



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 08:04 PM UTC

PDB ID : 8W7E / pdb_00008w7e
Title : Design, synthesis and biological evaluations of novel small molecular hyper-activators of human caseinolytic peptidase P (hClpP)
Authors : Jiang, J.-X.; Ding, H.; Chen, M.-R.; Lu, M.-L.; Sun, H.-Y.; Xiao, Y.-B.
Deposited on : 2023-08-30
Resolution : 2.80 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

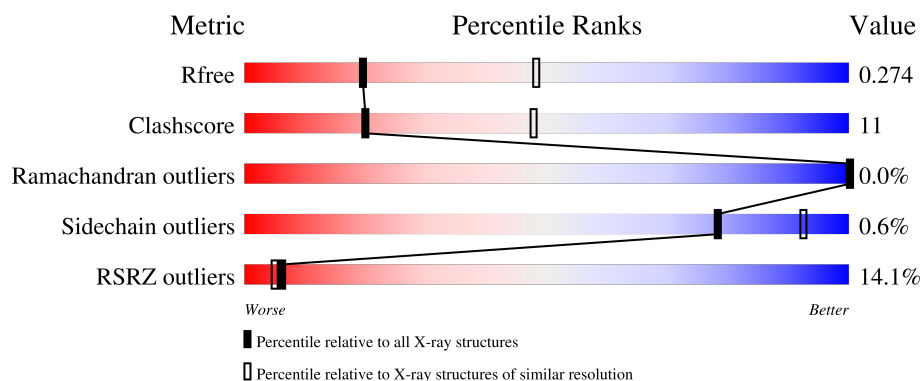
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	223	4% 61%18%22%
1	B	223	4% 63%15%21%
1	C	223	6% 62%17%22%
1	D	223	9% 64%15%21%
1	E	223	7% 61%17%22%

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Mol	Chain	Length	Quality of chain
1	F	223	
1	G	223	
1	H	223	
1	I	223	
1	J	223	
1	K	223	
1	L	223	
1	M	223	
1	N	223	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19090 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.

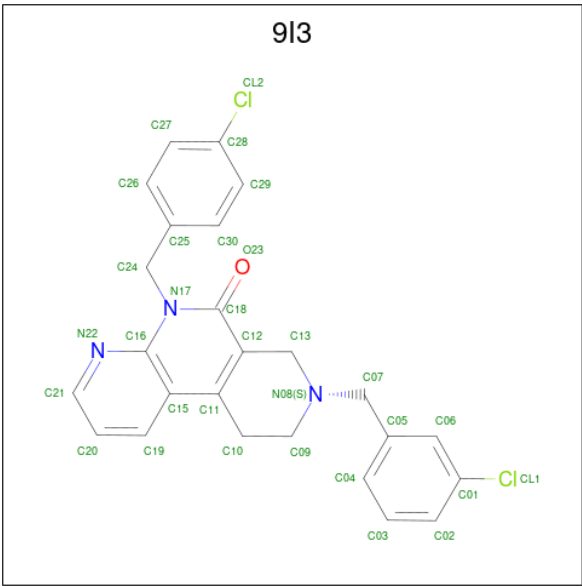
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	1	0
			1359	868	231	247	13			
1	B	176	Total	C	N	O	S	0	0	0
			1352	863	229	247	13			
1	C	175	Total	C	N	O	S	0	2	0
			1365	870	231	250	14			
1	D	176	Total	C	N	O	S	0	1	0
			1370	873	233	251	13			
1	E	174	Total	C	N	O	S	0	1	0
			1339	856	226	243	14			
1	F	177	Total	C	N	O	S	0	1	0
			1374	876	234	252	12			
1	G	176	Total	C	N	O	S	0	0	0
			1347	863	227	244	13			
1	H	175	Total	C	N	O	S	0	0	0
			1336	853	226	244	13			
1	I	169	Total	C	N	O	S	0	0	0
			1296	828	219	236	13			
1	J	168	Total	C	N	O	S	0	0	0
			1276	818	216	229	13			
1	K	172	Total	C	N	O	S	0	0	0
			1314	841	222	238	13			
1	L	172	Total	C	N	O	S	0	0	0
			1330	852	223	242	13			
1	M	170	Total	C	N	O	S	0	1	0
			1283	823	212	236	12			
1	N	171	Total	C	N	O	S	0	0	0
			1315	844	219	239	13			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	GLY	-	linker	UNP Q16740
A	56	SER	-	linker	UNP Q16740
A	57	SER	-	linker	UNP Q16740
B	55	GLY	-	linker	UNP Q16740
B	56	SER	-	linker	UNP Q16740
B	57	SER	-	linker	UNP Q16740
C	55	GLY	-	linker	UNP Q16740
C	56	SER	-	linker	UNP Q16740
C	57	SER	-	linker	UNP Q16740
D	55	GLY	-	linker	UNP Q16740
D	56	SER	-	linker	UNP Q16740
D	57	SER	-	linker	UNP Q16740
E	55	GLY	-	linker	UNP Q16740
E	56	SER	-	linker	UNP Q16740
E	57	SER	-	linker	UNP Q16740
F	55	GLY	-	linker	UNP Q16740
F	56	SER	-	linker	UNP Q16740
F	57	SER	-	linker	UNP Q16740
G	55	GLY	-	linker	UNP Q16740
G	56	SER	-	linker	UNP Q16740
G	57	SER	-	linker	UNP Q16740
H	55	GLY	-	linker	UNP Q16740
H	56	SER	-	linker	UNP Q16740
H	57	SER	-	linker	UNP Q16740
I	55	GLY	-	linker	UNP Q16740
I	56	SER	-	linker	UNP Q16740
I	57	SER	-	linker	UNP Q16740
J	55	GLY	-	linker	UNP Q16740
J	56	SER	-	linker	UNP Q16740
J	57	SER	-	linker	UNP Q16740
K	55	GLY	-	linker	UNP Q16740
K	56	SER	-	linker	UNP Q16740
K	57	SER	-	linker	UNP Q16740
L	55	GLY	-	linker	UNP Q16740
L	56	SER	-	linker	UNP Q16740
L	57	SER	-	linker	UNP Q16740
M	55	GLY	-	linker	UNP Q16740
M	56	SER	-	linker	UNP Q16740
M	57	SER	-	linker	UNP Q16740
N	55	GLY	-	linker	UNP Q16740
N	56	SER	-	linker	UNP Q16740
N	57	SER	-	linker	UNP Q16740

- Molecule 2 is 3-[(3-chlorophenyl)methyl]-6-[(4-chlorophenyl)methyl]-2,4-dihydro-1H-pyrido[

2,3-c[[2,7]naphthyridin-5-one (CCD ID: 9I3) (formula: C₂₅H₂₁Cl₂N₃O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			31	25	2	3	1		
2	B	1	Total	C	Cl	N	O	0	0
			31	25	2	3	1		
2	C	1	Total	C	Cl	N	O	0	0
			31	25	2	3	1		
2	D	1	Total	C	Cl	N	O	0	0
			31	25	2	3	1		
2	E	1	Total	C	Cl	N	O	0	0
			31	25	2	3	1		
2	E	1	Total	C	Cl	N	O	0	0
			31	25	2	3	1		
2	F	1	Total	C	Cl	N	O	0	0
			31	25	2	3	1		
2	G	1	Total	C	Cl	N	O	0	0
			31	25	2	3	1		
2	H	1	Total	C	Cl	N	O	0	0
			31	25	2	3	1		
2	I	1	Total	C	Cl	N	O	0	0
			31	25	2	3	1		
2	K	1	Total	C	Cl	N	O	0	0
			31	25	2	3	1		
2	L	1	Total	C	Cl	N	O	0	0
			31	25	2	3	1		
2	M	1	Total	C	Cl	N	O	0	0
			31	25	2	3	1		

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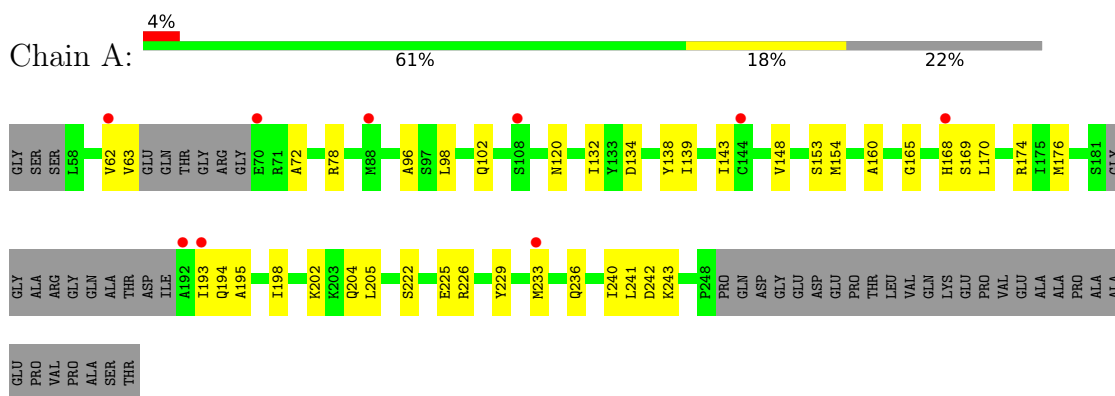
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	N	1	31	25	2	3	1	0	0

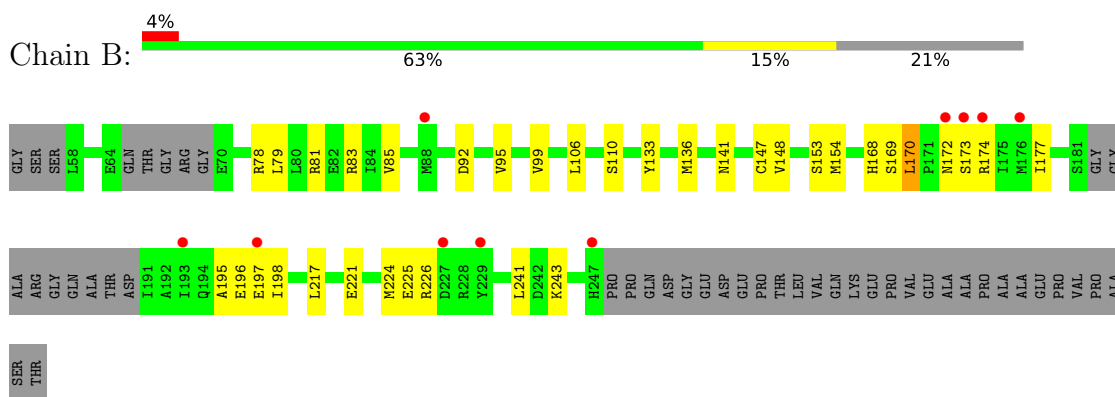
3 Residue-property plots

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

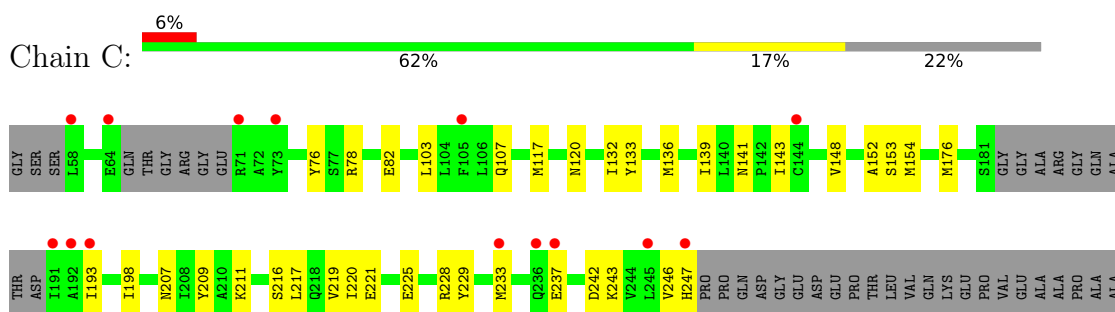
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



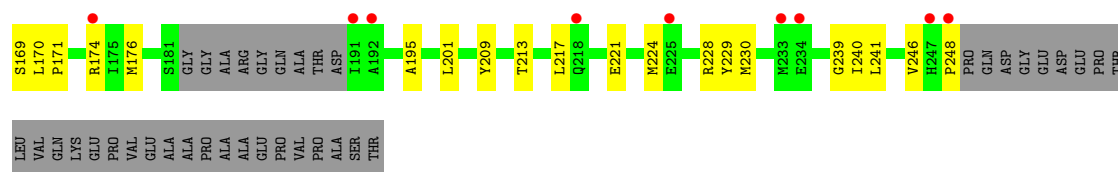
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



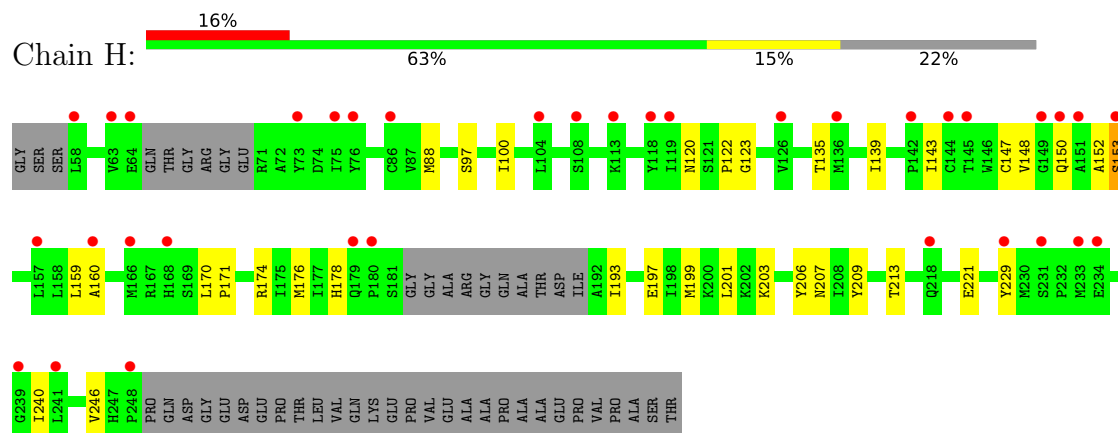
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



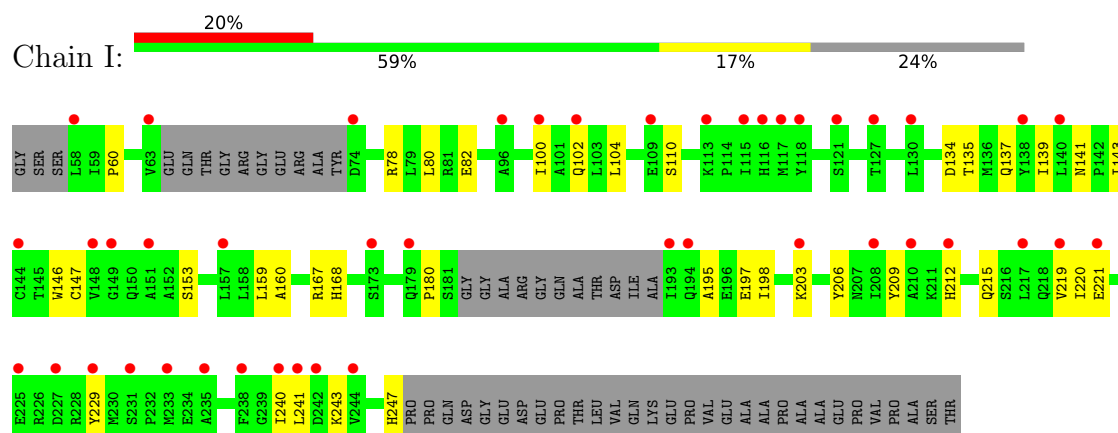
[illegible]



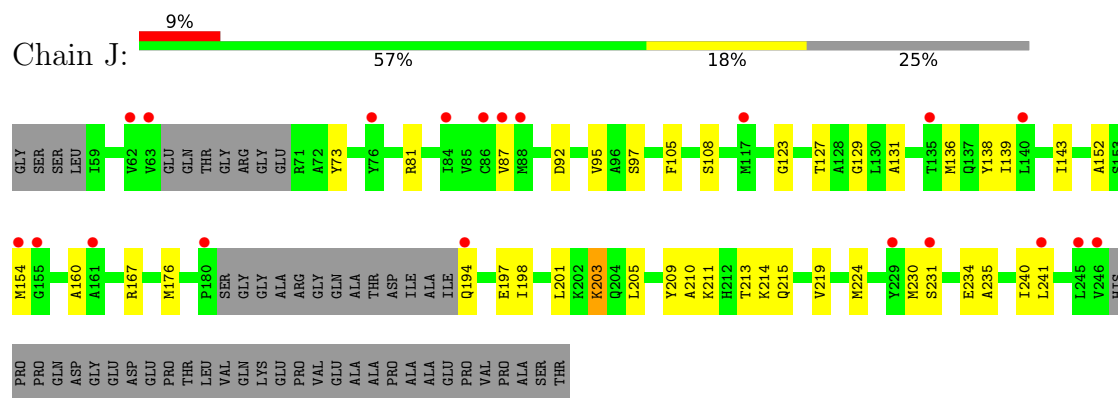
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



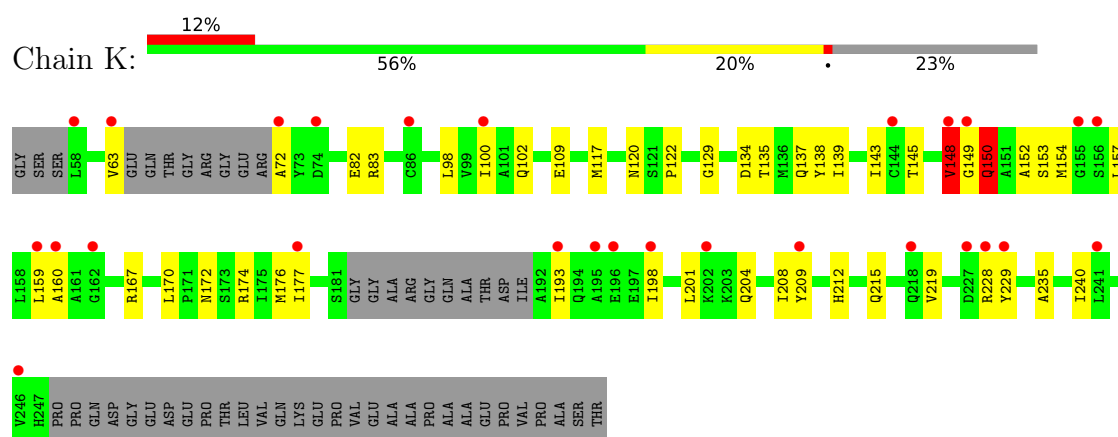
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



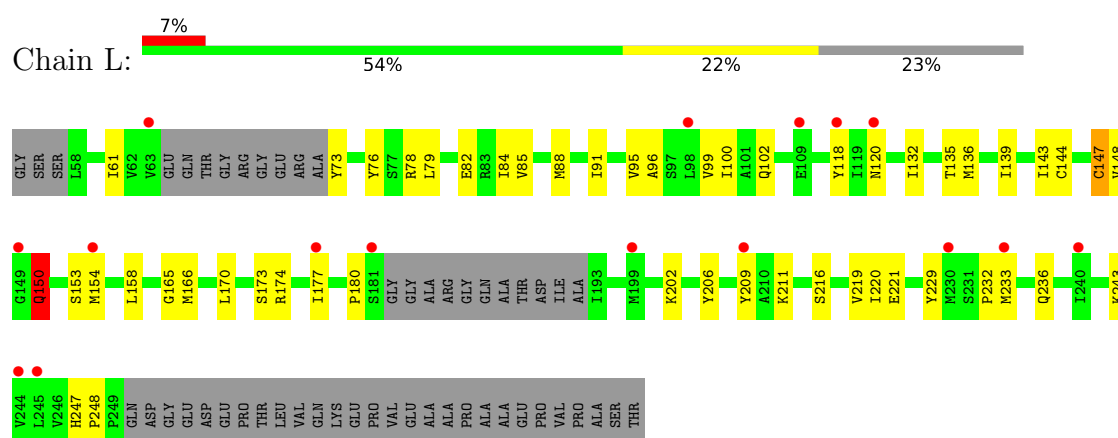
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



