



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:47 PM UTC

PDB ID : 9MZA / pdb_00009mza
Title : Chemically Hijacked BCL6-TCIP3-p300 Complex
Authors : Hinshaw, S.M.; Gray, N.S.; Nix, M.N.; Gourisankar, S.; Martinez, M.; Crabtree, G.R.
Deposited on : 2025-01-22
Resolution : 2.10 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

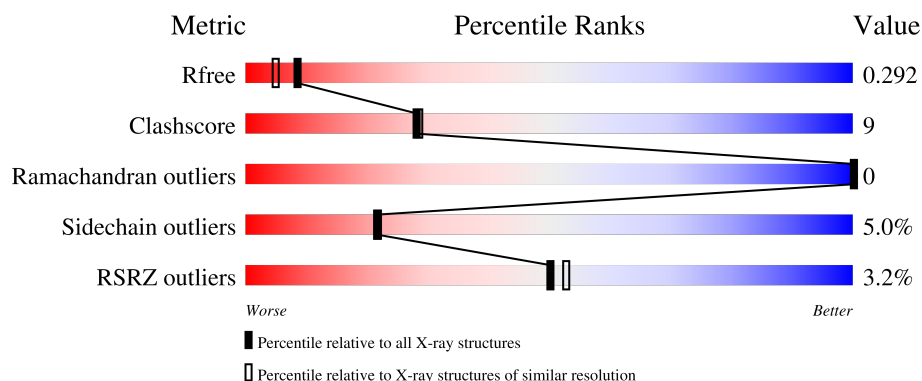
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	128	2% 81% 11% 5%
1	C	128	2% 80% 16% • •
2	B	145	5% 59% 17% • 23%
2	D	145	3% 59% 17% • • 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4493 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 B-cell lymphoma 6 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			985	624	175	178	8			
1	C	123	Total	C	N	O	S	0	1	0
			1005	635	179	183	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP P41182
A	3	PRO	-	expression tag	UNP P41182
A	4	GLY	-	expression tag	UNP P41182
A	8	GLN	CYS	conflict	UNP P41182
A	67	ARG	CYS	conflict	UNP P41182
A	84	ASN	CYS	conflict	UNP P41182
C	2	GLY	-	expression tag	UNP P41182
C	3	PRO	-	expression tag	UNP P41182
C	4	GLY	-	expression tag	UNP P41182
C	8	GLN	CYS	conflict	UNP P41182
C	67	ARG	CYS	conflict	UNP P41182
C	84	ASN	CYS	conflict	UNP P41182

- Molecule 2 is a protein called Histone acetyltransferase p300.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	112	Total	C	N	O	S	0	2	0
			958	620	153	180	5			
2	D	113	Total	C	N	O	S	0	0	0
			955	619	154	177	5			

There are 46 discrepancies between the modelled and reference sequences:

