



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 10:05 PM EDT

PDB ID : 3LIN  
Title : crystal structure of HTLV protease complexed with the inhibitor, KNI-10562  
Authors : Satoh, T.; Li, M.; Nguyen, J.; Kiso, Y.; Wlodawer, A.; Gustchina, A.  
Deposited on : 2010-01-25  
Resolution : 1.96 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
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) : 2.35

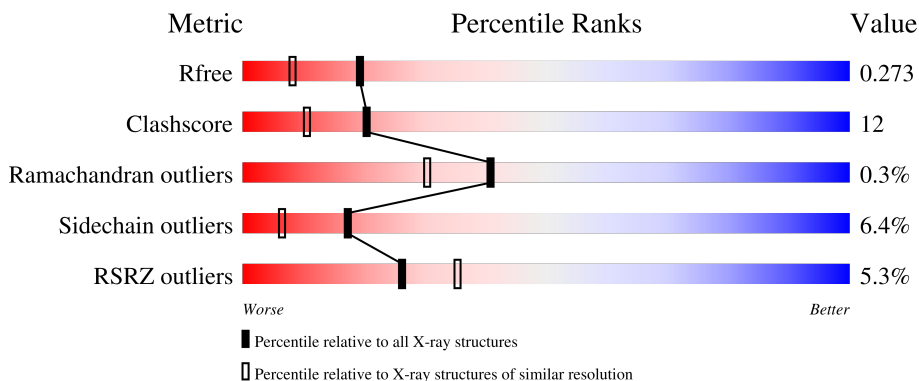
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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.




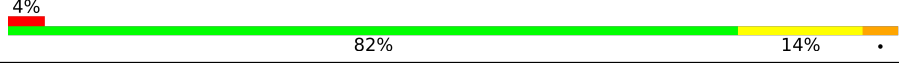
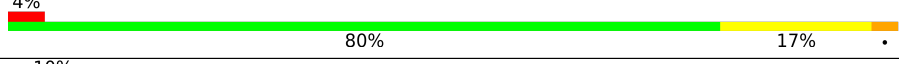


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	116	 4% 78% 21% .
1	B	116	 8% 79% 17% ..
1	C	116	 4% 84% 13% .
1	D	116	 2% 78% 19% ..
1	E	116	 5% 75% 22% .

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Mol	Chain	Length	Quality of chain
1	F	116	
1	G	116	
1	H	116	
1	I	116	
1	J	116	
1	K	116	
1	L	116	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11892 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 Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	116	883	564	152	164	3	0	0	0
1	B	116	883	564	152	164	3	0	0	0
1	C	116	896	576	152	165	3	0	3	0
1	D	116	901	576	155	167	3	0	3	0
1	E	116	883	564	152	164	3	0	0	0
1	F	116	883	564	152	164	3	0	0	0
1	G	116	883	564	152	164	3	0	0	0
1	H	116	882	564	152	163	3	0	0	0
1	I	116	896	576	152	165	3	0	3	0
1	J	116	901	576	155	167	3	0	3	0
1	K	116	883	564	152	164	3	0	0	0
1	L	116	883	564	152	164	3	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

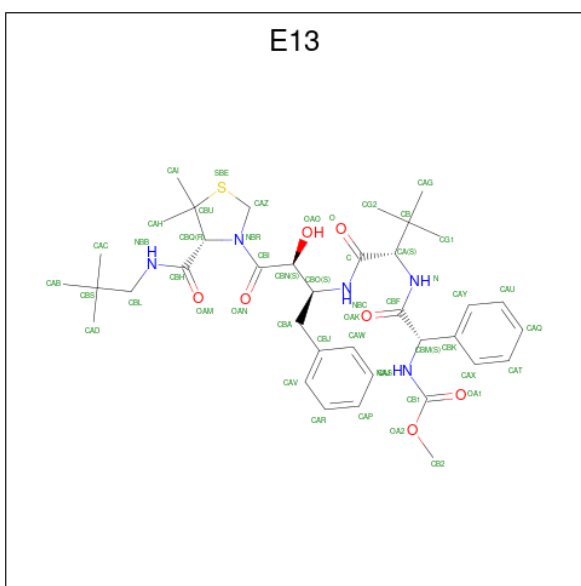
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ILE	LEU	engineered mutation	UNP Q82134
B	40	ILE	LEU	engineered mutation	UNP Q82134
C	40	ILE	LEU	engineered mutation	UNP Q82134
D	40	ILE	LEU	engineered mutation	UNP Q82134
E	40	ILE	LEU	engineered mutation	UNP Q82134

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Chain	Residue	Modelled	Actual	Comment	Reference
F	40	ILE	LEU	engineered mutation	UNP Q82134
G	40	ILE	LEU	engineered mutation	UNP Q82134
H	40	ILE	LEU	engineered mutation	UNP Q82134
I	40	ILE	LEU	engineered mutation	UNP Q82134
J	40	ILE	LEU	engineered mutation	UNP Q82134
K	40	ILE	LEU	engineered mutation	UNP Q82134
L	40	ILE	LEU	engineered mutation	UNP Q82134

- Molecule 2 is N-[(2S,3S)-4-[(4R)-4-[(2,2-dimethylpropyl)carbamoyl]-5,5-dimethyl-1,3-thiazolidin-3-yl]-3-hydroxy-4-oxo-1-phenylbutan-2-yl]-N 2 -[(2S)-2-[(methoxycarbonyl)amino]-2-phenylacetyl]-3-methyl-L-valinamide (three-letter code: E13) (formula: C<sub>37</sub>H<sub>53</sub>N<sub>5</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	Total	C	N	O	S	0	0
			50	37	5	7	1		
2	C	1	Total	C	N	O	S	0	1
			100	74	10	14	2		
2	E	1	Total	C	N	O	S	0	0
			50	37	5	7	1		
2	H	1	Total	C	N	O	S	0	1
			100	74	10	14	2		
2	I	1	Total	C	N	O	S	0	1
			100	74	10	14	2		
2	L	1	Total	C	N	O	S	0	0
			50	37	5	7	1		

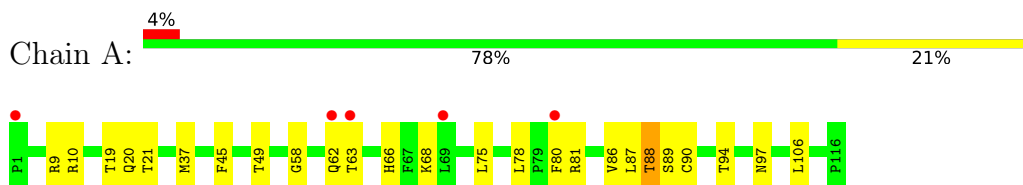
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	63	Total O 63 63	0	0
3	B	65	Total O 65 65	0	0
3	C	68	Total O 68 68	0	3
3	D	55	Total O 55 55	0	0
3	E	85	Total O 85 85	0	0
3	F	60	Total O 60 60	0	0
3	G	63	Total O 63 63	0	0
3	H	54	Total O 54 54	0	0
3	I	79	Total O 79 79	0	0
3	J	59	Total O 59 59	0	0
3	K	64	Total O 64 64	0	0
3	L	70	Total O 70 70	0	0

