



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:32 am BST

PDB ID : 4A98
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) in complex with bromoflurazepam
Authors : Spurny, R.; Brams, M.; Nury, H.; Legrand, P.; Ulens, C.
Deposited on : 2011-11-24
Resolution : 3.61 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 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 : 2.11
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) : 2.11

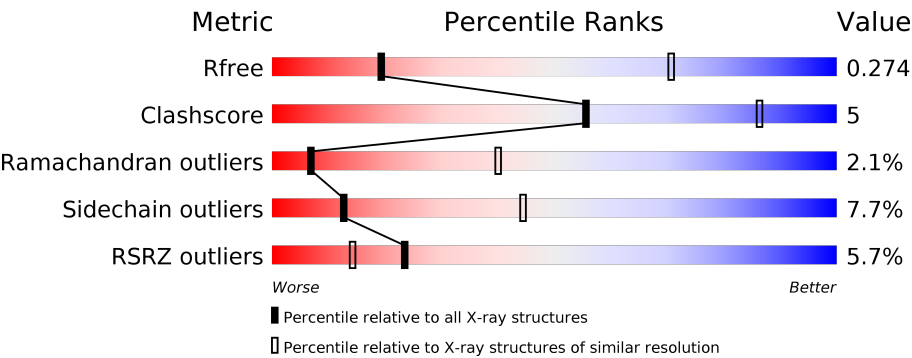
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.61 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.






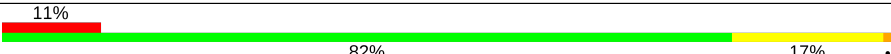
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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 on 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	307	<div><div>7%</div><div><div></div><div>81%</div><div>17%</div><div>.</div></div></div>
1	B	307	<div><div>4%</div><div><div></div><div>79%</div><div>19%</div><div>.</div></div></div>
1	C	307	<div><div>4%</div><div><div></div><div>81%</div><div>17%</div><div>.</div></div></div>
1	D	307	<div><div>6%</div><div><div></div><div>82%</div><div>16%</div><div>.</div></div></div>
1	E	307	<div><div>4%</div><div><div></div><div>81%</div><div>17%</div><div>.</div></div></div>
1	F	307	<div><div>6%</div><div><div></div><div>82%</div><div>16%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	307	
1	H	307	
1	I	307	
1	J	307	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BFZ	A	1318	-	-	-	X
2	BFZ	B	1318	-	-	X	-
2	BFZ	C	1318	-	-	X	-
2	BFZ	D	1318	-	-	X	X
2	BFZ	F	1318	-	-	X	-
2	BFZ	I	1318	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25120 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 CYS-LOOP LIGAND-GATED ION CHANNEL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2485	1622	412	445	6			
1	B	307	Total	C	N	O	S	0	0	0
			2485	1622	412	445	6			
1	C	307	Total	C	N	O	S	0	0	0
			2485	1622	412	445	6			
1	D	307	Total	C	N	O	S	0	0	0
			2485	1622	412	445	6			
1	E	307	Total	C	N	O	S	0	0	0
			2485	1622	412	445	6			
1	F	307	Total	C	N	O	S	0	0	0
			2485	1622	412	445	6			
1	G	307	Total	C	N	O	S	0	0	0
			2485	1622	412	445	6			
1	H	307	Total	C	N	O	S	0	0	0
			2485	1622	412	445	6			
1	I	307	Total	C	N	O	S	0	0	0
			2485	1622	412	445	6			
1	J	307	Total	C	N	O	S	0	0	0
			2485	1622	412	445	6			

There are 20 discrepancies between the modelled and reference sequences:

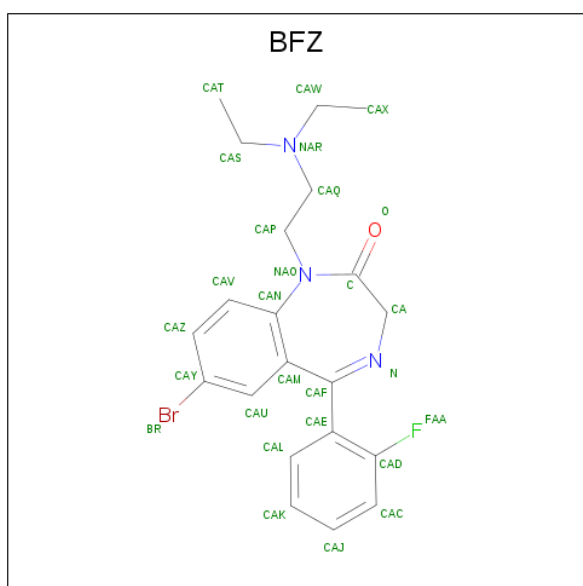
Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	insertion	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	289	ASN	MET	conflict	UNP P0C7B7
C	164	GLY	-	insertion	UNP P0C7B7
C	289	ASN	MET	conflict	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
E	164	GLY	-	insertion	UNP P0C7B7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	289	ASN	MET	conflict	UNP P0C7B7
F	164	GLY	-	insertion	UNP P0C7B7
F	289	ASN	MET	conflict	UNP P0C7B7
G	164	GLY	-	insertion	UNP P0C7B7
G	289	ASN	MET	conflict	UNP P0C7B7
H	164	GLY	-	insertion	UNP P0C7B7
H	289	ASN	MET	conflict	UNP P0C7B7
I	164	GLY	-	insertion	UNP P0C7B7
I	289	ASN	MET	conflict	UNP P0C7B7
J	164	GLY	-	insertion	UNP P0C7B7
J	289	ASN	MET	conflict	UNP P0C7B7

- Molecule 2 is 7-BROMO-1-[2-(DIETHYLAMINO)ETHYL]-5-(2-FLUOROPHENYL)-1,3-DIHYDRO-2H-1,4-BENZODIAZEPIN-2-ONE (three-letter code: BFZ) (formula: $C_{21}H_{23}BrFN_3O$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	F	N	O	0	0
			27	1	21	1	3	1		
2	B	1	Total	Br	C	F	N	O	0	0
			27	1	21	1	3	1		
2	C	1	Total	Br	C	F	N	O	0	0
			27	1	21	1	3	1		
2	D	1	Total	Br	C	F	N	O	0	0
			27	1	21	1	3	1		
2	E	1	Total	Br	C	F	N	O	0	0
			27	1	21	1	3	1		

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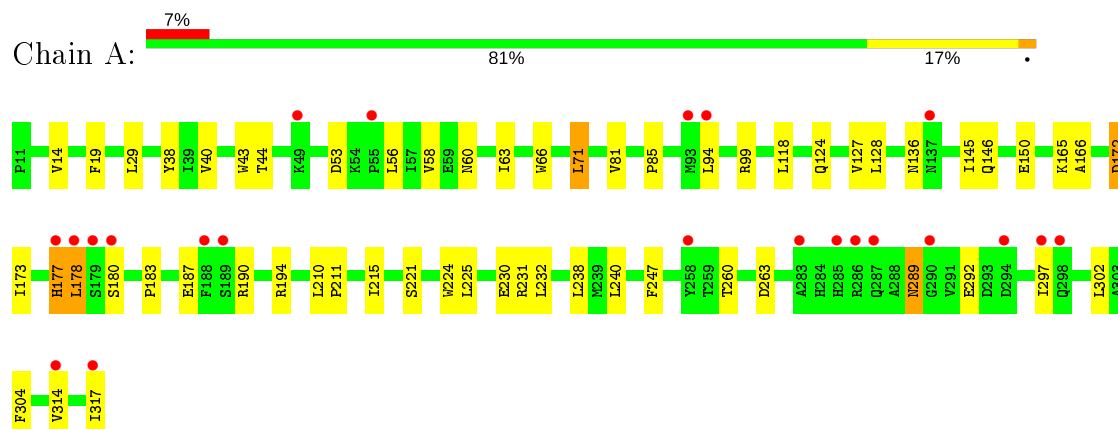
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	F	1	Total	Br	C	F	N	O	0	0
			27	1	21	1	3	1		
2	G	1	Total	Br	C	F	N	O	0	0
			27	1	21	1	3	1		
2	H	1	Total	Br	C	F	N	O	0	0
			27	1	21	1	3	1		
2	I	1	Total	Br	C	F	N	O	0	0
			27	1	21	1	3	1		
2	J	1	Total	Br	C	F	N	O	0	0
			27	1	21	1	3	1		

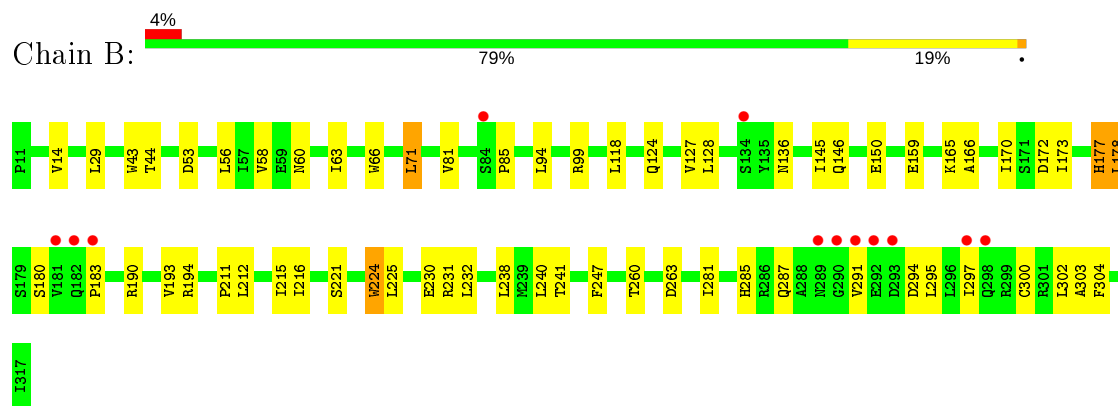
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

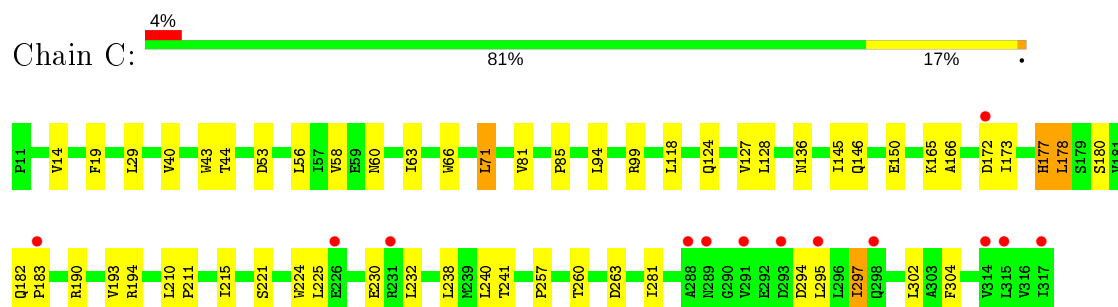
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL




• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

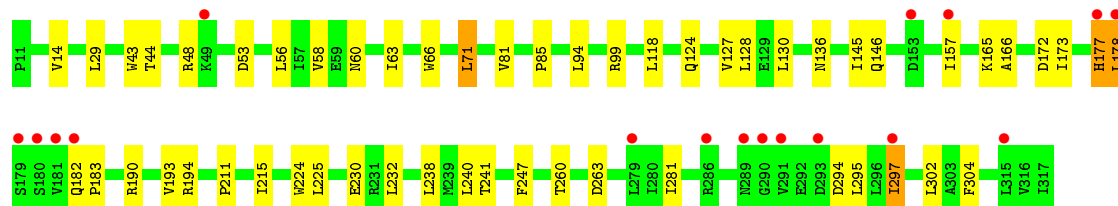


• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL




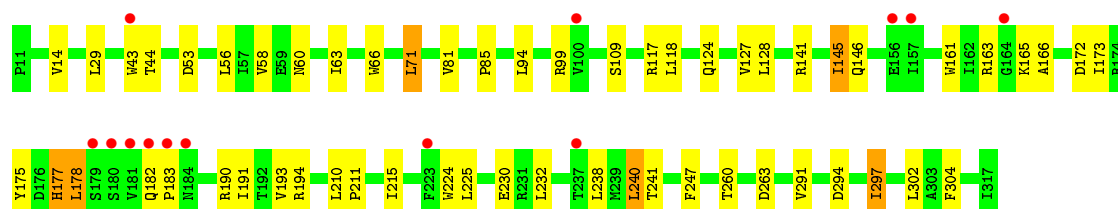
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain D: 




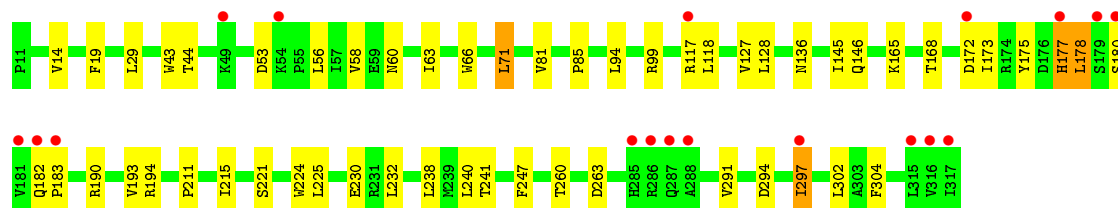
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain E: 




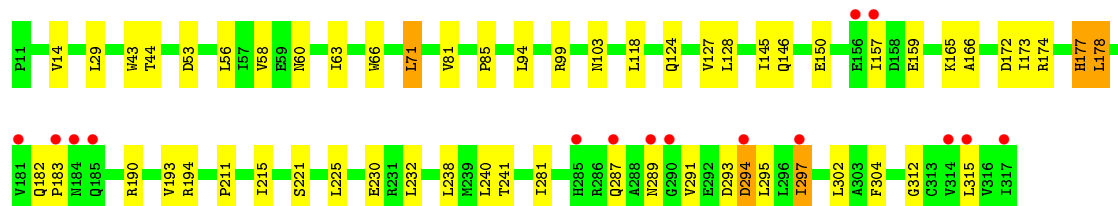
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain F: 




• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

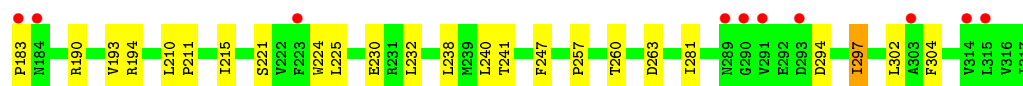
Chain G: 



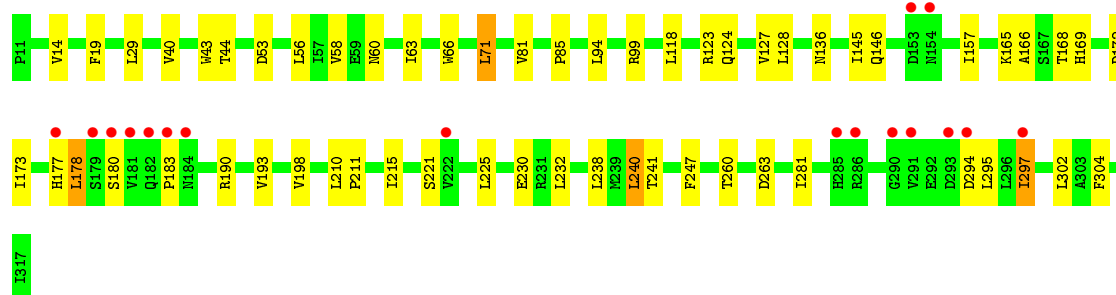
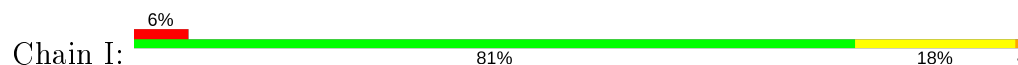
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain H: 

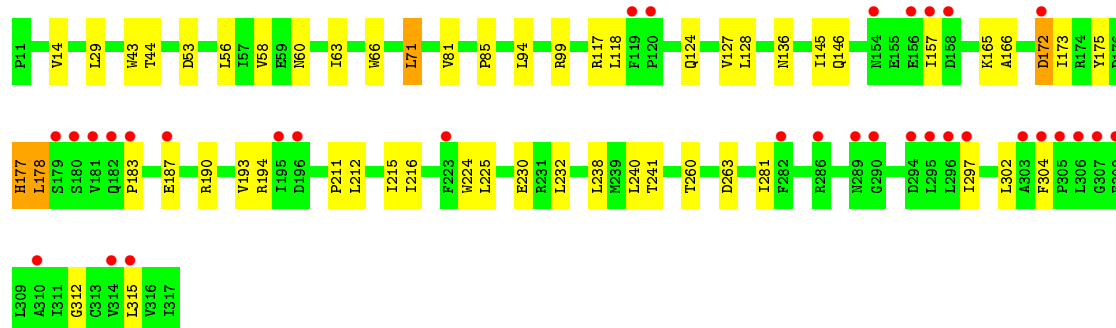
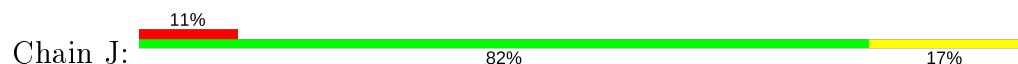




• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.40Å 268.20Å 111.40Å 90.00° 108.10° 90.00°	Depositor
Resolution (Å)	25.47 – 3.61 49.69 – 3.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.47-3.61) 99.5 (49.69-3.61)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.57Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.231 , 0.245 0.249 , 0.274	Depositor DCC
R_{free} test set	3421 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	115.9	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 120.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.043 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	25120	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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

5.1 Standard geometry

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

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	0.40	0/2553	0.58	0/3481
1	B	0.40	0/2553	0.58	0/3481
1	C	0.40	0/2553	0.57	0/3481
1	D	0.40	0/2553	0.58	0/3481
1	E	0.40	0/2553	0.58	0/3481
1	F	0.40	0/2553	0.57	0/3481
1	G	0.40	0/2553	0.58	0/3481
1	H	0.40	0/2553	0.57	0/3481
1	I	0.41	0/2553	0.58	0/3481
1	J	0.40	0/2553	0.57	0/3481
All	All	0.40	0/25530	0.58	0/34810

There are no bond length outliers.

