



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2022 – 12:09 PM JST

PDB ID : 7VDS
Title : The structure of cyclin-dependent kinase 5 (CDK5) in complex with p25 and Compound 24
Authors : Malojcic, G.; Clugston, S.L.; Daniels, M.; Harmange, J.C.; Ledeborner, M.
Deposited on : 2021-09-07
Resolution : 3.05 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

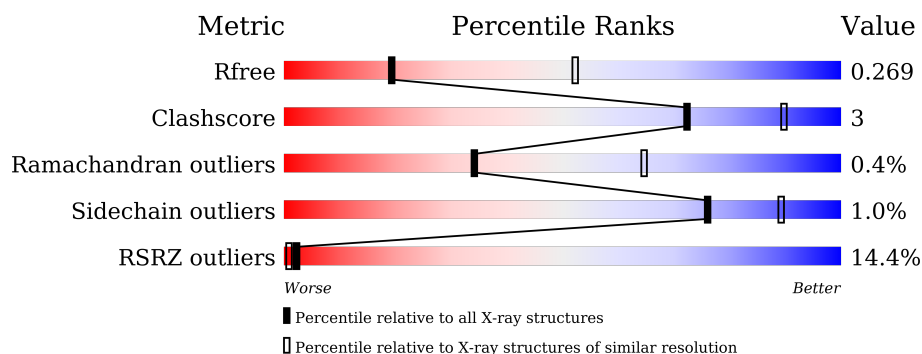
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	292	<div> <div></div> <div>92%</div> <div>7%</div> <div></div> </div>
1	B	292	<div> <div>17%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
2	C	209	<div> <div>63%</div> <div>8%</div> <div>29%</div> </div>
2	D	209	<div> <div>33%</div> <div>62%</div> <div>8%</div> <div>30%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	302	-	-	-	X
4	GOL	A	304	-	-	-	X
4	GOL	C	401	-	-	-	X
5	EDO	A	311	-	-	-	X
5	EDO	A	312	-	-	-	X
5	EDO	A	313	-	-	-	X
5	EDO	A	317	-	-	-	X
5	EDO	B	303	-	-	-	X
5	EDO	C	402	-	-	-	X
5	EDO	C	406	-	-	-	X
5	EDO	C	407	-	-	-	X
5	EDO	C	408	-	-	-	X
5	EDO	C	409	-	-	-	X
6	CL	A	320	-	-	-	X
6	CL	A	322	-	-	-	X
6	CL	A	327	-	-	-	X
6	CL	C	416	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7215 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-like kinase 5, p25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2330	1495	400	424	11			
1	B	278	Total	C	N	O	S	0	0	0
			2235	1434	386	405	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q00535
B	1	SER	-	expression tag	UNP Q00535

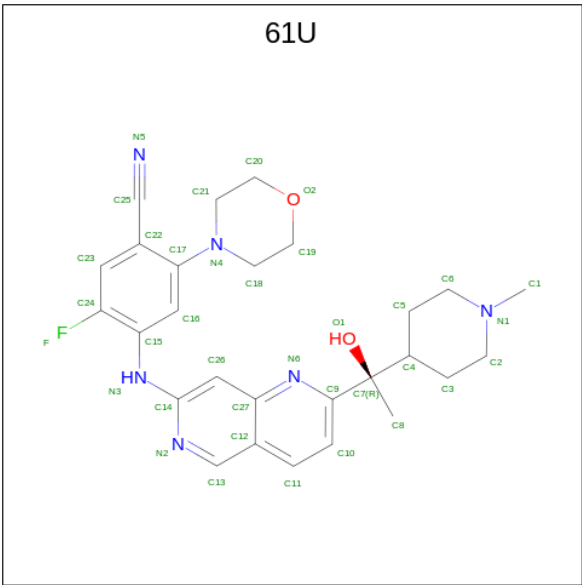
- Molecule 2 is a protein called Cyclin-dependent kinase 5 activator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	148	Total	C	N	O	S	0	1	0
			1207	774	201	221	11			
2	D	147	Total	C	N	O	S	0	0	0
			1191	765	196	219	11			

There are 2 discrepancies between the modelled and reference sequences:

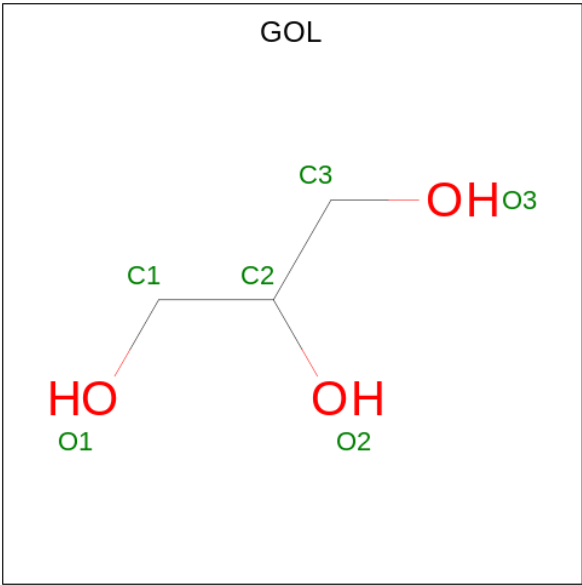
Chain	Residue	Modelled	Actual	Comment	Reference
C	99	MET	-	initiating methionine	UNP Q15078
D	99	MET	-	initiating methionine	UNP Q15078

