



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2026 – 10:45 AM EDT

PDB ID : 9PNC / pdb_00009pnc
Title : Crystal structure of human mitochondrial ClpP protease C144R mutant in complex with imipridone compound, TR-65
Authors : Mabanglo, M.F.; Houry, W.A.
Deposited on : 2025-07-19
Resolution : 2.70 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

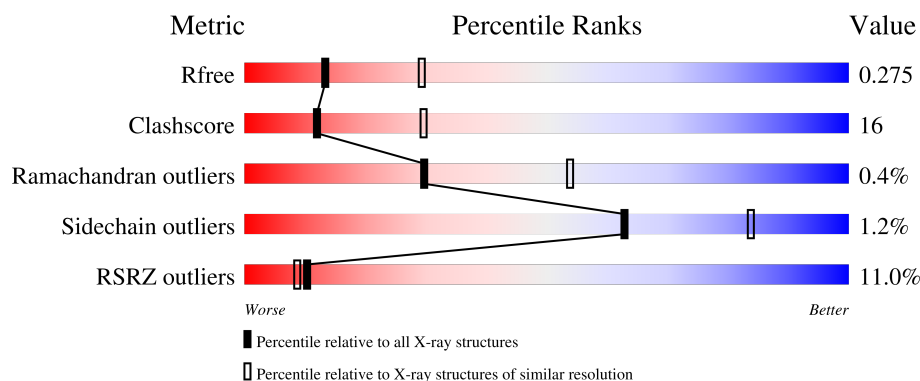
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	2% 57% 19% 24%
1	B	221	5% 55% 20% 24%
1	C	221	8% 56% 19% 24%
1	D	221	6% 52% 23% 24%
1	E	221	6% 59% 17% 24%

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Mol	Chain	Length	Quality of chain
1	F	221	
1	G	221	
1	H	221	
1	I	221	
1	J	221	
1	K	221	
1	L	221	
1	M	221	
1	N	221	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18941 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.

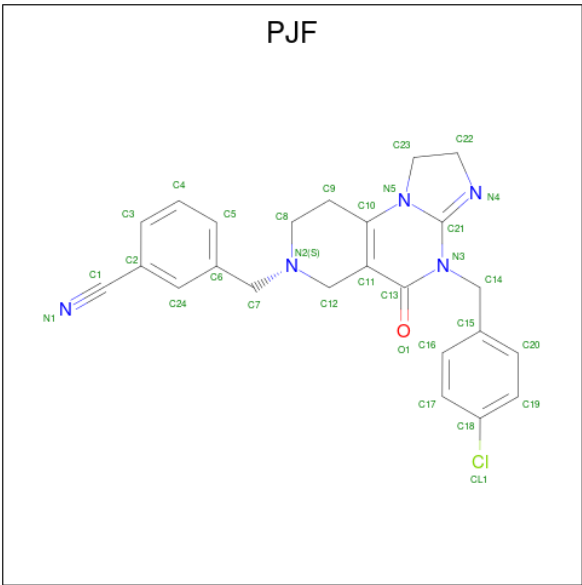
- Molecule 1 is a protein called ATP-dependent Clp protease proteolytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1312	835	226	239	12			
1	B	167	Total	C	N	O	S	0	0	0
			1304	831	225	236	12			
1	C	167	Total	C	N	O	S	0	0	0
			1305	830	225	238	12			
1	D	168	Total	C	N	O	S	0	0	0
			1312	835	226	239	12			
1	E	169	Total	C	N	O	S	0	0	0
			1321	840	228	241	12			
1	F	166	Total	C	N	O	S	0	0	0
			1296	825	224	235	12			
1	G	168	Total	C	N	O	S	0	0	0
			1313	834	227	240	12			
1	H	166	Total	C	N	O	S	0	0	0
			1296	825	224	235	12			
1	I	165	Total	C	N	O	S	0	0	0
			1289	820	223	234	12			
1	J	167	Total	C	N	O	S	0	0	0
			1306	831	225	238	12			
1	K	170	Total	C	N	O	S	0	0	0
			1324	842	228	242	12			
1	L	164	Total	C	N	O	S	0	0	0
			1282	815	222	233	12			
1	M	166	Total	C	N	O	S	0	0	0
			1296	827	224	233	12			
1	N	168	Total	C	N	O	S	0	0	0
			1309	833	226	238	12			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	SER	-	expression tag	UNP Q16740
A	144	ARG	CYS	engineered mutation	UNP Q16740
B	57	SER	-	expression tag	UNP Q16740
B	144	ARG	CYS	engineered mutation	UNP Q16740
C	57	SER	-	expression tag	UNP Q16740
C	144	ARG	CYS	engineered mutation	UNP Q16740
D	57	SER	-	expression tag	UNP Q16740
D	144	ARG	CYS	engineered mutation	UNP Q16740
E	57	SER	-	expression tag	UNP Q16740
E	144	ARG	CYS	engineered mutation	UNP Q16740
F	57	SER	-	expression tag	UNP Q16740
F	144	ARG	CYS	engineered mutation	UNP Q16740
G	57	SER	-	expression tag	UNP Q16740
G	144	ARG	CYS	engineered mutation	UNP Q16740
H	57	SER	-	expression tag	UNP Q16740
H	144	ARG	CYS	engineered mutation	UNP Q16740
I	57	SER	-	expression tag	UNP Q16740
I	144	ARG	CYS	engineered mutation	UNP Q16740
J	57	SER	-	expression tag	UNP Q16740
J	144	ARG	CYS	engineered mutation	UNP Q16740
K	57	SER	-	expression tag	UNP Q16740
K	144	ARG	CYS	engineered mutation	UNP Q16740
L	57	SER	-	expression tag	UNP Q16740
L	144	ARG	CYS	engineered mutation	UNP Q16740
M	57	SER	-	expression tag	UNP Q16740
M	144	ARG	CYS	engineered mutation	UNP Q16740
N	57	SER	-	expression tag	UNP Q16740
N	144	ARG	CYS	engineered mutation	UNP Q16740

- Molecule 2 is 3-{[(10R)-4-[(4-chlorophenyl)methyl]-5-oxo-1,2,4,5,8,9-hexahydroimidazo[1,2-a]pyrido[3,4-e]pyrimidin-7(6H)-yl)methyl}benzonitrile (CCD ID: P.JF) (formula: C₂₄H₂₂ClN₅O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			31	24	1	5	1		
2	B	1	Total	C	Cl	N	O	0	0
			31	24	1	5	1		
2	C	1	Total	C	Cl	N	O	0	0
			31	24	1	5	1		
2	D	1	Total	C	Cl	N	O	0	0
			31	24	1	5	1		
2	E	1	Total	C	Cl	N	O	0	0
			31	24	1	5	1		
2	F	1	Total	C	Cl	N	O	0	0
			31	24	1	5	1		
2	G	1	Total	C	Cl	N	O	0	0
			31	24	1	5	1		
2	H	1	Total	C	Cl	N	O	0	0
			31	24	1	5	1		
2	I	1	Total	C	Cl	N	O	0	0
			31	24	1	5	1		
2	J	1	Total	C	Cl	N	O	0	0
			31	24	1	5	1		
2	K	1	Total	C	Cl	N	O	0	0
			31	24	1	5	1		
2	L	1	Total	C	Cl	N	O	0	0
			31	24	1	5	1		
2	M	1	Total	C	Cl	N	O	0	0
			31	24	1	5	1		
2	N	1	Total	C	Cl	N	O	0	0
			31	24	1	5	1		

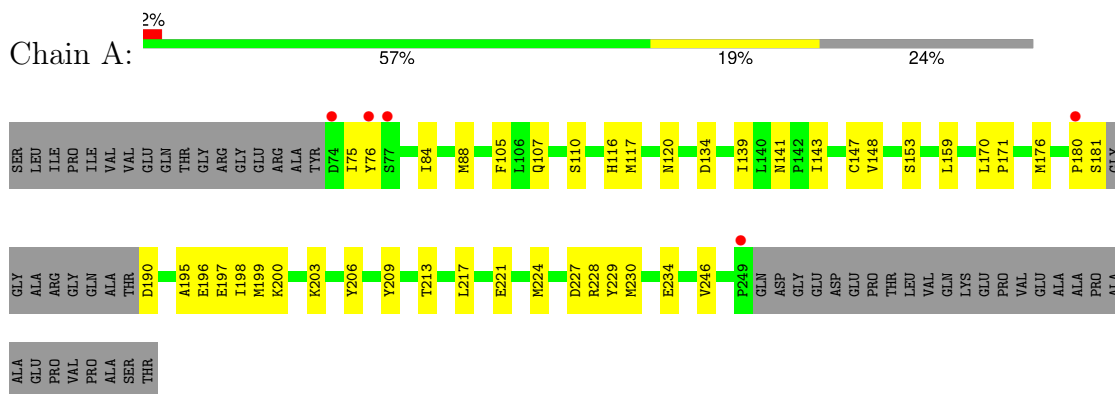
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total 22	O 22	0	0
3	B	18	Total 18	O 18	0	0
3	C	15	Total 15	O 15	0	0
3	D	14	Total 14	O 14	0	0
3	E	24	Total 24	O 24	0	0
3	F	28	Total 28	O 28	0	0
3	G	27	Total 27	O 27	0	0
3	H	16	Total 16	O 16	0	0
3	I	14	Total 14	O 14	0	0
3	J	8	Total 8	O 8	0	0
3	K	12	Total 12	O 12	0	0
3	L	11	Total 11	O 11	0	0
3	M	19	Total 19	O 19	0	0
3	N	14	Total 14	O 14	0	0

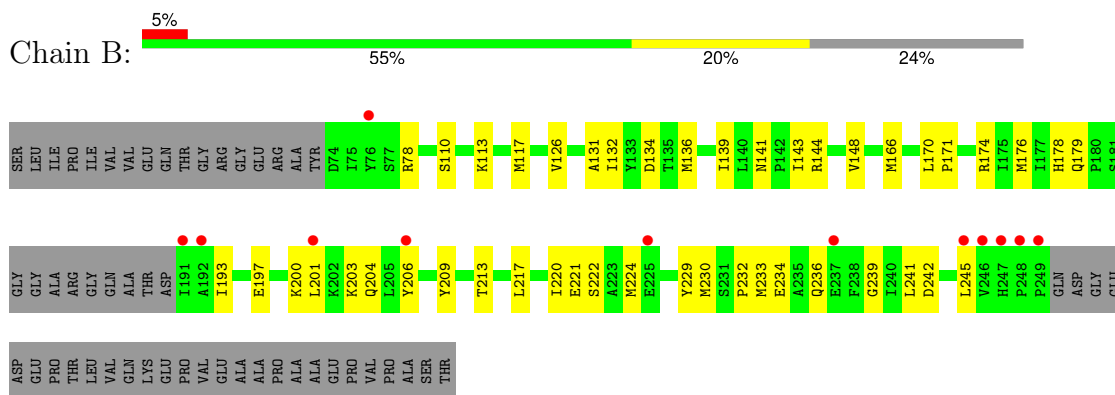
3 Residue-property plots

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.

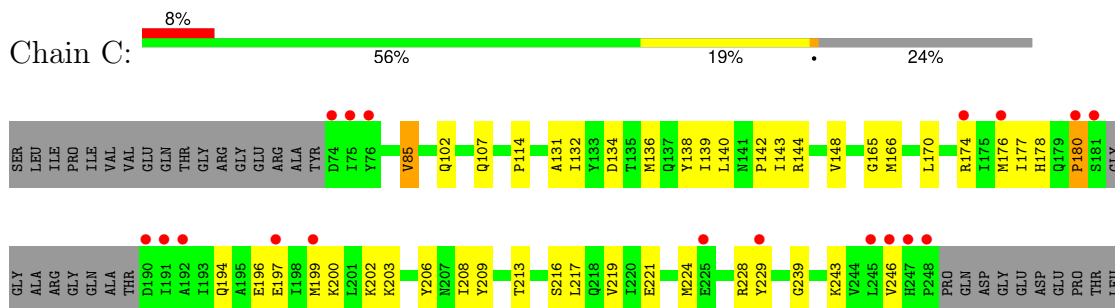
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



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



VAL
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ALA
THR

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



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D74
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Y76
S77
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L79
I84
V85
Q102
S110
H116
V126
I132
M136
I139
L140
N141
P142
I143
R144
V148
A160
G165
H168
S169
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P171
N172
S173
R174
I175

M176
S181
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Q204
Y205
Y206
Y209
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T213
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S222
Y229
M230
S231
P232
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V246
E247
P248
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- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



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I198

L201
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Y206
N207
Y209
T213
S216
L217
Q218
V219
E221
L220
R226
M230
M233
E234
A235
E237
L241
L245
V246
H247
P248
P249
Q250
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VAL
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ALA
SER
THR

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



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D74
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V85
Q102
D134
I139
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R144
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M166
S169
L170
P171
R174
I177
P180
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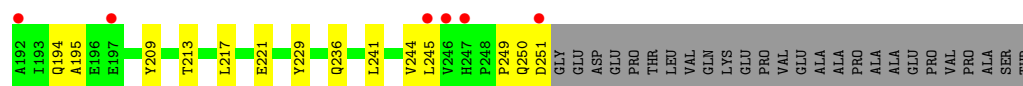
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I198
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T213
L217
Q218
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S222
A223
M224
E225
R228
S231
P232
M233
E234
E237
F238
G239
I240
L241
V246
P249
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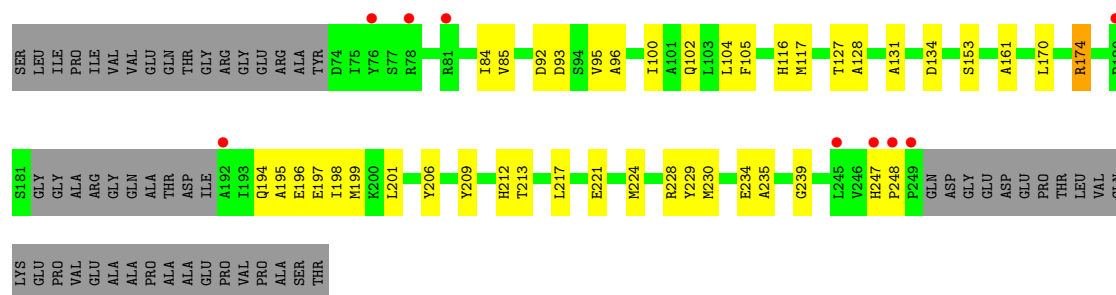
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



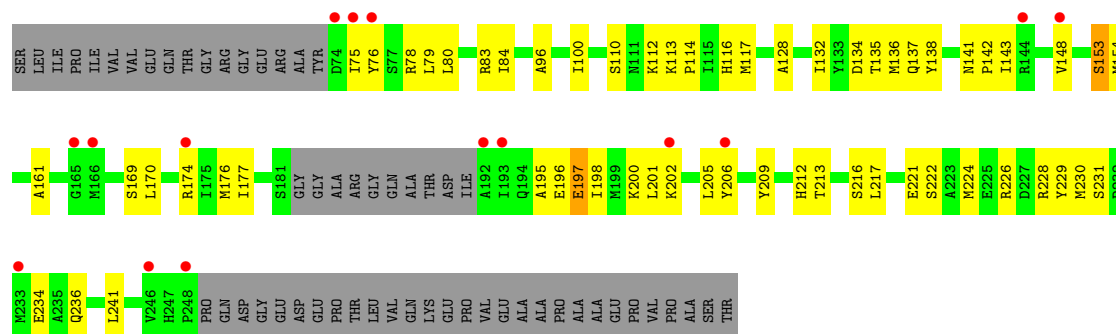
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I75
Y76
L80
R81
L88
P114
I132
M136
I139
P142
I143
V146
C147
V148
L159
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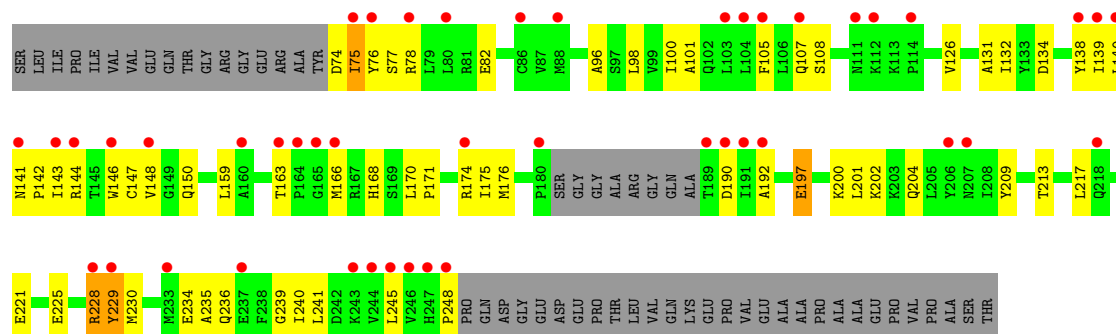
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



