



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:32 PM EDT

PDB ID : 3PEO / pdb_00003peo
Title : Crystal structure of acetylcholine binding protein complexed with metocurine
Authors : Talley, T.T.; Harel, M.; Yamauchi, G.J.; Radic, Z.; Hansen, S.; Huxford, T.; Taylor, P.W.
Deposited on : 2010-10-27
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

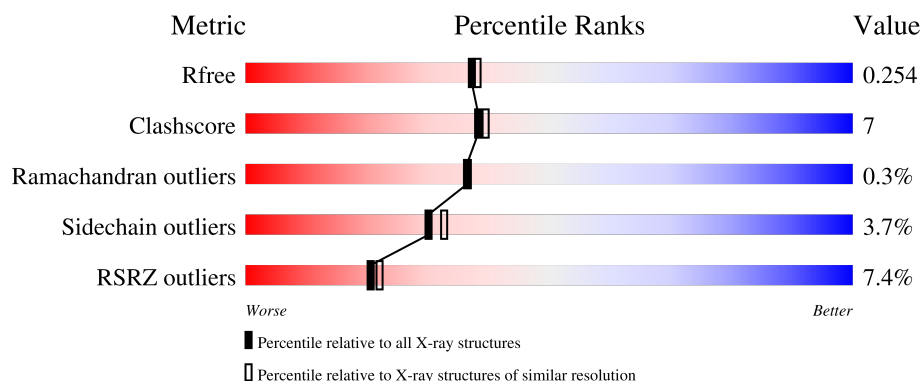
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	228	9% 70% 16% • 11%
1	B	228	3% 76% 13% • 9%
1	C	228	4% 81% 11% 7%
1	D	228	11% 68% 18% • 11%
1	E	228	6% 73% 16% 10%

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Mol	Chain	Length	Quality of chain
1	F	228	9% 76% 11% • 11%
1	G	228	7% 77% 9% • 9%
1	H	228	% 81% 11% 7%
1	I	228	11% 75% 13% • 11%
1	J	228	5% 76% 13% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18224 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	203	Total	C	N	O	S	0	0	0
			1617	1022	264	323	8			
1	B	208	Total	C	N	O	S	0	2	0
			1673	1058	278	329	8			
1	C	211	Total	C	N	O	S	0	1	0
			1689	1065	278	338	8			
1	D	204	Total	C	N	O	S	0	3	0
			1639	1037	268	326	8			
1	E	205	Total	C	N	O	S	0	0	0
			1636	1033	269	325	9			
1	F	202	Total	C	N	O	S	0	2	0
			1621	1027	265	321	8			
1	G	207	Total	C	N	O	S	0	4	0
			1678	1062	280	328	8			
1	H	211	Total	C	N	O	S	0	1	0
			1689	1065	278	338	8			
1	I	204	Total	C	N	O	S	0	3	0
			1639	1037	268	326	8			
1	J	207	Total	C	N	O	S	0	0	0
			1649	1041	271	328	9			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP Q8WSF8
A	-7	TYR	-	expression tag	UNP Q8WSF8
A	-6	LYS	-	expression tag	UNP Q8WSF8
A	-5	ASP	-	expression tag	UNP Q8WSF8
A	-4	ASP	-	expression tag	UNP Q8WSF8
A	-3	ASP	-	expression tag	UNP Q8WSF8
A	-2	ASP	-	expression tag	UNP Q8WSF8
A	-1	LYS	-	expression tag	UNP Q8WSF8
A	0	LEU	-	expression tag	UNP Q8WSF8

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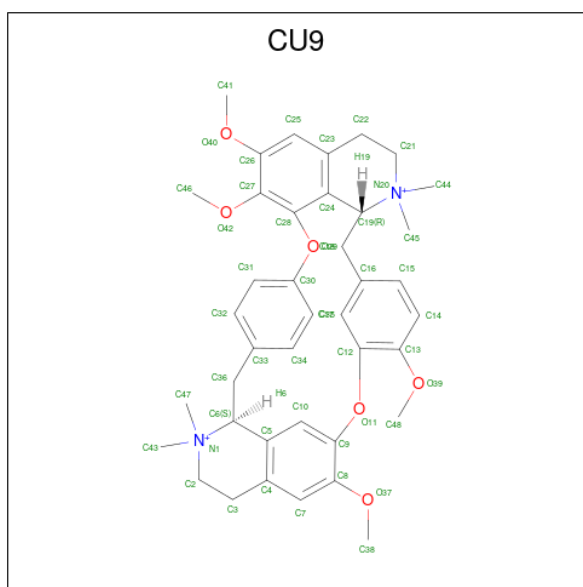
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	ASP	-	expression tag	UNP Q8WSF8
B	-7	TYR	-	expression tag	UNP Q8WSF8
B	-6	LYS	-	expression tag	UNP Q8WSF8
B	-5	ASP	-	expression tag	UNP Q8WSF8
B	-4	ASP	-	expression tag	UNP Q8WSF8
B	-3	ASP	-	expression tag	UNP Q8WSF8
B	-2	ASP	-	expression tag	UNP Q8WSF8
B	-1	LYS	-	expression tag	UNP Q8WSF8
B	0	LEU	-	expression tag	UNP Q8WSF8
C	-8	ASP	-	expression tag	UNP Q8WSF8
C	-7	TYR	-	expression tag	UNP Q8WSF8
C	-6	LYS	-	expression tag	UNP Q8WSF8
C	-5	ASP	-	expression tag	UNP Q8WSF8
C	-4	ASP	-	expression tag	UNP Q8WSF8
C	-3	ASP	-	expression tag	UNP Q8WSF8
C	-2	ASP	-	expression tag	UNP Q8WSF8
C	-1	LYS	-	expression tag	UNP Q8WSF8
C	0	LEU	-	expression tag	UNP Q8WSF8
D	-8	ASP	-	expression tag	UNP Q8WSF8
D	-7	TYR	-	expression tag	UNP Q8WSF8
D	-6	LYS	-	expression tag	UNP Q8WSF8
D	-5	ASP	-	expression tag	UNP Q8WSF8
D	-4	ASP	-	expression tag	UNP Q8WSF8
D	-3	ASP	-	expression tag	UNP Q8WSF8
D	-2	ASP	-	expression tag	UNP Q8WSF8
D	-1	LYS	-	expression tag	UNP Q8WSF8
D	0	LEU	-	expression tag	UNP Q8WSF8
E	-8	ASP	-	expression tag	UNP Q8WSF8
E	-7	TYR	-	expression tag	UNP Q8WSF8
E	-6	LYS	-	expression tag	UNP Q8WSF8
E	-5	ASP	-	expression tag	UNP Q8WSF8
E	-4	ASP	-	expression tag	UNP Q8WSF8
E	-3	ASP	-	expression tag	UNP Q8WSF8
E	-2	ASP	-	expression tag	UNP Q8WSF8
E	-1	LYS	-	expression tag	UNP Q8WSF8
E	0	LEU	-	expression tag	UNP Q8WSF8
F	-8	ASP	-	expression tag	UNP Q8WSF8
F	-7	TYR	-	expression tag	UNP Q8WSF8
F	-6	LYS	-	expression tag	UNP Q8WSF8
F	-5	ASP	-	expression tag	UNP Q8WSF8
F	-4	ASP	-	expression tag	UNP Q8WSF8
F	-3	ASP	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	ASP	-	expression tag	UNP Q8WSF8
F	-1	LYS	-	expression tag	UNP Q8WSF8
F	0	LEU	-	expression tag	UNP Q8WSF8
G	-8	ASP	-	expression tag	UNP Q8WSF8
G	-7	TYR	-	expression tag	UNP Q8WSF8
G	-6	LYS	-	expression tag	UNP Q8WSF8
G	-5	ASP	-	expression tag	UNP Q8WSF8
G	-4	ASP	-	expression tag	UNP Q8WSF8
G	-3	ASP	-	expression tag	UNP Q8WSF8
G	-2	ASP	-	expression tag	UNP Q8WSF8
G	-1	LYS	-	expression tag	UNP Q8WSF8
G	0	LEU	-	expression tag	UNP Q8WSF8
H	-8	ASP	-	expression tag	UNP Q8WSF8
H	-7	TYR	-	expression tag	UNP Q8WSF8
H	-6	LYS	-	expression tag	UNP Q8WSF8
H	-5	ASP	-	expression tag	UNP Q8WSF8
H	-4	ASP	-	expression tag	UNP Q8WSF8
H	-3	ASP	-	expression tag	UNP Q8WSF8
H	-2	ASP	-	expression tag	UNP Q8WSF8
H	-1	LYS	-	expression tag	UNP Q8WSF8
H	0	LEU	-	expression tag	UNP Q8WSF8
I	-8	ASP	-	expression tag	UNP Q8WSF8
I	-7	TYR	-	expression tag	UNP Q8WSF8
I	-6	LYS	-	expression tag	UNP Q8WSF8
I	-5	ASP	-	expression tag	UNP Q8WSF8
I	-4	ASP	-	expression tag	UNP Q8WSF8
I	-3	ASP	-	expression tag	UNP Q8WSF8
I	-2	ASP	-	expression tag	UNP Q8WSF8
I	-1	LYS	-	expression tag	UNP Q8WSF8
I	0	LEU	-	expression tag	UNP Q8WSF8
J	-8	ASP	-	expression tag	UNP Q8WSF8
J	-7	TYR	-	expression tag	UNP Q8WSF8
J	-6	LYS	-	expression tag	UNP Q8WSF8
J	-5	ASP	-	expression tag	UNP Q8WSF8
J	-4	ASP	-	expression tag	UNP Q8WSF8
J	-3	ASP	-	expression tag	UNP Q8WSF8
J	-2	ASP	-	expression tag	UNP Q8WSF8
J	-1	LYS	-	expression tag	UNP Q8WSF8
J	0	LEU	-	expression tag	UNP Q8WSF8

- Molecule 2 is 6,6',7',12'-tetramethoxy-2,2',2'-tetramethyltubocuraran-2,2'-dium (CCD ID: CU9) (formula: C₄₀H₄₈N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			48	40	2	6		
2	B	1	Total	C	N	O	0	0
			48	40	2	6		
2	C	1	Total	C	N	O	0	0
			48	40	2	6		
2	D	1	Total	C	N	O	0	0
			48	40	2	6		
2	F	1	Total	C	N	O	0	0
			48	40	2	6		
2	F	1	Total	C	N	O	0	0
			48	40	2	6		
2	H	1	Total	C	N	O	0	0
			48	40	2	6		
2	J	1	Total	C	N	O	0	0
			48	40	2	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	148	Total	O	0	0
			148	148		
3	B	155	Total	O	0	0
			155	155		
3	C	125	Total	O	0	0
			125	125		
3	D	117	Total	O	0	0
			117	117		

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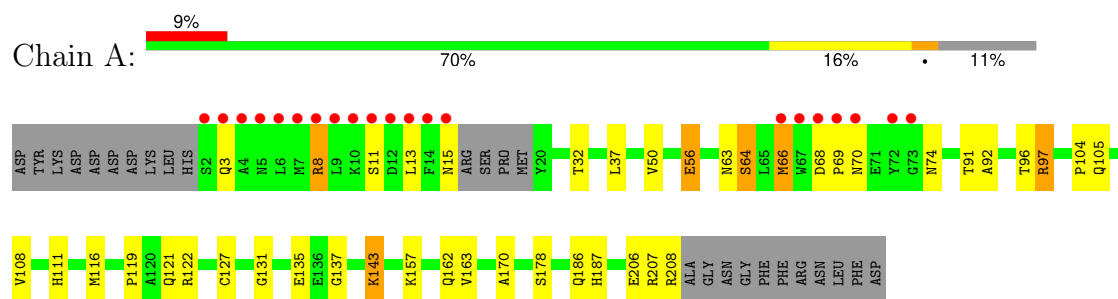
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	112	Total 112	O 112	0	0
3	F	138	Total 138	O 138	0	0
3	G	166	Total 166	O 166	0	0
3	H	133	Total 133	O 133	0	0
3	I	110	Total 110	O 110	0	0
3	J	106	Total 106	O 106	0	0

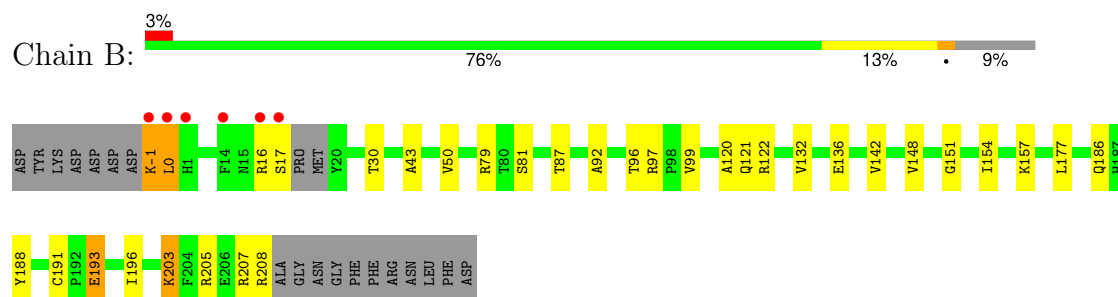
3 Residue-property plots [i](#)

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.

