



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2020 – 10:13 AM JST

PDB ID : 7C8A  
Title : Peroxiredoxin from *Aeropyrum pernix* K1 (ApPrx) C50S/F80C/C207S/C213  
S mutant modified with 2-(bromoacetyl)naphthalene(Naph@ApPrx\*)  
Authors : Himiyama, T.; Nakamura, T.  
Deposited on : 2020-05-29  
Resolution : 2.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

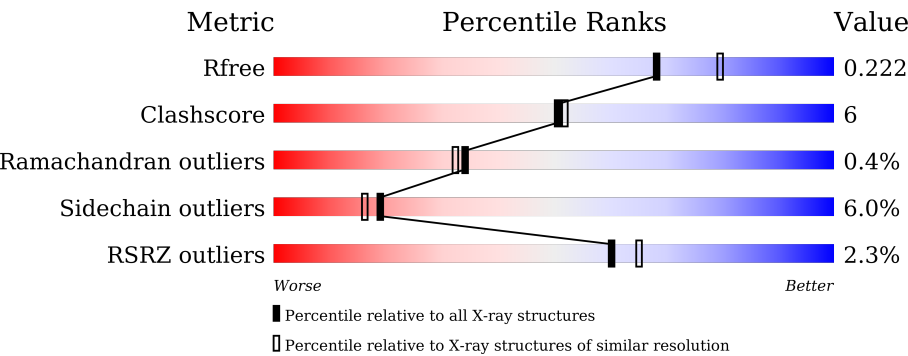
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	250	<div><div>2%</div><div><div></div><div>82%</div><div>14%</div><div>..</div></div></div>
1	B	250	<div><div>%</div><div><div></div><div>83%</div><div>13%</div><div>..</div></div></div>
1	C	250	<div><div>3%</div><div><div></div><div>80%</div><div>15%</div><div>..</div></div></div>
1	D	250	<div><div>%</div><div><div></div><div>79%</div><div>18%</div><div>.</div></div></div>
1	E	250	<div><div>2%</div><div><div></div><div>81%</div><div>14%</div><div>..</div></div></div>
1	F	250	<div><div>3%</div><div><div></div><div>84%</div><div>12%</div><div>..</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	250	<div><div>%</div><div><div></div><div>83%</div><div>12%</div><div></div></div><div></div></div>
1	H	250	<div><div>4%</div><div><div></div><div>85%</div><div>12%</div><div></div></div><div></div></div>
1	I	250	<div><div>4%</div><div><div></div><div>81%</div><div>14%</div><div></div></div><div></div></div>
1	J	250	<div><div>2%</div><div><div></div><div>84%</div><div>11%</div><div></div></div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20794 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 Peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total 1968	C 1262	N 347	O 354	S 5	0	0	0
1	B	244	Total 1968	C 1262	N 347	O 354	S 5	0	0	0
1	C	244	Total 1968	C 1262	N 347	O 354	S 5	0	0	0
1	D	244	Total 1968	C 1262	N 347	O 354	S 5	0	0	0
1	E	244	Total 1968	C 1262	N 347	O 354	S 5	0	0	0
1	F	244	Total 1968	C 1262	N 347	O 354	S 5	0	0	0
1	G	244	Total 1968	C 1262	N 347	O 354	S 5	0	0	0
1	H	244	Total 1968	C 1262	N 347	O 354	S 5	0	0	0
1	I	244	Total 1968	C 1262	N 347	O 354	S 5	0	0	0
1	J	244	Total 1968	C 1262	N 347	O 354	S 5	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

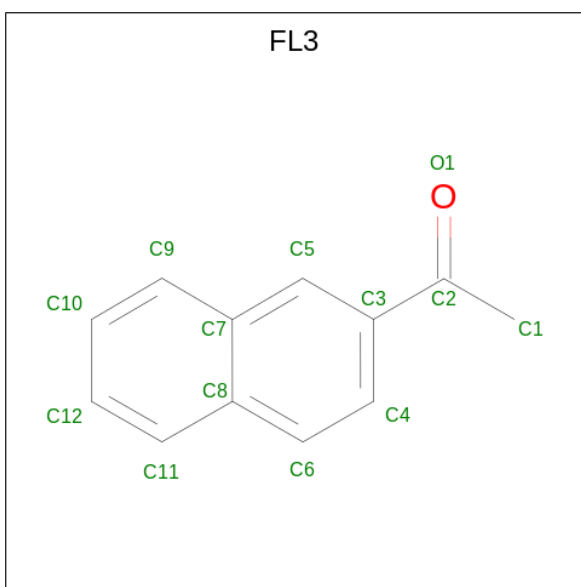
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	SER	CYS	engineered mutation	UNP Q9Y9L0
A	80	CYS	PHE	engineered mutation	UNP Q9Y9L0
A	207	SER	CYS	engineered mutation	UNP Q9Y9L0
A	213	SER	CYS	engineered mutation	UNP Q9Y9L0
B	50	SER	CYS	engineered mutation	UNP Q9Y9L0
B	80	CYS	PHE	engineered mutation	UNP Q9Y9L0
B	207	SER	CYS	engineered mutation	UNP Q9Y9L0
B	213	SER	CYS	engineered mutation	UNP Q9Y9L0
C	50	SER	CYS	engineered mutation	UNP Q9Y9L0

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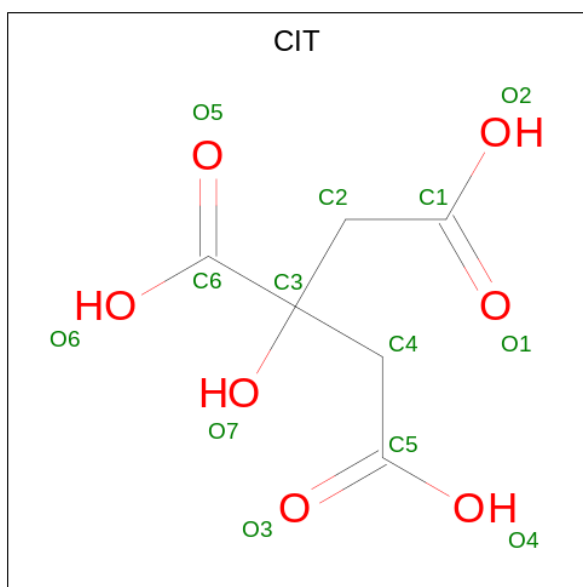
Chain	Residue	Modelled	Actual	Comment	Reference
C	80	CYS	PHE	engineered mutation	UNP Q9Y9L0
C	207	SER	CYS	engineered mutation	UNP Q9Y9L0
C	213	SER	CYS	engineered mutation	UNP Q9Y9L0
D	50	SER	CYS	engineered mutation	UNP Q9Y9L0
D	80	CYS	PHE	engineered mutation	UNP Q9Y9L0
D	207	SER	CYS	engineered mutation	UNP Q9Y9L0
D	213	SER	CYS	engineered mutation	UNP Q9Y9L0
E	50	SER	CYS	engineered mutation	UNP Q9Y9L0
E	80	CYS	PHE	engineered mutation	UNP Q9Y9L0
E	207	SER	CYS	engineered mutation	UNP Q9Y9L0
E	213	SER	CYS	engineered mutation	UNP Q9Y9L0
F	50	SER	CYS	engineered mutation	UNP Q9Y9L0
F	80	CYS	PHE	engineered mutation	UNP Q9Y9L0
F	207	SER	CYS	engineered mutation	UNP Q9Y9L0
F	213	SER	CYS	engineered mutation	UNP Q9Y9L0
G	50	SER	CYS	engineered mutation	UNP Q9Y9L0
G	80	CYS	PHE	engineered mutation	UNP Q9Y9L0
G	207	SER	CYS	engineered mutation	UNP Q9Y9L0
G	213	SER	CYS	engineered mutation	UNP Q9Y9L0
H	50	SER	CYS	engineered mutation	UNP Q9Y9L0
H	80	CYS	PHE	engineered mutation	UNP Q9Y9L0
H	207	SER	CYS	engineered mutation	UNP Q9Y9L0
H	213	SER	CYS	engineered mutation	UNP Q9Y9L0
I	50	SER	CYS	engineered mutation	UNP Q9Y9L0
I	80	CYS	PHE	engineered mutation	UNP Q9Y9L0
I	207	SER	CYS	engineered mutation	UNP Q9Y9L0
I	213	SER	CYS	engineered mutation	UNP Q9Y9L0
J	50	SER	CYS	engineered mutation	UNP Q9Y9L0
J	80	CYS	PHE	engineered mutation	UNP Q9Y9L0
J	207	SER	CYS	engineered mutation	UNP Q9Y9L0
J	213	SER	CYS	engineered mutation	UNP Q9Y9L0

- Molecule 2 is 1-naphthalen-2-ylethanone (three-letter code: FL3) (formula: C<sub>12</sub>H<sub>10</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	12	1		
2	B	1	Total	C	O	0	0
			13	12	1		
2	C	1	Total	C	O	0	0
			13	12	1		
2	D	1	Total	C	O	0	0
			13	12	1		
2	E	1	Total	C	O	0	0
			13	12	1		
2	F	1	Total	C	O	0	0
			13	12	1		
2	G	1	Total	C	O	0	0
			13	12	1		
2	H	1	Total	C	O	0	0
			13	12	1		
2	I	1	Total	C	O	0	0
			13	12	1		
2	J	1	Total	C	O	0	0
			13	12	1		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		
3	G	1	Total	C	O	0	0
			13	6	7		
3	H	1	Total	C	O	0	0
			13	6	7		
3	I	1	Total	C	O	0	0
			13	6	7		
3	J	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	90	Total	O	0	0
			90	90		

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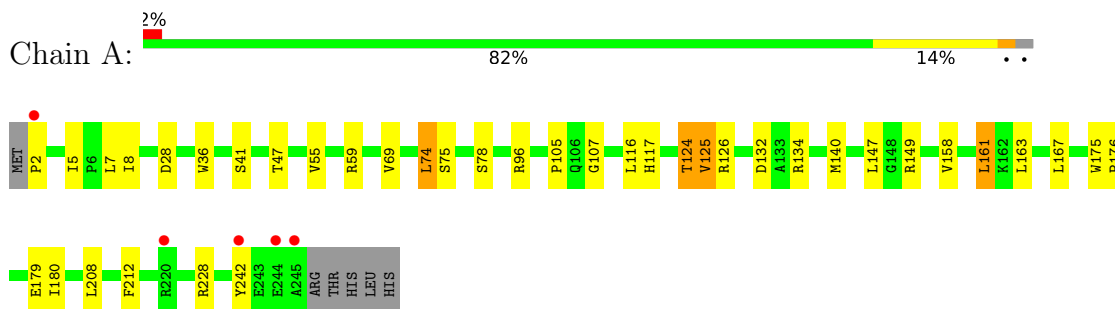
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	99	Total 99	O 99	0	0
4	D	68	Total 68	O 68	0	0
4	E	71	Total 71	O 71	0	0
4	F	80	Total 80	O 80	0	0
4	G	86	Total 86	O 86	0	0
4	H	86	Total 86	O 86	0	0
4	I	92	Total 92	O 92	0	0
4	J	73	Total 73	O 73	0	0



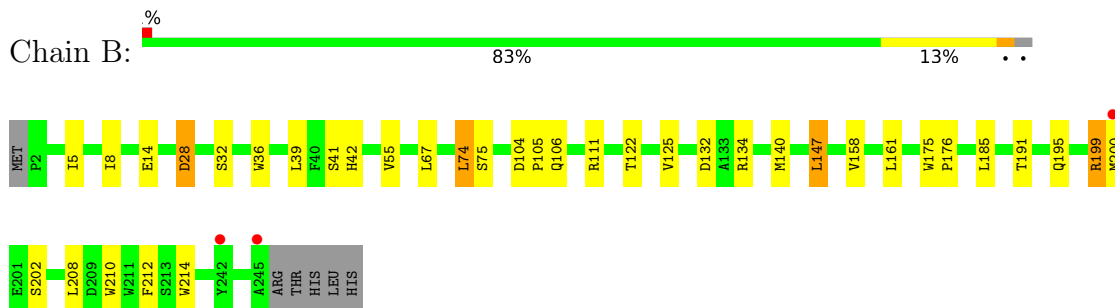
### 3 Residue-property plots [i](#)

