



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:37 AM UTC

PDB ID : 1U54 / pdb_00001u54
Title : Crystal Structures of the Phosphorylated and Unphosphorylated Kinase Domains of the CDC42-associated Tyrosine Kinase ACK1 bound to AMP-PCP
Authors : Loughheed, J.C.; Chen, R.H.; Mak, P.; Stout, T.J.
Deposited on : 2004-07-26
Resolution : 2.80 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

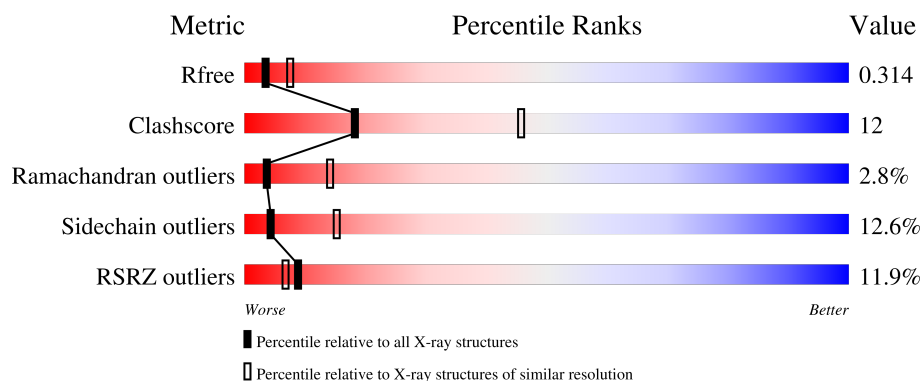
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	291	13% 60% 25% 5% 10%
2	B	291	8% 58% 26% 5% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4293 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 Activated CDC42 kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	263	2117	1345	377	379	1	15	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	GLY	-	cloning artifact	UNP Q07912
A	108	SER	-	cloning artifact	UNP Q07912
A	284	PTR	TYR	modified residue	UNP Q07912
A	396	GLU	-	cloning artifact	UNP Q07912
A	397	PHE	-	cloning artifact	UNP Q07912

- Molecule 2 is a protein called Activated CDC42 kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	261	2100	1338	374	373	15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	107	GLY	-	cloning artifact	UNP Q07912
B	108	SER	-	cloning artifact	UNP Q07912
B	396	GLU	-	cloning artifact	UNP Q07912
B	397	PHE	-	cloning artifact	UNP Q07912

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

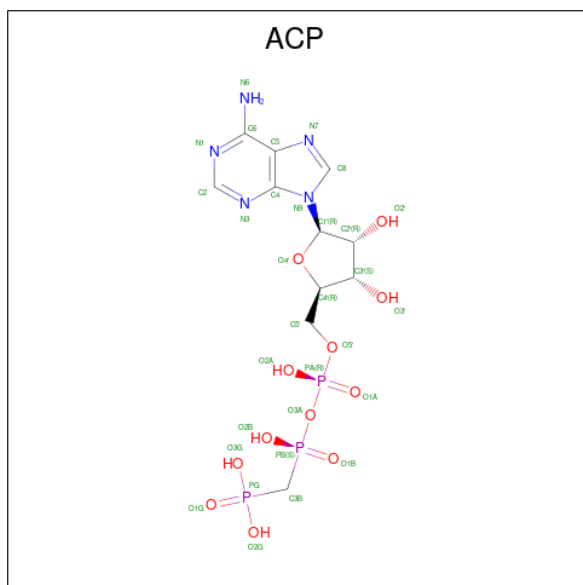
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 11	N 5	O 12	P 3	0	0
4	B	1	Total 31	C 11	N 5	O 12	P 3	0	0