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

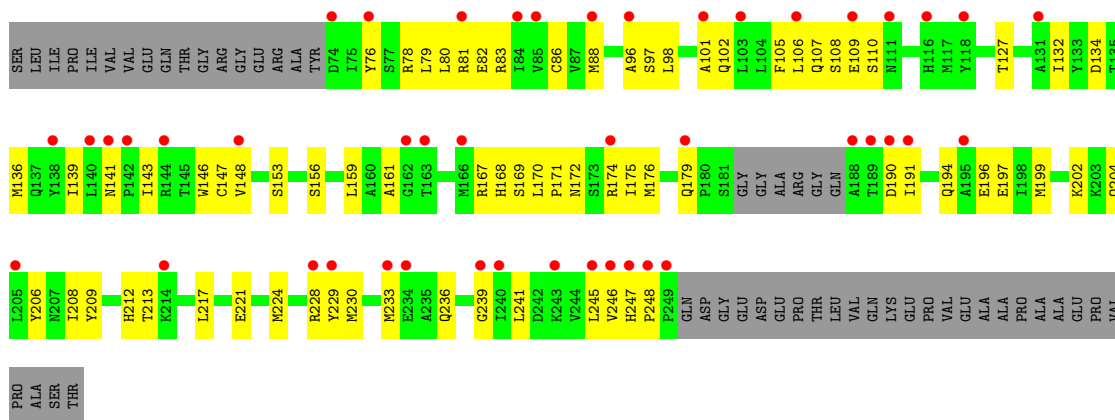


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

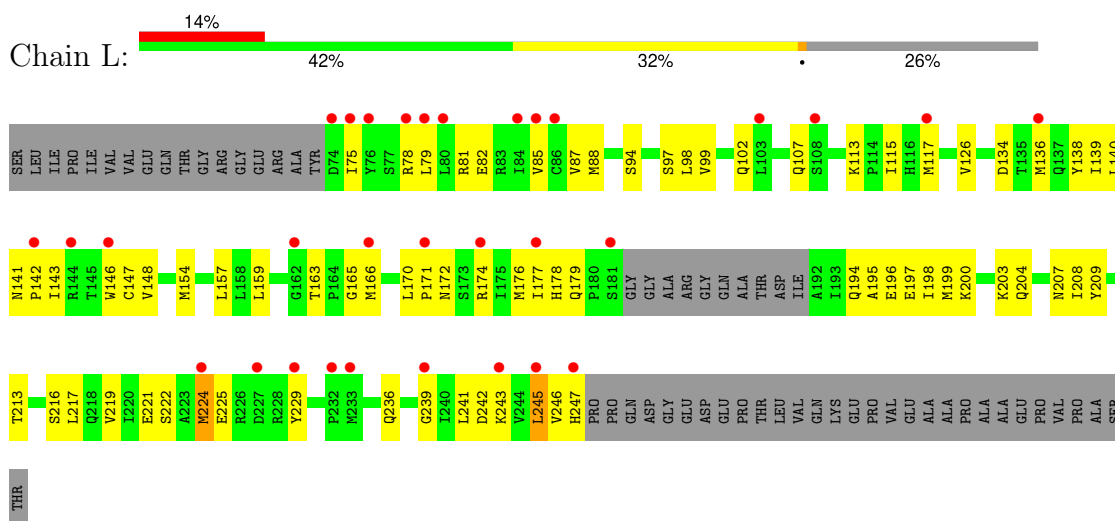


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

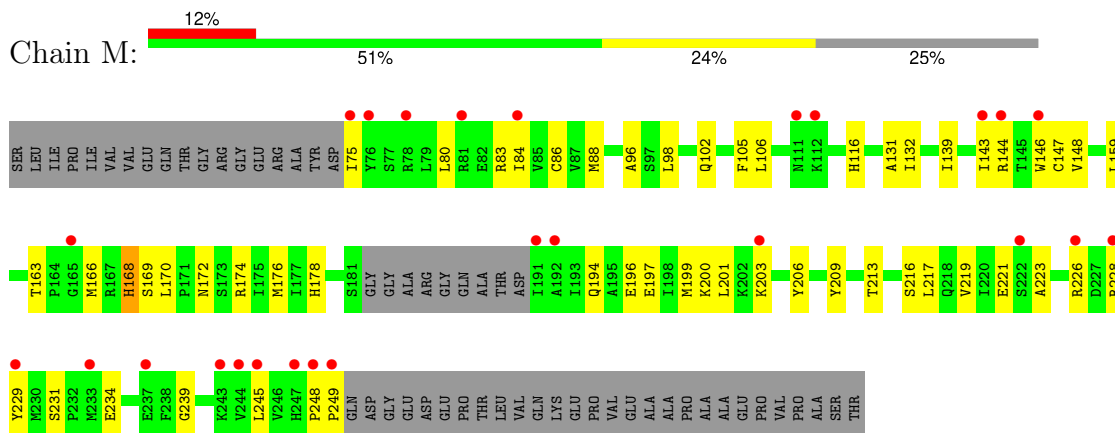




- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

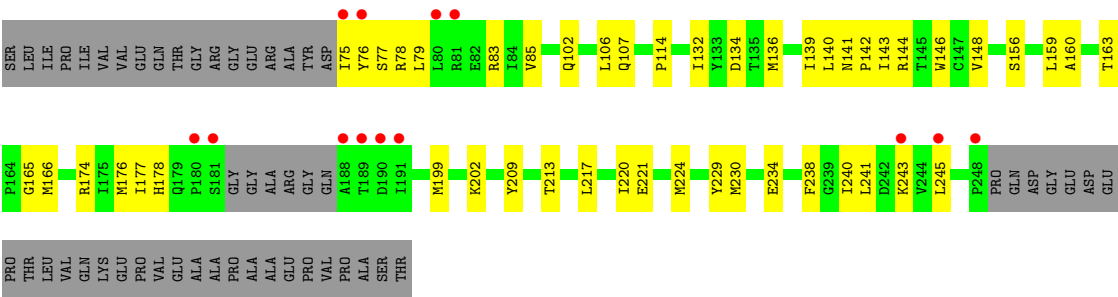


- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



- 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	181.23Å 148.50Å 151.33Å 90.00° 101.44° 90.00°	Depositor
Resolution (Å)	49.44 – 2.70 49.44 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.44-2.70) 85.6 (49.44-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.236 , 0.276 0.236 , 0.275	Depositor DCC
R_{free} test set	2000 reflections (1.85%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18941	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 5.26% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.22	0/1336	0.53	0/1806
1	B	0.24	0/1328	0.55	0/1795
1	C	0.20	0/1328	0.52	0/1794
1	D	0.31	1/1336 (0.1%)	0.55	1/1806 (0.1%)
1	E	0.30	1/1345 (0.1%)	0.53	0/1818
1	F	0.19	0/1320	0.50	0/1784
1	G	0.21	0/1337	0.52	0/1807
1	H	0.22	0/1320	0.52	0/1784
1	I	0.27	0/1312	0.54	2/1772 (0.1%)
1	J	0.33	0/1329	0.67	3/1796 (0.2%)
1	K	0.35	0/1348	0.67	0/1823
1	L	0.28	0/1304	0.65	1/1760 (0.1%)
1	M	0.26	0/1320	0.59	0/1784
1	N	0.23	0/1332	0.58	0/1800
All	All	0.26	2/18595 (0.0%)	0.57	7/25129 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	174	ARG	CB-CG	-5.52	1.35	1.52
1	D	204	GLN	CD-NE2	5.03	1.43	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	197	GLU	CA-CB-CG	-8.38	97.33	114.10
1	L	224	MET	CB-CG-SD	-6.50	93.21	112.70
1	J	229	TYR	CA-CB-CG	6.42	125.46	113.90
1	D	204	GLN	CA-CB-CG	-6.18	101.74	114.10
1	J	228	ARG	CA-C-N	-5.60	113.14	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	228	ARG	C-N-CA	-5.60	113.14	122.21
1	I	137	GLN	N-CA-C	-5.23	105.27	110.97

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	1312	0	1349	33	0
1	B	1304	0	1345	41	0
1	C	1305	0	1342	46	0
1	D	1312	0	1349	45	0
1	E	1321	0	1357	37	0
1	F	1296	0	1334	35	0
1	G	1313	0	1346	26	0
1	H	1296	0	1334	34	0
1	I	1289	0	1327	52	0
1	J	1306	0	1344	74	0
1	K	1324	0	1361	83	0
1	L	1282	0	1320	83	0
1	M	1296	0	1341	57	0
1	N	1309	0	1350	49	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
2	C	31	0	0	1	0
2	D	31	0	0	1	0
2	E	31	0	0	0	0
2	F	31	0	0	0	0
2	G	31	0	0	0	0
2	H	31	0	0	0	0
2	I	31	0	0	0	0
2	J	31	0	0	1	0
2	K	31	0	0	4	0
2	L	31	0	0	6	0
2	M	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	31	0	0	0	0
3	A	22	0	0	2	0
3	B	18	0	0	0	0
3	C	15	0	0	3	0
3	D	14	0	0	2	0
3	E	24	0	0	0	0
3	F	28	0	0	2	0
3	G	27	0	0	1	0
3	H	16	0	0	3	0
3	I	14	0	0	0	0
3	J	8	0	0	1	0
3	K	12	0	0	1	0
3	L	11	0	0	6	0
3	M	19	0	0	2	0
3	N	14	0	0	0	0
All	All	18941	0	18799	589	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 16.

