



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:20 AM UTC

PDB ID : 6GUF / pdb_00006guf
Title : CDK2/CyclinA in complex with CGP74514A
Authors : Wood, D.J.; Korolchuk, S.; Tatum, N.J.; Wang, L.Z.; Endicott, J.A.; Noble, M.E.M.; Martin, M.P.
Deposited on : 2018-06-19
Resolution : 2.65 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

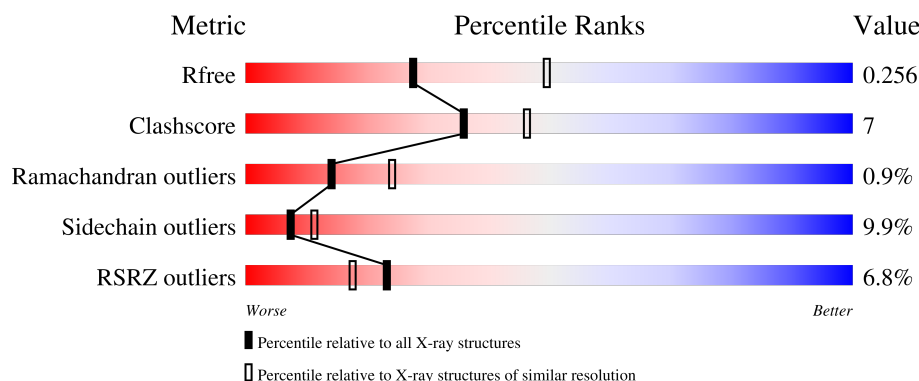
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	302	4% 79% 14% • • •
1	C	302	16% 76% 18% • •
2	B	268	% 81% 13% • •
2	D	268	4% 82% 12% • •

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
3	23D	A	301	X	-	-	-
3	23D	C	301	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9172 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	P	S	0	0	0
			2383	1549	406	419	1	8			
1	C	298	Total	C	N	O	P	S	0	0	0
			2399	1556	408	426	1	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P24941
A	-2	PRO	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-3	GLY	-	expression tag	UNP P24941
C	-2	PRO	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	261	Total	C	N	O	S		0	0	0
			2106	1364	343	389	10				
2	D	261	Total	C	N	O	S		0	0	0
			2106	1364	343	389	10				

There are 14 discrepancies between the modelled and reference sequences:

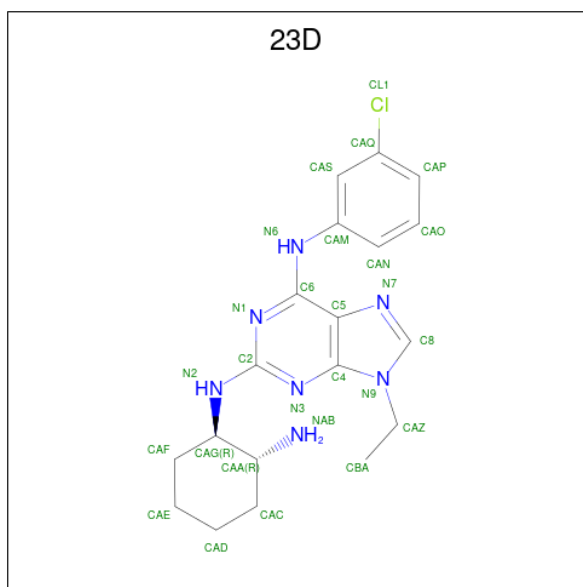
Chain	Residue	Modelled	Actual	Comment	Reference
B	171	GLY	-	expression tag	UNP P30274
B	433	HIS	-	expression tag	UNP P30274
B	434	HIS	-	expression tag	UNP P30274
B	435	HIS	-	expression tag	UNP P30274

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Chain	Residue	Modelled	Actual	Comment	Reference
B	436	HIS	-	expression tag	UNP P30274
B	437	HIS	-	expression tag	UNP P30274
B	438	HIS	-	expression tag	UNP P30274
D	171	GLY	-	expression tag	UNP P30274
D	433	HIS	-	expression tag	UNP P30274
D	434	HIS	-	expression tag	UNP P30274
D	435	HIS	-	expression tag	UNP P30274
D	436	HIS	-	expression tag	UNP P30274
D	437	HIS	-	expression tag	UNP P30274
D	438	HIS	-	expression tag	UNP P30274

- Molecule 3 is N2-[(1R,2S)-2-AMINOCYCLOHEXYL]-N6-(3-CHLOROPHENYL)-9-ETHYL-L-9H-PURINE-2,6-DIAMINE (CCD ID: 23D) (formula: C₁₉H₂₄ClN₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0
			27	19	1	7	
3	C	1	Total	C	Cl	N	0
			27	19	1	7	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		

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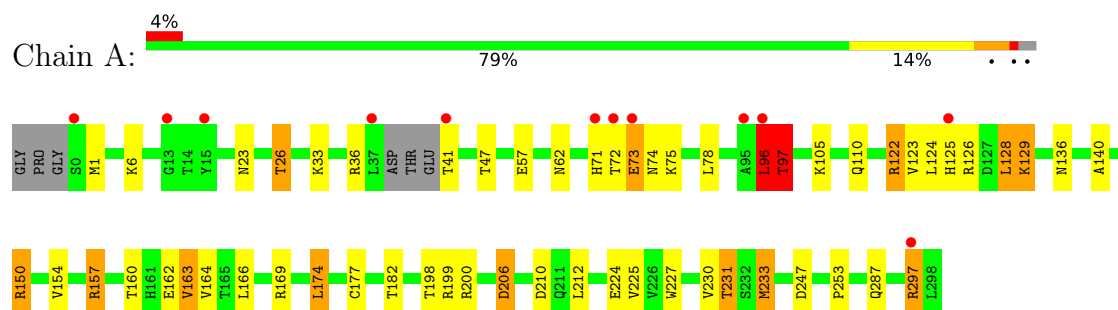
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	36	Total 36	O 36	0	0
4	C	23	Total 23	O 23	0	0
4	D	18	Total 18	O 18	0	0

