Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 01:14 pm GMT

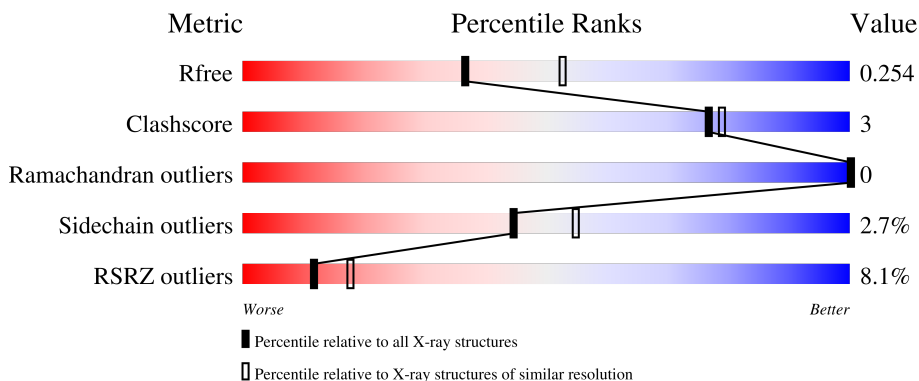|		
PDB ID	:	5LXB
Title	:	Crystal structure of a mutant binding protein (5HTBP-AChBP) in complex with palonosetron
Authors	:	Ulens, C.
Deposited on	:	2016-09-20
Resolution	:	2.34 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.34 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	Percentile Ranks	Value
Rfree		0.254
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		2.7%
RSRZ outliers		8.1%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	242	6% / 76% 7% · 15%
1	B	242	6% / 76% 8% · 15%
1	C	242	11% / 76% 8% 15%
1	D	242	5% / 78% 6% · 15%
1	E	242	4% / 75% 10% 15%

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Mol	Chain	Length	Quality of chain
1	F	242	5% ▇ 76% 7% · 15%
1	G	242	10% ▇ 75% 8% · 15%
1	H	242	9% ▇ 76% 8% · 15%
1	I	242	8% ▇ 77% 6% · 15%
1	J	242	6% ▇ 77% 7% · 15%

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
2	NAG	C	301	-	-	-	X
2	NAG	E	301	-	-	-	X
2	NAG	G	301	-	-	-	X
2	NAG	J	301	-	-	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 16946 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
			1640	1039	269	323	9			
1	B	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	C	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	D	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	E	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	F	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	G	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	H	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	I	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			
1	J	205	Total	C	N	O	S	0	0	0
			1640	1039	269	323	9			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	VAL	ALA	conflict	UNP Q8WSF8
A	53	TRP	TYR	conflict	UNP Q8WSF8
A	55	ARG	GLN	conflict	UNP Q8WSF8
A	136	VAL	ALA	conflict	UNP Q8WSF8
A	218	HIS	-	expression tag	UNP Q8WSF8
A	219	HIS	-	expression tag	UNP Q8WSF8
A	220	HIS	-	expression tag	UNP Q8WSF8
A	221	HIS	-	expression tag	UNP Q8WSF8
A	222	HIS	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	223	HIS	-	expression tag	UNP Q8WSF8
B	41	VAL	ALA	conflict	UNP Q8WSF8
B	53	TRP	TYR	conflict	UNP Q8WSF8
B	55	ARG	GLN	conflict	UNP Q8WSF8
B	136	VAL	ALA	conflict	UNP Q8WSF8
B	218	HIS	-	expression tag	UNP Q8WSF8
B	219	HIS	-	expression tag	UNP Q8WSF8
B	220	HIS	-	expression tag	UNP Q8WSF8
B	221	HIS	-	expression tag	UNP Q8WSF8
B	222	HIS	-	expression tag	UNP Q8WSF8
B	223	HIS	-	expression tag	UNP Q8WSF8
C	41	VAL	ALA	conflict	UNP Q8WSF8
C	53	TRP	TYR	conflict	UNP Q8WSF8
C	55	ARG	GLN	conflict	UNP Q8WSF8
C	136	VAL	ALA	conflict	UNP Q8WSF8
C	218	HIS	-	expression tag	UNP Q8WSF8
C	219	HIS	-	expression tag	UNP Q8WSF8
C	220	HIS	-	expression tag	UNP Q8WSF8
C	221	HIS	-	expression tag	UNP Q8WSF8
C	222	HIS	-	expression tag	UNP Q8WSF8
C	223	HIS	-	expression tag	UNP Q8WSF8
D	41	VAL	ALA	conflict	UNP Q8WSF8
D	53	TRP	TYR	conflict	UNP Q8WSF8
D	55	ARG	GLN	conflict	UNP Q8WSF8
D	136	VAL	ALA	conflict	UNP Q8WSF8
D	218	HIS	-	expression tag	UNP Q8WSF8
D	219	HIS	-	expression tag	UNP Q8WSF8
D	220	HIS	-	expression tag	UNP Q8WSF8
D	221	HIS	-	expression tag	UNP Q8WSF8
D	222	HIS	-	expression tag	UNP Q8WSF8
D	223	HIS	-	expression tag	UNP Q8WSF8
E	41	VAL	ALA	conflict	UNP Q8WSF8
E	53	TRP	TYR	conflict	UNP Q8WSF8
E	55	ARG	GLN	conflict	UNP Q8WSF8
E	136	VAL	ALA	conflict	UNP Q8WSF8
E	218	HIS	-	expression tag	UNP Q8WSF8
E	219	HIS	-	expression tag	UNP Q8WSF8
E	220	HIS	-	expression tag	UNP Q8WSF8
E	221	HIS	-	expression tag	UNP Q8WSF8
E	222	HIS	-	expression tag	UNP Q8WSF8
E	223	HIS	-	expression tag	UNP Q8WSF8
F	41	VAL	ALA	conflict	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	53	TRP	TYR	conflict	UNP Q8WSF8
F	55	ARG	GLN	conflict	UNP Q8WSF8
F	136	VAL	ALA	conflict	UNP Q8WSF8
F	218	HIS	-	expression tag	UNP Q8WSF8
F	219	HIS	-	expression tag	UNP Q8WSF8
F	220	HIS	-	expression tag	UNP Q8WSF8
F	221	HIS	-	expression tag	UNP Q8WSF8
F	222	HIS	-	expression tag	UNP Q8WSF8
F	223	HIS	-	expression tag	UNP Q8WSF8
G	41	VAL	ALA	conflict	UNP Q8WSF8
G	53	TRP	TYR	conflict	UNP Q8WSF8
G	55	ARG	GLN	conflict	UNP Q8WSF8
G	136	VAL	ALA	conflict	UNP Q8WSF8
G	218	HIS	-	expression tag	UNP Q8WSF8
G	219	HIS	-	expression tag	UNP Q8WSF8
G	220	HIS	-	expression tag	UNP Q8WSF8
G	221	HIS	-	expression tag	UNP Q8WSF8
G	222	HIS	-	expression tag	UNP Q8WSF8
G	223	HIS	-	expression tag	UNP Q8WSF8
H	41	VAL	ALA	conflict	UNP Q8WSF8
H	53	TRP	TYR	conflict	UNP Q8WSF8
H	55	ARG	GLN	conflict	UNP Q8WSF8
H	136	VAL	ALA	conflict	UNP Q8WSF8
H	218	HIS	-	expression tag	UNP Q8WSF8
H	219	HIS	-	expression tag	UNP Q8WSF8
H	220	HIS	-	expression tag	UNP Q8WSF8
H	221	HIS	-	expression tag	UNP Q8WSF8
H	222	HIS	-	expression tag	UNP Q8WSF8
H	223	HIS	-	expression tag	UNP Q8WSF8
I	41	VAL	ALA	conflict	UNP Q8WSF8
I	53	TRP	TYR	conflict	UNP Q8WSF8
I	55	ARG	GLN	conflict	UNP Q8WSF8
I	136	VAL	ALA	conflict	UNP Q8WSF8
I	218	HIS	-	expression tag	UNP Q8WSF8
I	219	HIS	-	expression tag	UNP Q8WSF8
I	220	HIS	-	expression tag	UNP Q8WSF8
I	221	HIS	-	expression tag	UNP Q8WSF8
I	222	HIS	-	expression tag	UNP Q8WSF8
I	223	HIS	-	expression tag	UNP Q8WSF8
J	41	VAL	ALA	conflict	UNP Q8WSF8
J	53	TRP	TYR	conflict	UNP Q8WSF8
J	55	ARG	GLN	conflict	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	136	VAL	ALA	conflict	UNP Q8WSF8
J	218	HIS	-	expression tag	UNP Q8WSF8
J	219	HIS	-	expression tag	UNP Q8WSF8
J	220	HIS	-	expression tag	UNP Q8WSF8
J	221	HIS	-	expression tag	UNP Q8WSF8
J	222	HIS	-	expression tag	UNP Q8WSF8
J	223	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	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is palonosetron (three-letter code: 7A9) (formula: $C_{19}H_{24}N_2O$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 22	C 19	N 2	O 1	0	0
3	C	1	Total 22	C 19	N 2	O 1	0	0
3	D	1	Total 22	C 19	N 2	O 1	0	0
3	E	1	Total 22	C 19	N 2	O 1	0	0
3	G	1	Total 22	C 19	N 2	O 1	0	0
3	H	1	Total 22	C 19	N 2	O 1	0	0
3	J	1	Total 22	C 19	N 2	O 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total 29	O 29	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	27	Total 27	O 27	0	0
4	C	11	Total 11	O 11	0	0
4	D	34	Total 34	O 34	0	0
4	E	54	Total 54	O 54	0	0
4	F	46	Total 46	O 46	0	0
4	G	20	Total 20	O 20	0	0
4	H	14	Total 14	O 14	0	0
4	I	20	Total 20	O 20	0	0
4	J	25	Total 25	O 25	0	0

3 Residue-property plots ⓘ

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.
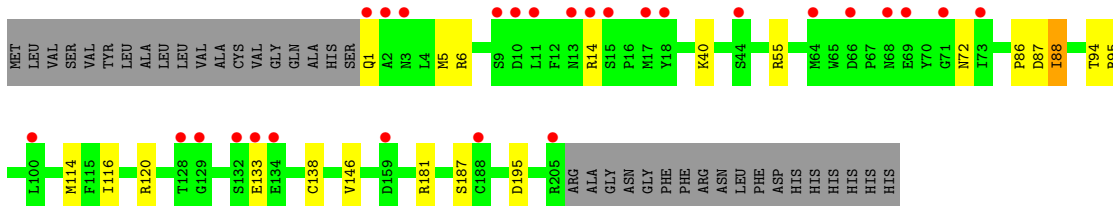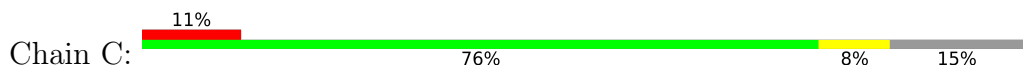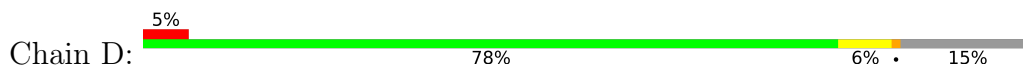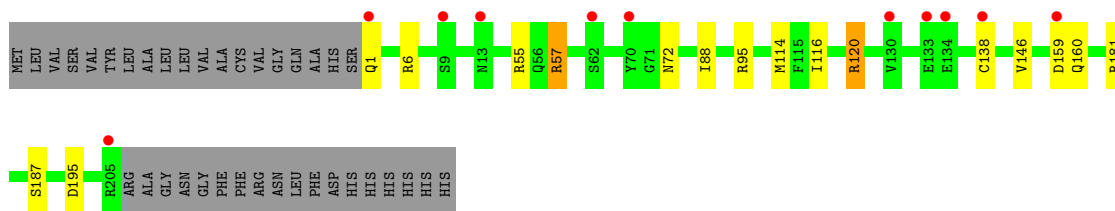
- Molecule 1: Soluble acetylcholine receptor