All (589) 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:J:176:MET:SD	1:J:229:TYR:CE1	2.50	1.05
1:N:78:ARG:H	1:N:78:ARG:HD2	1.22	1.04
1:J:176:MET:HB2	1:J:229:TYR:CD1	1.92	1.03
1:K:80:LEU:HD11	1:K:106:LEU:HD21	1.43	0.99
1:M:176:MET:HB2	1:M:229:TYR:CE1	1.97	0.98
1:A:228:ARG:NH2	1:A:234:GLU:OE2	1.95	0.97
1:J:201:LEU:HD12	1:K:174:ARG:HH21	1.30	0.96
1:N:165:GLY:O	1:N:243:LYS:NZ	2.00	0.94
1:L:78:ARG:HH12	1:L:82:GLU:HB2	1.33	0.91
1:J:176:MET:SD	1:J:229:TYR:HE1	1.91	0.90
1:M:203:LYS:HD3	1:M:206:TYR:HD2	1.39	0.87
1:J:174:ARG:NH2	1:J:229:TYR:CD2	2.43	0.87
1:J:201:LEU:HD12	1:K:174:ARG:NH2	1.90	0.87
1:M:176:MET:HB2	1:M:229:TYR:CD1	2.12	0.85
1:K:78:ARG:NH1	1:K:81:ARG:HH11	1.77	0.83
1:A:200:LYS:NZ	3:A:402:HOH:O	2.12	0.82
1:K:176:MET:HB2	1:K:229:TYR:HD1	1.45	0.82
1:M:197:GLU:OE2	1:N:174:ARG:NH1	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:141:ASN:OD1	3:L:401:HOH:O	1.97	0.81
1:J:176:MET:HB2	1:J:229:TYR:CG	2.16	0.80
1:J:176:MET:CB	1:J:229:TYR:CD1	2.66	0.78
1:K:179:GLN:NE2	3:K:401:HOH:O	2.15	0.78
1:K:78:ARG:O	1:K:81:ARG:N	2.17	0.78
1:A:227:ASP:OD2	3:A:401:HOH:O	2.01	0.77
1:F:153:SER:OG	3:F:401:HOH:O	2.02	0.77
1:J:176:MET:SD	1:J:229:TYR:CD1	2.77	0.77
1:C:246:VAL:O	3:C:401:HOH:O	2.03	0.77
1:B:236:GLN:NE2	1:B:242:ASP:O	2.16	0.77
1:J:175:ILE:O	1:J:229:TYR:HB3	1.85	0.77
1:G:139:ILE:HD11	1:G:143:ILE:HD11	1.67	0.76
1:A:196:GLU:HG3	1:M:199:MET:HE1	1.65	0.76
1:K:98:LEU:HD13	1:K:102:GLN:NE2	1.99	0.76
1:M:176:MET:HB2	1:M:229:TYR:HE1	1.46	0.76
1:D:78:ARG:NH1	3:D:401:HOH:O	2.19	0.76
1:L:75:ILE:H	1:L:75:ILE:HD12	1.50	0.75
1:A:228:ARG:HH22	1:A:234:GLU:CD	1.95	0.74
1:L:78:ARG:NH1	1:L:82:GLU:HB2	2.03	0.74
1:N:142:PRO:HA	1:N:163:THR:HG21	1.70	0.73
1:K:197:GLU:OE2	1:L:229:TYR:HB2	1.88	0.73
1:L:78:ARG:NH1	1:L:78:ARG:O	2.21	0.73
1:B:200:LYS:HA	1:B:203:LYS:HE3	1.70	0.73
1:L:197:GLU:OE2	3:L:402:HOH:O	2.06	0.73
1:L:176:MET:HB2	1:L:229:TYR:CD2	2.24	0.73
1:K:176:MET:HB2	1:K:229:TYR:CD1	2.24	0.72
1:J:176:MET:CE	1:J:229:TYR:CE1	2.73	0.72
1:L:139:ILE:HD11	1:L:143:ILE:HD11	1.72	0.71
1:J:176:MET:CG	1:J:229:TYR:CD1	2.74	0.71
1:M:226:ARG:CZ	1:M:228:ARG:HH21	2.04	0.71
1:K:80:LEU:CD1	1:K:106:LEU:HD21	2.20	0.71
1:K:102:GLN:O	1:K:106:LEU:HD23	1.90	0.71
1:K:78:ARG:HD2	1:K:78:ARG:C	2.15	0.70
1:N:77:SER:H	1:N:78:ARG:HH11	1.40	0.70
1:D:148:VAL:HG13	1:D:170:LEU:HD12	1.74	0.70
1:B:134:ASP:HB3	1:C:170:LEU:HD13	1.73	0.69
1:G:217:LEU:O	1:G:221:GLU:HG3	1.92	0.69
1:D:139:ILE:HD11	1:D:143:ILE:HD11	1.76	0.68
1:I:132:ILE:O	1:I:136:MET:HG3	1.93	0.68
1:G:250:GLN:NE2	3:G:403:HOH:O	2.26	0.67
1:F:194:GLN:O	1:F:198:ILE:HD12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:78:ARG:O	1:K:78:ARG:HD2	1.95	0.67
1:F:148:VAL:HG23	1:F:170:LEU:HD12	1.75	0.67
1:J:107:GLN:NE2	1:J:140:LEU:H	1.92	0.67
1:H:230:MET:HE3	1:H:234:GLU:HG2	1.76	0.67
1:J:228:ARG:HH22	1:J:230:MET:HG2	1.60	0.67
1:L:82:GLU:OE2	2:L:301:PJF:C15	2.43	0.66
1:L:204:GLN:O	1:L:208:ILE:HD12	1.95	0.66
1:M:84:ILE:HG12	1:M:116:HIS:HB2	1.76	0.66
1:H:93:ASP:OD1	3:H:401:HOH:O	2.14	0.66
1:B:230:MET:HB3	1:B:234:GLU:HB2	1.75	0.66
1:J:176:MET:HE2	1:J:229:TYR:CE1	2.30	0.66
1:A:197:GLU:HA	1:A:200:LYS:HG3	1.76	0.66
1:F:225:GLU:OE2	1:I:226:ARG:NE	2.28	0.66
1:K:78:ARG:HH12	1:K:81:ARG:NH1	1.94	0.66
1:K:175:ILE:O	1:K:230:MET:N	2.24	0.66
1:M:203:LYS:HD3	1:M:206:TYR:CD2	2.27	0.66
1:E:196:GLU:OE1	1:I:206:TYR:OH	2.14	0.65
1:N:75:ILE:HA	1:N:78:ARG:HD3	1.77	0.65
1:F:209:TYR:O	1:F:213:THR:OG1	2.14	0.65
1:K:153:SER:HA	1:K:179:GLN:HE22	1.60	0.65
1:C:139:ILE:HD11	1:C:143:ILE:HD11	1.78	0.65
1:L:140:LEU:N	3:L:401:HOH:O	2.28	0.65
1:M:200:LYS:HD2	1:N:174:ARG:HH12	1.62	0.65
1:L:217:LEU:O	1:L:221:GLU:HG3	1.97	0.64
1:N:144:ARG:HG2	1:N:166:MET:HB3	1.80	0.64
1:D:194:GLN:O	1:D:198:ILE:HD12	1.98	0.64
1:G:148:VAL:HG23	1:G:170:LEU:HD12	1.80	0.64
1:K:174:ARG:HB3	1:K:229:TYR:CD2	2.33	0.64
1:M:223:ALA:HA	1:M:226:ARG:HH21	1.61	0.64
1:C:200:LYS:NZ	3:C:402:HOH:O	2.31	0.64
1:G:159:LEU:HD21	1:G:241:LEU:HD21	1.80	0.64
1:H:201:LEU:HD11	1:I:174:ARG:NH1	2.13	0.64
1:L:78:ARG:HH12	1:L:82:GLU:CB	2.08	0.64
1:M:200:LYS:CD	1:N:174:ARG:HH12	2.11	0.63
1:L:78:ARG:HH12	1:L:82:GLU:N	1.94	0.63
1:L:176:MET:HE3	1:L:229:TYR:CE2	2.33	0.63
1:A:181:SER:OG	1:M:194:GLN:NE2	2.27	0.63
1:K:78:ARG:NH1	1:K:81:ARG:NH1	2.46	0.63
1:C:209:TYR:O	1:C:213:THR:OG1	2.13	0.63
1:M:217:LEU:O	1:M:221:GLU:HG3	1.98	0.63
1:L:143:ILE:H	1:L:163:THR:HG23	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:217:LEU:O	1:J:221:GLU:HG3	1.98	0.62
1:N:78:ARG:HD2	1:N:78:ARG:N	2.06	0.62
1:L:146:TRP:HZ3	1:L:245:LEU:HD11	1.64	0.62
1:I:197:GLU:OE2	1:I:200:LYS:HD2	1.99	0.62
1:M:197:GLU:OE2	3:M:401:HOH:O	2.16	0.62
1:F:218:GLN:O	1:F:218:GLN:NE2	2.33	0.62
1:E:196:GLU:OE2	1:E:196:GLU:N	2.29	0.62
1:N:77:SER:H	1:N:78:ARG:NH1	1.96	0.62
1:D:204:GLN:HE22	1:E:174:ARG:NH2	1.98	0.62
1:J:176:MET:CE	1:J:229:TYR:HE1	2.12	0.62
1:K:228:ARG:HG2	1:K:229:TYR:H	1.65	0.62
1:H:153:SER:HB2	3:H:413:HOH:O	1.99	0.62
1:J:209:TYR:O	1:J:213:THR:OG1	2.12	0.62
1:I:134:ASP:HB3	1:J:170:LEU:HD13	1.81	0.61
1:C:114:PRO:HB3	1:C:142:PRO:HG2	1.82	0.61
1:E:209:TYR:O	1:E:213:THR:OG1	2.13	0.61
1:L:209:TYR:O	1:L:213:THR:OG1	2.14	0.61
1:M:174:ARG:HH11	1:M:229:TYR:HB2	1.66	0.61
1:F:202:LYS:HD2	1:H:195:ALA:HB3	1.82	0.61
1:M:98:LEU:O	1:M:102:GLN:HG3	2.00	0.61
1:C:176:MET:SD	1:C:178:HIS:HB3	2.40	0.61
1:D:217:LEU:O	1:D:221:GLU:HG3	1.99	0.61
1:K:78:ARG:HH11	1:K:81:ARG:HD3	1.65	0.61
1:G:74:ASP:O	1:G:75:ILE:HG22	2.01	0.61
1:D:204:GLN:NE2	1:E:174:ARG:HH22	1.99	0.61
1:I:231:SER:OG	1:I:234:GLU:HG3	2.01	0.61
1:H:194:GLN:O	1:H:198:ILE:HD12	2.01	0.61
1:K:233:MET:HE1	1:K:236:GLN:OE1	2.01	0.61
1:J:142:PRO:HA	1:J:163:THR:HG21	1.84	0.60
1:K:139:ILE:HD11	1:K:143:ILE:HD11	1.82	0.60
1:D:132:ILE:O	1:D:136:MET:HG3	2.00	0.60
1:M:139:ILE:HD11	1:M:143:ILE:HD11	1.83	0.60
1:C:148:VAL:HG21	2:C:301:PJF:C1	2.31	0.60
1:A:75:ILE:HD11	1:G:80:LEU:HD21	1.82	0.60
1:I:209:TYR:O	1:I:213:THR:OG1	2.17	0.60
1:J:171:PRO:HG3	1:J:245:LEU:O	2.02	0.59
1:K:147:CYS:HB2	1:K:159:LEU:HD13	1.83	0.59
1:G:146:TRP:CH2	1:G:245:LEU:HD21	2.37	0.59
1:L:78:ARG:NH2	1:L:82:GLU:OE1	2.36	0.59
1:M:176:MET:SD	1:M:178:HIS:HB3	2.43	0.59
1:F:144:ARG:HH21	1:F:166:MET:HE2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:108:SER:HB3	2:K:301:PJF:C20	2.32	0.59
1:E:247:HIS:HB3	1:E:248:PRO:HD2	1.85	0.59
1:F:80:LEU:HD13	1:F:102:GLN:HE21	1.68	0.59
1:N:217:LEU:O	1:N:221:GLU:HG3	2.03	0.59
1:J:139:ILE:HD11	1:J:143:ILE:HD11	1.84	0.58
1:J:144:ARG:HG2	1:J:166:MET:HB3	1.84	0.58
1:L:176:MET:HG2	1:L:178:HIS:N	2.17	0.58
1:L:146:TRP:CZ3	1:L:245:LEU:HD11	2.37	0.58
1:B:217:LEU:O	1:B:221:GLU:HG3	2.02	0.58
1:D:126:VAL:CG1	1:D:201:LEU:HD22	2.34	0.58
1:L:82:GLU:OE2	2:L:301:PJF:N4	2.36	0.58
1:I:177:ILE:O	1:I:224:MET:HE3	2.03	0.58
1:K:78:ARG:NH2	1:K:82:GLU:OE2	2.35	0.58
1:N:159:LEU:HD21	1:N:241:LEU:HD21	1.85	0.58
1:G:174:ARG:HB3	1:G:229:TYR:CD2	2.38	0.58
1:M:102:GLN:HA	1:N:75:ILE:HD13	1.86	0.58
1:B:233:MET:HE1	1:B:236:GLN:OE1	2.03	0.58
1:G:194:GLN:HG3	1:G:195:ALA:N	2.19	0.57
1:K:228:ARG:CZ	1:K:229:TYR:O	2.51	0.57
1:K:101:ALA:HB1	1:L:79:LEU:HD21	1.86	0.57
1:K:134:ASP:HB3	1:L:170:LEU:HD23	1.86	0.57
1:L:142:PRO:HA	1:L:163:THR:HG21	1.87	0.57
1:C:131:ALA:HB1	1:D:148:VAL:HG12	1.87	0.57
1:J:126:VAL:HG11	1:J:201:LEU:HG	1.87	0.57
1:B:193:ILE:HG21	1:C:229:TYR:HE1	1.70	0.57
1:N:177:ILE:O	1:N:224:MET:HE3	2.05	0.57
1:K:228:ARG:NH1	1:K:229:TYR:O	2.38	0.57
1:C:206:TYR:CZ	1:C:221:GLU:HG2	2.39	0.57
1:E:126:VAL:HG11	1:E:201:LEU:HG	1.87	0.57
1:L:176:MET:HB2	1:L:229:TYR:CE2	2.41	0.56
1:E:216:SER:OG	1:E:219:VAL:HG23	2.04	0.56
1:J:201:LEU:HA	1:K:174:ARG:HH21	1.69	0.56
1:M:105:PHE:CB	1:N:75:ILE:HD11	2.34	0.56
1:K:176:MET:HE3	1:K:229:TYR:CD1	2.41	0.56
1:E:217:LEU:O	1:E:221:GLU:HG3	2.05	0.56
1:G:194:GLN:HG3	1:G:195:ALA:H	1.70	0.56
1:K:204:GLN:HE21	1:L:172:ASN:HD22	1.53	0.56
1:H:209:TYR:O	1:H:213:THR:OG1	2.20	0.56
1:C:107:GLN:NE2	1:C:140:LEU:HG	2.21	0.56
1:C:138:TYR:CZ	1:D:248:PRO:HG3	2.41	0.56
1:E:176:MET:HB2	1:E:229:TYR:CD1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:117:MET:HE1	1:I:136:MET:SD	2.46	0.56
1:K:132:ILE:O	1:K:136:MET:HG3	2.05	0.56
1:J:78:ARG:NH1	1:J:82:GLU:OE2	2.38	0.56
1:N:114:PRO:HG3	1:N:142:PRO:HG2	1.87	0.56
1:I:153:SER:OG	1:I:154:MET:N	2.32	0.55
1:D:204:GLN:NE2	1:E:174:ARG:NH2	2.54	0.55
1:H:213:THR:HG22	1:H:239:GLY:C	2.31	0.55
1:M:146:TRP:CE2	1:M:168:HIS:NE2	2.73	0.55
1:J:200:LYS:HZ3	1:K:228:ARG:CZ	2.19	0.55
1:E:171:PRO:HD3	1:E:245:LEU:O	2.07	0.55
1:N:107:GLN:NE2	1:N:140:LEU:H	2.05	0.55
1:G:132:ILE:O	1:G:136:MET:HG3	2.07	0.55
1:B:201:LEU:HA	1:C:174:ARG:NH2	2.22	0.55
1:B:204:GLN:CD	1:C:174:ARG:HH12	2.15	0.55
1:C:216:SER:OG	1:C:219:VAL:HG23	2.07	0.55
1:I:148:VAL:HG23	1:I:170:LEU:HD12	1.89	0.55
1:K:97:SER:CB	1:L:88:MET:HE1	2.37	0.55
1:M:144:ARG:HG2	1:M:166:MET:HB3	1.88	0.55
1:B:204:GLN:NE2	1:C:174:ARG:HH12	2.05	0.55
1:M:216:SER:OG	1:M:219:VAL:HG23	2.07	0.54
1:B:220:ILE:O	1:B:224:MET:HG3	2.07	0.54
1:D:209:TYR:O	1:D:213:THR:OG1	2.26	0.54
1:N:176:MET:HE2	1:N:229:TYR:CZ	2.42	0.54
1:F:177:ILE:HG13	1:F:224:MET:HG2	1.89	0.54
1:J:204:GLN:NE2	1:K:172:ASN:OD1	2.41	0.54
1:F:171:PRO:HG3	1:F:246:VAL:HG22	1.89	0.54
1:J:144:ARG:HE	1:J:168:HIS:HE1	1.55	0.54
1:I:197:GLU:OE2	1:I:197:GLU:HA	2.05	0.53
1:B:176:MET:HE3	1:B:178:HIS:O	2.08	0.53
1:G:209:TYR:O	1:G:213:THR:OG1	2.20	0.53
1:L:102:GLN:HE21	1:M:75:ILE:CD1	2.22	0.53
1:B:110:SER:OG	1:B:113:LYS:HG3	2.08	0.53
1:B:233:MET:HA	1:B:233:MET:HE3	1.90	0.53
1:B:201:LEU:HA	1:C:174:ARG:HH21	1.72	0.53
1:M:245:LEU:HD13	1:M:249:PRO:HD3	1.91	0.53
1:F:225:GLU:OE2	1:I:228:ARG:HD2	2.08	0.53
1:J:170:LEU:CD2	1:J:245:LEU:HD11	2.38	0.53
1:M:147:CYS:HB3	1:M:169:SER:HB2	1.91	0.53
1:D:74:ASP:O	1:D:78:ARG:HG2	2.08	0.53
1:L:165:GLY:O	1:L:243:LYS:NZ	2.42	0.53
1:E:201:LEU:HD13	1:F:174:ARG:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:ALA:C	1:N:199:MET:HE1	2.34	0.52
1:M:231:SER:OG	1:M:234:GLU:HG3	2.09	0.52
1:A:76:TYR:OH	1:G:98:LEU:HD13	2.09	0.52
1:D:201:LEU:HG	1:E:174:ARG:HH21	1.75	0.52
1:E:134:ASP:HB3	1:F:170:LEU:HD13	1.91	0.52
1:L:147:CYS:HB2	1:L:159:LEU:HD13	1.91	0.52
1:B:132:ILE:O	1:B:136:MET:HG3	2.09	0.52
1:C:132:ILE:O	1:C:136:MET:HG3	2.08	0.52
1:H:174:ARG:HG3	1:H:229:TYR:CD2	2.45	0.52
1:J:131:ALA:HB1	1:K:148:VAL:HG22	1.91	0.52
1:K:78:ARG:O	1:K:79:LEU:C	2.52	0.52
1:N:230:MET:HB3	1:N:234:GLU:HB2	1.91	0.52
1:B:171:PRO:HG3	1:B:245:LEU:O	2.10	0.52
1:E:150:GLN:CB	1:E:174:ARG:HB2	2.38	0.52
1:H:217:LEU:O	1:H:221:GLU:HG3	2.10	0.52
1:J:148:VAL:HG11	2:J:301:PJF:C1	2.39	0.52
1:F:213:THR:HG22	1:F:239:GLY:C	2.35	0.52
1:G:143:ILE:H	1:G:163:THR:HG22	1.75	0.52
1:N:77:SER:N	1:N:78:ARG:HH11	2.08	0.52
1:I:76:TYR:HD1	1:I:79:LEU:HD12	1.74	0.51
1:I:114:PRO:HB3	1:I:142:PRO:HG2	1.92	0.51
1:K:236:GLN:HB2	1:K:241:LEU:HD12	1.92	0.51
1:A:209:TYR:O	1:A:213:THR:OG1	2.15	0.51
1:D:236:GLN:HB2	1:D:241:LEU:HD12	1.91	0.51
1:J:144:ARG:HE	1:J:168:HIS:CE1	2.28	0.51
1:K:153:SER:HA	1:K:179:GLN:NE2	2.24	0.51
1:C:165:GLY:O	1:C:243:LYS:HE3	2.10	0.51
1:L:75:ILE:H	1:L:75:ILE:CD1	2.21	0.51
1:L:78:ARG:NH1	1:L:82:GLU:N	2.57	0.51
1:J:174:ARG:CZ	1:J:229:TYR:CD2	2.93	0.51
1:L:134:ASP:HB3	1:M:170:LEU:HD23	1.92	0.51
1:M:209:TYR:O	1:M:213:THR:OG1	2.18	0.51
1:C:134:ASP:HB3	1:D:170:LEU:HD13	1.91	0.51
1:M:148:VAL:HG22	1:M:170:LEU:HD22	1.93	0.51
1:E:144:ARG:HE	1:E:166:MET:HG2	1.76	0.51
1:K:96:ALA:HA	1:K:132:ILE:HD11	1.93	0.51
1:C:177:ILE:HD12	1:C:224:MET:HG3	1.92	0.51
1:J:78:ARG:CZ	1:J:82:GLU:OE2	2.59	0.51
1:K:217:LEU:O	1:K:221:GLU:HG3	2.11	0.51
1:L:87:VAL:HG22	1:L:99:VAL:HG21	1.93	0.51
1:B:148:VAL:HG23	1:B:170:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:161:ALA:HA	1:I:212:HIS:ND1	2.27	0.51
1:K:197:GLU:CD	1:L:229:TYR:HB2	2.35	0.51
1:K:202:LYS:HE2	1:K:224:MET:HE3	1.93	0.51
1:L:78:ARG:CZ	1:L:81:ARG:HG2	2.41	0.51
1:L:179:GLN:OE1	3:L:403:HOH:O	2.17	0.51
1:N:160:ALA:HB2	1:N:240:ILE:HG23	1.92	0.51
1:E:176:MET:HE3	1:E:229:TYR:CE1	2.46	0.50
1:H:230:MET:HE2	1:H:235:ALA:HA	1.93	0.50
1:H:247:HIS:HB2	1:H:248:PRO:HD2	1.93	0.50
1:J:228:ARG:HG2	1:J:229:TYR:N	2.26	0.50
1:D:160:ALA:HB2	1:D:240:ILE:HG23	1.92	0.50
1:F:228:ARG:NH2	1:F:234:GLU:OE1	2.44	0.50
1:K:228:ARG:HG2	1:K:229:TYR:N	2.25	0.50
1:M:131:ALA:HB1	1:N:148:VAL:HG12	1.93	0.50
1:L:176:MET:HB2	1:L:229:TYR:HD2	1.75	0.50
1:K:107:GLN:HA	1:K:141:ASN:HD21	1.74	0.50
1:L:216:SER:OG	1:L:219:VAL:HG23	2.12	0.50
1:G:146:TRP:HH2	1:G:245:LEU:HD21	1.76	0.50
1:D:213:THR:HG22	1:D:239:GLY:C	2.36	0.50
1:I:112:LYS:HG3	1:I:113:LYS:N	2.26	0.50
1:C:148:VAL:HG13	1:C:170:LEU:HD12	1.94	0.50
1:B:213:THR:HG22	1:B:239:GLY:C	2.37	0.50
1:D:196:GLU:OE1	1:D:196:GLU:N	2.37	0.50
1:K:78:ARG:HD3	1:K:81:ARG:HB3	1.94	0.50
1:D:126:VAL:HG11	1:D:201:LEU:HD22	1.93	0.49
1:K:105:PHE:CD2	1:K:106:LEU:HD22	2.47	0.49
1:M:196:GLU:O	1:M:200:LYS:HG3	2.12	0.49
1:J:107:GLN:HE21	1:J:140:LEU:H	1.59	0.49
1:J:230:MET:HB3	1:J:234:GLU:HB2	1.94	0.49
1:F:180:PRO:HG3	3:F:401:HOH:O	2.12	0.49
1:M:176:MET:HG2	1:M:178:HIS:N	2.28	0.49
1:K:141:ASN:OD1	1:K:141:ASN:N	2.46	0.49
1:E:233:MET:O	1:E:237:GLU:HG3	2.12	0.49
1:F:231:SER:OG	1:F:234:GLU:HG3	2.13	0.49
1:C:196:GLU:HG3	1:K:199:MET:HE1	1.95	0.49
1:D:85:VAL:HG13	1:D:102:GLN:OE1	2.12	0.49
1:E:203:LYS:HA	1:E:206:TYR:CD2	2.48	0.49
1:J:228:ARG:O	1:J:229:TYR:HD1	1.96	0.49
1:L:113:LYS:O	1:L:141:ASN:ND2	2.43	0.49
1:A:139:ILE:HD11	1:A:143:ILE:HD11	1.94	0.48
1:K:156:SER:OG	1:K:209:TYR:OH	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:156:SER:HG	1:N:209:TYR:HH	1.61	0.48
1:D:176:MET:HE3	1:D:229:TYR:CE1	2.48	0.48
1:H:102:GLN:HG3	1:I:75:ILE:CD1	2.42	0.48
1:H:197:GLU:OE1	1:I:229:TYR:HB2	2.14	0.48
1:M:105:PHE:HB3	1:N:75:ILE:HD11	1.95	0.48
1:F:196:GLU:OE2	1:H:199:MET:HE1	2.14	0.48
1:H:228:ARG:NH2	1:H:234:GLU:OE1	2.46	0.48
1:J:74:ASP:C	1:J:76:TYR:H	2.22	0.48
1:L:85:VAL:O	1:L:117:MET:HA	2.14	0.48
1:B:117:MET:HB2	1:B:117:MET:HE3	1.67	0.48
1:E:206:TYR:OH	1:I:196:GLU:OE2	2.26	0.48
1:K:97:SER:HB2	1:L:88:MET:HE1	1.96	0.48
1:G:194:GLN:HE21	1:N:202:LYS:NZ	2.12	0.48
1:J:159:LEU:HD21	1:J:241:LEU:HD23	1.96	0.48
1:I:96:ALA:HB2	1:I:128:ALA:HB1	1.95	0.48
1:A:171:PRO:HG3	1:A:246:VAL:HG12	1.95	0.48
1:K:86:CYS:HB3	1:K:88:MET:HG2	1.95	0.48
1:K:176:MET:HE3	1:K:229:TYR:CE1	2.49	0.48
1:L:143:ILE:H	1:L:163:THR:CG2	2.25	0.48
1:N:144:ARG:NH2	1:N:166:MET:HG2	2.29	0.48
1:G:147:CYS:HB2	1:G:159:LEU:HD13	1.96	0.48
1:I:154:MET:HE1	1:I:205:LEU:HD11	1.95	0.48
1:F:139:ILE:HD11	1:F:143:ILE:HD11	1.96	0.47
1:G:81:ARG:HG2	1:G:81:ARG:HH11	1.79	0.47
1:I:169:SER:HB2	1:I:241:LEU:HD22	1.96	0.47
1:L:199:MET:O	1:L:203:LYS:HG2	2.14	0.47
1:A:84:ILE:HG12	1:A:116:HIS:HB2	1.96	0.47
1:B:209:TYR:O	1:B:213:THR:OG1	2.21	0.47
1:E:194:GLN:OE1	1:I:202:LYS:NZ	2.48	0.47
1:H:134:ASP:HB3	1:I:170:LEU:HD13	1.95	0.47
1:K:204:GLN:O	1:K:208:ILE:HD13	2.13	0.47
1:A:176:MET:HB2	1:A:229:TYR:CD2	2.49	0.47
1:I:202:LYS:HG3	1:I:206:TYR:CZ	2.49	0.47
1:I:141:ASN:OD1	1:I:141:ASN:N	2.47	0.47
1:I:230:MET:HA	1:I:234:GLU:OE1	2.14	0.47
1:J:105:PHE:HA	2:K:301:PJF:C19	2.43	0.47
1:J:197:GLU:HG2	1:K:228:ARG:HG3	1.95	0.47
1:A:199:MET:HE2	1:A:203:LYS:HE3	1.97	0.47
1:A:197:GLU:HG2	1:B:229:TYR:CD2	2.49	0.47
1:B:236:GLN:HB2	1:B:241:LEU:HD12	1.97	0.47
1:D:168:HIS:HD2	1:D:245:LEU:HD11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:ASP:HB3	1:G:170:LEU:HD13	1.95	0.47
1:F:218:GLN:NE2	1:F:222:SER:OG	2.48	0.47
1:I:201:LEU:HD21	1:J:174:ARG:HD3	1.96	0.47
1:K:197:GLU:OE2	1:L:229:TYR:HD1	1.97	0.47
1:K:206:TYR:CE1	1:K:224:MET:HE2	2.50	0.47
1:K:213:THR:HG22	1:K:239:GLY:C	2.40	0.47
1:H:161:ALA:HA	1:H:212:HIS:ND1	2.29	0.47
1:K:171:PRO:HG3	1:K:246:VAL:HG22	1.97	0.47
1:M:201:LEU:HG	3:M:401:HOH:O	2.14	0.47
1:N:176:MET:SD	1:N:178:HIS:HB3	2.54	0.47
1:N:78:ARG:H	1:N:78:ARG:CD	2.03	0.47
1:N:144:ARG:HH21	1:N:166:MET:HG2	1.80	0.47
1:B:179:GLN:O	1:L:194:GLN:NE2	2.32	0.47
1:K:80:LEU:HD11	1:K:106:LEU:CD2	2.31	0.47
1:C:199:MET:O	1:C:203:LYS:HG3	2.15	0.46
1:J:134:ASP:HB3	1:K:170:LEU:HD12	1.97	0.46
1:D:76:TYR:HD1	1:D:79:LEU:HD12	1.80	0.46
1:L:94:SER:O	1:L:97:SER:OG	2.28	0.46
1:M:226:ARG:NH2	1:M:228:ARG:HH21	2.13	0.46
1:L:197:GLU:OE1	1:M:174:ARG:NH1	2.49	0.46
1:A:195:ALA:HA	1:A:198:ILE:HD12	1.98	0.46
1:L:126:VAL:O	1:L:154:MET:HE2	2.15	0.46
1:L:222:SER:O	1:L:225:GLU:HG2	2.15	0.46
1:F:217:LEU:O	1:F:221:GLU:HG3	2.16	0.46
1:A:105:PHE:HE1	1:B:78:ARG:NH1	2.13	0.46
1:C:206:TYR:OH	1:K:196:GLU:OE1	2.32	0.46
1:D:231:SER:OG	1:D:234:GLU:HG3	2.15	0.46
1:M:176:MET:CB	1:M:229:TYR:HE1	2.23	0.46
1:J:190:ASP:HB2	3:J:402:HOH:O	2.16	0.46
1:L:157:LEU:HD21	1:L:208:ILE:HG21	1.98	0.46
1:L:213:THR:HG22	1:L:239:GLY:C	2.41	0.46
1:F:199:MET:O	1:F:203:LYS:HG3	2.15	0.46
1:H:84:ILE:HG12	1:H:116:HIS:HB2	1.97	0.46
1:H:170:LEU:HD23	1:H:170:LEU:HA	1.76	0.46
1:I:176:MET:HE2	1:I:229:TYR:CZ	2.51	0.46
1:L:82:GLU:OE2	2:L:301:PJF:C16	2.63	0.46
1:D:171:PRO:HG3	1:D:246:VAL:HG22	1.98	0.45
1:K:105:PHE:HA	2:L:301:PJF:C19	2.46	0.45
1:N:132:ILE:O	1:N:136:MET:HG3	2.16	0.45
1:K:105:PHE:HD2	1:K:106:LEU:HD22	1.80	0.45
1:L:170:LEU:HB3	1:L:171:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:MET:HE1	1:H:196:GLU:OE2	2.15	0.45
1:I:138:TYR:CE1	1:J:248:PRO:HD3	2.51	0.45
1:I:197:GLU:CD	1:J:174:ARG:NH2	2.74	0.45
1:M:102:GLN:HA	1:N:75:ILE:CD1	2.47	0.45
1:D:126:VAL:HG12	1:D:201:LEU:HD22	1.98	0.45
1:E:174:ARG:HA	1:E:174:ARG:HD3	1.60	0.45
1:E:176:MET:SD	1:E:178:HIS:HB3	2.57	0.45
1:F:144:ARG:HE	1:F:166:MET:HE2	1.81	0.45
1:H:170:LEU:HD13	1:N:134:ASP:HB3	1.98	0.45
1:K:78:ARG:CD	1:K:81:ARG:HB3	2.47	0.45
1:L:178:HIS:HA	1:L:224:MET:SD	2.56	0.45
1:H:100:ILE:O	1:H:104:LEU:HD22	2.17	0.45
1:A:148:VAL:HG12	1:A:170:LEU:HD12	1.99	0.45
1:B:144:ARG:HE	1:B:166:MET:HE2	1.82	0.45
1:F:144:ARG:HG2	1:F:166:MET:HB3	1.99	0.45
1:I:197:GLU:CD	1:J:174:ARG:CZ	2.90	0.45
1:I:236:GLN:HB2	1:I:241:LEU:HD12	1.99	0.45
1:J:146:TRP:HZ3	1:J:245:LEU:CD2	2.29	0.45
1:K:209:TYR:O	1:K:213:THR:OG1	2.27	0.45
1:M:96:ALA:HA	1:M:132:ILE:HD11	1.98	0.45
1:M:203:LYS:HE3	1:M:221:GLU:OE2	2.17	0.45
1:N:220:ILE:O	1:N:224:MET:HG3	2.16	0.45
1:I:134:ASP:CB	1:J:170:LEU:HD13	2.47	0.45
1:L:176:MET:HG2	1:L:178:HIS:H	1.82	0.45
1:B:139:ILE:HD11	1:B:143:ILE:HD11	1.98	0.44
1:L:177:ILE:HG13	1:L:224:MET:SD	2.57	0.44
1:J:96:ALA:HA	1:J:132:ILE:HD11	1.98	0.44
1:C:144:ARG:HE	1:C:166:MET:HG2	1.83	0.44
1:H:85:VAL:HG13	1:H:102:GLN:OE1	2.18	0.44
1:I:100:ILE:HG23	1:I:135:THR:HG21	1.99	0.44
1:L:142:PRO:HB3	1:L:166:MET:HE1	1.99	0.44
1:A:197:GLU:OE2	1:B:174:ARG:NE	2.44	0.44
1:N:76:TYR:O	1:N:79:LEU:HB2	2.18	0.44
1:N:107:GLN:HG3	1:N:141:ASN:OD1	2.18	0.44
1:A:75:ILE:HD11	1:G:80:LEU:CD2	2.46	0.44
1:D:168:HIS:CD2	1:D:243:LYS:HD2	2.53	0.44
1:J:144:ARG:HH21	1:J:168:HIS:CE1	2.34	0.44
1:J:150:GLN:CB	1:J:174:ARG:HB2	2.48	0.44
1:L:136:MET:C	1:L:138:TYR:H	2.25	0.44
1:M:147:CYS:HB2	1:M:159:LEU:HD13	2.00	0.44
1:F:199:MET:HG2	1:H:199:MET:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:235:ALA:HB1	1:J:240:ILE:HB	1.99	0.44
1:L:97:SER:OG	1:L:98:LEU:N	2.51	0.44
1:A:206:TYR:CD1	1:A:224:MET:HE2	2.53	0.44
1:F:225:GLU:OE2	1:I:226:ARG:NH2	2.51	0.44
1:H:127:THR:OG1	3:H:401:HOH:O	2.21	0.44
1:N:230:MET:HE1	1:N:238:PHE:CG	2.53	0.44
1:D:204:GLN:HE22	1:E:174:ARG:CZ	2.29	0.44
1:J:236:GLN:HB2	1:J:241:LEU:HD12	1.99	0.44
1:K:236:GLN:HB2	1:K:241:LEU:CD1	2.47	0.44
1:L:176:MET:SD	1:L:178:HIS:HB3	2.58	0.44
1:C:107:GLN:HE21	1:C:140:LEU:HG	1.81	0.43
1:F:74:ASP:CG	1:F:75:ILE:H	2.25	0.43
1:I:217:LEU:O	1:I:221:GLU:HG3	2.18	0.43
1:F:169:SER:HB2	1:F:241:LEU:HD22	1.99	0.43
1:C:107:GLN:HE21	1:C:140:LEU:H	1.66	0.43
1:F:217:LEU:HD12	1:F:217:LEU:HA	1.84	0.43
1:H:131:ALA:HB1	1:I:148:VAL:HG22	2.01	0.43
1:J:74:ASP:OD1	1:J:76:TYR:HB2	2.18	0.43
1:N:176:MET:HB2	1:N:229:TYR:CD2	2.54	0.43
1:A:110:SER:O	1:A:141:ASN:ND2	2.48	0.43
1:B:201:LEU:HD23	1:C:174:ARG:NH2	2.33	0.43
1:D:230:MET:HB3	1:D:234:GLU:HB2	1.98	0.43
1:J:138:TYR:CE1	1:K:248:PRO:HG3	2.53	0.43
1:J:228:ARG:NH1	1:J:229:TYR:O	2.51	0.43
1:B:203:LYS:HA	1:B:206:TYR:HD2	1.84	0.43
1:C:196:GLU:OE2	1:K:199:MET:HE1	2.19	0.43
1:E:203:LYS:O	1:E:207:ASN:ND2	2.44	0.43
1:E:226:ARG:HH21	1:J:225:GLU:CD	2.27	0.43
1:K:83:ARG:HA	1:K:106:LEU:CD1	2.49	0.43
1:L:236:GLN:NE2	1:L:242:ASP:O	2.52	0.43
1:M:102:GLN:O	1:M:106:LEU:HD13	2.18	0.43
1:N:139:ILE:HD11	1:N:143:ILE:HD11	2.00	0.43
1:I:136:MET:HB3	1:I:143:ILE:HD13	2.00	0.43
1:K:167:ARG:HE	1:K:167:ARG:HB2	1.64	0.43
1:M:146:TRP:CD2	1:M:168:HIS:CD2	3.07	0.43
1:C:217:LEU:CD1	1:C:221:GLU:OE2	2.67	0.43
1:E:169:SER:HB2	1:E:241:LEU:HD22	2.00	0.43
1:N:83:ARG:HG2	1:N:106:LEU:HD12	2.01	0.43
1:D:110:SER:O	1:D:141:ASN:ND2	2.46	0.43
1:M:86:CYS:HB3	1:M:88:MET:HG2	2.00	0.43
1:A:88:MET:SD	1:A:120:ASN:HB3	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:MET:HB2	1:A:117:MET:HE3	1.72	0.43
1:A:147:CYS:HB2	1:A:159:LEU:HD13	2.01	0.43
1:F:202:LYS:HD2	1:H:195:ALA:CB	2.49	0.43
1:H:105:PHE:CE1	1:I:78:ARG:NH2	2.87	0.43
1:L:195:ALA:HA	1:L:198:ILE:HD12	2.01	0.43
1:L:197:GLU:OE1	1:M:174:ARG:HD2	2.19	0.43
1:N:146:TRP:CZ3	1:N:245:LEU:HD12	2.54	0.43
1:N:209:TYR:O	1:N:213:THR:OG1	2.21	0.43
1:B:110:SER:O	1:B:141:ASN:ND2	2.48	0.42
1:I:84:ILE:HA	1:I:116:HIS:O	2.19	0.42
1:J:174:ARG:NH2	1:J:229:TYR:CG	2.86	0.42
1:L:78:ARG:HH12	1:L:82:GLU:H	1.64	0.42
1:M:248:PRO:HA	1:M:249:PRO:HD2	1.75	0.42
1:A:134:ASP:HB3	1:B:170:LEU:HD13	2.01	0.42
1:B:236:GLN:HE21	1:B:242:ASP:C	2.19	0.42
1:C:107:GLN:HB3	3:C:404:HOH:O	2.19	0.42
1:G:170:LEU:HD23	1:G:170:LEU:HA	1.86	0.42
1:K:161:ALA:HA	1:K:212:HIS:ND1	2.33	0.42
1:J:100:ILE:HG21	2:K:301:PJF:N1	2.34	0.42
1:L:115:ILE:HD12	1:L:139:ILE:HD12	2.02	0.42
1:E:201:LEU:HD12	1:E:201:LEU:HA	1.71	0.42
1:H:117:MET:HB2	1:H:117:MET:HE3	1.75	0.42
1:J:105:PHE:HB2	2:K:301:PJF:CL1	2.57	0.42
1:L:148:VAL:HG22	1:L:170:LEU:HD22	2.01	0.42
1:A:107:GLN:HG3	1:A:141:ASN:OD1	2.19	0.42
1:D:144:ARG:HH22	1:D:243:LYS:NZ	2.16	0.42
1:D:148:VAL:HG21	2:D:301:PJF:C1	2.50	0.42
1:J:101:ALA:HB1	1:K:79:LEU:HD11	2.01	0.42
1:J:107:GLN:HG3	1:J:141:ASN:OD1	2.18	0.42
1:K:107:GLN:HG3	1:K:141:ASN:OD1	2.20	0.42
1:B:200:LYS:HA	1:B:203:LYS:CE	2.46	0.42
1:K:147:CYS:HB3	1:K:169:SER:HB2	2.02	0.42
1:M:213:THR:HG22	1:M:239:GLY:C	2.45	0.42
1:D:165:GLY:N	1:D:242:ASP:OD2	2.53	0.42
1:H:92:ASP:OD1	1:H:95:VAL:HG23	2.20	0.42
1:J:98:LEU:HD13	1:K:76:TYR:OH	2.20	0.42
1:L:171:PRO:HG3	1:L:246:VAL:HG12	2.02	0.42
1:L:236:GLN:HB2	1:L:241:LEU:CD1	2.50	0.42
1:B:131:ALA:HB1	1:C:148:VAL:HG12	2.02	0.42
1:D:201:LEU:HD23	1:E:174:ARG:NH2	2.35	0.42
1:L:236:GLN:HB2	1:L:241:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:MET:HE3	1:C:202:LYS:HB3	2.01	0.42
1:D:84:ILE:HG12	1:D:116:HIS:HB2	2.01	0.42
1:F:171:PRO:CG	1:F:246:VAL:HG22	2.48	0.42
1:K:127:THR:HG21	1:L:174:ARG:CZ	2.49	0.42
1:L:78:ARG:HH12	1:L:82:GLU:CA	2.32	0.42
1:L:177:ILE:C	1:L:224:MET:SD	3.03	0.42
1:M:200:LYS:HD3	1:N:174:ARG:HH12	1.85	0.42
1:B:171:PRO:O	1:B:232:PRO:HG2	2.20	0.42
1:A:206:TYR:CE2	1:A:221:GLU:HG2	2.55	0.41
1:C:85:VAL:HG13	1:C:102:GLN:OE1	2.19	0.41
1:C:170:LEU:HD23	1:C:170:LEU:HA	1.80	0.41
1:C:208:ILE:HD11	1:D:172:ASN:OD1	2.20	0.41
1:D:206:TYR:HB3	1:D:217:LEU:CD2	2.50	0.41
1:I:230:MET:HB3	1:I:234:GLU:HB2	2.01	0.41
1:J:213:THR:HG22	1:J:239:GLY:C	2.45	0.41
1:L:82:GLU:HG2	2:L:301:PJF:C22	2.50	0.41
1:M:83:ARG:NH1	1:M:106:LEU:O	2.47	0.41
1:E:75:ILE:HD12	1:E:75:ILE:HA	1.95	0.41
1:H:96:ALA:HB2	1:H:128:ALA:HB1	2.01	0.41
1:K:168:HIS:HD2	1:K:245:LEU:HD11	1.85	0.41
1:N:141:ASN:OD1	1:N:141:ASN:N	2.53	0.41
1:F:170:LEU:HD23	1:F:170:LEU:HA	1.80	0.41
1:J:150:GLN:HB2	1:J:174:ARG:HB2	2.01	0.41
1:K:83:ARG:HH12	1:K:109:GLU:HB2	1.85	0.41
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.74	0.41
1:L:148:VAL:HG21	2:L:301:PJF:C1	2.51	0.41
1:L:207:ASN:ND2	3:L:405:HOH:O	2.53	0.41
1:A:171:PRO:CG	1:A:246:VAL:HG12	2.50	0.41
1:A:230:MET:HB3	1:A:234:GLU:HB3	2.02	0.41
1:B:197:GLU:OE2	1:C:228:ARG:HB2	2.21	0.41
1:C:107:GLN:NE2	1:C:140:LEU:H	2.18	0.41
1:G:114:PRO:HB3	1:G:142:PRO:HG2	2.01	0.41
1:I:196:GLU:O	1:I:200:LYS:HG3	2.20	0.41
1:K:80:LEU:HA	1:K:80:LEU:HD12	1.60	0.41
1:L:134:ASP:OD2	1:M:172:ASN:N	2.35	0.41
1:N:240:ILE:HG22	1:N:241:LEU:HD23	2.02	0.41
1:C:134:ASP:CG	1:D:171:PRO:HD2	2.46	0.41
1:K:146:TRP:HH2	1:K:245:LEU:HD22	1.85	0.41
1:C:213:THR:HG22	1:C:239:GLY:C	2.45	0.41
1:E:236:GLN:HB2	1:E:241:LEU:CD1	2.50	0.41
1:H:206:TYR:CD1	1:H:224:MET:HE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:LEU:HA	1:I:80:LEU:HD12	1.81	0.41
1:M:80:LEU:HD12	1:M:80:LEU:HA	1.92	0.41
1:N:85:VAL:HG13	1:N:102:GLN:OE1	2.21	0.41
1:A:153:SER:HB2	1:A:180:PRO:HD3	2.02	0.41
1:J:74:ASP:HB3	1:J:77:SER:OG	2.21	0.41
1:C:180:PRO:O	1:K:194:GLN:NE2	2.54	0.41
1:D:232:PRO:HG2	3:D:407:HOH:O	2.20	0.41
1:E:195:ALA:CB	1:I:198:ILE:HG22	2.51	0.41
1:E:198:ILE:HG22	1:I:195:ALA:CB	2.51	0.41
1:E:198:ILE:HG22	1:I:195:ALA:HB2	2.03	0.41
1:H:105:PHE:HE1	1:I:78:ARG:NH2	2.19	0.41
1:J:204:GLN:HE21	1:J:204:GLN:HB3	1.58	0.41
1:L:107:GLN:HG3	3:L:401:HOH:O	2.20	0.41
1:L:134:ASP:HB3	1:M:170:LEU:HB3	2.03	0.41
1:C:197:GLU:HG2	1:D:229:TYR:CD1	2.56	0.41
1:D:169:SER:HB2	1:D:241:LEU:HD22	2.02	0.41
1:J:228:ARG:NH2	1:J:230:MET:HG2	2.30	0.41
1:L:196:GLU:O	1:L:200:LYS:HG3	2.21	0.41
1:E:170:LEU:HB3	1:E:171:PRO:HD2	2.02	0.40
1:E:230:MET:HB3	1:E:234:GLU:HB2	2.03	0.40
1:M:176:MET:HB2	1:M:229:TYR:HD1	1.75	0.40
1:A:197:GLU:OE1	1:B:229:TYR:HB2	2.21	0.40
1:B:126:VAL:HG11	1:B:201:LEU:HD22	2.04	0.40
1:B:236:GLN:HB2	1:B:241:LEU:CD1	2.50	0.40
1:C:194:GLN:HA	1:C:194:GLN:HE21	1.86	0.40
1:J:147:CYS:HB2	1:J:159:LEU:HD13	2.03	0.40
1:L:224:MET:HB3	1:L:224:MET:HE3	1.76	0.40
1:D:211:LYS:HG2	1:D:212:HIS:CD2	2.57	0.40
1:G:251:ASP:OD2	1:G:251:ASP:N	2.55	0.40
1:J:138:TYR:CD1	1:J:138:TYR:C	3.00	0.40
1:M:176:MET:CG	1:M:178:HIS:HB3	2.52	0.40
1:C:144:ARG:HE	1:C:166:MET:CG	2.34	0.40
1:D:217:LEU:HD23	1:D:217:LEU:HA	1.84	0.40
1:G:236:GLN:NE2	1:G:244:VAL:HG23	2.37	0.40
1:I:83:ARG:HH21	1:I:141:ASN:HD22	1.69	0.40
1:I:84:ILE:HG12	1:I:116:HIS:HB2	2.04	0.40
1:M:105:PHE:HB2	1:N:75:ILE:HD11	2.02	0.40
1:N:76:TYR:N	1:N:78:ARG:NH1	2.70	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%)	160 (98%)	4 (2%)	0	100	100
1	B	163/221 (74%)	159 (98%)	4 (2%)	0	100	100
1	C	163/221 (74%)	156 (96%)	6 (4%)	1 (1%)	21	44
1	D	164/221 (74%)	160 (98%)	4 (2%)	0	100	100
1	E	165/221 (75%)	160 (97%)	4 (2%)	1 (1%)	21	44
1	F	162/221 (73%)	158 (98%)	4 (2%)	0	100	100
1	G	164/221 (74%)	156 (95%)	6 (4%)	2 (1%)	10	27
1	H	162/221 (73%)	158 (98%)	4 (2%)	0	100	100
1	I	161/221 (73%)	155 (96%)	6 (4%)	0	100	100
1	J	163/221 (74%)	156 (96%)	5 (3%)	2 (1%)	10	27
1	K	166/221 (75%)	158 (95%)	6 (4%)	2 (1%)	10	27
1	L	160/221 (72%)	154 (96%)	6 (4%)	0	100	100
1	M	162/221 (73%)	158 (98%)	4 (2%)	0	100	100
1	N	164/221 (74%)	160 (98%)	4 (2%)	0	100	100
All	All	2283/3094 (74%)	2208 (97%)	67 (3%)	8 (0%)	30	54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	180	PRO
1	G	75	ILE
1	J	75	ILE
1	K	191	ILE
1	G	249	PRO
1	J	192	ALA
1	K	190	ASP
1	E	249	PRO

