Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2022 – 04:22 am BST

PDB ID	:	6SGV
Title	:	Crystal structure of AcAChBP in complex with hosieine
Authors	:	Hunter, W.N.; Dawson, A.; Parker, H.
Deposited on	:	2019-08-05
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

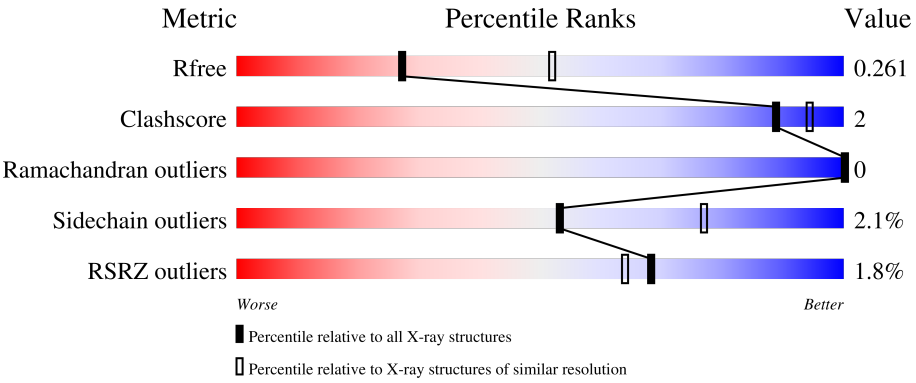
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	249	2% 78% • • 18%
1	B	249	3% 76% 5% • 18%
1	C	249	% 78% • • 18%
1	D	249	% 77% 5% • 18%
1	E	249	2% 78% • • 18%

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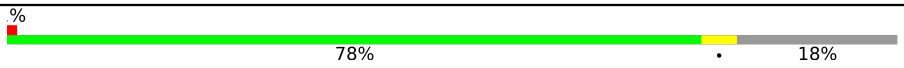
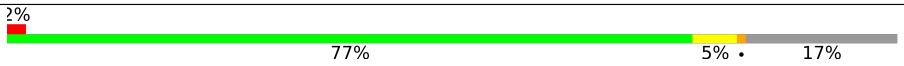
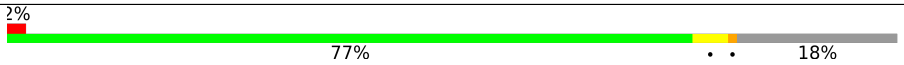
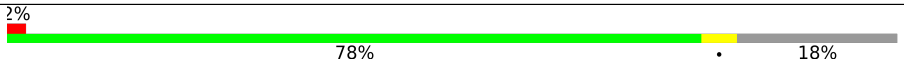
Mol	Chain	Length	Quality of chain
1	F	249	
1	G	249	
1	H	249	
1	I	249	
1	J	249	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	301	-	-	-	X
4	ACT	I	301	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17086 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	B	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	C	205	Total	C	N	O	S	0	1	0
			1645	1041	270	325	9			
1	D	205	Total	C	N	O	S	0	2	0
			1651	1044	273	325	9			
1	E	205	Total	C	N	O	S	0	1	0
			1642	1039	269	325	9			
1	F	205	Total	C	N	O	S	0	1	0
			1644	1041	269	325	9			
1	G	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	H	206	Total	C	N	O	S	0	1	0
			1655	1047	273	326	9			
1	I	205	Total	C	N	O	S	0	1	0
			1645	1041	270	325	9			
1	J	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	VAL	ALA	conflict	UNP Q8WSF8
A	155	VAL	ALA	conflict	UNP Q8WSF8
A	237	GLU	-	expression tag	UNP Q8WSF8
A	238	ASN	-	expression tag	UNP Q8WSF8
A	239	LEU	-	expression tag	UNP Q8WSF8
A	240	TYR	-	expression tag	UNP Q8WSF8
A	241	PHE	-	expression tag	UNP Q8WSF8
A	242	GLN	-	expression tag	UNP Q8WSF8
A	243	GLY	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	244	HIS	-	expression tag	UNP Q8WSF8
A	245	HIS	-	expression tag	UNP Q8WSF8
A	246	HIS	-	expression tag	UNP Q8WSF8
A	247	HIS	-	expression tag	UNP Q8WSF8
A	248	HIS	-	expression tag	UNP Q8WSF8
A	249	HIS	-	expression tag	UNP Q8WSF8
B	60	VAL	ALA	conflict	UNP Q8WSF8
B	155	VAL	ALA	conflict	UNP Q8WSF8
B	237	GLU	-	expression tag	UNP Q8WSF8
B	238	ASN	-	expression tag	UNP Q8WSF8
B	239	LEU	-	expression tag	UNP Q8WSF8
B	240	TYR	-	expression tag	UNP Q8WSF8
B	241	PHE	-	expression tag	UNP Q8WSF8
B	242	GLN	-	expression tag	UNP Q8WSF8
B	243	GLY	-	expression tag	UNP Q8WSF8
B	244	HIS	-	expression tag	UNP Q8WSF8
B	245	HIS	-	expression tag	UNP Q8WSF8
B	246	HIS	-	expression tag	UNP Q8WSF8
B	247	HIS	-	expression tag	UNP Q8WSF8
B	248	HIS	-	expression tag	UNP Q8WSF8
B	249	HIS	-	expression tag	UNP Q8WSF8
C	60	VAL	ALA	conflict	UNP Q8WSF8
C	155	VAL	ALA	conflict	UNP Q8WSF8
C	237	GLU	-	expression tag	UNP Q8WSF8
C	238	ASN	-	expression tag	UNP Q8WSF8
C	239	LEU	-	expression tag	UNP Q8WSF8
C	240	TYR	-	expression tag	UNP Q8WSF8
C	241	PHE	-	expression tag	UNP Q8WSF8
C	242	GLN	-	expression tag	UNP Q8WSF8
C	243	GLY	-	expression tag	UNP Q8WSF8
C	244	HIS	-	expression tag	UNP Q8WSF8
C	245	HIS	-	expression tag	UNP Q8WSF8
C	246	HIS	-	expression tag	UNP Q8WSF8
C	247	HIS	-	expression tag	UNP Q8WSF8
C	248	HIS	-	expression tag	UNP Q8WSF8
C	249	HIS	-	expression tag	UNP Q8WSF8
D	60	VAL	ALA	conflict	UNP Q8WSF8
D	155	VAL	ALA	conflict	UNP Q8WSF8
D	237	GLU	-	expression tag	UNP Q8WSF8
D	238	ASN	-	expression tag	UNP Q8WSF8
D	239	LEU	-	expression tag	UNP Q8WSF8
D	240	TYR	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	241	PHE	-	expression tag	UNP Q8WSF8
D	242	GLN	-	expression tag	UNP Q8WSF8
D	243	GLY	-	expression tag	UNP Q8WSF8
D	244	HIS	-	expression tag	UNP Q8WSF8
D	245	HIS	-	expression tag	UNP Q8WSF8
D	246	HIS	-	expression tag	UNP Q8WSF8
D	247	HIS	-	expression tag	UNP Q8WSF8
D	248	HIS	-	expression tag	UNP Q8WSF8
D	249	HIS	-	expression tag	UNP Q8WSF8
E	60	VAL	ALA	conflict	UNP Q8WSF8
E	155	VAL	ALA	conflict	UNP Q8WSF8
E	237	GLU	-	expression tag	UNP Q8WSF8
E	238	ASN	-	expression tag	UNP Q8WSF8
E	239	LEU	-	expression tag	UNP Q8WSF8
E	240	TYR	-	expression tag	UNP Q8WSF8
E	241	PHE	-	expression tag	UNP Q8WSF8
E	242	GLN	-	expression tag	UNP Q8WSF8
E	243	GLY	-	expression tag	UNP Q8WSF8
E	244	HIS	-	expression tag	UNP Q8WSF8
E	245	HIS	-	expression tag	UNP Q8WSF8
E	246	HIS	-	expression tag	UNP Q8WSF8
E	247	HIS	-	expression tag	UNP Q8WSF8
E	248	HIS	-	expression tag	UNP Q8WSF8
E	249	HIS	-	expression tag	UNP Q8WSF8
F	60	VAL	ALA	conflict	UNP Q8WSF8
F	155	VAL	ALA	conflict	UNP Q8WSF8
F	237	GLU	-	expression tag	UNP Q8WSF8
F	238	ASN	-	expression tag	UNP Q8WSF8
F	239	LEU	-	expression tag	UNP Q8WSF8
F	240	TYR	-	expression tag	UNP Q8WSF8
F	241	PHE	-	expression tag	UNP Q8WSF8
F	242	GLN	-	expression tag	UNP Q8WSF8
F	243	GLY	-	expression tag	UNP Q8WSF8
F	244	HIS	-	expression tag	UNP Q8WSF8
F	245	HIS	-	expression tag	UNP Q8WSF8
F	246	HIS	-	expression tag	UNP Q8WSF8
F	247	HIS	-	expression tag	UNP Q8WSF8
F	248	HIS	-	expression tag	UNP Q8WSF8
F	249	HIS	-	expression tag	UNP Q8WSF8
G	60	VAL	ALA	conflict	UNP Q8WSF8
G	155	VAL	ALA	conflict	UNP Q8WSF8
G	237	GLU	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	238	ASN	-	expression tag	UNP Q8WSF8
G	239	LEU	-	expression tag	UNP Q8WSF8
G	240	TYR	-	expression tag	UNP Q8WSF8
G	241	PHE	-	expression tag	UNP Q8WSF8
G	242	GLN	-	expression tag	UNP Q8WSF8
G	243	GLY	-	expression tag	UNP Q8WSF8
G	244	HIS	-	expression tag	UNP Q8WSF8
G	245	HIS	-	expression tag	UNP Q8WSF8
G	246	HIS	-	expression tag	UNP Q8WSF8
G	247	HIS	-	expression tag	UNP Q8WSF8
G	248	HIS	-	expression tag	UNP Q8WSF8
G	249	HIS	-	expression tag	UNP Q8WSF8
H	60	VAL	ALA	conflict	UNP Q8WSF8
H	155	VAL	ALA	conflict	UNP Q8WSF8
H	237	GLU	-	expression tag	UNP Q8WSF8
H	238	ASN	-	expression tag	UNP Q8WSF8
H	239	LEU	-	expression tag	UNP Q8WSF8
H	240	TYR	-	expression tag	UNP Q8WSF8
H	241	PHE	-	expression tag	UNP Q8WSF8
H	242	GLN	-	expression tag	UNP Q8WSF8
H	243	GLY	-	expression tag	UNP Q8WSF8
H	244	HIS	-	expression tag	UNP Q8WSF8
H	245	HIS	-	expression tag	UNP Q8WSF8
H	246	HIS	-	expression tag	UNP Q8WSF8
H	247	HIS	-	expression tag	UNP Q8WSF8
H	248	HIS	-	expression tag	UNP Q8WSF8
H	249	HIS	-	expression tag	UNP Q8WSF8
I	60	VAL	ALA	conflict	UNP Q8WSF8
I	155	VAL	ALA	conflict	UNP Q8WSF8
I	237	GLU	-	expression tag	UNP Q8WSF8
I	238	ASN	-	expression tag	UNP Q8WSF8
I	239	LEU	-	expression tag	UNP Q8WSF8
I	240	TYR	-	expression tag	UNP Q8WSF8
I	241	PHE	-	expression tag	UNP Q8WSF8
I	242	GLN	-	expression tag	UNP Q8WSF8
I	243	GLY	-	expression tag	UNP Q8WSF8
I	244	HIS	-	expression tag	UNP Q8WSF8
I	245	HIS	-	expression tag	UNP Q8WSF8
I	246	HIS	-	expression tag	UNP Q8WSF8
I	247	HIS	-	expression tag	UNP Q8WSF8
I	248	HIS	-	expression tag	UNP Q8WSF8
I	249	HIS	-	expression tag	UNP Q8WSF8