- Molecule 1: Soluble acetylcholine receptor

- Molecule 1: Soluble acetylcholine receptor

- Molecule 1: Soluble acetylcholine receptor

MET LEU VAL SER VAL TYR LEU ALA LEU LEU VAL ALA CYS VAL GLY GLN ALA HIS SER Q1 R6 S9 N13 R55 Q56 R57 S62 Y70 G71 N72 I88 R95 M114 F115 I116 R120 V130 E133 E134 C138 V146 D159 Q160 R181
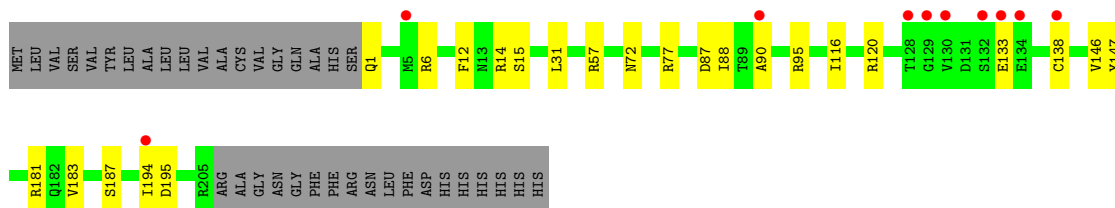
S187 D195 R205 ARG ALA GLY ASN GLY PHE PHE ARG ASN LEU PHE ASP HIS HIS HIS HIS HIS HIS

• Molecule 1: Soluble acetylcholine receptor

Chain E:

4%
75% 10% 15%

MET LEU VAL SER VAL TYR LEU ALA LEU LEU VAL ALA CYS VAL GLY GLN ALA HIS SER Q1 M5 R6 F12 N13 R14 S15 L31 R57 N72 R77 D87 I88 T89 A90 R95 I116 R120 T128 G129 V130 D131 S132 E133 E134 C138 V146 Y147

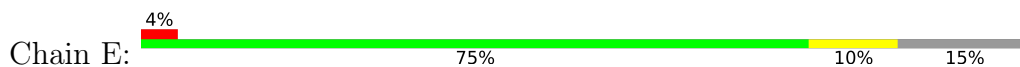R181 Q182 V183 S187 I194 D195 R205 ARG ALA GLY ASN GLY PHE PHE ARG ASN LEU PHE ASP HIS HIS HIS HIS HIS HIS

• Molecule 1: Soluble acetylcholine receptor

Chain F:

5%
76% 7% • 15%

MET LEU VAL SER VAL TYR LEU ALA LEU LEU VAL ALA CYS VAL GLY GLN ALA HIS SER Q1 M5 R6 L7 S15 P16 K23 I50 R55 D66 N72 P86 D87 I88 R95 I116 R120 L121 T128 S132 E133 E134 C138 D153 R181

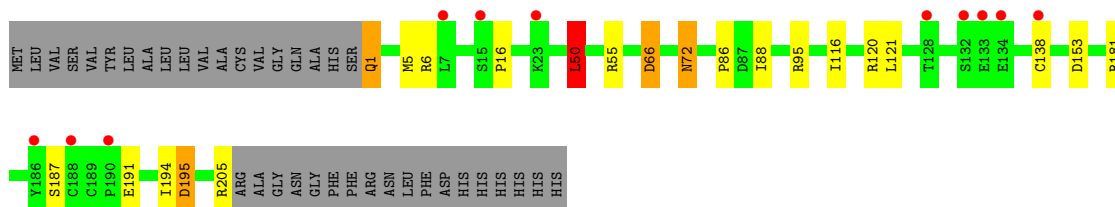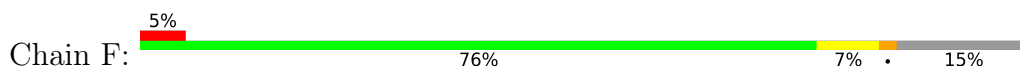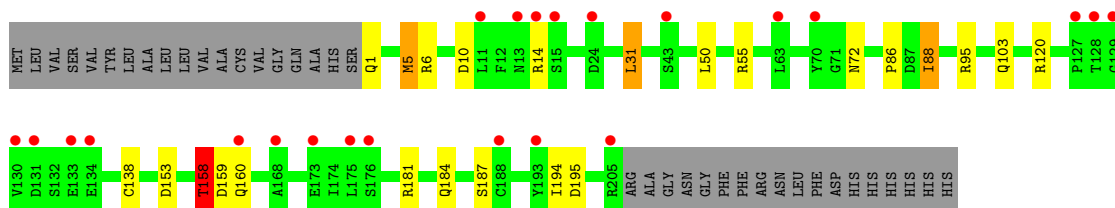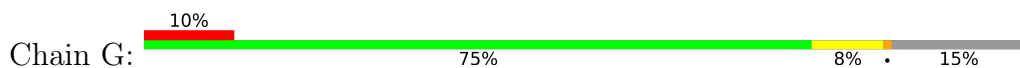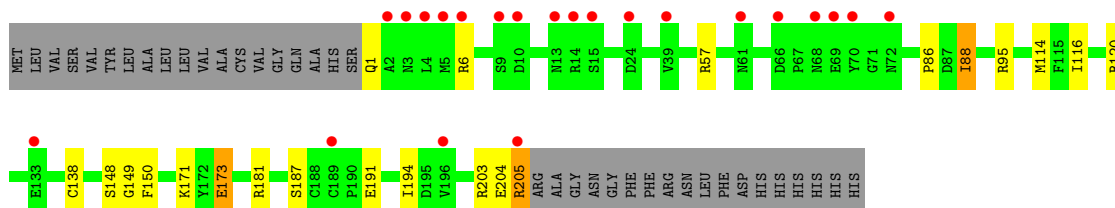Y186 S187 C188 C189 P190 E191 I194 D195 R205 ARG ALA GLY ASN GLY PHE PHE ARG ASN LEU PHE ASP HIS HIS HIS HIS HIS HIS

• Molecule 1: Soluble acetylcholine receptor

Chain G:

10%
75% 8% • 15%

MET LEU VAL SER VAL TYR LEU ALA LEU LEU VAL ALA CYS VAL GLY GLN ALA HIS SER Q1 M5 R6 D10 L11 F12 N13 R14 S15 D24 L31 S43 L50 R55 L63 Y70 G71 N72 P86 D87 I88 R95 Q103 R120 P127 T128 G129

V130 D131 S132 E133 E134 C138 D153 T158 D159 Q160 A168 E173 I174 L175 S176 R181 Q184 S187 C188 Y193 I194 D195 R205 ARG ALA GLY ASN GLY PHE PHE ARG ASN LEU PHE ASP HIS HIS HIS HIS HIS HIS

• Molecule 1: Soluble acetylcholine receptor

Chain H:

9%
76% 8% • 15%

MET LEU VAL SER VAL TYR LEU ALA LEU LEU VAL ALA CYS VAL GLY GLN ALA HIS SER Q1 A2 N3 L4 M5 R6 S9 D10 N13 R14 S15 D24 V39 R57 N61 D66 P67 N68 E69 Y70 G71 N72 P86 D87 I88 R95 M114 F115 I116 R120

E133 C138 S148 G149 F150 K171 Y172 E173 R181 S187 C188 C189 P190 E191 I194 D195 V196 R203 E204 R205 ARG ALA GLY ASN GLY PHE PHE ARG ASN LEU PHE ASP HIS HIS HIS HIS HIS HIS

• Molecule 1: Soluble acetylcholine receptor

Chain I:

• Molecule 1: Soluble acetylcholine receptor

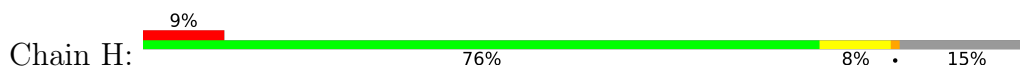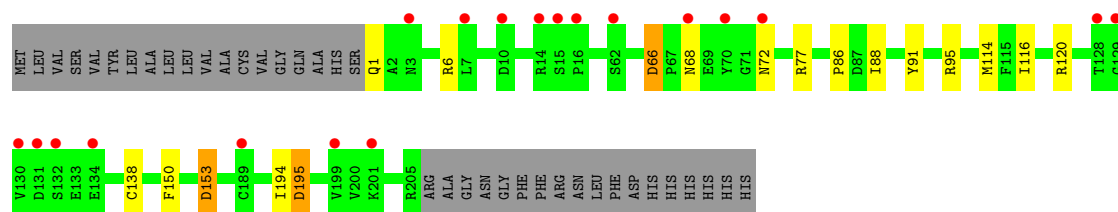Chain J:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.22Å 137.05Å 131.25Å 90.00° 93.78° 90.00°	Depositor
Resolution (Å)	130.96 – 2.34 47.34 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.8 (130.96-2.34) 98.8 (47.34-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0157	Depositor
R, R_{free}	0.218 , 0.245 0.226 , 0.254	Depositor DCC
R_{free} test set	5294 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	47.2	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16946	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 7A9, NAG

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	0.86	2/1681 (0.1%)	0.98	11/2294 (0.5%)
1	B	0.80	2/1681 (0.1%)	0.94	6/2294 (0.3%)
1	C	0.76	1/1681 (0.1%)	0.92	7/2294 (0.3%)
1	D	0.80	0/1681	1.02	8/2294 (0.3%)
1	E	0.96	2/1681 (0.1%)	0.98	8/2294 (0.3%)
1	F	0.85	1/1681 (0.1%)	1.06	13/2294 (0.6%)
1	G	0.82	1/1681 (0.1%)	1.00	11/2294 (0.5%)
1	H	0.80	1/1681 (0.1%)	0.97	10/2294 (0.4%)
1	I	0.75	0/1681	0.97	12/2294 (0.5%)
1	J	0.81	0/1681	0.94	6/2294 (0.3%)
All	All	0.82	10/16810 (0.1%)	0.98	92/22940 (0.4%)

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	E	0	1
1	F	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	GLU	CD-OE1	-9.19	1.15	1.25
1	G	158	THR	CB-CG2	-8.64	1.23	1.52
1	E	187	SER	CB-OG	-7.33	1.32	1.42
1	H	150	PHE	CG-CD2	6.52	1.48	1.38
1	A	89	THR	CB-CG2	-6.32	1.31	1.52
1	F	191	GLU	CD-OE1	-6.18	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	187	SER	CB-OG	-5.59	1.34	1.42
1	E	14	ARG	C-O	-5.52	1.12	1.23
1	B	191	GLU	CG-CD	5.43	1.60	1.51
1	B	193	TYR	CG-CD2	5.03	1.45	1.39