- Molecule 3 is 5-fluoranyl-4-[[2-[(1R)-1-(1-methylpiperidin-4-yl)-1-oxidanyl-ethyl]-1,6-naphthylridin-7-yl]amino]-2-morpholin-4-yl-benzenecarbonitrile (three-letter code: 61U) (formula: C₂₇H₃₁FN₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			36	27	1	6	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



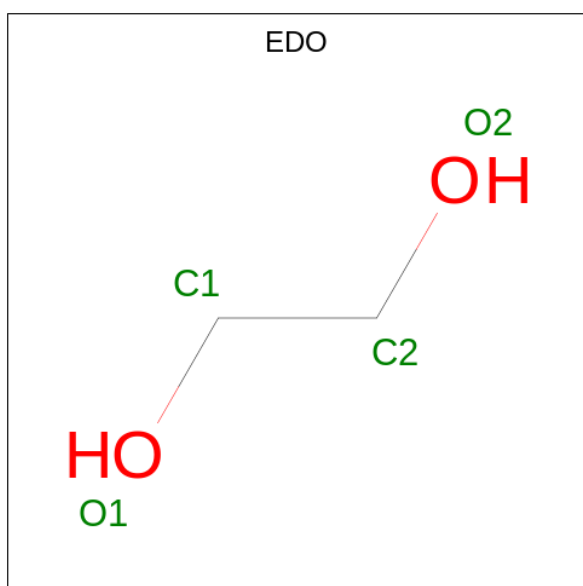
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	10	Total Cl 10 10	0	0
6	C	9	Total Cl 9 9	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	48	Total O 48 48	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	4	Total	O	0	0
			4	4		
7	C	17	Total	O	0	0
			17	17		

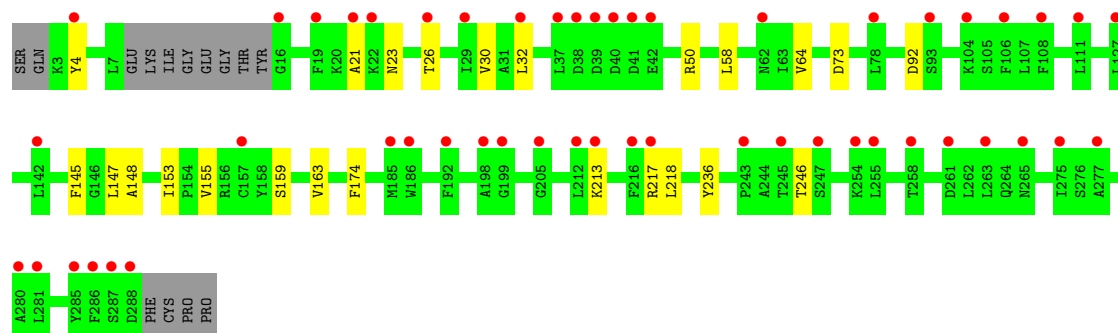
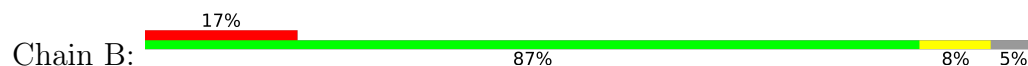
3 Residue-property plots [i](#)

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.

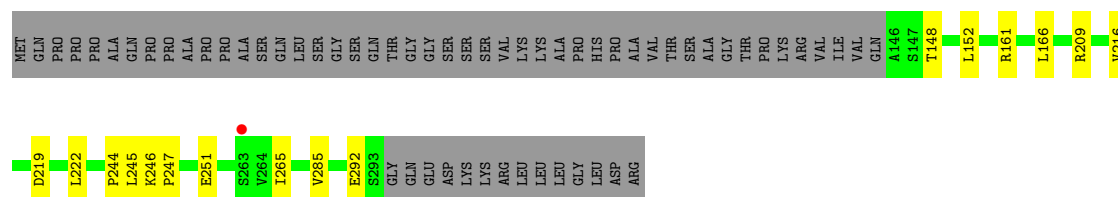
- Molecule 1: Cyclin-dependent-like kinase 5, p25