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

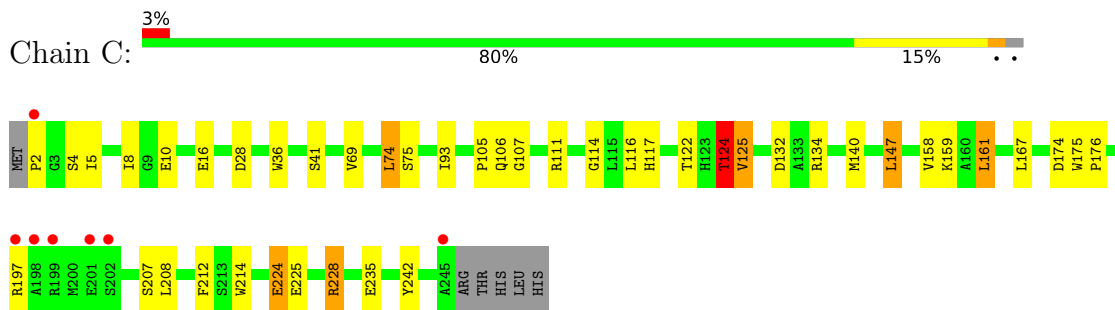
#### • Molecule 1: Peroxiredoxin



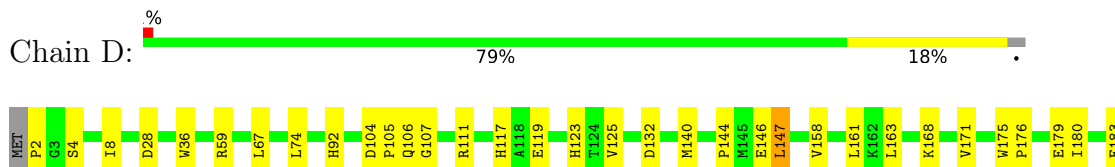
#### • Molecule 1: Peroxiredoxin



#### • Molecule 1: Peroxiredoxin

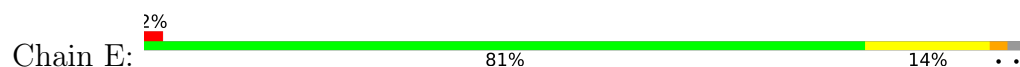


#### • Molecule 1: Peroxiredoxin

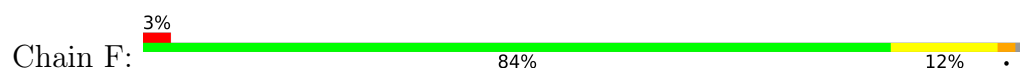




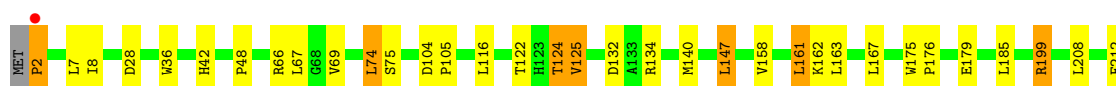
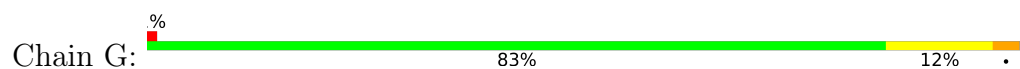
● Molecule 1: Peroxiredoxin



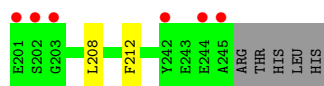
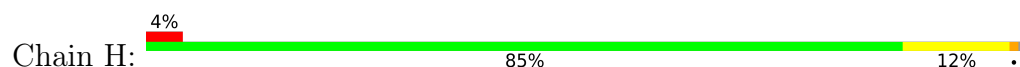
● Molecule 1: Peroxiredoxin



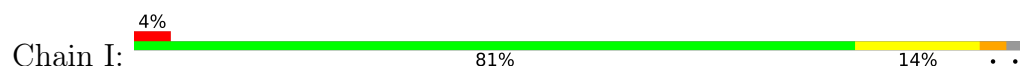
● Molecule 1: Peroxiredoxin

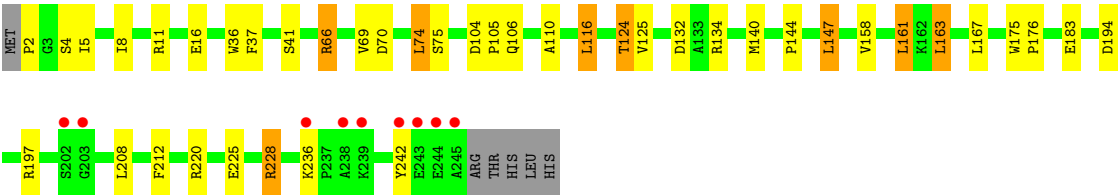


● Molecule 1: Peroxiredoxin

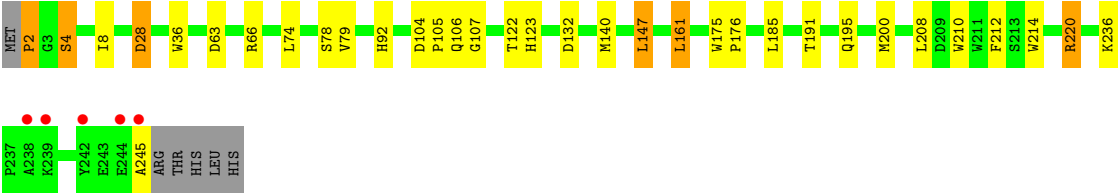
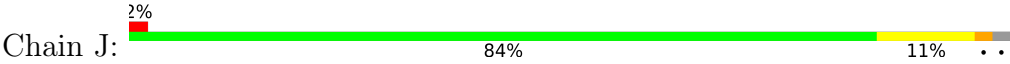


● Molecule 1: Peroxiredoxin





● Molecule 1: Peroxiredoxin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.00Å 103.08Å 105.03Å 105.94° 104.94° 92.38°	Depositor
Resolution (Å)	49.24 – 2.10 49.20 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.24-2.10) 97.9 (49.20-2.09)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.166 , 0.217 0.175 , 0.222	Depositor DCC
$R_{free}$ test set	8444 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20794	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FL3, CIT

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	0.74	1/2022 (0.0%)	0.90	3/2749 (0.1%)
1	B	0.71	0/2022	0.88	2/2749 (0.1%)
1	C	0.70	0/2022	0.90	3/2749 (0.1%)
1	D	0.70	1/2022 (0.0%)	0.87	1/2749 (0.0%)
1	E	0.70	0/2022	0.88	0/2749
1	F	0.69	0/2022	0.86	0/2749
1	G	0.69	0/2022	0.92	2/2749 (0.1%)
1	H	0.68	0/2022	0.87	0/2749
1	I	0.68	0/2022	0.87	2/2749 (0.1%)
1	J	0.70	0/2022	0.84	0/2749
All	All	0.70	2/20220 (0.0%)	0.88	13/27490 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	GLU	CD-OE1	10.61	1.37	1.25
1	D	179	GLU	CD-OE1	9.36	1.35	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	PRO	CA-N-CD	-6.75	102.05	111.50
1	A	134	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	C	134	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	G	2	PRO	CA-N-CD	-6.08	102.99	111.50
1	G	134	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	I	228	ARG	CB-CA-C	5.69	121.79	110.40
1	C	2	PRO	CA-N-CD	-5.52	103.78	111.50
1	D	220	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	B	199	ARG	NE-CZ-NH2	-5.43	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	I	2	PRO	CA-N-CD	-5.30	104.08	111.50
1	B	134	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	124	THR	N-CA-CB	-5.02	100.77	110.30

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	1968	0	1954	25	0
1	B	1968	0	1954	27	0
1	C	1968	0	1954	36	0
1	D	1968	0	1954	28	0
1	E	1968	0	1954	25	0
1	F	1968	0	1954	26	0
1	G	1968	0	1954	31	0
1	H	1968	0	1954	22	0
1	I	1968	0	1954	27	0
1	J	1968	0	1954	25	0
2	A	13	0	0	0	0
2	B	13	0	0	0	0
2	C	13	0	0	0	0
2	D	13	0	0	0	0
2	E	13	0	0	0	0
2	F	13	0	0	1	0
2	G	13	0	0	0	0
2	H	13	0	0	0	0
2	I	13	0	0	1	0
2	J	13	0	0	0	0
3	A	13	0	5	2	0
3	B	13	0	5	0	0
3	C	13	0	5	0	0
3	D	13	0	5	0	0
3	E	13	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	13	0	5	0	0
3	G	13	0	5	1	0
3	H	13	0	5	0	0
3	I	13	0	5	0	0
3	J	13	0	5	0	0
4	A	109	0	0	1	0
4	B	90	0	0	0	0
4	C	99	0	0	4	0
4	D	68	0	0	2	0
4	E	71	0	0	1	0
4	F	80	0	0	4	0
4	G	86	0	0	1	0
4	H	86	0	0	2	0
4	I	92	0	0	0	0
4	J	73	0	0	1	0
All	All	20794	0	19590	226	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 6.