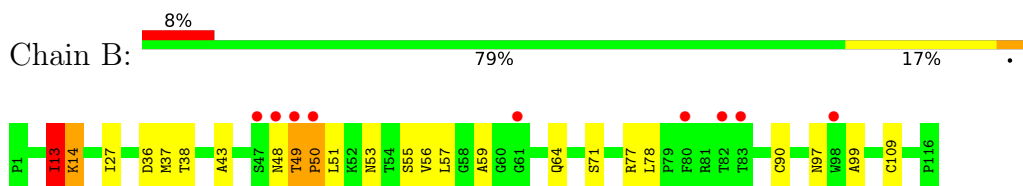
### 3 Residue-property plots [i](#)

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.

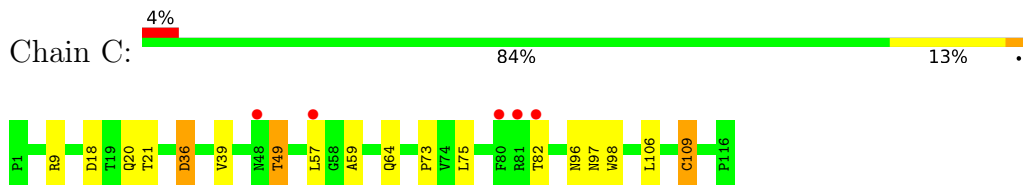
- Molecule 1: Protease



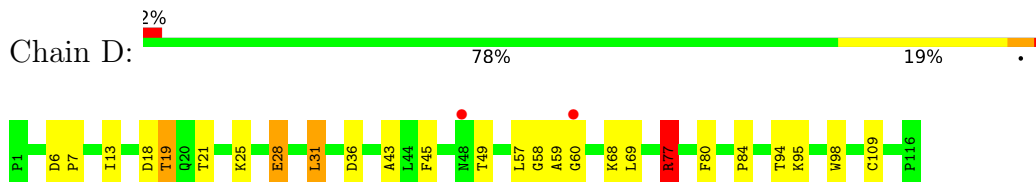
- Molecule 1: Protease



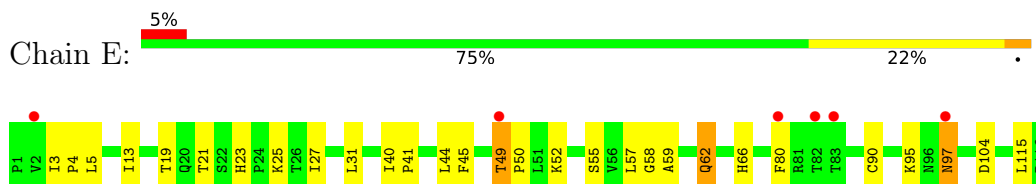
- Molecule 1: Protease



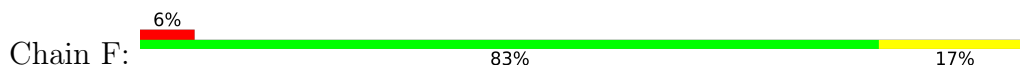
- Molecule 1: Protease



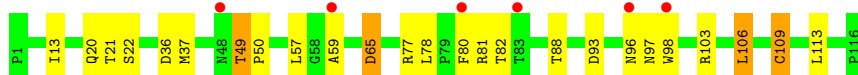
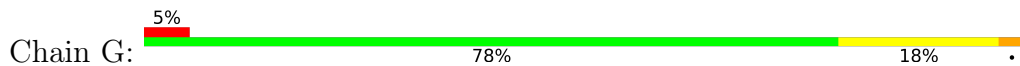
- Molecule 1: Protease



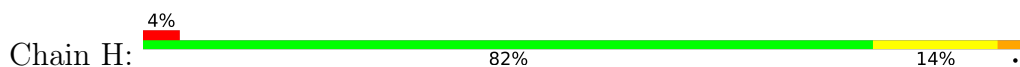
- Molecule 1: Protease



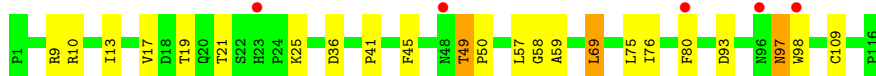
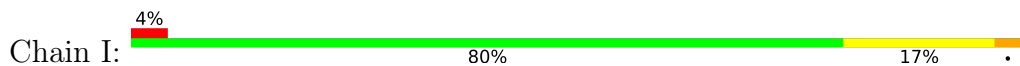
● Molecule 1: Protease



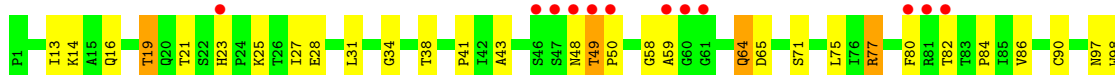
● Molecule 1: Protease



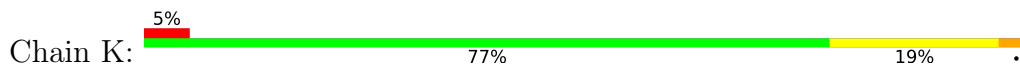
● Molecule 1: Protease



● Molecule 1: Protease



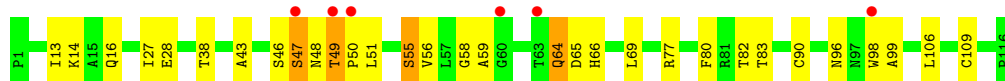
● Molecule 1: Protease



● Molecule 1: Protease







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.36Å 77.31Å 159.17Å 90.00° 95.09° 90.00°	Depositor
Resolution (Å)	50.00 – 1.96 49.03 – 1.96	Depositor EDS
% Data completeness (in resolution range)	96.9 (50.00-1.96) 96.9 (49.03-1.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 1.97Å)	Xtrriage
Refinement program	REFMAC 5.5.0104	Depositor
R, $R_{free}$	0.213 , 0.262 0.225 , 0.273	Depositor DCC
$R_{free}$ test set	3393 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtrriage
Anisotropy	0.103	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3703e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: E13

