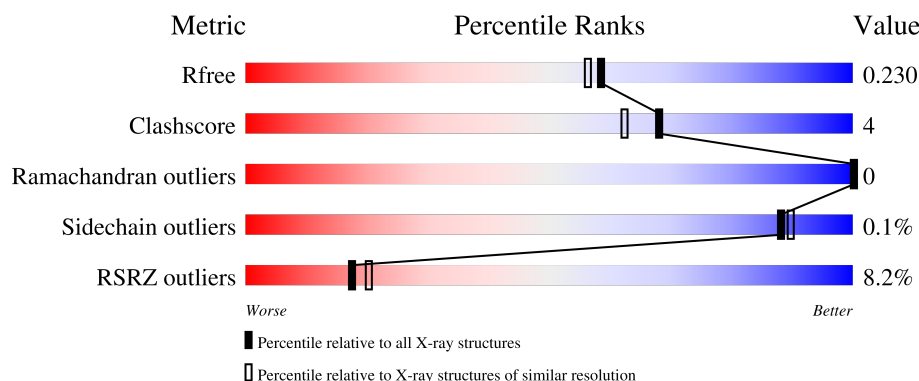
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	296	8% 88% 10% .
1	B	296	8% 88% 11% .
1	C	296	7% 89% 7% .
1	D	296	9% 86% 10% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	303	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10341 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 Casein kinase I isoform delta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	P	S	0	2	0
			2400	1535	422	427	1	15			
1	B	292	Total	C	N	O	P	S	0	1	0
			2397	1533	422	427	1	14			
1	C	285	Total	C	N	O	P	S	0	5	0
			2355	1512	409	417	1	16			
1	D	285	Total	C	N	O	P	S	0	4	0
			2347	1507	406	417	1	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P48730
A	0	MET	-	expression tag	UNP P48730
B	-1	SER	-	expression tag	UNP P48730
B	0	MET	-	expression tag	UNP P48730
C	-1	SER	-	expression tag	UNP P48730
C	0	MET	-	expression tag	UNP P48730
D	-1	SER	-	expression tag	UNP P48730
D	0	MET	-	expression tag	UNP P48730

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



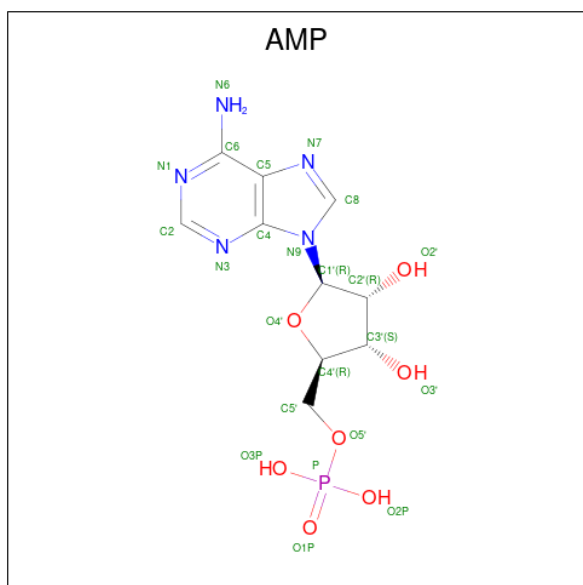
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total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

Continued on next page...

Continued from previous page...

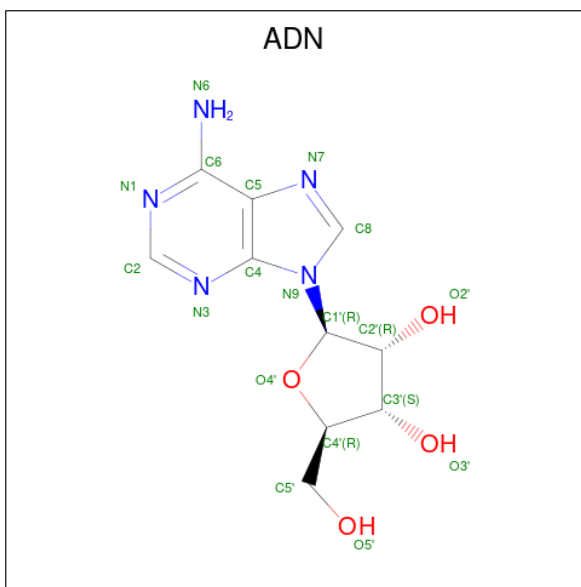
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