All (226) 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:B:14:GLU:OE1	1:B:28:ASP:OD1	1.83	0.95
1:B:105:PRO:O	1:C:105:PRO:O	1.86	0.93
1:C:235:GLU:CD	4:C:401:HOH:O	2.09	0.90
1:A:105:PRO:O	1:F:105:PRO:O	1.92	0.88
1:C:69:VAL:HG21	1:C:158:VAL:HG11	1.56	0.86
1:E:69:VAL:HG21	1:E:158:VAL:HG11	1.59	0.85
1:E:106:GLN:O	1:E:111:ARG:NH2	2.11	0.83
1:F:235:GLU:HG2	4:F:475:HOH:O	1.79	0.82
1:C:235:GLU:OE2	4:C:401:HOH:O	1.96	0.81
1:I:69:VAL:HG21	1:I:158:VAL:HG11	1.63	0.80
1:A:107:GLY:HA3	1:F:106:GLN:HE22	1.47	0.80
1:A:69:VAL:HG21	1:A:158:VAL:HG11	1.65	0.79
1:J:8:ILE:HG13	1:J:140:MET:HE2	1.64	0.78
1:G:69:VAL:HG21	1:G:158:VAL:HG11	1.68	0.75
1:E:140:MET:HE1	1:F:117:HIS:CE1	2.23	0.74
1:A:8:ILE:HG13	1:A:140:MET:CE	2.19	0.72
1:H:11:ARG:NH1	1:H:14:GLU:OE2	2.22	0.71
1:H:91:ARG:NH2	4:H:401:HOH:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ILE:HG13	1:B:140:MET:HE2	1.71	0.71
1:E:105:PRO:O	1:H:105:PRO:O	2.07	0.71
1:D:105:PRO:O	1:J:105:PRO:O	2.09	0.70
1:G:105:PRO:O	1:I:105:PRO:O	2.11	0.68
1:E:4:SER:HA	1:F:4:SER:HA	1.75	0.68
1:D:228:ARG:NH2	4:D:401:HOH:O	2.27	0.68
1:J:8:ILE:HG13	1:J:140:MET:CE	2.23	0.68
1:F:14:GLU:OE1	1:F:28:ASP:OD1	2.13	0.67
1:A:41:SER:HB2	1:A:124:THR:HG21	1.76	0.66
1:E:140:MET:CE	1:F:117:HIS:HE1	2.08	0.66
1:C:41:SER:HB2	1:C:124:THR:HG21	1.78	0.66
1:I:242:TYR:CD1	1:J:214:TRP:HH2	2.13	0.66
1:B:106:GLN:HE22	1:C:107:GLY:HA3	1.61	0.65
1:D:8:ILE:HG13	1:D:140:MET:HE2	1.79	0.64
1:G:7:LEU:HA	1:G:140:MET:HE1	1.80	0.63
1:A:8:ILE:HG13	1:A:140:MET:HE2	1.80	0.63
1:D:220:ARG:HG3	1:D:220:ARG:HH21	1.64	0.63
1:I:8:ILE:HG13	1:I:140:MET:CE	2.28	0.63
1:A:124:THR:HB	4:A:448:HOH:O	1.99	0.62
1:I:161:LEU:HD13	1:J:147:LEU:HG	1.82	0.61
1:C:106:GLN:O	1:C:111:ARG:NH2	2.34	0.61
1:G:147:LEU:HG	1:H:161:LEU:HD13	1.82	0.60
1:H:106:GLN:O	1:H:111:ARG:NH2	2.35	0.60
3:G:302:CIT:O5	2:I:301:FL3:C10	2.50	0.59
1:B:8:ILE:HG13	1:B:140:MET:CE	2.32	0.59
1:F:74:LEU:HD13	1:F:74:LEU:C	2.23	0.59
1:H:8:ILE:HG13	1:H:140:MET:CE	2.33	0.58
1:C:8:ILE:HG13	1:C:140:MET:HE2	1.85	0.57
1:I:4:SER:HA	1:J:4:SER:HA	1.85	0.57
1:A:161:LEU:HD13	1:B:147:LEU:HG	1.87	0.57
1:J:191:THR:H	1:J:195:GLN:NE2	2.03	0.57
1:D:8:ILE:HG13	1:D:140:MET:CE	2.35	0.57
1:E:140:MET:CE	1:F:117:HIS:CE1	2.86	0.56
1:D:220:ARG:CG	1:D:220:ARG:HH21	2.18	0.56
1:H:7:LEU:HA	1:H:140:MET:HE1	1.86	0.56
1:A:55:VAL:O	1:A:59:ARG:HG3	2.05	0.56
1:A:7:LEU:HA	1:A:140:MET:HE1	1.88	0.56
1:C:74:LEU:HD13	1:C:75:SER:N	2.20	0.56
1:G:8:ILE:HG13	1:G:140:MET:CE	2.35	0.56
1:I:41:SER:HB2	1:I:124:THR:HG21	1.86	0.56
1:E:69:VAL:CG2	1:E:158:VAL:HG11	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:TRP:CG	1:B:176:PRO:HA	2.42	0.55
1:G:67:LEU:O	1:G:162:LYS:HE3	2.06	0.55
1:B:67:LEU:HD13	1:B:158:VAL:HG23	1.89	0.55
1:H:8:ILE:HG13	1:H:140:MET:HE3	1.88	0.55
1:J:185:LEU:O	1:J:214:TRP:HB2	2.06	0.54
1:F:231:ARG:O	1:F:235:GLU:HG3	2.08	0.54
1:A:180:ILE:HD11	1:B:55:VAL:HG21	1.89	0.54
1:G:208:LEU:CD1	1:G:214:TRP:HZ3	2.21	0.53
1:D:185:LEU:O	1:D:214:TRP:HB2	2.07	0.53
1:I:147:LEU:HG	1:J:161:LEU:HD13	1.91	0.52
1:A:41:SER:HB2	1:A:124:THR:CG2	2.38	0.52
1:B:200:MET:HG2	1:B:210:TRP:HB3	1.92	0.52
1:B:122:THR:HB	1:C:105:PRO:HG2	1.91	0.52
1:C:124:THR:HB	4:C:446:HOH:O	2.10	0.51
1:C:74:LEU:HD13	1:C:74:LEU:C	2.30	0.51
1:B:191:THR:H	1:B:195:GLN:NE2	2.08	0.51
1:E:78:SER:OG	1:H:123:HIS:HE1	1.94	0.51
1:F:175:TRP:CG	1:F:176:PRO:HA	2.46	0.51
1:J:175:TRP:CG	1:J:176:PRO:HA	2.45	0.51
1:A:124:THR:HG23	1:A:125:VAL:O	2.11	0.51
1:B:74:LEU:HD13	1:B:75:SER:N	2.25	0.51
1:C:5:ILE:HG22	1:C:114:GLY:HA3	1.93	0.51
1:B:42:HIS:CE1	1:B:75:SER:HB3	2.46	0.51
1:D:106:GLN:HE22	1:J:107:GLY:HA3	1.75	0.51
1:D:107:GLY:HA3	1:J:106:GLN:HE22	1.76	0.51
1:D:188:PRO:O	1:D:199:ARG:NH2	2.44	0.50
1:G:8:ILE:HG13	1:G:140:MET:HE3	1.93	0.50
1:A:175:TRP:CG	1:A:176:PRO:HA	2.47	0.50
1:D:123:HIS:HE1	1:J:78:SER:OG	1.94	0.50
1:F:174:ASP:HB3	4:F:414:HOH:O	2.10	0.50
1:J:220:ARG:HD3	4:J:455:HOH:O	2.11	0.50
1:E:36:TRP:CD2	1:E:132:ASP:HA	2.47	0.50
1:E:124:THR:HB	4:E:439:HOH:O	2.11	0.50
1:F:191:THR:H	1:F:195:GLN:NE2	2.10	0.50
1:D:104:ASP:N	1:D:105:PRO:HD3	2.27	0.49
1:E:74:LEU:HD13	1:E:75:SER:N	2.28	0.49
1:A:8:ILE:HG13	1:A:140:MET:HE3	1.93	0.49
1:I:74:LEU:HD13	1:I:75:SER:N	2.27	0.49
1:D:106:GLN:O	1:D:111:ARG:NH2	2.46	0.49
1:G:208:LEU:CD1	1:G:214:TRP:CZ3	2.96	0.49
1:C:124:THR:HG23	1:C:125:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:MET:HE3	1:D:117:HIS:HE1	1.77	0.49
1:A:126:ARG:HB3	1:A:149:ARG:CZ	2.43	0.49
1:C:228:ARG:HH11	1:C:228:ARG:CG	2.26	0.49
1:B:106:GLN:O	1:B:111:ARG:NH2	2.46	0.48
1:G:185:LEU:O	1:G:214:TRP:HB2	2.12	0.48
1:D:67:LEU:HD13	1:D:158:VAL:HG23	1.94	0.48
1:F:126:ARG:HB3	1:F:149:ARG:CZ	2.44	0.48
1:F:36:TRP:CD2	1:F:132:ASP:HA	2.48	0.48
1:I:242:TYR:CD1	1:J:214:TRP:CH2	2.99	0.48
1:E:122:THR:HB	1:H:105:PRO:HG2	1.94	0.48
1:E:175:TRP:CG	1:E:176:PRO:HA	2.49	0.48
1:G:104:ASP:N	1:G:105:PRO:HD3	2.28	0.48
1:C:208:LEU:HD22	1:C:214:TRP:HZ3	1.78	0.48
1:F:74:LEU:HD13	1:F:75:SER:N	2.29	0.47
1:G:228:ARG:HH11	1:G:228:ARG:HG2	1.79	0.47
1:C:117:HIS:CE1	1:D:140:MET:HE1	2.49	0.47
1:C:8:ILE:HG13	1:C:140:MET:CE	2.43	0.47
1:C:4:SER:HA	1:D:4:SER:HA	1.94	0.47
1:F:74:LEU:CD1	1:F:74:LEU:C	2.83	0.47
1:G:228:ARG:HH11	1:G:228:ARG:CG	2.26	0.47
1:J:92:HIS:O	1:J:245:ALA:HB1	2.14	0.47
1:C:74:LEU:CD1	1:C:74:LEU:C	2.82	0.47
1:A:117:HIS:CE1	1:B:140:MET:HE1	2.49	0.47
1:C:69:VAL:CG2	1:C:158:VAL:HG11	2.37	0.47
1:D:36:TRP:CD2	1:D:132:ASP:HA	2.49	0.47
1:D:175:TRP:CG	1:D:176:PRO:HA	2.50	0.47
1:I:36:TRP:CD2	1:I:132:ASP:HA	2.49	0.47
1:B:104:ASP:N	1:B:105:PRO:CD	2.78	0.47
1:C:10:GLU:OE2	1:D:2:PRO:N	2.48	0.47
1:J:104:ASP:N	1:J:105:PRO:HD3	2.30	0.47
1:I:110:ALA:HB1	1:I:116:LEU:HD13	1.96	0.46
1:I:11:ARG:HG2	1:I:11:ARG:HH11	1.81	0.46
1:I:74:LEU:C	1:I:74:LEU:CD1	2.84	0.46
1:G:161:LEU:HD13	1:H:147:LEU:HG	1.97	0.46
1:B:39:LEU:C	1:B:39:LEU:HD23	2.36	0.46
1:I:8:ILE:HG13	1:I:140:MET:HE2	1.97	0.46
1:C:224:GLU:HG2	4:C:402:HOH:O	2.15	0.46
1:G:36:TRP:CD2	1:G:132:ASP:HA	2.51	0.46
1:D:92:HIS:O	1:D:245:ALA:HB1	2.16	0.46
1:J:200:MET:HG2	1:J:210:TRP:HB3	1.97	0.46
1:E:41:SER:HB2	1:E:124:THR:HG21	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:122:THR:OG1	1:J:123:HIS:CD2	2.69	0.45
1:G:175:TRP:CG	1:G:176:PRO:HA	2.51	0.45
1:A:74:LEU:HD13	1:A:75:SER:N	2.31	0.45
1:D:119:GLU:OE1	1:D:146:GLU:OE2	2.34	0.45
1:B:200:MET:CE	1:B:200:MET:HA	2.47	0.45
1:B:185:LEU:O	1:B:214:TRP:HB2	2.16	0.45
1:I:41:SER:HB2	1:I:124:THR:CG2	2.46	0.45
1:E:124:THR:HG23	1:E:125:VAL:O	2.16	0.45
1:I:175:TRP:CG	1:I:176:PRO:HA	2.51	0.45
1:C:36:TRP:CD2	1:C:132:ASP:HA	2.52	0.45
1:C:41:SER:HB2	1:C:124:THR:CG2	2.46	0.45
1:H:39:LEU:C	1:H:39:LEU:HD23	2.36	0.45
1:E:74:LEU:CD1	1:E:74:LEU:C	2.85	0.45
1:C:175:TRP:CG	1:C:176:PRO:HA	2.52	0.44
1:D:163:LEU:HD12	1:D:175:TRP:CH2	2.52	0.44
1:J:28:ASP:N	1:J:28:ASP:OD1	2.51	0.44
1:C:161:LEU:HD13	1:D:147:LEU:HG	1.99	0.44
1:H:74:LEU:C	1:H:74:LEU:HD13	2.38	0.44
1:H:175:TRP:CG	1:H:176:PRO:HA	2.53	0.44
1:G:163:LEU:CD2	1:G:175:TRP:CH2	3.01	0.44
1:G:8:ILE:N	1:G:140:MET:HE2	2.34	0.43
1:E:208:LEU:HD12	1:E:208:LEU:HA	1.91	0.43
1:C:159:LYS:NZ	1:C:225:GLU:OE2	2.42	0.43
1:F:8:ILE:N	1:F:140:MET:CE	2.81	0.43
1:H:79:VAL:HG12	4:H:465:HOH:O	2.18	0.43
1:A:36:TRP:CD2	1:A:132:ASP:HA	2.53	0.43
1:A:74:LEU:C	1:A:74:LEU:HD13	2.39	0.43
1:I:104:ASP:N	1:I:105:PRO:HD3	2.33	0.43
1:B:36:TRP:CD2	1:B:132:ASP:HA	2.54	0.43
1:B:74:LEU:C	1:B:74:LEU:HD13	2.38	0.43
1:J:8:ILE:CG1	1:J:140:MET:HE2	2.41	0.43
1:F:7:LEU:C	1:F:140:MET:HE1	2.39	0.43
3:A:302:CIT:O5	2:F:301:FL3:C10	2.67	0.43
1:F:67:LEU:CD1	1:F:158:VAL:HG23	2.49	0.43
1:F:8:ILE:HG13	1:F:140:MET:HE2	2.00	0.42
1:I:74:LEU:HD13	1:I:74:LEU:C	2.39	0.42
1:C:147:LEU:HD23	1:D:171:VAL:HB	2.00	0.42
1:G:147:LEU:HD23	1:H:171:VAL:HB	2.01	0.42
1:G:69:VAL:CG2	1:G:158:VAL:HG11	2.44	0.42
1:I:37:PHE:HA	1:I:70:ASP:O	2.19	0.42
1:G:74:LEU:HD13	1:G:74:LEU:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HG21	1:B:5:ILE:HD13	2.01	0.42
1:B:175:TRP:CD1	1:B:176:PRO:HA	2.54	0.42
1:E:16:GLU:HG2	1:E:23:VAL:CG1	2.50	0.42
1:H:36:TRP:CD2	1:H:132:ASP:HA	2.54	0.42
1:A:74:LEU:C	1:A:74:LEU:CD1	2.88	0.42
1:C:41:SER:HA	1:C:74:LEU:O	2.20	0.42
1:G:122:THR:HA	1:I:106:GLN:HG2	2.00	0.42
1:D:194:ASP:OD1	1:D:197:ARG:NH2	2.52	0.42
1:G:74:LEU:HD13	1:G:75:SER:N	2.34	0.42
1:I:66:ARG:NH2	1:I:225:GLU:OE1	2.53	0.42
1:G:42:HIS:O	1:G:124:THR:HG22	2.19	0.42
1:G:8:ILE:HG13	1:G:140:MET:HE2	2.02	0.42
1:J:36:TRP:CD2	1:J:132:ASP:HA	2.54	0.42
1:E:161:LEU:HD13	1:F:147:LEU:HG	2.00	0.42
1:J:63:ASP:OD1	1:J:66:ARG:NH1	2.50	0.42
1:C:208:LEU:HD22	1:C:214:TRP:CZ3	2.56	0.41
1:G:48:PRO:HG2	1:H:186:ILE:HG21	2.01	0.41
1:I:163:LEU:HD12	1:I:163:LEU:HA	1.79	0.41
1:E:3:GLY:HA3	1:F:7:LEU:HD21	2.02	0.41
1:G:208:LEU:HD23	1:H:93:ILE:CD1	2.50	0.41
1:F:36:TRP:HB2	1:F:69:VAL:HG22	2.03	0.41
1:I:194:ASP:OD1	1:I:197:ARG:NH2	2.51	0.41
1:C:93:ILE:HD13	1:D:180:ILE:HD13	2.01	0.41
1:A:78:SER:HB3	1:F:123:HIS:HE1	1.86	0.41
1:I:161:LEU:HD12	1:I:161:LEU:HA	1.87	0.41
1:H:126:ARG:HB3	1:H:149:ARG:CZ	2.50	0.41
1:G:124:THR:HG23	1:G:125:VAL:O	2.20	0.41
1:J:200:MET:HA	1:J:200:MET:CE	2.51	0.41
1:B:41:SER:HA	1:B:74:LEU:O	2.21	0.41
1:C:140:MET:HE3	1:D:117:HIS:CE1	2.55	0.41
1:F:111:ARG:HG2	4:F:480:HOH:O	2.20	0.40
1:G:179:GLU:HG2	1:H:59:ARG:NH1	2.36	0.40
1:E:107:GLY:HA3	1:H:106:GLN:HE22	1.86	0.40
1:A:117:HIS:CE1	1:B:140:MET:CE	3.04	0.40
1:G:199:ARG:NH1	4:G:409:HOH:O	2.54	0.40
1:G:42:HIS:CE1	1:G:75:SER:HB3	2.56	0.40
1:I:175:TRP:CD1	1:I:176:PRO:HA	2.56	0.40
1:I:5:ILE:O	1:J:2:PRO:HB3	2.20	0.40
1:E:164:GLY:HA3	4:F:467:HOH:O	2.20	0.40
1:E:47:THR:HB	3:E:302:CIT:C5	2.52	0.40
1:A:47:THR:HB	3:A:302:CIT:C5	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:PRO:HG2	1:C:122:THR:HB	2.03	0.40
1:C:174:ASP:HB3	4:D:434:HOH:O	2.20	0.40
1:E:55:VAL:O	1:E:59:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/250 (97%)	236 (98%)	5 (2%)	1 (0%)	34	32
1	B	242/250 (97%)	238 (98%)	3 (1%)	1 (0%)	34	32
1	C	242/250 (97%)	236 (98%)	5 (2%)	1 (0%)	34	32
1	D	242/250 (97%)	236 (98%)	5 (2%)	1 (0%)	34	32
1	E	242/250 (97%)	235 (97%)	6 (2%)	1 (0%)	34	32
1	F	242/250 (97%)	235 (97%)	6 (2%)	1 (0%)	34	32
1	G	242/250 (97%)	234 (97%)	7 (3%)	1 (0%)	34	32
1	H	242/250 (97%)	236 (98%)	5 (2%)	1 (0%)	34	32
1	I	242/250 (97%)	236 (98%)	5 (2%)	1 (0%)	34	32
1	J	242/250 (97%)	236 (98%)	6 (2%)	0	100	100
All	All	2420/2500 (97%)	2358 (97%)	53 (2%)	9 (0%)	34	32