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	6	ARG	NE-CZ-NH2	16.05	128.32	120.30
1	D	6	ARG	NE-CZ-NH2	15.05	127.83	120.30
1	F	6	ARG	NE-CZ-NH2	14.27	127.43	120.30
1	D	181	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	B	6	ARG	NE-CZ-NH2	10.04	125.32	120.30
1	A	6	ARG	NE-CZ-NH2	9.85	125.22	120.30
1	C	6	ARG	NE-CZ-NH2	9.59	125.09	120.30
1	J	6	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	I	6	ARG	NE-CZ-NH2	9.31	124.96	120.30
1	H	6	ARG	NE-CZ-NH2	9.10	124.85	120.30
1	H	181	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	E	95	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	F	55	ARG	NE-CZ-NH2	8.43	124.51	120.30
1	I	66	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	G	6	ARG	NH1-CZ-NH2	-8.36	110.20	119.40
1	F	50	LEU	CB-CG-CD1	-8.36	96.79	111.00
1	D	6	ARG	NH1-CZ-NH2	-8.32	110.25	119.40
1	E	95	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	E	6	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	F	6	ARG	NH1-CZ-NH2	-8.08	110.52	119.40
1	E	181	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	F	66	ASP	CB-CG-OD2	7.62	125.15	118.30
1	H	95	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	F	66	ASP	CB-CG-OD1	-7.42	111.63	118.30
1	I	150	PHE	CB-CG-CD2	-7.40	115.62	120.80
1	F	95	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	I	150	PHE	CB-CG-CD1	7.16	125.81	120.80
1	A	77	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	D	55	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	A	95	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	D	57	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	I	77	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	95	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	D	120	ARG	NE-CZ-NH1	6.79	123.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	195	ASP	CB-CG-OD2	6.76	124.38	118.30
1	A	150	PHE	CB-CG-CD2	-6.71	116.10	120.80
1	B	31	LEU	CA-CB-CG	6.69	130.69	115.30
1	E	6	ARG	CG-CD-NE	-6.46	98.24	111.80
1	C	181	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	G	95	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	F	95	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	H	120	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	E	31	LEU	CA-CB-CG	6.10	129.34	115.30
1	G	31	LEU	CA-CB-CG	6.10	129.34	115.30
1	J	55	ARG	NE-CZ-NH2	5.99	123.30	120.30
1	H	120	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	I	195	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	193	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	A	138	CYS	CA-CB-SG	-5.87	103.43	114.00
1	F	120	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	95	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	J	95	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	95	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	J	95	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	181	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	I	153	ASP	CB-CG-OD1	5.66	123.39	118.30
1	I	95	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	I	120	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	5	MET	CG-SD-CE	5.61	109.18	100.20
1	H	173	GLU	CA-CB-CG	5.60	125.71	113.40
1	G	181	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	95	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	G	120	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	95	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	120	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	I	95	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	F	181	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	E	120	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	H	205	ARG	CA-CB-CG	5.45	125.40	113.40
1	J	114	MET	CG-SD-CE	5.42	108.87	100.20
1	E	12	PHE	CB-CG-CD1	-5.41	117.01	120.80
1	C	95	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	89	THR	CA-CB-CG2	-5.34	104.93	112.40
1	G	95	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	H	95	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	F	55	ARG	CB-CG-CD	5.31	125.40	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	120	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	I	66	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	95	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	I	91	TYR	CB-CG-CD1	5.26	124.16	121.00
1	A	6	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	G	88	ILE	CG1-CB-CG2	-5.19	99.98	111.40
1	B	120	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	H	203	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	G	184	GLN	CA-CB-CG	5.13	124.69	113.40
1	H	88	ILE	CG1-CB-CG2	-5.10	100.18	111.40
1	B	181	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	G	103	GLN	CA-CB-CG	-5.04	102.31	113.40
1	A	120	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	114	MET	CG-SD-CE	-5.03	92.16	100.20
1	G	5	MET	CG-SD-CE	5.03	108.24	100.20
1	J	120	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	15	SER	Peptide
1	F	72	ASN	Sidechain

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	1640	0	1580	17	0
1	B	1640	0	1578	12	0
1	C	1640	0	1578	7	0
1	D	1640	0	1578	9	0
1	E	1640	0	1578	10	0
1	F	1640	0	1578	12	0
1	G	1640	0	1578	11	0
1	H	1640	0	1578	13	0
1	I	1640	0	1578	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1640	0	1578	7	0
2	A	14	0	13	3	0
2	C	14	0	13	1	0
2	D	14	0	13	1	0
2	E	14	0	13	1	0
2	F	14	0	13	2	0
2	G	14	0	13	1	0
2	I	14	0	13	3	0
2	J	14	0	13	0	0
3	B	22	0	0	0	0
3	C	22	0	0	0	0
3	D	22	0	0	0	0
3	E	22	0	0	0	0
3	G	22	0	0	0	0
3	H	22	0	0	0	0
3	J	22	0	0	0	0
4	A	29	0	0	0	0
4	B	27	0	0	0	0
4	C	11	0	0	0	0
4	D	34	0	0	0	0
4	E	54	0	0	1	0
4	F	46	0	0	0	0
4	G	20	0	0	0	0
4	H	14	0	0	0	0
4	I	20	0	0	0	0
4	J	25	0	0	0	0
All	All	16946	0	15886	97	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (97) 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:F:72:ASN:HD21	2:F:301:NAG:C1	1.75	0.99
1:A:125:CYS:SG	1:A:138:CYS:HB3	2.16	0.85
1:A:89:THR:HG21	1:B:102:PRO:HD3	1.67	0.76
1:F:72:ASN:ND2	2:F:301:NAG:C1	2.50	0.74
1:E:1:GLN:N	1:E:1:GLN:OE1	2.22	0.73
1:D:159:ASP:OD1	1:D:160:GLN:NE2	2.22	0.73
1:G:1:GLN:OE1	1:G:1:GLN:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ASN:OD1	2:D:301:NAG:C1	2.38	0.71
1:H:1:GLN:N	1:H:1:GLN:OE1	2.23	0.71
1:C:1:GLN:OE1	1:C:1:GLN:N	2.23	0.71
1:A:1:GLN:N	1:A:1:GLN:OE1	2.24	0.71
1:B:149:GLY:CA	1:B:194:ILE:CD1	2.69	0.71
1:F:1:GLN:OE1	1:F:1:GLN:N	2.23	0.70
1:H:149:GLY:CA	1:H:194:ILE:CD1	2.69	0.70
1:B:149:GLY:HA2	1:B:194:ILE:CD1	2.22	0.70
1:H:149:GLY:HA2	1:H:194:ILE:CD1	2.22	0.69
1:J:1:GLN:OE1	1:J:1:GLN:N	2.25	0.69
1:G:158:THR:HG23	1:G:160:GLN:H	1.59	0.67
1:B:1:GLN:OE1	1:B:1:GLN:N	2.22	0.67
1:H:149:GLY:HA2	1:H:194:ILE:HD13	1.78	0.66
1:I:1:GLN:OE1	1:I:1:GLN:N	2.23	0.65
1:E:90:ALA:O	4:E:401:HOH:O	2.13	0.65
1:A:72:ASN:HD21	2:A:301:NAG:C1	2.10	0.64
1:B:149:GLY:HA2	1:B:194:ILE:HD13	1.79	0.64
1:B:149:GLY:HA3	1:B:194:ILE:HD11	1.80	0.64
1:F:5:MET:CE	1:J:16:PRO:HD2	2.29	0.62
1:H:173:GLU:HG3	1:H:205:ARG:C	2.21	0.61
1:H:149:GLY:HA3	1:H:194:ILE:HD11	1.83	0.60
1:C:86:PRO:HB2	1:C:88:ILE:HD13	1.83	0.60
1:B:86:PRO:HB2	1:B:88:ILE:HD13	1.85	0.58
1:D:1:GLN:N	1:D:1:GLN:OE1	2.34	0.58
1:F:16:PRO:HD2	1:G:5:MET:HE3	1.84	0.58
1:J:184:GLN:HG3	1:J:195:ASP:OD2	2.03	0.58
1:H:86:PRO:HB2	1:H:88:ILE:HD13	1.86	0.57
1:H:149:GLY:HA3	1:H:194:ILE:CD1	2.33	0.57
1:B:149:GLY:HA3	1:B:194:ILE:CD1	2.33	0.57
1:G:153:ASP:OD1	1:G:194:ILE:HD13	2.04	0.56
1:H:204:GLU:O	1:H:205:ARG:HG3	2.05	0.56
1:G:158:THR:CG2	1:G:160:GLN:H	2.19	0.55
1:F:153:ASP:OD1	1:F:194:ILE:HD13	2.06	0.55
1:H:148:SER:HB3	1:H:191:GLU:HG3	1.88	0.55
1:E:72:ASN:OD1	2:E:301:NAG:C1	2.56	0.54
1:I:153:ASP:OD1	1:I:194:ILE:HD13	2.08	0.53
1:A:16:PRO:HD2	1:B:5:MET:CE	2.39	0.53
1:F:86:PRO:HB2	1:F:88:ILE:HD13	1.90	0.53
1:A:114:MET:HG3	1:A:116:ILE:HD11	1.89	0.53
1:I:72:ASN:HD21	2:I:301:NAG:C1	2.21	0.52
1:D:114:MET:HG3	1:D:116:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:MET:HG3	1:H:116:ILE:HD11	1.93	0.51
1:G:86:PRO:HB2	1:G:88:ILE:HD13	1.91	0.51
1:A:148:SER:HB3	1:A:191:GLU:HG3	1.93	0.51
1:I:86:PRO:HB2	1:I:88:ILE:HD13	1.93	0.50
1:I:72:ASN:ND2	2:I:301:NAG:C1	2.75	0.50
1:A:183:VAL:HG22	1:A:194:ILE:HD12	1.93	0.50
1:G:72:ASN:HD21	2:G:301:NAG:C1	2.25	0.50
1:A:125:CYS:SG	1:A:138:CYS:CB	2.94	0.49
1:A:72:ASN:HD21	2:A:301:NAG:C2	2.24	0.49
1:A:16:PRO:HG2	1:B:5:MET:HE2	1.94	0.48
1:B:184:GLN:HG3	1:B:195:ASP:OD2	2.14	0.48
1:I:114:MET:HG3	1:I:116:ILE:HD11	1.96	0.48
1:J:86:PRO:HB2	1:J:88:ILE:HD13	1.95	0.47
1:A:72:ASN:HD21	2:A:301:NAG:H2	1.79	0.47
1:E:133:GLU:N	1:E:133:GLU:OE1	2.48	0.47
1:C:72:ASN:OD1	2:C:301:NAG:C7	2.63	0.47
1:A:77:ARG:HD3	1:E:147:TYR:CE1	2.50	0.46
1:C:55:ARG:HG2	1:C:116:ILE:HD13	1.97	0.46
1:B:55:ARG:HG2	1:B:116:ILE:HD13	1.97	0.46
1:F:50:LEU:HD11	1:F:121:LEU:HD23	1.99	0.45
1:I:72:ASN:OD1	2:I:301:NAG:C7	2.66	0.44
1:F:1:GLN:N	1:F:1:GLN:CD	2.72	0.44
1:A:148:SER:CB	1:A:191:GLU:HG3	2.48	0.43
1:F:16:PRO:HD2	1:G:5:MET:CE	2.47	0.43
1:H:116:ILE:N	1:H:116:ILE:HD12	2.33	0.43
1:E:116:ILE:HD12	1:E:116:ILE:N	2.33	0.43
1:I:66:ASP:CG	1:I:68:ASN:OD1	2.56	0.43
1:I:116:ILE:HD12	1:I:116:ILE:N	2.34	0.43
1:D:146:VAL:HG23	1:E:77:ARG:HG2	1.99	0.43
1:F:116:ILE:HD12	1:F:116:ILE:N	2.34	0.43
1:J:183:VAL:HG22	1:J:194:ILE:HD12	2.01	0.43
1:G:1:GLN:N	1:G:1:GLN:CD	2.72	0.43
1:D:116:ILE:HD12	1:D:116:ILE:N	2.34	0.43
1:D:1:GLN:N	1:D:1:GLN:CD	2.73	0.42
1:C:1:GLN:N	1:C:1:GLN:CD	2.73	0.42
1:J:1:GLN:N	1:J:1:GLN:CD	2.72	0.42
1:A:116:ILE:N	1:A:116:ILE:HD12	2.33	0.42
1:H:1:GLN:N	1:H:1:GLN:CD	2.73	0.42
1:I:1:GLN:N	1:I:1:GLN:CD	2.73	0.42
1:G:10:ASP:HA	1:G:14:ARG:HD3	2.02	0.42
1:G:158:THR:HG23	1:G:159:ASP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:VAL:HG22	1:E:194:ILE:HD12	2.02	0.41
1:A:1:GLN:N	1:A:1:GLN:CD	2.73	0.41
1:A:77:ARG:HG2	1:E:146:VAL:HG23	2.03	0.41
1:C:94:THR:O	1:D:120:ARG:HD2	2.21	0.41
1:E:87:ASP:OD2	1:E:146:VAL:HG22	2.21	0.41
1:D:159:ASP:OD1	1:D:159:ASP:C	2.58	0.40
1:C:87:ASP:OD2	1:C:146:VAL:HG22	2.22	0.40
1:F:5:MET:HE1	1:J:16:PRO:HD2	1.99	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	203/242 (84%)	200 (98%)	3 (2%)	0	100	100
1	B	203/242 (84%)	201 (99%)	2 (1%)	0	100	100
1	C	203/242 (84%)	201 (99%)	2 (1%)	0	100	100
1	D	203/242 (84%)	200 (98%)	3 (2%)	0	100	100
1	E	203/242 (84%)	200 (98%)	3 (2%)	0	100	100
1	F	203/242 (84%)	201 (99%)	2 (1%)	0	100	100
1	G	203/242 (84%)	200 (98%)	3 (2%)	0	100	100
1	H	203/242 (84%)	201 (99%)	2 (1%)	0	100	100
1	I	203/242 (84%)	199 (98%)	4 (2%)	0	100	100
1	J	203/242 (84%)	200 (98%)	3 (2%)	0	100	100
All	All	2030/2420 (84%)	2003 (99%)	27 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/218 (86%)	186 (99%)	2 (1%)	73	83
1	B	188/218 (86%)	183 (97%)	5 (3%)	44	55
1	C	188/218 (86%)	182 (97%)	6 (3%)	39	47
1	D	188/218 (86%)	183 (97%)	5 (3%)	44	55
1	E	188/218 (86%)	184 (98%)	4 (2%)	53	65
1	F	188/218 (86%)	181 (96%)	7 (4%)	34	43
1	G	188/218 (86%)	181 (96%)	7 (4%)	34	43
1	H	188/218 (86%)	184 (98%)	4 (2%)	53	65
1	I	188/218 (86%)	186 (99%)	2 (1%)	73	83
1	J	188/218 (86%)	179 (95%)	9 (5%)	25	32
All	All	1880/2180 (86%)	1829 (97%)	51 (3%)	44	55

