



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2026 – 06:04 PM EDT

PDB ID : 10OT / pdb_000010ot
Title : Crystal structure of mouse CD38 in complex with compound 6
Authors : Jain, R.; Bigelow, L.
Deposited on : 2026-01-29
Resolution : 2.15 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 Phenix2.2
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.2
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

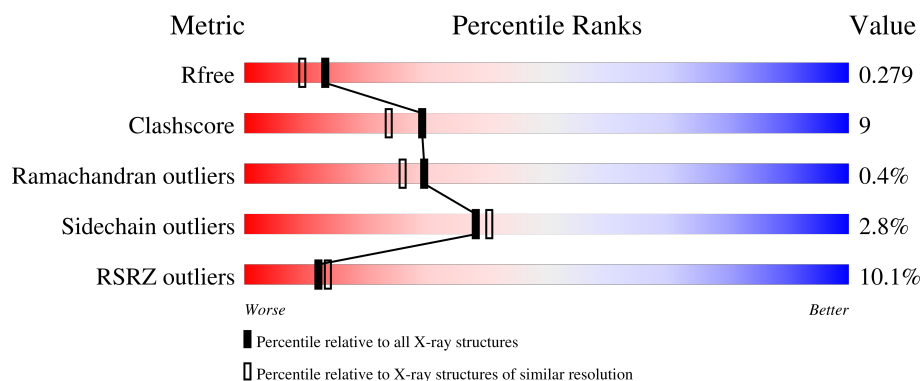
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	263	10% 72% 21% • 5%
1	B	263	9% 72% 21% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4367 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 ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase 1.

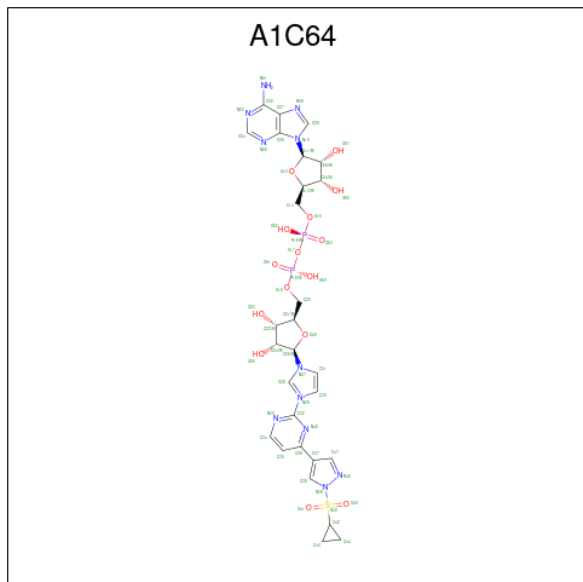
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	2	1	0
			2013	1282	342	370	19			
1	B	247	Total	C	N	O	S	0	2	0
			2007	1279	341	368	19			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	ASP	ASN	engineered mutation	UNP P56528
A	124	ASP	ASN	engineered mutation	UNP P56528
A	213	ASP	ASN	engineered mutation	UNP P56528
A	223	ASP	ASN	engineered mutation	UNP P56528
A	230	GLN	GLU	engineered mutation	UNP P56528
A	305	LEU	-	expression tag	UNP P56528
A	306	GLU	-	expression tag	UNP P56528
A	307	VAL	-	expression tag	UNP P56528
A	308	LEU	-	expression tag	UNP P56528
A	309	PHE	-	expression tag	UNP P56528
A	310	GLN	-	expression tag	UNP P56528
B	104	ASP	ASN	engineered mutation	UNP P56528
B	124	ASP	ASN	engineered mutation	UNP P56528
B	213	ASP	ASN	engineered mutation	UNP P56528
B	223	ASP	ASN	engineered mutation	UNP P56528
B	230	GLN	GLU	engineered mutation	UNP P56528
B	305	LEU	-	expression tag	UNP P56528
B	306	GLU	-	expression tag	UNP P56528
B	307	VAL	-	expression tag	UNP P56528
B	308	LEU	-	expression tag	UNP P56528
B	309	PHE	-	expression tag	UNP P56528
B	310	GLN	-	expression tag	UNP P56528

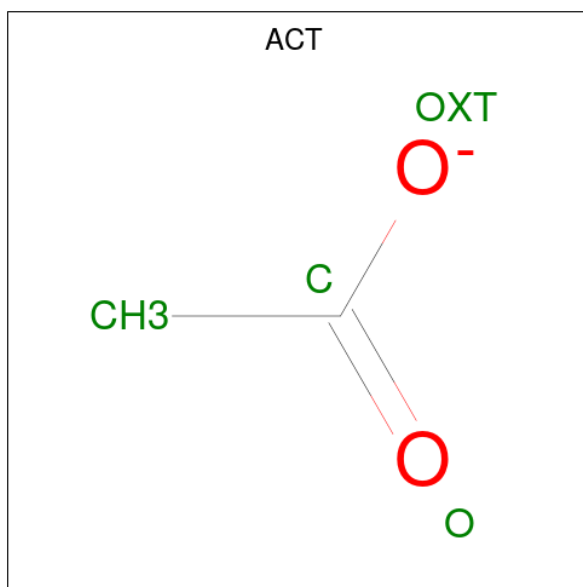
- Molecule 2 is [(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl [(2 {R},3 {S},4 {R},5 {R})-5-[3-[4-(1-cyclopropylsulfon

ylpyrazol-4-yl]pyrimidin-2-yl]imidazol-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methyl hydrogen phosphate (CCD ID: A1C64) (formula: $C_{28}H_{34}N_{11}O_{15}P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			57	28	11	15	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			57	28	11	15	2	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