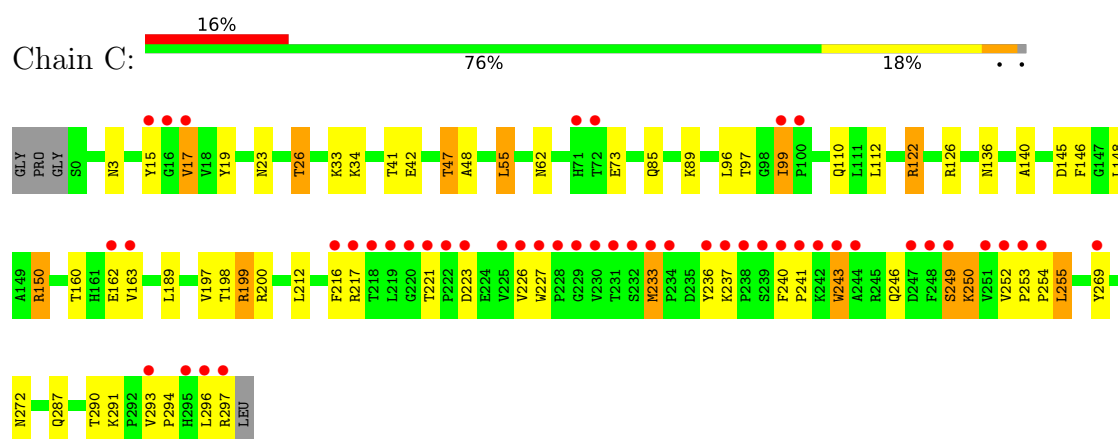
3 Residue-property plots [i](#)

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.

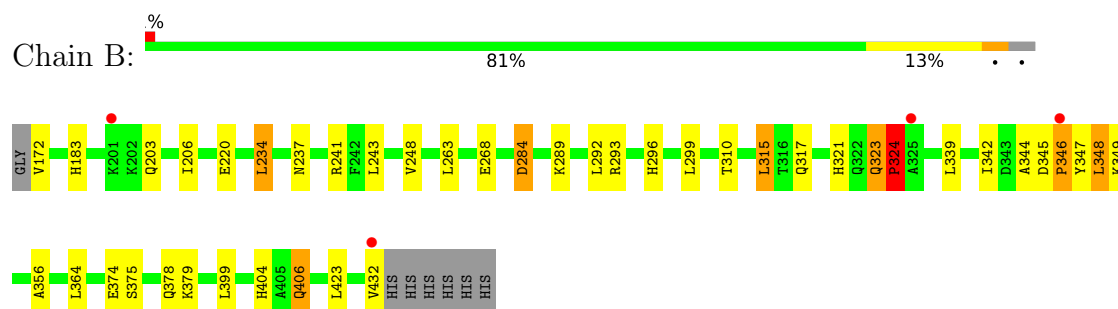
• Molecule 1: Cyclin-dependent kinase 2



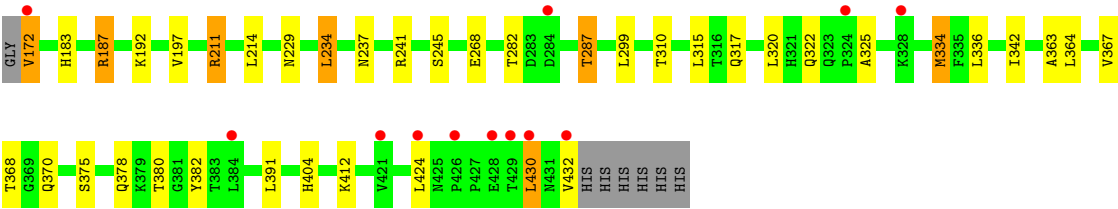
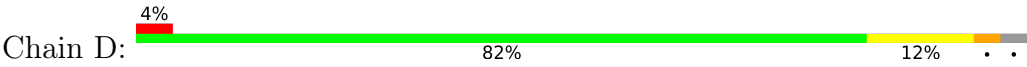
• Molecule 1: Cyclin-dependent kinase 2



• Molecule 2: Cyclin-A2



• Molecule 2: Cyclin-A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.32Å 136.69Å 150.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.17 – 2.65 101.17 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (101.17-2.65) 99.9 (101.17-2.65)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.203 , 0.255 0.208 , 0.256	Depositor DCC
R_{free} test set	2244 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9172	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: 23D, TPO

