Full wwPDB X-ray Structure Validation Report ⓘ

May 8, 2024 – 06:12 PM JST

PDB ID	:	8YLB
Title	:	Cocrystal structures of agonists compound 1 with HsClpP
Authors	:	Zhao, N.; Zhu, Y.; Bao, R.
Deposited on	:	2024-03-06
Resolution	:	2.15 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:

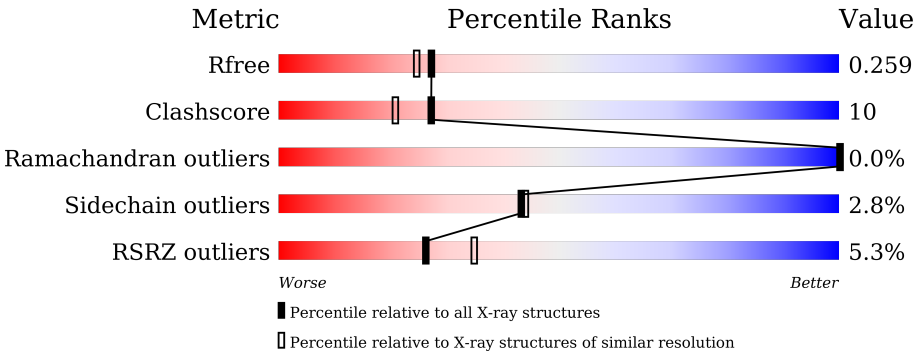
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 <=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	220	5% 61% 18% • 20%
1	B	220	5% 63% 15% 21%
1	C	220	4% 58% 18% • 22%
1	D	220	5% 63% 14% • 22%
1	E	220	2% 65% 11% • 22%
1	F	220	2% 65% 9% • 25%

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Mol	Chain	Length	Quality of chain
1	G	220	3% 65% 11% 23%
1	H	220	7% 51% 23% 25%
1	I	220	4% 59% 19% 22%
1	J	220	6% 59% 18% 23%
1	K	220	3% 60% 18% 22%
1	L	220	3% 69% 9% 23%
1	M	220	5% 65% 13% 22%
1	N	220	5% 55% 21% 22%

2 Entry composition (i)

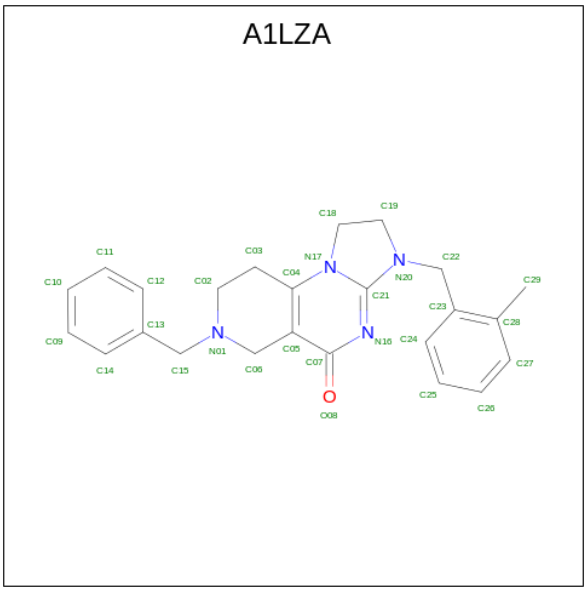
There are 3 unique types of molecules in this entry. The entry contains 19734 atoms, of which 294 are hydrogens and 0 are deuteriums.

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	176	Total	C	N	O	S	0	1	0
			1383	882	236	252	13			
1	B	173	Total	C	N	O	S	0	0	0
			1346	862	228	243	13			
1	C	171	Total	C	N	O	S	0	0	0
			1335	856	226	240	13			
1	D	171	Total	C	N	O	S	0	0	0
			1333	854	226	240	13			
1	E	171	Total	C	N	O	S	0	0	0
			1333	854	226	240	13			
1	F	166	Total	C	N	O	S	0	0	0
			1298	831	219	235	13			
1	G	170	Total	C	N	O	S	0	1	0
			1334	854	226	241	13			
1	H	166	Total	C	N	O	S	0	2	0
			1307	834	221	238	14			
1	I	172	Total	C	N	O	S	0	1	0
			1349	864	228	244	13			
1	J	169	Total	C	N	O	S	0	1	0
			1327	850	224	240	13			
1	K	171	Total	C	N	O	S	0	0	0
			1338	855	227	243	13			
1	L	170	Total	C	N	O	S	0	0	0
			1327	850	225	239	13			
1	M	171	Total	C	N	O	S	0	1	0
			1340	858	227	242	13			
1	N	172	Total	C	N	O	S	0	1	0
			1347	861	228	245	13			

- Molecule 2 is 5-[(2-methylphenyl)methyl]-11-(phenylmethyl)-2,5,7,11-tetrazatricyclo[7.4.0.0^{2,6}]trideca-1(9),6-dien-8-one (three-letter code: A1LZA) (formula: $C_{24}H_{26}N_4O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	B	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	C	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	D	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	E	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	F	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	G	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	H	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	I	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	J	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	K	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	L	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	M	1	Total	C	H	N	O	0	0
			50	24	21	4	1		
2	N	1	Total	C	H	N	O	0	0
			50	24	21	4	1		

- Molecule 3 is water.

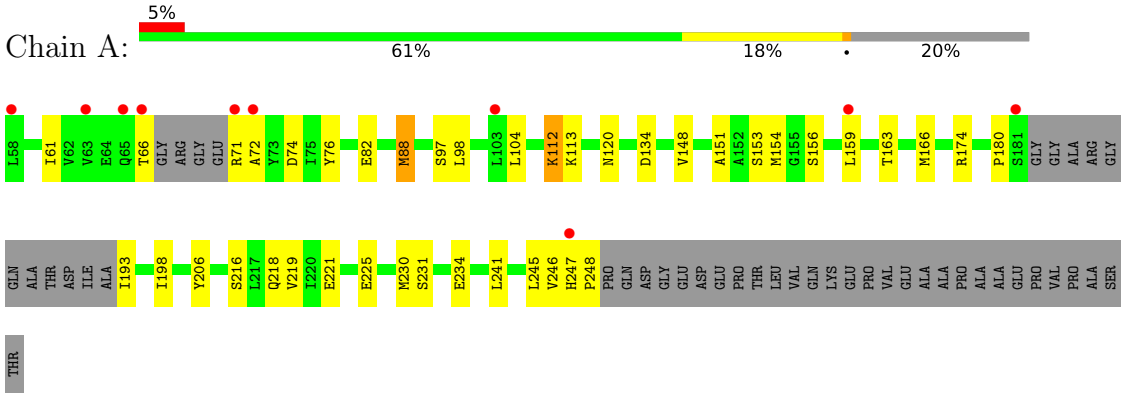
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	30	Total O 30 30	0	0
3	B	25	Total O 25 25	0	0
3	C	12	Total O 12 12	0	0
3	D	16	Total O 16 16	0	0
3	E	33	Total O 33 33	0	0
3	F	31	Total O 31 31	0	0
3	G	28	Total O 28 28	0	0
3	H	9	Total O 9 9	0	0
3	I	17	Total O 17 17	0	0
3	J	20	Total O 20 20	0	0
3	K	30	Total O 30 30	0	0
3	L	37	Total O 37 37	0	0
3	M	39	Total O 39 39	0	0
3	N	10	Total O 10 10	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.

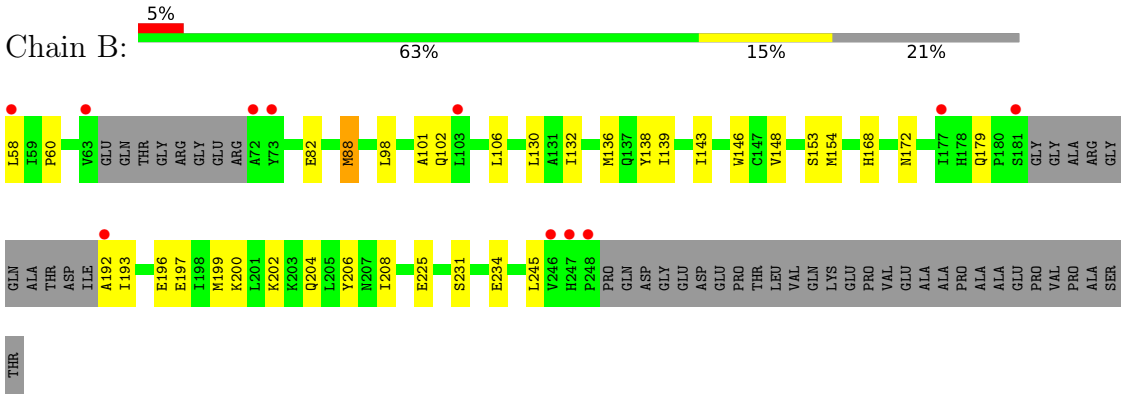
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain A:



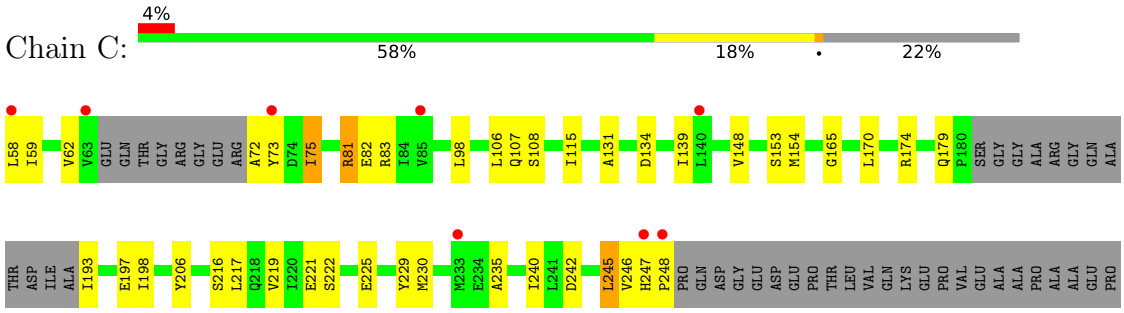
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain B:



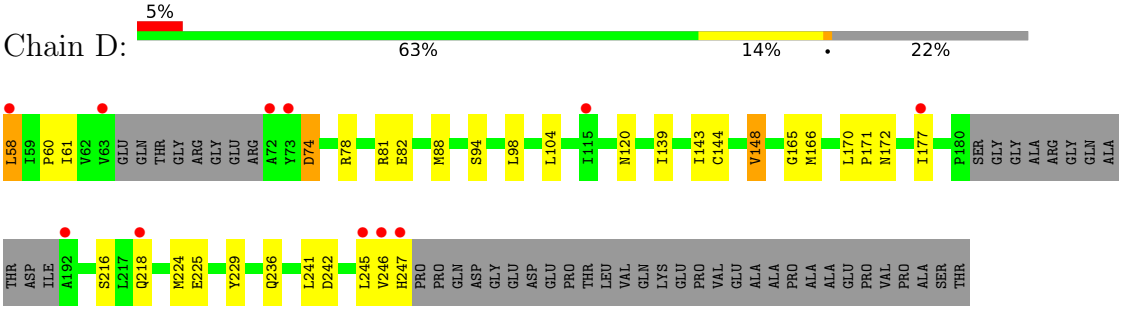
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain C:



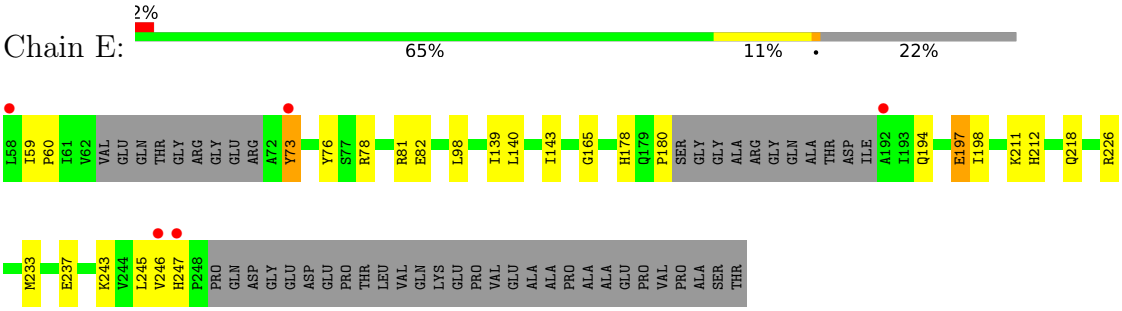
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain D:



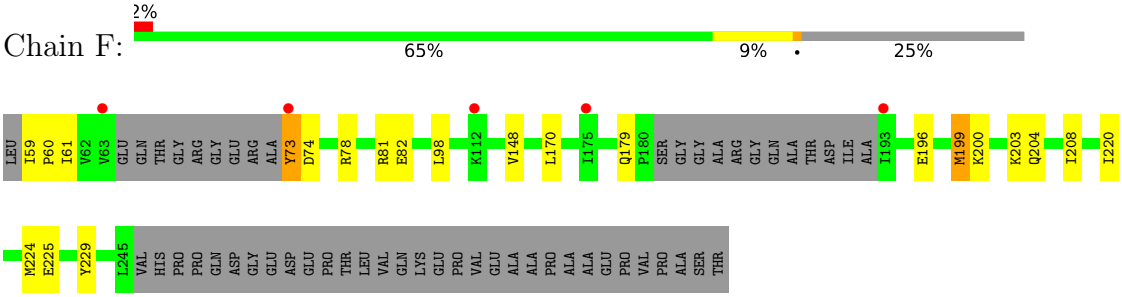
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain E:



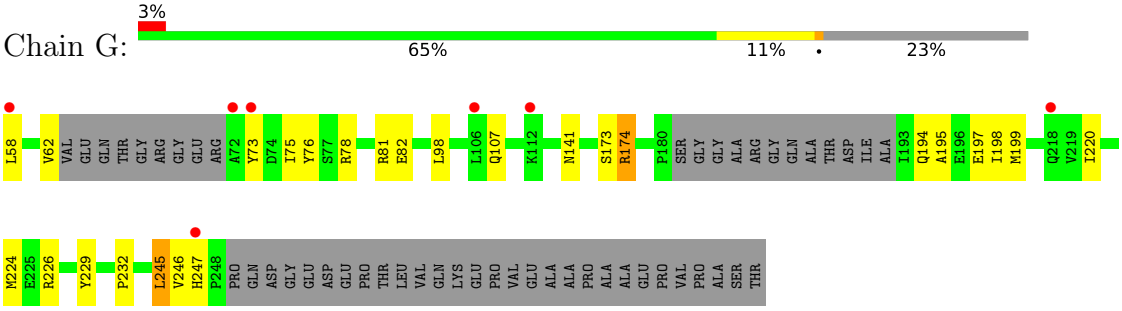
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain F:



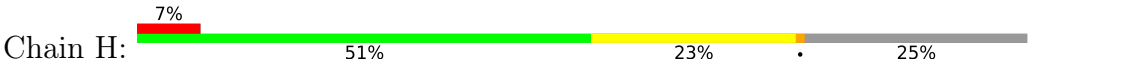
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

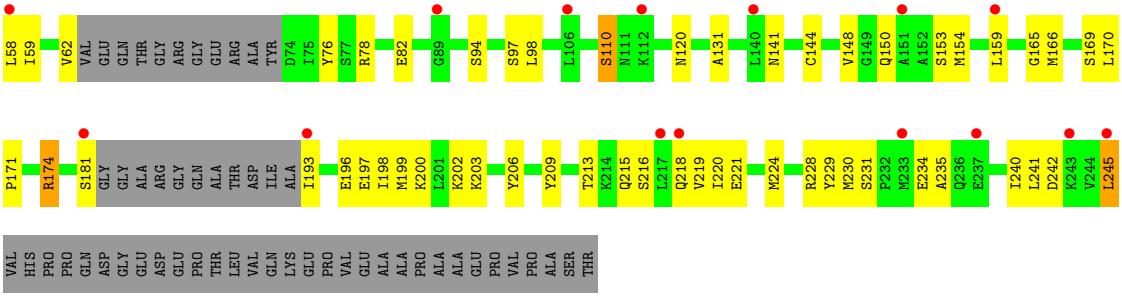
Chain G:



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

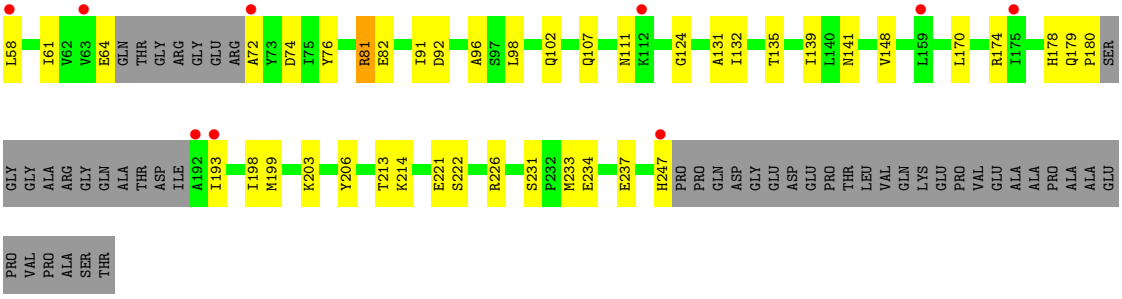
Chain H:





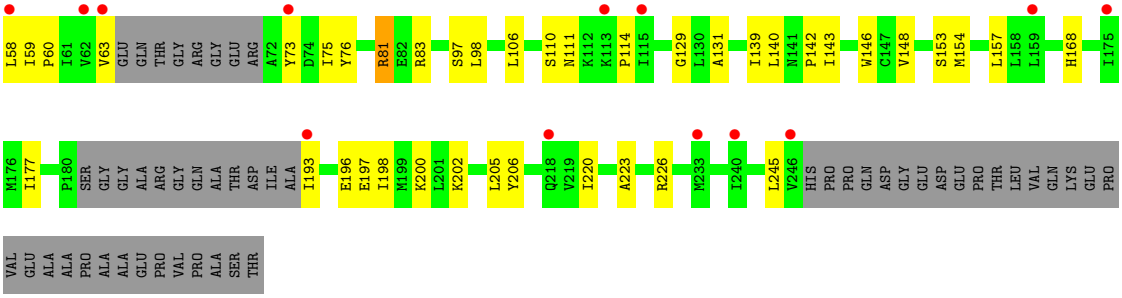
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain I:



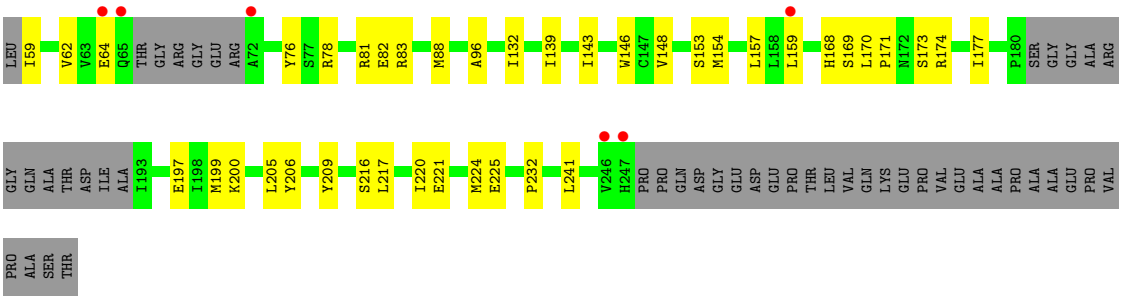
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain J:



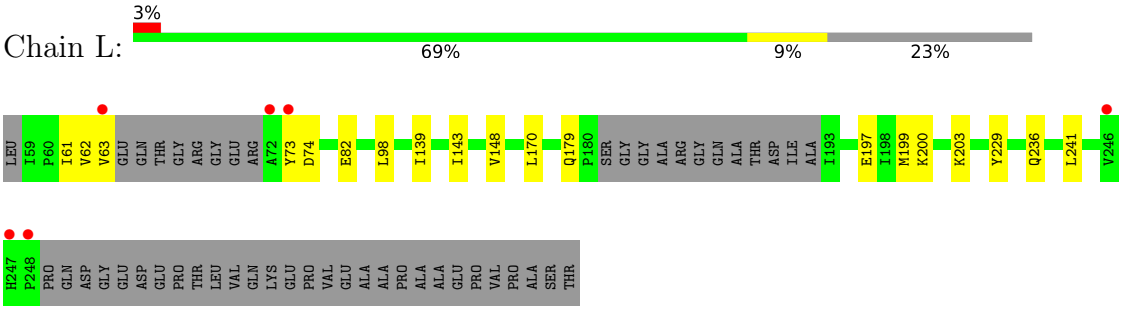
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain K:



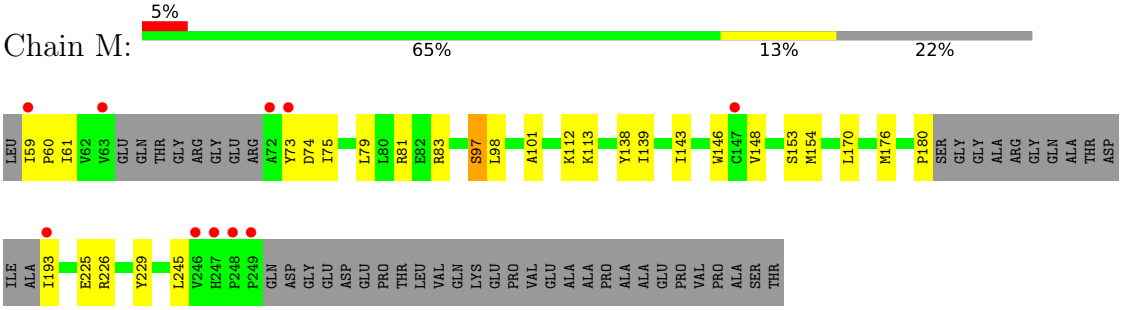
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain L:



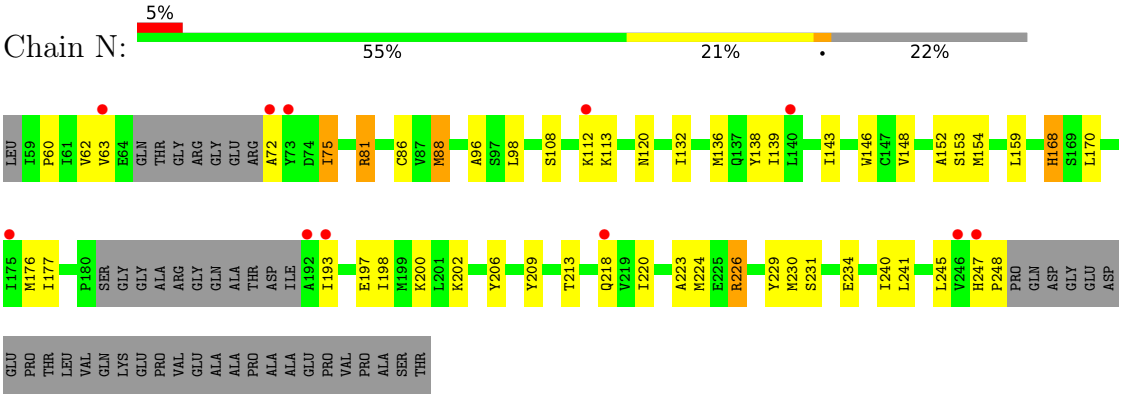
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain M:



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

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.24Å 96.74Å 124.54Å 90.00° 94.44° 90.00°	Depositor
Resolution (Å)	19.88 – 2.15 19.88 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.88-2.15) 99.6 (19.88-2.15)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.15Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.207 , 0.260 0.208 , 0.259	Depositor DCC
R_{free} test set	2016 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19734	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1LZA

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	0.42	0/1407	0.61	0/1902
1	B	0.40	0/1370	0.61	0/1853
1	C	0.37	0/1359	0.59	0/1838
1	D	0.43	0/1356	0.62	0/1833
1	E	0.41	0/1357	0.61	0/1835
1	F	0.43	0/1320	0.62	0/1783
1	G	0.39	0/1358	0.62	0/1836
1	H	0.37	0/1328	0.59	0/1792
1	I	0.35	0/1372	0.57	0/1855
1	J	0.39	0/1349	0.59	0/1823
1	K	0.41	0/1361	0.61	0/1839
1	L	0.40	0/1351	0.62	0/1827
1	M	0.45	0/1365	0.64	0/1847
1	N	0.37	0/1371	0.60	0/1854
All	All	0.40	0/19024	0.61	0/25717

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

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	1383	0	1423	35	0
1	B	1346	0	1390	33	0
1	C	1335	0	1380	43	0
1	D	1333	0	1378	33	0
1	E	1333	0	1376	26	0
1	F	1298	0	1341	18	0
1	G	1334	0	1375	21	0
1	H	1307	0	1351	70	0
1	I	1349	0	1392	34	0
1	J	1327	0	1373	32	0
1	K	1338	0	1376	28	0
1	L	1327	0	1369	14	0
1	M	1340	0	1380	34	0
1	N	1347	0	1384	47	0
2	A	29	21	0	1	0
2	B	29	21	0	2	0
2	C	29	21	0	1	0
2	D	29	21	0	1	0
2	E	29	21	0	1	0
2	F	29	21	0	0	0
2	G	29	21	0	1	0
2	H	29	21	0	1	0
2	I	29	21	0	1	0
2	J	29	21	0	0	0
2	K	29	21	0	0	0
2	L	29	21	0	1	0
2	M	29	21	0	0	0
2	N	29	21	0	0	0
3	A	30	0	0	4	0
3	B	25	0	0	0	0
3	C	12	0	0	1	0
3	D	16	0	0	0	0
3	E	33	0	0	1	0
3	F	31	0	0	1	0
3	G	28	0	0	2	0
3	H	9	0	0	0	0
3	I	17	0	0	2	0
3	J	20	0	0	3	0
3	K	30	0	0	1	0
3	L	37	0	0	0	0
3	M	39	0	0	1	0
3	N	10	0	0	1	0
All	All	19440	294	19288	386	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 10.

All (386) 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:J:73:TYR:OH	1:J:81:ARG:NH1	1.76	1.16
1:B:192:ALA:HB1	1:H:181:SER:HB3	1.40	1.01
1:H:193:ILE:HD11	1:H:198:ILE:HD13	1.42	0.99
1:B:196:GLU:HA	1:H:199:MET:HE1	1.45	0.94
1:H:148:VAL:HG12	1:H:170:LEU:HD12	1.49	0.94
1:B:192:ALA:HB1	1:H:181:SER:CB	1.97	0.93
1:H:148:VAL:HG12	1:H:170:LEU:CD1	2.03	0.88
1:C:230:MET:HE3	1:C:235:ALA:HA	1.60	0.84
1:H:230:MET:HE1	1:H:235:ALA:HA	1.58	0.84
1:J:98:LEU:HD12	1:K:76:TYR:OH	1.78	0.83
1:N:230:MET:HE1	1:N:240:ILE:HD12	1.61	0.82
1:E:194:GLN:O	1:E:198:ILE:HD12	1.79	0.82
1:C:148:VAL:HG12	1:C:170:LEU:HD23	1.60	0.81
1:D:88:MET:HG2	1:D:120:ASN:HB3	1.63	0.81
1:A:71:ARG:HG3	1:A:72:ALA:N	1.93	0.81
1:D:236:GLN:NE2	1:D:242:ASP:O	2.12	0.81
1:C:246:VAL:HG12	1:C:247:HIS:CD2	2.16	0.81
1:F:73:TYR:OH	1:F:81:ARG:HG3	1.82	0.79
1:G:197:GLU:OE1	3:G:401:HOH:O	1.98	0.79
1:E:139:ILE:HD11	1:E:143:ILE:HD11	1.66	0.78
1:M:97:SER:HB2	1:N:88:MET:HG3	1.67	0.76
1:E:78:ARG:NH1	1:E:82:GLU:OE2	2.19	0.75
1:I:64:GLU:OE2	1:I:81:ARG:NH1	2.20	0.74
1:D:98:LEU:HD22	1:E:76:TYR:OH	1.89	0.73
1:N:230:MET:HE1	1:N:240:ILE:CD1	2.19	0.73
1:D:98:LEU:HD21	1:E:59:ILE:HD12	1.71	0.73
1:H:110:SER:O	1:H:141:ASN:ND2	2.21	0.72
1:N:148:VAL:HG12	1:N:170:LEU:HD23	1.71	0.72
1:C:230:MET:CE	1:C:235:ALA:HA	2.20	0.72
1:C:179:GLN:NE2	3:C:401:HOH:O	2.03	0.72
1:A:61:ILE:CG2	1:A:72:ALA:HB1	2.21	0.71
1:N:152:ALA:HB1	1:N:176:MET:CE	2.20	0.71
1:I:64:GLU:CD	1:I:81:ARG:HH11	1.94	0.71
1:I:72:ALA:HB1	3:I:417:HOH:O	1.89	0.70
1:L:139:ILE:HD11	1:L:143:ILE:HD11	1.73	0.70
1:H:131:ALA:HB1	1:I:148[A]:VAL:HG22	1.72	0.70
1:H:148:VAL:CG1	1:H:170:LEU:HD12	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:131:ALA:HB1	1:J:148:VAL:HG22	1.74	0.70
1:J:131:ALA:HB1	1:K:148:VAL:HG22	1.73	0.70
1:N:220:ILE:O	1:N:224:MET:HG3	1.92	0.69
1:H:206:TYR:CE2	1:H:221:GLU:HG2	2.27	0.69
1:N:152:ALA:HB1	1:N:176:MET:HE3	1.73	0.69
1:C:131:ALA:HB1	1:D:148:VAL:HG23	1.74	0.69
1:H:174:ARG:NH2	1:N:200:LYS:HE3	2.06	0.69
1:J:153:SER:OG	3:J:401:HOH:O	2.10	0.69
1:C:131:ALA:HB1	1:D:148:VAL:CG2	2.23	0.68
1:M:148:VAL:HG12	1:M:170:LEU:HD23	1.75	0.68
1:A:71:ARG:HG3	1:A:72:ALA:H	1.59	0.68
1:H:193:ILE:CD1	1:H:198:ILE:HD13	2.23	0.67
1:G:246:VAL:HG12	1:G:247:HIS:CE1	2.30	0.67
1:D:216:SER:OG	1:D:218:GLN:HG2	1.95	0.66
1:M:138:TYR:CZ	1:N:248:PRO:HG3	2.30	0.66
1:H:153[A]:SER:OG	1:H:154:MET:N	2.29	0.66
1:E:197:GLU:HG2	1:F:229:TYR:HD1	1.62	0.65
1:G:174:ARG:HG3	1:G:229:TYR:CD2	2.31	0.65
1:B:196:GLU:HG3	1:H:199:MET:HE3	1.79	0.64
1:B:196:GLU:HA	1:H:199:MET:CE	2.22	0.64
1:G:174:ARG:HH11	1:G:174:ARG:HB3	1.62	0.64
1:E:197:GLU:HG3	3:E:433:HOH:O	1.96	0.64
1:H:131:ALA:CB	1:I:148[A]:VAL:HG22	2.27	0.64
1:G:73:TYR:CZ	1:G:81:ARG:HD2	2.33	0.64
1:H:245:LEU:HD23	1:H:245:LEU:O	1.98	0.63
1:J:58:LEU:HD23	1:J:59:ILE:O	1.98	0.63
1:M:73:TYR:OH	1:M:81:ARG:NH1	2.30	0.63
1:B:196:GLU:CA	1:H:199:MET:HE1	2.23	0.63
1:C:230:MET:HE1	1:C:240:ILE:HD12	1.80	0.63
1:M:73:TYR:CZ	1:M:81:ARG:HD3	2.34	0.63
1:N:62:VAL:O	1:N:72:ALA:HA	1.98	0.63
1:M:146:TRP:HZ3	1:M:245:LEU:HD21	1.64	0.63
1:C:73:TYR:OH	1:C:81:ARG:NH2	2.28	0.62
1:E:178:HIS:O	1:E:180:PRO:HD3	1.98	0.62
1:K:157:LEU:HD13	1:K:205:LEU:HD22	1.81	0.62
1:C:206:TYR:CZ	1:C:221:GLU:HG3	2.35	0.62
1:A:218:GLN:HG2	3:A:426:HOH:O	2.00	0.61
1:I:61:ILE:HD13	1:I:74:ASP:HA	1.82	0.61
1:L:63:VAL:HG22	1:L:73:TYR:CD1	2.34	0.61
1:B:196:GLU:HG3	1:H:199:MET:CE	2.30	0.61
1:L:148:VAL:HG12	1:L:170:LEU:HD23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:230:MET:CE	1:H:235:ALA:HA	2.27	0.61
1:C:230:MET:CE	1:C:240:ILE:HD12	2.30	0.60
1:K:78:ARG:NH1	1:K:82:GLU:OE2	2.29	0.60
1:M:193:ILE:HG22	1:N:229:TYR:HE1	1.65	0.60
1:B:98:LEU:HD21	1:C:59:ILE:HD12	1.83	0.60
1:F:148:VAL:HG12	1:F:170:LEU:HD23	1.84	0.60
1:C:62:VAL:O	1:C:72:ALA:HA	2.00	0.60
1:J:98:LEU:HD11	1:K:59:ILE:HD12	1.84	0.60
1:E:73:TYR:HE2	1:E:81:ARG:HE	1.49	0.59
1:E:245:LEU:HD12	1:E:245:LEU:O	2.02	0.59
1:H:220:ILE:O	1:H:224:MET:HG3	2.02	0.59
1:A:153[B]:SER:OG	1:A:180:PRO:HD2	2.02	0.59
1:I:231:SER:OG	1:I:234:GLU:HG3	2.02	0.59
1:F:220:ILE:O	1:F:224:MET:HG3	2.02	0.59
1:K:217:LEU:O	1:K:221:GLU:HG3	2.02	0.59
1:H:170:LEU:HD23	1:H:245:LEU:CD2	2.32	0.59
1:H:206:TYR:CZ	1:H:221:GLU:HG2	2.37	0.59
1:L:61:ILE:HG23	1:L:73:TYR:HB3	1.85	0.59
1:I:98:LEU:O	1:I:102:GLN:HG3	2.02	0.58
1:J:111:ASN:HB2	1:J:140:LEU:HD12	1.84	0.58
1:K:139:ILE:HD11	1:K:143:ILE:HD11	1.85	0.58
1:I:206:TYR:CE2	1:I:221:GLU:HG3	2.38	0.58
1:I:206:TYR:CZ	1:I:221:GLU:HG3	2.39	0.58
1:J:73:TYR:HH	1:J:81:ARG:NH1	2.00	0.58
1:H:169:SER:HB2	1:H:241:LEU:HD22	1.86	0.58
1:J:58:LEU:HD23	1:J:59:ILE:N	2.18	0.57
1:M:146:TRP:CZ3	1:M:245:LEU:HD21	2.39	0.57
1:J:131:ALA:CB	1:K:148:VAL:HG22	2.34	0.57
1:D:236:GLN:HB2	1:D:241:LEU:HD11	1.85	0.57
1:C:230:MET:HE3	1:C:235:ALA:CA	2.34	0.57
1:L:197:GLU:OE2	1:M:229:TYR:HB2	2.05	0.57
1:J:98:LEU:HD12	1:K:76:TYR:CZ	2.39	0.57
1:I:58:LEU:N	1:I:58:LEU:HD22	2.20	0.57
1:M:226:ARG:NH1	3:M:402:HOH:O	2.32	0.57
1:A:193:ILE:HD11	1:A:198:ILE:HG12	1.86	0.56
1:E:98:LEU:HD11	1:F:59:ILE:HD12	1.88	0.56
1:H:98:LEU:HD22	1:I:76:TYR:OH	2.04	0.56
1:H:174:ARG:HH22	1:N:200:LYS:HE3	1.70	0.56
1:G:195:ALA:HB3	1:J:202:LYS:HD3	1.87	0.56
1:H:229:TYR:HD1	1:N:197:GLU:HG3	1.69	0.56
3:J:412:HOH:O	1:K:171:PRO:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:153[A]:SER:OG	1:M:154:MET:N	2.37	0.56
1:H:159:LEU:HD21	1:H:241:LEU:HD23	1.87	0.55
1:N:231:SER:OG	1:N:234:GLU:HG2	2.05	0.55
1:M:138:TYR:O	1:N:248:PRO:HD3	2.07	0.55
1:J:197:GLU:HB2	3:J:411:HOH:O	2.06	0.55
1:A:231:SER:OG	1:A:234:GLU:HG3	2.06	0.55
1:I:64:GLU:CD	1:I:81:ARG:NH1	2.59	0.55
1:A:112:LYS:HG2	1:A:113:LYS:N	2.22	0.55
1:K:200:LYS:HD3	3:K:417:HOH:O	2.07	0.55
1:H:245:LEU:HD23	1:H:245:LEU:C	2.27	0.54
1:I:135:THR:O	1:I:139:ILE:HG23	2.08	0.54
1:M:148:VAL:HG12	1:M:170:LEU:CD2	2.35	0.54
1:D:139:ILE:HD11	1:D:143:ILE:HD11	1.89	0.54
1:H:230:MET:HE1	1:H:240:ILE:HD12	1.88	0.54
1:I:92:ASP:HB2	3:I:410:HOH:O	2.05	0.54
1:D:236:GLN:HB2	1:D:241:LEU:CD1	2.37	0.54
1:C:131:ALA:CB	1:D:148:VAL:HG23	2.36	0.54
1:E:233:MET:O	1:E:237:GLU:HG3	2.08	0.54
1:A:82:GLU:HG3	2:A:301:A1LZA:C25	2.39	0.53
1:G:174:ARG:HG3	1:G:229:TYR:CE2	2.43	0.53
1:A:61:ILE:HG21	1:A:72:ALA:HB1	1.89	0.53
1:F:199:MET:HG2	1:K:199:MET:HG3	1.89	0.53
1:L:63:VAL:HG22	1:L:73:TYR:CE1	2.44	0.53
1:B:139:ILE:HD11	1:B:143:ILE:HD11	1.90	0.53
1:G:174:ARG:NH1	3:G:402:HOH:O	2.35	0.53
1:N:139:ILE:HD11	1:N:143:ILE:HD11	1.90	0.53
1:C:58:LEU:O	1:C:58:LEU:HD12	2.08	0.52
1:D:104:LEU:HD22	2:E:301:A1LZA:O08	2.08	0.52
1:C:216:SER:OG	1:C:219:VAL:HG23	2.09	0.52
1:K:62:VAL:HG21	1:K:78:ARG:HG2	1.91	0.52
1:A:76:TYR:CZ	1:G:98:LEU:HD23	2.45	0.52
1:C:197:GLU:OE1	1:D:229:TYR:HB2	2.08	0.52
1:A:193:ILE:CD1	1:A:198:ILE:HG12	2.39	0.52
1:F:98:LEU:HD23	1:G:76:TYR:OH	2.09	0.52
1:H:59:ILE:HD12	1:N:98:LEU:HD11	1.90	0.52
1:H:199:MET:O	1:H:203:LYS:HG3	2.09	0.52
1:G:194:GLN:O	1:G:198:ILE:HG13	2.09	0.52
1:H:169:SER:HB2	1:H:241:LEU:CD2	2.40	0.52
1:J:73:TYR:N	1:J:73:TYR:CD1	2.78	0.52
1:E:73:TYR:CE2	1:E:81:ARG:HD3	2.45	0.52
1:G:220:ILE:O	1:G:224:MET:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:209:TYR:O	1:N:213:THR:HG23	2.10	0.52
1:D:82:GLU:HG3	2:D:301:A1LZA:C24	2.40	0.52
1:E:226:ARG:HD3	1:M:225:GLU:OE1	2.10	0.51
1:K:146:TRP:CE3	1:K:168:HIS:HB2	2.45	0.51
1:J:129:GLY:HA3	1:J:154:MET:HE2	1.92	0.51
1:L:236:GLN:HB2	1:L:241:LEU:CD1	2.40	0.51
1:E:246:VAL:HG12	1:E:247:HIS:CE1	2.46	0.51
1:I:233:MET:HE3	1:I:233:MET:HA	1.93	0.51
1:M:245:LEU:HD12	1:M:245:LEU:O	2.09	0.51
1:C:225:GLU:OE2	1:H:228:ARG:HD2	2.11	0.51
1:A:104:LEU:HD22	2:B:301:A1LZA:O08	2.11	0.51
1:A:88:MET:HG3	1:A:120:ASN:HB3	1.94	0.50
1:M:98:LEU:HD11	1:N:60:PRO:HD2	1.93	0.50
1:J:157:LEU:HD13	1:J:205:LEU:HD22	1.93	0.50
1:C:134:ASP:OD2	1:D:172:ASN:HB2	2.11	0.50
1:D:61:ILE:HD13	1:D:74:ASP:HA	1.93	0.50
1:N:202:LYS:HE2	1:N:206:TYR:OH	2.11	0.50
1:E:211:LYS:HD3	1:E:212:HIS:NE2	2.26	0.50
1:E:73:TYR:HE2	1:E:81:ARG:NE	2.08	0.50
1:C:107:GLN:OE1	1:C:139:ILE:HA	2.12	0.50
1:H:148:VAL:CG1	1:H:170:LEU:CD1	2.81	0.49
1:B:199:MET:CE	1:H:196:GLU:HA	2.42	0.49
1:C:193:ILE:HD11	1:C:198:ILE:HG12	1.95	0.49
1:F:196:GLU:OE2	1:K:206:TYR:OH	2.28	0.49
1:A:61:ILE:HD13	1:A:74:ASP:HA	1.94	0.49
1:F:59:ILE:CG2	1:F:74:ASP:HB2	2.43	0.49
1:N:81:ARG:O	1:N:81:ARG:HG3	2.13	0.49
1:H:196:GLU:O	1:H:200:LYS:HG3	2.13	0.49
1:I:131:ALA:CB	1:J:148:VAL:HG22	2.42	0.49
1:N:153[A]:SER:OG	1:N:154:MET:N	2.46	0.49
1:H:215:GLN:HB3	1:H:219:VAL:CG2	2.43	0.48
1:A:247:HIS:HB2	3:A:412:HOH:O	2.13	0.48
1:C:206:TYR:CE2	1:C:221:GLU:HG3	2.48	0.48
1:L:63:VAL:HG22	1:L:73:TYR:HD1	1.78	0.48
1:C:98:LEU:HD11	1:D:60:PRO:HD2	1.95	0.48
1:B:202:LYS:HE2	1:B:206:TYR:OH	2.14	0.48
1:H:62:VAL:HG21	1:H:78:ARG:HG2	1.95	0.48
1:M:139:ILE:HD11	1:M:143:ILE:HD11	1.95	0.48
1:D:81:ARG:HG2	1:D:81:ARG:HH11	1.78	0.48
1:H:144:CYS:HA	1:H:166:MET:O	2.14	0.48
1:M:170:LEU:HD22	1:M:170:LEU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ILE:HG13	1:D:58:LEU:HD21	1.94	0.48
1:E:73:TYR:CZ	1:E:81:ARG:HD3	2.48	0.48
1:K:209:TYR:HB3	1:K:220:ILE:HD12	1.95	0.48
1:B:153:SER:OG	1:B:154:MET:N	2.45	0.48
1:M:59:ILE:N	1:M:59:ILE:HD12	2.28	0.48
1:M:138:TYR:HE2	1:N:245:LEU:HD21	1.78	0.48
1:N:86:CYS:HB3	1:N:88:MET:HG2	1.96	0.48
1:B:58:LEU:HD23	1:B:58:LEU:N	2.29	0.47
1:F:98:LEU:HD23	1:G:76:TYR:CZ	2.49	0.47
1:H:245:LEU:HD11	1:N:138:TYR:CE1	2.49	0.47
1:G:107:GLN:HG3	1:G:141:ASN:OD1	2.15	0.47
1:C:59:ILE:N	1:C:59:ILE:HD13	2.30	0.47
1:C:153:SER:OG	1:C:154:MET:N	2.48	0.47
1:N:136:MET:HG2	1:N:143:ILE:HD13	1.97	0.47
1:M:153[B]:SER:OG	1:M:180:PRO:HD2	2.15	0.47
1:N:152:ALA:HB1	1:N:176:MET:HE2	1.95	0.47
1:H:165:GLY:N	1:H:242:ASP:OD2	2.48	0.47
1:M:73:TYR:CZ	1:M:81:ARG:CD	2.98	0.47
1:D:245:LEU:HD12	1:D:245:LEU:HA	1.61	0.47
1:I:111:ASN:OD1	1:I:111:ASN:C	2.53	0.47
1:I:213:THR:O	1:I:214:LYS:HB2	2.15	0.47
1:N:146:TRP:HZ3	1:N:245:LEU:HD22	1.80	0.46
1:A:71:ARG:CG	1:A:72:ALA:N	2.71	0.46
1:G:173:SER:O	1:G:232:PRO:HD3	2.15	0.46
1:H:230:MET:CE	1:H:235:ALA:CA	2.92	0.46
1:L:199:MET:CE	1:L:203:LYS:HE2	2.46	0.46
1:N:146:TRP:CZ3	1:N:245:LEU:HD22	2.51	0.46
1:A:98:LEU:HD21	1:B:60:PRO:HD3	1.96	0.46
1:A:163:THR:O	1:A:166:MET:HB2	2.15	0.46
1:D:78:ARG:HH12	1:D:82:GLU:HG2	1.81	0.46
1:D:246:VAL:HG13	1:D:247:HIS:H	1.80	0.46
1:N:177:ILE:HD11	1:N:223:ALA:HB1	1.96	0.46
1:A:134:ASP:OD2	1:B:172:ASN:HB2	2.16	0.46
1:N:148:VAL:HG12	1:N:170:LEU:CD2	2.43	0.46
1:J:193:ILE:CD1	1:J:198:ILE:HB	2.45	0.46
1:H:245:LEU:HD11	1:N:138:TYR:HE1	1.81	0.45
1:H:82:GLU:HG3	2:H:301:A1LZA:C25	2.45	0.45
1:H:170:LEU:HB3	1:H:171:PRO:CD	2.47	0.45
1:D:98:LEU:CD2	1:E:76:TYR:OH	2.62	0.45
1:C:217:LEU:HD23	1:C:217:LEU:HA	1.82	0.45
1:H:230:MET:HE1	1:H:240:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:N	1:D:170:LEU:HD22	2.32	0.45
1:D:171:PRO:HG3	1:D:246:VAL:HA	1.99	0.45
1:H:174:ARG:NH1	1:H:231:SER:HA	2.32	0.45
1:H:193:ILE:HD12	1:H:197:GLU:CB	2.46	0.45
1:K:82:GLU:O	1:K:83:ARG:HB2	2.16	0.45
1:H:170:LEU:HD23	1:H:245:LEU:HD22	1.99	0.45
1:J:83:ARG:HG2	1:J:106:LEU:HD22	1.99	0.45
1:H:174:ARG:HB3	1:H:229:TYR:CD2	2.52	0.45
1:I:193:ILE:HG13	1:I:198:ILE:HG13	1.98	0.45
1:B:101:ALA:HB1	1:C:75:ILE:HG12	1.98	0.45
1:H:76:TYR:OH	1:N:98:LEU:HD12	2.17	0.45
1:B:225:GLU:OE1	1:I:226:ARG:HD3	2.16	0.44
1:I:178:HIS:O	1:I:180:PRO:HD3	2.18	0.44
1:L:98:LEU:HD21	1:M:59:ILE:HG13	1.99	0.44
1:A:247:HIS:HB3	1:A:248:PRO:HD2	2.00	0.44
1:J:206:TYR:HA	1:J:220:ILE:HG21	1.99	0.44
1:D:98:LEU:HD22	1:E:76:TYR:CZ	2.53	0.44
1:J:139:ILE:HD11	1:J:143:ILE:HD11	1.98	0.44
1:B:82:GLU:HG3	2:B:301:A1LZA:C26	2.47	0.44
1:F:78:ARG:NH1	1:F:82:GLU:OE2	2.47	0.44
1:H:193:ILE:HD12	1:H:197:GLU:HB2	2.00	0.44
1:H:230:MET:HB3	1:H:230:MET:HE3	1.83	0.44
1:H:230:MET:HB3	1:H:234:GLU:HB2	2.00	0.44
1:N:96:ALA:HA	1:N:132:ILE:HD11	1.99	0.44
1:C:59:ILE:HG13	1:D:58:LEU:CD2	2.47	0.44
1:G:58:LEU:C	1:G:58:LEU:HD13	2.38	0.44
1:H:174:ARG:HD2	1:H:174:ARG:HA	1.68	0.44
1:M:176:MET:HB2	1:M:229:TYR:CD2	2.52	0.44
1:B:146:TRP:CE3	1:B:168:HIS:HB2	2.53	0.44
1:H:209:TYR:O	1:H:213:THR:HG23	2.18	0.44
1:J:177:ILE:HD11	1:J:223:ALA:HB1	2.00	0.44
1:B:98:LEU:O	1:B:102:GLN:HG3	2.18	0.44
1:B:245:LEU:C	1:B:245:LEU:HD12	2.38	0.44
1:C:206:TYR:HB3	1:C:217:LEU:CD2	2.48	0.44
1:J:97:SER:HB2	1:K:88:MET:HG2	1.99	0.44
1:L:62:VAL:N	1:L:73:TYR:O	2.35	0.44
1:M:112:LYS:HD2	1:M:112:LYS:HA	1.41	0.44
1:M:113:LYS:HB3	1:M:113:LYS:HE3	1.83	0.44
1:A:97:SER:HB3	1:B:88:MET:HG2	1.98	0.43
1:A:206:TYR:CE2	1:A:221:GLU:HG3	2.53	0.43
1:B:197:GLU:OE2	1:C:229:TYR:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:SER:OG	1:B:234:GLU:HG3	2.18	0.43
1:H:58:LEU:N	1:H:58:LEU:HD22	2.33	0.43
1:C:148:VAL:HG12	1:C:170:LEU:CD2	2.40	0.43
1:A:159:LEU:HD21	1:A:241:LEU:HD23	2.00	0.43
1:E:73:TYR:OH	1:E:81:ARG:HD3	2.19	0.43
1:F:225:GLU:HG2	3:F:411:HOH:O	2.18	0.43
1:B:193:ILE:HG22	1:C:229:TYR:HE1	1.83	0.43
1:G:62:VAL:HG21	1:G:78:ARG:HG2	2.00	0.43
1:D:165:GLY:N	1:D:242:ASP:OD2	2.52	0.43
1:N:63:VAL:HA	1:N:72:ALA:HA	2.01	0.43
1:A:151:ALA:O	1:A:156:SER:HB3	2.19	0.43
1:E:98:LEU:HD21	1:F:60:PRO:HD3	2.00	0.43
1:I:91:ILE:O	1:I:124:GLY:HA3	2.19	0.43
1:J:196:GLU:O	1:J:200:LYS:HG3	2.19	0.43
1:C:58:LEU:C	1:C:59:ILE:HD13	2.39	0.43
1:N:193:ILE:HD12	1:N:198:ILE:HG13	2.01	0.43
1:N:230:MET:CE	1:N:240:ILE:CD1	2.95	0.43
1:A:71:ARG:CG	1:A:72:ALA:H	2.28	0.43
1:I:96:ALA:HA	1:I:132:ILE:HD11	1.99	0.43
1:J:58:LEU:HD23	1:J:59:ILE:H	1.82	0.43
1:N:159:LEU:HD21	1:N:241:LEU:HD23	2.01	0.43
1:A:230:MET:HB3	1:A:234:GLU:HB2	2.01	0.42
1:K:173:SER:O	1:K:232:PRO:HD3	2.19	0.42
1:F:203:LYS:HE3	1:F:203:LYS:HB2	1.86	0.42
1:N:148:VAL:CG1	1:N:170:LEU:HD23	2.46	0.42
1:B:199:MET:HE1	1:H:196:GLU:N	2.34	0.42
1:D:177:ILE:HD12	1:D:224:MET:HG3	2.00	0.42
1:I:98:LEU:CD2	1:J:76:TYR:OH	2.67	0.42
1:M:61:ILE:N	1:M:61:ILE:HD13	2.34	0.42
1:G:226:ARG:HD3	1:K:225:GLU:OE1	2.18	0.42
1:H:229:TYR:HE1	1:N:193:ILE:HG22	1.84	0.42
1:F:61:ILE:HD13	1:F:74:ASP:HA	2.01	0.42
1:H:59:ILE:CD1	1:N:98:LEU:HD11	2.48	0.42
1:L:82:GLU:HG3	2:L:301:A1LZA:C25	2.50	0.42
1:B:130:LEU:HD23	1:B:130:LEU:HA	1.91	0.42
1:H:120:ASN:HB2	1:H:148:VAL:O	2.19	0.42
1:I:98:LEU:CD1	1:J:60:PRO:HD2	2.49	0.42
1:K:153:SER:OG	1:K:154:MET:N	2.52	0.42
1:N:146:TRP:CE3	1:N:168:HIS:HB2	2.54	0.42
1:B:138:TYR:O	1:C:248:PRO:HD3	2.20	0.42
1:C:245:LEU:HD12	1:C:245:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:193:ILE:CG1	1:H:198:ILE:CD1	2.98	0.42
1:M:60:PRO:C	1:M:61:ILE:HD13	2.40	0.42
1:A:120:ASN:HB2	1:A:148:VAL:O	2.20	0.42
1:B:197:GLU:O	1:B:197:GLU:HG3	2.18	0.42
1:D:170:LEU:N	1:D:170:LEU:CD2	2.83	0.42
1:D:225:GLU:HG2	1:N:226:ARG:HG2	2.01	0.42
1:H:150:GLN:HA	1:H:174:ARG:O	2.20	0.42
1:I:102:GLN:HG2	1:J:75:ILE:HD13	2.01	0.42
1:L:199:MET:HE3	1:L:203:LYS:HE2	2.02	0.42
1:M:112:LYS:HD2	1:M:112:LYS:O	2.20	0.42
1:H:216:SER:O	1:H:219:VAL:HG22	2.19	0.42
1:E:73:TYR:OH	1:E:81:ARG:CD	2.68	0.41
1:K:177:ILE:HG13	1:K:224:MET:HG2	2.03	0.41
1:A:225:GLU:OE1	1:J:226:ARG:NE	2.53	0.41
1:C:106:LEU:CB	1:C:115:ILE:HD11	2.50	0.41
1:M:81:ARG:HE	1:M:81:ARG:HB3	1.59	0.41
1:B:132:ILE:O	1:B:136:MET:HG3	2.20	0.41
1:C:165:GLY:N	1:C:242:ASP:OD2	2.54	0.41
1:F:204:GLN:O	1:F:208:ILE:HG13	2.20	0.41
1:G:245:LEU:HD22	1:G:247:HIS:O	2.20	0.41
1:H:94:SER:O	1:H:98:LEU:HD23	2.21	0.41
1:J:114:PRO:HB3	1:J:142:PRO:HG2	2.02	0.41
1:D:98:LEU:HD11	1:E:60:PRO:HD2	2.01	0.41
1:I:148[B]:VAL:HG12	1:I:170:LEU:HD23	2.02	0.41
1:M:73:TYR:OH	1:M:81:ARG:CD	2.68	0.41
1:B:200:LYS:HE2	1:C:174:ARG:NH2	2.35	0.41
1:H:202:LYS:HE2	1:H:224:MET:HE2	2.02	0.41
1:K:169:SER:HB2	1:K:241:LEU:HD22	2.01	0.41
1:B:102:GLN:O	1:B:106:LEU:HG	2.20	0.41
1:B:204:GLN:O	1:B:208:ILE:HG13	2.20	0.41
1:I:82:GLU:HG3	2:I:301:A1LZA:C25	2.49	0.41
1:I:199:MET:CE	1:I:203:LYS:HE2	2.50	0.41
1:M:83:ARG:HD3	1:M:113:LYS:HE3	2.03	0.41
1:M:101:ALA:HB1	1:N:75:ILE:HD12	2.02	0.41
1:A:153[A]:SER:OG	1:A:154:MET:N	2.53	0.41
3:A:409:HOH:O	1:I:179:GLN:HB2	2.20	0.41
1:H:59:ILE:HD13	1:N:98:LEU:HD21	2.03	0.41
1:H:215:GLN:HB3	1:H:219:VAL:HG21	2.02	0.41
1:K:96:ALA:HA	1:K:132:ILE:HD11	2.03	0.41
1:A:216:SER:HB3	1:A:219:VAL:H	1.85	0.41
1:A:246:VAL:HG12	1:A:247:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:GLU:O	1:C:83:ARG:HB2	2.21	0.41
1:F:59:ILE:HG22	1:F:74:ASP:HB2	2.02	0.41
1:J:146:TRP:CE3	1:J:168:HIS:HB2	2.56	0.41
1:K:197:GLU:OE1	1:L:229:TYR:HB2	2.21	0.41
1:N:120:ASN:ND2	3:N:401:HOH:O	2.44	0.41
1:A:206:TYR:CZ	1:A:221:GLU:HG3	2.55	0.41
1:C:247:HIS:HB3	1:C:248:PRO:CD	2.51	0.41
1:G:82:GLU:HG3	2:G:301:A1LZA:C24	2.51	0.41
1:K:159:LEU:HD21	1:K:241:LEU:HD23	2.03	0.41
1:C:82:GLU:HG3	2:C:301:A1LZA:C25	2.51	0.40
1:K:170:LEU:N	1:K:170:LEU:HD22	2.36	0.40
1:D:144:CYS:HA	1:D:166:MET:O	2.21	0.40
1:I:107:GLN:HG3	1:I:141:ASN:OD1	2.21	0.40
1:I:214:LYS:HD3	1:I:214:LYS:HA	1.49	0.40
1:M:75:ILE:O	1:M:79:LEU:HD13	2.21	0.40
1:N:112:LYS:HG3	1:N:113:LYS:N	2.35	0.40
1:A:76:TYR:OH	1:G:98:LEU:HD23	2.21	0.40
1:A:248:PRO:C	3:A:412:HOH:O	2.60	0.40
1:E:165:GLY:O	1:E:243:LYS:HE3	2.21	0.40
1:E:98:LEU:CD1	1:F:59:ILE:HD12	2.51	0.40
1:K:170:LEU:HB3	1:K:171:PRO:CD	2.51	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	171/220 (78%)	168 (98%)	3 (2%)	0	100	100
1	B	167/220 (76%)	162 (97%)	5 (3%)	0	100	100
1	C	165/220 (75%)	159 (96%)	6 (4%)	0	100	100
1	D	165/220 (75%)	162 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	165/220 (75%)	161 (98%)	4 (2%)	0	100	100
1	F	160/220 (73%)	155 (97%)	5 (3%)	0	100	100
1	G	165/220 (75%)	161 (98%)	4 (2%)	0	100	100
1	H	162/220 (74%)	155 (96%)	7 (4%)	0	100	100
1	I	167/220 (76%)	162 (97%)	5 (3%)	0	100	100
1	J	164/220 (74%)	159 (97%)	4 (2%)	1 (1%)	25	18
1	K	165/220 (75%)	161 (98%)	4 (2%)	0	100	100
1	L	164/220 (74%)	161 (98%)	3 (2%)	0	100	100
1	M	166/220 (76%)	159 (96%)	7 (4%)	0	100	100
1	N	167/220 (76%)	161 (96%)	6 (4%)	0	100	100
All	All	2313/3080 (75%)	2246 (97%)	66 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	110	SER