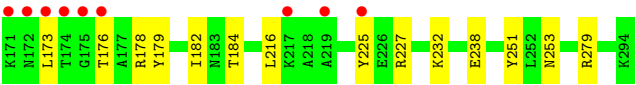
- Molecule 5 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			19	10	5	4		
5	D	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	140	Total	O	0	0
			140	140		
6	B	165	Total	O	0	0
			165	165		
6	C	176	Total	O	0	0
			176	176		
6	D	158	Total	O	0	0
			158	158		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.06Å 81.81Å 89.09Å 90.27° 105.95° 93.60°	Depositor
Resolution (Å)	47.09 – 1.96 47.09 – 1.96	Depositor EDS
% Data completeness (in resolution range)	93.0 (47.09-1.96) 93.0 (47.09-1.96)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.188 , 0.221 0.200 , 0.230	Depositor DCC
R_{free} test set	4541 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,h+1	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10341	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: AMP, SO4, TPO, EDO, ADN

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	1.12	2/2449 (0.1%)	1.25	0/3286
1	B	1.13	4/2443 (0.2%)	1.24	0/3278
1	C	1.11	1/2410 (0.0%)	1.24	1/3229 (0.0%)
1	D	1.13	2/2400 (0.1%)	1.26	1/3218 (0.0%)
All	All	1.12	9/9702 (0.1%)	1.25	2/13011 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	ASP	CG-OD1	6.93	1.38	1.25
1	A	132	ASP	CG-OD1	6.09	1.36	1.25
1	D	19	SER	C-O	5.80	1.30	1.24
1	C	140	LYS	C-O	-5.67	1.16	1.24
1	B	180	ALA	C-O	5.40	1.30	1.23
1	B	87	PRO	C-O	-5.19	1.17	1.23
1	D	253	ASN	C-O	5.14	1.30	1.24
1	B	253	ASN	C-O	5.13	1.30	1.24
1	A	180	ALA	C-O	5.01	1.29	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	15	ILE	N-CA-C	-5.39	107.87	113.10
1	D	15	ILE	N-CA-C	-5.16	108.09	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	77	TYR	Peptide
1	D	77	TYR	Peptide

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	2400	0	2402	21	0
1	B	2397	0	2397	21	0
1	C	2355	0	2371	10	0
1	D	2347	0	2358	17	0
2	A	15	0	0	1	0
2	B	15	0	0	2	0
2	C	15	0	0	1	0
2	D	10	0	0	0	0
3	A	4	0	6	0	0
3	B	24	0	36	0	0
3	C	12	0	18	1	0
3	D	24	0	36	1	0
4	A	23	0	12	1	0
4	B	23	0	12	3	0
5	C	19	0	13	1	0
5	D	19	0	13	0	0
6	A	140	0	0	4	0
6	B	165	0	0	4	0
6	C	176	0	0	0	0
6	D	158	0	0	1	0
All	All	10341	0	9674	69	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 4.