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	146/185 (79%)	144 (99%)	2 (1%)	59	82
1	B	145/185 (78%)	144 (99%)	1 (1%)	76	90
1	C	145/185 (78%)	144 (99%)	1 (1%)	76	90
1	D	146/185 (79%)	145 (99%)	1 (1%)	76	90
1	E	147/185 (80%)	147 (100%)	0	100	100
1	F	144/185 (78%)	142 (99%)	2 (1%)	59	82
1	G	146/185 (79%)	144 (99%)	2 (1%)	59	82
1	H	144/185 (78%)	143 (99%)	1 (1%)	76	90
1	I	143/185 (77%)	139 (97%)	4 (3%)	38	68
1	J	145/185 (78%)	142 (98%)	3 (2%)	47	75
1	K	147/185 (80%)	144 (98%)	3 (2%)	48	76
1	L	142/185 (77%)	140 (99%)	2 (1%)	59	82
1	M	144/185 (78%)	142 (99%)	2 (1%)	59	82
1	N	145/185 (78%)	145 (100%)	0	100	100
All	All	2029/2590 (78%)	2005 (99%)	24 (1%)	63	84

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

Mol	Chain	Res	Type
1	A	190	ASP
1	A	217	LEU
1	B	222	SER
1	C	85	VAL
1	D	222	SER
1	F	85	VAL
1	F	202	LYS
1	G	74	ASP
1	G	163	THR
1	H	174	ARG
1	I	110	SER

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Mol	Chain	Res	Type
1	I	153	SER
1	I	216	SER
1	I	222	SER
1	J	75	ILE
1	J	197	GLU
1	J	202	LYS
1	K	108	SER
1	K	110	SER
1	K	247	HIS
1	L	245	LEU
1	L	247	HIS
1	M	163	THR
1	M	168	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	B	107	GLN
1	B	247	HIS
1	C	107	GLN
1	C	137	GLN
1	C	179	GLN
1	C	247	HIS
1	D	111	ASN
1	D	137	GLN
1	D	172	ASN
1	D	204	GLN
1	D	215	GLN
1	D	247	HIS
1	E	137	GLN
1	E	179	GLN
1	E	218	GLN
1	E	236	GLN
1	E	247	HIS
1	F	102	GLN
1	F	107	GLN
1	F	137	GLN
1	F	218	GLN
1	F	236	GLN
1	G	111	ASN
1	G	179	GLN

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Mol	Chain	Res	Type
1	G	194	GLN
1	G	247	HIS
1	H	218	GLN
1	H	247	HIS
1	I	102	GLN
1	J	107	GLN
1	J	172	ASN
1	J	204	GLN
1	K	102	GLN
1	K	107	GLN
1	K	137	GLN
1	K	172	ASN
1	K	179	GLN
1	K	204	GLN
1	K	247	HIS
1	L	102	GLN
1	L	116	HIS
1	L	120	ASN
1	M	172	ASN
1	M	179	GLN
1	M	194	GLN
1	M	247	HIS
1	N	107	GLN
1	N	179	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	PJF	J	301	-	35,35,35	0.73	1 (2%)	43,50,50	0.96	3 (6%)
2	PJF	M	301	-	35,35,35	0.80	2 (5%)	43,50,50	1.06	4 (9%)
2	PJF	I	301	-	35,35,35	0.71	1 (2%)	43,50,50	1.00	3 (6%)
2	PJF	D	301	-	35,35,35	0.76	2 (5%)	43,50,50	1.07	3 (6%)
2	PJF	G	301	-	35,35,35	0.77	1 (2%)	43,50,50	0.96	3 (6%)
2	PJF	E	301	-	35,35,35	0.73	1 (2%)	43,50,50	0.91	3 (6%)
2	PJF	A	301	-	35,35,35	0.75	1 (2%)	43,50,50	0.94	3 (6%)
2	PJF	H	301	-	35,35,35	0.75	1 (2%)	43,50,50	0.99	3 (6%)
2	PJF	N	301	-	35,35,35	0.73	1 (2%)	43,50,50	1.00	3 (6%)
2	PJF	K	301	-	35,35,35	0.80	2 (5%)	43,50,50	1.01	4 (9%)
2	PJF	L	301	-	35,35,35	0.88	2 (5%)	43,50,50	1.40	5 (11%)
2	PJF	B	301	-	35,35,35	0.72	1 (2%)	43,50,50	1.11	4 (9%)
2	PJF	F	301	-	35,35,35	0.72	1 (2%)	43,50,50	1.10	5 (11%)
2	PJF	C	301	-	35,35,35	0.70	1 (2%)	43,50,50	1.03	4 (9%)

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	PJF	J	301	-	-	0/10/25/25	0/5/5/5
2	PJF	M	301	-	-	0/10/25/25	0/5/5/5
2	PJF	I	301	-	-	0/10/25/25	0/5/5/5
2	PJF	D	301	-	-	0/10/25/25	0/5/5/5
2	PJF	G	301	-	-	0/10/25/25	0/5/5/5
2	PJF	E	301	-	-	1/10/25/25	0/5/5/5
2	PJF	A	301	-	-	0/10/25/25	0/5/5/5
2	PJF	H	301	-	-	0/10/25/25	0/5/5/5
2	PJF	N	301	-	-	1/10/25/25	0/5/5/5
2	PJF	K	301	-	-	0/10/25/25	0/5/5/5
2	PJF	L	301	-	-	0/10/25/25	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PJF	B	301	-	-	2/10/25/25	0/5/5/5
2	PJF	F	301	-	-	0/10/25/25	0/5/5/5
2	PJF	C	301	-	-	0/10/25/25	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	301	PJF	C13-N3	-3.15	1.34	1.40
2	L	301	PJF	C13-N3	-3.09	1.34	1.40
2	D	301	PJF	C13-N3	-2.70	1.35	1.40
2	M	301	PJF	C13-N3	-2.39	1.36	1.40
2	G	301	PJF	C13-N3	-2.39	1.36	1.40
2	E	301	PJF	C13-N3	-2.37	1.36	1.40
2	H	301	PJF	C13-N3	-2.33	1.36	1.40
2	N	301	PJF	C13-N3	-2.28	1.36	1.40
2	I	301	PJF	C13-N3	-2.27	1.36	1.40
2	A	301	PJF	C13-N3	-2.22	1.36	1.40
2	B	301	PJF	C13-N3	-2.16	1.36	1.40
2	J	301	PJF	C13-N3	-2.15	1.36	1.40
2	F	301	PJF	C13-N3	-2.15	1.36	1.40
2	M	301	PJF	C13-C11	-2.10	1.39	1.44
2	C	301	PJF	C13-N3	-2.09	1.36	1.40
2	D	301	PJF	C13-C11	-2.06	1.39	1.44
2	K	301	PJF	C13-C11	-2.06	1.39	1.44
2	L	301	PJF	C13-C11	-2.05	1.39	1.44