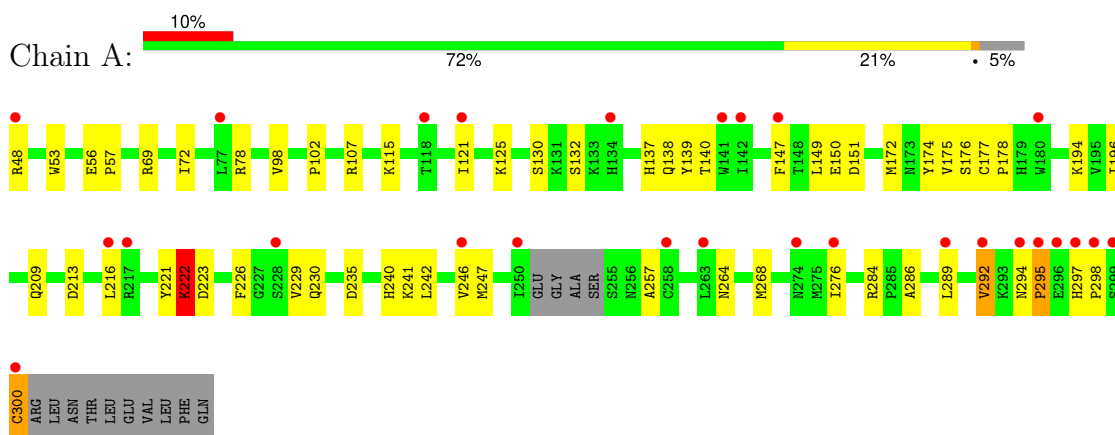
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total 114	O 114	0	0
4	B	111	Total 111	O 111	0	0

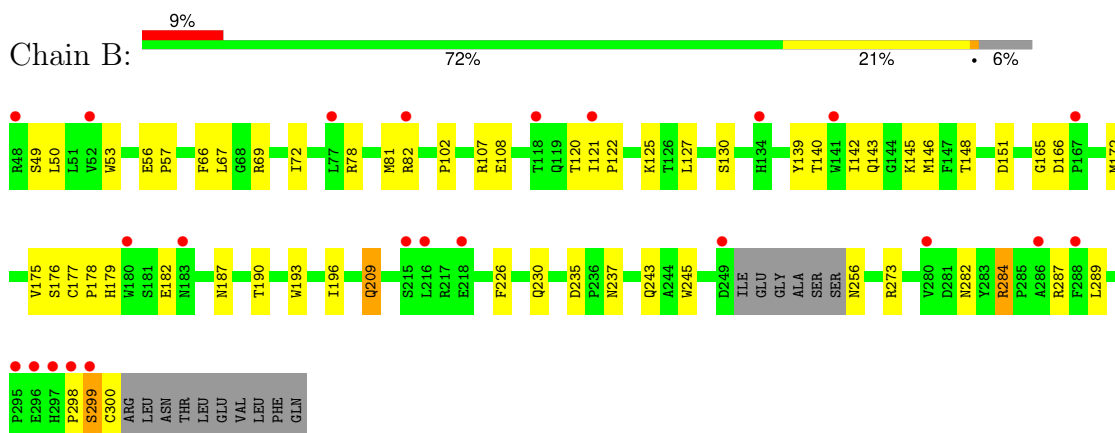
3 Residue-property plots

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: ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase 1



- Molecule 1: ADP-ribosyl cyclase/cyclic ADP-ribose hydrolase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	128.97Å 58.15Å 87.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.61 – 2.15 72.61 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (72.61-2.15) 99.3 (72.61-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.264 , 0.280 0.266 , 0.279	Depositor DCC
R_{free} test set	1832 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4367	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4721e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ACT, A1C64

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	0.86	6/2066 (0.3%)	0.94	10/2804 (0.4%)
1	B	0.80	2/2060 (0.1%)	0.98	3/2796 (0.1%)
All	All	0.83	8/4126 (0.2%)	0.96	13/5600 (0.2%)