All (69) 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:54:LYS:HE2	1:A:58:MET:HE1	1.65	0.78
1:D:238:GLU:OE2	6:D:401:HOH:O	2.14	0.65
1:B:270:ARG:NH2	2:B:303:SO4:O3	2.31	0.63
1:B:82:MET:HE2	4:B:310:AMP:HN61	1.65	0.62
1:A:171:LYS:NZ	2:A:302:SO4:O3	2.33	0.62
1:A:54:LYS:HE2	1:A:58:MET:CE	2.33	0.58
1:D:173:LEU:HD22	1:D:184:THR:HG22	1.87	0.57
1:D:279[A]:ARG:HG2	1:D:279[A]:ARG:HH11	1.69	0.56
1:A:5:VAL:HG11	1:A:79:VAL:HG11	1.87	0.54
1:B:91:ASP:HA	6:B:407:HOH:O	2.06	0.54
1:A:10:ARG:NH2	6:A:408:HOH:O	2.42	0.53
1:D:279[A]:ARG:HG2	1:D:279[A]:ARG:NH1	2.24	0.53
1:B:216:LEU:HD13	1:B:227:ARG:HG2	1.93	0.51
1:C:82[A]:MET:HE2	5:C:307:ADN:HN61	1.75	0.51
1:B:119:ILE:HD11	1:B:147:ILE:HG21	1.93	0.51
1:D:176:THR:O	3:D:303:EDO:H22	2.09	0.50
1:B:5:VAL:HG11	1:B:79:VAL:HG11	1.93	0.50
1:A:216:LEU:HD13	1:A:227:ARG:HG2	1.94	0.50
1:C:5:VAL:HG11	1:C:79:VAL:HG11	1.94	0.49
1:D:216:LEU:HD13	1:D:227:ARG:HG2	1.94	0.48
1:A:176:THR:HA	6:A:484:HOH:O	2.13	0.48
1:D:173:LEU:HD12	1:D:225:TYR:CD2	2.48	0.48
1:A:5:VAL:CG1	1:A:79:VAL:HG11	2.44	0.48
1:A:216:LEU:HB3	1:A:227:ARG:HD3	1.94	0.48
1:A:119:ILE:HD11	1:A:147:ILE:HG21	1.96	0.47
1:D:56:TYR:CE1	1:D:66:PRO:HG2	2.50	0.47
1:B:5:VAL:CG1	1:B:79:VAL:HG11	2.45	0.47
1:C:173:LEU:HD21	1:C:177:ALA:HA	1.96	0.47
1:A:70:TRP:CH2	1:A:72:GLY:HA3	2.49	0.47
1:B:263:LYS:NZ	6:B:413:HOH:O	2.48	0.46
1:B:56:TYR:OH	6:B:401:HOH:O	2.18	0.46
1:C:123:ASN:OD1	1:C:157[A]:ARG:NE	2.39	0.46
1:A:178:ARG:HD2	1:A:179:TYR:CZ	2.52	0.45
1:A:23:ILE:HG13	4:A:305:AMP:C8	2.52	0.45
1:B:178:ARG:HD2	1:B:179:TYR:CZ	2.52	0.45
1:D:173:LEU:HD12	1:D:225:TYR:HD2	1.82	0.45
1:C:56:TYR:CE1	1:C:66:PRO:HG2	2.52	0.45
1:A:56:TYR:O	1:A:60:GLN:HG2	2.17	0.45
1:D:5:VAL:HG11	1:D:79:VAL:HG11	1.99	0.44
1:B:173:LEU:HD13	1:B:225:TYR:CD2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:VAL:HG23	1:C:43:LYS:HG3	1.98	0.44
1:B:70:TRP:CH2	1:B:72:GLY:HA3	2.52	0.44
1:D:178:ARG:HD2	1:D:179:TYR:CZ	2.53	0.44
1:D:68:ILE:CD1	1:D:82[B]:MET:HG2	2.48	0.43
1:D:119:ILE:HD11	1:D:147:ILE:HG21	1.99	0.43
1:A:279[B]:ARG:NH1	2:C:301:SO4:O1	2.51	0.43
1:C:229:SER:O	1:C:233:MET:HG3	2.19	0.43
1:C:119:ILE:HD11	1:C:147:ILE:HG21	1.99	0.43
1:B:42:VAL:HG23	1:B:43:LYS:HG3	2.01	0.43
1:B:23:ILE:HG13	4:B:310:AMP:O4'	2.19	0.42
1:B:56:TYR:CE1	1:B:66:PRO:HG2	2.54	0.42
1:C:178:ARG:HD2	1:C:179:TYR:CZ	2.54	0.42
1:A:183:ASN:ND2	6:A:404:HOH:O	2.35	0.42
1:B:23:ILE:HG13	4:B:310:AMP:C8	2.54	0.42
1:D:182:ILE:HD11	1:D:232:LYS:HB3	2.01	0.42
1:A:173:LEU:HD13	1:A:225:TYR:CD2	2.55	0.42
1:C:238:GLU:CD	3:C:305:EDO:H22	2.45	0.42
1:A:118:TYR:CZ	1:A:122:LYS:HE3	2.55	0.42
1:A:183:ASN:HB2	6:A:404:HOH:O	2.19	0.41
1:B:63:VAL:CG1	1:B:144:LEU:HD11	2.50	0.41
1:D:42:VAL:HG23	1:D:43:LYS:HG3	2.02	0.41
1:D:251:TYR:CD1	1:D:251:TYR:C	2.98	0.41
1:A:154:LYS:NZ	1:A:189:GLU:OE2	2.53	0.41
1:A:42:VAL:HG23	1:A:43:LYS:HG3	2.03	0.41
1:D:48:GLN:HA	1:D:51:ILE:HD12	2.03	0.41
1:B:251:TYR:CD1	1:B:251:TYR:C	2.99	0.40
1:B:69:ARG:HD2	6:B:446:HOH:O	2.21	0.40
1:B:158:ASP:HB3	1:B:161:THR:OG1	2.21	0.40
1:B:270:ARG:NE	2:B:303:SO4:O3	2.52	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	291/296 (98%)	283 (97%)	8 (3%)	0	100	100
1	B	290/296 (98%)	281 (97%)	9 (3%)	0	100	100
1	C	284/296 (96%)	277 (98%)	7 (2%)	0	100	100
1	D	284/296 (96%)	276 (97%)	8 (3%)	0	100	100
All	All	1149/1184 (97%)	1117 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	256/259 (99%)	256 (100%)	0	100	100
1	B	255/259 (98%)	254 (100%)	1 (0%)	84	85
1	C	253/259 (98%)	253 (100%)	0	100	100
1	D	252/259 (97%)	252 (100%)	0	100	100
All	All	1016/1036 (98%)	1015 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	48	GLN
1	B	271	GLN
1	C	190	GLN
1	D	190	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	TPO	A	220	1	8,10,11	1.09	1 (12%)	10,14,16	0.80	0
1	TPO	B	220	1	8,10,11	0.90	1 (12%)	10,14,16	0.89	0
1	TPO	D	220	1	8,10,11	0.76	0	10,14,16	0.89	0
1	TPO	C	220	1	8,10,11	0.57	0	10,14,16	1.04	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
1	TPO	A	220	1	-	5/9/11/13	-
1	TPO	B	220	1	-	5/9/11/13	-
1	TPO	D	220	1	-	0/9/11/13	-
1	TPO	C	220	1	-	0/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	TPO	P-OG1	2.32	1.63	1.59
1	B	220	TPO	P-OG1	2.14	1.63	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	220	TPO	N-CA-CB-OG1
1	A	220	TPO	CG2-CB-OG1-P
1	B	220	TPO	N-CA-CB-CG2
1	B	220	TPO	N-CA-CB-OG1
1	B	220	TPO	C-CA-CB-CG2
1	B	220	TPO	CG2-CB-OG1-P
1	A	220	TPO	C-CA-CB-CG2
1	A	220	TPO	N-CA-CB-CG2
1	A	220	TPO	O-C-CA-CB
1	B	220	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