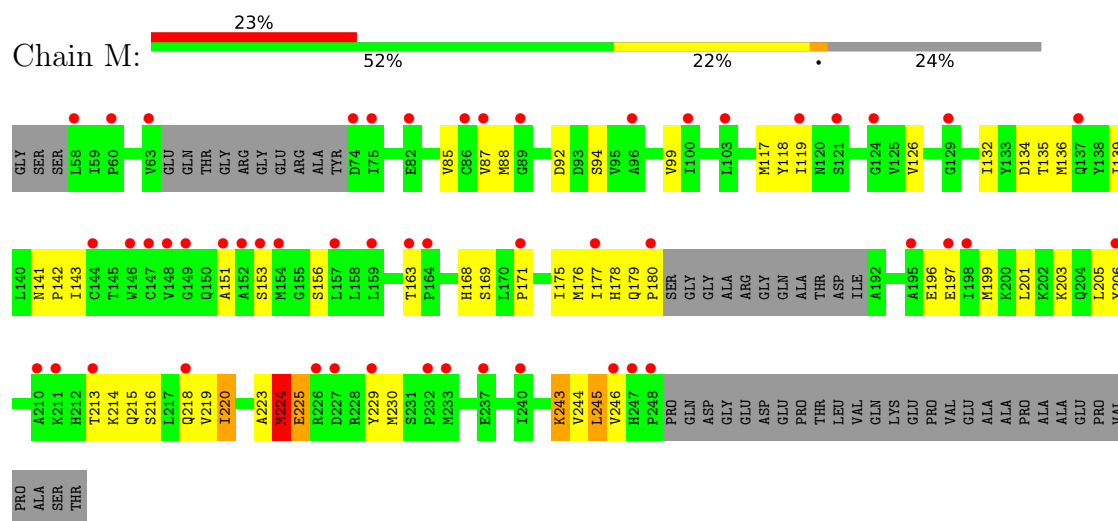
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



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

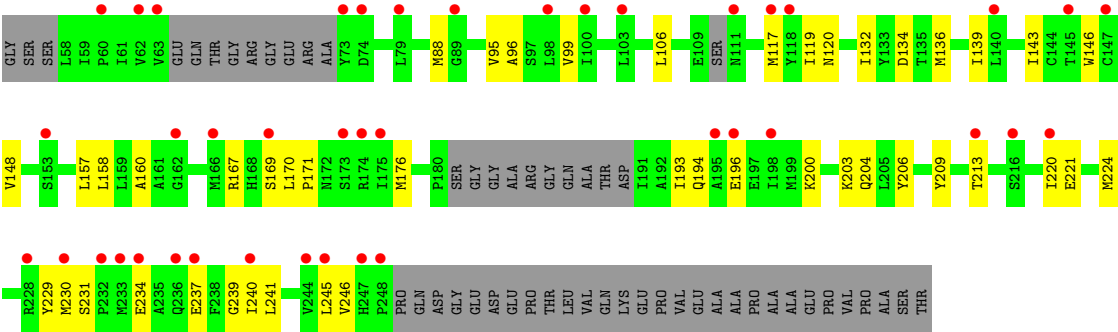


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.77Å 119.22Å 152.81Å 90.00° 100.82° 90.00°	Depositor
Resolution (Å)	46.65 – 2.80 46.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.65-2.80) 88.0 (46.65-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.20 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.266 , 0.274 0.268 , 0.274	Depositor DCC
R_{free} test set	1993 reflections (2.74%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	19090	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: 9I3

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	0.43	0/1383	0.49	0/1871
1	B	0.25	0/1375	0.36	0/1861
1	C	0.15	0/1388	0.39	0/1877
1	D	0.22	0/1393	0.46	0/1883
1	E	0.33	0/1362	0.53	1/1843 (0.1%)
1	F	0.41	1/1398 (0.1%)	0.57	2/1892 (0.1%)
1	G	0.18	0/1371	0.39	0/1858
1	H	0.14	0/1359	0.44	1/1841 (0.1%)
1	I	0.17	0/1318	0.50	0/1785
1	J	0.55	0/1298	0.60	0/1760
1	K	0.55	1/1336 (0.1%)	0.66	2/1808 (0.1%)
1	L	0.33	0/1355	0.56	1/1836 (0.1%)
1	M	0.45	0/1306	0.65	4/1775 (0.2%)
1	N	0.22	0/1338	0.46	0/1812
All	All	0.34	2/18980 (0.0%)	0.51	11/25702 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	91	ILE	C-N	-6.55	1.25	1.33
1	K	148	VAL	CA-C	-5.95	1.44	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	148	VAL	N-CA-C	-9.39	100.76	111.00
1	E	80	LEU	N-CA-C	-6.26	105.77	113.41
1	M	243	LYS	N-CA-C	5.86	117.59	107.93
1	L	150	GLN	N-CA-C	5.81	118.20	110.53
1	H	153	SER	CB-CA-C	-5.63	110.06	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	224	MET	N-CA-C	-5.38	105.82	112.38
1	M	225	GLU	CA-C-N	-5.17	112.08	120.72
1	M	225	GLU	C-N-CA	-5.17	112.08	120.72
1	K	153	SER	CB-CA-C	-5.07	110.34	117.23
1	F	192	ALA	CA-C-N	-5.06	116.24	123.17
1	F	192	ALA	C-N-CA	-5.06	116.24	123.17

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	1359	0	1389	30	0
1	B	1352	0	1369	26	0
1	C	1365	0	1385	27	0
1	D	1370	0	1396	31	0
1	E	1339	0	1367	29	0
1	F	1374	0	1396	60	0
1	G	1347	0	1370	33	0
1	H	1336	0	1356	22	0
1	I	1296	0	1318	24	0
1	J	1276	0	1292	34	0
1	K	1314	0	1338	45	0
1	L	1330	0	1356	44	0
1	M	1283	0	1285	46	0
1	N	1315	0	1334	38	0
2	A	31	0	0	0	0
2	B	31	0	0	1	0
2	C	31	0	0	0	0
2	D	31	0	0	1	0
2	E	62	0	0	1	0
2	F	31	0	0	0	0
2	G	31	0	0	1	0
2	H	31	0	0	1	0
2	I	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	31	0	0	1	0
2	L	31	0	0	3	0
2	M	31	0	0	0	0
2	N	31	0	0	1	0
All	All	19090	0	18951	435	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 11.