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	0.65	0/901	0.78	0/1233
1	B	0.69	0/901	0.84	1/1233 (0.1%)
1	C	0.78	1/923 (0.1%)	0.85	2/1263 (0.2%)
1	D	0.79	1/928 (0.1%)	1.02	6/1269 (0.5%)
1	E	0.74	0/901	0.82	1/1233 (0.1%)
1	F	0.67	0/901	0.83	2/1233 (0.2%)
1	G	0.78	1/901 (0.1%)	0.89	4/1233 (0.3%)
1	H	0.73	1/900 (0.1%)	0.81	0/1233
1	I	0.78	1/923 (0.1%)	0.89	2/1263 (0.2%)
1	J	0.71	1/928 (0.1%)	0.82	1/1269 (0.1%)
1	K	0.72	1/901 (0.1%)	0.82	0/1233
1	L	0.70	0/901	0.85	1/1233 (0.1%)
All	All	0.73	7/10909 (0.1%)	0.85	20/14928 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	109	CYS	CB-SG	-11.83	1.62	1.82
1	C	109	CYS	CB-SG	-11.76	1.62	1.82
1	D	109	CYS	CB-SG	-10.03	1.65	1.82
1	J	109	CYS	CB-SG	-6.46	1.71	1.82
1	I	109	CYS	CB-SG	-6.12	1.71	1.82
1	K	109	CYS	CB-SG	-5.13	1.73	1.81
1	H	109	CYS	CB-SG	-5.01	1.73	1.81

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	77[A]	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	D	77[B]	ARG	NE-CZ-NH2	-7.21	116.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	ILE	CB-CA-C	-6.19	99.22	111.60
1	D	109	CYS	CB-CA-C	-6.11	98.19	110.40
1	D	6	ASP	CB-CG-OD1	5.93	123.64	118.30
1	G	36	ASP	CB-CG-OD1	5.87	123.58	118.30
1	D	18	ASP	CB-CG-OD1	5.77	123.49	118.30
1	C	36	ASP	CB-CG-OD1	5.72	123.44	118.30
1	I	36	ASP	CB-CG-OD1	5.71	123.44	118.30
1	C	109	CYS	CB-CA-C	-5.70	99.00	110.40
1	L	69	LEU	CA-CB-CG	5.58	128.14	115.30
1	G	37	MET	CG-SD-CE	-5.46	91.47	100.20
1	E	104	ASP	CB-CG-OD1	5.44	123.19	118.30
1	J	104	ASP	CB-CG-OD1	5.32	123.08	118.30
1	D	31	LEU	CB-CG-CD1	5.28	119.98	111.00
1	F	98	TRP	CA-CB-CG	5.19	123.57	113.70
1	I	69	LEU	CA-CB-CG	5.17	127.19	115.30
1	G	109	CYS	CB-CA-C	-5.12	100.17	110.40
1	G	113	LEU	CA-CB-CG	5.07	126.95	115.30
1	F	69	LEU	CA-CB-CG	5.06	126.95	115.30

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	883	0	926	19	0
1	B	883	0	926	18	0
1	C	896	0	953	16	0
1	D	901	0	952	25	0
1	E	883	0	926	25	0
1	F	883	0	926	11	0
1	G	883	0	926	22	0
1	H	882	0	926	15	0
1	I	896	0	953	27	0
1	J	901	0	952	30	0
1	K	883	0	926	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	883	0	926	28	0
2	B	50	0	53	2	0
2	C	100	0	106	24	0
2	E	50	0	52	2	0
2	H	100	0	106	16	0
2	I	100	0	106	21	0
2	L	50	0	53	1	0
3	A	63	0	0	8	1
3	B	65	0	0	10	0
3	C	68	0	0	13	0
3	D	55	0	0	5	0
3	E	85	0	0	9	1
3	F	60	0	0	4	0
3	G	63	0	0	8	0
3	H	54	0	0	9	0
3	I	79	0	0	7	0
3	J	59	0	0	5	0
3	K	64	0	0	10	0
3	L	70	0	0	11	0
All	All	11892	0	11694	283	1

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 12.