There are no bond angle outliers.

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	2485	0	2439	28	0
1	B	2485	0	2439	25	0
1	C	2485	0	2439	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2485	0	2439	19	0
1	E	2485	0	2439	24	0
1	F	2485	0	2439	26	0
1	G	2485	0	2439	25	0
1	H	2485	0	2439	23	0
1	I	2485	0	2439	22	0
1	J	2485	0	2439	23	0
2	A	27	0	23	5	0
2	B	27	0	23	9	0
2	C	27	0	23	14	0
2	D	27	0	23	12	0
2	E	27	0	23	8	0
2	F	27	0	23	14	0
2	G	27	0	23	8	0
2	H	27	0	23	7	0
2	I	27	0	23	5	0
2	J	27	0	23	7	0
All	All	25120	0	24620	253	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 5.

All (253) 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:A:150:GLU:OE2	2:B:1318:BFZ:BR	2.20	1.15
1:E:182:GLN:CB	2:E:1318:BFZ:HAW2	1.96	0.95
1:C:177:HIS:HB3	2:C:1318:BFZ:HAV	1.52	0.89
1:G:177:HIS:HB2	2:G:1318:BFZ:HAT1	1.54	0.88
1:H:150:GLU:OE2	2:I:1318:BFZ:BR	2.48	0.86
2:D:1318:BFZ:HAS2	2:D:1318:BFZ:HAV	1.59	0.84
2:H:1318:BFZ:HAV	2:H:1318:BFZ:HAS2	1.59	0.83
1:H:150:GLU:OE1	2:I:1318:BFZ:BR	2.50	0.83
1:C:180:SER:CB	2:C:1318:BFZ:HAS1	2.06	0.83
2:G:1318:BFZ:HAV	2:G:1318:BFZ:HAS2	1.63	0.79
2:G:1318:BFZ:FAA	2:G:1318:BFZ:HAU	1.73	0.79
1:C:177:HIS:HB3	2:C:1318:BFZ:CAV	2.12	0.78
1:A:40:VAL:HG21	2:B:1318:BFZ:HA2C	1.66	0.77
1:F:177:HIS:HB3	2:F:1318:BFZ:HAV	1.67	0.77
1:D:177:HIS:HB2	2:D:1318:BFZ:HAT1	1.69	0.74
1:H:150:GLU:CD	2:I:1318:BFZ:BR	2.83	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1318:BFZ:FAA	2:A:1318:BFZ:HAU	1.79	0.71
1:C:150:GLU:OE2	2:D:1318:BFZ:BR	2.63	0.71
1:J:177:HIS:HB2	2:J:1318:BFZ:HAT1	1.73	0.71
2:C:1318:BFZ:FAA	2:C:1318:BFZ:HAU	1.80	0.71
2:D:1318:BFZ:O	2:D:1318:BFZ:HAQ1	1.90	0.70
1:H:177:HIS:HB2	2:H:1318:BFZ:HAT1	1.73	0.69
1:E:177:HIS:HB3	2:E:1318:BFZ:HAZ	1.73	0.69
1:J:177:HIS:HB3	2:J:1318:BFZ:HAV	1.75	0.69
1:F:180:SER:CB	2:F:1318:BFZ:HAS1	2.25	0.67
1:A:150:GLU:CD	2:B:1318:BFZ:BR	2.88	0.66
1:C:182:GLN:H	2:C:1318:BFZ:CAW	2.09	0.66
1:C:177:HIS:CB	2:C:1318:BFZ:HAV	2.27	0.64
1:D:157:ILE:HD11	1:E:117:ARG:HE	1.62	0.64
1:B:170:ILE:HB	1:I:169:HIS:ND1	2.12	0.64
1:A:40:VAL:HG21	2:B:1318:BFZ:CA	2.29	0.63
1:G:177:HIS:HB3	2:G:1318:BFZ:HAZ	1.79	0.63
1:B:177:HIS:HB3	2:B:1318:BFZ:HAV	1.83	0.60
1:F:177:HIS:HB3	2:F:1318:BFZ:CAV	2.31	0.60
2:D:1318:BFZ:FAA	2:D:1318:BFZ:HAU	1.91	0.60
1:C:40:VAL:CG2	2:D:1318:BFZ:HA2C	2.31	0.60
1:I:44:THR:HA	1:I:99:ARG:HA	1.83	0.60
1:C:177:HIS:HB3	2:C:1318:BFZ:CAZ	2.31	0.59
1:E:161:TRP:HB3	1:E:163:ARG:HH21	1.68	0.59
1:G:294:ASP:HB2	1:G:297:ILE:HG22	1.83	0.59
1:C:182:GLN:CB	2:C:1318:BFZ:HAW2	2.32	0.58
1:E:177:HIS:HB3	2:E:1318:BFZ:CAZ	2.33	0.58
1:I:157:ILE:HD11	1:J:117:ARG:HE	1.67	0.58
2:J:1318:BFZ:FAA	2:J:1318:BFZ:HAU	1.93	0.58
1:C:44:THR:HA	1:C:99:ARG:HA	1.86	0.56
1:I:180:SER:CB	2:I:1318:BFZ:HAT1	2.36	0.56
1:B:44:THR:HA	1:B:99:ARG:HA	1.88	0.55
2:G:1318:BFZ:HAV	2:G:1318:BFZ:CAS	2.35	0.55
1:A:40:VAL:CG2	2:B:1318:BFZ:HA2C	2.35	0.55
1:C:40:VAL:HG21	2:D:1318:BFZ:HA2C	1.88	0.54
1:A:221:SER:HB2	1:B:281:ILE:HD11	1.90	0.54
1:A:180:SER:CB	2:A:1318:BFZ:HAS2	2.38	0.53
1:E:44:THR:HA	1:E:99:ARG:HA	1.91	0.53
1:H:294:ASP:HB2	1:H:297:ILE:HG22	1.91	0.53
1:G:44:THR:HA	1:G:99:ARG:HA	1.90	0.53
1:J:44:THR:HA	1:J:99:ARG:HA	1.90	0.52
1:C:182:GLN:H	2:C:1318:BFZ:HAW2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:HG22	1:B:194:ARG:HG2	1.92	0.52
1:F:44:THR:HA	1:F:99:ARG:HA	1.90	0.52
1:A:44:THR:HA	1:A:99:ARG:HA	1.90	0.52
1:B:241:THR:HA	1:C:240:LEU:HD23	1.92	0.52
1:F:294:ASP:HB2	1:F:297:ILE:HG22	1.92	0.52
1:A:19:PHE:CE1	2:B:1318:BFZ:HA1C	2.45	0.52
1:I:19:PHE:CE1	2:J:1318:BFZ:HA1C	2.45	0.52
1:F:180:SER:CB	2:F:1318:BFZ:HAW1	2.40	0.51
2:F:1318:BFZ:HAU	2:F:1318:BFZ:CAD	2.40	0.51
1:D:44:THR:HA	1:D:99:ARG:HA	1.91	0.51
1:C:127:VAL:HG22	1:C:194:ARG:HG2	1.93	0.51
1:B:150:GLU:OE2	2:C:1318:BFZ:BR	2.84	0.51
1:H:14:VAL:HG22	1:H:43:TRP:HB3	1.93	0.51
1:J:127:VAL:HG22	1:J:194:ARG:HG2	1.93	0.51
1:F:14:VAL:HG22	1:F:43:TRP:HB3	1.93	0.51
1:E:127:VAL:HG22	1:E:194:ARG:HG2	1.93	0.50
1:A:240:LEU:HD23	1:E:241:THR:HA	1.94	0.50
1:B:180:SER:CB	2:B:1318:BFZ:HAT1	2.42	0.50
1:J:14:VAL:HG22	1:J:43:TRP:HB3	1.93	0.50
1:A:14:VAL:HG22	1:A:43:TRP:HB3	1.94	0.50
1:B:300:CYS:HB2	1:B:303:ALA:HB3	1.92	0.50
1:D:14:VAL:HG22	1:D:43:TRP:HB3	1.94	0.50
1:A:127:VAL:HG22	1:A:194:ARG:HG2	1.93	0.49
1:C:40:VAL:HG21	2:D:1318:BFZ:CA	2.42	0.49
1:H:127:VAL:HG22	1:H:194:ARG:HG2	1.93	0.49
1:D:127:VAL:HG22	1:D:194:ARG:HG2	1.94	0.49
1:G:127:VAL:HG22	1:G:194:ARG:HG2	1.92	0.49
1:E:14:VAL:HG22	1:E:43:TRP:HB3	1.94	0.49
1:G:103:ASN:ND2	2:H:1318:BFZ:HA2C	2.27	0.49
2:C:1318:BFZ:CAD	2:C:1318:BFZ:HAU	2.42	0.49
1:E:294:ASP:HB2	1:E:297:ILE:HG22	1.93	0.49
1:C:14:VAL:HG22	1:C:43:TRP:HB3	1.94	0.49
1:B:14:VAL:HG22	1:B:43:TRP:HB3	1.94	0.49
1:E:175:TYR:CD1	2:E:1318:BFZ:BR	3.21	0.49
1:G:14:VAL:HG22	1:G:43:TRP:HB3	1.94	0.49
1:D:58:VAL:HG12	1:D:63:ILE:HG13	1.95	0.48
1:H:241:THR:HA	1:I:240:LEU:HD23	1.94	0.48
1:G:58:VAL:HG12	1:G:63:ILE:HG13	1.94	0.48
1:F:19:PHE:CE2	2:G:1318:BFZ:BR	3.22	0.48
1:F:241:THR:HA	1:G:240:LEU:HD23	1.96	0.48
1:I:14:VAL:HG22	1:I:43:TRP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:HIS:HB3	2:E:1318:BFZ:CAV	2.44	0.48
1:C:177:HIS:HB3	2:C:1318:BFZ:HAZ	1.95	0.48
1:B:225:LEU:HD22	1:B:230:GLU:HB3	1.96	0.47
2:F:1318:BFZ:HAU	2:F:1318:BFZ:FAA	2.04	0.47
1:I:40:VAL:HG21	2:J:1318:BFZ:HA2C	1.96	0.47
1:J:312:GLY:HA2	1:J:315:LEU:HD12	1.96	0.47
1:E:225:LEU:HD22	1:E:230:GLU:HB3	1.97	0.47
1:H:81:VAL:HG21	1:H:85:PRO:HG3	1.96	0.47
1:G:71:LEU:HD11	1:G:94:LEU:HD21	1.96	0.47
1:A:71:LEU:HD11	1:A:94:LEU:HD21	1.97	0.47
1:D:225:LEU:HD22	1:D:230:GLU:HB3	1.97	0.47
1:F:182:GLN:CB	2:F:1318:BFZ:HAW2	2.44	0.47
1:F:225:LEU:HD22	1:F:230:GLU:HB3	1.97	0.47
1:F:58:VAL:HG12	1:F:63:ILE:HG13	1.97	0.47
1:C:58:VAL:HG12	1:C:63:ILE:HG13	1.97	0.47
2:H:1318:BFZ:HAU	2:H:1318:BFZ:FAA	2.05	0.46
1:A:225:LEU:HD22	1:A:230:GLU:HB3	1.97	0.46
1:H:225:LEU:HD22	1:H:230:GLU:HB3	1.97	0.46
1:I:225:LEU:HD22	1:I:230:GLU:HB3	1.97	0.46
1:J:225:LEU:HD22	1:J:230:GLU:HB3	1.97	0.46
1:C:225:LEU:HD22	1:C:230:GLU:HB3	1.97	0.46
2:H:1318:BFZ:HAP2	2:H:1318:BFZ:HAS2	1.61	0.46
1:A:81:VAL:HG21	1:A:85:PRO:HG3	1.98	0.46
1:B:71:LEU:HD11	1:B:94:LEU:HD21	1.98	0.46
2:A:1318:BFZ:HAV	2:A:1318:BFZ:CAQ	2.45	0.46
1:B:58:VAL:HG12	1:B:63:ILE:HG13	1.98	0.46
1:A:289:ASN:HD21	1:A:292:GLU:HB2	1.79	0.46
1:D:182:GLN:H	2:D:1318:BFZ:HAX1	1.81	0.46
1:G:177:HIS:CB	2:G:1318:BFZ:HAT1	2.36	0.46
1:H:44:THR:HA	1:H:99:ARG:HA	1.97	0.46
1:E:81:VAL:HG21	1:E:85:PRO:HG3	1.97	0.46
1:I:81:VAL:HG21	1:I:85:PRO:HG3	1.97	0.46
2:D:1318:BFZ:HAS2	2:D:1318:BFZ:HAP2	1.48	0.46
1:D:81:VAL:HG21	1:D:85:PRO:HG3	1.96	0.46
1:F:71:LEU:HD11	1:F:94:LEU:HD21	1.97	0.46
1:H:58:VAL:HG12	1:H:63:ILE:HG13	1.98	0.46
1:H:71:LEU:HD11	1:H:94:LEU:HD21	1.97	0.46
1:D:71:LEU:HD11	1:D:94:LEU:HD21	1.98	0.45
1:G:221:SER:HB2	1:H:281:ILE:HD11	1.99	0.45
1:G:150:GLU:OE2	2:H:1318:BFZ:BR	2.89	0.45
1:J:81:VAL:HG21	1:J:85:PRO:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:VAL:HG12	1:E:63:ILE:HG13	1.98	0.45
1:B:81:VAL:HG21	1:B:85:PRO:HG3	1.98	0.45
2:F:1318:BFZ:HAV	2:F:1318:BFZ:HAP2	1.61	0.45
1:F:221:SER:HB2	1:G:281:ILE:HD11	1.98	0.45
1:G:81:VAL:HG21	1:G:85:PRO:HG3	1.98	0.45
2:A:1318:BFZ:HAQ2	2:A:1318:BFZ:HAV	1.99	0.45
1:A:58:VAL:HG12	1:A:63:ILE:HG13	1.97	0.45
1:I:71:LEU:HD11	1:I:94:LEU:HD21	1.98	0.45
1:C:180:SER:CB	2:C:1318:BFZ:CAS	2.88	0.45
1:G:182:GLN:CB	2:G:1318:BFZ:HAW2	2.46	0.45
1:E:71:LEU:HD11	1:E:94:LEU:HD21	1.98	0.45
1:C:221:SER:HB2	1:D:281:ILE:HD11	1.98	0.45
1:F:66:TRP:HB3	1:F:71:LEU:HD12	1.99	0.45
1:J:58:VAL:HG12	1:J:63:ILE:HG13	1.98	0.45
1:C:211:PRO:O	1:C:215:ILE:HG12	2.18	0.44
1:A:314:VAL:HA	1:A:317:ILE:HD12	1.99	0.44
1:C:294:ASP:HB2	1:C:297:ILE:HG22	1.98	0.44
2:F:1318:BFZ:HAP2	2:F:1318:BFZ:HAS2	1.72	0.44
1:G:225:LEU:HD22	1:G:230:GLU:HB3	1.97	0.44
1:E:177:HIS:HB3	2:E:1318:BFZ:HAV	1.98	0.44
2:I:1318:BFZ:HAP2	2:I:1318:BFZ:HAS2	1.79	0.44
1:J:71:LEU:HD11	1:J:94:LEU:HD21	1.99	0.44
1:D:294:ASP:HB2	1:D:297:ILE:HG22	1.99	0.44
1:I:211:PRO:O	1:I:215:ILE:HG12	2.18	0.44
1:B:211:PRO:O	1:B:215:ILE:HG12	2.18	0.44
1:C:66:TRP:HB3	1:C:71:LEU:HD12	2.00	0.44
2:C:1318:BFZ:HAS2	2:C:1318:BFZ:HAP2	1.77	0.44
1:I:221:SER:HB2	1:J:281:ILE:HD11	1.98	0.44
1:I:58:VAL:HG12	1:I:63:ILE:HG13	1.99	0.44
2:J:1318:BFZ:CAQ	2:J:1318:BFZ:O	2.66	0.44
1:J:172:ASP:HB3	1:J:187:GLU:HG2	1.98	0.44
1:B:225:LEU:HB2	1:B:231:ARG:HG3	1.99	0.44
1:F:81:VAL:HG21	1:F:85:PRO:HG3	1.99	0.44
1:G:159:GLU:HG3	1:H:257:PRO:HB3	1.99	0.44
1:J:66:TRP:HB3	1:J:71:LEU:HD12	2.00	0.44
1:F:240:LEU:HD23	1:J:241:THR:HA	2.00	0.43
1:G:211:PRO:O	1:G:215:ILE:HG12	2.18	0.43
1:E:66:TRP:HB3	1:E:71:LEU:HD12	2.00	0.43
1:H:211:PRO:O	1:H:215:ILE:HG12	2.18	0.43
1:I:294:ASP:HB2	1:I:297:ILE:HG22	2.01	0.43
1:C:71:LEU:HD11	1:C:94:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:PRO:O	1:A:215:ILE:HG12	2.18	0.43
1:D:211:PRO:O	1:D:215:ILE:HG12	2.18	0.43
2:E:1318:BFZ:HAU	2:E:1318:BFZ:FAA	2.08	0.43
2:F:1318:BFZ:CAQ	2:F:1318:BFZ:O	2.66	0.43
1:A:172:ASP:HB3	1:A:187:GLU:HG2	2.01	0.43
1:A:66:TRP:HB3	1:A:71:LEU:HD12	2.00	0.43
1:B:66:TRP:HB3	1:B:71:LEU:HD12	2.00	0.43
1:C:241:THR:HA	1:D:240:LEU:HD23	2.01	0.43
1:F:177:HIS:CB	2:F:1318:BFZ:HAV	2.43	0.43
1:H:221:SER:HB2	1:I:281:ILE:HD11	2.00	0.43
1:D:66:TRP:HB3	1:D:71:LEU:HD12	2.01	0.43
1:F:211:PRO:O	1:F:215:ILE:HG12	2.18	0.43
1:A:221:SER:HA	1:A:224:TRP:HE3	1.84	0.43
1:F:127:VAL:HG22	1:F:194:ARG:HG2	2.00	0.42
1:G:157:ILE:HD11	1:H:115:ASP:OD2	2.18	0.42
1:J:211:PRO:O	1:J:215:ILE:HG12	2.18	0.42
1:D:241:THR:HA	1:E:240:LEU:HD23	2.00	0.42
1:G:312:GLY:HA2	1:G:315:LEU:HD12	2.00	0.42
1:B:221:SER:HA	1:B:224:TRP:HE3	1.84	0.42
1:E:211:PRO:O	1:E:215:ILE:HG12	2.18	0.42
1:G:66:TRP:HB3	1:G:71:LEU:HD12	2.01	0.42
1:H:66:TRP:HB3	1:H:71:LEU:HD12	2.00	0.42
1:A:173:ILE:HD13	1:A:190:ARG:HB3	2.02	0.42
1:B:127:VAL:HA	1:B:193:VAL:O	2.20	0.42
1:C:19:PHE:CE1	2:D:1318:BFZ:HA1C	2.55	0.42
1:F:173:ILE:HD13	1:F:190:ARG:HB3	2.01	0.42
1:A:38:TYR:CZ	2:B:1318:BFZ:HAC	2.55	0.42
1:C:260:THR:H	1:C:263:ASP:HB2	1.85	0.42
1:H:173:ILE:HD13	1:H:190:ARG:HB3	2.02	0.42
1:E:173:ILE:HD13	1:E:190:ARG:HB3	2.02	0.42
1:F:260:THR:H	1:F:263:ASP:HB2	1.85	0.42
1:I:66:TRP:HB3	1:I:71:LEU:HD12	2.01	0.42
1:J:260:THR:H	1:J:263:ASP:HB2	1.85	0.42
1:A:177:HIS:HB3	2:A:1318:BFZ:HAZ	2.01	0.42
1:J:173:ILE:HD13	1:J:190:ARG:HB3	2.02	0.42
1:B:159:GLU:HG3	1:C:257:PRO:HB3	2.02	0.41
1:B:260:THR:H	1:B:263:ASP:HB2	1.85	0.41
1:F:177:HIS:HB3	2:F:1318:BFZ:CAZ	2.50	0.41
2:D:1318:BFZ:HAV	2:D:1318:BFZ:HAP2	1.79	0.41
1:I:123:ARG:HD2	1:I:198:VAL:HG22	2.02	0.41
1:G:241:THR:HA	1:H:240:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:175:TYR:HB3	2:J:1318:BFZ:CAZ	2.50	0.41
1:C:127:VAL:HA	1:C:193:VAL:O	2.21	0.41
1:C:81:VAL:HG21	1:C:85:PRO:HG3	2.01	0.41
1:D:127:VAL:HA	1:D:193:VAL:O	2.21	0.41
1:D:260:THR:H	1:D:263:ASP:HB2	1.85	0.41
1:D:173:ILE:HD13	1:D:190:ARG:HB3	2.03	0.41
1:I:260:THR:H	1:I:263:ASP:HB2	1.85	0.41
1:I:241:THR:HA	1:J:240:LEU:HD23	2.02	0.41
1:F:117:ARG:HE	1:J:157:ILE:HD11	1.85	0.41
2:F:1318:BFZ:HAV	2:F:1318:BFZ:HAS2	2.03	0.41
1:A:260:THR:H	1:A:263:ASP:HB2	1.85	0.41
1:I:173:ILE:HD13	1:I:190:ARG:HB3	2.02	0.41
1:G:173:ILE:HD13	1:G:190:ARG:HB3	2.01	0.41
1:C:173:ILE:HD13	1:C:190:ARG:HB3	2.02	0.41
1:E:127:VAL:HA	1:E:193:VAL:O	2.21	0.41
1:E:260:THR:H	1:E:263:ASP:HB2	1.85	0.41
1:G:127:VAL:HA	1:G:193:VAL:O	2.20	0.41
2:H:1318:BFZ:HAV	2:H:1318:BFZ:CAS	2.39	0.41
1:I:127:VAL:HA	1:I:193:VAL:O	2.21	0.41
1:B:173:ILE:HD13	1:B:190:ARG:HB3	2.01	0.41
1:F:127:VAL:HA	1:F:193:VAL:O	2.21	0.41
1:H:127:VAL:HA	1:H:193:VAL:O	2.21	0.41
1:B:212:LEU:O	1:B:216:ILE:HG12	2.21	0.40
1:A:224:TRP:HD1	1:B:285:HIS:CE1	2.38	0.40
1:H:260:THR:H	1:H:263:ASP:HB2	1.85	0.40
1:J:127:VAL:HA	1:J:193:VAL:O	2.21	0.40
1:J:212:LEU:O	1:J:216:ILE:HG12	2.22	0.40
1:E:145:ILE:HG13	1:E:191:ILE:HD13	2.03	0.40
1:F:175:TYR:CD1	2:F:1318:BFZ:BR	3.30	0.40
1:A:225:LEU:HB2	1:A:231:ARG:HG3	2.04	0.40
1:B:221:SER:HB2	1:C:281:ILE:HD11	2.03	0.40
2:E:1318:BFZ:NAR	2:E:1318:BFZ:O	2.55	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	305/307 (99%)	275 (90%)	23 (8%)	7 (2%)	6	38
1	B	305/307 (99%)	275 (90%)	22 (7%)	8 (3%)	5	35
1	C	305/307 (99%)	278 (91%)	21 (7%)	6 (2%)	7	41
1	D	305/307 (99%)	277 (91%)	22 (7%)	6 (2%)	7	41
1	E	305/307 (99%)	276 (90%)	23 (8%)	6 (2%)	7	41
1	F	305/307 (99%)	279 (92%)	21 (7%)	5 (2%)	9	45
1	G	305/307 (99%)	278 (91%)	19 (6%)	8 (3%)	5	35
1	H	305/307 (99%)	277 (91%)	22 (7%)	6 (2%)	7	41
1	I	305/307 (99%)	276 (90%)	23 (8%)	6 (2%)	7	41
1	J	305/307 (99%)	277 (91%)	22 (7%)	6 (2%)	7	41
All	All	3050/3070 (99%)	2768 (91%)	218 (7%)	64 (2%)	7	40