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	0.97	3/2432 (0.1%)	1.09	7/3297 (0.2%)
1	C	0.93	0/2449	1.10	5/3322 (0.2%)
2	B	0.88	0/2156	1.08	4/2932 (0.1%)
2	D	0.84	0/2156	1.04	1/2932 (0.0%)
All	All	0.91	3/9193 (0.0%)	1.08	17/12483 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	VAL	C-O	-5.99	1.17	1.24
1	A	129	LYS	C-O	-5.50	1.18	1.24
1	A	154	VAL	CA-C	5.14	1.57	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	323	GLN	CA-C-N	10.36	132.78	119.84
2	B	323	GLN	C-N-CA	10.36	132.78	119.84
1	A	96	LEU	N-CA-C	-7.07	99.08	110.32
1	A	253	PRO	N-CA-C	6.37	118.47	110.70
1	A	123	VAL	N-CA-C	6.34	117.25	108.12
1	C	253	PRO	N-CA-C	6.24	118.31	110.70
1	A	136	ASN	CA-C-N	5.80	128.33	120.38
1	A	136	ASN	C-N-CA	5.80	128.33	120.38
1	A	1	MET	N-CA-C	5.69	119.32	112.38
1	C	249	SER	N-CA-C	-5.46	101.76	109.96
2	B	347	TYR	N-CA-C	5.25	119.31	113.01
2	B	324	PRO	N-CA-C	-5.14	101.88	112.47
1	A	163	VAL	N-CA-C	5.05	117.10	108.86
1	C	136	ASN	CA-C-N	5.05	127.30	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	ASN	C-N-CA	5.05	127.30	120.38
1	C	126	ARG	N-CA-C	5.05	119.02	112.86
2	D	430	LEU	N-CA-C	5.02	119.54	113.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2383	0	2436	37	0
1	C	2399	0	2443	46	0
2	B	2106	0	2125	33	0
2	D	2106	0	2125	25	0
3	A	27	0	24	0	0
3	C	27	0	24	0	0
4	A	47	0	0	2	0
4	B	36	0	0	2	0
4	C	23	0	0	0	0
4	D	18	0	0	2	0
All	All	9172	0	9177	133	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:323:GLN:CB	2:B:324:PRO:HD3	1.54	1.34
1:C:15:TYR:CE2	1:C:47:THR:CG2	2.24	1.20
1:C:15:TYR:CZ	1:C:47:THR:HG23	1.80	1.16
1:C:17:VAL:HG11	1:C:19:TYR:CE1	1.83	1.13
1:C:15:TYR:CD2	1:C:47:THR:CG2	2.33	1.11
2:B:323:GLN:HB2	2:B:324:PRO:HD3	1.20	1.08
1:C:15:TYR:CE2	1:C:47:THR:HG22	1.86	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:VAL:CG1	1:C:19:TYR:CE1	2.40	1.04
1:A:125:HIS:CE1	1:A:128:LEU:HD13	1.94	1.02
2:B:323:GLN:CB	2:B:324:PRO:CD	2.37	1.01
2:B:323:GLN:HB2	2:B:324:PRO:CD	1.91	0.99
2:B:323:GLN:HB3	2:B:324:PRO:HD3	1.47	0.96
1:C:17:VAL:HG11	1:C:19:TYR:HE1	1.15	0.95
1:C:17:VAL:CG1	1:C:19:TYR:HE1	1.77	0.94
1:C:15:TYR:CE2	1:C:47:THR:HG23	1.99	0.91
1:A:125:HIS:ND1	1:A:128:LEU:HD13	1.86	0.91
2:D:187:ARG:HH11	2:D:187:ARG:HG2	1.35	0.88
1:C:15:TYR:CD2	1:C:47:THR:HG21	2.09	0.87
1:C:15:TYR:CE1	1:C:47:THR:HG23	2.11	0.85
1:C:249:SER:O	1:C:250:LYS:HG2	1.81	0.81
2:B:237:ASN:HD21	2:B:241:ARG:HH11	1.29	0.80
1:C:15:TYR:CG	1:C:47:THR:HG21	2.16	0.79
2:D:237:ASN:HD21	2:D:241:ARG:HH11	1.29	0.78
1:A:125:HIS:O	1:A:126:ARG:HB2	1.86	0.74
2:B:346:PRO:HB2	2:B:349:LYS:HZ2	1.52	0.73
1:C:17:VAL:HG13	1:C:19:TYR:CE1	2.23	0.73
1:A:96:LEU:O	1:A:97:THR:HG23	1.89	0.72
2:D:187:ARG:HG2	2:D:187:ARG:NH1	2.02	0.72
2:D:363:ALA:O	2:D:367:VAL:HG12	1.89	0.72
1:A:26:THR:HG21	4:A:406:HOH:O	1.89	0.72
2:B:323:GLN:N	2:B:323:GLN:OE1	2.24	0.71
1:A:177:CYS:SG	1:A:233:MET:HE3	2.30	0.70
2:B:234:LEU:HD13	2:B:310:THR:HG21	1.74	0.70
1:A:297:ARG:HH11	1:A:297:ARG:HG2	1.58	0.69
1:C:15:TYR:CD2	1:C:47:THR:HG22	2.11	0.69
1:A:110:GLN:HE22	1:A:140:ALA:HA	1.56	0.68
2:B:346:PRO:HB2	2:B:349:LYS:NZ	2.09	0.68
1:C:15:TYR:CG	1:C:47:THR:CG2	2.75	0.66
1:C:110:GLN:HE22	1:C:140:ALA:HA	1.60	0.66
2:D:234:LEU:HD13	2:D:310:THR:HG21	1.77	0.66
1:C:197:VAL:HG11	1:C:252:VAL:HG13	1.78	0.65
1:C:15:TYR:CZ	1:C:47:THR:CG2	2.57	0.65
1:A:150:ARG:NH1	2:B:268:GLU:O	2.29	0.64
2:D:187:ARG:NH2	2:D:382:TYR:CZ	2.67	0.63
1:A:227:TRP:CH2	1:A:233:MET:HE1	2.34	0.62
1:A:125:HIS:CE1	1:A:128:LEU:CD1	2.78	0.62
1:A:224:GLU:OE2	1:A:231:THR:HB	2.00	0.61
1:C:99:ILE:CD1	1:C:199:ARG:HD2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ILE:HD13	1:C:199:ARG:HD2	1.83	0.60
1:C:122:ARG:O	1:C:122:ARG:HG2	2.02	0.59
1:C:150:ARG:NH1	2:D:268:GLU:O	2.34	0.59
1:A:122:ARG:HG2	1:A:122:ARG:O	2.03	0.59
1:A:177:CYS:SG	1:A:233:MET:HG2	2.43	0.59
1:A:71:HIS:O	1:A:73:GLU:N	2.36	0.58