All (435) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:ARG:CZ	1:K:201:LEU:HD21	1.79	1.11
1:F:193:ILE:CG2	1:F:197:GLU:HB3	1.94	0.95
1:N:88:MET:HG2	1:N:120:ASN:HB3	1.48	0.94
1:J:213:THR:HG23	1:J:215:GLN:H	1.31	0.93
1:L:139:ILE:HD11	1:L:143:ILE:HD11	1.57	0.86
1:K:129:GLY:HA3	1:K:154:MET:CE	2.06	0.85
1:F:203:LYS:HA	1:F:206:TYR:CD2	2.11	0.85
1:H:123:GLY:HA3	1:H:153:SER:HB3	1.59	0.85
1:K:129:GLY:HA3	1:K:154:MET:HE2	1.60	0.84
1:G:174:ARG:CZ	1:K:201:LEU:CD2	2.56	0.83
1:F:203:LYS:HA	1:F:206:TYR:HD2	1.42	0.83
1:G:88:MET:HG2	1:G:120:ASN:HB3	1.61	0.82
1:D:213:THR:HG22	1:D:215:GLN:HG2	1.59	0.82
1:I:139:ILE:HD11	1:I:143:ILE:HD11	1.59	0.81
1:F:91:ILE:CD1	1:F:121:SER:OG	2.32	0.78
1:F:193:ILE:HG22	1:F:194:GLN:N	1.97	0.78
1:G:160:ALA:HB2	1:G:240:ILE:HG23	1.66	0.78
1:A:148:VAL:HG12	1:A:170:LEU:HD12	1.66	0.78
1:L:61:ILE:HG23	1:L:73:TYR:HB3	1.66	0.78
1:N:139:ILE:HD11	1:N:143:ILE:HD11	1.65	0.77
1:F:193:ILE:HG21	1:F:197:GLU:HB3	1.67	0.77
1:N:171:PRO:HG3	1:N:246:VAL:HG12	1.67	0.77
1:J:160:ALA:HB2	1:J:240:ILE:HG23	1.69	0.74
1:I:160:ALA:HB2	1:I:240:ILE:HG23	1.69	0.73
1:H:139:ILE:HD11	1:H:143:ILE:HD11	1.69	0.73
1:K:139:ILE:HD11	1:K:143:ILE:HD11	1.71	0.73
1:F:193:ILE:CG2	1:F:194:GLN:N	2.52	0.72
1:D:213:THR:CG2	1:D:238:PHE:O	2.37	0.72
1:C:233[A]:MET:SD	1:E:217:LEU:HB3	2.29	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:ARG:NE	1:K:201:LEU:HD21	2.04	0.72
1:I:100:ILE:HG23	1:I:135:THR:HG21	1.71	0.71
1:C:233[B]:MET:HG3	1:E:218:GLN:HA	1.73	0.70
1:L:100:ILE:HG23	1:L:135:THR:HG21	1.72	0.70
1:J:139:ILE:HD11	1:J:143:ILE:HD11	1.73	0.70
1:F:91:ILE:HD12	1:F:121:SER:OG	1.91	0.70
1:I:197:GLU:HG2	1:N:229:TYR:HD1	1.57	0.69
1:E:142:PRO:HB2	1:E:166:MET:HE1	1.72	0.69
1:J:136:MET:HE3	1:J:143:ILE:HG21	1.74	0.69
1:H:122:PRO:HA	1:H:152:ALA:HB3	1.75	0.69
1:E:209:TYR:HB3	1:E:220:ILE:HD12	1.74	0.68
1:B:168:HIS:HD2	1:B:243:LYS:HB2	1.58	0.68
1:A:134:ASP:HB3	1:F:170:LEU:HD23	1.74	0.68
1:J:210:ALA:HA	1:J:213:THR:HG22	1.75	0.67
1:F:91:ILE:HD11	1:F:121:SER:OG	1.95	0.67
1:L:96:ALA:O	1:L:100:ILE:HG12	1.95	0.67
1:M:215:GLN:HB3	1:M:219:VAL:HG21	1.77	0.66
1:F:142:PRO:HB2	1:F:166:MET:HE1	1.76	0.66
1:J:131:ALA:HB1	1:L:148:VAL:HG22	1.78	0.66
1:A:236:GLN:NE2	1:A:242:ASP:O	2.29	0.66
1:D:96:ALA:O	1:D:100:ILE:HG12	1.96	0.66
1:L:100:ILE:HD12	1:L:135:THR:HG21	1.78	0.66
1:F:193:ILE:CG2	1:F:194:GLN:H	2.09	0.65
1:N:234:GLU:HA	1:N:237:GLU:HB3	1.78	0.65
1:E:160:ALA:HB2	1:E:240:ILE:HG23	1.78	0.65
1:C:132:ILE:HG22	1:C:136:MET:HE2	1.78	0.65
1:D:86:CYS:HA	1:D:118:TYR:HB2	1.79	0.65
1:D:213:THR:HG23	1:D:239:GLY:HA3	1.80	0.64
1:E:107:GLN:HG3	1:E:111:ASN:HB3	1.80	0.64
1:G:170:LEU:HD23	1:K:134:ASP:HB3	1.79	0.64
1:C:133:TYR:HA	1:C:136:MET:HE3	1.78	0.64
1:F:193:ILE:HG22	1:F:197:GLU:HB3	1.79	0.64
1:C:152:ALA:HB1	1:C:176:MET:HE2	1.80	0.64
1:F:218:GLN:CD	1:F:218:GLN:H	2.07	0.63
1:A:139:ILE:HD11	1:A:143:ILE:HD11	1.79	0.63
1:E:139:ILE:HD11	1:E:143:ILE:HD11	1.81	0.63
1:M:171:PRO:HG3	1:M:246:VAL:HG22	1.80	0.63
1:F:199:MET:HE1	1:M:196:GLU:HA	1.79	0.62
1:M:179:GLN:HE21	1:M:205:LEU:CD1	2.12	0.62
1:D:213:THR:HG22	1:D:215:GLN:CG	2.28	0.61
1:L:78:ARG:NH1	1:L:82:GLU:OE2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:179:GLN:HE21	1:M:205:LEU:HD11	1.64	0.61
1:F:88:MET:HE3	1:F:118:TYR:HB3	1.83	0.61
1:L:209:TYR:HB3	1:L:220:ILE:HD13	1.81	0.61
1:M:177:ILE:HD12	1:M:224:MET:HE2	1.83	0.61
1:F:123:GLY:HA3	1:F:153[B]:SER:HB2	1.83	0.61
1:K:177:ILE:HB	1:K:209:TYR:HE2	1.66	0.61
1:N:117:MET:HE2	1:N:119:ILE:HD11	1.82	0.61
1:K:193:ILE:HD12	1:K:198:ILE:HB	1.82	0.61
1:J:231:SER:HB2	1:J:234:GLU:H	1.66	0.61
1:L:100:ILE:HD11	1:L:132:ILE:HA	1.84	0.60
1:F:123:GLY:HA3	1:F:153[A]:SER:HB3	1.82	0.60
1:H:160:ALA:HB2	1:H:240:ILE:HG23	1.83	0.59
1:C:209:TYR:HB3	1:C:220:ILE:HD12	1.84	0.59
1:D:213:THR:HG23	1:D:238:PHE:O	2.03	0.59
1:G:169:SER:HB2	1:G:241:LEU:HD22	1.85	0.59
1:K:129:GLY:HA3	1:K:154:MET:HE3	1.85	0.59
1:B:110:SER:O	1:B:141:ASN:ND2	2.31	0.59
1:K:100:ILE:HG23	1:K:135:THR:HG21	1.84	0.59
1:K:167:ARG:NH1	1:K:240:ILE:O	2.35	0.58
1:I:80:LEU:HD11	1:I:102:GLN:HG2	1.85	0.58
1:E:157:LEU:HD13	1:E:205:LEU:HD22	1.85	0.58
1:J:97:SER:OG	1:L:76:TYR:OH	2.20	0.58
1:G:73:TYR:OH	1:G:81:ARG:NH1	2.36	0.58
1:I:134:ASP:HB3	1:N:170:LEU:HD13	1.85	0.58
1:C:139:ILE:HD11	1:C:143:ILE:HD11	1.85	0.58
1:H:206:TYR:CZ	1:H:221:GLU:HG3	2.39	0.58
1:J:73:TYR:CE2	1:J:81:ARG:HD2	2.39	0.57
1:M:85:VAL:HG11	1:M:99:VAL:HG13	1.87	0.57
1:N:200:LYS:HA	1:N:203:LYS:HE2	1.85	0.57
1:K:148:VAL:HA	1:K:170:LEU:HD23	1.85	0.57
1:L:100:ILE:HD12	1:L:135:THR:CG2	2.34	0.57
1:M:139:ILE:HD12	1:M:141:ASN:HB2	1.86	0.57
1:M:171:PRO:HD3	1:M:245:LEU:O	2.05	0.57
1:F:193:ILE:HG21	1:F:197:GLU:CB	2.35	0.56
1:K:160:ALA:HA	1:K:167:ARG:HH11	1.70	0.56
1:B:147:CYS:SG	1:B:173:SER:HB3	2.45	0.56
1:J:92:ASP:H	1:J:95:VAL:HG12	1.69	0.56
1:N:146:TRP:HZ3	1:N:245:LEU:HD21	1.70	0.56
1:N:193:ILE:HG22	1:N:194:GLN:H	1.71	0.56
1:F:85:VAL:O	1:F:117:MET:HA	2.06	0.55
1:L:91:ILE:HA	1:L:95:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:196:GLU:O	1:N:200:LYS:HG3	2.05	0.55
1:M:216:SER:H	1:M:219:VAL:CG2	2.19	0.55
1:B:177:ILE:HD12	1:B:224:MET:HG3	1.89	0.55
1:J:194:GLN:O	1:J:198:ILE:HG12	2.07	0.55
1:M:215:GLN:HB3	1:M:219:VAL:CG2	2.37	0.55
1:N:167:ARG:NH2	1:N:239:GLY:O	2.40	0.55
1:K:120:ASN:HB2	1:K:149:GLY:HA3	1.89	0.55
1:A:63:VAL:HG12	1:A:72:ALA:HB2	1.89	0.54
1:B:133:TYR:HA	1:B:136:MET:HE3	1.90	0.54
1:J:123:GLY:HA2	1:J:154:MET:HB2	1.90	0.54
1:L:165:GLY:O	1:L:243:LYS:NZ	2.36	0.54
1:A:176:MET:HE3	1:A:229:TYR:CE1	2.43	0.54
1:B:217:LEU:O	1:B:221:GLU:HG3	2.07	0.53
1:L:153:SER:OG	1:L:180:PRO:HD3	2.07	0.53
1:L:154:MET:O	1:L:158:LEU:HD12	2.09	0.53
1:M:142:PRO:HA	1:M:163:THR:HG21	1.90	0.53
1:F:193:ILE:HG21	1:F:197:GLU:CG	2.39	0.53
1:K:215:GLN:HB3	1:K:219:VAL:CG2	2.38	0.53
1:E:111:ASN:HA	1:E:141:ASN:ND2	2.23	0.53
1:F:231:SER:N	1:F:234:GLU:OE1	2.35	0.53
1:I:110:SER:O	1:I:141:ASN:ND2	2.34	0.53
1:M:216:SER:OG	1:M:219:VAL:HG22	2.09	0.53
1:A:98:LEU:O	1:A:102:GLN:HG3	2.09	0.53
1:I:137:GLN:HE22	1:I:212:HIS:CE1	2.27	0.53
1:N:169:SER:HB2	1:N:241:LEU:HD22	1.90	0.53
1:B:148:VAL:HG23	1:B:170:LEU:HD12	1.90	0.53
1:C:217:LEU:O	1:C:221:GLU:HG3	2.09	0.53
1:I:168:HIS:CD2	1:I:243:LYS:HD2	2.44	0.53
1:M:223:ALA:C	1:M:225:GLU:N	2.65	0.53
1:A:63:VAL:HA	1:A:72:ALA:HA	1.91	0.53
1:K:235:ALA:HB1	1:K:240:ILE:HB	1.91	0.53
1:B:170:LEU:HD13	1:G:134:ASP:HB3	1.91	0.52
1:M:177:ILE:O	1:M:224:MET:HG3	2.09	0.52
1:F:87:VAL:N	1:F:118:TYR:O	2.42	0.52
1:C:78:ARG:NH1	1:C:82:GLU:OE2	2.35	0.52
1:K:145:THR:HB	1:K:159:LEU:HD12	1.90	0.52
1:D:103:LEU:HD11	1:D:117:MET:CE	2.39	0.52
1:M:151:ALA:O	1:M:156:SER:OG	2.26	0.52
1:M:175:ILE:O	1:M:230:MET:N	2.43	0.52
1:M:216:SER:H	1:M:219:VAL:HG22	1.75	0.52
1:C:176:MET:HG3	1:C:228:ARG:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:149:GLY:O	1:K:150:GLN:C	2.52	0.52
1:M:176:MET:HE2	1:M:178:HIS:HD2	1.74	0.52
1:G:82:GLU:HG3	2:G:301:9I3:C27	2.40	0.52
1:F:139:ILE:HD11	1:F:143:ILE:HD11	1.92	0.52
1:M:199:MET:O	1:M:203:LYS:HG2	2.10	0.52
1:N:160:ALA:HB2	1:N:240:ILE:HG23	1.91	0.52
1:K:129:GLY:CA	1:K:154:MET:HE2	2.37	0.51
1:M:218:GLN:O	1:M:219:VAL:C	2.49	0.51
1:A:174:ARG:NH2	1:B:197:GLU:OE1	2.41	0.51
1:F:216:SER:O	1:F:219:VAL:HG22	2.11	0.51
1:B:83:ARG:HG2	1:B:106:LEU:HD22	1.92	0.51
1:C:237:GLU:HG3	1:E:203:LYS:HE3	1.91	0.51
1:G:171:PRO:HG3	1:G:246:VAL:HG22	1.92	0.51
1:E:79:LEU:HD12	2:E:301:9I3:CL2	2.47	0.51
1:H:199:MET:HE2	1:H:199:MET:HA	1.92	0.51
1:J:197:GLU:OE2	1:L:229:TYR:HB2	2.11	0.51
1:I:203:LYS:HA	1:I:206:TYR:CD2	2.46	0.51
1:E:82:GLU:O	1:E:84:ILE:HG13	2.10	0.51
1:L:177:ILE:HB	1:L:209:TYR:HE2	1.74	0.51
1:F:92:ASP:C	1:F:92:ASP:OD1	2.53	0.51
1:M:117:MET:HE2	1:M:119:ILE:HD11	1.92	0.51
1:E:85:VAL:O	1:E:117:MET:HA	2.11	0.51
1:M:139:ILE:HD11	1:M:143:ILE:HD11	1.91	0.51
1:J:138:TYR:CE2	1:L:248:PRO:HD3	2.46	0.50
1:K:159:LEU:O	1:K:160:ALA:C	2.51	0.50
1:K:176:MET:HG3	1:K:228:ARG:O	2.11	0.50
1:D:199:MET:HG3	1:D:203:LYS:HZ2	1.76	0.50
1:F:102:GLN:NE2	1:I:60:PRO:HG2	2.26	0.50
1:D:213:THR:HG22	1:D:213:THR:O	2.11	0.50
1:E:157:LEU:CD1	1:E:205:LEU:HD22	2.40	0.50
1:H:176:MET:HE2	1:H:178:HIS:HB3	1.92	0.50
1:K:157:LEU:HA	1:K:209:TYR:CE1	2.45	0.50
1:N:120:ASN:HB2	1:N:148:VAL:HG13	1.93	0.50
1:B:225:GLU:OE2	1:C:228:ARG:HD2	2.11	0.50
1:D:199:MET:HG3	1:D:203:LYS:NZ	2.27	0.49
1:D:213:THR:HG23	1:D:239:GLY:CA	2.42	0.49
1:F:117:MET:SD	1:F:136:MET:HE3	2.51	0.49
1:G:230:MET:HE1	1:G:240:ILE:HD12	1.94	0.49
1:M:176:MET:HE2	1:M:178:HIS:CD2	2.47	0.49
1:A:153[A]:SER:OG	1:A:154:MET:N	2.43	0.49
1:E:100:ILE:HG23	1:E:135:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:MET:SD	1:H:120:ASN:HB3	2.52	0.49
1:J:127:THR:HG23	1:L:150:GLN:H	1.76	0.49
1:N:230:MET:HE1	1:N:240:ILE:CD1	2.42	0.49
1:A:138:TYR:CZ	1:F:248:PRO:HG3	2.47	0.49
1:F:193:ILE:CG2	1:F:197:GLU:CB	2.80	0.49
1:J:152:ALA:HA	1:J:176:MET:HB3	1.94	0.49
1:L:85:VAL:HG11	1:L:99:VAL:HG13	1.93	0.49
1:B:78:ARG:O	1:B:81:ARG:HB2	2.11	0.49
1:K:122:PRO:HA	1:K:152:ALA:HB3	1.94	0.49
1:L:88:MET:HE2	1:L:148:VAL:HG11	1.95	0.49
1:L:120:ASN:HB2	1:L:148:VAL:HG13	1.94	0.49
1:I:195:ALA:O	1:I:198:ILE:HG22	2.12	0.49
1:F:192:ALA:C	1:F:193:ILE:HG13	2.37	0.49
1:L:95:VAL:O	1:L:99:VAL:HG23	2.12	0.49
1:M:88:MET:HE2	1:M:118:TYR:HB3	1.95	0.49
1:F:169:SER:HB2	1:F:241:LEU:HD22	1.94	0.49
1:I:215:GLN:HB3	1:I:219:VAL:CG2	2.43	0.48
1:L:85:VAL:HG13	1:L:102:GLN:NE2	2.28	0.48
1:B:169:SER:OG	1:B:173:SER:HB2	2.13	0.48
1:C:207:ASN:O	1:C:211:LYS:HB2	2.14	0.48
1:M:224:MET:HE3	1:M:224:MET:HB2	1.64	0.48
1:N:136:MET:HG2	1:N:143:ILE:HD13	1.95	0.48
1:A:62:VAL:O	1:A:72:ALA:HA	2.13	0.48
1:A:165:GLY:O	1:A:243:LYS:NZ	2.46	0.48
1:H:150:GLN:HB2	1:H:174:ARG:HB3	1.96	0.48
1:J:213:THR:OG1	1:J:215:GLN:HG2	2.13	0.48
1:J:131:ALA:HB1	1:L:148:VAL:CG2	2.42	0.48
1:N:136:MET:CE	1:N:158:LEU:HD12	2.43	0.48
1:I:153:SER:OG	1:I:180:PRO:HD3	2.13	0.48
1:J:209:TYR:O	1:J:213:THR:HG22	2.12	0.48
1:N:206:TYR:HA	1:N:220:ILE:HG21	1.95	0.48
1:G:209:TYR:O	1:G:213:THR:OG1	2.26	0.48
1:H:171:PRO:HG3	1:H:246:VAL:HG12	1.94	0.48
1:F:196:GLU:OE2	1:M:199:MET:HE1	2.13	0.47
1:G:98:LEU:O	1:G:102:GLN:HG3	2.14	0.47
1:N:230:MET:HE1	1:N:240:ILE:HD12	1.96	0.47
1:E:228:ARG:HH22	1:E:234:GLU:CD	2.22	0.47
1:F:110:SER:O	1:F:141:ASN:ND2	2.41	0.47
1:K:174:ARG:HB3	1:K:229:TYR:CD2	2.48	0.47
1:B:226:ARG:NH1	1:C:225:GLU:OE2	2.45	0.47
1:F:214:LYS:O	1:F:214:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:GLN:HB3	1:F:219:VAL:CG2	2.45	0.47
1:L:206:TYR:CZ	1:L:221:GLU:HG2	2.50	0.47
1:B:195:ALA:O	1:B:198:ILE:HG22	2.15	0.47
1:G:105:PHE:O	1:G:108:SER:OG	2.31	0.47
1:K:157:LEU:HD12	1:K:209:TYR:CE1	2.49	0.47
1:L:118:TYR:HE2	2:L:301:9I3:CL1	2.34	0.47
1:B:196:GLU:OE1	1:D:202:LYS:NZ	2.48	0.47
1:J:213:THR:O	1:J:214:LYS:HB2	2.15	0.47
1:A:120:ASN:HB2	1:A:148:VAL:HG23	1.96	0.47
1:D:76:TYR:OH	1:H:97:SER:OG	2.32	0.47
1:F:217:LEU:HD12	1:F:217:LEU:H	1.79	0.47
1:M:169:SER:O	1:M:245:LEU:HD23	2.15	0.47
1:A:202:LYS:HD2	1:A:205:LEU:HD12	1.97	0.47
1:G:217:LEU:O	1:G:221:GLU:HG3	2.14	0.47
1:M:229:TYR:O	1:M:230:MET:HG3	2.15	0.47
1:I:197:GLU:HG2	1:N:229:TYR:CD1	2.44	0.47
1:J:129:GLY:HA3	1:J:154:MET:SD	2.55	0.47
1:D:115:ILE:HD12	1:D:139:ILE:HD12	1.95	0.46
1:G:167:ARG:NH1	1:G:239:GLY:O	2.42	0.46
1:N:209:TYR:O	1:N:213:THR:HG22	2.15	0.46
1:B:172:ASN:N	1:G:134:ASP:OD2	2.46	0.46
1:C:148:VAL:HG22	1:D:131:ALA:HB1	1.97	0.46
1:C:193:ILE:HD11	1:C:198:ILE:HG12	1.97	0.46
1:N:176:MET:HE3	1:N:229:TYR:CE1	2.51	0.46
1:A:168:HIS:CE1	1:A:243:LYS:HD2	2.51	0.46
1:B:170:LEU:CD1	1:G:134:ASP:HB3	2.45	0.46
1:B:85:VAL:HG11	1:B:99:VAL:HG13	1.98	0.46
1:C:246:VAL:HG21	1:E:222:SER:OG	2.15	0.46
1:H:100:ILE:HG23	1:H:135:THR:HG21	1.97	0.46
1:J:215:GLN:HB3	1:J:219:VAL:CG2	2.46	0.46
1:K:120:ASN:CB	1:K:149:GLY:HA3	2.45	0.46
1:K:172:ASN:ND2	1:N:134:ASP:OD1	2.48	0.46
1:D:217:LEU:O	1:D:221:GLU:HG3	2.16	0.46
1:H:203:LYS:O	1:H:207:ASN:ND2	2.46	0.46
1:N:157:LEU:HA	1:N:209:TYR:HE1	1.80	0.46
1:B:92:ASP:H	1:B:95:VAL:HG22	1.81	0.46
1:E:203:LYS:HA	1:E:206:TYR:CD2	2.50	0.46
1:E:206:TYR:HB3	1:E:217:LEU:CD2	2.46	0.46
1:M:135:THR:O	1:M:139:ILE:HG23	2.16	0.46
1:F:65:GLN:HA	1:F:70:GLU:HB2	1.98	0.45
1:L:206:TYR:CE2	1:L:221:GLU:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:194:GLN:OE1	1:J:194:GLN:HA	2.16	0.45
1:M:179:GLN:OE1	1:M:180:PRO:HD2	2.16	0.45
1:E:87:VAL:N	1:E:118:TYR:O	2.47	0.45
1:A:226:ARG:HD2	1:D:225:GLU:CD	2.41	0.45
1:A:233:MET:HE3	1:L:247:HIS:CE1	2.52	0.45
1:N:160:ALA:HA	1:N:167:ARG:HD2	1.97	0.45
1:C:153[A]:SER:OG	1:C:154:MET:N	2.47	0.45
1:C:229:TYR:HB2	1:D:197:GLU:HG3	1.99	0.45
1:I:209:TYR:HB3	1:I:220:ILE:HD13	1.99	0.45
1:J:131:ALA:CB	1:L:148:VAL:HG22	2.44	0.45
1:A:225:GLU:OE2	1:D:228:ARG:HD2	2.17	0.45
1:L:79:LEU:O	1:L:84:ILE:HB	2.17	0.45
1:L:144:CYS:HA	1:L:166:MET:O	2.16	0.45
1:J:215:GLN:HB3	1:J:219:VAL:HG21	1.99	0.45
1:J:230:MET:HE3	1:J:235:ALA:HA	1.98	0.45
1:M:206:TYR:HA	1:M:220:ILE:HG21	1.98	0.45
1:H:147:CYS:HB2	1:H:159:LEU:HD13	1.99	0.45
1:J:210:ALA:HA	1:J:213:THR:CG2	2.46	0.45
1:E:92:ASP:OD1	1:E:94:SER:N	2.50	0.44
1:G:248:PRO:HG3	1:K:138:TYR:CE1	2.52	0.44
1:L:147:CYS:SG	1:L:173:SER:HB3	2.57	0.44
1:D:153[A]:SER:OG	1:D:154:MET:N	2.51	0.44
1:B:172:ASN:HB3	1:G:130:LEU:HD13	2.00	0.44
1:F:206:TYR:CE1	1:F:221:GLU:HG2	2.52	0.44
1:K:204:GLN:O	1:K:208:ILE:HG13	2.17	0.44
1:L:233:MET:O	1:L:236:GLN:HB3	2.17	0.44
1:M:132:ILE:O	1:M:136:MET:HG3	2.17	0.44
1:F:122:PRO:HA	1:F:152:ALA:HB3	2.00	0.44
1:N:95:VAL:O	1:N:99:VAL:HG23	2.16	0.44
1:A:169:SER:HB2	1:A:241:LEU:HD22	2.00	0.44
1:B:172:ASN:HB3	1:G:130:LEU:HB3	1.99	0.44
1:D:213:THR:CG2	1:D:215:GLN:CG	2.96	0.44
1:E:196:GLU:H	1:E:196:GLU:CD	2.26	0.44
1:E:203:LYS:O	1:E:206:TYR:HB2	2.17	0.44
1:F:215:GLN:HB2	1:F:220:ILE:HD11	1.99	0.44
1:L:173:SER:O	1:L:232:PRO:HD3	2.18	0.44
1:L:211:LYS:HB2	1:L:211:LYS:HE2	1.85	0.44
1:F:217:LEU:O	1:F:221:GLU:HG3	2.18	0.44
1:G:224:MET:HE2	1:G:224:MET:HB3	1.77	0.44
1:K:193:ILE:CD1	1:K:198:ILE:HB	2.47	0.44
1:C:247:HIS:CE1	1:D:137:GLN:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:230:MET:HE1	1:G:240:ILE:CD1	2.48	0.43
1:E:238:PHE:HD2	1:E:240:ILE:HG13	1.84	0.43
1:G:78:ARG:HD2	1:G:78:ARG:O	2.18	0.43
1:K:120:ASN:CG	1:K:149:GLY:HA3	2.44	0.43
1:D:79:LEU:HD12	2:D:301:9I3:CL2	2.55	0.43
1:K:137:GLN:HE22	1:K:212:HIS:CE1	2.36	0.43
1:N:230:MET:HB3	1:N:234:GLU:HG2	2.00	0.43
1:A:194:GLN:O	1:A:198:ILE:HD12	2.18	0.43
1:E:176:MET:HB2	1:E:229:TYR:CD2	2.53	0.43
1:F:138:TYR:CD1	1:I:247:HIS:HA	2.54	0.43
1:E:202:LYS:O	1:E:203:LYS:C	2.61	0.43
1:K:148:VAL:HG22	1:K:149:GLY:N	2.33	0.43
1:K:215:GLN:HB3	1:K:219:VAL:HG21	2.00	0.43
1:M:153[B]:SER:OG	1:M:180:PRO:HD3	2.19	0.43
1:B:79:LEU:HD12	2:B:301:9I3:CL2	2.55	0.43
1:F:236:GLN:NE2	1:F:242:ASP:O	2.48	0.43
1:I:146:TRP:CE3	1:I:168:HIS:HB2	2.54	0.43
1:L:132:ILE:O	1:L:135:THR:OG1	2.30	0.43
1:C:76:TYR:OH	1:D:98:LEU:HD12	2.19	0.43
1:H:170:LEU:HD13	1:M:134:ASP:HB3	2.00	0.43
1:M:153[A]:SER:OG	1:M:179:GLN:OE1	2.23	0.43
1:D:129:GLY:HA3	1:D:154:MET:HE2	2.01	0.43
1:F:201:LEU:HD23	1:F:201:LEU:HA	1.90	0.43
1:M:87:VAL:HB	1:M:119:ILE:HD13	2.01	0.43
1:A:226:ARG:HH11	1:D:225:GLU:CD	2.27	0.43
1:B:174:ARG:HH11	1:G:201:LEU:HD21	1.84	0.43
1:F:197:GLU:OE1	1:I:229:TYR:HB2	2.19	0.43
1:G:176:MET:HG3	1:G:228:ARG:O	2.19	0.43
1:H:201:LEU:HD23	1:H:201:LEU:HA	1.91	0.43
1:K:160:ALA:HA	1:K:167:ARG:NH1	2.33	0.43
1:L:202:LYS:HG3	1:L:206:TYR:CE2	2.54	0.43
1:F:100:ILE:HG23	1:F:135:THR:HG21	2.00	0.42
1:F:213:THR:OG1	1:F:220:ILE:HD11	2.19	0.42
1:H:148:VAL:HG11	2:H:301:9I3:CL1	2.55	0.42
1:J:230:MET:SD	1:J:234:GLU:HG2	2.59	0.42
1:K:82:GLU:HG3	2:K:301:9I3:C29	2.48	0.42
1:B:169:SER:HB3	1:B:241:LEU:HD22	2.01	0.42
1:F:98:LEU:O	1:F:102:GLN:HG3	2.18	0.42
1:K:174:ARG:NH2	1:N:204:GLN:OE1	2.35	0.42
1:M:213:THR:O	1:M:214:LYS:HB2	2.17	0.42
1:A:225:GLU:OE1	1:D:226:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:LEU:O	1:E:84:ILE:HB	2.20	0.42
1:G:230:MET:HE3	1:G:230:MET:HB2	1.87	0.42
1:H:193:ILE:HG21	1:H:197:GLU:HG2	2.01	0.42
1:L:170:LEU:HD11	2:L:301:9I3:C02	2.50	0.42
1:C:216:SER:OG	1:C:219:VAL:HG23	2.20	0.42
1:J:87:VAL:HG12	1:J:87:VAL:O	2.19	0.42
1:M:168:HIS:HA	1:M:243:LYS:O	2.19	0.42
1:A:193:ILE:HD11	1:A:198:ILE:HG13	2.02	0.42
1:C:242:ASP:O	1:C:243:LYS:HG3	2.20	0.42
1:D:100:ILE:HD12	1:D:135:THR:OG1	2.19	0.42
1:L:136:MET:HG2	1:L:143:ILE:HD13	2.02	0.42
1:N:106:LEU:HD23	1:N:106:LEU:HA	1.91	0.42
1:N:193:ILE:HG22	1:N:194:GLN:N	2.35	0.42
1:B:153:SER:OG	1:B:154:MET:N	2.52	0.42
1:A:195:ALA:C	1:H:199:MET:HE3	2.44	0.42
1:K:98:LEU:O	1:K:102:GLN:HG3	2.19	0.42
1:A:96:ALA:HA	1:A:132:ILE:HD11	2.01	0.42
1:A:160:ALA:HB2	1:A:240:ILE:HG23	2.01	0.42
1:F:83:ARG:HH12	1:F:109:GLU:HB2	1.85	0.42
1:F:153[A]:SER:OG	1:F:154:MET:N	2.53	0.42
1:I:206:TYR:CZ	1:I:221:GLU:HG3	2.53	0.42
1:D:175:ILE:O	1:D:230:MET:N	2.43	0.42
1:J:167:ARG:HB2	1:J:241:LEU:HA	2.01	0.42
1:K:145:THR:OG1	1:K:167:ARG:HG2	2.20	0.42
1:N:148:VAL:HG23	1:N:170:LEU:HD12	2.02	0.42
1:N:224:MET:HE2	1:N:224:MET:HB3	1.92	0.42
1:H:206:TYR:CE2	1:H:221:GLU:HG3	2.55	0.41
1:N:176:MET:HE3	1:N:229:TYR:CZ	2.55	0.41
1:I:78:ARG:HH12	1:I:82:GLU:HG2	1.85	0.41
1:J:203:LYS:HE2	1:J:203:LYS:HB2	1.70	0.41
1:K:129:GLY:CA	1:K:154:MET:CE	2.90	0.41
1:M:229:TYR:C	1:M:230:MET:HG3	2.45	0.41
1:A:195:ALA:HA	1:A:198:ILE:HD13	2.02	0.41
1:I:167:ARG:HE	1:I:241:LEU:HA	1.84	0.41
1:K:63:VAL:HA	1:K:72:ALA:HA	2.02	0.41
1:L:118:TYR:CE2	2:L:301:9I3:CL1	3.10	0.41
1:M:92:ASP:OD1	1:M:94:SER:N	2.53	0.41
1:M:220:ILE:HG23	1:M:224:MET:CE	2.50	0.41
1:E:107:GLN:CG	1:E:111:ASN:HB3	2.49	0.41
1:M:220:ILE:HG23	1:M:224:MET:HE1	2.01	0.41
1:L:150:GLN:HA	1:L:174:ARG:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:HIS:ND1	1:F:224:MET:O	2.39	0.41
1:J:201:LEU:O	1:J:205:LEU:HG	2.20	0.41
1:K:83:ARG:HH12	1:K:109:GLU:HB2	1.86	0.41
1:I:104:LEU:HD22	2:N:301:9I3:O23	2.21	0.41
1:N:96:ALA:HA	1:N:132:ILE:HD11	2.03	0.41
1:C:107:GLN:HG3	1:C:141:ASN:OD1	2.20	0.41
1:D:224:MET:HE2	1:D:224:MET:HB3	1.98	0.41
1:F:193:ILE:HG23	1:F:194:GLN:H	1.83	0.41
1:G:176:MET:HB2	1:G:229:TYR:CD2	2.55	0.41
1:H:209:TYR:O	1:H:213:THR:HG23	2.21	0.41
1:J:224:MET:HB3	1:J:224:MET:HE2	1.81	0.41
1:L:216:SER:OG	1:L:219:VAL:HG22	2.20	0.41
1:M:126:VAL:HG11	1:M:201:LEU:HD13	2.03	0.41
1:N:206:TYR:CZ	1:N:221:GLU:HB3	2.55	0.41
1:C:120:ASN:HB2	1:C:148:VAL:HG13	2.02	0.41
1:C:198:ILE:HG22	1:G:195:ALA:HB2	2.03	0.41
1:F:75:ILE:HD12	1:F:75:ILE:HA	1.90	0.41
1:G:174:ARG:NH2	1:K:201:LEU:CD2	2.82	0.41
1:N:230:MET:HB3	1:N:234:GLU:CG	2.51	0.41
1:E:75:ILE:O	1:E:79:LEU:HD13	2.20	0.40
1:F:157:LEU:HD12	1:F:209:TYR:CE1	2.56	0.40
1:H:229:TYR:CD1	1:M:197:GLU:HG2	2.56	0.40
1:J:105:PHE:O	1:J:108:SER:HB3	2.21	0.40
1:L:132:ILE:HB	1:L:158:LEU:HD21	2.04	0.40
1:M:219:VAL:HG23	1:M:220:ILE:N	2.36	0.40
1:F:118:TYR:HD1	1:F:146:TRP:HB2	1.87	0.40
1:F:148:VAL:HG23	1:F:170:LEU:HD22	2.04	0.40
1:G:96:ALA:HA	1:G:132:ILE:HD11	2.02	0.40
1:A:204:GLN:HE22	1:F:174:ARG:HD3	1.86	0.40
1:N:231:SER:HB2	1:N:234:GLU:OE2	2.22	0.40
1:A:78:ARG:O	1:A:78:ARG:HD2	2.21	0.40
1:C:103:LEU:HD21	1:C:117:MET:HE3	2.04	0.40
1:G:62:VAL:HG21	1:G:78:ARG:HG2	2.03	0.40
1:I:147:CYS:HB2	1:I:159:LEU:HD22	2.04	0.40
1:F:106:LEU:HD23	1:F:106:LEU:HA	1.86	0.40
1:F:120:ASN:CG	1:F:149:GLY:HA3	2.47	0.40
1:K:117:MET:HE3	1:K:117:MET:HB2	1.95	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	170/223 (76%)	164 (96%)	6 (4%)	0	100	100
1	B	170/223 (76%)	162 (95%)	8 (5%)	0	100	100
1	C	171/223 (77%)	164 (96%)	7 (4%)	0	100	100
1	D	171/223 (77%)	164 (96%)	7 (4%)	0	100	100
1	E	169/223 (76%)	164 (97%)	5 (3%)	0	100	100
1	F	172/223 (77%)	166 (96%)	6 (4%)	0	100	100
1	G	170/223 (76%)	164 (96%)	6 (4%)	0	100	100
1	H	169/223 (76%)	161 (95%)	8 (5%)	0	100	100
1	I	163/223 (73%)	155 (95%)	8 (5%)	0	100	100
1	J	162/223 (73%)	155 (96%)	7 (4%)	0	100	100
1	K	166/223 (74%)	160 (96%)	5 (3%)	1 (1%)	21	51
1	L	166/223 (74%)	161 (97%)	5 (3%)	0	100	100
1	M	165/223 (74%)	154 (93%)	11 (7%)	0	100	100
1	N	163/223 (73%)	152 (93%)	11 (7%)	0	100	100
All	All	2347/3122 (75%)	2246 (96%)	100 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	150	GLN