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ILE
1	A	195	ASP
1	B	57	ARG
1	B	88	ILE
1	B	138	CYS
1	B	187	SER
1	B	195	ASP
1	C	14	ARG
1	C	40	LYS
1	C	88	ILE
1	C	133	GLU
1	C	138	CYS
1	C	195	ASP
1	D	57	ARG
1	D	88	ILE
1	D	138	CYS

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Mol	Chain	Res	Type
1	D	187	SER
1	D	195	ASP
1	E	57	ARG
1	E	88	ILE
1	E	138	CYS
1	E	195	ASP
1	F	1	GLN
1	F	50	LEU
1	F	66	ASP
1	F	138	CYS
1	F	187	SER
1	F	195	ASP
1	F	205	ARG
1	G	31	LEU
1	G	50	LEU
1	G	55	ARG
1	G	138	CYS
1	G	158	THR
1	G	187	SER
1	G	195	ASP
1	H	57	ARG
1	H	138	CYS
1	H	171	LYS
1	H	187	SER
1	I	138	CYS
1	I	195	ASP
1	J	1	GLN
1	J	15	SER
1	J	50	LEU
1	J	55	ARG
1	J	57	ARG
1	J	69	GLU
1	J	138	CYS
1	J	187	SER
1	J	195	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	182	GLN
1	A	184	GLN

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Mol	Chain	Res	Type
1	B	103	GLN
1	B	182	GLN
1	C	103	GLN
1	C	182	GLN
1	D	103	GLN
1	D	182	GLN
1	E	182	GLN
1	F	72	ASN
1	F	182	GLN
1	G	182	GLN
1	H	182	GLN
1	I	72	ASN
1	I	182	GLN

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 ⓘ

15 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	NAG	A	301	-	14,14,15	0.65	0	17,19,21	1.80	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	NAG	I	301	-	14,14,15	0.73	0	17,19,21	1.77	4 (23%)
3	7A9	H	301	-	26,26,26	0.91	1 (3%)	33,39,39	0.93	0
3	7A9	D	302	-	26,26,26	0.98	2 (7%)	33,39,39	0.96	2 (6%)
3	7A9	G	302	-	26,26,26	0.73	0	33,39,39	0.97	2 (6%)
2	NAG	D	301	-	14,14,15	0.72	0	17,19,21	2.37	6 (35%)
2	NAG	E	301	-	14,14,15	0.72	0	17,19,21	1.83	4 (23%)
2	NAG	G	301	-	14,14,15	0.43	0	17,19,21	1.04	1 (5%)
3	7A9	J	302	-	26,26,26	0.91	0	33,39,39	1.14	3 (9%)
3	7A9	C	302	-	26,26,26	1.17	4 (15%)	33,39,39	1.43	5 (15%)
3	7A9	B	301	-	26,26,26	0.77	0	33,39,39	1.32	4 (12%)
2	NAG	F	301	-	14,14,15	0.81	0	17,19,21	3.24	8 (47%)
3	7A9	E	302	-	26,26,26	0.72	0	33,39,39	1.08	3 (9%)
2	NAG	J	301	-	14,14,15	0.58	0	17,19,21	1.01	1 (5%)
2	NAG	C	301	-	14,14,15	0.60	0	17,19,21	1.35	3 (17%)

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	NAG	A	301	-	-	1/6/23/26	0/1/1/1
2	NAG	I	301	-	-	1/6/23/26	0/1/1/1
3	7A9	H	301	-	-	3/4/44/44	0/6/5/5
3	7A9	D	302	-	-	3/4/44/44	0/6/5/5
3	7A9	G	302	-	-	2/4/44/44	0/6/5/5
2	NAG	D	301	-	-	4/6/23/26	0/1/1/1
2	NAG	E	301	-	-	0/6/23/26	0/1/1/1
2	NAG	G	301	-	-	0/6/23/26	0/1/1/1
3	7A9	J	302	-	-	2/4/44/44	0/6/5/5
3	7A9	C	302	-	-	4/4/44/44	0/6/5/5
3	7A9	B	301	-	-	2/4/44/44	0/6/5/5
2	NAG	F	301	-	-	5/6/23/26	0/1/1/1
3	7A9	E	302	-	-	2/4/44/44	0/6/5/5
2	NAG	J	301	-	-	3/6/23/26	0/1/1/1
2	NAG	C	301	-	-	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	7A9	C09-C03	-2.74	1.47	1.51
3	H	301	7A9	C08-C06	2.38	1.52	1.47
3	C	302	7A9	C16-N17	2.37	1.50	1.46
3	D	302	7A9	C09-C03	-2.36	1.47	1.51
3	C	302	7A9	C16-C15	2.29	1.57	1.53
3	C	302	7A9	C04-C03	-2.15	1.51	1.53
3	D	302	7A9	C06-N05	-2.05	1.32	1.36

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	NAG	C2-N2-C7	7.13	133.06	122.90
2	F	301	NAG	O5-C1-C2	-6.97	100.28	111.29
2	F	301	NAG	C1-O5-C5	-5.38	104.91	112.19
2	D	301	NAG	C2-N2-C7	4.92	129.91	122.90
2	D	301	NAG	C1-O5-C5	4.40	118.15	112.19
2	A	301	NAG	C1-O5-C5	4.34	118.07	112.19
3	C	302	7A9	O07-C06-N05	4.29	125.30	121.96
2	I	301	NAG	O4-C4-C5	3.99	119.20	109.30
2	E	301	NAG	C1-O5-C5	-3.89	106.92	112.19
2	A	301	NAG	C4-C3-C2	-3.85	105.38	111.02
2	C	301	NAG	C1-O5-C5	3.55	117.00	112.19
2	E	301	NAG	C2-N2-C7	3.50	127.89	122.90
2	D	301	NAG	O5-C1-C2	3.44	116.72	111.29
2	F	301	NAG	C1-C2-N2	3.42	116.33	110.49
2	D	301	NAG	C4-C3-C2	3.29	115.84	111.02
2	G	301	NAG	C1-O5-C5	3.26	116.61	112.19
3	C	302	7A9	C08-C06-N05	3.25	119.51	116.24
2	F	301	NAG	O7-C7-N2	-3.12	116.21	121.95
2	D	301	NAG	C1-C2-N2	3.08	115.75	110.49
3	B	301	7A9	C19-C20-C21	-3.07	104.02	109.44
2	F	301	NAG	C8-C7-N2	3.02	121.22	116.10
3	C	302	7A9	O07-C06-C08	-2.95	115.13	122.99
2	I	301	NAG	C1-O5-C5	2.91	116.13	112.19
2	F	301	NAG	C4-C3-C2	-2.66	107.11	111.02
3	B	301	7A9	C08-C06-N05	2.66	118.91	116.24
2	I	301	NAG	C3-C4-C5	-2.64	105.53	110.24
3	B	301	7A9	O07-C06-N05	2.54	123.94	121.96
3	J	302	7A9	C19-C20-C21	-2.53	104.99	109.44
3	E	302	7A9	O07-C06-N05	2.52	123.92	121.96
2	F	301	NAG	O5-C5-C6	2.46	111.06	107.20
2	E	301	NAG	O3-C3-C2	2.44	114.52	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	301	NAG	C4-C3-C2	2.44	114.59	111.02
3	J	302	7A9	C15-C16-N17	-2.44	107.07	111.29
3	G	302	7A9	C03-C04-N05	2.43	115.81	110.96
2	D	301	NAG	O7-C7-N2	2.36	126.30	121.95
2	I	301	NAG	C6-C5-C4	2.33	118.45	113.00
3	E	302	7A9	C03-C04-N05	2.27	115.50	110.96
3	C	302	7A9	C09-C08-C06	-2.25	119.15	121.22
3	B	301	7A9	O07-C06-C08	-2.20	117.13	122.99
3	E	302	7A9	C19-C20-C21	-2.15	105.64	109.44
2	C	301	NAG	C3-C4-C5	2.15	114.08	110.24
3	D	302	7A9	C03-C04-N05	2.11	115.18	110.96
2	C	301	NAG	C2-N2-C7	2.11	125.91	122.90
2	E	301	NAG	O7-C7-N2	2.08	125.78	121.95
3	G	302	7A9	C08-C06-N05	2.07	118.33	116.24
3	D	302	7A9	O07-C06-N05	2.05	123.56	121.96
3	C	302	7A9	C02-C03-C09	2.04	112.51	108.05
3	J	302	7A9	C02-C03-C04	-2.01	107.93	111.38

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	NAG	C3-C2-N2-C7
3	B	301	7A9	C20-C15-N05-C04
3	C	302	7A9	C16-C15-N05-C06
3	C	302	7A9	C16-C15-N05-C04
3	C	302	7A9	C20-C15-N05-C04
3	D	302	7A9	C16-C15-N05-C04
3	D	302	7A9	C20-C15-N05-C04
3	E	302	7A9	C16-C15-N05-C04
3	E	302	7A9	C20-C15-N05-C04
3	G	302	7A9	C16-C15-N05-C04
3	G	302	7A9	C20-C15-N05-C04
3	H	301	7A9	C16-C15-N05-C04
3	H	301	7A9	C20-C15-N05-C04
2	D	301	NAG	O5-C5-C6-O6
2	J	301	NAG	O5-C5-C6-O6
2	F	301	NAG	O5-C5-C6-O6
2	D	301	NAG	C4-C5-C6-O6
2	J	301	NAG	C4-C5-C6-O6
2	F	301	NAG	C8-C7-N2-C2
2	F	301	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	F	301	NAG	C4-C5-C6-O6
2	F	301	NAG	C1-C2-N2-C7
3	B	301	7A9	C16-C15-N05-C04
2	I	301	NAG	O5-C5-C6-O6
2	A	301	NAG	O5-C5-C6-O6
2	C	301	NAG	O5-C5-C6-O6
3	D	302	7A9	C16-C15-N05-C06
3	H	301	7A9	C16-C15-N05-C06
3	J	302	7A9	C20-C15-N05-C04
2	D	301	NAG	C1-C2-N2-C7
3	J	302	7A9	C16-C15-N05-C04
3	C	302	7A9	C20-C15-N05-C06
2	J	301	NAG	C3-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAG	3	0
2	I	301	NAG	3	0
2	D	301	NAG	1	0
2	E	301	NAG	1	0
2	G	301	NAG	1	0
2	F	301	NAG	2	0
2	C	301	NAG	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 7A9 H 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7A9 D 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 7A9 G 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 7A9 J 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 7A9 C 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 7A9 B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 7A9 E 302