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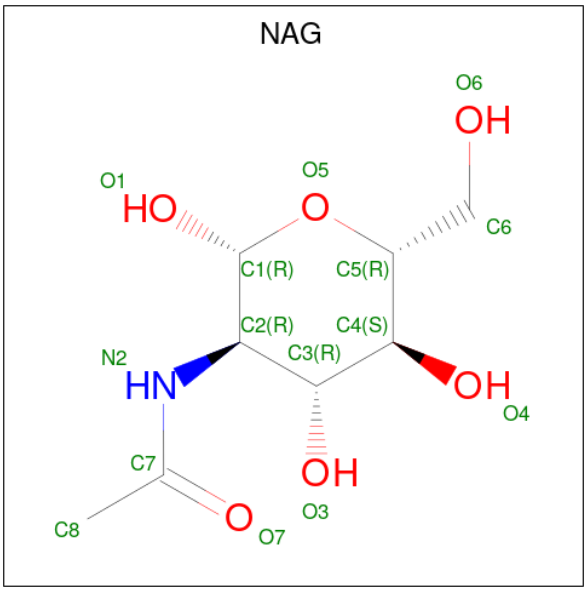
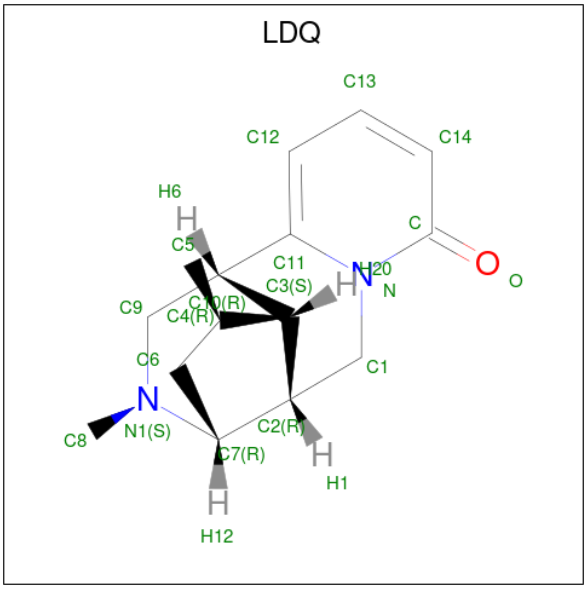
Chain	Residue	Modelled	Actual	Comment	Reference
J	60	VAL	ALA	conflict	UNP Q8WSF8
J	155	VAL	ALA	conflict	UNP Q8WSF8
J	237	GLU	-	expression tag	UNP Q8WSF8
J	238	ASN	-	expression tag	UNP Q8WSF8
J	239	LEU	-	expression tag	UNP Q8WSF8
J	240	TYR	-	expression tag	UNP Q8WSF8
J	241	PHE	-	expression tag	UNP Q8WSF8
J	242	GLN	-	expression tag	UNP Q8WSF8
J	243	GLY	-	expression tag	UNP Q8WSF8
J	244	HIS	-	expression tag	UNP Q8WSF8
J	245	HIS	-	expression tag	UNP Q8WSF8
J	246	HIS	-	expression tag	UNP Q8WSF8
J	247	HIS	-	expression tag	UNP Q8WSF8
J	248	HIS	-	expression tag	UNP Q8WSF8
J	249	HIS	-	expression tag	UNP Q8WSF8

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



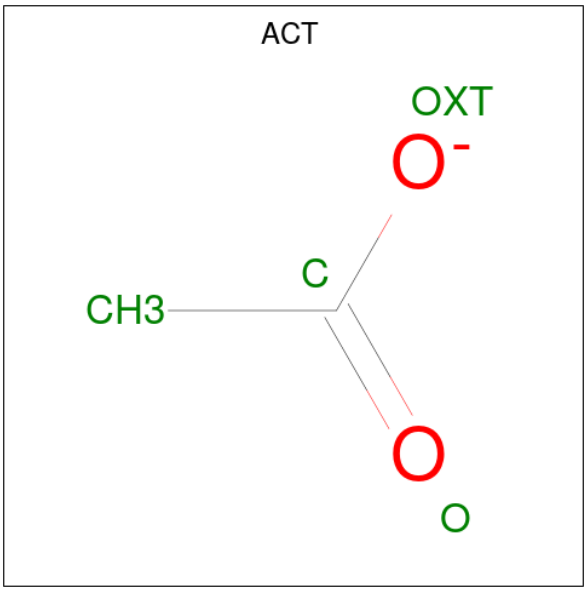
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is Hosieine (three-letter code: LDQ) (formula: $C_{15}H_{20}N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 18 15 2 1	0	0
3	B	1	Total C N O 18 15 2 1	0	0
3	C	1	Total C N O 18 15 2 1	0	0
3	D	1	Total C N O 18 15 2 1	0	0
3	E	1	Total C N O 18 15 2 1	0	0
3	F	1	Total C N O 18 15 2 1	0	0
3	G	1	Total C N O 18 15 2 1	0	0
3	H	1	Total C N O 18 15 2 1	0	0
3	I	1	Total C N O 18 15 2 1	0	0
3	J	1	Total C N O 18 15 2 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is water.

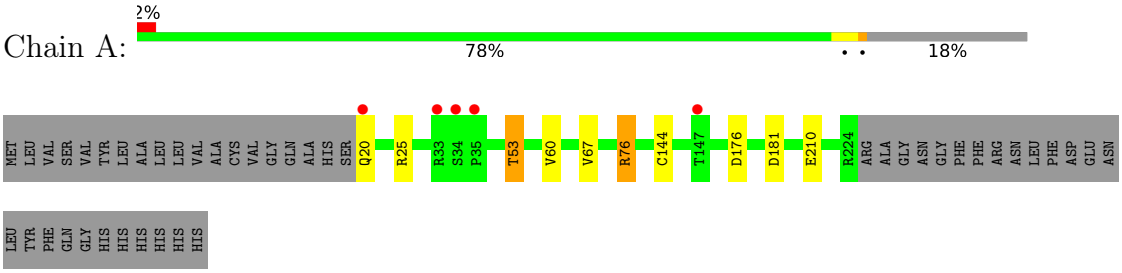
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	38	Total O 38 38	0	0
5	B	36	Total O 36 36	0	0
5	C	44	Total O 44 44	0	0
5	D	47	Total O 47 47	0	0
5	E	52	Total O 52 52	0	0
5	F	46	Total O 46 46	0	0
5	G	53	Total O 53 53	0	0
5	H	39	Total O 39 39	0	0
5	I	43	Total O 43 43	0	0
5	J	36	Total O 36 36	0	0

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.

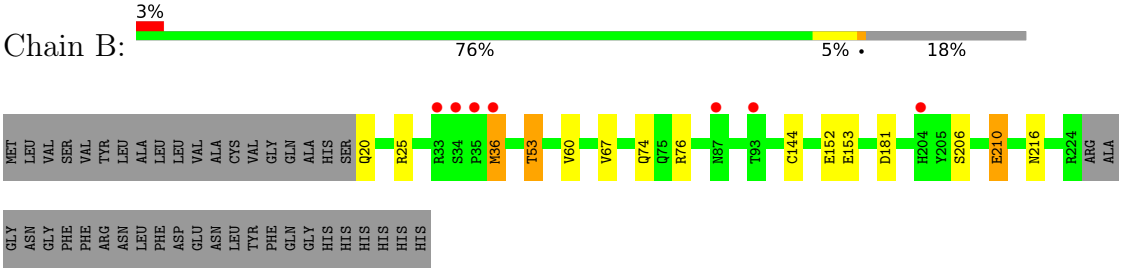
• Molecule 1: Soluble acetylcholine receptor

Chain A:



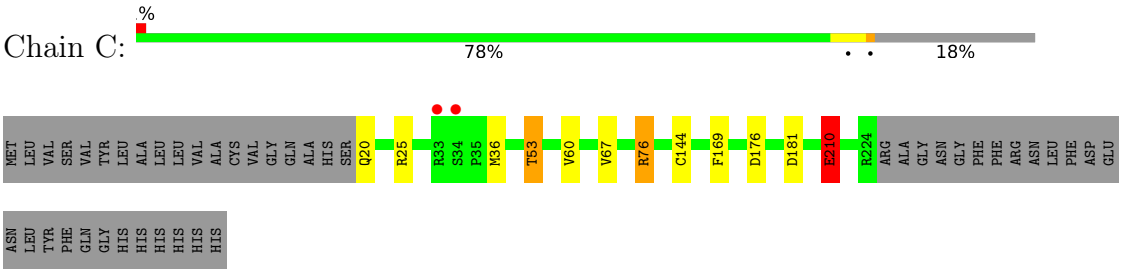
• Molecule 1: Soluble acetylcholine receptor

Chain B:



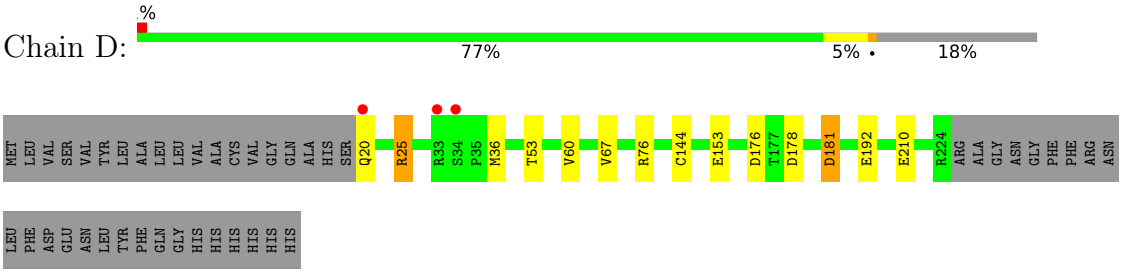
• Molecule 1: Soluble acetylcholine receptor

Chain C:



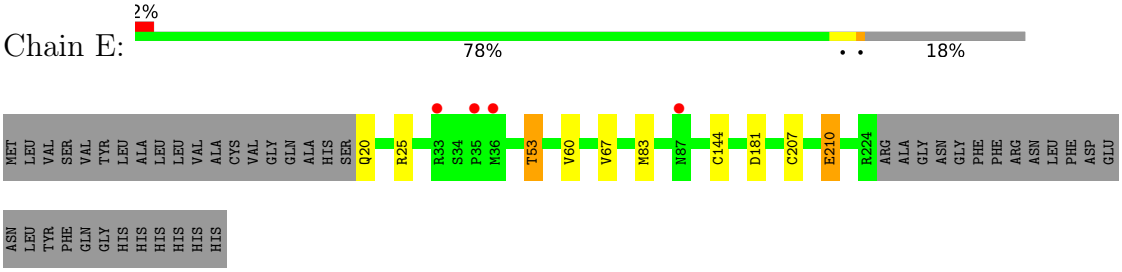
• Molecule 1: Soluble acetylcholine receptor

Chain D:



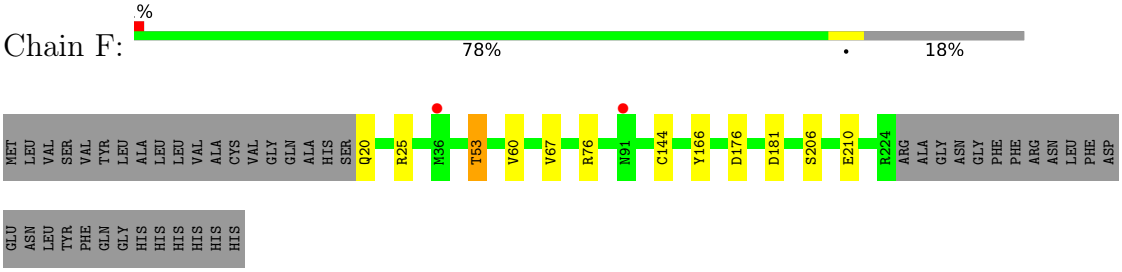
• Molecule 1: Soluble acetylcholine receptor

Chain E:



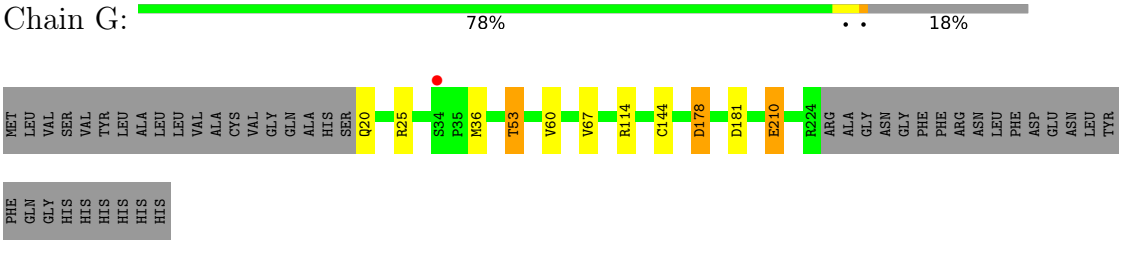
• Molecule 1: Soluble acetylcholine receptor

Chain F:



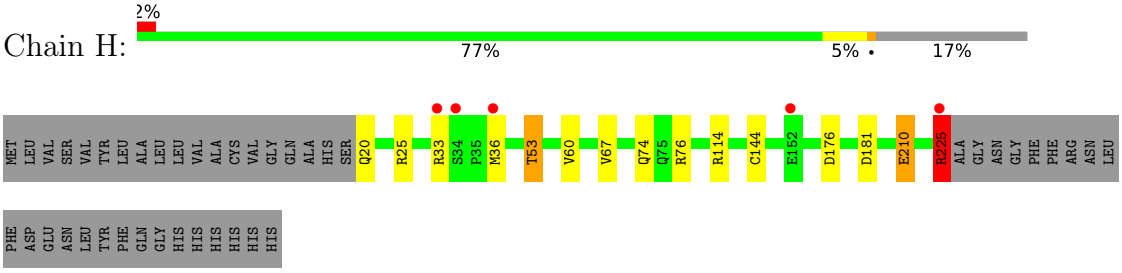
• Molecule 1: Soluble acetylcholine receptor

Chain G:



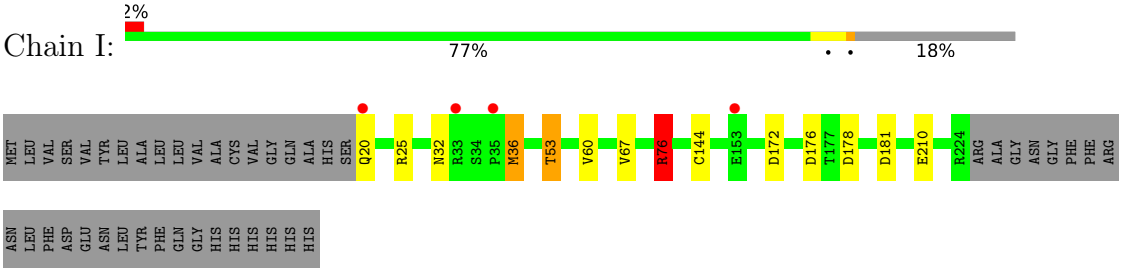
• Molecule 1: Soluble acetylcholine receptor