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	PRO
1	B	166	ALA
1	B	183	PRO
1	C	183	PRO
1	D	183	PRO
1	E	183	PRO
1	F	183	PRO
1	G	183	PRO
1	H	183	PRO
1	I	183	PRO
1	J	183	PRO
1	A	60	ASN
1	A	177	HIS
1	B	60	ASN
1	B	177	HIS
1	B	295	LEU
1	C	166	ALA
1	C	177	HIS
1	D	60	ASN
1	D	166	ALA

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Mol	Chain	Res	Type
1	D	177	HIS
1	E	60	ASN
1	E	166	ALA
1	E	177	HIS
1	F	60	ASN
1	F	177	HIS
1	G	60	ASN
1	G	166	ALA
1	G	177	HIS
1	H	60	ASN
1	H	166	ALA
1	H	177	HIS
1	I	166	ALA
1	I	177	HIS
1	J	60	ASN
1	J	177	HIS
1	B	294	ASP
1	C	60	ASN
1	G	294	ASP
1	I	60	ASN
1	J	166	ALA
1	A	53	ASP
1	A	289	ASN
1	B	53	ASP
1	C	53	ASP
1	D	53	ASP
1	E	53	ASP
1	E	178	LEU
1	F	53	ASP
1	G	53	ASP
1	G	289	ASN
1	H	53	ASP
1	I	53	ASP
1	J	53	ASP
1	J	178	LEU
1	A	178	LEU
1	B	178	LEU
1	C	178	LEU
1	D	178	LEU
1	F	178	LEU
1	G	178	LEU
1	H	178	LEU

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Mol	Chain	Res	Type
1	I	178	LEU
1	A	166	ALA

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	268/275 (98%)	249 (93%)	19 (7%)	14	47
1	B	268/275 (98%)	246 (92%)	22 (8%)	11	42
1	C	268/275 (98%)	248 (92%)	20 (8%)	13	45
1	D	268/275 (98%)	246 (92%)	22 (8%)	11	42
1	E	268/275 (98%)	245 (91%)	23 (9%)	10	41
1	F	268/275 (98%)	248 (92%)	20 (8%)	13	45
1	G	268/275 (98%)	247 (92%)	21 (8%)	12	44
1	H	268/275 (98%)	248 (92%)	20 (8%)	13	45
1	I	268/275 (98%)	246 (92%)	22 (8%)	11	42
1	J	268/275 (98%)	250 (93%)	18 (7%)	16	50
All	All	2680/2750 (98%)	2473 (92%)	207 (8%)	13	44

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	56	LEU
1	A	71	LEU
1	A	118	LEU
1	A	124	GLN
1	A	128	LEU
1	A	136	ASN
1	A	145	ILE
1	A	146	GLN
1	A	165	LYS
1	A	172	ASP

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Mol	Chain	Res	Type
1	A	178	LEU
1	A	210	LEU
1	A	232	LEU
1	A	238	LEU
1	A	247	PHE
1	A	297	ILE
1	A	302	LEU
1	A	304	PHE
1	B	29	LEU
1	B	56	LEU
1	B	71	LEU
1	B	118	LEU
1	B	124	GLN
1	B	128	LEU
1	B	136	ASN
1	B	145	ILE
1	B	146	GLN
1	B	165	LYS
1	B	172	ASP
1	B	178	LEU
1	B	224	TRP
1	B	232	LEU
1	B	238	LEU
1	B	240	LEU
1	B	247	PHE
1	B	287	GLN
1	B	291	VAL
1	B	297	ILE
1	B	302	LEU
1	B	304	PHE
1	C	29	LEU
1	C	56	LEU
1	C	71	LEU
1	C	118	LEU
1	C	124	GLN
1	C	128	LEU
1	C	136	ASN
1	C	145	ILE
1	C	146	GLN
1	C	165	LYS
1	C	172	ASP
1	C	178	LEU

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Mol	Chain	Res	Type
1	C	210	LEU
1	C	224	TRP
1	C	232	LEU
1	C	238	LEU
1	C	295	LEU
1	C	297	ILE
1	C	302	LEU
1	C	304	PHE
1	D	29	LEU
1	D	48	ARG
1	D	56	LEU
1	D	71	LEU
1	D	118	LEU
1	D	124	GLN
1	D	128	LEU
1	D	130	LEU
1	D	136	ASN
1	D	145	ILE
1	D	146	GLN
1	D	165	LYS
1	D	172	ASP
1	D	178	LEU
1	D	224	TRP
1	D	232	LEU
1	D	238	LEU
1	D	247	PHE
1	D	295	LEU
1	D	297	ILE
1	D	302	LEU
1	D	304	PHE
1	E	29	LEU
1	E	56	LEU
1	E	71	LEU
1	E	109	SER
1	E	118	LEU
1	E	124	GLN
1	E	128	LEU
1	E	141	ARG
1	E	145	ILE
1	E	146	GLN
1	E	165	LYS
1	E	172	ASP

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Mol	Chain	Res	Type
1	E	178	LEU
1	E	210	LEU
1	E	224	TRP
1	E	232	LEU
1	E	238	LEU
1	E	240	LEU
1	E	247	PHE
1	E	291	VAL
1	E	297	ILE
1	E	302	LEU
1	E	304	PHE
1	F	29	LEU
1	F	56	LEU
1	F	71	LEU
1	F	118	LEU
1	F	128	LEU
1	F	136	ASN
1	F	145	ILE
1	F	146	GLN
1	F	165	LYS
1	F	168	THR
1	F	172	ASP
1	F	178	LEU
1	F	224	TRP
1	F	232	LEU
1	F	238	LEU
1	F	247	PHE
1	F	291	VAL
1	F	297	ILE
1	F	302	LEU
1	F	304	PHE
1	G	29	LEU
1	G	56	LEU
1	G	71	LEU
1	G	118	LEU
1	G	124	GLN
1	G	128	LEU
1	G	145	ILE
1	G	146	GLN
1	G	165	LYS
1	G	172	ASP
1	G	174	ARG

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Mol	Chain	Res	Type
1	G	178	LEU
1	G	232	LEU
1	G	238	LEU
1	G	287	GLN
1	G	291	VAL
1	G	293	ASP
1	G	295	LEU
1	G	297	ILE
1	G	302	LEU
1	G	304	PHE
1	H	29	LEU
1	H	56	LEU
1	H	71	LEU
1	H	118	LEU
1	H	124	GLN
1	H	128	LEU
1	H	136	ASN
1	H	145	ILE
1	H	146	GLN
1	H	165	LYS
1	H	172	ASP
1	H	178	LEU
1	H	210	LEU
1	H	224	TRP
1	H	232	LEU
1	H	238	LEU
1	H	247	PHE
1	H	297	ILE
1	H	302	LEU
1	H	304	PHE
1	I	29	LEU
1	I	56	LEU
1	I	71	LEU
1	I	118	LEU
1	I	124	GLN
1	I	128	LEU
1	I	136	ASN
1	I	145	ILE
1	I	146	GLN
1	I	165	LYS
1	I	168	THR
1	I	172	ASP

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Mol	Chain	Res	Type
1	I	178	LEU
1	I	210	LEU
1	I	232	LEU
1	I	238	LEU
1	I	240	LEU
1	I	247	PHE
1	I	295	LEU
1	I	297	ILE
1	I	302	LEU
1	I	304	PHE
1	J	29	LEU
1	J	56	LEU
1	J	71	LEU
1	J	118	LEU
1	J	124	GLN
1	J	128	LEU
1	J	136	ASN
1	J	145	ILE
1	J	146	GLN
1	J	165	LYS
1	J	172	ASP
1	J	178	LEU
1	J	224	TRP
1	J	232	LEU
1	J	238	LEU
1	J	297	ILE
1	J	302	LEU
1	J	304	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	GLN
1	B	62	GLN
1	B	298	GLN
1	C	284	HIS
1	D	42	GLN
1	E	298	GLN
1	F	103	ASN
1	G	103	ASN
1	G	285	HIS
1	H	284	HIS

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Mol	Chain	Res	Type
1	H	298	GLN
1	J	124	GLN
1	J	298	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