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	150/186 (81%)	149 (99%)	1 (1%)	76	91
1	B	147/186 (79%)	146 (99%)	1 (1%)	76	91
1	C	150/186 (81%)	150 (100%)	0	100	100
1	D	151/186 (81%)	151 (100%)	0	100	100
1	E	147/186 (79%)	147 (100%)	0	100	100
1	F	151/186 (81%)	150 (99%)	1 (1%)	76	91
1	G	147/186 (79%)	147 (100%)	0	100	100
1	H	146/186 (78%)	146 (100%)	0	100	100
1	I	143/186 (77%)	143 (100%)	0	100	100
1	J	137/186 (74%)	135 (98%)	2 (2%)	57	84
1	K	143/186 (77%)	141 (99%)	2 (1%)	59	85
1	L	148/186 (80%)	146 (99%)	2 (1%)	59	85
1	M	139/186 (75%)	135 (97%)	4 (3%)	37	73
1	N	144/186 (77%)	144 (100%)	0	100	100
All	All	2043/2604 (78%)	2030 (99%)	13 (1%)	78	92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	SER
1	B	170	LEU
1	F	70	GLU
1	J	203	LYS
1	J	211	LYS
1	K	148	VAL
1	K	150	GLN
1	L	147	CYS
1	L	150	GLN
1	M	220	ILE
1	M	224	MET
1	M	244	VAL
1	M	245	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	194	GLN
1	A	204	GLN
1	A	247	HIS
1	B	102	GLN
1	C	107	GLN
1	C	168	HIS
1	C	247	HIS
1	D	137	GLN
1	E	120	ASN
1	E	204	GLN
1	E	247	HIS
1	G	120	ASN
1	G	194	GLN
1	G	207	ASN
1	H	179	GLN
1	H	194	GLN
1	H	218	GLN
1	H	236	GLN
1	I	107	GLN
1	I	137	GLN
1	I	179	GLN
1	J	179	GLN
1	J	215	GLN
1	K	179	GLN
1	K	194	GLN
1	L	141	ASN
1	L	150	GLN
1	L	194	GLN
1	M	137	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

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	9I3	A	301	-	35,35,35	3.32	7 (20%)	43,50,50	1.32	8 (18%)
2	9I3	B	301	-	35,35,35	3.28	8 (22%)	43,50,50	1.35	9 (20%)
2	9I3	H	301	-	35,35,35	3.29	8 (22%)	43,50,50	1.46	10 (23%)
2	9I3	L	301	-	35,35,35	3.26	8 (22%)	43,50,50	1.56	11 (25%)
2	9I3	G	301	-	35,35,35	3.32	8 (22%)	43,50,50	1.35	9 (20%)
2	9I3	K	301	-	35,35,35	3.28	7 (20%)	43,50,50	1.35	9 (20%)
2	9I3	C	301	-	35,35,35	3.29	7 (20%)	43,50,50	1.33	8 (18%)
2	9I3	E	302	-	35,35,35	3.34	8 (22%)	43,50,50	1.30	9 (20%)
2	9I3	E	301	-	35,35,35	3.33	7 (20%)	43,50,50	1.34	9 (20%)
2	9I3	F	301	-	35,35,35	3.31	8 (22%)	43,50,50	1.33	8 (18%)
2	9I3	D	301	-	35,35,35	3.28	7 (20%)	43,50,50	1.40	10 (23%)
2	9I3	M	301	-	35,35,35	3.33	7 (20%)	43,50,50	1.29	7 (16%)
2	9I3	I	301	-	35,35,35	3.29	8 (22%)	43,50,50	1.35	9 (20%)
2	9I3	N	301	-	35,35,35	3.32	8 (22%)	43,50,50	1.37	10 (23%)

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	9I3	A	301	-	-	0/8/17/17	0/5/5/5
2	9I3	B	301	-	-	0/8/17/17	0/5/5/5
2	9I3	H	301	-	-	2/8/17/17	0/5/5/5
2	9I3	L	301	-	-	0/8/17/17	0/5/5/5
2	9I3	G	301	-	-	1/8/17/17	0/5/5/5
2	9I3	K	301	-	-	0/8/17/17	0/5/5/5
2	9I3	C	301	-	-	0/8/17/17	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9I3	E	302	-	-	0/8/17/17	0/5/5/5
2	9I3	E	301	-	-	0/8/17/17	0/5/5/5
2	9I3	F	301	-	-	0/8/17/17	0/5/5/5
2	9I3	D	301	-	-	0/8/17/17	0/5/5/5
2	9I3	M	301	-	-	2/8/17/17	0/5/5/5
2	9I3	I	301	-	-	0/8/17/17	0/5/5/5
2	9I3	N	301	-	-	2/8/17/17	0/5/5/5

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	301	9I3	C13-N08	-14.07	1.34	1.46
2	E	301	9I3	C13-N08	-14.05	1.34	1.46
2	E	302	9I3	C13-N08	-14.01	1.34	1.46
2	G	301	9I3	C13-N08	-13.88	1.34	1.46
2	N	301	9I3	C13-N08	-13.86	1.34	1.46
2	F	301	9I3	C13-N08	-13.86	1.34	1.46
2	A	301	9I3	C13-N08	-13.82	1.34	1.46
2	I	301	9I3	C13-N08	-13.78	1.34	1.46
2	H	301	9I3	C13-N08	-13.71	1.34	1.46
2	C	301	9I3	C13-N08	-13.68	1.34	1.46
2	K	301	9I3	C13-N08	-13.63	1.34	1.46
2	B	301	9I3	C13-N08	-13.63	1.34	1.46
2	D	301	9I3	C13-N08	-13.58	1.34	1.46
2	L	301	9I3	C13-N08	-13.38	1.34	1.46
2	F	301	9I3	C07-N08	-9.23	1.29	1.47
2	M	301	9I3	C07-N08	-9.22	1.29	1.47
2	A	301	9I3	C07-N08	-9.19	1.30	1.47
2	N	301	9I3	C07-N08	-9.19	1.30	1.47
2	D	301	9I3	C07-N08	-9.15	1.30	1.47
2	E	302	9I3	C07-N08	-9.15	1.30	1.47
2	K	301	9I3	C07-N08	-9.14	1.30	1.47
2	G	301	9I3	C07-N08	-9.14	1.30	1.47
2	E	301	9I3	C07-N08	-9.08	1.30	1.47
2	C	301	9I3	C07-N08	-9.08	1.30	1.47
2	H	301	9I3	C07-N08	-9.07	1.30	1.47
2	B	301	9I3	C07-N08	-9.04	1.30	1.47
2	I	301	9I3	C07-N08	-8.99	1.30	1.47
2	L	301	9I3	C07-N08	-8.91	1.30	1.47
2	L	301	9I3	C15-C11	-5.80	1.36	1.46
2	A	301	9I3	C15-C11	-5.69	1.36	1.46
2	C	301	9I3	C15-C11	-5.65	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	9I3	C15-C11	-5.62	1.36	1.46
2	G	301	9I3	C15-C11	-5.60	1.36	1.46
2	I	301	9I3	C15-C11	-5.59	1.36	1.46
2	B	301	9I3	C15-C11	-5.58	1.36	1.46
2	F	301	9I3	C15-C11	-5.58	1.36	1.46
2	E	302	9I3	C15-C11	-5.57	1.36	1.46
2	K	301	9I3	C15-C11	-5.55	1.36	1.46
2	H	301	9I3	C15-C11	-5.55	1.36	1.46
2	M	301	9I3	C15-C11	-5.54	1.36	1.46
2	N	301	9I3	C15-C11	-5.50	1.37	1.46
2	E	301	9I3	C15-C11	-5.50	1.37	1.46
2	A	301	9I3	C09-N08	-4.77	1.34	1.46
2	K	301	9I3	C09-N08	-4.70	1.34	1.46
2	C	301	9I3	C09-N08	-4.69	1.34	1.46
2	I	301	9I3	C09-N08	-4.68	1.34	1.46
2	F	301	9I3	C09-N08	-4.66	1.34	1.46
2	D	301	9I3	C09-N08	-4.66	1.34	1.46
2	E	302	9I3	C09-N08	-4.65	1.34	1.46
2	M	301	9I3	C09-N08	-4.65	1.34	1.46
2	B	301	9I3	C09-N08	-4.63	1.34	1.46
2	E	301	9I3	C09-N08	-4.63	1.34	1.46
2	L	301	9I3	C09-N08	-4.62	1.34	1.46
2	N	301	9I3	C09-N08	-4.62	1.34	1.46
2	G	301	9I3	C09-N08	-4.62	1.34	1.46
2	H	301	9I3	C09-N08	-4.58	1.34	1.46
2	E	301	9I3	C16-N17	-3.57	1.33	1.39
2	D	301	9I3	C16-N17	-3.56	1.33	1.39
2	K	301	9I3	C16-N17	-3.51	1.34	1.39
2	A	301	9I3	C16-N17	-3.48	1.34	1.39
2	N	301	9I3	C16-N17	-3.48	1.34	1.39
2	B	301	9I3	C16-N17	-3.47	1.34	1.39
2	M	301	9I3	C16-N17	-3.47	1.34	1.39
2	E	302	9I3	C16-N17	-3.43	1.34	1.39
2	H	301	9I3	C16-N17	-3.43	1.34	1.39
2	G	301	9I3	C16-N17	-3.41	1.34	1.39
2	L	301	9I3	C16-N17	-3.39	1.34	1.39
2	C	301	9I3	C16-N17	-3.36	1.34	1.39
2	F	301	9I3	C16-N17	-3.33	1.34	1.39
2	I	301	9I3	C16-N17	-3.26	1.34	1.39
2	G	301	9I3	C19-C15	-2.60	1.36	1.39
2	A	301	9I3	C19-C15	-2.57	1.36	1.39
2	M	301	9I3	C19-C15	-2.57	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	301	9I3	C19-C15	-2.53	1.36	1.39
2	L	301	9I3	C19-C15	-2.53	1.36	1.39
2	C	301	9I3	C19-C15	-2.52	1.36	1.39
2	F	301	9I3	C19-C15	-2.52	1.36	1.39
2	I	301	9I3	C19-C15	-2.51	1.36	1.39
2	N	301	9I3	C19-C15	-2.50	1.36	1.39
2	B	301	9I3	C19-C15	-2.50	1.36	1.39
2	H	301	9I3	C19-C15	-2.50	1.36	1.39
2	E	302	9I3	C19-C15	-2.48	1.36	1.39
2	E	301	9I3	C19-C15	-2.44	1.36	1.39
2	I	301	9I3	C12-C11	-2.43	1.32	1.36
2	D	301	9I3	C19-C15	-2.42	1.36	1.39
2	E	302	9I3	C12-C11	-2.42	1.32	1.36
2	N	301	9I3	C12-C11	-2.42	1.32	1.36
2	B	301	9I3	C12-C11	-2.39	1.33	1.36
2	L	301	9I3	C12-C11	-2.34	1.33	1.36
2	A	301	9I3	C12-C11	-2.34	1.33	1.36
2	H	301	9I3	C12-C11	-2.32	1.33	1.36
2	G	301	9I3	C12-C11	-2.32	1.33	1.36
2	M	301	9I3	C12-C11	-2.30	1.33	1.36
2	C	301	9I3	C12-C11	-2.30	1.33	1.36
2	D	301	9I3	C12-C11	-2.30	1.33	1.36
2	E	301	9I3	C12-C11	-2.29	1.33	1.36
2	F	301	9I3	C12-C11	-2.29	1.33	1.36
2	K	301	9I3	C12-C11	-2.24	1.33	1.36
2	N	301	9I3	O23-C18	-2.17	1.18	1.23
2	H	301	9I3	O23-C18	-2.03	1.18	1.23
2	L	301	9I3	C01-CL1	2.03	1.79	1.74
2	I	301	9I3	O23-C18	-2.02	1.18	1.23
2	G	301	9I3	O23-C18	-2.02	1.19	1.23
2	F	301	9I3	O23-C18	-2.01	1.19	1.23
2	B	301	9I3	O23-C18	-2.01	1.19	1.23
2	E	302	9I3	O23-C18	-2.01	1.19	1.23