All (283) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:117[A]:E13:HAS	2:I:117[A]:E13:CAX	1.43	1.49
2:I:117[A]:E13:CAX	2:I:117[A]:E13:CAS	2.10	1.28
2:C:117[B]:E13:CBM	3:C:840:HOH:O	1.68	1.28
2:H:117[A]:E13:CB2	3:H:838:HOH:O	1.66	1.27
2:H:117[B]:E13:CB1	3:H:839:HOH:O	1.73	1.27
2:C:117[B]:E13:CBK	3:C:840:HOH:O	1.75	1.19
2:C:117[B]:E13:HBM	3:C:840:HOH:O	1.29	1.18
2:H:117[A]:E13:HB2	3:H:838:HOH:O	1.17	1.18
2:C:117[A]:E13:CB1	3:C:843:HOH:O	1.94	1.13
2:I:117[A]:E13:HAS	2:I:117[A]:E13:CBK	1.81	1.11
1:B:36:ASP:OD1	3:B:146:HOH:O	1.69	1.09
1:A:63:THR:HG22	3:A:442:HOH:O	1.50	1.09
1:A:37:MET:SD	3:A:382:HOH:O	2.11	1.08
2:C:117[A]:E13:OA1	3:C:843:HOH:O	1.73	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:117[A]:E13:HAS	2:I:117[A]:E13:HAX	1.37	1.06
1:C:57[B]:LEU:HB2	3:C:840:HOH:O	1.53	1.06
2:C:117[A]:E13:HB2A	3:C:842:HOH:O	0.88	1.05
1:K:81:ARG:NH2	3:K:622:HOH:O	1.88	1.04
2:I:117[A]:E13:HAS	2:I:117[A]:E13:CBF	1.88	1.03
1:K:76:ILE:HG12	3:K:475:HOH:O	1.57	1.02
2:I:117[A]:E13:NBC	2:I:117[A]:E13:CAW	2.19	1.02
2:C:117[B]:E13:CAY	3:C:840:HOH:O	1.99	0.94
1:K:37:MET:SD	3:K:139:HOH:O	2.24	0.94
1:L:55:SER:HB2	1:L:64:GLN:HG3	1.47	0.94
1:I:21:THR:HG21	1:I:49:THR:HG21	1.51	0.92
1:A:90:CYS:SG	3:A:590:HOH:O	1.92	0.91
1:K:96:ASN:HB2	3:K:282:HOH:O	1.72	0.90
1:K:21:THR:HG21	1:K:49:THR:HG21	1.51	0.90
1:A:90:CYS:HA	3:A:382:HOH:O	1.72	0.89
1:C:36:ASP:HA	3:D:749:HOH:O	1.76	0.86
1:J:77[A]:ARG:HD3	1:J:84:PRO:HB3	1.58	0.86
3:B:120:HOH:O	1:E:49:THR:HG23	1.77	0.85
1:J:14:LYS:HG3	3:J:491:HOH:O	1.78	0.83
1:L:55:SER:HB2	1:L:64:GLN:CG	2.09	0.82
1:I:75:LEU:O	3:I:786:HOH:O	1.97	0.81
1:E:3:ILE:HG22	3:E:812:HOH:O	1.78	0.81
1:H:98:TRP:CZ3	2:H:117[B]:E13:HAR	2.17	0.80
2:C:117[A]:E13:HAR	1:D:59:ALA:HA	1.63	0.80
1:C:20:GLN:O	1:F:25:LYS:HE2	1.82	0.80
3:C:448:HOH:O	1:D:60:GLY:HA3	1.82	0.80
1:I:97:ASN:HD22	1:I:97:ASN:H	1.26	0.79
1:L:55:SER:CB	1:L:64:GLN:HG3	2.12	0.79
2:I:117[A]:E13:CAW	2:I:117[A]:E13:HNBC	1.97	0.78
2:I:117[A]:E13:HNBC	2:I:117[A]:E13:HAW	1.49	0.77
2:I:117[A]:E13:CAS	2:I:117[A]:E13:CBF	2.61	0.77
1:B:49:THR:O	3:B:598:HOH:O	2.03	0.77
1:I:25:LYS:HE2	3:I:500:HOH:O	1.85	0.75
1:C:98:TRP:CZ2	2:C:117[A]:E13:HAP	2.22	0.74
1:K:21:THR:CG2	1:K:49:THR:HG21	2.19	0.73
1:L:16:GLN:HG3	3:L:220:HOH:O	1.89	0.73
2:I:117[A]:E13:CAS	2:I:117[A]:E13:CBK	2.55	0.72
2:C:117[B]:E13:HAR	1:D:98:TRP:CZ3	2.24	0.72
1:F:27:ILE:HD12	1:F:99:ALA:HB1	1.71	0.72
1:B:55:SER:HB3	3:B:499:HOH:O	1.89	0.71
1:E:4:PRO:O	3:E:812:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19[A]:THR:HG23	1:D:45:PHE:CE2	2.25	0.71
1:I:93:ASP:OD2	1:I:98:TRP:CD1	2.43	0.71
1:G:21:THR:HG21	1:G:49:THR:HG21	1.74	0.70
1:B:55:SER:CB	3:B:499:HOH:O	2.39	0.70
1:K:85:ILE:HG12	3:K:389:HOH:O	1.92	0.70
1:I:21:THR:CG2	1:I:49:THR:HG21	2.21	0.69
1:K:57:LEU:HD11	1:L:98:TRP:CZ2	2.26	0.69
1:C:9:ARG:NH2	3:C:226:HOH:O	2.26	0.69
1:G:98:TRP:CZ2	2:H:117[A]:E13:HAP	2.27	0.69
1:C:57[A]:LEU:HB3	3:C:840:HOH:O	1.92	0.69
1:L:55:SER:HB2	1:L:64:GLN:CD	2.14	0.68
1:E:21:THR:HG21	1:E:49:THR:HG21	1.75	0.68
1:F:108:GLN:OE1	3:F:213:HOH:O	2.12	0.67
1:K:57:LEU:HD11	1:L:98:TRP:HZ2	1.59	0.67
1:L:27:ILE:HD12	1:L:99:ALA:HB1	1.77	0.67
2:C:117[B]:E13:HAS	2:C:117[B]:E13:CAX	2.26	0.66
3:G:789:HOH:O	1:J:27:ILE:CG2	2.43	0.66
1:I:93:ASP:OD2	1:I:98:TRP:HD1	1.78	0.66
1:L:50:PRO:HA	3:L:510:HOH:O	1.96	0.66
1:I:97:ASN:HD22	1:I:97:ASN:N	1.93	0.65
2:I:117[A]:E13:HAS	2:I:117[A]:E13:CBM	2.25	0.65
2:H:117[B]:E13:NAJ	3:H:839:HOH:O	2.10	0.65
1:E:25:LYS:HE2	3:E:588:HOH:O	1.96	0.65
1:D:77[B]:ARG:HG3	1:D:77[B]:ARG:HH11	1.61	0.64
1:G:81:ARG:NH1	3:G:315:HOH:O	2.29	0.64
2:H:117[A]:E13:HAX	2:H:117[A]:E13:OAK	1.97	0.64
1:C:98:TRP:CH2	2:C:117[A]:E13:CAP	2.81	0.63
1:I:58:GLY:HA3	1:J:59:ALA:HB3	1.79	0.63
1:B:109:CYS:HB2	3:B:579:HOH:O	1.99	0.62
1:H:59:ALA:HA	2:H:117[A]:E13:HAR	1.80	0.62
2:H:117[A]:E13:HB2A	3:H:838:HOH:O	1.57	0.62
1:K:40:ILE:HD12	1:K:90:CYS:SG	2.39	0.62
1:I:76:ILE:HG12	3:I:786:HOH:O	2.00	0.61
1:D:19[A]:THR:HG21	1:D:45:PHE:CD2	2.35	0.61
1:K:61:GLY:HA2	3:L:743:HOH:O	2.00	0.61
1:K:17:VAL:HG13	3:K:475:HOH:O	2.01	0.61
2:C:117[B]:E13:HAS	2:C:117[B]:E13:CAT	2.31	0.61