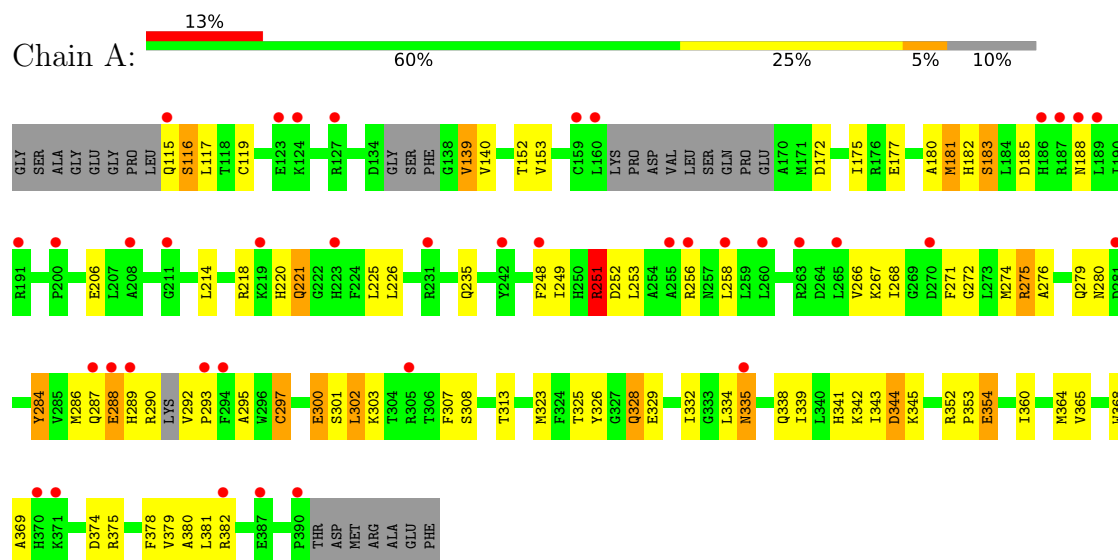
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	6	Total O 6 6	0	0
5	B	4	Total O 4 4	0	0

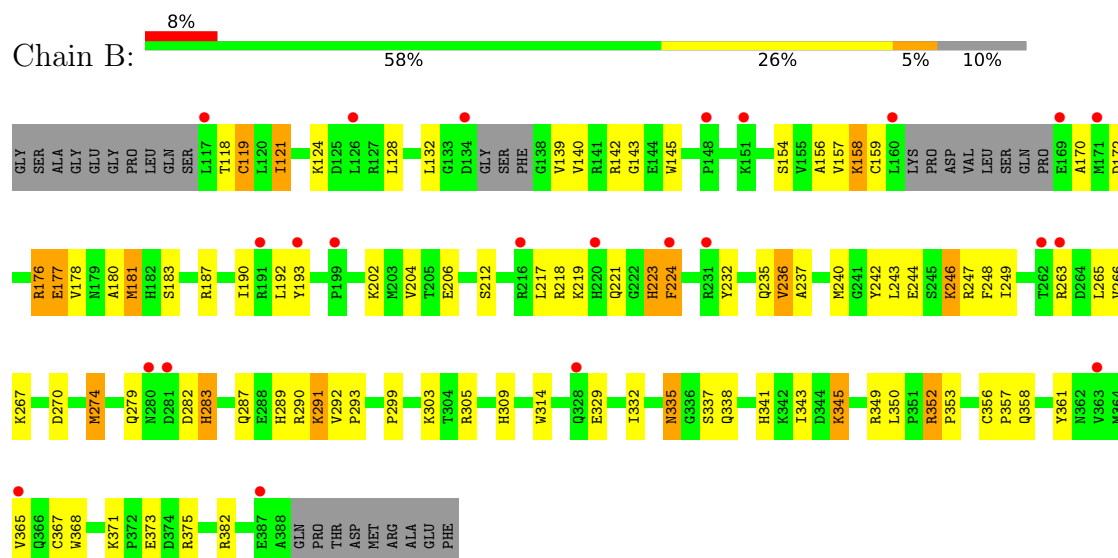
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Activated CDC42 kinase 1



• Molecule 2: Activated CDC42 kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	200.38Å 42.33Å 70.85Å 90.00° 96.28° 90.00°	Depositor
Resolution (Å)	38.71 – 2.80 38.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.71-2.80) 98.3 (38.71-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.222 , 0.322 0.226 , 0.314	Depositor DCC
R_{free} test set	684 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 56.4	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	0.89	EDS
Total number of atoms	4293	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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: ACP, PTR, 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	1.10	4/2147 (0.2%)	1.19	8/2900 (0.3%)
2	B	1.09	4/2148 (0.2%)	1.16	8/2903 (0.3%)
All	All	1.10	8/4295 (0.2%)	1.18	16/5803 (0.3%)

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	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	ASP	CA-C	8.12	1.56	1.52
2	B	274	MET	SD-CE	-6.50	1.63	1.79
2	B	178	VAL	CA-CB	6.27	1.60	1.54
1	A	293	PRO	CA-C	6.14	1.58	1.52
1	A	323	MET	SD-CE	-5.93	1.64	1.79
2	B	181	MET	SD-CE	-5.55	1.65	1.79
2	B	240	MET	SD-CE	-5.42	1.66	1.79
1	A	364	MET	SD-CE	-5.22	1.66	1.79

