



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2022 – 12:15 PM JST

PDB ID : 7VDP
Title : The structure of cyclin-dependent kinase 5 (CDK5) in complex with p25 and Compound 1
Authors : Malojcic, G.; Clugston, S.L.; Daniels, M.; Harmange, J.C.; Ledeborner, M.
Deposited on : 2021-09-07
Resolution : 2.09 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

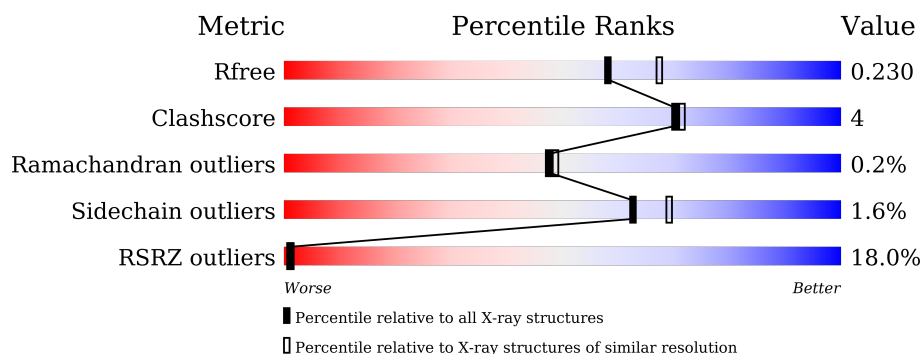
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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	292	<div> <div>3%</div> <div>90%</div> <div>8%</div> <div>..</div> </div>
1	B	292	<div> <div>15%</div> <div>83%</div> <div>12%</div> <div>.</div> </div>
2	C	209	<div> <div>69%</div> <div>29%</div> </div>
2	D	209	<div> <div>47%</div> <div>53%</div> <div>10%</div> <div>37%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7321 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2307	1480	397	419	11			
1	B	279	Total	C	N	O	S	0	0	0
			2248	1447	388	403	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

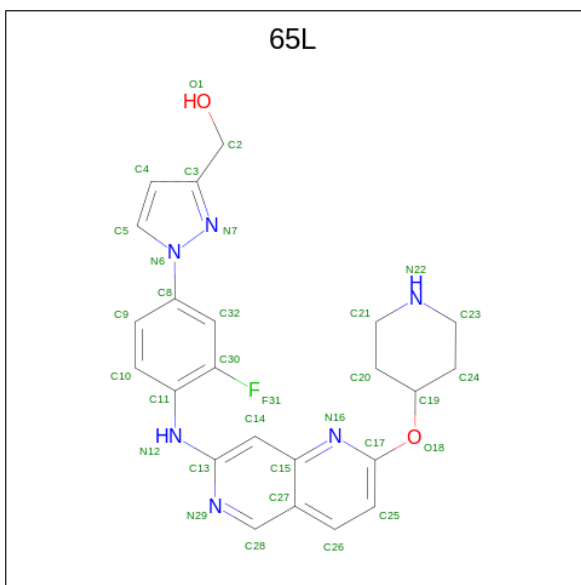
- Molecule 2 is a protein called Cyclin-dependent kinase 5 activator 1, p25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	148	Total	C	N	O	S	0	0	0
			1196	768	197	220	11			
2	D	131	Total	C	N	O	S	0	0	0
			1067	689	174	196	8			

There are 2 discrepancies between the modelled and reference sequences:

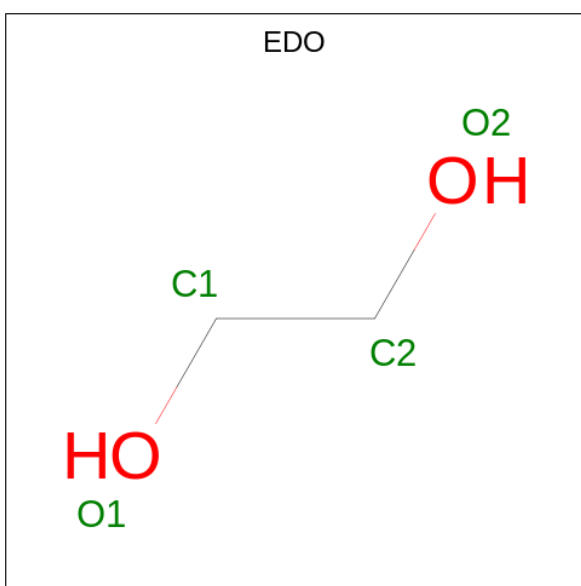
Chain	Residue	Modelled	Actual	Comment	Reference
C	99	MET	-	initiating methionine	UNP Q15078
D	99	MET	-	initiating methionine	UNP Q15078