Bond lengths

Bond angles

Torsions

Rings
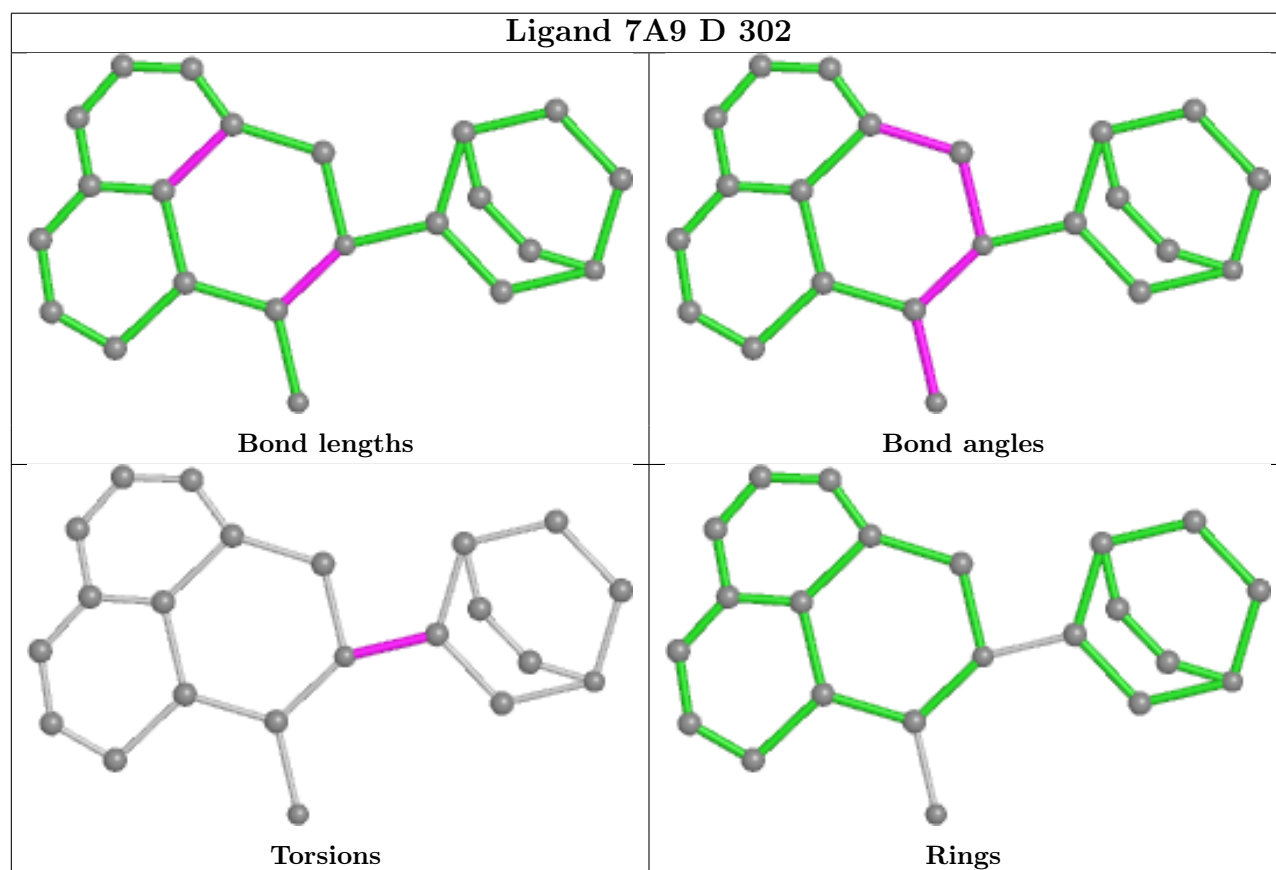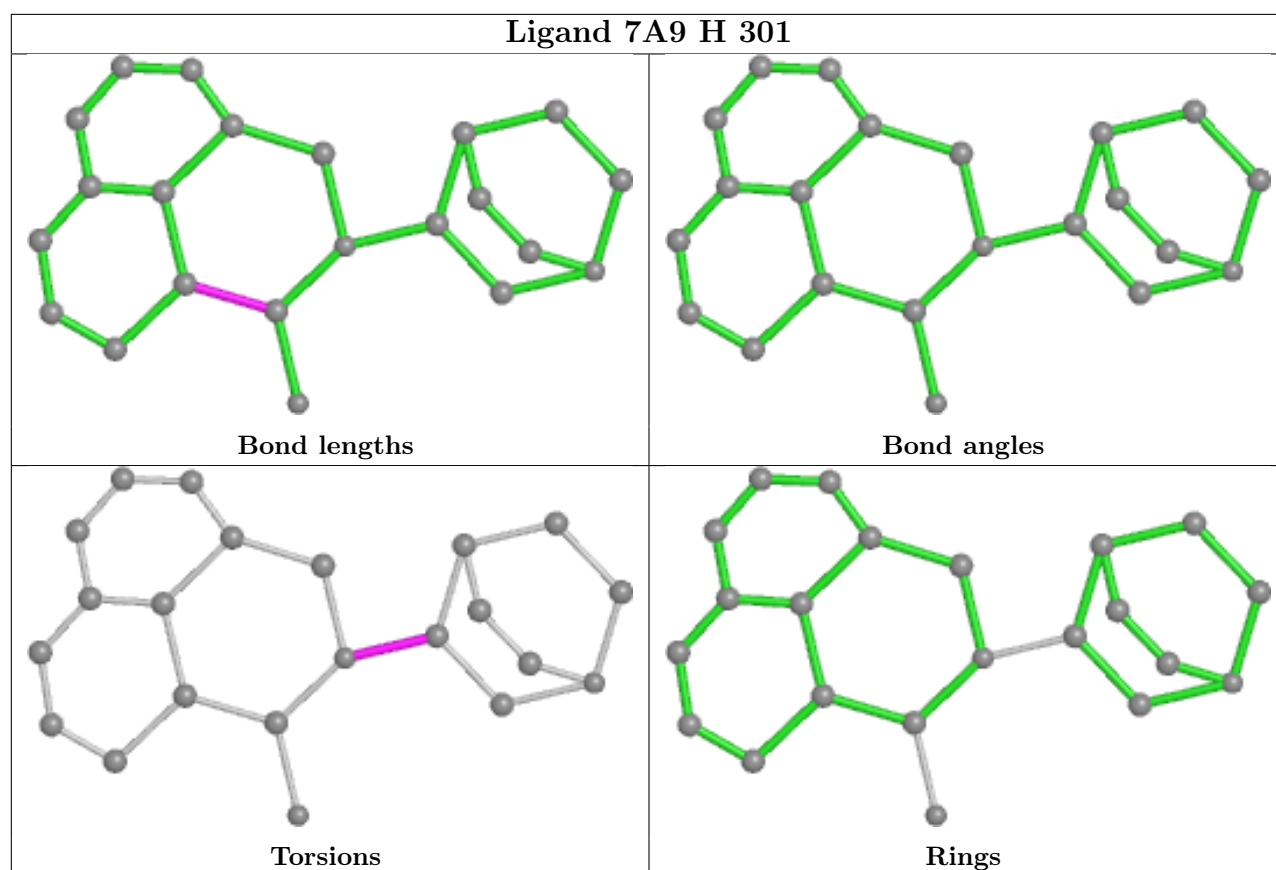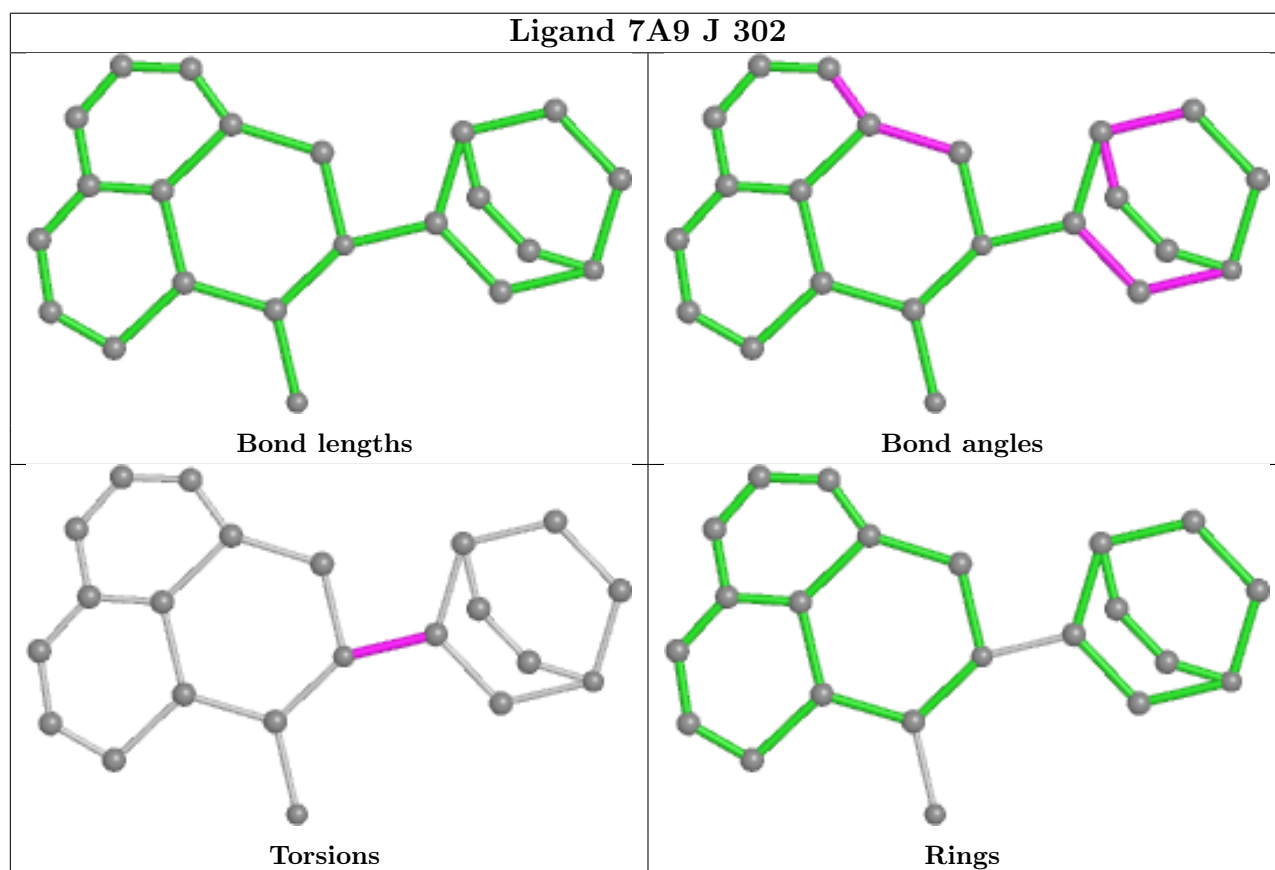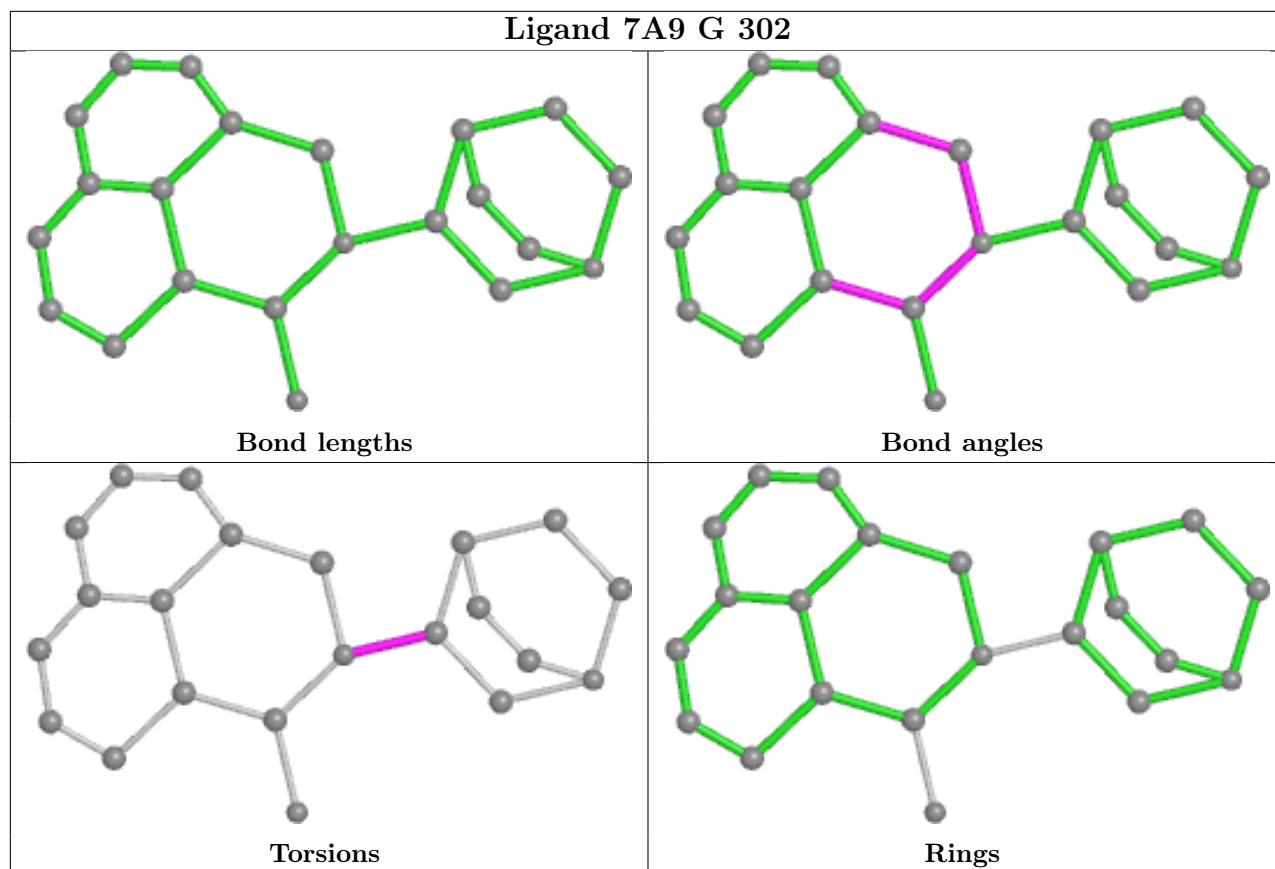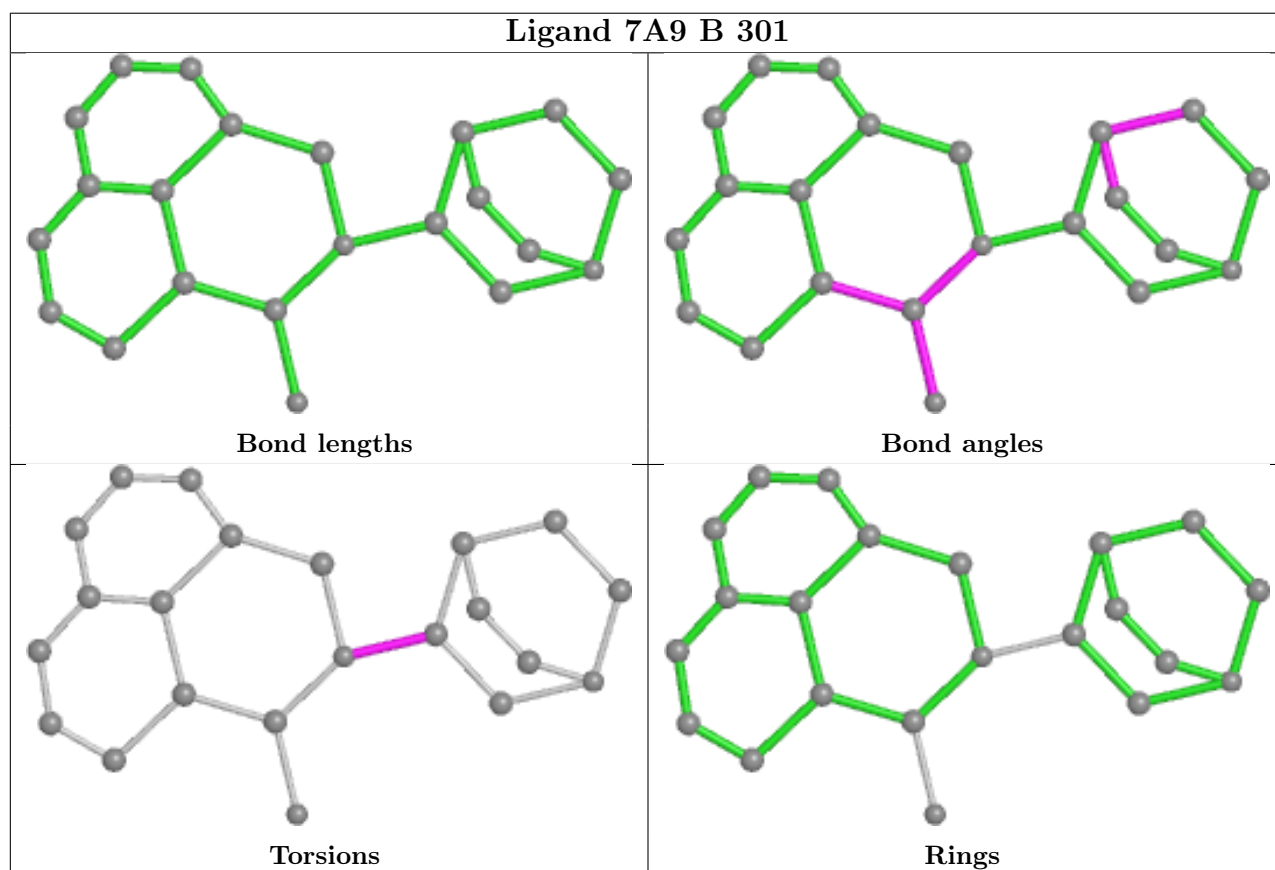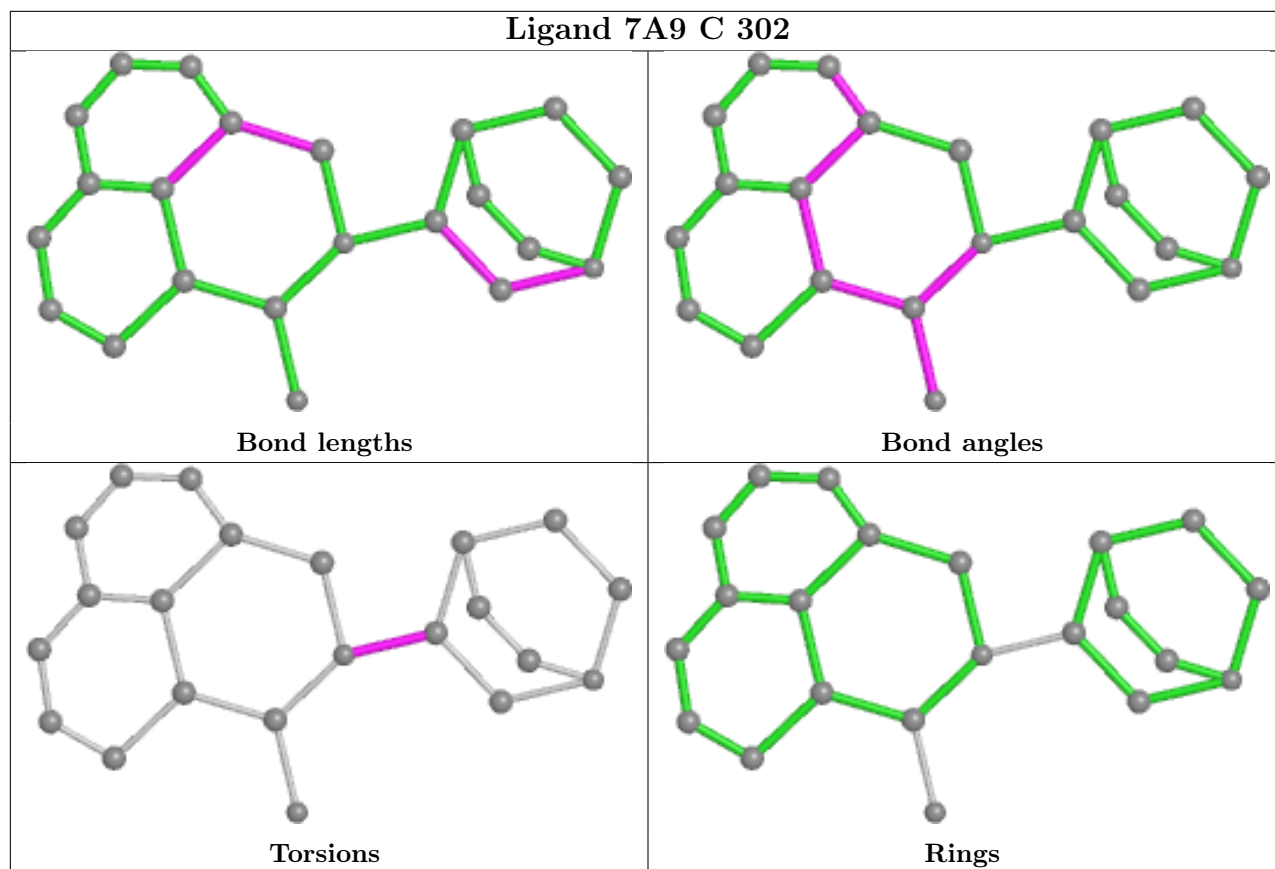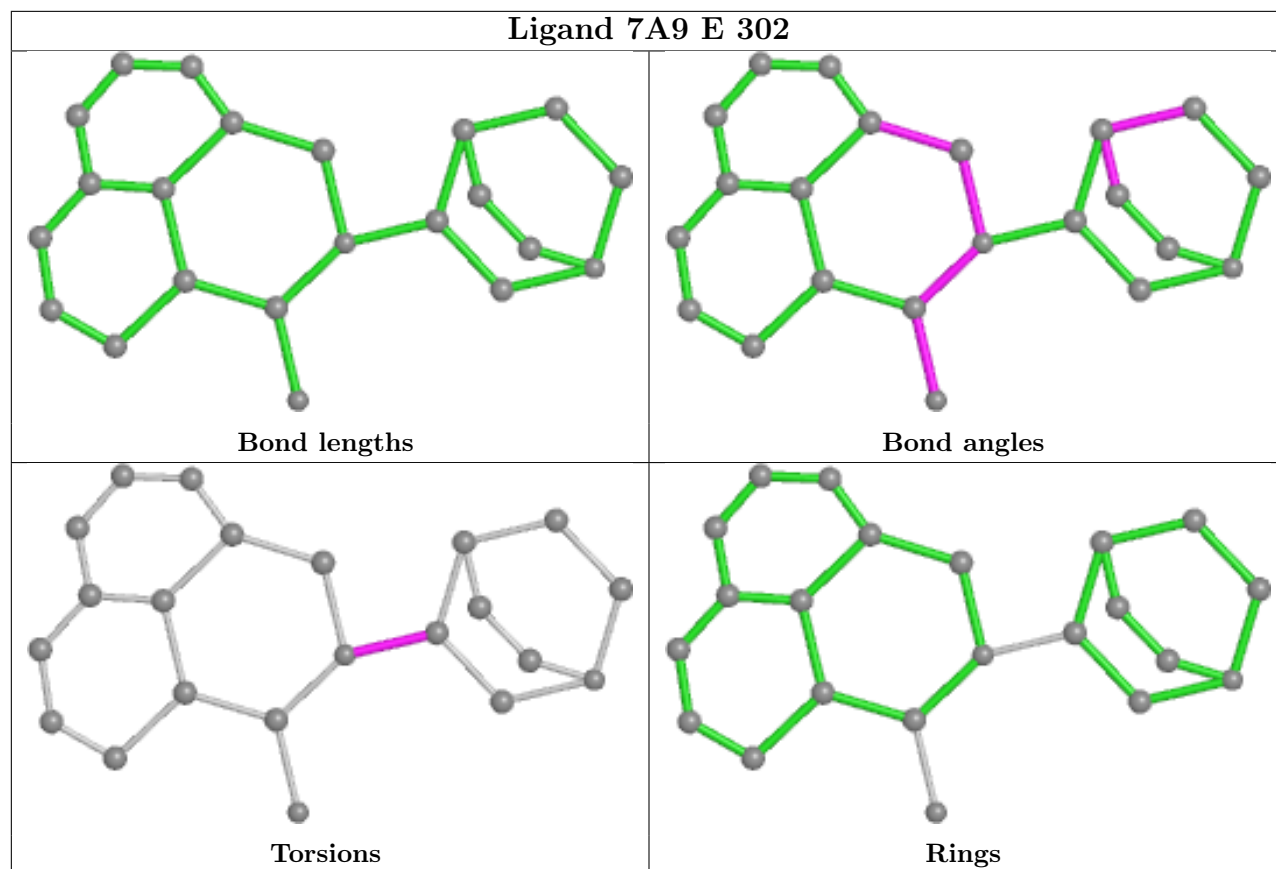
5.7 Other polymers ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	205/242 (84%)	0.76	15 (7%)	15	22	35, 51, 76, 96	0
1	B	205/242 (84%)	0.85	15 (7%)	15	22	38, 52, 80, 99	0
1	C	205/242 (84%)	0.91	27 (13%)	3	5	37, 55, 78, 113	0
1	D	205/242 (84%)	0.68	11 (5%)	25	36	35, 50, 72, 104	0
1	E	205/242 (84%)	0.78	10 (4%)	29	40	32, 46, 68, 94	0
1	F	205/242 (84%)	0.70	11 (5%)	25	36	36, 51, 80, 94	0
1	G	205/242 (84%)	0.97	23 (11%)	5	8	40, 59, 88, 108	0
1	H	205/242 (84%)	1.00	22 (10%)	6	9	41, 58, 83, 102	0
1	I	205/242 (84%)	0.86	19 (9%)	8	14	40, 56, 84, 105	0
1	J	205/242 (84%)	0.84	14 (6%)	17	25	36, 52, 79, 99	0
All	All	2050/2420 (84%)	0.84	167 (8%)	12	18	32, 53, 80, 113	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	134	GLU	5.1
1	H	68	ASN	5.1
1	G	14	ARG	5.0
1	F	133	GLU	4.9
1	H	133	GLU	4.9
1	H	72	ASN	4.6
1	I	14	ARG	4.6
1	I	68	ASN	4.6
1	C	15	SER	4.5
1	C	128	THR	4.4
1	F	134	GLU	4.4
1	C	11	LEU	4.3
1	A	134	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	68	ASN	4.1
1	H	69	GLU	4.1
1	G	205	ARG	4.1
1	C	18	TYR	4.0
1	B	14	ARG	4.0
1	G	129	GLY	4.0
1	G	133	GLU	4.0
1	B	15	SER	4.0
1	E	133	GLU	3.7
1	C	188	CYS	3.7
1	G	131	ASP	3.7
1	I	132	SER	3.6
1	G	130	VAL	3.6