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	119	CYS	N-CA-C	8.41	121.67	109.14
2	B	159	CYS	N-CA-C	7.08	120.55	110.14
1	A	251	ARG	N-CA-CB	-5.88	107.46	114.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	177	GLU	CA-C-N	5.85	128.43	120.77
2	B	177	GLU	C-N-CA	5.85	128.43	120.77
1	A	188	ASN	N-CA-C	5.83	120.01	113.02
1	A	375	ARG	N-CA-C	-5.76	102.78	109.93
1	A	258	LEU	N-CA-C	-5.75	100.34	109.76
2	B	246	LYS	N-CA-C	-5.74	105.77	112.89
1	A	182	HIS	N-CA-C	-5.40	104.81	111.40
2	B	236	VAL	N-CA-C	-5.34	105.40	110.42
2	B	156	ALA	N-CA-C	-5.23	101.75	110.17
1	A	272	GLY	N-CA-C	5.13	118.88	112.73
1	A	119	CYS	N-CA-C	5.12	116.62	108.79
2	B	350	LEU	N-CA-C	-5.10	103.60	109.93
1	A	341	HIS	N-CA-C	-5.06	105.66	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	ILE	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	2117	0	2105	49	0
2	B	2100	0	2099	47	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	31	0	14	1	0
4	B	31	0	14	3	0
5	A	6	0	0	0	0
5	B	4	0	0	1	0
All	All	4293	0	4232	97	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 12.