Chain H:



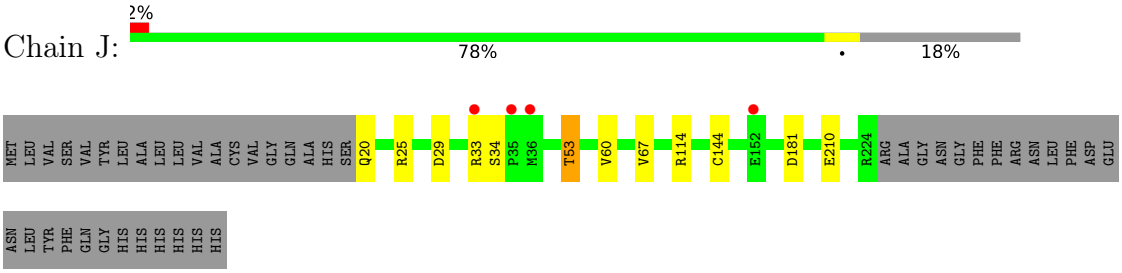
• Molecule 1: Soluble acetylcholine receptor

Chain I:



• Molecule 1: Soluble acetylcholine receptor

Chain J:


2%
78%
18%
MET LEU VAL SER VAL TYR LEU ALA LEU LEU VAL ALA CYS VAL GLY GLN ALA HIS SER Q20 R25 D29 R33 S34 P35 M36 T53 V60 V67 R114 C144 E152 D181 E210 R224 ARG ALA GLY ASN GLY PHE PHE ARG ASN LEU PHE ASP GLU
ASN LEU TYR PHE GLN GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	209.80Å 133.41Å 131.16Å 90.00° 102.51° 90.00°	Depositor
Resolution (Å)	45.03 – 2.60 45.03 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.03-2.60) 100.0 (45.03-2.60)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.232 , 0.257 0.238 , 0.261	Depositor DCC
R_{free} test set	5457 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	17086	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: ACT, NAG, LDQ

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	0.56	0/1676	0.79	3/2287 (0.1%)
1	B	0.56	0/1676	0.80	3/2287 (0.1%)
1	C	0.58	1/1687 (0.1%)	0.84	6/2301 (0.3%)
1	D	0.62	0/1697	0.86	7/2312 (0.3%)
1	E	0.57	0/1687	0.81	3/2301 (0.1%)
1	F	0.63	1/1687 (0.1%)	0.83	2/2301 (0.1%)
1	G	0.61	0/1676	0.82	4/2287 (0.2%)
1	H	0.56	0/1698	0.81	5/2315 (0.2%)
1	I	0.60	0/1687	0.85	7/2301 (0.3%)
1	J	0.58	1/1676 (0.1%)	0.80	3/2287 (0.1%)
All	All	0.59	3/16847 (0.0%)	0.82	43/22979 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	210	GLU	CD-OE1	-6.68	1.18	1.25
1	C	210	GLU	CD-OE2	-5.58	1.19	1.25
1	F	166	TYR	CG-CD2	5.53	1.46	1.39

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	76[A]	ARG	CA-CB-CG	8.85	132.87	113.40
1	I	76[B]	ARG	CA-CB-CG	8.85	132.87	113.40
1	G	178	ASP	CB-CG-OD1	8.69	126.12	118.30
1	D	178	ASP	CB-CG-OD2	-8.52	110.64	118.30
1	E	83	MET	CG-SD-CE	8.40	113.64	100.20
1	A	76	ARG	CA-CB-CG	7.98	130.96	113.40
1	D	25	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	C	210	GLU	OE1-CD-OE2	-7.12	114.76	123.30
1	H	225	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	G	178	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	D	178	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	25	ARG	NE-CZ-NH2	6.47	123.53	120.30
1	C	25	ARG	NE-CZ-NH2	6.37	123.49	120.30
1	G	25	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	B	25	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	H	25	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	C	210	GLU	CG-CD-OE1	6.21	130.71	118.30
1	J	25	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	D	181	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	F	25	ARG	NE-CZ-NH1	-5.95	117.32	120.30
1	J	210	GLU	CG-CD-OE2	5.90	130.11	118.30
1	I	172	ASP	CB-CG-OD1	5.87	123.58	118.30
1	E	25[A]	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	E	25[B]	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	F	25	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	I	25	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	I	36	MET	CA-CB-CG	5.66	122.92	113.30
1	H	114	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	I	178	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	B	36	MET	CA-CB-CG	5.55	122.74	113.30
1	D	192	GLU	OE1-CD-OE2	-5.43	116.79	123.30
1	I	172	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	25	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	J	114	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	H	225	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	G	25	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	D	153	GLU	CA-CB-CG	5.20	124.85	113.40
1	C	25	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	B	153	GLU	CA-CB-CG	5.14	124.71	113.40
1	H	25	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	C	76[A]	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	C	76[B]	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	D	25	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	181	ASP	Sidechain
1	E	207	CYS	Peptide

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	1636	0	1568	5	0
1	B	1636	0	1569	6	1
1	C	1645	0	1581	6	0
1	D	1651	0	1591	6	0
1	E	1642	0	1577	4	0
1	F	1644	0	1582	4	0
1	G	1636	0	1569	6	1
1	H	1655	0	1595	9	0
1	I	1645	0	1582	11	0
1	J	1636	0	1569	6	0
2	A	14	0	13	0	0
2	C	14	0	13	0	0
2	E	14	0	13	0	0
3	A	18	0	0	0	0
3	B	18	0	0	0	0
3	C	18	0	0	0	0
3	D	18	0	0	0	0
3	E	18	0	0	0	0
3	F	18	0	0	0	0
3	G	18	0	0	0	0
3	H	18	0	0	0	0
3	I	18	0	0	0	0
3	J	18	0	0	0	0
4	I	4	0	3	4	0
5	A	38	0	0	1	0
5	B	36	0	0	2	0
5	C	44	0	0	0	0
5	D	47	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	52	0	0	1	0
5	F	46	0	0	1	1
5	G	53	0	0	2	1
5	H	39	0	0	2	0
5	I	43	0	0	3	0
5	J	36	0	0	2	0
All	All	17086	0	15825	63	2

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 2.

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:B:74:GLN:OE1	1:B:76:ARG:NH1	1.99	0.94
1:D:76[B]:ARG:HH11	1:D:76[B]:ARG:HG3	1.39	0.87
1:H:76[B]:ARG:NH1	1:H:176:ASP:OD1	2.15	0.78
1:G:210:GLU:HG3	5:G:742:HOH:O	1.92	0.69
1:I:76[A]:ARG:NH2	1:I:176:ASP:OD1	2.30	0.65
1:H:74:GLN:OE1	1:H:76[B]:ARG:NH2	2.30	0.65
1:C:76[A]:ARG:NH1	1:C:176:ASP:OD1	2.30	0.64
1:F:76[A]:ARG:NH2	1:F:176:ASP:OD1	2.31	0.64
1:A:76:ARG:NH2	1:A:176:ASP:OD1	2.31	0.63
1:D:76[B]:ARG:NH2	1:D:176:ASP:OD1	2.30	0.63
1:D:76[B]:ARG:HH11	1:D:76[B]:ARG:CG	2.11	0.61
1:C:169:PHE:CD2	1:C:210:GLU:HG2	2.35	0.61
1:J:34:SER:HB2	5:J:732:HOH:O	2.05	0.57
1:I:32:ASN:HD21	4:I:301:ACT:CH3	2.17	0.57
1:I:32:ASN:HD21	4:I:301:ACT:H1	1.69	0.56
1:E:210:GLU:HG3	5:E:444:HOH:O	2.08	0.53
1:H:33:ARG:NH1	5:H:701:HOH:O	2.42	0.52
1:I:76[A]:ARG:HG3	5:I:437:HOH:O	2.12	0.49
1:B:216:ASN:ND2	5:B:701:HOH:O	2.47	0.48
1:I:32:ASN:ND2	4:I:301:ACT:CH3	2.77	0.48
1:H:225:ARG:HH11	1:H:225:ARG:HG3	1.80	0.47
1:C:20:GLN:N	1:C:20:GLN:OE1	2.48	0.47
1:C:169:PHE:HD2	1:C:210:GLU:HG2	1.76	0.47
5:F:742:HOH:O	1:G:114:ARG:HD2	2.13	0.47
1:A:20:GLN:N	1:A:20:GLN:OE1	2.48	0.46
1:D:20:GLN:OE1	1:D:20:GLN:N	2.48	0.46
1:F:20:GLN:N	1:F:20:GLN:OE1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:GLN:OE1	1:H:20:GLN:N	2.49	0.46
1:E:20:GLN:N	1:E:20:GLN:OE1	2.48	0.46
1:G:20:GLN:N	1:G:20:GLN:OE1	2.48	0.46
1:B:20:GLN:N	1:B:20:GLN:OE1	2.48	0.46
1:D:25:ARG:HD3	5:D:742:HOH:O	2.16	0.46
1:J:20:GLN:N	1:J:20:GLN:OE1	2.48	0.45
1:F:67:VAL:HG21	1:F:144:CYS:SG	2.57	0.45
1:I:20:GLN:N	1:I:20:GLN:OE1	2.49	0.45
1:J:53:THR:HG23	5:J:728:HOH:O	2.16	0.45
1:H:53:THR:HB	1:H:181:ASP:HB3	1.99	0.45
1:F:53:THR:HB	1:F:181:ASP:HB3	2.00	0.44
1:D:67:VAL:HG21	1:D:144:CYS:SG	2.57	0.44
1:G:53:THR:HB	1:G:181:ASP:HB3	2.00	0.44
1:C:53:THR:HB	1:C:181:ASP:HB3	1.99	0.44
1:H:76[B]:ARG:HG3	1:H:76[B]:ARG:HH21	1.83	0.44
1:A:53:THR:HB	1:A:181:ASP:HB3	1.99	0.43
1:I:53:THR:HB	1:I:181:ASP:HB3	2.00	0.43
1:J:53:THR:HB	1:J:181:ASP:HB3	2.00	0.43
1:A:67:VAL:HG21	1:A:144:CYS:SG	2.59	0.43
1:B:210:GLU:HG3	5:B:732:HOH:O	2.18	0.43
1:B:67:VAL:HG21	1:B:144:CYS:SG	2.59	0.43
1:G:53:THR:HG23	5:G:728:HOH:O	2.19	0.43
1:E:53:THR:HB	1:E:181:ASP:HB3	1.99	0.43
1:E:67:VAL:HG21	1:E:144:CYS:SG	2.59	0.43
1:J:67:VAL:HG21	1:J:144:CYS:SG	2.59	0.43
1:H:67:VAL:HG21	1:H:144:CYS:SG	2.58	0.43
1:I:32:ASN:ND2	4:I:301:ACT:H1	2.34	0.42
1:B:53:THR:HB	1:B:181:ASP:HB3	2.00	0.42
1:I:67:VAL:HG21	1:I:144:CYS:SG	2.59	0.42
1:C:67:VAL:HG21	1:C:144:CYS:SG	2.60	0.42
1:J:29:ASP:HA	1:J:33:ARG:HD2	2.02	0.42
1:I:53:THR:HG23	5:I:434:HOH:O	2.19	0.41
1:A:76:ARG:HG3	5:A:436:HOH:O	2.20	0.41
1:H:210:GLU:HG3	5:H:736:HOH:O	2.20	0.41
1:G:67:VAL:HG21	1:G:144:CYS:SG	2.60	0.41
1:I:53:THR:CG2	5:I:434:HOH:O	2.69	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLU:OE1	1:G:178:ASP:OD2[4_556]	2.04	0.16
5:F:740:HOH:O	5:G:748:HOH:O[2_656]	2.16	0.04

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	203/249 (82%)	200 (98%)	3 (2%)	0	100	100
1	B	203/249 (82%)	200 (98%)	3 (2%)	0	100	100
1	C	204/249 (82%)	201 (98%)	3 (2%)	0	100	100
1	D	204/249 (82%)	201 (98%)	3 (2%)	0	100	100
1	E	204/249 (82%)	201 (98%)	3 (2%)	0	100	100
1	F	204/249 (82%)	201 (98%)	3 (2%)	0	100	100
1	G	203/249 (82%)	200 (98%)	3 (2%)	0	100	100
1	H	205/249 (82%)	202 (98%)	3 (2%)	0	100	100
1	I	204/249 (82%)	201 (98%)	3 (2%)	0	100	100
1	J	203/249 (82%)	200 (98%)	3 (2%)	0	100	100
All	All	2037/2490 (82%)	2007 (98%)	30 (2%)	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	188/224 (84%)	185 (98%)	3 (2%)	62	82
1	B	188/224 (84%)	183 (97%)	5 (3%)	44	71
1	C	189/224 (84%)	185 (98%)	4 (2%)	53	77
1	D	190/224 (85%)	186 (98%)	4 (2%)	53	77
1	E	189/224 (84%)	186 (98%)	3 (2%)	62	82
1	F	189/224 (84%)	185 (98%)	4 (2%)	53	77
1	G	188/224 (84%)	184 (98%)	4 (2%)	53	77
1	H	190/224 (85%)	185 (97%)	5 (3%)	46	72
1	I	189/224 (84%)	183 (97%)	6 (3%)	39	65
1	J	188/224 (84%)	186 (99%)	2 (1%)	73	88
All	All	1888/2240 (84%)	1848 (98%)	40 (2%)	53	77