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	301	9I3	C24-N17-C18	3.47	120.42	116.72
2	D	301	9I3	C24-N17-C18	3.41	120.36	116.72
2	A	301	9I3	C24-N17-C18	3.34	120.28	116.72
2	K	301	9I3	C24-N17-C18	3.33	120.26	116.72
2	B	301	9I3	C24-N17-C18	3.32	120.25	116.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	301	9I3	C07-N08-C09	-3.29	103.98	111.07
2	H	301	9I3	C24-N17-C18	3.09	120.02	116.72
2	L	301	9I3	C19-C15-C16	2.97	120.15	117.23
2	L	301	9I3	C24-N17-C18	2.96	119.87	116.72
2	C	301	9I3	C24-N17-C18	2.95	119.87	116.72
2	G	301	9I3	C24-N17-C18	2.91	119.82	116.72
2	N	301	9I3	C12-C18-N17	2.90	120.73	115.17
2	L	301	9I3	C18-C12-C11	-2.89	118.94	121.92
2	D	301	9I3	C07-N08-C09	-2.87	104.89	111.07
2	E	302	9I3	C24-N17-C18	2.86	119.77	116.72
2	F	301	9I3	O23-C18-C12	-2.77	119.80	125.06
2	A	301	9I3	C19-C15-C16	2.75	119.94	117.23
2	C	301	9I3	C12-C18-N17	2.75	120.44	115.17
2	H	301	9I3	C12-C18-N17	2.74	120.44	115.17
2	I	301	9I3	C12-C18-N17	2.74	120.43	115.17
2	F	301	9I3	C12-C18-N17	2.74	120.43	115.17
2	D	301	9I3	O23-C18-C12	-2.74	119.86	125.06
2	F	301	9I3	C24-N17-C18	2.73	119.63	116.72
2	I	301	9I3	O23-C18-C12	-2.73	119.87	125.06
2	G	301	9I3	C12-C18-N17	2.72	120.40	115.17
2	G	301	9I3	O23-C18-C12	-2.72	119.89	125.06
2	B	301	9I3	C12-C18-N17	2.72	120.39	115.17
2	C	301	9I3	O23-C18-C12	-2.72	119.89	125.06
2	L	301	9I3	C12-C18-N17	2.71	120.38	115.17
2	K	301	9I3	C12-C18-N17	2.71	120.38	115.17
2	H	301	9I3	O23-C18-C12	-2.70	119.92	125.06
2	D	301	9I3	C12-C18-N17	2.69	120.33	115.17
2	I	301	9I3	C19-C15-C16	2.68	119.87	117.23
2	H	301	9I3	C07-N08-C09	-2.68	105.29	111.07
2	M	301	9I3	O23-C18-C12	-2.68	119.97	125.06
2	K	301	9I3	O23-C18-C12	-2.67	119.98	125.06
2	B	301	9I3	O23-C18-C12	-2.66	120.00	125.06
2	H	301	9I3	C10-C09-N08	2.66	113.56	111.19
2	N	301	9I3	C24-N17-C18	2.65	119.54	116.72
2	L	301	9I3	C25-C24-N17	-2.65	109.15	113.46
2	L	301	9I3	C06-C01-CL1	2.65	122.49	119.17
2	A	301	9I3	O23-C18-C12	-2.64	120.04	125.06
2	E	302	9I3	O23-C18-C12	-2.63	120.06	125.06
2	N	301	9I3	O23-C18-C12	-2.62	120.08	125.06
2	M	301	9I3	C12-C18-N17	2.62	120.20	115.17
2	B	301	9I3	C07-N08-C09	-2.61	105.45	111.07
2	L	301	9I3	O23-C18-C12	-2.61	120.11	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	9I3	O23-C18-C12	-2.60	120.12	125.06
2	E	301	9I3	C10-C11-C15	2.59	120.66	118.13
2	I	301	9I3	C24-N17-C18	2.59	119.48	116.72
2	E	302	9I3	C12-C18-N17	2.59	120.14	115.17
2	A	301	9I3	C12-C18-N17	2.58	120.13	115.17
2	C	301	9I3	C19-C15-C16	2.56	119.75	117.23
2	H	301	9I3	C18-C12-C11	-2.56	119.27	121.92
2	E	302	9I3	C19-C15-C16	2.54	119.73	117.23
2	K	301	9I3	C18-C12-C11	-2.53	119.30	121.92
2	E	301	9I3	C12-C18-N17	2.53	120.03	115.17
2	F	301	9I3	C19-C15-C16	2.51	119.70	117.23
2	C	301	9I3	C18-C12-C11	-2.51	119.33	121.92
2	D	301	9I3	C18-C12-C11	-2.48	119.35	121.92
2	F	301	9I3	C10-C11-C15	2.48	120.55	118.13
2	B	301	9I3	C18-C12-C11	-2.47	119.36	121.92
2	I	301	9I3	C07-N08-C09	-2.47	105.76	111.07
2	N	301	9I3	C18-C12-C11	-2.47	119.37	121.92
2	M	301	9I3	C19-C15-C16	2.44	119.63	117.23
2	G	301	9I3	C18-C12-C11	-2.44	119.40	121.92
2	D	301	9I3	C19-C15-C16	2.44	119.63	117.23
2	M	301	9I3	C10-C11-C15	2.41	120.48	118.13
2	H	301	9I3	C19-C15-C16	2.41	119.60	117.23
2	A	301	9I3	C18-C12-C11	-2.40	119.44	121.92
2	N	301	9I3	C10-C11-C15	2.40	120.47	118.13
2	C	301	9I3	C07-N08-C09	-2.39	105.92	111.07
2	F	301	9I3	C18-C12-C11	-2.39	119.45	121.92
2	B	301	9I3	C19-C15-C16	2.38	119.58	117.23
2	K	301	9I3	C19-C15-C16	2.35	119.55	117.23
2	I	301	9I3	C18-C12-C11	-2.34	119.50	121.92
2	G	301	9I3	C20-C21-N22	-2.32	119.75	123.42
2	G	301	9I3	C07-N08-C09	-2.32	106.08	111.07
2	N	301	9I3	C19-C15-C16	2.31	119.51	117.23
2	E	301	9I3	C19-C15-C16	2.31	119.50	117.23
2	C	301	9I3	C21-N22-C16	2.30	120.25	115.05
2	N	301	9I3	C10-C09-N08	2.29	113.23	111.19
2	E	301	9I3	C24-N17-C18	2.29	119.16	116.72
2	K	301	9I3	C21-N22-C16	2.29	120.23	115.05
2	I	301	9I3	C21-N22-C16	2.29	120.23	115.05
2	G	301	9I3	C19-C15-C16	2.29	119.48	117.23
2	G	301	9I3	C21-N22-C16	2.29	120.23	115.05
2	K	301	9I3	C20-C21-N22	-2.29	119.80	123.42
2	E	301	9I3	C18-C12-C11	-2.28	119.56	121.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	9I3	C20-C21-N22	-2.28	119.81	123.42
2	F	301	9I3	C21-N22-C16	2.28	120.20	115.05
2	H	301	9I3	C21-N22-C16	2.28	120.20	115.05
2	K	301	9I3	C10-C11-C15	2.28	120.35	118.13
2	D	301	9I3	C20-C21-N22	-2.28	119.82	123.42
2	G	301	9I3	C10-C11-C15	2.27	120.34	118.13
2	D	301	9I3	C21-N22-C16	2.25	120.15	115.05
2	N	301	9I3	C07-N08-C09	-2.25	106.22	111.07
2	M	301	9I3	C20-C21-N22	-2.25	119.85	123.42
2	A	301	9I3	C21-N22-C16	2.25	120.14	115.05
2	N	301	9I3	C20-C21-N22	-2.23	119.89	123.42
2	D	301	9I3	C10-C09-N08	2.23	113.17	111.19
2	N	301	9I3	C21-N22-C16	2.22	120.08	115.05
2	M	301	9I3	C21-N22-C16	2.22	120.08	115.05
2	C	301	9I3	C20-C21-N22	-2.22	119.90	123.42
2	I	301	9I3	C10-C11-C15	2.22	120.30	118.13
2	E	301	9I3	C21-N22-C16	2.22	120.07	115.05
2	F	301	9I3	C20-C21-N22	-2.22	119.91	123.42
2	H	301	9I3	C20-C21-N22	-2.22	119.91	123.42
2	B	301	9I3	C21-N22-C16	2.22	120.06	115.05
2	H	301	9I3	C10-C11-C15	2.21	120.29	118.13
2	E	302	9I3	C21-N22-C16	2.21	120.05	115.05
2	B	301	9I3	C20-C21-N22	-2.20	119.94	123.42
2	E	302	9I3	C10-C11-C15	2.19	120.27	118.13
2	I	301	9I3	C20-C21-N22	-2.18	119.97	123.42
2	E	302	9I3	C18-C12-C11	-2.17	119.67	121.92
2	L	301	9I3	C21-N22-C16	2.16	119.93	115.05
2	A	301	9I3	C20-C21-N22	-2.15	120.01	123.42
2	L	301	9I3	C05-C07-N08	2.15	117.56	113.15
2	K	301	9I3	C25-C24-N17	-2.15	109.97	113.46
2	E	302	9I3	C20-C21-N22	-2.14	120.03	123.42
2	A	301	9I3	C07-N08-C09	-2.12	106.51	111.07
2	B	301	9I3	C10-C11-C15	2.12	120.19	118.13
2	D	301	9I3	C10-C11-C15	2.06	120.14	118.13
2	E	301	9I3	C07-N08-C09	-2.05	106.65	111.07
2	L	301	9I3	C19-C15-C11	-2.05	119.88	123.22
2	E	302	9I3	C07-N08-C09	-2.01	106.75	111.07

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	301	9I3	C05-C07-N08-C09
2	M	301	9I3	C05-C07-N08-C13
2	N	301	9I3	C05-C07-N08-C13
2	H	301	9I3	C05-C07-N08-C13
2	N	301	9I3	C05-C07-N08-C09
2	H	301	9I3	C05-C07-N08-C09
2	G	301	9I3	C05-C07-N08-C13

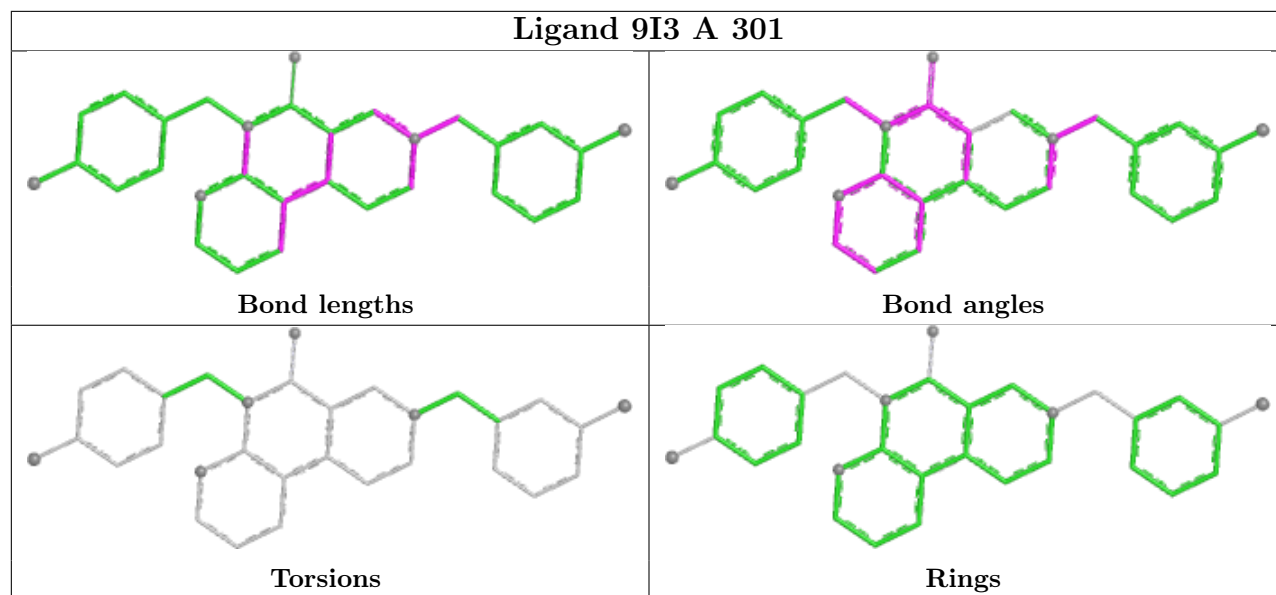
There are no ring outliers.

8 monomers are involved in 10 short contacts:

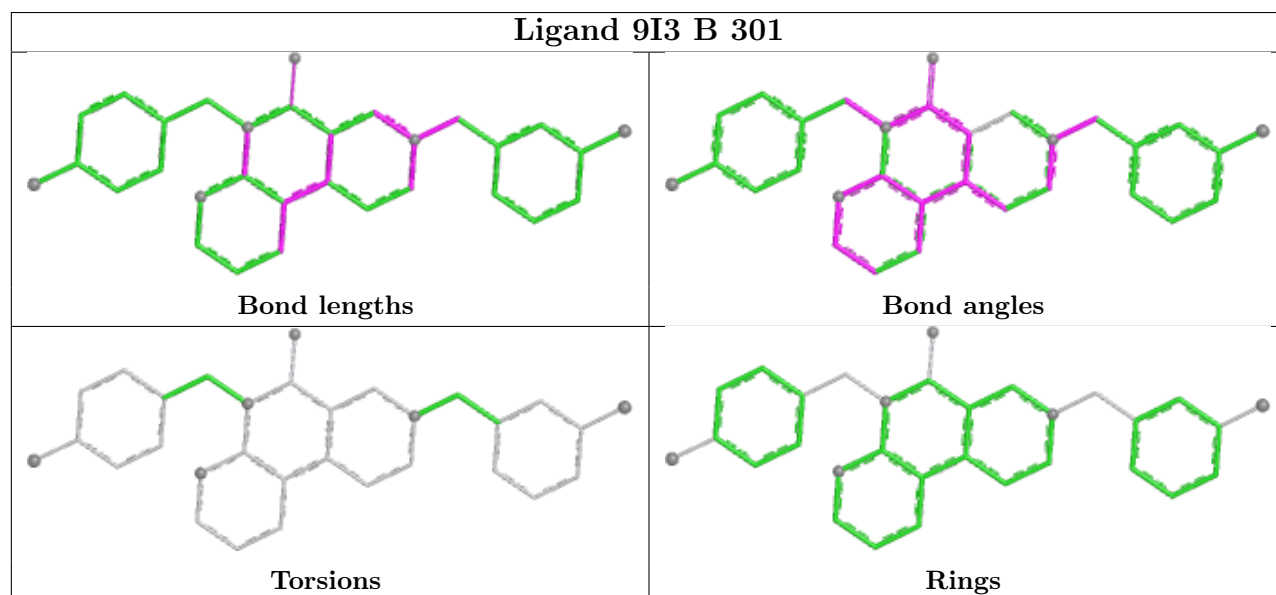
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	9I3	1	0
2	H	301	9I3	1	0
2	L	301	9I3	3	0
2	G	301	9I3	1	0
2	K	301	9I3	1	0
2	E	301	9I3	1	0
2	D	301	9I3	1	0
2	N	301	9I3	1	0

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.