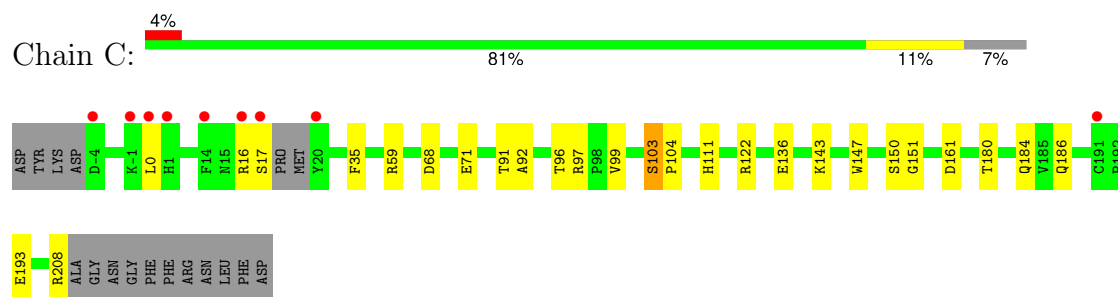
- Molecule 1: Soluble acetylcholine receptor



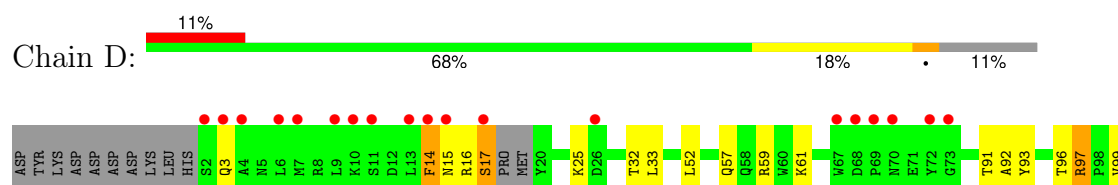
- Molecule 1: Soluble acetylcholine receptor

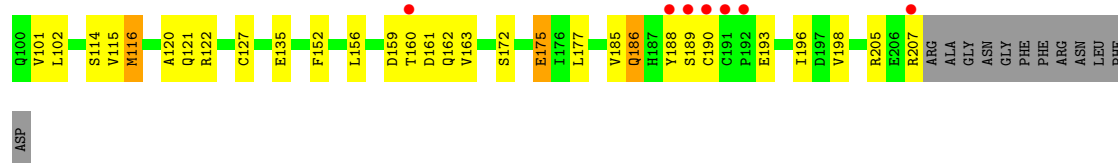


- Molecule 1: Soluble acetylcholine receptor

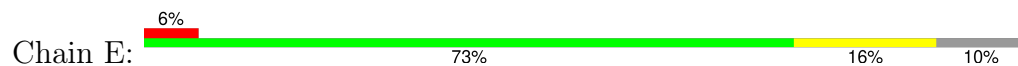


- Molecule 1: Soluble acetylcholine receptor

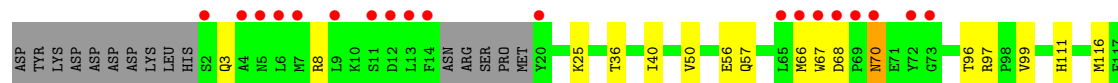
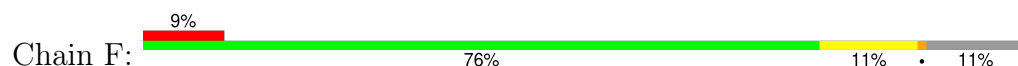




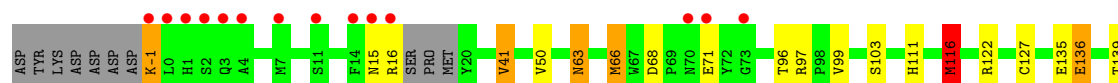
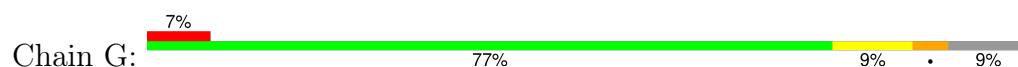
- Molecule 1: Soluble acetylcholine receptor



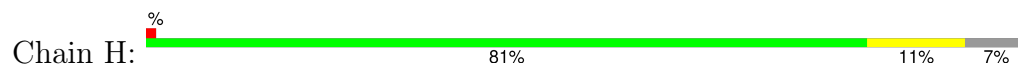
- Molecule 1: Soluble acetylcholine receptor



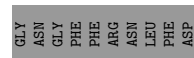
- Molecule 1: Soluble acetylcholine receptor

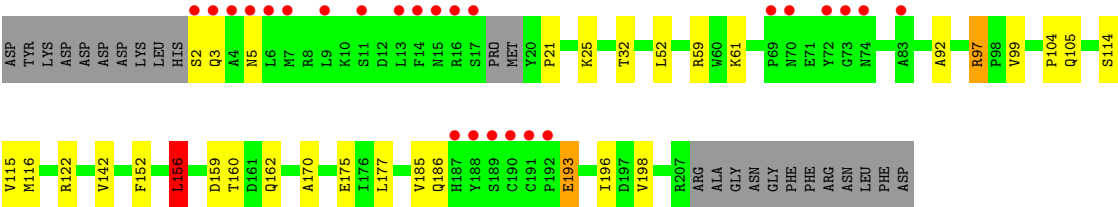


- Molecule 1: Soluble acetylcholine receptor

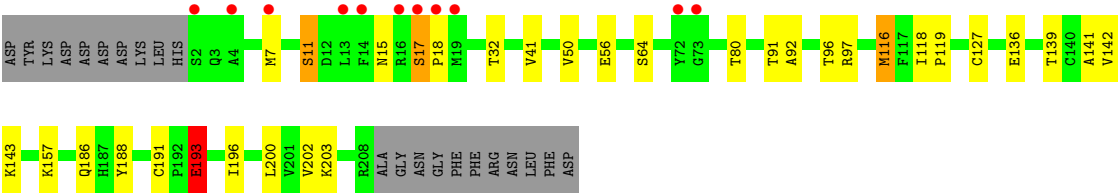
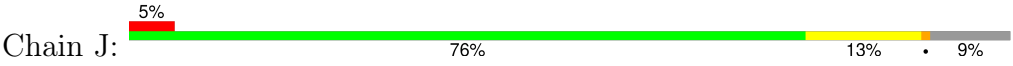


- Molecule 1: Soluble acetylcholine receptor





● Molecule 1: Soluble acetylcholine receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.70Å 147.57Å 148.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	104.83 – 2.10 104.80 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (104.83-2.10) 99.3 (104.80-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.255 0.207 , 0.254	Depositor DCC
R_{free} test set	1593 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18224	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0521e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CU9

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	1.41	4/1655 (0.2%)	1.23	7/2256 (0.3%)
1	B	1.43	7/1718 (0.4%)	1.22	1/2340 (0.0%)
1	C	1.38	4/1731 (0.2%)	1.17	3/2358 (0.1%)
1	D	1.31	3/1686 (0.2%)	1.22	5/2299 (0.2%)
1	E	1.38	4/1674 (0.2%)	1.19	2/2280 (0.1%)
1	F	1.38	3/1665 (0.2%)	1.18	2/2270 (0.1%)
1	G	1.35	6/1729 (0.3%)	1.25	6/2354 (0.3%)
1	H	1.34	3/1731 (0.2%)	1.18	0/2358
1	I	1.30	4/1686 (0.2%)	1.20	2/2299 (0.1%)
1	J	1.33	2/1689 (0.1%)	1.16	2/2303 (0.1%)
All	All	1.36	40/16964 (0.2%)	1.20	30/23117 (0.1%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	ALA	CA-CB	7.31	1.64	1.53
1	F	154	ILE	CA-CB	6.94	1.63	1.54
1	D	101	VAL	CA-CB	6.49	1.62	1.54
1	C	103	SER	N-CA	6.19	1.50	1.45
1	E	99	VAL	CA-CB	6.16	1.61	1.54
1	E	201	VAL	CA-CB	5.96	1.61	1.54
1	B	30	THR	CA-CB	5.96	1.61	1.53
1	E	121	GLN	CA-C	-5.95	1.45	1.52
1	C	151	GLY	C-O	-5.95	1.17	1.24
1	G	141	ALA	C-O	5.85	1.30	1.23
1	I	142	VAL	CA-CB	5.78	1.62	1.54
1	D	163	VAL	CA-C	5.76	1.59	1.52
1	B	120	ALA	CA-CB	5.72	1.61	1.53
1	D	127	CYS	N-CA	-5.72	1.39	1.46
1	A	178	SER	C-O	-5.71	1.16	1.23
1	J	202	VAL	C-O	-5.69	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	GLU	C-O	5.67	1.30	1.23
1	B	148	VAL	N-CA	5.60	1.53	1.46
1	F	208	ARG	NE-CZ	5.60	1.39	1.33
1	H	58	GLN	CA-C	-5.50	1.46	1.52
1	G	63	ASN	C-O	-5.46	1.17	1.24
1	H	56	GLU	N-CA	-5.40	1.39	1.46
1	H	103	SER	N-CA	5.40	1.50	1.45
1	I	92	ALA	CA-CB	-5.35	1.45	1.53
1	C	35	PHE	N-CA	5.30	1.52	1.46
1	E	103	SER	N-CA	5.29	1.49	1.46
1	I	92	ALA	CA-C	5.24	1.59	1.52
1	A	170	ALA	CA-CB	5.21	1.62	1.53
1	F	40	ILE	CA-C	-5.20	1.46	1.52
1	B	87	THR	N-CA	5.20	1.50	1.45
1	G	146	SER	N-CA	-5.14	1.39	1.46
1	B	203	LYS	CA-C	-5.10	1.46	1.52
1	B	154	ILE	CA-CB	5.08	1.60	1.54
1	I	170	ALA	CA-CB	5.07	1.62	1.53
1	G	157	LYS	N-CA	-5.07	1.39	1.45
1	J	97	ARG	N-CA	5.06	1.52	1.46
1	G	150	SER	CA-C	-5.03	1.46	1.53
1	C	97	ARG	N-CA	5.02	1.50	1.45
1	A	32	THR	CA-CB	5.01	1.60	1.53
1	G	116	MET	N-CA	-5.01	1.39	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	193	GLU	N-CA-C	6.94	118.54	109.93
1	G	103	SER	CA-C-N	6.57	126.52	119.76
1	G	103	SER	C-N-CA	6.57	126.52	119.76
1	C	103	SER	CA-C-N	6.47	126.42	119.76
1	C	103	SER	C-N-CA	6.47	126.42	119.76
1	A	108	VAL	N-CA-C	-6.38	98.43	107.75
1	A	143	LYS	N-CA-C	-6.09	100.26	109.95
1	B	0	LEU	N-CA-C	-6.06	104.79	111.82
1	E	103	SER	CA-C-N	5.98	125.92	119.76
1	E	103	SER	C-N-CA	5.98	125.92	119.76
1	A	13	LEU	N-CA-C	5.78	117.66	111.36
1	G	41	VAL	CB-CA-C	-5.75	102.78	112.16
1	D	3	GLN	N-CA-C	-5.74	105.11	111.71
1	A	97	ARG	CA-C-N	-5.71	113.88	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ARG	C-N-CA	-5.71	113.88	119.76
1	F	208	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	F	36	THR	CA-CB-OG1	-5.53	101.31	109.60
1	I	156	LEU	CB-CA-C	-5.38	101.07	109.84
1	A	163	VAL	N-CA-C	-5.33	102.71	109.58
1	C	111	HIS	N-CA-C	5.30	117.81	111.71
1	G	195	TYR	CA-CB-CG	-5.22	104.50	113.90
1	D	161	ASP	CA-C-N	-5.18	115.85	123.00
1	D	161	ASP	C-N-CA	-5.18	115.85	123.00
1	G	116	MET	CA-CB-CG	-5.11	103.89	114.10
1	G	111	HIS	N-CA-C	5.09	117.56	111.71
1	D	102	LEU	CA-C-N	-5.08	116.64	123.96
1	D	102	LEU	C-N-CA	-5.08	116.64	123.96
1	A	143	LYS	CA-CB-CG	5.04	124.17	114.10
1	J	41	VAL	CB-CA-C	-5.03	105.45	112.04
1	I	177	LEU	N-CA-C	-5.00	106.87	113.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1617	0	1544	35	0
1	B	1673	0	1618	17	0
1	C	1689	0	1617	16	0
1	D	1639	0	1578	35	0
1	E	1636	0	1566	21	0
1	F	1621	0	1560	24	0
1	G	1678	0	1631	20	0
1	H	1689	0	1617	16	0
1	I	1639	0	1578	23	0
1	J	1649	0	1579	14	0
2	A	48	0	48	2	0
2	B	48	0	48	2	0
2	C	48	0	48	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	48	0	48	8	0
2	F	96	0	96	6	0
2	H	48	0	48	0	0
2	J	48	0	48	12	0
3	A	148	0	0	11	0
3	B	155	0	0	1	0
3	C	125	0	0	4	0
3	D	117	0	0	5	0
3	E	112	0	0	1	0
3	F	138	0	0	12	0
3	G	166	0	0	4	0
3	H	133	0	0	2	0
3	I	110	0	0	6	0
3	J	106	0	0	1	0
All	All	18224	0	16272	229	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 7.