- Molecule 3 is [1-[3-fluoranyl-4-[(2-piperidin-4-yloxy-1,6-naphthyridin-7-yl)amino]phenyl]pyrazol-3-yl]methanol (three-letter code: 65L) (formula: C₂₃H₂₃FN₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			32	23	1	6	2		
3	B	1	Total	C	F	N	O	0	0
			32	23	1	6	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



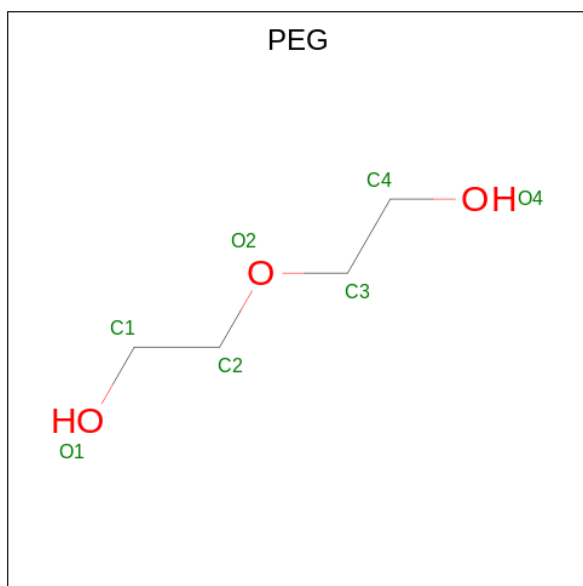
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

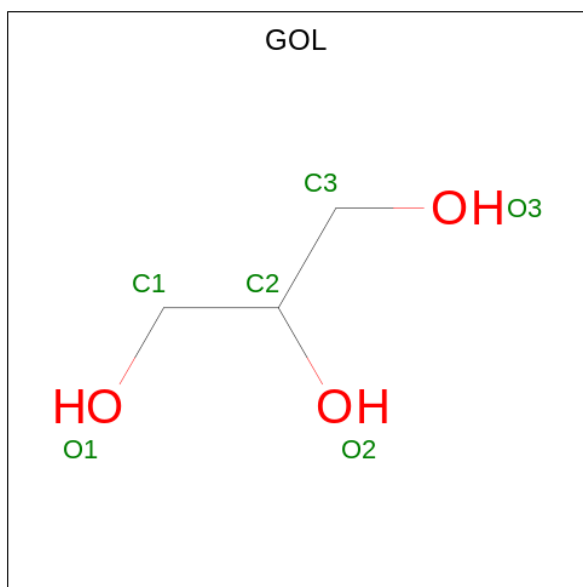


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total Cl 6 6	0	0
6	C	1	Total Cl 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	183	Total O 183 183	0	0
8	B	86	Total O 86 86	0	0
8	C	97	Total O 97 97	0	0
8	D	6	Total O 6 6	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.

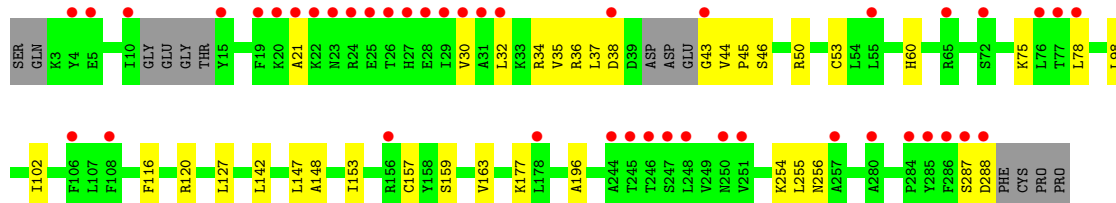
• Molecule 1: Cyclin-dependent-like kinase 5

Chain A: 



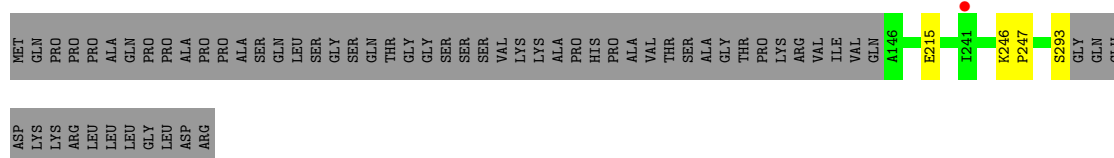
• Molecule 1: Cyclin-dependent-like kinase 5

Chain B: 



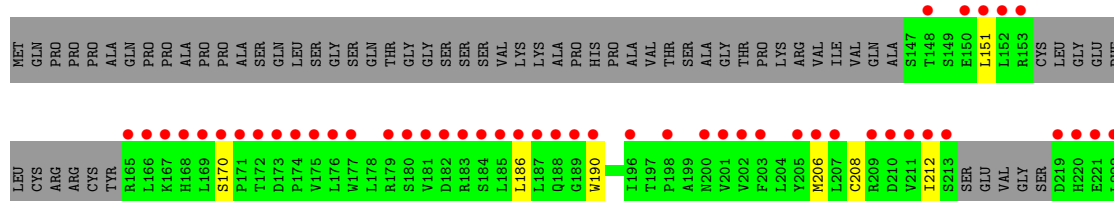
• Molecule 2: Cyclin-dependent kinase 5 activator 1, p25