All (97) 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:284:PTR:HE2	1:A:286:MET:HB2	1.40	1.03
2:B:235:GLN:HE21	2:B:266:VAL:HG12	1.42	0.84
2:B:180:ALA:HB1	2:B:274:MET:HE2	1.61	0.82
2:B:232:TYR:OH	2:B:263:ARG:O	1.99	0.80
4:A:101:ACP:O1G	4:A:101:ACP:O3A	2.02	0.76
1:A:284:PTR:CE2	1:A:286:MET:HB2	2.20	0.67
2:B:223:HIS:O	2:B:224:PHE:C	2.39	0.64
1:A:288:GLU:O	1:A:290:ARG:N	2.31	0.63
1:A:206:GLU:OE2	1:A:267:LYS:NZ	2.26	0.62
2:B:282:ASP:OD1	2:B:283:HIS:HB3	2.00	0.60
1:A:248:PHE:CG	1:A:274:MET:HE3	2.39	0.58
1:A:185:ASP:OD1	1:A:185:ASP:C	2.46	0.58
2:B:244:GLU:HG3	2:B:309:HIS:ND1	2.18	0.57
2:B:361:TYR:O	2:B:365:VAL:HG23	2.04	0.57
2:B:299:PRO:HG3	2:B:343:ILE:HD12	1.87	0.56
1:A:181:MET:HE2	1:A:271:PHE:HB2	1.87	0.56
2:B:248:PHE:CD2	2:B:274:MET:HE3	2.39	0.56
2:B:180:ALA:HB1	2:B:274:MET:CE	2.36	0.54
1:A:177:GLU:CG	1:A:181:MET:HE1	2.39	0.53
1:A:248:PHE:CE1	1:A:276:ALA:HB2	2.44	0.53
1:A:248:PHE:CD1	1:A:274:MET:HE3	2.44	0.52
1:A:275:ARG:NE	1:A:284:PTR:O3P	2.43	0.52
1:A:353:PRO:O	1:A:354:GLU:C	2.51	0.52
1:A:368:TRP:O	1:A:369:ALA:C	2.50	0.52
1:A:214:LEU:HD21	1:A:218:ARG:NH2	2.25	0.52
2:B:128:LEU:HD21	2:B:157:VAL:HG11	1.93	0.51
1:A:221:GLN:NE2	1:A:326:TYR:CB	2.74	0.50
1:A:177:GLU:HG3	1:A:181:MET:HE1	1.94	0.49
2:B:158:LYS:HE3	4:B:400:ACP:O3A	2.12	0.49
2:B:367:CYS:O	2:B:375:ARG:HD3	2.11	0.49
1:A:307:PHE:CD2	1:A:307:PHE:N	2.81	0.49
2:B:248:PHE:HD2	2:B:274:MET:HE3	1.78	0.49
2:B:358:GLN:HG3	5:B:1:HOH:O	2.12	0.49
2:B:181:MET:HE3	2:B:190:ILE:O	2.13	0.48
1:A:286:MET:HG2	1:A:287:GLN:N	2.29	0.48
2:B:217:LEU:HA	2:B:224:PHE:CE2	2.49	0.48
2:B:121:ILE:HG12	2:B:145:TRP:NE1	2.29	0.47
1:A:253:LEU:HD12	1:A:253:LEU:HA	1.73	0.47
2:B:290:ARG:C	2:B:291:LYS:HG2	2.39	0.47
2:B:341:HIS:HA	2:B:345:LYS:HB2	1.96	0.47
1:A:181:MET:HE2	1:A:271:PHE:HD1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ILE:O	1:A:342:LYS:HB2	2.15	0.47
1:A:235:GLN:OE1	1:A:266:VAL:HG12	2.15	0.46
2:B:236:VAL:O	2:B:237:ALA:C	2.58	0.46
1:A:344:ASP:O	1:A:345:LYS:C	2.59	0.46
2:B:192:LEU:HD12	2:B:204:VAL:O	2.15	0.46
1:A:328:GLN:HA	2:B:303:LYS:O	2.16	0.46
2:B:121:ILE:HD13	2:B:204:VAL:HG21	1.98	0.46
2:B:265:LEU:HD21	2:B:267:LYS:HE2	1.97	0.46
2:B:287:GLN:O	2:B:305:ARG:NH1	2.49	0.46
1:A:335:ASN:HB2	1:A:338:GLN:HG3	1.96	0.46
2:B:172:ASP:O	2:B:176:ARG:HB2	2.16	0.46
1:A:115:GLN:O	1:A:116:SER:CB	2.63	0.45
1:A:252:ASP:OD1	1:A:256:ARG:NH2	2.49	0.45
1:A:300:GLU:HG2	1:A:301:SER:N	2.30	0.45
2:B:223:HIS:ND1	2:B:224:PHE:N	2.64	0.45
2:B:244:GLU:HA	2:B:309:HIS:CE1	2.52	0.45
2:B:193:TYR:HE1	2:B:206:GLU:HA	1.81	0.45
1:A:378:PHE:O	1:A:379:VAL:C	2.59	0.45
1:A:220:HIS:O	1:A:221:GLN:C	2.59	0.45
1:A:221:GLN:NE2	1:A:326:TYR:HB2	2.32	0.45
1:A:274:MET:O	1:A:275:ARG:NH1	2.48	0.45
2:B:314:TRP:CD1	2:B:314:TRP:C	2.95	0.45
1:A:221:GLN:O	1:A:326:TYR:CE1	2.70	0.45
2:B:314:TRP:CE3	2:B:368:TRP:HA	2.52	0.44
1:A:181:MET:HE2	1:A:271:PHE:CD1	2.52	0.44
1:A:180:ALA:O	1:A:183:SER:OG	2.35	0.44
1:A:177:GLU:O	1:A:181:MET:HE3	2.18	0.44
1:A:325:THR:HB	1:A:328:GLN:CB	2.49	0.43
2:B:142:ARG:HG2	2:B:143:GLY:N	2.33	0.43
1:A:139:VAL:CG1	1:A:140:VAL:N	2.82	0.43
1:A:325:THR:CB	1:A:328:GLN:HB3	2.49	0.43
1:A:221:GLN:NE2	1:A:326:TYR:HB3	2.34	0.43
2:B:242:TYR:O	2:B:243:LEU:C	2.62	0.42
2:B:352:ARG:HB2	2:B:361:TYR:CD2	2.53	0.42
2:B:181:MET:HE2	2:B:192:LEU:HB2	2.01	0.42
2:B:292:VAL:O	2:B:293:PRO:C	2.62	0.42
2:B:132:LEU:HD13	4:B:400:ACP:C2	2.50	0.42
2:B:177:GLU:O	2:B:180:ALA:HB3	2.20	0.42
2:B:235:GLN:NE2	2:B:266:VAL:HG12	2.22	0.42
1:A:286:MET:HG2	1:A:287:GLN:H	1.85	0.41
1:A:328:GLN:HE21	1:A:328:GLN:HB2	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:HIS:ND1	2:B:223:HIS:C	2.78	0.41
1:A:251:ARG:HH12	1:A:286:MET:HE3	1.85	0.41
1:A:380:ALA:O	1:A:381:LEU:C	2.63	0.41
2:B:206:GLU:OE2	2:B:267:LYS:NZ	2.54	0.41
4:B:400:ACP:O1G	4:B:400:ACP:O2B	2.39	0.41
1:A:325:THR:OG1	1:A:328:GLN:HB3	2.20	0.41
1:A:381:LEU:O	1:A:382:ARG:C	2.64	0.41
1:A:302:LEU:CD1	1:A:343:ILE:HD11	2.51	0.41
2:B:287:GLN:OE1	2:B:289:HIS:HE1	2.03	0.41
2:B:335:ASN:ND2	2:B:338:GLN:H	2.19	0.41
1:A:297:CYS:HB2	1:A:301:SER:HB2	2.03	0.40
2:B:187:ARG:HH11	2:B:187:ARG:HG3	1.86	0.40
1:A:225:LEU:HG	1:A:226:LEU:N	2.35	0.40
2:B:249:ILE:HD13	2:B:249:ILE:HG21	1.85	0.40
2:B:352:ARG:HA	2:B:353:PRO:HD2	1.90	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	254/291 (87%)	221 (87%)	25 (10%)	8 (3%)	3	12
2	B	255/291 (88%)	232 (91%)	17 (7%)	6 (2%)	4	17
All	All	509/582 (88%)	453 (89%)	42 (8%)	14 (3%)	4	14

