



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 02:08 AM UTC

PDB ID : 7VP9 / pdb_00007vp9
Title : Crystal structure of human ClpP in complex with ZG111
Authors : Wang, P.Y.; Gan, J.H.; Yang, C.-G.
Deposited on : 2021-10-15
Resolution : 2.55 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

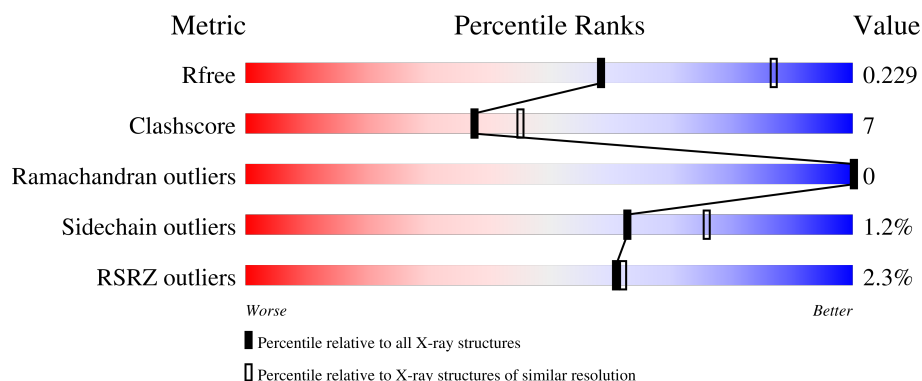
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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

Mol	Chain	Length	Quality of chain
1	A	221	0% 67% 10% 23%
1	B	221	3% 64% 13% 23%
1	C	221	4% 60% 15% 24%
1	D	221	5% 52% 24% 23%
1	E	221	2% 63% 13% 23%

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Mol	Chain	Length	Quality of chain
1	F	221	 3% 60% 17% 23%
1	G	221	 % 63% 14% 23%
1	H	221	 75% 6% 19%
1	I	221	 % 69% 12% 19%
1	J	221	 70% 11% 19%
1	K	221	 % 70% 10% 20%
1	L	221	 % 73% 8% 19%
1	M	221	 % 71% 10% 19%
1	N	221	 % 70% 11% 19%

2 Entry composition

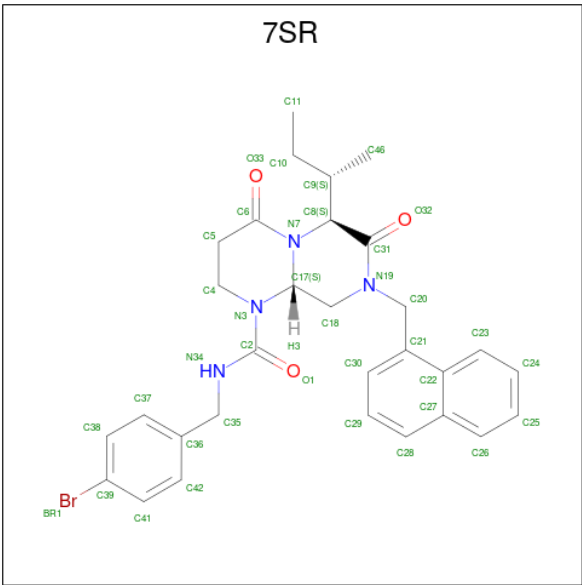
There are 4 unique types of molecules in this entry. The entry contains 19269 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP-dependent Clp protease proteolytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1306	836	219	238	13			
1	B	170	Total	C	N	O	S	0	0	0
			1300	831	221	236	12			
1	C	168	Total	C	N	O	S	0	0	0
			1266	809	215	229	13			
1	D	170	Total	C	N	O	S	0	0	0
			1288	821	220	235	12			
1	E	171	Total	C	N	O	S	0	0	0
			1309	839	220	237	13			
1	F	171	Total	C	N	O	S	0	0	0
			1312	841	221	237	13			
1	G	170	Total	C	N	O	S	0	0	0
			1314	843	219	239	13			
1	H	180	Total	C	N	O	S	0	0	0
			1395	887	240	255	13			
1	I	178	Total	C	N	O	S	0	0	0
			1366	874	232	247	13			
1	J	178	Total	C	N	O	S	0	0	0
			1360	870	227	250	13			
1	K	176	Total	C	N	O	S	0	0	0
			1334	857	225	239	13			
1	L	179	Total	C	N	O	S	0	0	0
			1385	882	237	254	12			
1	M	179	Total	C	N	O	S	0	0	0
			1358	866	230	249	13			
1	N	179	Total	C	N	O	S	0	0	0
			1375	875	236	251	13			

- Molecule 2 is (6S,9aS)-N-[(4-bromophenyl)methyl]-6-[(2S)-butan-2-yl]-8-(naphthalen-1-ylmethyl)-4,7-bis(oxidanylidene)-3,6,9,9a-tetrahydro-2H-pyrazino[1,2-a]pyrimidine-1-carboxamide (CCD ID: 7SR) (formula: C₃₀H₃₃BrN₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			38	1	30	4	3		
2	A	1	Total	Br	C	N	O	0	0
			38	1	30	4	3		
2	B	1	Total	Br	C	N	O	0	0
			38	1	30	4	3		
2	D	1	Total	Br	C	N	O	0	0
			38	1	30	4	3		
2	D	1	Total	Br	C	N	O	0	0
			38	1	30	4	3		
2	E	1	Total	Br	C	N	O	0	0
			38	1	30	4	3		
2	G	1	Total	Br	C	N	O	0	0
			38	1	30	4	3		
2	H	1	Total	Br	C	N	O	0	0
			38	1	30	4	3		
2	I	1	Total	Br	C	N	O	0	0
			38	1	30	4	3		
2	I	1	Total	Br	C	N	O	0	0
			38	1	30	4	3		
2	K	1	Total	Br	C	N	O	0	0
			38	1	30	4	3		
2	K	1	Total	Br	C	N	O	0	0
			38	1	30	4	3		
2	L	1	Total	Br	C	N	O	0	0
			38	1	30	4	3		
2	N	1	Total	Br	C	N	O	0	0
			38	1	30	4	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0
3	K	1	Total Mg 1 1	0	0
3	L	1	Total Mg 1 1	0	0
3	M	1	Total Mg 1 1	0	0
3	N	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	B	3	Total O 3 3	0	0
4	C	2	Total O 2 2	0	0
4	F	1	Total O 1 1	0	0
4	G	4	Total O 4 4	0	0

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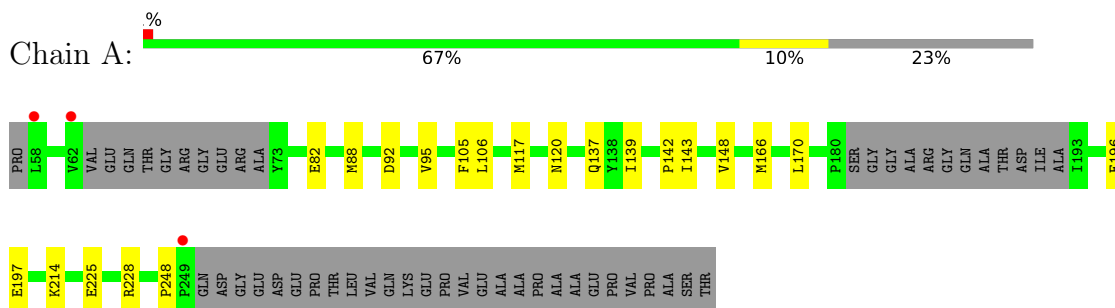
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	7	Total 7	O 7	0	0
4	I	13	Total 13	O 13	0	0
4	J	10	Total 10	O 10	0	0
4	K	4	Total 4	O 4	0	0
4	L	2	Total 2	O 2	0	0
4	M	3	Total 3	O 3	0	0
4	N	3	Total 3	O 3	0	0

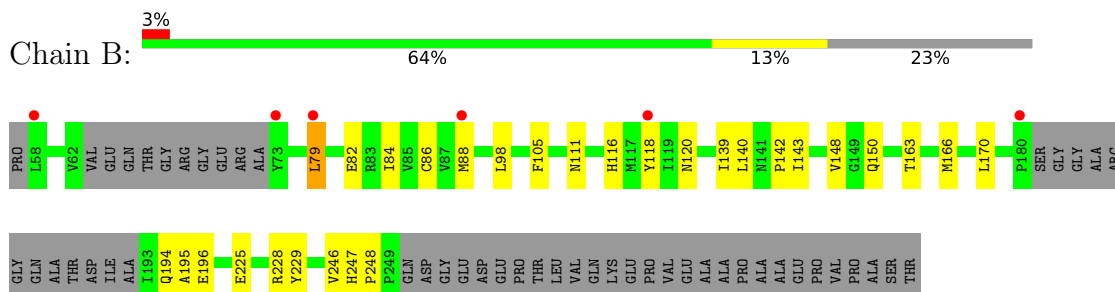
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

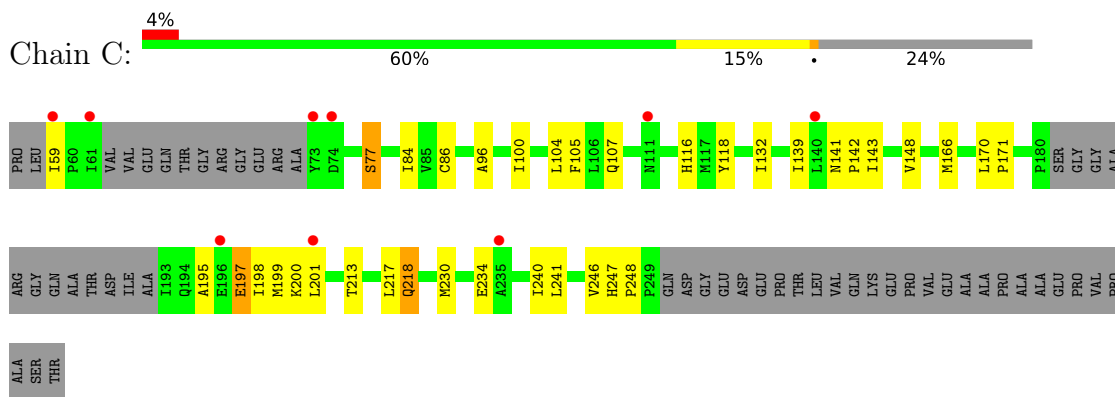
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



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

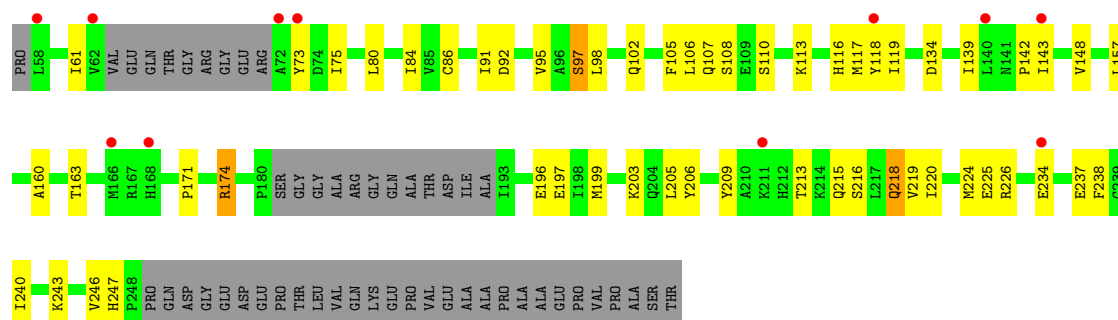


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

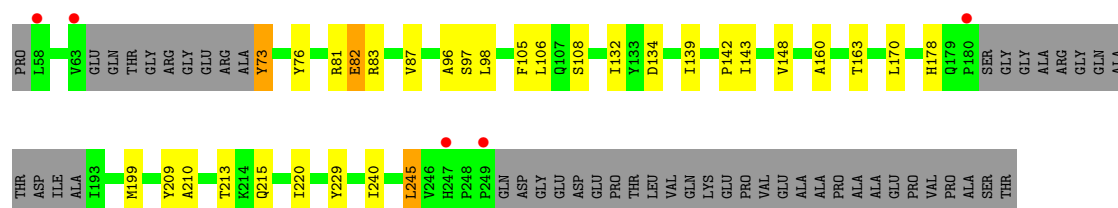


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

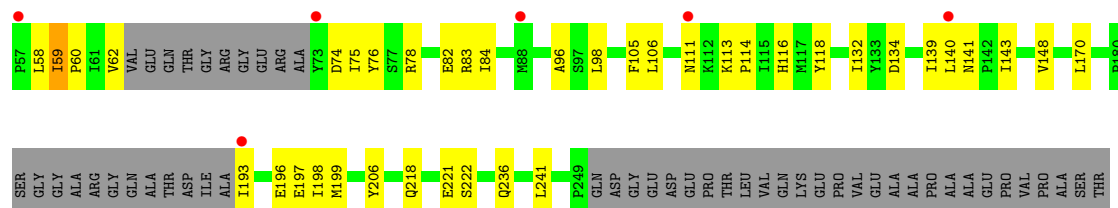




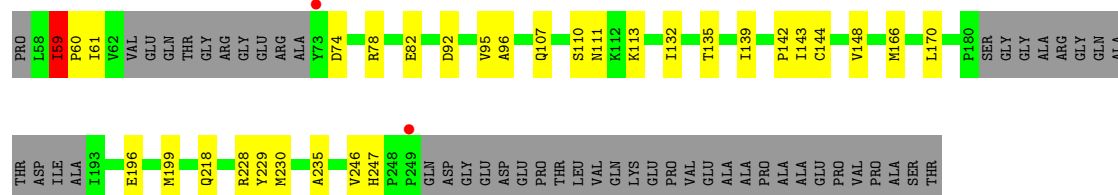
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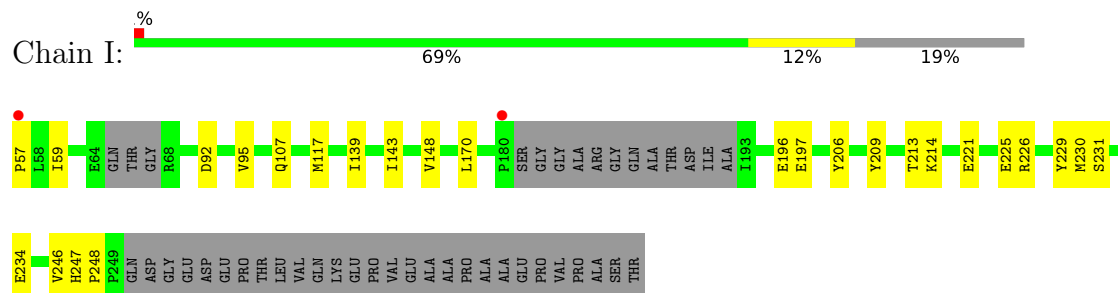


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

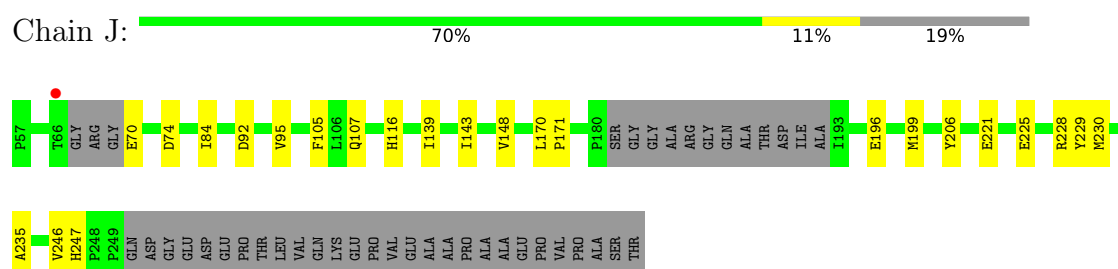


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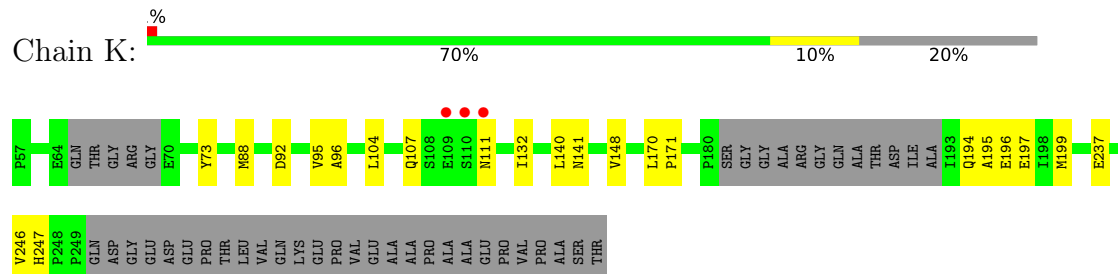
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



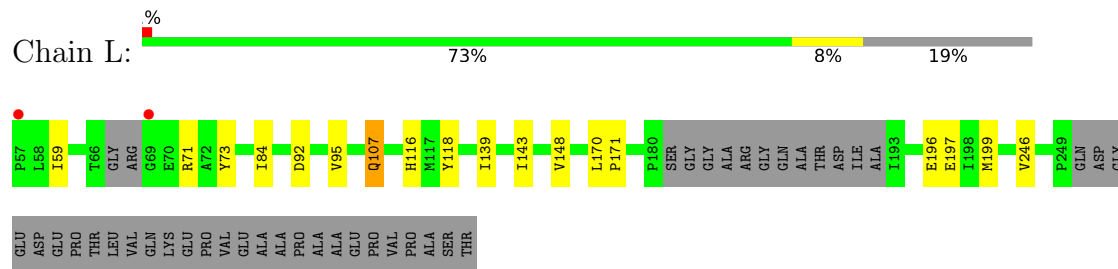
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



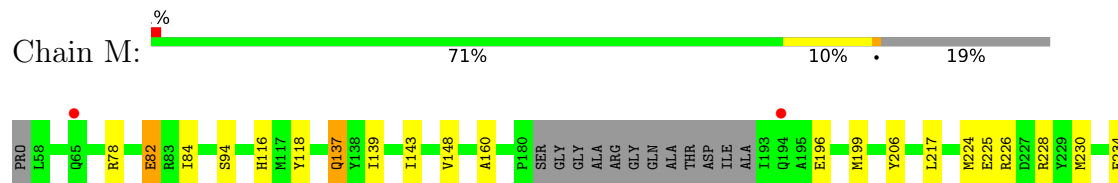
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

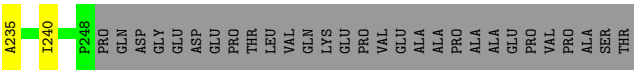


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

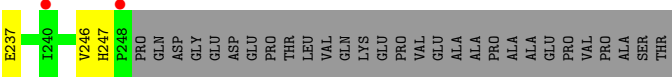


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.81Å 97.41Å 146.69Å 90.00° 90.63° 90.00°	Depositor
Resolution (Å)	28.84 – 2.55 28.84 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.2 (28.84-2.55) 95.1 (28.84-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.202 , 0.232 0.201 , 0.229	Depositor DCC
R_{free} test set	4644 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19269	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 7SR, MG