- Molecule 1: Cyclin-dependent-like kinase 5, p25

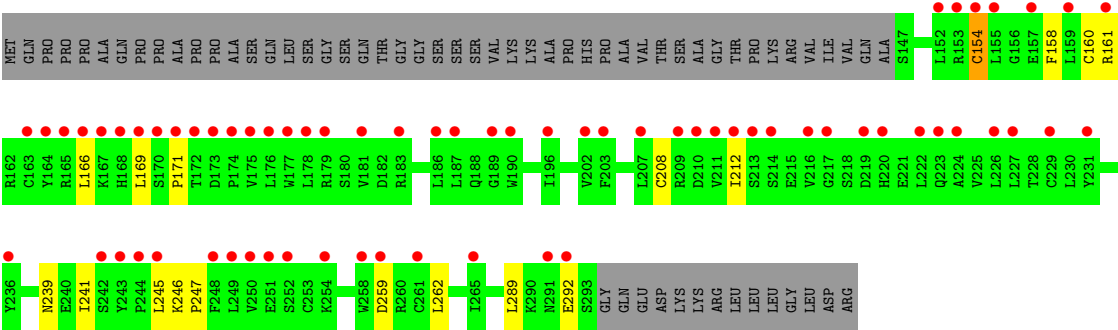


- Molecule 2: Cyclin-dependent kinase 5 activator 1



- Molecule 2: Cyclin-dependent kinase 5 activator 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.06Å 118.06Å 153.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.51 – 3.05 48.51 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.51-3.05) 99.9 (48.51-3.05)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.225 , 0.272 0.224 , 0.269	Depositor DCC
R_{free} test set	1207 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	106.0	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 98.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7215	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 61U, CL, GOL, EDO

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	0/2385	0.74	0/3229
1	B	0.65	0/2286	0.73	0/3094
2	C	0.64	0/1235	0.69	0/1674
2	D	0.66	0/1219	0.70	0/1653
All	All	0.64	0/7125	0.72	0/9650

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2330	0	2344	13	0
1	B	2235	0	2256	15	0
2	C	1207	0	1197	10	0
2	D	1191	0	1180	17	0
3	A	36	0	0	0	0
4	A	42	0	56	0	0
4	C	6	0	8	0	0
5	A	36	0	54	0	0
5	B	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	48	0	0
6	A	10	0	0	0	0
6	C	9	0	0	0	0
7	A	48	0	0	1	0
7	B	4	0	0	0	0
7	C	17	0	0	0	0
All	All	7215	0	7161	48	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 3.

All (48) 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:D:160:CYS:SG	2:D:169:LEU:HG	2.10	0.92
2:D:154:CYS:SG	2:D:289:LEU:O	2.36	0.84
1:B:50:ARG:HH22	2:D:241:ILE:HG23	1.50	0.75
2:D:158:PHE:HB2	2:D:292:GLU:HG2	1.69	0.74
2:D:208:CYS:O	2:D:212:ILE:HG22	1.87	0.72
2:C:148:THR:O	2:C:152:LEU:HD23	1.94	0.68
1:A:83:CYS:HA	1:A:135:ASN:OD1	1.94	0.67
1:B:147:LEU:HD23	2:D:241:ILE:HG21	1.76	0.67
2:D:241:ILE:HG22	2:D:241:ILE:O	1.98	0.64
2:D:166:LEU:O	2:D:169:LEU:HD13	1.98	0.64
1:B:147:LEU:CD2	2:D:241:ILE:HG21	2.30	0.62
1:B:58:LEU:HD13	1:B:145:PHE:HE2	1.66	0.60