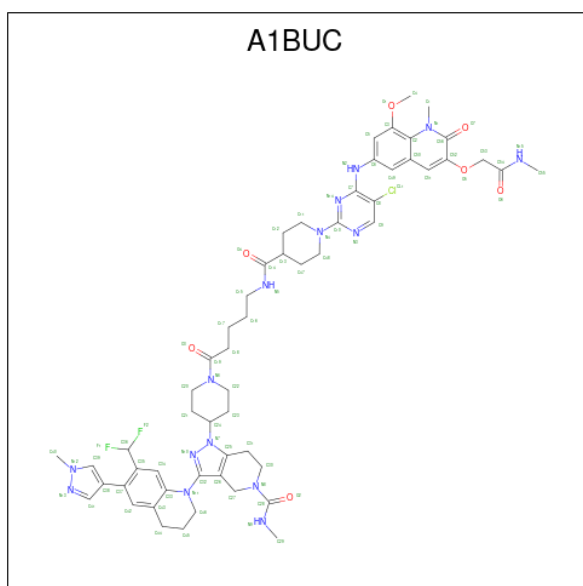
Chain	Residue	Modelled	Actual	Comment	Reference
B	1017	MET	-	initiating methionine	UNP Q09472
B	1018	HIS	-	expression tag	UNP Q09472
B	1019	HIS	-	expression tag	UNP Q09472
B	1020	HIS	-	expression tag	UNP Q09472
B	1021	HIS	-	expression tag	UNP Q09472
B	1022	HIS	-	expression tag	UNP Q09472
B	1023	HIS	-	expression tag	UNP Q09472
B	1024	SER	-	expression tag	UNP Q09472
B	1025	SER	-	expression tag	UNP Q09472
B	1026	GLY	-	expression tag	UNP Q09472
B	1027	VAL	-	expression tag	UNP Q09472
B	1028	ASP	-	expression tag	UNP Q09472
B	1029	LEU	-	expression tag	UNP Q09472
B	1030	GLY	-	expression tag	UNP Q09472
B	1031	THR	-	expression tag	UNP Q09472
B	1032	GLU	-	expression tag	UNP Q09472
B	1033	ASN	-	expression tag	UNP Q09472
B	1034	LEU	-	expression tag	UNP Q09472
B	1035	TYR	-	expression tag	UNP Q09472
B	1036	PHE	-	expression tag	UNP Q09472
B	1037	GLN	-	expression tag	UNP Q09472
B	1038	SER	-	expression tag	UNP Q09472
B	1039	MET	-	expression tag	UNP Q09472
D	1017	MET	-	initiating methionine	UNP Q09472
D	1018	HIS	-	expression tag	UNP Q09472
D	1019	HIS	-	expression tag	UNP Q09472
D	1020	HIS	-	expression tag	UNP Q09472
D	1021	HIS	-	expression tag	UNP Q09472
D	1022	HIS	-	expression tag	UNP Q09472
D	1023	HIS	-	expression tag	UNP Q09472
D	1024	SER	-	expression tag	UNP Q09472
D	1025	SER	-	expression tag	UNP Q09472
D	1026	GLY	-	expression tag	UNP Q09472
D	1027	VAL	-	expression tag	UNP Q09472
D	1028	ASP	-	expression tag	UNP Q09472
D	1029	LEU	-	expression tag	UNP Q09472
D	1030	GLY	-	expression tag	UNP Q09472
D	1031	THR	-	expression tag	UNP Q09472
D	1032	GLU	-	expression tag	UNP Q09472
D	1033	ASN	-	expression tag	UNP Q09472
D	1034	LEU	-	expression tag	UNP Q09472
D	1035	TYR	-	expression tag	UNP Q09472
D	1036	PHE	-	expression tag	UNP Q09472

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1037	GLN	-	expression tag	UNP Q09472
D	1038	SER	-	expression tag	UNP Q09472
D	1039	MET	-	expression tag	UNP Q09472

- Molecule 3 is 1-{1-[5-({1-[5-chloro-4-({8-methoxy-1-methyl-3-[2-(methylamino)-2-oxoethoxy]-2-oxo-1,2-dihydroquinolin-6-yl}amino)pyrimidin-2-yl]piperidine-4-carbonyl}amino)pentanoyl]piperidin-4-yl}-3-[(6M)-7-(difluoromethyl)-6-(1-methyl-1H-pyrazol-4-yl)-3,4-dihydroquinolin-1(2H)-yl]-N-methyl-1,4,6,7-tetrahydro-5H-pyrazolo[4,3-c]pyridine-5-carboxamide (CCD ID: A1BUC) (formula: C₅₆H₆₈ClF₂N₁₅O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			81	56	1	2	15	7		
3	C	1	Total	C	Cl	F	N	O	0	0
			81	56	1	2	15	7		

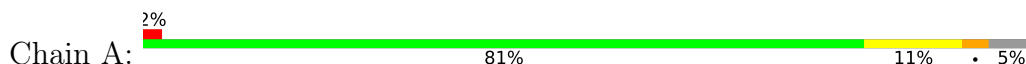
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	128	Total	O	0	0
			128	128		
4	B	86	Total	O	0	0
			86	86		
4	C	132	Total	O	0	0
			132	132		
4	D	82	Total	O	0	0
			82	82		

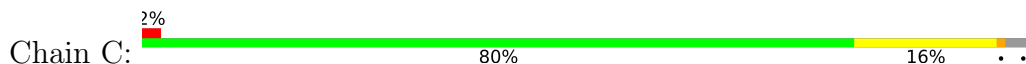
3 Residue-property plots [i](#)

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.