Chain C: 



• Molecule 2: Cyclin-dependent kinase 5 activator 1, p25

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.37Å 118.37Å 155.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.79 – 2.09 51.79 – 2.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (51.79-2.09) 100.0 (51.79-2.09)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.201 , 0.229 0.207 , 0.230	Depositor DCC
R_{free} test set	3645 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7321	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: EDO, GOL, 65L, PEG, CL

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	0.68	0/2360	0.77	0/3193
1	B	0.68	0/2299	0.76	0/3109
2	C	0.74	2/1224 (0.2%)	0.74	0/1660
2	D	0.66	0/1091	0.69	0/1479
All	All	0.69	2/6974 (0.0%)	0.75	0/9441

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	215	GLU	CG-CD	7.54	1.63	1.51
2	C	215	GLU	CD-OE2	6.00	1.32	1.25

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	2307	0	2324	19	0
1	B	2248	0	2280	24	0
2	C	1196	0	1185	1	0
2	D	1067	0	1060	13	0
3	A	32	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	32	0	0	0	0
4	A	28	0	42	4	0
4	C	12	0	18	0	0
5	A	14	0	20	2	0
6	A	6	0	0	0	0
6	C	1	0	0	0	0
7	A	6	0	8	0	0
8	A	183	0	0	3	0
8	B	86	0	0	1	0
8	C	97	0	0	0	0
8	D	6	0	0	1	0
All	All	7321	0	6937	50	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 4.

All (50) 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:249:LEU:HD21	2:D:254:LYS:HE3	1.78	0.66
2:D:261:CYS:SG	8:D:404:HOH:O	2.53	0.66
1:B:157:CYS:HB2	1:B:177:LYS:HB3	1.81	0.63
1:B:153:ILE:HD12	2:D:276:ASN:HA	1.82	0.62
1:B:21:ALA:HB3	1:B:32:LEU:HD13	1.85	0.57
2:D:249:LEU:HD21	2:D:254:LYS:CE	2.38	0.54
1:A:61:LYS:NZ	8:A:403:HOH:O	2.41	0.53
1:B:43:GLY:O	1:B:46:SER:OG	2.27	0.52
1:A:260:ARG:HB2	5:A:310:PEG:H12	1.91	0.52
1:B:287:SER:O	1:B:288:ASP:OD1	2.27	0.52
1:A:12:GLU:HA	1:A:17:THR:HA	1.93	0.50
1:A:241:MET:HE3	8:A:469:HOH:O	2.11	0.50
3:A:301:65L:C10	4:A:302:EDO:H12	2.41	0.49
1:A:136:ARG:HA	4:A:307:EDO:H11	1.94	0.49
1:B:78:LEU:N	1:B:78:LEU:HD23	2.28	0.48
2:D:208:CYS:HA	2:D:212:ILE:HD13	1.96	0.48
1:B:256:ASN:OD1	1:B:256:ASN:N	2.47	0.48
1:B:53:CYS:SG	2:D:265:ILE:HG12	2.53	0.47
1:A:78:LEU:HD12	1:A:78:LEU:N	2.29	0.47
1:B:159:SER:HB2	2:D:239:ASN:O	2.14	0.47
1:A:135:ASN:O	4:A:307:EDO:H22	2.15	0.47
1:B:37:LEU:HD23	2:D:258:TRP:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ARG:NH1	1:B:148:ALA:O	2.47	0.47
1:B:30:VAL:HG23	1:B:32:LEU:CD1	2.46	0.46
1:A:40:ASP:OD2	1:B:36:ARG:NH2	2.49	0.46
1:A:162:VAL:HG21	1:A:179:TYR:OH	2.17	0.45
1:B:98:LEU:O	1:B:254:LYS:HE3	2.15	0.45
1:B:34:ARG:CG	1:B:75:LYS:HD2	2.47	0.45
2:D:255:GLU:O	2:D:259:ASP:HB2	2.17	0.45
2:D:151:LEU:HD22	2:D:289:LEU:HD23	2.00	0.44
1:B:196:ALA:HB1	1:B:255:LEU:HG	1.98	0.44
1:B:120:ARG:O	2:D:273:LEU:HD11	2.17	0.44
1:B:35:VAL:HG13	1:B:44:VAL:HG12	2.00	0.43
1:A:136:ARG:N	1:A:136:ARG:HD2	2.32	0.43
1:A:36:ARG:CZ	1:B:36:ARG:HD2	2.49	0.43
1:B:60:HIS:O	8:B:401:HOH:O	2.21	0.43
2:D:190:TRP:CE3	2:D:190:TRP:HA	2.54	0.43
1:B:127:LEU:CD2	1:B:142:LEU:HD11	2.48	0.43
1:A:39:ASP:HB2	1:A:42:GLU:HA	2.01	0.43
2:D:228:THR:HG21	2:D:260:ARG:HD2	2.01	0.42
1:A:44:VAL:N	1:A:45:PRO:CD	2.83	0.42
1:A:257:ALA:HA	5:A:310:PEG:H11	2.02	0.42
1:B:116:PHE:O	1:B:120:ARG:HG2	2.19	0.42
1:A:36:ARG:CD	1:B:36:ARG:CZ	2.98	0.42
2:C:246:LYS:HB3	2:C:247:PRO:HD3	2.01	0.42
1:A:180:SER:HB2	8:A:554:HOH:O	2.20	0.42
1:A:136:ARG:HA	4:A:307:EDO:C1	2.50	0.41
1:B:44:VAL:HB	1:B:45:PRO:HD3	2.03	0.41
1:A:213:LYS:O	1:A:217:ARG:HB2	2.21	0.41
1:A:55:LEU:HD23	1:A:55:LEU:HA	1.96	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	283/292 (97%)	270 (95%)	12 (4%)	1 (0%)	34	32
1	B	273/292 (94%)	262 (96%)	10 (4%)	1 (0%)	34	32
2	C	146/209 (70%)	146 (100%)	0	0	100	100
2	D	125/209 (60%)	122 (98%)	3 (2%)	0	100	100
All	All	827/1002 (82%)	800 (97%)	25 (3%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