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	155/184 (84%)	150 (97%)	5 (3%)	39	38
1	B	150/184 (82%)	147 (98%)	3 (2%)	55	59
1	C	149/184 (81%)	144 (97%)	5 (3%)	37	35
1	D	148/184 (80%)	144 (97%)	4 (3%)	44	46
1	E	148/184 (80%)	144 (97%)	4 (3%)	44	46
1	F	145/184 (79%)	141 (97%)	4 (3%)	43	44
1	G	149/184 (81%)	145 (97%)	4 (3%)	44	46
1	H	147/184 (80%)	142 (97%)	5 (3%)	37	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	150/184 (82%)	145 (97%)	5 (3%)	38 37
1	J	148/184 (80%)	145 (98%)	3 (2%)	55 59
1	K	149/184 (81%)	145 (97%)	4 (3%)	44 46
1	L	148/184 (80%)	145 (98%)	3 (2%)	55 59
1	M	150/184 (82%)	148 (99%)	2 (1%)	69 74
1	N	150/184 (82%)	142 (95%)	8 (5%)	22 19
All	All	2086/2576 (81%)	2027 (97%)	59 (3%)	43 44

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	88	MET
1	A	112	LYS
1	A	174	ARG
1	A	245	LEU
1	B	88	MET
1	B	148	VAL
1	B	179	GLN
1	C	75	ILE
1	C	81	ARG
1	C	108	SER
1	C	222	SER
1	C	245	LEU
1	D	58	LEU
1	D	74	ASP
1	D	94	SER
1	D	148	VAL
1	E	73	TYR
1	E	140	LEU
1	E	197	GLU
1	E	218	GLN
1	F	73	TYR
1	F	179	GLN
1	F	199	MET
1	F	200	LYS
1	G	75	ILE
1	G	174	ARG
1	G	199	MET
1	G	245	LEU

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Mol	Chain	Res	Type
1	H	97	SER
1	H	110	SER
1	H	174	ARG
1	H	218	GLN
1	H	245	LEU
1	I	81	ARG
1	I	174	ARG
1	I	222	SER
1	I	237	GLU
1	I	247	HIS
1	J	63	VAL
1	J	81	ARG
1	J	245	LEU
1	K	64	GLU
1	K	81	ARG
1	K	174	ARG
1	K	216	SER
1	L	74	ASP
1	L	179	GLN
1	L	200	LYS
1	M	74	ASP
1	M	97	SER
1	N	75	ILE
1	N	81	ARG
1	N	88	MET
1	N	108	SER
1	N	168	HIS
1	N	218	GLN
1	N	226	ARG
1	N	247	HIS

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

Mol	Chain	Res	Type
1	B	247	HIS
1	C	247	HIS
1	E	179	GLN
1	G	107	GLN
1	H	137	GLN
1	L	204	GLN
1	M	247	HIS

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

14 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	A1LZA	C	301	-	33,33,33	3.78	13 (39%)	39,47,47	3.19	14 (35%)
2	A1LZA	D	301	-	33,33,33	3.66	13 (39%)	39,47,47	3.08	11 (28%)
2	A1LZA	N	301	-	33,33,33	3.73	13 (39%)	39,47,47	3.25	13 (33%)
2	A1LZA	G	301	-	33,33,33	3.91	14 (42%)	39,47,47	3.16	12 (30%)
2	A1LZA	K	301	-	33,33,33	3.68	12 (36%)	39,47,47	3.30	11 (28%)
2	A1LZA	M	301	-	33,33,33	3.90	14 (42%)	39,47,47	3.19	11 (28%)
2	A1LZA	J	301	-	33,33,33	3.63	13 (39%)	39,47,47	3.15	10 (25%)
2	A1LZA	H	301	-	33,33,33	3.83	13 (39%)	39,47,47	3.19	11 (28%)
2	A1LZA	I	301	-	33,33,33	3.75	13 (39%)	39,47,47	3.22	13 (33%)
2	A1LZA	B	301	-	33,33,33	3.97	14 (42%)	39,47,47	3.19	10 (25%)
2	A1LZA	A	301	-	33,33,33	3.86	15 (45%)	39,47,47	3.23	12 (30%)
2	A1LZA	E	301	-	33,33,33	3.66	13 (39%)	39,47,47	3.25	12 (30%)
2	A1LZA	L	301	-	33,33,33	3.95	15 (45%)	39,47,47	3.22	12 (30%)
2	A1LZA	F	301	-	33,33,33	3.81	13 (39%)	39,47,47	3.15	12 (30%)

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	A1LZA	C	301	-	-	3/8/26/26	0/5/5/5
2	A1LZA	D	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	N	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	G	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	K	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	M	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	J	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	H	301	-	-	1/8/26/26	0/5/5/5
2	A1LZA	I	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	B	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	A	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	E	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	L	301	-	-	2/8/26/26	0/5/5/5
2	A1LZA	F	301	-	-	2/8/26/26	0/5/5/5