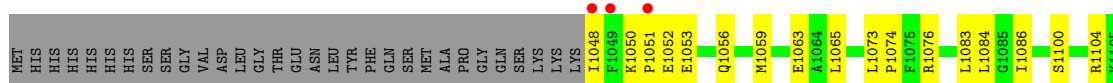
- Molecule 1: B-cell lymphoma 6 protein



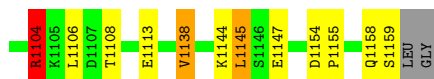
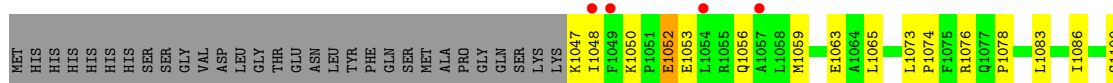
- Molecule 1: B-cell lymphoma 6 protein



- Molecule 2: Histone acetyltransferase p300



- Molecule 2: Histone acetyltransferase p300



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.39Å 94.79Å 97.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 2.10 60.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (60.00-2.10) 98.9 (60.00-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.217 , 0.277 0.245 , 0.292	Depositor DCC
R_{free} test set	2021 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4493	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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 30.18 % 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 1.3659e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: A1BUC

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	0.64	0/999	1.20	2/1347 (0.1%)
1	C	0.64	0/1020	1.20	3/1374 (0.2%)
2	B	0.57	0/988	1.13	1/1343 (0.1%)
2	D	0.57	0/982	1.16	3/1333 (0.2%)
All	All	0.60	0/3989	1.17	9/5397 (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	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1108	THR	CA-CB-OG1	-7.08	98.97	109.60
1	C	88	ASP	CA-CB-CG	6.59	119.19	112.60
2	B	1152	GLU	CB-CG-CD	-6.25	101.97	112.60
2	D	1147	GLU	CB-CA-C	-5.99	101.23	110.81
1	C	26	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	A	26	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	A	32	THR	CA-CB-OG1	-5.34	101.60	109.60
2	D	1104	ARG	N-CA-CB	5.25	117.62	110.01
1	C	103	MET	CG-SD-CE	-5.06	89.76	100.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	ARG	Sidechain
1	C	94	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	985	0	1008	14	0
1	C	1005	0	1020	28	0
2	B	958	0	937	15	0
2	D	955	0	940	14	0
3	A	81	0	0	2	0
3	C	81	0	0	1	0
4	A	128	0	0	8	0
4	B	86	0	0	5	0
4	C	132	0	0	15	0
4	D	82	0	0	3	0
All	All	4493	0	3905	71	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 (71) 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:123:LYS:O	4:A:301:HOH:O	1.96	0.84
1:C:39:SER:O	4:C:301:HOH:O	1.98	0.82
1:A:88:ASP:CG	4:A:303:HOH:O	2.34	0.71
1:A:17:ASP:OD2	4:A:302:HOH:O	2.09	0.70
2:B:1159:SER:N	4:B:1201:HOH:O	2.23	0.69
2:B:1104:ARG:HD3	4:B:1265:HOH:O	1.92	0.69
1:C:116[A]:HIS:ND1	4:C:304:HOH:O	2.24	0.69
3:A:201:A1BUC:C1	3:A:201:A1BUC:O1	2.40	0.69
1:C:17:ASP:OD2	4:C:302:HOH:O	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ILE:HG12	1:C:125:ILE:CD1	2.24	0.67
1:A:98:ARG:HD3	4:A:373:HOH:O	1.94	0.66
3:C:201:A1BUC:O1	3:C:201:A1BUC:C1	2.44	0.66
1:C:33:ASP:O	4:C:303:HOH:O	2.12	0.66
1:A:88:ASP:OD2	4:A:303:HOH:O	2.14	0.65
1:C:116[A]:HIS:CE1	4:C:304:HOH:O	2.52	0.62
2:D:1138:VAL:HG12	4:D:1251:HOH:O	2.00	0.62
1:C:102:ILE:HG12	1:C:125:ILE:HD13	1.82	0.62