All (229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:220:CU9:H47	3:F:822:HOH:O	1.41	1.19
1:D:97[A]:ARG:HH11	1:D:97[A]:ARG:CG	1.57	1.18
1:D:97[A]:ARG:HG2	1:D:97[A]:ARG:NH1	1.41	1.02
2:J:301:CU9:C30	2:J:301:CU9:H46B	1.99	0.93
1:F:143:LYS:HE3	3:F:280:HOH:O	1.67	0.91
1:A:97:ARG:HD2	3:A:448:HOH:O	1.71	0.89
2:J:301:CU9:H35	2:J:301:CU9:H18	1.55	0.88
1:I:160[A]:THR:HG22	1:I:162:GLN:H	1.37	0.87
1:D:25:LYS:HE3	1:D:152:PHE:HD2	1.38	0.87
1:A:15:ASN:HB3	1:G:16:ARG:HD2	1.55	0.86
1:B:97[B]:ARG:NH1	3:B:965:HOH:O	2.06	0.85
2:J:301:CU9:C30	2:J:301:CU9:C46	2.58	0.82
2:J:301:CU9:H46B	2:J:301:CU9:C31	2.11	0.81
1:D:25:LYS:HE3	1:D:152:PHE:CD2	2.16	0.80
1:D:160[A]:THR:HG22	1:D:162:GLN:H	1.45	0.79
1:A:143:LYS:NZ	3:A:239:HOH:O	2.16	0.79
1:I:32:THR:CG2	1:I:159:ASP:HB3	2.14	0.78
1:A:3:GLN:HG2	3:E:372:HOH:O	1.83	0.77
1:C:59:ARG:HG3	3:C:608:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:59:ARG:HD2	3:I:535:HOH:O	1.85	0.76
2:J:301:CU9:C46	2:J:301:CU9:C31	2.64	0.76
1:F:57:GLN:CD	3:F:822:HOH:O	2.29	0.76
1:D:175:GLU:HG2	1:D:207:ARG:HG3	1.67	0.76
1:I:21:PRO:HD3	1:J:7:MET:HE2	1.68	0.75
1:A:50:VAL:HG21	1:A:127:CYS:SG	2.27	0.75
1:F:143:LYS:NZ	3:F:867:HOH:O	2.20	0.74
1:B:186:GLN:HG2	1:B:188:TYR:OH	1.87	0.73
1:F:97[B]:ARG:NH1	1:F:124:SER:OG	2.20	0.73
1:A:143:LYS:HE3	3:A:295:HOH:O	1.88	0.73
1:A:104:PRO:O	3:A:1125:HOH:O	2.05	0.72
1:A:116:MET:SD	2:A:301:CU9:H43B	2.32	0.70
1:B:186:GLN:HG2	1:B:188:TYR:CZ	2.27	0.69
1:I:105:GLN:HG2	3:I:943:HOH:O	1.93	0.69
1:G:68:ASP:HB3	1:G:71:GLU:HG3	1.74	0.68
2:J:301:CU9:H18	2:J:301:CU9:C35	2.23	0.68
2:J:301:CU9:C46	2:J:301:CU9:O29	2.42	0.68
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.34	0.67
1:D:97[A]:ARG:CG	1:D:97[A]:ARG:NH1	2.28	0.66
2:D:301:CU9:H18	2:D:301:CU9:H35	1.75	0.66
1:I:185:VAL:HG22	1:I:196:ILE:HD12	1.78	0.65
1:F:99[B]:VAL:HG22	3:F:231:HOH:O	1.96	0.65
1:F:187:HIS:HD2	3:F:235:HOH:O	1.79	0.65
1:C:143:LYS:HE2	3:C:1127:HOH:O	1.96	0.65
1:D:186:GLN:HG2	1:D:188:TYR:CZ	2.32	0.65
1:B:191:CYS:HB3	1:B:193:GLU:OE1	1.98	0.64
1:G:191:CYS:HB3	1:G:193:GLU:OE1	1.97	0.64
2:D:301:CU9:H44A	1:E:166:SER:O	1.97	0.64
1:A:207:ARG:O	1:A:208:ARG:HG3	1.96	0.64
1:G:139:THR:OG1	1:G:203:LYS:HG2	1.98	0.63
1:A:97:ARG:CD	3:A:448:HOH:O	2.38	0.62
1:A:187:HIS:HD2	3:A:242:HOH:O	1.81	0.62
1:G:97[B]:ARG:NH1	3:G:1013:HOH:O	2.33	0.62
1:C:59:ARG:HD3	1:C:59:ARG:C	2.25	0.61
1:G:186:GLN:HE21	1:G:186:GLN:HA	1.66	0.61
1:D:172:SER:O	1:D:207:ARG:HD3	2.01	0.61
1:F:50:VAL:HG21	1:F:127:CYS:SG	2.41	0.61
1:I:97[A]:ARG:NH1	1:I:97[A]:ARG:HG2	2.15	0.61
2:A:301:CU9:H46A	1:E:188:TYR:CD2	2.36	0.60
1:F:97[B]:ARG:NH1	3:F:746:HOH:O	2.35	0.60
1:F:99[B]:VAL:HG23	3:F:1175:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ASP:OD2	1:D:159:ASP:N	2.34	0.59
1:I:2:SER:HA	1:I:5:ASN:ND2	2.18	0.59
1:H:20:TYR:N	3:H:1136:HOH:O	2.35	0.59
1:H:63:ASN:O	1:H:66:MET:HG2	2.02	0.59
1:F:3:GLN:HG2	3:J:1141:HOH:O	2.02	0.59
1:I:32:THR:HG21	1:I:159:ASP:HB3	1.83	0.59
1:D:59:ARG:HG3	1:D:116:MET:HE3	1.84	0.59
1:J:191:CYS:HB3	1:J:193:GLU:OE1	2.03	0.59
1:B:177:LEU:HB2	1:B:203:LYS:HD2	1.85	0.58
1:I:97[A]:ARG:HG2	1:I:97[A]:ARG:HH11	1.69	0.58
1:F:96:THR:O	1:G:122:ARG:HD2	2.04	0.57
1:I:97[B]:ARG:NH1	3:I:645:HOH:O	2.37	0.57
1:A:121:GLN:NE2	3:A:492:HOH:O	2.38	0.57
1:I:152:PHE:CD2	1:I:193:GLU:HB3	2.39	0.57
1:A:97:ARG:NE	3:A:448:HOH:O	2.38	0.56
1:F:56:GLU:O	1:F:119:PRO:HD2	2.05	0.56
1:F:116:MET:SD	2:F:220:CU9:H43B	2.45	0.56
1:I:97[A]:ARG:HH11	1:I:97[A]:ARG:CG	2.17	0.56
1:G:99[A]:VAL:HG23	3:G:250:HOH:O	2.05	0.56
1:G:96:THR:O	1:H:122:ARG:HD2	2.05	0.56
1:H:110:THR:HG22	1:H:111:HIS:N	2.21	0.55
1:F:68:ASP:C	1:F:70:ASN:H	2.14	0.55
1:I:32:THR:HG22	3:I:228:HOH:O	2.06	0.55
1:J:50:VAL:HG21	1:J:127:CYS:SG	2.47	0.55
1:J:141:ALA:HA	1:J:200:LEU:O	2.07	0.55
1:A:63:ASN:O	1:A:66:MET:HG3	2.06	0.55
1:G:135:GLU:HG3	1:G:208:ARG:HH12	1.71	0.55
1:D:25:LYS:HG2	1:D:152:PHE:HB3	1.89	0.55
1:D:32:THR:CG2	1:D:159:ASP:HB3	2.37	0.55
3:I:469:HOH:O	2:J:301:CU9:H43A	2.06	0.55
2:J:301:CU9:O29	2:J:301:CU9:H46A	2.07	0.55
1:A:97:ARG:HG2	1:A:97:ARG:HH11	1.72	0.54
1:D:96:THR:O	1:E:122:ARG:HD2	2.07	0.54
1:J:116:MET:HE3	1:J:118:ILE:HD11	1.89	0.54
1:E:139:THR:OG1	1:E:203:LYS:HG2	2.08	0.54
1:A:122:ARG:HD2	1:E:96:THR:O	2.08	0.53
1:H:191:CYS:HB3	1:H:193:GLU:OE2	2.08	0.53
1:H:20:TYR:N	3:H:686:HOH:O	2.42	0.53
1:F:162:GLN:NE2	3:F:825:HOH:O	2.42	0.53
1:I:156:LEU:HD13	1:I:198:VAL:HG23	1.91	0.53
1:E:81:SER:O	1:E:84:ASP:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:159:ASP:OD2	1:I:159:ASP:N	2.41	0.53
2:J:301:CU9:C31	2:J:301:CU9:H46A	2.36	0.53
2:B:301:CU9:H45A	2:B:301:CU9:C16	2.38	0.53
1:D:190:CYS:HB3	3:D:633:HOH:O	2.08	0.53
1:I:193:GLU:CD	1:I:193:GLU:H	2.16	0.53
1:C:16:ARG:HG2	1:C:17:SER:H	1.74	0.53
1:A:96:THR:O	1:B:122:ARG:HD2	2.09	0.52
1:D:99[A]:VAL:HG23	3:D:459:HOH:O	2.08	0.52
1:E:50:VAL:CG2	1:E:127:CYS:SG	2.98	0.52
1:D:93:TYR:CZ	2:D:301:CU9:H47	2.45	0.52
1:B:193:GLU:CD	1:B:193:GLU:H	2.18	0.52
1:J:136:GLU:CD	1:J:136:GLU:H	2.18	0.52
1:D:186:GLN:HG2	1:D:188:TYR:OH	2.09	0.51
1:C:150:SER:HB2	1:C:193:GLU:HG3	1.92	0.51
2:D:301:CU9:H18	2:D:301:CU9:C35	2.39	0.51
1:A:8:ARG:O	1:A:11:SER:HB3	2.11	0.51
2:F:220:CU9:H46A	1:J:188:TYR:CD2	2.46	0.51
1:F:162:GLN:NE2	3:F:748:HOH:O	2.45	0.50
2:D:301:CU9:H43A	3:D:556:HOH:O	2.11	0.50
1:E:11:SER:O	1:E:15:ASN:HB2	2.11	0.50
1:A:206:GLU:OE1	1:A:208:ARG:NH2	2.45	0.50
1:G:207[B]:ARG:NH2	3:G:985:HOH:O	2.43	0.50
1:B:151:GLY:HA2	1:B:196:ILE:HD12	1.93	0.49
1:A:56:GLU:O	1:A:119:PRO:HD2	2.12	0.49
1:A:187:HIS:HE1	3:A:224:HOH:O	1.94	0.49
1:G:50:VAL:HG21	1:G:127:CYS:SG	2.52	0.49
1:A:162:GLN:NE2	3:A:839:HOH:O	2.44	0.49
1:D:32:THR:HG22	3:D:221:HOH:O	2.12	0.48
1:D:59:ARG:HD3	3:D:594:HOH:O	2.12	0.48
1:J:91:THR:HG22	1:J:92:ALA:O	2.13	0.48
1:F:68:ASP:C	1:F:70:ASN:N	2.69	0.48
1:G:193:GLU:CD	1:G:193:GLU:H	2.19	0.48
1:J:11:SER:O	1:J:15:ASN:HB2	2.13	0.48
1:A:68:ASP:C	1:A:70:ASN:H	2.22	0.48
1:A:104:PRO:HG2	1:E:89:ASP:HB2	1.95	0.48
1:F:136:GLU:CD	1:F:136:GLU:H	2.21	0.48
1:D:59:ARG:HA	1:D:115:VAL:O	2.13	0.48
1:G:-1:LYS:HE3	1:G:-1:LYS:HB3	1.71	0.48
1:B:96:THR:O	1:C:122:ARG:HD2	2.14	0.47
2:B:301:CU9:C16	2:B:301:CU9:C45	2.92	0.47
1:F:67:TRP:CE3	1:F:111:HIS:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:GLN:HE21	1:G:186:GLN:CA	2.28	0.47
1:H:189:SER:O	1:H:190:CYS:C	2.58	0.47
2:J:301:CU9:H46A	2:J:301:CU9:H31	1.95	0.47
1:F:187:HIS:HE1	3:F:309:HOH:O	1.98	0.47
1:A:69:PRO:O	1:A:74:ASN:HA	2.15	0.46
1:A:105:GLN:HA	1:A:105:GLN:NE2	2.30	0.46
1:H:96:THR:O	1:I:122:ARG:HD2	2.15	0.46
1:D:177:LEU:HD11	1:D:205:ARG:HD3	1.97	0.46
1:B:207:ARG:NH2	1:B:207:ARG:HG3	2.30	0.46
2:J:301:CU9:C30	2:J:301:CU9:H46A	2.45	0.46
1:D:97[A]:ARG:HH11	1:D:97[A]:ARG:HG2	0.61	0.46
1:G:136:GLU:H	1:G:136:GLU:CD	2.24	0.45
1:E:41:VAL:HG23	1:E:53:VAL:HG23	1.97	0.45
1:B:-1:LYS:HB3	1:B:-1:LYS:HE3	1.49	0.45
1:A:157:LYS:HE3	3:A:770:HOH:O	2.17	0.45
1:E:208:ARG:HA	1:E:208:ARG:HD3	1.58	0.45
1:H:110:THR:CG2	1:H:111:HIS:N	2.80	0.45
1:A:37:LEU:HD12	1:A:37:LEU:HA	1.79	0.45
1:B:132:VAL:HG23	1:B:205:ARG:HA	1.97	0.45
2:D:301:CU9:H47	2:D:301:CU9:H36A	1.48	0.45
1:F:97[B]:ARG:HH11	1:F:97[B]:ARG:HD2	1.60	0.45
1:A:131:GLY:O	1:A:137:GLY:HA2	2.18	0.44
1:B:207:ARG:HG3	1:B:207:ARG:HH21	1.82	0.44
2:D:301:CU9:H44B	2:D:301:CU9:C23	2.48	0.44
1:E:175:GLU:HB2	1:E:207:ARG:HG3	1.99	0.44
1:H:89:ASP:HB2	1:I:104:PRO:HG2	2.00	0.44
1:F:97[B]:ARG:NH2	3:F:1233:HOH:O	2.49	0.44
1:D:32:THR:HG21	1:D:159:ASP:HB3	1.99	0.43
1:E:137:GLY:HA2	1:E:205:ARG:HB3	2.00	0.43
1:E:41:VAL:CG2	1:E:53:VAL:HG23	2.48	0.43
1:A:66:MET:HA	1:A:111:HIS:O	2.18	0.43
1:E:91:THR:HG22	1:E:92:ALA:O	2.18	0.43
1:D:14:PHE:C	1:D:16:ARG:H	2.27	0.43
1:D:156:LEU:HD13	1:D:198:VAL:HG23	2.00	0.43
1:H:150:SER:HB2	1:H:193:GLU:HG3	1.99	0.43
1:J:139:THR:OG1	1:J:203:LYS:HG2	2.19	0.43
1:E:136:GLU:CD	1:E:136:GLU:H	2.26	0.43
1:F:122:ARG:HD2	1:J:96:THR:O	2.18	0.43
1:H:163:VAL:HG21	1:H:200:LEU:CD1	2.48	0.43
1:C:91:THR:HG22	1:C:92:ALA:O	2.17	0.43
1:J:56:GLU:O	1:J:119:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LYS:HA	1:D:114:SER:HA	2.01	0.43
1:D:186:GLN:HG2	1:D:188:TYR:CE2	2.53	0.43
2:D:301:CU9:H32	1:E:55:TYR:OH	2.19	0.43
1:A:116:MET:HB2	1:A:116:MET:HE3	1.40	0.43
1:C:103:SER:HB2	1:C:104:PRO:HD2	2.00	0.43
1:H:178:SER:OG	1:H:203:LYS:HD2	2.19	0.43
1:B:177:LEU:HD12	1:B:203:LYS:HD3	1.99	0.42
1:C:136:GLU:CD	1:C:136:GLU:H	2.27	0.42
2:F:220:CU9:H18A	2:F:220:CU9:H21	1.75	0.42
1:A:68:ASP:C	1:A:70:ASN:N	2.78	0.42
1:C:103:SER:HB2	1:C:104:PRO:CD	2.49	0.42
1:A:50:VAL:CG2	1:A:127:CYS:SG	3.01	0.42
1:E:163:VAL:HG21	1:E:200:LEU:CD1	2.49	0.42
1:I:59:ARG:HA	1:I:115:VAL:O	2.19	0.42
1:B:79:ARG:HD2	1:B:79:ARG:N	2.34	0.42
1:B:43:ALA:HA	1:B:50:VAL:HG22	2.02	0.42
1:C:68:ASP:HB3	1:C:71:GLU:HG3	2.00	0.42
1:D:185:VAL:HG22	1:D:196:ILE:HD12	2.01	0.42
2:F:220:CU9:C23	2:F:220:CU9:H44B	2.50	0.42
1:I:61:LYS:HA	1:I:114:SER:HA	2.01	0.42
1:D:120:ALA:C	1:D:121:GLN:HG3	2.45	0.41
1:C:161:ASP:O	1:C:180:THR:HA	2.20	0.41
1:C:96:THR:O	1:D:122:ARG:HD2	2.19	0.41
1:A:3:GLN:NE2	1:E:27:ASP:OD2	2.44	0.41
1:D:16:ARG:O	1:D:17:SER:HB2	2.21	0.41
1:G:99[B]:VAL:HG22	3:G:250:HOH:O	2.20	0.41
1:I:105:GLN:CG	3:I:943:HOH:O	2.60	0.41
1:E:161:ASP:OD1	1:E:161:ASP:C	2.64	0.41
1:H:59:ARG:HD3	1:H:59:ARG:C	2.46	0.41
1:J:32:THR:OG1	1:J:157:LYS:HE3	2.21	0.41
1:J:143:LYS:NZ	1:J:186:GLN:NE2	2.68	0.41
1:B:99[A]:VAL:CG1	1:B:121:GLN:HB3	2.51	0.41
1:D:91:THR:HG22	1:D:92:ALA:O	2.21	0.41
1:C:143:LYS:CE	3:C:1127:HOH:O	2.63	0.40
2:C:301:CU9:C38	1:D:57:GLN:HE21	2.34	0.40
1:D:14:PHE:O	1:D:16:ARG:N	2.54	0.40
1:I:116:MET:HE2	1:I:116:MET:HB2	1.82	0.40
1:C:147:TRP:O	2:C:301:CU9:H2	2.21	0.40
1:C:99:VAL:HG12	3:C:952:HOH:O	2.20	0.40
1:G:63:ASN:O	1:G:66:MET:HG3	2.21	0.40
1:H:136:GLU:CD	1:H:136:GLU:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:THR:HG22	1:A:92:ALA:O	2.21	0.40
1:F:118:ILE:HG13	2:F:220:CU9:H48B	2.02	0.40
1:G:41:VAL:O	1:G:41:VAL:HG12	2.20	0.40
1:G:116:MET:HE3	1:G:116:MET:HB2	1.95	0.40
1:H:50:VAL:HG21	1:H:127:CYS:SG	2.61	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	199/228 (87%)	187 (94%)	11 (6%)	1 (0%)	24	22
1	B	206/228 (90%)	199 (97%)	7 (3%)	0	100	100
1	C	208/228 (91%)	204 (98%)	4 (2%)	0	100	100
1	D	203/228 (89%)	198 (98%)	3 (2%)	2 (1%)	12	9
1	E	201/228 (88%)	191 (95%)	9 (4%)	1 (0%)	24	22
1	F	200/228 (88%)	192 (96%)	8 (4%)	0	100	100
1	G	207/228 (91%)	201 (97%)	6 (3%)	0	100	100
1	H	208/228 (91%)	204 (98%)	4 (2%)	0	100	100
1	I	203/228 (89%)	195 (96%)	8 (4%)	0	100	100
1	J	205/228 (90%)	195 (95%)	7 (3%)	3 (2%)	8	4
All	All	2040/2280 (90%)	1966 (96%)	67 (3%)	7 (0%)	36	36

