



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2026 – 10:10 AM EDT

PDB ID : 9Z3C / pdb_00009z3c
Title : Human ClpP with drug
Authors : Majaesic, E.; Barghash, M.; Lee, J.; Houry, W.A.
Deposited on : 2025-11-06
Resolution : 2.78 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

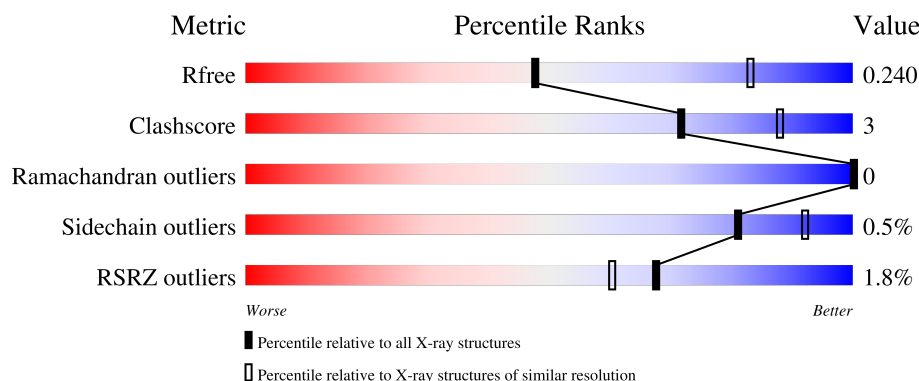
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	221	% 70% 9% 21%
1	B	221	% 71% 7% 22%
1	C	221	% 72% 7% 21%
1	D	221	74% 6% 20%
1	E	221	% 76% • 20%

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Mol	Chain	Length	Quality of chain
1	F	221	4% 71% 9% 21%
1	G	221	% 72% 6% 21%

2 Entry composition

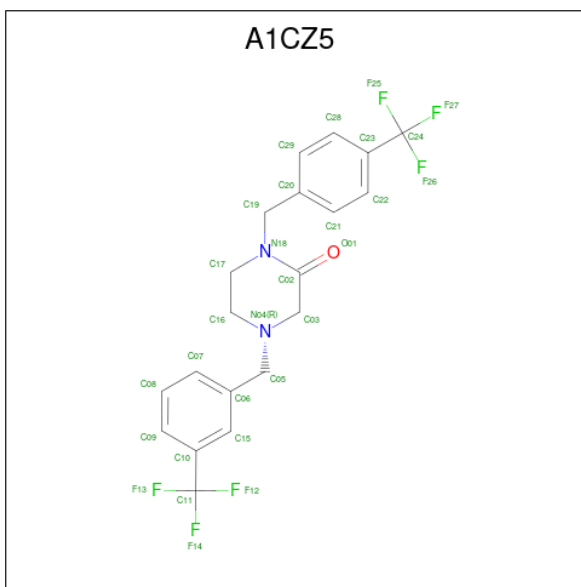
There are 4 unique types of molecules in this entry. The entry contains 9818 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent Clp protease proteolytic subunit, mitochondrial.

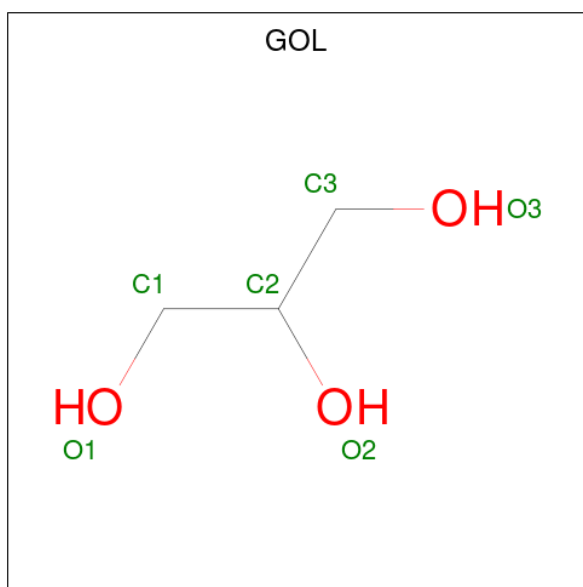
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	1	0
			1346	860	228	246	12			
1	B	173	Total	C	N	O	S	0	0	0
			1335	854	225	243	13			
1	C	175	Total	C	N	O	S	0	0	0
			1355	867	229	246	13			
1	D	176	Total	C	N	O	S	0	1	0
			1367	873	235	246	13			
1	E	176	Total	C	N	O	S	0	0	0
			1357	868	231	245	13			
1	F	175	Total	C	N	O	S	0	1	0
			1364	873	231	247	13			
1	G	174	Total	C	N	O	S	0	1	0
			1355	866	230	246	13			

- Molecule 2 is 4-{{3-(trifluoromethyl)phenyl}methyl}-1-{{4-(trifluoromethyl)phenyl}methyl}piperazin-2-one (CCD ID: A1CZ5) (formula: C₂₀H₁₈F₆N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			29	20	6	2	1		
2	B	1	Total	C	F	N	O	0	0
			29	20	6	2	1		
2	C	1	Total	C	F	N	O	0	0
			29	20	6	2	1		
2	D	1	Total	C	F	N	O	0	0
			29	20	6	2	1		
2	E	1	Total	C	F	N	O	0	0
			29	20	6	2	1		
2	F	1	Total	C	F	N	O	0	0
			29	20	6	2	1		
2	G	1	Total	C	F	N	O	0	0
			29	20	6	2	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

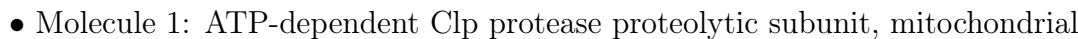
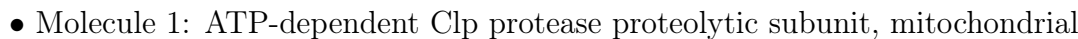
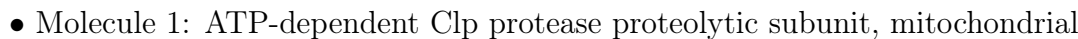


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

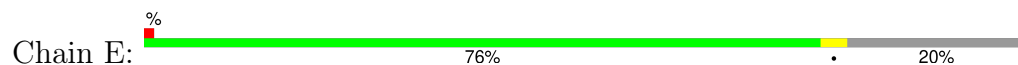
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	22	Total	O	0	0
			22	22		
4	C	13	Total	O	0	0
			13	13		
4	D	23	Total	O	0	0
			23	23		
4	E	17	Total	O	0	0
			17	17		
4	F	20	Total	O	0	0
			20	20		
4	G	18	Total	O	0	0
			18	18		

- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



LYS
GLU
PRO
VAL
GLU
ALA
ALA
PRO
ALA
ALA
GLU
PRO
VAL
PRO
ALA
SER
THR

- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



PE7
V63
GLN
THR
GLY
ARG
GLY
E70
Y73
R78
S97
V126
I139
I143
M176
P180
SER
GLY
GLY
ALA
ALA
ARG
GLN
ALA
THR
ASP
ILE
A192
P248
P249
GLN
ASP
GLY
GLY
ASP
GLY
PRO
THR
LEU
VAL
GLN
LYS
PRO
GLU
VAL
ALA
PRO

ALA
ALA
GLU
PRO
PRO
ALA
SER
THR

- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



PRO
L58
V63
GLN
THR
GLY
ARG
GLY
GLY
ARG
A72
Y73
I84
M88
H116
G123
I139
I143
C144
V148
S153
M166
H167
H168
S169
M176
I177
H178
S181
GLY
GLY
ALA
ARG
GLY
GLN
ALA
THR
ASP
I191
Q194
E197
I198
L241
D242

K243
V244
I245
V246
P249
GLN
ASP
GLY
GLY
ASP
GLY
PRO
THR
LEU
VAL
GLN
LYS
GLU
PRO
VAL
GLU
ALA
ALA
PRO
ALA
ALA
GLU
PRO
VAL
PRO
ALA
SER
THR

- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



PRO
L58
V63
GLN
THR
GLY
ARG
GLY
GLY
ARG
A72
Y73
R78
E82
R83
I84
V87
K113
H116
D134
A152
P171
M176
P180
S181
GLY
GLY
ALA
ARG
GLY
GLN
ALA
THR
ASP
I191
Y229
V246
H247
P248
PRO
GLN
ASP
GLY
GLU
ASP
GLU

PRO
THR
LEU
VAL
GLN
GLU
PRO
VAL
GLU
ALA
ALA
PRO
ALA
ALA
GLU
VAL
PRO
PRO
ALA
SER
THR

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.06Å 121.14Å 100.83Å 90.00° 116.58° 90.00°	Depositor
Resolution (Å)	34.41 – 2.78 34.41 – 2.78	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.41-2.78) 99.9 (34.41-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.190 , 0.240 0.190 , 0.240	Depositor DCC
R_{free} test set	2307 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9818	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: GOL, A1CZ5

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	0.09	0/1369	0.26	0/1855
1	B	0.09	0/1359	0.28	0/1839
1	C	0.09	0/1379	0.25	0/1867
1	D	0.10	0/1391	0.29	0/1881
1	E	0.10	0/1382	0.26	0/1871
1	F	0.13	0/1389	0.28	0/1880
1	G	0.10	0/1379	0.28	0/1865
All	All	0.10	0/9648	0.27	0/13058

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	1346	0	1360	12	0
1	B	1335	0	1363	11	0
1	C	1355	0	1384	10	0
1	D	1367	0	1400	9	0
1	E	1357	0	1382	6	0
1	F	1364	0	1403	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1355	0	1389	10	0
2	A	29	0	0	0	0
2	B	29	0	0	0	0
2	C	29	0	0	0	0
2	D	29	0	0	0	0
2	E	29	0	0	0	0
2	F	29	0	0	1	0
2	G	29	0	0	0	0
3	E	6	0	8	1	0
4	A	17	0	0	0	0
4	B	22	0	0	0	0
4	C	13	0	0	0	0
4	D	23	0	0	0	0
4	E	17	0	0	0	0
4	F	20	0	0	0	0
4	G	18	0	0	0	0
All	All	9818	0	9689	63	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 (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:VAL:H	3:E:302:GOL:H31	1.53	0.73
1:C:86:CYS:HB3	1:C:88:MET:HE2	1.81	0.62
1:A:139:ILE:HD11	1:A:143:ILE:HD11	1.84	0.59
1:F:139:ILE:HD11	1:F:143:ILE:HD11	1.86	0.57
1:F:144:CYS:SG	1:F:166:MET:HE2	2.47	0.54
1:C:139:ILE:HD11	1:C:143:ILE:HD11	1.89	0.54
1:A:78:ARG:HH12	1:A:82:GLU:HG2	1.73	0.52
1:D:148:VAL:HG23	1:D:170:LEU:HD12	1.92	0.52
1:B:59:ILE:HG23	1:B:75:ILE:HG22	1.92	0.51
1:E:73:TYR:CE1	1:E:78:ARG:HD3	2.46	0.51
1:A:160:ALA:HB2	1:A:240:ILE:HG23	1.93	0.50
1:F:148:VAL:HG11	2:F:301:A1CZ5:F12	2.03	0.49
1:F:197:GLU:HG2	1:G:229:TYR:CD1	2.48	0.49
1:A:148:VAL:HG23	1:A:170:LEU:HD12	1.95	0.49
1:A:84:ILE:HG12	1:A:116:HIS:HB2	1.94	0.49
1:B:169:SER:HB2	1:B:241:LEU:HD22	1.95	0.48
1:G:152:ALA:HB1	1:G:176:MET:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD13	1:G:134:ASP:HB3	1.95	0.48
1:E:97:SER:HB2	1:F:88:MET:HE3	1.94	0.48
1:F:123:GLY:HA3	1:F:153[A]:SER:HB3	1.95	0.48
1:D:191:ILE:HD11	1:E:176:MET:HE1	1.95	0.48
1:F:84:ILE:HG12	1:F:116:HIS:HB2	1.94	0.48
1:F:123:GLY:HA3	1:F:153[B]:SER:HB2	1.94	0.48
1:G:84:ILE:HG12	1:G:116:HIS:HB2	1.96	0.47
1:A:206:TYR:CE2	1:A:221:GLU:HG2	2.50	0.46
1:F:169:SER:HB2	1:F:241:LEU:HD22	1.96	0.46
1:F:176:MET:HE2	1:F:178:HIS:HD2	1.80	0.46
1:A:78:ARG:NH1	1:A:82:GLU:HG2	2.29	0.46
1:A:136:MET:HE3	1:A:143:ILE:HG21	1.98	0.46
1:A:85:VAL:HG11	1:A:99:VAL:HG13	1.98	0.45
1:B:146:TRP:HZ3	1:B:245:LEU:HD11	1.82	0.45
1:C:134:ASP:HB3	1:D:170:LEU:HD13	1.98	0.45
1:C:73:TYR:CE2	1:C:81:ARG:HD2	2.52	0.45
1:F:197:GLU:HG2	1:G:229:TYR:HD1	1.82	0.45
1:D:160:ALA:HB2	1:D:240:ILE:HG23	1.98	0.45
1:B:134:ASP:HB3	1:C:170:LEU:HD13	1.97	0.44
1:B:194:GLN:O	1:B:198:ILE:HG13	2.18	0.44
1:A:194:GLN:O	1:A:198:ILE:HG13	2.18	0.44
1:B:154:MET:HA	1:B:154:MET:HE2	1.98	0.43
1:A:169:SER:HB2	1:A:241:LEU:HD22	1.99	0.43
1:G:78:ARG:NH1	1:G:82:GLU:HG2	2.33	0.43
1:F:176:MET:HE2	1:F:178:HIS:CD2	2.53	0.43
1:B:230:MET:HB3	1:B:234:GLU:HB2	2.01	0.43
1:C:98:LEU:HD12	1:C:98:LEU:HA	1.84	0.42
1:D:138:TYR:O	1:E:248:PRO:HD3	2.19	0.42
1:G:83:ARG:HD2	1:G:113:LYS:HD3	2.01	0.42
1:B:78:ARG:HH12	1:B:82:GLU:HG2	1.85	0.42
1:B:206:TYR:CE2	1:B:221:GLU:HG2	2.55	0.42
1:F:168:HIS:CD2	1:F:243:LYS:HD2	2.54	0.42
1:D:176:MET:HE2	1:D:178:HIS:CD2	2.55	0.42
1:F:197:GLU:CD	1:G:229:TYR:HB2	2.44	0.42
1:B:231:SER:OG	1:B:234:GLU:HG3	2.20	0.41
1:G:176:MET:HE3	1:G:180:PRO:HG3	2.02	0.41
1:B:78:ARG:NH1	1:B:82:GLU:HG2	2.36	0.41
1:C:88:MET:HG2	1:C:120:ASN:N	2.35	0.41
1:C:169:SER:HB2	1:C:241:LEU:HD22	2.02	0.41
1:D:117:MET:HE3	1:D:117:MET:HB2	1.94	0.41
1:D:139:ILE:HD11	1:D:143:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:ILE:HD11	1:E:143:ILE:HD11	2.02	0.41
1:F:194:GLN:O	1:F:198:ILE:HG13	2.21	0.41
1:G:171:PRO:HG3	1:G:246:VAL:HG22	2.03	0.41
1:C:130:LEU:HD13	1:D:172:ASN:HB3	2.04	0.40
1:C:151:ALA:O	1:C:156:SER:HB3	2.21	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	169/221 (76%)	163 (96%)	6 (4%)	0	100	100
1	B	167/221 (76%)	160 (96%)	7 (4%)	0	100	100
1	C	169/221 (76%)	165 (98%)	4 (2%)	0	100	100
1	D	171/221 (77%)	162 (95%)	9 (5%)	0	100	100
1	E	170/221 (77%)	163 (96%)	7 (4%)	0	100	100
1	F	170/221 (77%)	159 (94%)	11 (6%)	0	100	100
1	G	169/221 (76%)	163 (96%)	6 (4%)	0	100	100
All	All	1185/1547 (77%)	1135 (96%)	50 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	146/185 (79%)	145 (99%)	1 (1%)	76	90
1	B	147/185 (80%)	146 (99%)	1 (1%)	76	90
1	C	149/185 (80%)	149 (100%)	0	100	100
1	D	150/185 (81%)	149 (99%)	1 (1%)	76	90
1	E	148/185 (80%)	147 (99%)	1 (1%)	76	90
1	F	152/185 (82%)	152 (100%)	0	100	100
1	G	150/185 (81%)	149 (99%)	1 (1%)	76	90
All	All	1042/1295 (80%)	1037 (100%)	5 (0%)	81	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	LEU
1	B	245	LEU
1	D	245	LEU
1	E	73	TYR
1	G	87	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	ASN
1	B	107	GLN
1	B	150	GLN
1	B	247	HIS
1	C	204	GLN
1	D	172	ASN
1	D	179	GLN
1	D	247	HIS
1	E	204	GLN
1	F	218	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
2	A1CZ5	B	301	-	31,31,31	1.46	4 (12%)	44,46,46	1.23	6 (13%)
2	A1CZ5	C	301	-	31,31,31	1.47	4 (12%)	44,46,46	1.21	6 (13%)
2	A1CZ5	G	301	-	31,31,31	1.42	4 (12%)	44,46,46	1.18	6 (13%)
2	A1CZ5	E	301	-	31,31,31	1.44	4 (12%)	44,46,46	1.26	6 (13%)
2	A1CZ5	A	301	-	31,31,31	1.43	4 (12%)	44,46,46	1.20	6 (13%)
2	A1CZ5	F	301	-	31,31,31	1.52	4 (12%)	44,46,46	1.25	6 (13%)
2	A1CZ5	D	301	-	31,31,31	1.48	4 (12%)	44,46,46	1.22	6 (13%)
3	GOL	E	302	-	5,5,5	0.34	0	5,5,5	0.52	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
2	A1CZ5	B	301	-	-	1/20/33/33	0/3/3/3
2	A1CZ5	C	301	-	-	0/20/33/33	0/3/3/3
2	A1CZ5	G	301	-	-	2/20/33/33	0/3/3/3
2	A1CZ5	E	301	-	-	0/20/33/33	0/3/3/3
2	A1CZ5	A	301	-	-	1/20/33/33	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1CZ5	F	301	-	-	1/20/33/33	0/3/3/3
2	A1CZ5	D	301	-	-	3/20/33/33	0/3/3/3
3	GOL	E	302	-	-	4/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	A1CZ5	C02-N18	6.45	1.42	1.34
2	G	301	A1CZ5	C02-N18	6.40	1.42	1.34
2	F	301	A1CZ5	C02-N18	6.36	1.42	1.34
2	B	301	A1CZ5	C02-N18	6.18	1.42	1.34
2	C	301	A1CZ5	C02-N18	6.18	1.42	1.34
2	A	301	A1CZ5	C02-N18	6.11	1.42	1.34
2	E	301	A1CZ5	C02-N18	5.88	1.42	1.34
2	F	301	A1CZ5	C03-N04	3.01	1.49	1.46
2	C	301	A1CZ5	C03-N04	2.98	1.49	1.46
2	B	301	A1CZ5	C03-N04	2.64	1.49	1.46
2	A	301	A1CZ5	C03-N04	2.64	1.49	1.46
2	D	301	A1CZ5	C03-N04	2.60	1.49	1.46
2	E	301	A1CZ5	C03-N04	2.51	1.48	1.46
2	E	301	A1CZ5	C24-C23	2.50	1.54	1.49
2	F	301	A1CZ5	C24-C23	2.42	1.54	1.49
2	D	301	A1CZ5	C24-C23	2.37	1.54	1.49
2	C	301	A1CZ5	C24-C23	2.35	1.54	1.49
2	A	301	A1CZ5	C24-C23	2.34	1.54	1.49
2	G	301	A1CZ5	C24-C23	2.33	1.54	1.49
2	B	301	A1CZ5	C11-C10	2.29	1.54	1.49
2	B	301	A1CZ5	C24-C23	2.29	1.54	1.49
2	E	301	A1CZ5	C11-C10	2.29	1.54	1.49
2	G	301	A1CZ5	C03-N04	2.27	1.48	1.46
2	D	301	A1CZ5	C11-C10	2.26	1.54	1.49
2	G	301	A1CZ5	C11-C10	2.25	1.54	1.49
2	C	301	A1CZ5	C11-C10	2.23	1.54	1.49
2	F	301	A1CZ5	C11-C10	2.18	1.54	1.49
2	A	301	A1CZ5	C11-C10	2.05	1.54	1.49