1:C:98:ARG:HD2	4:C:354:HOH:O	1.99	0.61
1:A:115:GLU:HG3	4:A:408:HOH:O	2.02	0.60
2:D:1052:GLU:OE2	2:D:1056:GLN:HG3	2.04	0.56
1:C:106:MET:CE	1:C:121:CYS:HB3	2.36	0.55
1:C:102:ILE:CG1	1:C:125:ILE:HD11	2.37	0.55
1:C:102:ILE:HG12	1:C:125:ILE:HD11	1.90	0.54
1:A:51:MET:SD	1:C:31:LEU:HD12	2.47	0.54
1:C:98:ARG:CD	4:C:354:HOH:O	2.55	0.54
1:C:67:ARG:NH1	4:C:306:HOH:O	2.40	0.53
1:A:58:TYR:O	1:A:62:THR:HB	2.08	0.52
2:B:1158:GLN:HB2	4:B:1201:HOH:O	2.09	0.52
1:C:88:ASP:HB3	4:C:363:HOH:O	2.09	0.52
1:A:116:HIS:HB2	4:A:379:HOH:O	2.10	0.51
2:D:1078:PRO:HG2	4:D:1279:HOH:O	2.10	0.51
2:B:1138:VAL:HG12	4:B:1244:HOH:O	2.09	0.51
1:C:106:MET:HE2	1:C:121:CYS:CB	2.41	0.51
2:D:1104:ARG:HD3	4:D:1261:HOH:O	2.12	0.49
1:A:94:ARG:NH2	4:A:304:HOH:O	2.33	0.49
1:A:31:LEU:HD12	1:C:51:MET:SD	2.52	0.48
2:D:1154:ASP:HB2	2:D:1155:PRO:HD3	1.95	0.48
2:B:1153:ILE:HG13	2:B:1157:MET:HG2	1.96	0.48
1:C:75:ASP:HB2	4:C:375:HOH:O	2.14	0.47
2:B:1086:ILE:HG13	2:B:1086:ILE:O	2.15	0.47
2:D:1086:ILE:O	2:D:1086:ILE:HG13	2.14	0.47
2:B:1059:MET:HE2	2:B:1106:LEU:HD13	1.96	0.47
1:C:106:MET:HE2	1:C:121:CYS:HB3	1.98	0.46
1:C:116[B]:HIS:CD2	4:C:318:HOH:O	2.67	0.46
1:C:106:MET:HE3	1:C:121:CYS:HB3	1.97	0.46
1:C:115:GLU:HG3	4:C:410:HOH:O	2.16	0.46
2:B:1065:LEU:HD22	2:B:1145:LEU:HD22	1.98	0.45
2:D:1158:GLN:CG	2:D:1159:SER:N	2.79	0.45
2:D:1059:MET:HE2	2:D:1106:LEU:HD13	1.99	0.45
2:B:1052:GLU:OE2	2:B:1056:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1076:ARG:O	2:D:1100:SER:HB3	2.16	0.44
2:D:1050:LYS:O	2:D:1053:GLU:HB2	2.16	0.44
1:C:88:ASP:CG	4:C:363:HOH:O	2.61	0.44
1:A:8:GLN:HG2	1:C:96:ASN:HA	1.99	0.44
1:C:116[B]:HIS:CG	4:C:362:HOH:O	2.71	0.44
2:B:1050:LYS:H	2:B:1053:GLU:CD	2.27	0.43
2:B:1084:LEU:HD11	4:B:1246:HOH:O	2.18	0.42
2:B:1076:ARG:O	2:B:1100:SER:HB3	2.19	0.42
2:B:1059:MET:O	2:B:1063[B]:GLU:HG2	2.20	0.42
2:D:1065:LEU:HD22	2:D:1145:LEU:HD22	2.02	0.42
1:C:88:ASP:CB	4:C:363:HOH:O	2.68	0.41
2:D:1158:GLN:HG2	2:D:1159:SER:N	2.35	0.41
2:B:1073:LEU:N	2:B:1074:PRO:CD	2.84	0.41
2:B:1050:LYS:O	2:B:1051:PRO:C	2.64	0.41
2:D:1059:MET:O	2:D:1063:GLU:HG2	2.21	0.41
2:D:1073:LEU:N	2:D:1074:PRO:CD	2.84	0.41
1:A:60:ILE:HG23	1:A:66:LYS:HD3	2.03	0.40
1:C:121:CYS:O	1:C:125:ILE:HG12	2.21	0.40
1:A:26:ARG:HH11	1:A:26:ARG:HD2	1.61	0.40
3:A:201:A1BUC:C41	3:A:201:A1BUC:F1	2.59	0.40
1:C:102:ILE:HG13	1:C:125:ILE:HD11	2.03	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	120/128 (94%)	116 (97%)	4 (3%)	0	100	100
1	C	122/128 (95%)	118 (97%)	4 (3%)	0	100	100
2	B	112/145 (77%)	110 (98%)	2 (2%)	0	100	100
2	D	111/145 (77%)	108 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	465/546 (85%)	452 (97%)	13 (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	112/115 (97%)	108 (96%)	4 (4%)	31	34
1	C	114/115 (99%)	112 (98%)	2 (2%)	51	60
2	B	109/135 (81%)	102 (94%)	7 (6%)	16	14
2	D	108/135 (80%)	99 (92%)	9 (8%)	10	8
All	All	443/500 (89%)	421 (95%)	22 (5%)	22	22