1:G:49:THR:HG23	3:J:498:HOH:O	2.01	0.61
1:I:17:VAL:HG13	3:I:786:HOH:O	2.01	0.61
2:I:117[A]:E13:HAX	2:I:117[A]:E13:OAK	2.01	0.61
1:G:93:ASP:OD2	1:G:97:ASN:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ASP:HB3	1:C:75:LEU:HB2	1.84	0.60
1:C:98:TRP:CH2	2:C:117[A]:E13:HAP	2.35	0.60
1:G:13:ILE:HD11	1:G:80:PHE:HE1	1.65	0.60
2:I:117[A]:E13:CAS	2:I:117[A]:E13:HAX	2.08	0.59
1:I:98:TRP:HE3	3:I:663:HOH:O	1.85	0.59
1:B:51:LEU:HA	3:B:298:HOH:O	2.01	0.59
1:L:49:THR:HG22	1:L:50:PRO:HD2	1.85	0.59
2:I:117[A]:E13:CAW	2:I:117[A]:E13:C	2.81	0.58
1:B:50:PRO:HB2	3:B:328:HOH:O	2.02	0.58
1:J:43:ALA:H	1:J:97:ASN:ND2	2.02	0.58
1:J:65:ASP:N	1:J:65:ASP:OD1	2.37	0.58
1:D:19[A]:THR:CG2	1:D:45:PHE:CE2	2.87	0.57
1:E:21:THR:CG2	1:E:49:THR:HG21	2.33	0.57
1:I:59:ALA:HA	2:I:117[B]:E13:HAR	1.86	0.57
1:L:49:THR:HG22	1:L:50:PRO:CD	2.34	0.57
1:C:21:THR:HG21	1:C:49:THR:HG21	1.87	0.57
1:E:95:LYS:HE2	3:E:512:HOH:O	2.03	0.57
1:A:97:ASN:ND2	3:A:294:HOH:O	2.35	0.57
1:D:60:GLY:N	3:D:119:HOH:O	2.37	0.57
1:E:115:LEU:HD22	3:F:428:HOH:O	2.05	0.56
1:E:41:PRO:HB3	1:E:97:ASN:HB2	1.86	0.56
1:E:55:SER:OG	1:E:62:GLN:OE1	2.20	0.56
2:I:117[A]:E13:CAS	2:I:117[A]:E13:N	2.68	0.56
1:L:27:ILE:HD12	1:L:99:ALA:CB	2.36	0.56
1:B:53:ASN:ND2	3:B:228:HOH:O	2.38	0.56
1:C:98:TRP:CZ2	2:C:117[A]:E13:CAP	2.88	0.56
1:H:98:TRP:CZ3	2:H:117[B]:E13:CAR	2.87	0.55
1:I:59:ALA:HB3	1:J:58:GLY:HA3	1.89	0.55
1:L:66:HIS:HB3	3:L:288:HOH:O	2.07	0.55
1:H:95:LYS:NZ	3:H:344:HOH:O	2.39	0.55
1:J:64:GLN:HG2	3:J:188:HOH:O	2.06	0.55
1:D:13:ILE:HD11	1:D:80:PHE:HE1	1.72	0.54
1:F:27:ILE:HD12	1:F:99:ALA:CB	2.36	0.54
1:G:96:ASN:OD1	1:G:96:ASN:O	2.26	0.54
1:I:98:TRP:CH2	2:I:117[A]:E13:HAR	2.42	0.54
1:G:96:ASN:O	1:G:97:ASN:HB3	2.07	0.54
1:E:13:ILE:HD11	1:E:80:PHE:HE1	1.72	0.53
1:L:14:LYS:HG2	3:L:474:HOH:O	2.08	0.53
1:A:80:PHE:CE2	1:A:81:ARG:HD2	2.43	0.53
1:K:40:ILE:CD1	1:K:90:CYS:SG	2.97	0.53
1:H:50:PRO:O	1:H:71:SER:OG	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:LEU:HD22	1:F:86:VAL:HG22	1.91	0.52
1:A:75:LEU:HD22	1:A:86:VAL:HG22	1.91	0.52
1:K:27:ILE:HD12	1:K:99:ALA:CB	2.39	0.52
3:G:789:HOH:O	1:J:27:ILE:HG22	2.06	0.52
1:A:58:GLY:HA3	1:B:59:ALA:HB3	1.92	0.52
1:D:19[A]:THR:CG2	1:D:45:PHE:CD2	2.92	0.52
1:I:49:THR:HG22	1:I:50:PRO:HD2	1.91	0.52
1:L:109:CYS:HB2	3:L:388:HOH:O	2.08	0.52
1:A:10:ARG:HD2	3:A:561:HOH:O	2.09	0.51
1:G:49:THR:HG22	3:G:119:HOH:O	2.10	0.51
1:J:75:LEU:HD23	1:J:86:VAL:HG13	1.93	0.51
1:A:87:LEU:HD12	3:A:590:HOH:O	2.09	0.51
2:C:117[B]:E13:CAX	2:C:117[B]:E13:CAS	2.88	0.51
1:K:58:GLY:HA3	1:L:59:ALA:HB3	1.93	0.50
1:L:49:THR:O	3:L:510:HOH:O	2.19	0.50
1:K:74:VAL:HG12	3:K:475:HOH:O	2.10	0.50
1:G:49:THR:HG22	1:G:50:PRO:HD2	1.94	0.50
1:I:41:PRO:HB3	1:I:97:ASN:HB3	1.94	0.50
1:A:68:LYS:HG2	1:A:94:THR:CG2	2.41	0.50
1:E:49:THR:HG22	3:E:122:HOH:O	2.12	0.50
1:H:98:TRP:HZ3	2:H:117[B]:E13:HAR	1.75	0.50
1:L:65:ASP:HB3	1:L:66:HIS:HD2	1.76	0.49
1:J:50:PRO:O	1:J:71:SER:OG	2.30	0.49
1:L:28:GLU:HG3	3:L:474:HOH:O	2.10	0.49
1:H:48:ASN:OD1	1:H:48:ASN:N	2.45	0.49
1:B:55:SER:OG	1:B:64:GLN:NE2	2.45	0.49
1:B:59:ALA:HA	2:B:117:E13:HAR	1.94	0.49
1:H:95:LYS:HD2	3:H:299:HOH:O	2.12	0.49
1:J:27:ILE:HD12	1:J:99:ALA:HB1	1.94	0.49
1:H:27:ILE:HD12	1:H:99:ALA:HB1	1.93	0.49
1:D:7:PRO:HA	3:D:749:HOH:O	2.13	0.49
1:C:106:LEU:O	1:C:109:CYS:HB2	2.12	0.48
1:G:103:ARG:HA	1:G:106:LEU:HB2	1.95	0.48
1:J:41:PRO:HB3	1:J:97:ASN:HB3	1.94	0.48
2:C:117[A]:E13:HB2B	1:D:36:ASP:OD2	2.13	0.48
1:I:49:THR:CG2	3:L:125:HOH:O	2.61	0.48
1:B:43:ALA:H	1:B:97:ASN:ND2	2.11	0.48
2:C:117[A]:E13:OAK	2:C:117[A]:E13:HAX	2.12	0.48
1:G:98:TRP:CH2	2:H:117[A]:E13:HAP	2.48	0.48
1:J:13:ILE:HD11	1:J:80:PHE:HE1	1.79	0.48
1:K:13:ILE:HD11	1:K:80:PHE:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:109:CYS:N	3:K:389:HOH:O	2.46	0.48
1:E:58:GLY:HA3	1:F:59:ALA:HB3	1.95	0.48
1:K:97:ASN:N	3:K:722:HOH:O	2.47	0.48
1:E:66:HIS:CD2	1:E:95:LYS:HE3	2.49	0.48
1:B:27:ILE:HD12	1:B:99:ALA:HB1	1.96	0.47
2:I:117[A]:E13:HAW	1:J:34:GLY:O	2.14	0.47
1:J:77[A]:ARG:HE	1:J:77[A]:ARG:HB2	1.21	0.47
1:K:27:ILE:HD13	1:K:44:LEU:HD11	1.96	0.47
1:J:21:THR:HG21	1:J:49:THR:HG21	1.94	0.47