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	A1CZ5	C17-N18-C02	-4.33	119.02	123.60
2	A	301	A1CZ5	C17-N18-C02	-4.21	119.15	123.60
2	D	301	A1CZ5	C17-N18-C02	-4.18	119.18	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	A1CZ5	C17-N18-C02	-4.18	119.18	123.60
2	G	301	A1CZ5	C17-N18-C02	-4.17	119.19	123.60
2	B	301	A1CZ5	C17-N18-C02	-4.15	119.21	123.60
2	C	301	A1CZ5	C17-N18-C02	-4.13	119.23	123.60
2	E	301	A1CZ5	C20-C19-N18	3.36	118.44	113.15
2	F	301	A1CZ5	C20-C19-N18	3.26	118.28	113.15
2	B	301	A1CZ5	C03-N04-C16	-3.25	105.44	110.10
2	D	301	A1CZ5	C03-N04-C16	-3.24	105.45	110.10
2	E	301	A1CZ5	C03-N04-C16	-3.14	105.59	110.10
2	A	301	A1CZ5	C03-N04-C16	-3.07	105.69	110.10
2	G	301	A1CZ5	C03-N04-C16	-3.07	105.70	110.10
2	C	301	A1CZ5	C20-C19-N18	2.94	117.78	113.15
2	D	301	A1CZ5	C20-C19-N18	2.93	117.75	113.15
2	C	301	A1CZ5	C03-N04-C16	-2.92	105.91	110.10
2	F	301	A1CZ5	C03-N04-C16	-2.91	105.92	110.10
2	B	301	A1CZ5	C20-C19-N18	2.84	117.62	113.15
2	A	301	A1CZ5	C20-C19-N18	2.58	117.21	113.15
2	G	301	A1CZ5	C20-C19-N18	2.58	117.21	113.15
2	E	301	A1CZ5	C16-C17-N18	2.49	115.36	110.42
2	B	301	A1CZ5	C16-C17-N18	2.42	115.23	110.42
2	F	301	A1CZ5	C08-C09-C10	-2.41	118.31	120.75
2	C	301	A1CZ5	C08-C09-C10	-2.40	118.31	120.75
2	A	301	A1CZ5	C08-C09-C10	-2.36	118.35	120.75
2	A	301	A1CZ5	C19-N18-C17	2.34	120.75	116.24
2	B	301	A1CZ5	C08-C09-C10	-2.33	118.39	120.75
2	F	301	A1CZ5	C19-N18-C17	2.30	120.67	116.24
2	D	301	A1CZ5	C16-C17-N18	2.30	114.99	110.42
2	C	301	A1CZ5	C19-N18-C17	2.30	120.67	116.24
2	G	301	A1CZ5	C08-C09-C10	-2.28	118.44	120.75
2	E	301	A1CZ5	C19-N18-C17	2.27	120.61	116.24
2	B	301	A1CZ5	C19-N18-C17	2.26	120.59	116.24
2	D	301	A1CZ5	C08-C09-C10	-2.24	118.48	120.75
2	E	301	A1CZ5	C08-C09-C10	-2.23	118.49	120.75
2	D	301	A1CZ5	C19-N18-C17	2.21	120.49	116.24
2	A	301	A1CZ5	C16-C17-N18	2.18	114.74	110.42
2	G	301	A1CZ5	C19-N18-C17	2.14	120.36	116.24
2	C	301	A1CZ5	C16-C17-N18	2.11	114.62	110.42
2	F	301	A1CZ5	C16-C17-N18	2.04	114.47	110.42
2	G	301	A1CZ5	C16-C17-N18	2.02	114.43	110.42