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	15	ASN
1	A	64	SER

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Mol	Chain	Res	Type
1	J	64	SER
1	E	64	SER
1	J	18	PRO
1	D	14	PHE
1	J	17	SER

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	184/206 (89%)	179 (97%)	5 (3%)	39	45
1	B	191/206 (93%)	181 (95%)	10 (5%)	21	20
1	C	193/206 (94%)	189 (98%)	4 (2%)	47	54
1	D	188/206 (91%)	177 (94%)	11 (6%)	18	16
1	E	186/206 (90%)	180 (97%)	6 (3%)	34	38
1	F	185/206 (90%)	180 (97%)	5 (3%)	39	45
1	G	192/206 (93%)	182 (95%)	10 (5%)	21	20
1	H	193/206 (94%)	189 (98%)	4 (2%)	47	54
1	I	188/206 (91%)	178 (95%)	10 (5%)	20	19
1	J	188/206 (91%)	181 (96%)	7 (4%)	30	33
All	All	1888/2060 (92%)	1816 (96%)	72 (4%)	30	32

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	64	SER
1	A	66	MET
1	A	135	GLU
1	A	186	GLN
1	B	-1	LYS
1	B	0	LEU
1	B	16	ARG

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Mol	Chain	Res	Type
1	B	17	SER
1	B	81	SER
1	B	136	GLU
1	B	142	VAL
1	B	157	LYS
1	B	193	GLU
1	B	208	ARG
1	C	0	LEU
1	C	184	GLN
1	C	186	GLN
1	C	208	ARG
1	D	17	SER
1	D	33	LEU
1	D	52	LEU
1	D	97[A]	ARG
1	D	97[B]	ARG
1	D	116	MET
1	D	135	GLU
1	D	175	GLU
1	D	186	GLN
1	D	189	SER
1	D	193	GLU
1	E	16	ARG
1	E	25	LYS
1	E	80	THR
1	E	160	THR
1	E	193	GLU
1	E	208	ARG
1	F	8	ARG
1	F	25	LYS
1	F	66	MET
1	F	70	ASN
1	F	136	GLU
1	G	-1	LYS
1	G	15	ASN
1	G	66	MET
1	G	116	MET
1	G	136	GLU
1	G	157	LYS
1	G	186	GLN
1	G	207[A]	ARG
1	G	207[B]	ARG

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Mol	Chain	Res	Type
1	G	208	ARG
1	H	17	SER
1	H	136	GLU
1	H	186	GLN
1	H	207	ARG
1	I	3	GLN
1	I	25	LYS
1	I	52	LEU
1	I	97[A]	ARG
1	I	97[B]	ARG
1	I	99	VAL
1	I	156	LEU
1	I	175	GLU
1	I	186	GLN
1	I	193	GLU
1	J	11	SER
1	J	17	SER
1	J	80	THR
1	J	116	MET
1	J	142	VAL
1	J	193	GLU
1	J	196	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	74	ASN
1	A	105	GLN
1	A	121	GLN
1	A	162	GLN
1	A	187	HIS
1	B	1	HIS
1	B	15	ASN
1	B	58	GLN
1	B	162	GLN
1	C	15	ASN
1	C	48	ASN
1	C	184	GLN
1	D	57	GLN
1	D	100	GLN
1	E	3	GLN

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Mol	Chain	Res	Type
1	F	63	ASN
1	F	74	ASN
1	F	105	GLN
1	F	162	GLN
1	F	184	GLN
1	F	186	GLN
1	F	187	HIS
1	G	5	ASN
1	G	58	GLN
1	G	121	GLN
1	G	186	GLN
1	H	105	GLN
1	H	184	GLN
1	H	186	GLN
1	I	5	ASN
1	I	58	GLN
1	J	3	GLN
1	J	121	GLN
1	J	186	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CU9	B	301	-	54,54,54	1.12	5 (9%)	80,82,82	1.66	13 (16%)
2	CU9	A	301	-	54,54,54	1.05	2 (3%)	80,82,82	1.60	12 (15%)
2	CU9	J	301	-	54,54,54	0.96	1 (1%)	80,82,82	2.10	19 (23%)
2	CU9	C	301	-	54,54,54	1.33	5 (9%)	80,82,82	1.92	9 (11%)
2	CU9	F	301	-	54,54,54	1.15	3 (5%)	80,82,82	1.40	9 (11%)
2	CU9	H	301	-	54,54,54	1.04	2 (3%)	80,82,82	1.91	12 (15%)
2	CU9	F	220	-	54,54,54	1.11	3 (5%)	80,82,82	1.78	15 (18%)
2	CU9	D	301	-	54,54,54	1.03	4 (7%)	80,82,82	2.01	18 (22%)

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	CU9	B	301	-	-	3/24/56/56	-
2	CU9	A	301	-	-	0/24/56/56	-
2	CU9	J	301	-	-	6/24/56/56	-
2	CU9	C	301	-	-	2/24/56/56	-
2	CU9	F	301	-	-	1/24/56/56	-
2	CU9	H	301	-	-	2/24/56/56	-
2	CU9	F	220	-	-	3/24/56/56	-
2	CU9	D	301	-	-	8/24/56/56	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	CU9	C25-C23	3.30	1.44	1.39
2	C	301	CU9	C15-C14	3.08	1.43	1.38
2	F	220	CU9	C22-C23	2.89	1.56	1.51
2	H	301	CU9	C25-C26	2.86	1.43	1.38
2	C	301	CU9	C25-C26	2.84	1.43	1.38
2	F	301	CU9	C10-C5	2.83	1.44	1.39
2	C	301	CU9	C6-N1	-2.82	1.45	1.54
2	A	301	CU9	O37-C8	2.67	1.41	1.37
2	F	301	CU9	C19-N20	-2.59	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	CU9	C28-C24	2.54	1.43	1.39
2	H	301	CU9	C6-N1	-2.48	1.46	1.54
2	B	301	CU9	O40-C26	2.42	1.41	1.37
2	C	301	CU9	C18-C16	2.38	1.56	1.51
2	A	301	CU9	C13-C12	-2.37	1.35	1.40
2	C	301	CU9	C25-C23	2.34	1.43	1.39
2	J	301	CU9	C6-N1	-2.32	1.47	1.54
2	D	301	CU9	C6-N1	-2.30	1.47	1.54
2	F	220	CU9	C25-C26	2.27	1.42	1.38
2	B	301	CU9	C34-C33	2.26	1.43	1.38
2	F	220	CU9	O40-C26	2.25	1.40	1.37
2	D	301	CU9	C35-C30	2.12	1.42	1.38
2	B	301	CU9	O37-C8	2.12	1.40	1.37
2	F	301	CU9	C34-C33	2.09	1.43	1.38
2	B	301	CU9	C35-C34	2.08	1.42	1.38
2	D	301	CU9	O39-C13	2.01	1.40	1.37

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	CU9	C48-O39-C13	9.02	130.74	117.51
2	C	301	CU9	C30-O29-C28	8.61	131.99	118.40
2	F	220	CU9	C30-O29-C28	8.11	131.20	118.40
2	D	301	CU9	C48-O39-C13	7.65	128.73	117.51
2	H	301	CU9	C38-O37-C8	7.13	127.97	117.51
2	F	301	CU9	C30-O29-C28	6.89	129.27	118.40
2	J	301	CU9	C48-O39-C13	6.86	127.57	117.51
2	H	301	CU9	C30-O29-C28	6.75	129.05	118.40
2	H	301	CU9	C48-O39-C13	6.68	127.31	117.51
2	J	301	CU9	O39-C13-C12	6.63	124.39	115.40
2	D	301	CU9	C46-O42-C27	6.43	132.20	114.74
2	B	301	CU9	C30-O29-C28	6.34	128.40	118.40
2	A	301	CU9	C30-O29-C28	5.65	127.31	118.40
2	B	301	CU9	C48-O39-C13	5.52	125.61	117.51
2	C	301	CU9	C38-O37-C8	5.52	125.60	117.51
2	D	301	CU9	O39-C13-C12	5.44	122.79	115.40
2	H	301	CU9	C46-O42-C27	5.43	129.49	114.74
2	F	220	CU9	C38-O37-C8	5.08	124.96	117.51
2	F	301	CU9	C48-O39-C13	4.99	124.83	117.51
2	J	301	CU9	O40-C26-C27	4.96	123.64	115.14
2	J	301	CU9	C30-O29-C28	4.92	126.17	118.40
2	J	301	CU9	O40-C26-C25	-4.44	116.44	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	220	CU9	C46-O42-C27	4.37	126.60	114.74
2	A	301	CU9	C41-O40-C26	4.27	123.77	117.51
2	J	301	CU9	C46-O42-C27	4.18	126.10	114.74
2	B	301	CU9	O37-C8-C9	4.02	120.85	115.40
2	J	301	CU9	C2-C3-C4	-4.00	103.55	113.56
2	J	301	CU9	O39-C13-C14	-3.99	117.57	124.30
2	J	301	CU9	O37-C8-C9	3.99	120.82	115.40
2	A	301	CU9	C46-O42-C27	3.94	125.44	114.74
2	D	301	CU9	C3-C2-N1	3.88	124.00	112.60
2	J	301	CU9	C38-O37-C8	3.87	123.19	117.51
2	D	301	CU9	C38-O37-C8	3.80	123.08	117.51
2	F	220	CU9	C41-O40-C26	3.75	123.01	117.51
2	C	301	CU9	C41-O40-C26	3.67	122.89	117.51
2	H	301	CU9	O37-C8-C9	3.63	120.33	115.40
2	D	301	CU9	O37-C8-C9	3.63	120.33	115.40
2	B	301	CU9	C10-C5-C4	-3.61	115.45	119.39
2	D	301	CU9	O42-C27-C26	-3.60	114.95	120.12
2	B	301	CU9	C35-C34-C33	-3.59	116.28	121.00
2	F	220	CU9	C48-O39-C13	3.43	122.55	117.51
2	A	301	CU9	O37-C8-C9	3.39	120.00	115.40
2	A	301	CU9	C12-O11-C9	3.28	125.93	118.09
2	C	301	CU9	O37-C8-C9	3.28	119.85	115.40
2	A	301	CU9	C2-N1-C6	3.24	117.03	109.50
2	H	301	CU9	C10-C5-C4	-3.20	115.90	119.39
2	D	301	CU9	O40-C26-C25	-3.13	118.68	124.08
2	D	301	CU9	C36-C6-N1	-3.13	105.56	112.39
2	D	301	CU9	C2-N1-C6	3.10	116.70	109.50
2	B	301	CU9	C7-C8-C9	-2.97	116.02	119.83
2	J	301	CU9	C3-C4-C7	-2.97	114.05	119.91
2	F	220	CU9	C34-C35-C30	-2.95	116.36	119.73
2	D	301	CU9	O40-C26-C27	2.93	120.16	115.14
2	J	301	CU9	O29-C28-C27	-2.90	114.26	120.32
2	D	301	CU9	C28-C24-C19	2.83	122.07	117.95
2	D	301	CU9	O42-C27-C28	2.82	126.78	120.35
2	J	301	CU9	C28-C24-C19	2.81	122.04	117.95
2	D	301	CU9	O39-C13-C14	-2.81	119.56	124.30
2	C	301	CU9	C46-O42-C27	2.75	122.20	114.74
2	H	301	CU9	C41-O40-C26	2.72	121.51	117.51
2	H	301	CU9	C7-C4-C5	2.64	122.81	119.49
2	H	301	CU9	C34-C35-C30	-2.60	116.76	119.73
2	F	220	CU9	C34-C33-C32	2.55	122.02	118.23
2	J	301	CU9	O37-C8-C7	-2.53	119.72	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	CU9	O42-C27-C26	-2.53	116.50	120.12
2	H	301	CU9	C17-C12-C13	2.52	123.07	119.83
2	B	301	CU9	C45-N20-C44	2.47	114.48	107.34
2	D	301	CU9	C36-C33-C32	-2.44	116.36	120.90
2	A	301	CU9	C3-C4-C7	-2.38	115.21	119.91
2	A	301	CU9	C12-C17-C16	-2.38	116.52	120.04
2	F	220	CU9	O42-C27-C26	-2.38	116.72	120.12
2	B	301	CU9	C41-O40-C26	-2.34	114.09	117.51
2	F	301	CU9	O37-C8-C9	2.33	118.57	115.40
2	A	301	CU9	C10-C9-C8	2.33	122.82	119.83
2	B	301	CU9	C46-O42-C27	2.33	121.06	114.74
2	A	301	CU9	C17-C12-C13	2.29	122.77	119.83
2	F	220	CU9	C28-C24-C19	2.27	121.25	117.95
2	F	301	CU9	O39-C13-C12	2.25	118.46	115.40
2	F	301	CU9	O29-C28-C27	-2.24	115.63	120.32
2	J	301	CU9	O29-C28-C24	2.22	123.28	117.28
2	A	301	CU9	C3-C2-N1	2.21	119.09	112.60
2	F	220	CU9	C31-C32-C33	-2.20	118.11	121.00
2	F	220	CU9	C15-C14-C13	-2.19	115.91	120.06
2	B	301	CU9	O42-C27-C26	-2.19	116.99	120.12
2	F	220	CU9	C45-N20-C44	-2.16	101.08	107.34
2	F	301	CU9	O29-C28-C24	2.16	123.12	117.28
2	C	301	CU9	C28-C24-C19	2.14	121.07	117.95
2	D	301	CU9	C4-C5-C6	2.14	124.81	122.12
2	D	301	CU9	C18-C16-C17	2.13	124.09	120.43
2	H	301	CU9	C27-C28-C24	2.11	124.23	120.19
2	J	301	CU9	C22-C23-C25	-2.09	115.79	119.91
2	F	301	CU9	C12-O11-C9	-2.09	113.10	118.09
2	B	301	CU9	C45-N20-C19	-2.09	104.57	110.97
2	J	301	CU9	C18-C16-C17	2.09	124.01	120.43
2	J	301	CU9	C12-O11-C9	-2.06	113.16	118.09
2	B	301	CU9	O40-C26-C27	2.06	118.67	115.14
2	F	220	CU9	C12-O11-C9	2.06	123.01	118.09
2	D	301	CU9	C10-C5-C4	-2.06	117.14	119.39
2	H	301	CU9	O29-C28-C27	-2.04	116.05	120.32
2	F	301	CU9	C10-C5-C6	2.03	121.70	118.08
2	C	301	CU9	C27-C28-C24	2.03	124.08	120.19
2	B	301	CU9	C36-C33-C32	-2.02	117.14	120.90
2	C	301	CU9	O11-C9-C8	2.02	123.29	117.04
2	F	220	CU9	C35-C30-C31	2.02	123.11	120.16
2	F	220	CU9	C10-C5-C6	2.02	121.67	118.08
2	J	301	CU9	C3-C4-C5	2.02	124.11	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	CU9	C45-N20-C19	2.02	117.16	110.97