1:L:46:SER:C	1:L:48:ASN:H	2.17	0.47
1:A:21:THR:HB	1:A:49:THR:HG21	1.96	0.47
1:B:27:ILE:HD12	1:B:99:ALA:CB	2.45	0.47
2:C:117[A]:E13:HAS	2:C:117[A]:E13:CAX	2.44	0.47
1:I:10:ARG:HD2	3:I:163:HOH:O	2.14	0.47
1:I:17:VAL:HA	3:I:786:HOH:O	2.15	0.47
1:B:13:ILE:HD12	1:B:78:LEU:HD22	1.95	0.47
1:E:19:THR:HB	1:E:45:PHE:CE2	2.50	0.47
1:D:21:THR:HG21	1:D:49:THR:HG21	1.97	0.47
1:D:77[B]:ARG:HG3	1:D:77[B]:ARG:NH1	2.29	0.47
1:L:51:LEU:HA	3:L:394:HOH:O	2.15	0.47
1:A:19:THR:HB	1:A:45:PHE:CE1	2.50	0.46
2:C:117[A]:E13:HAY	1:D:57:LEU:HB3	1.98	0.46
1:E:27:ILE:HD13	1:E:44:LEU:HD11	1.96	0.46
1:J:49:THR:HG22	1:J:50:PRO:HD2	1.95	0.46
1:G:77:ARG:NH1	3:G:776:HOH:O	2.38	0.46
1:J:16:GLN:HG3	3:J:680:HOH:O	2.15	0.46
3:H:562:HOH:O	1:K:49:THR:HG23	2.14	0.46
1:C:21:THR:CG2	1:C:49:THR:HG21	2.45	0.46
1:E:3:ILE:HD13	1:E:31:LEU:CD1	2.45	0.46
1:G:21:THR:CG2	1:G:49:THR:HG21	2.44	0.46
1:E:49:THR:HG22	1:E:50:PRO:HD2	1.98	0.46
1:J:27:ILE:HD12	1:J:99:ALA:CB	2.46	0.46
2:C:117[B]:E13:CAT	2:C:117[B]:E13:CAS	2.93	0.46
1:I:98:TRP:CH2	2:I:117[A]:E13:CAR	2.98	0.46
1:G:98:TRP:CH2	2:H:117[A]:E13:CAP	3.00	0.45
1:H:55:SER:OG	1:H:62:GLN:OE1	2.30	0.45
1:E:52:LYS:NZ	3:E:199:HOH:O	2.45	0.45
1:G:20:GLN:O	1:J:25:LYS:HE2	2.16	0.45
1:A:21:THR:CB	1:A:49:THR:HG21	2.47	0.45
1:C:59:ALA:HB3	1:D:58:GLY:HA3	1.99	0.45
3:G:148:HOH:O	1:J:23:HIS:HE1	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57[B]:LEU:HD12	3:C:836:HOH:O	2.17	0.44
2:E:117:E13:CAT	1:F:10:ARG:HD3	2.47	0.44
1:I:49:THR:HG23	3:L:125:HOH:O	2.18	0.44
1:B:56:VAL:CG1	2:B:117:E13:HG1B	2.46	0.44
1:E:59:ALA:HB3	1:F:58:GLY:HA3	2.00	0.44
1:K:38:THR:O	1:K:90:CYS:HB2	2.18	0.44
1:E:5:LEU:HD23	3:E:812:HOH:O	2.18	0.44
1:H:66:HIS:CD2	3:H:464:HOH:O	2.70	0.44
1:H:77:ARG:HE	1:H:77:ARG:HB2	1.49	0.44
2:H:117[B]:E13:OAK	2:H:117[B]:E13:HAX	2.17	0.44
1:I:13:ILE:HD11	1:I:80:PHE:HE1	1.83	0.44
2:I:117[A]:E13:CBK	2:I:117[A]:E13:CAP	2.96	0.44
1:I:19:THR:HB	1:I:45:PHE:CE2	2.53	0.43
1:F:89:SER:HA	3:F:422:HOH:O	2.16	0.43
1:D:68:LYS:HG3	1:D:94:THR:HG21	2.01	0.43
1:A:21:THR:HG21	1:A:49:THR:HG21	1.99	0.43
1:E:40:ILE:HD12	1:E:90:CYS:SG	2.59	0.43
1:E:80:PHE:HE2	3:E:834:HOH:O	2.01	0.43
1:A:20:GLN:O	1:D:25:LYS:HE2	2.18	0.43
1:H:28:GLU:CD	1:K:88:THR:HG21	2.38	0.43
1:A:81:ARG:NH1	3:A:647:HOH:O	2.42	0.43
1:C:39:VAL:HG21	2:C:117[A]:E13:HAC	2.01	0.43
1:G:59:ALA:CB	2:H:117[A]:E13:HG1A	2.48	0.43
1:I:50:PRO:HG2	1:L:43:ALA:HB2	2.00	0.43
1:F:75:LEU:HB2	3:F:501:HOH:O	2.19	0.43
2:C:117[B]:E13:CAX	2:C:117[B]:E13:HAW	2.49	0.42
1:K:5:LEU:HD13	1:L:106:LEU:HD13	2.01	0.42
1:A:68:LYS:HG2	1:A:94:THR:HG21	2.01	0.42
1:E:59:ALA:HA	2:E:117:E13:HAR	2.02	0.42
3:C:682:HOH:O	1:F:14:LYS:HE2	2.19	0.42
1:E:49:THR:CG2	3:E:122:HOH:O	2.68	0.42
1:H:21:THR:HG21	1:H:49:THR:HG21	2.01	0.42
1:B:14:LYS:HG2	3:B:346:HOH:O	2.19	0.42
1:L:13:ILE:HD11	1:L:80:PHE:HE1	1.85	0.41
1:L:59:ALA:HA	2:L:117:E13:HAR	2.02	0.41
1:K:27:ILE:HD12	1:K:99:ALA:HB1	2.01	0.41
1:D:28[A]:GLU:HA	1:D:28[A]:GLU:OE1	2.20	0.41
1:G:65:ASP:OD1	1:G:65:ASP:N	2.53	0.41
1:I:57[A]:LEU:HD11	1:J:98:TRP:CH2	2.55	0.41
1:A:88:THR:HG23	1:D:28[A]:GLU:HG3	2.02	0.41
1:D:95:LYS:NZ	3:D:756:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:96:ASN:HB3	1:L:98:TRP:NE1	2.35	0.41
1:D:43:ALA:HB1	3:D:533:HOH:O	2.19	0.41
1:G:88:THR:HG23	1:J:28[A]:GLU:HG3	2.02	0.41
1:J:38:THR:O	1:J:90:CYS:HB2	2.20	0.41
1:K:59:ALA:HB3	1:L:58:GLY:HA3	2.01	0.41
1:L:38:THR:O	1:L:90:CYS:HB2	2.20	0.41
1:G:49:THR:CG2	3:G:119:HOH:O	2.66	0.41
1:K:80:PHE:CD2	1:K:81:ARG:HG3	2.56	0.41
1:B:38:THR:O	1:B:90:CYS:HB2	2.21	0.41
1:D:77[A]:ARG:HD3	1:D:84:PRO:HB3	2.02	0.41
1:D:77[B]:ARG:HH11	1:D:77[B]:ARG:CG	2.33	0.41
3:G:789:HOH:O	1:J:41:PRO:HG2	2.20	0.41
1:J:23:HIS:HB3	3:J:186:HOH:O	2.21	0.41
1:K:85:ILE:CD1	3:K:389:HOH:O	2.68	0.41
1:G:98:TRP:CZ2	2:H:117[A]:E13:CAP	3.03	0.41
1:J:19[A]:THR:HG22	1:J:21:THR:H	1.86	0.41
1:G:59:ALA:HB3	1:H:58:GLY:HA3	2.03	0.40
1:J:43:ALA:H	1:J:97:ASN:HD21	1.70	0.40
1:J:75:LEU:CD2	1:J:86:VAL:HG13	2.51	0.40
1:D:77[A]:ARG:HE	1:D:77[A]:ARG:HB2	1.34	0.40
1:I:41:PRO:HB3	1:I:97:ASN:CB	2.50	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:535:HOH:O	3:E:237:HOH:O[1_545]	2.13	0.07