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	HIS
1	A	354	GLU
2	B	170	ALA

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Mol	Chain	Res	Type
1	A	116	SER
1	A	221	GLN
1	A	332	ILE
2	B	270	ASP
1	A	288	GLU
1	A	295	ALA
1	A	335	ASN
2	B	219	LYS
2	B	224	PHE
2	B	332	ILE
2	B	357	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	227/249 (91%)	200 (88%)	27 (12%)	5	17
2	B	226/250 (90%)	196 (87%)	30 (13%)	4	14
All	All	453/499 (91%)	396 (87%)	57 (13%)	4	15

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	139	VAL
1	A	152	THR
1	A	153	VAL
1	A	172	ASP
1	A	175	ILE
1	A	181	MET
1	A	183	SER
1	A	249	ILE
1	A	251	ARG
1	A	275	ARG
1	A	279	GLN

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Mol	Chain	Res	Type
1	A	280	ASN
1	A	292	VAL
1	A	297	CYS
1	A	300	GLU
1	A	302	LEU
1	A	303	LYS
1	A	308	SER
1	A	313	THR
1	A	328	GLN
1	A	329	GLU
1	A	334	LEU
1	A	352	ARG
1	A	360	ILE
1	A	365	VAL
1	A	374	ASP
2	B	118	THR
2	B	119	CYS
2	B	121	ILE
2	B	124	LYS
2	B	139	VAL
2	B	140	VAL
2	B	154	SER
2	B	158	LYS
2	B	176	ARG
2	B	183	SER
2	B	202	LYS
2	B	212	SER
2	B	218	ARG
2	B	221	GLN
2	B	223	HIS
2	B	246	LYS
2	B	247	ARG
2	B	279	GLN
2	B	283	HIS
2	B	291	LYS
2	B	329	GLU
2	B	335	ASN
2	B	337	SER
2	B	345	LYS
2	B	349	ARG
2	B	352	ARG
2	B	356	CYS

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Mol	Chain	Res	Type
2	B	371	LYS
2	B	373	GLU
2	B	382	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	A	221	GLN
1	A	257	ASN
1	A	309	HIS
1	A	328	GLN
1	A	366	GLN
2	B	235	GLN
2	B	289	HIS
2	B	335	ASN
2	B	341	HIS
2	B	362	ASN

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	PTR	A	284	1	15,16,17	1.93	1 (6%)	17,22,24	0.82	1 (5%)

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	PTR	A	284	1	-	1/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	PTR	OH-CZ	-7.04	1.24	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	PTR	O3P-P-OH	2.24	111.95	105.32

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	284	PTR	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	284	PTR	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
4	ACP	A	101	3	31,33,33	2.42	9 (29%)	47,52,52	2.65	16 (34%)
4	ACP	B	400	3	31,33,33	2.59	9 (29%)	47,52,52	1.67	14 (29%)