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	301	CU9	C27-C26-O40-C41
2	J	301	CU9	C12-C13-O39-C48
2	J	301	CU9	C26-C27-O42-C46
2	D	301	CU9	C26-C27-O42-C46
2	J	301	CU9	C14-C13-O39-C48
2	J	301	CU9	C25-C26-O40-C41
2	D	301	CU9	C25-C26-O40-C41
2	D	301	CU9	C27-C26-O40-C41
2	D	301	CU9	C9-C8-O37-C38
2	B	301	CU9	C9-C8-O37-C38
2	J	301	CU9	C28-C27-O42-C46
2	D	301	CU9	C7-C8-O37-C38
2	B	301	CU9	C7-C8-O37-C38
2	D	301	CU9	C28-C27-O42-C46
2	D	301	CU9	C12-C13-O39-C48
2	D	301	CU9	C14-C13-O39-C48
2	F	301	CU9	C27-C26-O40-C41
2	H	301	CU9	C15-C16-C18-C19
2	F	220	CU9	C14-C13-O39-C48
2	F	220	CU9	C17-C16-C18-C19
2	C	301	CU9	C17-C16-C18-C19
2	H	301	CU9	C17-C16-C18-C19
2	C	301	CU9	C15-C16-C18-C19
2	B	301	CU9	C15-C16-C18-C19
2	F	220	CU9	C26-C27-O42-C46

There are no ring outliers.

6 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	CU9	2	0
2	A	301	CU9	2	0
2	J	301	CU9	12	0
2	C	301	CU9	2	0
2	F	220	CU9	6	0

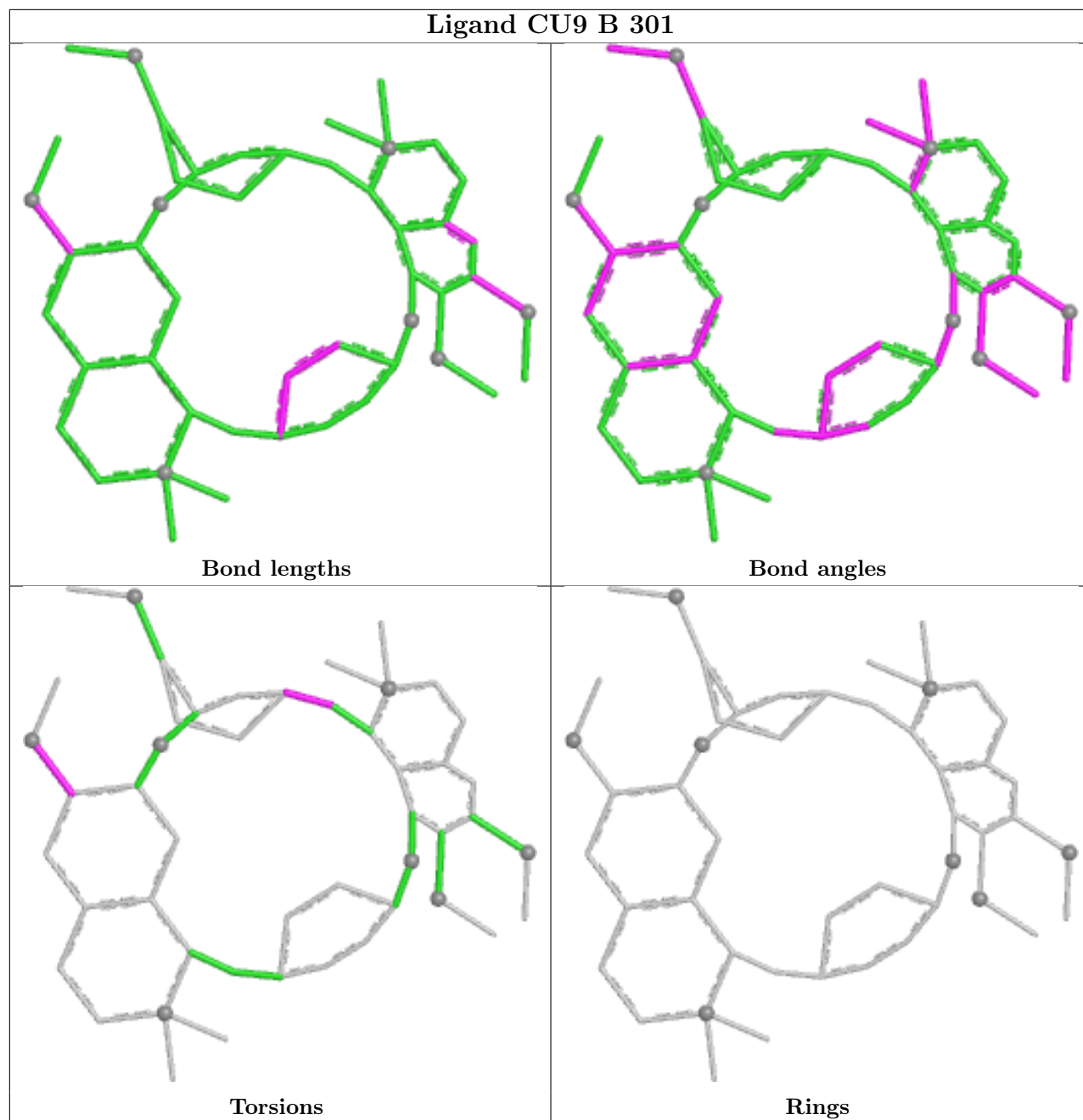
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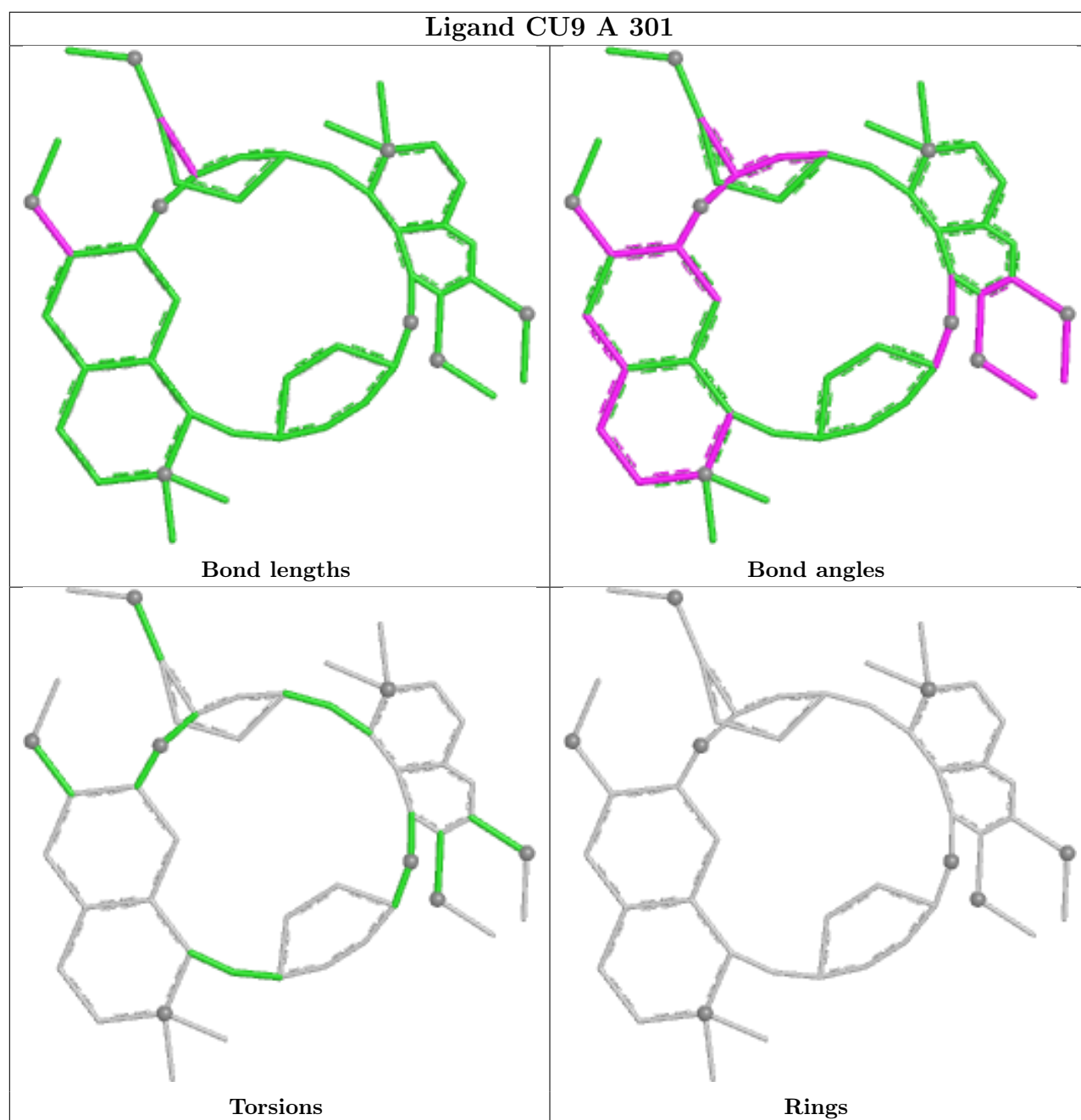
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	CU9	8	0