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	THR
1	A	60	VAL
1	A	210	GLU
1	B	36	MET
1	B	53	THR
1	B	60	VAL
1	B	206	SER
1	B	210	GLU
1	C	36	MET
1	C	53	THR
1	C	60	VAL
1	C	210	GLU
1	D	36	MET
1	D	53	THR
1	D	60	VAL
1	D	210	GLU
1	E	53	THR
1	E	60	VAL
1	E	210	GLU
1	F	53	THR
1	F	60	VAL
1	F	206	SER
1	F	210	GLU
1	G	36	MET

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Mol	Chain	Res	Type
1	G	53	THR
1	G	60	VAL
1	G	210	GLU
1	H	36	MET
1	H	53	THR
1	H	60	VAL
1	H	210	GLU
1	H	225	ARG
1	I	36	MET
1	I	53	THR
1	I	60	VAL
1	I	76[A]	ARG
1	I	76[B]	ARG
1	I	210	GLU
1	J	53	THR
1	J	60	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	B	32	ASN
1	B	216	ASN
1	C	32	ASN
1	D	32	ASN
1	E	32	ASN
1	E	216	ASN
1	F	32	ASN
1	G	32	ASN
1	G	204	HIS
1	G	216	ASN
1	H	32	ASN
1	H	91	ASN
1	I	32	ASN
1	J	32	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	LDQ	G	601	-	20,21,21	0.42	0	24,33,33	0.72	1 (4%)
3	LDQ	J	601	-	20,21,21	0.39	0	24,33,33	0.46	0
3	LDQ	B	601	-	20,21,21	0.24	0	24,33,33	0.71	1 (4%)
2	NAG	A	301	1	14,14,15	0.84	0	17,19,21	2.58	6 (35%)
3	LDQ	F	601	-	20,21,21	0.50	0	24,33,33	0.74	1 (4%)
3	LDQ	C	302	-	20,21,21	0.44	0	24,33,33	0.59	0
3	LDQ	E	302	-	20,21,21	0.41	0	24,33,33	0.66	0
3	LDQ	A	302	-	20,21,21	0.51	0	24,33,33	0.55	0
3	LDQ	H	601	-	20,21,21	0.46	0	24,33,33	0.48	0
4	ACT	I	301	-	3,3,3	1.04	0	3,3,3	0.48	0
3	LDQ	D	601	-	20,21,21	0.51	0	24,33,33	0.67	1 (4%)
2	NAG	C	301	1	14,14,15	1.22	1 (7%)	17,19,21	2.08	4 (23%)
2	NAG	E	301	1	14,14,15	0.94	0	17,19,21	2.06	5 (29%)
3	LDQ	I	302	-	20,21,21	0.44	0	24,33,33	0.73	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LDQ	G	601	-	-	-	0/4/4/4
3	LDQ	J	601	-	-	-	0/4/4/4
3	LDQ	B	601	-	-	-	0/4/4/4
2	NAG	A	301	1	-	1/6/23/26	0/1/1/1
3	LDQ	F	601	-	-	-	0/4/4/4
3	LDQ	C	302	-	-	-	0/4/4/4
3	LDQ	E	302	-	-	-	0/4/4/4
3	LDQ	A	302	-	-	-	0/4/4/4
3	LDQ	H	601	-	-	-	0/4/4/4
3	LDQ	D	601	-	-	-	0/4/4/4
2	NAG	C	301	1	-	0/6/23/26	0/1/1/1
2	NAG	E	301	1	-	3/6/23/26	0/1/1/1
3	LDQ	I	302	-	-	-	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAG	C1-C2	3.09	1.57	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	NAG	C1-O5-C5	8.85	124.18	112.19
2	C	301	NAG	C1-O5-C5	5.98	120.30	112.19
2	E	301	NAG	C2-N2-C7	5.12	130.19	122.90
2	E	301	NAG	C8-C7-N2	3.98	122.84	116.10
2	C	301	NAG	O5-C1-C2	3.05	116.10	111.29
2	A	301	NAG	O5-C5-C6	2.96	111.85	107.20
3	B	601	LDQ	C10-C9-N1	2.62	113.82	110.40
3	F	601	LDQ	C10-C9-N1	2.61	113.81	110.40
2	A	301	NAG	C4-C3-C2	2.57	114.79	111.02
2	E	301	NAG	C3-C4-C5	2.56	114.80	110.24
2	C	301	NAG	C2-N2-C7	2.47	126.42	122.90
3	G	601	LDQ	C10-C9-N1	2.45	113.59	110.40
2	E	301	NAG	C1-O5-C5	2.43	115.48	112.19
2	A	301	NAG	C3-C4-C5	2.42	114.56	110.24
3	I	302	LDQ	C10-C9-N1	2.40	113.53	110.40
2	C	301	NAG	O4-C4-C5	2.39	115.24	109.30
2	A	301	NAG	C2-N2-C7	2.16	125.98	122.90
2	E	301	NAG	O7-C7-N2	-2.12	118.06	121.95
2	A	301	NAG	O5-C1-C2	2.08	114.58	111.29
3	D	601	LDQ	C10-C9-N1	2.01	113.02	110.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

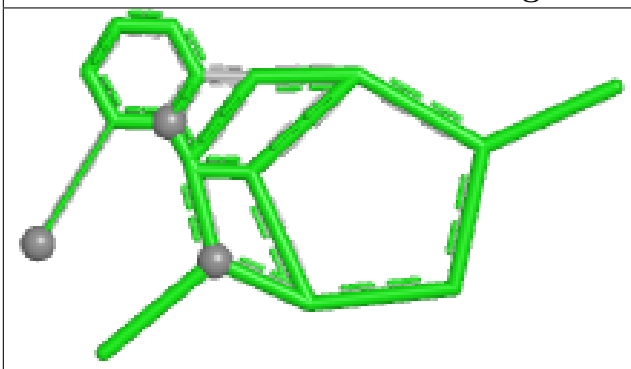
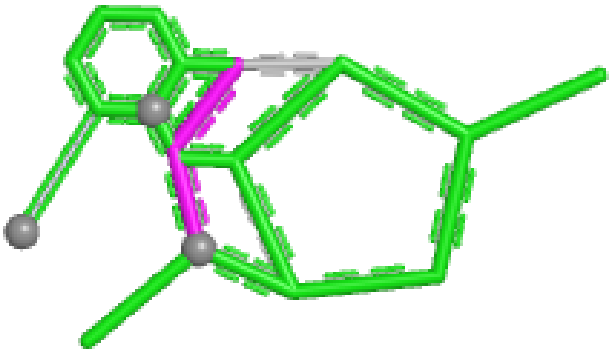
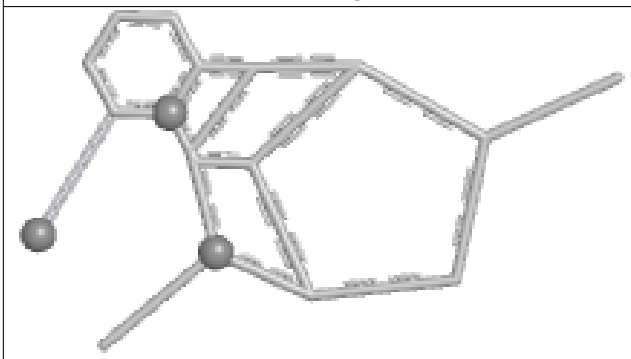
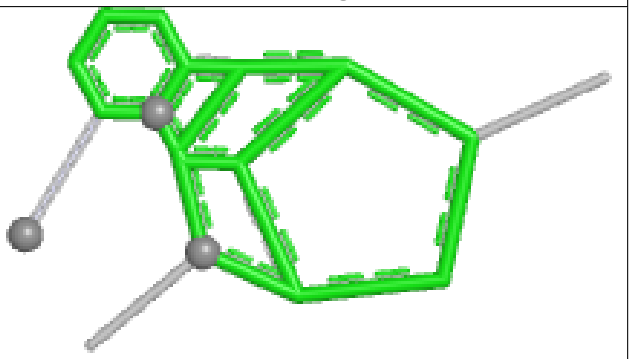
Mol	Chain	Res	Type	Atoms
2	E	301	NAG	C8-C7-N2-C2
2	E	301	NAG	O7-C7-N2-C2
2	A	301	NAG	O5-C5-C6-O6
2	E	301	NAG	C1-C2-N2-C7

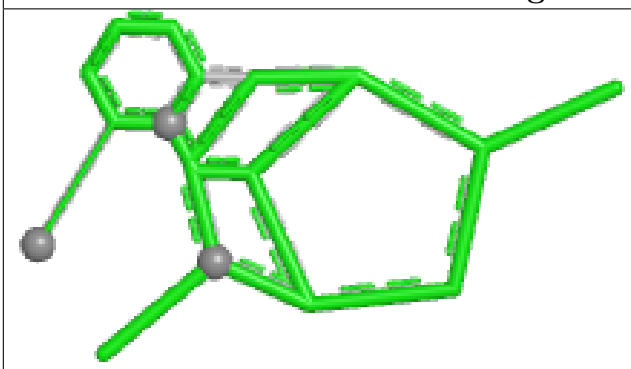
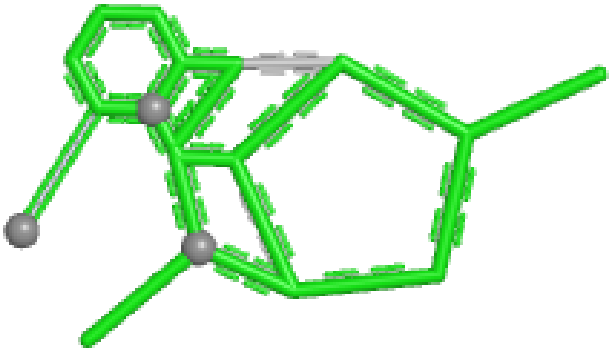
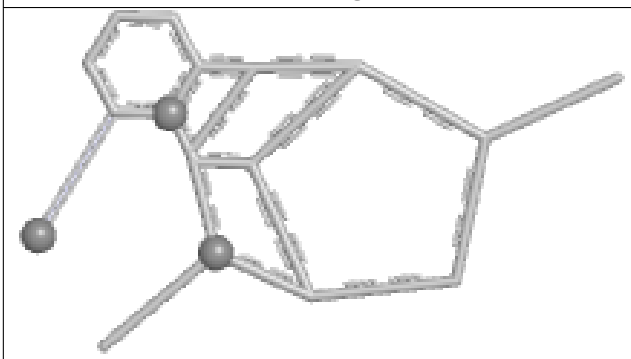
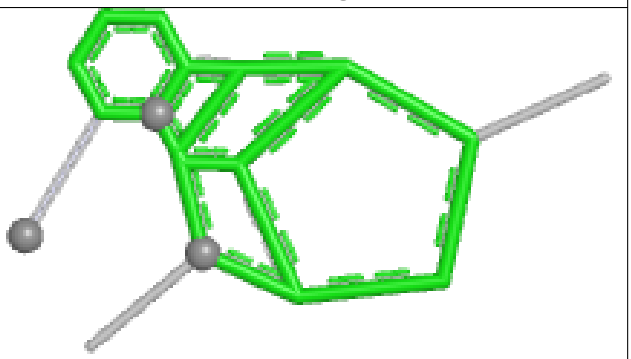
There are no ring outliers.

1 monomer is involved in 4 short contacts:

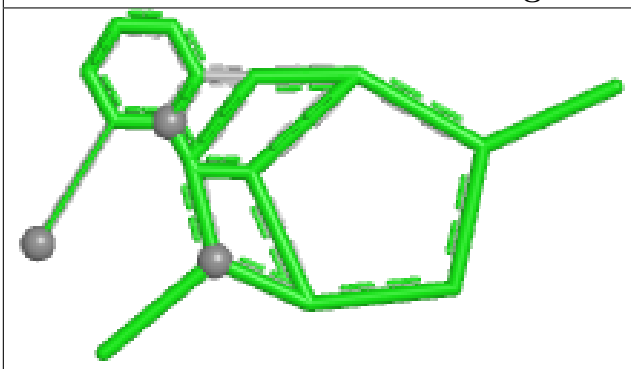
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	301	ACT	4	0

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.