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

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	256/260 (98%)	252 (98%)	4 (2%)	62	69
1	B	249/260 (96%)	246 (99%)	3 (1%)	71	77
2	C	138/187 (74%)	137 (99%)	1 (1%)	84	88
2	D	124/187 (66%)	120 (97%)	4 (3%)	39	41
All	All	767/894 (86%)	755 (98%)	12 (2%)	62	69

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	39	ASP
1	A	136	ARG
1	A	141	LYS
1	B	38	ASP
1	B	102	ILE
1	B	147	LEU
2	C	293	SER
2	D	170	SER

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Mol	Chain	Res	Type
2	D	186	LEU
2	D	206	MET
2	D	283	THR

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	206	ASN
1	B	282	GLN
2	C	188	GLN
2	C	266	ASN
2	D	188	GLN
2	D	239	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	307	-	3,3,3	0.08	0	2,2,2	0.36	0
4	EDO	A	306	-	3,3,3	0.07	0	2,2,2	0.24	0
4	EDO	A	303	-	3,3,3	0.09	0	2,2,2	0.24	0
3	65L	A	301	-	35,36,36	0.72	0	42,50,50	2.35	14 (33%)
3	65L	B	301	-	35,36,36	0.83	2 (5%)	42,50,50	2.34	14 (33%)
4	EDO	C	403	-	3,3,3	0.02	0	2,2,2	0.17	0
7	GOL	A	317	-	5,5,5	0.10	0	5,5,5	0.29	0
4	EDO	C	402	-	3,3,3	0.06	0	2,2,2	0.20	0
5	PEG	A	310	-	6,6,6	0.18	0	5,5,5	0.25	0
4	EDO	C	401	-	3,3,3	0.25	0	2,2,2	0.19	0
4	EDO	A	308	-	3,3,3	0.03	0	2,2,2	0.10	0
4	EDO	A	302	-	3,3,3	0.25	0	2,2,2	0.71	0
5	PEG	A	309	-	6,6,6	0.19	0	5,5,5	0.13	0
4	EDO	A	305	-	3,3,3	0.09	0	2,2,2	0.19	0
4	EDO	A	304	-	3,3,3	0.09	0	2,2,2	0.20	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
4	EDO	A	307	-	-	1/1/1/1	-
4	EDO	A	306	-	-	0/1/1/1	-
4	EDO	A	303	-	-	0/1/1/1	-
3	65L	A	301	-	-	2/12/22/22	0/5/5/5
3	65L	B	301	-	-	2/12/22/22	0/5/5/5
4	EDO	C	403	-	-	1/1/1/1	-
7	GOL	A	317	-	-	0/4/4/4	-
4	EDO	C	402	-	-	1/1/1/1	-
5	PEG	A	310	-	-	3/4/4/4	-
4	EDO	C	401	-	-	1/1/1/1	-
4	EDO	A	308	-	-	0/1/1/1	-
4	EDO	A	302	-	-	1/1/1/1	-
5	PEG	A	309	-	-	3/4/4/4	-
4	EDO	A	305	-	-	0/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	65L	C17-N16	2.11	1.33	1.30
3	B	301	65L	C3-N7	-2.02	1.31	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	65L	C17-N16-C15	7.81	121.51	115.79
3	B	301	65L	C17-N16-C15	7.63	121.37	115.79
3	A	301	65L	C5-N6-N7	-5.74	106.87	112.72
3	B	301	65L	C5-N6-N7	-5.23	107.38	112.72
3	B	301	65L	C28-N29-C13	5.10	122.97	117.81
3	A	301	65L	C25-C17-N16	-4.89	120.71	125.57
3	B	301	65L	C25-C17-N16	-4.39	121.20	125.57
3	A	301	65L	C28-N29-C13	4.30	122.16	117.81
3	A	301	65L	C17-O18-C19	3.02	120.84	117.75
3	B	301	65L	C17-O18-C19	2.87	120.69	117.75
3	B	301	65L	C32-C30-C11	-2.86	120.78	123.50
3	A	301	65L	C3-N7-N6	2.83	108.94	105.66
3	A	301	65L	C14-C15-N16	2.71	122.84	118.72
3	B	301	65L	C5-C4-C3	2.67	107.65	105.54
3	B	301	65L	C2-C3-C4	-2.52	125.61	129.89
3	A	301	65L	C5-C4-C3	2.51	107.52	105.54
3	B	301	65L	C9-C8-C32	-2.51	118.77	121.74
3	A	301	65L	O18-C17-N16	2.43	121.76	119.63
3	B	301	65L	C3-N7-N6	2.36	108.40	105.66
3	B	301	65L	C14-C15-N16	2.32	122.25	118.72
3	A	301	65L	C26-C25-C17	2.32	120.25	117.67
3	B	301	65L	C9-C8-N6	2.27	121.14	119.15
3	B	301	65L	O18-C17-N16	2.20	121.56	119.63
3	A	301	65L	C4-C3-N7	-2.13	108.21	110.44
3	B	301	65L	C26-C25-C17	2.07	119.97	117.67
3	A	301	65L	C14-C13-N29	-2.07	119.85	122.75
3	A	301	65L	C32-C30-C11	-2.06	121.53	123.50
3	A	301	65L	C9-C8-C32	-2.04	119.32	121.74