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	A1LZA	C06-N01	-15.69	1.32	1.46
2	M	301	A1LZA	C06-N01	-15.55	1.32	1.46
2	B	301	A1LZA	C06-N01	-15.50	1.32	1.46
2	G	301	A1LZA	C06-N01	-15.48	1.32	1.46
2	A	301	A1LZA	C06-N01	-15.24	1.32	1.46
2	H	301	A1LZA	C06-N01	-15.07	1.32	1.46
2	I	301	A1LZA	C06-N01	-14.49	1.33	1.46
2	F	301	A1LZA	C06-N01	-14.20	1.33	1.46
2	C	301	A1LZA	C06-N01	-13.85	1.34	1.46
2	N	301	A1LZA	C06-N01	-13.82	1.34	1.46
2	K	301	A1LZA	C06-N01	-13.73	1.34	1.46
2	J	301	A1LZA	C06-N01	-13.60	1.34	1.46
2	E	301	A1LZA	C06-N01	-13.48	1.34	1.46
2	D	301	A1LZA	C06-N01	-13.47	1.34	1.46
2	C	301	A1LZA	C18-N17	-7.60	1.36	1.47
2	F	301	A1LZA	C18-N17	-7.38	1.36	1.47
2	D	301	A1LZA	C18-N17	-7.06	1.37	1.47
2	H	301	A1LZA	C18-N17	-7.02	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	301	A1LZA	C18-N17	-6.95	1.37	1.47
2	M	301	A1LZA	C18-N17	-6.94	1.37	1.47
2	E	301	A1LZA	C18-N17	-6.93	1.37	1.47
2	A	301	A1LZA	C18-N17	-6.80	1.37	1.47
2	I	301	A1LZA	C18-N17	-6.78	1.37	1.47
2	B	301	A1LZA	C18-N17	-6.78	1.37	1.47
2	L	301	A1LZA	C18-N17	-6.75	1.37	1.47
2	J	301	A1LZA	C18-N17	-6.75	1.37	1.47
2	B	301	A1LZA	C06-C05	-6.68	1.41	1.51
2	N	301	A1LZA	C19-N20	-6.52	1.33	1.47
2	C	301	A1LZA	C19-N20	-6.51	1.33	1.47
2	I	301	A1LZA	C19-N20	-6.40	1.33	1.47
2	G	301	A1LZA	C19-N20	-6.36	1.33	1.47
2	E	301	A1LZA	C19-N20	-6.33	1.33	1.47
2	L	301	A1LZA	C06-C05	-6.32	1.41	1.51
2	G	301	A1LZA	C18-N17	-6.32	1.38	1.47
2	B	301	A1LZA	C19-N20	-6.31	1.33	1.47
2	K	301	A1LZA	C19-N20	-6.31	1.33	1.47
2	D	301	A1LZA	C19-N20	-6.26	1.33	1.47
2	A	301	A1LZA	C19-N20	-6.24	1.33	1.47
2	K	301	A1LZA	C18-N17	-6.18	1.38	1.47
2	M	301	A1LZA	C06-C05	-6.17	1.41	1.51
2	J	301	A1LZA	C19-N20	-6.16	1.34	1.47
2	F	301	A1LZA	C19-N20	-6.11	1.34	1.47
2	F	301	A1LZA	C06-C05	-6.11	1.42	1.51
2	L	301	A1LZA	C19-N20	-6.09	1.34	1.47
2	H	301	A1LZA	C19-N20	-5.96	1.34	1.47
2	M	301	A1LZA	C19-N20	-5.88	1.34	1.47
2	H	301	A1LZA	C06-C05	-5.83	1.42	1.51
2	D	301	A1LZA	C06-C05	-5.79	1.42	1.51
2	K	301	A1LZA	C06-C05	-5.74	1.42	1.51
2	G	301	A1LZA	C06-C05	-5.71	1.42	1.51
2	E	301	A1LZA	C06-C05	-5.65	1.42	1.51
2	A	301	A1LZA	C06-C05	-5.54	1.42	1.51
2	J	301	A1LZA	C06-C05	-5.49	1.42	1.51
2	I	301	A1LZA	C06-C05	-5.37	1.43	1.51
2	C	301	A1LZA	C06-C05	-5.28	1.43	1.51
2	N	301	A1LZA	C06-C05	-5.13	1.43	1.51
2	F	301	A1LZA	C21-N16	5.07	1.38	1.31
2	N	301	A1LZA	C03-C04	-5.03	1.42	1.49
2	N	301	A1LZA	C02-N01	-5.02	1.33	1.46
2	C	301	A1LZA	C02-N01	-4.94	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	A1LZA	C02-C03	-4.92	1.39	1.52
2	M	301	A1LZA	C02-C03	-4.89	1.39	1.52
2	C	301	A1LZA	C02-C03	-4.78	1.39	1.52
2	E	301	A1LZA	C02-C03	-4.76	1.39	1.52
2	F	301	A1LZA	C02-C03	-4.76	1.39	1.52
2	F	301	A1LZA	C02-N01	-4.75	1.33	1.46
2	E	301	A1LZA	C02-N01	-4.74	1.33	1.46
2	K	301	A1LZA	C02-C03	-4.73	1.39	1.52
2	J	301	A1LZA	C02-N01	-4.71	1.33	1.46
2	G	301	A1LZA	C21-N16	4.70	1.38	1.31
2	G	301	A1LZA	C02-N01	-4.68	1.34	1.46
2	J	301	A1LZA	C02-C03	-4.65	1.40	1.52
2	L	301	A1LZA	C02-C03	-4.64	1.40	1.52
2	N	301	A1LZA	C02-C03	-4.64	1.40	1.52
2	D	301	A1LZA	C02-N01	-4.63	1.34	1.46
2	M	301	A1LZA	C02-N01	-4.62	1.34	1.46
2	K	301	A1LZA	C02-N01	-4.61	1.34	1.46
2	C	301	A1LZA	C03-C04	-4.60	1.43	1.49
2	I	301	A1LZA	C02-N01	-4.60	1.34	1.46
2	I	301	A1LZA	C02-C03	-4.59	1.40	1.52
2	D	301	A1LZA	C19-C18	-4.57	1.40	1.51
2	A	301	A1LZA	C02-C03	-4.56	1.40	1.52
2	B	301	A1LZA	C02-C03	-4.56	1.40	1.52
2	H	301	A1LZA	C19-C18	-4.53	1.40	1.51
2	F	301	A1LZA	C19-C18	-4.51	1.40	1.51
2	C	301	A1LZA	C21-N16	4.50	1.38	1.31
2	L	301	A1LZA	C02-N01	-4.49	1.34	1.46
2	B	301	A1LZA	C02-N01	-4.49	1.34	1.46
2	C	301	A1LZA	C19-C18	-4.47	1.40	1.51
2	K	301	A1LZA	C21-N16	4.47	1.38	1.31
2	G	301	A1LZA	C03-C04	-4.46	1.43	1.49
2	D	301	A1LZA	C02-C03	-4.45	1.40	1.52
2	H	301	A1LZA	C02-N01	-4.45	1.34	1.46
2	G	301	A1LZA	C19-C18	-4.45	1.40	1.51
2	N	301	A1LZA	C19-C18	-4.45	1.40	1.51
2	J	301	A1LZA	C03-C04	-4.38	1.43	1.49
2	K	301	A1LZA	C03-C04	-4.38	1.43	1.49
2	M	301	A1LZA	C19-C18	-4.38	1.40	1.51
2	A	301	A1LZA	C03-C04	-4.37	1.43	1.49
2	H	301	A1LZA	C02-C03	-4.37	1.40	1.52
2	E	301	A1LZA	C19-C18	-4.37	1.40	1.51
2	K	301	A1LZA	C19-C18	-4.36	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	A1LZA	C19-C18	-4.34	1.40	1.51
2	J	301	A1LZA	C19-C18	-4.32	1.41	1.51
2	H	301	A1LZA	C21-N16	4.31	1.37	1.31
2	B	301	A1LZA	C19-C18	-4.30	1.41	1.51
2	B	301	A1LZA	C21-N16	4.30	1.37	1.31
2	B	301	A1LZA	C03-C04	-4.29	1.43	1.49
2	A	301	A1LZA	C02-N01	-4.25	1.35	1.46
2	L	301	A1LZA	C19-C18	-4.24	1.41	1.51
2	A	301	A1LZA	C19-C18	-4.23	1.41	1.51
2	F	301	A1LZA	C03-C04	-4.22	1.43	1.49
2	E	301	A1LZA	C03-C04	-4.19	1.43	1.49
2	L	301	A1LZA	C21-N16	4.19	1.37	1.31
2	L	301	A1LZA	C03-C04	-4.17	1.43	1.49
2	D	301	A1LZA	C21-N16	4.12	1.37	1.31
2	M	301	A1LZA	C03-C04	-4.12	1.43	1.49
2	I	301	A1LZA	C03-C04	-4.10	1.43	1.49
2	D	301	A1LZA	C03-C04	-4.09	1.43	1.49
2	J	301	A1LZA	C21-N16	4.03	1.37	1.31
2	A	301	A1LZA	C21-N16	4.01	1.37	1.31
2	H	301	A1LZA	C03-C04	-3.96	1.44	1.49
2	N	301	A1LZA	C21-N17	-3.83	1.30	1.37
2	G	301	A1LZA	C21-N17	-3.83	1.30	1.37
2	A	301	A1LZA	O08-C07	-3.79	1.17	1.23
2	E	301	A1LZA	C21-N16	3.78	1.37	1.31
2	K	301	A1LZA	O08-C07	-3.78	1.17	1.23
2	N	301	A1LZA	C21-N16	3.55	1.36	1.31
2	B	301	A1LZA	C21-N17	-3.52	1.30	1.37
2	I	301	A1LZA	C21-N16	3.50	1.36	1.31
2	I	301	A1LZA	C21-N17	-3.50	1.30	1.37
2	E	301	A1LZA	O08-C07	-3.46	1.18	1.23
2	C	301	A1LZA	C21-N17	-3.44	1.30	1.37
2	J	301	A1LZA	C21-N17	-3.41	1.31	1.37
2	B	301	A1LZA	O08-C07	-3.39	1.18	1.23
2	D	301	A1LZA	O08-C07	-3.37	1.18	1.23
2	M	301	A1LZA	C07-N16	-3.36	1.32	1.38
2	M	301	A1LZA	C21-N17	-3.27	1.31	1.37
2	E	301	A1LZA	C21-N17	-3.25	1.31	1.37
2	A	301	A1LZA	C21-N17	-3.19	1.31	1.37
2	D	301	A1LZA	C21-N17	-3.18	1.31	1.37
2	K	301	A1LZA	C21-N17	-3.17	1.31	1.37
2	H	301	A1LZA	C07-N16	-3.16	1.32	1.38
2	H	301	A1LZA	O08-C07	-3.12	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	301	A1LZA	C07-N16	-3.11	1.32	1.38
2	F	301	A1LZA	C21-N17	-3.11	1.31	1.37
2	M	301	A1LZA	O08-C07	-3.10	1.18	1.23
2	L	301	A1LZA	C21-N17	-3.10	1.31	1.37
2	L	301	A1LZA	O08-C07	-3.10	1.18	1.23
2	H	301	A1LZA	C21-N17	-3.03	1.31	1.37
2	B	301	A1LZA	C07-N16	-3.03	1.32	1.38
2	M	301	A1LZA	C21-N16	2.98	1.35	1.31
2	D	301	A1LZA	C07-N16	-2.96	1.32	1.38
2	F	301	A1LZA	C22-C23	2.94	1.56	1.51
2	J	301	A1LZA	O08-C07	-2.92	1.19	1.23
2	I	301	A1LZA	O08-C07	-2.89	1.19	1.23
2	N	301	A1LZA	O08-C07	-2.89	1.19	1.23
2	C	301	A1LZA	C22-C23	2.85	1.56	1.51
2	J	301	A1LZA	C07-N16	-2.84	1.33	1.38
2	G	301	A1LZA	C15-C13	2.84	1.56	1.51
2	L	301	A1LZA	C07-N16	-2.83	1.33	1.38
2	A	301	A1LZA	C07-N16	-2.83	1.33	1.38
2	K	301	A1LZA	C07-N16	-2.79	1.33	1.38
2	I	301	A1LZA	C22-C23	2.74	1.56	1.51
2	L	301	A1LZA	C22-C23	2.72	1.56	1.51
2	L	301	A1LZA	C07-C05	-2.72	1.43	1.45
2	N	301	A1LZA	C07-N16	-2.72	1.33	1.38
2	B	301	A1LZA	C22-C23	2.71	1.56	1.51
2	C	301	A1LZA	C07-N16	-2.68	1.33	1.38
2	E	301	A1LZA	C07-N16	-2.63	1.33	1.38
2	C	301	A1LZA	O08-C07	-2.52	1.19	1.23
2	B	301	A1LZA	C07-C05	-2.50	1.43	1.45
2	A	301	A1LZA	C22-C23	2.42	1.55	1.51
2	G	301	A1LZA	C07-N16	-2.42	1.33	1.38
2	F	301	A1LZA	O08-C07	-2.41	1.20	1.23
2	N	301	A1LZA	C15-C13	2.41	1.55	1.51
2	M	301	A1LZA	C22-C23	2.36	1.55	1.51
2	F	301	A1LZA	C07-N16	-2.29	1.33	1.38
2	D	301	A1LZA	C22-C23	2.29	1.55	1.51
2	G	301	A1LZA	C22-C23	2.28	1.55	1.51
2	L	301	A1LZA	C15-C13	2.23	1.55	1.51
2	A	301	A1LZA	C15-C13	2.21	1.55	1.51
2	G	301	A1LZA	O08-C07	-2.18	1.20	1.23
2	M	301	A1LZA	C15-C13	2.14	1.55	1.51
2	H	301	A1LZA	C22-C23	2.14	1.55	1.51
2	J	301	A1LZA	C22-C23	2.08	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	A1LZA	C15-C13	2.08	1.55	1.51
2	A	301	A1LZA	C07-C05	-2.02	1.43	1.45

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	A1LZA	C03-C02-N01	11.28	121.48	111.23
2	N	301	A1LZA	C03-C02-N01	10.97	121.19	111.23
2	E	301	A1LZA	C03-C02-N01	10.88	121.12	111.23
2	J	301	A1LZA	C03-C02-N01	10.83	121.07	111.23
2	K	301	A1LZA	C03-C02-N01	10.71	120.96	111.23
2	G	301	A1LZA	C03-C02-N01	10.60	120.86	111.23
2	L	301	A1LZA	C03-C02-N01	10.46	120.73	111.23
2	F	301	A1LZA	C03-C02-N01	10.45	120.72	111.23
2	H	301	A1LZA	C03-C02-N01	10.45	120.72	111.23
2	C	301	A1LZA	C03-C02-N01	10.33	120.61	111.23
2	M	301	A1LZA	C06-N01-C02	10.31	123.30	109.95
2	B	301	A1LZA	C06-N01-C02	10.26	123.24	109.95
2	I	301	A1LZA	C03-C02-N01	10.25	120.54	111.23
2	B	301	A1LZA	C03-C02-N01	10.13	120.43	111.23
2	C	301	A1LZA	C06-N01-C02	10.12	123.06	109.95
2	M	301	A1LZA	C03-C02-N01	10.05	120.36	111.23
2	D	301	A1LZA	C06-N01-C02	10.01	122.92	109.95
2	F	301	A1LZA	C06-N01-C02	10.00	122.90	109.95
2	D	301	A1LZA	C03-C02-N01	9.84	120.17	111.23
2	H	301	A1LZA	C06-N01-C02	9.71	122.53	109.95
2	I	301	A1LZA	C06-N01-C02	9.70	122.51	109.95
2	G	301	A1LZA	C06-N01-C02	9.68	122.49	109.95
2	L	301	A1LZA	C06-N01-C02	9.53	122.29	109.95
2	K	301	A1LZA	C06-N01-C02	9.52	122.29	109.95
2	E	301	A1LZA	C06-N01-C02	9.52	122.28	109.95
2	J	301	A1LZA	C06-N01-C02	9.38	122.11	109.95
2	A	301	A1LZA	C06-N01-C02	9.36	122.07	109.95
2	N	301	A1LZA	C06-N01-C02	8.96	121.55	109.95
2	H	301	A1LZA	C03-C04-N17	8.30	123.43	117.25
2	L	301	A1LZA	C03-C04-N17	8.03	123.22	117.25
2	B	301	A1LZA	C03-C04-N17	7.50	122.83	117.25
2	K	301	A1LZA	C03-C04-N17	7.44	122.79	117.25
2	M	301	A1LZA	C03-C04-N17	7.38	122.74	117.25
2	N	301	A1LZA	C15-N01-C06	7.29	120.12	110.53
2	A	301	A1LZA	C03-C04-N17	7.22	122.62	117.25
2	I	301	A1LZA	C03-C04-N17	7.00	122.46	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	A1LZA	C15-N01-C06	6.93	119.64	110.53
2	K	301	A1LZA	C15-N01-C06	6.66	119.29	110.53
2	C	301	A1LZA	C15-N01-C06	6.63	119.26	110.53
2	J	301	A1LZA	C15-N01-C06	6.38	118.92	110.53
2	I	301	A1LZA	C15-N01-C06	6.31	118.83	110.53
2	D	301	A1LZA	C03-C04-N17	6.25	121.90	117.25
2	E	301	A1LZA	C03-C04-N17	6.23	121.89	117.25
2	A	301	A1LZA	C15-N01-C06	6.04	118.47	110.53
2	N	301	A1LZA	C03-C04-N17	5.98	121.70	117.25
2	G	301	A1LZA	C15-N01-C06	5.84	118.22	110.53
2	J	301	A1LZA	C03-C04-N17	5.80	121.57	117.25
2	N	301	A1LZA	C02-C03-C04	5.73	119.27	108.47
2	D	301	A1LZA	C15-N01-C06	5.72	118.06	110.53
2	I	301	A1LZA	C02-C03-C04	5.63	119.10	108.47
2	F	301	A1LZA	C15-N01-C06	5.62	117.92	110.53
2	K	301	A1LZA	C02-C03-C04	5.59	119.02	108.47
2	M	301	A1LZA	C15-N01-C06	5.52	117.79	110.53
2	C	301	A1LZA	C02-C03-C04	5.46	118.76	108.47
2	E	301	A1LZA	C02-C03-C04	5.41	118.68	108.47
2	L	301	A1LZA	C02-C03-C04	5.40	118.66	108.47
2	D	301	A1LZA	C02-C03-C04	5.39	118.64	108.47
2	J	301	A1LZA	C02-C03-C04	5.35	118.56	108.47
2	M	301	A1LZA	C02-C03-C04	5.26	118.40	108.47
2	H	301	A1LZA	C02-C03-C04	5.26	118.39	108.47
2	L	301	A1LZA	C15-N01-C06	5.26	117.45	110.53
2	F	301	A1LZA	C03-C04-N17	5.23	121.14	117.25
2	G	301	A1LZA	C02-C03-C04	5.10	118.10	108.47
2	K	301	A1LZA	C19-C18-N17	5.10	107.73	102.95
2	F	301	A1LZA	C02-C03-C04	5.09	118.07	108.47
2	C	301	A1LZA	C03-C04-N17	5.08	121.03	117.25
2	A	301	A1LZA	C02-C03-C04	5.06	118.01	108.47
2	B	301	A1LZA	C02-C03-C04	5.05	118.00	108.47
2	B	301	A1LZA	C15-N01-C06	5.03	117.15	110.53
2	G	301	A1LZA	C03-C04-N17	4.91	120.90	117.25
2	H	301	A1LZA	C15-N01-C06	4.72	116.74	110.53
2	N	301	A1LZA	C19-C18-N17	4.71	107.37	102.95
2	B	301	A1LZA	C19-C18-N17	4.62	107.29	102.95
2	J	301	A1LZA	C19-C18-N17	4.54	107.21	102.95
2	L	301	A1LZA	C19-C18-N17	4.38	107.06	102.95
2	H	301	A1LZA	C19-C18-N17	4.37	107.06	102.95
2	I	301	A1LZA	C19-C18-N17	4.34	107.02	102.95
2	H	301	A1LZA	C15-N01-C02	4.32	120.67	111.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	A1LZA	C19-C18-N17	4.25	106.94	102.95
2	E	301	A1LZA	C19-C18-N17	4.22	106.91	102.95
2	M	301	A1LZA	C19-C18-N17	4.19	106.88	102.95
2	G	301	A1LZA	C19-C18-N17	4.18	106.88	102.95
2	A	301	A1LZA	C19-C18-N17	4.14	106.83	102.95
2	L	301	A1LZA	C15-N01-C02	4.13	120.25	111.06
2	F	301	A1LZA	C19-C18-N17	4.12	106.82	102.95
2	D	301	A1LZA	C19-C18-N17	3.90	106.61	102.95
2	B	301	A1LZA	C15-N01-C02	3.77	119.45	111.06
2	A	301	A1LZA	C15-N01-C02	3.71	119.32	111.06
2	G	301	A1LZA	C15-N01-C02	3.66	119.20	111.06
2	F	301	A1LZA	C15-N01-C02	3.63	119.14	111.06
2	F	301	A1LZA	C22-C23-C28	3.60	127.00	120.51
2	D	301	A1LZA	C15-N01-C02	3.57	119.01	111.06
2	J	301	A1LZA	C15-N01-C02	3.55	118.97	111.06
2	M	301	A1LZA	C15-N01-C02	3.50	118.86	111.06
2	I	301	A1LZA	C15-N01-C02	3.36	118.55	111.06
2	G	301	A1LZA	C22-C23-C28	3.32	126.50	120.51
2	K	301	A1LZA	C15-N01-C02	3.30	118.41	111.06
2	N	301	A1LZA	C15-N01-C02	3.23	118.26	111.06
2	E	301	A1LZA	C15-N01-C02	3.14	118.05	111.06
2	C	301	A1LZA	C22-C23-C28	3.12	126.13	120.51
2	G	301	A1LZA	N20-C21-N16	3.07	129.32	125.60
2	E	301	A1LZA	C22-C23-C28	3.02	125.95	120.51
2	G	301	A1LZA	N17-C21-N16	-2.98	121.60	124.41
2	M	301	A1LZA	C22-N20-C19	2.92	128.68	121.02
2	C	301	A1LZA	C15-N01-C02	2.91	117.54	111.06
2	G	301	A1LZA	C22-C23-C24	-2.84	114.50	120.11
2	B	301	A1LZA	C22-N20-C19	2.74	128.21	121.02
2	A	301	A1LZA	C22-N20-C19	2.69	128.08	121.02
2	J	301	A1LZA	C22-N20-C19	2.66	127.99	121.02
2	F	301	A1LZA	C29-C28-C27	-2.60	115.24	120.31
2	H	301	A1LZA	C22-N20-C19	2.54	127.67	121.02
2	I	301	A1LZA	C22-N20-C19	2.54	127.67	121.02
2	M	301	A1LZA	C21-N17-C04	-2.50	118.98	123.30
2	I	301	A1LZA	C22-C23-C28	2.48	124.97	120.51
2	L	301	A1LZA	C22-N20-C19	2.47	127.49	121.02
2	F	301	A1LZA	C22-C23-C24	-2.47	115.25	120.11
2	E	301	A1LZA	C22-C23-C24	-2.42	115.34	120.11
2	A	301	A1LZA	C22-C23-C28	2.38	124.80	120.51
2	N	301	A1LZA	C22-C23-C28	2.37	124.77	120.51
2	D	301	A1LZA	C22-N20-C19	2.36	127.20	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	A1LZA	C21-N17-C04	-2.34	119.27	123.30
2	N	301	A1LZA	C22-N20-C19	2.34	127.15	121.02
2	F	301	A1LZA	N20-C21-N16	2.33	128.43	125.60
2	G	301	A1LZA	C29-C28-C27	-2.33	115.77	120.31
2	N	301	A1LZA	C13-C15-N01	-2.32	108.61	113.12
2	K	301	A1LZA	C22-N20-C19	2.32	127.10	121.02
2	H	301	A1LZA	C21-N17-C04	-2.32	119.31	123.30
2	L	301	A1LZA	C21-N17-C04	-2.29	119.35	123.30
2	J	301	A1LZA	C21-N17-C04	-2.29	119.36	123.30
2	M	301	A1LZA	C22-C23-C28	2.28	124.62	120.51
2	I	301	A1LZA	C29-C28-C27	-2.27	115.89	120.31
2	E	301	A1LZA	C29-C28-C27	-2.26	115.89	120.31
2	K	301	A1LZA	C22-C23-C28	2.26	124.59	120.51
2	C	301	A1LZA	N17-C21-N16	-2.24	122.30	124.41
2	D	301	A1LZA	C18-C19-N20	2.21	107.26	103.06
2	L	301	A1LZA	C22-C23-C28	2.21	124.50	120.51
2	I	301	A1LZA	C21-N17-C04	-2.20	119.50	123.30
2	C	301	A1LZA	C22-N20-C19	2.20	126.78	121.02
2	E	301	A1LZA	N17-C21-N16	-2.20	122.34	124.41
2	F	301	A1LZA	C21-N17-C04	-2.19	119.52	123.30
2	A	301	A1LZA	C21-N17-C04	-2.19	119.53	123.30
2	L	301	A1LZA	C27-C28-C23	2.18	121.23	118.55
2	C	301	A1LZA	C21-N17-C04	-2.18	119.54	123.30
2	D	301	A1LZA	C22-C23-C28	2.18	124.43	120.51
2	C	301	A1LZA	C18-C19-N20	2.17	107.19	103.06
2	N	301	A1LZA	C21-N17-C04	-2.15	119.59	123.30
2	E	301	A1LZA	C07-C05-C04	-2.15	117.24	119.71
2	A	301	A1LZA	C29-C28-C27	-2.15	116.11	120.31
2	I	301	A1LZA	N17-C21-N16	-2.13	122.40	124.41
2	B	301	A1LZA	C22-C23-C28	2.13	124.36	120.51
2	K	301	A1LZA	C18-N17-C21	-2.12	106.90	110.94
2	N	301	A1LZA	C07-C05-C04	-2.08	117.33	119.71
2	M	301	A1LZA	C29-C28-C27	-2.08	116.25	120.31
2	N	301	A1LZA	N17-C21-N16	-2.07	122.46	124.41
2	K	301	A1LZA	C21-N17-C04	-2.07	119.74	123.30
2	J	301	A1LZA	C22-C23-C28	2.06	124.22	120.51
2	A	301	A1LZA	C27-C28-C23	2.05	121.06	118.55
2	D	301	A1LZA	C21-N17-C04	-2.03	119.80	123.30
2	C	301	A1LZA	C29-C28-C27	-2.02	116.38	120.31
2	H	301	A1LZA	C05-C04-N17	-2.02	118.43	120.63
2	L	301	A1LZA	C29-C28-C27	-2.01	116.38	120.31
2	C	301	A1LZA	C27-C28-C23	2.00	121.01	118.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	301	A1LZA	C18-C19-N20	2.00	106.87	103.06
2	I	301	A1LZA	C27-C28-C23	2.00	121.00	118.55