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	0.32	1/1331 (0.1%)	0.61	3/1805 (0.2%)
1	B	0.42	1/1324 (0.1%)	0.71	4/1795 (0.2%)
1	C	0.62	1/1290 (0.1%)	0.77	3/1749 (0.2%)
1	D	0.46	0/1311	0.81	2/1779 (0.1%)
1	E	0.51	0/1334	0.71	2/1810 (0.1%)
1	F	0.33	0/1337	0.59	1/1813 (0.1%)
1	G	0.54	0/1339	0.56	3/1814 (0.2%)
1	H	0.39	0/1421	0.49	1/1925 (0.1%)
1	I	0.49	2/1392 (0.1%)	0.53	1/1886 (0.1%)
1	J	0.43	1/1386 (0.1%)	0.51	0/1880
1	K	0.59	1/1360 (0.1%)	0.69	4/1846 (0.2%)
1	L	0.46	1/1411 (0.1%)	0.60	0/1911
1	M	0.30	0/1383	0.60	1/1876 (0.1%)
1	N	0.37	0/1400	0.62	1/1896 (0.1%)
All	All	0.46	8/19019 (0.0%)	0.63	26/25785 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	248	PRO	CA-C	11.74	1.60	1.52
1	I	59	ILE	CA-C	-7.03	1.47	1.53
1	B	248	PRO	CA-C	6.50	1.56	1.52
1	I	248	PRO	CA-C	-6.12	1.48	1.52
1	K	140	LEU	CA-C	-5.62	1.47	1.53
1	L	59	ILE	CA-C	-5.49	1.48	1.53
1	A	248	PRO	CA-C	-5.34	1.48	1.52
1	J	74	ASP	C-O	-5.25	1.17	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	248	PRO	O-C-N	11.87	126.73	121.15
1	B	88	MET	CB-CA-C	-8.18	94.65	109.38
1	M	137	GLN	CA-CB-CG	7.65	129.41	114.10
1	N	69	GLY	N-CA-C	7.64	124.29	112.60
1	A	214	LYS	CA-CB-CG	-7.12	99.87	114.10
1	B	248	PRO	O-C-N	7.10	124.48	121.15
1	K	111	ASN	N-CA-C	-7.06	101.76	110.65
1	B	88	MET	N-CA-CB	6.78	121.61	110.69
1	E	82	GLU	N-CA-C	-6.78	105.00	112.72
1	I	248	PRO	O-C-N	-6.59	118.05	121.15
1	K	237	GLU	CB-CA-C	-6.34	100.27	110.79
1	G	59	ILE	CA-C-N	6.12	128.22	120.51
1	G	59	ILE	C-N-CA	6.12	128.22	120.51
1	A	248	PRO	O-C-N	-6.05	118.31	121.15
1	C	197	GLU	N-CA-CB	-6.05	101.24	110.26
1	E	245	LEU	N-CA-C	6.03	118.24	108.41
1	K	88	MET	CB-CG-SD	-6.01	94.66	112.70
1	A	137	GLN	CA-CB-CG	-5.82	102.47	114.10
1	B	88	MET	N-CA-C	5.77	118.88	109.59
1	K	88	MET	CA-CB-CG	5.76	125.62	114.10
1	G	218	GLN	CA-CB-CG	-5.42	103.26	114.10
1	H	203	LYS	CB-CG-CD	5.29	123.48	111.30
1	D	218	GLN	CB-CG-CD	-5.16	103.83	112.60
1	F	82	GLU	N-CA-CB	5.14	117.66	110.56
1	D	174	ARG	CB-CG-CD	-5.04	99.70	111.30
1	C	218	GLN	CB-CA-C	5.04	120.34	110.67

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	1306	0	1316	16	0
1	B	1300	0	1315	25	0
1	C	1266	0	1263	29	0
1	D	1288	0	1282	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1309	0	1321	27	0
1	F	1312	0	1337	36	0
1	G	1314	0	1337	22	0
1	H	1395	0	1416	9	0
1	I	1366	0	1386	18	0
1	J	1360	0	1360	14	0
1	K	1334	0	1339	11	0
1	L	1385	0	1402	11	0
1	M	1358	0	1358	20	0
1	N	1375	0	1390	18	0
2	A	76	0	0	4	0
2	B	38	0	0	1	0
2	D	76	0	0	8	0
2	E	38	0	0	1	0
2	G	38	0	0	1	0
2	H	38	0	0	0	0
2	I	76	0	0	1	0
2	K	76	0	0	1	0
2	L	38	0	0	0	0
2	N	38	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	F	1	0	0	0	0
4	G	4	0	0	0	0
4	H	7	0	0	0	0
4	I	13	0	0	0	0
4	J	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	4	0	0	0	0
4	L	2	0	0	0	0
4	M	3	0	0	0	0
4	N	3	0	0	0	0
All	All	19269	0	18822	265	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 (265) 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:A:302:7SR:BR1	1:B:79:LEU:HD12	2.32	0.84
1:F:111:ASN:HD21	1:F:140:LEU:HD12	1.43	0.83
1:A:105:PHE:HB2	2:A:302:7SR:BR1	2.34	0.83
1:E:213:THR:HG21	1:E:220:ILE:HD11	1.60	0.82
1:G:142:PRO:HB2	1:G:166:MET:HE1	1.62	0.81
1:D:139:ILE:HD11	1:D:143:ILE:HD11	1.66	0.77
1:C:118:TYR:HE1	1:C:148:VAL:HG22	1.50	0.76
1:C:148:VAL:HG12	1:C:170:LEU:HG	1.67	0.76
1:N:66:THR:HG21	1:N:71:ARG:HD2	1.69	0.73
1:G:148:VAL:HG13	1:G:170:LEU:HD12	1.70	0.72
1:D:234:GLU:HA	1:D:237:GLU:HG2	1.72	0.71
1:F:196:GLU:HG3	1:J:199:MET:HE1	1.71	0.71
1:B:142:PRO:HA	1:B:163:THR:HG21	1.74	0.70
1:D:196:GLU:HA	1:L:199:MET:HE1	1.74	0.69
1:E:213:THR:HG23	1:E:215:GLN:H	1.57	0.69
1:E:142:PRO:HA	1:E:163:THR:HG21	1.75	0.68
1:G:59:ILE:HG22	1:G:60:PRO:HD2	1.74	0.68
1:B:84:ILE:HG12	1:B:116:HIS:HB2	1.75	0.68
1:A:139:ILE:HD11	1:A:143:ILE:HD11	1.75	0.68
1:D:134:ASP:HB3	1:E:170:LEU:HD23	1.74	0.68
1:E:97:SER:HB2	1:F:118:TYR:HE2	1.59	0.67
1:C:199:MET:HE1	1:M:196:GLU:HA	1.78	0.66
1:M:94:SER:HA	1:N:88:MET:HE2	1.78	0.66
1:C:84:ILE:HG12	1:C:116:HIS:HB2	1.78	0.66
1:M:94:SER:HA	1:N:88:MET:CE	2.26	0.65
1:K:148:VAL:HG13	1:K:170:LEU:HD12	1.79	0.65
2:D:301:7SR:C17	2:D:301:7SR:C10	2.74	0.65
1:F:118:TYR:HE1	1:F:148:VAL:HG22	1.62	0.65
1:A:148:VAL:HG13	1:A:170:LEU:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:MET:SD	1:A:120:ASN:HB3	2.37	0.64
1:I:230:MET:HB3	1:I:234:GLU:HG3	1.79	0.64
1:D:226:ARG:HD2	1:M:225:GLU:OE2	1.97	0.64
1:A:142:PRO:HB2	1:A:166:MET:HE1	1.79	0.63
1:D:213:THR:HG23	1:D:215:GLN:H	1.63	0.63
1:C:200:LYS:HB3	1:D:174:ARG:HH21	1.62	0.63
1:D:213:THR:HG21	1:D:220:ILE:HD11	1.80	0.63
1:E:98:LEU:HD21	1:F:60:PRO:HD3	1.80	0.62
1:C:105:PHE:HB2	2:D:302:7SR:BR1	2.54	0.62
1:F:111:ASN:HD21	1:F:140:LEU:CD1	2.13	0.62
1:C:142:PRO:HB2	1:C:166:MET:HE1	1.80	0.62
1:F:59:ILE:HD11	1:F:76:TYR:CD2	2.34	0.61
1:C:200:LYS:HB3	1:D:174:ARG:NH2	2.15	0.61
1:D:197:GLU:OE1	1:E:229:TYR:HB2	2.00	0.61
1:A:88:MET:HE1	1:A:120:ASN:HB3	1.82	0.61
1:M:217:LEU:H	1:M:217:LEU:HD12	1.66	0.61
1:H:84:ILE:HG12	1:H:116:HIS:HB2	1.81	0.60
1:M:78:ARG:NH2	1:M:82:GLU:OE1	2.34	0.60
1:D:142:PRO:HA	1:D:163:THR:HG21	1.83	0.60
1:C:118:TYR:HE1	1:C:148:VAL:CG2	2.14	0.60
1:F:74:ASP:OD1	1:F:76:TYR:N	2.30	0.60
1:C:139:ILE:HD11	1:C:143:ILE:HD11	1.84	0.60
1:D:91:ILE:HA	1:D:95:VAL:HG21	1.84	0.60
1:B:139:ILE:HD11	1:B:143:ILE:HD11	1.85	0.59
1:J:230:MET:HE2	1:J:235:ALA:HA	1.84	0.59
1:J:148:VAL:HG13	1:J:170:LEU:HD12	1.84	0.59
1:E:97:SER:HB2	1:F:118:TYR:CE2	2.38	0.58
1:G:78:ARG:NH2	1:G:82:GLU:HG2	2.18	0.58
1:E:96:ALA:HA	1:E:132:ILE:HD11	1.86	0.58
1:F:111:ASN:OD1	1:F:140:LEU:HB2	2.03	0.58
1:D:157:LEU:HD13	1:D:205:LEU:HD22	1.86	0.57
1:N:118:TYR:HE1	1:N:148:VAL:CG2	2.16	0.57
1:I:197:GLU:OE2	1:J:228:ARG:HA	2.04	0.57
1:F:139:ILE:HD11	1:F:143:ILE:HD11	1.87	0.57
1:B:143:ILE:H	1:B:163:THR:HG23	1.71	0.56
1:B:98:LEU:HD11	1:C:59:ILE:HG22	1.88	0.56
1:E:83:ARG:HA	1:E:106:LEU:HD13	1.88	0.56
1:G:139:ILE:HD11	1:G:143:ILE:HD11	1.87	0.56
1:K:246:VAL:HG12	1:K:247:HIS:CE1	2.41	0.55
1:D:118:TYR:HE1	1:D:148:VAL:CG1	2.19	0.55
1:F:118:TYR:HE1	1:F:148:VAL:CG2	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:118:TYR:HE1	1:L:148:VAL:HB	1.72	0.54
1:G:107:GLN:HA	1:G:110:SER:O	2.07	0.54
1:D:215:GLN:HB3	1:D:219:VAL:HG11	1.89	0.54
1:B:105:PHE:HB2	2:B:301:7SR:BR1	2.63	0.54
1:F:83:ARG:NH2	1:F:113:LYS:O	2.41	0.53
1:G:78:ARG:HH22	1:G:82:GLU:HG2	1.74	0.53
1:C:171:PRO:HG3	1:C:246:VAL:HG22	1.90	0.53
1:E:105:PHE:HB2	2:E:301:7SR:BR1	2.64	0.53
1:E:209:TYR:O	1:E:213:THR:HG22	2.08	0.53
1:G:135:THR:O	1:G:139:ILE:HG23	2.08	0.53
1:D:92:ASP:H	1:D:95:VAL:HG22	1.73	0.52
1:F:148:VAL:HG12	1:F:170:LEU:HG	1.91	0.52
1:F:84:ILE:HG12	1:F:116:HIS:HB2	1.91	0.52
1:H:148:VAL:HG13	1:H:170:LEU:HD12	1.90	0.52
1:B:79:LEU:HD23	1:B:84:ILE:HB	1.91	0.52
1:C:246:VAL:HG12	1:C:247:HIS:CE1	2.45	0.52
1:A:88:MET:CE	1:A:120:ASN:HB3	2.40	0.52
1:B:148:VAL:HG23	1:B:170:LEU:HD12	1.91	0.52
1:I:107:GLN:HE22	2:I:301:7SR:C11	2.22	0.52
1:B:143:ILE:H	1:B:163:THR:CG2	2.24	0.51
1:E:73:TYR:N	1:E:73:TYR:CD2	2.72	0.51
1:M:139:ILE:HD11	1:M:143:ILE:HD11	1.92	0.51
1:N:237:GLU:O	1:N:237:GLU:HG3	2.10	0.51
1:D:216:SER:OG	1:D:218:GLN:HB2	2.11	0.51
1:E:139:ILE:HD11	1:E:143:ILE:HD11	1.91	0.51
1:D:84:ILE:HG12	1:D:116:HIS:HB2	1.93	0.51
1:E:148:VAL:HG12	1:E:170:LEU:HB2	1.93	0.51
1:F:98:LEU:HD21	1:G:59:ILE:HG23	1.93	0.51
1:E:199:MET:HE1	1:K:196:GLU:HA	1.92	0.50
1:F:83:ARG:NH1	1:F:106:LEU:O	2.44	0.50
1:C:118:TYR:CE1	1:C:148:VAL:HG22	2.40	0.50
1:I:57:PRO:O	1:I:57:PRO:HG2	2.11	0.50
1:I:197:GLU:CD	1:J:229:TYR:H	2.19	0.50
1:I:148:VAL:HG13	1:I:170:LEU:HD12	1.93	0.50
1:D:209:TYR:O	1:D:213:THR:HG22	2.11	0.50
1:A:92:ASP:OD1	1:A:95:VAL:HG23	2.12	0.49
1:F:83:ARG:NH2	1:F:114:PRO:O	2.45	0.49
1:F:62:VAL:HG21	1:F:78:ARG:HG2	1.92	0.49
1:D:110:SER:OG	1:D:113:LYS:HG3	2.12	0.49
1:N:118:TYR:CE1	1:N:148:VAL:HG22	2.47	0.49
1:D:108:SER:HB3	2:D:301:7SR:C35	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:VAL:HG12	1:D:247:HIS:ND1	2.27	0.49
1:G:196:GLU:OE2	1:I:206:TYR:OH	2.27	0.49
1:N:104:LEU:O	1:N:107:GLN:HG3	2.13	0.49
1:I:231:SER:OG	1:I:234:GLU:HG2	2.12	0.49
1:I:246:VAL:HG12	1:I:247:HIS:CD2	2.48	0.49
1:D:105:PHE:HB2	2:D:301:7SR:BR1	2.68	0.49
1:B:118:TYR:HE1	1:B:148:VAL:CG1	2.26	0.48
1:N:171:PRO:HG3	1:N:246:VAL:HG22	1.95	0.48
1:D:61:ILE:HD12	1:D:73:TYR:C	2.38	0.48
1:B:86:CYS:HG	1:B:118:TYR:HD2	1.60	0.48
1:N:79:LEU:HG	1:N:84:ILE:HB	1.96	0.48
1:D:171:PRO:HG3	1:D:246:VAL:HG22	1.96	0.48
1:N:246:VAL:HG12	1:N:247:HIS:CD2	2.49	0.48
1:N:139:ILE:HD11	1:N:143:ILE:HD11	1.95	0.48
1:B:225:GLU:OE2	1:H:226:ARG:NH2	2.39	0.47
1:G:199:MET:HE1	1:I:196:GLU:OE2	2.14	0.47
1:G:246:VAL:HG12	1:G:247:HIS:CD2	2.49	0.47
1:M:230:MET:HE3	1:M:235:ALA:HA	1.96	0.47
1:F:111:ASN:ND2	1:F:140:LEU:HD12	2.21	0.47
1:B:120:ASN:HA	1:B:150:GLN:O	2.15	0.47
1:N:118:TYR:HE1	1:N:148:VAL:HG21	1.79	0.47
1:C:107:GLN:HE22	2:D:302:7SR:C11	2.27	0.47
1:C:195:ALA:O	1:M:199:MET:HE1	2.14	0.47
1:H:197:GLU:CD	1:I:229:TYR:HB2	2.40	0.47
1:C:199:MET:HB2	1:M:199:MET:HE3	1.97	0.47
1:D:102:GLN:O	1:D:106:LEU:HD13	2.14	0.47
1:I:139:ILE:HD11	1:I:143:ILE:HD11	1.96	0.47
1:L:84:ILE:HG12	1:L:116:HIS:HB2	1.96	0.47
1:C:217:LEU:N	1:C:217:LEU:HD12	2.30	0.47
1:A:105:PHE:HD2	1:A:106:LEU:HD12	1.80	0.47
1:D:117:MET:HG2	1:D:119:ILE:CD1	2.45	0.47
1:D:225:GLU:OE1	1:M:226:ARG:NH1	2.44	0.47
1:B:118:TYR:HE1	1:B:148:VAL:HG12	1.80	0.46
1:D:143:ILE:H	1:D:163:THR:HG23	1.80	0.46
1:K:92:ASP:OD1	1:K:95:VAL:HG23	2.15	0.46
1:G:96:ALA:HA	1:G:132:ILE:HD11	1.97	0.46
1:M:228:ARG:HH12	1:M:234:GLU:CD	2.21	0.46
1:B:196:GLU:OE1	1:N:199:MET:HE1	2.15	0.46
1:B:148:VAL:CG2	1:B:170:LEU:HD12	2.45	0.46
1:D:196:GLU:CA	1:L:199:MET:HE1	2.45	0.46
1:B:163:THR:OG1	1:B:166:MET:SD	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:MET:HG2	1:D:119:ILE:HD11	1.97	0.46
1:E:210:ALA:HA	1:E:213:THR:HG22	1.98	0.46
1:N:206:TYR:CE2	1:N:221:GLU:HG2	2.51	0.45
2:A:302:7SR:C37	1:B:82:GLU:HG3	2.46	0.45
1:D:107:GLN:NE2	2:D:301:7SR:C11	2.79	0.45
1:D:209:TYR:CD2	1:D:224:MET:HE2	2.52	0.45
1:F:74:ASP:OD1	1:F:75:ILE:N	2.49	0.45
1:G:230:MET:HE2	1:G:235:ALA:HA	1.99	0.45
1:M:206:TYR:CE1	1:M:224:MET:HE2	2.52	0.45
1:D:97:SER:HB3	1:E:76:TYR:OH	2.17	0.45
1:D:199:MET:HE1	1:L:196:GLU:HG3	1.99	0.45
1:F:96:ALA:HA	1:F:132:ILE:HD11	1.99	0.44
1:N:209:TYR:O	1:N:213:THR:HG23	2.16	0.44
1:F:199:MET:HE1	1:J:196:GLU:OE2	2.17	0.44
1:E:199:MET:HE1	1:K:195:ALA:C	2.42	0.44
1:D:160:ALA:HB2	1:D:240:ILE:HG23	2.00	0.44
1:H:171:PRO:HG3	1:H:246:VAL:HG22	1.99	0.44
1:D:243:LYS:HA	1:D:243:LYS:HD3	1.74	0.44
1:K:104:LEU:O	1:K:107:GLN:HG3	2.18	0.44
1:C:96:ALA:HA	1:C:132:ILE:HD11	1.99	0.44
1:F:236:GLN:HB2	1:F:241:LEU:HD11	2.00	0.44
1:J:246:VAL:HG12	1:J:247:HIS:CD2	2.52	0.44
1:C:77:SER:OG	1:D:61:ILE:HG22	2.18	0.43
1:C:213:THR:HG22	1:C:240:ILE:HA	2.00	0.43
1:D:203:LYS:HA	1:D:206:TYR:CD2	2.53	0.43
1:F:134:ASP:HB3	1:G:170:LEU:HD13	2.00	0.43
1:F:111:ASN:HA	1:F:141:ASN:HD21	1.83	0.43
1:M:84:ILE:HG12	1:M:116:HIS:HB2	2.01	0.43
1:A:225:GLU:CD	1:I:226:ARG:HH21	2.27	0.43
1:D:75:ILE:HG13	2:D:302:7SR:BR1	2.73	0.43
1:H:206:TYR:CE2	1:H:221:GLU:HG2	2.53	0.43
1:J:92:ASP:OD1	1:J:95:VAL:HG23	2.18	0.43
1:B:194:GLN:HG3	1:B:195:ALA:N	2.34	0.43
1:F:105:PHE:HB2	2:G:301:7SR:BR1	2.73	0.43
1:G:78:ARG:HH22	1:G:82:GLU:CG	2.31	0.43
1:J:139:ILE:HD11	1:J:143:ILE:HD11	2.00	0.43
1:K:171:PRO:HG3	1:K:246:VAL:HG22	2.00	0.43
1:F:206:TYR:CE2	1:F:221:GLU:HG2	2.53	0.43
1:E:160:ALA:HB2	1:E:240:ILE:HG23	2.00	0.43
1:C:195:ALA:C	1:M:199:MET:HE1	2.43	0.43
1:E:199:MET:HE3	1:K:199:MET:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:LEU:CD1	1:D:106:LEU:HD11	2.49	0.43
1:I:92:ASP:OD1	1:I:95:VAL:HG23	2.19	0.43
1:L:92:ASP:OD1	1:L:95:VAL:HG23	2.19	0.43
1:F:74:ASP:OD1	1:F:74:ASP:C	2.61	0.42
1:D:213:THR:OG1	1:D:238:PHE:O	2.38	0.42
2:D:302:7SR:C17	2:D:302:7SR:C10	2.97	0.42
1:F:118:TYR:CE1	1:F:148:VAL:HG22	2.50	0.42
1:A:196:GLU:HG3	1:H:199:MET:HE1	2.00	0.42
1:L:171:PRO:HG3	1:L:246:VAL:HG22	2.01	0.42
1:D:98:LEU:HA	1:D:98:LEU:HD12	1.81	0.42
1:F:111:ASN:OD1	1:F:111:ASN:O	2.36	0.42
1:F:193:ILE:HG12	1:F:198:ILE:HG13	2.01	0.42
1:G:144:CYS:SG	1:G:166:MET:HE2	2.59	0.42
1:G:228:ARG:HD2	1:J:225:GLU:OE2	2.19	0.42
1:J:84:ILE:HG12	1:J:116:HIS:HB2	2.01	0.42
1:B:194:GLN:HG3	1:B:195:ALA:H	1.85	0.42
1:F:197:GLU:OE2	1:G:229:TYR:HB2	2.20	0.42
1:N:92:ASP:OD1	1:N:95:VAL:HG23	2.20	0.42
1:B:140:LEU:HG	1:B:140:LEU:O	2.20	0.42
1:G:61:ILE:HG22	1:G:74:ASP:HA	2.00	0.42
1:J:206:TYR:CE2	1:J:221:GLU:HG2	2.54	0.42
1:N:118:TYR:CE1	1:N:148:VAL:CG2	2.99	0.42
1:D:105:PHE:CD2	1:D:106:LEU:HD12	2.55	0.42
1:J:171:PRO:HG3	1:J:246:VAL:HG22	2.02	0.42
1:L:107:GLN:HE21	1:L:107:GLN:HB3	1.45	0.42
1:C:141:ASN:OD1	1:C:141:ASN:N	2.51	0.42
1:D:118:TYR:CE1	1:D:148:VAL:CG1	3.01	0.42
1:M:118:TYR:HE1	1:M:148:VAL:HB	1.85	0.42
1:M:160:ALA:HB2	1:M:240:ILE:HG23	2.01	0.42
1:C:171:PRO:CG	1:C:246:VAL:HG22	2.50	0.41
1:D:215:GLN:HB3	1:D:219:VAL:CG1	2.49	0.41
1:E:87:VAL:HG23	1:E:87:VAL:O	2.19	0.41
1:E:178:HIS:CE1	1:K:194:GLN:NE2	2.88	0.41
1:L:139:ILE:HD11	1:L:143:ILE:HD11	2.01	0.41
1:E:83:ARG:HA	1:E:106:LEU:CD1	2.49	0.41
1:K:96:ALA:HA	1:K:132:ILE:HD11	2.02	0.41
1:C:230:MET:HB3	1:C:234:GLU:HB3	2.01	0.41
1:D:216:SER:OG	1:D:218:GLN:OE1	2.30	0.41
1:A:120:ASN:HB2	1:A:148:VAL:O	2.20	0.41
1:E:134:ASP:HB3	1:F:170:LEU:HD13	2.02	0.41
1:K:197:GLU:HA	1:K:197:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:SER:CB	1:D:61:ILE:HG22	2.51	0.41
1:C:197:GLU:O	1:C:201:LEU:HD12	2.21	0.41
1:G:92:ASP:OD1	1:G:95:VAL:HG23	2.20	0.41
1:I:209:TYR:O	1:I:213:THR:HG23	2.21	0.41
1:L:170:LEU:HA	1:L:170:LEU:HD23	1.74	0.41
1:A:82:GLU:HG3	2:A:301:7SR:C37	2.51	0.41
1:D:80:LEU:HD11	1:D:106:LEU:HD11	2.02	0.41
1:E:143:ILE:H	1:E:163:THR:HG23	1.84	0.41
1:B:228:ARG:HD2	1:H:225:GLU:OE2	2.20	0.41
1:D:143:ILE:H	1:D:163:THR:CG2	2.32	0.41
1:F:58:LEU:HD22	1:F:58:LEU:HA	1.67	0.41
1:B:246:VAL:HG22	1:B:247:HIS:CD2	2.56	0.41
1:C:86:CYS:SG	1:C:118:TYR:HD2	2.44	0.41
1:D:216:SER:O	1:D:219:VAL:HG12	2.21	0.41
1:D:220:ILE:HG22	1:D:224:MET:HE3	2.03	0.41
1:I:117:MET:HE3	1:I:117:MET:HB2	1.97	0.41
1:D:86:CYS:SG	1:D:118:TYR:HD2	2.44	0.41
1:F:218:GLN:O	1:F:222:SER:HB2	2.20	0.41
1:M:217:LEU:HD12	1:M:217:LEU:N	2.33	0.41
1:C:100:ILE:O	1:C:104:LEU:HD23	2.21	0.40
1:A:197:GLU:OE1	1:B:229:TYR:HB2	2.20	0.40
1:J:105:PHE:HB2	2:K:302:7SR:BR1	2.76	0.40
1:A:117:MET:HE3	1:A:117:MET:HB2	1.98	0.40
1:E:106:LEU:HD23	1:E:106:LEU:HA	1.84	0.40
1:G:59:ILE:HG22	1:G:60:PRO:CD	2.46	0.40
1:H:229:TYR:H	1:N:197:GLU:CD	2.29	0.40
1:I:206:TYR:CE2	1:I:221:GLU:HG2	2.56	0.40
1:A:228:ARG:HD2	1:I:225:GLU:OE2	2.21	0.40
1:L:71:ARG:HD2	1:L:73:TYR:OH	2.21	0.40
1:M:137:GLN:OE1	1:M:137:GLN:HA	2.22	0.40
1:M:199:MET:HB2	1:M:199:MET:HE2	1.71	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	164/221 (74%)	159 (97%)	5 (3%)	0	100	100
1	B	164/221 (74%)	159 (97%)	5 (3%)	0	100	100
1	C	162/221 (73%)	158 (98%)	4 (2%)	0	100	100
1	D	164/221 (74%)	158 (96%)	6 (4%)	0	100	100
1	E	165/221 (75%)	160 (97%)	5 (3%)	0	100	100
1	F	165/221 (75%)	161 (98%)	4 (2%)	0	100	100
1	G	164/221 (74%)	161 (98%)	3 (2%)	0	100	100
1	H	176/221 (80%)	169 (96%)	7 (4%)	0	100	100
1	I	172/221 (78%)	167 (97%)	5 (3%)	0	100	100
1	J	172/221 (78%)	167 (97%)	5 (3%)	0	100	100
1	K	170/221 (77%)	164 (96%)	6 (4%)	0	100	100
1	L	173/221 (78%)	168 (97%)	5 (3%)	0	100	100
1	M	175/221 (79%)	170 (97%)	5 (3%)	0	100	100
1	N	175/221 (79%)	170 (97%)	5 (3%)	0	100	100
All	All	2361/3094 (76%)	2291 (97%)	70 (3%)	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	143/185 (77%)	143 (100%)	0	100	100
1	B	142/185 (77%)	140 (99%)	2 (1%)	59	73
1	C	135/185 (73%)	131 (97%)	4 (3%)	36	51
1	D	137/185 (74%)	136 (99%)	1 (1%)	76	84
1	E	143/185 (77%)	138 (96%)	5 (4%)	32	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	145/185 (78%)	144 (99%)	1 (1%)	76	84
1	G	145/185 (78%)	142 (98%)	3 (2%)	47	63
1	H	153/185 (83%)	153 (100%)	0	100	100
1	I	149/185 (80%)	148 (99%)	1 (1%)	76	84
1	J	147/185 (80%)	145 (99%)	2 (1%)	59	73
1	K	142/185 (77%)	140 (99%)	2 (1%)	59	73
1	L	152/185 (82%)	150 (99%)	2 (1%)	61	74
1	M	145/185 (78%)	144 (99%)	1 (1%)	76	84
1	N	149/185 (80%)	149 (100%)	0	100	100
All	All	2027/2590 (78%)	2003 (99%)	24 (1%)	63	76