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	B	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	ASP	C-N	14.24	1.50	1.34
1	A	177	CYS	C-N	12.60	1.48	1.33
1	A	56	GLU	C-N	6.70	1.49	1.33
1	B	176	SER	C-O	-5.88	1.16	1.23
1	A	176	SER	C-O	-5.63	1.16	1.23
1	B	122	PRO	C-O	-5.43	1.17	1.23
1	A	132	SER	C-O	-5.15	1.19	1.24
1	A	295	PRO	N-CD	-5.05	1.40	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ASP	CA-C-N	10.43	130.72	119.87
1	A	235	ASP	C-N-CA	10.43	130.72	119.87
1	A	56	GLU	CA-C-N	8.70	130.72	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	GLU	C-N-CA	8.70	130.72	119.84
1	A	177	CYS	CA-C-N	8.13	128.44	119.90
1	A	177	CYS	C-N-CA	8.13	128.44	119.90
1	A	177	CYS	O-C-N	-8.04	113.78	121.57
1	A	292	VAL	N-CA-C	-6.91	103.58	110.62
1	B	182	GLU	O-C-N	-6.10	114.47	122.59
1	A	235	ASP	O-C-N	-5.94	115.89	121.35
1	A	222	LYS	CB-CA-C	-5.14	101.12	110.63
1	B	151	ASP	CB-CA-C	5.04	120.34	110.67
1	B	120	THR	CA-CB-OG1	-5.04	102.05	109.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	273	ARG	Sidechain
1	B	66	PHE	Mainchain
1	B	82	ARG	Sidechain

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	2013	0	1955	40	0
1	B	2007	0	1949	35	0
2	A	57	0	0	0	0
2	B	57	0	0	1	0
3	A	4	0	3	0	0
3	B	4	0	3	1	0
4	A	114	0	0	2	0
4	B	111	0	0	0	0
All	All	4367	0	3910	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 9.

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:222:LYS:H	1:A:222:LYS:CD	1.93	0.79
1:A:78:ARG:HH21	1:A:147:PHE:HE1	1.32	0.77
1:B:282:ASN:HB3	1:B:287:ARG:HD3	1.67	0.76
1:B:102:PRO:HB2	1:B:178:PRO:HG3	1.73	0.69
1:B:146:MET:HE3	1:B:245:TRP:HH2	1.61	0.66
1:A:48:ARG:HH11	1:A:48:ARG:HG3	1.59	0.65
1:A:140:THR:HG21	1:A:151:ASP:OD2	1.96	0.65
1:A:264:ASN:O	1:A:268:MET:HG3	1.95	0.65
1:A:294:ASN:N	1:A:295:PRO:HD3	2.11	0.65
1:A:242:LEU:C	1:A:242:LEU:HD23	2.25	0.62
1:A:48:ARG:HG3	1:A:48:ARG:NH1	2.17	0.59
1:A:222:LYS:H	1:A:222:LYS:HD3	1.67	0.58
1:A:284:ARG:HH22	1:B:300:CYS:C	2.12	0.58
1:B:226:PHE:HA	1:B:230:GLN:HB2	1.85	0.58
1:B:284:ARG:HA	1:B:287:ARG:HB3	1.86	0.56
1:A:246:VAL:HG11	1:A:257:ALA:HB3	1.87	0.56
1:A:102:PRO:HB2	1:A:178:PRO:HG3	1.88	0.55
1:B:127:LEU:HD12	1:B:148:THR:HG22	1.88	0.55
1:A:221:TYR:CZ	1:A:223:ASP:HB2	2.43	0.54
1:A:297:HIS:CG	1:A:298:PRO:HD2	2.42	0.54
1:A:300:CYS:C	1:B:284:ARG:HH22	2.15	0.54
1:A:48:ARG:HH11	1:A:48:ARG:CG	2.20	0.54