10 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	BFZ	C	1318	-	29,29,29	2.37	5 (17%)	39,40,40	2.43	16 (41%)
2	BFZ	E	1318	-	29,29,29	2.24	5 (17%)	39,40,40	2.69	18 (46%)
2	BFZ	G	1318	-	29,29,29	2.34	5 (17%)	39,40,40	2.22	15 (38%)
2	BFZ	I	1318	-	29,29,29	2.42	4 (13%)	39,40,40	2.18	12 (30%)
2	BFZ	F	1318	-	29,29,29	2.63	5 (17%)	39,40,40	2.47	13 (33%)
2	BFZ	B	1318	-	29,29,29	2.84	5 (17%)	39,40,40	2.34	14 (35%)
2	BFZ	D	1318	-	29,29,29	2.68	5 (17%)	39,40,40	2.57	18 (46%)
2	BFZ	H	1318	-	29,29,29	2.57	5 (17%)	39,40,40	2.37	18 (46%)
2	BFZ	J	1318	1	29,29,29	2.59	5 (17%)	39,40,40	2.66	17 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BFZ	A	1318	-	29,29,29	2.35	5 (17%)	39,40,40	2.20	13 (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	BFZ	C	1318	-	-	7/13/30/30	0/3/3/3
2	BFZ	E	1318	-	-	7/13/30/30	0/3/3/3
2	BFZ	G	1318	-	-	5/13/30/30	0/3/3/3
2	BFZ	I	1318	-	-	6/13/30/30	0/3/3/3
2	BFZ	F	1318	-	-	10/13/30/30	0/3/3/3
2	BFZ	B	1318	-	-	8/13/30/30	0/3/3/3
2	BFZ	D	1318	-	-	7/13/30/30	0/3/3/3
2	BFZ	H	1318	-	-	7/13/30/30	0/3/3/3
2	BFZ	J	1318	1	-	5/13/30/30	0/3/3/3
2	BFZ	A	1318	-	-	3/13/30/30	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1318	BFZ	CAN-NAO	-11.10	1.33	1.43
2	J	1318	BFZ	CAN-NAO	-10.39	1.33	1.43
2	D	1318	BFZ	CAN-NAO	-10.36	1.33	1.43
2	F	1318	BFZ	CAN-NAO	-10.12	1.34	1.43
2	H	1318	BFZ	CAN-NAO	-9.12	1.34	1.43
2	A	1318	BFZ	CAN-NAO	-8.96	1.35	1.43
2	G	1318	BFZ	CAN-NAO	-8.91	1.35	1.43
2	I	1318	BFZ	CAN-NAO	-8.55	1.35	1.43
2	C	1318	BFZ	CAN-NAO	-8.51	1.35	1.43
2	E	1318	BFZ	CAN-NAO	-7.06	1.36	1.43
2	B	1318	BFZ	CAM-CAF	-6.45	1.39	1.49
2	E	1318	BFZ	CAM-CAF	-6.38	1.39	1.49
2	B	1318	BFZ	CAE-CAF	-6.35	1.37	1.49
2	F	1318	BFZ	CAM-CAF	-6.22	1.40	1.49
2	D	1318	BFZ	CAE-CAF	-5.90	1.38	1.49
2	I	1318	BFZ	CAM-CAF	-5.89	1.40	1.49
2	H	1318	BFZ	CAM-CAF	-5.71	1.40	1.49
2	F	1318	BFZ	CAE-CAF	-5.68	1.38	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1318	BFZ	CAE-CAF	-5.65	1.38	1.49
2	H	1318	BFZ	CAE-CAF	-5.60	1.38	1.49
2	C	1318	BFZ	CAM-CAF	-5.58	1.41	1.49
2	D	1318	BFZ	CAM-CAF	-5.45	1.41	1.49
2	G	1318	BFZ	CAM-CAF	-5.34	1.41	1.49
2	A	1318	BFZ	CAM-CAF	-5.23	1.41	1.49
2	J	1318	BFZ	CAE-CAF	-5.13	1.39	1.49
2	J	1318	BFZ	CAM-CAF	-5.05	1.41	1.49
2	C	1318	BFZ	CAE-CAF	-5.04	1.39	1.49
2	E	1318	BFZ	CAE-CAF	-4.82	1.40	1.49
2	A	1318	BFZ	CAE-CAF	-4.69	1.40	1.49
2	H	1318	BFZ	CA-C	4.68	1.57	1.51
2	G	1318	BFZ	CAE-CAF	-4.43	1.41	1.49
2	J	1318	BFZ	CAF-N	3.73	1.33	1.28
2	G	1318	BFZ	CAF-N	3.72	1.33	1.28
2	D	1318	BFZ	CA-C	3.62	1.56	1.51
2	F	1318	BFZ	CAF-N	3.59	1.33	1.28
2	C	1318	BFZ	CA-C	3.46	1.56	1.51
2	C	1318	BFZ	CAF-N	3.38	1.33	1.28
2	A	1318	BFZ	CAF-N	3.15	1.32	1.28
2	E	1318	BFZ	CAF-N	3.01	1.32	1.28
2	B	1318	BFZ	CA-C	2.91	1.55	1.51
2	H	1318	BFZ	CAF-N	2.89	1.32	1.28
2	J	1318	BFZ	CA-C	2.80	1.55	1.51
2	I	1318	BFZ	CAF-N	2.77	1.32	1.28
2	D	1318	BFZ	CAF-N	2.73	1.32	1.28
2	B	1318	BFZ	CAF-N	2.66	1.32	1.28
2	E	1318	BFZ	CA-C	2.59	1.54	1.51
2	G	1318	BFZ	CA-C	2.58	1.54	1.51
2	A	1318	BFZ	CA-C	2.46	1.54	1.51
2	F	1318	BFZ	CA-C	2.22	1.54	1.51

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1318	BFZ	CAV-CAN-NAO	-6.57	112.02	119.24
2	E	1318	BFZ	O-C-CA	-6.16	114.95	122.61
2	J	1318	BFZ	CAV-CAN-NAO	-6.16	112.46	119.24
2	B	1318	BFZ	CAV-CAN-NAO	-6.02	112.61	119.24
2	J	1318	BFZ	CAP-NAO-C	6.02	126.51	118.08
2	F	1318	BFZ	CA-N-CAF	5.99	124.30	117.47
2	D	1318	BFZ	CAV-CAN-NAO	-5.88	112.77	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1318	BFZ	CA-N-CAF	5.71	123.99	117.47
2	F	1318	BFZ	CAV-CAN-NAO	-5.71	112.96	119.24
2	C	1318	BFZ	CAP-NAO-C	5.69	126.06	118.08
2	J	1318	BFZ	CA-N-CAF	5.61	123.87	117.47
2	G	1318	BFZ	CA-N-CAF	5.58	123.83	117.47
2	H	1318	BFZ	CAV-CAN-NAO	-5.57	113.12	119.24
2	F	1318	BFZ	CAP-NAO-C	5.53	125.84	118.08
2	H	1318	BFZ	CAE-CAF-CAM	5.48	125.36	117.64
2	A	1318	BFZ	CAV-CAN-NAO	-5.46	113.23	119.24
2	I	1318	BFZ	CA-N-CAF	5.38	123.61	117.47
2	A	1318	BFZ	CA-N-CAF	5.32	123.54	117.47
2	C	1318	BFZ	CAV-CAN-NAO	-5.19	113.53	119.24
2	D	1318	BFZ	CAP-NAO-C	5.07	125.19	118.08
2	B	1318	BFZ	CAP-NAO-C	5.05	125.16	118.08
2	J	1318	BFZ	CAE-CAF-CAM	5.05	124.75	117.64
2	J	1318	BFZ	CAP-NAO-CAN	-4.91	112.95	118.41
2	E	1318	BFZ	CAP-NAO-C	4.86	124.89	118.08
2	C	1318	BFZ	O-C-CA	-4.85	116.58	122.61
2	F	1318	BFZ	CAP-NAO-CAN	-4.82	113.05	118.41
2	D	1318	BFZ	CAE-CAF-CAM	4.82	124.42	117.64
2	D	1318	BFZ	CAC-CAD-CAE	-4.54	118.17	123.11
2	A	1318	BFZ	CAE-CAF-CAM	4.54	124.03	117.64
2	C	1318	BFZ	CA-N-CAF	4.39	122.48	117.47
2	G	1318	BFZ	CAV-CAN-NAO	-4.33	114.47	119.24
2	I	1318	BFZ	CAE-CAF-CAM	4.32	123.73	117.64
2	E	1318	BFZ	CAE-CAF-CAM	4.22	123.59	117.64
2	H	1318	BFZ	CAP-NAO-C	4.20	123.97	118.08
2	B	1318	BFZ	CAL-CAE-CAD	4.16	121.40	116.67
2	I	1318	BFZ	CA-C-NAO	4.13	124.57	115.74
2	G	1318	BFZ	CAP-NAO-C	4.12	123.86	118.08
2	H	1318	BFZ	CAN-NAO-C	-4.06	118.30	123.09
2	A	1318	BFZ	O-C-NAO	-4.06	117.13	121.86
2	C	1318	BFZ	CA-C-NAO	4.05	124.39	115.74
2	B	1318	BFZ	CA-N-CAF	4.02	122.06	117.47
2	B	1318	BFZ	CAP-NAO-CAN	-4.01	113.96	118.41
2	D	1318	BFZ	CAL-CAE-CAD	4.00	121.22	116.67
2	F	1318	BFZ	O-C-CA	-3.99	117.65	122.61
2	G	1318	BFZ	CAE-CAF-CAM	3.94	123.19	117.64
2	I	1318	BFZ	O-C-CA	-3.94	117.72	122.61
2	J	1318	BFZ	CAC-CAD-CAE	-3.90	118.86	123.11
2	D	1318	BFZ	FAA-CAD-CAC	3.89	127.27	118.59
2	C	1318	BFZ	CAQ-CAP-NAO	3.89	118.44	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1318	BFZ	CAM-CAN-NAO	3.80	128.75	121.26
2	H	1318	BFZ	O-C-NAO	-3.78	117.46	121.86
2	G	1318	BFZ	C-CA-N	-3.76	104.48	108.93
2	F	1318	BFZ	CAL-CAE-CAD	3.73	120.91	116.67
2	J	1318	BFZ	O-C-CA	-3.73	117.98	122.61
2	F	1318	BFZ	CAC-CAD-CAE	-3.71	119.07	123.11
2	D	1318	BFZ	CA-C-NAO	3.70	123.65	115.74
2	D	1318	BFZ	O-C-CA	-3.69	118.03	122.61
2	E	1318	BFZ	CAN-NAO-C	-3.69	118.74	123.09
2	D	1318	BFZ	CAN-NAO-C	-3.65	118.78	123.09
2	I	1318	BFZ	O-C-NAO	-3.62	117.64	121.86
2	I	1318	BFZ	CAV-CAN-NAO	-3.61	115.27	119.24
2	H	1318	BFZ	CA-N-CAF	3.60	121.58	117.47
2	A	1318	BFZ	CA-C-NAO	3.58	123.39	115.74
2	B	1318	BFZ	CAC-CAD-CAE	-3.56	119.24	123.11
2	H	1318	BFZ	CA-C-NAO	3.53	123.28	115.74
2	B	1318	BFZ	O-C-CA	-3.51	118.26	122.61
2	A	1318	BFZ	CAC-CAD-CAE	-3.47	119.33	123.11
2	I	1318	BFZ	CAL-CAE-CAD	3.47	120.61	116.67
2	F	1318	BFZ	CA-C-NAO	3.46	123.13	115.74
2	B	1318	BFZ	CA-C-NAO	3.43	123.06	115.74
2	E	1318	BFZ	CA-C-NAO	3.36	122.93	115.74
2	E	1318	BFZ	BR-CAY-CAU	3.34	123.91	119.27
2	C	1318	BFZ	CAN-NAO-C	-3.34	119.15	123.09
2	C	1318	BFZ	CAP-NAO-CAN	-3.31	114.73	118.41
2	I	1318	BFZ	CAC-CAD-CAE	-3.29	119.53	123.11
2	B	1318	BFZ	C-CA-N	-3.17	105.17	108.93
2	J	1318	BFZ	C-CA-N	-3.17	105.18	108.93
2	G	1318	BFZ	CA-C-NAO	3.16	122.50	115.74
2	G	1318	BFZ	O-C-CA	-3.14	118.71	122.61
2	J	1318	BFZ	CAQ-CAP-NAO	3.13	117.10	111.56
2	E	1318	BFZ	CAL-CAE-CAD	3.10	120.19	116.67
2	J	1318	BFZ	CA-C-NAO	3.08	122.33	115.74
2	D	1318	BFZ	O-C-NAO	-3.07	118.28	121.86
2	E	1318	BFZ	CAQ-CAP-NAO	3.04	116.94	111.56
2	D	1318	BFZ	FAA-CAD-CAE	-3.04	114.52	119.67
2	H	1318	BFZ	CAL-CAE-CAD	3.00	120.08	116.67
2	D	1318	BFZ	CA-N-CAF	2.98	120.88	117.47
2	J	1318	BFZ	CAE-CAF-N	-2.97	112.80	116.80
2	A	1318	BFZ	CAM-CAF-N	-2.96	120.14	125.08
2	I	1318	BFZ	FAA-CAD-CAC	2.95	125.17	118.59
2	F	1318	BFZ	CAQ-CAP-NAO	2.94	116.77	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1318	BFZ	CAM-CAF-N	-2.92	120.20	125.08
2	C	1318	BFZ	CAL-CAE-CAD	2.89	119.95	116.67
2	F	1318	BFZ	CAM-CAN-NAO	2.87	126.92	121.26
2	I	1318	BFZ	C-CA-N	-2.84	105.56	108.93
2	B	1318	BFZ	O-C-NAO	-2.84	118.55	121.86
2	G	1318	BFZ	CAC-CAD-CAE	-2.83	120.03	123.11
2	E	1318	BFZ	CAU-CAM-CAF	-2.82	114.80	118.88
2	A	1318	BFZ	CAU-CAM-CAF	-2.82	114.80	118.88
2	G	1318	BFZ	CAQ-CAP-NAO	2.80	116.52	111.56
2	C	1318	BFZ	CAE-CAF-CAM	2.78	121.55	117.64
2	H	1318	BFZ	O-C-CA	-2.75	119.20	122.61
2	H	1318	BFZ	CAE-CAF-N	-2.73	113.11	116.80
2	G	1318	BFZ	O-C-NAO	-2.70	118.71	121.86
2	C	1318	BFZ	CAU-CAM-CAF	-2.70	114.97	118.88
2	G	1318	BFZ	CAN-NAO-C	-2.65	119.96	123.09
2	B	1318	BFZ	BR-CAY-CAZ	-2.63	115.48	119.30
2	E	1318	BFZ	CAM-CAF-N	-2.61	120.73	125.08
2	A	1318	BFZ	CAM-CAN-NAO	2.60	126.39	121.26
2	I	1318	BFZ	FAA-CAD-CAE	-2.60	115.26	119.67
2	C	1318	BFZ	CAC-CAD-CAE	-2.59	120.29	123.11
2	C	1318	BFZ	CAM-CAF-N	-2.59	120.76	125.08
2	J	1318	BFZ	CAM-CAN-NAO	2.57	126.32	121.26
2	C	1318	BFZ	CAM-CAN-NAO	2.57	126.32	121.26
2	C	1318	BFZ	CAN-CAM-CAF	2.57	126.26	122.73
2	H	1318	BFZ	CAM-CAN-NAO	2.55	126.29	121.26
2	E	1318	BFZ	FAA-CAD-CAE	-2.54	115.35	119.67
2	A	1318	BFZ	O-C-CA	-2.54	119.46	122.61
2	H	1318	BFZ	BR-CAY-CAU	2.52	122.77	119.27
2	H	1318	BFZ	CAC-CAD-CAE	-2.50	120.39	123.11
2	A	1318	BFZ	CAN-CAM-CAF	2.50	126.17	122.73
2	H	1318	BFZ	FAA-CAD-CAE	-2.47	115.47	119.67
2	A	1318	BFZ	CAL-CAE-CAD	2.46	119.47	116.67
2	C	1318	BFZ	O-C-NAO	-2.45	119.00	121.86
2	H	1318	BFZ	FAA-CAD-CAC	2.44	124.04	118.59
2	F	1318	BFZ	CAE-CAF-CAM	2.44	121.08	117.64
2	E	1318	BFZ	FAA-CAD-CAC	2.43	124.00	118.59
2	I	1318	BFZ	CAE-CAF-N	-2.40	113.56	116.80
2	H	1318	BFZ	CAU-CAM-CAF	-2.39	115.41	118.88
2	A	1318	BFZ	CAN-NAO-C	-2.39	120.27	123.09
2	D	1318	BFZ	CAE-CAF-N	-2.35	113.63	116.80
2	B	1318	BFZ	FAA-CAD-CAC	2.32	123.76	118.59
2	B	1318	BFZ	CAM-CAN-NAO	2.31	125.82	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1318	BFZ	CAC-CAD-CAE	-2.31	120.60	123.11
2	D	1318	BFZ	BR-CAY-CAU	2.31	122.47	119.27
2	J	1318	BFZ	CAN-NAO-C	-2.30	120.38	123.09
2	F	1318	BFZ	CAU-CAM-CAF	-2.29	115.56	118.88
2	F	1318	BFZ	O-C-NAO	-2.29	119.19	121.86
2	J	1318	BFZ	CAL-CAE-CAD	2.27	119.25	116.67
2	D	1318	BFZ	CAQ-CAP-NAO	2.27	115.57	111.56
2	D	1318	BFZ	CAU-CAM-CAF	-2.27	115.60	118.88
2	H	1318	BFZ	CAM-CAF-N	-2.26	121.30	125.08
2	G	1318	BFZ	CAM-CAN-NAO	2.26	125.72	121.26
2	J	1318	BFZ	CAL-CAE-CAF	-2.23	115.98	119.92
2	E	1318	BFZ	CAP-NAO-CAN	-2.22	115.94	118.41
2	G	1318	BFZ	CAP-NAO-CAN	-2.20	115.97	118.41
2	J	1318	BFZ	CAM-CAF-N	-2.17	121.46	125.08
2	G	1318	BFZ	CAU-CAM-CAF	-2.15	115.76	118.88
2	D	1318	BFZ	CAP-NAO-CAN	-2.15	116.03	118.41
2	D	1318	BFZ	CAM-CAN-NAO	2.13	125.46	121.26
2	B	1318	BFZ	BR-CAY-CAU	2.13	122.23	119.27
2	E	1318	BFZ	CAL-CAE-CAF	2.05	123.53	119.92
2	H	1318	BFZ	C-CA-N	-2.04	106.52	108.93
2	J	1318	BFZ	BR-CAY-CAU	2.03	122.09	119.27