1:A:32:LEU:HD22	1:A:77:THR:CG2	2.33	0.59
2:D:212:ILE:O	2:D:212:ILE:HG23	2.03	0.59
2:C:161[B]:ARG:NH1	2:C:292:GLU:OE2	2.38	0.57
2:D:160:CYS:SG	2:D:171:PRO:HB3	2.45	0.56
2:C:161[A]:ARG:NH1	2:C:292:GLU:O	2.39	0.56
1:B:218:LEU:HD12	1:B:246:THR:HG21	1.88	0.55
2:D:161:ARG:NH1	2:D:292:GLU:O	2.40	0.55
1:A:63:ILE:HG12	1:A:142:LEU:HD21	1.88	0.54
1:B:21:ALA:HB3	1:B:32:LEU:HD13	1.89	0.54
1:A:62:ASN:O	1:A:142:LEU:HD23	2.08	0.53
2:C:161[A]:ARG:CZ	2:C:161[A]:ARG:HB2	2.40	0.52
1:A:166:TRP:CZ3	1:B:92:ASP:HB3	2.49	0.48
1:A:174:PHE:CD1	1:A:236:TYR:HA	2.48	0.48
1:B:174:PHE:CD1	1:B:236:TYR:HA	2.49	0.47
1:B:213:LYS:O	1:B:217:ARG:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:160:CYS:HG	2:D:169:LEU:HG	1.79	0.46
2:C:209:ARG:NH1	2:C:285:VAL:HG22	2.31	0.46
1:B:159:SER:HB2	2:D:239:ASN:O	2.15	0.46
2:C:246:LYS:N	2:C:247:PRO:HD2	2.30	0.46
1:A:42:GLU:HB2	2:C:244:PRO:HB3	1.99	0.45
1:B:153:ILE:O	1:B:155:VAL:HG23	2.17	0.44
1:B:23:ASN:HB3	1:B:26:THR:O	2.18	0.44
1:B:4:TYR:CE1	1:B:30:VAL:HG21	2.52	0.44
1:B:50:ARG:NH1	1:B:148:ALA:O	2.48	0.44
2:D:259:ASP:O	2:D:262:LEU:HG	2.19	0.43
1:A:213:LYS:O	1:A:217:ARG:HB2	2.19	0.43
2:D:246:LYS:HB3	2:D:247:PRO:HD3	2.01	0.43
2:C:216:VAL:HG11	2:C:222:LEU:HB2	2.01	0.42
1:A:23:ASN:O	1:A:27:HIS:N	2.51	0.42
2:D:212:ILE:O	2:D:212:ILE:CG2	2.68	0.41
1:A:53:CYS:SG	2:C:265:ILE:HG12	2.60	0.41
1:A:142:LEU:HD23	1:A:142:LEU:H	1.84	0.41
1:B:4:TYR:CE1	1:B:23:ASN:HB2	2.55	0.41
1:A:209:ASP:OD2	1:A:213:LYS:NZ	2.53	0.41
2:C:161[A]:ARG:HB2	2:C:161[A]:ARG:NH2	2.37	0.40
1:A:102:ILE:HD12	7:A:432:HOH:O	2.22	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	288/292 (99%)	269 (93%)	18 (6%)	1 (0%)	41	70
1	B	274/292 (94%)	255 (93%)	17 (6%)	2 (1%)	22	52
2	C	147/209 (70%)	143 (97%)	4 (3%)	0	100	100
2	D	145/209 (69%)	136 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	854/1002 (85%)	803 (94%)	48 (6%)	3 (0%)	34 64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	VAL
1	B	163	VAL
1	B	73	ASP