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	79	LEU
1	B	111	ASN
1	C	77	SER
1	C	198	ILE
1	C	218	GLN
1	C	241	LEU
1	D	97	SER
1	E	73	TYR
1	E	81	ARG
1	E	82	GLU
1	E	108	SER
1	E	245	LEU
1	F	59	ILE
1	G	59	ILE
1	G	111	ASN
1	G	113	LYS
1	I	214	LYS
1	J	70	GLU
1	J	107	GLN
1	K	73	TYR
1	K	141	ASN
1	L	107	GLN
1	L	197	GLU
1	M	82	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	236	GLN
1	C	107	GLN
1	C	204	GLN
1	E	204	GLN
1	F	111	ASN
1	F	172	ASN
1	I	107	GLN
1	I	168	HIS
1	L	107	GLN
1	L	168	HIS
1	L	178	HIS
1	L	204	GLN
1	M	172	ASN
1	N	204	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 for Mogul analysis.

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	7SR	K	302	-	41,42,42	3.12	9 (21%)	52,60,60	1.30	7 (13%)
2	7SR	I	301	-	41,42,42	3.21	8 (19%)	52,60,60	1.37	6 (11%)
2	7SR	H	301	-	41,42,42	3.12	8 (19%)	52,60,60	1.31	7 (13%)
2	7SR	E	301	-	41,42,42	3.26	10 (24%)	52,60,60	1.78	5 (9%)
2	7SR	L	301	-	41,42,42	3.19	10 (24%)	52,60,60	1.40	7 (13%)
2	7SR	N	301	-	41,42,42	3.35	15 (36%)	52,60,60	1.70	8 (15%)
2	7SR	A	301	-	41,42,42	3.24	9 (21%)	52,60,60	1.19	5 (9%)
2	7SR	B	301	-	41,42,42	3.10	14 (34%)	52,60,60	2.04	10 (19%)
2	7SR	D	302	-	41,42,42	3.30	12 (29%)	52,60,60	1.41	5 (9%)
2	7SR	K	301	-	41,42,42	3.44	18 (43%)	52,60,60	1.86	12 (23%)
2	7SR	A	302	-	41,42,42	3.29	10 (24%)	52,60,60	1.60	9 (17%)
2	7SR	I	302	-	41,42,42	3.13	18 (43%)	52,60,60	1.66	8 (15%)
2	7SR	D	301	-	41,42,42	3.13	10 (24%)	52,60,60	2.30	13 (25%)
2	7SR	G	301	-	41,42,42	3.24	9 (21%)	52,60,60	1.21	4 (7%)

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	7SR	K	302	-	-	0/19/52/52	0/5/5/5
2	7SR	I	301	-	-	0/19/52/52	0/5/5/5
2	7SR	H	301	-	-	0/19/52/52	0/5/5/5
2	7SR	E	301	-	-	6/19/52/52	0/5/5/5
2	7SR	L	301	-	-	2/19/52/52	0/5/5/5
2	7SR	N	301	-	-	1/19/52/52	0/5/5/5
2	7SR	A	301	-	-	3/19/52/52	0/5/5/5
2	7SR	B	301	-	-	2/19/52/52	0/5/5/5
2	7SR	D	302	-	-	5/19/52/52	0/5/5/5
2	7SR	K	301	-	-	0/19/52/52	0/5/5/5
2	7SR	A	302	-	-	4/19/52/52	0/5/5/5
2	7SR	I	302	-	-	1/19/52/52	0/5/5/5
2	7SR	D	301	-	-	6/19/52/52	0/5/5/5
2	7SR	G	301	-	-	7/19/52/52	0/5/5/5

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	7SR	C6-N7	16.04	1.49	1.35
2	I	301	7SR	C6-N7	15.97	1.49	1.35
2	A	301	7SR	C6-N7	15.96	1.49	1.35
2	A	302	7SR	C6-N7	15.72	1.49	1.35
2	G	301	7SR	C6-N7	15.71	1.49	1.35
2	L	301	7SR	C6-N7	15.67	1.49	1.35
2	K	302	7SR	C6-N7	15.04	1.48	1.35
2	D	301	7SR	C6-N7	14.91	1.48	1.35
2	H	301	7SR	C6-N7	14.87	1.48	1.35
2	D	302	7SR	C6-N7	14.82	1.48	1.35
2	N	301	7SR	C6-N7	12.75	1.46	1.35
2	K	301	7SR	C6-N7	12.18	1.46	1.35
2	B	301	7SR	C6-N7	12.18	1.46	1.35
2	I	302	7SR	C6-N7	10.00	1.44	1.35
2	K	301	7SR	C8-N7	-9.02	1.31	1.47
2	B	301	7SR	C8-N7	-8.92	1.31	1.47
2	N	301	7SR	C8-N7	-8.59	1.32	1.47
2	K	301	7SR	C18-N19	-8.35	1.37	1.46
2	I	302	7SR	C8-N7	-8.33	1.32	1.47
2	D	302	7SR	C8-N7	-8.04	1.33	1.47
2	N	301	7SR	C18-N19	-7.82	1.38	1.46
2	I	302	7SR	C18-N19	-7.20	1.38	1.46
2	H	301	7SR	C31-N19	6.76	1.49	1.35
2	A	301	7SR	C31-N19	6.67	1.49	1.35
2	G	301	7SR	C31-N19	6.65	1.49	1.35
2	I	301	7SR	C31-N19	6.60	1.49	1.35
2	E	301	7SR	C31-N19	6.53	1.49	1.35
2	A	302	7SR	C31-N19	6.50	1.49	1.35
2	D	301	7SR	C31-N19	6.42	1.49	1.35
2	G	301	7SR	C8-N7	-6.39	1.36	1.47
2	K	302	7SR	C31-N19	6.39	1.49	1.35
2	K	302	7SR	C8-N7	-6.33	1.36	1.47
2	A	301	7SR	C8-N7	-6.32	1.36	1.47
2	D	302	7SR	C18-N19	-6.29	1.39	1.46
2	B	301	7SR	C18-N19	-6.28	1.39	1.46
2	H	301	7SR	C8-N7	-6.23	1.36	1.47
2	E	301	7SR	C8-N7	-6.19	1.36	1.47
2	L	301	7SR	C31-N19	6.18	1.48	1.35
2	L	301	7SR	C8-N7	-6.17	1.36	1.47
2	A	302	7SR	C8-N7	-6.07	1.36	1.47
2	I	301	7SR	C8-N7	-6.01	1.36	1.47
2	D	301	7SR	C8-N7	-5.98	1.37	1.47
2	I	302	7SR	C17-N7	-5.03	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	7SR	C18-N19	-4.98	1.41	1.46
2	D	302	7SR	C31-N19	4.96	1.46	1.35
2	L	301	7SR	C18-N19	-4.96	1.41	1.46
2	B	301	7SR	C31-N19	4.91	1.45	1.35
2	I	301	7SR	C18-N19	-4.75	1.41	1.46
2	E	301	7SR	C18-N19	-4.75	1.41	1.46
2	A	301	7SR	C18-N19	-4.74	1.41	1.46
2	H	301	7SR	C18-N19	-4.73	1.41	1.46
2	G	301	7SR	C18-N19	-4.68	1.41	1.46
2	N	301	7SR	C31-N19	4.59	1.45	1.35
2	K	302	7SR	C18-N19	-4.53	1.41	1.46
2	N	301	7SR	C17-N7	-4.52	1.41	1.47
2	K	301	7SR	C8-C31	-4.50	1.43	1.52
2	I	302	7SR	C8-C31	-4.49	1.43	1.52
2	N	301	7SR	C8-C31	-4.47	1.43	1.52
2	K	301	7SR	C17-N7	-4.36	1.41	1.47
2	G	301	7SR	C2-N3	4.20	1.49	1.37
2	D	301	7SR	C2-N3	4.19	1.49	1.37
2	K	301	7SR	C22-C27	-4.15	1.35	1.43
2	A	302	7SR	C2-N3	4.14	1.49	1.37
2	D	302	7SR	C17-N7	-4.10	1.42	1.47
2	K	302	7SR	C2-N3	4.03	1.49	1.37
2	H	301	7SR	C2-N3	4.02	1.49	1.37
2	B	301	7SR	C22-C27	-4.00	1.35	1.43
2	L	301	7SR	C2-N3	3.99	1.48	1.37
2	D	301	7SR	C18-N19	-3.94	1.42	1.46
2	K	301	7SR	C31-N19	3.94	1.43	1.35
2	A	302	7SR	C10-C9	-3.93	1.40	1.53
2	I	301	7SR	C2-N3	3.93	1.48	1.37
2	I	302	7SR	C22-C27	-3.92	1.35	1.43
2	E	301	7SR	C2-N3	3.91	1.48	1.37
2	K	301	7SR	C4-N3	-3.84	1.40	1.47
2	A	301	7SR	C2-N3	3.79	1.48	1.37
2	I	302	7SR	C4-N3	-3.61	1.40	1.47
2	I	302	7SR	C31-N19	3.57	1.43	1.35
2	N	301	7SR	C22-C27	-3.56	1.36	1.43
2	B	301	7SR	C17-N7	-3.46	1.43	1.47
2	D	302	7SR	C2-N3	3.45	1.47	1.37
2	K	301	7SR	C23-C22	-3.39	1.35	1.42
2	D	302	7SR	C8-C31	-3.37	1.45	1.52
2	N	301	7SR	C23-C22	-3.35	1.35	1.42
2	E	301	7SR	BR1-C39	3.31	1.96	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	7SR	BR1-C39	3.26	1.96	1.90
2	B	301	7SR	C4-N3	-3.24	1.41	1.47
2	I	302	7SR	O1-C2	-3.18	1.17	1.23
2	A	302	7SR	BR1-C39	3.15	1.96	1.90
2	B	301	7SR	C2-N3	3.12	1.46	1.37
2	D	302	7SR	C22-C27	-3.09	1.37	1.43
2	K	301	7SR	C42-C41	-3.01	1.33	1.38
2	I	302	7SR	C21-C22	-3.00	1.35	1.42
2	K	302	7SR	BR1-C39	2.99	1.96	1.90
2	B	301	7SR	C8-C31	-2.96	1.46	1.52
2	N	301	7SR	O1-C2	-2.95	1.17	1.23
2	H	301	7SR	BR1-C39	2.94	1.96	1.90
2	L	301	7SR	BR1-C39	2.94	1.96	1.90
2	H	301	7SR	C2-N34	2.92	1.46	1.34
2	A	301	7SR	BR1-C39	2.91	1.96	1.90
2	K	301	7SR	C2-N3	2.90	1.45	1.37
2	D	301	7SR	C2-N34	2.90	1.46	1.34
2	N	301	7SR	C21-C22	-2.87	1.35	1.42
2	K	301	7SR	O33-C6	-2.87	1.16	1.23
2	N	301	7SR	C28-C27	-2.87	1.35	1.42
2	K	301	7SR	C21-C22	-2.85	1.35	1.42
2	K	302	7SR	C2-N34	2.84	1.45	1.34
2	E	301	7SR	C17-N7	-2.83	1.43	1.47
2	I	301	7SR	C2-N34	2.82	1.45	1.34
2	D	301	7SR	C17-N3	2.81	1.50	1.46
2	L	301	7SR	C2-N34	2.79	1.45	1.34
2	G	301	7SR	C2-N34	2.78	1.45	1.34
2	I	302	7SR	C23-C22	-2.78	1.36	1.42
2	A	302	7SR	C2-N34	2.76	1.45	1.34
2	I	302	7SR	C28-C27	-2.75	1.36	1.42
2	A	301	7SR	C2-N34	2.74	1.45	1.34
2	D	302	7SR	C23-C22	-2.72	1.36	1.42
2	N	301	7SR	C4-N3	-2.71	1.42	1.47
2	K	301	7SR	O1-C2	-2.70	1.18	1.23
2	N	301	7SR	C2-N3	2.62	1.44	1.37
2	I	302	7SR	O32-C31	-2.62	1.17	1.22
2	E	301	7SR	C2-N34	2.59	1.44	1.34
2	K	301	7SR	C28-C27	-2.59	1.36	1.42
2	K	301	7SR	O32-C31	-2.55	1.17	1.22
2	I	302	7SR	O33-C6	-2.47	1.17	1.23
2	B	301	7SR	C23-C22	-2.41	1.37	1.42
2	B	301	7SR	C28-C27	-2.41	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	7SR	C17-N3	2.41	1.49	1.46
2	D	301	7SR	C17-N7	-2.40	1.44	1.47
2	D	302	7SR	C4-N3	-2.40	1.42	1.47
2	D	302	7SR	C2-N34	2.38	1.44	1.34
2	A	301	7SR	C17-N7	-2.36	1.44	1.47
2	G	301	7SR	C17-N7	-2.35	1.44	1.47
2	B	301	7SR	C9-C8	-2.32	1.50	1.54
2	G	301	7SR	C8-C31	-2.30	1.47	1.52
2	N	301	7SR	C9-C8	-2.30	1.50	1.54
2	L	301	7SR	C8-C31	-2.29	1.47	1.52
2	D	301	7SR	C42-C41	2.29	1.42	1.38
2	I	302	7SR	C4-C5	-2.21	1.46	1.52
2	H	301	7SR	C8-C31	-2.20	1.48	1.52
2	A	302	7SR	C8-C31	-2.20	1.48	1.52
2	I	302	7SR	C38-C37	-2.20	1.35	1.38
2	A	301	7SR	C8-C31	-2.18	1.48	1.52
2	D	302	7SR	C28-C27	-2.18	1.37	1.42
2	B	301	7SR	C2-N34	2.16	1.43	1.34
2	I	301	7SR	C8-C31	-2.16	1.48	1.52
2	B	301	7SR	C21-C22	-2.15	1.37	1.42
2	K	302	7SR	C17-N7	-2.15	1.44	1.47
2	D	301	7SR	C10-C9	-2.13	1.46	1.53
2	N	301	7SR	C42-C41	-2.12	1.35	1.38
2	L	301	7SR	C17-N3	2.10	1.49	1.46
2	I	301	7SR	BR1-C39	2.09	1.94	1.90
2	E	301	7SR	C8-C31	-2.09	1.48	1.52
2	K	301	7SR	C29-C30	-2.08	1.35	1.38
2	L	301	7SR	C17-N7	-2.06	1.44	1.47
2	I	302	7SR	C20-N19	-2.04	1.43	1.46
2	K	302	7SR	C22-C27	-2.03	1.39	1.43
2	I	302	7SR	C9-C8	-2.03	1.50	1.54
2	K	301	7SR	C42-C36	-2.02	1.34	1.38
2	E	301	7SR	C5-C6	2.00	1.55	1.51