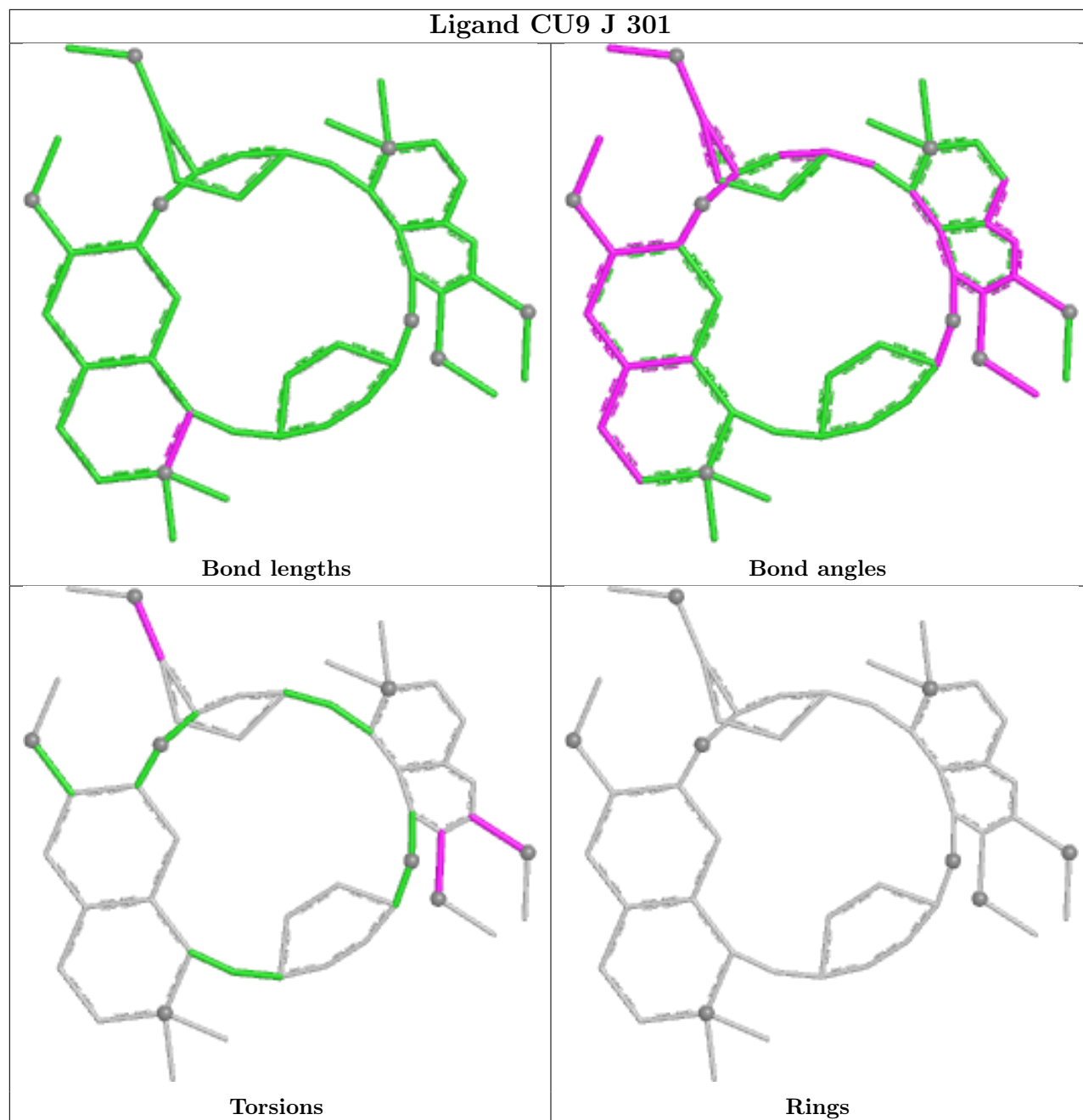
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