5.3.2 Protein sidechains [i](#)

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	258/260 (99%)	257 (100%)	1 (0%)	91 95
1	B	248/260 (95%)	247 (100%)	1 (0%)	91 95
2	C	139/187 (74%)	135 (97%)	4 (3%)	42 70
2	D	138/187 (74%)	136 (99%)	2 (1%)	67 84
All	All	783/894 (88%)	775 (99%)	8 (1%)	76 89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	B	64	VAL
2	C	166	LEU
2	C	219	ASP
2	C	245	LEU
2	C	251	GLU
2	D	154	CYS
2	D	245	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	GLN
2	D	274	GLN
2	D	276	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 48 ligands modelled in this entry, 19 are monoatomic - leaving 29 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
5	EDO	C	403	-	3,3,3	0.08	0	2,2,2	0.20	0
4	GOL	A	302	-	5,5,5	0.08	0	5,5,5	0.26	0
3	61U	A	301	-	38,40,40	0.69	2 (5%)	52,58,58	1.98	14 (26%)
5	EDO	A	310	-	3,3,3	0.10	0	2,2,2	0.25	0
5	EDO	B	302	-	3,3,3	0.09	0	2,2,2	0.13	0
5	EDO	A	315	-	3,3,3	0.08	0	2,2,2	0.22	0
4	GOL	A	303	-	5,5,5	0.10	0	5,5,5	0.31	0
5	EDO	A	312	-	3,3,3	0.07	0	2,2,2	0.17	0
5	EDO	A	317	-	3,3,3	0.08	0	2,2,2	0.28	0
5	EDO	C	408	-	3,3,3	0.10	0	2,2,2	0.23	0
4	GOL	A	308	-	5,5,5	0.09	0	5,5,5	0.23	0
5	EDO	A	316	-	3,3,3	0.08	0	2,2,2	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	C	402	-	3,3,3	0.07	0	2,2,2	0.21	0
5	EDO	B	303	-	3,3,3	0.05	0	2,2,2	0.20	0
5	EDO	C	406	-	3,3,3	0.08	0	2,2,2	0.19	0
4	GOL	A	306	-	5,5,5	0.11	0	5,5,5	0.31	0
5	EDO	A	314	-	3,3,3	0.06	0	2,2,2	0.17	0
4	GOL	A	305	-	5,5,5	0.12	0	5,5,5	0.41	0
4	GOL	C	401	-	5,5,5	0.12	0	5,5,5	0.36	0
4	GOL	A	307	-	5,5,5	0.11	0	5,5,5	0.28	0
5	EDO	A	311	-	3,3,3	0.08	0	2,2,2	0.18	0
4	GOL	A	304	-	5,5,5	0.11	0	5,5,5	0.28	0
5	EDO	C	404	-	3,3,3	0.07	0	2,2,2	0.25	0
5	EDO	C	405	-	3,3,3	0.08	0	2,2,2	0.12	0
5	EDO	A	309	-	3,3,3	0.04	0	2,2,2	0.10	0
5	EDO	C	409	-	3,3,3	0.09	0	2,2,2	0.22	0
5	EDO	C	407	-	3,3,3	0.08	0	2,2,2	0.19	0
5	EDO	B	301	-	3,3,3	0.05	0	2,2,2	0.19	0
5	EDO	A	313	-	3,3,3	0.09	0	2,2,2	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	403	-	-	1/1/1/1	-
4	GOL	A	302	-	-	1/4/4/4	-
3	61U	A	301	-	-	3/21/40/40	0/5/5/5
5	EDO	A	310	-	-	1/1/1/1	-
5	EDO	B	302	-	-	0/1/1/1	-
5	EDO	A	315	-	-	1/1/1/1	-
4	GOL	A	303	-	-	2/4/4/4	-
5	EDO	A	312	-	-	1/1/1/1	-
5	EDO	A	317	-	-	0/1/1/1	-
5	EDO	C	408	-	-	0/1/1/1	-
4	GOL	A	308	-	-	2/4/4/4	-
5	EDO	A	316	-	-	0/1/1/1	-
5	EDO	C	402	-	-	1/1/1/1	-
5	EDO	B	303	-	-	1/1/1/1	-
5	EDO	C	406	-	-	1/1/1/1	-
4	GOL	A	306	-	-	2/4/4/4	-
5	EDO	A	314	-	-	1/1/1/1	-
4	GOL	A	305	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	401	-	-	4/4/4/4	-
4	GOL	A	307	-	-	2/4/4/4	-
5	EDO	A	311	-	-	1/1/1/1	-
4	GOL	A	304	-	-	1/4/4/4	-
5	EDO	C	404	-	-	1/1/1/1	-
5	EDO	C	405	-	-	1/1/1/1	-
5	EDO	A	309	-	-	0/1/1/1	-
5	EDO	C	409	-	-	0/1/1/1	-
5	EDO	C	407	-	-	0/1/1/1	-
5	EDO	B	301	-	-	1/1/1/1	-
5	EDO	A	313	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	61U	C15-C24	2.19	1.41	1.38
3	A	301	61U	C27-N6	-2.07	1.34	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	61U	C13-N2-C14	5.47	123.34	117.81
3	A	301	61U	F-C24-C15	5.29	124.14	117.50
3	A	301	61U	C9-N6-C27	4.44	120.68	117.36
3	A	301	61U	C24-C15-N3	4.05	126.38	118.49
3	A	301	61U	C23-C24-C15	-3.72	119.96	123.50
3	A	301	61U	C26-C27-N6	3.24	123.65	118.72
3	A	301	61U	C16-C15-N3	-2.96	114.91	121.05
3	A	301	61U	C10-C9-C7	-2.85	117.60	122.14
3	A	301	61U	C16-C17-N4	-2.82	118.34	122.52
3	A	301	61U	C22-C23-C24	2.66	121.16	119.40
3	A	301	61U	O2-C20-C21	-2.15	107.06	111.80
3	A	301	61U	C12-C13-N2	-2.08	120.16	124.08
3	A	301	61U	C12-C27-N6	-2.06	119.20	122.26
3	A	301	61U	C5-C6-N1	-2.00	108.54	111.22