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	41	GLU
1	A	62	THR
1	A	88	ASP
2	B	1048	ILE
2	B	1083	LEU
2	B	1138	VAL
2	B	1145	LEU
2	B	1147	GLU
2	B	1151	GLN
2	B	1159	SER
1	C	16	SER
1	C	40	ARG
2	D	1047	LYS
2	D	1048	ILE
2	D	1052	GLU
2	D	1083	LEU

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Mol	Chain	Res	Type
2	D	1104	ARG
2	D	1113	GLU
2	D	1138	VAL
2	D	1144	LYS
2	D	1145	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	42	GLN
1	A	116	HIS
2	B	1068	GLN
1	C	8	GLN
2	D	1077	GLN
2	D	1158	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	A1BUC	A	201	-	89,90,90	0.87	4 (4%)	110,130,130	1.31	11 (10%)
3	A1BUC	C	201	-	89,90,90	0.87	3 (3%)	110,130,130	1.25	11 (10%)

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	A1BUC	A	201	-	-	11/53/94/94	0/10/10/10
3	A1BUC	C	201	-	-	10/53/94/94	0/10/10/10

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	A1BUC	C26-C32	-4.10	1.39	1.46
3	A	201	A1BUC	C28-N9	-3.26	1.29	1.34
3	C	201	A1BUC	C51-C52	3.14	1.37	1.33
3	A	201	A1BUC	C26-C32	-2.97	1.41	1.46
3	C	201	A1BUC	C28-N9	-2.97	1.30	1.34
3	A	201	A1BUC	C51-C52	2.77	1.36	1.33
3	A	201	A1BUC	C52-C56	-2.36	1.41	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	A1BUC	C8-C7-N2	5.83	125.45	120.23
3	C	201	A1BUC	C7-C8-CL1	4.25	122.87	119.76
3	C	201	A1BUC	C15-N5-C14	3.84	129.45	122.55
3	A	201	A1BUC	F1-C36-C35	3.72	114.58	110.64
3	A	201	A1BUC	C7-C8-CL1	3.72	122.48	119.76
3	C	201	A1BUC	C33-N11-C32	-3.66	118.52	125.11
3	A	201	A1BUC	C33-N11-C32	-3.19	119.37	125.11
3	C	201	A1BUC	C8-C7-N2	3.17	123.07	120.23
3	C	201	A1BUC	C40-N12-C39	2.82	130.78	127.94
3	A	201	A1BUC	N2-C7-N14	-2.75	115.02	119.08
3	A	201	A1BUC	C11-N4-C10	-2.59	116.55	121.67
3	A	201	A1BUC	C48-N4-C10	-2.53	116.67	121.67
3	C	201	A1BUC	C40-N12-N13	-2.52	118.00	120.03
3	C	201	A1BUC	C22-C23-C24	-2.46	106.28	110.78
3	A	201	A1BUC	C11-C12-C13	-2.36	106.80	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	A1BUC	C50-C49-C6	2.26	121.47	119.00
3	C	201	A1BUC	C46-N11-C33	2.24	121.95	115.40
3	C	201	A1BUC	C48-C47-C13	2.18	113.99	110.54
3	A	201	A1BUC	C50-C49-C6	2.15	121.35	119.00
3	C	201	A1BUC	C25-N7-N10	-2.13	109.69	112.40
3	A	201	A1BUC	C40-N12-N13	-2.10	118.34	120.03
3	A	201	A1BUC	C53-O5-C52	2.00	120.04	117.48

There are no chirality outliers.