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	7SR	C35-N34-C2	-9.35	110.67	120.79
2	D	301	7SR	C38-C37-C36	-7.50	111.14	121.00
2	I	302	7SR	C20-N19-C18	6.99	126.78	115.82
2	K	301	7SR	C20-N19-C18	6.67	126.28	115.82
2	D	301	7SR	C35-N34-C2	-6.50	113.75	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	7SR	C20-N19-C18	6.34	125.75	115.82
2	D	302	7SR	C20-N19-C18	5.79	124.89	115.82
2	N	301	7SR	C20-N19-C18	5.68	124.72	115.82
2	D	301	7SR	C37-C38-C39	5.60	125.88	119.18
2	B	301	7SR	C10-C9-C8	-5.52	100.85	111.51
2	D	301	7SR	C20-N19-C18	5.48	124.42	115.82
2	B	301	7SR	C35-N34-C2	-5.21	115.14	120.79
2	L	301	7SR	C20-N19-C18	5.20	123.98	115.82
2	A	302	7SR	C20-N19-C18	4.73	123.23	115.82
2	N	301	7SR	C35-N34-C2	-4.67	115.73	120.79
2	K	301	7SR	C20-N19-C31	-4.64	115.42	119.80
2	K	302	7SR	C20-N19-C18	4.47	122.83	115.82
2	H	301	7SR	C20-N19-C18	4.28	122.54	115.82
2	I	302	7SR	C20-N19-C31	-4.24	115.80	119.80
2	K	301	7SR	C5-C4-N3	-4.24	98.69	111.52
2	B	301	7SR	O32-C31-N19	-4.06	117.80	122.53
2	N	301	7SR	C5-C4-N3	-4.00	99.41	111.52
2	E	301	7SR	C20-N19-C18	3.99	122.08	115.82
2	G	301	7SR	C20-N19-C18	3.99	122.07	115.82
2	I	301	7SR	C20-N19-C18	3.97	122.05	115.82
2	K	301	7SR	C10-C9-C8	3.96	119.16	111.51
2	N	301	7SR	C21-C20-N19	3.87	120.20	113.51
2	A	301	7SR	C20-N19-C18	3.87	121.89	115.82
2	A	302	7SR	C9-C8-N7	3.85	119.18	111.95
2	B	301	7SR	C5-C4-N3	-3.83	99.92	111.52
2	B	301	7SR	C20-N19-C31	-3.73	116.28	119.80
2	A	302	7SR	C21-C20-N19	3.73	119.94	113.51
2	A	302	7SR	C46-C9-C8	-3.61	102.28	110.36
2	D	301	7SR	C42-C36-C37	3.46	123.38	118.23
2	D	301	7SR	C18-C17-N3	3.42	118.49	112.61
2	I	302	7SR	C5-C4-N3	-3.42	101.18	111.52
2	G	301	7SR	C35-N34-C2	-3.40	117.11	120.79
2	A	302	7SR	C35-N34-C2	-3.36	117.14	120.79
2	L	301	7SR	C20-N19-C31	-3.32	116.66	119.80
2	A	302	7SR	C20-N19-C31	-3.31	116.67	119.80
2	I	301	7SR	C42-C36-C37	3.26	123.08	118.23
2	I	302	7SR	O33-C6-N7	-3.16	118.21	122.36
2	B	301	7SR	C42-C36-C37	3.12	122.87	118.23
2	K	301	7SR	O32-C31-N19	-3.11	118.91	122.53
2	D	301	7SR	C9-C8-N7	-3.07	106.18	111.95
2	D	301	7SR	BR1-C39-C38	3.05	123.45	119.30
2	I	301	7SR	C5-C4-N3	-3.01	102.41	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	301	7SR	C21-C20-N19	3.01	118.71	113.51
2	D	301	7SR	C9-C8-C31	2.95	116.94	110.90
2	K	301	7SR	BR1-C39-C41	-2.91	115.33	119.30
2	D	302	7SR	O32-C31-N19	-2.91	119.14	122.53
2	D	302	7SR	C42-C36-C37	2.88	122.52	118.23
2	D	302	7SR	C5-C4-N3	-2.81	103.01	111.52
2	K	302	7SR	C5-C4-N3	-2.80	103.06	111.52
2	K	301	7SR	C21-C20-N19	2.79	118.32	113.51
2	I	302	7SR	O32-C31-N19	-2.78	119.29	122.53
2	D	301	7SR	C42-C41-C39	-2.78	115.85	119.18
2	H	301	7SR	C21-C20-N19	2.74	118.24	113.51
2	K	302	7SR	C9-C8-C31	2.67	116.38	110.90
2	B	301	7SR	C17-C18-N19	-2.66	107.86	111.04
2	I	301	7SR	C18-C17-N3	2.59	117.06	112.61
2	E	301	7SR	C42-C36-C37	2.56	122.03	118.23
2	K	302	7SR	O32-C31-N19	-2.55	119.56	122.53
2	N	301	7SR	C23-C22-C21	-2.53	118.31	122.55
2	I	302	7SR	C21-C20-N19	2.53	117.88	113.51
2	D	301	7SR	O32-C31-N19	-2.50	119.61	122.53
2	L	301	7SR	C35-N34-C2	-2.48	118.10	120.79
2	K	302	7SR	C10-C9-C8	2.48	116.30	111.51
2	N	301	7SR	C42-C36-C37	2.46	121.90	118.23
2	D	302	7SR	C20-N19-C31	-2.46	117.48	119.80
2	D	301	7SR	C20-N19-C31	-2.46	117.48	119.80
2	A	301	7SR	C35-N34-C2	-2.46	118.13	120.79
2	H	301	7SR	C5-C4-N3	-2.46	104.09	111.52
2	K	301	7SR	C42-C36-C37	2.45	121.88	118.23
2	I	301	7SR	C35-N34-C2	-2.42	118.17	120.79
2	A	302	7SR	C10-C9-C8	2.42	116.18	111.51
2	H	301	7SR	C42-C36-C37	2.38	121.77	118.23
2	N	301	7SR	C23-C22-C27	2.37	120.99	117.92
2	A	301	7SR	C42-C36-C37	2.35	121.73	118.23
2	E	301	7SR	C18-C17-N3	2.35	116.65	112.61
2	A	301	7SR	C10-C9-C8	2.34	116.04	111.51
2	K	301	7SR	C35-N34-C2	-2.34	118.25	120.79
2	K	302	7SR	C42-C36-C37	2.34	121.71	118.23
2	L	301	7SR	O32-C31-N19	-2.33	119.81	122.53
2	A	302	7SR	O32-C31-N19	-2.33	119.82	122.53
2	A	302	7SR	C46-C9-C10	-2.33	105.94	111.81
2	I	302	7SR	C46-C9-C10	-2.27	106.08	111.81
2	H	301	7SR	C10-C9-C8	2.27	115.89	111.51
2	H	301	7SR	O33-C6-N7	-2.25	119.41	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	7SR	C41-C39-C38	2.20	124.67	121.33
2	A	301	7SR	C9-C8-C31	2.18	115.36	110.90
2	L	301	7SR	C42-C36-C37	2.15	121.44	118.23
2	H	301	7SR	C18-C17-N3	2.14	116.30	112.61
2	G	301	7SR	C42-C36-C37	2.10	121.36	118.23
2	N	301	7SR	C41-C42-C36	-2.09	118.25	121.00
2	K	301	7SR	BR1-C39-C38	2.08	122.13	119.30
2	K	301	7SR	C9-C8-C31	2.08	115.17	110.90
2	I	301	7SR	C41-C42-C36	-2.08	118.27	121.00
2	K	301	7SR	C35-C36-C42	-2.06	116.73	120.94
2	I	302	7SR	C9-C8-N7	2.04	115.78	111.95
2	K	302	7SR	O33-C6-N7	-2.03	119.69	122.36
2	D	301	7SR	O1-C2-N34	-2.03	118.08	123.35
2	L	301	7SR	C5-C4-N3	-2.03	105.36	111.52
2	B	301	7SR	C9-C8-C31	2.02	115.03	110.90
2	E	301	7SR	O1-C2-N34	-2.01	118.16	123.35
2	G	301	7SR	C46-C9-C8	2.00	114.85	110.36

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	302	7SR	C31-C8-C9-C46
2	E	301	7SR	C11-C10-C9-C8
2	E	301	7SR	N7-C8-C9-C10
2	E	301	7SR	N7-C8-C9-C46
2	G	301	7SR	C11-C10-C9-C8
2	G	301	7SR	N7-C8-C9-C10
2	G	301	7SR	N7-C8-C9-C46
2	A	302	7SR	C11-C10-C9-C46
2	B	301	7SR	C11-C10-C9-C8
2	A	302	7SR	C11-C10-C9-C8
2	G	301	7SR	C11-C10-C9-C46
2	D	301	7SR	C21-C20-N19-C18
2	E	301	7SR	C11-C10-C9-C46
2	D	302	7SR	N7-C8-C9-C46
2	D	301	7SR	C21-C20-N19-C31
2	D	301	7SR	C11-C10-C9-C8
2	I	302	7SR	N7-C8-C9-C46
2	D	301	7SR	C11-C10-C9-C46
2	B	301	7SR	C11-C10-C9-C46
2	E	301	7SR	C31-C8-C9-C46

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Mol	Chain	Res	Type	Atoms
2	G	301	7SR	C31-C8-C9-C46
2	A	301	7SR	C31-C8-C9-C10
2	D	302	7SR	C31-C8-C9-C10
2	E	301	7SR	C31-C8-C9-C10
2	G	301	7SR	C31-C8-C9-C10
2	A	301	7SR	N7-C8-C9-C10
2	D	302	7SR	N7-C8-C9-C10
2	L	301	7SR	N7-C8-C9-C10
2	A	302	7SR	C21-C20-N19-C18
2	D	301	7SR	N19-C20-C21-C22
2	D	302	7SR	N19-C20-C21-C22
2	G	301	7SR	N19-C20-C21-C22
2	A	301	7SR	N7-C8-C9-C46
2	D	301	7SR	C31-C8-C9-C10
2	L	301	7SR	C31-C8-C9-C10
2	N	301	7SR	C31-C8-C9-C10
2	A	302	7SR	N19-C20-C21-C22

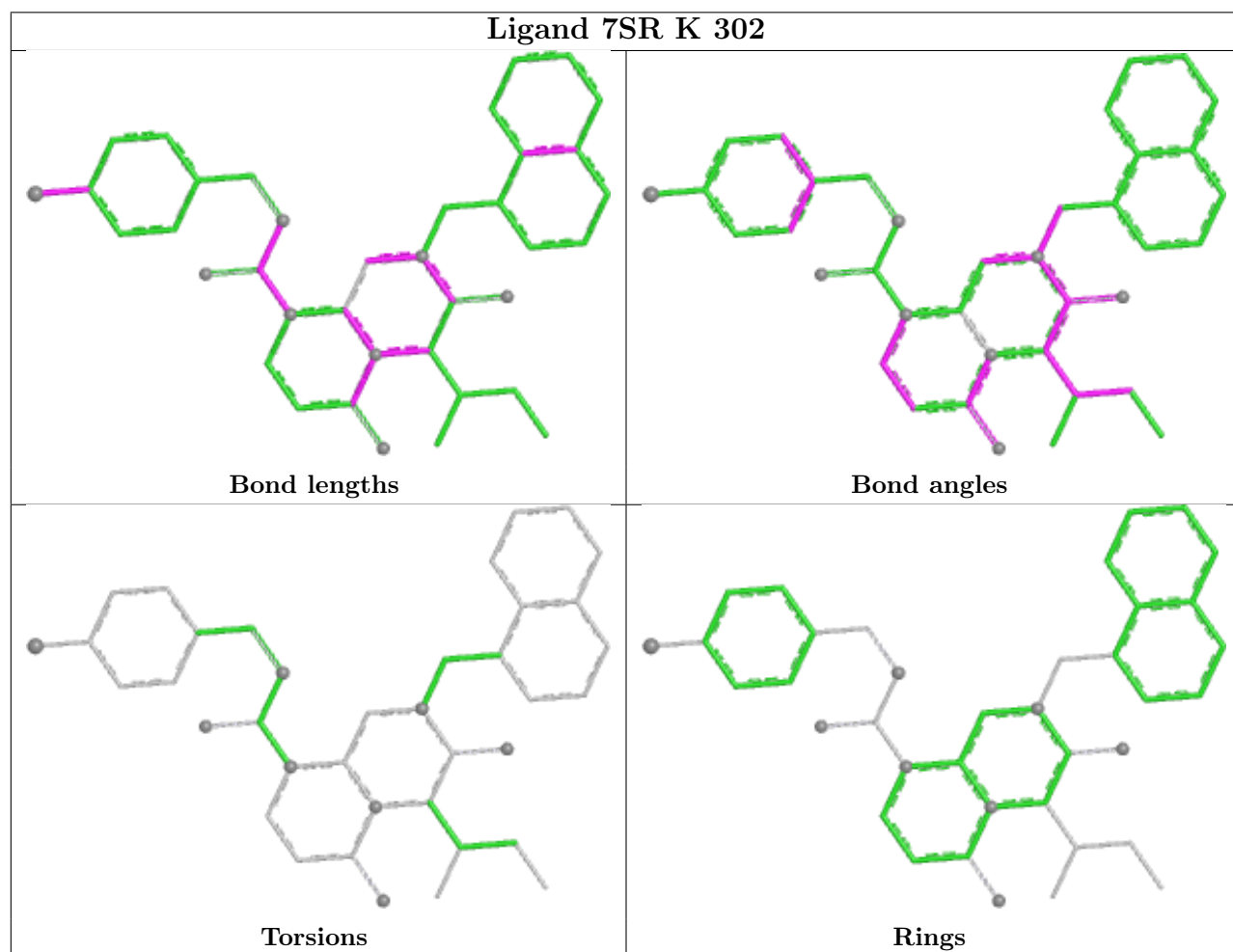
There are no ring outliers.