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	302	GOL	O1-C1-C2-O2
3	E	302	GOL	O1-C1-C2-C3
3	E	302	GOL	C1-C2-C3-O3
3	E	302	GOL	O2-C2-C3-O3
2	A	301	A1CZ5	C20-C19-N18-C02
2	B	301	A1CZ5	C20-C19-N18-C02
2	F	301	A1CZ5	C20-C19-N18-C02
2	D	301	A1CZ5	C20-C19-N18-C02
2	D	301	A1CZ5	N18-C19-C20-C21
2	G	301	A1CZ5	N18-C19-C20-C29
2	D	301	A1CZ5	N18-C19-C20-C29
2	G	301	A1CZ5	N18-C19-C20-C21

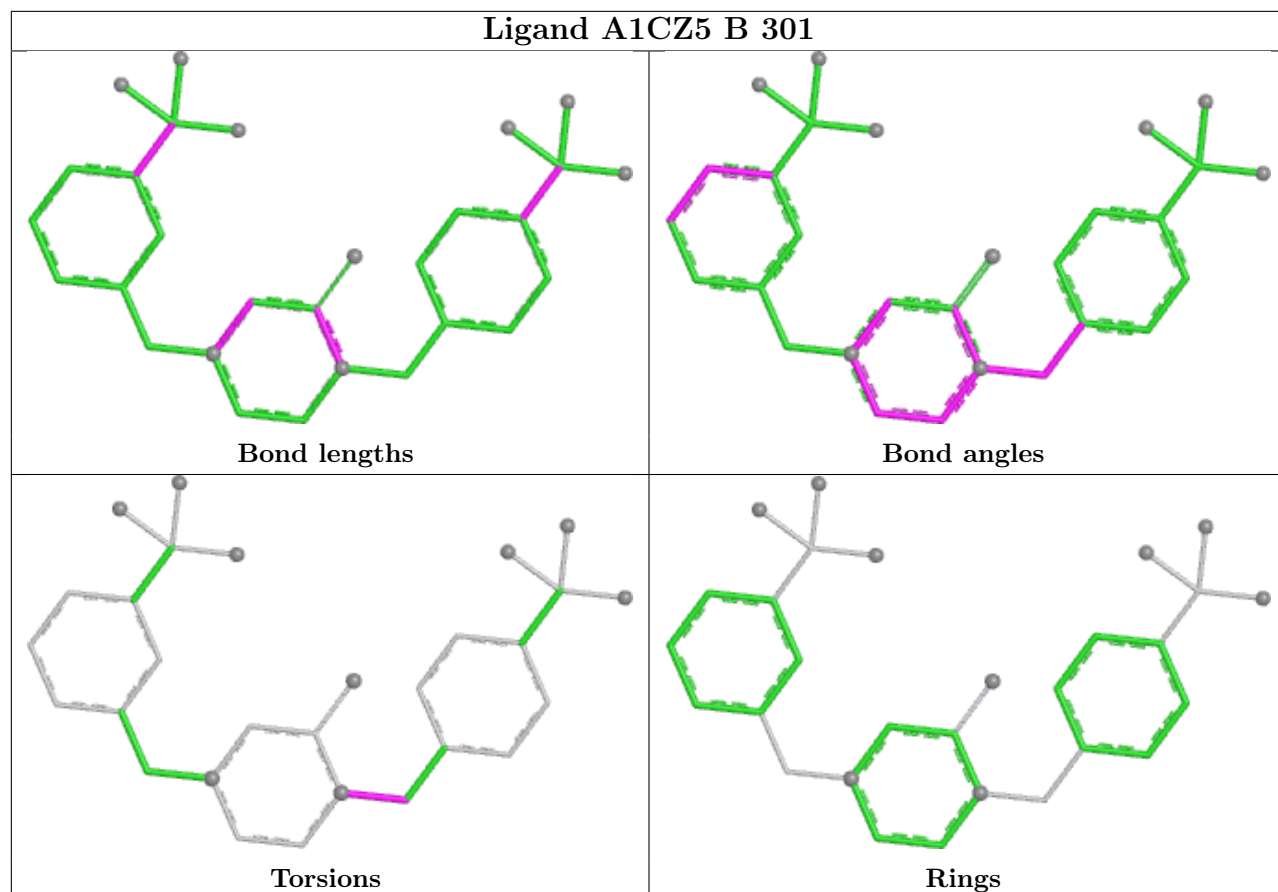
There are no ring outliers.

2 monomers are involved in 2 short contacts:

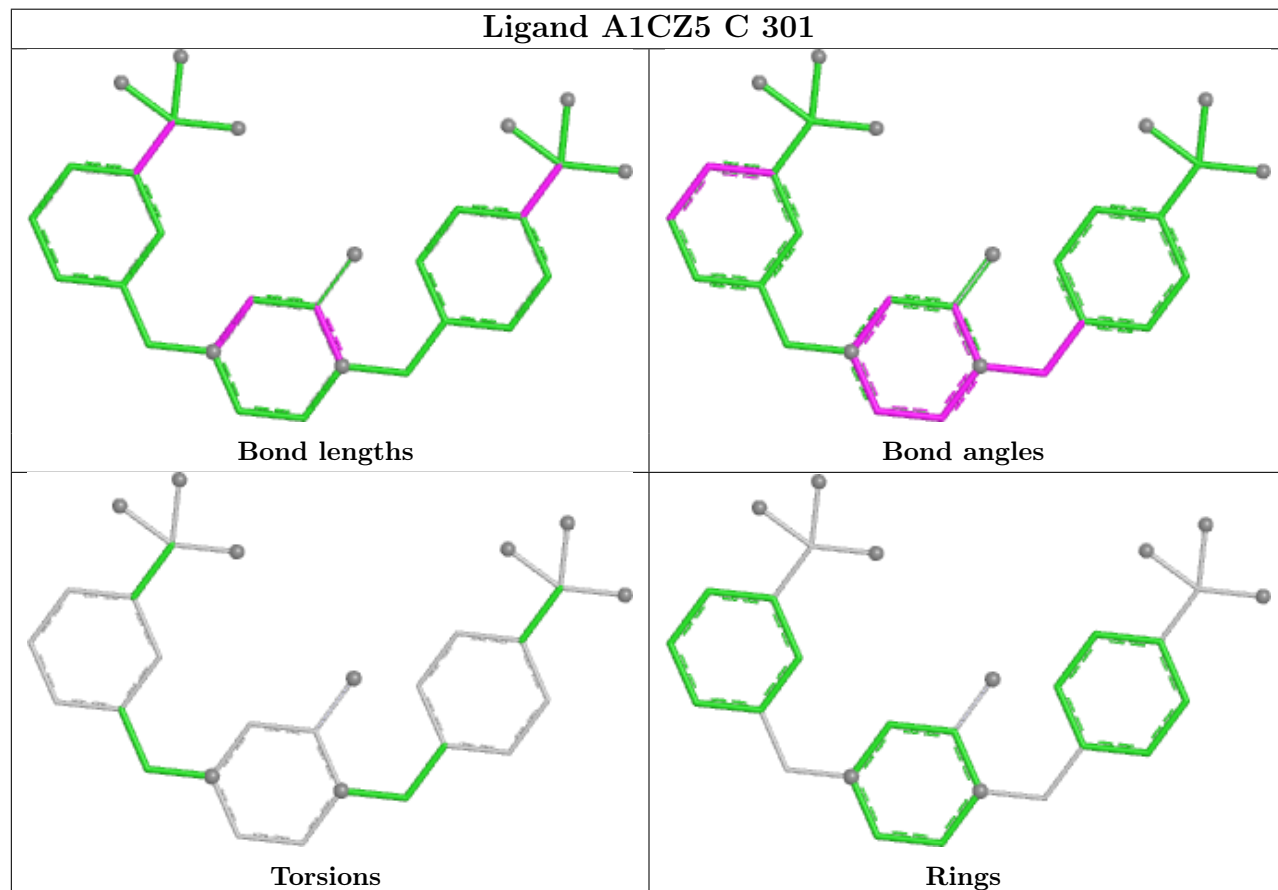
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	A1CZ5	1	0
3	E	302	GOL	1	0

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.