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	125	VAL
1	D	125	VAL
1	F	125	VAL
1	H	125	VAL

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Mol	Chain	Res	Type
1	G	125	VAL
1	A	125	VAL
1	B	125	VAL
1	I	125	VAL
1	E	125	VAL

### 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	210/216 (97%)	197 (94%)	13 (6%)	18	15
1	B	210/216 (97%)	201 (96%)	9 (4%)	29	29
1	C	210/216 (97%)	196 (93%)	14 (7%)	16	13
1	D	210/216 (97%)	197 (94%)	13 (6%)	18	15
1	E	210/216 (97%)	193 (92%)	17 (8%)	11	8
1	F	210/216 (97%)	200 (95%)	10 (5%)	25	24
1	G	210/216 (97%)	197 (94%)	13 (6%)	18	15
1	H	210/216 (97%)	201 (96%)	9 (4%)	29	29
1	I	210/216 (97%)	193 (92%)	17 (8%)	11	8
1	J	210/216 (97%)	199 (95%)	11 (5%)	23	21
All	All	2100/2160 (97%)	1974 (94%)	126 (6%)	19	16

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	74	LEU
1	A	96	ARG
1	A	116	LEU
1	A	124	THR
1	A	147	LEU
1	A	161	LEU
1	A	163	LEU

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Mol	Chain	Res	Type
1	A	167	LEU
1	A	208	LEU
1	A	212	PHE
1	A	228	ARG
1	A	242	TYR
1	B	28	ASP
1	B	32	SER
1	B	74	LEU
1	B	147	LEU
1	B	161	LEU
1	B	199	ARG
1	B	202	SER
1	B	208	LEU
1	B	212	PHE
1	C	16	GLU
1	C	28	ASP
1	C	74	LEU
1	C	116	LEU
1	C	124	THR
1	C	147	LEU
1	C	161	LEU
1	C	167	LEU
1	C	197	ARG
1	C	207	SER
1	C	212	PHE
1	C	224	GLU
1	C	228	ARG
1	C	242	TYR
1	D	28	ASP
1	D	59	ARG
1	D	74	LEU
1	D	144	PRO
1	D	147	LEU
1	D	161	LEU
1	D	168	LYS
1	D	183	GLU
1	D	202	SER
1	D	208	LEU
1	D	212	PHE
1	D	220	ARG
1	D	244	GLU
1	E	11	ARG

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Mol	Chain	Res	Type
1	E	25	LYS
1	E	28	ASP
1	E	74	LEU
1	E	96	ARG
1	E	116	LEU
1	E	124	THR
1	E	147	LEU
1	E	161	LEU
1	E	167	LEU
1	E	183	GLU
1	E	199	ARG
1	E	207	SER
1	E	208	LEU
1	E	212	PHE
1	E	236	LYS
1	E	242	TYR
1	F	4	SER
1	F	28	ASP
1	F	74	LEU
1	F	79	VAL
1	F	147	LEU
1	F	161	LEU
1	F	197	ARG
1	F	199	ARG
1	F	212	PHE
1	F	220	ARG
1	G	2	PRO
1	G	28	ASP
1	G	66	ARG
1	G	74	LEU
1	G	116	LEU
1	G	124	THR
1	G	147	LEU
1	G	161	LEU
1	G	167	LEU
1	G	199	ARG
1	G	212	PHE
1	G	228	ARG
1	G	236	LYS
1	H	25	LYS
1	H	28	ASP
1	H	79	VAL

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Mol	Chain	Res	Type
1	H	147	LEU
1	H	161	LEU
1	H	193	GLU
1	H	197	ARG
1	H	208	LEU
1	H	212	PHE
1	I	16	GLU
1	I	66	ARG
1	I	74	LEU
1	I	116	LEU
1	I	124	THR
1	I	134	ARG
1	I	144	PRO
1	I	147	LEU
1	I	161	LEU
1	I	163	LEU
1	I	167	LEU
1	I	183	GLU
1	I	208	LEU
1	I	212	PHE
1	I	220	ARG
1	I	228	ARG
1	I	236	LYS
1	J	2	PRO
1	J	4	SER
1	J	28	ASP
1	J	74	LEU
1	J	79	VAL
1	J	147	LEU
1	J	161	LEU
1	J	208	LEU
1	J	212	PHE
1	J	220	ARG
1	J	236	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	B	65	GLN
1	B	92	HIS
1	B	106	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
1	B	123	HIS
1	B	195	GLN
1	C	204	GLN
1	D	106	GLN
1	D	123	HIS
1	D	195	GLN
1	D	204	GLN
1	E	204	GLN
1	F	106	GLN
1	F	117	HIS
1	F	123	HIS
1	F	195	GLN
1	F	204	GLN
1	G	204	GLN
1	H	65	GLN
1	H	106	GLN
1	H	123	HIS
1	H	195	GLN
1	H	204	GLN
1	I	21	HIS
1	I	65	GLN
1	I	204	GLN
1	J	92	HIS
1	J	106	GLN
1	J	123	HIS
1	J	195	GLN
1	J	204	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

20 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	FL3	I	301	-	14,14,14	1.05	0	19,19,19	0.61	0
3	CIT	I	302	-	3,12,12	1.36	0	3,17,17	2.12	1 (33%)
3	CIT	D	302	-	3,12,12	1.16	0	3,17,17	1.41	1 (33%)
2	FL3	A	301	-	14,14,14	1.00	0	19,19,19	0.91	0
3	CIT	F	302	-	3,12,12	1.25	0	3,17,17	1.80	1 (33%)
2	FL3	H	301	-	14,14,14	1.26	2 (14%)	19,19,19	0.73	0
2	FL3	J	301	-	14,14,14	1.18	2 (14%)	19,19,19	0.92	0
2	FL3	G	301	-	14,14,14	1.16	1 (7%)	19,19,19	1.03	0
2	FL3	D	301	-	14,14,14	1.05	0	19,19,19	1.11	1 (5%)
2	FL3	F	301	-	14,14,14	1.11	1 (7%)	19,19,19	0.88	0
2	FL3	C	301	-	14,14,14	1.21	1 (7%)	19,19,19	0.64	0
2	FL3	E	301	-	14,14,14	1.08	0	19,19,19	0.80	0
2	FL3	B	301	-	14,14,14	1.16	0	19,19,19	0.73	0
3	CIT	C	302	-	3,12,12	1.25	0	3,17,17	1.78	1 (33%)
3	CIT	A	302	-	3,12,12	1.54	0	3,17,17	2.85	1 (33%)
3	CIT	G	302	-	3,12,12	1.11	0	3,17,17	1.81	1 (33%)
3	CIT	H	302	-	3,12,12	1.05	0	3,17,17	1.28	0
3	CIT	E	302	-	3,12,12	1.06	0	3,17,17	1.88	1 (33%)
3	CIT	J	302	-	3,12,12	1.39	0	3,17,17	2.10	1 (33%)
3	CIT	B	302	-	3,12,12	1.35	0	3,17,17	2.08	1 (33%)

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	FL3	I	301	-	-	2/4/4/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CIT	I	302	-	-	3/6/16/16	-
3	CIT	D	302	-	-	3/6/16/16	-
2	FL3	A	301	-	-	4/4/4/4	0/2/2/2
3	CIT	F	302	-	-	4/6/16/16	-
2	FL3	H	301	-	-	4/4/4/4	0/2/2/2
2	FL3	J	301	-	-	4/4/4/4	0/2/2/2
2	FL3	G	301	-	-	4/4/4/4	0/2/2/2
2	FL3	D	301	-	-	4/4/4/4	0/2/2/2
2	FL3	F	301	-	-	4/4/4/4	0/2/2/2
2	FL3	C	301	-	-	4/4/4/4	0/2/2/2
2	FL3	E	301	-	-	4/4/4/4	0/2/2/2
2	FL3	B	301	-	-	4/4/4/4	0/2/2/2
3	CIT	C	302	-	-	3/6/16/16	-
3	CIT	A	302	-	-	3/6/16/16	-
3	CIT	G	302	-	-	3/6/16/16	-
3	CIT	H	302	-	-	3/6/16/16	-
3	CIT	E	302	-	-	3/6/16/16	-
3	CIT	J	302	-	-	3/6/16/16	-
3	CIT	B	302	-	-	3/6/16/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	FL3	C3-C2	2.42	1.54	1.49
2	H	301	FL3	C5-C3	2.21	1.41	1.37
2	J	301	FL3	C5-C3	2.17	1.41	1.37
2	J	301	FL3	C10-C9	2.09	1.41	1.36
2	F	301	FL3	C10-C9	2.06	1.41	1.36
2	C	301	FL3	C5-C3	2.03	1.41	1.37
2	G	301	FL3	C10-C9	2.01	1.41	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	CIT	C3-C2-C1	-4.71	107.44	114.98
3	J	302	CIT	C3-C4-C5	-3.57	109.26	114.98
3	I	302	CIT	C3-C2-C1	-3.39	109.55	114.98
3	B	302	CIT	C3-C4-C5	-3.34	109.64	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	CIT	C3-C2-C1	-3.23	109.81	114.98
3	G	302	CIT	C3-C2-C1	-3.12	109.98	114.98
3	F	302	CIT	C3-C4-C5	-2.95	110.26	114.98
3	C	302	CIT	C3-C4-C5	-2.79	110.52	114.98
3	D	302	CIT	C3-C2-C1	-2.42	111.11	114.98
2	D	301	FL3	O1-C2-C3	-2.25	115.05	119.84

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	302	CIT	C1-C2-C3-O7
3	I	302	CIT	C1-C2-C3-C4
3	I	302	CIT	C1-C2-C3-C6
3	D	302	CIT	C1-C2-C3-C6
2	A	301	FL3	C1-C2-C3-C4
2	A	301	FL3	C1-C2-C3-C5
3	F	302	CIT	C2-C3-C4-C5
3	F	302	CIT	O7-C3-C4-C5
3	F	302	CIT	C6-C3-C4-C5
2	F	301	FL3	C1-C2-C3-C4
2	F	301	FL3	C1-C2-C3-C5
2	B	301	FL3	O1-C2-C3-C4
2	B	301	FL3	O1-C2-C3-C5
3	C	302	CIT	C2-C3-C4-C5
3	C	302	CIT	O7-C3-C4-C5
3	C	302	CIT	C6-C3-C4-C5
3	A	302	CIT	C1-C2-C3-C6
3	G	302	CIT	C1-C2-C3-C6
3	H	302	CIT	C2-C3-C4-C5
3	H	302	CIT	O7-C3-C4-C5
3	H	302	CIT	C6-C3-C4-C5
3	E	302	CIT	C1-C2-C3-O7
3	E	302	CIT	C1-C2-C3-C4
3	E	302	CIT	C1-C2-C3-C6
3	J	302	CIT	C2-C3-C4-C5
3	J	302	CIT	O7-C3-C4-C5
3	J	302	CIT	C6-C3-C4-C5
3	B	302	CIT	C6-C3-C4-C5
2	J	301	FL3	O1-C2-C3-C4
2	E	301	FL3	C1-C2-C3-C4
2	E	301	FL3	C1-C2-C3-C5