1:C:198:THR:HG22	1:C:200:ARG:HG2	1.85	0.58
2:D:237:ASN:ND2	2:D:241:ARG:HH11	2.00	0.58
1:A:125:HIS:CG	1:A:128:LEU:HD13	2.38	0.58
2:B:203:GLN:HG2	2:B:206:ILE:HG12	1.87	0.56
2:B:234:LEU:HD13	2:B:310:THR:CG2	2.35	0.56
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.72	0.55
1:C:23:ASN:HB3	1:C:26:THR:HG22	1.89	0.55
1:A:62:ASN:HD21	1:A:110:GLN:HE21	1.53	0.55
2:B:172:VAL:N	4:B:501:HOH:O	2.39	0.55
2:B:237:ASN:ND2	2:B:241:ARG:HH11	2.01	0.54
1:C:62:ASN:HD21	1:C:110:GLN:HE21	1.56	0.54
2:D:187:ARG:NH2	2:D:382:TYR:CE1	2.76	0.54
1:A:57:GLU:OE1	1:A:122:ARG:NH2	2.35	0.53
2:D:234:LEU:HD13	2:D:310:THR:CG2	2.38	0.53
2:D:380:THR:HG21	2:D:382:TYR:CD2	2.45	0.52
2:B:234:LEU:CD1	2:B:310:THR:CG2	2.87	0.52
1:C:17:VAL:HG13	1:C:19:TYR:CD1	2.45	0.52
1:C:17:VAL:HG12	1:C:34:LYS:HB3	1.93	0.51
2:B:203:GLN:HG2	2:B:206:ILE:CG1	2.41	0.51
2:D:404:HIS:CD2	4:D:511:HOH:O	2.64	0.51
2:D:364:LEU:HD22	2:D:370:GLN:HB2	1.94	0.50
1:A:71:HIS:CD2	2:B:296:HIS:NE2	2.80	0.49
1:C:252:VAL:HG11	1:C:255:LEU:HD22	1.94	0.49
1:A:126:ARG:HD2	1:A:163:VAL:HG11	1.94	0.49
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.77	0.49
1:A:71:HIS:CD2	2:B:296:HIS:CE1	3.01	0.48
1:C:15:TYR:OH	1:C:48:ALA:HA	2.13	0.48
1:A:162:GLU:HA	4:A:403:HOH:O	2.13	0.48
1:C:216:PHE:HE1	1:C:269:TYR:HH	1.62	0.48
2:B:345:ASP:HA	2:B:346:PRO:HA	1.54	0.47
2:D:234:LEU:CD1	2:D:310:THR:CG2	2.92	0.47
1:A:23:ASN:HB3	1:A:26:THR:HG22	1.97	0.47
1:A:206:ASP:OD1	1:A:210:ASP:OD2	2.31	0.47
2:B:293:ARG:NH2	1:C:3:ASN:ND2	2.62	0.47
2:D:287:THR:HG21	4:D:517:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:TRP:CZ2	1:A:233:MET:HE1	2.50	0.47
2:D:211:ARG:HE	2:D:211:ARG:HB3	1.42	0.46
1:A:157:ARG:NH1	2:B:268:GLU:OE2	2.46	0.46
2:B:404:HIS:CE1	2:B:406:GLN:HG2	2.51	0.46
2:D:380:THR:CG2	2:D:382:TYR:CD2	2.97	0.46
1:A:297:ARG:HG2	1:A:297:ARG:NH1	2.29	0.46
2:B:203:GLN:HE21	2:B:248:VAL:H	1.63	0.46
1:A:36:ARG:HD3	1:A:75:LYS:HG2	1.99	0.45
1:A:169:ARG:HD2	1:A:174:LEU:HD13	1.98	0.45
1:A:297:ARG:HH11	1:A:297:ARG:CG	2.26	0.45
1:A:96:LEU:C	1:A:97:THR:HG23	2.42	0.45
2:B:315:LEU:HD13	2:B:356:ALA:HB1	1.98	0.44
2:D:432:VAL:O	2:D:432:VAL:HG12	2.17	0.44
1:A:124:LEU:HD21	1:A:182:THR:HA	1.98	0.44
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.46	0.44
1:C:272:ASN:ND2	2:D:172:VAL:HG22	2.32	0.44
2:B:284:ASP:N	2:B:284:ASP:OD1	2.50	0.44
1:C:55:LEU:HD11	1:C:146:PHE:CD1	2.53	0.44
1:C:15:TYR:CD1	1:C:47:THR:CG2	3.01	0.44
1:C:293:VAL:HG12	1:C:294:PRO:O	2.18	0.44
2:D:322:GLN:HG3	2:D:325:ALA:HA	2.00	0.43
2:D:234:LEU:HD12	2:D:234:LEU:HA	1.78	0.43
2:B:378:GLN:HG3	4:B:515:HOH:O	2.18	0.43
2:D:187:ARG:NH1	2:D:187:ARG:CG	2.73	0.43
1:A:230:VAL:HA	1:A:233:MET:SD	2.58	0.43
1:C:237:LYS:HB3	1:C:240:PHE:CD1	2.54	0.43
1:A:125:HIS:O	1:A:126:ARG:CB	2.61	0.43
2:B:344:ALA:HB1	2:B:348:LEU:HD22	2.00	0.43
2:B:234:LEU:HD12	2:B:234:LEU:HA	1.78	0.42
1:C:221:THR:HG21	1:C:241:PRO:HB2	1.99	0.42
2:D:229:ASN:HD21	2:D:412:LYS:NZ	2.17	0.42
1:C:290:THR:HG22	1:C:291:LYS:H	1.84	0.42
1:A:71:HIS:NE2	2:B:296:HIS:NE2	2.67	0.42
1:C:249:SER:O	1:C:250:LYS:CG	2.62	0.42
1:C:216:PHE:HB3	1:C:221:THR:HG22	2.01	0.42
1:C:216:PHE:HE1	1:C:269:TYR:OH	2.03	0.42
2:B:315:LEU:HD12	2:B:315:LEU:HA	1.83	0.41
1:C:221:THR:OG1	1:C:243:TRP:N	2.49	0.41
1:A:297:ARG:NH1	1:A:297:ARG:CG	2.83	0.41
1:C:227:TRP:CZ2	1:C:233:MET:HE2	2.56	0.41
2:D:315:LEU:HD13	2:D:334:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:THR:HG22	1:A:200:ARG:HG3	2.02	0.40
2:B:321:HIS:HD2	2:B:375:SER:OG	2.03	0.40
1:C:290:THR:HG22	1:C:291:LYS:N	2.36	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	291/302 (96%)	275 (94%)	13 (4%)	3 (1%)	12	20
1	C	295/302 (98%)	280 (95%)	10 (3%)	5 (2%)	7	12
2	B	259/268 (97%)	252 (97%)	5 (2%)	2 (1%)	16	27
2	D	259/268 (97%)	255 (98%)	4 (2%)	0	100	100
All	All	1104/1140 (97%)	1062 (96%)	32 (3%)	10 (1%)	14	24