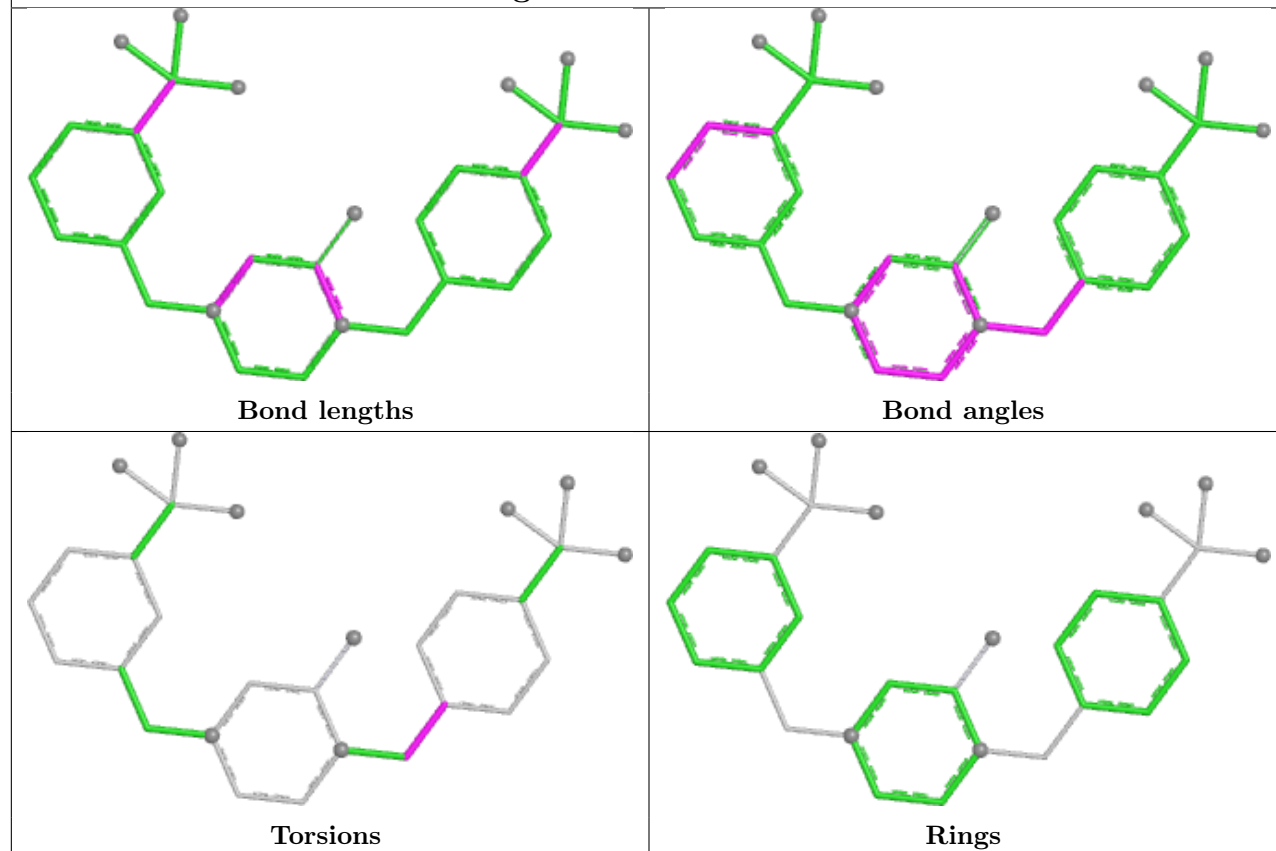
Ligand A1CZ5 B 301



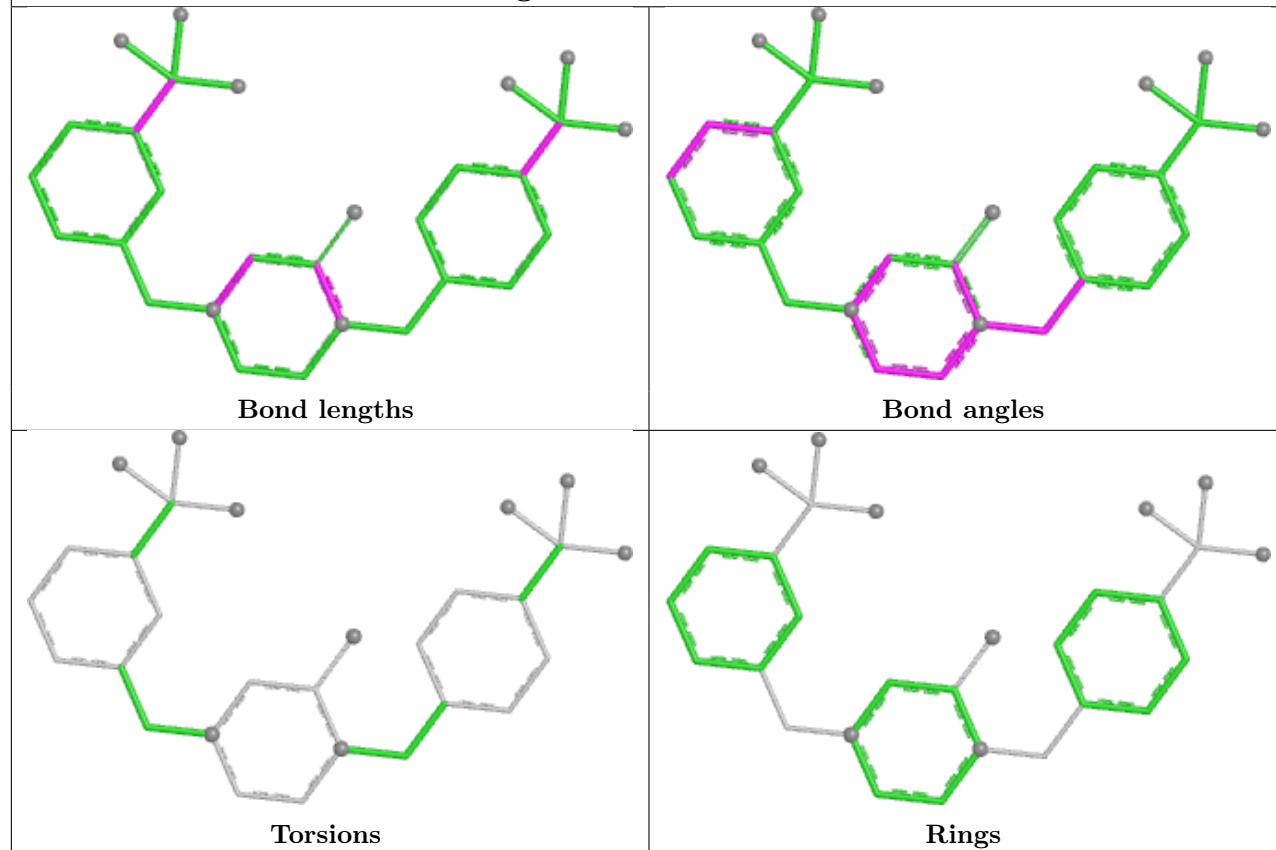
Ligand A1CZ5 C 301



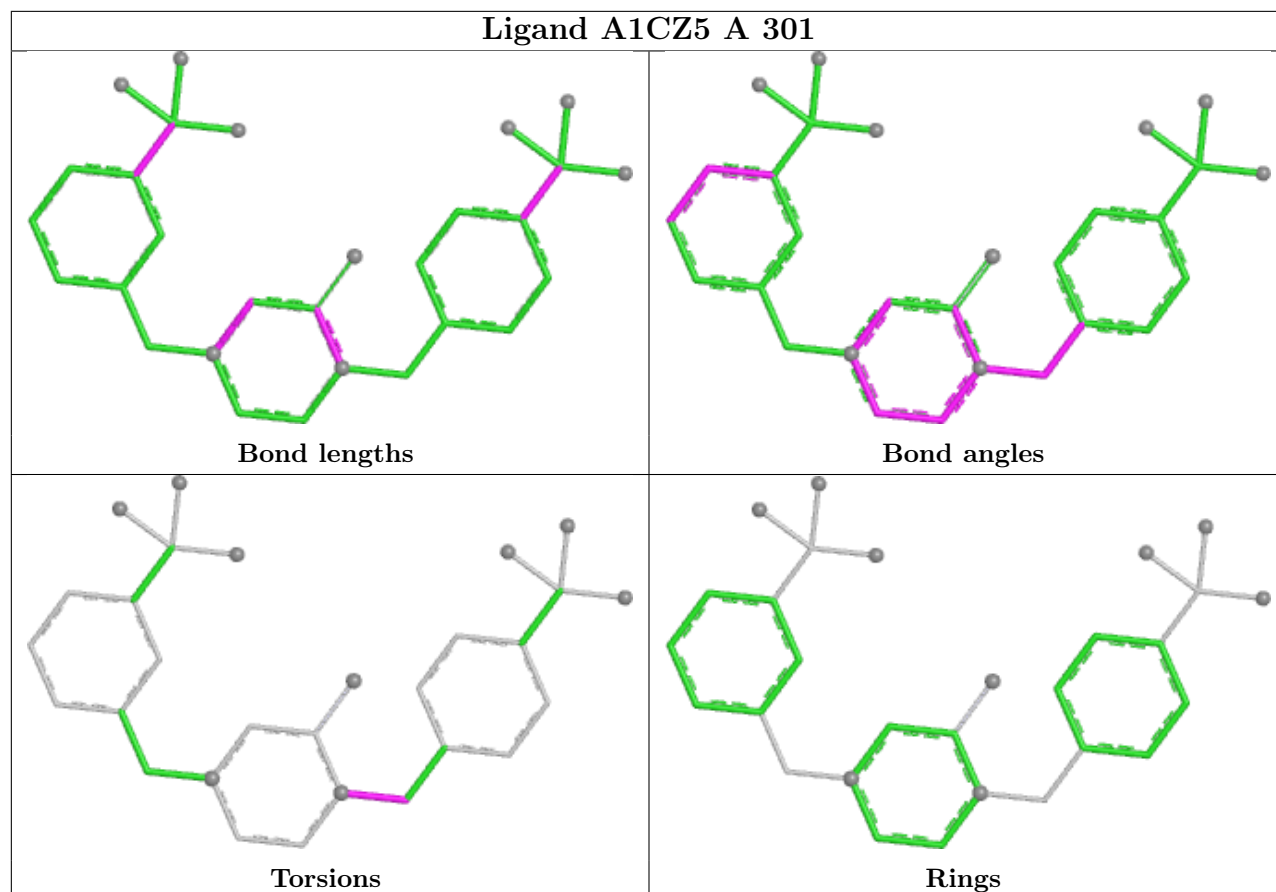
Ligand A1CZ5 G 301



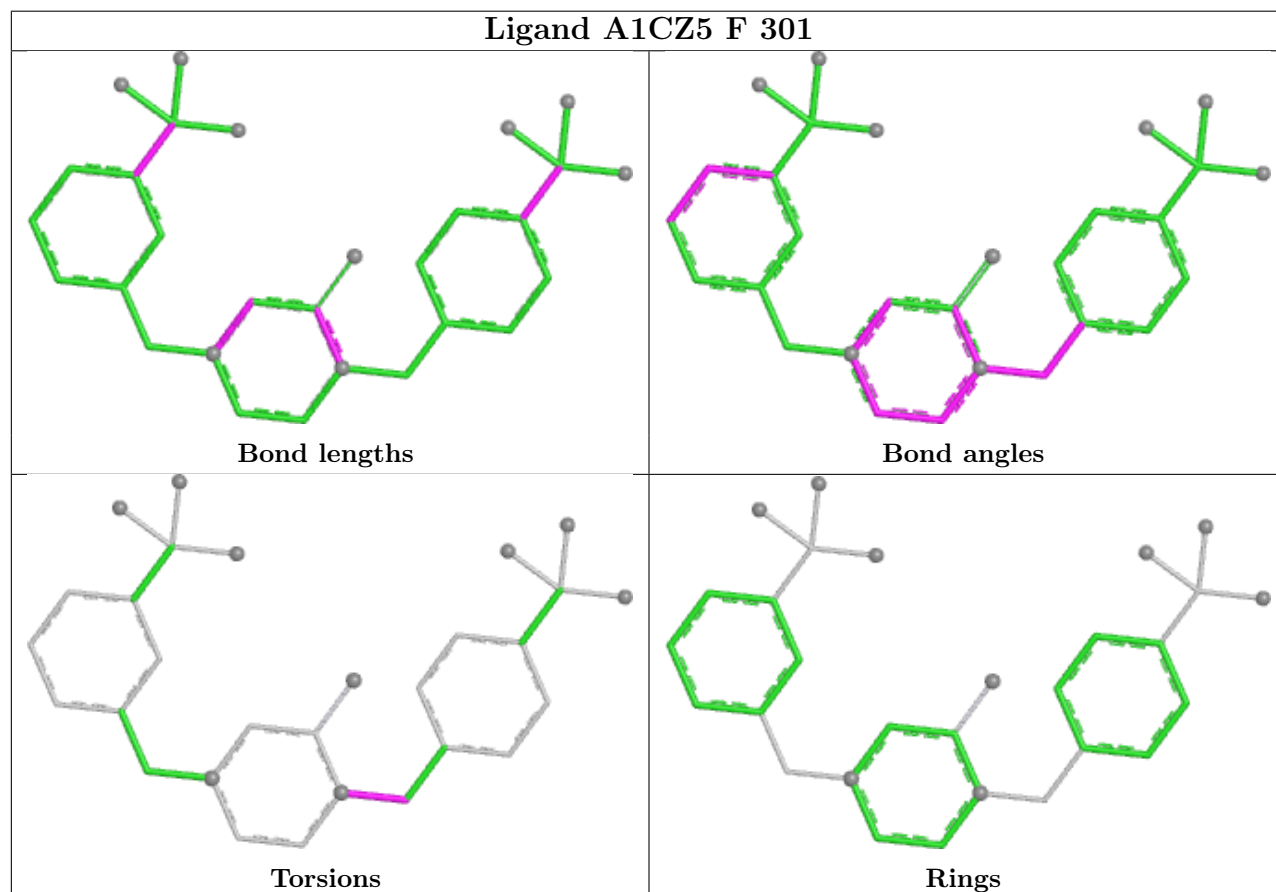
Ligand A1CZ5 E 301

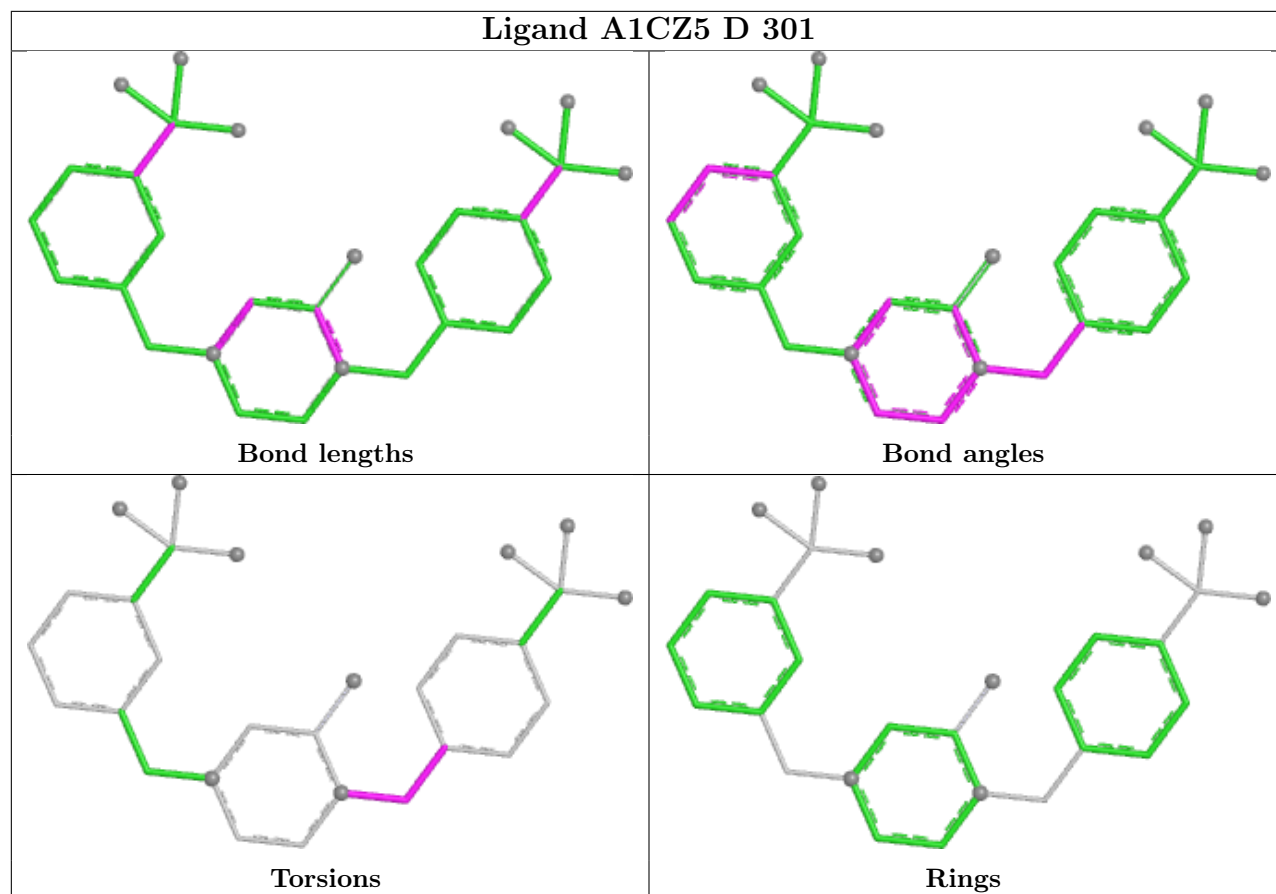


Ligand A1CZ5 A 301



Ligand A1CZ5 F 301





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	174/221 (78%)	-0.37	3 (1%) 69 62	20, 38, 59, 83	1 (0%)
1	B	173/221 (78%)	-0.32	2 (1%) 76 70	29, 42, 58, 76	0
1	C	175/221 (79%)	-0.25	3 (1%) 69 62	27, 41, 63, 86	0
1	D	176/221 (79%)	-0.51	1 (0%) 85 81	18, 35, 55, 81	1 (0%)
1	E	176/221 (79%)	-0.46	3 (1%) 69 62	22, 33, 61, 84	0