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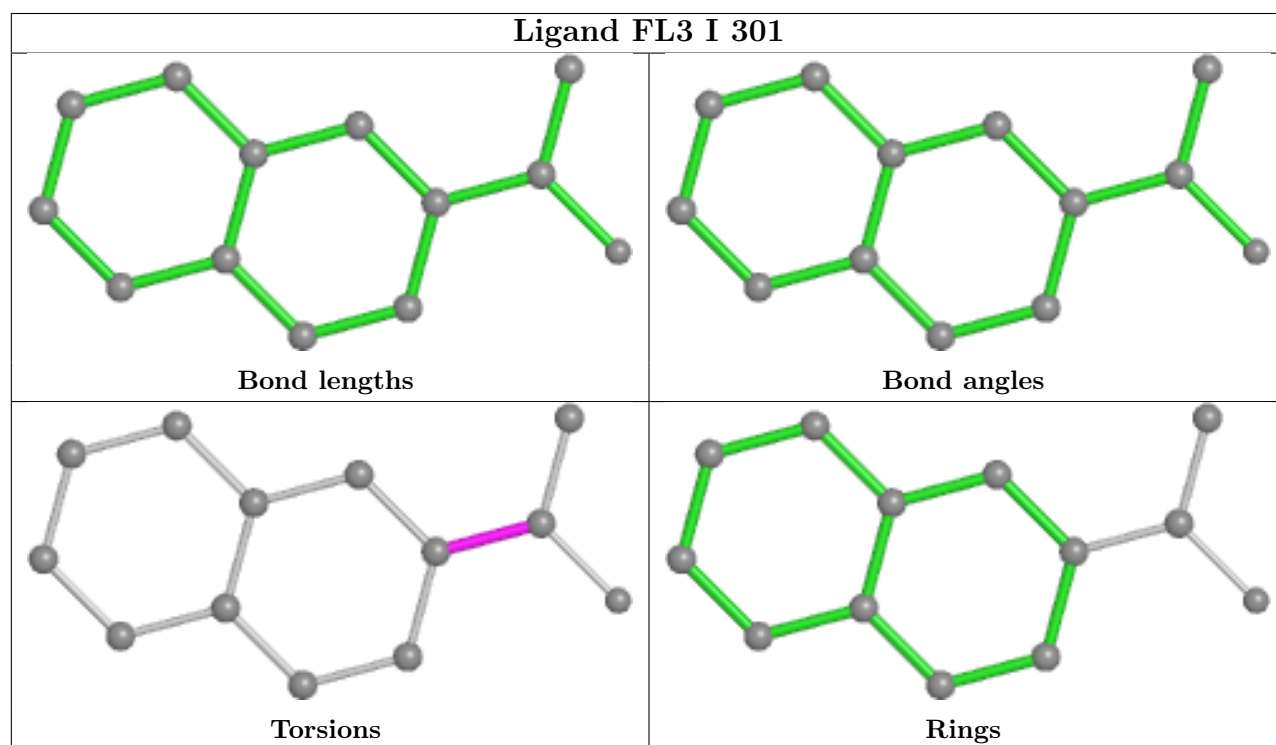
Mol	Chain	Res	Type	Atoms
2	J	301	FL3	O1-C2-C3-C5
2	A	301	FL3	O1-C2-C3-C4
2	A	301	FL3	O1-C2-C3-C5
2	F	301	FL3	O1-C2-C3-C4
2	F	301	FL3	O1-C2-C3-C5
2	E	301	FL3	O1-C2-C3-C4
2	B	301	FL3	C1-C2-C3-C4
2	C	301	FL3	O1-C2-C3-C5
2	E	301	FL3	O1-C2-C3-C5
2	B	301	FL3	C1-C2-C3-C5
2	C	301	FL3	O1-C2-C3-C4
3	G	302	CIT	C1-C2-C3-C4
2	J	301	FL3	C1-C2-C3-C4
2	J	301	FL3	C1-C2-C3-C5
3	D	302	CIT	C1-C2-C3-O7
3	D	302	CIT	C1-C2-C3-C4
3	A	302	CIT	C1-C2-C3-C4
3	G	302	CIT	C1-C2-C3-O7
3	B	302	CIT	C2-C3-C4-C5
3	B	302	CIT	O7-C3-C4-C5
2	C	301	FL3	C1-C2-C3-C5
2	D	301	FL3	O1-C2-C3-C5
2	C	301	FL3	C1-C2-C3-C4
2	G	301	FL3	O1-C2-C3-C5
2	D	301	FL3	O1-C2-C3-C4
3	A	302	CIT	C1-C2-C3-O7
2	G	301	FL3	O1-C2-C3-C4
2	D	301	FL3	C1-C2-C3-C5
2	G	301	FL3	C1-C2-C3-C4
2	G	301	FL3	C1-C2-C3-C5
2	D	301	FL3	C1-C2-C3-C4
2	H	301	FL3	O1-C2-C3-C4
2	H	301	FL3	O1-C2-C3-C5
2	H	301	FL3	C1-C2-C3-C4
3	F	302	CIT	C1-C2-C3-C4
2	H	301	FL3	C1-C2-C3-C5
2	I	301	FL3	O1-C2-C3-C4
2	I	301	FL3	O1-C2-C3-C5

There are no ring outliers.

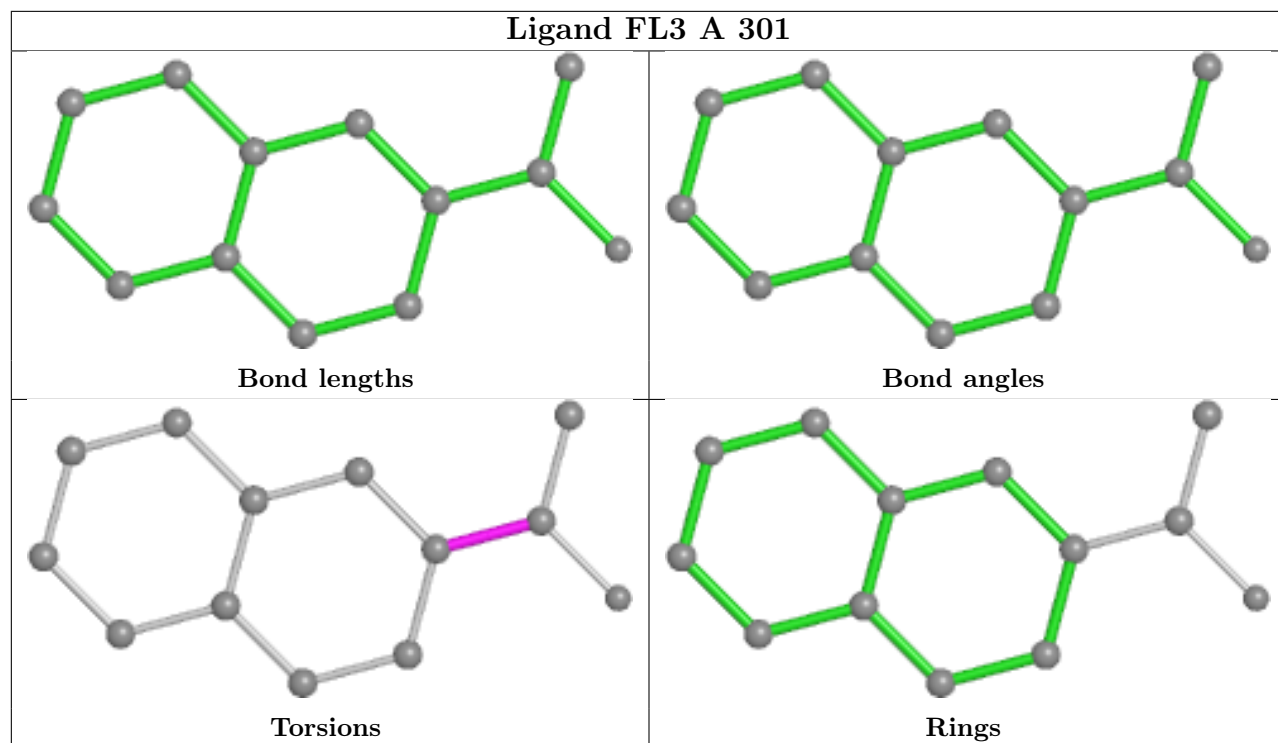
5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	301	FL3	1	0
2	F	301	FL3	1	0
3	A	302	CIT	2	0
3	G	302	CIT	1	0
3	E	302	CIT	1	0

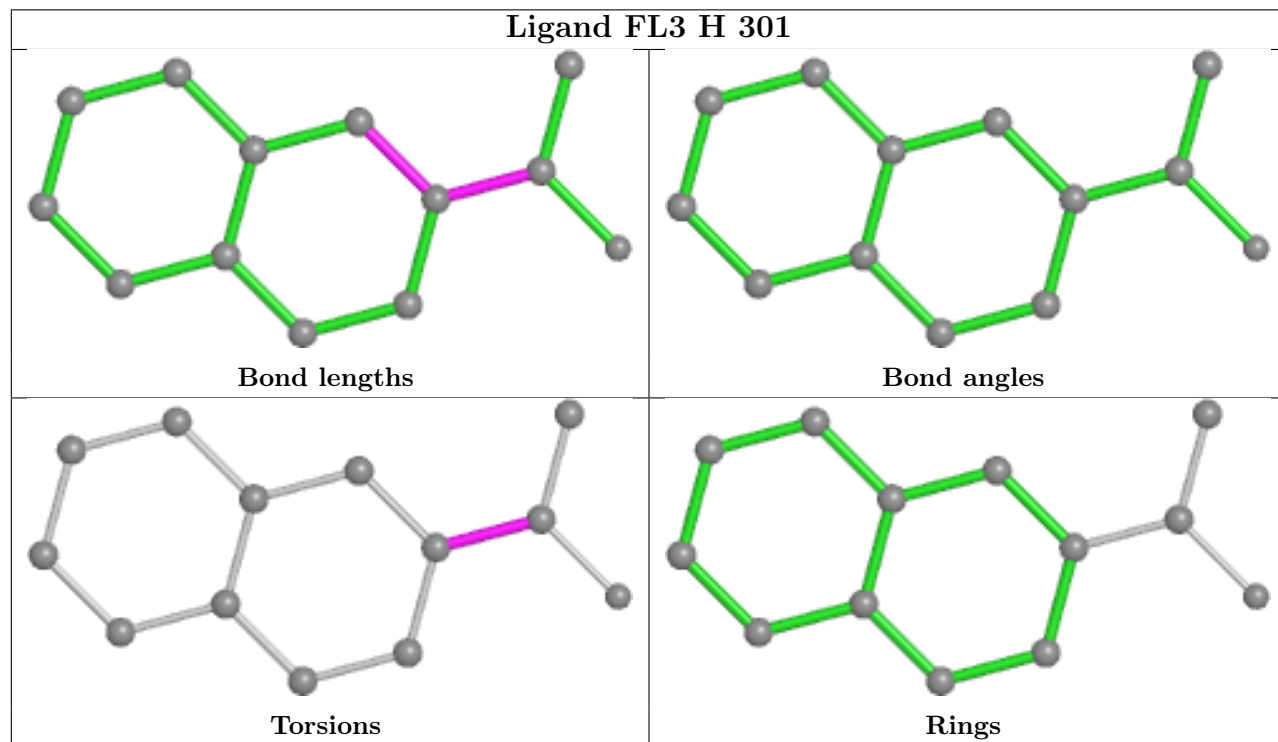
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 FL3 A 301