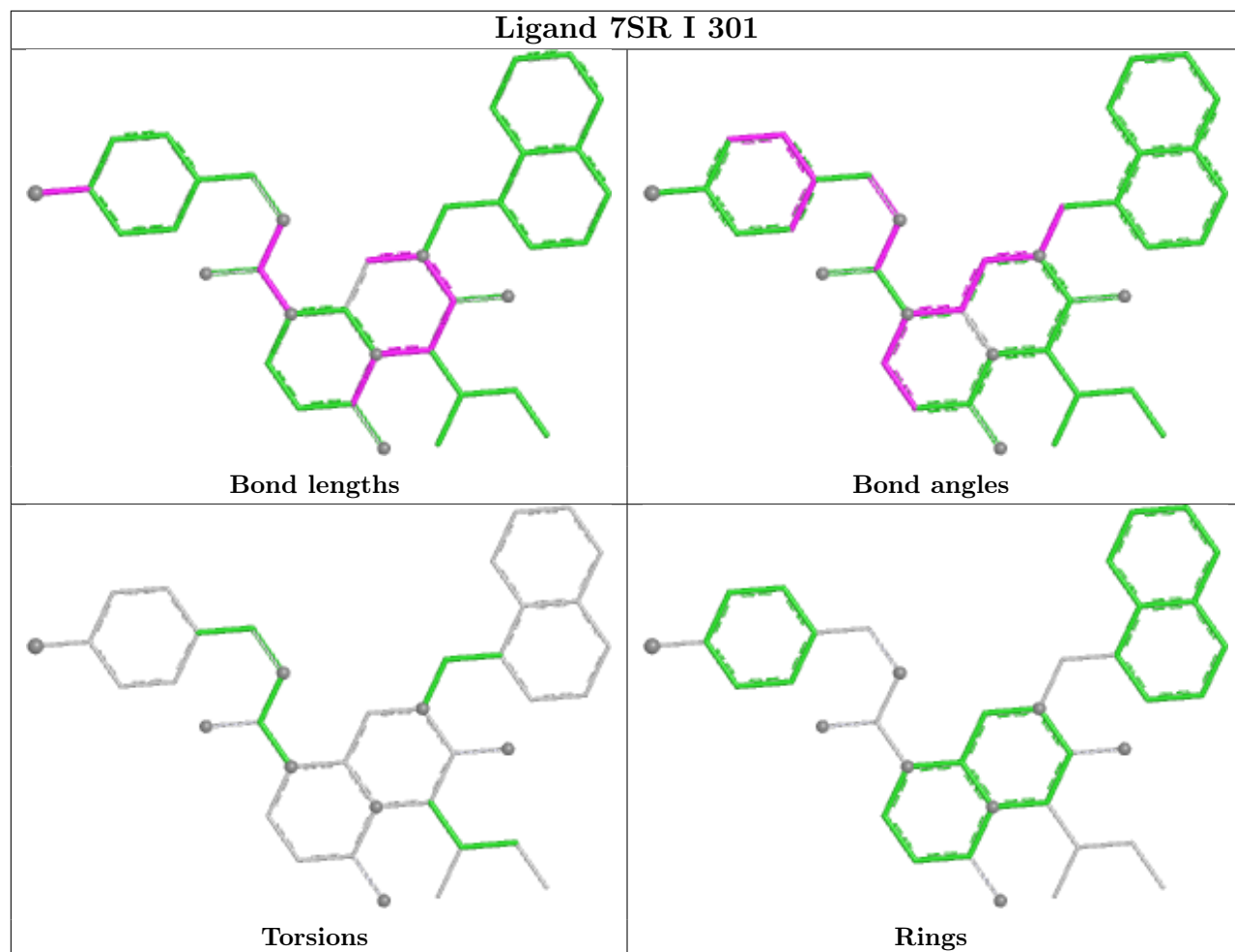
9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	302	7SR	1	0
2	I	301	7SR	1	0
2	E	301	7SR	1	0
2	A	301	7SR	1	0
2	B	301	7SR	1	0
2	D	302	7SR	4	0
2	A	302	7SR	3	0
2	D	301	7SR	4	0
2	G	301	7SR	1	0

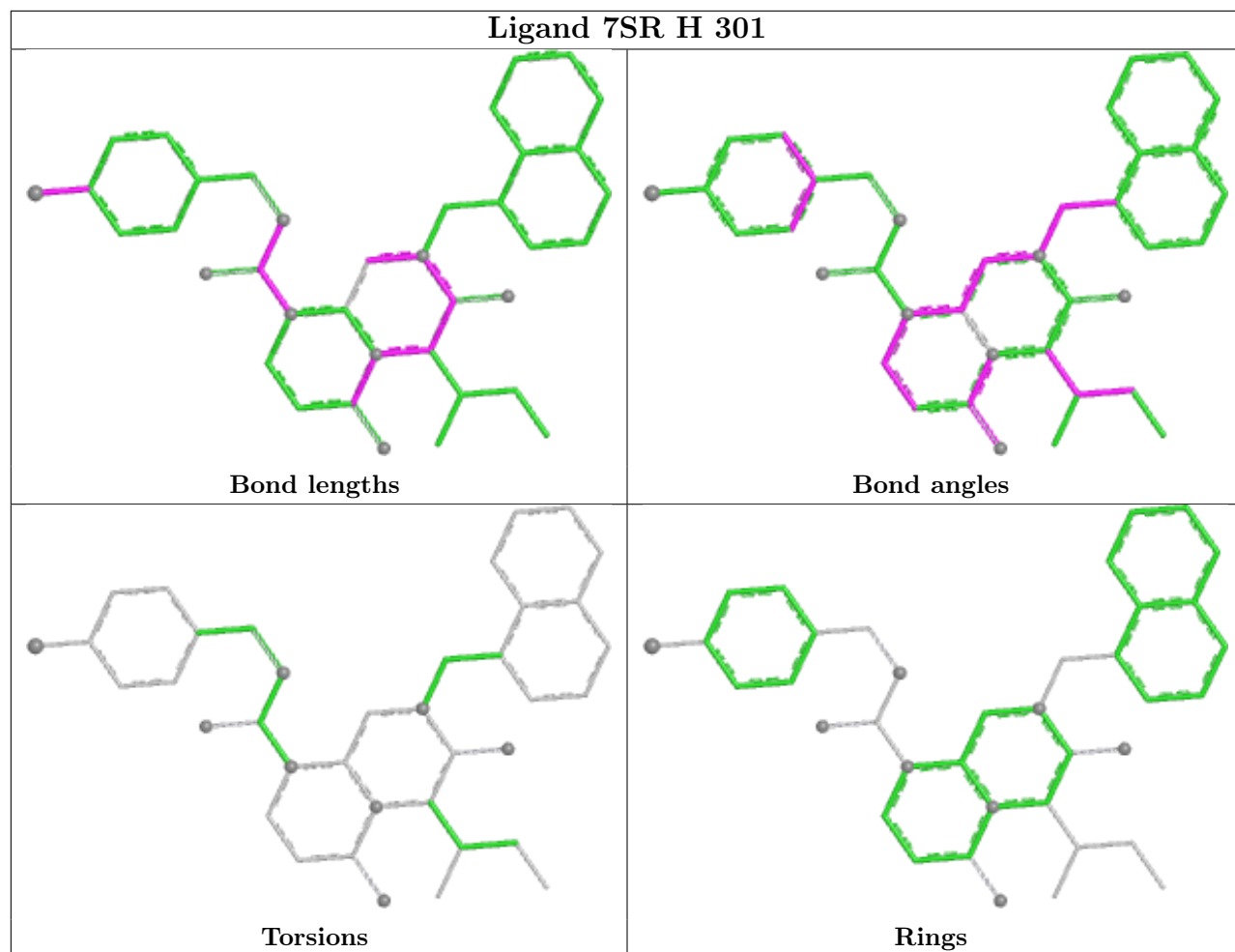
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