1	F	175/221 (79%)	-0.30	8 (4%) 37 31	19, 38, 64, 76	1 (0%)
1	G	174/221 (78%)	-0.45	2 (1%) 78 72	19, 35, 56, 66	1 (0%)
All	All	1223/1547 (79%)	-0.38	22 (1%) 67 60	18, 38, 60, 86	4 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	72	ALA	4.2
1	E	73	TYR	3.6
1	C	86	CYS	3.4
1	A	246	VAL	3.3
1	F	246	VAL	3.2
1	C	89	GLY	3.2
1	F	249	PRO	2.8
1	B	72	ALA	2.8
1	G	73	TYR	2.8
1	A	58	LEU	2.7
1	F	181	SER	2.5
1	B	192	ALA	2.5
1	F	63	VAL	2.4
1	E	63	VAL	2.4
1	F	245	LEU	2.3
1	F	191	ILE	2.3
1	D	58	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	63	VAL	2.2
1	G	63	VAL	2.1
1	C	72	ALA	2.0
1	E	249	PRO	2.0
1	F	73	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

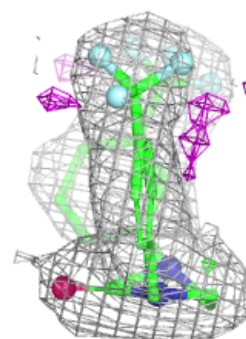
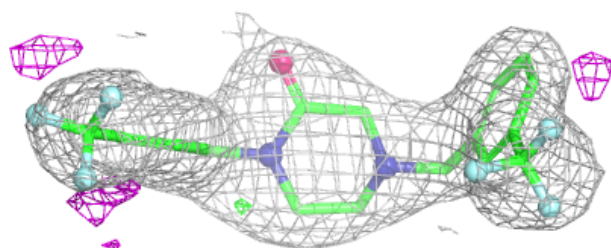