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	61U	C24-C15-N3-C14

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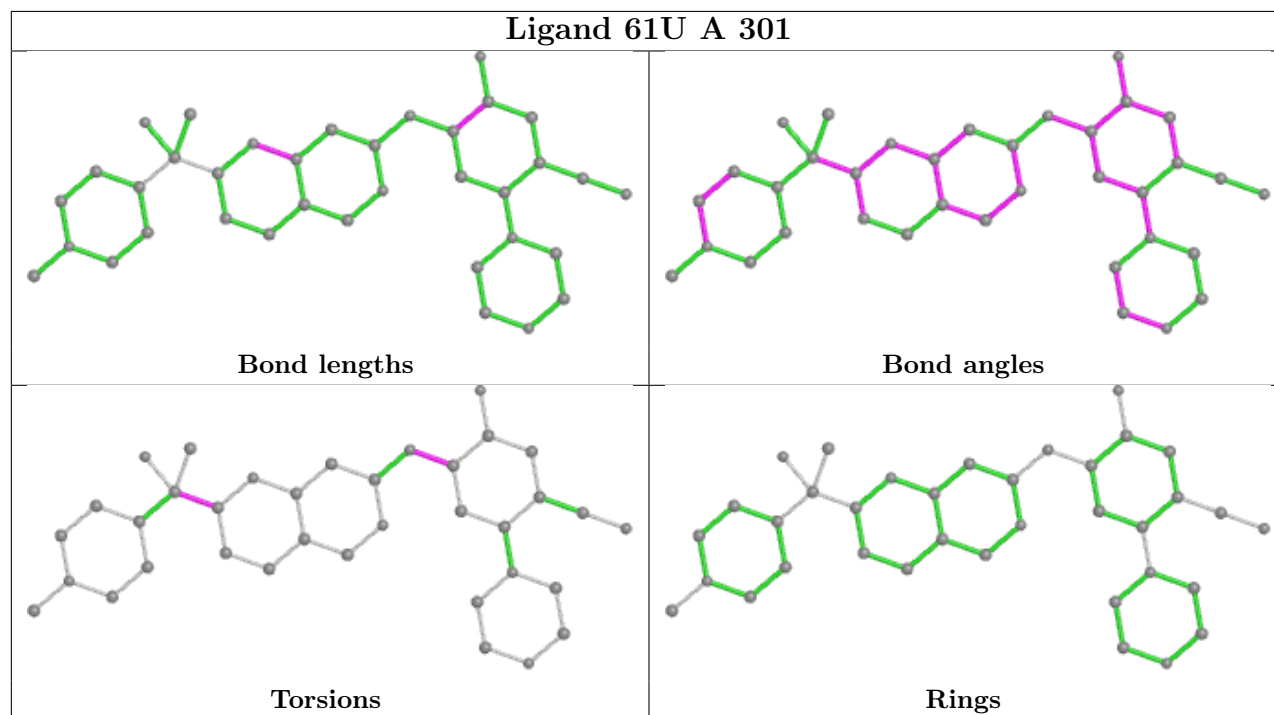
Mol	Chain	Res	Type	Atoms
3	A	301	61U	C16-C15-N3-C14
4	A	303	GOL	C1-C2-C3-O3
4	A	305	GOL	O1-C1-C2-O2
4	A	305	GOL	O1-C1-C2-C3
4	A	306	GOL	O1-C1-C2-O2
4	A	306	GOL	O1-C1-C2-C3
4	A	307	GOL	O1-C1-C2-C3
4	C	401	GOL	C1-C2-C3-O3
4	A	308	GOL	C1-C2-C3-O3
4	A	307	GOL	O1-C1-C2-O2
4	A	308	GOL	O2-C2-C3-O3
5	A	310	EDO	O1-C1-C2-O2
5	A	312	EDO	O1-C1-C2-O2
5	A	314	EDO	O1-C1-C2-O2
5	B	303	EDO	O1-C1-C2-O2
5	C	403	EDO	O1-C1-C2-O2
5	C	404	EDO	O1-C1-C2-O2
5	C	406	EDO	O1-C1-C2-O2
4	A	303	GOL	O2-C2-C3-O3
4	C	401	GOL	O2-C2-C3-O3
5	A	311	EDO	O1-C1-C2-O2
5	C	405	EDO	O1-C1-C2-O2
4	A	302	GOL	O1-C1-C2-O2
4	C	401	GOL	O1-C1-C2-C3
5	A	315	EDO	O1-C1-C2-O2
5	C	402	EDO	O1-C1-C2-O2
3	A	301	61U	C8-C7-C9-C10
4	C	401	GOL	O1-C1-C2-O2
4	A	304	GOL	O1-C1-C2-C3
5	B	301	EDO	O1-C1-C2-O2

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	290/292 (99%)	0.11	4 (1%) 75 53	75, 101, 155, 248	0
1	B	278/292 (95%)	0.93	51 (18%) 1 0	93, 154, 210, 236	0
2	C	148/209 (70%)	0.18	1 (0%) 87 72	75, 93, 127, 145	0
2	D	147/209 (70%)	2.44	68 (46%) 0 0	157, 233, 307, 362	0
All	All	863/1002 (86%)	0.78	124 (14%) 2 1	75, 127, 251, 362	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	175	VAL	20.5
2	D	213	SER	9.2
2	D	219	ASP	9.0
2	D	211	VAL	8.2
2	D	216	VAL	8.0
2	D	170	SER	7.5
2	D	173	ASP	7.5
2	D	212	ILE	7.3
1	B	245	THR	6.6
2	D	249	LEU	6.5
2	D	176	LEU	6.4
2	D	252	SER	6.4
2	D	248	PHE	6.2
2	D	226	LEU	6.1
2	D	159	LEU	6.0
1	B	42	GLU	5.6
2	D	177	TRP	5.4
2	D	243	TYR	5.4
2	D	163	CYS	5.3
2	D	174	PRO	5.2
2	D	244	PRO	5.2