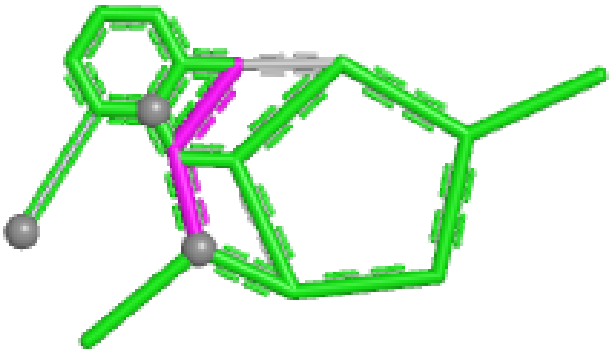
Ligand LDQ G 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LDQ J 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

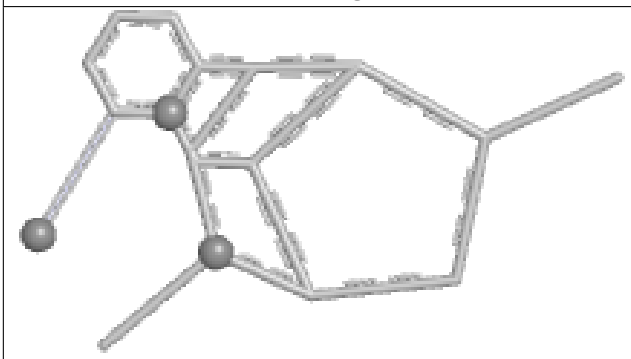
Ligand LDQ B 601



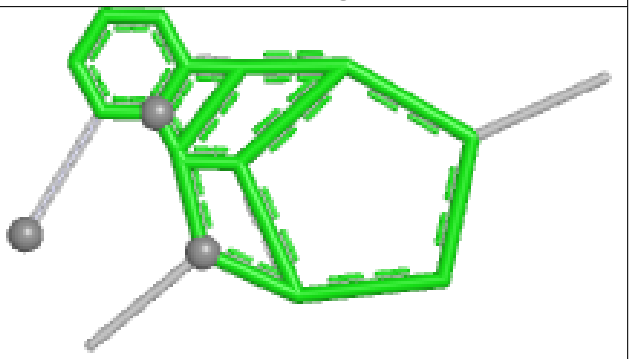
Bond lengths



Bond angles

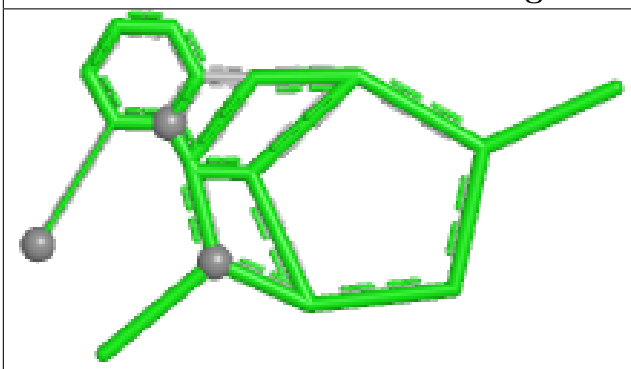


Torsions

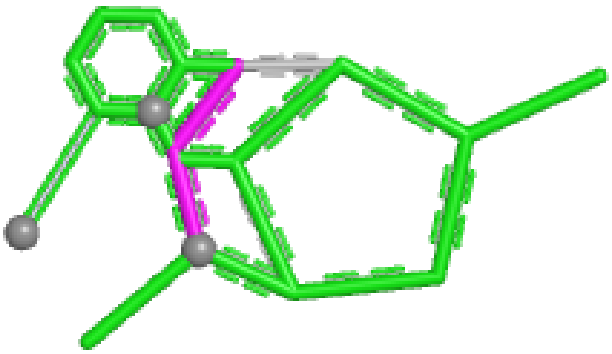


Rings

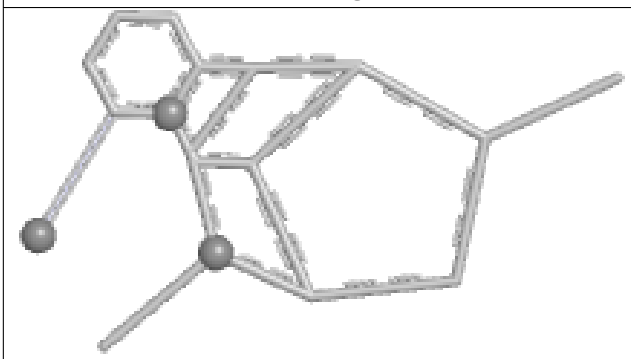
Ligand LDQ F 601



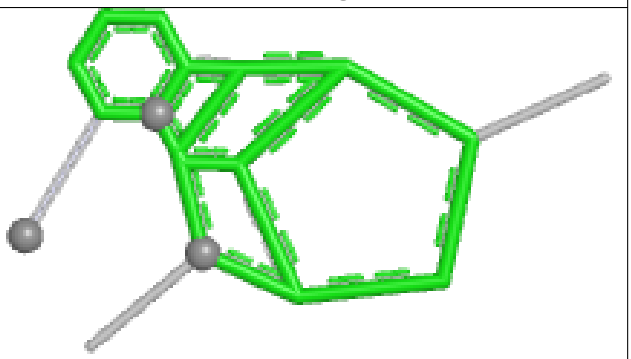
Bond lengths



Bond angles

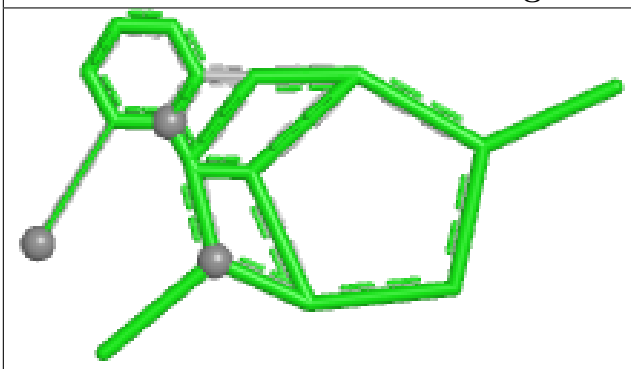


Torsions

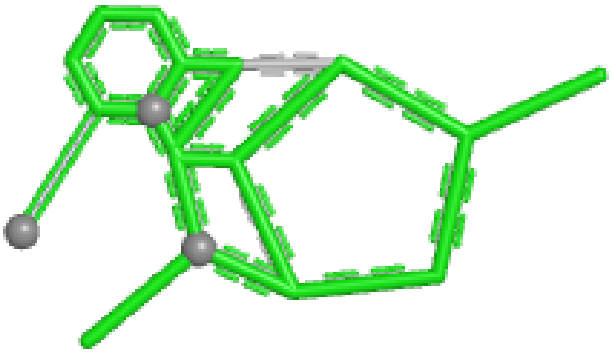


Rings

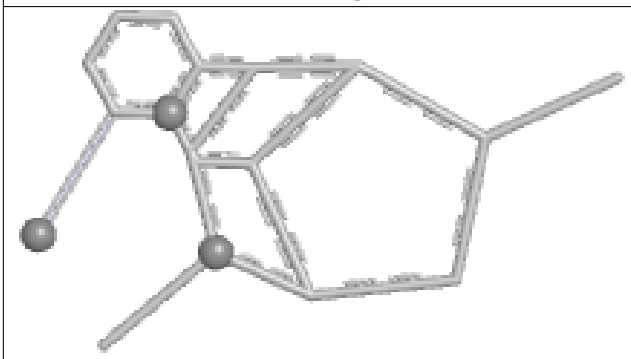
Ligand LDQ C 302



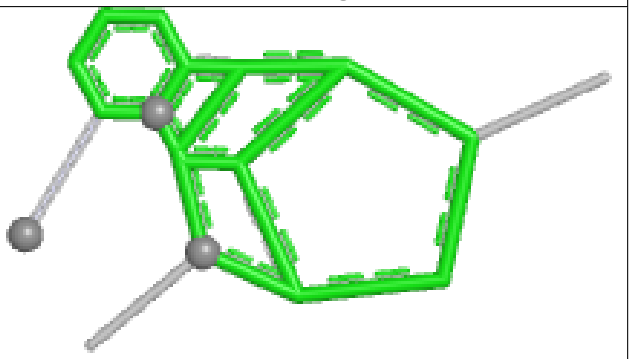
Bond lengths



Bond angles

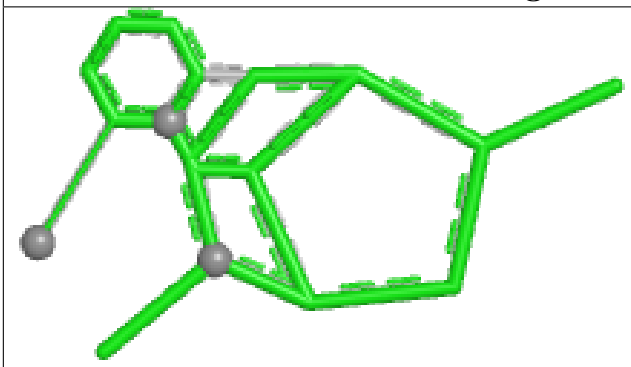


Torsions

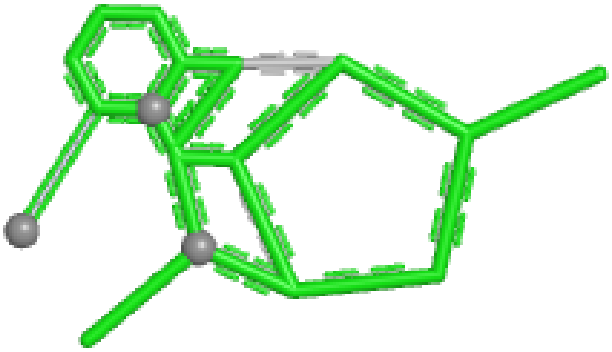


Rings

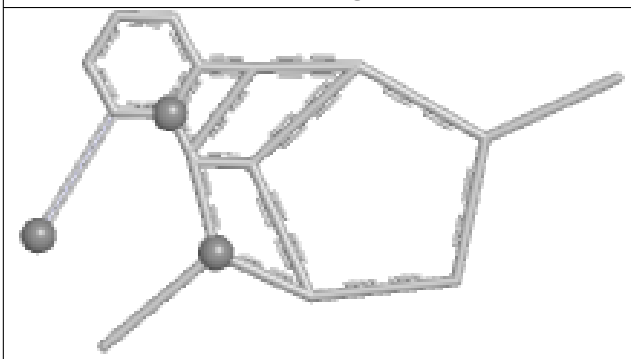
Ligand LDQ E 302



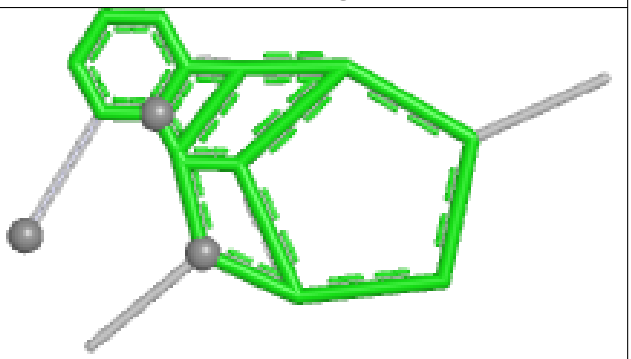
Bond lengths



Bond angles

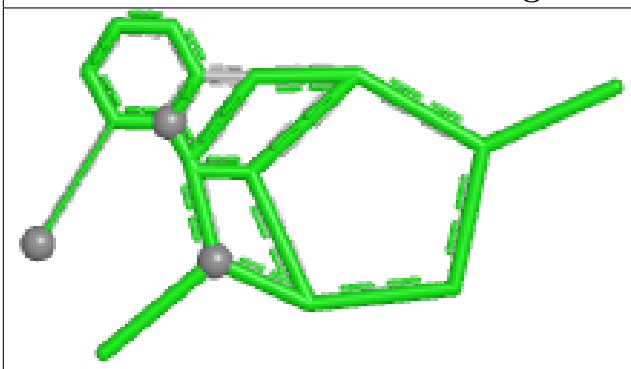


Torsions

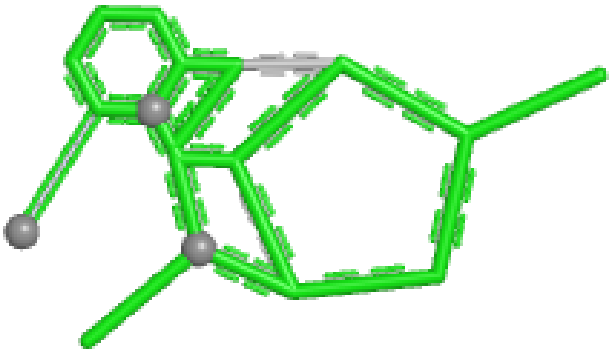


Rings

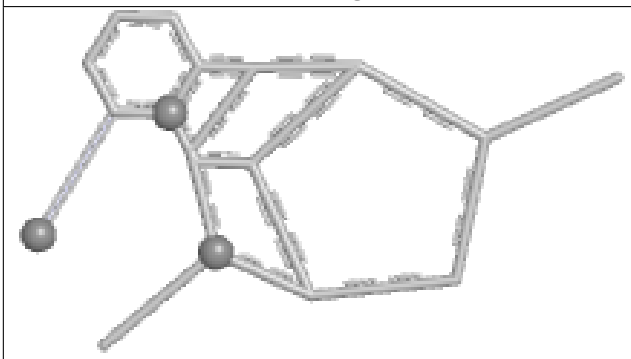
Ligand LDQ A 302



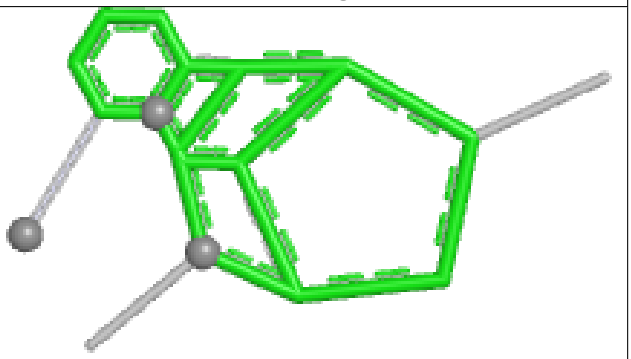
Bond lengths



Bond angles

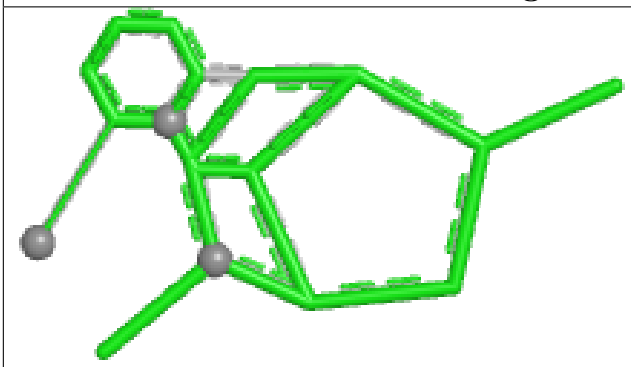


Torsions

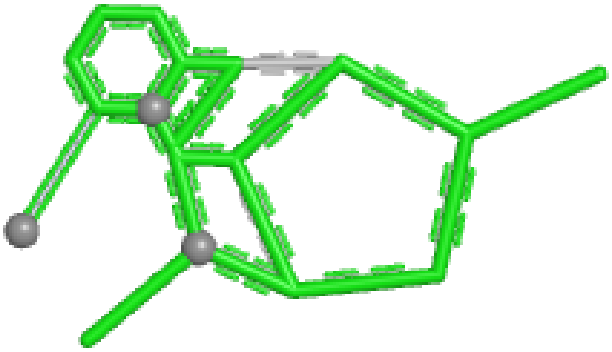


Rings

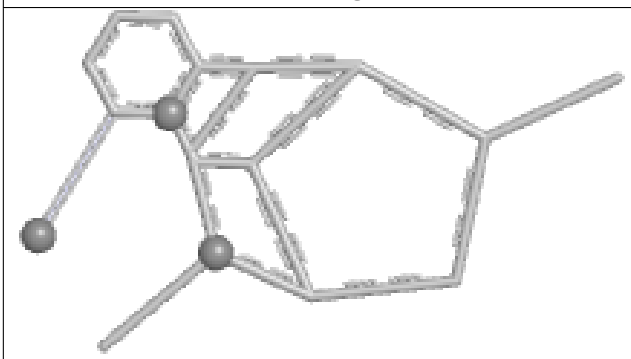
Ligand LDQ H 601



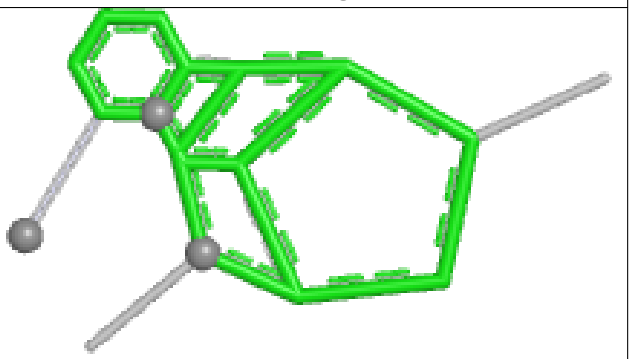
Bond lengths



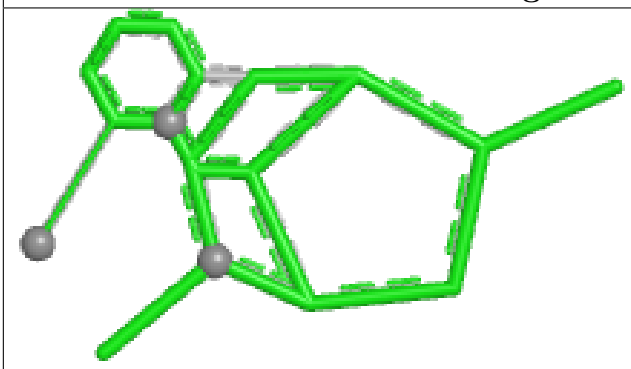
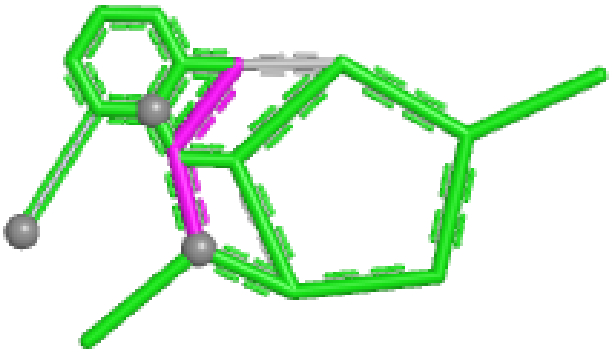
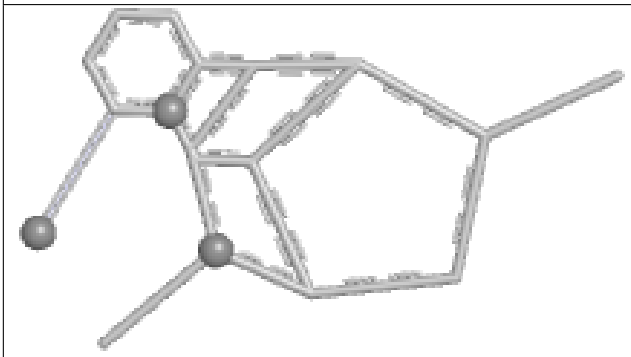
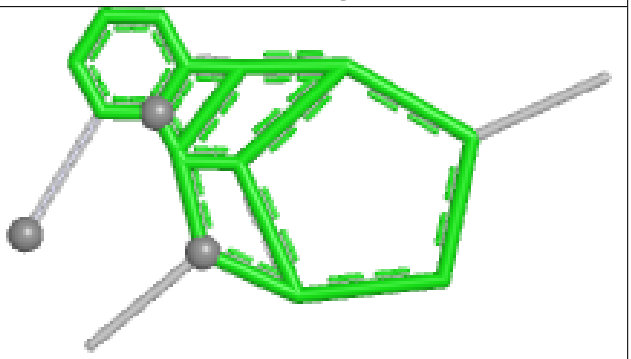
Bond angles

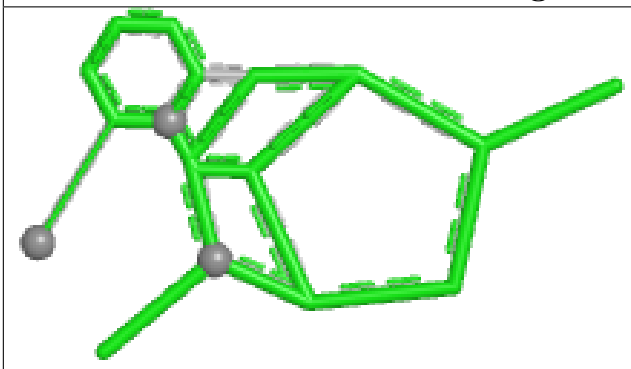