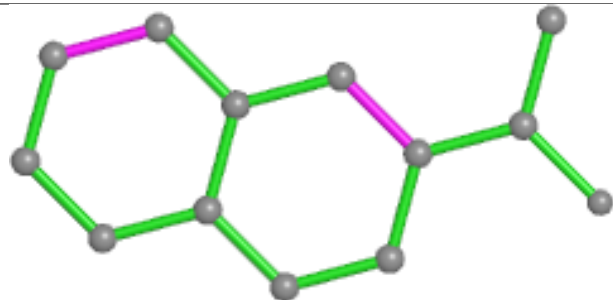


## Ligand FL3 H 301

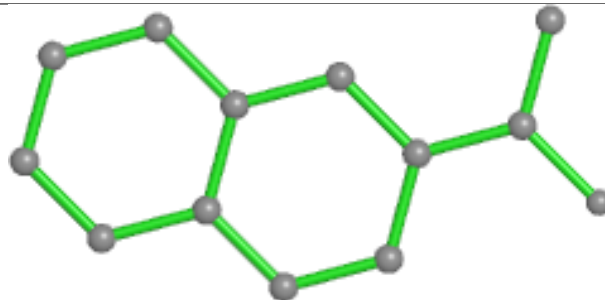




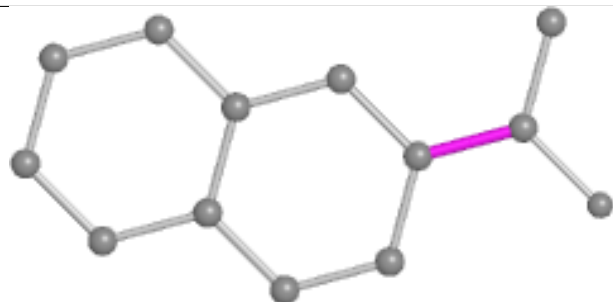
## Ligand FL3 J 301



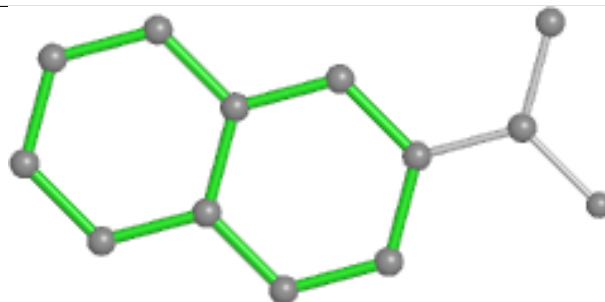
Bond lengths



Bond angles

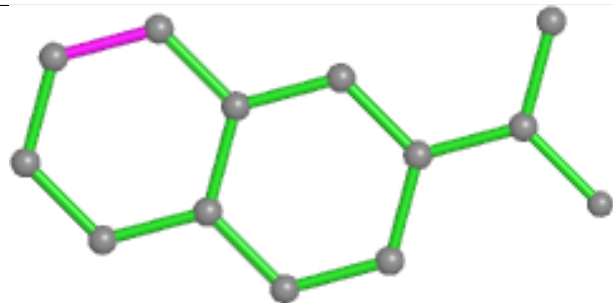


Torsions

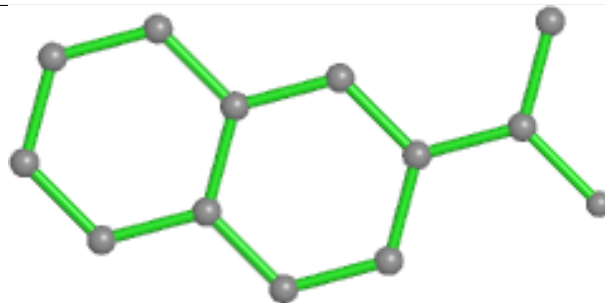


Rings

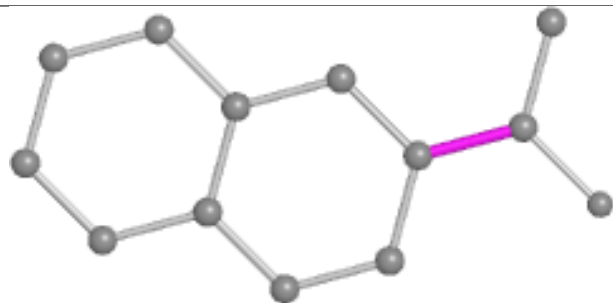
## Ligand FL3 G 301



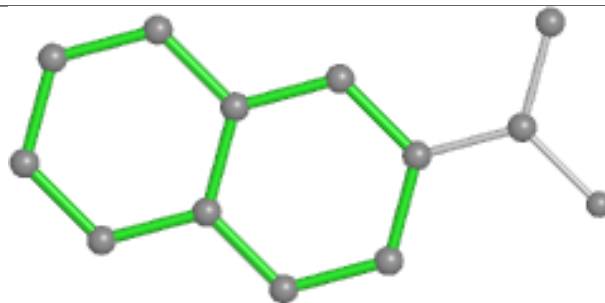
Bond lengths



Bond angles

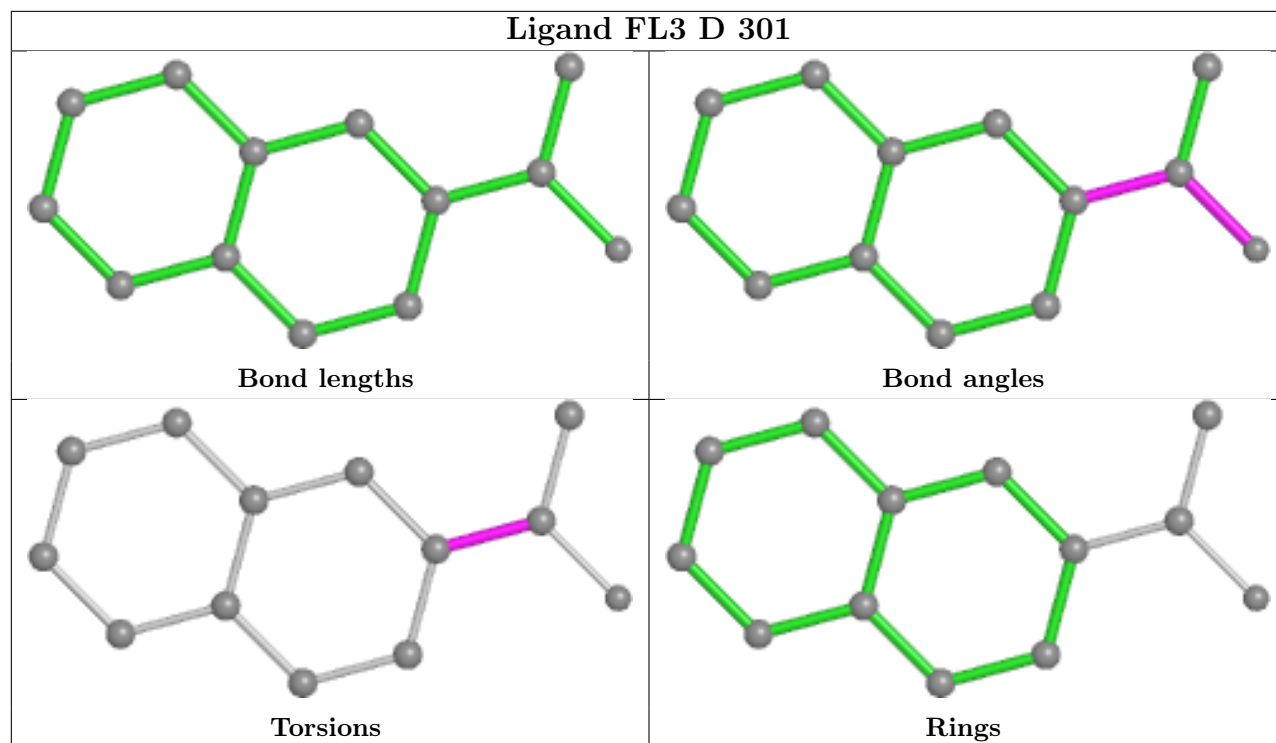


Torsions

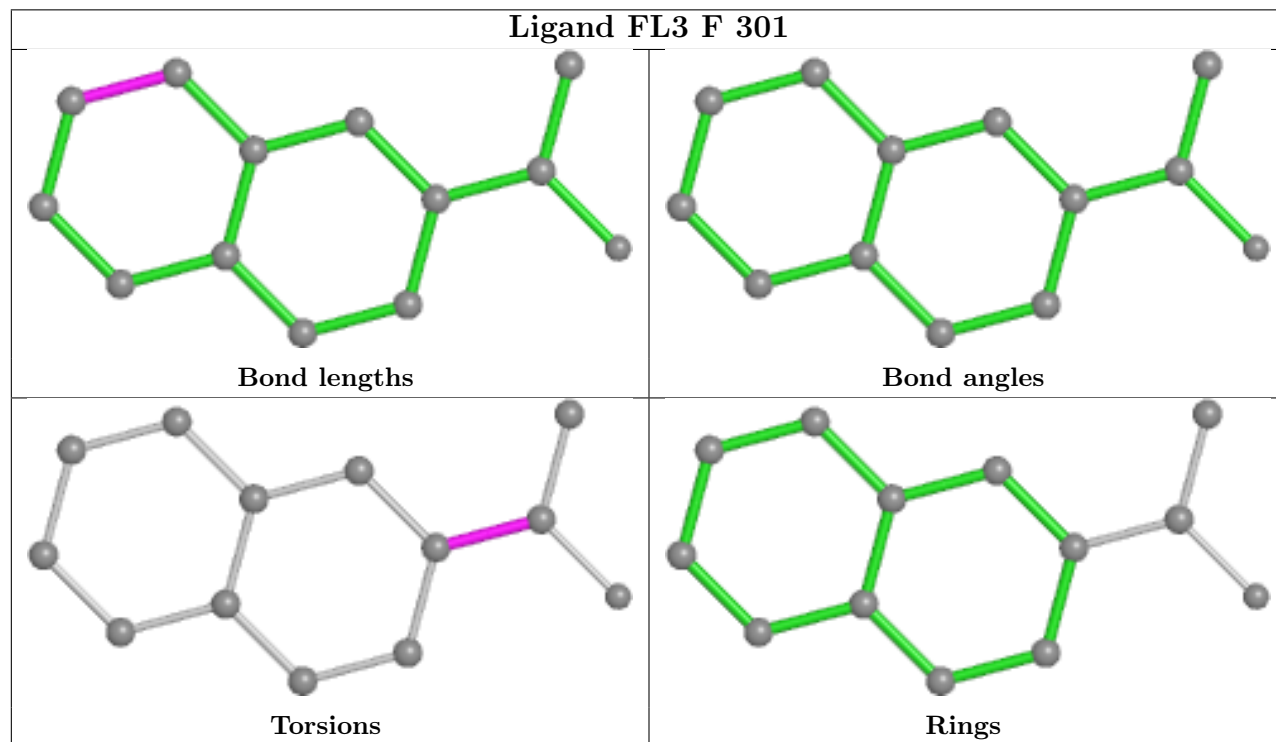


Rings

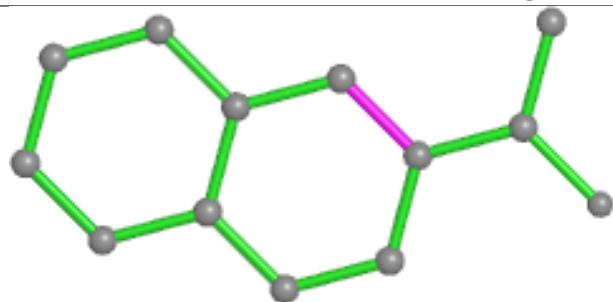
## Ligand FL3 D 301



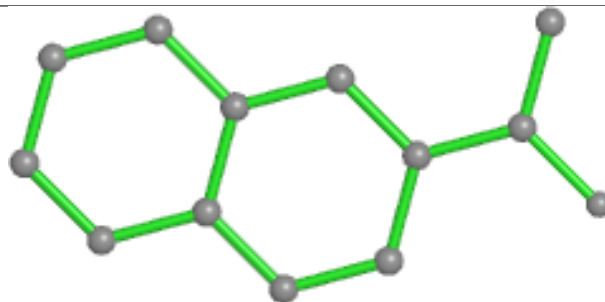
## Ligand FL3 F 301



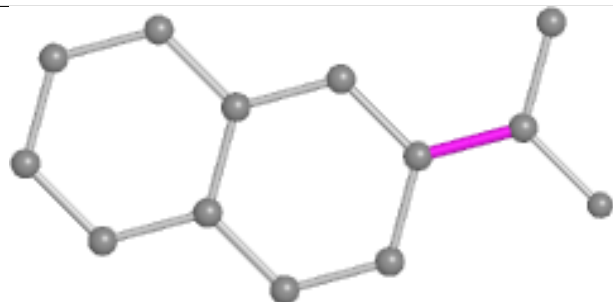
## Ligand FL3 C 301



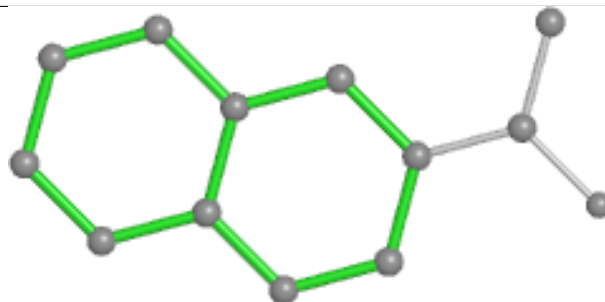
Bond lengths



Bond angles

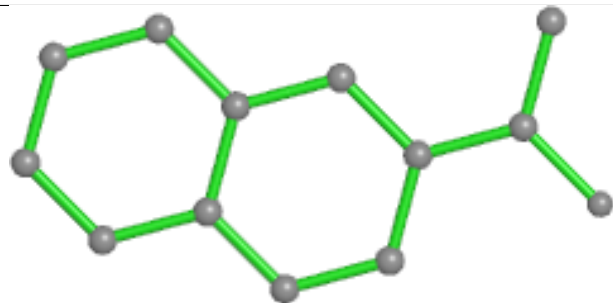


Torsions

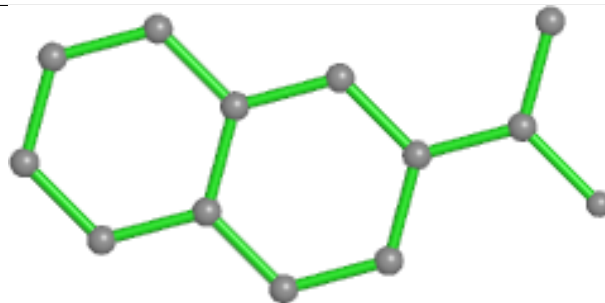


Rings

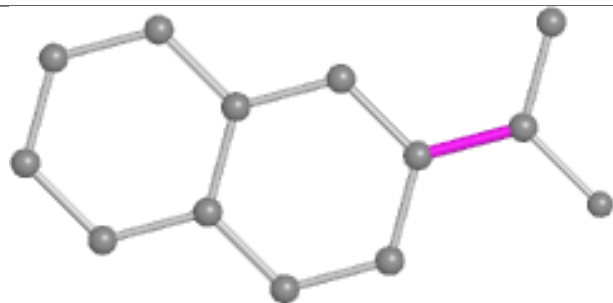
## Ligand FL3 E 301



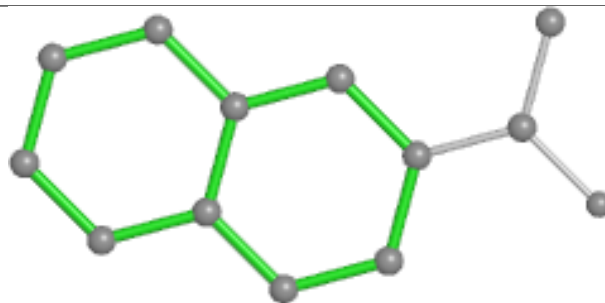
Bond lengths



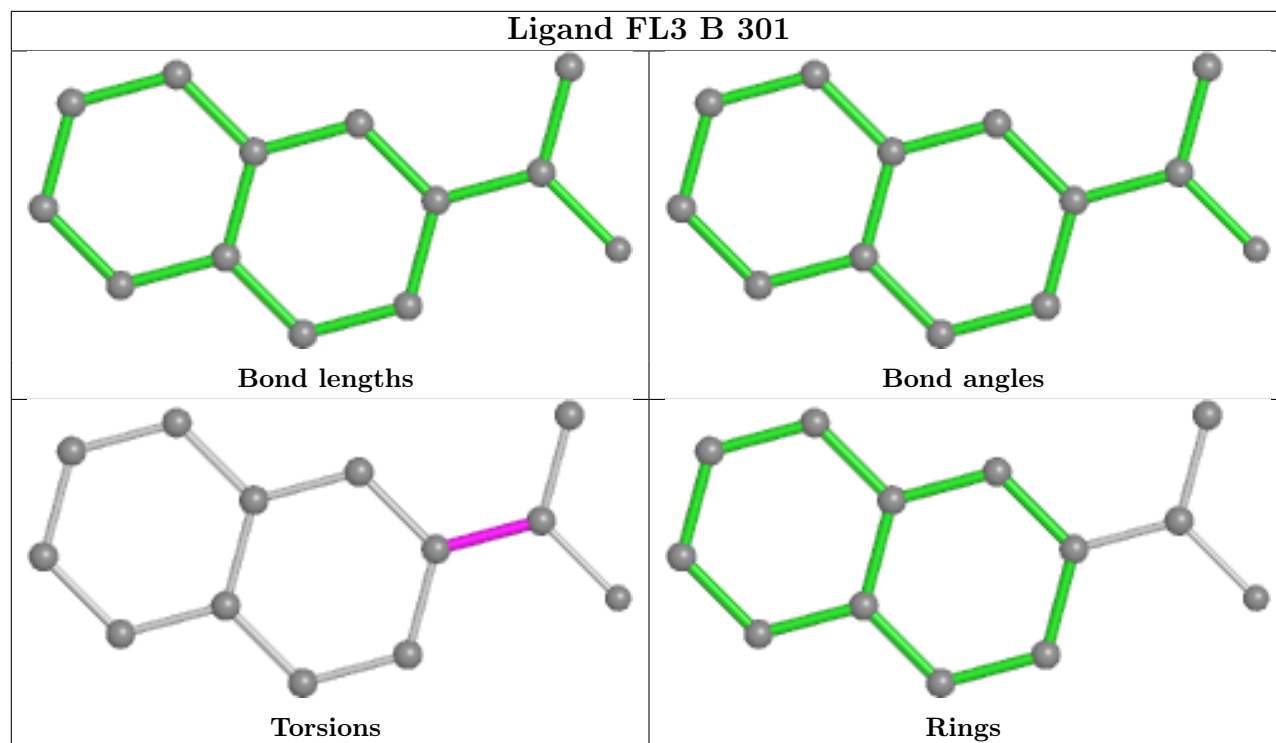
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	244/250 (97%)	-0.36	5 (2%) 65 69	25, 33, 61, 107	0
1	B	244/250 (97%)	-0.22	3 (1%) 79 82	25, 34, 61, 100	0
1	C	244/250 (97%)	-0.36	7 (2%) 51 57	28, 36, 63, 103	0
1	D	244/250 (97%)	-0.21	2 (0%) 86 88	29, 39, 64, 89	0
1	E	244/250 (97%)	-0.18	6 (2%) 57 62	28, 37, 67, 83	0
1	F	244/250 (97%)	-0.20	7 (2%) 51 57	27, 38, 65, 102	0
1	G	244/250 (97%)	-0.22	2 (0%) 86 88	28, 37, 66, 95	0
1	H	244/250 (97%)	-0.28	9 (3%) 41 48	29, 37, 67, 93	0
1	I	244/250 (97%)	-0.30	9 (3%) 41 48	29, 38, 68, 109	0
1	J	244/250 (97%)	-0.20	5 (2%) 65 69	31, 41, 70, 101	0
All	All	2440/2500 (97%)	-0.25	55 (2%) 60 65	25, 37, 66, 109	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	245	ALA	7.6
1	C	245	ALA	6.1
1	H	245	ALA	5.7
1	I	245	ALA	5.3
1	B	245	ALA	4.9
1	F	245	ALA	4.8
1	H	203	GLY	4.6
1	I	244	GLU	4.4
1	A	242	TYR	3.6
1	J	238	ALA	3.6
1	H	200	MET	3.6
1	A	244	GLU	3.5
1	I	242	TYR	3.5

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	G	244	GLU	3.2
1	F	242	TYR	3.2