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	ACP	A	101	3	-	3/19/38/38	0/3/3/3
4	ACP	B	400	3	-	7/19/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	ACP	PB-O3A	8.06	1.67	1.58
4	B	400	ACP	C4-N3	5.58	1.44	1.34
4	A	101	ACP	C8-N7	5.45	1.42	1.31
4	A	101	ACP	PB-O3A	5.41	1.64	1.58
4	A	101	ACP	PA-O3A	5.28	1.65	1.59
4	B	400	ACP	PA-O3A	5.06	1.65	1.59
4	B	400	ACP	PG-O1G	4.85	1.60	1.50
4	A	101	ACP	C5-C4	4.70	1.47	1.39
4	A	101	ACP	C4-N3	4.04	1.42	1.34
4	A	101	ACP	PG-O1G	3.65	1.57	1.50
4	B	400	ACP	C5-C4	3.52	1.45	1.39
4	B	400	ACP	C8-N7	3.28	1.38	1.31
4	B	400	ACP	PB-O1B	3.00	1.58	1.51
4	A	101	ACP	C5-N7	-2.91	1.33	1.39
4	B	400	ACP	C5-N7	-2.86	1.33	1.39
4	A	101	ACP	C4-N9	-2.30	1.32	1.37
4	A	101	ACP	C5'-C4'	2.25	1.58	1.51
4	B	400	ACP	C2-N1	2.06	1.37	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	101	ACP	C2'-C1'-N9	-7.86	93.78	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	101	ACP	O1G-PG-C3B	-6.88	96.36	111.37
4	A	101	ACP	O4'-C1'-N9	6.14	119.88	108.09
4	A	101	ACP	O2B-PB-O1B	5.61	128.20	109.95
4	A	101	ACP	C5-C4-N9	5.47	111.77	105.81
4	B	400	ACP	PB-O3A-PA	-3.79	120.00	132.37
4	A	101	ACP	C4-C5-N7	-3.68	106.38	110.58
4	A	101	ACP	C5-C4-N3	-3.54	121.85	126.72
4	A	101	ACP	O4'-C4'-C5'	3.23	119.67	109.33
4	A	101	ACP	C3'-C2'-C1'	3.15	107.42	101.46
4	A	101	ACP	PB-O3A-PA	-3.14	122.11	132.37
4	B	400	ACP	N6-C6-N1	3.07	125.20	118.38
4	B	400	ACP	C5-C4-N3	-3.01	122.57	126.72
4	A	101	ACP	N3-C2-N1	-2.99	124.05	128.58
4	B	400	ACP	O2'-C2'-C1'	2.95	120.27	110.10
4	A	101	ACP	C2-N1-C6	2.85	123.41	118.73
4	B	400	ACP	C5-C6-N6	-2.73	116.53	123.29
4	B	400	ACP	N3-C2-N1	-2.64	124.58	128.58
4	B	400	ACP	C2-N1-C6	2.61	123.03	118.73
4	A	101	ACP	C6-C5-N7	2.60	137.10	132.09
4	B	400	ACP	O3A-PA-O1A	2.37	117.83	110.70
4	A	101	ACP	C2'-C3'-C4'	2.26	106.97	102.61
4	B	400	ACP	O5'-PA-O1A	-2.22	100.15	108.94
4	B	400	ACP	C4-C5-N7	-2.15	108.12	110.58
4	B	400	ACP	C5-C4-N9	2.14	108.14	105.81
4	B	400	ACP	O2B-PB-O1B	2.12	116.86	109.95
4	B	400	ACP	O2'-C2'-C3'	-2.12	105.03	111.82
4	A	101	ACP	C4-N9-C8	-2.10	103.54	105.74
4	B	400	ACP	O3'-C3'-C4'	2.10	117.10	111.08
4	A	101	ACP	O2G-PG-O1G	2.01	117.58	112.39

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	101	ACP	PG-C3B-PB-O1B
4	A	101	ACP	PG-C3B-PB-O2B
4	A	101	ACP	PG-C3B-PB-O3A
4	B	400	ACP	PB-C3B-PG-O1G
4	B	400	ACP	PB-C3B-PG-O2G
4	B	400	ACP	PB-C3B-PG-O3G
4	B	400	ACP	PG-C3B-PB-O1B
4	B	400	ACP	PG-C3B-PB-O2B

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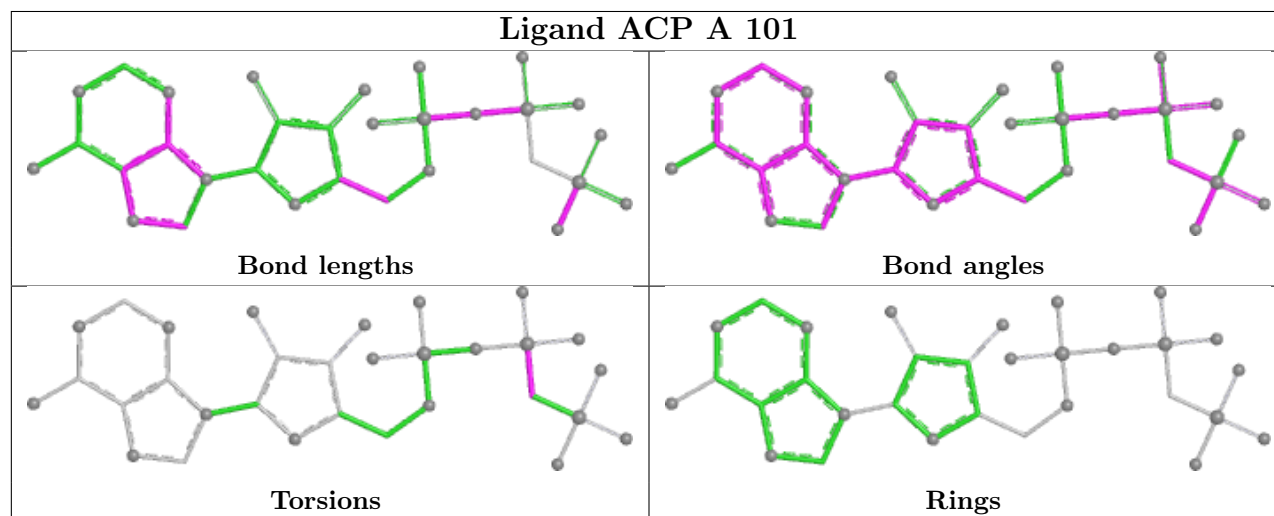
Mol	Chain	Res	Type	Atoms
4	B	400	ACP	PG-C3B-PB-O3A
4	B	400	ACP	PB-O3A-PA-O2A