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	THR
2	B	324	PRO
1	A	164	VAL
1	C	163	VAL
1	C	250	LYS
1	C	254	PRO
1	C	145	ASP
1	C	255	LEU
1	A	97	THR
2	B	346	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	260/264 (98%)	233 (90%)	27 (10%)	7	10
1	C	262/264 (99%)	231 (88%)	31 (12%)	5	7
2	B	234/240 (98%)	215 (92%)	19 (8%)	11	18
2	D	234/240 (98%)	213 (91%)	21 (9%)	9	14
All	All	990/1008 (98%)	892 (90%)	98 (10%)	7	11

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	26	THR
1	A	33	LYS
1	A	41	THR
1	A	47	THR
1	A	73	GLU
1	A	74	ASN
1	A	78	LEU
1	A	96	LEU
1	A	97	THR
1	A	105	LYS
1	A	122	ARG
1	A	128	LEU
1	A	129	LYS
1	A	150	ARG
1	A	157	ARG
1	A	166	LEU
1	A	174	LEU
1	A	199	ARG
1	A	206	ASP
1	A	212	LEU
1	A	225	VAL
1	A	231	THR
1	A	233	MET

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Mol	Chain	Res	Type
1	A	247	ASP
1	A	287	GLN
1	A	297	ARG
2	B	220	GLU
2	B	234	LEU
2	B	243	LEU
2	B	263	LEU
2	B	284	ASP
2	B	289	LYS
2	B	292	LEU
2	B	299	LEU
2	B	315	LEU
2	B	339	LEU
2	B	342	ILE
2	B	348	LEU
2	B	364	LEU
2	B	374	GLU
2	B	379	LYS
2	B	399	LEU
2	B	406	GLN
2	B	423	LEU
2	B	432	VAL
1	C	17	VAL
1	C	26	THR
1	C	33	LYS
1	C	41	THR
1	C	42	GLU
1	C	47	THR
1	C	55	LEU
1	C	73	GLU
1	C	85	GLN
1	C	89	LYS
1	C	96	LEU
1	C	97	THR
1	C	99	ILE
1	C	112	LEU
1	C	122	ARG
1	C	148	LEU
1	C	150	ARG
1	C	162	GLU
1	C	189	LEU
1	C	199	ARG

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Mol	Chain	Res	Type
1	C	212	LEU
1	C	217	ARG
1	C	223	ASP
1	C	226	VAL
1	C	233	MET
1	C	236	TYR
1	C	243	TRP
1	C	246	GLN
1	C	287	GLN
1	C	296	LEU
1	C	297	ARG
2	D	172	VAL
2	D	187	ARG
2	D	192	LYS
2	D	197	VAL
2	D	211	ARG
2	D	214	LEU
2	D	234	LEU
2	D	245	SER
2	D	282	THR
2	D	287	THR
2	D	299	LEU
2	D	320	LEU
2	D	334	MET
2	D	336	LEU
2	D	342	ILE
2	D	368	THR
2	D	375	SER
2	D	378	GLN
2	D	391	LEU
2	D	424	LEU
2	D	430	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	110	GLN
1	A	113	GLN
1	A	161	HIS
1	A	272	ASN
1	A	287	GLN

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Mol	Chain	Res	Type
2	B	173	ASN
2	B	179	HIS
2	B	203	GLN
2	B	208	ASN
2	B	233	HIS
2	B	237	ASN
2	B	313	GLN
2	B	317	GLN
2	B	321	HIS
1	C	3	ASN
1	C	110	GLN
1	C	265	GLN
1	C	272	ASN
2	D	208	ASN
2	D	229	ASN
2	D	233	HIS
2	D	237	ASN
2	D	296	HIS
2	D	313	GLN
2	D	317	GLN
2	D	321	HIS
2	D	370	GLN
2	D	395	HIS
2	D	404	HIS
2	D	415	ASN
2	D	431	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	C	160	1	8,10,11	0.86	0	10,14,16	1.67	1 (10%)
1	TPO	A	160	1	8,10,11	0.89	0	10,14,16	1.79	1 (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
1	TPO	C	160	1	-	1/9/11/13	-
1	TPO	A	160	1	-	1/9/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	160	TPO	P-OG1-CB	-4.33	111.55	123.33
1	C	160	TPO	P-OG1-CB	-3.61	113.52	123.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	O-C-CA-CB
1	A	160	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](#)