1	G	15	SER	3.6
1	I	131	ASP	3.6
1	H	15	SER	3.6
1	H	5	MET	3.5
1	G	13	ASN	3.5
1	H	70	TYR	3.5
1	J	11	LEU	3.5
1	C	14	ARG	3.5
1	H	66	ASP	3.4
1	I	128	THR	3.4
1	I	10	ASP	3.4
1	A	133	GLU	3.4
1	C	134	GLU	3.4
1	A	131	ASP	3.4
1	I	130	VAL	3.3
1	I	16	PRO	3.3
1	C	73	ILE	3.3
1	C	69	GLU	3.3
1	C	3	ASN	3.3
1	E	130	VAL	3.3
1	C	1	GLN	3.1
1	G	70	TYR	3.1
1	I	129	GLY	3.1
1	C	64	MET	3.1
1	B	5	MET	3.1
1	C	9	SER	3.1
1	J	9	SER	3.1
1	A	188	CYS	3.1
1	F	188	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	205	ARG	3.0
1	C	2	ALA	3.0
1	G	168	ALA	3.0
1	B	13	ASN	3.0
1	F	132	SER	3.0
1	B	1	GLN	3.0
1	H	196	VAL	3.0
1	B	22	THR	3.0
1	D	13	ASN	3.0
1	G	176	SER	2.9
1	I	201	LYS	2.9
1	J	73	ILE	2.8
1	H	3	ASN	2.8
1	D	130	VAL	2.8
1	B	3	ASN	2.8
1	C	13	ASN	2.8
1	D	133	GLU	2.8
1	I	3	ASN	2.8
1	A	5	MET	2.8
1	J	13	ASN	2.8
1	H	24	ASP	2.7
1	B	73	ILE	2.7
1	A	186	TYR	2.7
1	C	71	GLY	2.7
1	F	23	LYS	2.7
1	I	199	VAL	2.7
1	A	202	PHE	2.7
1	G	43	SER	2.6
1	H	9	SER	2.6
1	B	130	VAL	2.6
1	E	129	GLY	2.6
1	G	188	CYS	2.6
1	J	203	ARG	2.6
1	B	138	CYS	2.6
1	H	10	ASP	2.6
1	G	127	PRO	2.6
1	E	132	SER	2.6
1	F	128	THR	2.6
1	H	205	ARG	2.6
1	A	130	VAL	2.6
1	C	10	ASP	2.6
1	E	194	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	132	SER	2.5
1	D	1	GLN	2.5
1	D	159	ASP	2.5
1	G	175	LEU	2.5
1	H	4	LEU	2.5
1	J	22	THR	2.5
1	I	15	SER	2.5
1	C	17	MET	2.4
1	J	134	GLU	2.4
1	A	16	PRO	2.4
1	A	25	ASP	2.4
1	A	15	SER	2.4
1	J	131	ASP	2.4
1	D	9	SER	2.4
1	A	204	GLU	2.4
1	C	44	SER	2.4
1	H	13	ASN	2.4
1	A	129	GLY	2.4
1	C	133	GLU	2.4
1	B	129	GLY	2.4
1	H	6	ARG	2.4