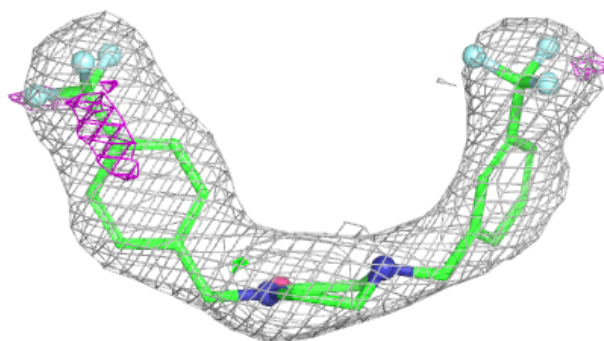
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	E	302	6/6	0.80	0.14	34,45,53,55	0
2	A1CZ5	C	301	29/29	0.90	0.12	40,51,65,74	0
2	A1CZ5	B	301	29/29	0.93	0.09	35,47,56,59	0
2	A1CZ5	G	301	29/29	0.94	0.09	28,42,49,56	0
2	A1CZ5	E	301	29/29	0.95	0.08	25,35,49,57	0
2	A1CZ5	A	301	29/29	0.95	0.07	29,39,47,51	0
2	A1CZ5	D	301	29/29	0.95	0.08	32,44,53,58	0
2	A1CZ5	F	301	29/29	0.96	0.07	23,38,48,51	0

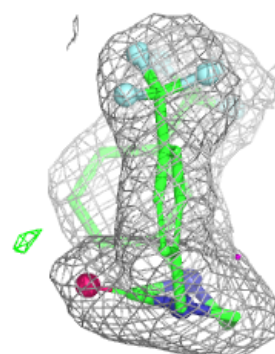
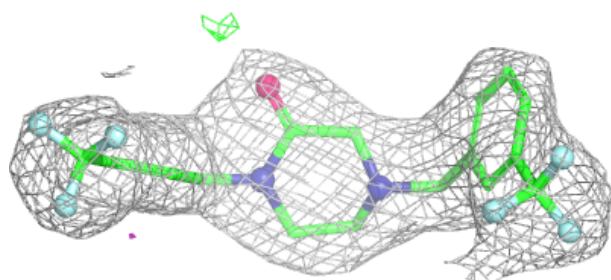
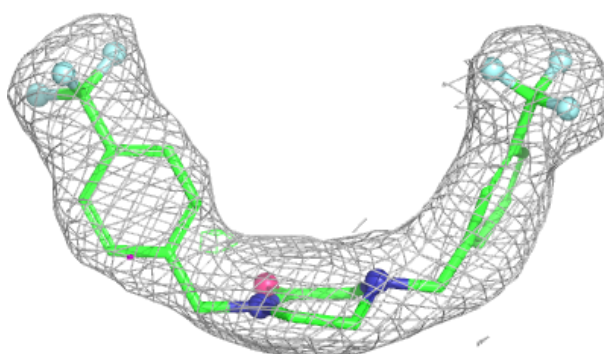
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1CZ5 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)