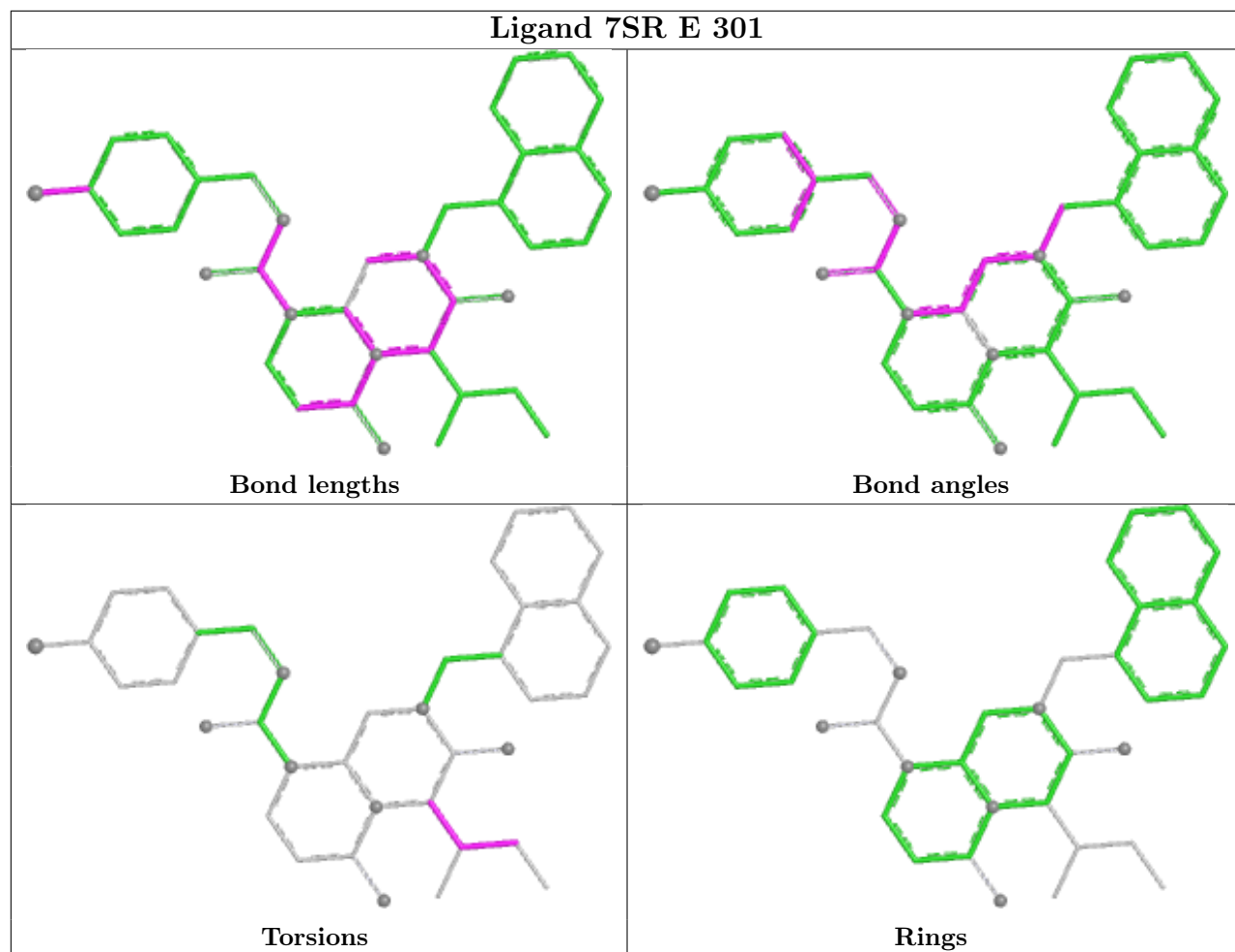




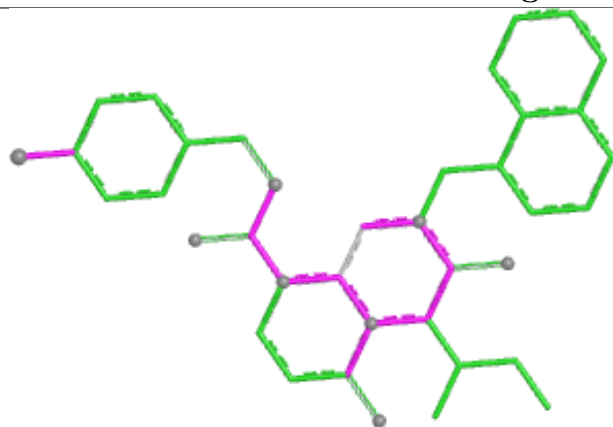
Ligand 7SR H 301



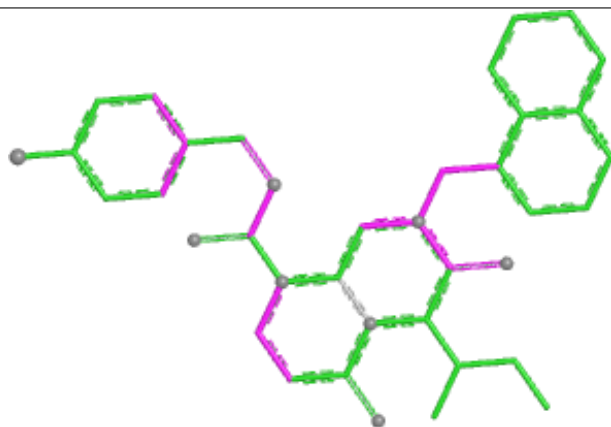
Ligand 7SR E 301



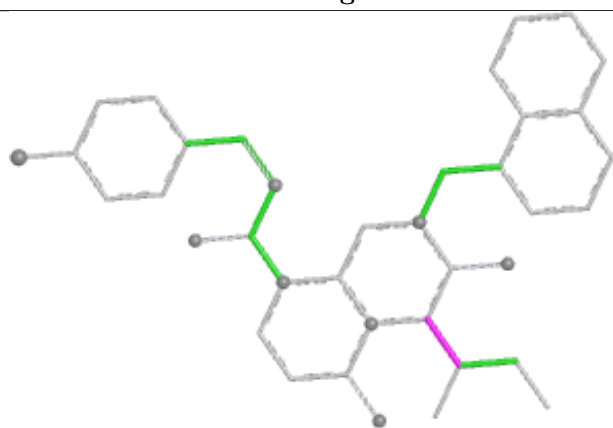
Ligand 7SR L 301



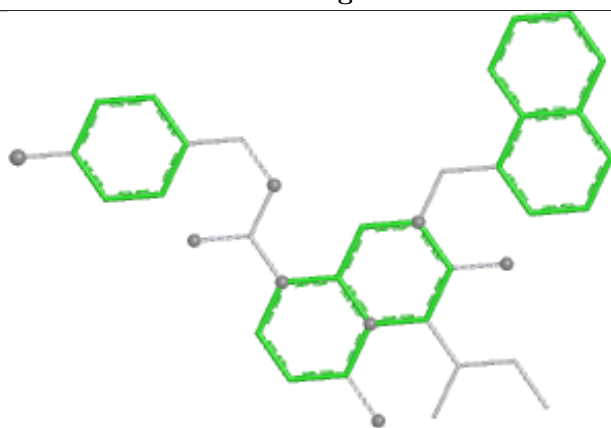
Bond lengths



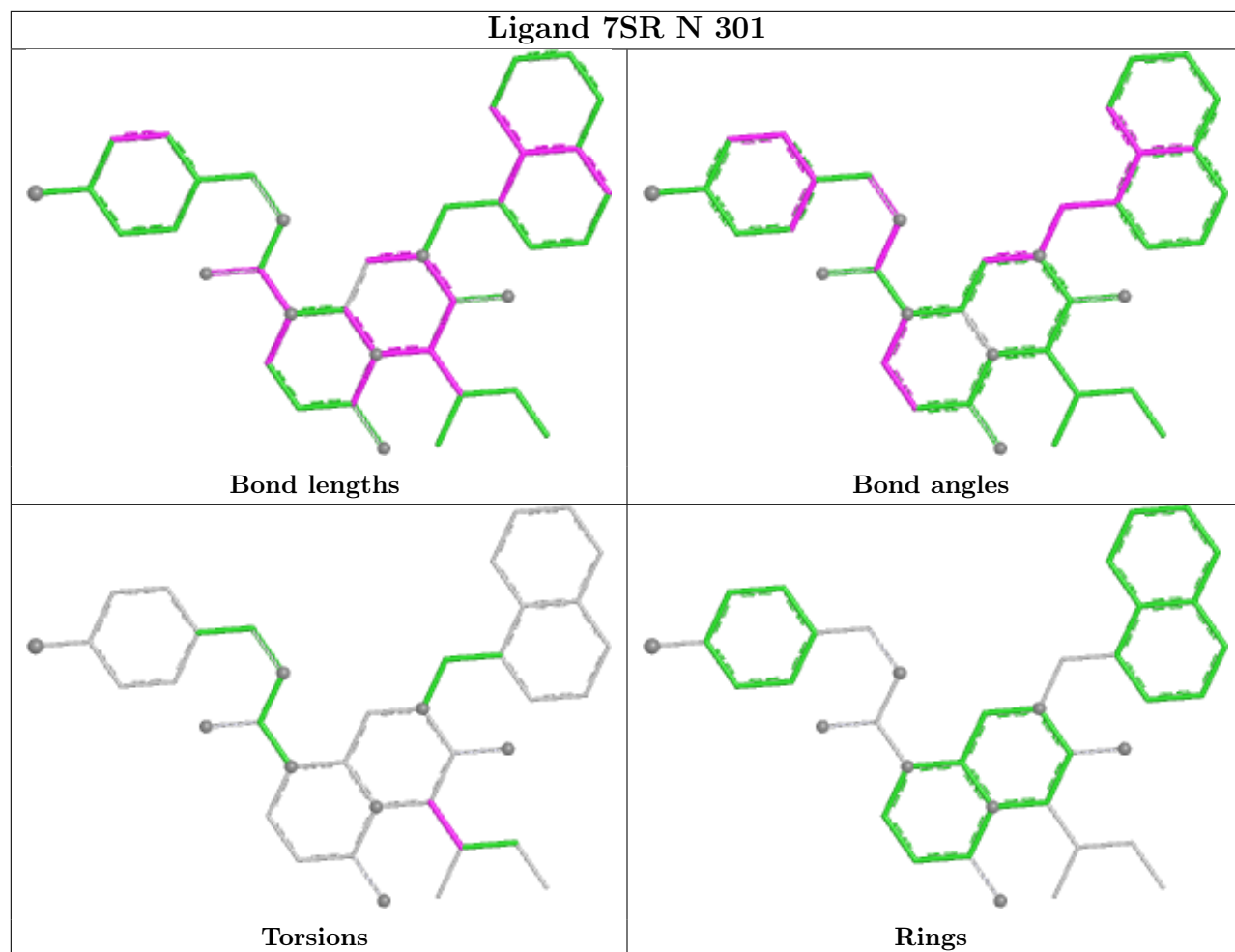
Bond angles

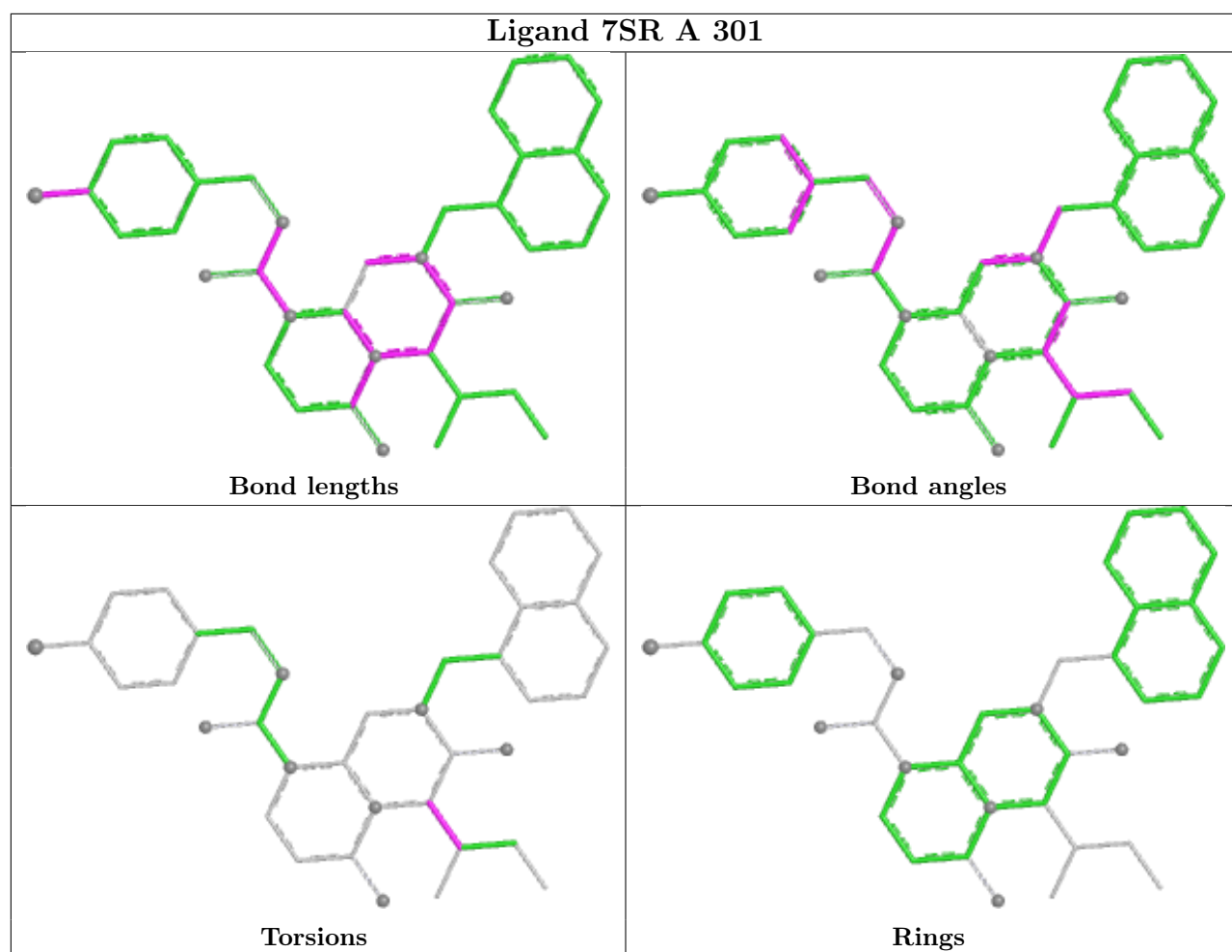


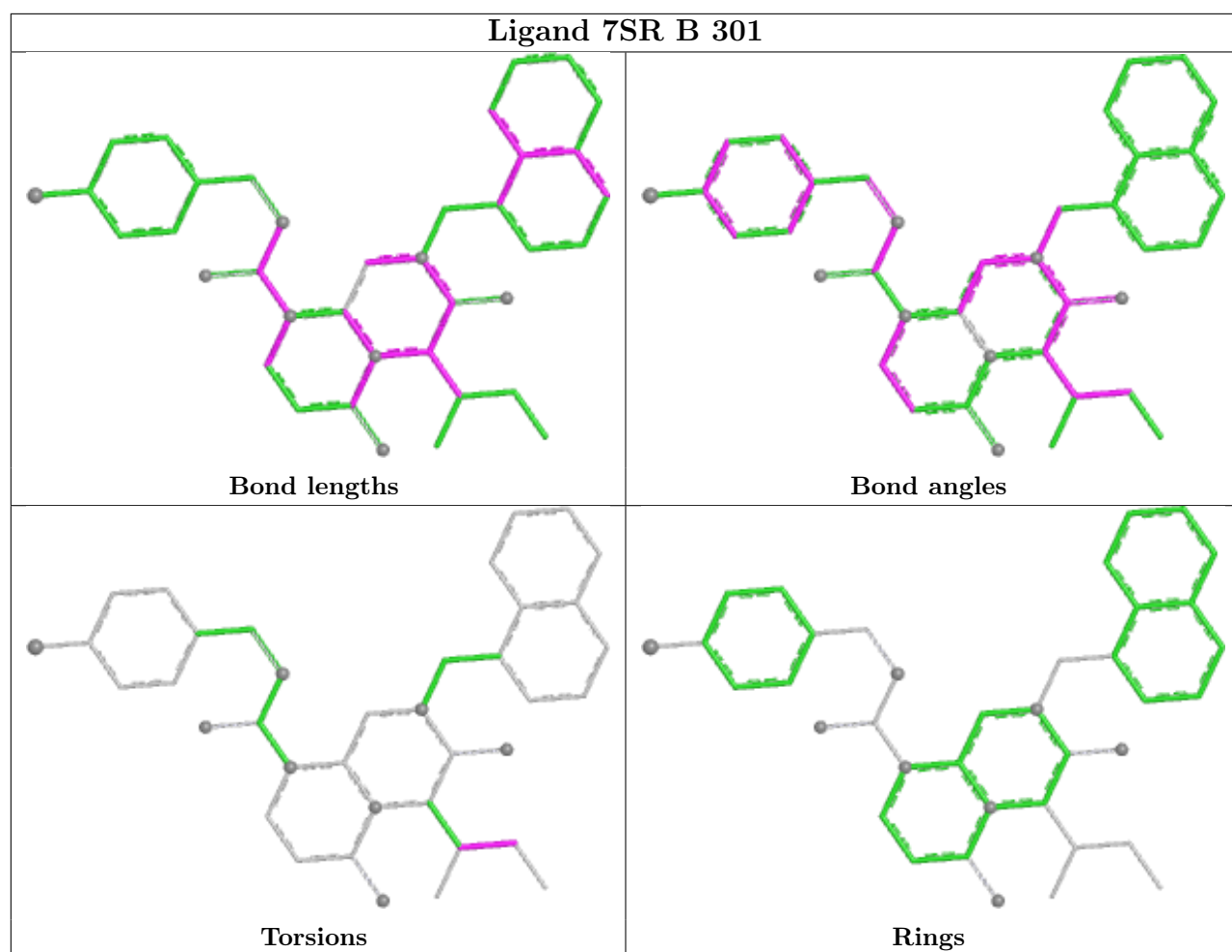
Torsions

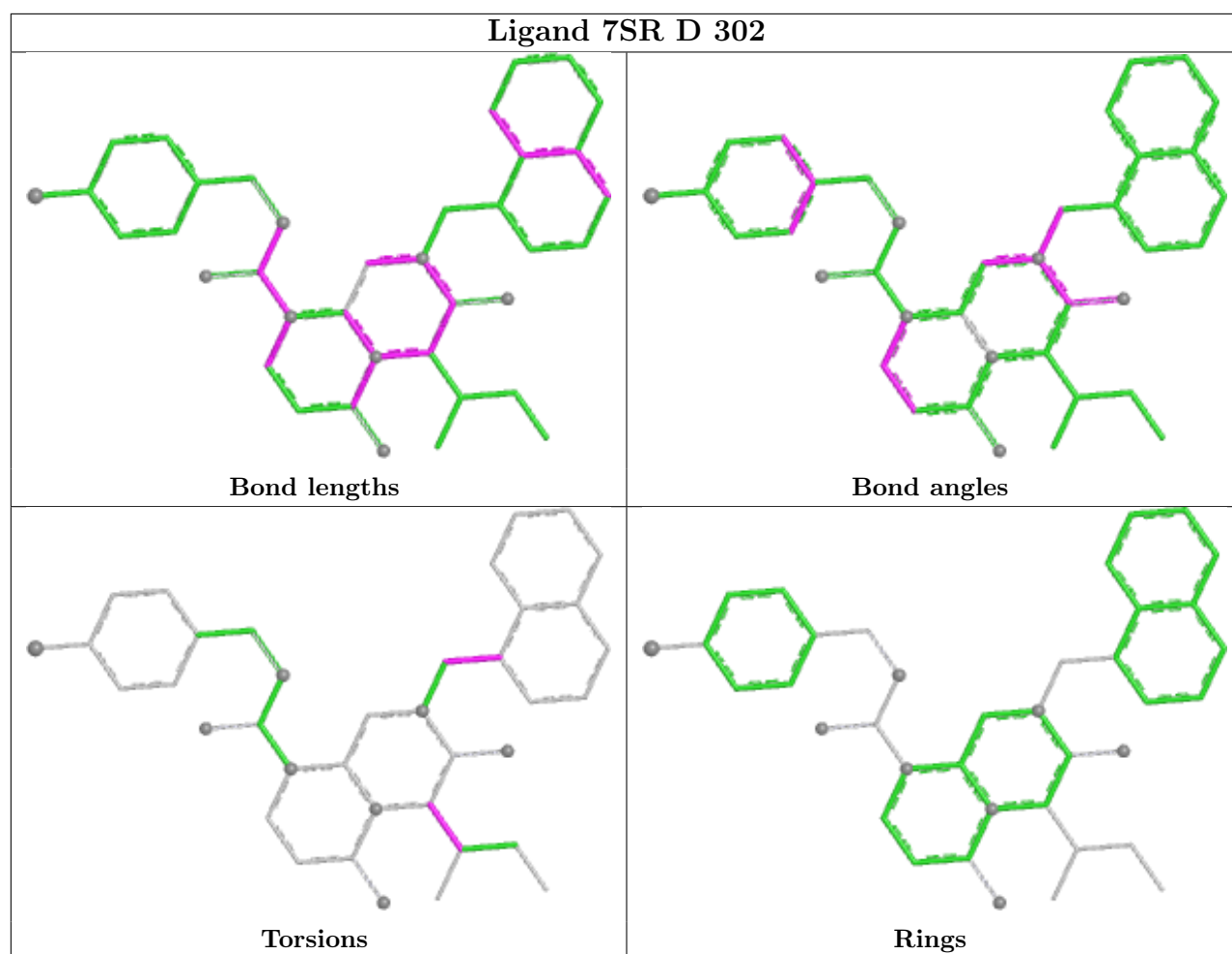


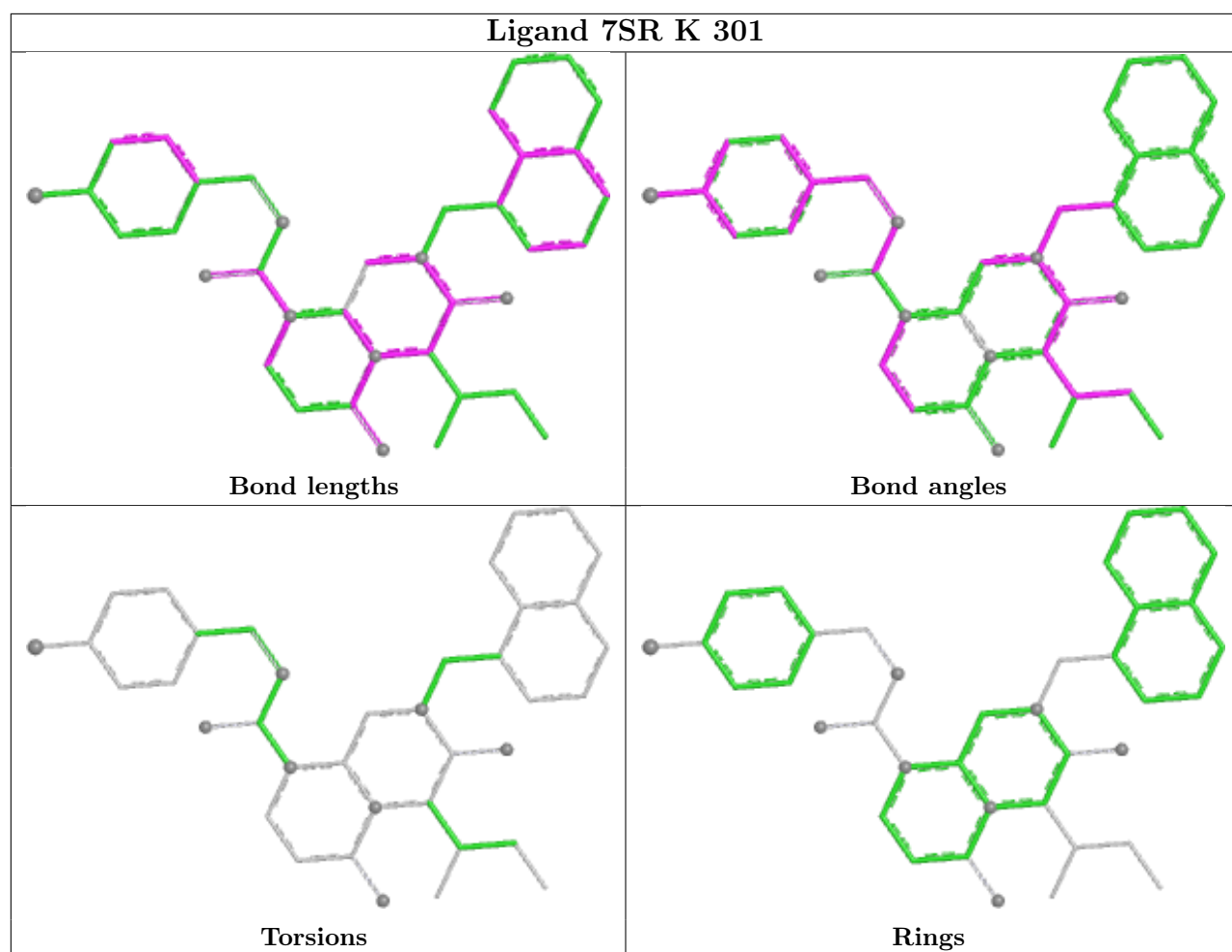
Rings



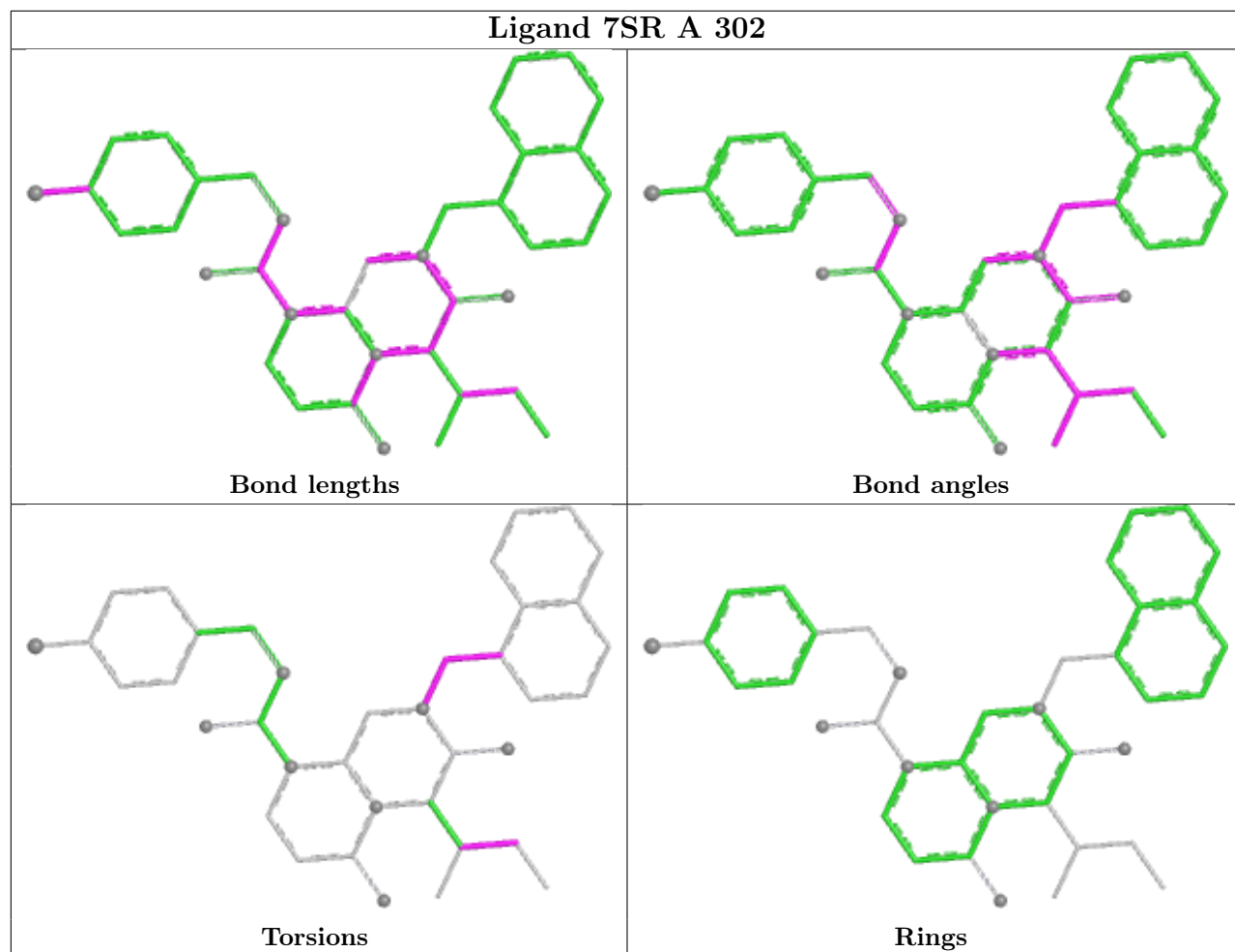


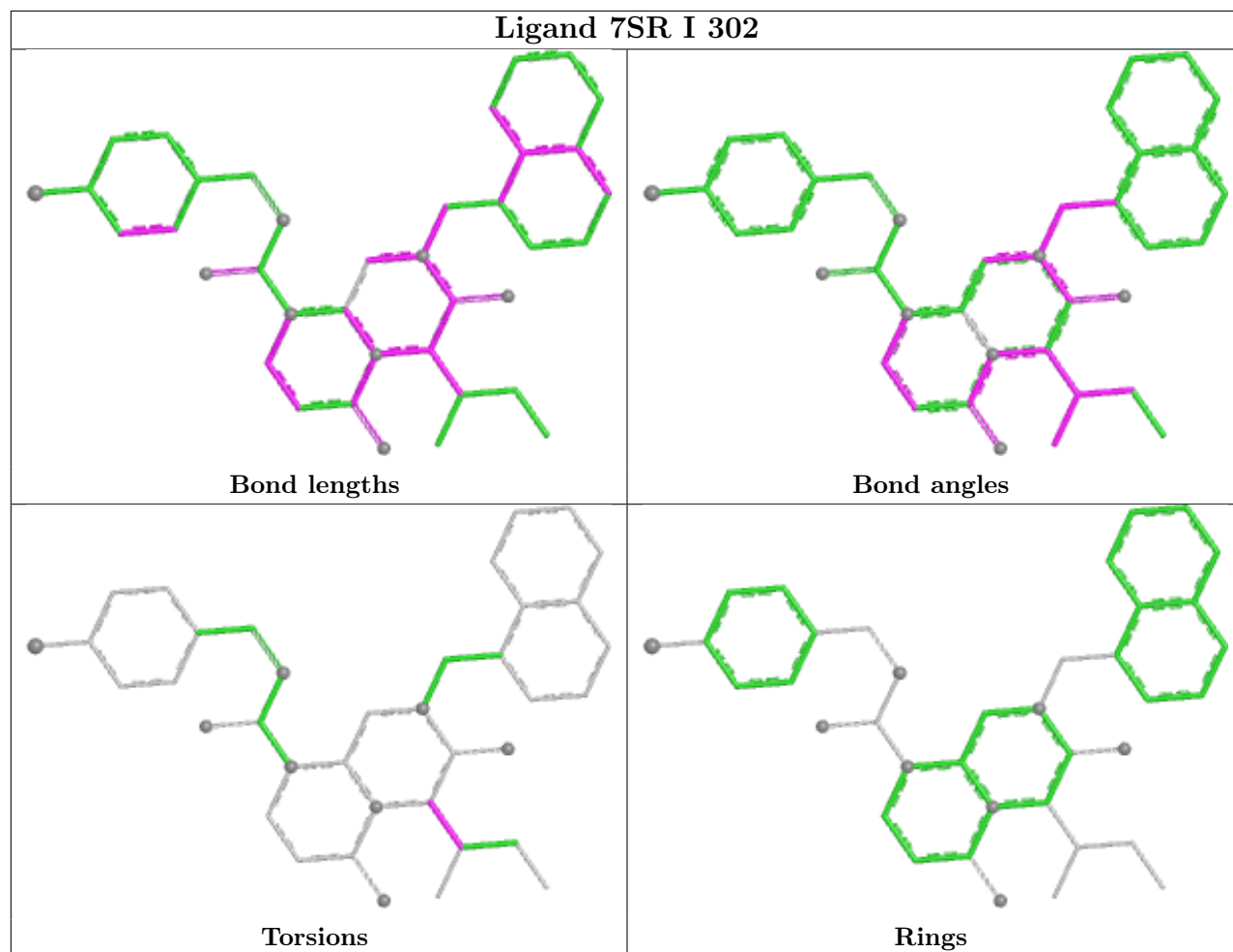




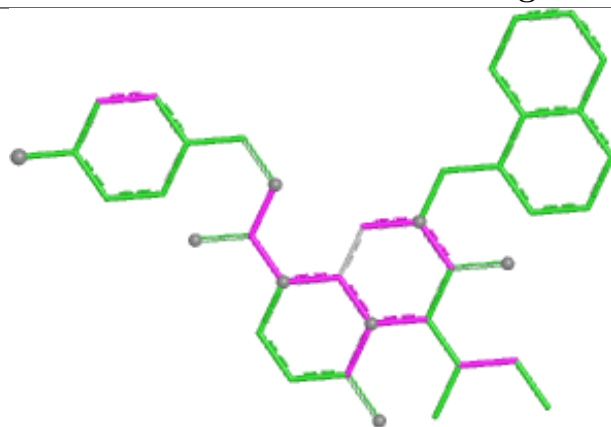


Ligand 7SR A 302

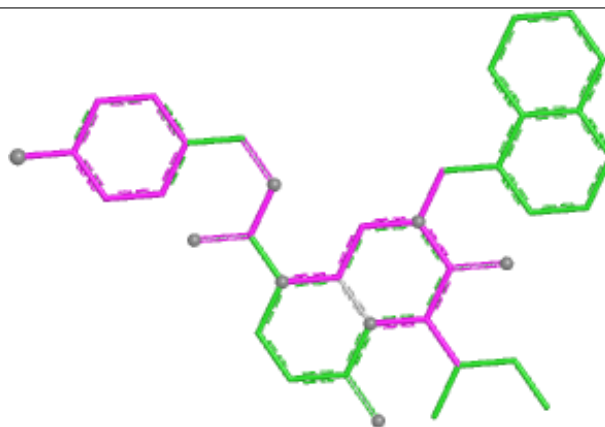




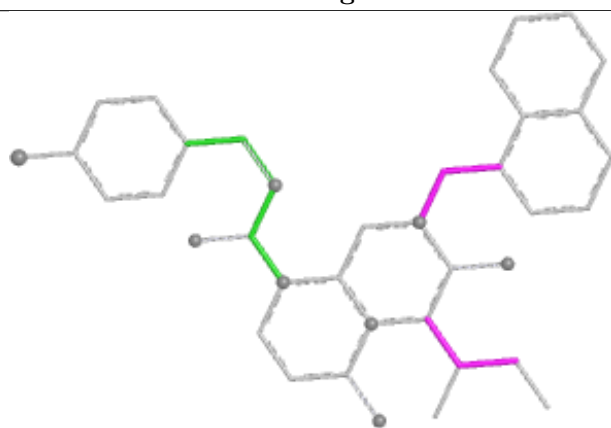
Ligand 7SR D 301



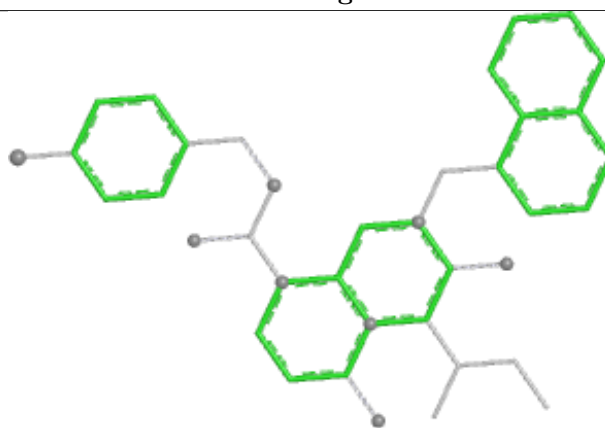
Bond lengths



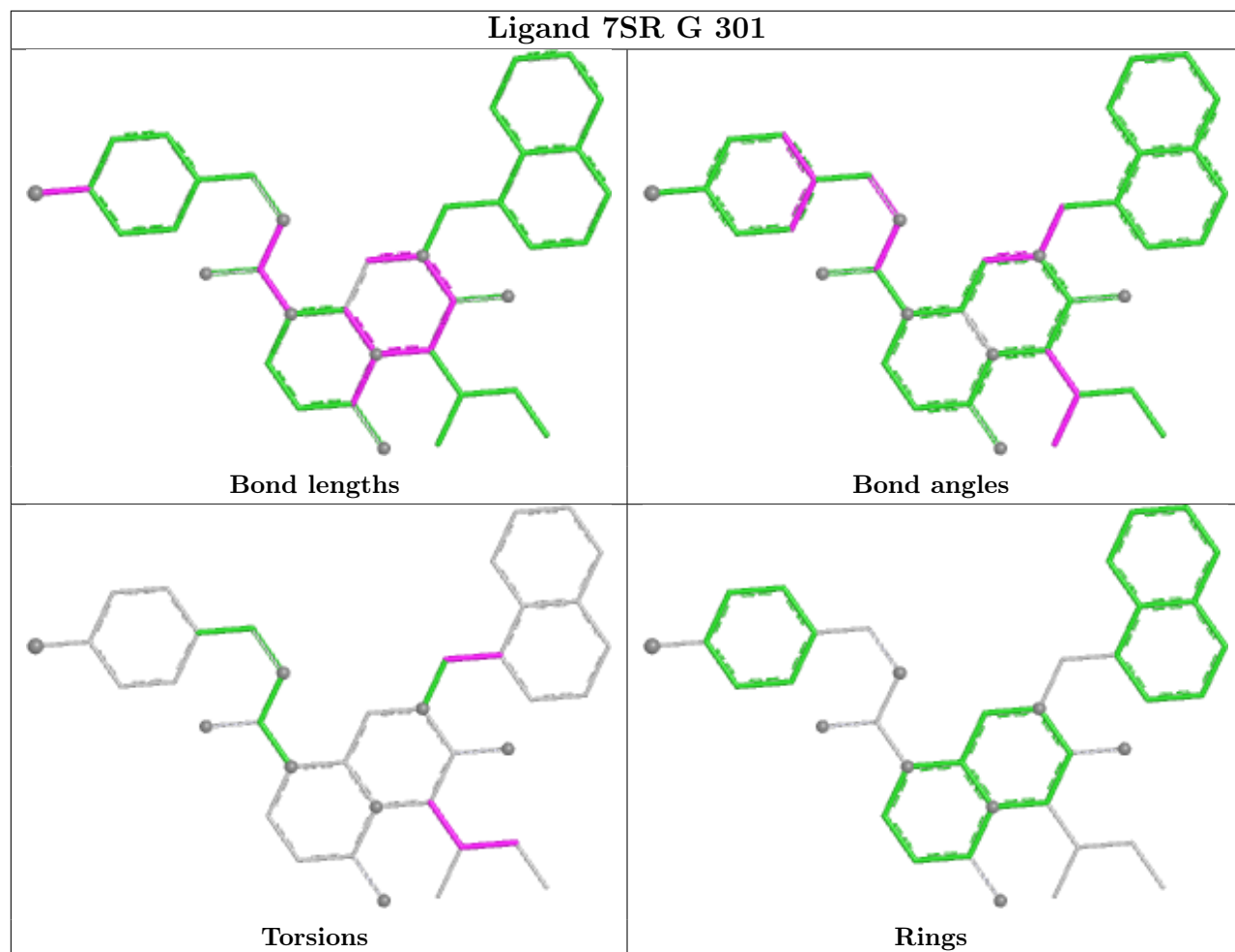
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	170/221 (76%)	-0.10	3 (1%) 67 69	43, 58, 79, 99	0
1	B	170/221 (76%)	0.04	6 (3%) 47 48	49, 66, 85, 101	0
1	C	168/221 (76%)	0.38	9 (5%) 31 31	59, 82, 99, 111	0
1	D	170/221 (76%)	0.53	11 (6%) 25 25	63, 86, 101, 127	0
1	E	171/221 (77%)	0.28	5 (2%) 53 55	59, 77, 94, 115	0
1	F	171/221 (77%)	0.13	6 (3%) 47 48	45, 64, 90, 111	0
1	G	170/221 (76%)	-0.24	2 (1%) 76 78	42, 55, 82, 98	0
1	H	180/221 (81%)	-0.41	1 (0%) 85 88	30, 47, 63, 84	0
1	I	178/221 (80%)	-0.50	2 (1%) 78 80	31, 41, 65, 87	0
1	J	178/221 (80%)	-0.50	1 (0%) 85 88	30, 40, 64, 79	0
1	K	176/221 (79%)	-0.26	3 (1%) 69 70	34, 45, 73, 89	0
1	L	179/221 (80%)	-0.18	2 (1%) 78 80	42, 58, 80, 93	0
1	M	179/221 (80%)	0.07	2 (1%) 78 80	45, 68, 90, 106	0
1	N	179/221 (80%)	-0.05	3 (1%) 69 70	42, 61, 79, 94	0
All	All	2439/3094 (78%)	-0.06	56 (2%) 61 62	30, 61, 92, 127	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	63	VAL	4.7
1	C	73	TYR	4.4
1	F	73	TYR	4.3
1	B	73	TYR	4.0
1	F	111	ASN	3.9
1	C	61	ILE	3.9
1	K	109	GLU	3.9
1	D	58	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	M	194	GLN	3.7
1	C	111	ASN	3.5
1	D	168	HIS	3.5
1	H	193	ILE	3.4
1	E	249	PRO	3.3
1	F	57	PRO	3.3
1	D	72	ALA	3.1
1	B	88	MET	3.0
1	B	118	TYR	3.0
1	C	196	GLU	2.9
1	M	65	GLN	2.8
1	E	58	LEU	2.7
1	D	118	TYR	2.7
1	D	140	LEU	2.7
1	D	62	VAL	2.6
1	A	62	VAL	2.6
1	K	110	SER	2.6
1	J	66	THR	2.6
1	F	140	LEU	2.6
1	I	180	PRO	2.4
1	K	111	ASN	2.4
1	A	58	LEU	2.4