All (21) torsion outliers are listed below:

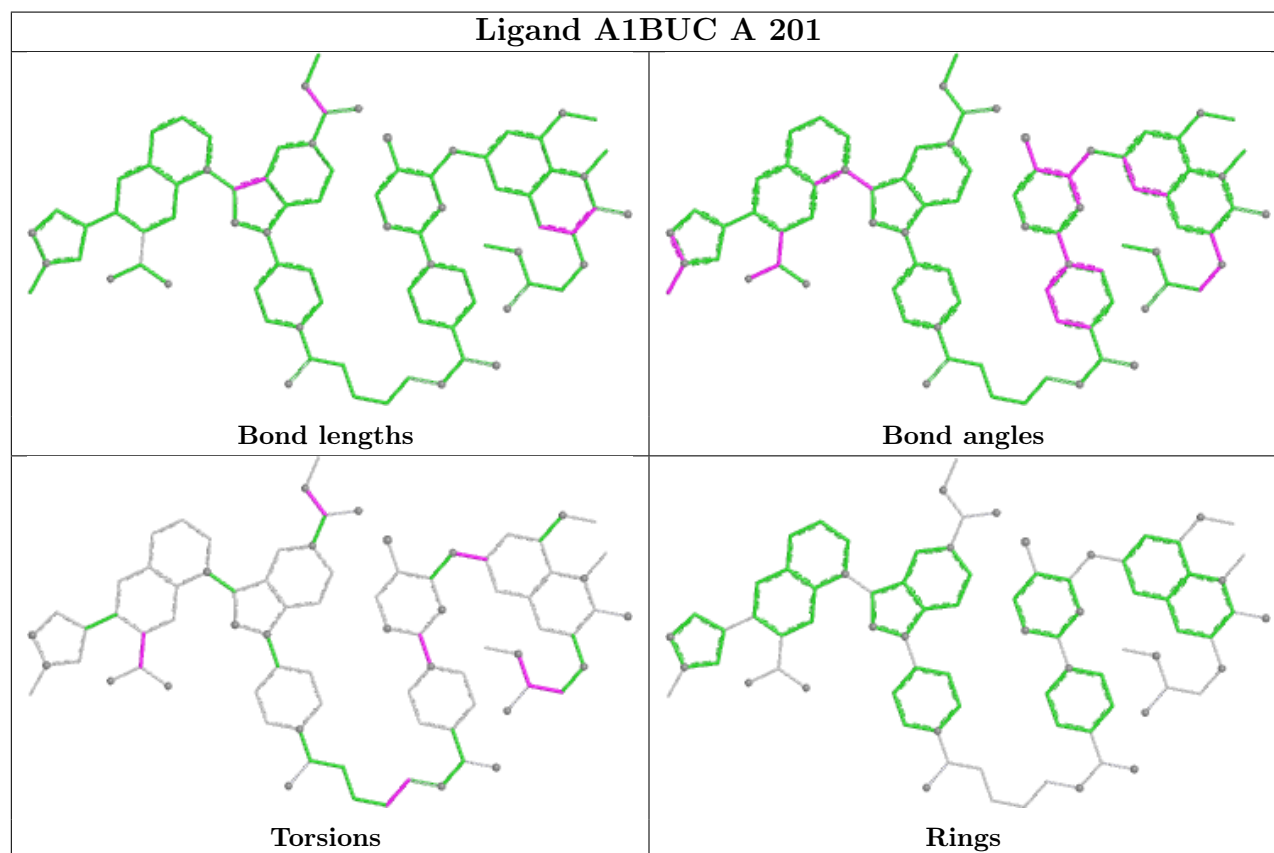
Mol	Chain	Res	Type	Atoms
3	A	201	A1BUC	N8-C28-N9-C29
3	A	201	A1BUC	N3-C10-N4-C48
3	C	201	A1BUC	C16-C17-C18-C19
3	C	201	A1BUC	N5-C15-C16-C17
3	A	201	A1BUC	N14-C10-N4-C48
3	A	201	A1BUC	N5-C15-C16-C17
3	C	201	A1BUC	O3-C19-N6-C20
3	A	201	A1BUC	O2-C28-N9-C29
3	C	201	A1BUC	C47-C13-C14-N5
3	C	201	A1BUC	C47-C13-C14-O4
3	C	201	A1BUC	C34-C35-C36-F1
3	A	201	A1BUC	O5-C53-C54-O6
3	A	201	A1BUC	O5-C53-C54-N15
3	C	201	A1BUC	C49-C6-N2-C7
3	C	201	A1BUC	O5-C53-C54-N15
3	C	201	A1BUC	O5-C53-C54-O6
3	C	201	A1BUC	O4-C14-N5-C15
3	A	201	A1BUC	C34-C35-C36-F1
3	A	201	A1BUC	C37-C35-C36-F1
3	A	201	A1BUC	C49-C6-N2-C7
3	A	201	A1BUC	O6-C54-N15-C55