1	A	245	ALA	3.1
1	I	236	LYS	3.0
1	G	2	PRO	3.0
1	J	242	TYR	2.9
1	F	220	ARG	2.9
1	B	242	TYR	2.8
1	C	198	ALA	2.8
1	C	202	SER	2.7
1	E	245	ALA	2.7
1	H	244	GLU	2.7
1	I	203	GLY	2.7
1	C	2	PRO	2.6
1	B	200	MET	2.5
1	I	238	ALA	2.4
1	F	2	PRO	2.4
1	E	141	LEU	2.4
1	F	66	ARG	2.4
1	C	201	GLU	2.4
1	I	239	LYS	2.4
1	I	243	GLU	2.3
1	E	2	PRO	2.3
1	A	220	ARG	2.3
1	C	197	ARG	2.3
1	D	242	TYR	2.3
1	H	197	ARG	2.3
1	A	2	PRO	2.3
1	J	239	LYS	2.2
1	E	203	GLY	2.2
1	H	202	SER	2.2
1	I	202	SER	2.2
1	D	203	GLY	2.2
1	H	201	GLU	2.2
1	J	244	GLU	2.2
1	H	242	TYR	2.2
1	H	2	PRO	2.1
1	E	242	TYR	2.1
1	F	201	GLU	2.1
1	C	199	ARG	2.0
1	E	200	MET	2.0
1	F	244	GLU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

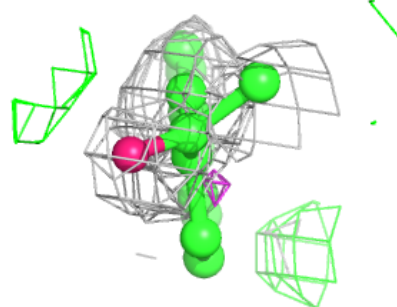
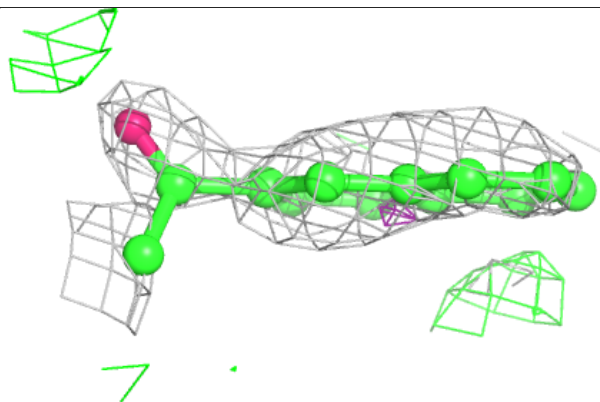
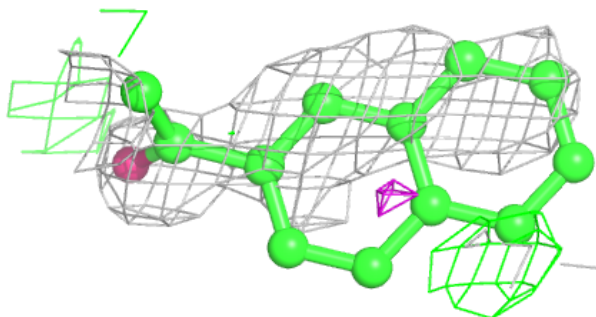
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	FL3	E	301	13/13	0.71	0.32	63,89,105,106	0
2	FL3	A	301	13/13	0.73	0.35	58,83,100,103	0
2	FL3	D	301	13/13	0.76	0.21	57,69,82,82	0
2	FL3	C	301	13/13	0.82	0.24	47,67,75,76	0
2	FL3	I	301	13/13	0.82	0.21	56,67,77,78	0
2	FL3	J	301	13/13	0.83	0.20	62,71,78,81	0
2	FL3	B	301	13/13	0.83	0.22	54,74,86,87	0
2	FL3	F	301	13/13	0.84	0.24	62,65,75,80	0
2	FL3	H	301	13/13	0.84	0.22	55,65,72,72	0
2	FL3	G	301	13/13	0.88	0.20	55,63,76,77	0
3	CIT	J	302	13/13	0.91	0.14	34,51,72,76	0
3	CIT	B	302	13/13	0.92	0.12	31,48,65,74	0
3	CIT	H	302	13/13	0.93	0.15	33,47,78,92	0
3	CIT	C	302	13/13	0.93	0.13	32,48,75,79	0
3	CIT	A	302	13/13	0.93	0.11	31,42,57,62	0
3	CIT	F	302	13/13	0.94	0.11	31,48,69,76	0
3	CIT	I	302	13/13	0.95	0.12	36,50,70,78	0
3	CIT	E	302	13/13	0.95	0.12	33,48,70,85	0
3	CIT	D	302	13/13	0.95	0.12	36,52,77,83	0
3	CIT	G	302	13/13	0.95	0.12	35,49,65,72	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 FL3 E 301:**

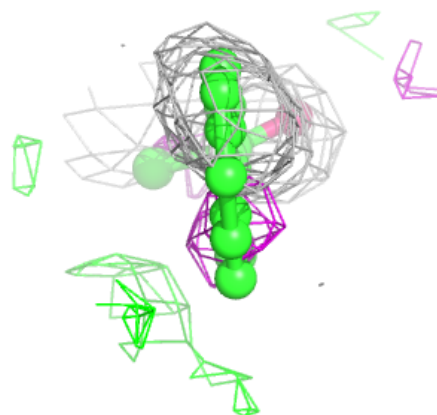
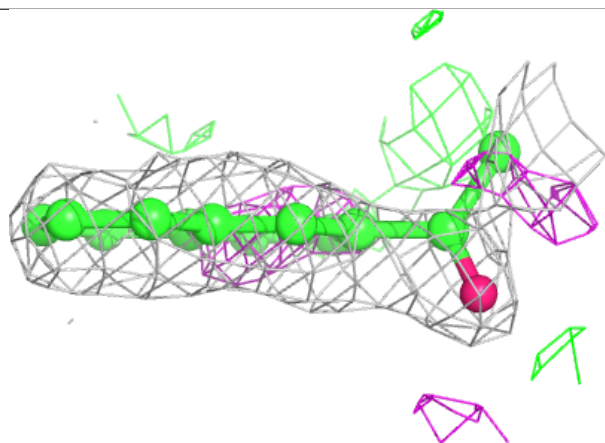
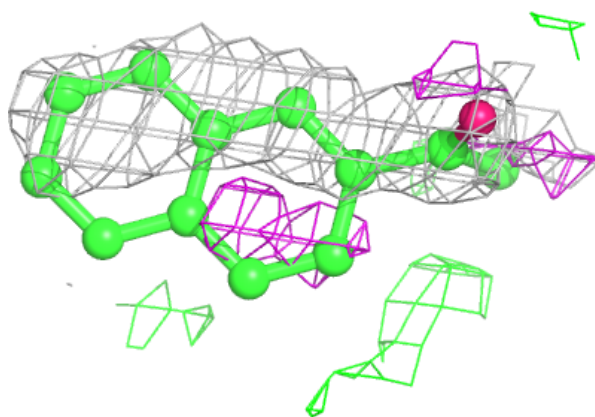
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





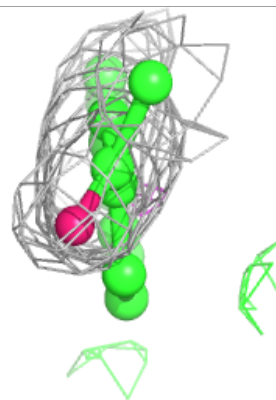
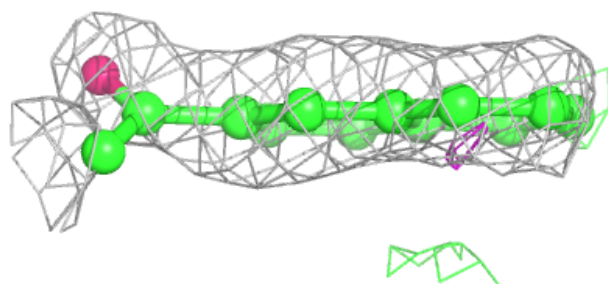
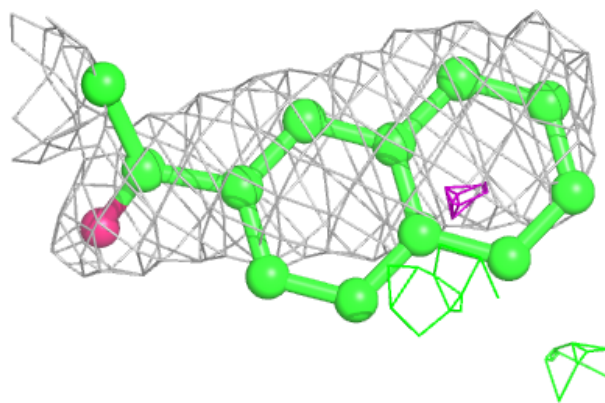
**Electron density around FL3 A 301:**