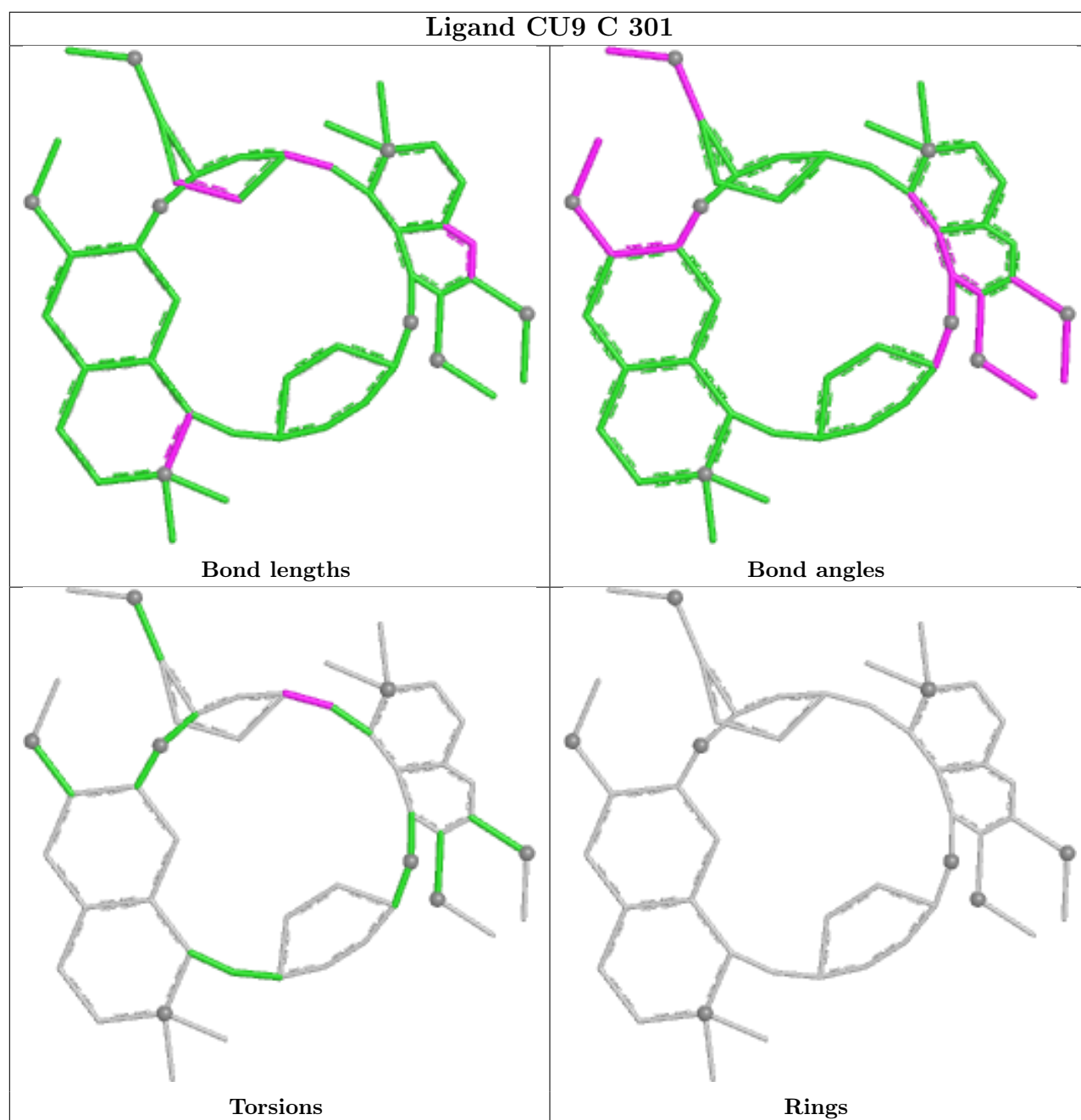
Ligand CU9 B 301



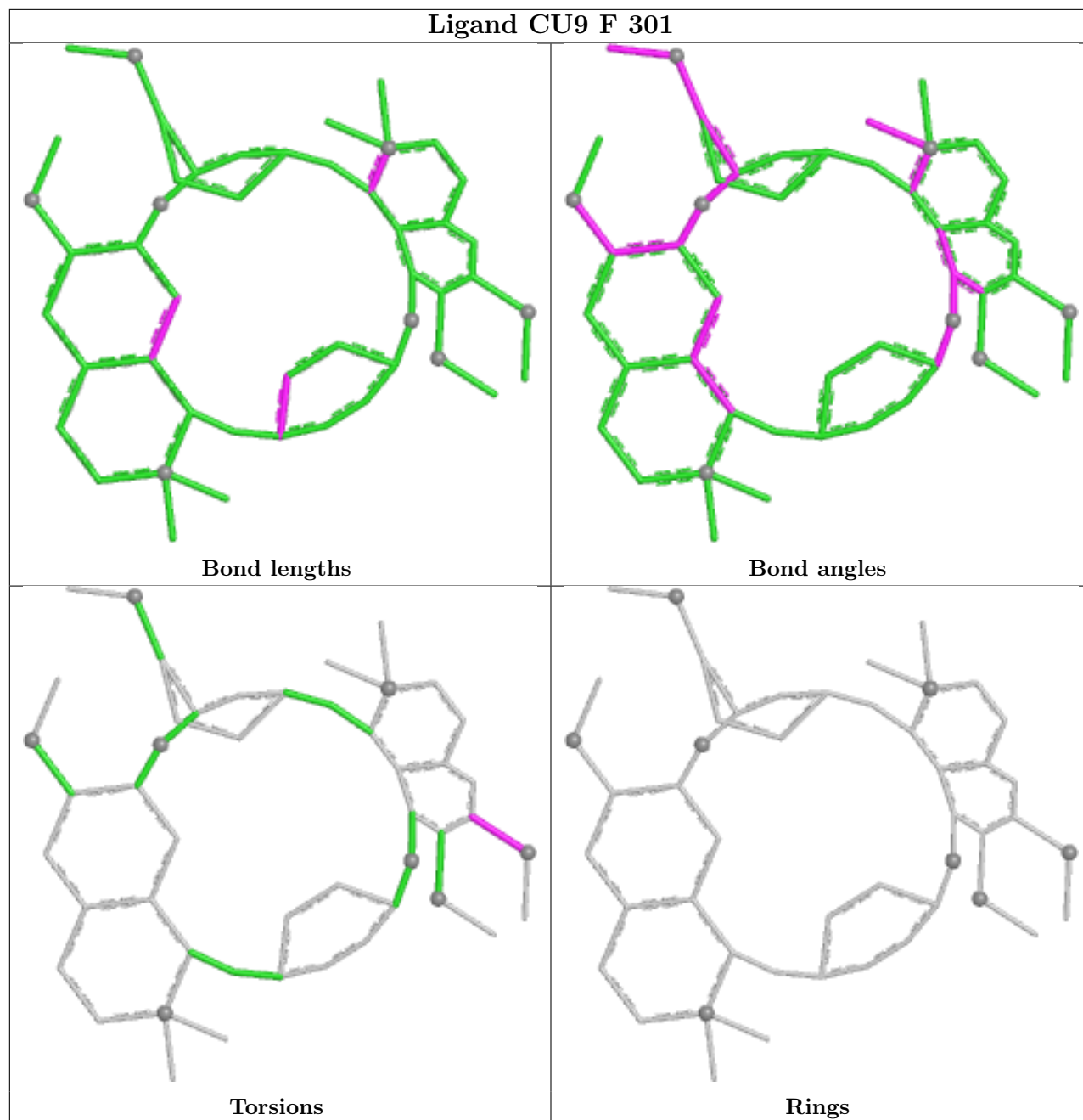


Ligand CU9 J 301

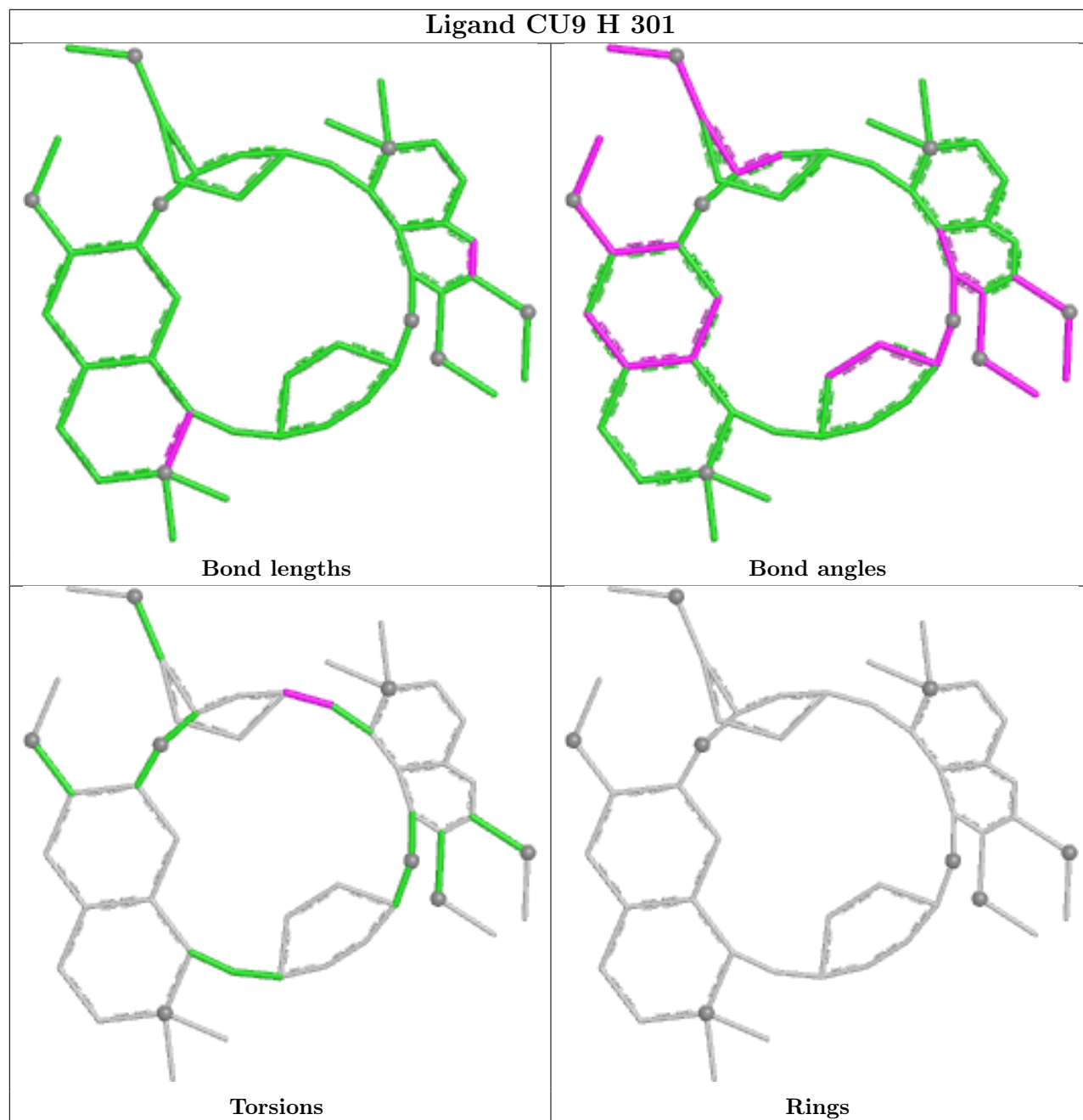


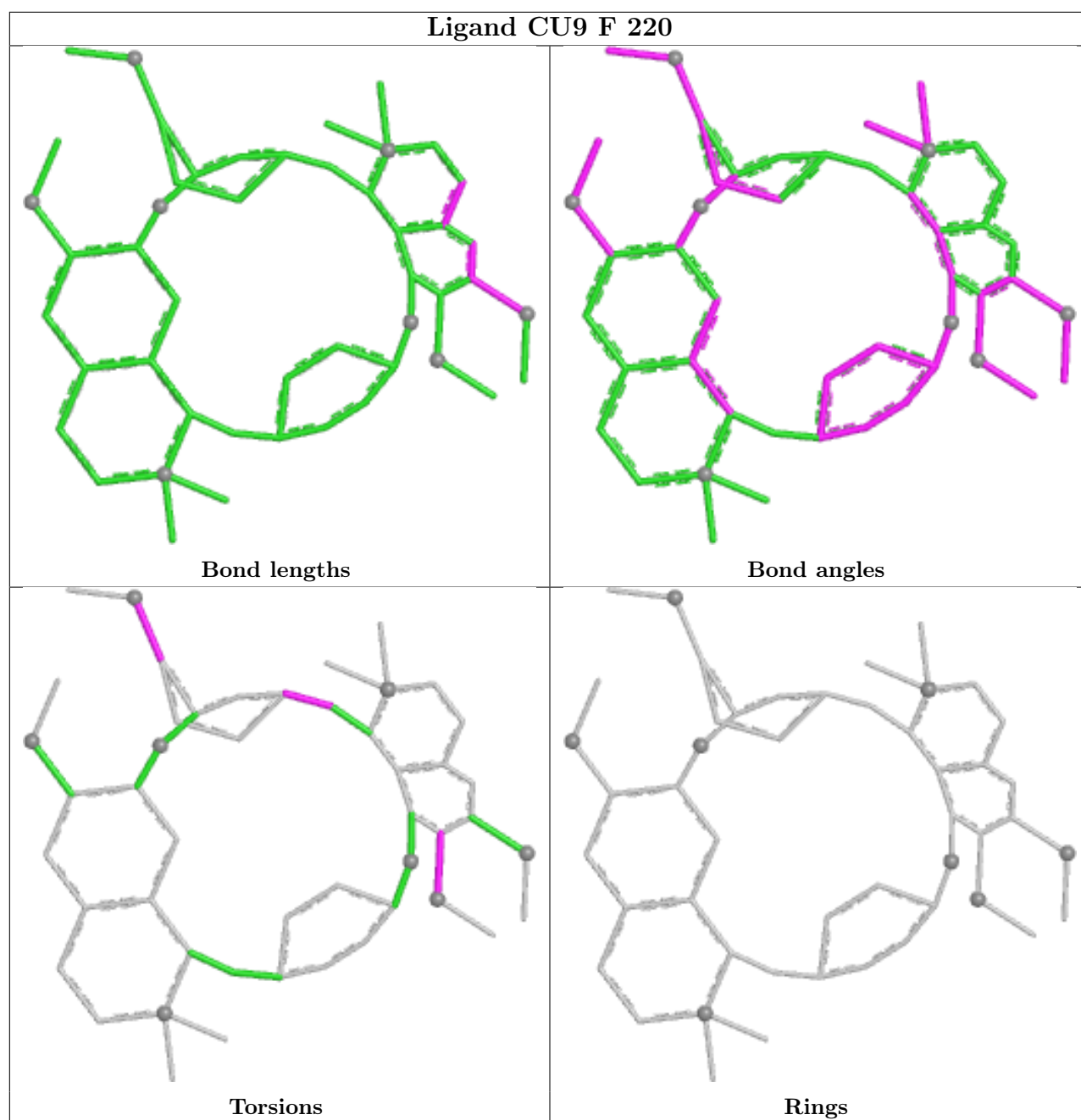


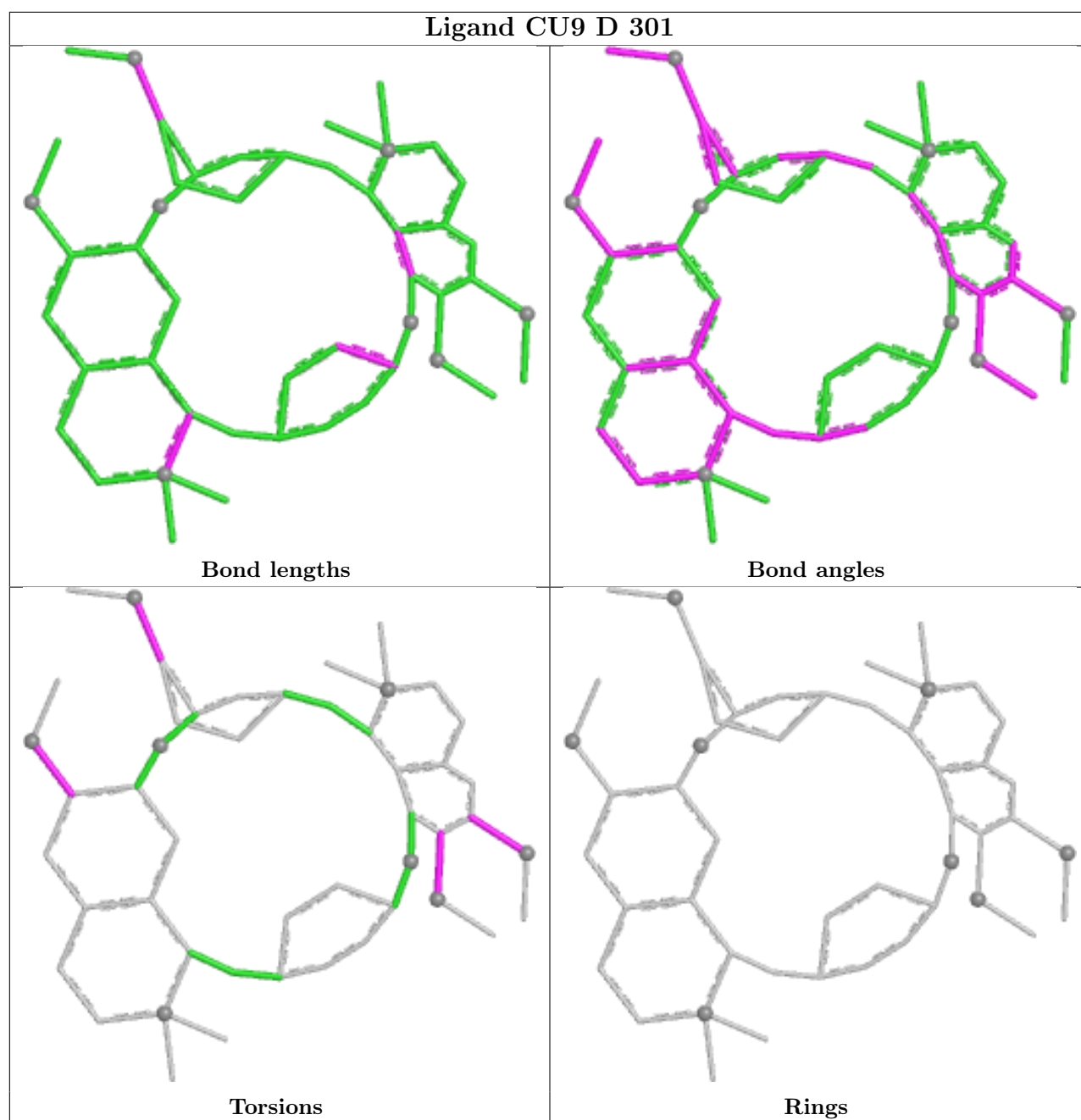
Ligand CU9 F 301



Ligand CU9 H 301







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	203/228 (89%)	0.18	21 (10%) 12 12	9, 20, 60, 79	0
1	B	208/228 (91%)	-0.07	6 (2%) 53 56	8, 19, 43, 70	2 (0%)
1	C	211/228 (92%)	-0.03	9 (4%) 40 41	9, 21, 50, 84	1 (0%)
1	D	204/228 (89%)	0.34	26 (12%) 8 8	9, 23, 68, 93	3 (1%)
1	E	205/228 (89%)	0.20	14 (6%) 23 25	11, 22, 56, 72	0
1	F	202/228 (88%)	0.20	20 (9%) 13 13	7, 20, 66, 75	2 (0%)
1	G	207/228 (90%)	0.00	17 (8%) 17 18	8, 19, 49, 75	4 (1%)
1	H	211/228 (92%)	-0.08	3 (1%) 73 75	9, 21, 45, 71	1 (0%)
1	I	204/228 (89%)	0.32	25 (12%) 8 8	7, 23, 64, 91	3 (1%)
1	J	207/228 (90%)	0.14	11 (5%) 32 34	10, 23, 58, 78	0
All	All	2062/2280 (90%)	0.12	152 (7%) 20 22	7, 21, 60, 93	16 (0%)

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	PHE	6.4
1	J	18	PRO	5.3
1	E	19	MET	5.2
1	B	17	SER	5.1
1	A	15	ASN	5.1
1	H	17	SER	4.9
1	D	188	TYR	4.8
1	G	0	LEU	4.8
1	D	14	PHE	4.5
1	A	4	ALA	4.5
1	J	19	MET	4.3
1	F	14	PHE	4.2
1	B	0	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	I	190	CYS	4.2
1	G	16	ARG	4.0
1	B	1	HIS	4.0
1	I	14	PHE	4.0
1	F	13	LEU	3.9
1	A	11	SER	3.9
1	I	188	TYR	3.9
1	I	7	MET	3.8
1	A	7	MET	3.8
1	A	70	ASN	3.7
1	I	13	LEU	3.7
1	J	7	MET	3.7
1	D	13	LEU	3.6
1	D	3	GLN	3.6
1	I	189	SER	3.6
1	A	13	LEU	3.5
1	D	17	SER	3.5
1	I	4	ALA	3.5
1	D	2	SER	3.4
1	I	191	CYS	3.4
1	C	-4	ASP	3.4
1	H	16	ARG	3.4
1	J	17	SER	3.4
1	I	192	PRO	3.4
1	D	4	ALA	3.4
1	F	9	LEU	3.4
1	G	1	HIS	3.3
1	E	16	ARG	3.3
1	B	16	ARG	3.2
1	E	20	TYR	3.2
1	D	192	PRO	3.2
1	E	7	MET	3.2
1	D	9	LEU	3.1
1	D	69	PRO	3.1
1	F	73	GLY	3.0
1	J	2	SER	3.0
1	F	69	PRO	3.0
1	D	7	MET	3.0
1	F	2	SER	3.0
1	A	12	ASP	3.0
1	F	7	MET	3.0
1	B	-1	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	67	TRP	3.0
1	D	15	ASN	2.9
1	F	6	LEU	2.9
1	D	73	GLY	2.9
1	A	69	PRO	2.9
1	D	191	CYS	2.9
1	H	-3	ASP	2.9
1	E	69	PRO	2.9
1	F	72	TYR	2.9
1	A	6	LEU	2.8
1	C	0	LEU	2.8
1	I	6	LEU	2.8
1	E	2	SER	2.7
1	G	-1	LYS	2.7
1	A	5	ASN	2.7
1	A	2	SER	2.7
1	J	4	ALA	2.7
1	A	9	LEU	2.7
1	F	208	ARG	2.7
1	I	70	ASN	2.7
1	A	73	GLY	2.7
1	D	72	TYR	2.6
1	G	73	GLY	2.6
1	F	4	ALA	2.6
1	G	4	ALA	2.6
1	I	69	PRO	2.6
1	I	17	SER	2.6
1	E	67	TRP	2.6
1	I	9	LEU	2.6
1	D	189	SER	2.6
1	A	72	TYR	2.6
1	I	5	ASN	2.6
1	I	15	ASN	2.6
1	A	67	TRP	2.6
1	C	1	HIS	2.5
1	D	70	ASN	2.5
1	E	73	GLY	2.5
1	G	15	ASN	2.5
1	I	74	ASN	2.5
1	F	20	TYR	2.4
1	G	11	SER	2.4
1	F	66	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	8	ARG	2.4
1	E	207	ARG	2.4
1	I	187	HIS	2.4
1	D	68	ASP	2.4
1	C	191	CYS	2.4
1	G	14	PHE	2.4
1	I	2	SER	2.4
1	I	72	TYR	2.4
1	G	3	GLN	2.4
1	I	3	GLN	2.4
1	E	13	LEU	2.3
1	F	70	ASN	2.3
1	D	207	ARG	2.3
1	D	190	CYS	2.3
1	F	12	ASP	2.3
1	C	14	PHE	2.3
1	J	13	LEU	2.3
1	J	72	TYR	2.3
1	B	14	PHE	2.3
1	G	70	ASN	2.3
1	F	5	ASN	2.2
1	D	6	LEU	2.2
1	I	16	ARG	2.2
1	D	26	ASP	2.2
1	E	66	MET	2.2
1	F	65	LEU	2.2
1	C	17	SER	2.2
1	F	11	SER	2.2
1	I	11	SER	2.2
1	E	15	ASN	2.2
1	G	71	GLU	2.2
1	I	83	ALA	2.2
1	A	66	MET	2.2
1	A	3	GLN	2.1
1	D	10	LYS	2.1
1	C	16	ARG	2.1
1	D	11	SER	2.1
1	G	2	SER	2.1
1	J	16	ARG	2.1
1	A	68	ASP	2.1
1	F	68	ASP	2.1
1	C	20	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	160[A]	THR	2.1
1	G	188	TYR	2.1
1	G	207[A]	ARG	2.1
1	A	10	LYS	2.1
1	G	191	CYS	2.0
1	I	73	GLY	2.0
1	J	73	GLY	2.0
1	E	14	PHE	2.0
1	J	14	PHE	2.0
1	G	7	MET	2.0
1	D	67	TRP	2.0
1	E	68	ASP	2.0
1	C	-1	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

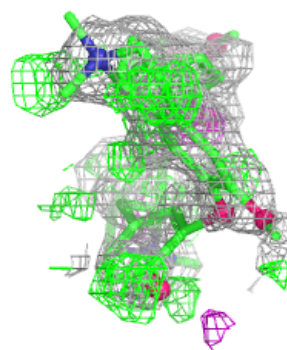
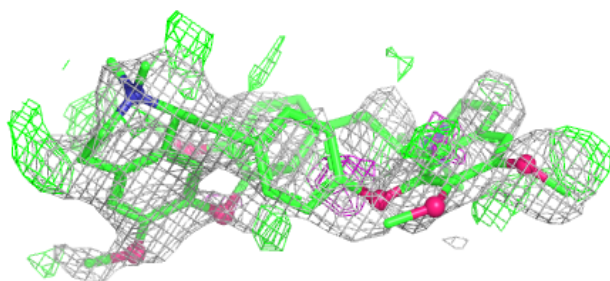
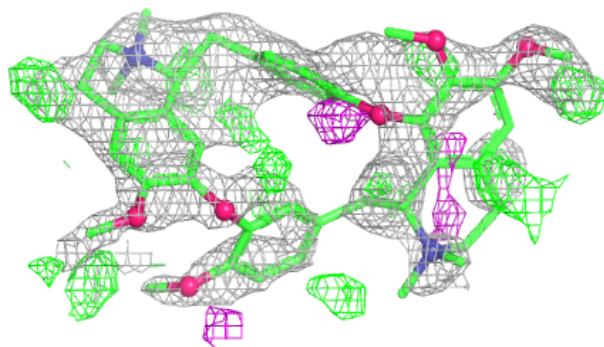
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CU9	J	301	48/48	0.64	0.26	30,39,45,49	48
2	CU9	D	301	48/48	0.67	0.26	31,42,46,47	48
2	CU9	A	301	48/48	0.90	0.10	8,22,27,29	48
2	CU9	C	301	48/48	0.90	0.10	17,28,32,34	0
2	CU9	F	220	48/48	0.91	0.11	6,23,28,31	48
2	CU9	H	301	48/48	0.93	0.09	14,19,25,30	48
2	CU9	B	301	48/48	0.96	0.06	5,12,15,18	0
2	CU9	F	301	48/48	0.97	0.05	4,13,17,19	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.