31 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	EDO	B	305	-	3,3,3	0.05	0	2,2,2	0.01	0
3	EDO	D	308	-	3,3,3	0.20	0	2,2,2	0.14	0
3	EDO	D	305	-	3,3,3	0.14	0	2,2,2	0.22	0
3	EDO	B	309	-	3,3,3	0.11	0	2,2,2	0.19	0
3	EDO	D	303	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	B	306	-	3,3,3	0.33	0	2,2,2	0.16	0
3	EDO	B	307	-	3,3,3	0.28	0	2,2,2	0.12	0
2	SO4	B	302	-	4,4,4	0.33	0	6,6,6	0.05	0
4	AMP	A	305	-	25,25,25	0.38	0	37,38,38	0.43	0
3	EDO	C	304	-	3,3,3	0.08	0	2,2,2	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	301	-	4,4,4	0.32	0	6,6,6	0.08	0
4	AMP	B	310	-	25,25,25	0.44	0	37,38,38	0.63	0
3	EDO	A	304	-	3,3,3	0.30	0	2,2,2	0.24	0
2	SO4	C	303	-	4,4,4	0.31	0	6,6,6	0.11	0
5	ADN	C	307	-	21,21,21	0.30	0	31,31,31	0.41	0
5	ADN	D	309	-	21,21,21	0.32	0	31,31,31	0.56	0
3	EDO	C	305	-	3,3,3	0.15	0	2,2,2	0.04	0
2	SO4	D	302	-	4,4,4	0.36	0	6,6,6	0.07	0
3	EDO	C	306	-	3,3,3	0.09	0	2,2,2	0.19	0
3	EDO	D	306	-	3,3,3	0.32	0	2,2,2	0.41	0
3	EDO	D	307	-	3,3,3	0.34	0	2,2,2	0.20	0
2	SO4	B	303	-	4,4,4	0.33	0	6,6,6	0.13	0
2	SO4	C	302	-	4,4,4	0.31	0	6,6,6	0.08	0
2	SO4	A	302	-	4,4,4	0.33	0	6,6,6	0.10	0
2	SO4	A	303	-	4,4,4	0.28	0	6,6,6	0.07	0
2	SO4	D	301	-	4,4,4	0.45	0	6,6,6	0.09	0
3	EDO	B	308	-	3,3,3	0.11	0	2,2,2	0.15	0
2	SO4	B	301	-	4,4,4	0.31	0	6,6,6	0.08	0
3	EDO	B	304	-	3,3,3	0.17	0	2,2,2	0.14	0
2	SO4	C	301	-	4,4,4	0.46	0	6,6,6	0.06	0
3	EDO	D	304	-	3,3,3	0.06	0	2,2,2	0.15	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
3	EDO	B	305	-	-	1/1/1/1	-
3	EDO	D	308	-	-	0/1/1/1	-
3	EDO	D	305	-	-	1/1/1/1	-
3	EDO	B	309	-	-	1/1/1/1	-
3	EDO	D	303	-	-	0/1/1/1	-
3	EDO	B	306	-	-	1/1/1/1	-
3	EDO	B	307	-	-	0/1/1/1	-
4	AMP	A	305	-	-	5/10/26/26	0/3/3/3
3	EDO	C	304	-	-	0/1/1/1	-
4	AMP	B	310	-	-	3/10/26/26	0/3/3/3
3	EDO	A	304	-	-	1/1/1/1	-
5	ADN	C	307	-	-	0/6/22/22	0/3/3/3
5	ADN	D	309	-	-	0/6/22/22	0/3/3/3
3	EDO	C	305	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	306	-	-	1/1/1/1	-
3	EDO	D	306	-	-	1/1/1/1	-
3	EDO	D	307	-	-	1/1/1/1	-
3	EDO	B	308	-	-	1/1/1/1	-
3	EDO	B	304	-	-	1/1/1/1	-
3	EDO	D	304	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	305	AMP	C5'-O5'-P-O2P
4	A	305	AMP	C5'-O5'-P-O3P
4	A	305	AMP	O4'-C4'-C5'-O5'
4	B	310	AMP	C5'-O5'-P-O2P
4	B	310	AMP	C5'-O5'-P-O3P
4	A	305	AMP	C3'-C4'-C5'-O5'
3	D	304	EDO	O1-C1-C2-O2
3	B	306	EDO	O1-C1-C2-O2
3	B	308	EDO	O1-C1-C2-O2
4	A	305	AMP	C5'-O5'-P-O1P
4	B	310	AMP	C5'-O5'-P-O1P
3	B	309	EDO	O1-C1-C2-O2
3	C	306	EDO	O1-C1-C2-O2
3	B	305	EDO	O1-C1-C2-O2
3	A	304	EDO	O1-C1-C2-O2
3	B	304	EDO	O1-C1-C2-O2
3	D	305	EDO	O1-C1-C2-O2
3	D	306	EDO	O1-C1-C2-O2
3	D	307	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 11 short contacts:

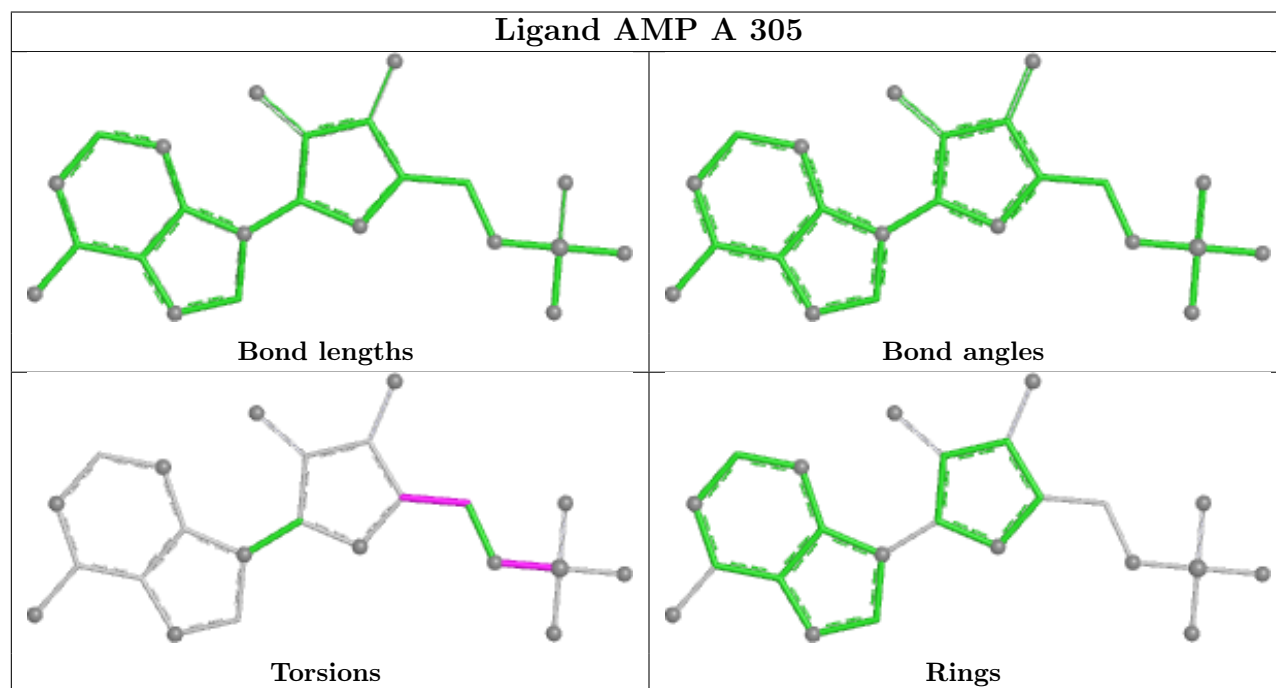
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	303	EDO	1	0
4	A	305	AMP	1	0
4	B	310	AMP	3	0