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	23D	C	301	-	29,30,30	0.50	0	39,42,42	0.68	0
3	23D	A	301	-	29,30,30	0.43	0	39,42,42	0.84	2 (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
3	23D	C	301	-	1/1/2/4	0/10/21/21	0/4/4/4
3	23D	A	301	-	1/1/2/4	2/10/21/21	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	23D	N6-C6-N1	2.92	123.39	119.08
3	A	301	23D	CAS-CAQ-CL1	-2.22	116.39	119.17

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	301	23D	CAA
3	C	301	23D	CAA

All (2) torsion outliers are listed below:

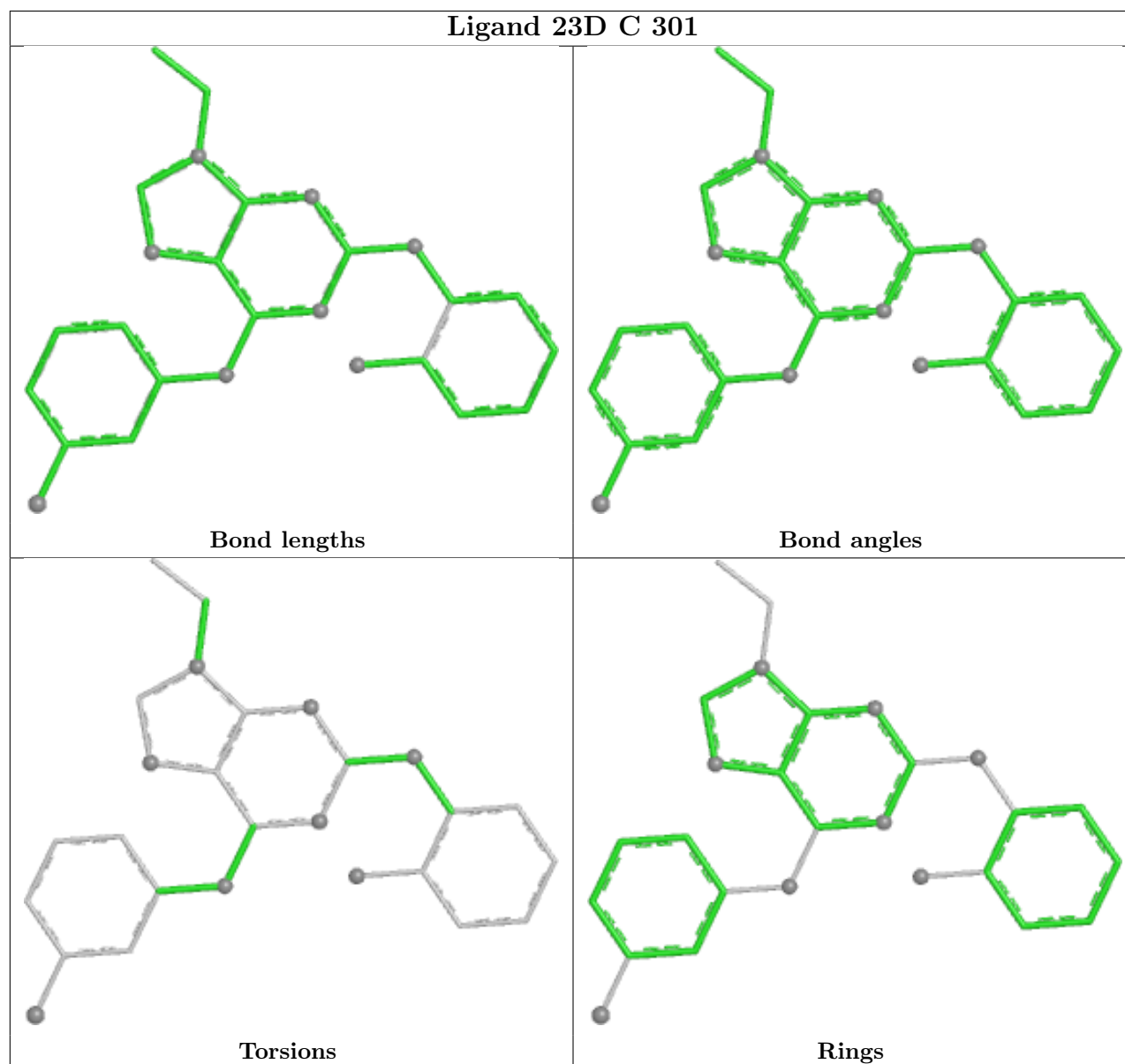
Mol	Chain	Res	Type	Atoms
3	A	301	23D	CBA-CAZ-N9-C8
3	A	301	23D	CBA-CAZ-N9-C4