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Mol	Chain	Res	Type	RSRZ
2	D	222	LEU	5.2
2	D	178	LEU	5.0
2	D	179	ARG	5.0
1	B	281	LEU	4.9
1	A	291	PRO	4.8
1	B	286	PHE	4.8
1	B	106	PHE	4.7
1	B	265	ASN	4.7
2	D	209	ARG	4.7
1	B	16	GLY	4.6
2	D	258	TRP	4.6
2	D	164	TYR	4.6
2	D	229	CYS	4.6
2	D	183	ARG	4.6
2	D	196	ILE	4.5
2	D	171	PRO	4.5
1	B	263	LEU	4.4
2	D	210	ASP	4.2
1	B	21	ALA	4.1
2	D	250	VAL	4.1
2	D	161	ARG	4.1
2	D	223	GLN	4.1
2	D	291	ASN	4.0
2	D	220	HIS	3.9
2	D	153	ARG	3.9
2	D	227	LEU	3.9
1	B	62	ASN	3.9
1	B	104	LYS	3.6
2	D	167	LYS	3.6
2	D	157	GLU	3.5
1	B	288	ASP	3.5
1	A	41	ASP	3.5
1	B	247	SER	3.5
2	D	152	LEU	3.4
1	B	93	SER	3.4
1	B	22	LYS	3.4
1	B	258	THR	3.4
2	D	214	SER	3.4
2	D	251	GLU	3.3
1	B	275	ILE	3.3
1	B	285	TYR	3.3
2	D	292	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	280	ALA	3.2
2	D	224	ALA	3.2
1	B	261	ASP	3.1
1	B	19	PHE	3.0
2	D	242	SER	3.0
1	B	198	ALA	3.0
1	B	213	LYS	3.0
2	D	217	GLY	2.9
1	B	142	LEU	2.9
2	D	231	TYR	2.9
1	B	4	TYR	2.8
2	D	207	LEU	2.8
1	B	192	PHE	2.8
2	D	265	ILE	2.8
1	B	185	MET	2.8
1	B	254	LYS	2.7
2	D	165	ARG	2.7
2	D	187	LEU	2.7
2	D	166	LEU	2.7
2	D	259	ASP	2.7
1	B	199	GLY	2.7
1	B	243	PRO	2.6
1	B	277	ALA	2.6
2	D	202	VAL	2.6
2	D	254	LYS	2.5
1	B	205	GLY	2.5
1	B	212	LEU	2.5
2	D	181	VAL	2.5
1	B	39	ASP	2.5
1	B	216	PHE	2.5
2	D	172	THR	2.5
1	B	37	LEU	2.5
2	D	245	LEU	2.5
1	B	108	PHE	2.4
2	C	263	SER	2.4
2	D	168	HIS	2.4
2	D	154	CYS	2.4
1	B	38	ASP	2.4
1	B	127	LEU	2.4
1	B	255	LEU	2.4
2	D	190	TRP	2.4
1	A	40	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	2	GLN	2.3
2	D	189	GLY	2.3
2	D	186	LEU	2.3
1	B	111	LEU	2.3
2	D	169	LEU	2.2
1	B	41	ASP	2.2
1	B	287	SER	2.2
1	B	29	ILE	2.2
2	D	236	TYR	2.2
1	B	32	LEU	2.2
2	D	261	CYS	2.2
2	D	203	PHE	2.2
1	B	78	LEU	2.2
2	D	155	LEU	2.2
1	B	186	TRP	2.1
1	B	40	ASP	2.1
1	B	26	THR	2.1
1	B	217	ARG	2.0
1	B	157	CYS	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 monosaccharides 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
5	EDO	B	303	4/4	0.39	0.75	141,142,143,146	0
5	EDO	A	313	4/4	0.44	0.52	134,134,140,141	0
6	CL	A	325	1/1	0.52	0.37	125,125,125,125	0
5	EDO	C	407	4/4	0.53	0.44	122,128,129,129	0