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	A1LZA	C13-C15-N01-C02
2	H	301	A1LZA	C13-C15-N01-C02
2	M	301	A1LZA	C13-C15-N01-C02
2	D	301	A1LZA	C13-C15-N01-C02
2	F	301	A1LZA	C13-C15-N01-C02
2	G	301	A1LZA	C13-C15-N01-C02
2	I	301	A1LZA	C13-C15-N01-C02
2	J	301	A1LZA	C13-C15-N01-C02
2	K	301	A1LZA	C13-C15-N01-C02
2	L	301	A1LZA	C13-C15-N01-C02
2	N	301	A1LZA	C13-C15-N01-C02
2	G	301	A1LZA	N20-C22-C23-C28
2	B	301	A1LZA	C13-C15-N01-C02
2	C	301	A1LZA	C13-C15-N01-C02
2	E	301	A1LZA	C13-C15-N01-C02
2	F	301	A1LZA	N20-C22-C23-C28
2	N	301	A1LZA	N20-C22-C23-C28
2	C	301	A1LZA	N20-C22-C23-C28
2	K	301	A1LZA	N20-C22-C23-C28
2	E	301	A1LZA	N20-C22-C23-C28
2	J	301	A1LZA	N20-C22-C23-C28
2	M	301	A1LZA	N20-C22-C23-C28
2	B	301	A1LZA	N20-C22-C23-C28
2	D	301	A1LZA	N20-C22-C23-C28
2	L	301	A1LZA	N20-C22-C23-C28
2	A	301	A1LZA	N20-C22-C23-C28
2	C	301	A1LZA	C13-C15-N01-C06
2	I	301	A1LZA	N20-C22-C23-C28

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	A1LZA	1	0

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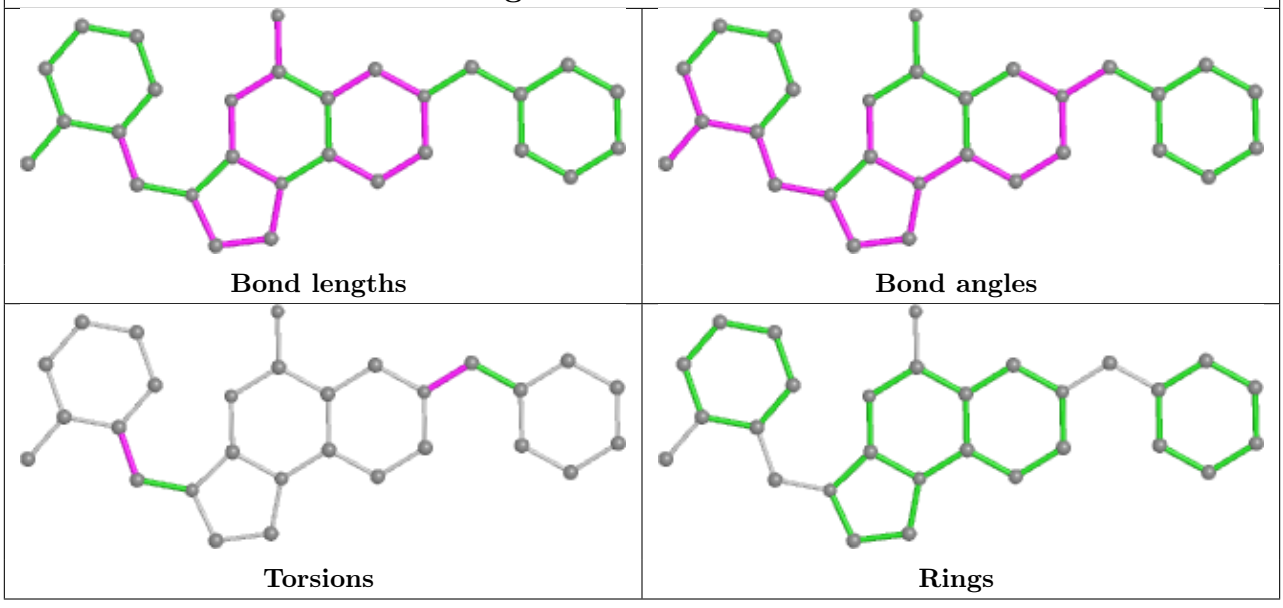
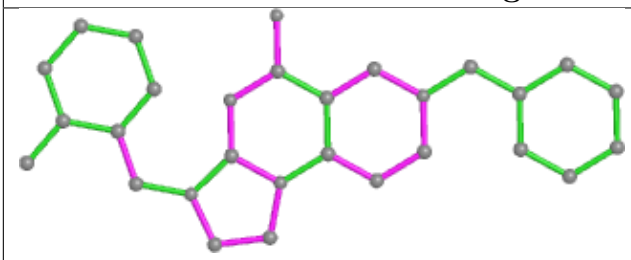
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	A1LZA	1	0
2	G	301	A1LZA	1	0
2	H	301	A1LZA	1	0
2	I	301	A1LZA	1	0
2	B	301	A1LZA	2	0
2	A	301	A1LZA	1	0
2	E	301	A1LZA	1	0
2	L	301	A1LZA	1	0

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 then 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.

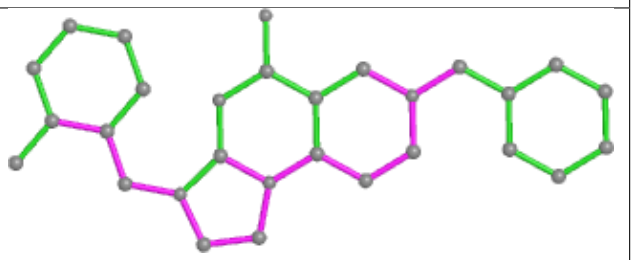
Ligand A1LZA C 301



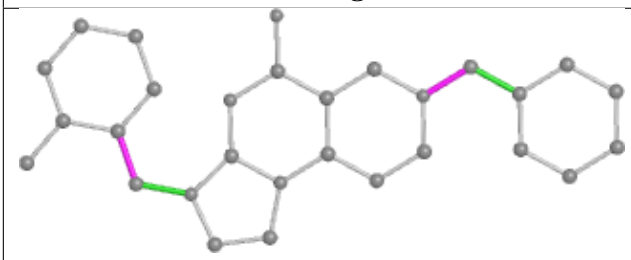
Ligand A1LZA D 301



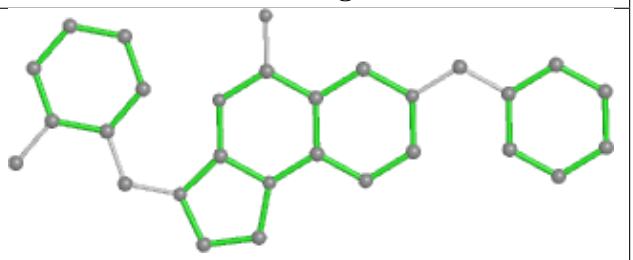
Bond lengths



Bond angles

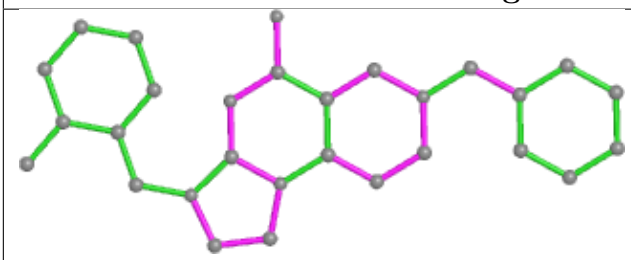


Torsions

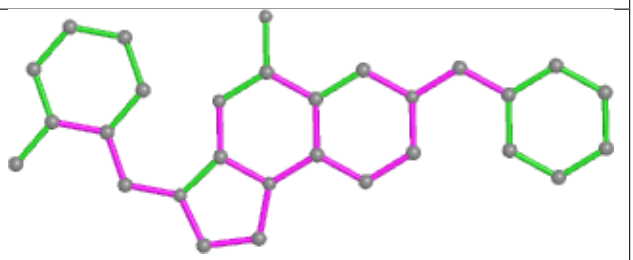


Rings

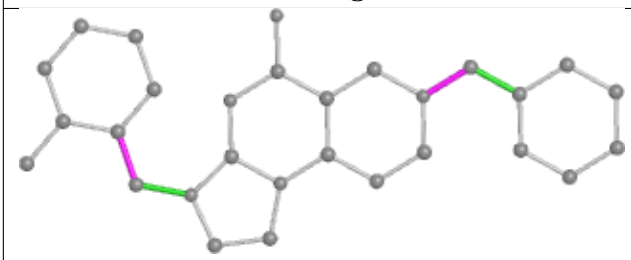
Ligand A1LZA N 301



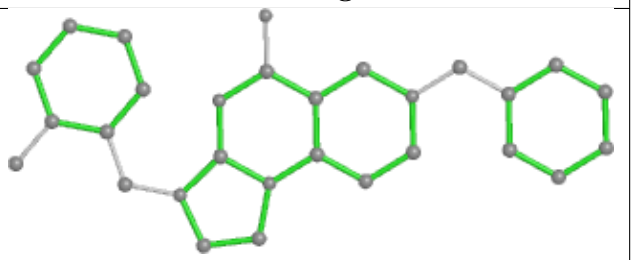
Bond lengths



Bond angles

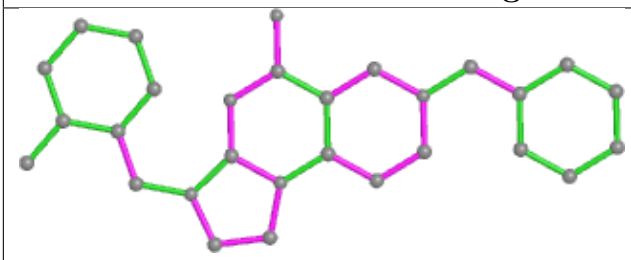


Torsions

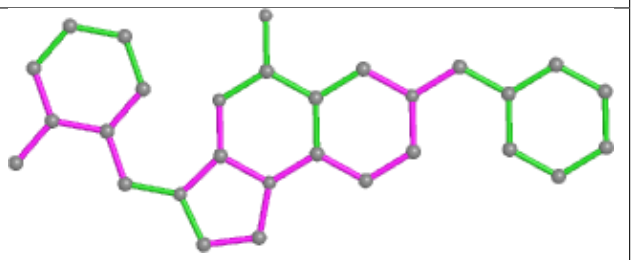


Rings

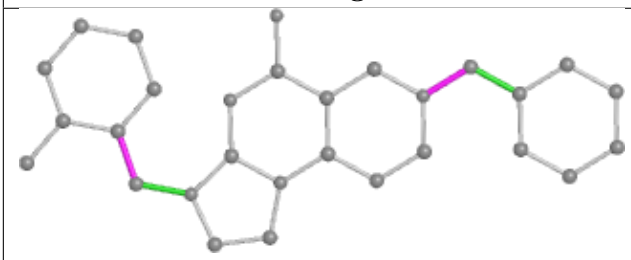
Ligand A1LZA G 301



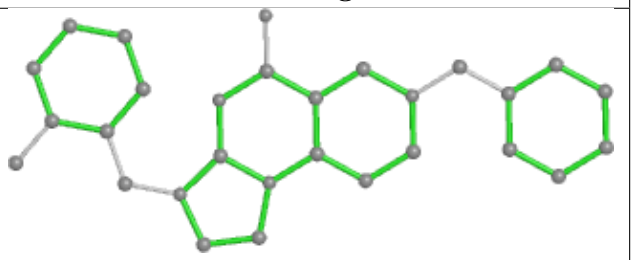
Bond lengths



Bond angles

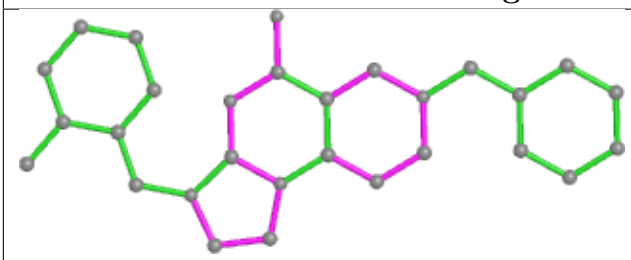


Torsions

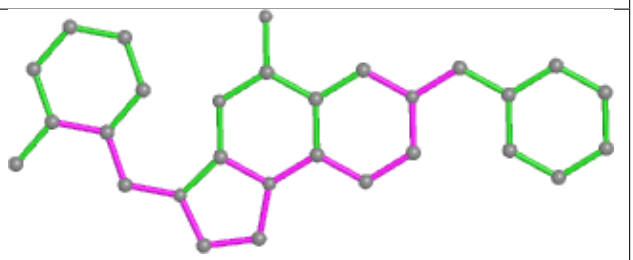


Rings

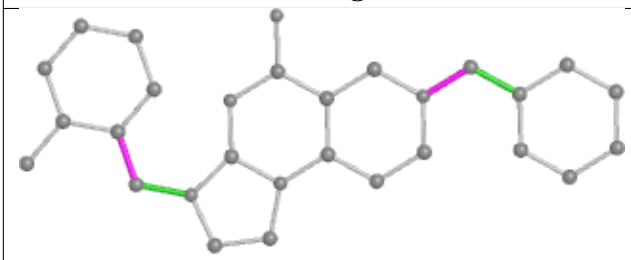
Ligand A1LZA K 301



Bond lengths



Bond angles



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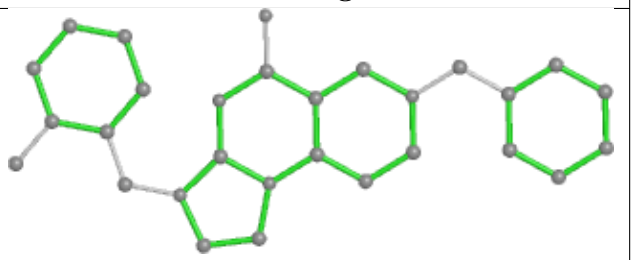
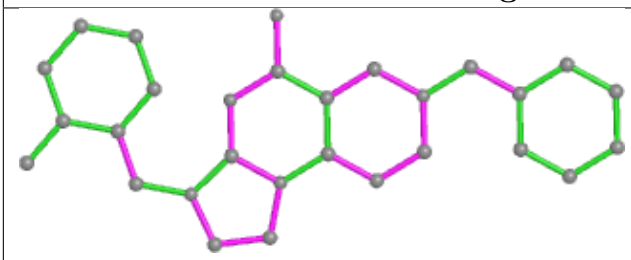


Rings

Ligand A1LZA M 301



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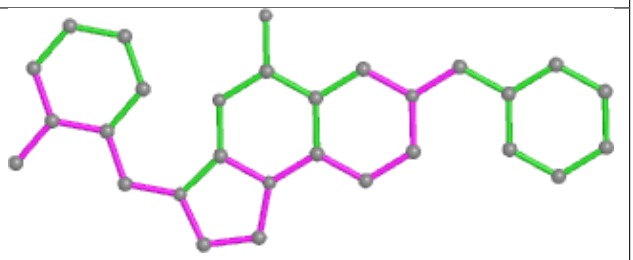
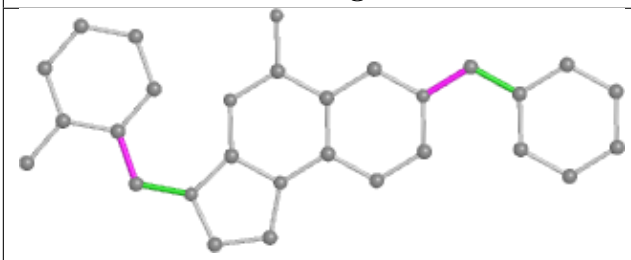


Bond angles



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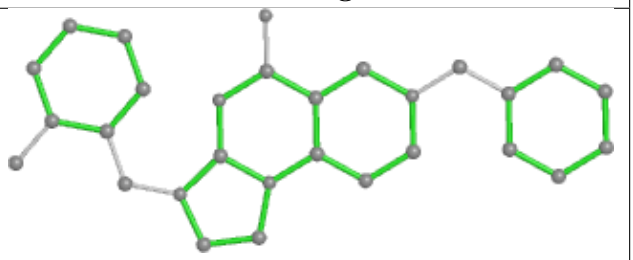
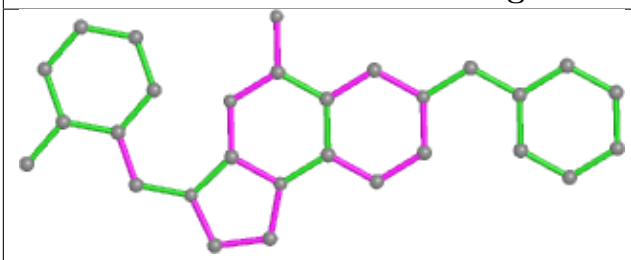