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1318	BFZ	CAQ-CAP-NAO-C
2	C	1318	BFZ	CAQ-CAP-NAO-CAN
2	E	1318	BFZ	CAQ-CAP-NAO-C
2	E	1318	BFZ	CAQ-CAP-NAO-CAN
2	G	1318	BFZ	CAQ-CAP-NAO-C
2	F	1318	BFZ	CAQ-CAP-NAO-C
2	F	1318	BFZ	CAQ-CAP-NAO-CAN
2	B	1318	BFZ	CAQ-CAP-NAO-C
2	D	1318	BFZ	CAP-CAQ-NAR-CAS
2	D	1318	BFZ	CAQ-CAP-NAO-C
2	D	1318	BFZ	CAQ-CAP-NAO-CAN
2	H	1318	BFZ	CAQ-CAP-NAO-C
2	J	1318	BFZ	CAQ-CAP-NAO-C
2	J	1318	BFZ	CAQ-CAP-NAO-CAN
2	C	1318	BFZ	CAP-CAQ-NAR-CAS
2	H	1318	BFZ	CAP-CAQ-NAR-CAS

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Mol	Chain	Res	Type	Atoms
2	E	1318	BFZ	CAP-CAQ-NAR-CAS
2	F	1318	BFZ	CAP-CAQ-NAR-CAS
2	J	1318	BFZ	CAP-CAQ-NAR-CAS
2	H	1318	BFZ	NAO-CAP-CAQ-NAR
2	B	1318	BFZ	CAP-CAQ-NAR-CAS
2	D	1318	BFZ	CAT-CAS-NAR-CAW
2	I	1318	BFZ	CAX-CAW-NAR-CAQ
2	F	1318	BFZ	CAX-CAW-NAR-CAS
2	F	1318	BFZ	CAX-CAW-NAR-CAQ
2	B	1318	BFZ	CAT-CAS-NAR-CAQ
2	D	1318	BFZ	CAT-CAS-NAR-CAQ
2	G	1318	BFZ	CAT-CAS-NAR-CAQ
2	F	1318	BFZ	CAT-CAS-NAR-CAW
2	F	1318	BFZ	CAT-CAS-NAR-CAQ
2	E	1318	BFZ	CAD-CAE-CAF-N
2	I	1318	BFZ	CAD-CAE-CAF-N
2	F	1318	BFZ	CAD-CAE-CAF-N
2	E	1318	BFZ	CAD-CAE-CAF-CAM
2	I	1318	BFZ	CAD-CAE-CAF-CAM
2	B	1318	BFZ	CAL-CAE-CAF-CAM
2	B	1318	BFZ	CAD-CAE-CAF-CAM
2	E	1318	BFZ	CAL-CAE-CAF-N
2	I	1318	BFZ	NAO-CAP-CAQ-NAR
2	G	1318	BFZ	CAT-CAS-NAR-CAW
2	I	1318	BFZ	CAX-CAW-NAR-CAS
2	B	1318	BFZ	CAT-CAS-NAR-CAW
2	C	1318	BFZ	CAT-CAS-NAR-CAQ
2	J	1318	BFZ	CAT-CAS-NAR-CAW
2	J	1318	BFZ	CAT-CAS-NAR-CAQ
2	G	1318	BFZ	CAP-CAQ-NAR-CAS
2	A	1318	BFZ	NAO-CAP-CAQ-NAR
2	C	1318	BFZ	CAX-CAW-NAR-CAS
2	C	1318	BFZ	CAT-CAS-NAR-CAW
2	D	1318	BFZ	CAP-CAQ-NAR-CAW
2	G	1318	BFZ	CAQ-CAP-NAO-CAN
2	B	1318	BFZ	CAQ-CAP-NAO-CAN
2	H	1318	BFZ	CAQ-CAP-NAO-CAN
2	C	1318	BFZ	CAX-CAW-NAR-CAQ
2	H	1318	BFZ	CAT-CAS-NAR-CAW
2	A	1318	BFZ	CAT-CAS-NAR-CAQ
2	H	1318	BFZ	CAD-CAE-CAF-CAM
2	F	1318	BFZ	CAL-CAE-CAF-N

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Mol	Chain	Res	Type	Atoms
2	B	1318	BFZ	CAL-CAE-CAF-N
2	H	1318	BFZ	CAX-CAW-NAR-CAS
2	D	1318	BFZ	NAO-CAP-CAQ-NAR
2	A	1318	BFZ	CAT-CAS-NAR-CAW
2	I	1318	BFZ	CAP-CAQ-NAR-CAS
2	E	1318	BFZ	CAL-CAE-CAF-CAM
2	F	1318	BFZ	CAD-CAE-CAF-CAM

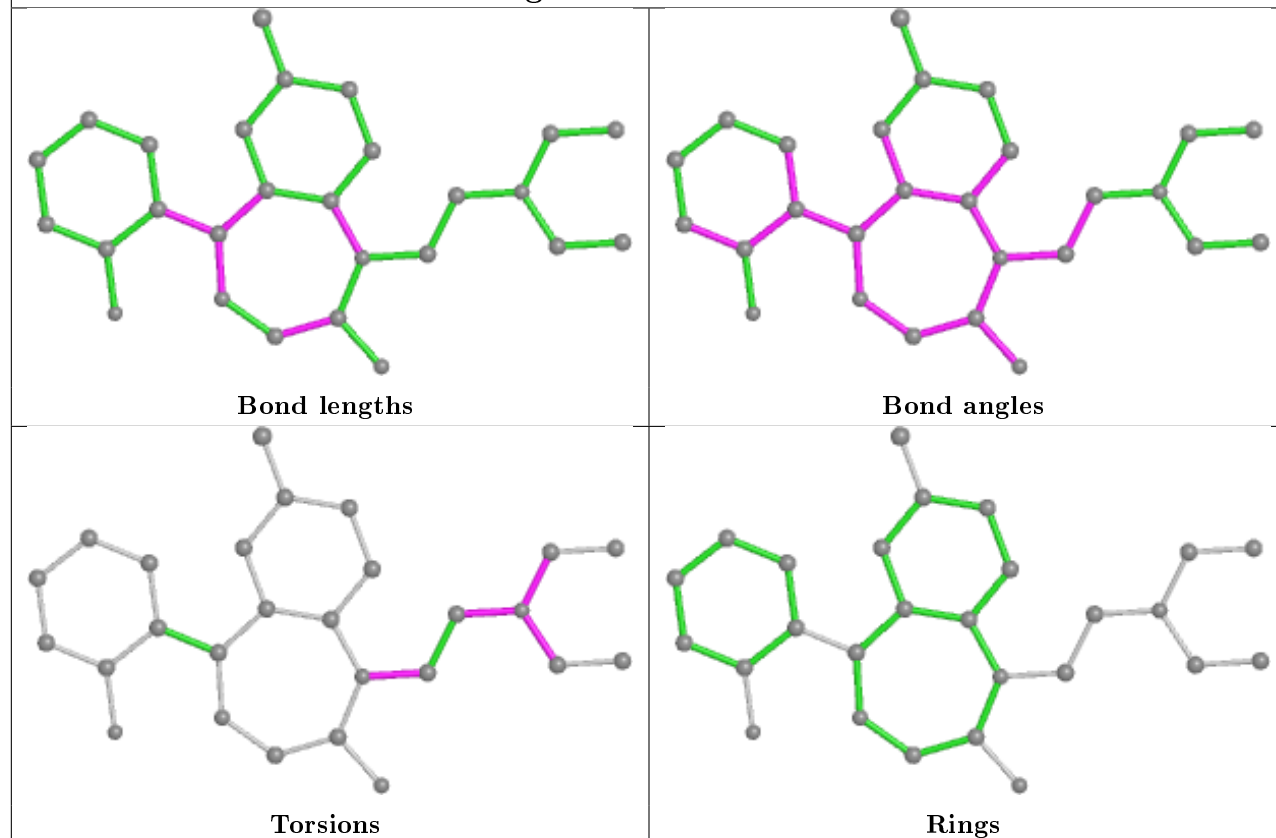
There are no ring outliers.

10 monomers are involved in 89 short contacts:

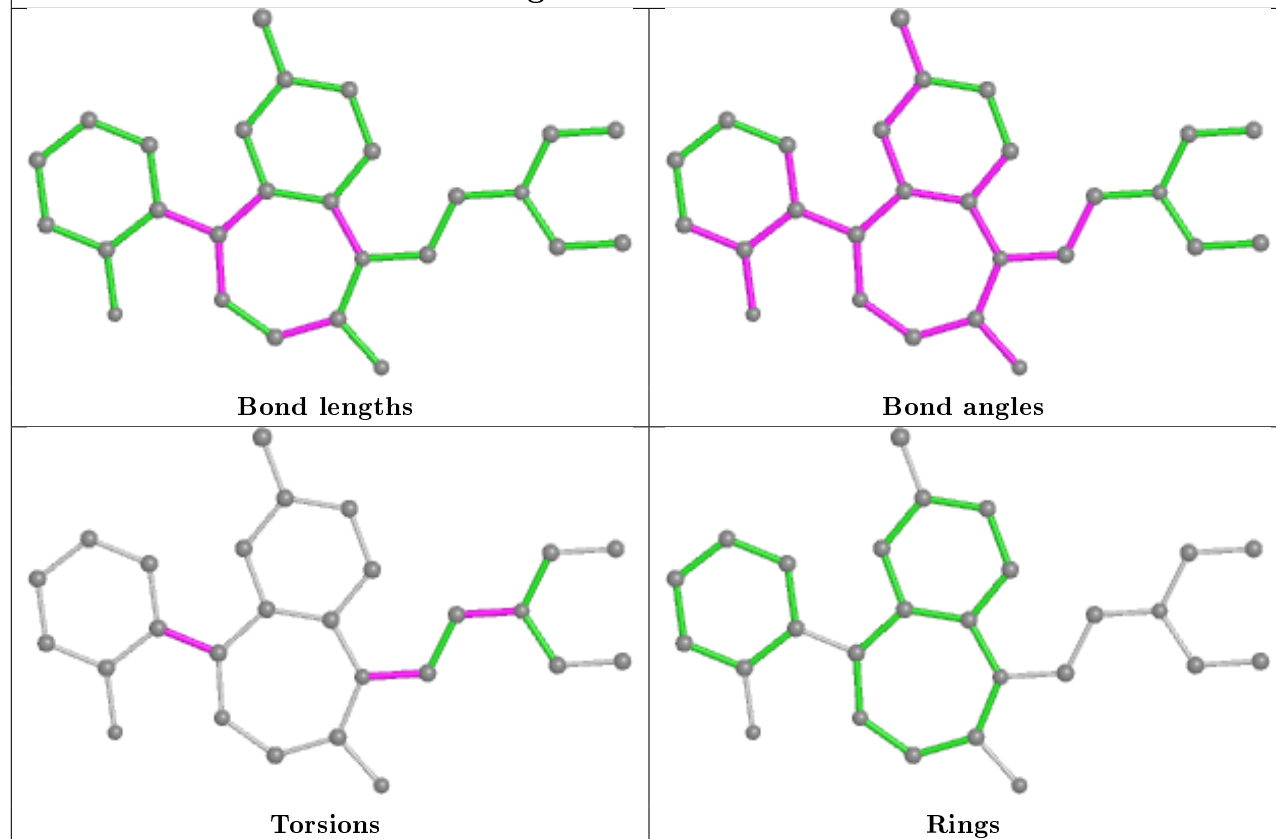
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1318	BFZ	14	0
2	E	1318	BFZ	8	0
2	G	1318	BFZ	8	0
2	I	1318	BFZ	5	0
2	F	1318	BFZ	14	0
2	B	1318	BFZ	9	0
2	D	1318	BFZ	12	0
2	H	1318	BFZ	7	0
2	J	1318	BFZ	7	0
2	A	1318	BFZ	5	0

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.