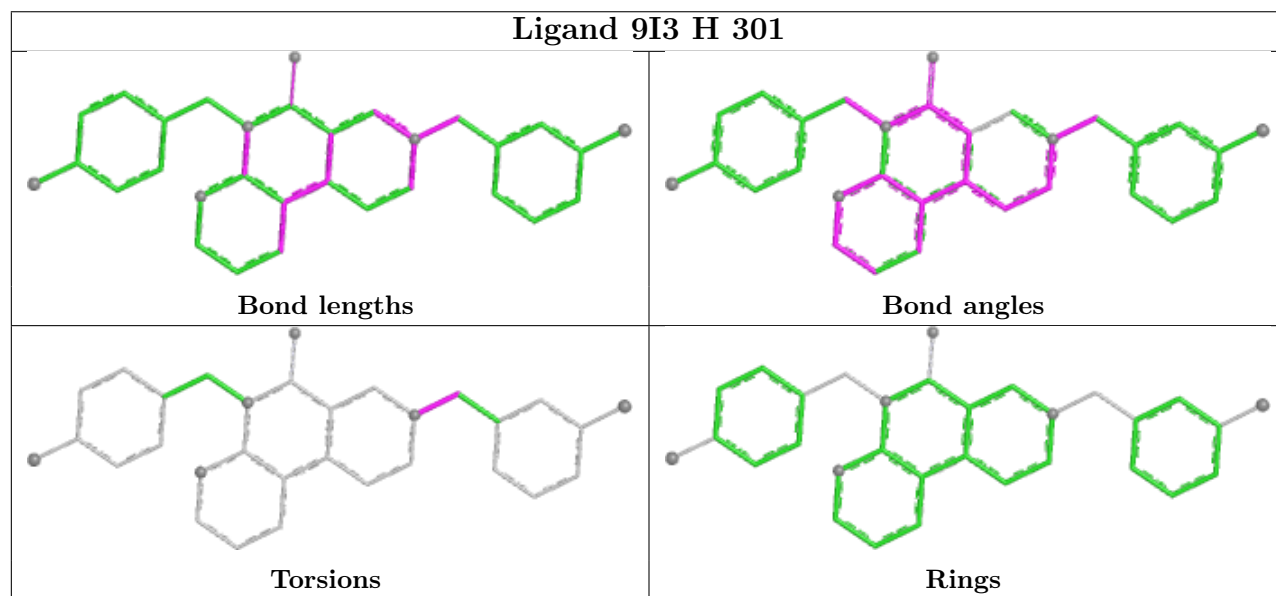
Ligand 9I3 A 301



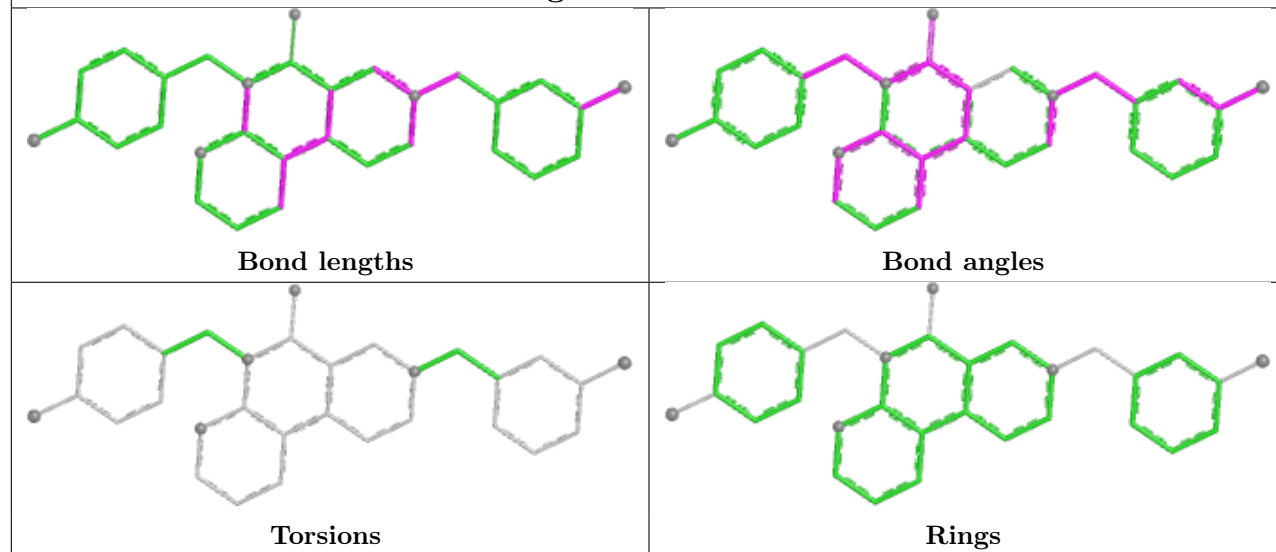
Ligand 9I3 B 301



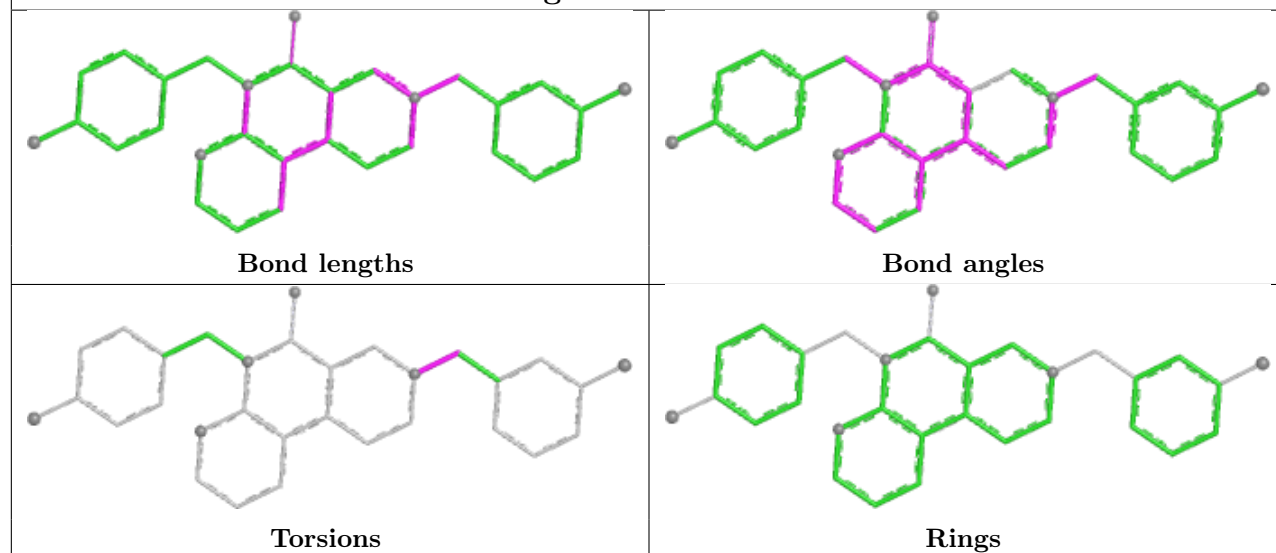
Ligand 9I3 H 301



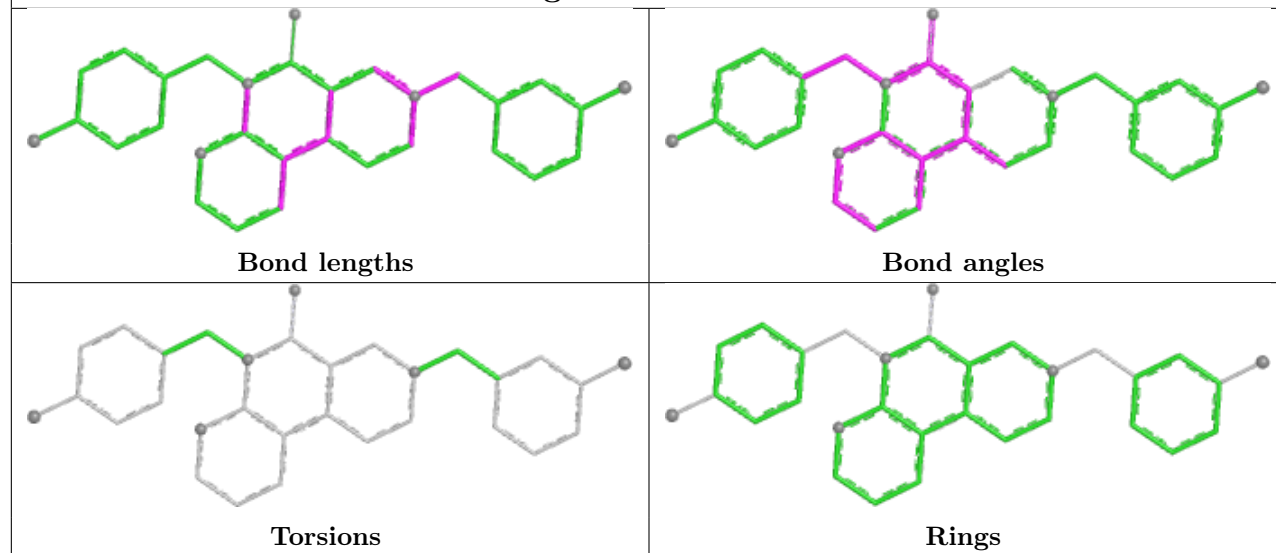
Ligand 9I3 L 301



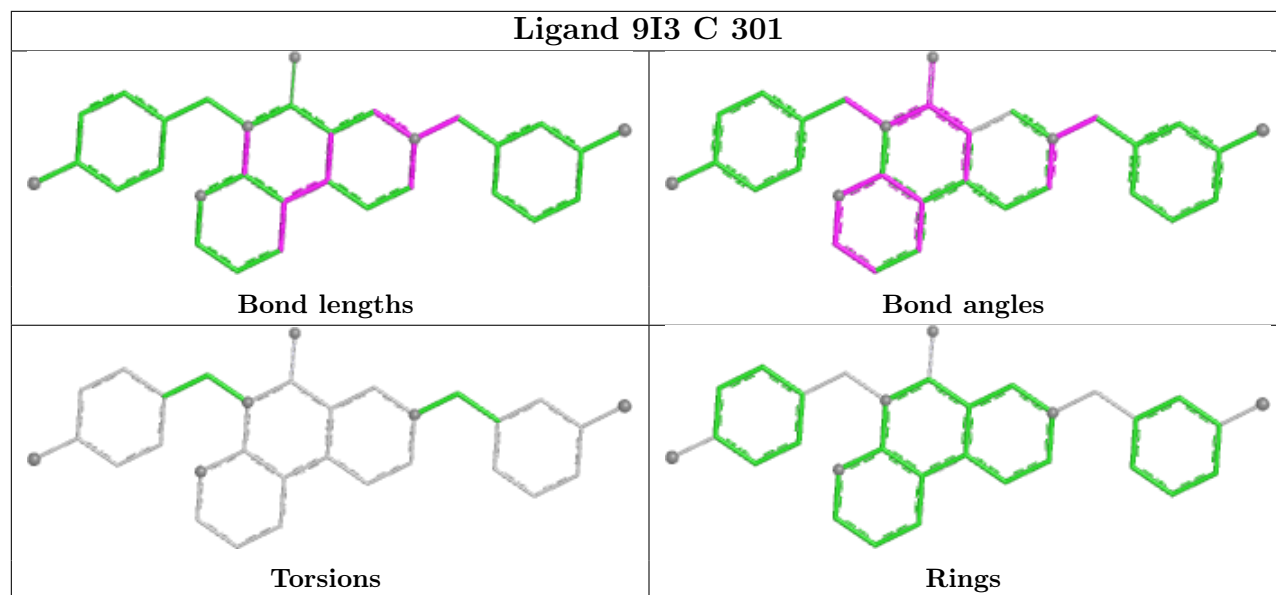
Ligand 9I3 G 301



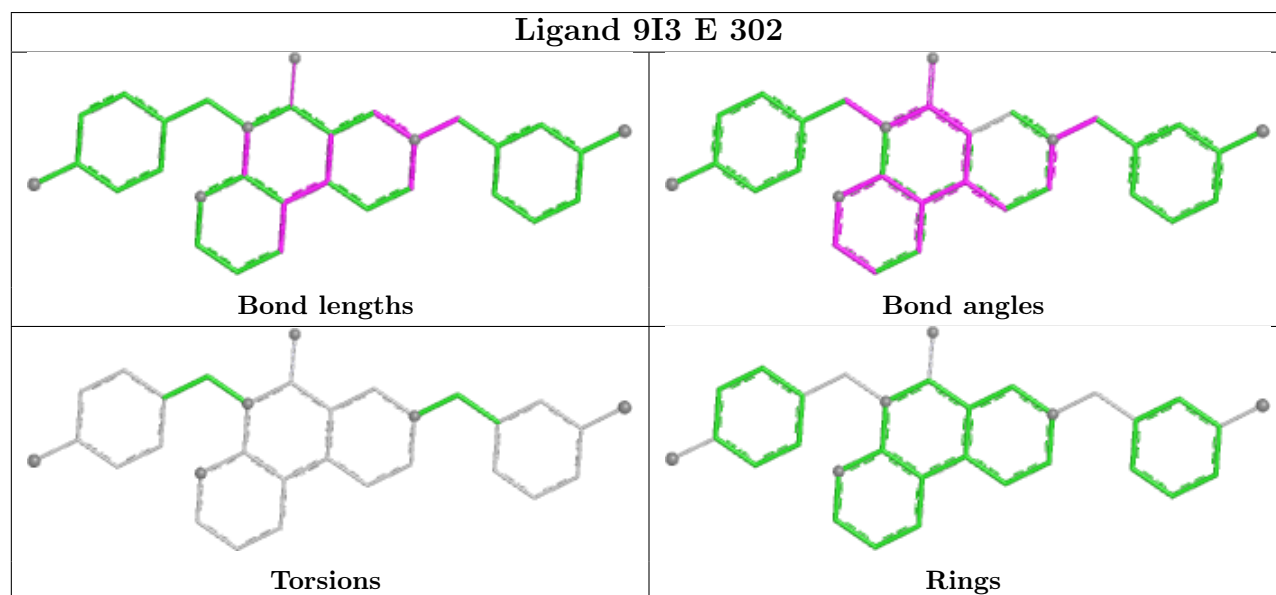
Ligand 9I3 K 301



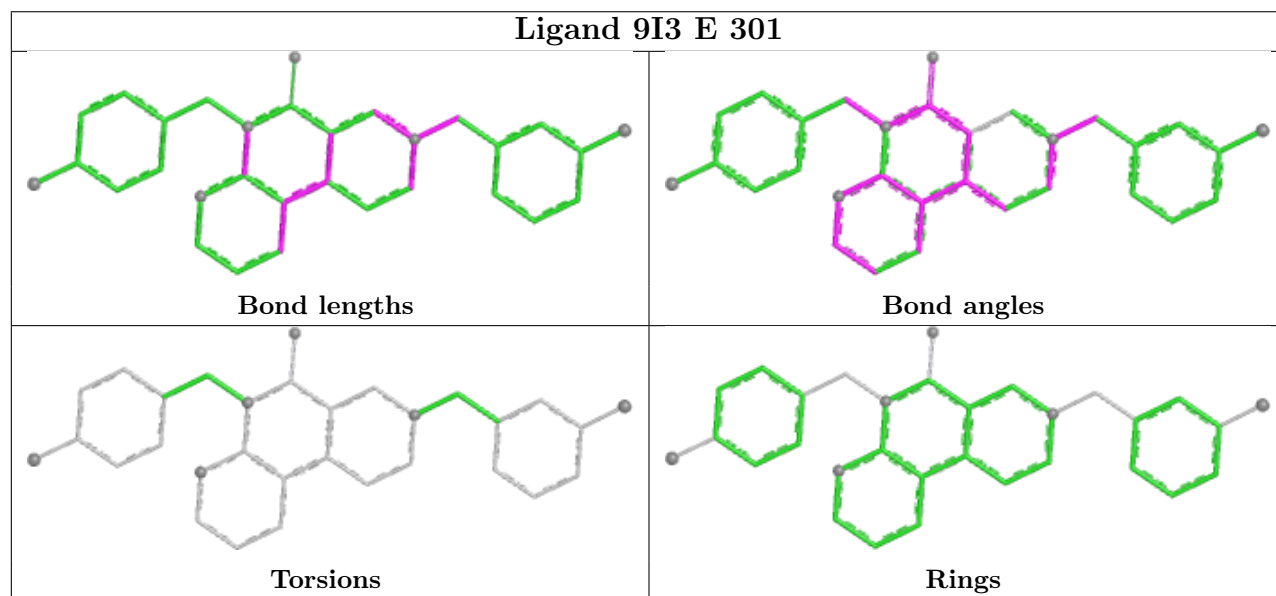
Ligand 9I3 C 301



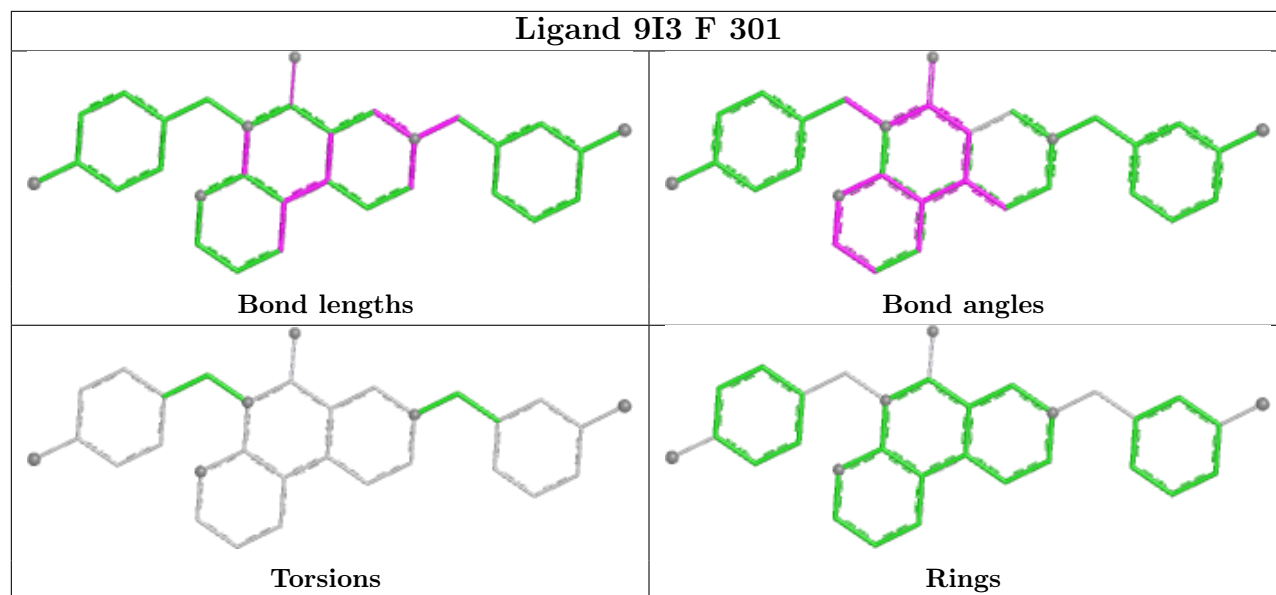
Ligand 9I3 E 302



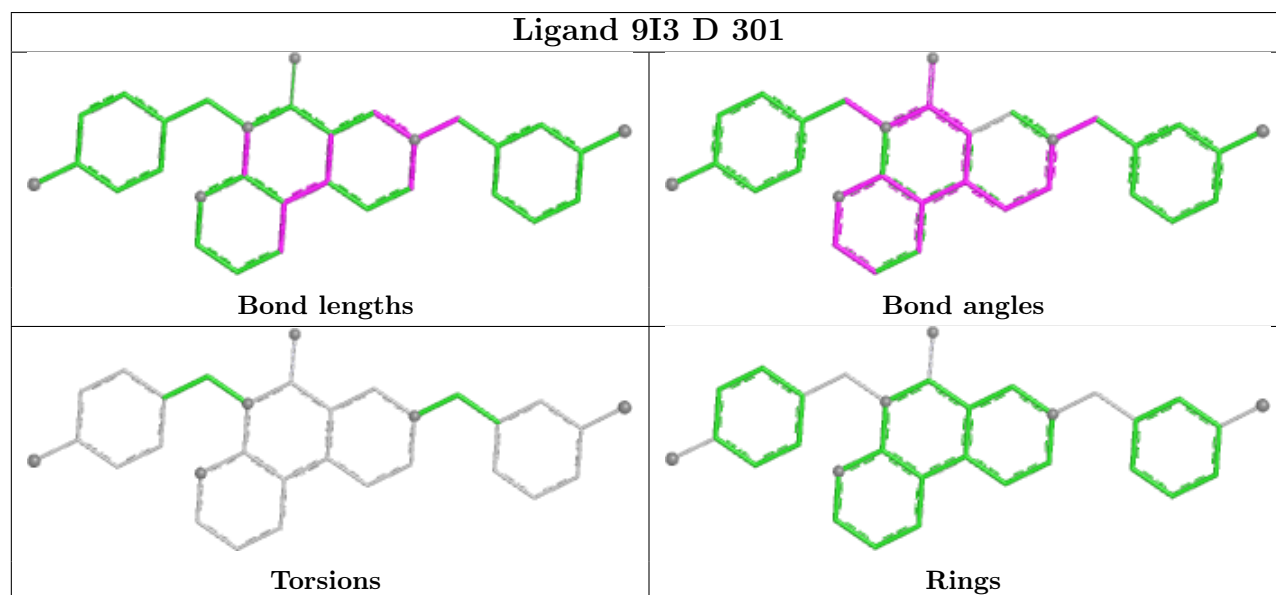
Ligand 9I3 E 301



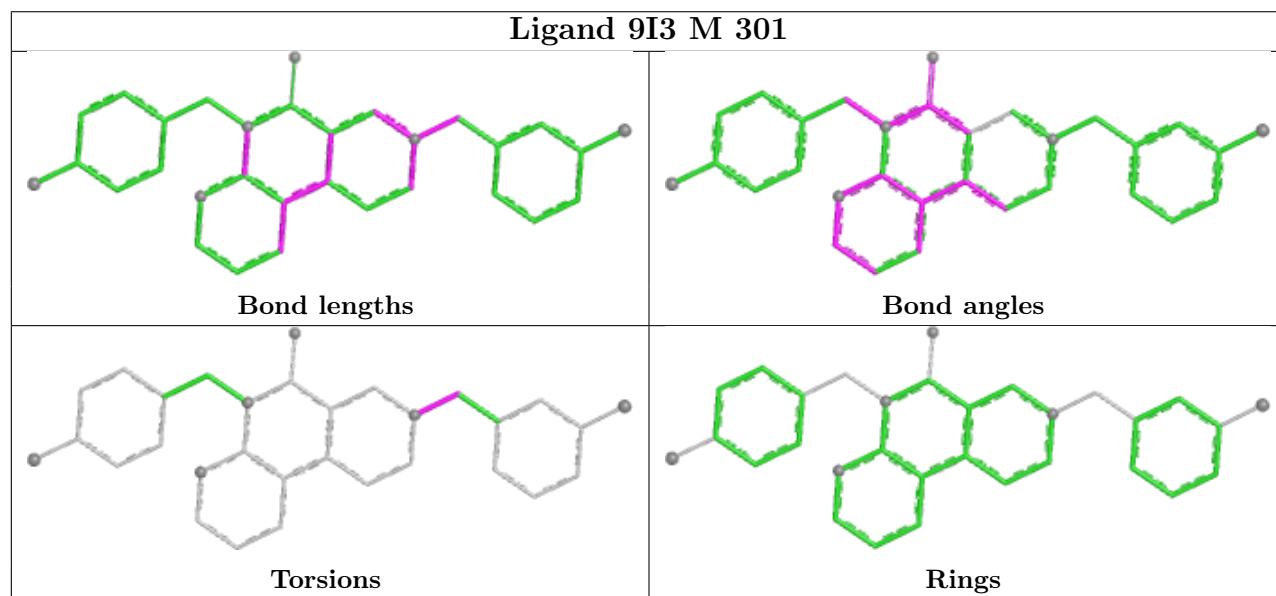
Ligand 9I3 F 301

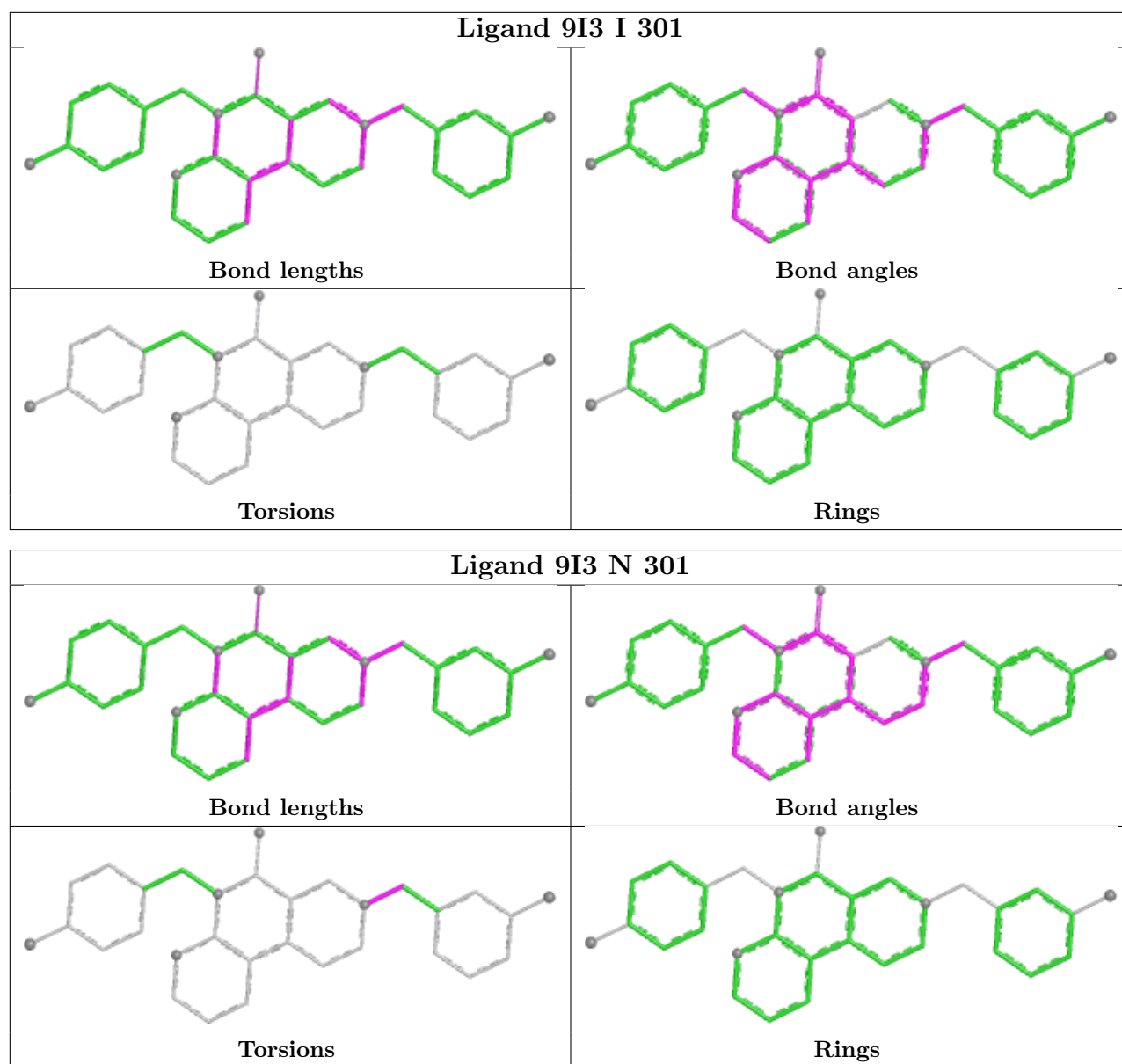


Ligand 9I3 D 301



Ligand 9I3 M 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(Å²)	Q<0.9
1	A	175/223 (78%)	0.72	9 (5%) 33 25	23, 51, 81, 107	1 (0%)
1	B	176/223 (78%)	0.60	10 (5%) 29 22	32, 53, 90, 130	0
1	C	175/223 (78%)	0.73	14 (8%) 18 13	26, 52, 88, 122	2 (1%)
1	D	176/223 (78%)	1.01	20 (11%) 10 7	28, 55, 83, 102	1 (0%)
1	E	174/223 (78%)	0.83	15 (8%) 16 12	26, 55, 85, 113	1 (0%)
1	F	177/223 (79%)	1.20	23 (12%) 7 6	30, 56, 87, 129	1 (0%)
1	G	176/223 (78%)	0.86	18 (10%) 12 9	35, 58, 90, 116	0
1	H	175/223 (78%)	1.42	35 (20%) 3 2	37, 61, 92, 119	0
1	I	169/223 (75%)	1.47	44 (26%) 1 1	41, 63, 86, 104	0
1	J	168/223 (75%)	1.00	20 (11%) 9 7	40, 63, 92, 126	0
1	K	172/223 (77%)	1.28	27 (15%) 5 4	44, 69, 95, 142	0
1	L	172/223 (77%)	1.14	16 (9%) 14 10	43, 68, 95, 121	0
1	M	170/223 (76%)	1.55	51 (30%) 1 1	38, 71, 101, 137	1 (0%)
1	N	171/223 (76%)	1.52	41 (23%) 2 1	44, 72, 104, 160	0
All	All	2426/3122 (77%)	1.09	343 (14%) 6 5	23, 60, 92, 160	7 (0%)