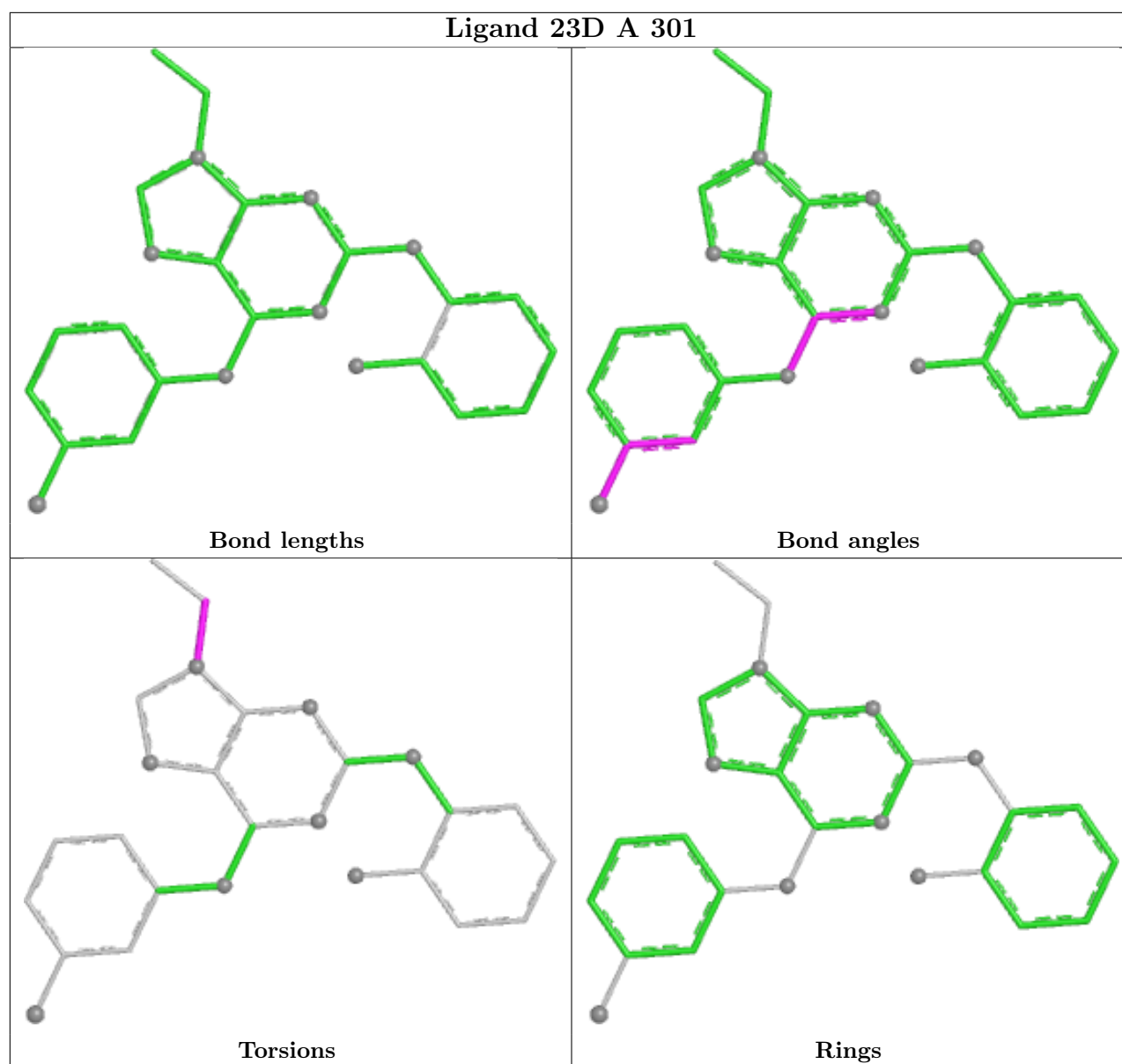
There are no ring outliers.

No monomer is involved in short contacts.

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	295/302 (97%)	-0.16	12 (4%) 41 33	20, 33, 72, 141	0
1	C	297/302 (98%)	0.75	48 (16%) 4 3	28, 52, 180, 223	0
2	B	261/268 (97%)	-0.12	4 (1%) 72 67	23, 38, 63, 90	0
2	D	261/268 (97%)	0.41	12 (4%) 37 29	26, 53, 88, 114	0
All	All	1114/1140 (97%)	0.23	76 (6%) 23 17	20, 44, 93, 223	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	VAL	7.3
1	C	240	PHE	7.0
1	C	15	TYR	6.3
1	C	238	PRO	6.0
1	C	296	LEU	5.9
1	C	243	TRP	5.7
1	C	241	PRO	5.6
1	C	222	PRO	5.3
1	C	221	THR	4.9
1	C	99	ILE	4.9
1	C	225	VAL	4.9
1	C	217	ARG	4.8
1	A	95	ALA	4.7
1	A	96	LEU	4.5
1	C	234	PRO	4.4
1	C	218	THR	4.2
1	C	244	ALA	3.9
2	D	432	VAL	3.9
1	C	17	VAL	3.7
1	C	251	VAL	3.7
1	C	233	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	16	GLY	3.6
1	C	239	SER	3.5
1	C	248	PHE	3.5
1	C	230	VAL	3.3
1	C	237	LYS	3.2
1	A	72	THR	3.2
1	C	236	TYR	3.2
1	A	37	LEU	3.2
1	C	269	TYR	3.2
2	B	346	PRO	3.1
1	C	216	PHE	3.1
2	D	424	LEU	3.1
1	C	297	ARG	3.0
1	A	41	THR	3.0
1	C	227	TRP	2.9
2	D	430	LEU	2.9
1	C	295	HIS	2.9
1	C	100	PRO	2.9
1	C	242	LYS	2.9
1	C	249	SER	2.8
2	B	432	VAL	2.8
1	C	229	GLY	2.8
1	C	72	THR	2.8
1	C	231	THR	2.8
2	D	324	PRO	2.7
1	C	228	PRO	2.7
1	C	223	ASP	2.7
1	A	125	HIS	2.6
1	C	253	PRO	2.6
1	C	162	GLU	2.5
2	D	428	GLU	2.5
1	A	297	ARG	2.5
1	A	73	GLU	2.5
1	C	220	GLY	2.5
1	A	71	HIS	2.4
1	C	219	LEU	2.4
2	B	325	ALA	2.4
2	D	426	PRO	2.3
2	D	429	THR	2.3
1	C	71	HIS	2.3
1	C	232	SER	2.3
1	C	252	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	15	TYR	2.2
1	A	0	SER	2.2
1	C	293	VAL	2.2
2	D	421	VAL	2.2
1	C	163	VAL	2.1
1	C	247	ASP	2.1
2	B	201	LYS	2.1
2	D	384	LEU	2.1
1	A	13	GLY	2.1
2	D	172	VAL	2.1
2	D	284	ASP	2.0
2	D	328	LYS	2.0
1	C	254	PRO	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	A	160	11/12	0.98	0.06	23,26,28,29	0
1	TPO	C	160	11/12	0.98	0.06	37,44,52,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