1	C	140	LEU	2.4
1	I	57	PRO	2.4
1	L	69	GLY	2.3
1	N	193	ILE	2.3
1	B	79	LEU	2.3
1	D	73	TYR	2.3
1	L	57	PRO	2.3
1	E	247	HIS	2.3
1	N	240	ILE	2.3
1	F	88	MET	2.3
1	A	249	PRO	2.3
1	N	248	PRO	2.2
1	G	249	PRO	2.2
1	D	166	MET	2.2
1	C	59	ILE	2.2
1	C	74	ASP	2.2
1	D	211	LYS	2.2
1	C	235	ALA	2.1
1	G	73	TYR	2.1
1	B	58	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	201	LEU	2.1
1	D	234	GLU	2.1
1	E	180	PRO	2.1
1	D	143	ILE	2.0
1	F	193	ILE	2.0
1	B	180	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	D	303	1/1	0.74	0.28	79,79,79,79	0
3	MG	C	301	1/1	0.83	0.14	98,98,98,98	0
3	MG	M	301	1/1	0.83	0.11	79,79,79,79	0
3	MG	N	302	1/1	0.84	0.19	77,77,77,77	0
2	7SR	A	302	38/38	0.85	0.14	59,89,112,114	0
3	MG	B	302	1/1	0.85	0.15	78,78,78,78	0
3	MG	J	301	1/1	0.87	0.14	55,55,55,55	0
2	7SR	E	301	38/38	0.88	0.12	75,96,115,120	0
3	MG	F	301	1/1	0.89	0.16	74,74,74,74	0
2	7SR	B	301	38/38	0.89	0.12	84,94,99,107	0
2	7SR	D	302	38/38	0.89	0.12	85,95,130,137	0
3	MG	E	302	1/1	0.89	0.19	67,67,67,67	0
2	7SR	D	301	38/38	0.90	0.13	79,91,106,106	0
3	MG	L	302	1/1	0.92	0.18	70,70,70,70	0
3	MG	G	302	1/1	0.94	0.16	60,60,60,60	0
3	MG	H	302	1/1	0.94	0.08	42,42,42,42	0
2	7SR	G	301	38/38	0.94	0.10	63,78,102,116	0

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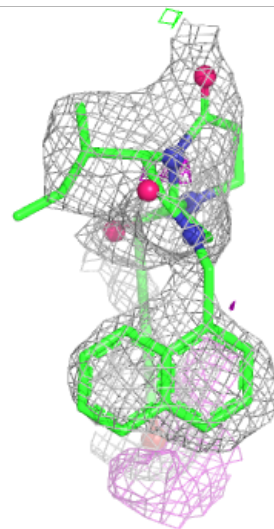
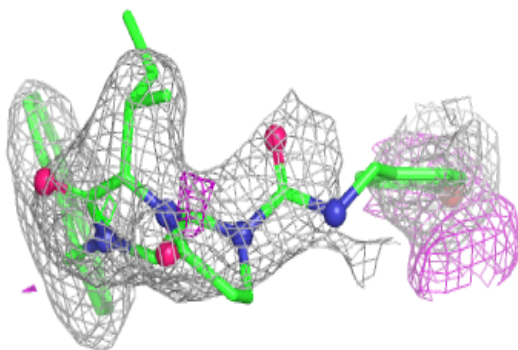
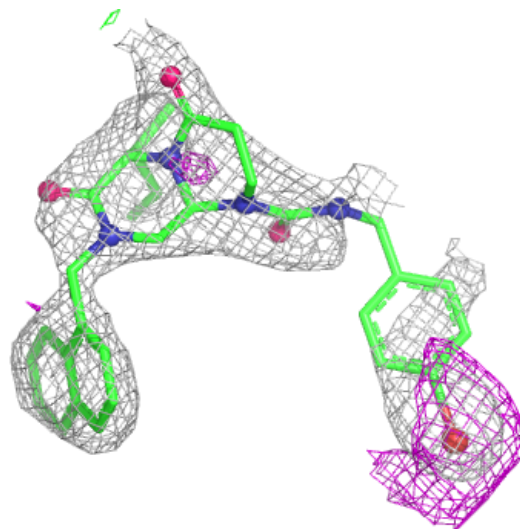
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	7SR	A	301	38/38	0.95	0.09	58,68,84,97	0
3	MG	A	303	1/1	0.96	0.22	65,65,65,65	0
3	MG	I	303	1/1	0.96	0.04	52,52,52,52	0
2	7SR	L	301	38/38	0.97	0.08	57,63,71,81	0
2	7SR	N	301	38/38	0.97	0.08	56,65,70,74	0
2	7SR	H	301	38/38	0.97	0.08	44,51,64,64	0
2	7SR	I	301	38/38	0.97	0.06	30,40,49,58	0
2	7SR	K	302	38/38	0.97	0.07	28,44,57,63	0
2	7SR	I	302	38/38	0.98	0.07	37,46,60,69	0
2	7SR	K	301	38/38	0.98	0.06	41,46,55,61	0
3	MG	K	303	1/1	0.99	0.07	45,45,45,45	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.

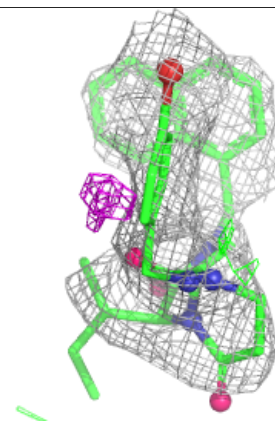
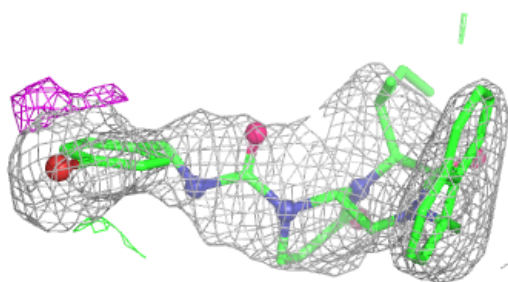
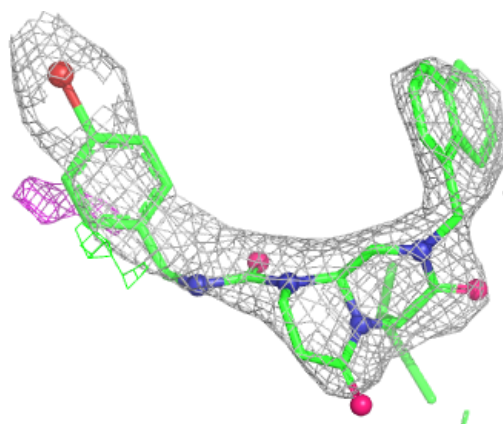
Electron density around 7SR A 302:

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



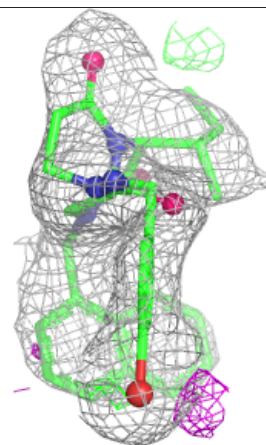
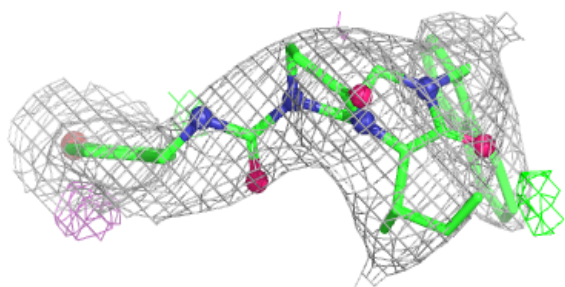
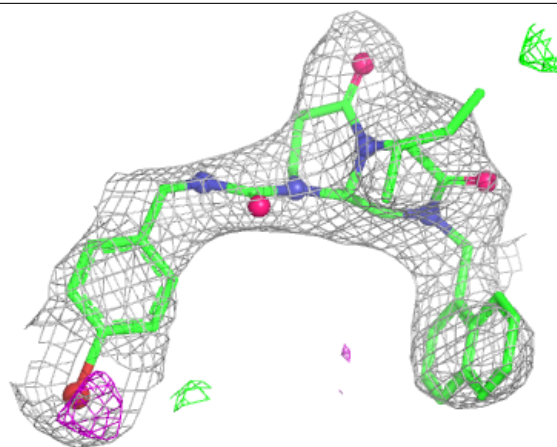
Electron density around 7SR E 301:

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



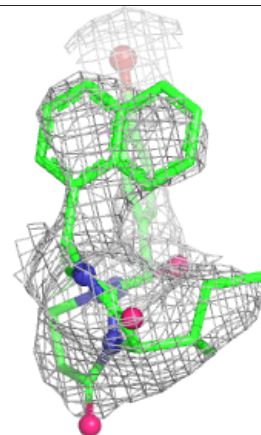
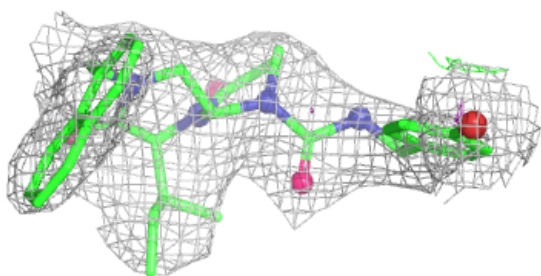
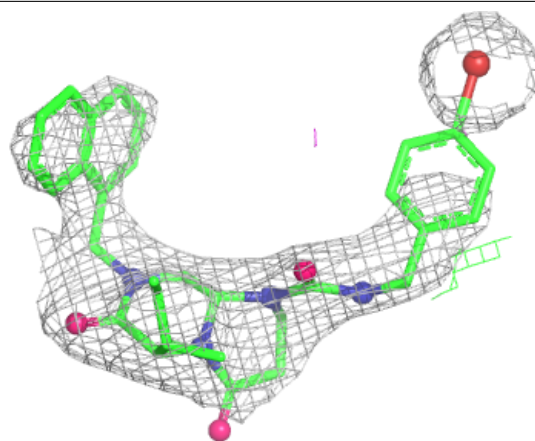
Electron density around 7SR B 301:

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



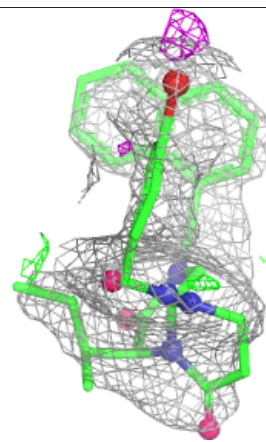
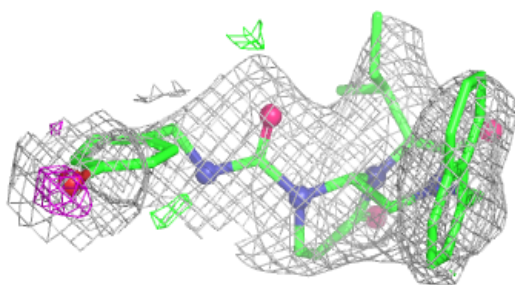
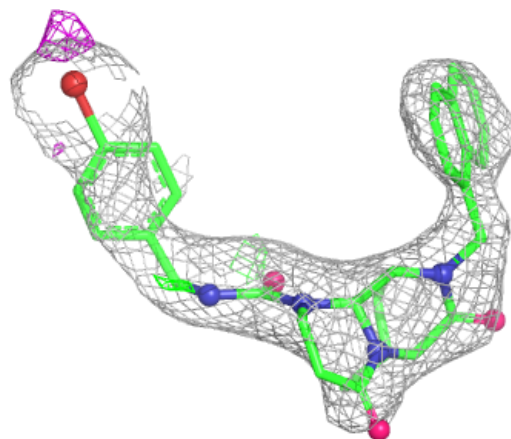
Electron density around 7SR D 302:

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



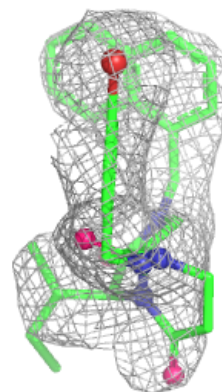
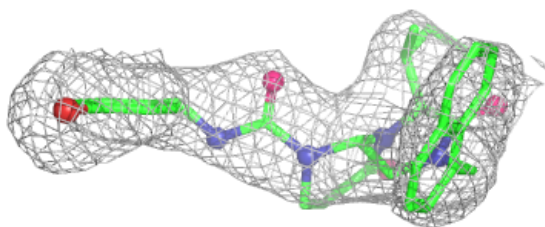
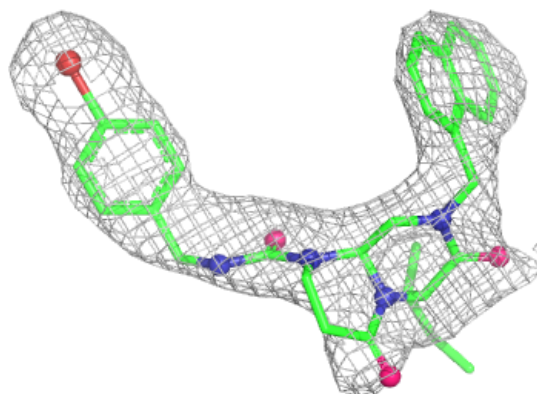
Electron density around 7SR D 301:

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



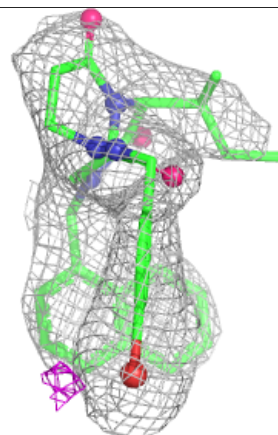
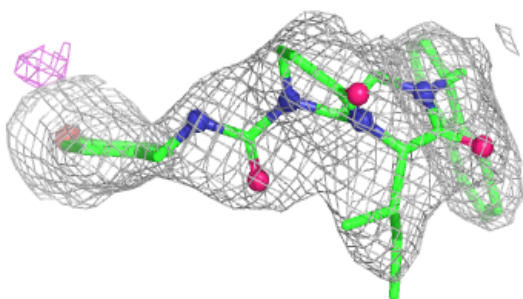
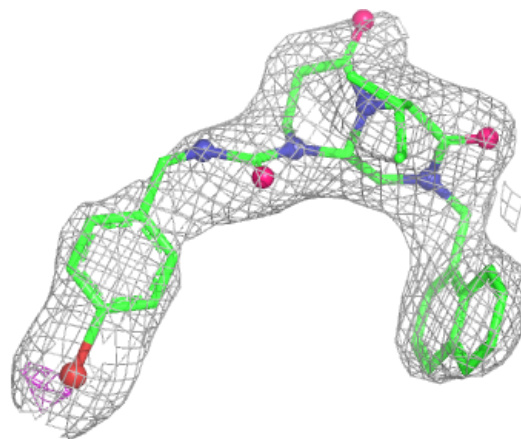
Electron density around 7SR G 301:

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and green (positive)



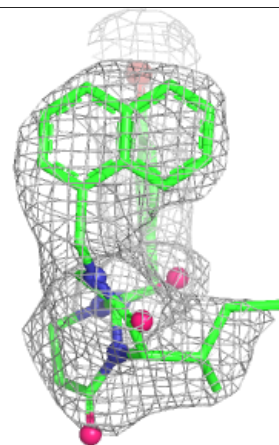
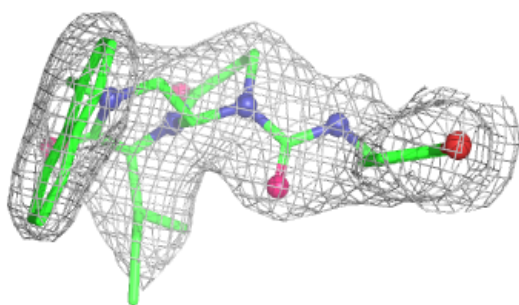
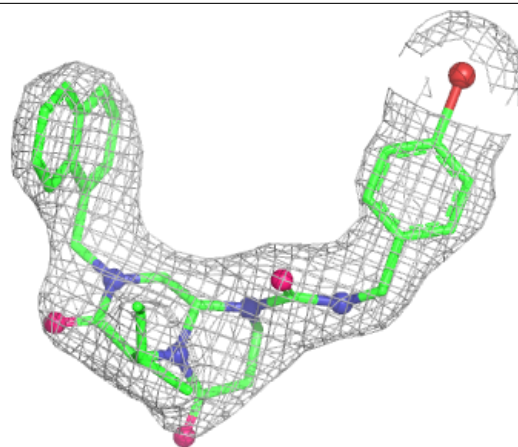
Electron density around 7SR A 301:

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



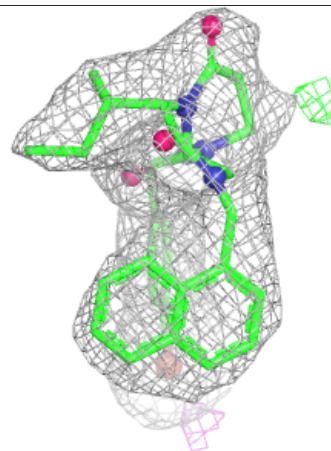
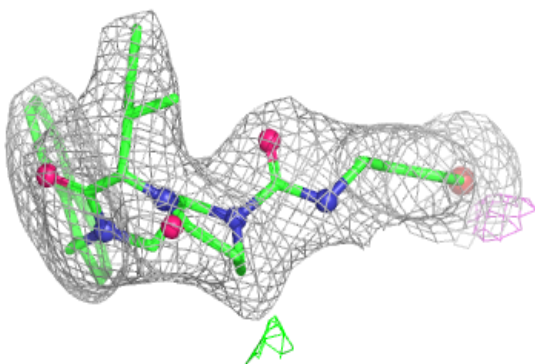
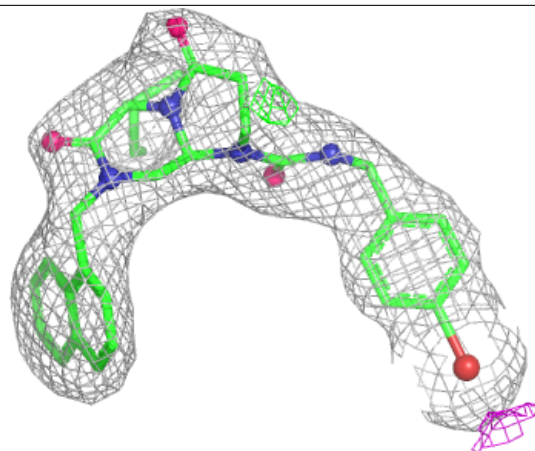
Electron density around 7SR L 301:

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and green (positive)



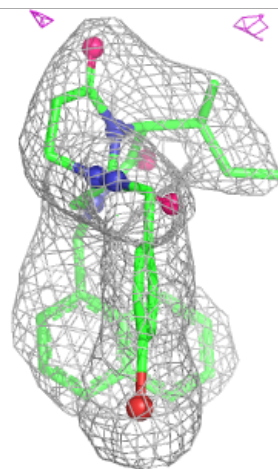
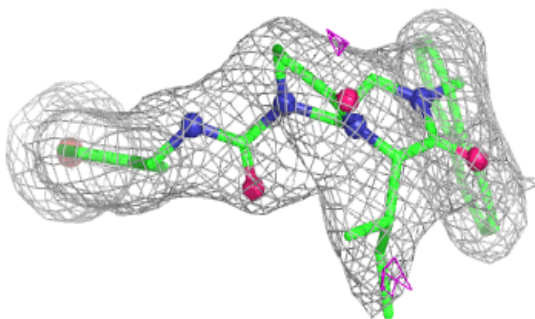
Electron density around 7SR N 301:

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



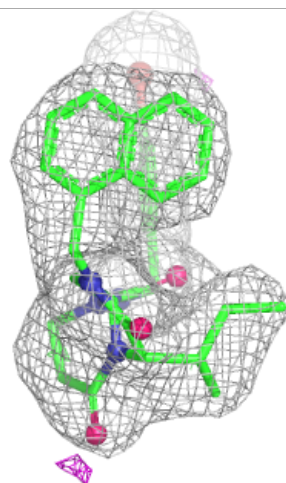
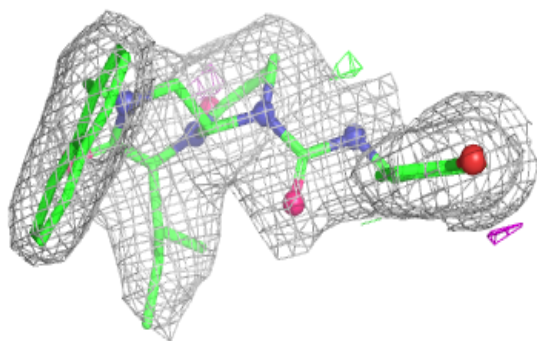
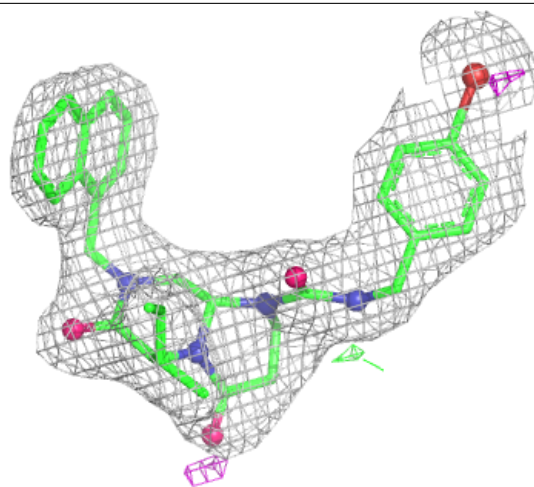
Electron density around 7SR H 301:

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and green (positive)



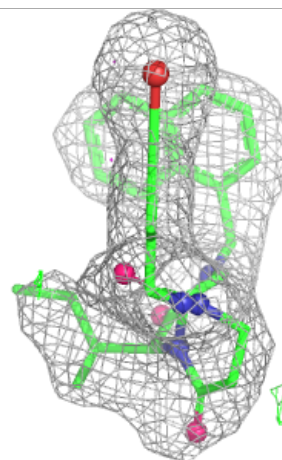
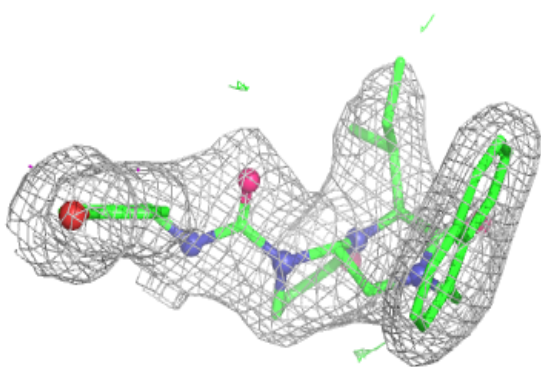
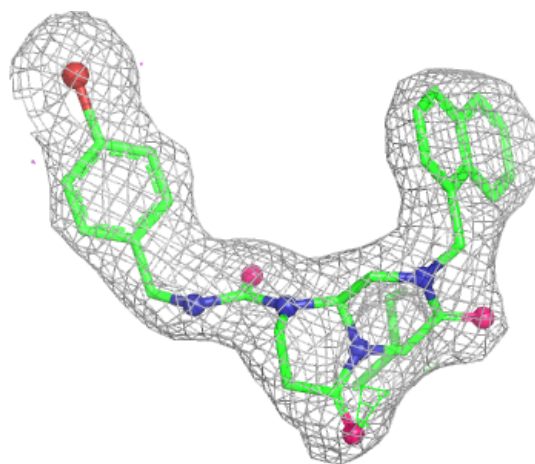
Electron density around 7SR I 301:

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



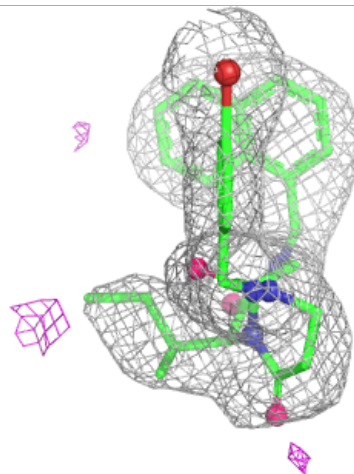
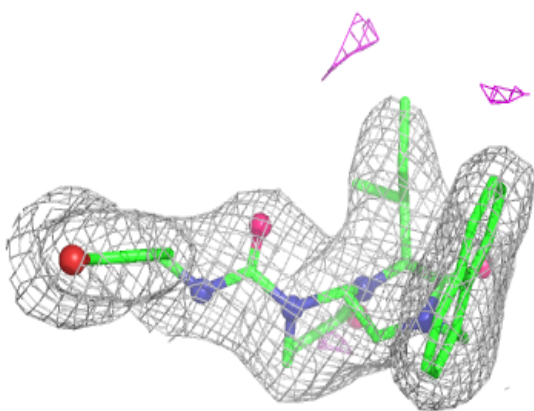
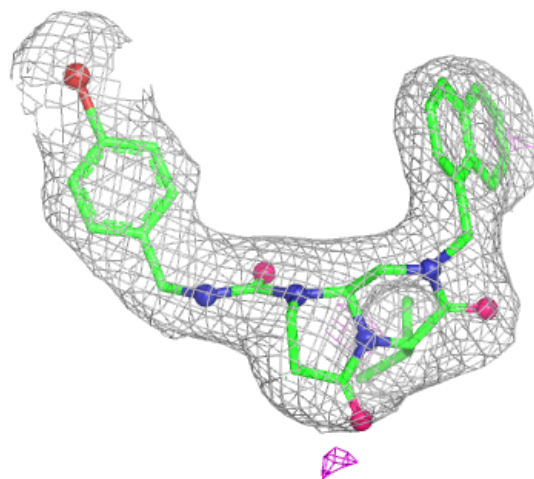
Electron density around 7SR K 302:

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



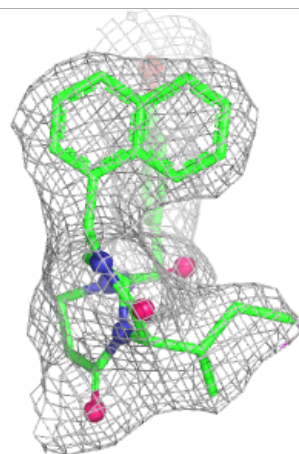
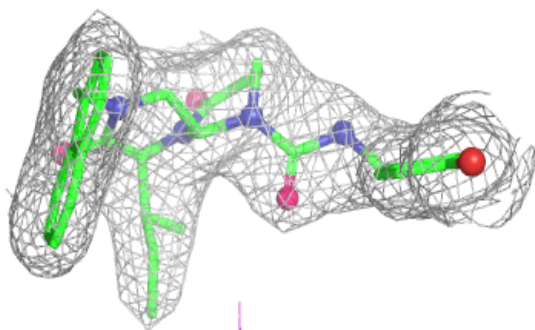
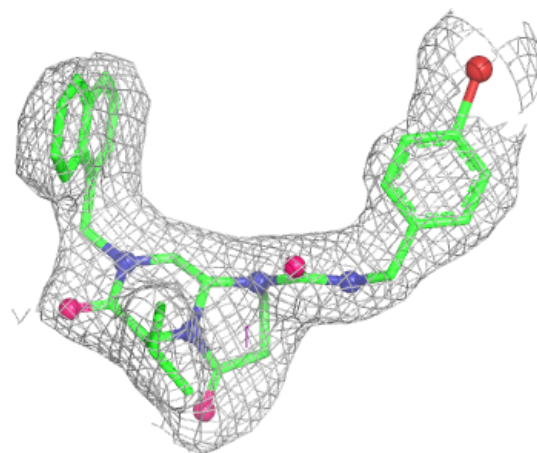
Electron density around 7SR I 302:

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



Electron density around 7SR K 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.