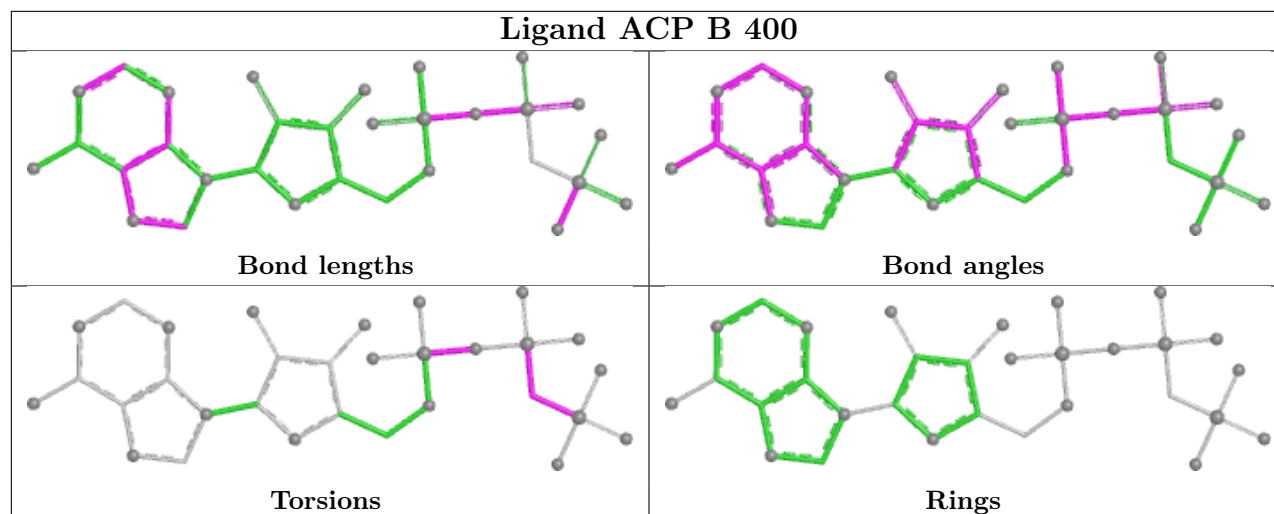
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	101	ACP	1	0
4	B	400	ACP	3	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	262/291 (90%)	0.91	39 (14%) 5 4	11, 28, 32, 36	29 (11%)
2	B	261/291 (89%)	0.64	23 (8%) 15 11	12, 27, 31, 40	21 (8%)
All	All	523/582 (89%)	0.77	62 (11%) 9 7	11, 27, 32, 40	50 (9%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	263	ARG	5.6
1	A	263	ARG	5.2
1	A	231	ARG	5.0
2	B	280	ASN	5.0
1	A	208	ALA	4.9
1	A	115	GLN	4.4
2	B	134	ASP	4.3
1	A	294	PHE	4.2
2	B	262	THR	4.0
1	A	287	GLN	3.9
2	B	220	HIS	3.9
1	A	223	HIS	3.9
1	A	191	ARG	3.9
2	B	328	GLN	3.8
1	A	371	LYS	3.7
1	A	200	PRO	3.6
2	B	281	ASP	3.5
1	A	187	ARG	3.4
1	A	305	ARG	3.3
2	B	169	GLU	3.3
2	B	126	LEU	3.2
1	A	289	HIS	3.2
1	A	281	ASP	3.2
1	A	127	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	387	GLU	2.9
1	A	260	LEU	2.9
2	B	171	MET	2.9
2	B	160	LEU	2.9
1	A	160	LEU	2.8
2	B	117	LEU	2.8
1	A	211	GLY	2.8
2	B	363	VAL	2.8
1	A	188	ASN	2.8
2	B	148	PRO	2.8
1	A	288	GLU	2.7
2	B	231	ARG	2.7
1	A	219	LYS	2.6
1	A	293	PRO	2.6
1	A	124	LYS	2.6
2	B	191	ARG	2.6
1	A	387	GLU	2.6
1	A	335	ASN	2.6
1	A	258	LEU	2.4
1	A	390	PRO	2.4
2	B	199	PRO	2.4
1	A	242	TYR	2.3
1	A	265	LEU	2.3
1	A	255	ALA	2.3
1	A	256	ARG	2.3
1	A	370	HIS	2.2
1	A	159	CYS	2.2
2	B	365	VAL	2.2
1	A	248	PHE	2.2
1	A	123	GLU	2.2
1	A	186	HIS	2.2
1	A	382	ARG	2.2
2	B	216	ARG	2.2
2	B	193	TYR	2.2
1	A	189	LEU	2.1
2	B	224	PHE	2.1
2	B	151	LYS	2.0
1	A	270	ASP	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	PTR	A	284	16/17	0.84	0.12	31,32,37,38	5