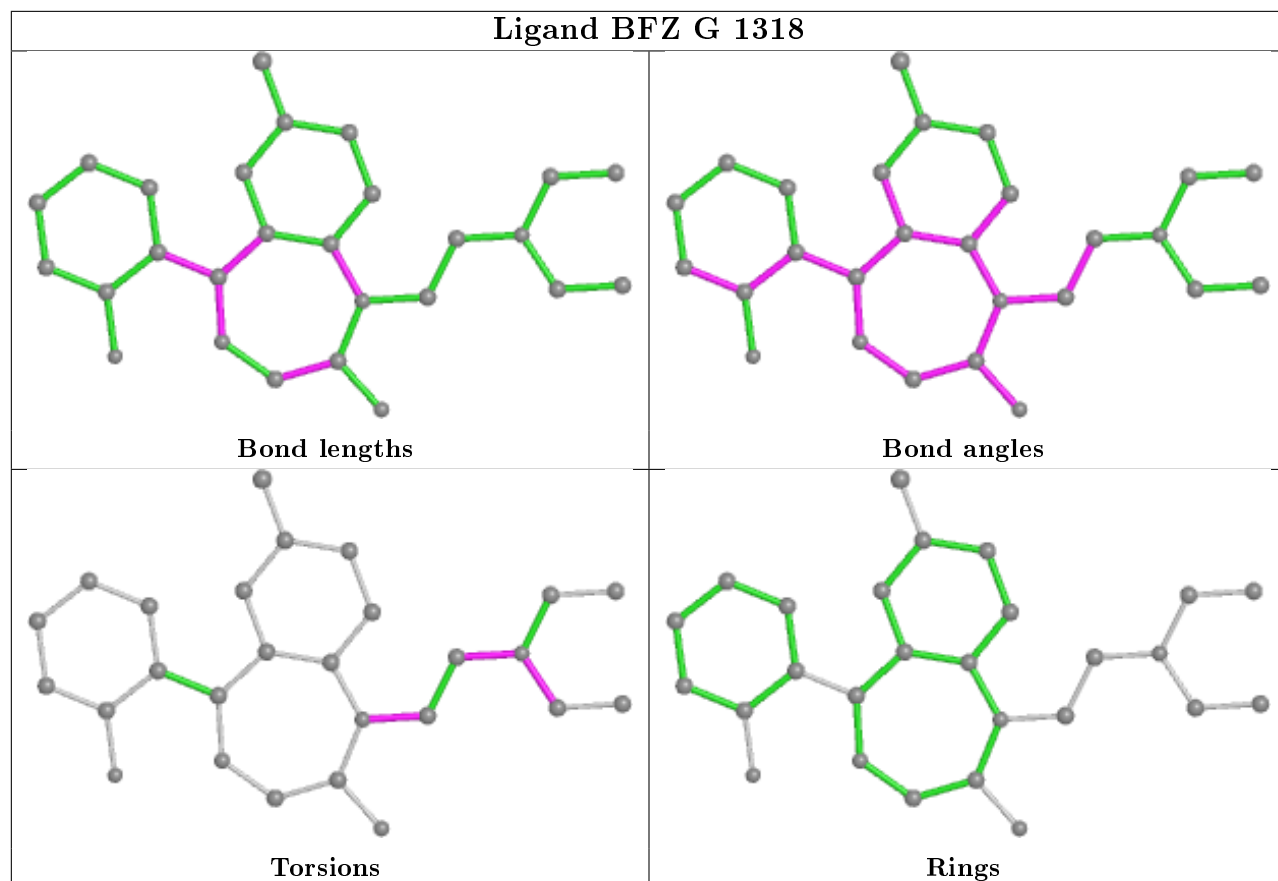
Ligand BFZ C 1318



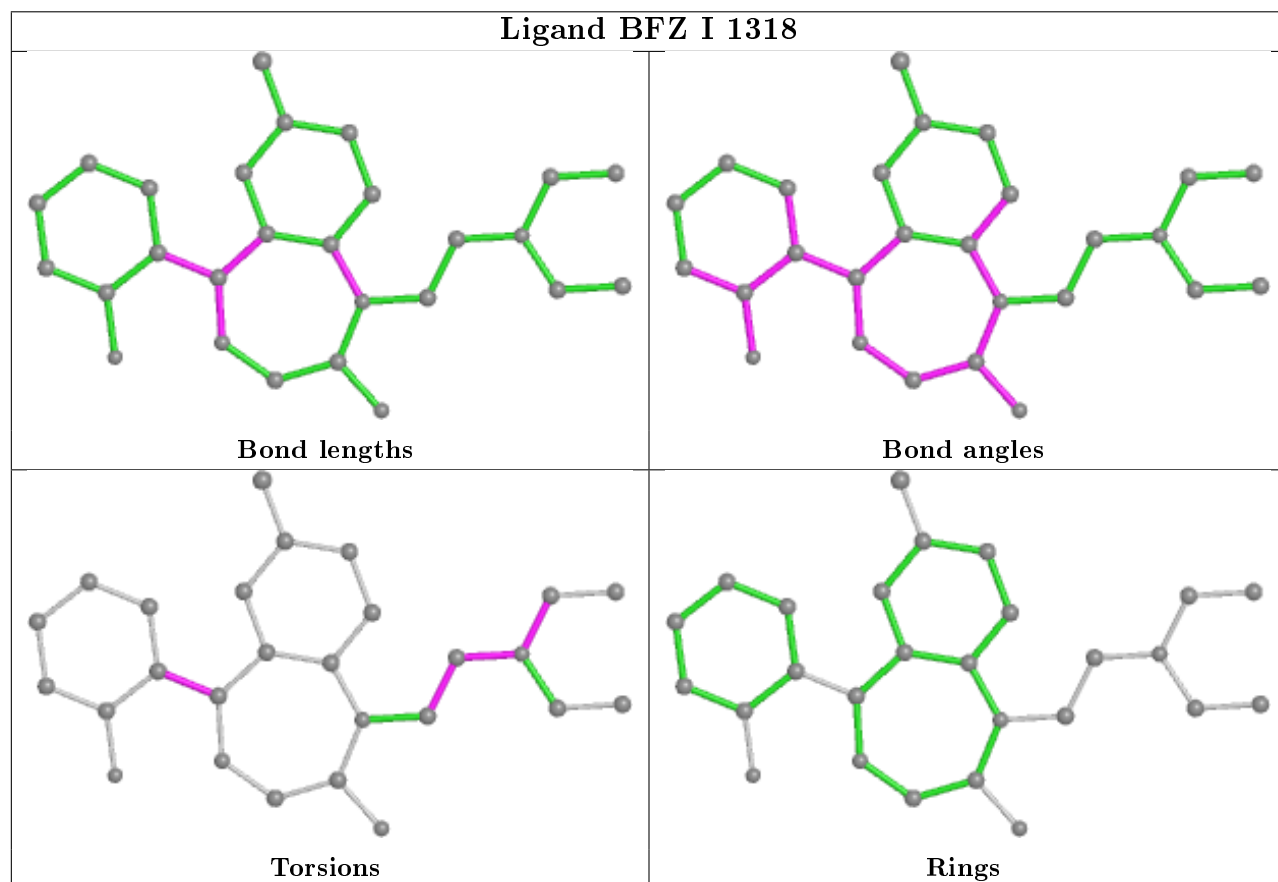
Ligand BFZ E 1318



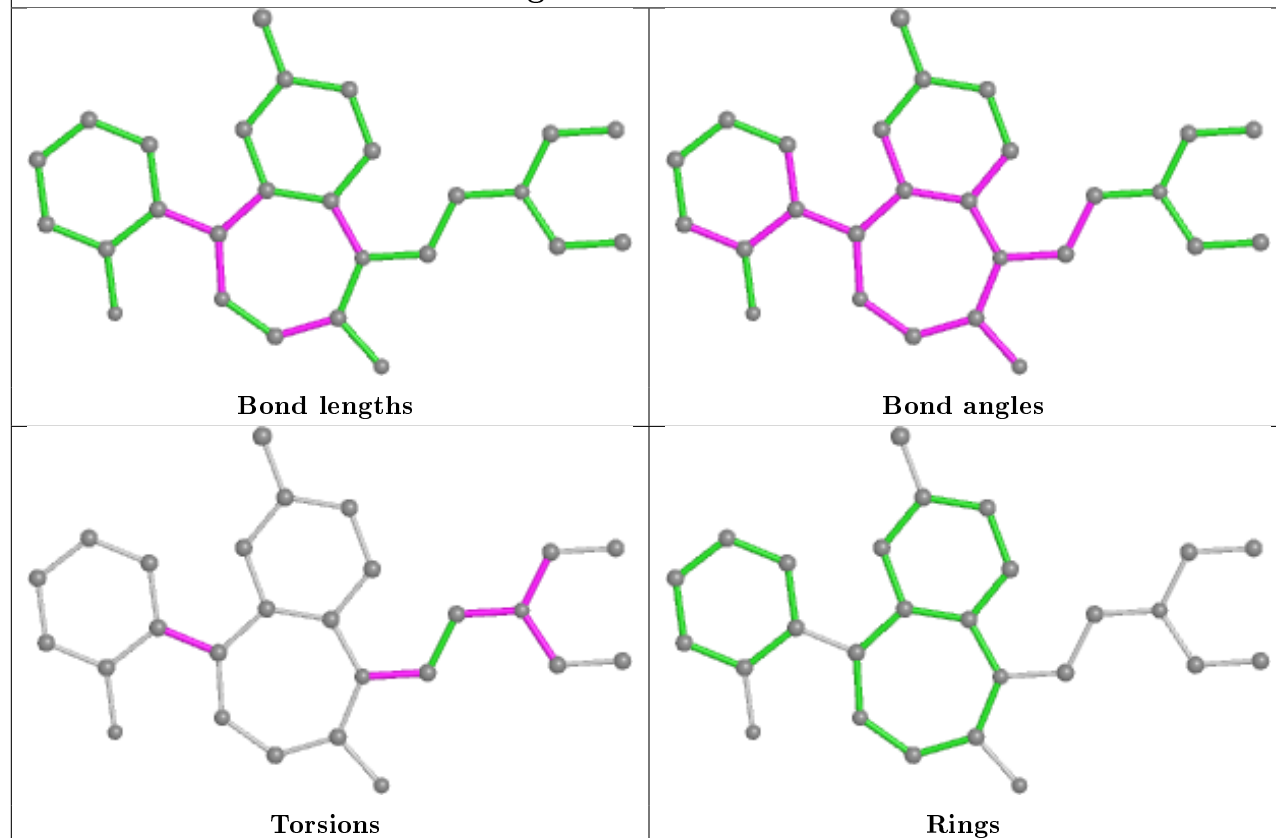
Ligand BFZ G 1318



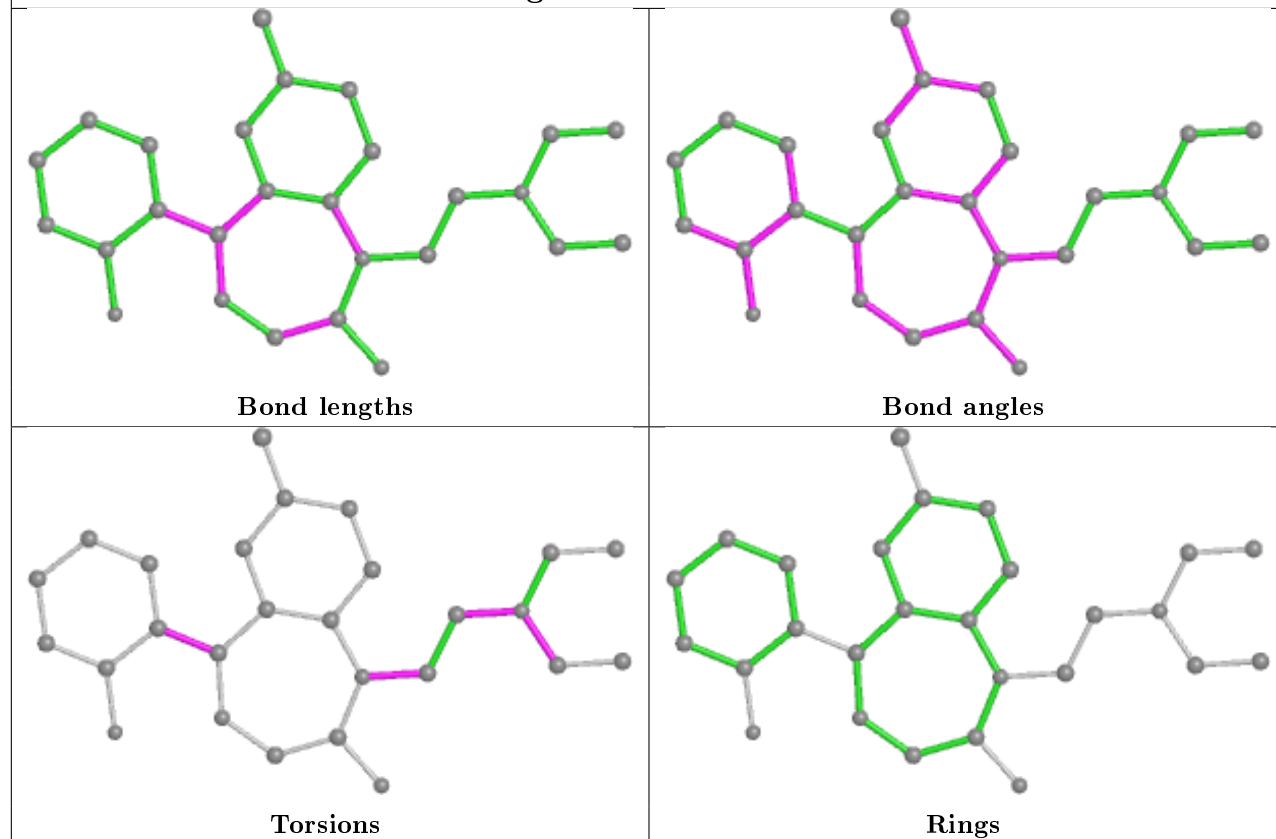
Ligand BFZ I 1318



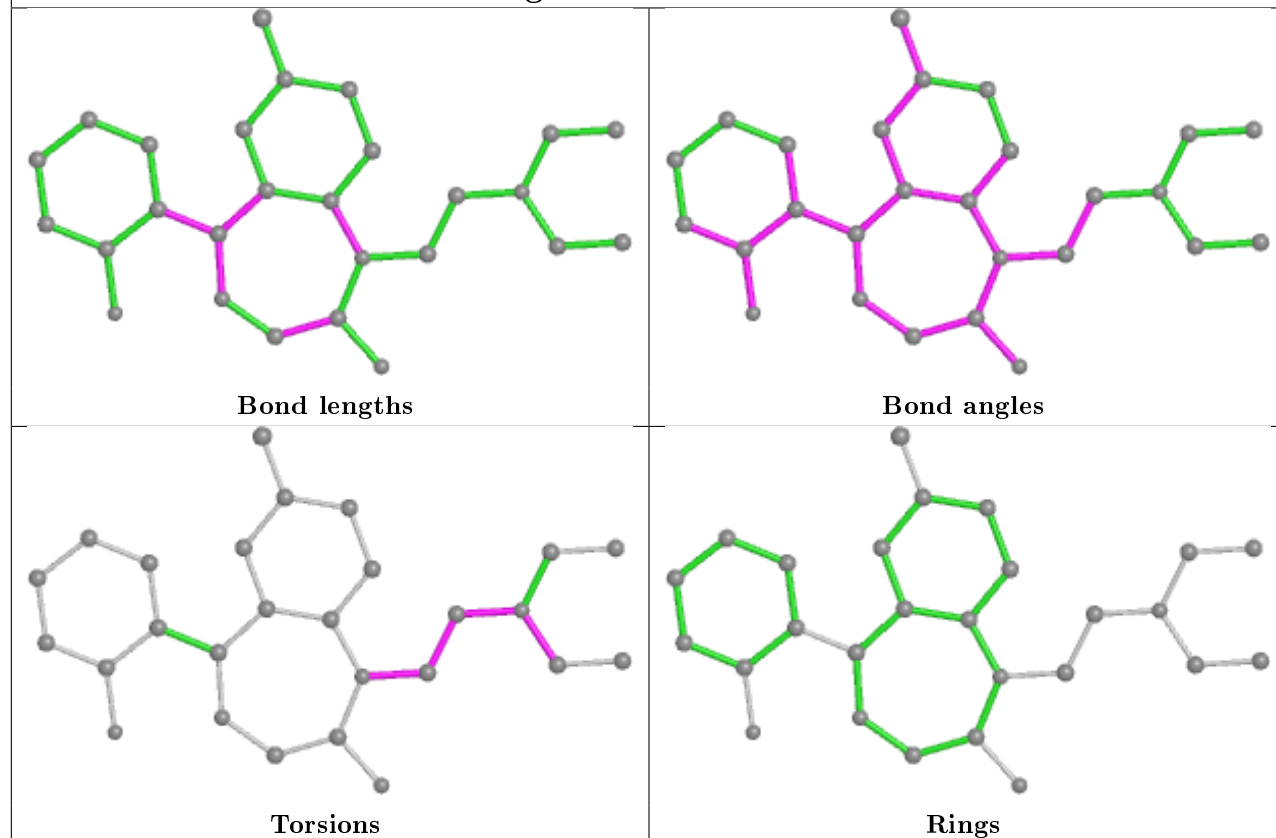
Ligand BFZ F 1318



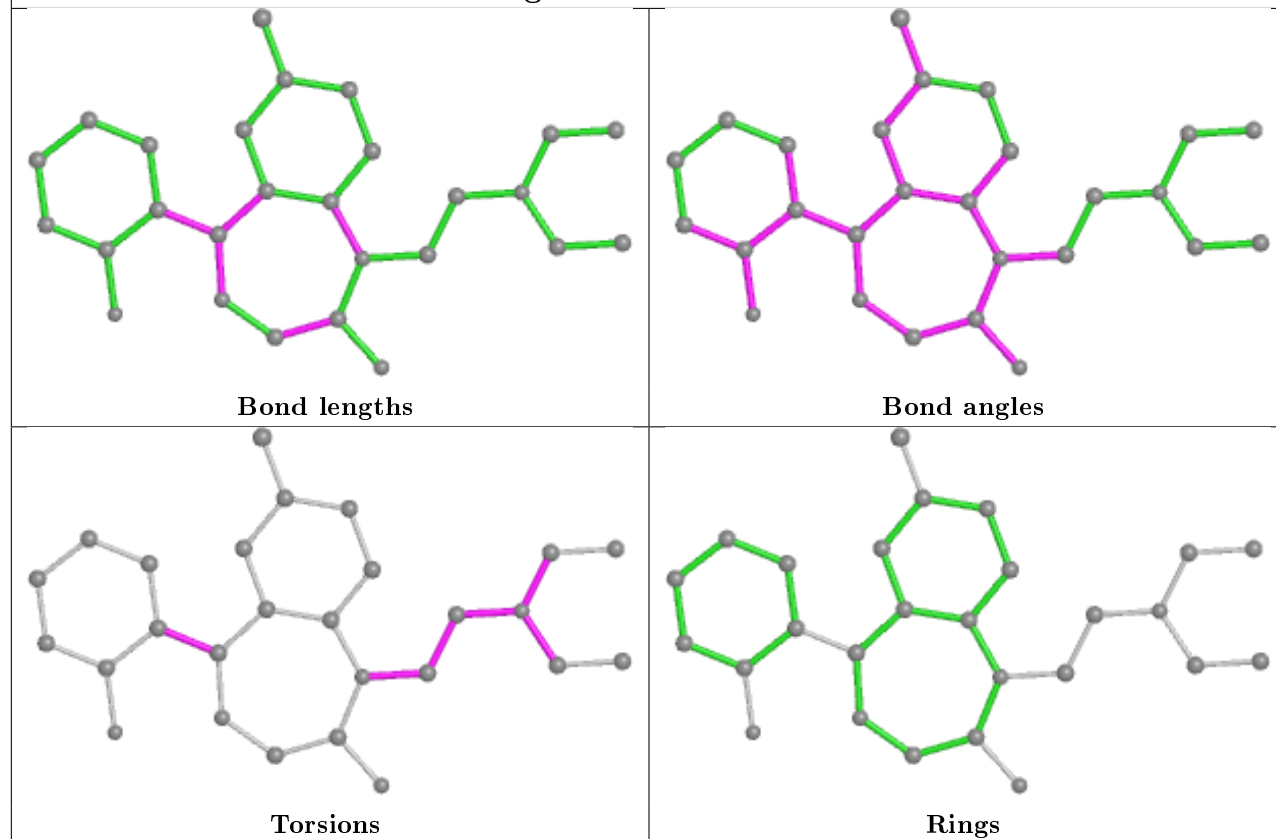
Ligand BFZ B 1318



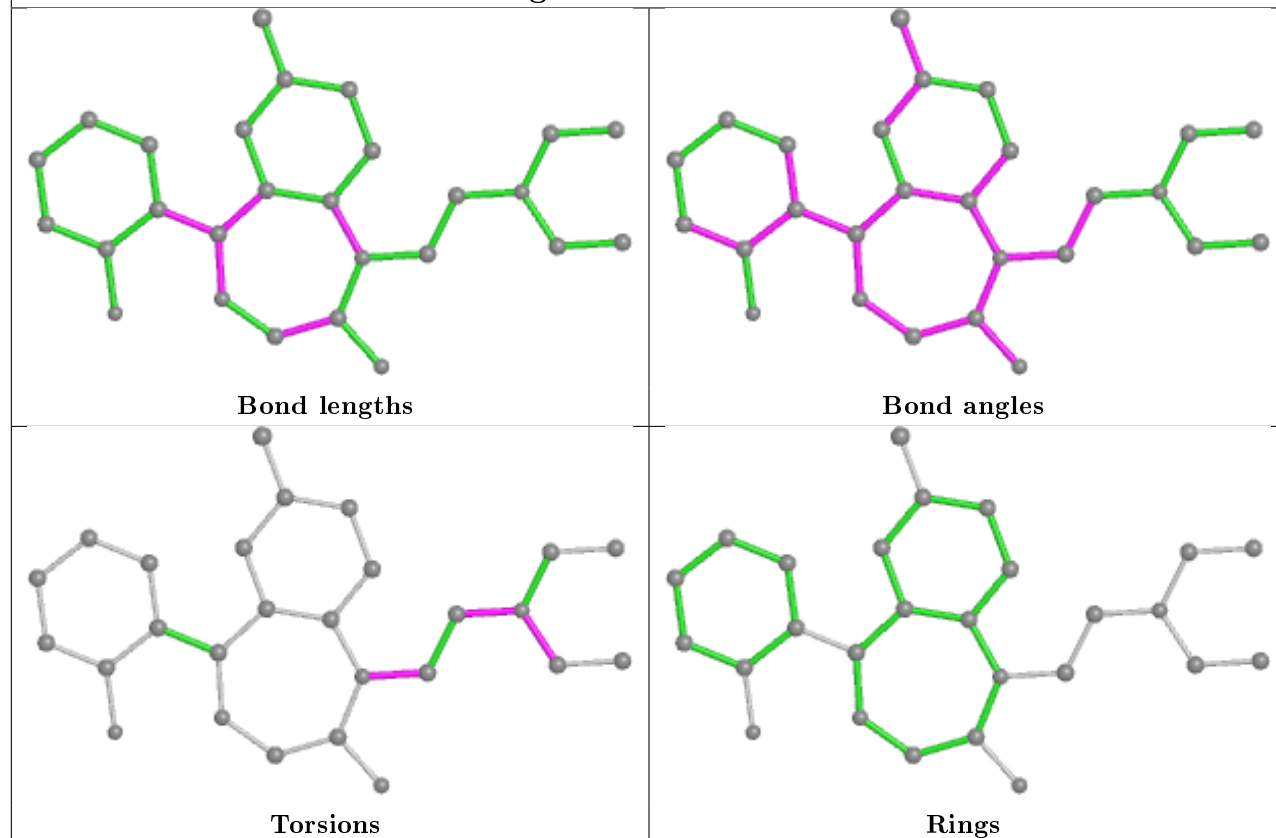
Ligand BFZ D 1318



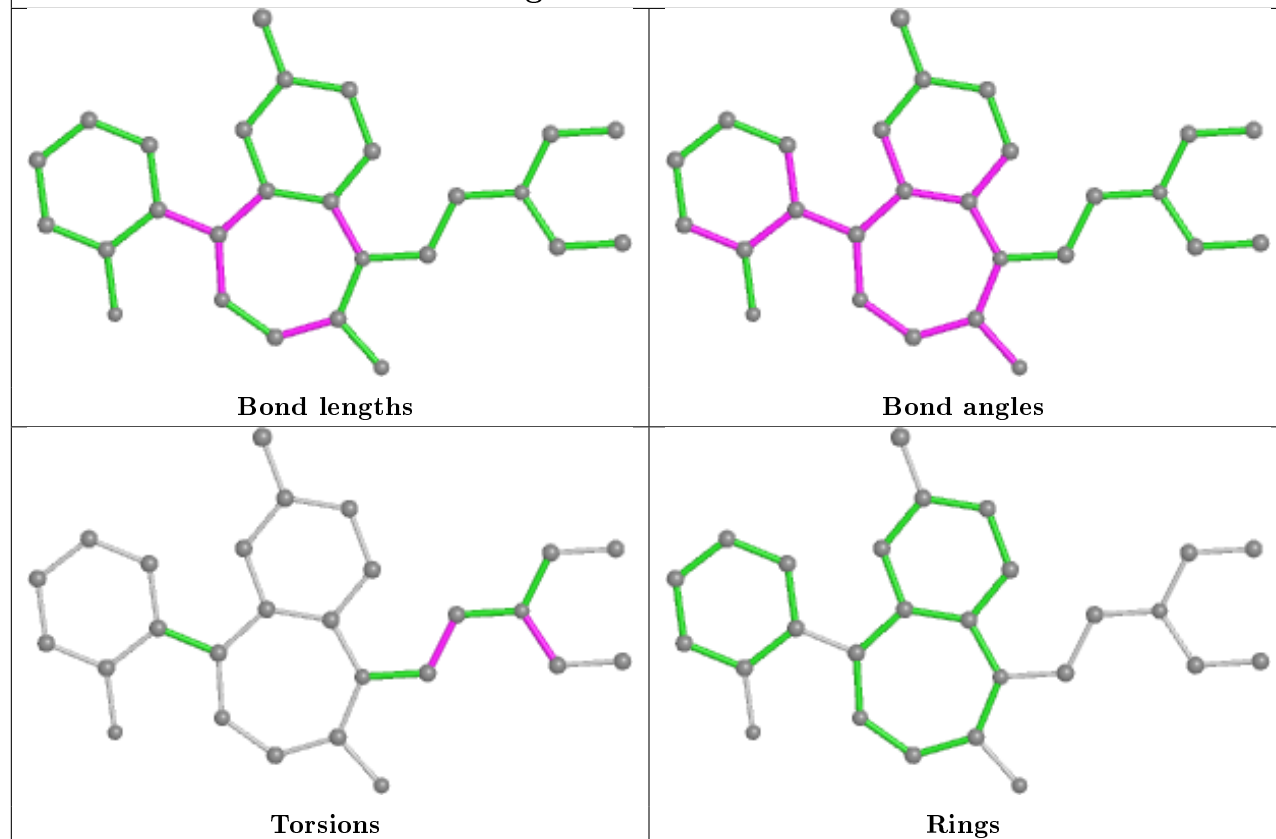
Ligand BFZ H 1318



Ligand BFZ J 1318



Ligand BFZ A 1318



5.7 Other polymers

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	307/307 (100%)	0.31	22 (7%) 15 9	103, 136, 185, 227	0
1	B	307/307 (100%)	0.11	12 (3%) 39 26	86, 124, 195, 207	0
1	C	307/307 (100%)	0.16	13 (4%) 36 24	90, 122, 197, 234	0
1	D	307/307 (100%)	0.19	17 (5%) 25 15	90, 123, 193, 226	0
1	E	307/307 (100%)	0.12	13 (4%) 36 24	101, 134, 185, 213	0
1	F	307/307 (100%)	0.25	18 (5%) 22 13	96, 141, 209, 240	0
1	G	307/307 (100%)	0.16	15 (4%) 29 19	94, 126, 198, 224	0
1	H	307/307 (100%)	0.20	14 (4%) 32 21	94, 132, 218, 243	0
1	I	307/307 (100%)	0.17	17 (5%) 25 15	91, 128, 203, 223	0
1	J	307/307 (100%)	0.42	33 (10%) 6 3	99, 141, 226, 250	0
All	All	3070/3070 (100%)	0.21	174 (5%) 23 14	86, 131, 203, 250	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	181	VAL	10.0
1	I	182	GLN	9.9
1	I	180	SER	7.3
1	D	181	VAL	7.3
1	J	303	ALA	7.2
1	B	289	ASN	5.7
1	H	183	PRO	5.2
1	I	183	PRO	5.2
1	B	290	GLY	5.1
1	G	290	GLY	5.0
1	D	179	SER	4.9
1	F	180	SER	4.9
1	I	297	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	H	289	ASN	4.7
1	J	156	GLU	4.6
1	E	181	VAL	4.5
1	B	291	VAL	4.4
1	D	297	ILE	4.4
1	H	182	GLN	4.4
1	D	180	SER	4.4
1	D	182	GLN	4.3
1	C	317	ILE	4.3
1	A	180	SER	4.3
1	H	293	ASP	4.3
1	I	179	SER	4.3
1	J	297	ILE	4.3
1	A	177	HIS	4.2
1	E	180	SER	4.2
1	I	154	ASN	4.1
1	J	304	PHE	4.1
1	E	182	GLN	4.1
1	I	177	HIS	4.0
1	E	183	PRO	3.9
1	I	291	VAL	3.9
1	C	231	ARG	3.9
1	C	226	GLU	3.8
1	E	157	ILE	3.8
1	H	291	VAL	3.8
1	C	291	VAL	3.7
1	A	179	SER	3.7
1	B	292	GLU	3.7
1	F	285	HIS	3.7
1	C	289	ASN	3.7
1	G	287	GLN	3.7
1	J	181	VAL	3.7
1	A	49	LYS	3.6
1	A	297	ILE	3.6
1	H	290	GLY	3.5
1	B	181	VAL	3.5
1	C	293	ASP	3.5
1	F	182	GLN	3.5
1	D	177	HIS	3.5
1	E	156	GLU	3.5
1	J	182	GLN	3.4
1	G	184	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	289	ASN	3.4
1	A	317	ILE	3.4
1	A	298	GLN	3.4
1	G	285	HIS	3.3
1	G	297	ILE	3.3
1	J	306	LEU	3.3
1	H	184	ASN	3.3
1	F	286	ARG	3.2
1	I	290	GLY	3.2
1	A	137	ASN	3.2
1	F	179	SER	3.2
1	J	180	SER	3.1
1	A	189	SER	3.1