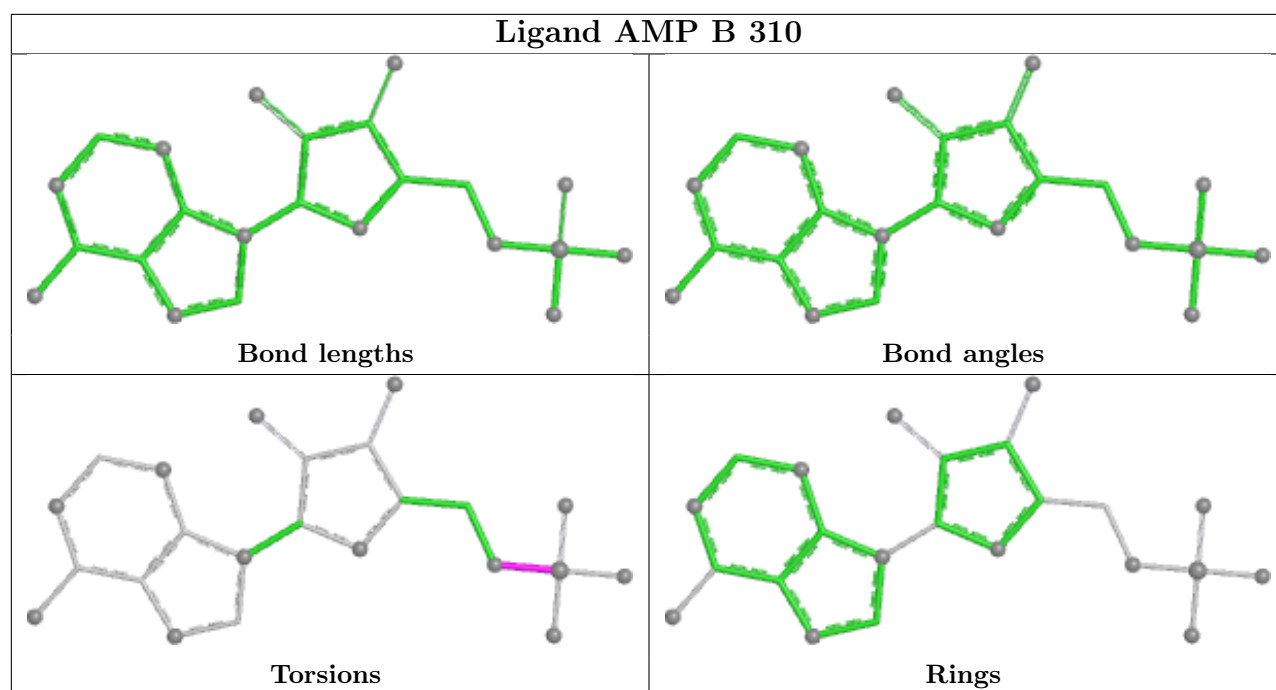
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	307	ADN	1	0
3	C	305	EDO	1	0
2	B	303	SO4	2	0
2	A	302	SO4	1	0
2	C	301	SO4	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	291/296 (98%)	0.49	23 (7%) 18 21	19, 38, 82, 113	2 (0%)
1	B	291/296 (98%)	0.45	23 (7%) 18 21	19, 38, 82, 122	1 (0%)
1	C	284/296 (95%)	0.42	21 (7%) 20 23	21, 34, 66, 93	5 (1%)
1	D	284/296 (95%)	0.51	27 (9%) 14 15	21, 35, 68, 101	4 (1%)
All	All	1150/1184 (97%)	0.47	94 (8%) 17 20	19, 36, 77, 122	12 (1%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	173	LEU	5.6
1	B	174	THR	5.2
1	C	6	GLY	4.8
1	C	173	LEU	4.6
1	D	19	SER	4.3
1	B	20	PHE	4.2
1	A	20	PHE	4.1
1	C	20	PHE	4.1
1	A	174	THR	4.0
1	B	218	ALA	3.9
1	D	6	GLY	3.8
1	A	3	LEU	3.7
1	B	17	SER	3.6
1	B	219	ALA	3.6
1	C	225	TYR	3.5
1	D	219	ALA	3.5
1	D	174	THR	3.4
1	D	167	TYR	3.4
1	D	170	ASN	3.3
1	B	3	LEU	3.3
1	A	95	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	219	ALA	3.3
1	B	19	SER	3.2
1	C	167	TYR	3.2
1	D	225	TYR	3.1
1	A	46	HIS	3.1
1	B	173	LEU	3.1
1	D	7	ASN	3.1
1	A	173	LEU	3.0
1	C	58	MET	3.0
1	D	169	GLU	3.0
1	C	174	THR	3.0
1	B	58	MET	3.0
1	B	42	VAL	2.9
1	C	19	SER	2.9
1	D	217	LYS	2.9
1	D	58	MET	2.9
1	C	170	ASN	2.9
1	C	166	PRO	2.9
1	A	225	TYR	2.8
1	C	171	LYS	2.7
1	B	225	TYR	2.7
1	C	219	ALA	2.7
1	D	175	GLY	2.7
1	C	44	THR	2.7
1	D	176	THR	2.7
1	A	226	GLU	2.7
1	A	223	GLN	2.6
1	D	171	LYS	2.6
1	A	51	ILE	2.6
1	A	17	SER	2.6
1	D	165	ILE	2.5
1	B	175	GLY	2.5
1	B	46	HIS	2.5
1	A	48	GLN	2.4
1	D	17	SER	2.4
1	D	73	ALA	2.4
1	C	45	LYS	2.4
1	D	166	PRO	2.4
1	C	7	ASN	2.4
1	C	157[A]	ARG	2.4
1	D	54	LYS	2.4
1	A	176	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	47	PRO	2.3
1	B	217	LYS	2.3
1	B	222	ARG	2.3
1	A	216	LEU	2.3
1	B	95	PHE	2.3
1	D	55	ILE	2.3
1	A	221	LYS	2.3
1	D	157	ARG	2.2
1	D	15	ILE	2.2
1	C	46	HIS	2.2
1	B	216	LEU	2.2
1	A	19	SER	2.2
1	B	73	ALA	2.2
1	D	20	PHE	2.2
1	B	51	ILE	2.2
1	D	5	VAL	2.2
1	A	41[A]	CYS	2.2
1	C	12	GLY	2.2
1	A	218	ALA	2.2
1	B	227	ARG	2.2
1	C	15	ILE	2.1
1	B	18	GLY	2.1
1	C	11	LEU	2.1
1	A	58	MET	2.1
1	B	223	GLN	2.1
1	C	164	HIS	2.1
1	B	45	LYS	2.1
1	A	227	ARG	2.0
1	A	292	MET	2.0
1	D	51	ILE	2.0
1	D	172	ASN	2.0