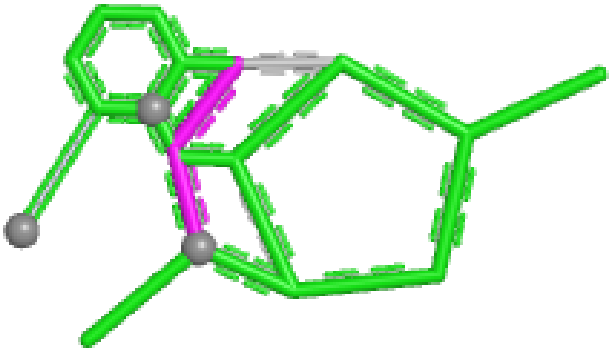
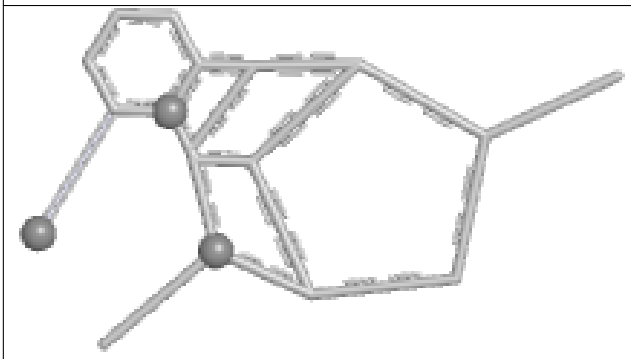
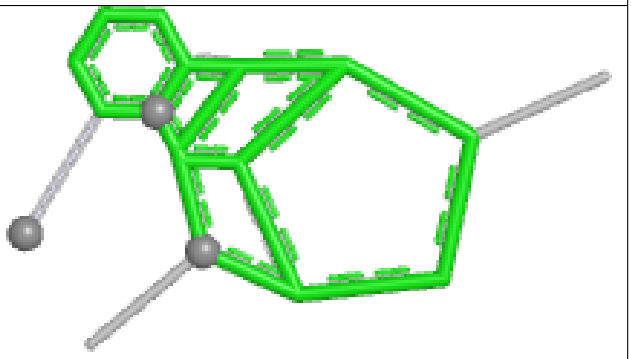


Torsions



Rings

Ligand LDQ D 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LDQ I 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 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	205/249 (82%)	0.11	5 (2%)	59	53	19, 29, 51, 91	0
1	B	205/249 (82%)	0.19	7 (3%)	45	38	19, 28, 50, 91	0
1	C	205/249 (82%)	0.01	2 (0%)	82	80	19, 27, 52, 89	0
1	D	205/249 (82%)	0.08	3 (1%)	73	70	16, 24, 49, 96	0
1	E	205/249 (82%)	0.04	4 (1%)	65	60	15, 26, 44, 84	0
1	F	205/249 (82%)	0.08	2 (0%)	82	80	16, 24, 45, 85	0
1	G	205/249 (82%)	0.02	1 (0%)	91	89	16, 25, 40, 80	0
1	H	206/249 (82%)	0.08	5 (2%)	59	53	18, 26, 53, 98	0
1	I	205/249 (82%)	0.01	4 (1%)	65	60	16, 25, 42, 90	0
1	J	205/249 (82%)	0.06	4 (1%)	65	60	17, 26, 52, 80	0
All	All	2051/2490 (82%)	0.07	37 (1%)	68	64	15, 26, 49, 98	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	ARG	4.2
1	A	33	ARG	4.0
1	B	34	SER	3.8
1	B	36	MET	3.8
1	D	33	ARG	3.8
1	H	34	SER	3.7
1	H	33	ARG	3.7
1	B	33	ARG	3.6
1	J	36	MET	3.5
1	D	34	SER	3.4
1	C	34	SER	3.2
1	E	33	ARG	3.2
1	I	35	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	35	PRO	3.0
1	A	34	SER	2.9
1	H	152	GLU	2.8
1	D	20	GLN	2.8
1	I	153	GLU	2.8
1	B	87	ASN	2.7
1	E	35	PRO	2.7
1	E	36	MET	2.6
1	A	35	PRO	2.6
1	H	225	ARG	2.5
1	I	20	GLN	2.5
1	A	147	THR	2.5
1	I	33	ARG	2.5
1	B	35	PRO	2.5
1	J	33	ARG	2.5
1	A	20	GLN	2.4
1	H	36	MET	2.3
1	J	152	GLU	2.1
1	G	34	SER	2.1
1	B	93	THR	2.1
1	F	91	ASN	2.1
1	F	36	MET	2.1
1	E	87	ASN	2.0
1	B	204	HIS	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)

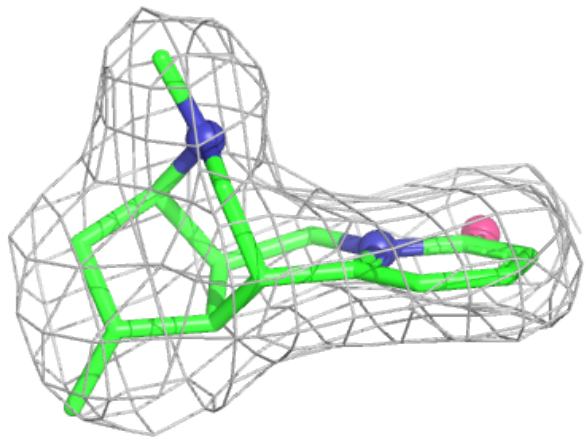
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