## 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	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
1	B	114/116 (98%)	112 (98%)	1 (1%)	1 (1%)	17	8
1	C	117/116 (101%)	116 (99%)	1 (1%)	0	100	100
1	D	117/116 (101%)	117 (100%)	0	0	100	100
1	E	114/116 (98%)	112 (98%)	1 (1%)	1 (1%)	17	8
1	F	114/116 (98%)	111 (97%)	2 (2%)	1 (1%)	17	8
1	G	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
1	H	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
1	I	117/116 (101%)	115 (98%)	2 (2%)	0	100	100
1	J	117/116 (101%)	116 (99%)	1 (1%)	0	100	100
1	K	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
1	L	114/116 (98%)	110 (96%)	3 (3%)	1 (1%)	17	8
All	All	1380/1392 (99%)	1358 (98%)	18 (1%)	4 (0%)	41	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	47	SER
1	E	97	ASN
1	F	47	SER
1	B	50	PRO

### 5.3.2 Protein sidechains [i](#)

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	102/102 (100%)	95 (93%)	7 (7%)	15	5
1	B	102/102 (100%)	94 (92%)	8 (8%)	12	3
1	C	105/102 (103%)	99 (94%)	6 (6%)	20	9
1	D	105/102 (103%)	97 (92%)	8 (8%)	13	4
1	E	102/102 (100%)	98 (96%)	4 (4%)	32	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	102/102 (100%)	96 (94%)	6 (6%)	19	8
1	G	102/102 (100%)	94 (92%)	8 (8%)	12	3
1	H	102/102 (100%)	93 (91%)	9 (9%)	10	2
1	I	105/102 (103%)	101 (96%)	4 (4%)	33	21
1	J	105/102 (103%)	96 (91%)	9 (9%)	10	3
1	K	102/102 (100%)	96 (94%)	6 (6%)	19	8
1	L	102/102 (100%)	94 (92%)	8 (8%)	12	3
All	All	1236/1224 (101%)	1153 (93%)	83 (7%)	17	5

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	62	GLN
1	A	66	HIS
1	A	78	LEU
1	A	88	THR
1	A	89	SER
1	A	106	LEU
1	B	13	ILE
1	B	14	LYS
1	B	37	MET
1	B	48	ASN
1	B	49	THR
1	B	57	LEU
1	B	71	SER
1	B	77	ARG
1	C	49	THR
1	C	64	GLN
1	C	73	PRO
1	C	82	THR
1	C	96	ASN
1	C	97	ASN
1	D	19[A]	THR
1	D	19[B]	THR
1	D	28[A]	GLU
1	D	28[B]	GLU
1	D	31	LEU
1	D	69	LEU
1	D	77[A]	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	77[B]	ARG
1	E	23	HIS
1	E	49	THR
1	E	57	LEU
1	E	62	GLN
1	F	48	ASN
1	F	71	SER
1	F	72	LEU
1	F	81	ARG
1	F	95	LYS
1	F	109	CYS
1	G	22	SER
1	G	49	THR
1	G	57	LEU
1	G	65	ASP
1	G	78	LEU
1	G	82	THR
1	G	106	LEU
1	G	109	CYS
1	H	14	LYS
1	H	47	SER
1	H	48	ASN
1	H	71	SER
1	H	77	ARG
1	H	83	THR
1	H	89	SER
1	H	95	LYS
1	H	109	CYS
1	I	9	ARG
1	I	49	THR
1	I	69	LEU
1	I	97	ASN
1	J	19[A]	THR
1	J	19[B]	THR
1	J	31	LEU
1	J	48	ASN
1	J	49	THR
1	J	64	GLN
1	J	77[A]	ARG
1	J	77[B]	ARG
1	J	82	THR
1	K	49	THR

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Mol	Chain	Res	Type
1	K	54	THR
1	K	57	LEU
1	K	88	THR
1	K	97	ASN
1	K	113	LEU
1	L	47	SER
1	L	49	THR
1	L	55	SER
1	L	56	VAL
1	L	64	GLN
1	L	77	ARG
1	L	82	THR
1	L	83	THR

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

Mol	Chain	Res	Type
1	B	64	GLN
1	B	97	ASN
1	D	62	GLN
1	D	64	GLN
1	F	64	GLN
1	I	62	GLN
1	I	66	HIS
1	I	97	ASN
1	J	23	HIS
1	J	96	ASN
1	J	97	ASN
1	L	23	HIS
1	L	64	GLN
1	L	66	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 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	E13	H	117[A]	-	52,52,52	5.10	26 (50%)	71,76,76	1.99	13 (18%)
2	E13	E	117	-	52,52,52	5.08	28 (53%)	71,76,76	2.11	19 (26%)
2	E13	I	117[B]	-	52,52,52	5.05	26 (50%)	71,76,76	2.29	15 (21%)
2	E13	L	117	-	52,52,52	5.17	26 (50%)	71,76,76	1.75	15 (21%)
2	E13	I	117[A]	-	52,52,52	5.18	26 (50%)	71,76,76	2.44	13 (18%)
2	E13	C	117[B]	-	52,52,52	5.08	25 (48%)	71,76,76	1.98	15 (21%)
2	E13	C	117[A]	-	52,52,52	5.02	24 (46%)	71,76,76	2.16	17 (23%)
2	E13	B	117	-	52,52,52	5.12	26 (50%)	71,76,76	1.84	15 (21%)
2	E13	H	117[B]	-	52,52,52	5.08	25 (48%)	71,76,76	2.13	18 (25%)