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	309	PEG	O1-C1-C2-O2
5	A	309	PEG	O2-C3-C4-O4
5	A	310	PEG	O1-C1-C2-O2

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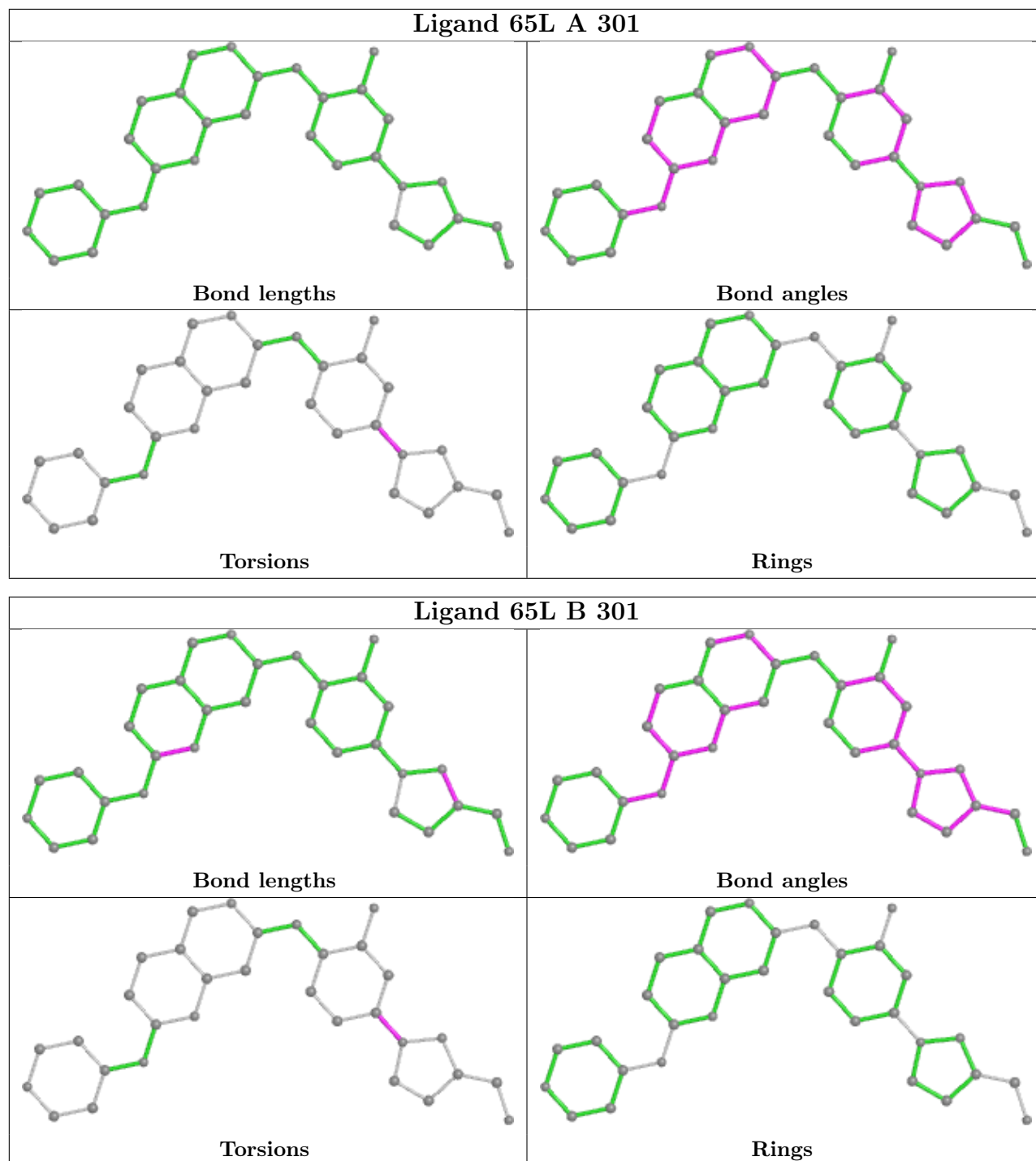
Mol	Chain	Res	Type	Atoms
4	A	307	EDO	O1-C1-C2-O2
4	C	402	EDO	O1-C1-C2-O2
4	A	302	EDO	O1-C1-C2-O2
5	A	309	PEG	C1-C2-O2-C3
3	A	301	65L	C9-C8-N6-C5
3	B	301	65L	C9-C8-N6-C5
3	B	301	65L	C32-C8-N6-C5
5	A	310	PEG	C1-C2-O2-C3
5	A	310	PEG	C4-C3-O2-C2
4	C	401	EDO	O1-C1-C2-O2
4	C	403	EDO	O1-C1-C2-O2
3	A	301	65L	C32-C8-N6-C5