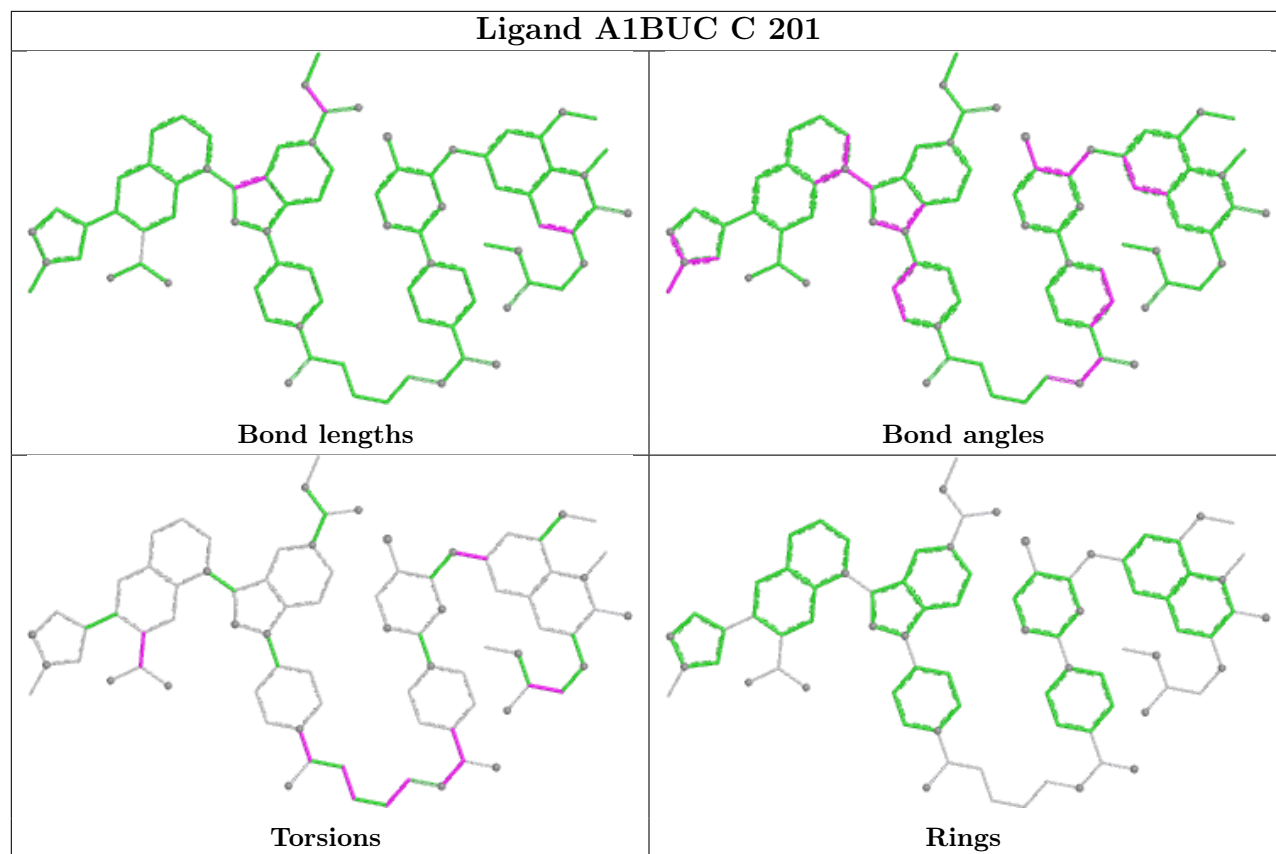
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	A1BUC	2	0
3	C	201	A1BUC	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	122/128 (95%)	0.57	2 (1%) 70 73	27, 43, 73, 90	0
1	C	123/128 (96%)	0.56	2 (1%) 70 73	21, 41, 80, 94	1 (0%)
2	B	112/145 (77%)	0.89	7 (6%) 26 27	28, 53, 88, 114	2 (1%)
2	D	113/145 (77%)	0.81	4 (3%) 47 49	31, 57, 100, 138	0
All	All	470/546 (86%)	0.70	15 (3%) 50 53	21, 47, 88, 138	3 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1048	ILE	3.8
2	B	1048	ILE	3.7
2	D	1049	PHE	3.5
2	B	1051	PRO	2.8
1	C	65	LEU	2.6
2	D	1057	ALA	2.6
2	B	1049	PHE	2.5
1	A	62	THR	2.4
1	A	65	LEU	2.2
1	C	7	SER	2.1
2	B	1125	PHE	2.1
2	B	1156	VAL	2.1
2	B	1144	LYS	2.1
2	B	1138	VAL	2.1
2	D	1054	LEU	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](#)