Rings

Ligand A1LZA J 301



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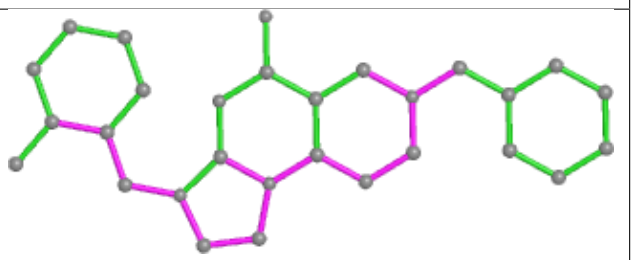
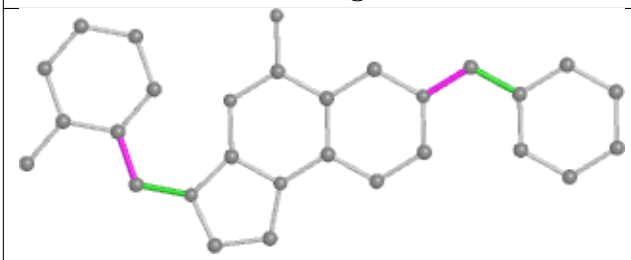


Bond angles



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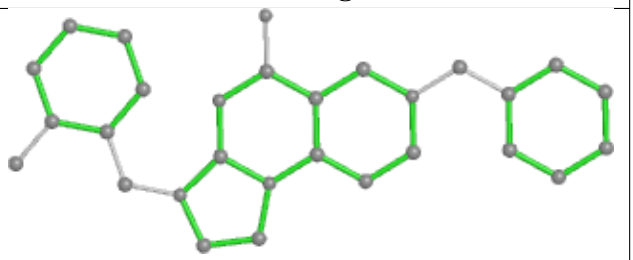
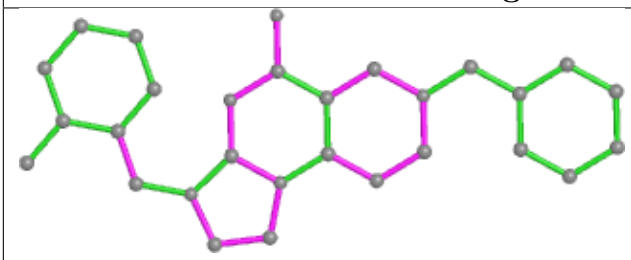
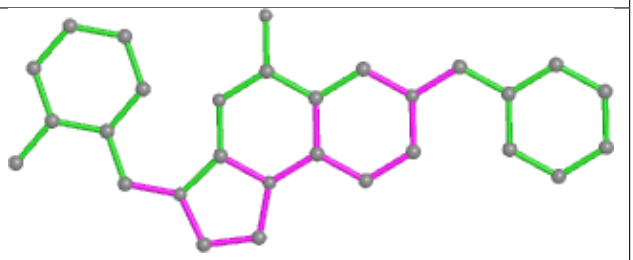


Rings

Ligand A1LZA H 301



Bond lengths



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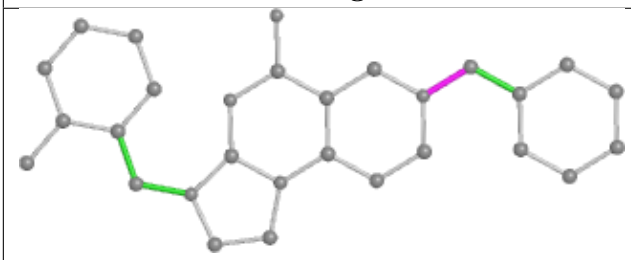

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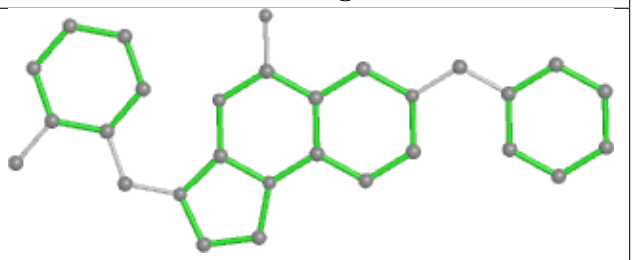
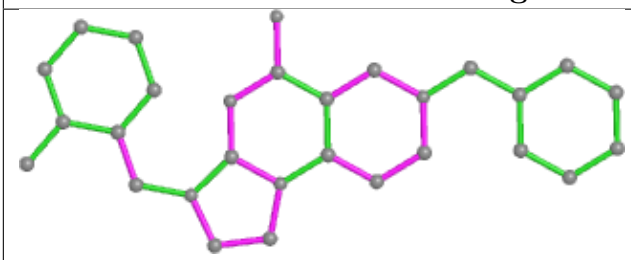


Rings

Ligand A1LZA I 301



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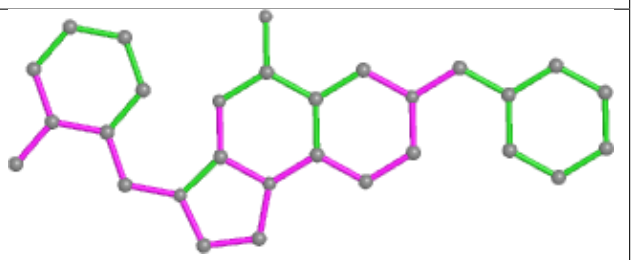
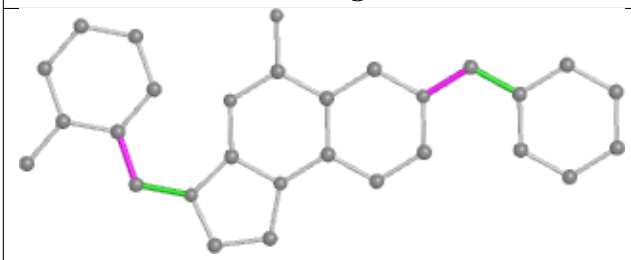
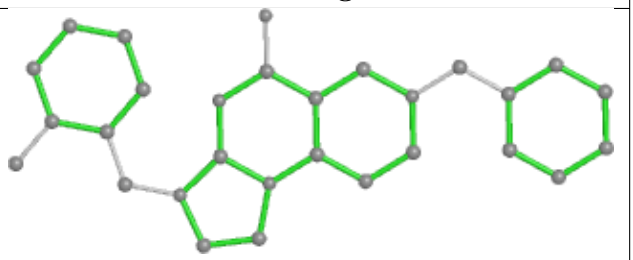


Bond angles

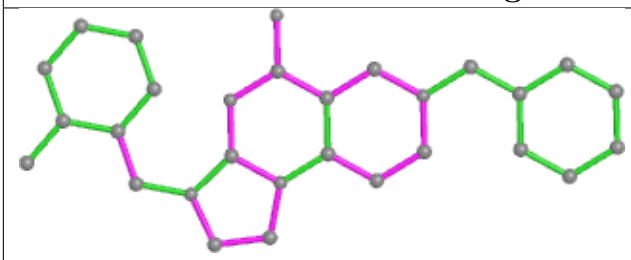


Torsions

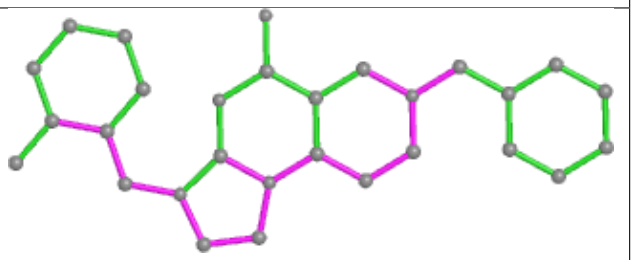


Rings

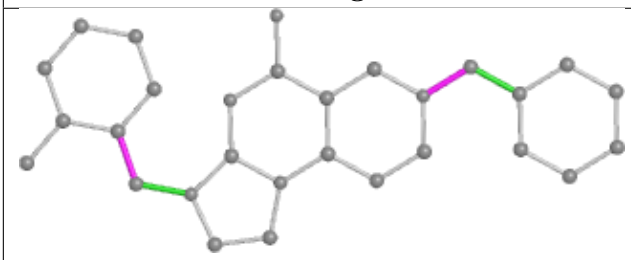
Ligand A1LZA B 301



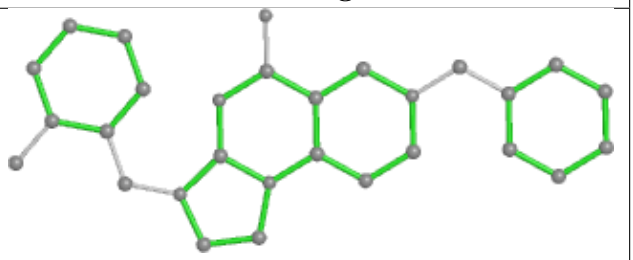
Bond lengths



Bond angles

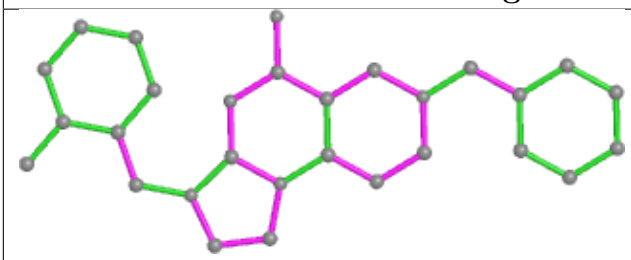


Torsions

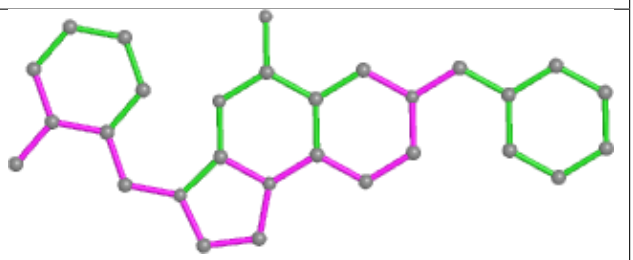


Rings

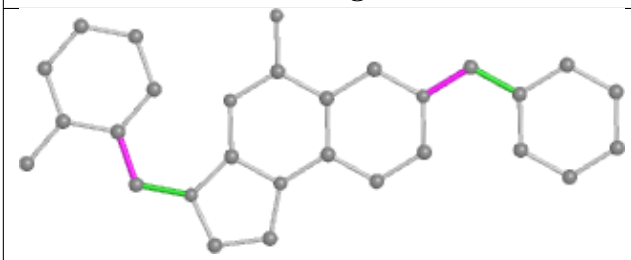
Ligand A1LZA A 301



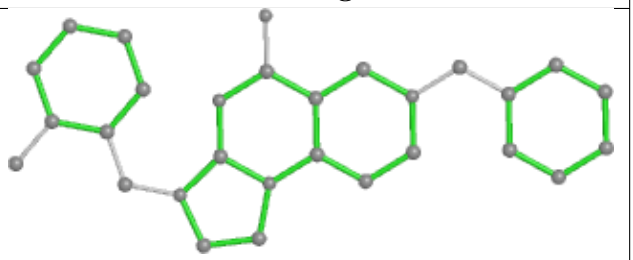
Bond lengths



Bond angles

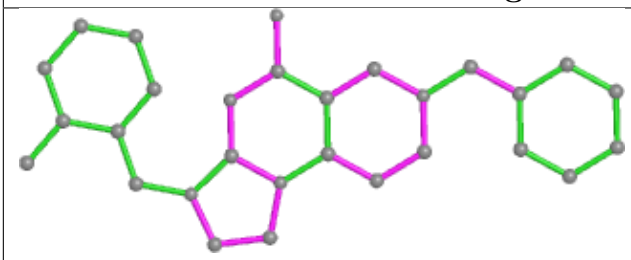


Torsions

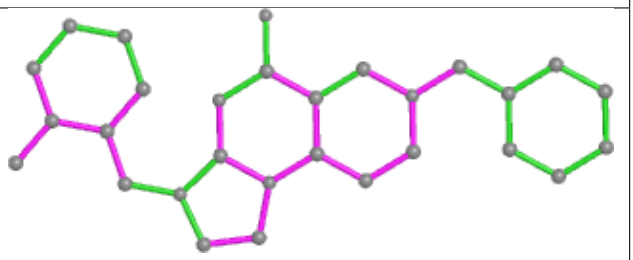


Rings

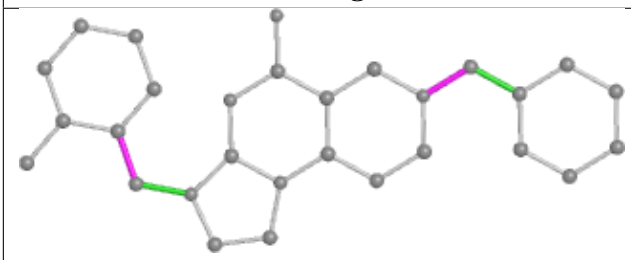
Ligand A1LZA E 301



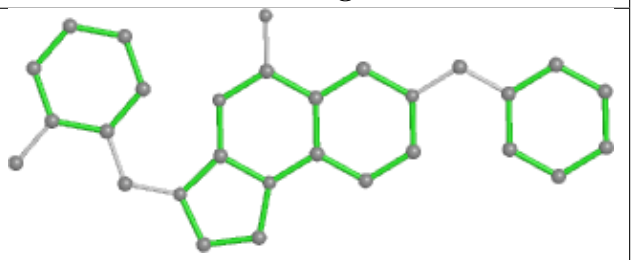
Bond lengths



Bond angles

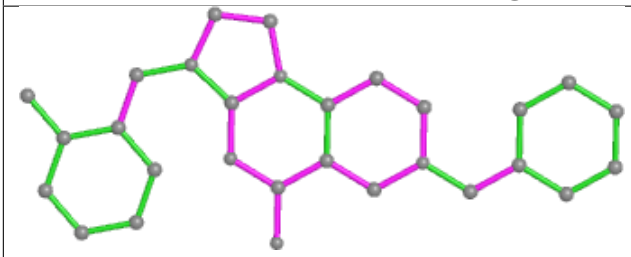


Torsions

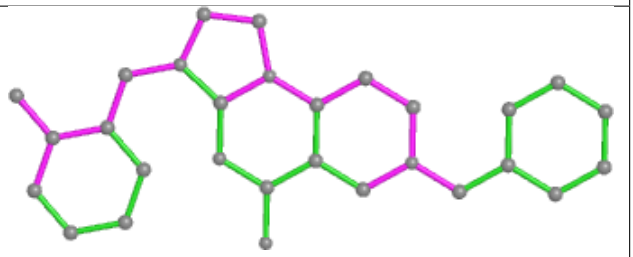


Rings

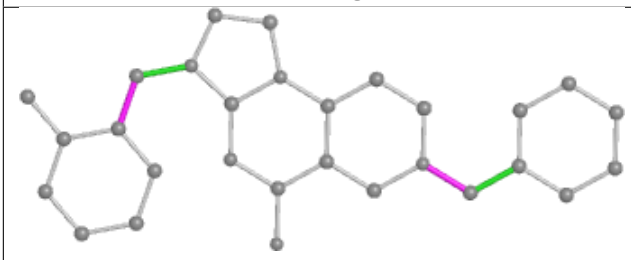
Ligand A1LZA L 301



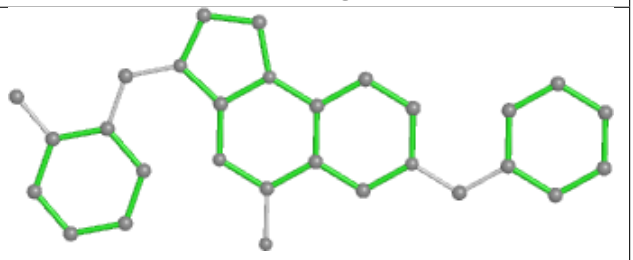
Bond lengths



Bond angles

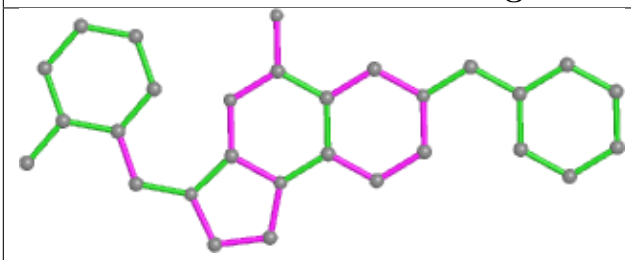


Torsions

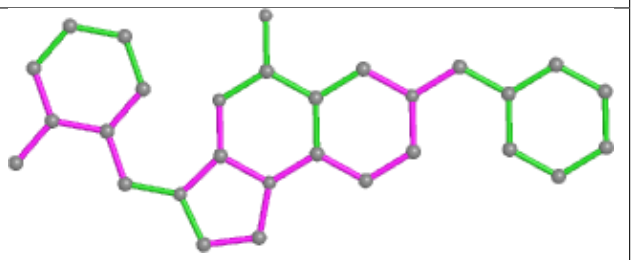


Rings

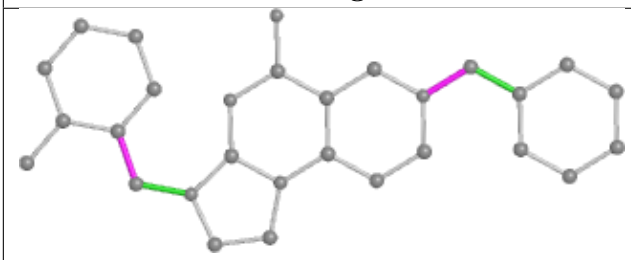
Ligand A1LZA F 301



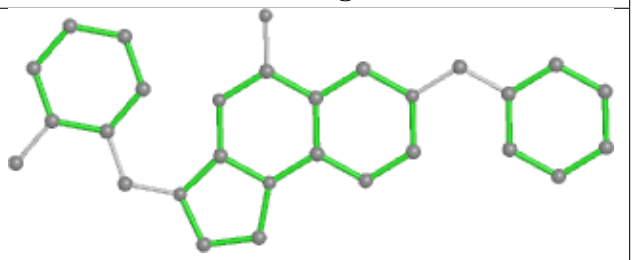
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	176/220 (80%)	0.26	10 (5%)	23	32	22, 33, 56, 75	0
1	B	173/220 (78%)	0.25	11 (6%)	19	26	27, 35, 55, 72	0
1	C	171/220 (77%)	0.32	8 (4%)	31	41	29, 38, 55, 69	0
1	D	171/220 (77%)	0.32	11 (6%)	19	26	27, 37, 54, 76	0
1	E	171/220 (77%)	0.17	5 (2%)	51	61	24, 33, 53, 69	0
1	F	166/220 (75%)	0.08	5 (3%)	50	59	23, 31, 46, 60	0
1	G	170/220 (77%)	0.17	7 (4%)	37	46	24, 34, 49, 64	0
1	H	166/220 (75%)	0.58	15 (9%)	9	14	33, 42, 55, 77	0
1	I	172/220 (78%)	0.36	9 (5%)	27	35	30, 39, 55, 70	0
1	J	169/220 (76%)	0.35	13 (7%)	13	18	29, 38, 55, 74	0
1	K	171/220 (77%)	0.19	6 (3%)	44	52	26, 35, 53, 75	0
1	L	170/220 (77%)	0.22	6 (3%)	44	52	21, 32, 48, 66	0
1	M	171/220 (77%)	0.19	10 (5%)	23	31	20, 31, 47, 72	0
1	N	172/220 (78%)	0.36	11 (6%)	19	26	26, 39, 54, 72	0
All	All	2389/3080 (77%)	0.27	127 (5%)	26	35	20, 36, 54, 77	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	58	LEU	8.8
1	M	63	VAL	5.6
1	N	63	VAL	5.2
1	H	181	SER	5.1
1	I	58	LEU	4.8
1	B	181	SER	4.8
1	D	192	ALA	4.8
1	D	58	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	N	218	GLN	4.6
1	M	249	PRO	4.5
1	N	73	TYR	4.5
1	C	73	TYR	4.4
1	L	73	TYR	4.3
1	D	247	HIS	4.3
1	I	192	ALA	4.3
1	A	71	ARG	4.1
1	E	73	TYR	4.1
1	J	63	VAL	4.0
1	N	72	ALA	4.0
1	B	63	VAL	4.0
1	K	247	HIS	4.0
1	B	72	ALA	4.0
1	C	63	VAL	4.0
1	A	247	HIS	3.9
1	J	58	LEU	3.9
1	D	63	VAL	3.9
1	E	192	ALA	3.8
1	M	59	ILE	3.8
1	L	247	HIS	3.7
1	H	233[A]	MET	3.6
1	B	73	TYR	3.5
1	J	73	TYR	3.5
1	A	66	THR	3.4
1	G	247	HIS	3.4
1	F	63	VAL	3.4
1	G	218	GLN	3.4
1	B	58	LEU	3.3
1	K	64	GLU	3.3
1	L	63	VAL	3.3
1	D	72	ALA	3.3
1	L	248	PRO	3.3
1	D	73	TYR	3.2
1	H	237	GLU	3.2
1	A	181	SER	3.2
1	N	192	ALA	3.2
1	C	58	LEU	3.2
1	N	112	LYS	3.1
1	I	63	VAL	3.1
1	H	245	LEU	3.0
1	I	247	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	72	ALA	3.0
1	E	247	HIS	3.0
1	J	240	ILE	2.9
1	D	246	VAL	2.9
1	K	246	VAL	2.9
1	F	73	TYR	2.9
1	F	175	ILE	2.9
1	L	72	ALA	2.9
1	J	233	MET	2.8
1	I	175	ILE	2.8
1	C	247	HIS	2.7
1	J	193	ILE	2.7
1	A	65	GLN	2.7
1	J	218[A]	GLN	2.7
1	G	58	LEU	2.7
1	K	72	ALA	2.7
1	C	248	PRO	2.7
1	H	218	GLN	2.7
1	G	73	TYR	2.6
1	H	217	LEU	2.6
1	E	58	LEU	2.6
1	J	175	ILE	2.6
1	B	248	PRO	2.6
1	M	248	PRO	2.6
1	I	112	LYS	2.6
1	C	140	LEU	2.6
1	N	140	LEU	2.6
1	J	159	LEU	2.5
1	I	72	ALA	2.5
1	H	112	LYS	2.5
1	B	247	HIS	2.5
1	N	175	ILE	2.5
1	A	58	LEU	2.4
1	H	159	LEU	2.4
1	A	63	VAL	2.4
1	B	246	VAL	2.4
1	M	73	TYR	2.4
1	B	192	ALA	2.4
1	D	245	LEU	2.4
1	J	246	VAL	2.3
1	D	218	GLN	2.3
1	C	233	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	193	ILE	2.3
1	G	106	LEU	2.3
1	G	112	LYS	2.3
1	E	246	VAL	2.3
1	N	247	HIS	2.3
1	D	177	ILE	2.3
1	H	106	LEU	2.2
1	M	72	ALA	2.2
1	B	103	LEU	2.2
1	K	159	LEU	2.2
1	M	246	VAL	2.2
1	L	246	VAL	2.2
1	H	243	LYS	2.2
1	A	103	LEU	2.2
1	I	193	ILE	2.1
1	N	193	ILE	2.1
1	I	159	LEU	2.1
1	M	147	CYS	2.1
1	N	246	VAL	2.1
1	J	115	ILE	2.1
1	J	62	VAL	2.1
1	A	159	LEU	2.1
1	J	113	LYS	2.1
1	M	247	HIS	2.1
1	D	115	ILE	2.1
1	H	193	ILE	2.1
1	H	140	LEU	2.1
1	F	112	LYS	2.1
1	B	177	ILE	2.0
1	H	89	GLY	2.0
1	K	65	GLN	2.0
1	A	72	ALA	2.0
1	H	151	ALA	2.0
1	M	193	ILE	2.0
1	C	85	VAL	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)