1:B:107:ARG:HD2	1:B:107:ARG:H	1.73	0.54
1:B:140:THR:HG21	1:B:148:THR:HG23	1.90	0.53
1:A:121:ILE:HD12	1:A:147:PHE:HB2	1.89	0.53
1:A:241:LYS:HG3	1:A:276:ILE:CG2	2.39	0.52
1:B:209:GLN:OE1	1:B:243:GLN:NE2	2.41	0.52
1:A:121:ILE:HD11	1:A:125:LYS:O	2.11	0.51
1:B:209:GLN:HB3	1:B:243:GLN:HG3	1.92	0.51
1:A:149:LEU:HD21	1:A:196:ILE:HG13	1.94	0.50
1:A:107:ARG:NH2	1:A:194:LYS:HE2	2.27	0.50
1:A:78:ARG:NH2	1:A:147:PHE:HE1	2.08	0.49
1:A:213:ASP:HB3	1:A:216:LEU:HD12	1.94	0.49
1:A:240:HIS:HD2	4:A:505:HOH:O	1.96	0.48
1:A:241:LYS:HG3	1:A:276:ILE:HG22	1.94	0.48
1:B:298:PRO:O	1:B:299:SER:HB3	2.13	0.48
1:B:179:HIS:HD2	3:B:402:ACT:H3	1.79	0.47
1:A:69:ARG:HG3	1:B:72:ILE:HD11	1.97	0.47
1:B:190:THR:HG23	2:B:401:A1C64:N46	2.29	0.47
1:A:300:CYS:O	1:B:284:ARG:NH2	2.41	0.46
1:A:53:TRP:CZ2	1:A:102:PRO:HG2	2.51	0.46
1:A:137:HIS:NE2	1:A:150:GLU:HB2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:TRP:CE3	1:B:196:ILE:HD11	2.51	0.45
1:A:222:LYS:H	1:A:222:LYS:HD2	1.78	0.45
1:B:67[B]:LEU:HD12	1:B:67[B]:LEU:HA	1.83	0.45
1:B:102:PRO:HG3	1:B:165:GLY:O	2.16	0.45
1:A:121:ILE:HG21	4:A:537:HOH:O	2.17	0.45
1:B:172:MET:H	1:B:172:MET:HG2	1.65	0.45
1:A:172:MET:HB2	1:A:174:TYR:CE2	2.52	0.45
1:A:115:LYS:HE3	1:A:115:LYS:HB3	1.72	0.44
1:A:138:GLN:CD	1:B:142:ILE:HD12	2.42	0.44
1:B:81:MET:HE2	1:B:81:MET:HB3	1.83	0.44
1:B:107:ARG:HD3	1:B:108:GLU:OE2	2.16	0.44
1:B:139:TYR:HA	1:B:289:LEU:HD11	2.00	0.44
1:B:143:GLN:HE22	1:B:145:LYS:HE2	1.82	0.44
1:A:57:PRO:HB3	1:A:175:VAL:C	2.44	0.43
1:B:67[A]:LEU:HD23	1:B:67[A]:LEU:HA	1.88	0.43
1:A:139:TYR:HA	1:A:289:LEU:HD11	1.99	0.43
1:A:292:VAL:O	1:A:295:PRO:HG3	2.19	0.43
1:A:247:MET:HE2	1:A:286:ALA:HB3	2.00	0.43
1:B:102:PRO:O	1:B:187:ASN:HA	2.19	0.42
1:A:226:PHE:HA	1:A:230:GLN:HB2	2.00	0.42
1:B:50:LEU:HD23	1:B:166:ASP:CG	2.44	0.42
1:B:56:GLU:O	1:B:177:CYS:HB2	2.20	0.42
1:B:146:MET:HE3	1:B:245:TRP:CH2	2.49	0.41
1:B:235:ASP:OD2	1:B:237:ASN:HB2	2.21	0.41
1:B:53:TRP:CE3	1:B:178:PRO:HB3	2.56	0.41
1:B:57:PRO:HB3	1:B:175:VAL:C	2.46	0.41
1:A:72:ILE:HD11	1:B:69:ARG:HG3	2.03	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	246/263 (94%)	240 (98%)	6 (2%)	0	100	100
1	B	245/263 (93%)	232 (95%)	11 (4%)	2 (1%)	16	10
All	All	491/526 (93%)	472 (96%)	17 (4%)	2 (0%)	30	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284	ARG
1	B	299	SER