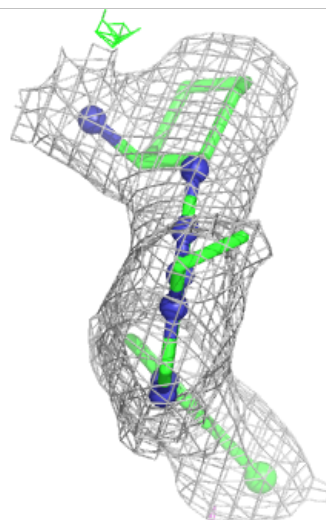
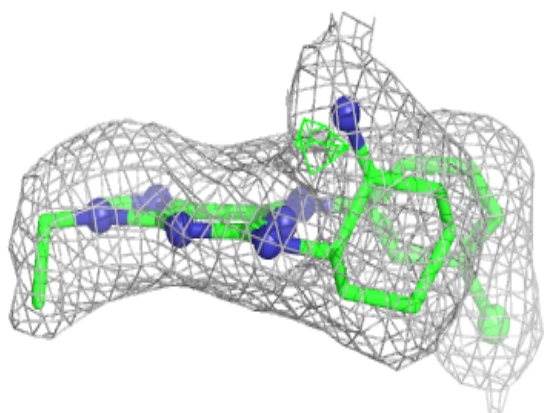
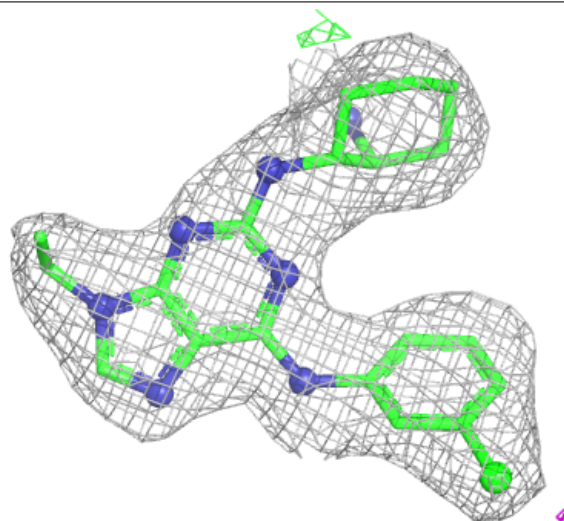
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	23D	C	301	27/27	0.92	0.10	36,42,50,64	0
3	23D	A	301	27/27	0.94	0.08	25,33,41,61	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.

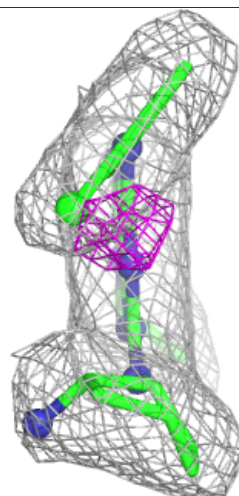
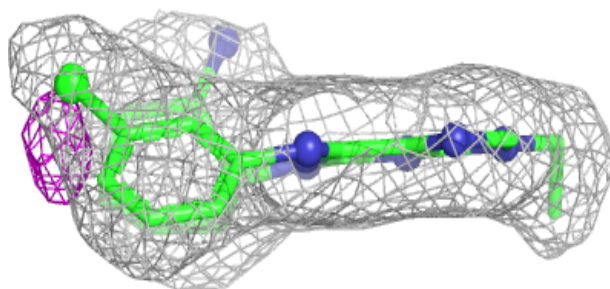
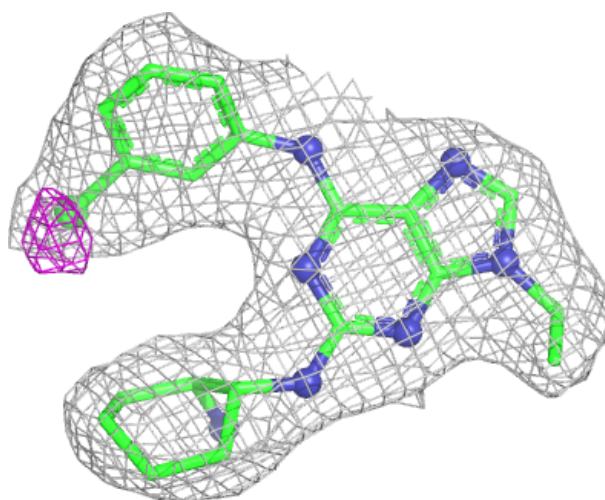
Electron density around 23D C 301:

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



Electron density around 23D A 301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.