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	B	220	11/12	0.71	0.15	85,96,108,109	0
1	TPO	A	220	11/12	0.73	0.14	97,103,107,109	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	TPO	C	220	11/12	0.84	0.13	75,84,88,88	0
1	TPO	D	220	11/12	0.89	0.11	64,70,75,77	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($\text{\AA}^2$)	Q<0.9
3	EDO	A	304	4/4	0.75	0.16	48,50,52,54	0
2	SO4	B	301	5/5	0.76	0.12	73,76,77,80	0
3	EDO	B	305	4/4	0.77	0.21	66,68,68,68	0
2	SO4	C	302	5/5	0.78	0.11	75,78,80,86	0
2	SO4	A	302	5/5	0.78	0.11	67,68,74,74	0
2	SO4	B	303	5/5	0.78	0.11	75,76,84,86	0
3	EDO	B	306	4/4	0.79	0.17	50,53,60,60	0
3	EDO	D	306	4/4	0.79	0.17	51,52,55,59	0
3	EDO	C	304	4/4	0.81	0.20	51,54,55,56	0
2	SO4	A	303	5/5	0.81	0.11	74,81,86,86	0
3	EDO	B	308	4/4	0.82	0.19	66,69,69,71	0
3	EDO	D	307	4/4	0.82	0.16	54,58,61,62	0
3	EDO	B	304	4/4	0.84	0.13	57,57,58,65	0
3	EDO	D	303	4/4	0.86	0.14	55,59,59,60	0
3	EDO	B	309	4/4	0.87	0.14	55,56,58,65	0
3	EDO	D	308	4/4	0.87	0.16	48,50,54,54	0
4	AMP	A	305	23/23	0.88	0.11	30,47,72,74	0
4	AMP	B	310	23/23	0.89	0.11	29,47,68,72	0
3	EDO	D	305	4/4	0.90	0.12	39,41,42,45	0
2	SO4	A	301	5/5	0.90	0.08	56,56,64,65	0
3	EDO	C	305	4/4	0.91	0.12	60,62,62,65	0
5	ADN	D	309	19/19	0.91	0.08	27,32,43,43	0
3	EDO	B	307	4/4	0.92	0.16	40,48,55,59	0
3	EDO	C	306	4/4	0.93	0.09	38,39,41,43	0
2	SO4	D	301	5/5	0.93	0.09	50,57,58,59	0
2	SO4	C	303	5/5	0.93	0.08	48,50,52,53	0

Continued on next page...