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	307	EDO	3	0
3	A	301	65L	1	0
5	A	310	PEG	2	0
4	A	302	EDO	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	287/292 (98%)	0.26	9 (3%) 49 55	29, 41, 79, 123	0
1	B	279/292 (95%)	0.81	44 (15%) 2 2	37, 68, 125, 161	0
2	C	148/209 (70%)	0.01	1 (0%) 87 89	31, 41, 63, 76	0
2	D	131/209 (62%)	4.26	98 (74%) 0 0	99, 134, 158, 174	0
All	All	845/1002 (84%)	1.02	152 (17%) 1 1	29, 53, 142, 174	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	226	LEU	18.1
2	D	222	LEU	16.8
2	D	211	VAL	15.6
2	D	175	VAL	12.2
1	B	22	LYS	11.5
2	D	207	LEU	11.2
1	B	245	THR	10.5
2	D	220	HIS	10.5
2	D	151	LEU	10.3
2	D	176	LEU	10.1
2	D	224	ALA	9.8
2	D	177	TRP	9.4
2	D	168	HIS	8.5
1	B	15	TYR	8.5
2	D	291	ASN	8.3
2	D	250	VAL	8.2
2	D	225	VAL	8.0
2	D	152	LEU	7.9
2	D	187	LEU	7.4
2	D	153	ARG	7.3
2	D	231	TYR	7.3