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

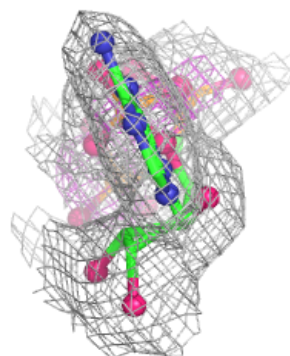
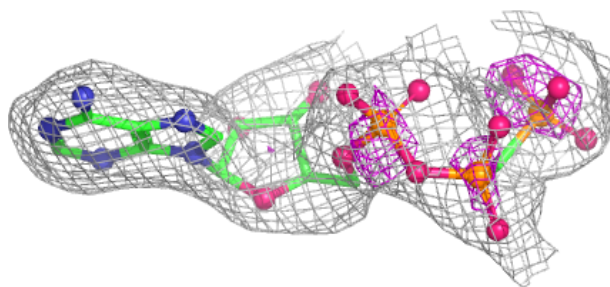
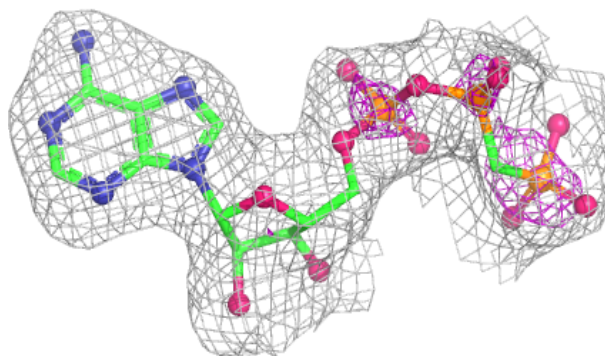
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	A	398	1/1	0.55	0.15	48,48,48,48	0
3	MG	A	399	1/1	0.66	0.16	48,48,48,48	0
3	MG	B	399	1/1	0.83	0.12	55,55,55,55	0
4	ACP	B	400	31/31	0.86	0.12	42,48,58,59	0
4	ACP	A	101	31/31	0.87	0.10	43,51,56,57	0
3	MG	B	398	1/1	0.90	0.13	57,57,57,57	0

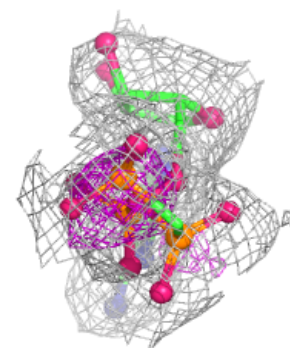
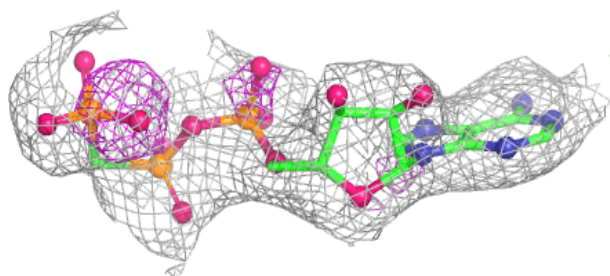
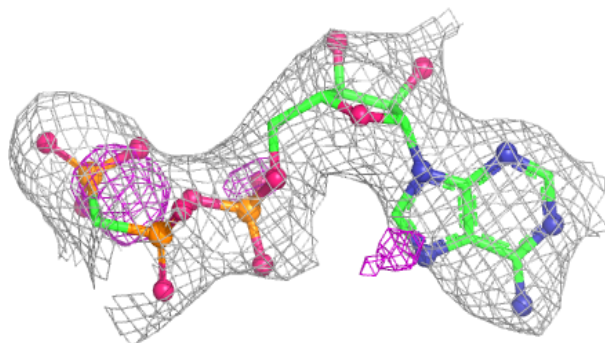
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP B 400:

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

**Electron density around ACP A 101:**

$2mF_o-DF_c$ (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.