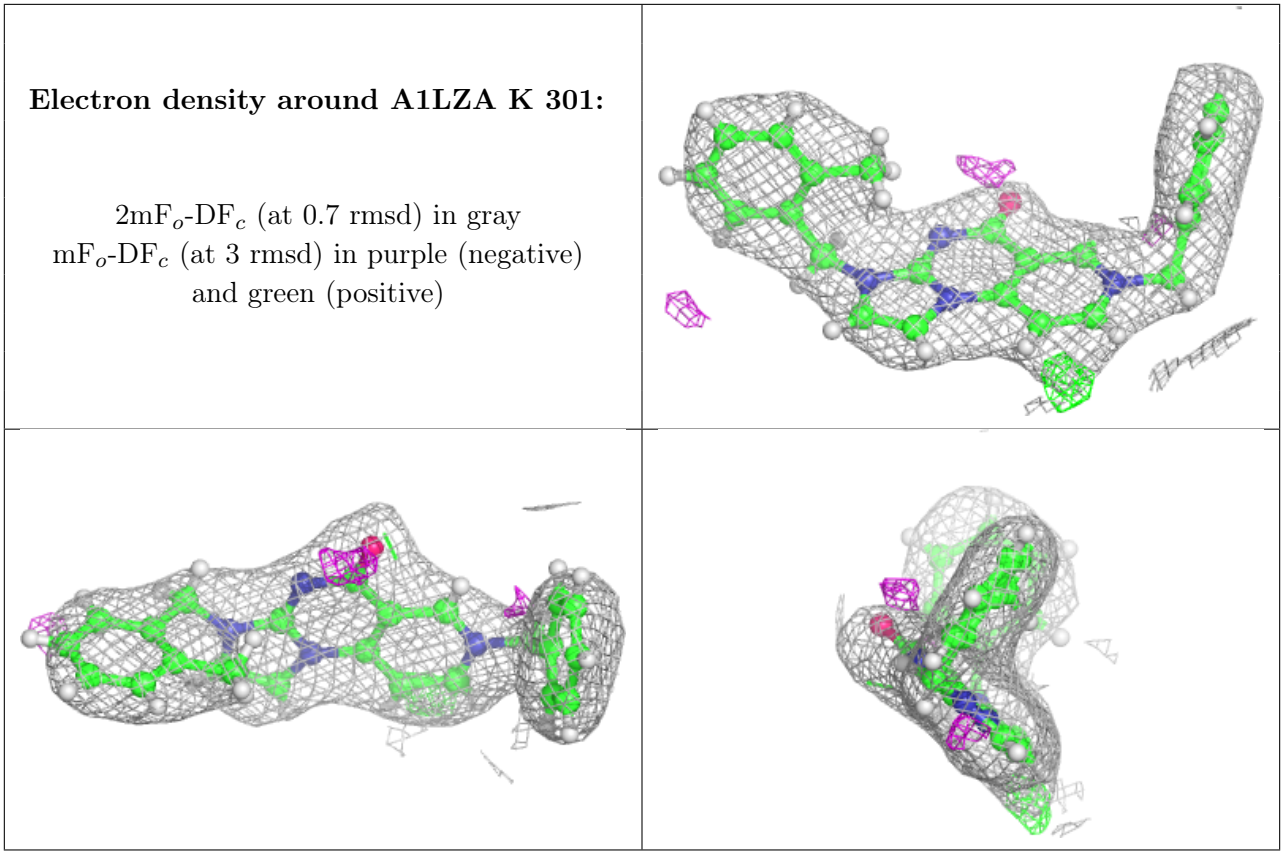
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	A1LZA	K	301	29/29	0.85	0.15	33,42,50,54	0
2	A1LZA	E	301	29/29	0.87	0.16	33,42,52,58	0
2	A1LZA	G	301	29/29	0.88	0.14	31,39,49,52	0
2	A1LZA	C	301	29/29	0.88	0.15	34,45,57,58	0
2	A1LZA	H	301	29/29	0.89	0.16	36,46,58,62	0
2	A1LZA	D	301	29/29	0.90	0.15	32,45,54,59	0
2	A1LZA	M	301	29/29	0.90	0.14	26,41,56,57	0
2	A1LZA	B	301	29/29	0.91	0.14	28,40,51,57	0
2	A1LZA	J	301	29/29	0.91	0.14	38,50,63,67	0
2	A1LZA	I	301	29/29	0.92	0.14	38,47,60,62	0
2	A1LZA	L	301	29/29	0.92	0.12	29,39,52,53	0
2	A1LZA	A	301	29/29	0.92	0.13	31,39,54,57	0
2	A1LZA	F	301	29/29	0.93	0.11	30,40,52,54	0
2	A1LZA	N	301	29/29	0.94	0.11	34,43,53,58	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.

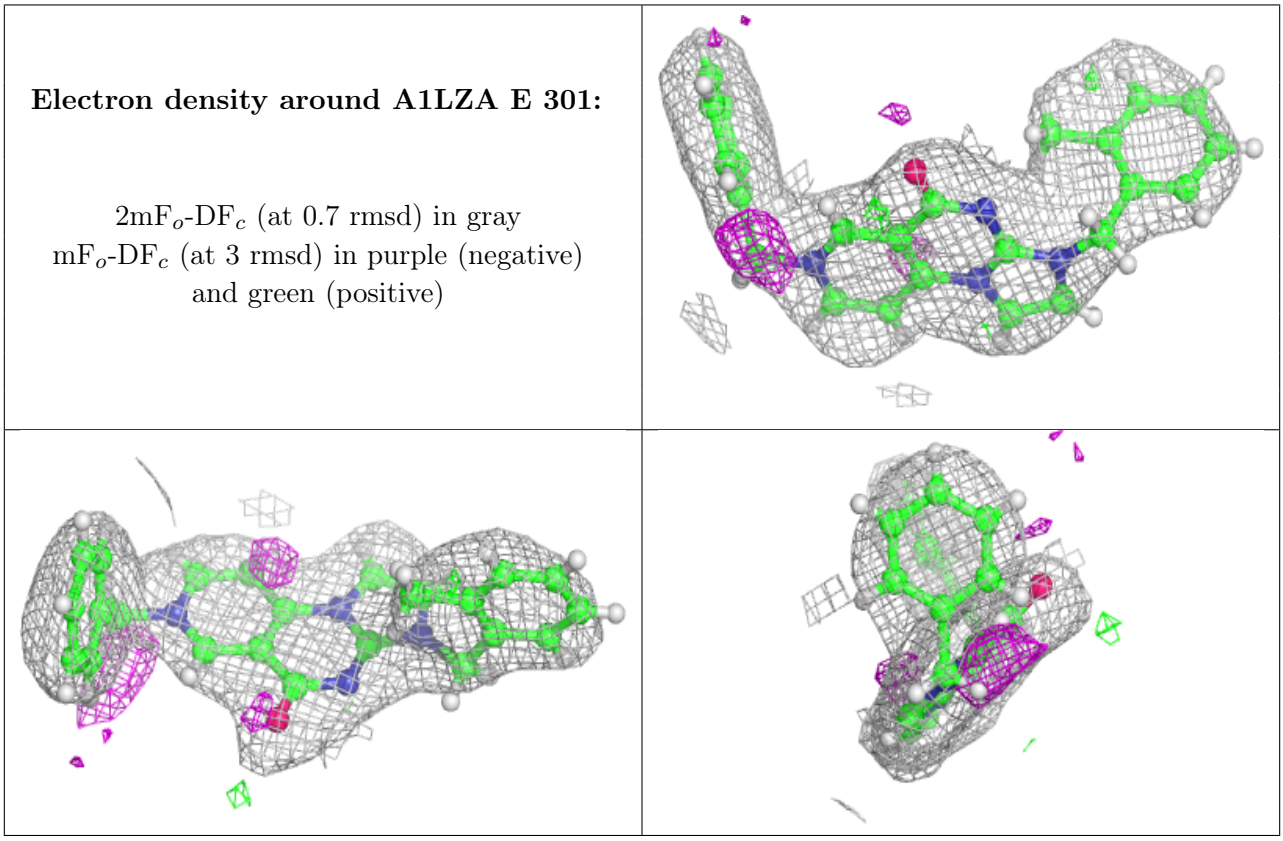
Electron density around A1LZA K 301:

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



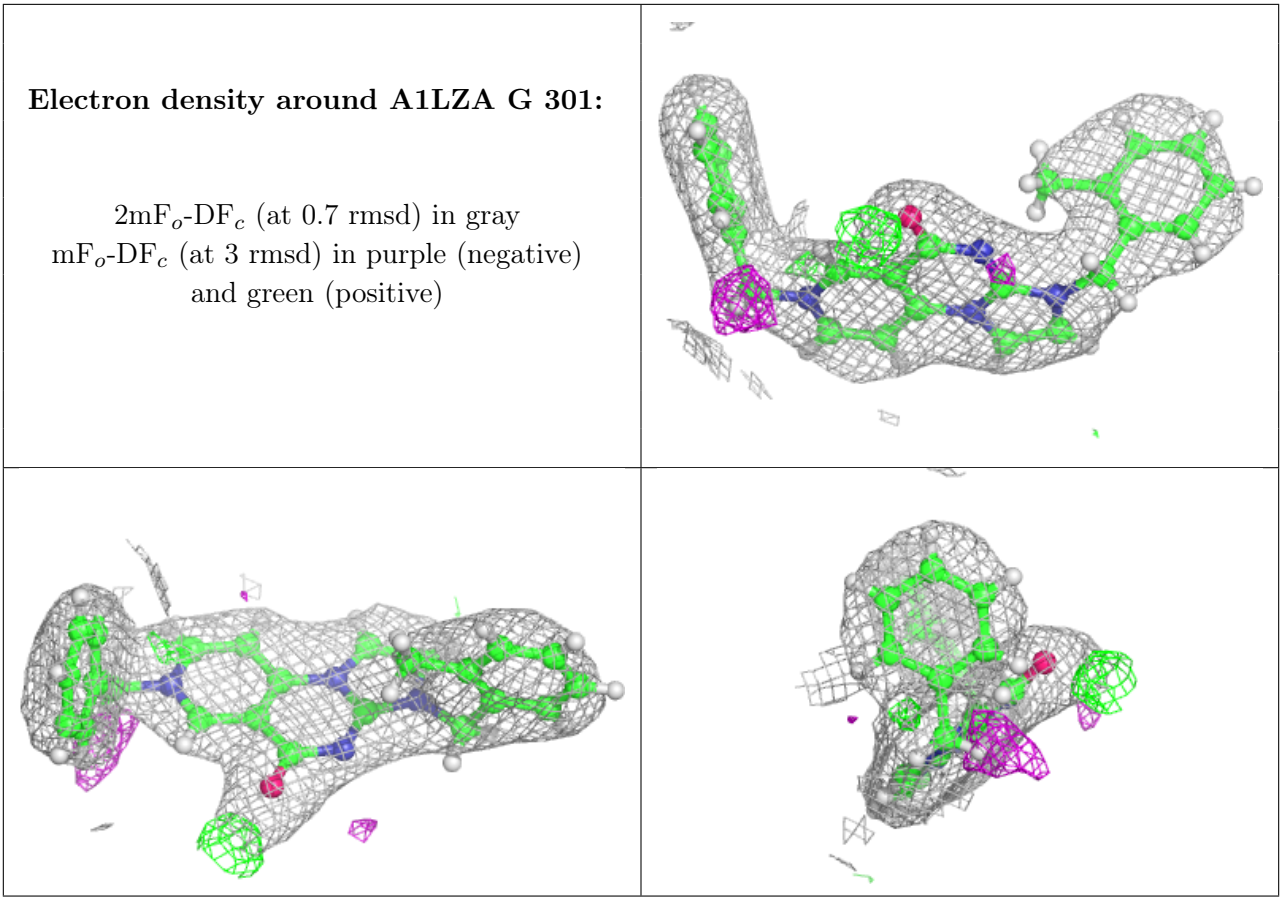
Electron density around A1LZA E 301:

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



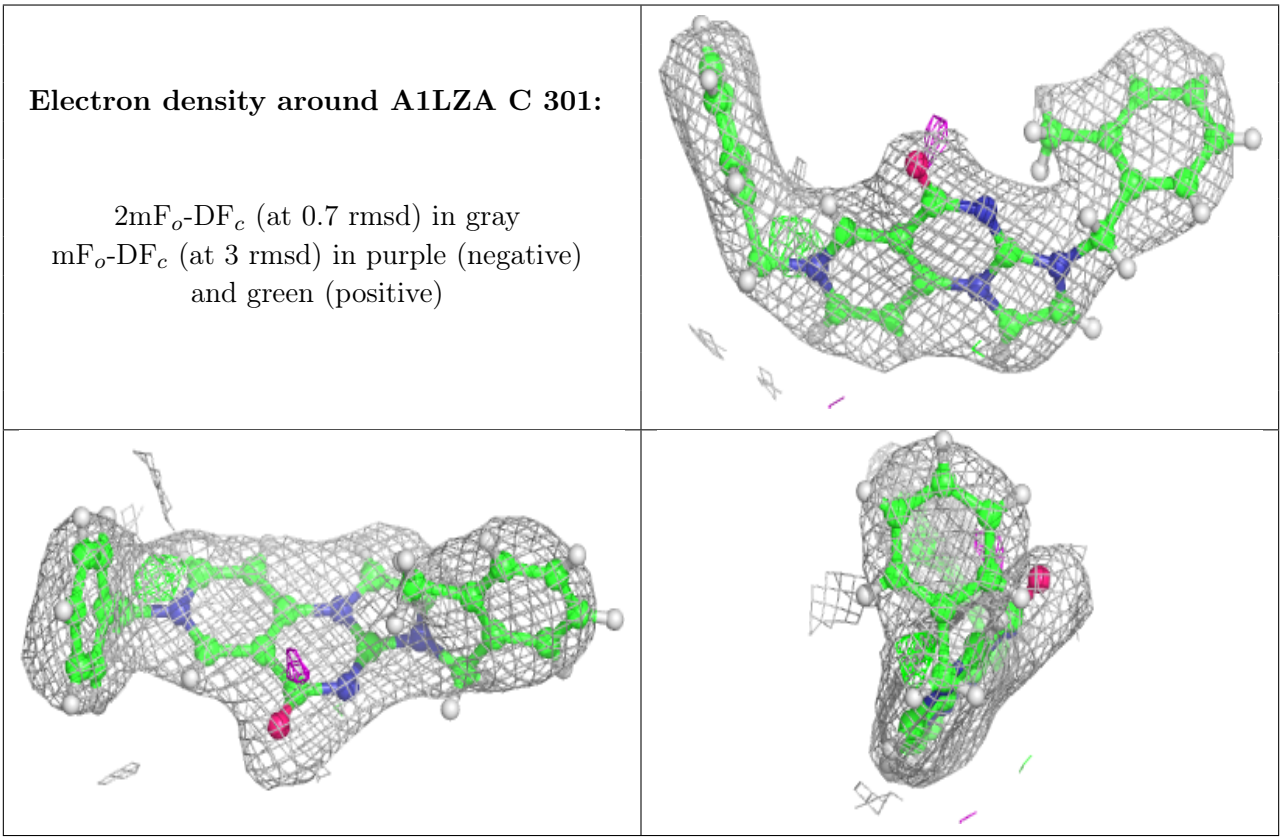
Electron density around A1LZA G 301:

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



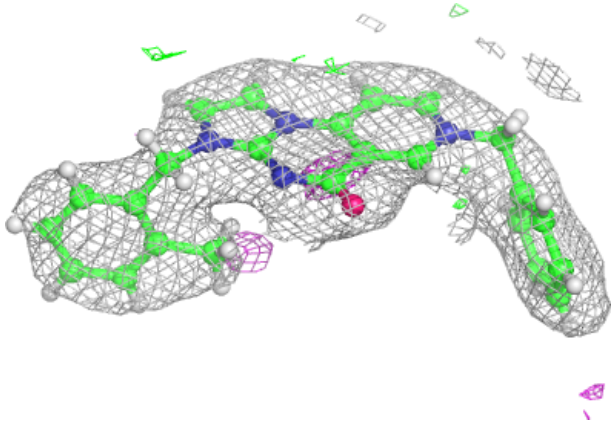
Electron density around A1LZA C 301:

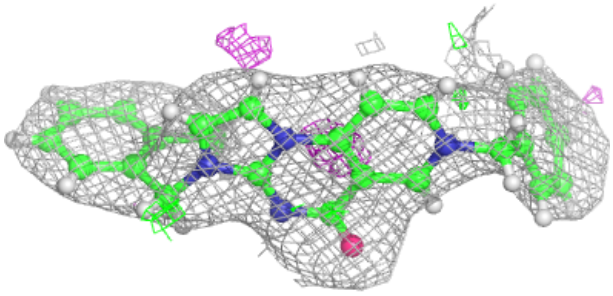
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

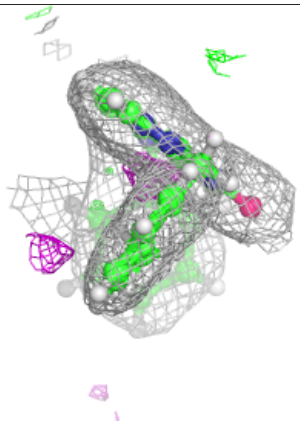


Electron density around A1LZA H 301:

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

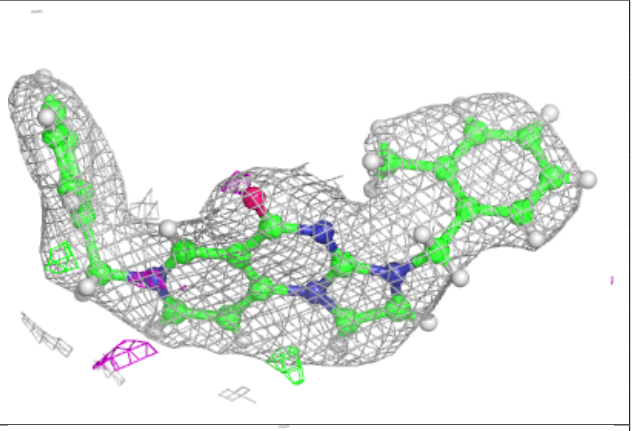


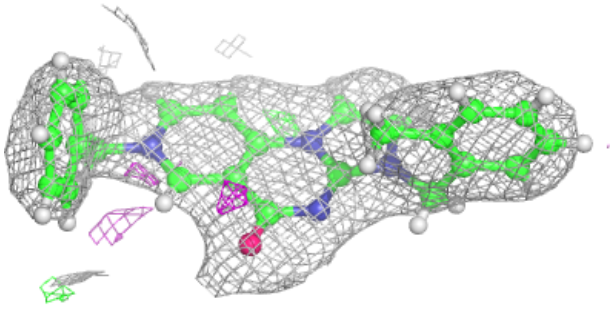


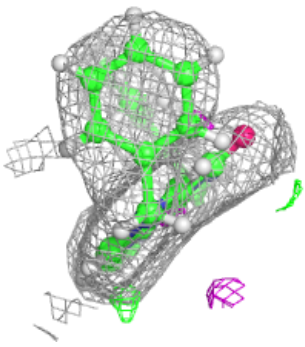


Electron density around A1LZA D 301:

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

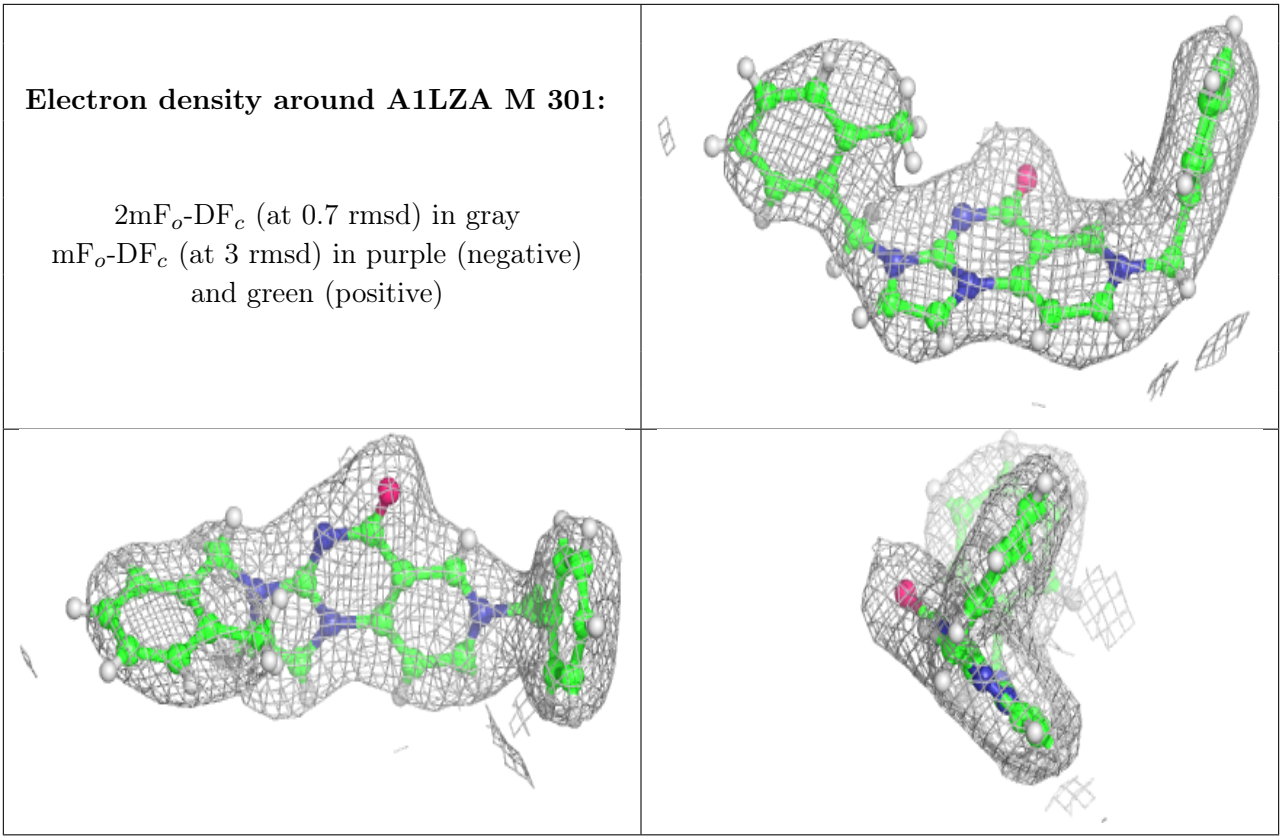






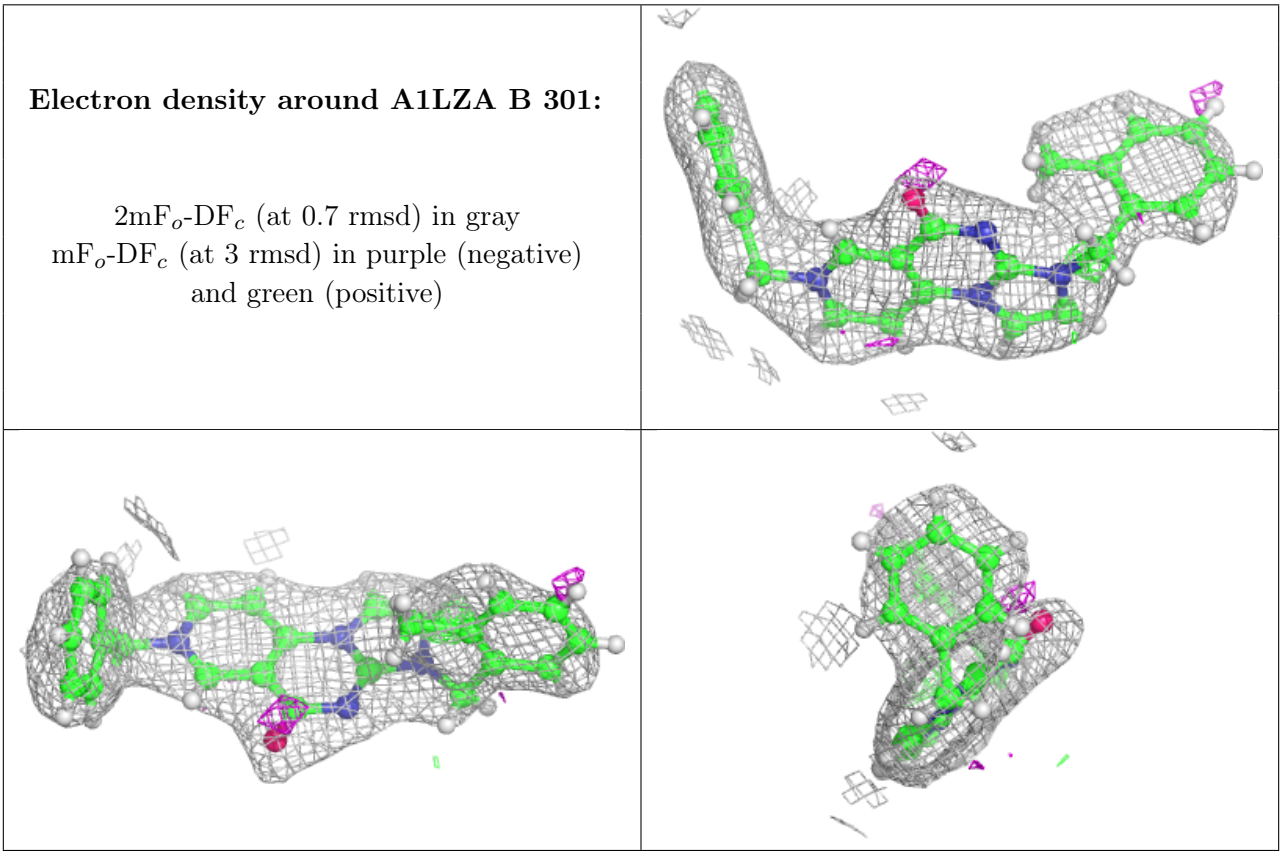
Electron density around A1LZA M 301:

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



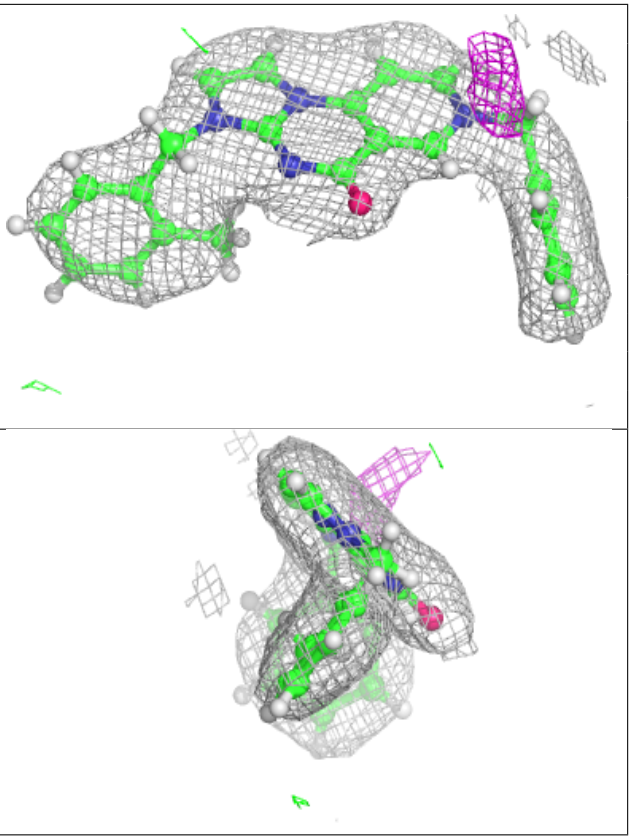
Electron density around A1LZA B 301:

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



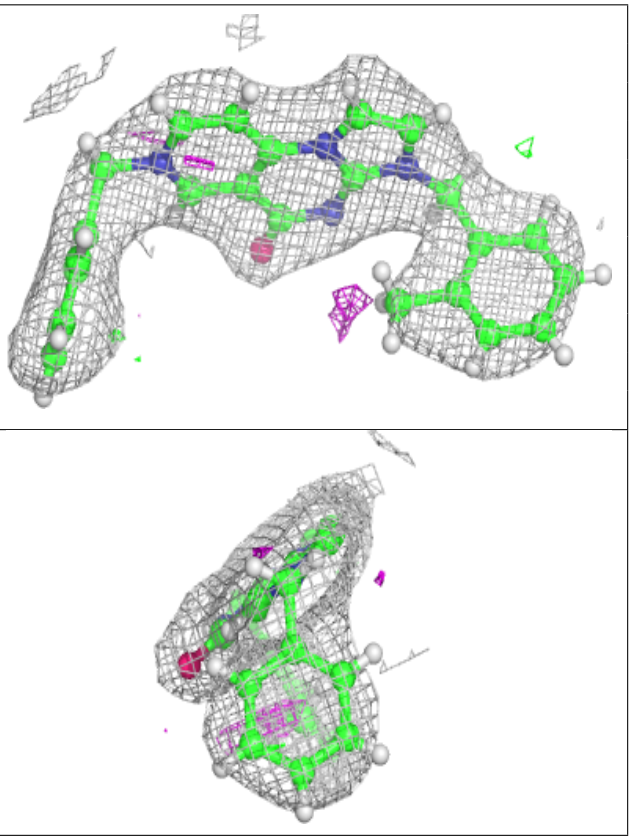
Electron density around A1LZA J 301:

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



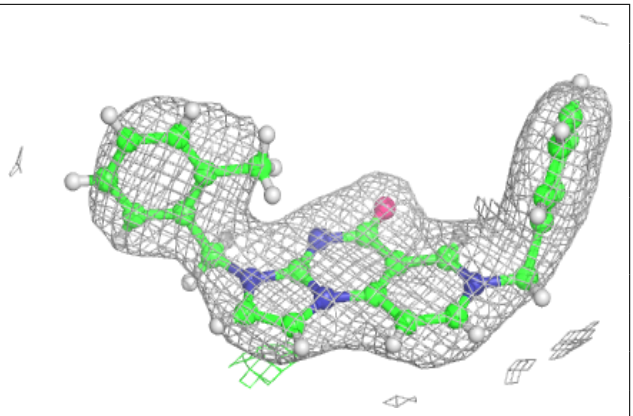
Electron density around A1LZA I 301:

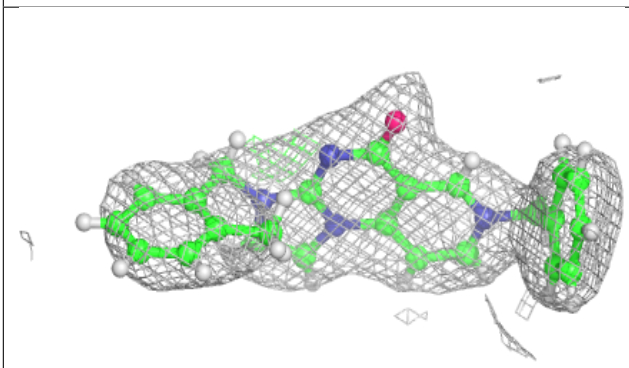
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

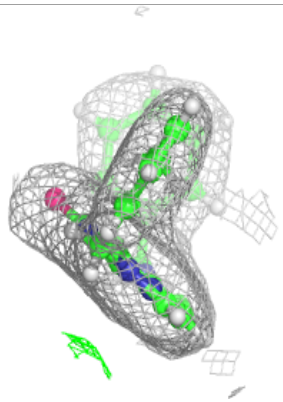


Electron density around A1LZA L 301:

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

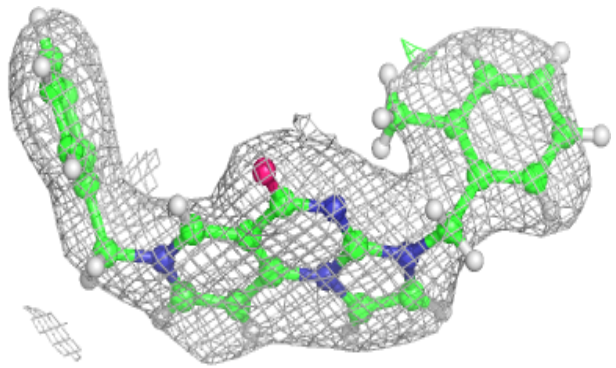


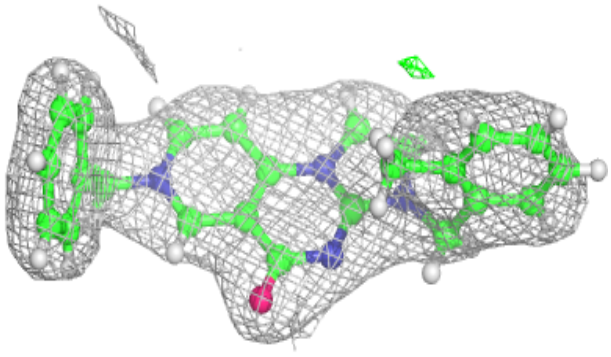


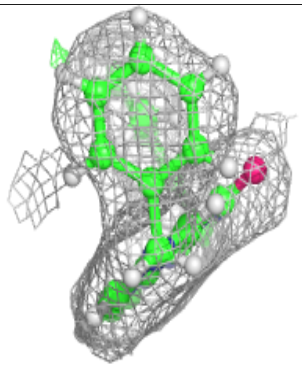


Electron density around A1LZA A 301:

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

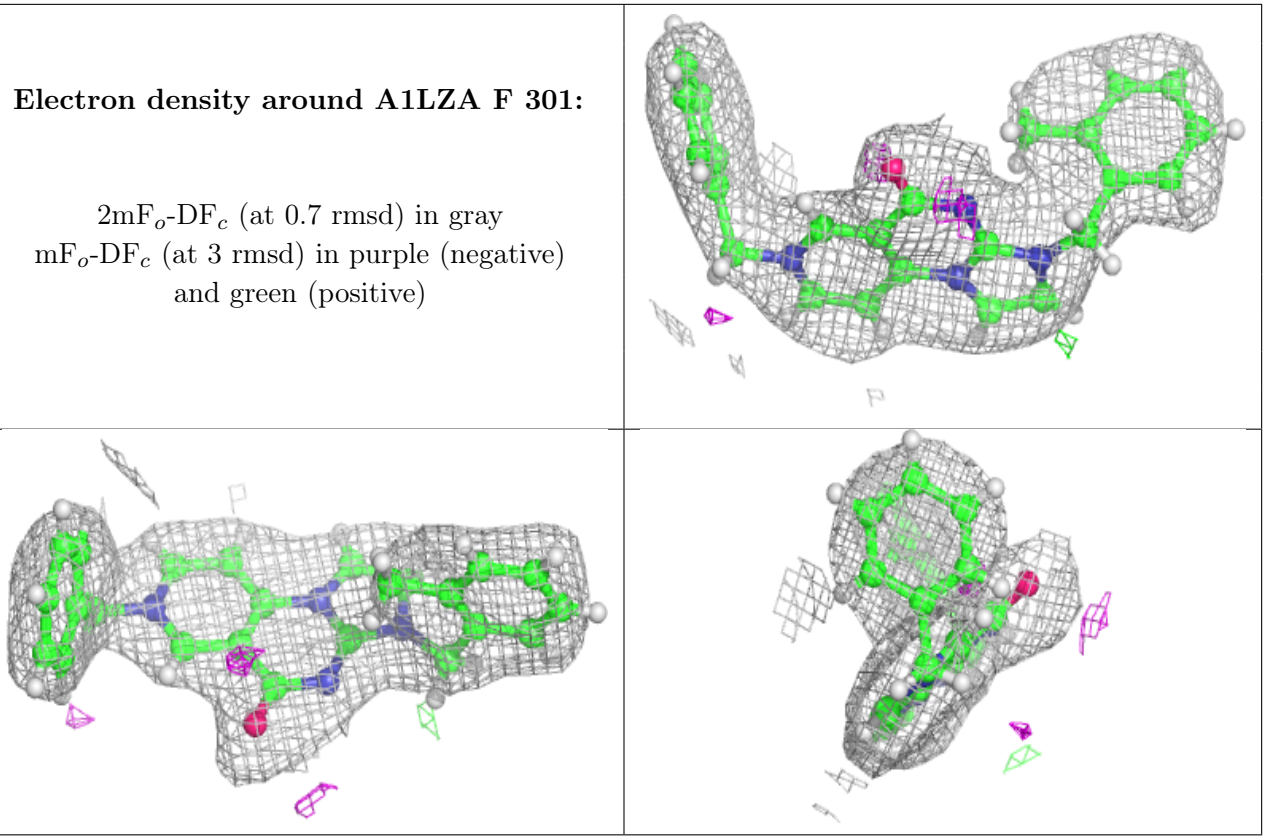






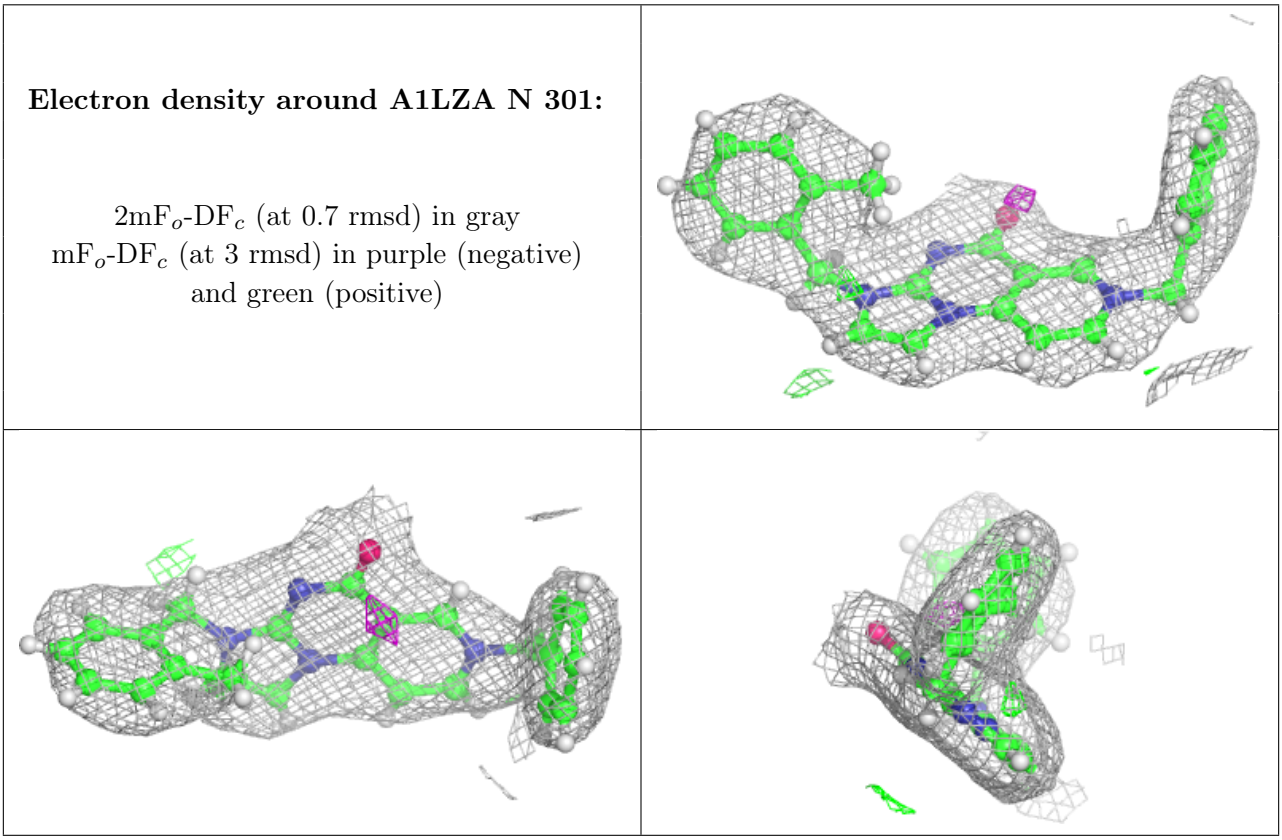
Electron density around A1LZA F 301:

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



Electron density around A1LZA N 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.