1	J	294	ASP	3.1
1	J	172	ASP	3.1
1	J	310	ALA	3.1
1	J	157	ILE	3.1
1	H	181	VAL	3.0
1	G	185	GLN	3.0
1	A	314	VAL	3.0
1	A	258	TYR	3.0
1	J	307	GLY	3.0
1	D	315	LEU	3.0
1	C	298	GLN	2.9
1	J	314	VAL	2.9
1	A	178	LEU	2.9
1	J	289	ASN	2.9
1	B	297	ILE	2.9
1	F	316	VAL	2.9
1	A	290	GLY	2.9
1	D	49	LYS	2.9
1	G	183	PRO	2.9
1	D	178	LEU	2.9
1	I	222	VAL	2.8
1	F	317	ILE	2.8
1	J	154	ASN	2.8
1	J	179	SER	2.8
1	J	290	GLY	2.8
1	F	49	LYS	2.8
1	J	282	PHE	2.8
1	B	182	GLN	2.7
1	F	297	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	294	ASP	2.7
1	J	187	GLU	2.7
1	A	188	PHE	2.7
1	D	291	VAL	2.6
1	F	181	VAL	2.6
1	H	314	VAL	2.6
1	F	177	HIS	2.6
1	H	123	ARG	2.6
1	J	183	PRO	2.6
1	C	314	VAL	2.6
1	A	283	ALA	2.6
1	I	293	ASP	2.6
1	J	158	ASP	2.6
1	F	287	GLN	2.6
1	A	294	ASP	2.6
1	J	286	ARG	2.5
1	F	172	ASP	2.5
1	G	317	ILE	2.5
1	G	181	VAL	2.5
1	C	183	PRO	2.5
1	I	184	ASN	2.5
1	H	315	LEU	2.5
1	I	153	ASP	2.5
1	J	195	ILE	2.5
1	C	172	ASP	2.5
1	A	286	ARG	2.5
1	J	120	PRO	2.5
1	A	93	MET	2.4
1	G	156	GLU	2.4
1	I	286	ARG	2.4
1	A	94	LEU	2.4
1	F	315	LEU	2.4
1	D	293	ASP	2.4
1	B	293	ASP	2.4
1	C	288	ALA	2.4
1	J	296	LEU	2.4
1	D	157	ILE	2.3
1	D	286	ARG	2.3
1	J	196	ASP	2.3
1	D	289	ASN	2.3
1	J	223	PHE	2.3
1	B	183	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	314	VAL	2.2
1	H	303	ALA	2.2
1	C	315	LEU	2.2
1	B	298	GLN	2.2
1	G	157	ILE	2.2
1	E	237	THR	2.2
1	A	287	GLN	2.2
1	B	134	SER	2.2
1	G	315	LEU	2.1
1	J	315	LEU	2.1
1	E	43	TRP	2.1
1	J	308	PHE	2.1
1	J	119	PHE	2.1
1	F	117	ARG	2.1
1	E	223	PHE	2.1
1	J	305	PRO	2.1
1	A	285	HIS	2.1
1	B	84	SER	2.1
1	E	184	ASN	2.1
1	F	183	PRO	2.1
1	F	54	LYS	2.1
1	E	164	GLY	2.1
1	E	179	SER	2.1
1	H	180	SER	2.1
1	D	279	LEU	2.1
1	I	285	HIS	2.1
1	F	288	ALA	2.1
1	D	290	GLY	2.1
1	H	223	PHE	2.1
1	D	153	ASP	2.1
1	A	55	PRO	2.0
1	E	100	VAL	2.0
1	J	295	LEU	2.0
1	C	295	LEU	2.0
1	G	294	ASP	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

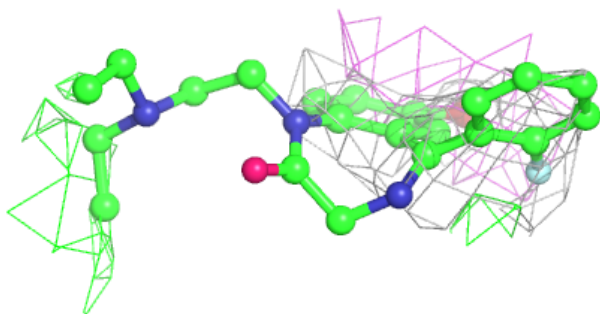
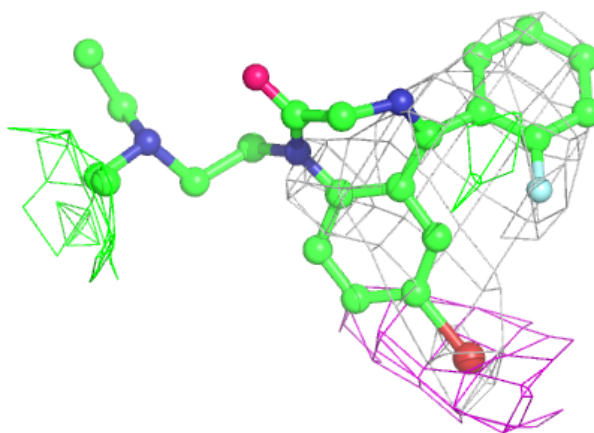
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BFZ	A	1318	27/27	0.73	0.72	47,165,300,300	27
2	BFZ	D	1318	27/27	0.79	0.49	22,140,300,300	27
2	BFZ	I	1318	27/27	0.79	0.50	6,115,299,300	27
2	BFZ	E	1318	27/27	0.84	0.48	26,113,300,300	27
2	BFZ	F	1318	27/27	0.84	0.45	28,187,300,300	27
2	BFZ	C	1318	27/27	0.86	0.30	25,167,300,300	27
2	BFZ	H	1318	27/27	0.88	0.35	3,121,300,300	27
2	BFZ	G	1318	27/27	0.88	0.37	25,164,292,300	27
2	BFZ	B	1318	27/27	0.90	0.30	25,152,299,300	27
2	BFZ	J	1318	27/27	0.92	0.36	3,148,299,300	27

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.