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	231/242 (96%)	225 (97%)	6 (3%)	40	43
1	B	230/242 (95%)	223 (97%)	7 (3%)	36	38
All	All	461/484 (95%)	448 (97%)	13 (3%)	38	40

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	VAL
1	A	130	SER
1	A	209	GLN
1	A	222	LYS
1	A	229	VAL
1	A	300	CYS
1	B	49	SER
1	B	78	ARG
1	B	121	ILE
1	B	125	LYS
1	B	130	SER
1	B	209	GLN
1	B	256	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	GLN
1	B	87	GLN
1	B	230	GLN
1	B	256	ASN
1	B	264	ASN
1	B	294	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	ACT	B	402	-	3,3,3	1.11	0	3,3,3	1.27	0
2	A1C64	B	401	-	62,64,64	3.26	32 (51%)	83,99,99	3.14	22 (26%)
3	ACT	A	402	-	3,3,3	1.11	0	3,3,3	1.26	0
2	A1C64	A	401	-	62,64,64	3.33	30 (48%)	83,99,99	3.83	27 (32%)

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	A1C64	B	401	-	-	9/46/80/80	0/8/8/8
2	A1C64	A	401	-	-	12/46/80/80	0/8/8/8

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	A1C64	C24-C22	-9.17	1.28	1.53
2	A	401	A1C64	C24-C22	-9.11	1.28	1.53
2	A	401	A1C64	O12-C13	-8.39	1.26	1.45
2	B	401	A1C64	N39-N46	-7.88	1.28	1.37
2	B	401	A1C64	O12-C13	-7.82	1.27	1.45
2	A	401	A1C64	O45-S40	-7.66	1.37	1.43
2	A	401	A1C64	N39-N46	-7.17	1.29	1.37
2	B	401	A1C64	O12-C11	7.07	1.58	1.42
2	A	401	A1C64	C56-C11	-6.97	1.31	1.53
2	B	401	A1C64	O49-C26	-6.36	1.27	1.42
2	A	401	A1C64	O49-C26	-6.30	1.27	1.42
2	B	401	A1C64	C56-C11	-6.22	1.33	1.53
2	A	401	A1C64	O12-C11	5.92	1.55	1.42
2	B	401	A1C64	O45-S40	-5.63	1.39	1.43
2	A	401	A1C64	C38-N39	-5.24	1.27	1.36
2	A	401	A1C64	O41-S40	-4.98	1.39	1.43
2	B	401	A1C64	C38-N39	-4.82	1.28	1.36
2	A	401	A1C64	C30-N29	-4.78	1.28	1.38
2	B	401	A1C64	C07-N08	-4.54	1.30	1.39
2	A	401	A1C64	C09-N10	-4.50	1.29	1.37
2	A	401	A1C64	C07-N08	-4.48	1.30	1.39
2	B	401	A1C64	O41-S40	-4.47	1.40	1.43
2	B	401	A1C64	C30-N29	-4.44	1.29	1.38
2	B	401	A1C64	C32-N33	-4.20	1.28	1.32
2	B	401	A1C64	C09-N10	-3.79	1.31	1.37
2	A	401	A1C64	C06-N10	-3.74	1.29	1.37
2	A	401	A1C64	C36-N48	-3.52	1.29	1.34
2	B	401	A1C64	C06-N10	-3.48	1.30	1.37
2	A	401	A1C64	C02-N01	3.45	1.43	1.34
2	B	401	A1C64	C36-N48	-3.41	1.29	1.34
2	B	401	A1C64	C02-N01	3.36	1.42	1.34
2	A	401	A1C64	O49-C21	3.31	1.52	1.45
2	B	401	A1C64	C31-N27	-3.27	1.28	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	A1C64	C47-N46	-3.23	1.28	1.32
2	A	401	A1C64	C31-N27	-3.21	1.28	1.37
2	B	401	A1C64	C28-N29	-3.02	1.28	1.33
2	A	401	A1C64	P18-O50	-2.96	1.41	1.55
2	A	401	A1C64	C56-C54	-2.94	1.45	1.53
2	A	401	A1C64	C07-C06	-2.84	1.34	1.39
2	B	401	A1C64	C28-N27	-2.82	1.29	1.33
2	B	401	A1C64	P18-O50	-2.75	1.42	1.55
2	A	401	A1C64	C32-N33	-2.64	1.29	1.32
2	A	401	A1C64	P16-O52	-2.47	1.43	1.55
2	A	401	A1C64	C04-N05	-2.44	1.29	1.33
2	A	401	A1C64	P18-O51	-2.43	1.42	1.50
2	B	401	A1C64	P18-O51	-2.37	1.42	1.50
2	B	401	A1C64	P16-O52	-2.30	1.44	1.55
2	B	401	A1C64	O23-C22	-2.30	1.37	1.43
2	B	401	A1C64	O49-C21	2.28	1.50	1.45
2	A	401	A1C64	C28-N27	-2.28	1.30	1.33
2	A	401	A1C64	C06-N05	-2.27	1.30	1.34
2	A	401	A1C64	C47-N46	-2.24	1.29	1.32
2	A	401	A1C64	C24-C26	2.24	1.60	1.53
2	B	401	A1C64	C24-C26	2.20	1.60	1.53
2	B	401	A1C64	O15-C14	-2.17	1.36	1.44
2	B	401	A1C64	C04-N05	-2.14	1.30	1.33
2	B	401	A1C64	C07-C06	-2.13	1.35	1.39
2	B	401	A1C64	C06-N05	-2.13	1.30	1.34
2	A	401	A1C64	O25-C24	-2.12	1.37	1.43
2	A	401	A1C64	C28-N29	-2.09	1.30	1.33
2	B	401	A1C64	C04-N03	-2.06	1.30	1.33
2	B	401	A1C64	C32-N48	-2.02	1.28	1.34