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Mol	Chain	Res	Type	RSRZ
2	D	167	LYS	7.0
2	D	229	CYS	7.0
2	D	189	GLY	6.9
2	D	174	PRO	6.7
2	D	173	ASP	6.6
1	B	29	ILE	6.6
2	D	170	SER	6.6
2	D	203	PHE	6.6
2	D	257	PHE	6.5
2	D	181	VAL	6.5
2	D	183	ARG	6.4
2	D	166	LEU	6.4
2	D	171	PRO	6.3
2	D	290	LYS	6.1
2	D	169	LEU	6.1
1	B	286	PHE	6.0
2	D	244	PRO	5.9
2	D	190	TRP	5.9
2	D	246	LYS	5.9
2	D	249	LEU	5.8
1	B	246	THR	5.8
2	D	205	TYR	5.6
2	D	253	CYS	5.6
2	D	248	PHE	5.5
2	D	287	SER	5.4
2	D	180	SER	5.2
2	D	285	VAL	5.1
1	B	288	ASP	5.1
2	D	292	GLU	5.1
2	D	258	TRP	5.1
2	D	227	LEU	4.9
2	D	165	ARG	4.9
2	D	245	LEU	4.8
2	D	267	LEU	4.8
1	B	25	GLU	4.8
2	D	188	GLN	4.5
2	D	179	ARG	4.3
2	D	172	THR	4.3
1	B	250	ASN	4.2
2	D	252	SER	4.2
1	B	257	ALA	4.2
2	D	219	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	241	ILE	4.2
1	B	287	SER	4.1
2	D	196	ILE	4.0
2	D	251	GLU	4.0
2	D	221	GLU	4.0
2	D	184	SER	3.9
2	D	201	VAL	3.9
1	B	284	PRO	3.9
1	B	30	VAL	3.9
1	A	156	ARG	3.8
2	D	260	ARG	3.7
1	B	247	SER	3.7
2	D	233	SER	3.7
1	A	162	VAL	3.7
2	D	202	VAL	3.7
2	D	263	SER	3.7
1	B	285	TYR	3.7
1	B	21	ALA	3.7
2	D	228	THR	3.7
2	D	259	ASP	3.6
2	D	254	LYS	3.6
1	B	32	LEU	3.5
1	B	248	LEU	3.5
2	D	213	SER	3.5
1	A	160	ALA	3.4
2	D	150	GLU	3.4
1	B	27	HIS	3.4
2	D	148	THR	3.3
2	D	186	LEU	3.3
1	A	11	GLY	3.2
1	B	10	ILE	3.2
2	D	234	TYR	3.2
2	D	286	PHE	3.2
2	D	283	THR	3.2
2	D	209	ARG	3.1
1	B	72	SER	3.1
1	B	65	ARG	3.0
1	B	156	ARG	3.0
2	D	223	GLN	3.0
1	B	178	LEU	3.0
2	D	212	ILE	3.0
1	B	24	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	41	ASP	2.9
1	B	43	GLY	2.9
1	B	55	LEU	2.9
2	D	256	ALA	2.8
1	A	42	GLU	2.8
2	D	266	ASN	2.8
1	A	39	ASP	2.8
1	B	38	ASP	2.8
1	A	40	ASP	2.8
1	B	76	LEU	2.8
2	D	232	LEU	2.7
1	B	28	GLU	2.7
1	B	5	GLU	2.7
2	D	206	MET	2.6
1	B	23	ASN	2.6
2	D	273	LEU	2.6
2	C	241	ILE	2.5
2	D	280	HIS	2.5
1	B	108	PHE	2.5
2	D	265	ILE	2.5
2	D	200	ASN	2.5
1	B	26	THR	2.4
2	D	242	SER	2.4
1	B	106	PHE	2.3
1	A	16	GLY	2.3
1	B	4	TYR	2.3
1	B	251	VAL	2.3
2	D	281	TYR	2.3
2	D	185	LEU	2.3
1	B	78	LEU	2.3
2	D	210	ASP	2.3
2	D	284	GLN	2.3
1	B	31	ALA	2.2
2	D	274	GLN	2.2
2	D	236	TYR	2.2
2	D	247	PRO	2.2
2	D	278	ASP	2.2
1	B	280	ALA	2.2
2	D	268	MET	2.2
2	D	262	LEU	2.1
1	B	244	ALA	2.1
2	D	269	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	20	LYS	2.1
2	D	182	ASP	2.1
1	B	19	PHE	2.1
1	B	77	THR	2.1
2	D	198	PRO	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
4	EDO	A	306	4/4	0.51	0.37	92,92,95,97	0
7	GOL	A	317	6/6	0.60	0.14	72,74,75,77	0
4	EDO	A	307	4/4	0.70	0.27	70,73,74,75	0
4	EDO	C	402	4/4	0.75	0.28	71,74,75,77	0
5	PEG	A	309	7/7	0.76	0.19	58,60,66,66	0
4	EDO	A	308	4/4	0.76	0.17	69,76,80,83	0
5	PEG	A	310	7/7	0.80	0.32	48,58,62,64	0
4	EDO	A	302	4/4	0.81	0.23	43,47,52,56	0
4	EDO	A	304	4/4	0.82	0.20	82,84,84,85	0
4	EDO	C	403	4/4	0.85	0.28	72,73,73,75	0
3	65L	B	301	32/32	0.86	0.13	53,69,74,76	0
4	EDO	A	303	4/4	0.89	0.12	58,64,66,67	0
6	CL	A	316	1/1	0.90	0.34	87,87,87,87	0
6	CL	A	315	1/1	0.90	0.11	75,75,75,75	0
6	CL	A	312	1/1	0.91	0.10	63,63,63,63	0
4	EDO	A	305	4/4	0.91	0.17	60,60,61,61	0
6	CL	C	404	1/1	0.93	0.25	73,73,73,73	0
6	CL	A	314	1/1	0.94	0.11	64,64,64,64	0