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	301	PJF	C22-C23-N5	-5.26	97.50	101.30
2	D	301	PJF	C2-C1-N1	-3.29	169.74	177.87
2	K	301	PJF	C11-C13-N3	3.00	120.37	115.16
2	B	301	PJF	C11-C13-N3	2.99	120.35	115.16
2	L	301	PJF	C11-C13-N3	2.98	120.34	115.16
2	F	301	PJF	C11-C13-N3	2.95	120.29	115.16
2	G	301	PJF	C11-C13-N3	2.94	120.27	115.16
2	H	301	PJF	C11-C13-N3	2.93	120.25	115.16
2	A	301	PJF	C11-C13-N3	2.91	120.21	115.16
2	N	301	PJF	C11-C13-N3	2.90	120.19	115.16
2	J	301	PJF	C11-C13-N3	2.89	120.18	115.16
2	C	301	PJF	C11-C13-N3	2.89	120.17	115.16
2	E	301	PJF	C11-C13-N3	2.88	120.16	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	301	PJF	C14-N3-C21	2.88	121.69	117.95
2	B	301	PJF	C7-N2-C12	2.88	114.16	110.51
2	D	301	PJF	C11-C13-N3	2.85	120.11	115.16
2	I	301	PJF	C11-C13-N3	2.81	120.05	115.16
2	K	301	PJF	C9-C10-N5	2.71	119.29	117.29
2	M	301	PJF	C11-C13-N3	2.67	119.79	115.16
2	B	301	PJF	O1-C13-C11	-2.66	120.01	125.06
2	F	301	PJF	O1-C13-C11	-2.65	120.01	125.06
2	H	301	PJF	O1-C13-C11	-2.64	120.05	125.06
2	A	301	PJF	O1-C13-C11	-2.63	120.06	125.06
2	J	301	PJF	O1-C13-C11	-2.63	120.07	125.06
2	G	301	PJF	O1-C13-C11	-2.62	120.08	125.06
2	D	301	PJF	O1-C13-C11	-2.61	120.09	125.06
2	I	301	PJF	O1-C13-C11	-2.60	120.11	125.06
2	M	301	PJF	O1-C13-C11	-2.60	120.11	125.06
2	L	301	PJF	O1-C13-C11	-2.60	120.12	125.06
2	L	301	PJF	C9-C10-N5	2.60	119.21	117.29
2	N	301	PJF	O1-C13-C11	-2.59	120.14	125.06
2	C	301	PJF	O1-C13-C11	-2.58	120.14	125.06
2	E	301	PJF	O1-C13-C11	-2.56	120.19	125.06
2	K	301	PJF	O1-C13-C11	-2.55	120.22	125.06
2	M	301	PJF	C22-C23-N5	-2.43	99.54	101.30
2	C	301	PJF	C2-C1-N1	-2.39	171.97	177.87
2	F	301	PJF	C2-C1-N1	-2.34	172.10	177.87
2	C	301	PJF	C14-N3-C13	2.29	120.95	117.72
2	F	301	PJF	C14-N3-C13	2.27	120.93	117.72
2	A	301	PJF	C14-N3-C13	2.27	120.92	117.72
2	I	301	PJF	C14-N3-C13	2.27	120.92	117.72
2	B	301	PJF	C14-N3-C13	2.26	120.91	117.72
2	J	301	PJF	C14-N3-C13	2.22	120.85	117.72
2	G	301	PJF	C14-N3-C13	2.20	120.83	117.72
2	E	301	PJF	C14-N3-C13	2.17	120.79	117.72
2	N	301	PJF	C14-N3-C13	2.12	120.71	117.72
2	K	301	PJF	C14-N3-C21	2.11	120.69	117.95
2	H	301	PJF	C14-N3-C13	2.10	120.68	117.72
2	F	301	PJF	C3-C2-C1	-2.07	116.60	119.97
2	M	301	PJF	C12-C11-C10	2.01	122.37	120.61

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	PJF	C6-C7-N2-C12
2	B	301	PJF	C6-C7-N2-C8
2	E	301	PJF	N1-C1-C2-C3
2	N	301	PJF	N1-C1-C2-C3

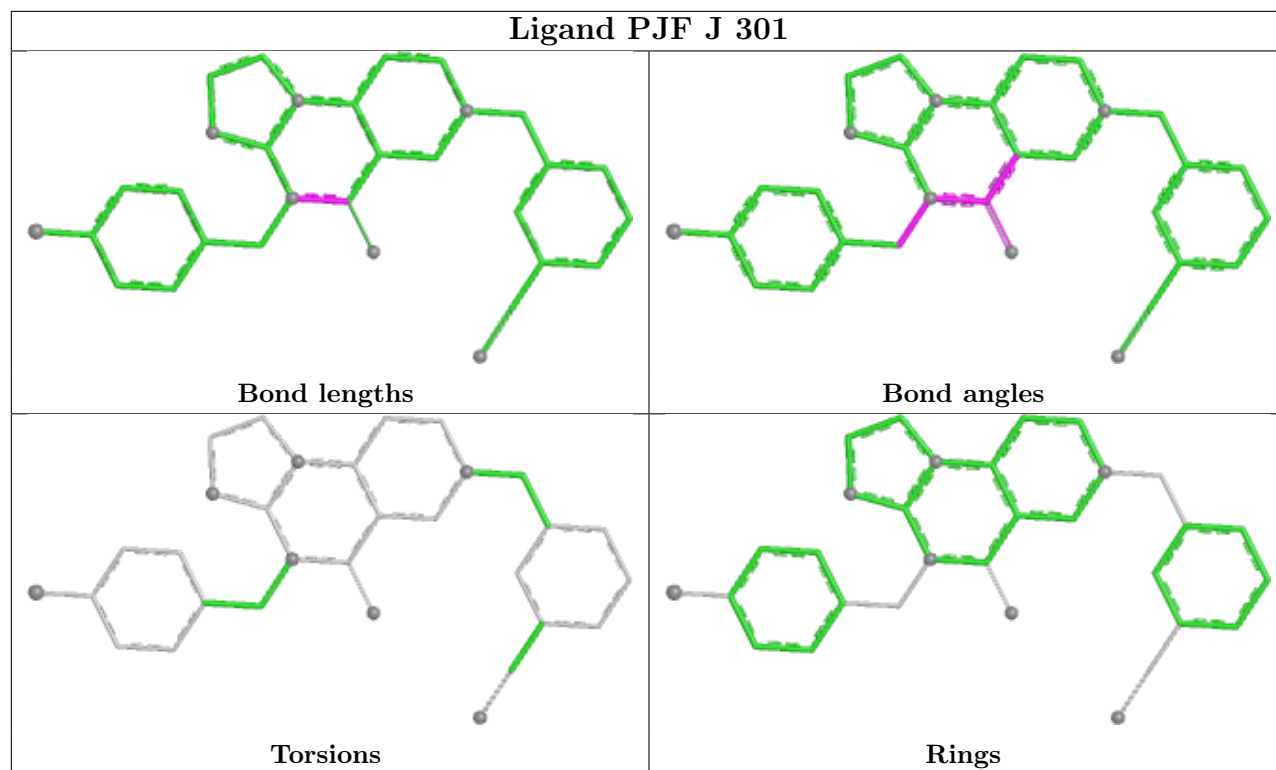
There are no ring outliers.

5 monomers are involved in 13 short contacts:

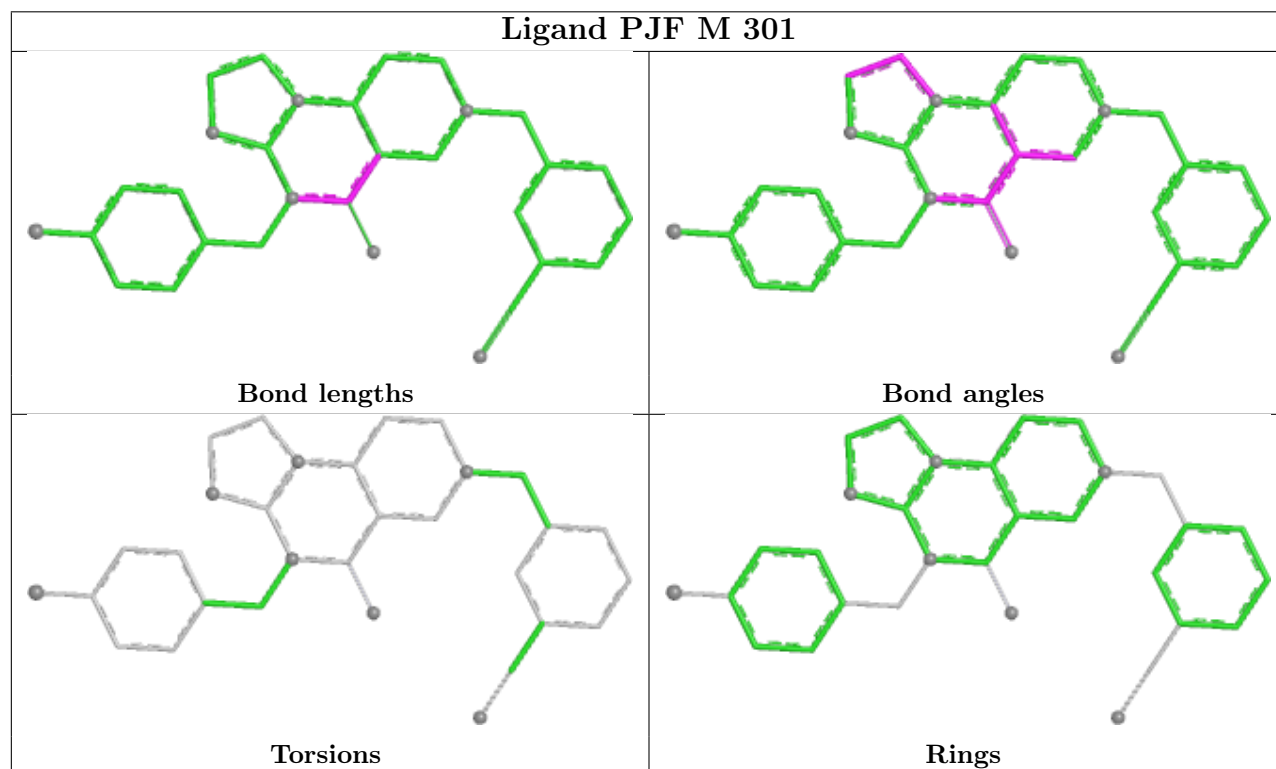
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	301	PJF	1	0
2	D	301	PJF	1	0
2	K	301	PJF	4	0
2	L	301	PJF	6	0
2	C	301	PJF	1	0

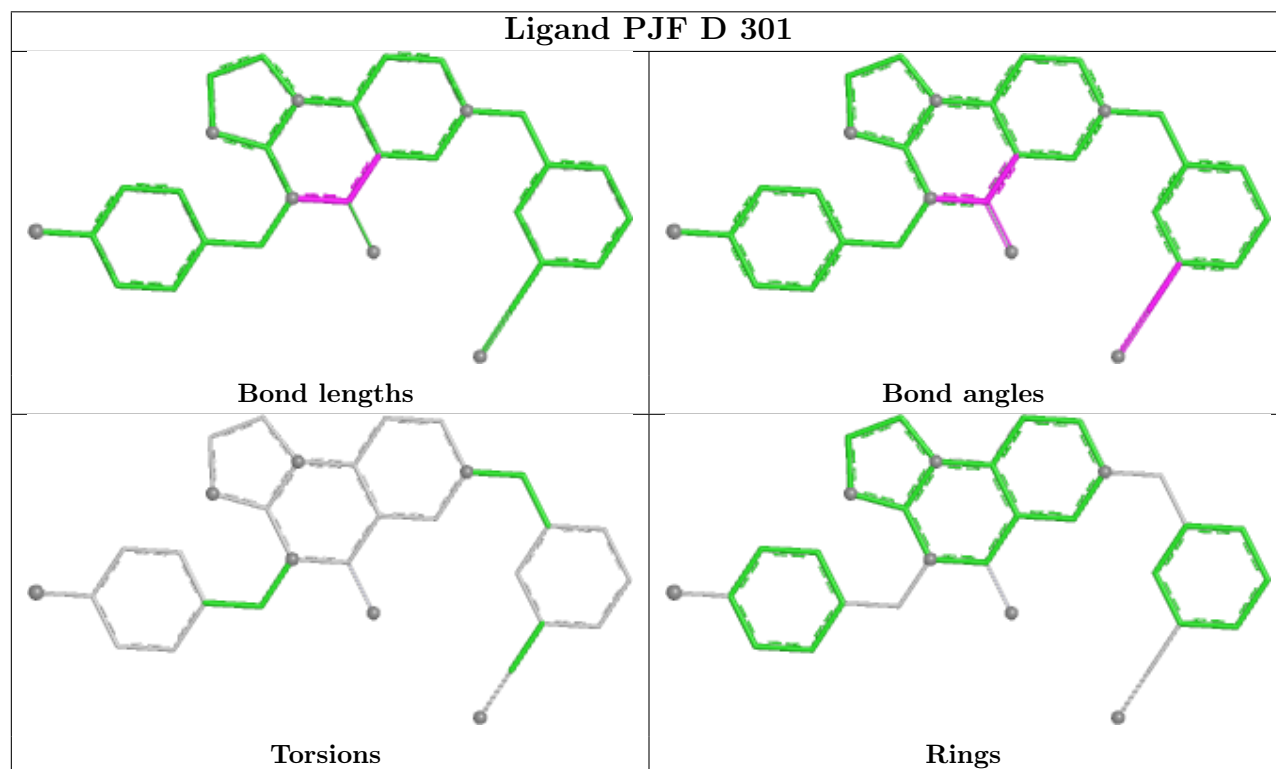
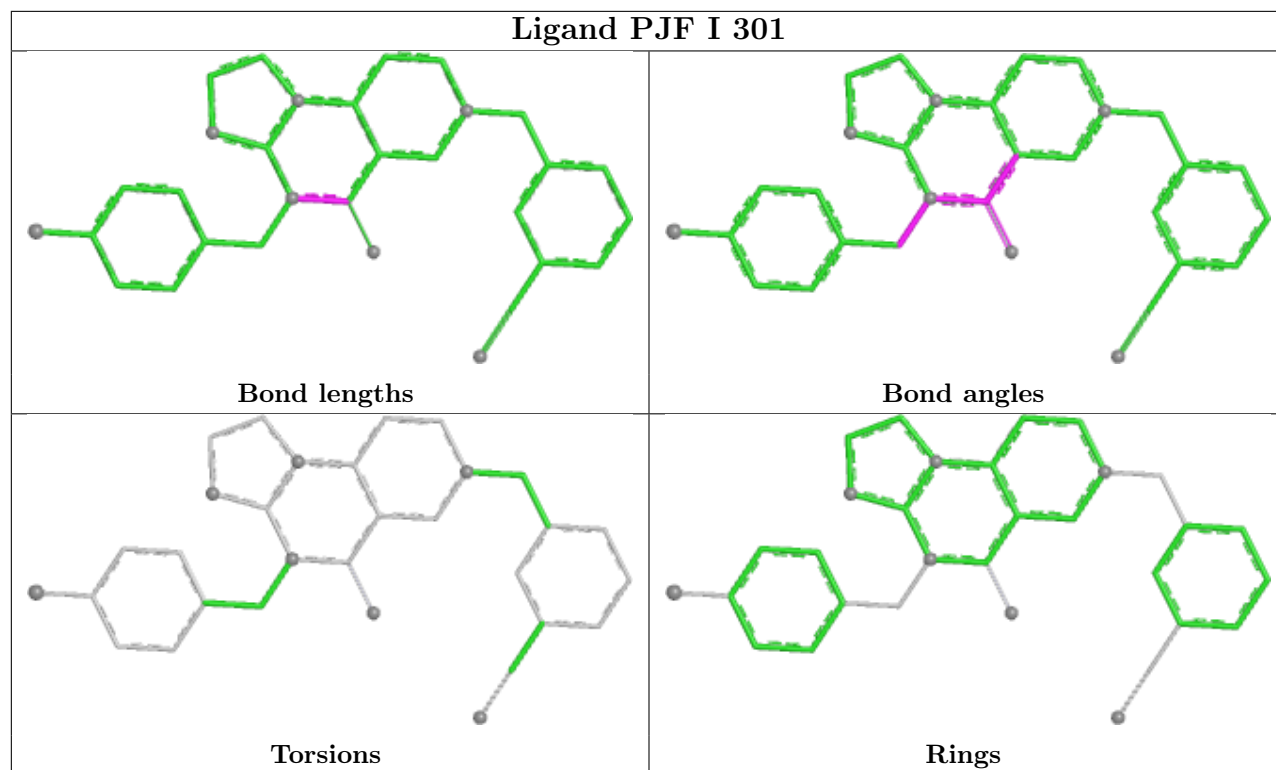
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

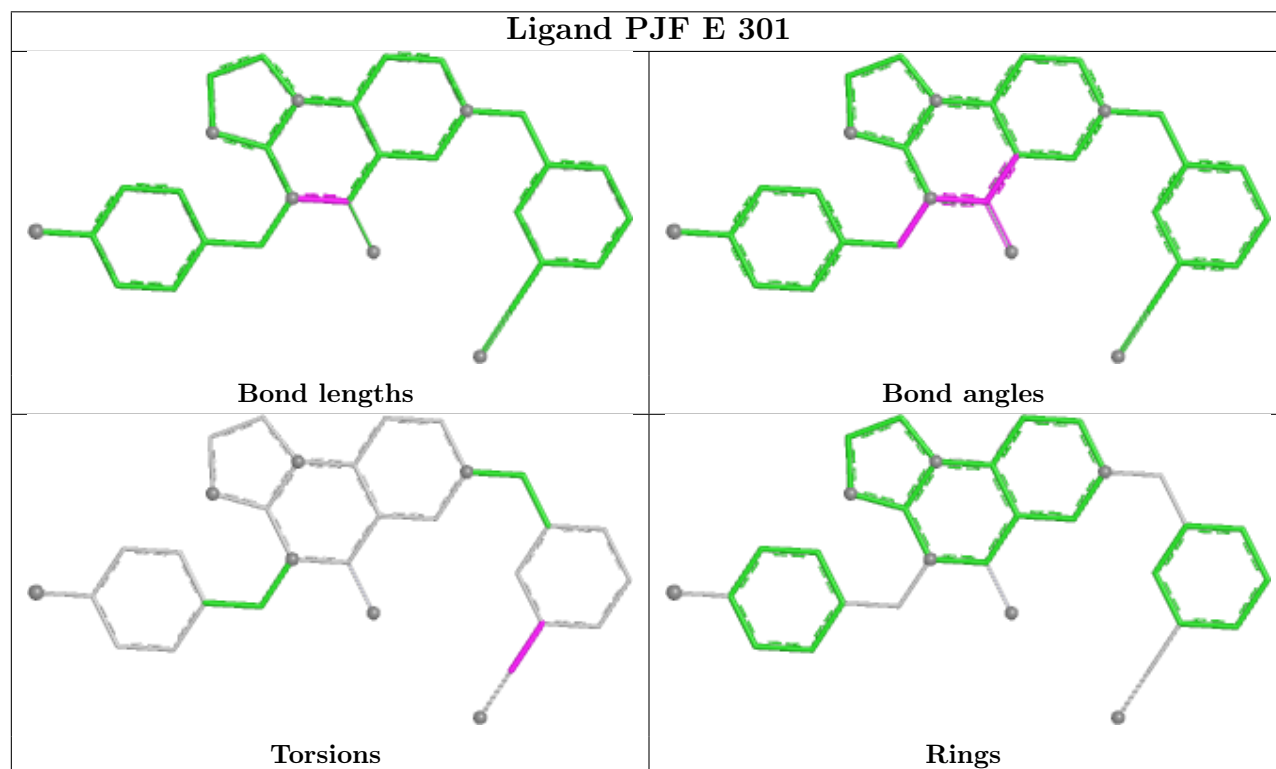
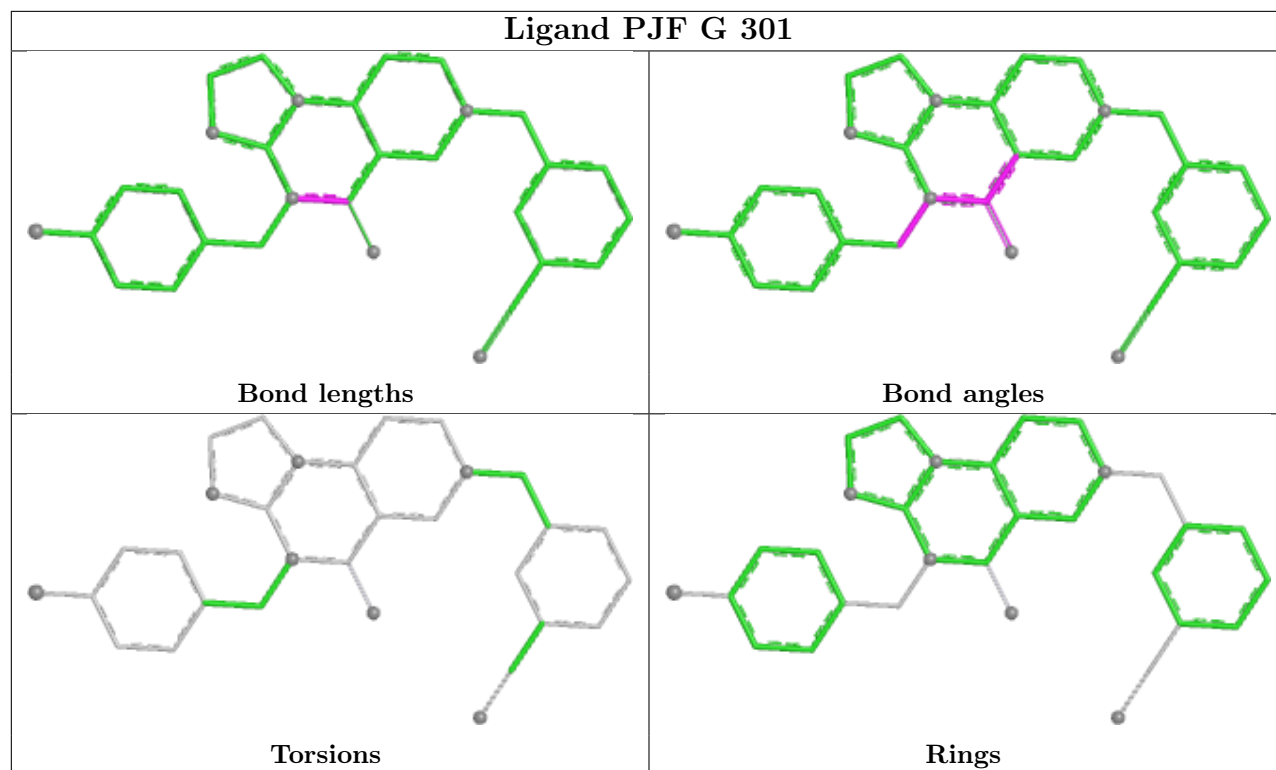
Ligand PJF J 301