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	A1C64	O45-S40-O41	-24.82	100.48	119.17
2	B	401	A1C64	O45-S40-O41	-20.43	103.79	119.17
2	A	401	A1C64	C34-N33-C32	12.89	121.58	114.36
2	B	401	A1C64	C34-N33-C32	10.41	120.19	114.36
2	A	401	A1C64	C24-C26-N27	7.32	131.31	113.31
2	A	401	A1C64	C36-N48-C32	6.01	121.22	115.99
2	A	401	A1C64	O41-S40-C42	5.74	115.14	107.82
2	B	401	A1C64	C24-C26-N27	5.35	126.45	113.31
2	A	401	A1C64	C54-C56-C11	5.25	111.39	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	A1C64	N05-C04-N03	-4.84	121.26	128.58
2	B	401	A1C64	C36-N48-C32	4.68	120.06	115.99
2	A	401	A1C64	C35-C34-N33	-4.63	118.30	123.97
2	B	401	A1C64	N05-C04-N03	-4.59	121.64	128.58
2	A	401	A1C64	N33-C32-N48	-4.55	121.10	126.18
2	B	401	A1C64	C07-C06-N05	-4.54	120.47	126.72
2	A	401	A1C64	C07-C06-N05	-4.35	120.72	126.72
2	B	401	A1C64	N33-C32-N29	4.12	119.62	115.35
2	A	401	A1C64	O49-C26-N27	-4.09	100.28	108.08
2	A	401	A1C64	N33-C32-N29	4.00	119.50	115.35
2	A	401	A1C64	N48-C32-N29	3.91	119.41	115.35
2	A	401	A1C64	C04-N05-C06	3.61	120.65	111.83
2	B	401	A1C64	C35-C34-N33	-3.57	119.59	123.97
2	B	401	A1C64	O49-C26-N27	-3.56	101.29	108.08
2	A	401	A1C64	C22-C24-C26	3.46	108.00	101.46
2	B	401	A1C64	C04-N05-C06	3.42	120.18	111.83
2	B	401	A1C64	N05-C06-N10	3.24	132.68	127.17
2	B	401	A1C64	O25-C24-C22	3.21	122.10	111.82
2	B	401	A1C64	N33-C32-N48	-2.88	122.96	126.18
2	B	401	A1C64	C24-C22-C21	2.80	108.03	102.61
2	A	401	A1C64	N05-C06-N10	2.78	131.89	127.17
2	B	401	A1C64	C26-N27-C31	-2.72	122.41	126.33
2	A	401	A1C64	C35-C36-N48	-2.70	119.77	122.92
2	A	401	A1C64	C56-C54-C13	-2.60	97.59	102.61
2	A	401	A1C64	C06-C07-N08	-2.55	107.67	110.58
2	B	401	A1C64	O50-P18-O17	2.54	114.13	107.27
2	B	401	A1C64	C54-C56-C11	2.53	106.24	101.46
2	A	401	A1C64	O12-C11-N10	2.46	112.82	108.09
2	B	401	A1C64	C32-N29-C30	2.45	128.30	124.94
2	B	401	A1C64	C22-C24-C26	2.42	106.03	101.46
2	A	401	A1C64	C24-C22-C21	2.36	107.17	102.61
2	A	401	A1C64	C07-N08-C09	2.28	107.03	103.45
2	B	401	A1C64	N10-C09-N08	-2.27	110.71	113.94
2	A	401	A1C64	N10-C09-N08	-2.24	110.76	113.94
2	A	401	A1C64	O25-C24-C22	2.19	118.83	111.82
2	A	401	A1C64	C37-C38-N39	-2.16	107.66	109.57
2	B	401	A1C64	N27-C28-N29	2.14	110.92	108.50
2	A	401	A1C64	O23-C22-C24	2.13	118.64	111.82
2	B	401	A1C64	O41-S40-C42	2.10	110.50	107.82
2	A	401	A1C64	O12-C11-C56	-2.04	102.25	106.62

There are no chirality outliers.

All (21) torsion outliers are listed below:

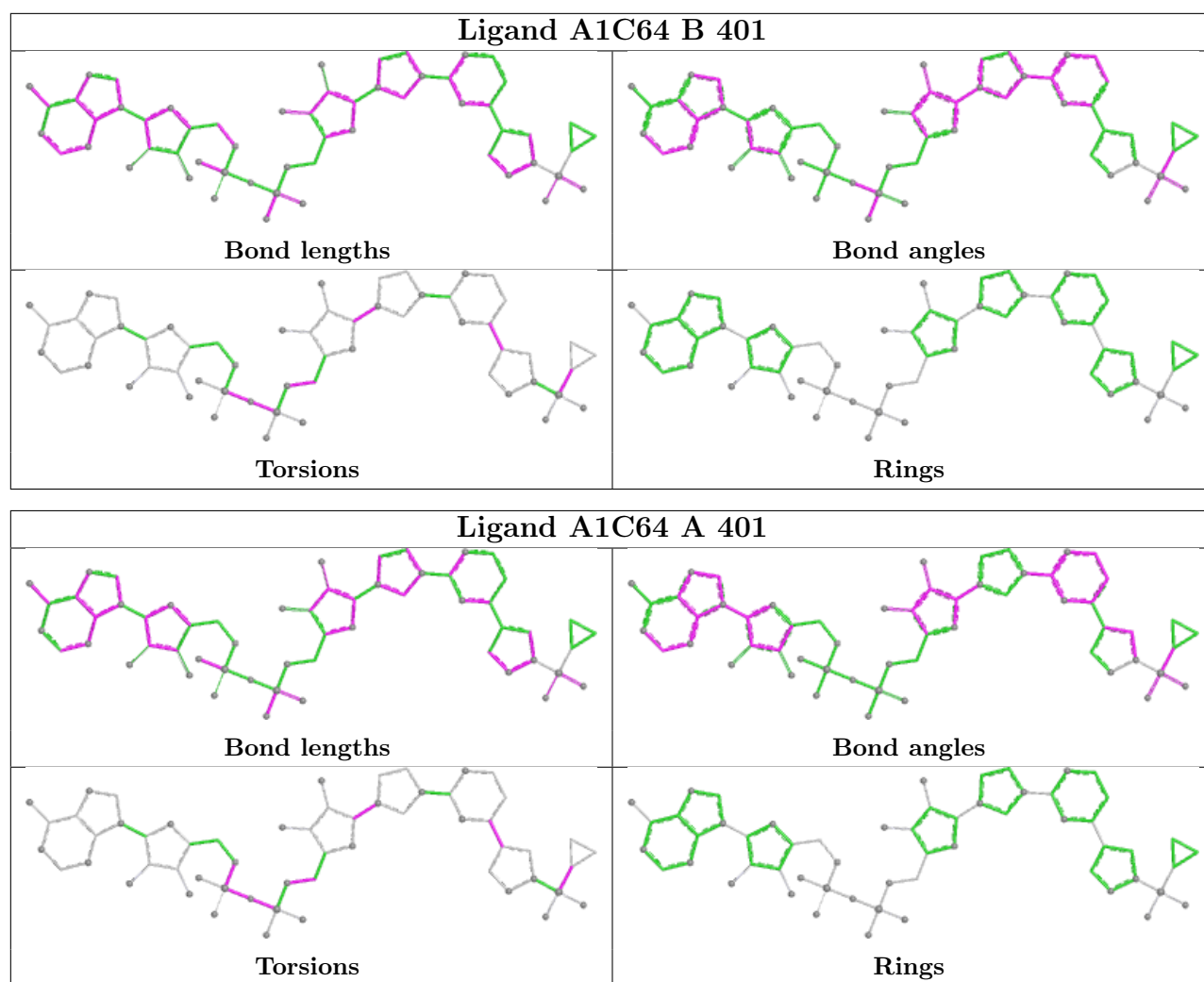
Mol	Chain	Res	Type	Atoms
2	A	401	A1C64	C35-C36-C37-C38
2	A	401	A1C64	C44-C42-S40-N39
2	B	401	A1C64	C43-C42-S40-N39
2	B	401	A1C64	C44-C42-S40-N39
2	B	401	A1C64	P16-O17-P18-O51
2	A	401	A1C64	P18-O17-P16-O15
2	B	401	A1C64	P18-O17-P16-O15
2	A	401	A1C64	C43-C42-S40-O41
2	A	401	A1C64	C24-C26-N27-C28
2	B	401	A1C64	C24-C26-N27-C28
2	A	401	A1C64	C14-O15-P16-O53
2	A	401	A1C64	N48-C36-C37-C38
2	B	401	A1C64	N48-C36-C37-C38
2	B	401	A1C64	C35-C36-C37-C38
2	B	401	A1C64	C21-C20-O19-P18
2	A	401	A1C64	C21-C20-O19-P18
2	A	401	A1C64	P16-O17-P18-O50
2	A	401	A1C64	P16-O17-P18-O51
2	B	401	A1C64	P16-O17-P18-O50
2	A	401	A1C64	C24-C26-N27-C31
2	A	401	A1C64	C44-C42-S40-O41

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	ACT	1	0
2	B	401	A1C64	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	249/263 (94%)	0.91	27 (10%)	11 12	19, 40, 60, 85	4 (1%)
1	B	247/263 (93%)	0.98	23 (9%)	14 16	17, 41, 59, 82	5 (2%)
All	All	496/526 (94%)	0.94	50 (10%)	12 14	17, 40, 60, 85	9 (1%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	LEU	4.5
1	A	250	ILE	4.5
1	A	299	SER	4.2
1	B	215	SER	4.2
1	B	141	TRP	4.0
1	B	183[A]	ASN	3.7
1	B	216	LEU	3.7
1	B	295	PRO	3.4
1	B	134	HIS	3.3
1	A	141	TRP	3.2
1	A	300	CYS	3.2
1	B	299	SER	3.1
1	A	258	CYS	3.0
1	A	289	LEU	3.0
1	B	118	THR	2.8
1	A	134	HIS	2.7
1	B	218	GLU	2.7
1	B	296	GLU	2.7
1	B	180	TRP	2.7
1	B	297	HIS	2.6
1	B	249	ASP	2.6
1	A	121	ILE	2.6
1	A	147	PHE	2.5
1	A	142	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	77	LEU	2.4
1	A	180	TRP	2.4
1	A	292	VAL	2.4
1	B	298	PRO	2.4
1	A	246	VAL	2.4
1	B	280	VAL	2.4
1	B	121	ILE	2.3
1	A	263	LEU	2.3
1	A	118	THR	2.3
1	A	298	PRO	2.3
1	A	217	ARG	2.3
1	B	286	ALA	2.2
1	B	288	PHE	2.2
1	A	295	PRO	2.2
1	B	52	VAL	2.1
1	A	48	ARG	2.1
1	A	228	SER	2.1
1	A	274[A]	ASN	2.1
1	B	82	ARG	2.1
1	A	276	ILE	2.1
1	A	294	ASN	2.1
1	B	167	PRO	2.1
1	A	296	GLU	2.0
1	A	77	LEU	2.0
1	B	48	ARG	2.0
1	A	297	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