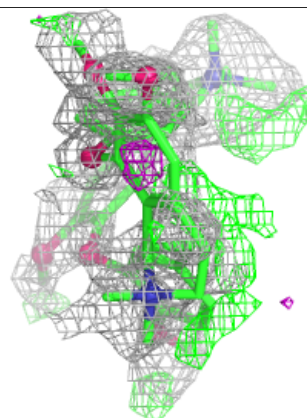
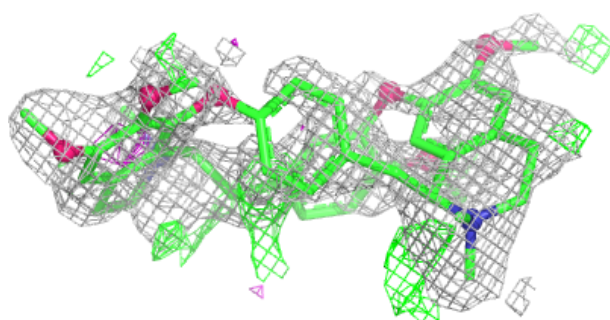
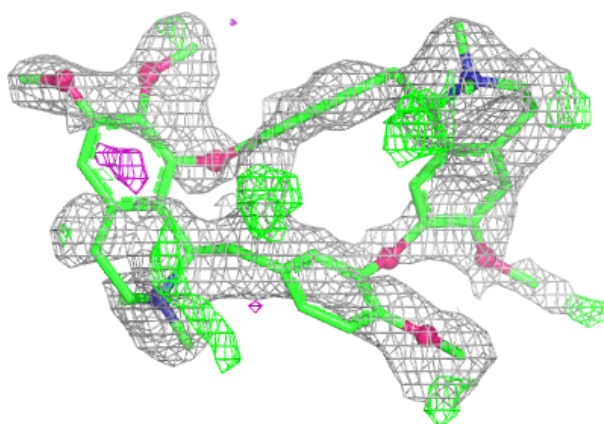
Electron density around CU9 J 301:

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

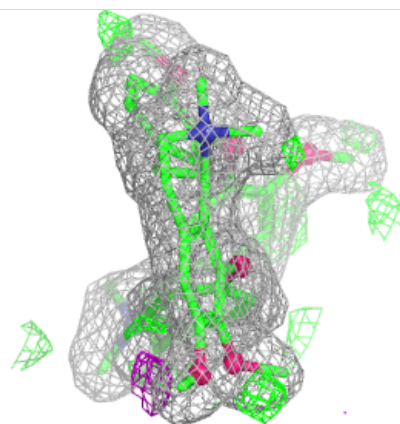
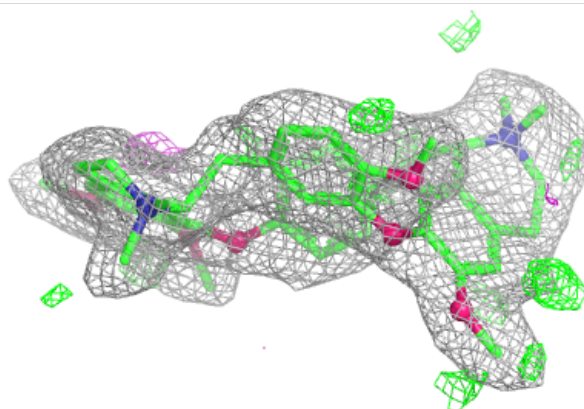
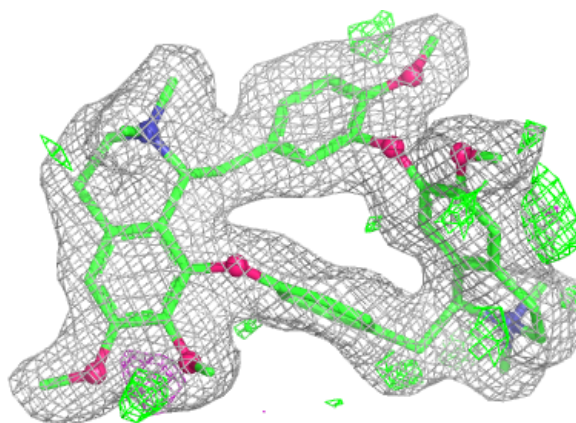


Electron density around CU9 D 301:

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

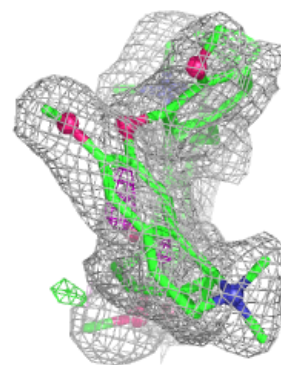
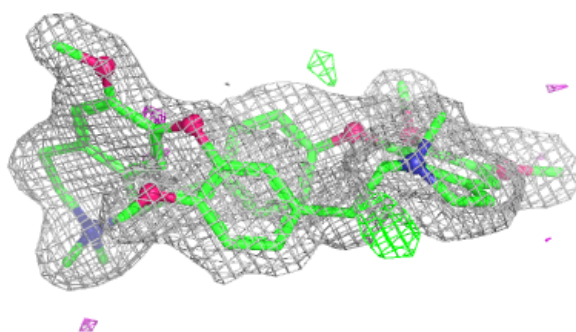
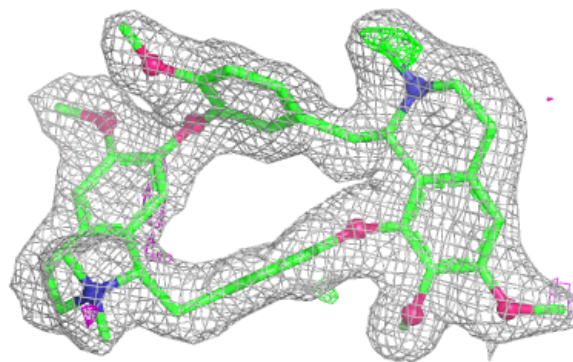
**Electron density around CU9 A 301:**

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

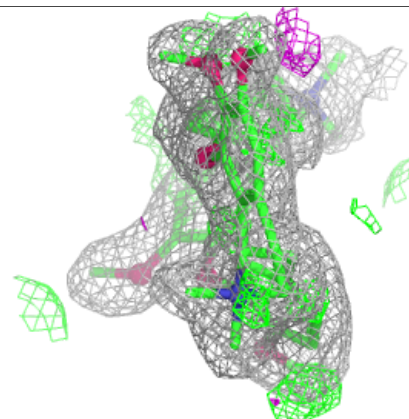
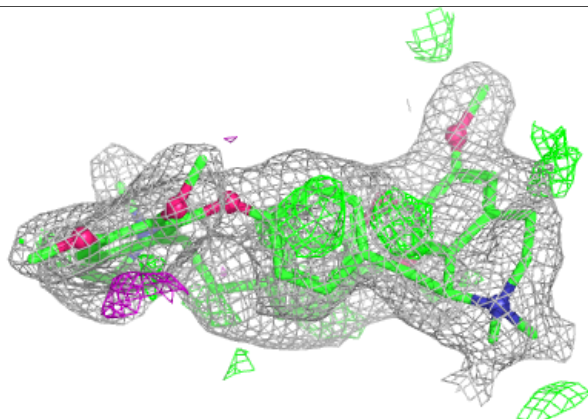
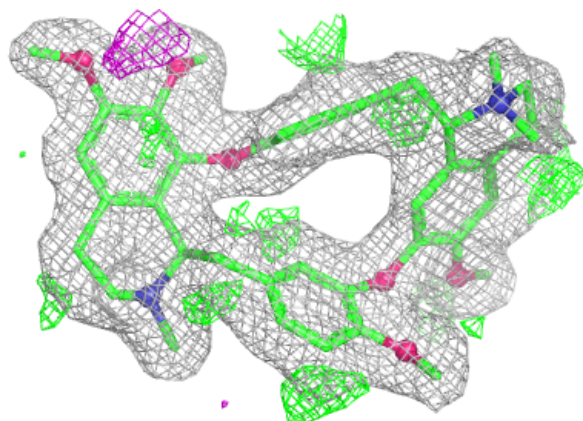


Electron density around CU9 C 301:

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

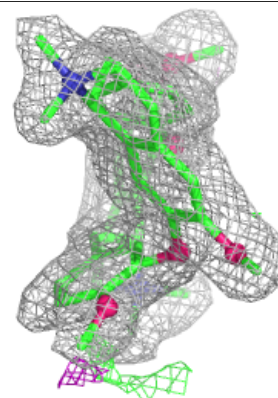
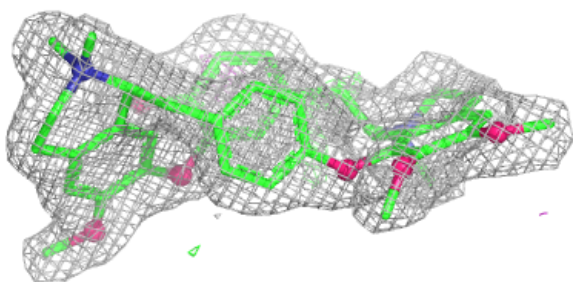
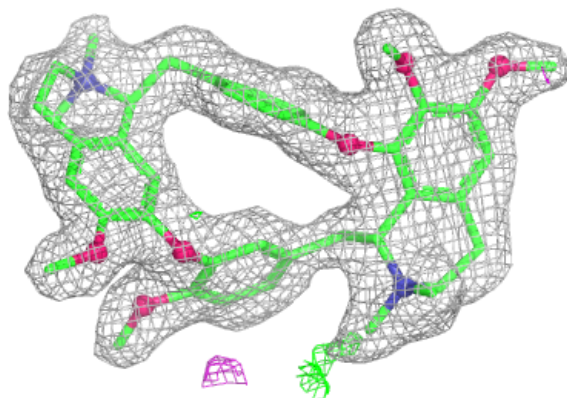
**Electron density around CU9 F 220:**

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

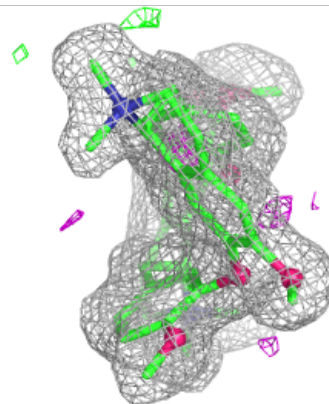
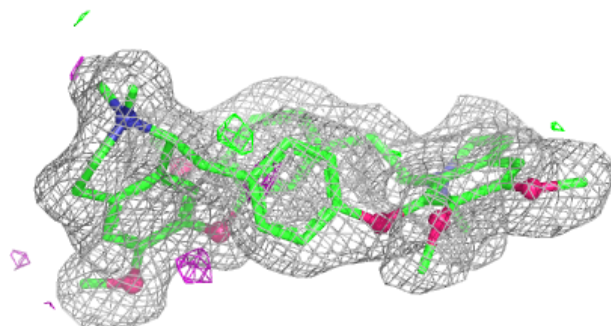
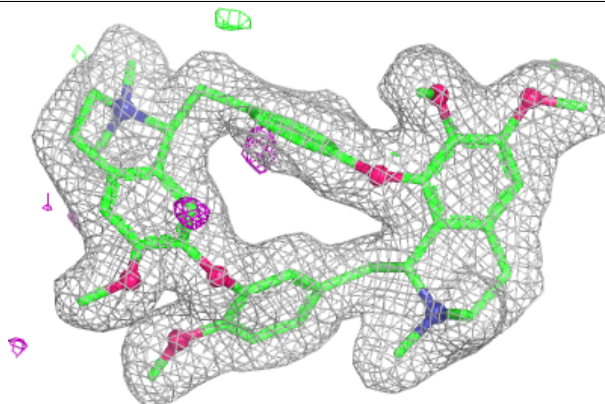


Electron density around CU9 H 301:

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

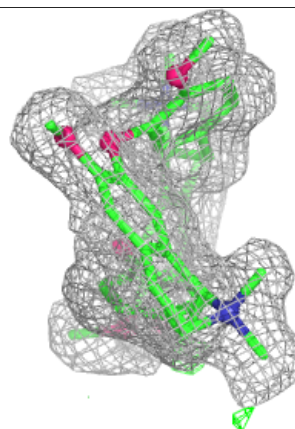
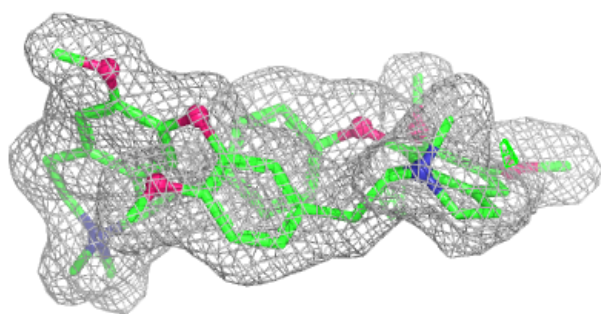
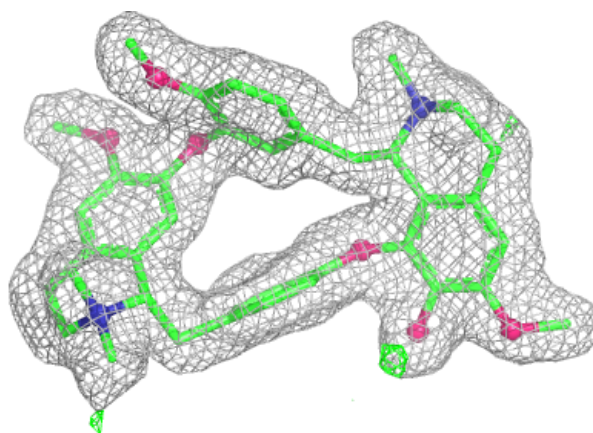
**Electron density around CU9 B 301:**

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



Electron density around CU9 F 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.