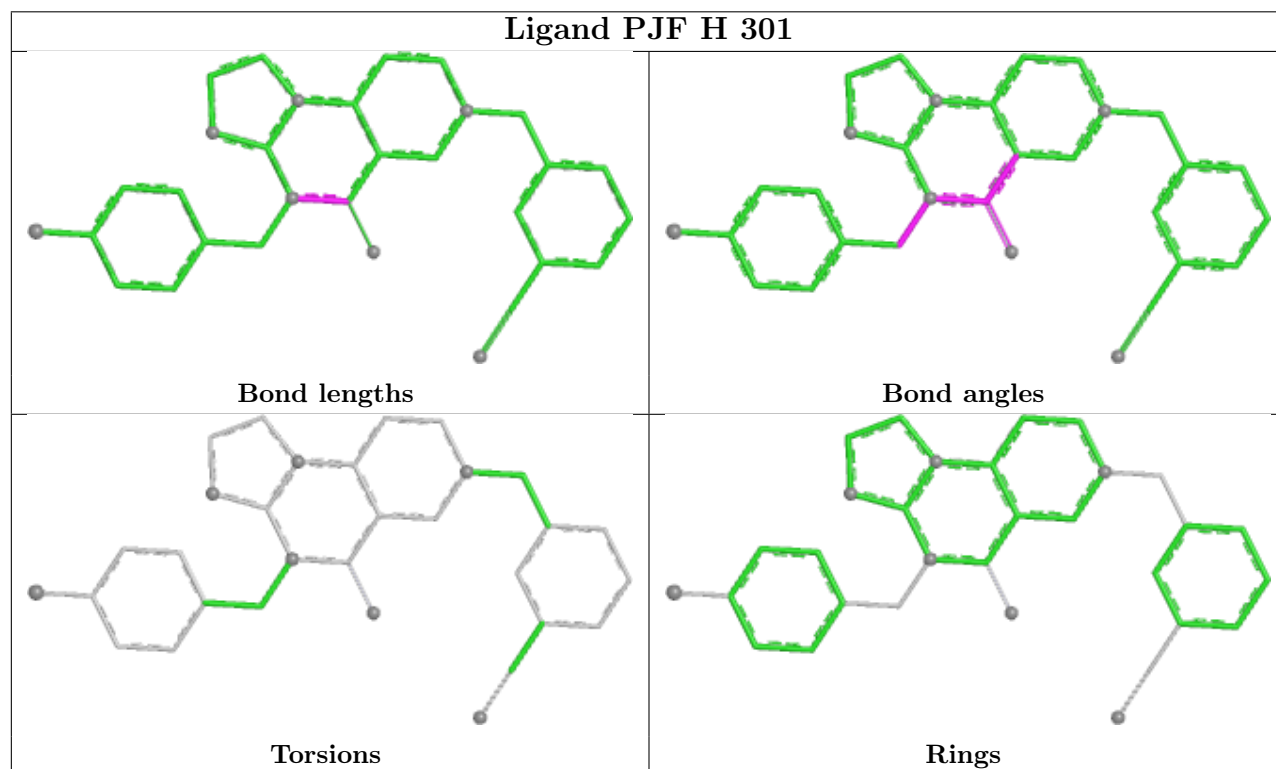
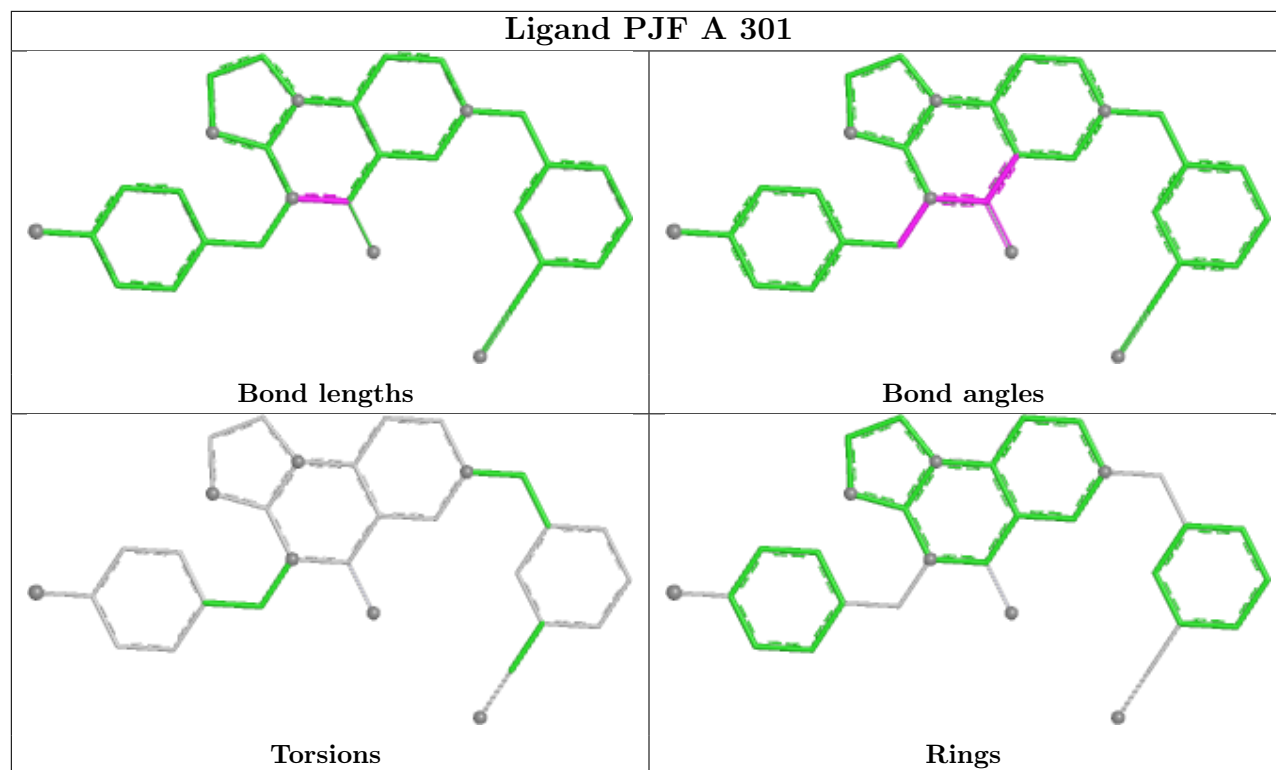


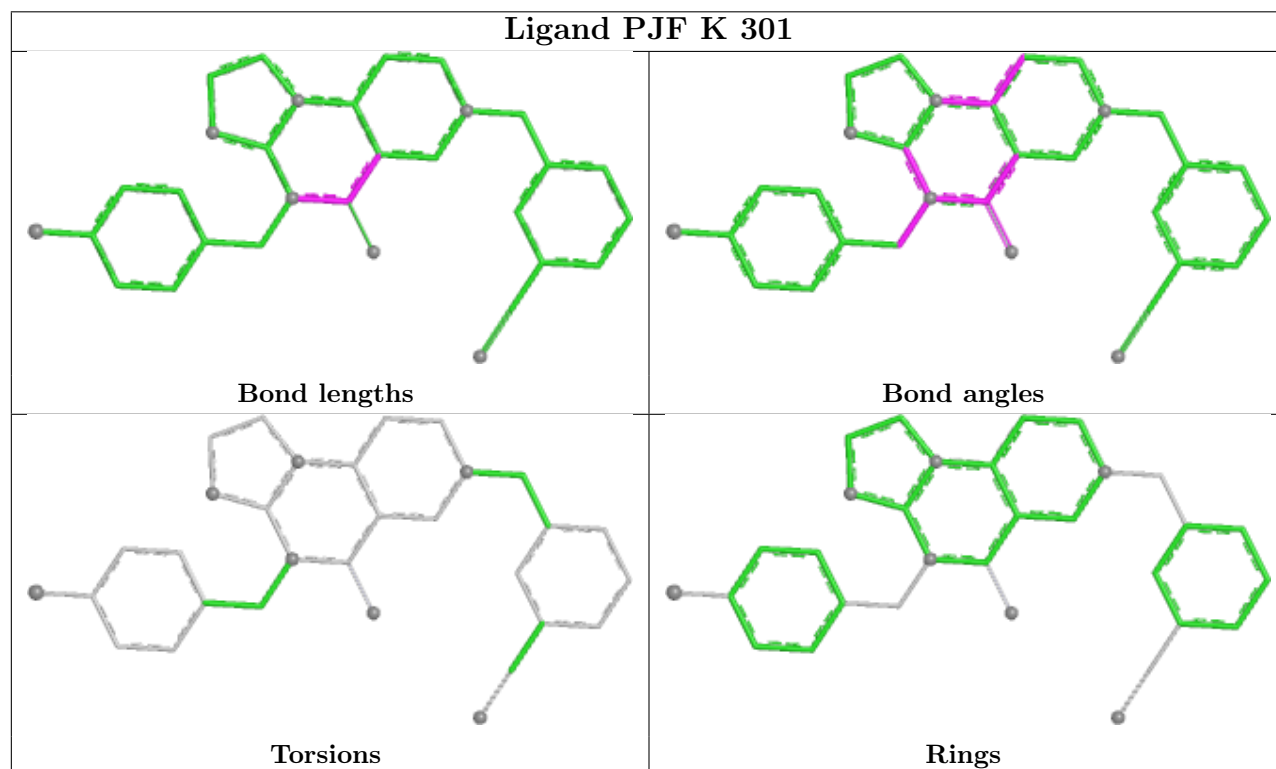
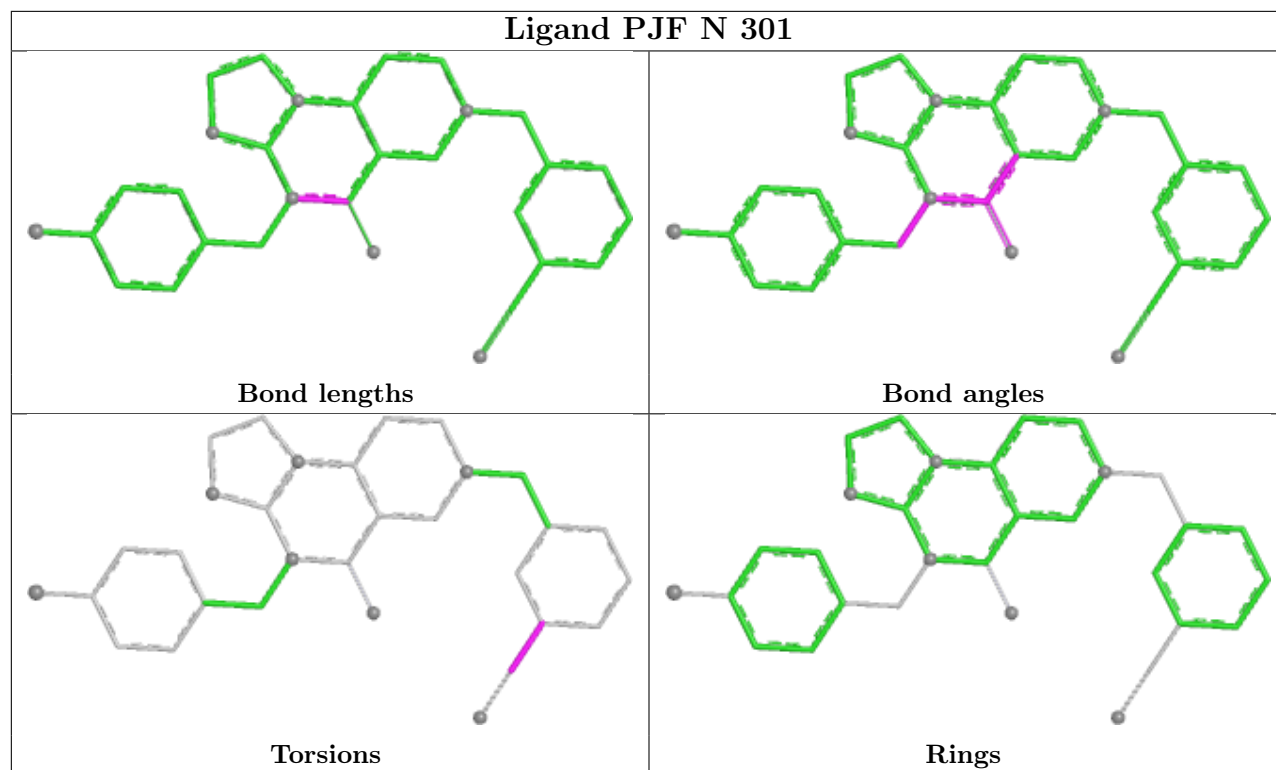
Ligand PJF M 301

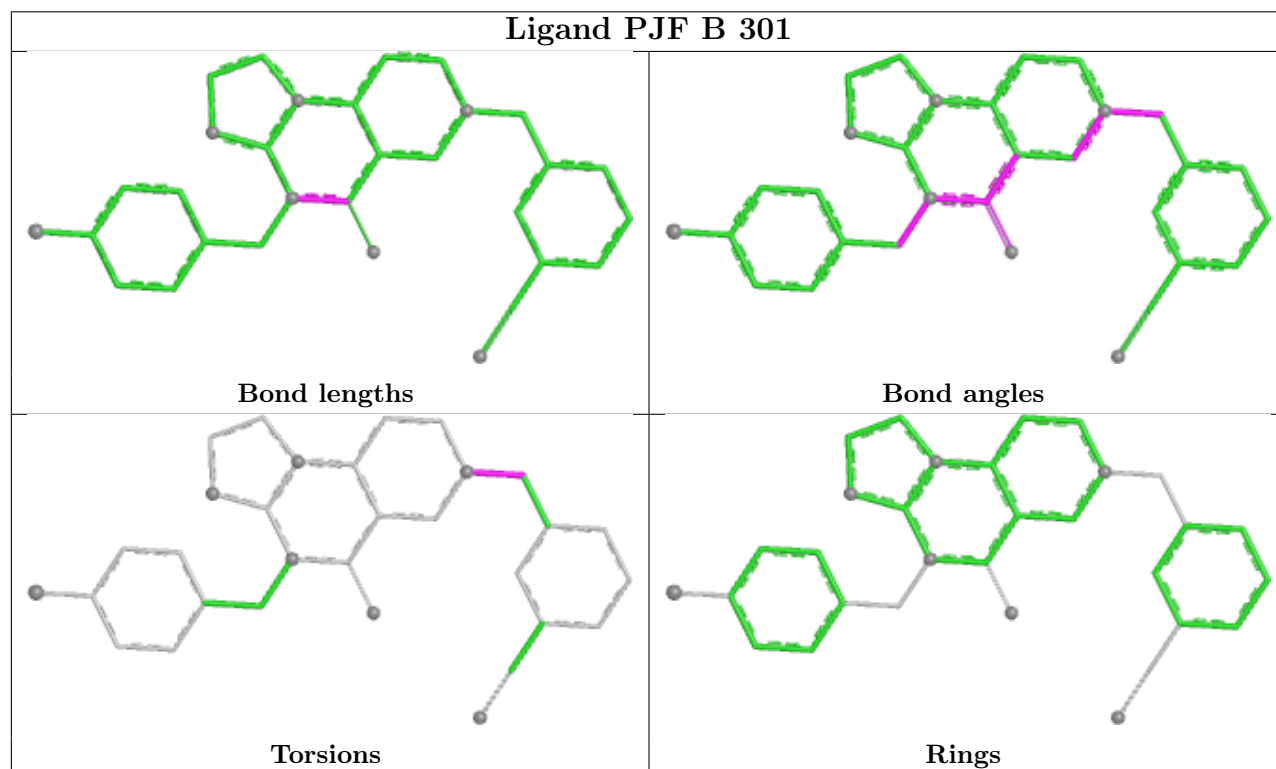
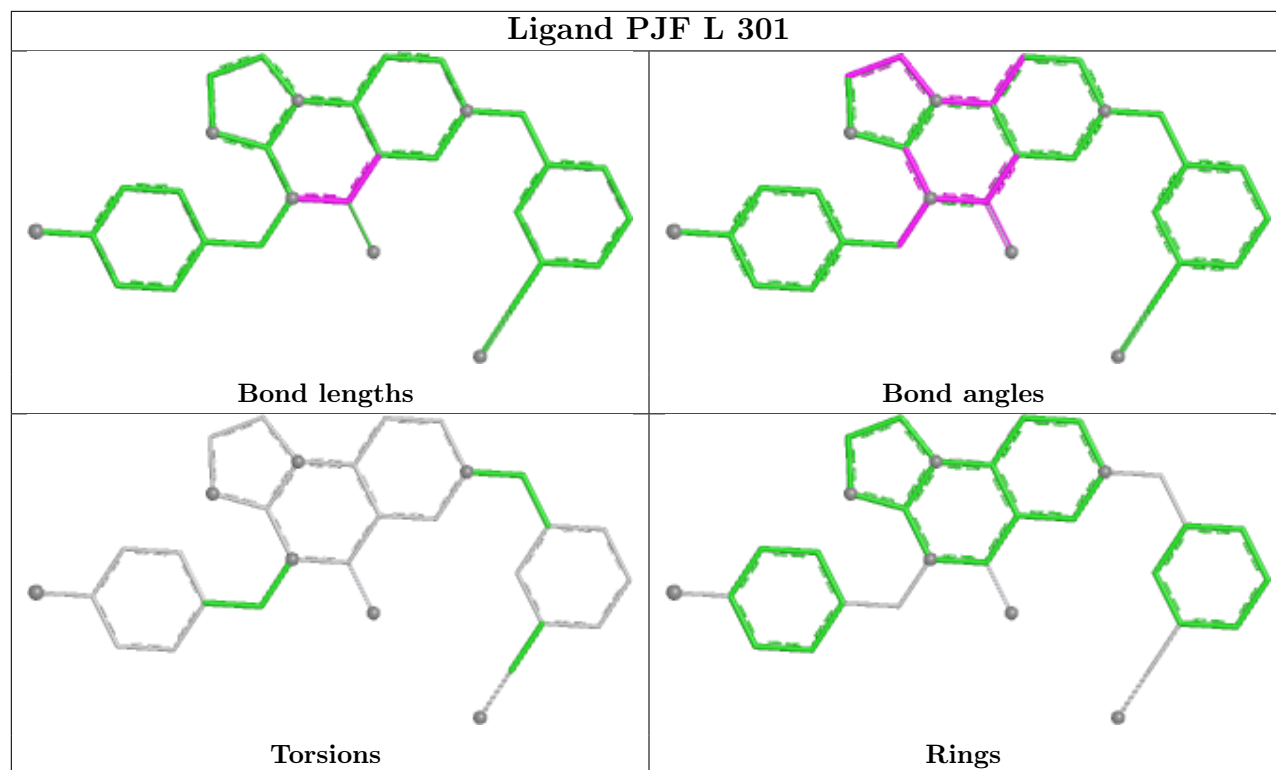