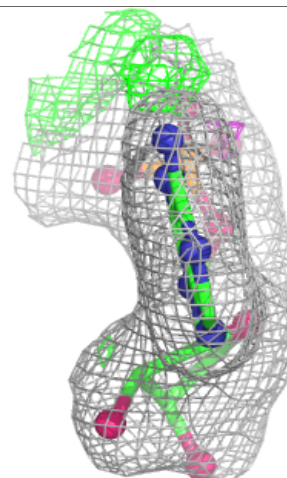
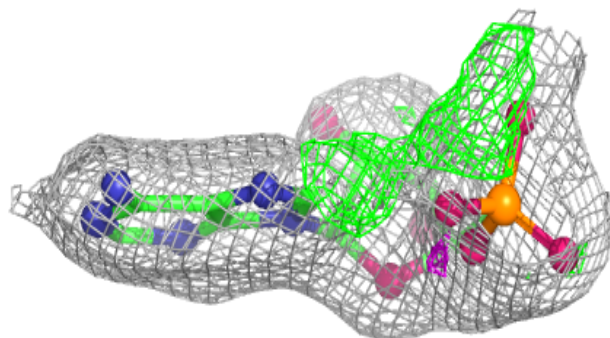
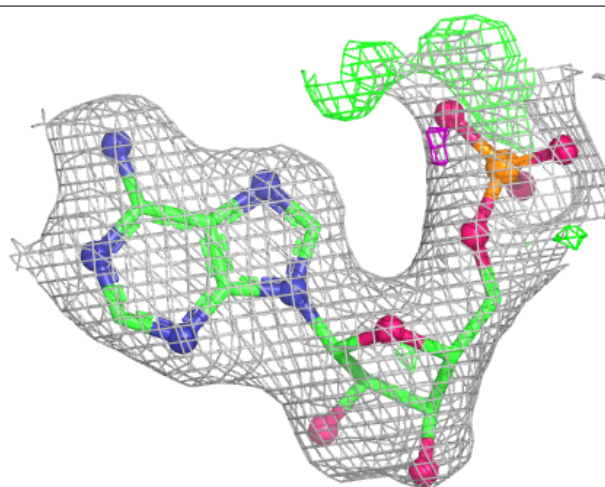
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	D	304	4/4	0.94	0.08	47,49,50,50	0
2	SO4	D	302	5/5	0.94	0.07	51,51,55,61	0
2	SO4	C	301	5/5	0.94	0.09	48,48,52,60	0
5	ADN	C	307	19/19	0.94	0.07	24,33,41,43	0
2	SO4	B	302	5/5	0.94	0.07	55,60,64,71	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.

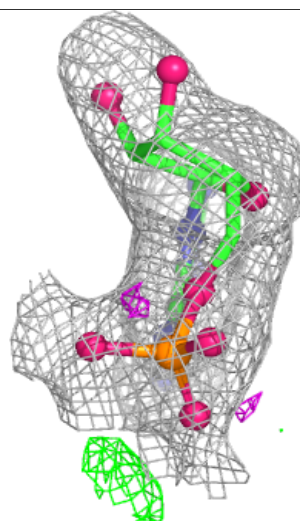
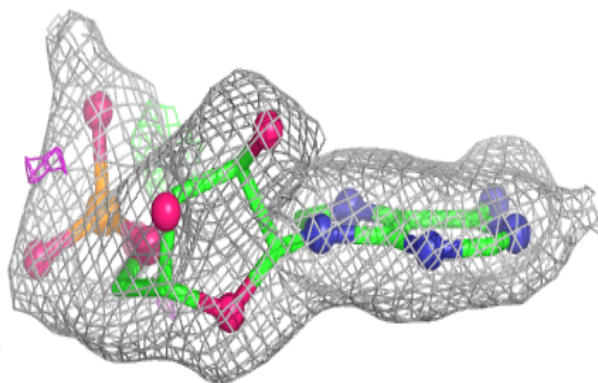
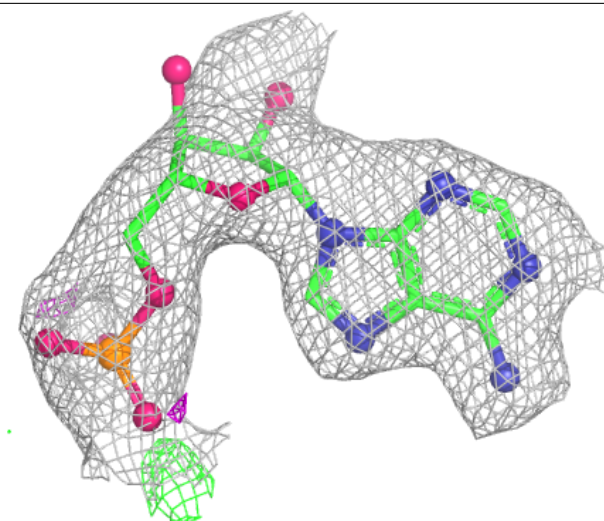
Electron density around AMP A 305:

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 B 310:

$2mF_o-DF_c$ (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.