All (343) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	149	GLY	7.0
1	K	149	GLY	6.8
1	B	173	SER	6.4
1	H	151	ALA	6.4
1	I	63	VAL	5.2
1	B	172	ASN	5.2
1	I	100	ILE	4.9
1	N	244	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	H	149	GLY	4.8
1	D	86	CYS	4.6
1	K	148	VAL	4.5
1	J	86	CYS	4.2
1	F	65	GLN	4.0
1	K	241	LEU	4.0
1	J	63	VAL	3.9
1	H	150	GLN	3.9
1	M	103	LEU	3.8
1	H	241	LEU	3.8
1	J	180	PRO	3.8
1	H	231	SER	3.7
1	D	84	ILE	3.7
1	J	87	VAL	3.7
1	L	245	LEU	3.6
1	N	216	SER	3.6
1	I	173	SER	3.6
1	M	211	LYS	3.6
1	N	162	GLY	3.6
1	G	225	GLU	3.6
1	F	148	VAL	3.6
1	M	229	TYR	3.6
1	C	144	CYS	3.6
1	N	230	MET	3.6
1	B	247	HIS	3.5
1	C	247	HIS	3.5
1	N	169	SER	3.5
1	N	89	GLY	3.5
1	N	63	VAL	3.5
1	J	231	SER	3.5
1	M	226	ARG	3.5
1	K	156	SER	3.5
1	M	227	ASP	3.4
1	J	88	MET	3.4
1	I	225	GLU	3.4
1	F	215	GLN	3.4
1	K	162	GLY	3.3
1	H	126	VAL	3.3
1	M	86	CYS	3.3
1	F	201	LEU	3.3
1	M	63	VAL	3.3
1	N	117	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	63	VAL	3.2
1	L	244	VAL	3.2
1	H	248	PRO	3.2
1	M	177	ILE	3.2
1	L	63	VAL	3.2
1	H	75	ILE	3.2
1	M	151	ALA	3.2
1	D	87	VAL	3.1
1	G	148	VAL	3.1
1	L	230	MET	3.1
1	K	144	CYS	3.1
1	G	174	ARG	3.1
1	H	58	LEU	3.1
1	M	213	THR	3.1
1	F	217	LEU	3.1
1	E	76	TYR	3.0
1	L	177	ILE	3.0
1	A	233	MET	3.0
1	N	175	ILE	3.0
1	F	221	GLU	3.0
1	N	237	GLU	3.0
1	D	247	HIS	3.0
1	J	117	MET	3.0
1	J	246	VAL	3.0
1	F	214	LYS	3.0
1	L	240	ILE	3.0
1	M	153[A]	SER	3.0
1	M	163	THR	3.0
1	A	193	ILE	3.0
1	K	195	ALA	3.0
1	J	62	VAL	3.0
1	M	60	PRO	2.9
1	N	248	PRO	2.9
1	M	246	VAL	2.9
1	N	245	LEU	2.9
1	E	233[A]	MET	2.9
1	C	105	PHE	2.9
1	K	246	VAL	2.9
1	H	73	TYR	2.9
1	M	96	ALA	2.9
1	M	100	ILE	2.9
1	I	241	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	233	MET	2.9
1	M	87	VAL	2.9
1	A	108	SER	2.9
1	F	174	ARG	2.9
1	H	239	GLY	2.8
1	H	179	GLN	2.8
1	H	113	LYS	2.8
1	F	161	ALA	2.8
1	I	58	LEU	2.8
1	I	149	GLY	2.8
1	K	209	TYR	2.8
1	L	209	TYR	2.8
1	D	245	LEU	2.8
1	F	213	THR	2.8
1	D	65	GLN	2.8
1	N	196	GLU	2.8
1	H	229	TYR	2.8
1	G	191	ILE	2.7
1	D	197	GLU	2.7
1	D	62	VAL	2.7
1	M	210	ALA	2.7
1	G	75	ILE	2.7
1	K	177	ILE	2.7
1	J	229	TYR	2.7
1	M	233	MET	2.7
1	M	248	PRO	2.7
1	H	233	MET	2.7
1	J	76	TYR	2.7
1	F	173	SER	2.7
1	I	121	SER	2.7
1	N	247	HIS	2.7
1	A	144	CYS	2.7
1	H	144	CYS	2.7
1	I	74	ASP	2.7
1	I	244	VAL	2.7
1	M	237	GLU	2.7
1	J	140	LEU	2.7
1	K	58	LEU	2.7
1	K	160	ALA	2.6
1	M	180	PRO	2.6
1	I	96	ALA	2.6
1	M	195	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	153	SER	2.6
1	M	89	GLY	2.6
1	I	144	CYS	2.6
1	H	104	LEU	2.6
1	H	218	GLN	2.6
1	M	152	ALA	2.6
1	N	74	ASP	2.6
1	M	149	GLY	2.6
1	C	58	LEU	2.6
1	C	245	LEU	2.6
1	F	245	LEU	2.5
1	F	70	GLU	2.5
1	H	180	PRO	2.5
1	L	118	TYR	2.5
1	E	111	ASN	2.5
1	N	103	LEU	2.5
1	N	166	MET	2.5
1	H	234	GLU	2.5
1	I	102	GLN	2.5
1	I	212	HIS	2.5
1	K	74	ASP	2.5
1	D	148	VAL	2.5
1	D	246	VAL	2.5
1	C	73	TYR	2.5
1	G	218	GLN	2.5
1	I	194	GLN	2.5
1	I	113	LYS	2.5
1	E	199	MET	2.4
1	J	245	LEU	2.4
1	L	154	MET	2.4
1	I	115	ILE	2.4
1	K	198	ILE	2.4
1	I	219	VAL	2.4
1	E	194	GLN	2.4
1	G	76	TYR	2.4
1	H	118	TYR	2.4
1	F	103	LEU	2.4
1	G	233	MET	2.4
1	H	157	LEU	2.4
1	M	159	LEU	2.4
1	D	60	PRO	2.4
1	M	119	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	192	ALA	2.4
1	K	72	ALA	2.4
1	D	73	TYR	2.4
1	M	137	GLN	2.4
1	N	213	THR	2.4
1	N	79	LEU	2.4
1	C	71	ARG	2.4
1	K	202	LYS	2.4
1	I	221	GLU	2.4
1	N	173	SER	2.4
1	B	176	MET	2.4
1	I	140	LEU	2.4
1	M	58	LEU	2.4
1	F	89	GLY	2.4
1	B	227	ASP	2.4
1	I	179	GLN	2.4
1	N	236	GLN	2.4
1	H	76	TYR	2.4
1	N	118	TYR	2.4
1	I	238	PHE	2.3
1	L	109	GLU	2.3
1	M	82	GLU	2.3
1	C	233[A]	MET	2.3
1	J	154	MET	2.3
1	M	121	SER	2.3
1	N	73	TYR	2.3
1	B	193	ILE	2.3
1	H	119	ILE	2.3
1	B	174	ARG	2.3
1	I	242	ASP	2.3
1	I	151	ALA	2.3
1	D	117	MET	2.3
1	I	157	LEU	2.3
1	I	127	THR	2.3
1	J	155	GLY	2.3
1	N	234	GLU	2.3
1	L	199	MET	2.3
1	E	86	CYS	2.3
1	H	86	CYS	2.3
1	K	100	ILE	2.3
1	K	193	ILE	2.3
1	N	100	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	N	220	ILE	2.3
1	N	232	PRO	2.3
1	L	120	ASN	2.3
1	A	192	ALA	2.3
1	D	233	MET	2.3
1	N	233	MET	2.3
1	F	134	ASP	2.3
1	J	84	ILE	2.3
1	F	216	SER	2.3
1	J	135	THR	2.3
1	N	228	ARG	2.3
1	G	248	PRO	2.3
1	N	62	VAL	2.3
1	B	88	MET	2.2
1	C	192	ALA	2.2
1	N	98	LEU	2.2
1	A	62	VAL	2.2
1	M	206	TYR	2.2
1	L	149	GLY	2.2
1	H	136	MET	2.2
1	F	195	ALA	2.2
1	H	64	GLU	2.2
1	N	195	ALA	2.2
1	L	98	LEU	2.2
1	C	193	ILE	2.2
1	I	193	ILE	2.2
1	M	240	ILE	2.2
1	K	228	ARG	2.2
1	M	129	GLY	2.2
1	N	140	LEU	2.2
1	F	218	GLN	2.2
1	I	240	ILE	2.2
1	A	168	HIS	2.2
1	E	247	HIS	2.2
1	M	74	ASP	2.2
1	D	85	VAL	2.2
1	E	248	PRO	2.2
1	L	233	MET	2.2
1	M	144	CYS	2.2
1	M	146	TRP	2.2
1	J	161	ALA	2.2
1	N	240	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	111	ASN	2.2
1	D	232	PRO	2.2
1	M	148	VAL	2.2
1	G	144	CYS	2.2
1	I	231	SER	2.2
1	G	192	ALA	2.2
1	I	210	ALA	2.2
1	K	196	GLU	2.2
1	I	208	ILE	2.1
1	J	194	GLN	2.1
1	M	247	HIS	2.1
1	M	164	PRO	2.1
1	G	117	MET	2.1
1	G	154	MET	2.1
1	K	229	TYR	2.1
1	H	108	SER	2.1
1	N	174	ARG	2.1
1	E	218	GLN	2.1
1	K	218	GLN	2.1
1	G	247	HIS	2.1
1	A	88	MET	2.1
1	I	130	LEU	2.1
1	J	241	LEU	2.1
1	M	157	LEU	2.1
1	E	223	ALA	2.1
1	G	73	TYR	2.1
1	C	237	GLU	2.1
1	G	234	GLU	2.1
1	I	109	GLU	2.1
1	K	86	CYS	2.1
1	M	75	ILE	2.1
1	N	153	SER	2.1
1	M	218	GLN	2.1
1	I	116	HIS	2.1
1	H	166	MET	2.1
1	I	203	LYS	2.1
1	M	171	PRO	2.1
1	I	227	ASP	2.1
1	K	227	ASP	2.1
1	D	138	TYR	2.1
1	F	193	ILE	2.1
1	I	235	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	198	ILE	2.1
1	L	181	SER	2.1
1	M	147	CYS	2.1
1	M	124	GLY	2.1
1	H	145	THR	2.1
1	H	160	ALA	2.1
1	N	198	ILE	2.1
1	A	70	GLU	2.1
1	B	197	GLU	2.1
1	E	225	GLU	2.1
1	I	118	TYR	2.1
1	I	138	TYR	2.1
1	C	236	GLN	2.0
1	F	224	MET	2.0
1	I	117	MET	2.0
1	N	147	CYS	2.0
1	E	85	VAL	2.0
1	H	142	PRO	2.0
1	D	241	LEU	2.0
1	G	124	GLY	2.0
1	C	191	ILE	2.0
1	E	193	ILE	2.0
1	N	145	THR	2.0
1	B	229	TYR	2.0
1	E	181	SER	2.0
1	F	244	VAL	2.0
1	G	97	SER	2.0
1	H	168	HIS	2.0
1	M	232	PRO	2.0
1	N	60	PRO	2.0
1	I	217	LEU	2.0
1	K	159	LEU	2.0
1	D	155	GLY	2.0
1	K	155	GLY	2.0
1	D	127	THR	2.0
1	C	64	GLU	2.0
1	M	197	GLU	2.0
1	M	154	MET	2.0
1	I	229	TYR	2.0
1	I	148	VAL	2.0
1	K	63	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

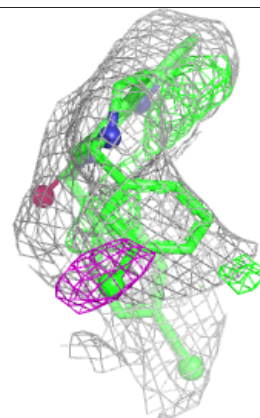
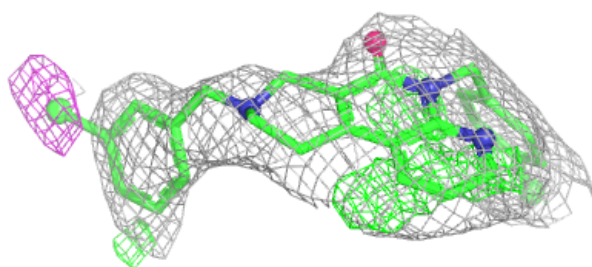
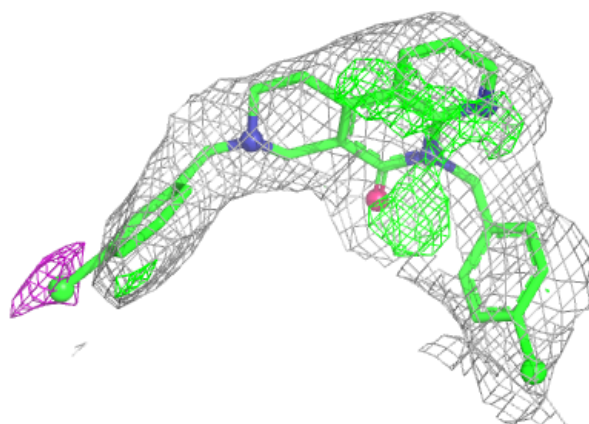
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	9I3	M	301	31/31	0.74	0.28	99,101,102,107	0
2	9I3	H	301	31/31	0.81	0.16	67,69,70,70	0
2	9I3	E	301	31/31	0.81	0.14	57,59,60,63	0
2	9I3	L	301	31/31	0.82	0.14	61,62,65,68	0
2	9I3	E	302	31/31	0.82	0.15	57,59,60,62	0
2	9I3	N	301	31/31	0.83	0.16	69,72,75,78	0
2	9I3	D	301	31/31	0.84	0.15	62,64,65,66	0
2	9I3	I	301	31/31	0.85	0.15	66,68,71,72	0
2	9I3	C	301	31/31	0.85	0.15	61,63,65,65	0
2	9I3	A	301	31/31	0.86	0.13	57,59,63,64	0
2	9I3	G	301	31/31	0.86	0.14	64,66,69,71	0
2	9I3	K	301	31/31	0.86	0.16	88,91,92,95	0
2	9I3	B	301	31/31	0.87	0.14	63,65,67,68	0
2	9I3	F	301	31/31	0.89	0.13	58,60,62,66	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.

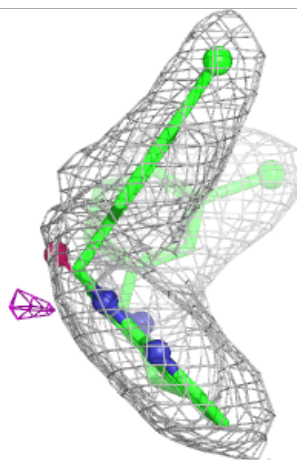
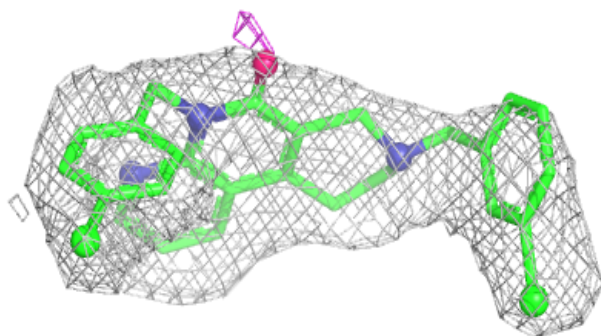
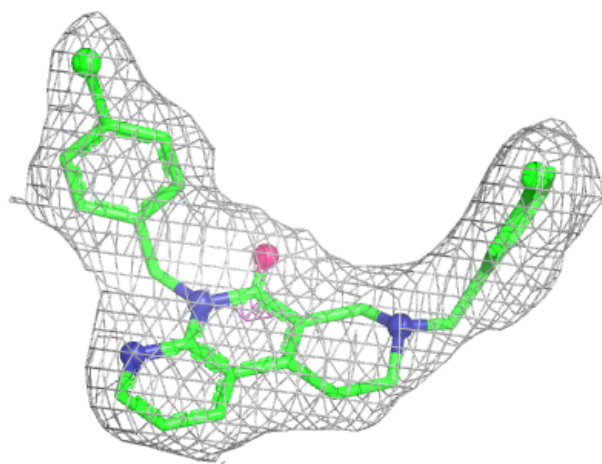
Electron density around 9I3 M 301:

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



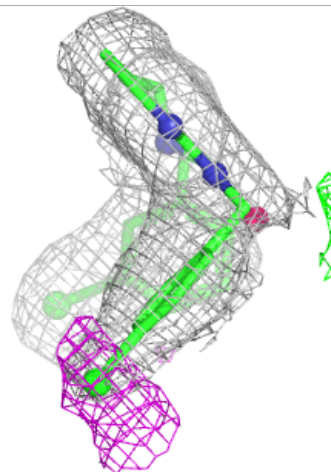
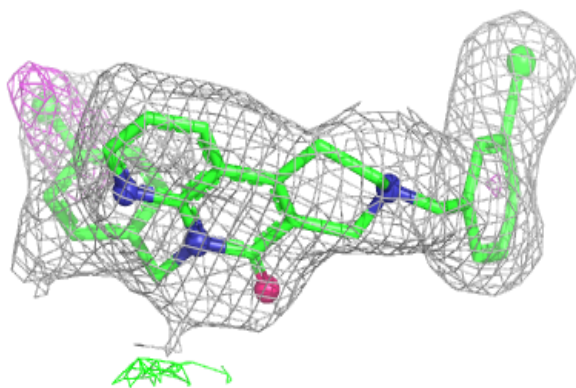
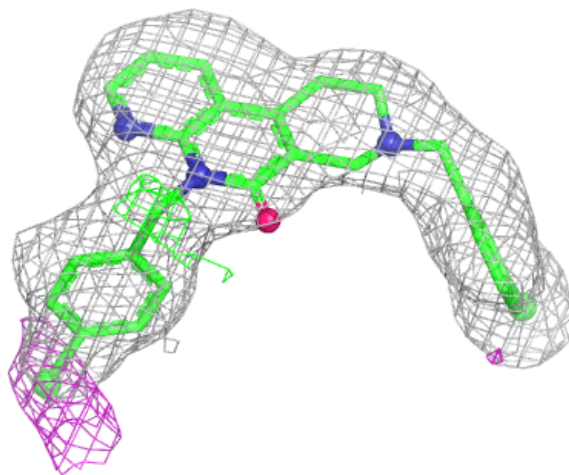
Electron density around 9I3 H 301:

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



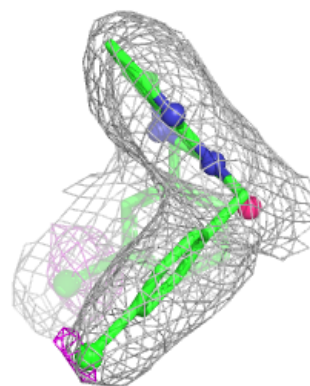
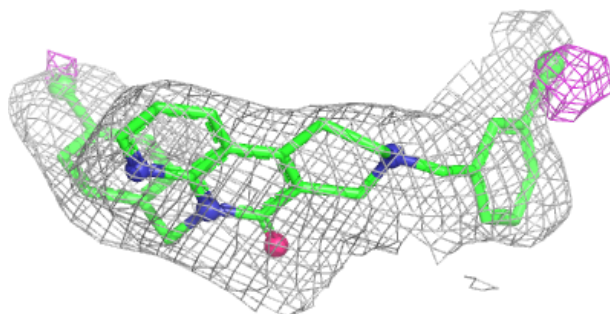
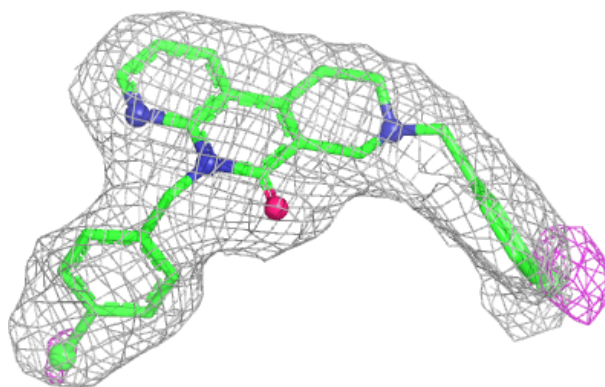
Electron density around 9I3 E 301:

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

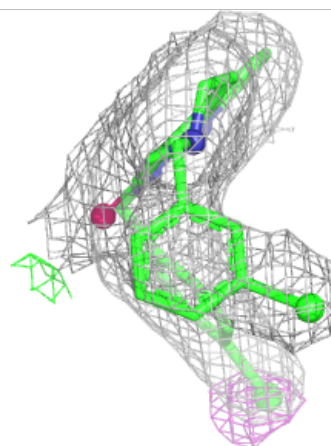
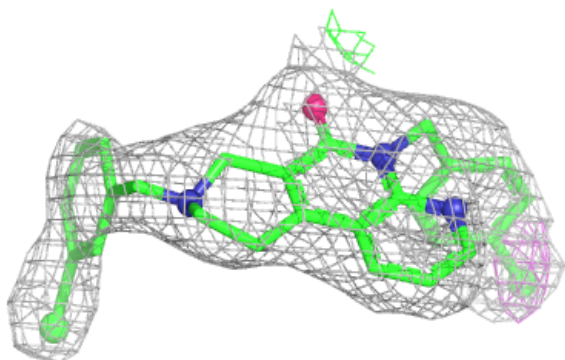
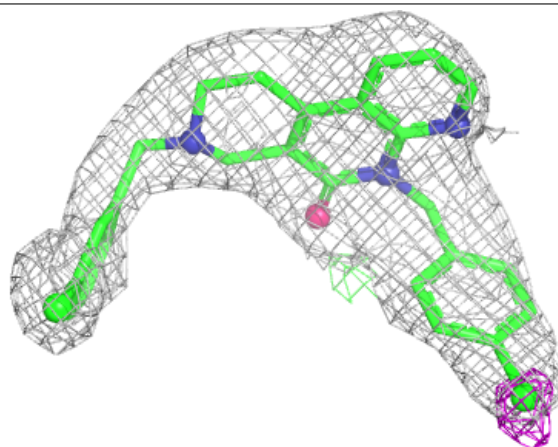


Electron density around 9I3 L 301:

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

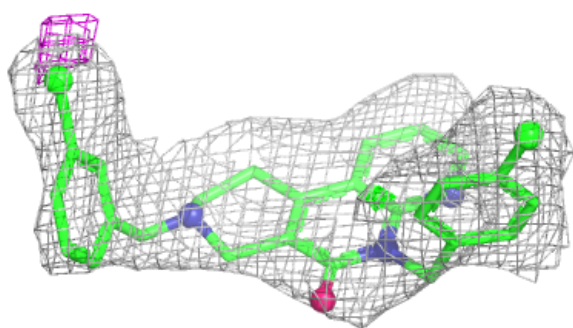
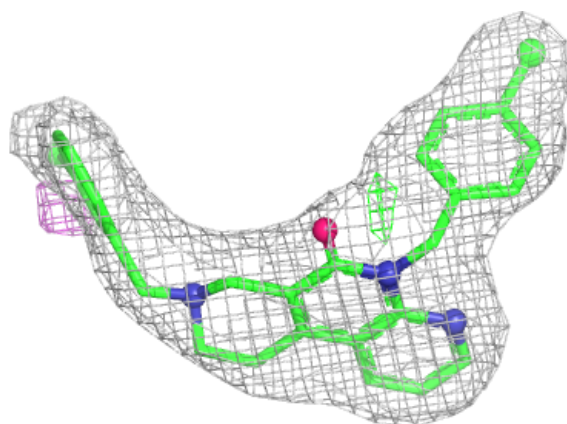
**Electron density around 9I3 E 302:**

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



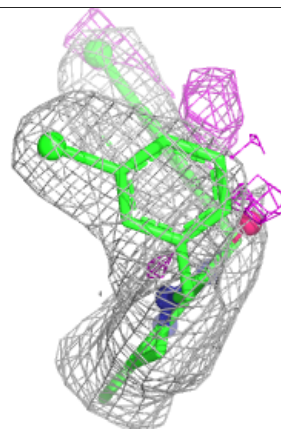
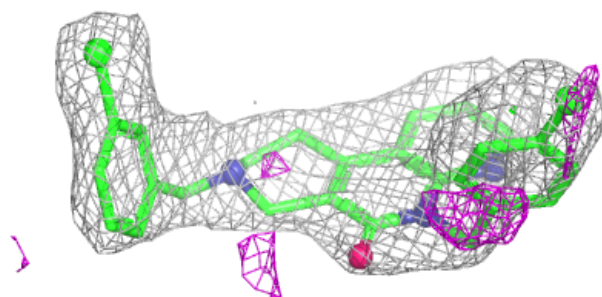
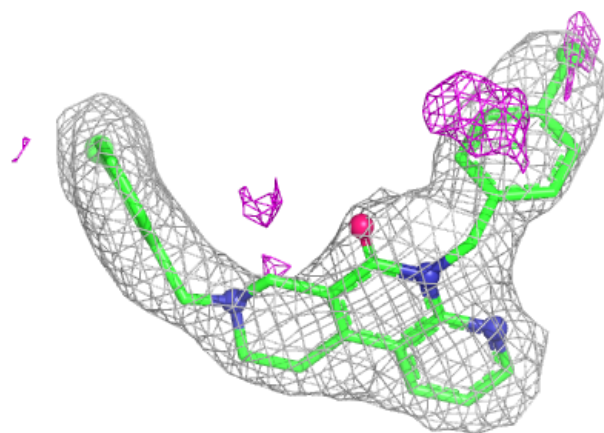
Electron density around 9I3 N 301:

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

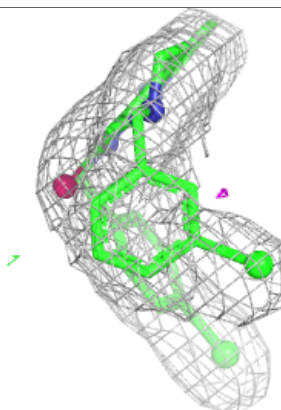
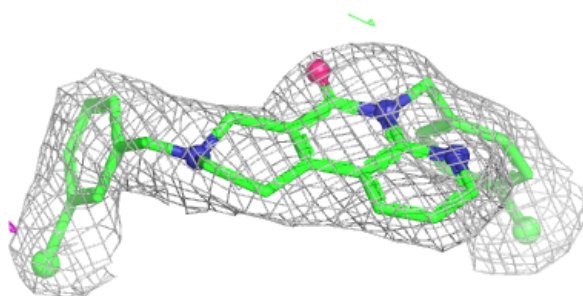
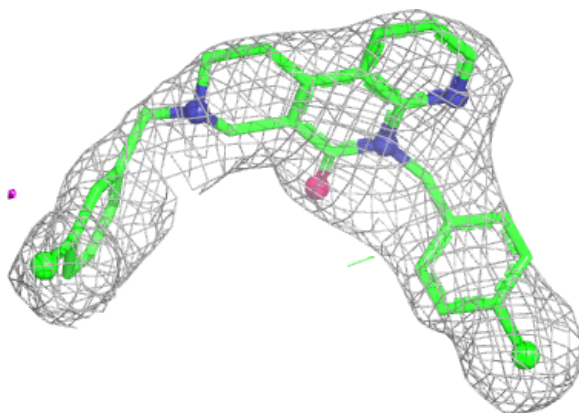


Electron density around 9I3 D 301:

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

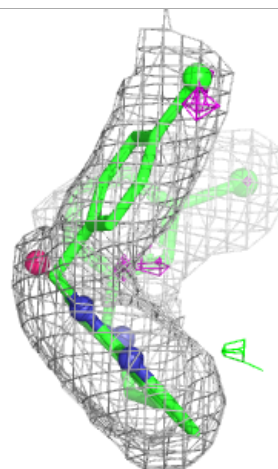
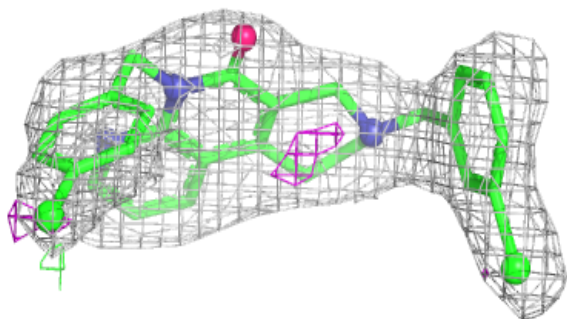
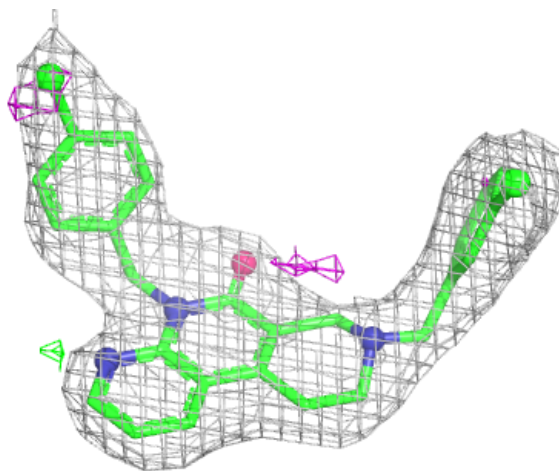
**Electron density around 9I3 I 301:**

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



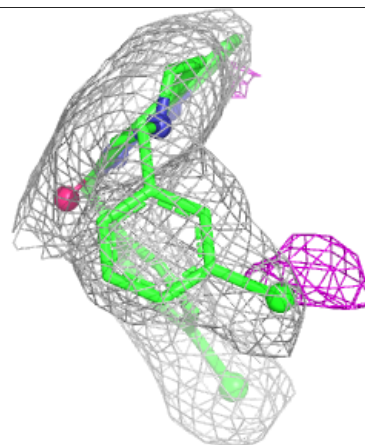
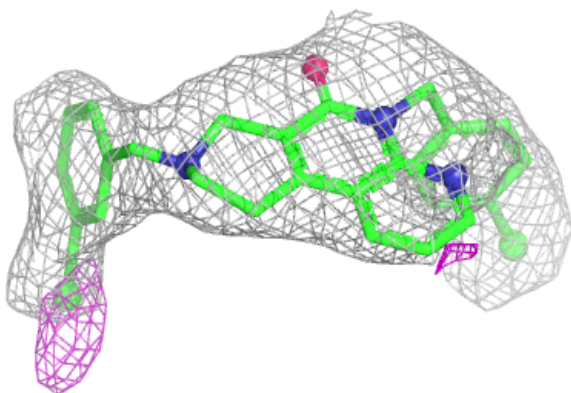
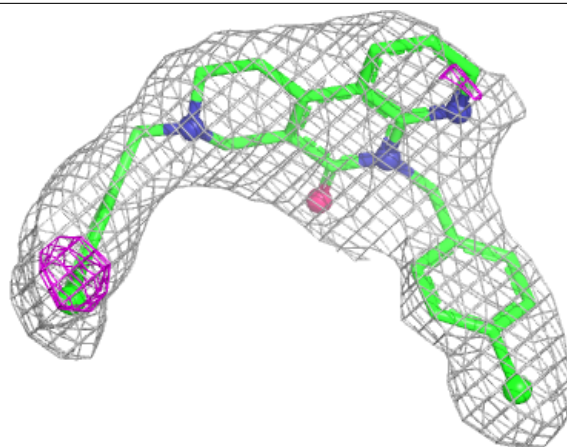
Electron density around 9I3 C 301:

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



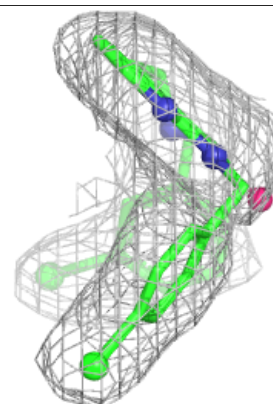
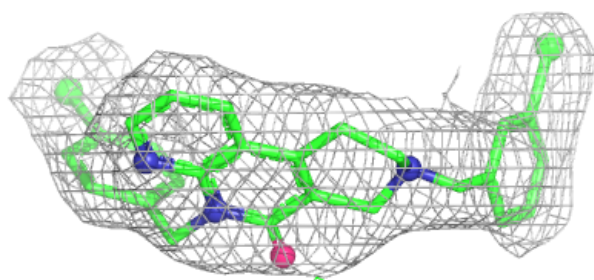
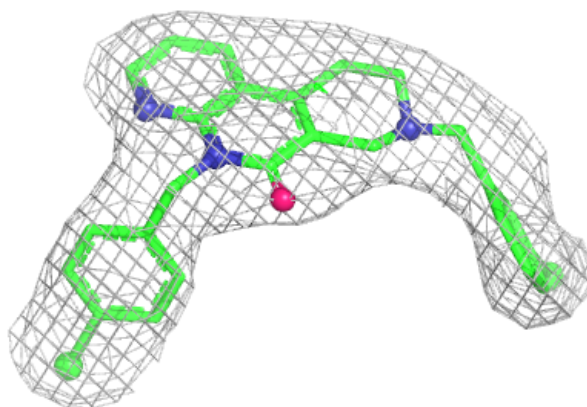
Electron density around 9I3 A 301:

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

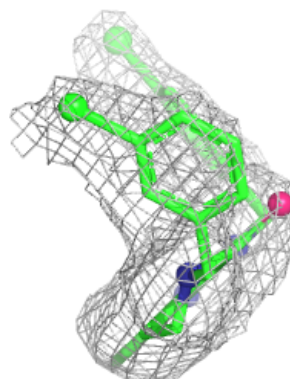
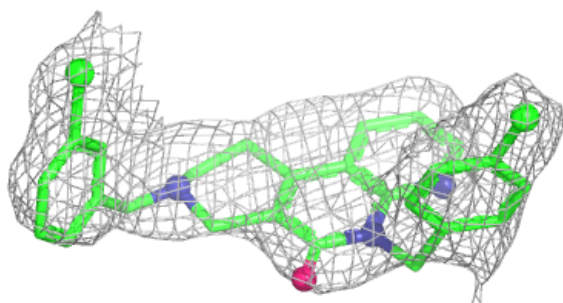
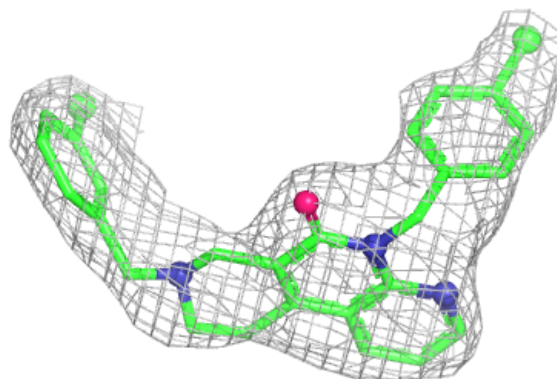


Electron density around 9I3 G 301:

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

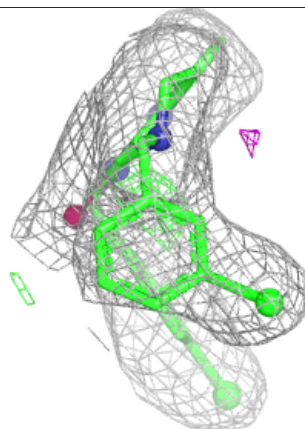
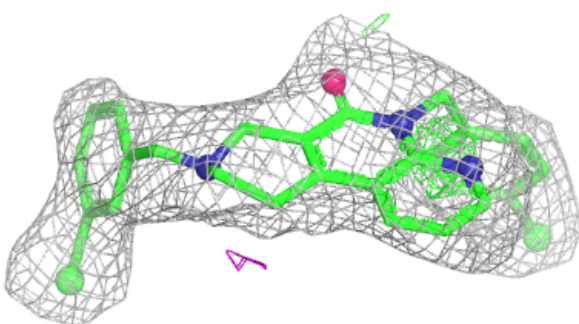
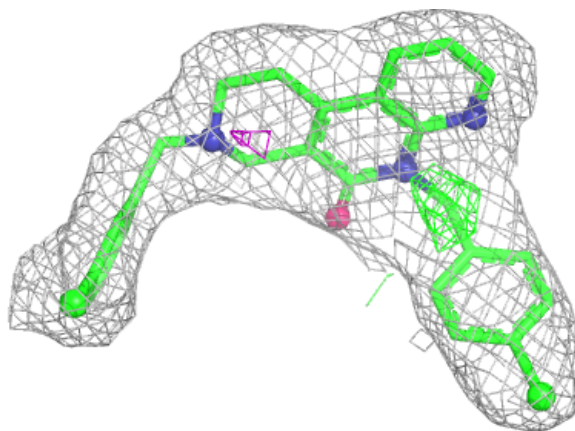
**Electron density around 9I3 K 301:**

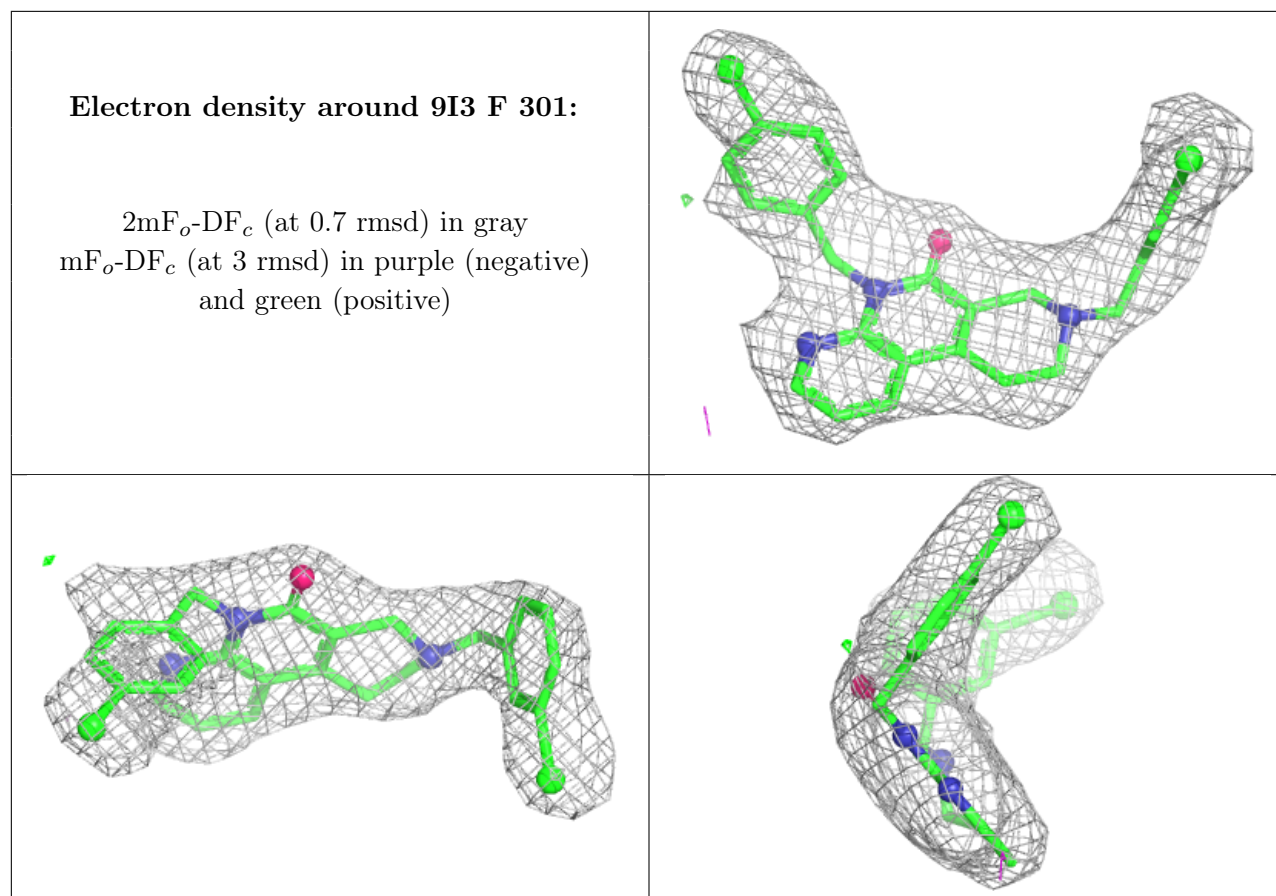
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 9I3 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.