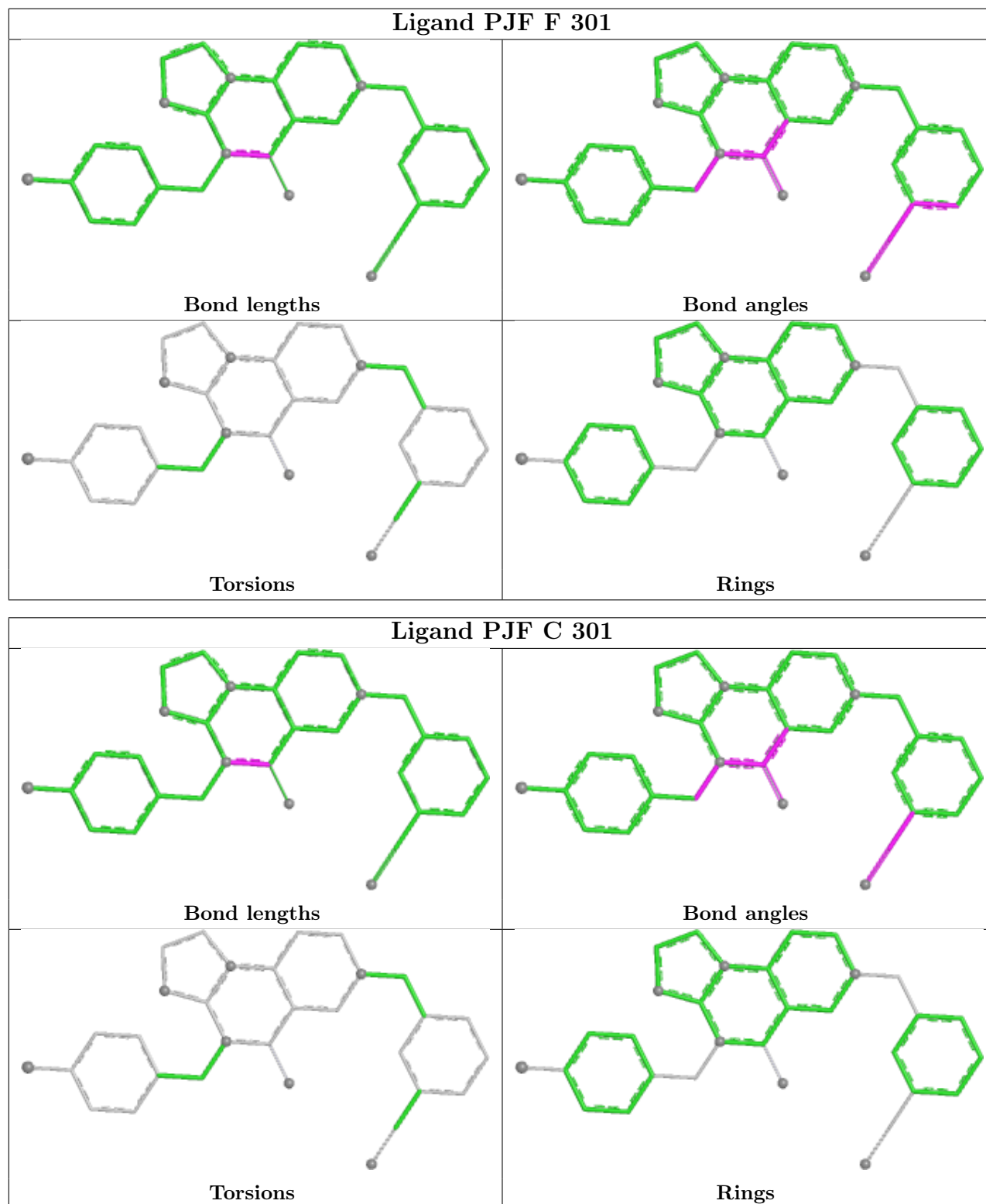












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	168/221 (76%)	0.57	5 (2%) 52 49	38, 50, 72, 96	0
1	B	167/221 (75%)	0.75	12 (7%) 21 18	43, 55, 83, 100	0
1	C	167/221 (75%)	0.91	18 (10%) 11 9	47, 61, 82, 107	0
1	D	168/221 (76%)	0.86	14 (8%) 17 14	46, 62, 86, 105	0
1	E	169/221 (76%)	0.79	13 (7%) 19 17	42, 56, 78, 95	0
1	F	166/221 (75%)	0.54	5 (3%) 52 49	40, 53, 70, 91	0
1	G	168/221 (76%)	0.40	7 (4%) 40 37	32, 46, 71, 88	0
1	H	166/221 (75%)	0.69	9 (5%) 31 27	46, 58, 77, 106	0
1	I	165/221 (74%)	0.93	15 (9%) 15 12	45, 63, 80, 95	0
1	J	167/221 (75%)	1.53	45 (26%) 1 1	49, 73, 94, 116	0
1	K	170/221 (76%)	1.65	45 (26%) 1 1	55, 73, 99, 116	0
1	L	164/221 (74%)	1.42	31 (18%) 3 3	43, 71, 88, 119	0
1	M	166/221 (75%)	1.21	26 (15%) 5 4	47, 63, 87, 103	0
1	N	168/221 (76%)	0.79	13 (7%) 19 17	45, 59, 76, 106	0
All	All	2339/3094 (75%)	0.93	258 (11%) 10 9	32, 61, 86, 119	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	75	ILE	6.9
1	M	191	ILE	6.4
1	A	76	TYR	6.2
1	N	76	TYR	5.8
1	K	249	PRO	5.6
1	B	191	ILE	5.4
1	J	248	PRO	5.2
1	K	229	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	76	TYR	5.1
1	K	76	TYR	5.1
1	L	76	TYR	4.9
1	J	247	HIS	4.9
1	B	76	TYR	4.5
1	B	246	VAL	4.5
1	D	249	PRO	4.5
1	K	188	ALA	4.5
1	H	249	PRO	4.4
1	N	190	ASP	4.2
1	L	174	ARG	4.1
1	C	190	ASP	4.1
1	M	245	LEU	4.1
1	J	245	LEU	4.0
1	J	246	VAL	4.0
1	F	249	PRO	4.0
1	M	229	TYR	4.0
1	C	245	LEU	4.0
1	I	144	ARG	4.0
1	I	76	TYR	4.0
1	C	191	ILE	3.9
1	M	249	PRO	3.8
1	J	229	TYR	3.8
1	M	247	HIS	3.8
1	H	76	TYR	3.8
1	B	247	HIS	3.8
1	L	74	ASP	3.8
1	K	101	ALA	3.8
1	L	75	ILE	3.7
1	K	228	ARG	3.7
1	J	76	TYR	3.6
1	K	174	ARG	3.6
1	G	246	VAL	3.6
1	J	233	MET	3.5
1	A	249	PRO	3.5
1	K	140	LEU	3.5
1	M	75	ILE	3.5
1	M	228	ARG	3.5
1	K	111	ASN	3.4
1	K	166	MET	3.4
1	G	251	ASP	3.4
1	C	76	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	76	TYR	3.4
1	J	140	LEU	3.4
1	K	191	ILE	3.3
1	M	76	TYR	3.3
1	J	192	ALA	3.3
1	M	192	ALA	3.3
1	L	243	LYS	3.3
1	L	247	HIS	3.3
1	K	245	LEU	3.3
1	L	80	LEU	3.3
1	L	171	PRO	3.3
1	N	189	THR	3.3
1	K	116	HIS	3.3
1	C	180	PRO	3.2
1	G	76	TYR	3.2
1	D	247	HIS	3.2
1	E	229	TYR	3.2
1	D	174	ARG	3.2
1	F	76	TYR	3.2
1	K	243	LYS	3.1
1	J	103	LEU	3.1
1	L	108	SER	3.1
1	J	244	VAL	3.1
1	I	192	ALA	3.1
1	J	191	ILE	3.1
1	L	84	ILE	3.1
1	K	246	VAL	3.1
1	E	174	ARG	3.1
1	E	245	LEU	3.0
1	J	78	ARG	3.0
1	C	246	VAL	3.0
1	J	112	LYS	3.0
1	B	192	ALA	3.0
1	C	247	HIS	3.0
1	E	250	GLN	3.0
1	K	233	MET	3.0
1	L	144	ARG	3.0
1	B	249	PRO	2.9
1	K	74	ASP	2.9
1	L	224	MET	2.9
1	J	206	TYR	2.9
1	J	80	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	192	ALA	2.9
1	M	165	GLY	2.8
1	K	109	GLU	2.8
1	J	166	MET	2.8
1	J	138	TYR	2.8
1	E	246	VAL	2.8
1	N	248	PRO	2.8
1	N	181	SER	2.8
1	J	207	ASN	2.8
1	C	74	ASP	2.8
1	E	190	ASP	2.8
1	J	144	ARG	2.8
1	J	190	ASP	2.8
1	I	233	MET	2.8
1	K	138	TYR	2.8
1	M	144	ARG	2.8
1	K	162	GLY	2.7
1	K	189	THR	2.7
1	D	194	GLN	2.7
1	M	243	LYS	2.7
1	G	192	ALA	2.7
1	M	112	LYS	2.7
1	M	248	PRO	2.7
1	J	104	LEU	2.7
1	I	174	ARG	2.7
1	L	181	SER	2.7
1	M	111	ASN	2.7
1	K	148	VAL	2.7
1	M	203	LYS	2.7
1	L	142	PRO	2.7
1	D	245	LEU	2.6
1	L	245	LEU	2.6
1	C	181	SER	2.6
1	K	190	ASP	2.6
1	J	174	ARG	2.6
1	H	192	ALA	2.6
1	K	85	VAL	2.6
1	N	245	LEU	2.6
1	C	174	ARG	2.6
1	H	81	ARG	2.6
1	L	78	ARG	2.6
1	M	226	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	244	VAL	2.6
1	A	77	SER	2.6
1	J	189	THR	2.6
1	F	233	MET	2.6
1	M	233	MET	2.6
1	J	75	ILE	2.6
1	N	188	ALA	2.6
1	L	166	MET	2.5
1	B	225	GLU	2.5
1	J	165	GLY	2.5
1	L	227	ASP	2.5
1	I	75	ILE	2.5
1	K	84	ILE	2.5
1	H	247	HIS	2.5
1	L	85	VAL	2.5
1	N	191	ILE	2.5
1	E	218	GLN	2.5
1	K	103	LEU	2.5
1	I	74	ASP	2.5
1	K	195	ALA	2.5
1	E	181	SER	2.4
1	C	248	PRO	2.4
1	K	239	GLY	2.4
1	E	206	TYR	2.4
1	I	202	LYS	2.4
1	K	144	ARG	2.4
1	C	229	TYR	2.4
1	G	197	GLU	2.4
1	I	148	VAL	2.4
1	I	246	VAL	2.4
1	B	245	LEU	2.4
1	J	139	ILE	2.4
1	N	80	LEU	2.4
1	E	74	ASP	2.4
1	L	239	GLY	2.4
1	M	84	ILE	2.3
1	J	141	ASN	2.3
1	B	237	GLU	2.3
1	K	214	LYS	2.3
1	L	146	TRP	2.3
1	B	248	PRO	2.3
1	L	162	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	228	ARG	2.3
1	D	238	PHE	2.3
1	J	105	PHE	2.3
1	K	205	LEU	2.3
1	J	88	MET	2.3
1	K	96	ALA	2.3
1	J	243	LYS	2.3
1	M	237	GLU	2.3
1	A	74	ASP	2.3
1	M	222	SER	2.3
1	J	107	GLN	2.3
1	D	74	ASP	2.3
1	H	180	PRO	2.3
1	I	165	GLY	2.3
1	E	191	ILE	2.2
1	L	86	CYS	2.2
1	C	225	GLU	2.2
1	N	81	ARG	2.2
1	A	180	PRO	2.2
1	J	160	ALA	2.2
1	K	247	HIS	2.2
1	C	197	GLU	2.2
1	B	206	TYR	2.2
1	J	111	ASN	2.2
1	H	248	PRO	2.2
1	K	248	PRO	2.2
1	M	146	TRP	2.2
1	K	240	ILE	2.2
1	C	192	ALA	2.2
1	M	81	ARG	2.2
1	J	164	PRO	2.2
1	L	232	PRO	2.2
1	K	106	LEU	2.2
1	L	103	LEU	2.2
1	C	176	MET	2.2
1	K	118	TYR	2.2
1	N	180	PRO	2.2
1	I	166	MET	2.2
1	K	88	MET	2.2
1	D	191	ILE	2.1
1	D	193	ILE	2.1
1	E	148	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	148	VAL	2.1
1	D	197	GLU	2.1
1	L	233	MET	2.1
1	I	193	ILE	2.1
1	J	143	ILE	2.1
1	K	131	ALA	2.1
1	F	197	GLU	2.1
1	K	234	GLU	2.1
1	L	117	MET	2.1
1	J	86	CYS	2.1
1	D	229	TYR	2.1
1	L	177	ILE	2.1
1	D	78	ARG	2.1
1	K	81	ARG	2.1
1	J	146	TRP	2.1
1	N	243	LYS	2.1
1	K	163	THR	2.1
1	J	114	PRO	2.1
1	B	201	LEU	2.1
1	G	245	LEU	2.1
1	L	79	LEU	2.1
1	K	141	ASN	2.1
1	G	247	HIS	2.1
1	I	206	TYR	2.1
1	F	237	GLU	2.0
1	M	78	ARG	2.0
1	K	142	PRO	2.0
1	L	136	MET	2.0
1	K	179	GLN	2.0
1	M	143	ILE	2.0
1	L	229	TYR	2.0
1	H	78	ARG	2.0
1	J	237	GLU	2.0
1	C	199	MET	2.0
1	I	248	PRO	2.0
1	J	163	THR	2.0
1	J	180	PRO	2.0
1	H	245	LEU	2.0
1	J	218	GLN	2.0
1	C	75	ILE	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](#)

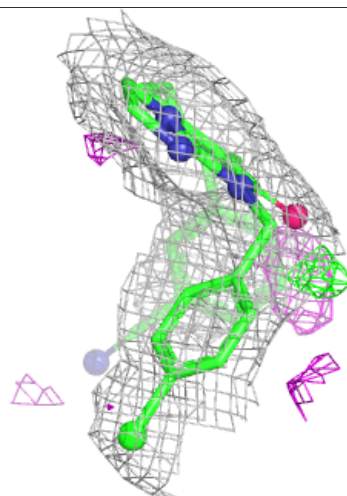
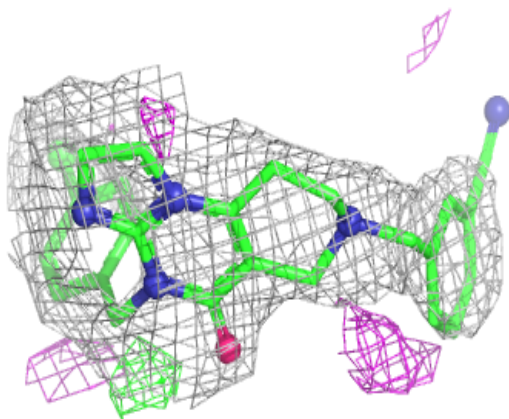
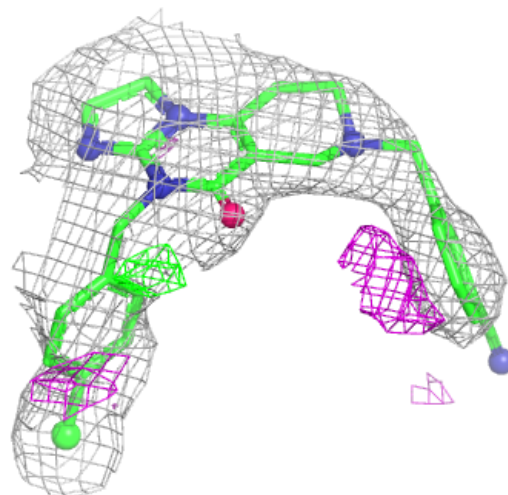
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PJF	K	301	31/31	0.84	0.17	66,79,91,97	0
2	PJF	L	301	31/31	0.85	0.18	71,82,93,105	0
2	PJF	M	301	31/31	0.88	0.14	54,64,78,84	0
2	PJF	J	301	31/31	0.91	0.14	64,76,83,89	0
2	PJF	H	301	31/31	0.92	0.12	49,62,69,75	0
2	PJF	B	301	31/31	0.93	0.11	36,51,60,70	0
2	PJF	I	301	31/31	0.93	0.12	57,65,70,72	0
2	PJF	D	301	31/31	0.93	0.11	50,60,66,69	0
2	PJF	N	301	31/31	0.93	0.11	48,61,69,80	0
2	PJF	A	301	31/31	0.94	0.10	40,46,53,69	0
2	PJF	E	301	31/31	0.94	0.12	51,56,65,66	0
2	PJF	C	301	31/31	0.94	0.10	43,51,58,60	0
2	PJF	G	301	31/31	0.95	0.10	39,46,52,58	0
2	PJF	F	301	31/31	0.95	0.10	40,47,54,66	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.

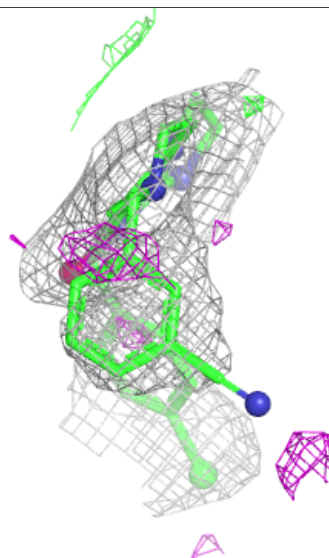
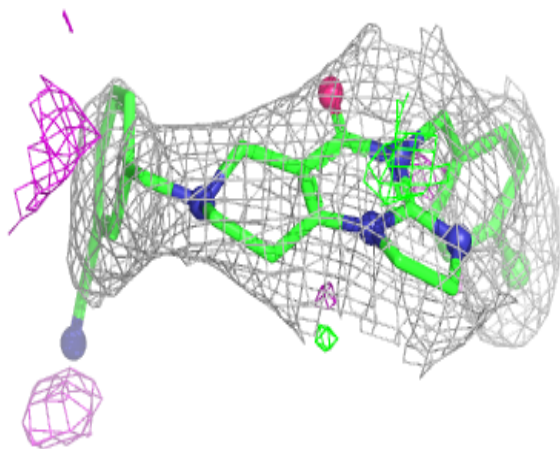
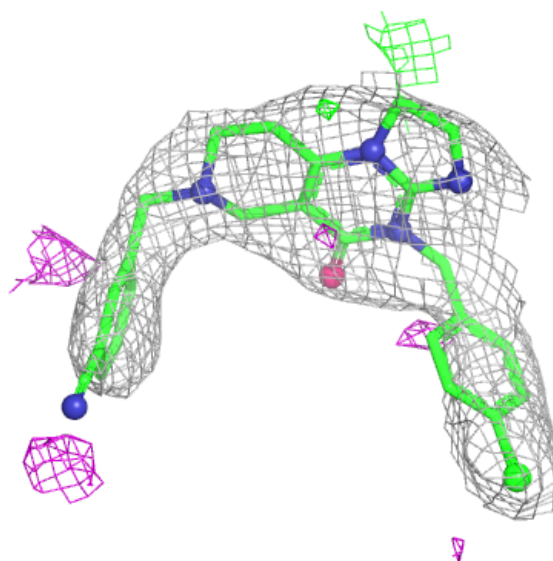
Electron density around PJF K 301:

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



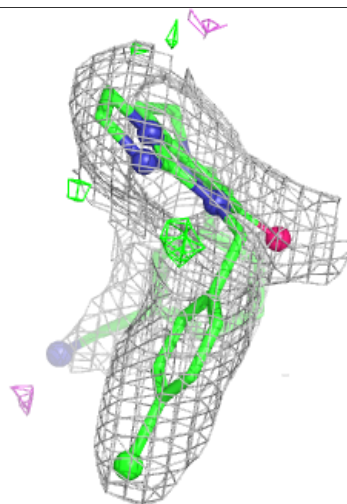
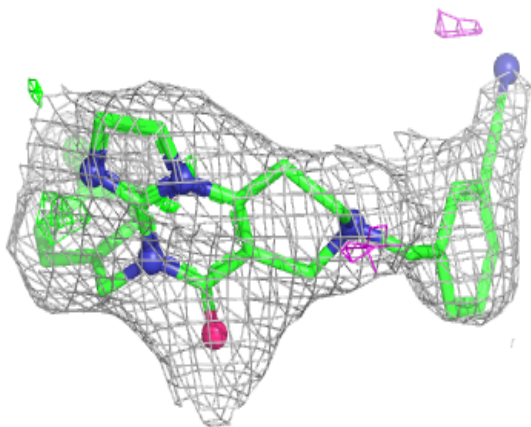
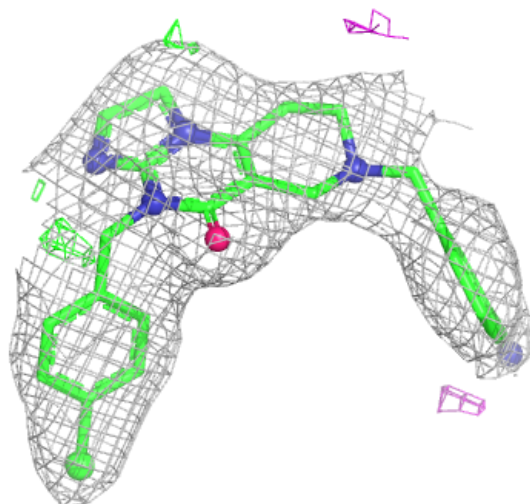
Electron density around PJF L 301:

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



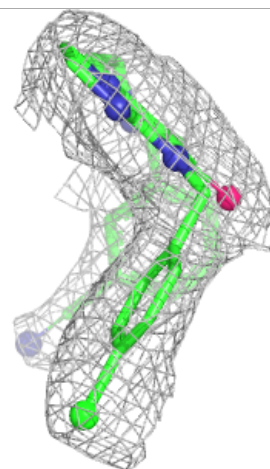
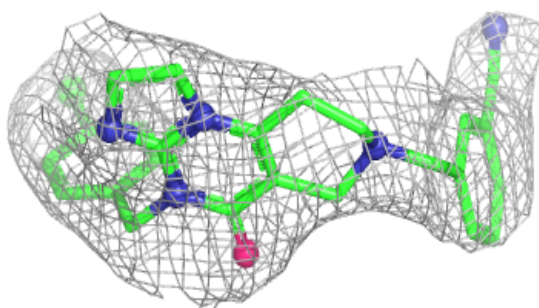
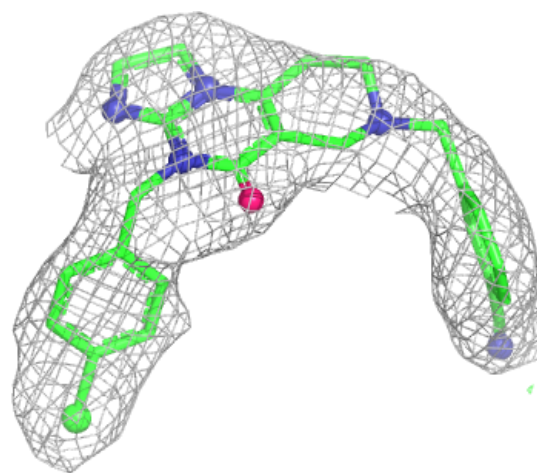
Electron density around PJF M 301:

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



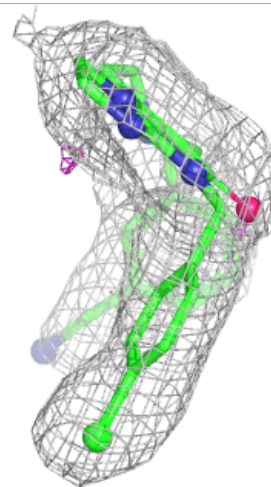
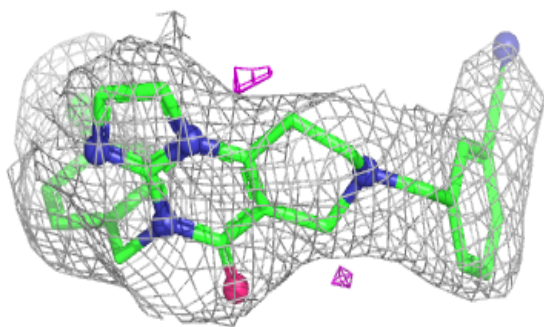
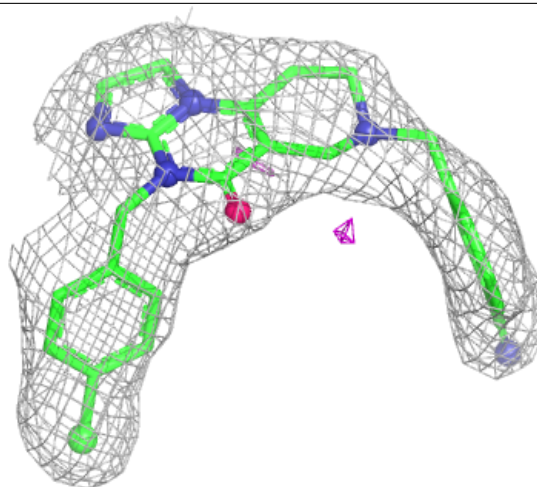
Electron density around PJF J 301:

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



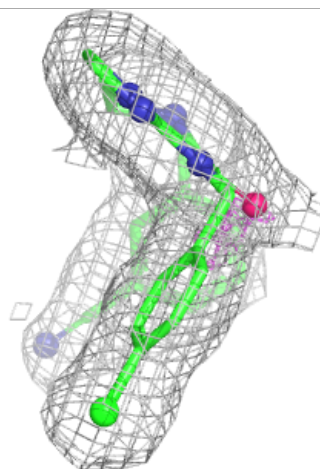
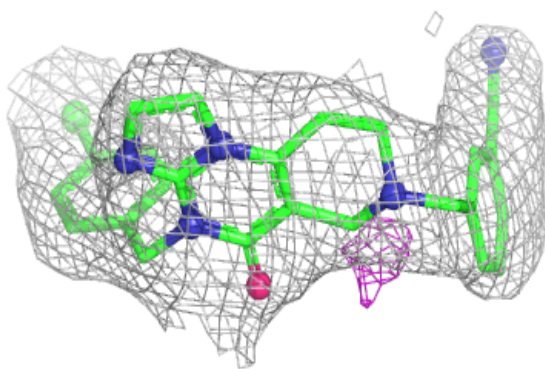
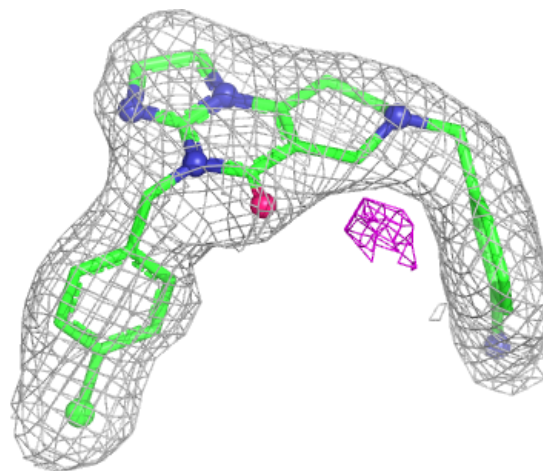
Electron density around PJF H 301:

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



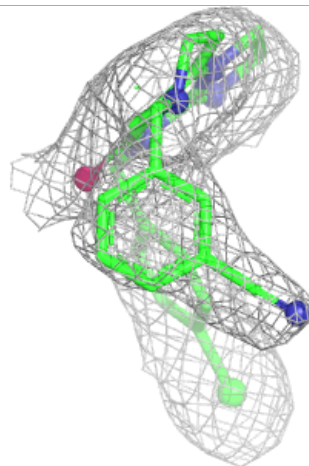
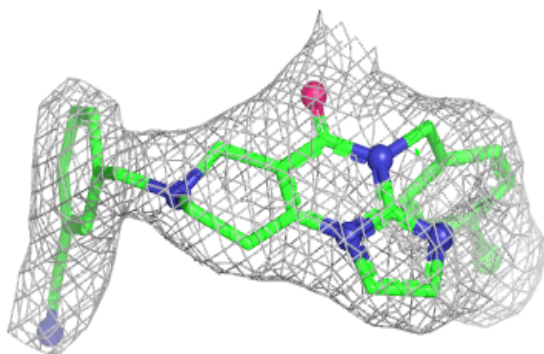
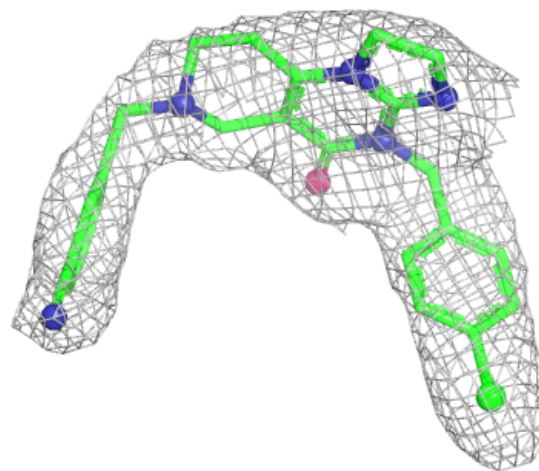
Electron density around PJF B 301:

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



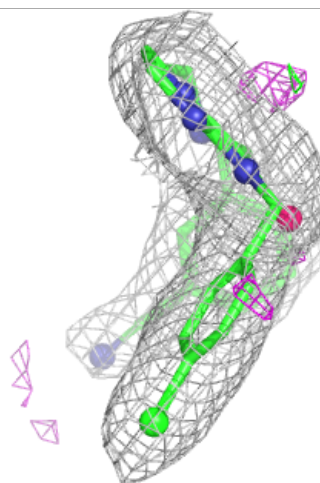
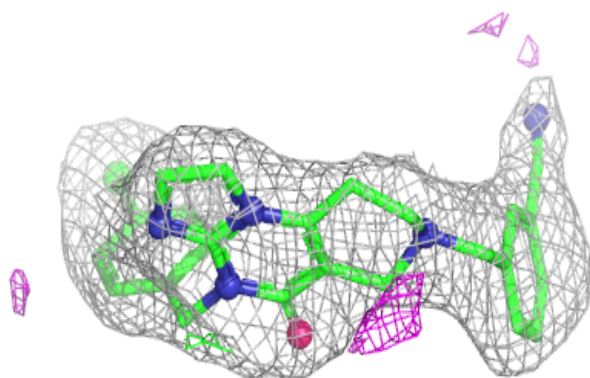
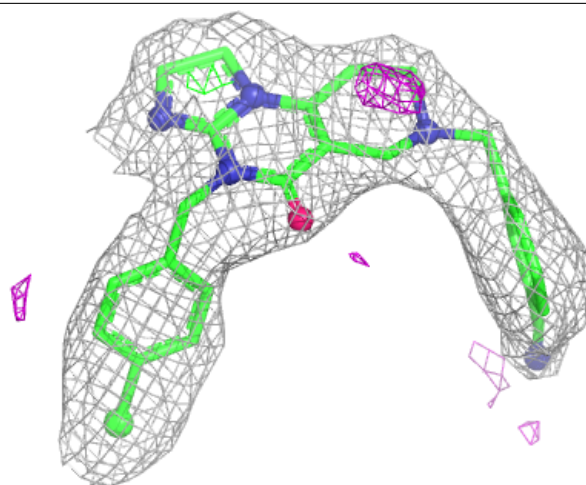
Electron density around PJF I 301:

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



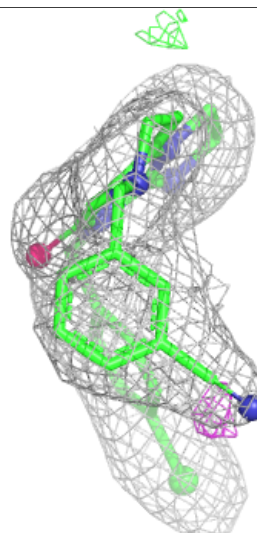
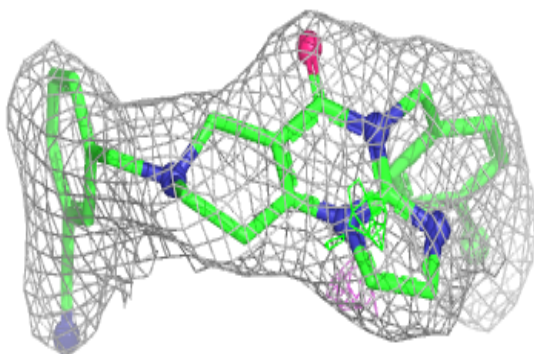
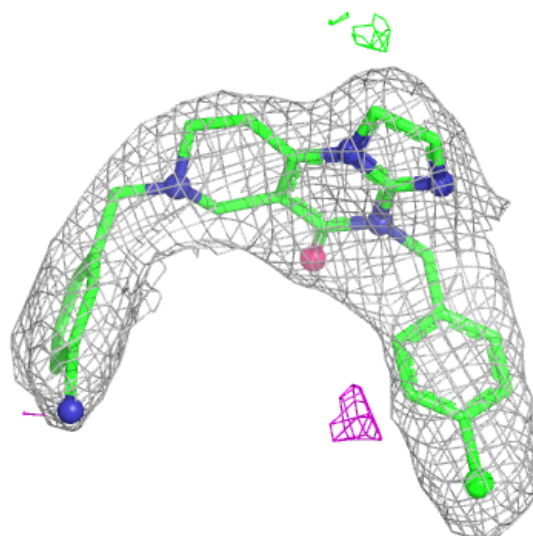
Electron density around PJF D 301:

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



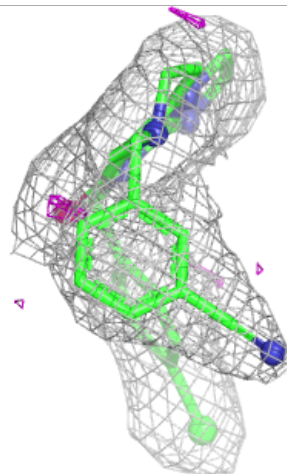
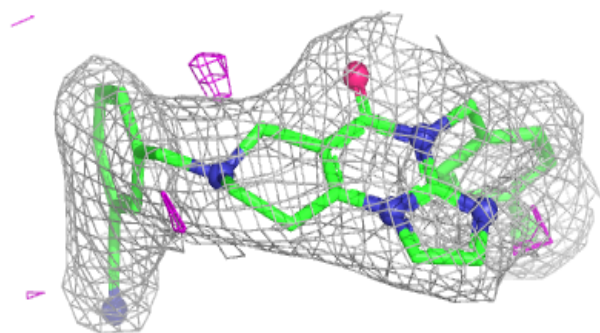
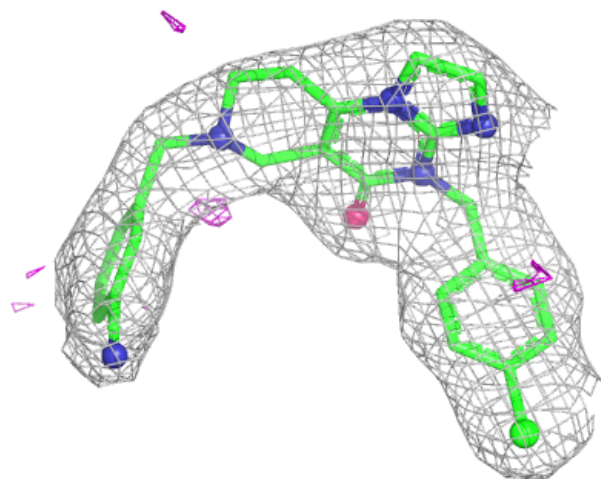
Electron density around PJF N 301:

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



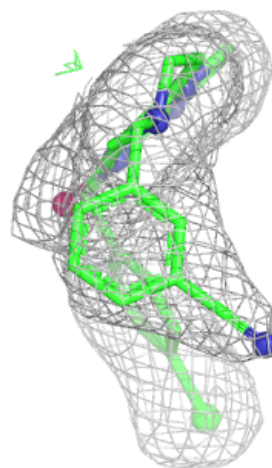
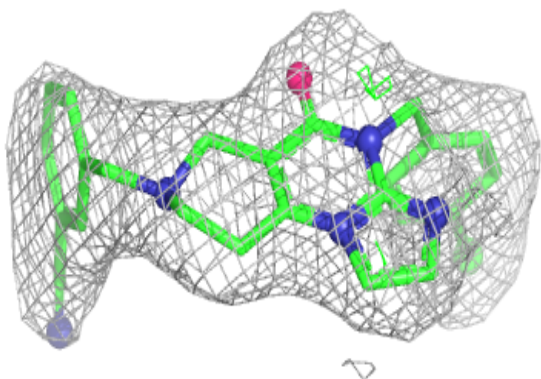
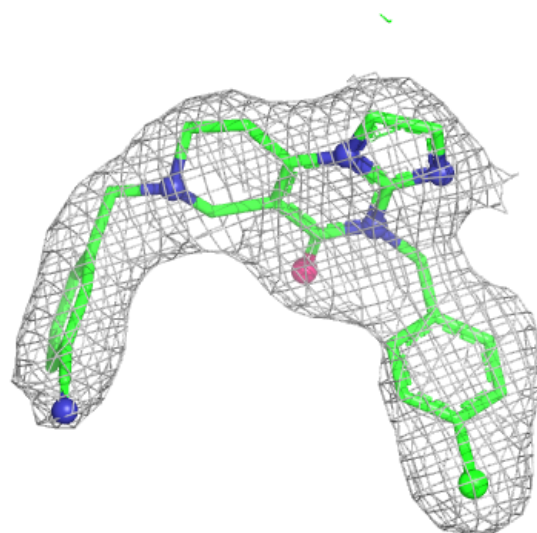
Electron density around PJF A 301:

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



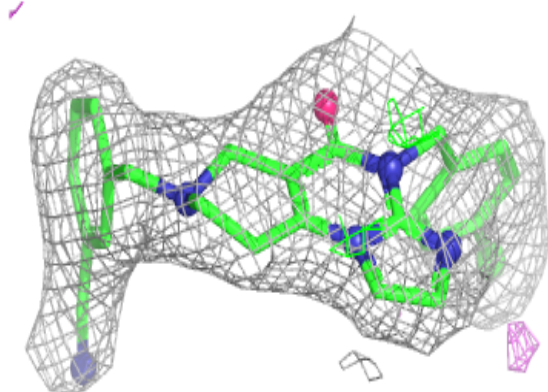
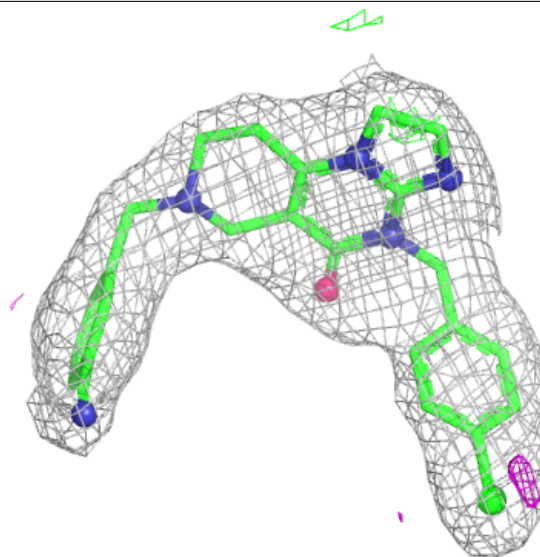
Electron density around PJF E 301:

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



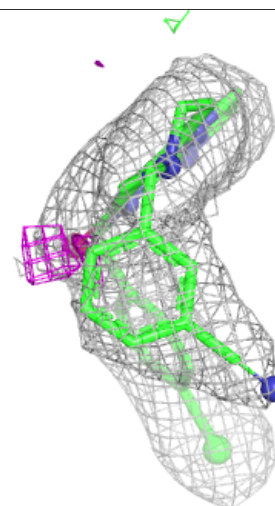
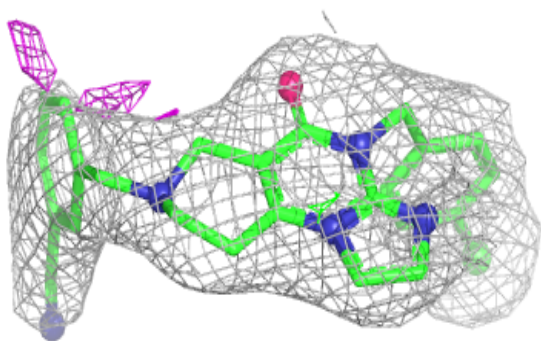
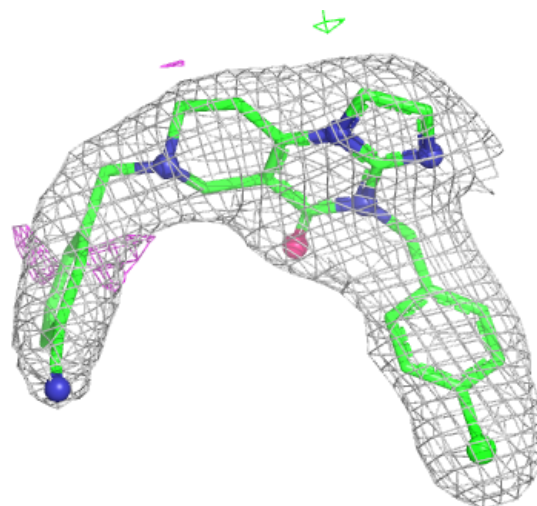
Electron density around PJF C 301:

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



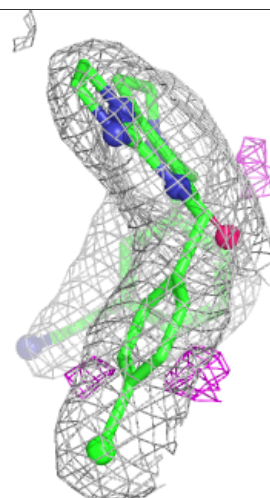
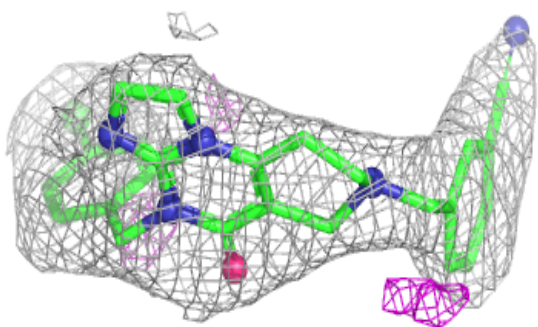
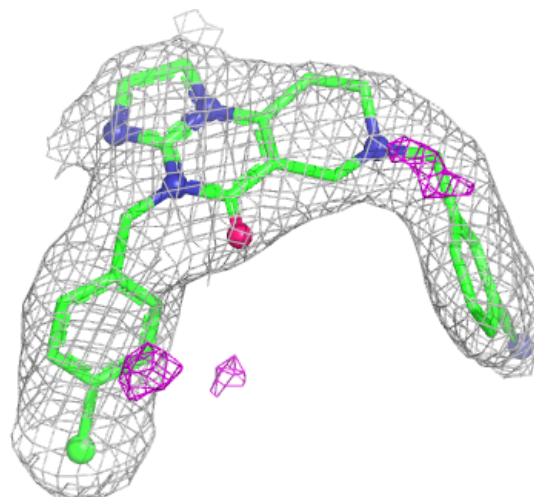
Electron density around PJF G 301:

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



Electron density around PJF F 301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.