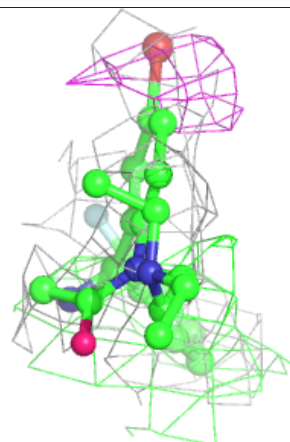
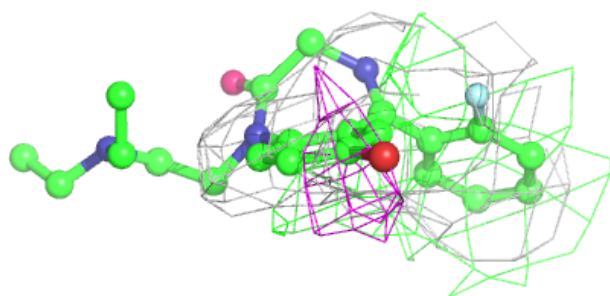
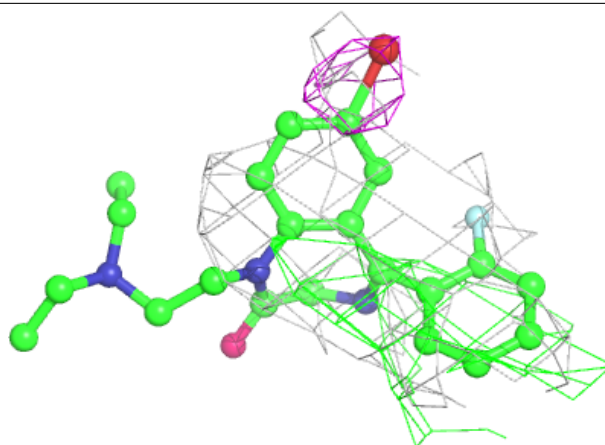
Electron density around BFZ A 1318:

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



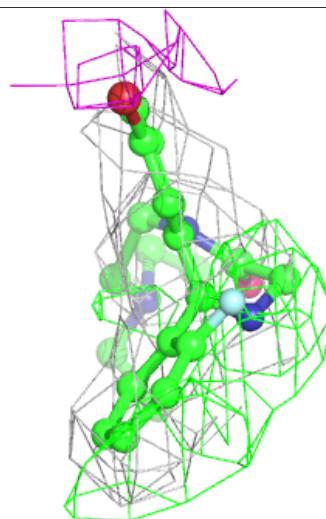
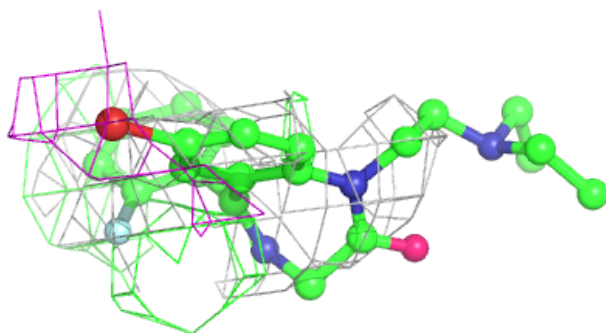
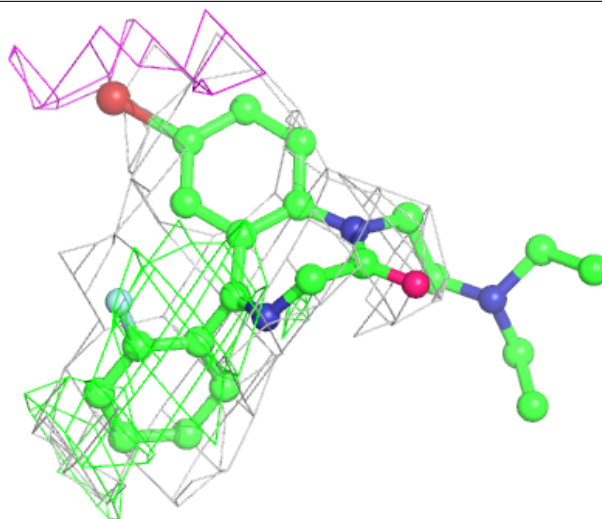
Electron density around BFZ D 1318:

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



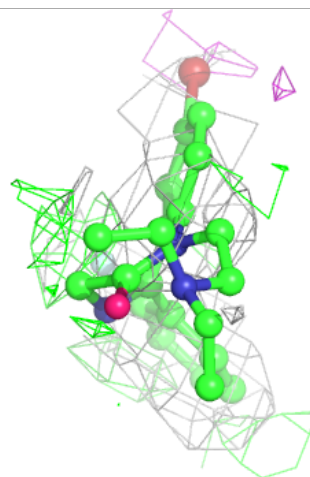
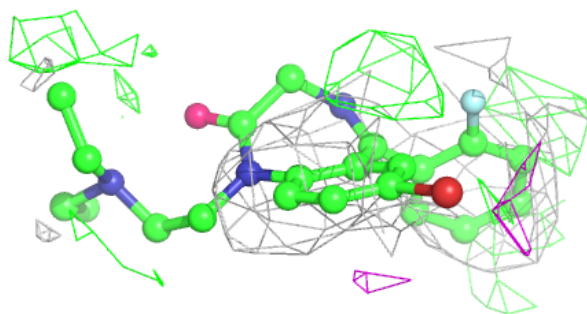
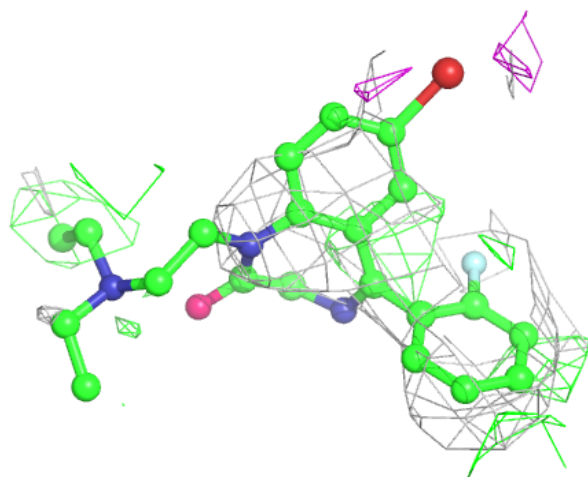
Electron density around BFZ I 1318:

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



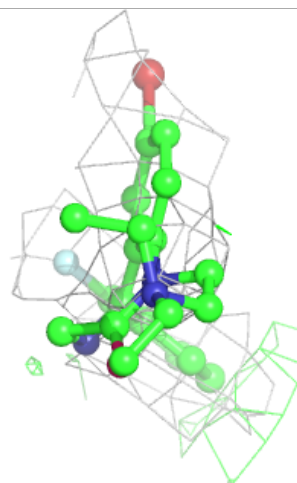
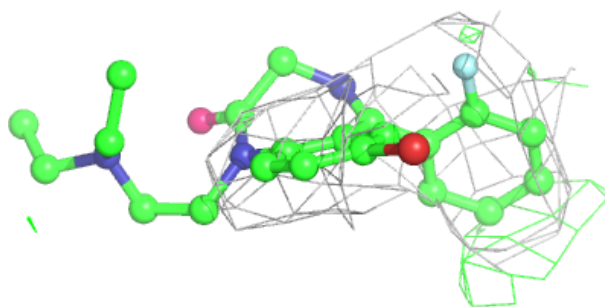
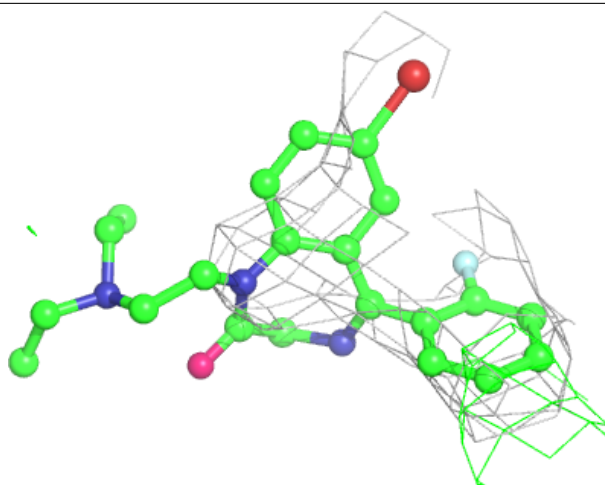
Electron density around BFZ E 1318:

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



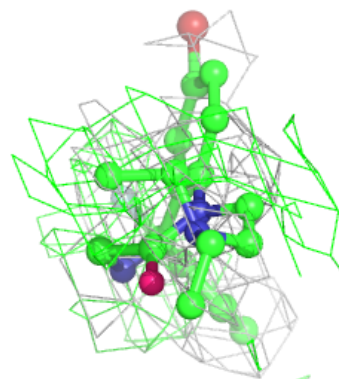
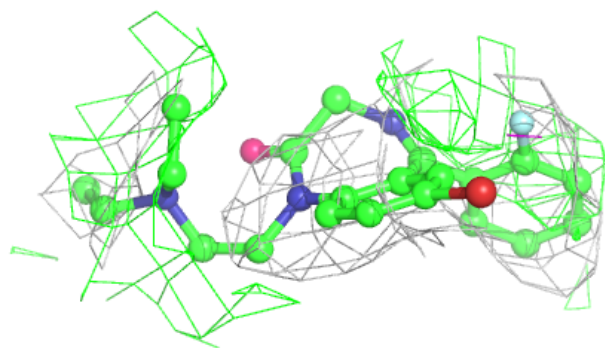
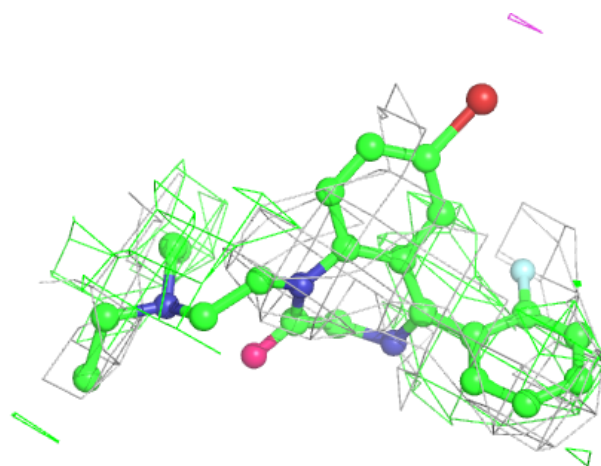
Electron density around BFZ F 1318:

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



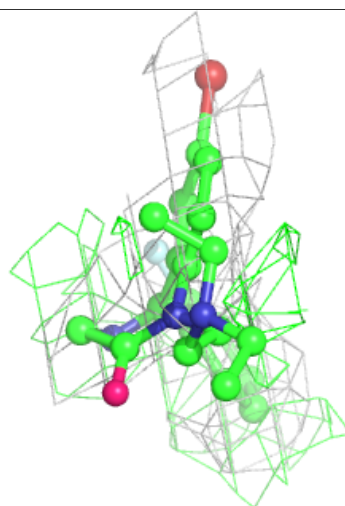
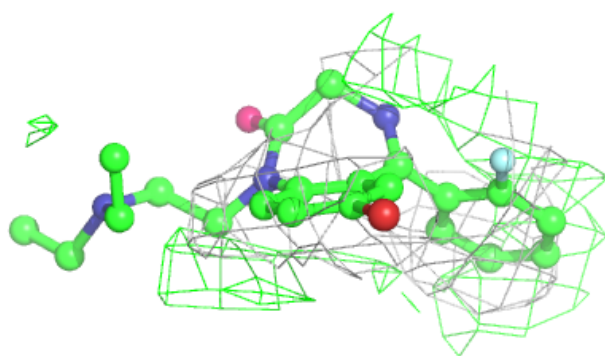
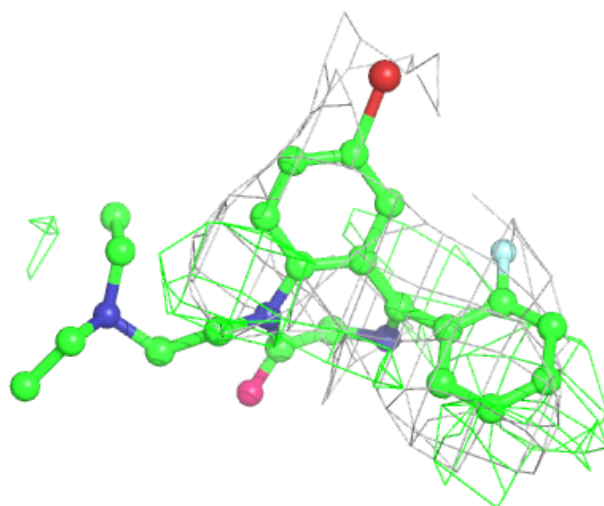
Electron density around BFZ C 1318:

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



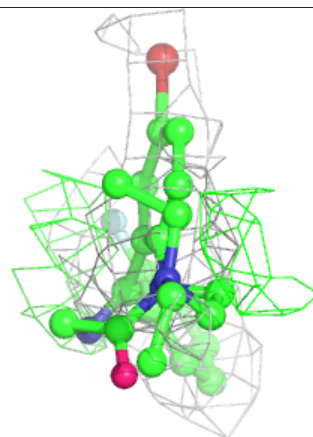
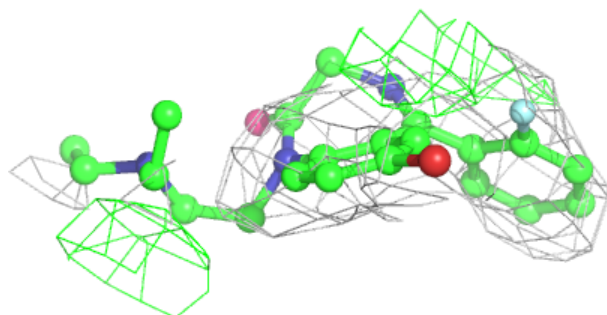
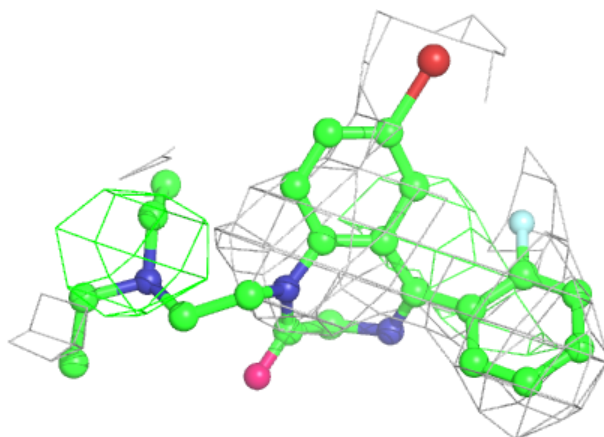
Electron density around BFZ H 1318:

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

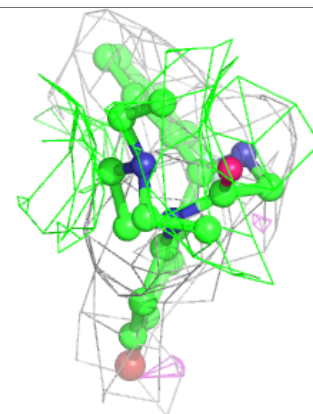
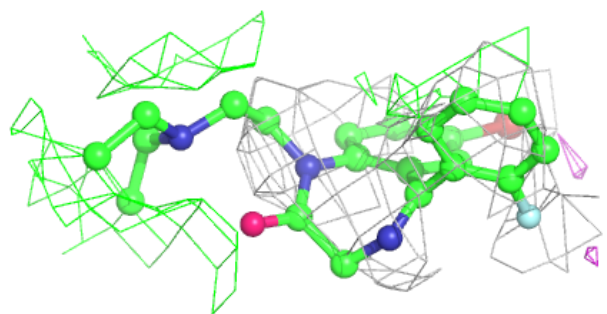
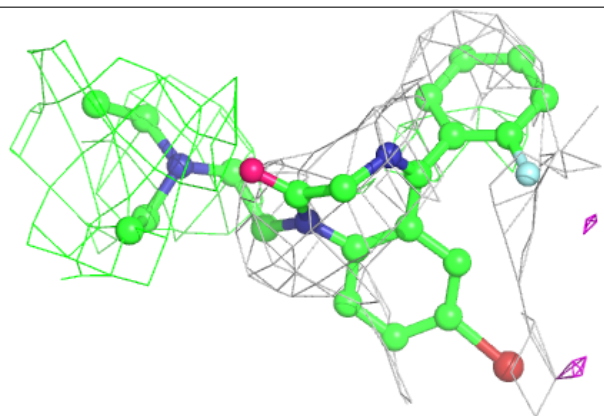


Electron density around BFZ G 1318:

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

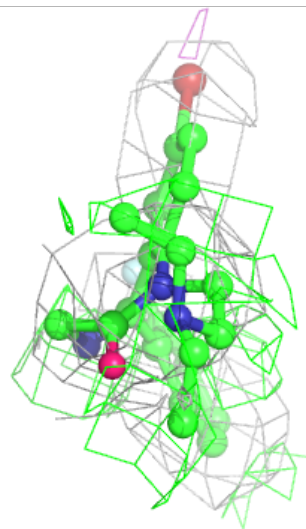
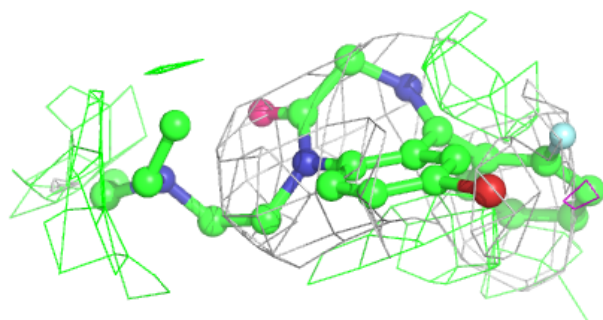
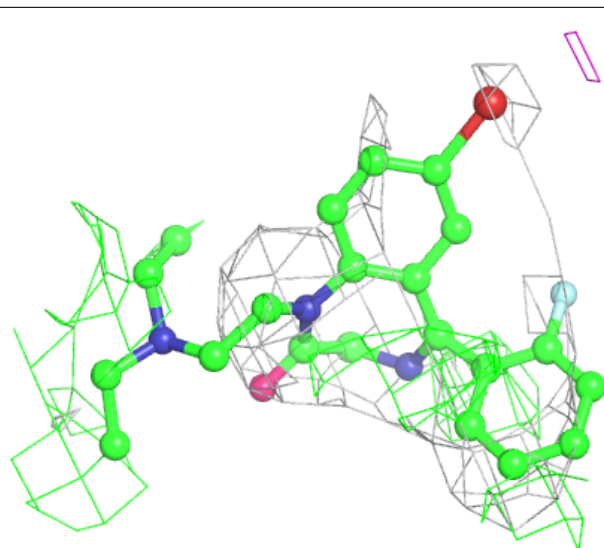
**Electron density around BFZ B 1318:**

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



Electron density around BFZ J 1318:

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.