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

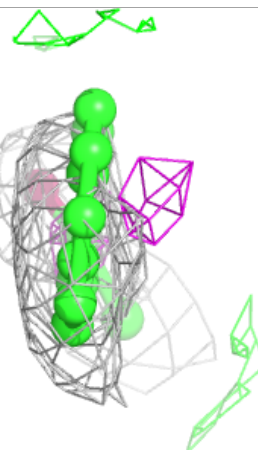
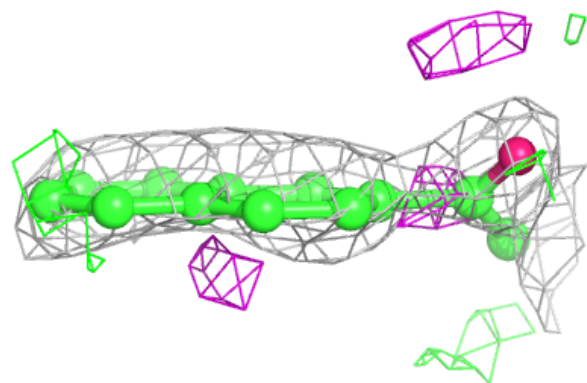
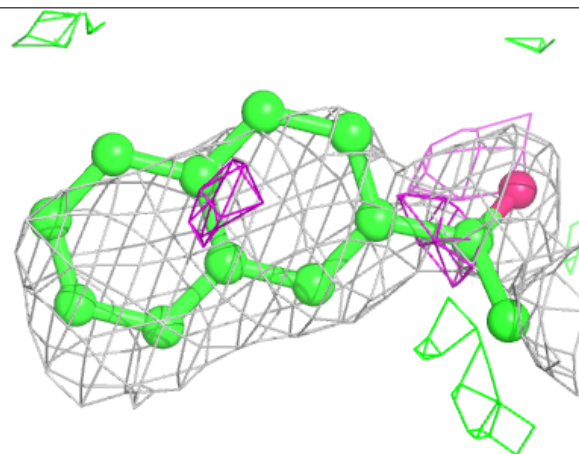


**Electron density around FL3 D 301:**

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

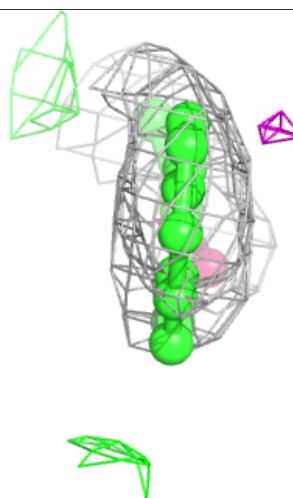
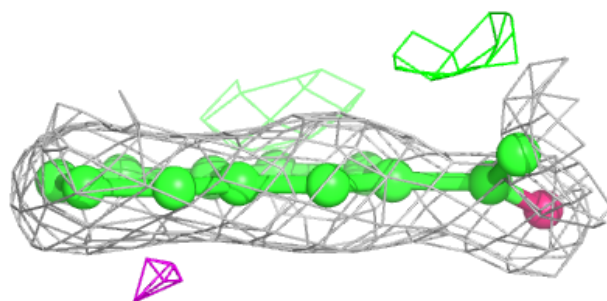
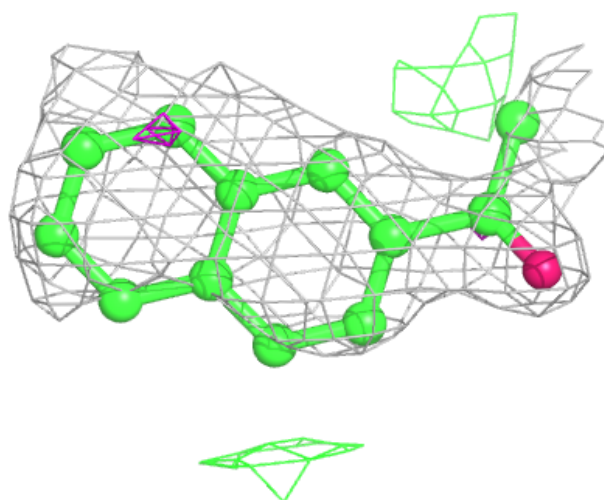
**Electron density around FL3 C 301:**

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



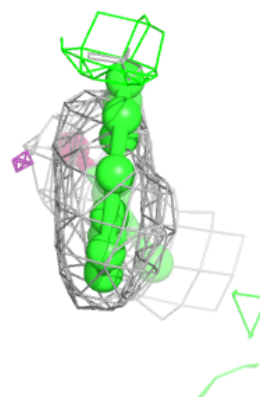
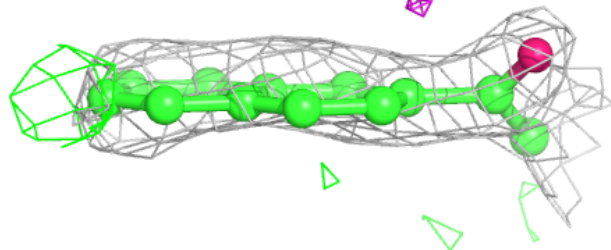
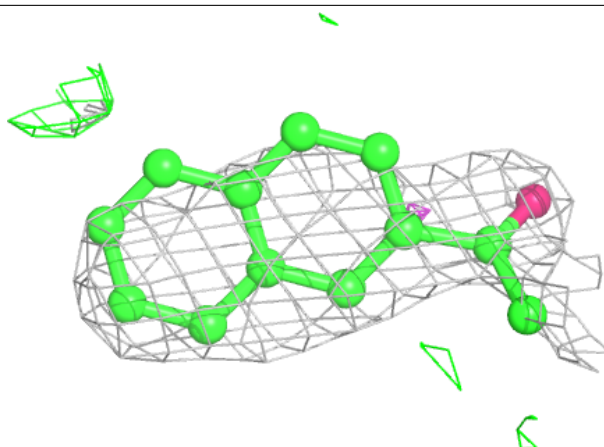
**Electron density around FL3 I 301:**

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



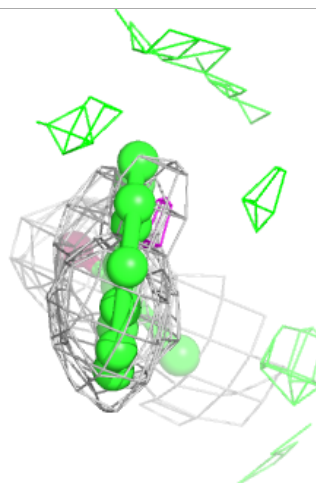
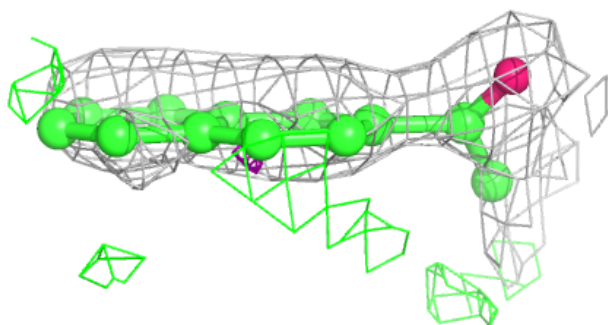
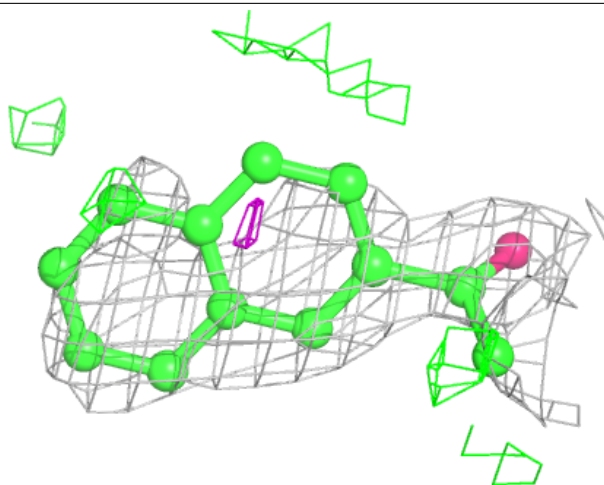
**Electron density around FL3 J 301:**

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



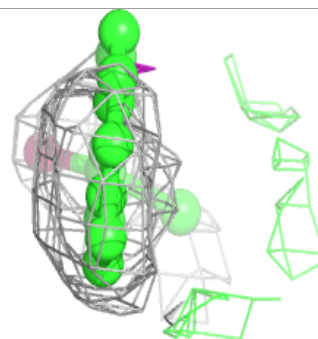
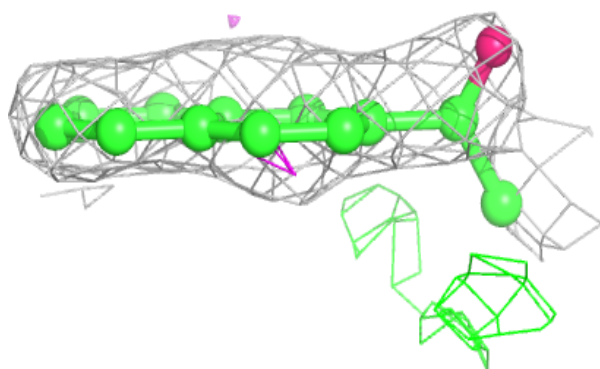
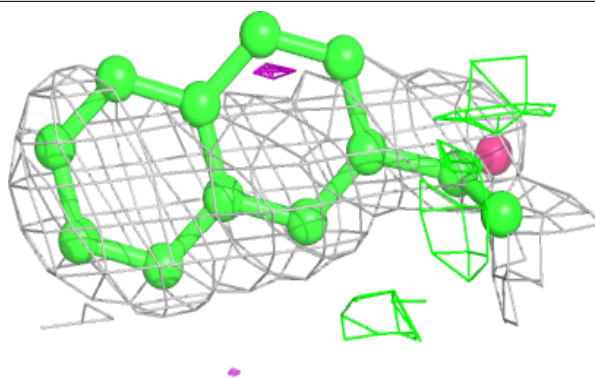
**Electron density around FL3 B 301:**

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

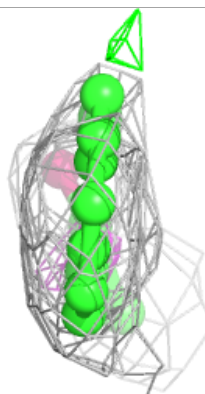
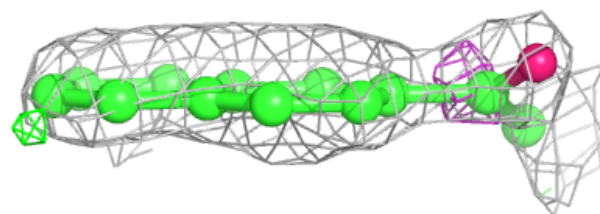
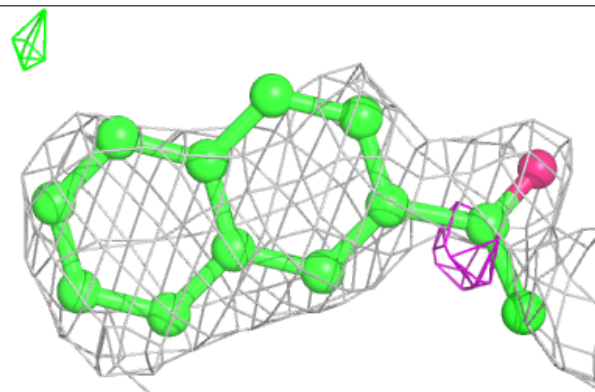


**Electron density around FL3 F 301:**

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

**Electron density around FL3 H 301:**

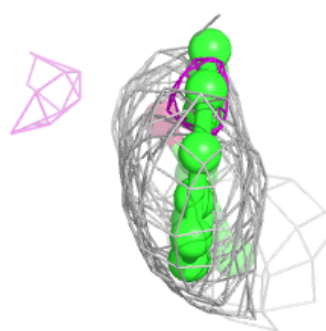
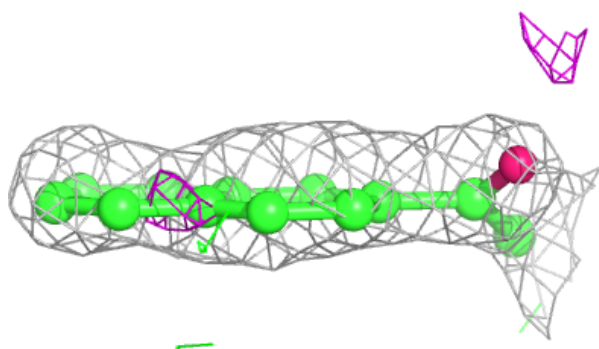
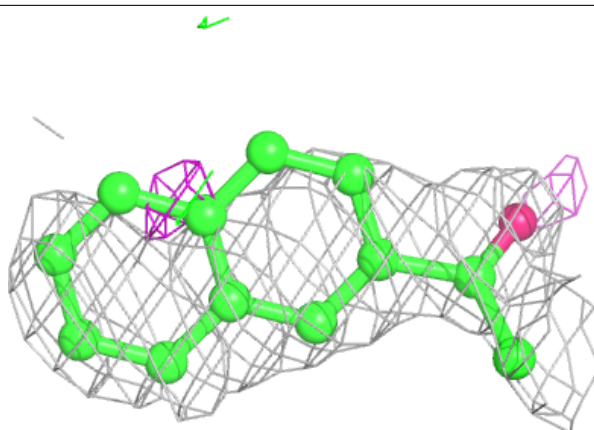
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around FL3 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.