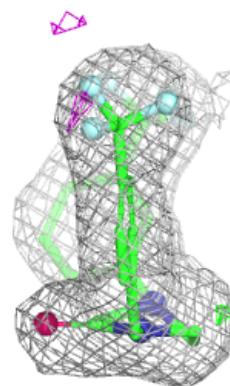
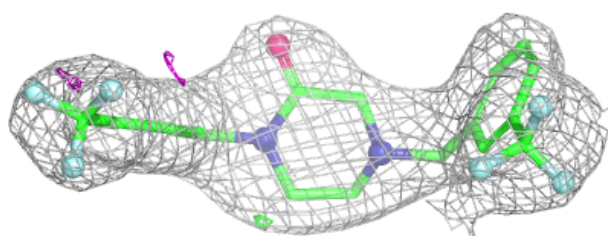
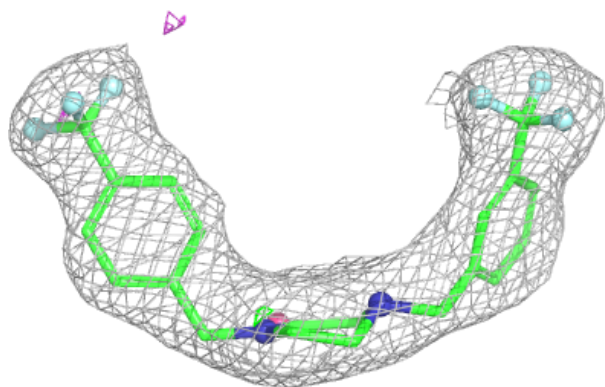
**Electron density around A1CZ5 B 301:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

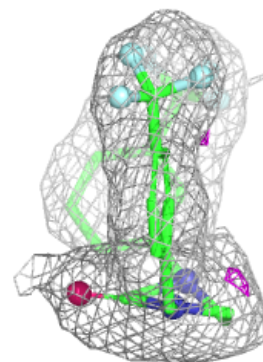
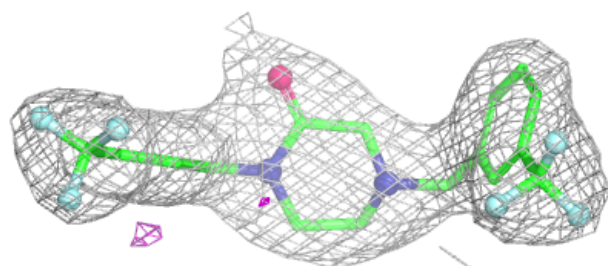
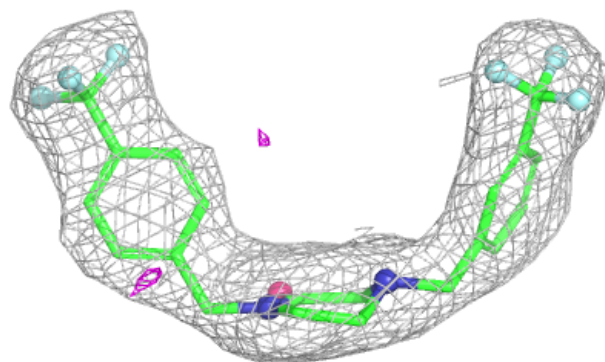


Electron density around A1CZ5 G 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

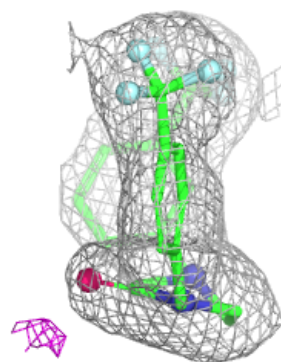
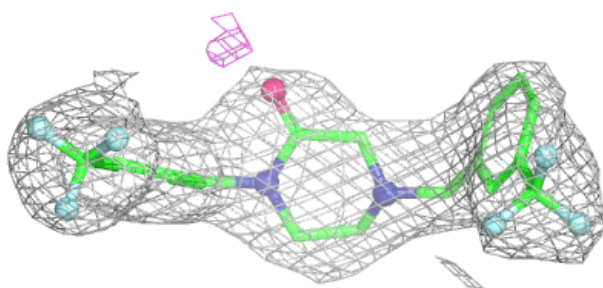
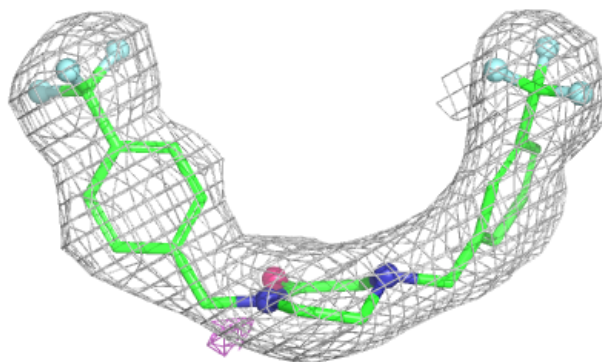
**Electron density around A1CZ5 E 301:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

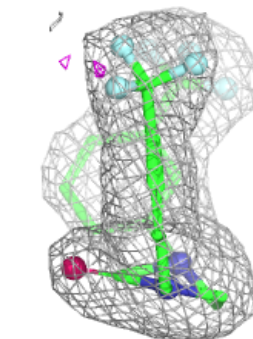
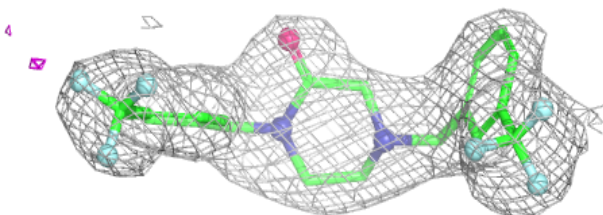
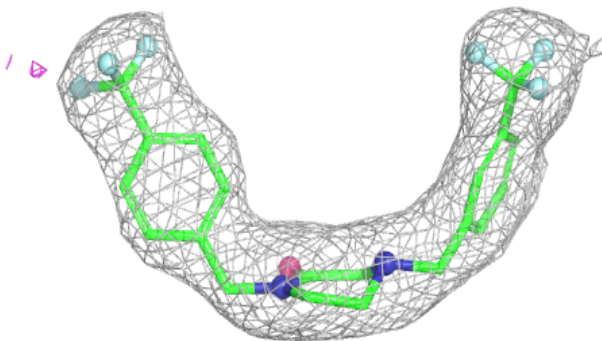


Electron density around A1CZ5 A 301:

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

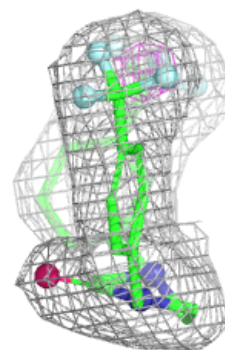
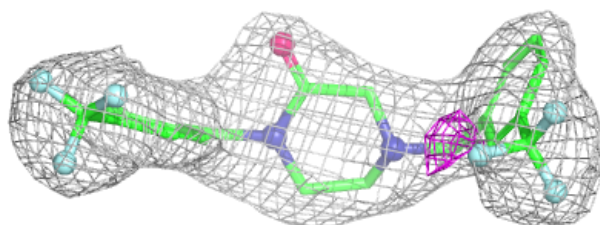
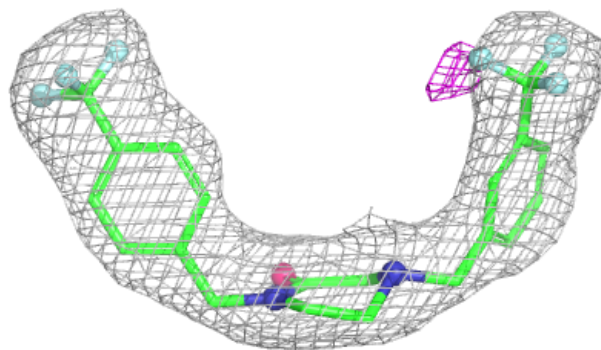
**Electron density around A1CZ5 D 301:**

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



Electron density around A1CZ5 F 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.