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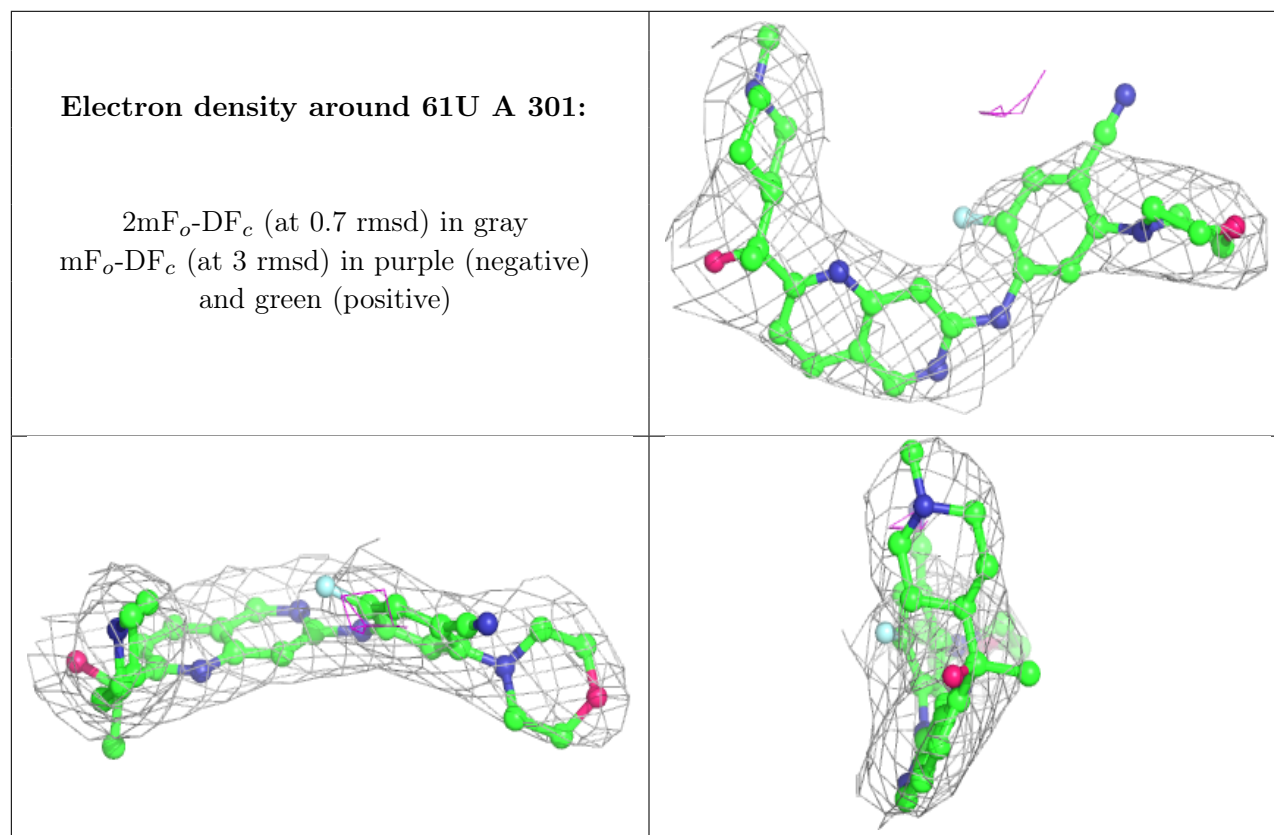
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CL	A	320	1/1	0.55	0.43	135,135,135,135	0
6	CL	A	327	1/1	0.55	0.96	111,111,111,111	0
4	GOL	C	401	6/6	0.61	0.84	128,141,149,151	0
6	CL	A	323	1/1	0.61	0.34	129,129,129,129	0
5	EDO	A	311	4/4	0.62	0.66	120,122,122,124	0
5	EDO	C	403	4/4	0.63	0.32	106,115,118,119	0
6	CL	C	411	1/1	0.63	0.14	160,160,160,160	0
6	CL	A	322	1/1	0.64	0.48	136,136,136,136	0
6	CL	C	418	1/1	0.67	0.31	124,124,124,124	0
4	GOL	A	308	6/6	0.68	0.36	148,149,151,152	0
6	CL	C	412	1/1	0.69	0.12	141,141,141,141	0
6	CL	C	416	1/1	0.71	0.43	151,151,151,151	0
5	EDO	C	408	4/4	0.71	0.79	122,133,140,141	0
4	GOL	A	305	6/6	0.73	0.37	104,120,127,128	0
5	EDO	A	309	4/4	0.74	0.38	123,130,131,133	0
4	GOL	A	304	6/6	0.74	0.66	136,142,145,145	0
5	EDO	A	317	4/4	0.75	0.89	124,133,137,144	0
5	EDO	C	406	4/4	0.75	0.55	118,125,130,135	0
5	EDO	C	409	4/4	0.75	0.76	137,142,142,144	0
5	EDO	C	402	4/4	0.76	0.93	119,124,126,126	0
5	EDO	A	310	4/4	0.78	0.33	118,126,126,129	0
4	GOL	A	306	6/6	0.78	0.25	114,126,130,133	0
5	EDO	A	312	4/4	0.78	0.75	127,128,128,129	0
4	GOL	A	302	6/6	0.79	0.77	115,128,133,135	0
5	EDO	C	405	4/4	0.82	0.30	126,129,132,137	0
5	EDO	B	301	4/4	0.82	0.56	129,144,150,159	0
4	GOL	A	307	6/6	0.82	0.43	104,114,118,120	0
6	CL	A	321	1/1	0.82	0.25	136,136,136,136	0
5	EDO	A	316	4/4	0.83	0.32	132,134,139,139	0
5	EDO	B	302	4/4	0.83	0.48	123,124,124,125	0
5	EDO	A	315	4/4	0.84	0.33	116,119,120,124	0
6	CL	A	324	1/1	0.84	0.50	133,133,133,133	0
6	CL	C	417	1/1	0.85	0.26	116,116,116,116	0
5	EDO	C	404	4/4	0.85	0.18	153,155,156,158	0
4	GOL	A	303	6/6	0.86	0.50	120,128,132,137	0
6	CL	C	415	1/1	0.87	0.18	117,117,117,117	0
6	CL	C	414	1/1	0.87	0.21	133,133,133,133	0
6	CL	C	413	1/1	0.88	0.50	125,125,125,125	0
6	CL	A	319	1/1	0.88	0.16	116,116,116,116	0
6	CL	A	318	1/1	0.88	0.33	108,108,108,108	0
5	EDO	A	314	4/4	0.89	0.45	108,109,109,112	0
6	CL	A	326	1/1	0.90	0.19	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	61U	A	301	36/36	0.93	0.29	70,95,129,142	0
6	CL	C	410	1/1	0.93	0.33	95,95,95,95	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.