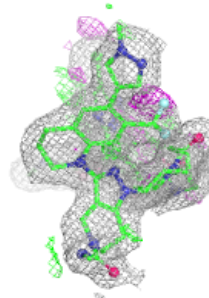
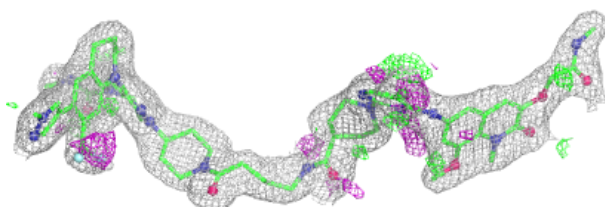
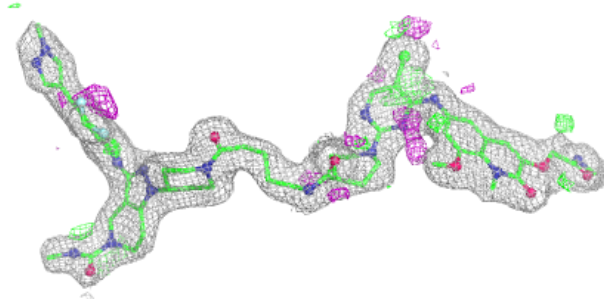
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1BUC	A	201	81/81	0.93	0.10	31,43,58,81	0
3	A1BUC	C	201	81/81	0.93	0.10	34,44,62,85	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.

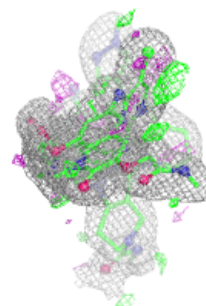
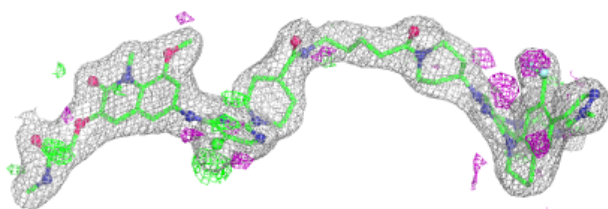
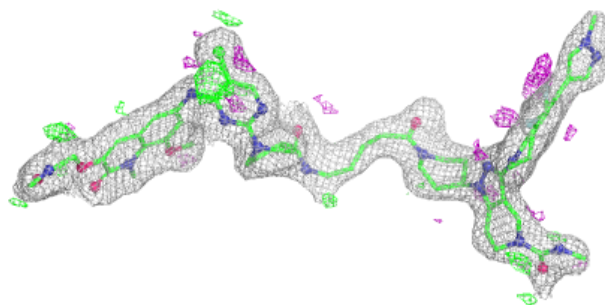
Electron density around A1BUC A 201:

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 A1BUC C 201:

$2mF_o-DF_c$ (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.