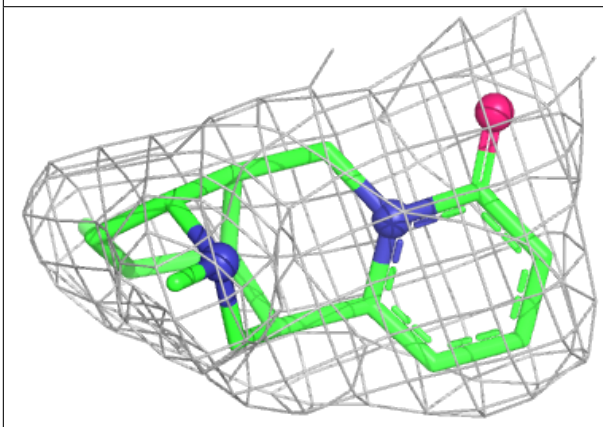
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	301	14/15	0.52	0.32	67,75,80,82	0
2	NAG	E	301	14/15	0.59	0.35	68,86,91,92	0
2	NAG	A	301	14/15	0.67	0.41	73,80,84,89	0
4	ACT	I	301	4/4	0.88	0.11	44,44,44,44	0
3	LDQ	F	601	18/18	0.90	0.19	20,22,24,24	0
3	LDQ	G	601	18/18	0.92	0.15	17,17,19,19	0
3	LDQ	E	302	18/18	0.92	0.18	16,17,19,20	0
3	LDQ	I	302	18/18	0.93	0.15	16,16,18,18	0
3	LDQ	C	302	18/18	0.93	0.14	22,24,24,24	0
3	LDQ	D	601	18/18	0.94	0.19	21,23,24,26	0
3	LDQ	H	601	18/18	0.94	0.17	18,18,20,20	0
3	LDQ	B	601	18/18	0.94	0.14	26,28,32,33	0
3	LDQ	J	601	18/18	0.94	0.14	19,20,21,21	0
3	LDQ	A	302	18/18	0.94	0.17	19,21,21,21	0

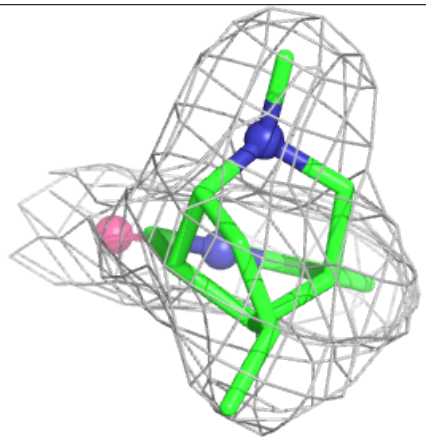
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LDQ F 601:

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

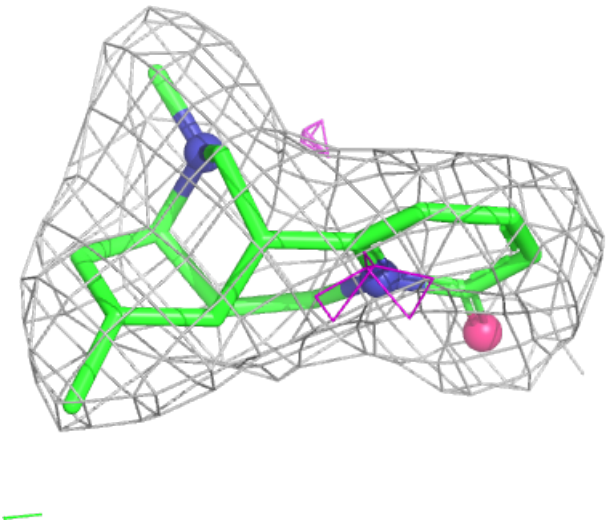


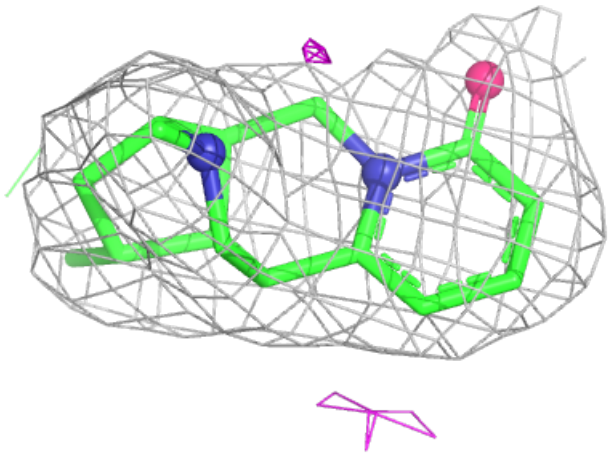


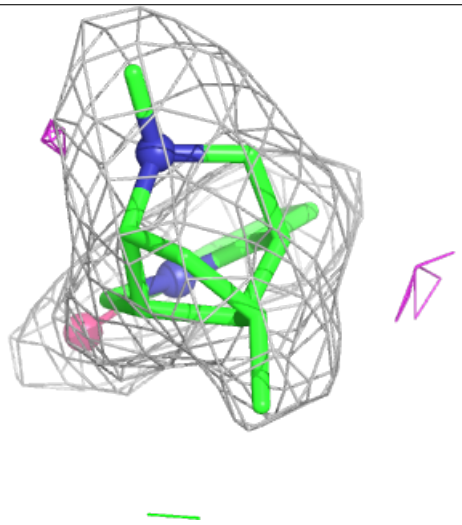


Electron density around LDQ G 601:

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

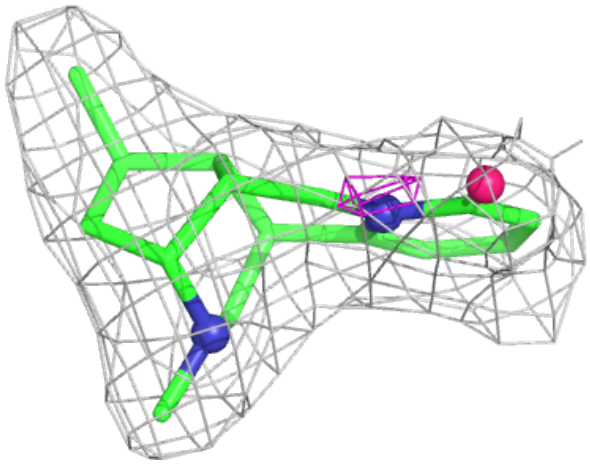


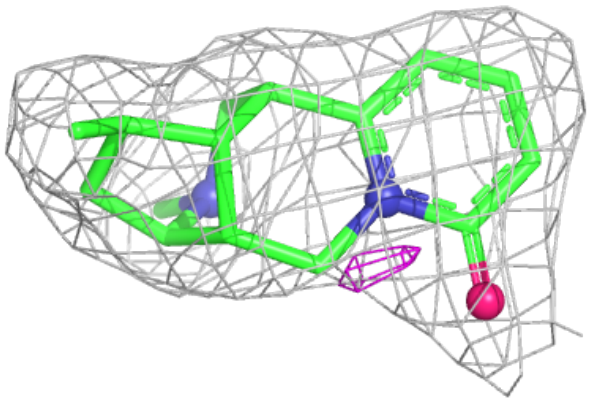


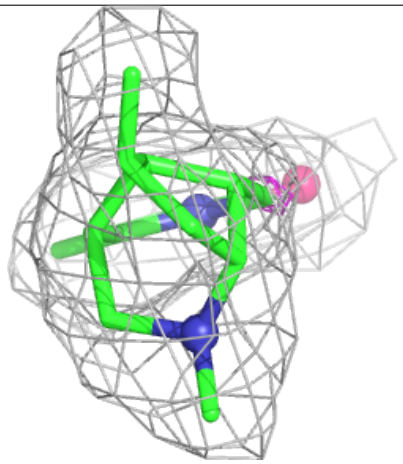


Electron density around LDQ E 302:

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

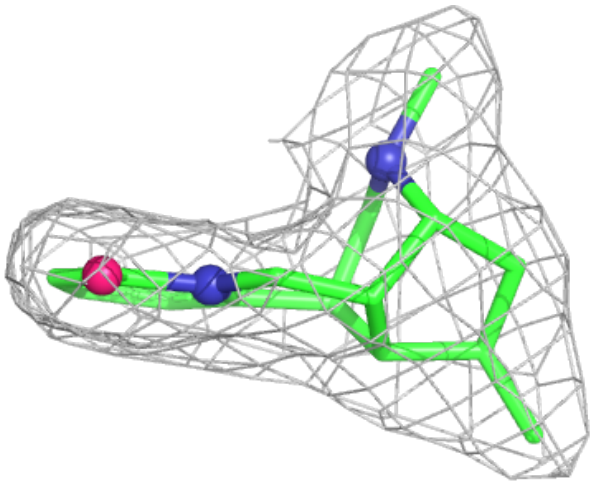


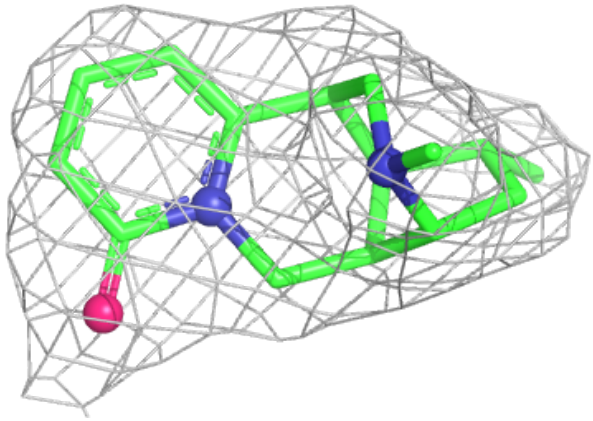


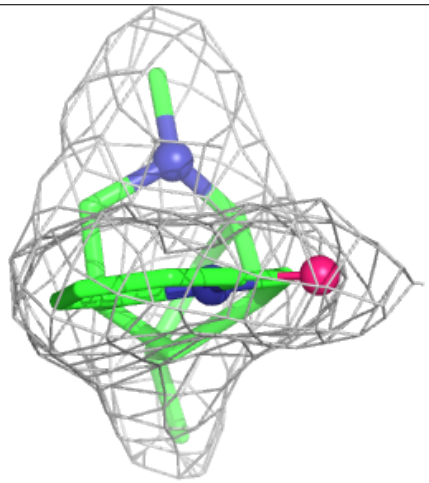


Electron density around LDQ I 302:

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

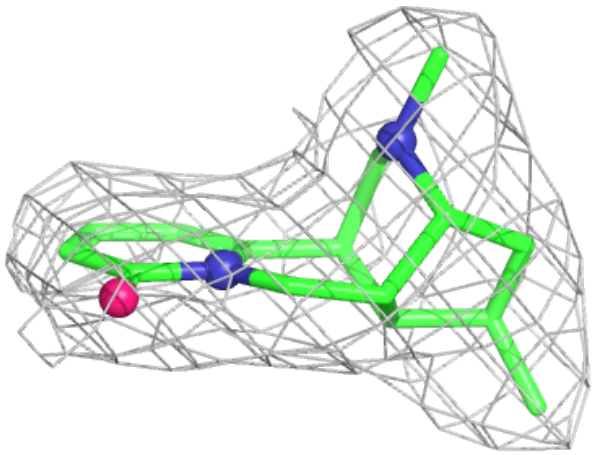


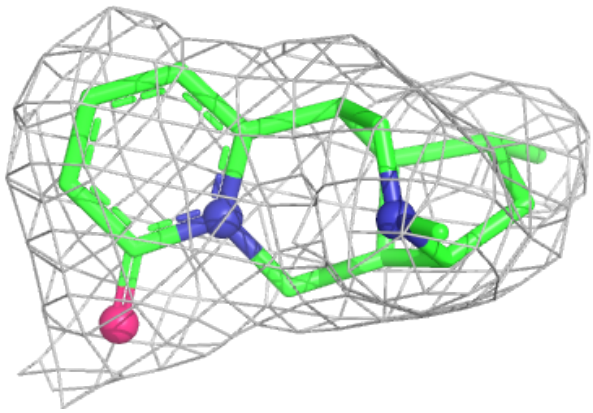


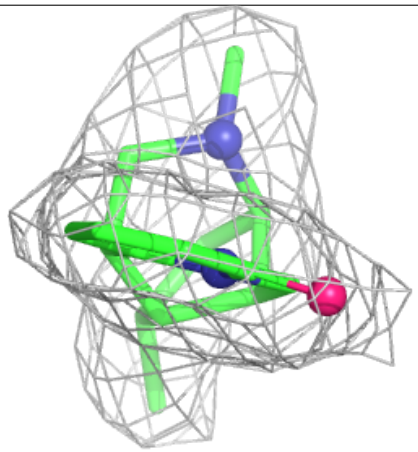


Electron density around LDQ C 302:

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

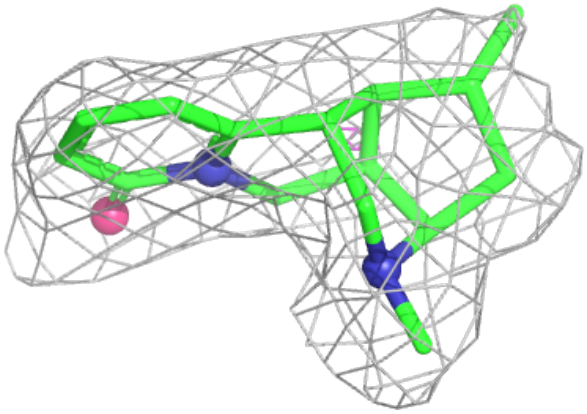


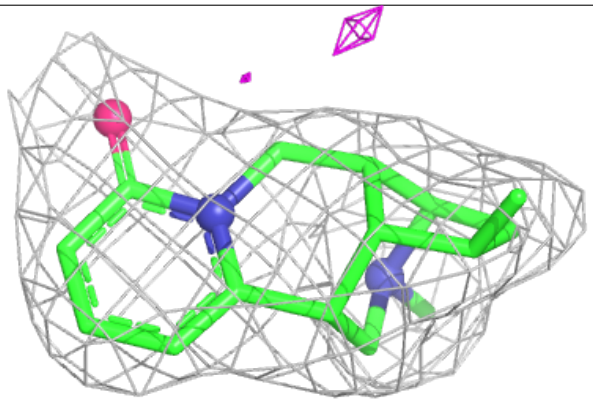


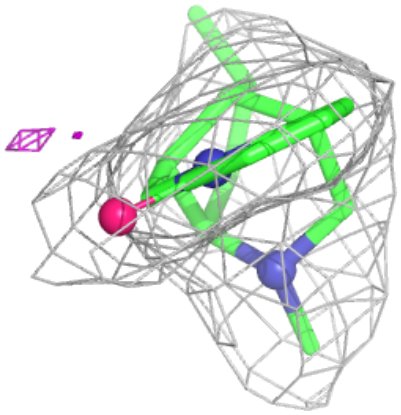


Electron density around LDQ D 601:

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

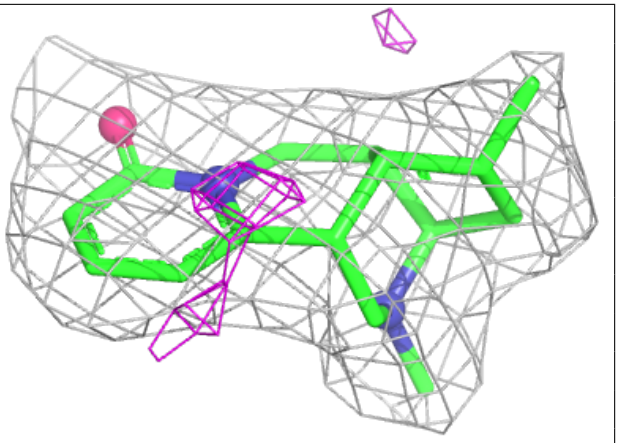


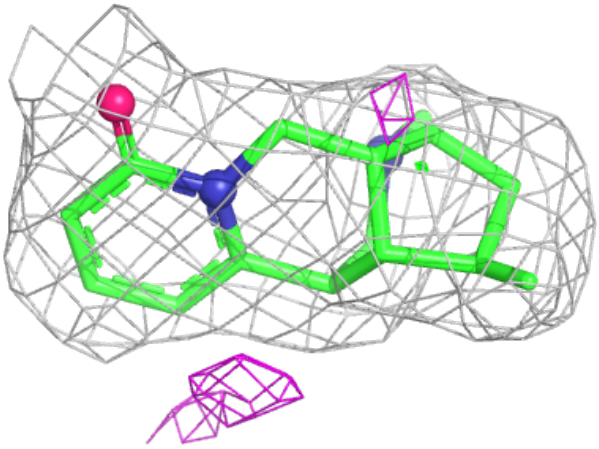


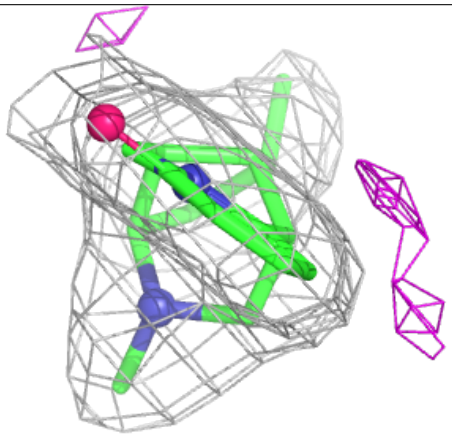


Electron density around LDQ H 601:

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

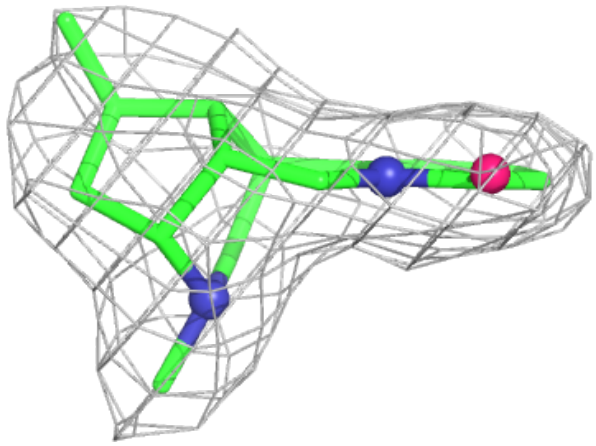


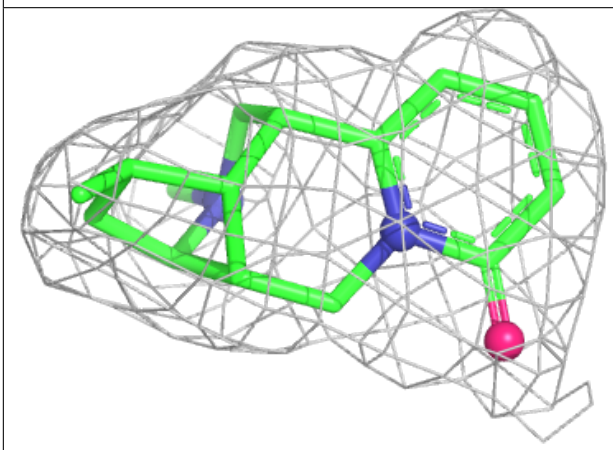


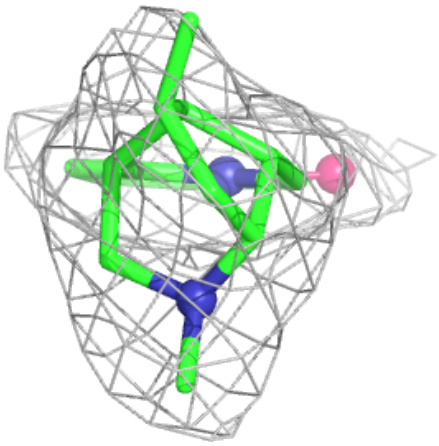


Electron density around LDQ B 601:

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

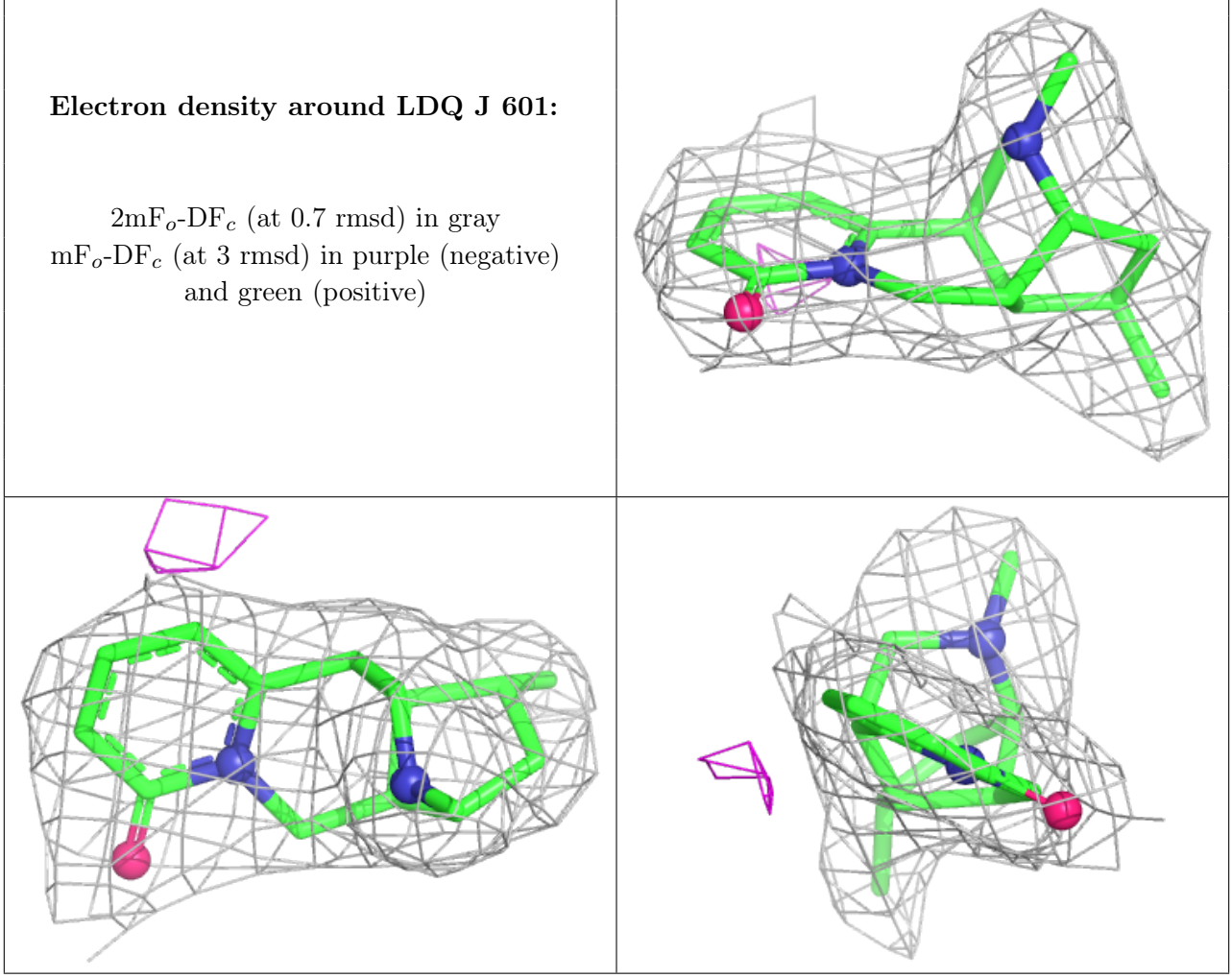






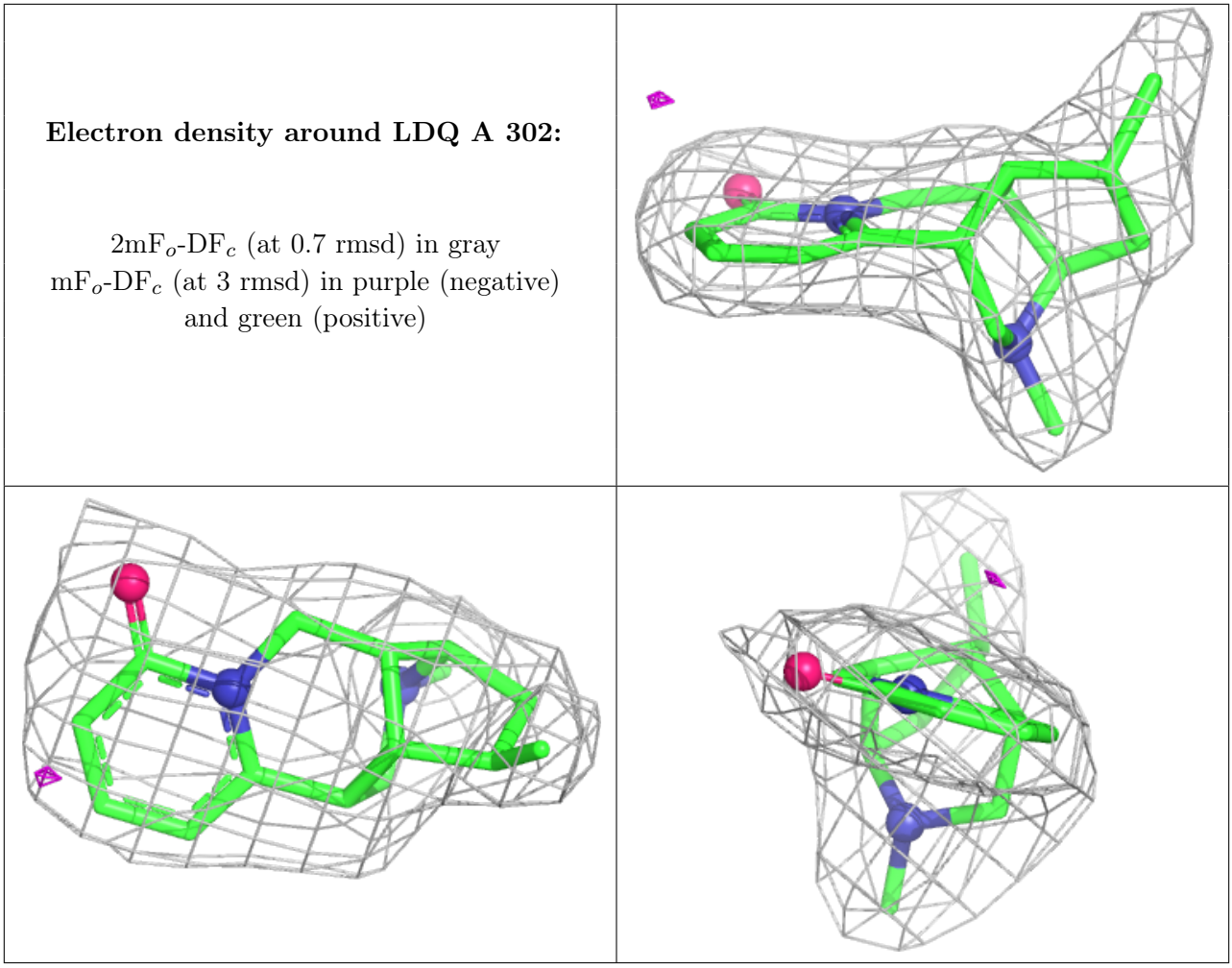
Electron density around LDQ J 601:

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



Electron density around LDQ A 302:

$2mF_o$-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.