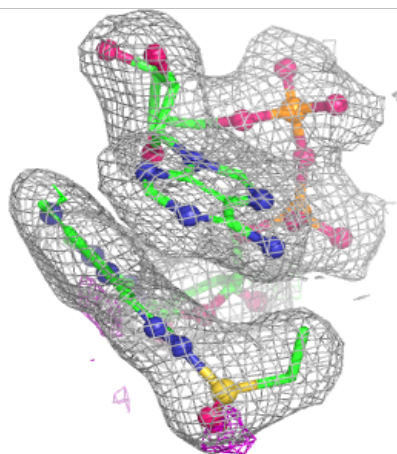
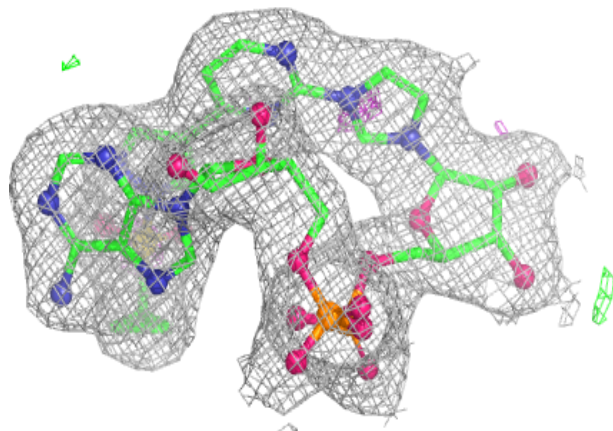
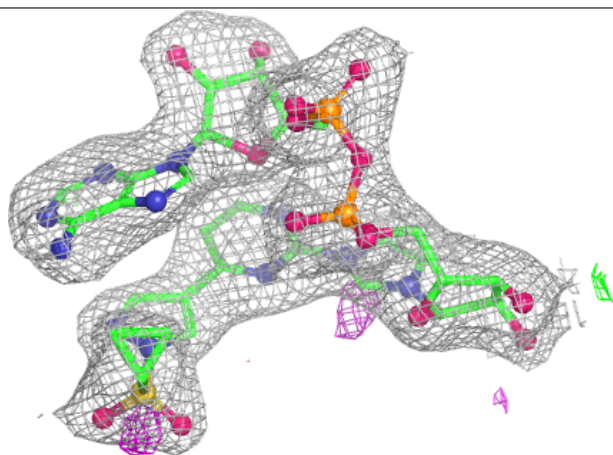
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	A	402	4/4	0.66	0.23	37,40,46,48	0
3	ACT	B	402	4/4	0.68	0.21	42,42,48,50	0
2	A1C64	B	401	57/57	0.94	0.09	29,39,48,53	0
2	A1C64	A	401	57/57	0.95	0.08	31,37,47,52	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.

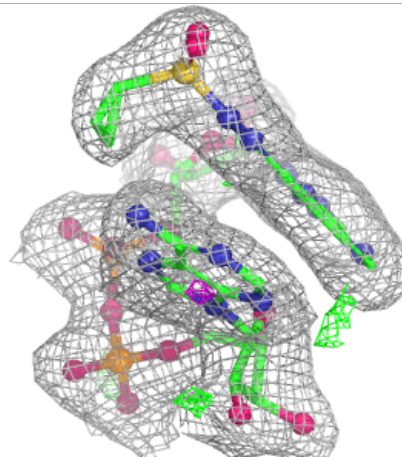
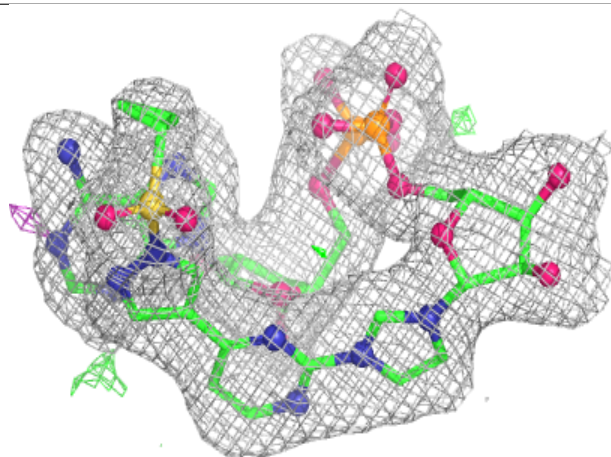
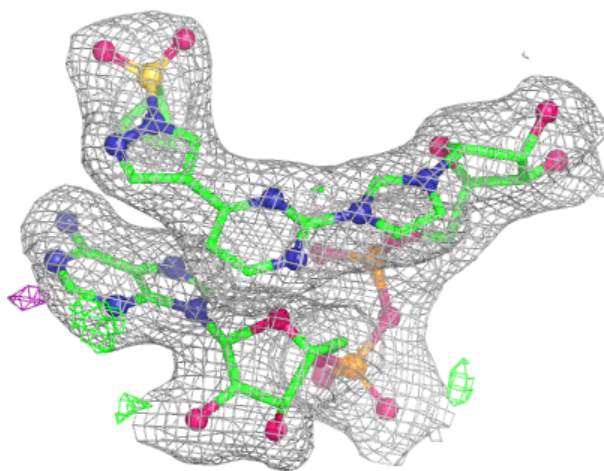
Electron density around A1C64 B 401:

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 A1C64 A 401:

$2mF_o-DF_c$ (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.