1	I	7	LEU	2.3
1	J	12	PHE	2.3
1	B	39	VAL	2.3
1	E	134	GLU	2.3
1	I	189	CYS	2.3
1	I	72	ASN	2.3
1	B	189	CYS	2.3
1	F	138	CYS	2.3
1	H	39	VAL	2.3
1	E	5	MET	2.2
1	D	138	CYS	2.2
1	G	160	GLN	2.2
1	G	128	THR	2.2
1	J	90	ALA	2.2
1	C	205	ARG	2.2
1	D	70	TYR	2.2
1	C	100	LEU	2.2
1	F	15	SER	2.2
1	H	61	ASN	2.2
1	G	63	LEU	2.2
1	E	128	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	189	CYS	2.1
1	F	7	LEU	2.1
1	I	134	GLU	2.1
1	G	193	TYR	2.1
1	I	70	TYR	2.1
1	J	66	ASP	2.1
1	J	72	ASN	2.1
1	G	11	LEU	2.1
1	H	189	CYS	2.1
1	F	186	TYR	2.1
1	C	129	GLY	2.1
1	F	190	PRO	2.1
1	J	129	GLY	2.1
1	C	66	ASP	2.1
1	D	205	ARG	2.1
1	E	138	CYS	2.1
1	B	70	TYR	2.1
1	C	132	SER	2.1
1	D	62	SER	2.1
1	I	62	SER	2.1
1	H	2	ALA	2.1
1	C	159	ASP	2.0
1	J	2	ALA	2.0
1	G	24	ASP	2.0
1	D	134	GLU	2.0
1	G	173	GLU	2.0
1	H	14	ARG	2.0
1	E	90	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	301	14/15	0.42	0.55	74,128,148,158	0
2	NAG	G	301	14/15	0.49	0.48	84,122,135,135	0
2	NAG	J	301	14/15	0.60	0.59	91,132,161,163	0
2	NAG	E	301	14/15	0.62	0.48	65,94,104,106	0
2	NAG	D	301	14/15	0.67	0.29	66,95,114,127	0
2	NAG	A	301	14/15	0.69	0.46	73,112,132,138	0
2	NAG	I	301	14/15	0.74	0.18	52,58,69,80	0
2	NAG	F	301	14/15	0.81	0.23	46,61,68,85	0
3	7A9	H	301	22/22	0.83	0.17	51,60,69,72	0
3	7A9	E	302	22/22	0.86	0.16	33,47,52,57	0
3	7A9	G	302	22/22	0.86	0.18	46,57,61,66	0
3	7A9	B	301	22/22	0.86	0.18	52,65,81,85	0
3	7A9	J	302	22/22	0.86	0.16	47,58,78,88	0
3	7A9	D	302	22/22	0.88	0.16	26,39,48,50	0