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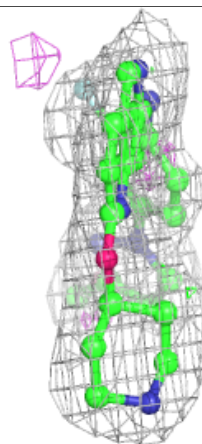
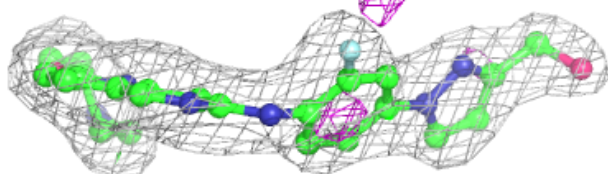
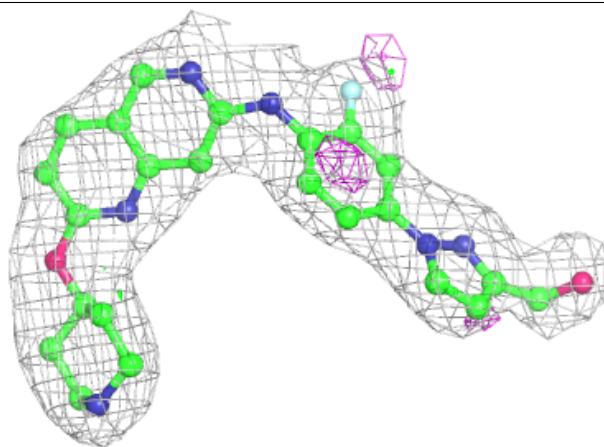
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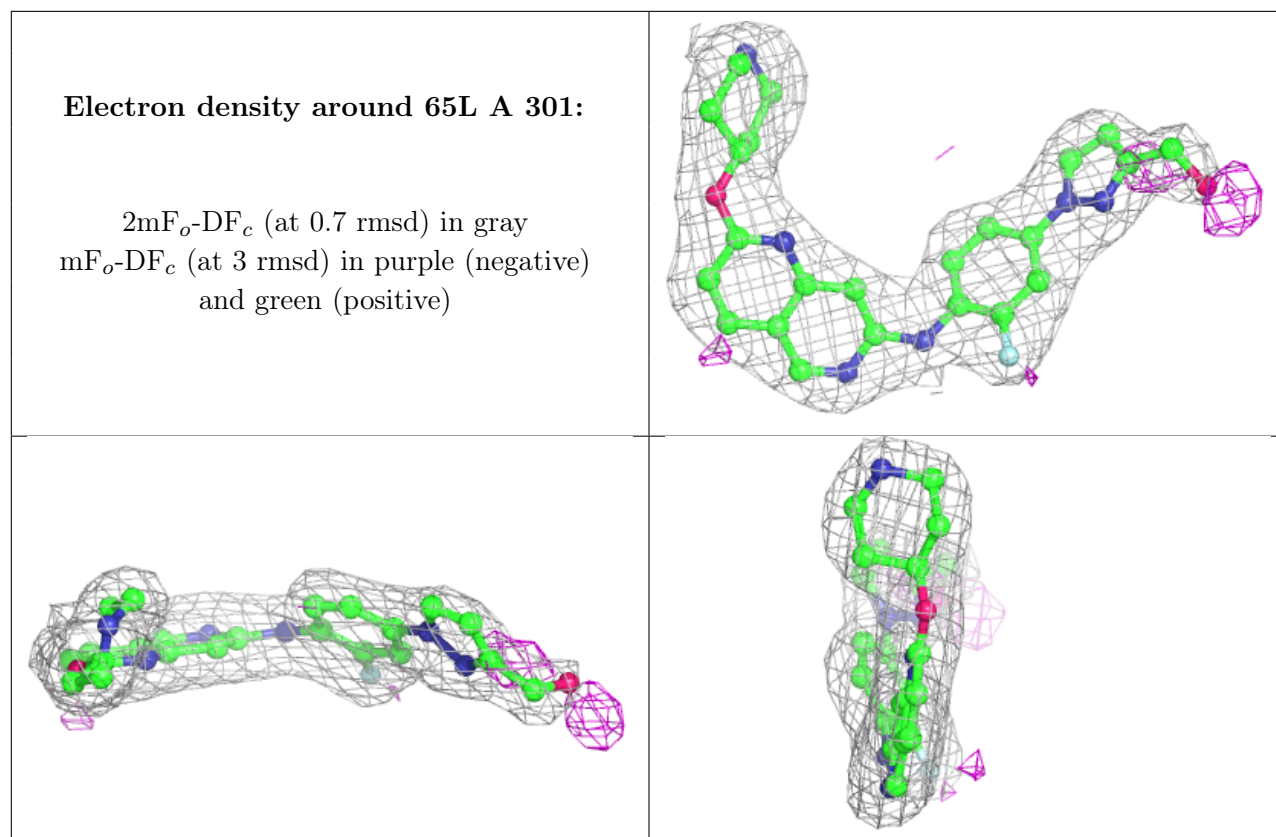
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	C	401	4/4	0.95	0.30	42,43,43,44	0
3	65L	A	301	32/32	0.96	0.12	32,39,55,61	0
6	CL	A	313	1/1	0.97	0.11	54,54,54,54	0
6	CL	A	311	1/1	0.97	0.11	44,44,44,44	0

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 65L B 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 [i](#)

There are no such residues in this entry.