3	7A9	C	302	22/22	0.93	0.14	30,41,52,53	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 7A9 H 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
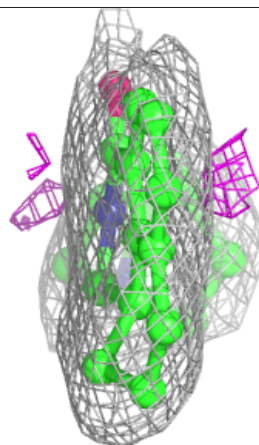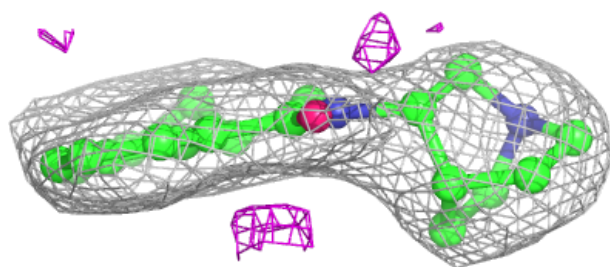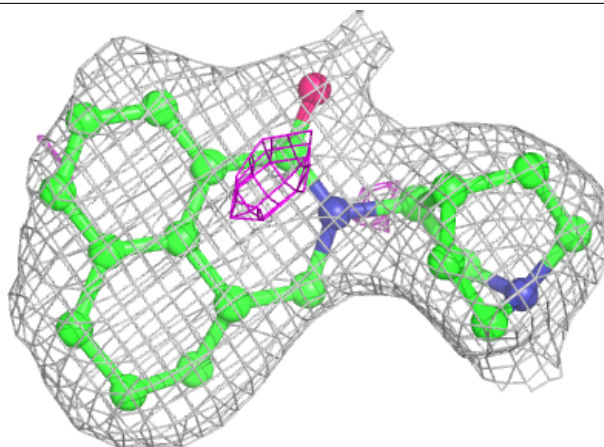
Electron density around 7A9 E 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
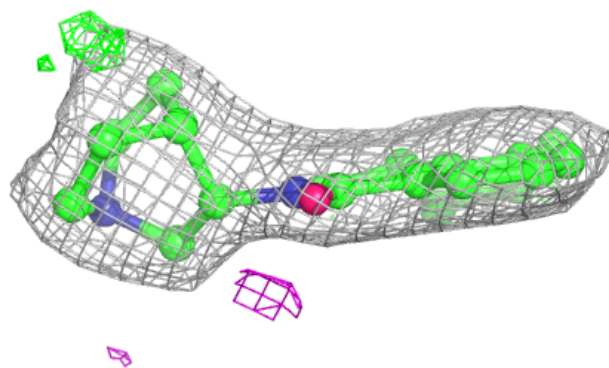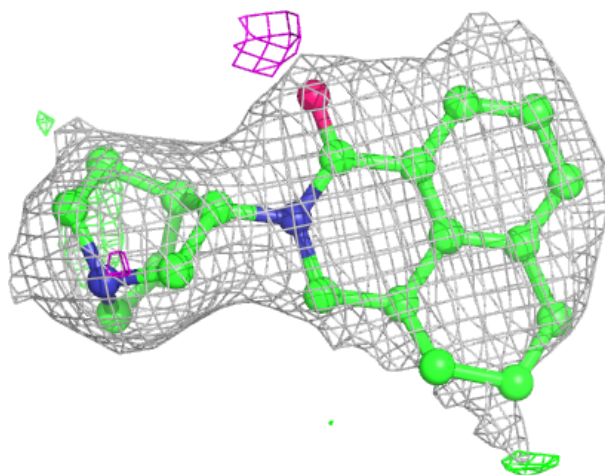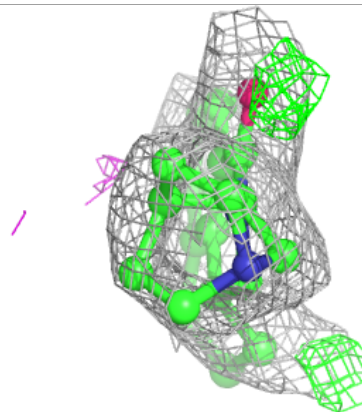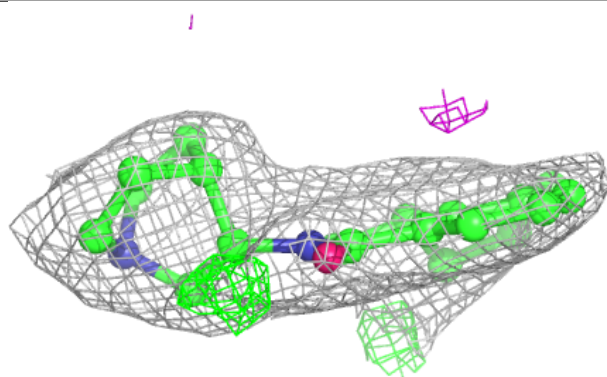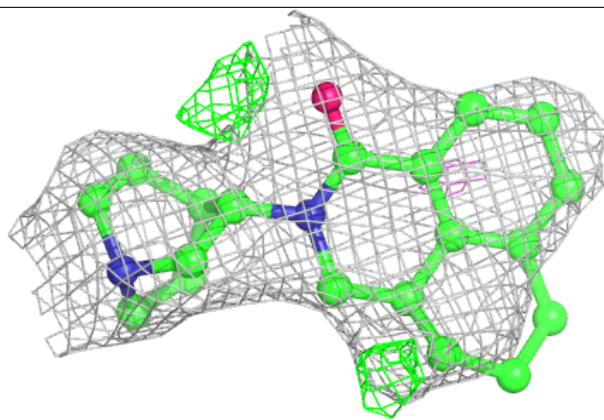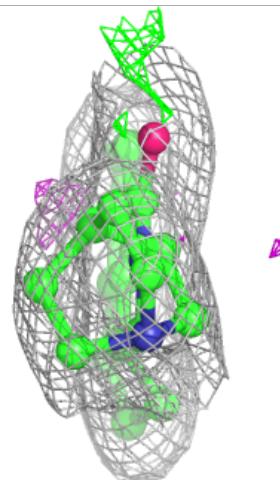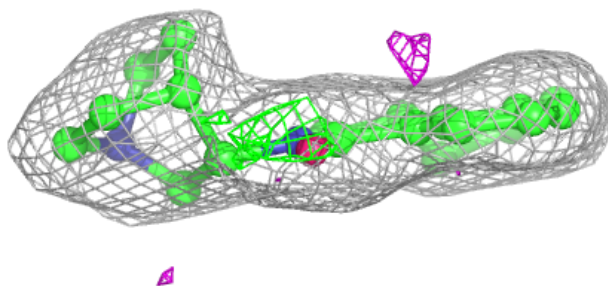$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
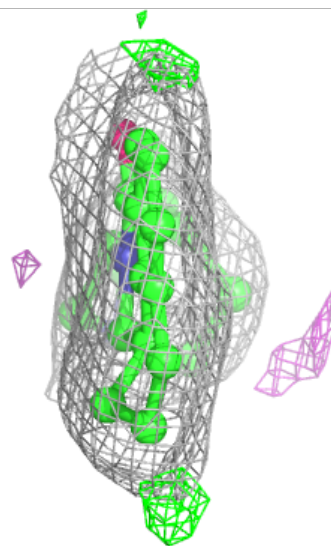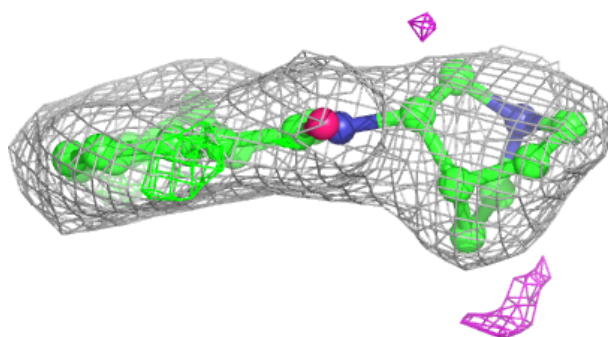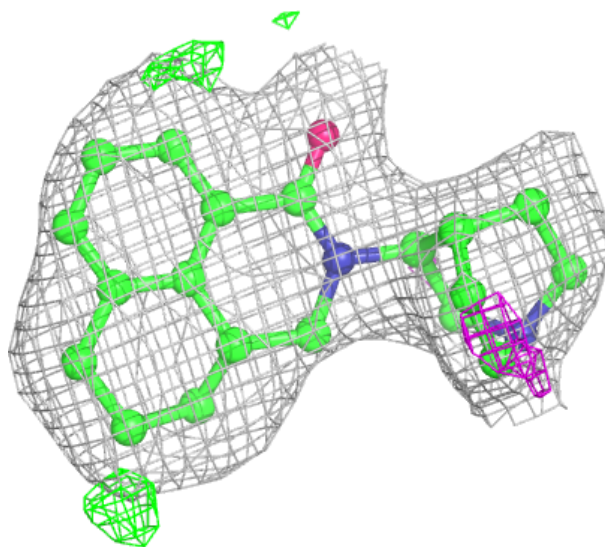
Electron density around 7A9 G 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
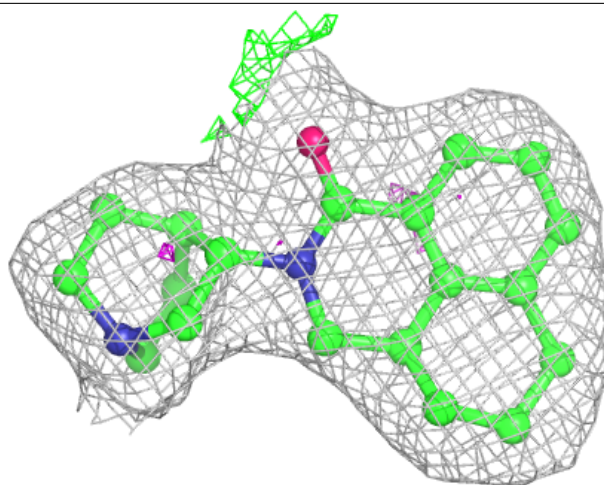and green (positive)
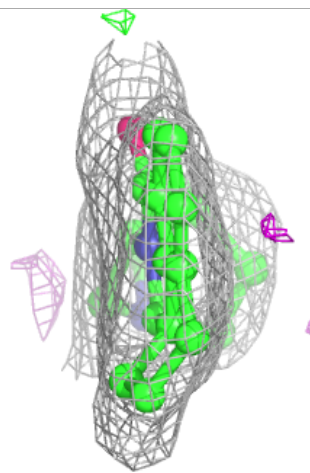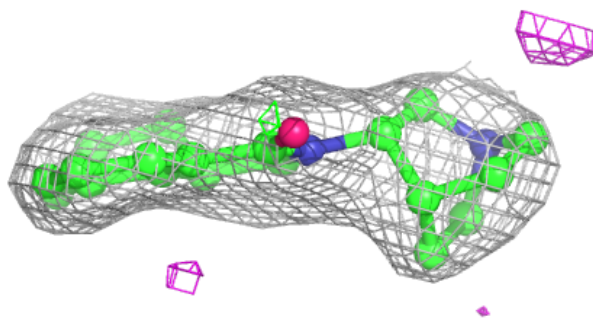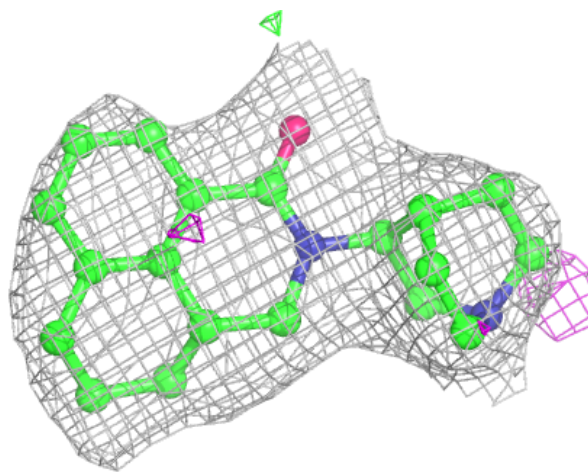
Electron density around 7A9 B 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
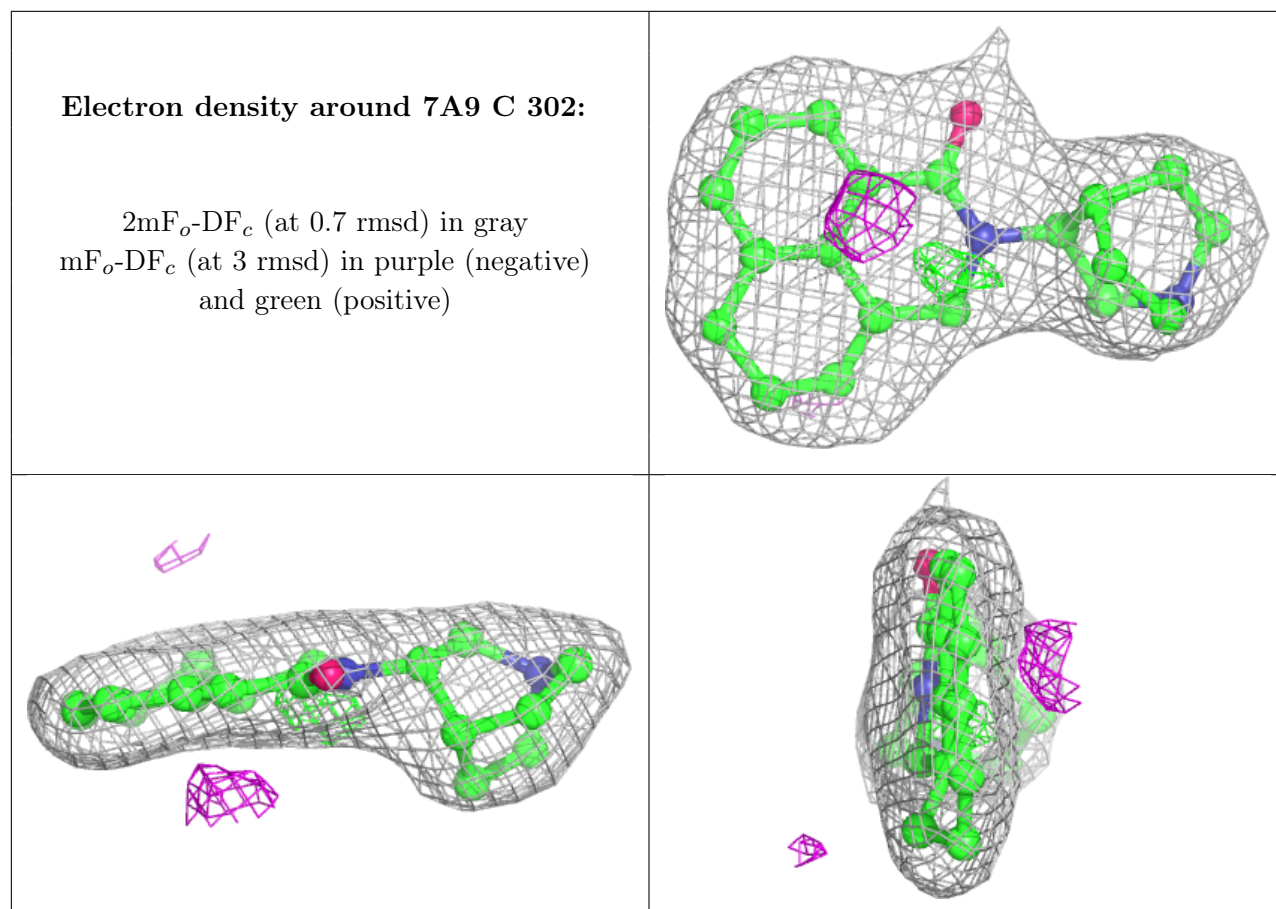and green (positive)
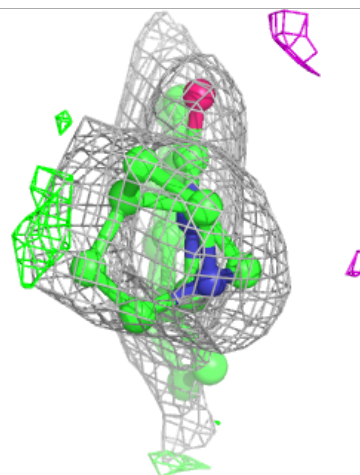
Electron density around 7A9 J 302:

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

Electron density around 7A9 D 302:

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

Electron density around 7A9 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.