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	E13	H	117[A]	-	-	10/58/74/74	0/3/3/3
2	E13	E	117	-	-	11/58/74/74	0/3/3/3
2	E13	I	117[B]	-	-	13/58/74/74	0/3/3/3
2	E13	L	117	-	-	10/58/74/74	0/3/3/3
2	E13	I	117[A]	-	-	11/58/74/74	0/3/3/3
2	E13	C	117[B]	-	-	9/58/74/74	0/3/3/3
2	E13	C	117[A]	-	-	8/58/74/74	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	E13	B	117	-	-	10/58/74/74	0/3/3/3
2	E13	H	117[B]	-	-	16/58/74/74	0/3/3/3

All (232) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	117	E13	CBQ-NBR	15.52	1.60	1.46
2	I	117[A]	E13	CBQ-NBR	14.20	1.58	1.46
2	C	117[A]	E13	CBQ-NBR	13.54	1.58	1.46
2	H	117[A]	E13	CBQ-NBR	13.49	1.58	1.46
2	B	117	E13	CBQ-NBR	13.40	1.58	1.46
2	I	117[B]	E13	CBQ-NBR	13.17	1.58	1.46
2	H	117[B]	E13	CBQ-NBR	12.90	1.57	1.46
2	E	117	E13	CBQ-NBR	12.58	1.57	1.46
2	H	117[B]	E13	OA1-CB1	12.14	1.44	1.21
2	L	117	E13	OA1-CB1	12.13	1.44	1.21
2	C	117[B]	E13	CBQ-NBR	12.00	1.57	1.46
2	B	117	E13	OA1-CB1	11.99	1.43	1.21
2	I	117[A]	E13	OA1-CB1	11.99	1.43	1.21
2	C	117[A]	E13	OA1-CB1	11.95	1.43	1.21
2	C	117[B]	E13	OA1-CB1	11.86	1.43	1.21
2	E	117	E13	OA1-CB1	11.78	1.43	1.21
2	H	117[A]	E13	OA1-CB1	11.74	1.43	1.21
2	I	117[B]	E13	OA1-CB1	11.26	1.42	1.21
2	C	117[B]	E13	CAY-CBK	10.85	1.56	1.39
2	B	117	E13	OA2-CB1	10.75	1.53	1.34
2	I	117[A]	E13	OA2-CB1	10.57	1.52	1.34
2	L	117	E13	OA2-CB1	10.53	1.52	1.34
2	E	117	E13	OA2-CB1	10.53	1.52	1.34
2	H	117[B]	E13	OA2-CB1	10.42	1.52	1.34
2	I	117[B]	E13	OA2-CB1	10.36	1.52	1.34
2	C	117[B]	E13	OA2-CB1	10.31	1.52	1.34
2	C	117[A]	E13	OA2-CB1	10.22	1.52	1.34
2	L	117	E13	CAY-CBK	10.22	1.55	1.39
2	B	117	E13	CAX-CBK	10.21	1.55	1.39
2	I	117[A]	E13	CAY-CBK	10.14	1.55	1.39
2	H	117[B]	E13	CAY-CBK	10.14	1.55	1.39
2	H	117[A]	E13	CAY-CBK	10.13	1.55	1.39
2	H	117[A]	E13	CAX-CBK	10.13	1.55	1.39
2	H	117[A]	E13	OA2-CB1	10.05	1.51	1.34
2	E	117	E13	CAY-CBK	9.97	1.55	1.39
2	L	117	E13	CAX-CBK	9.87	1.55	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	117[A]	E13	CAX-CBK	9.77	1.54	1.39
2	I	117[B]	E13	CAY-CBK	9.73	1.54	1.39
2	C	117[A]	E13	CAX-CBK	9.73	1.54	1.39
2	H	117[B]	E13	CAX-CBK	9.69	1.54	1.39
2	I	117[B]	E13	CAX-CBK	9.69	1.54	1.39
2	C	117[B]	E13	CAX-CBK	9.64	1.54	1.39
2	B	117	E13	CAY-CBK	9.63	1.54	1.39
2	E	117	E13	CAX-CBK	9.50	1.54	1.39
2	C	117[A]	E13	CAY-CBK	9.50	1.54	1.39
2	I	117[B]	E13	CAV-CBJ	7.77	1.55	1.38
2	E	117	E13	CAT-CAX	7.72	1.55	1.38
2	C	117[B]	E13	CAV-CBJ	7.69	1.55	1.38
2	H	117[B]	E13	CAV-CBJ	7.69	1.55	1.38
2	B	117	E13	CAT-CAX	7.67	1.55	1.38
2	I	117[B]	E13	CAT-CAX	7.66	1.55	1.38
2	H	117[B]	E13	CAT-CAX	7.65	1.55	1.38
2	I	117[A]	E13	CAT-CAX	7.65	1.55	1.38
2	B	117	E13	CAU-CAY	7.64	1.55	1.38
2	H	117[A]	E13	CAT-CAX	7.57	1.54	1.38
2	I	117[A]	E13	CAS-CAW	7.56	1.54	1.38
2	I	117[B]	E13	CAR-CAV	7.56	1.54	1.38
2	H	117[A]	E13	CAU-CAY	7.54	1.54	1.38
2	L	117	E13	CAU-CAY	7.53	1.54	1.38
2	I	117[B]	E13	CAS-CAW	7.50	1.54	1.38
2	C	117[B]	E13	CAW-CBJ	7.46	1.54	1.38
2	H	117[B]	E13	CAU-CAY	7.46	1.54	1.38
2	I	117[A]	E13	CAU-CAY	7.45	1.54	1.38
2	C	117[B]	E13	CAT-CAX	7.44	1.54	1.38
2	L	117	E13	CAS-CAW	7.43	1.54	1.38
2	I	117[A]	E13	CAW-CBJ	7.42	1.54	1.38
2	E	117	E13	CAR-CAV	7.41	1.54	1.38
2	B	117	E13	CAS-CAW	7.39	1.54	1.38
2	C	117[A]	E13	CAU-CAY	7.37	1.54	1.38
2	E	117	E13	CAW-CBJ	7.37	1.54	1.38
2	C	117[B]	E13	CAS-CAW	7.36	1.54	1.38
2	E	117	E13	CAU-CAY	7.34	1.54	1.38
2	E	117	E13	CAS-CAW	7.33	1.54	1.38
2	I	117[B]	E13	CAW-CBJ	7.33	1.54	1.38
2	H	117[B]	E13	CAS-CAW	7.28	1.54	1.38
2	C	117[A]	E13	CAT-CAX	7.28	1.54	1.38
2	H	117[A]	E13	CAV-CBJ	7.25	1.54	1.38
2	H	117[A]	E13	CAW-CBJ	7.24	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	117[B]	E13	CAU-CAY	7.23	1.54	1.38
2	B	117	E13	CAR-CAV	7.20	1.54	1.38
2	C	117[B]	E13	CAR-CAV	7.19	1.54	1.38
2	C	117[B]	E13	CAU-CAY	7.18	1.54	1.38
2	C	117[A]	E13	CAW-CBJ	7.18	1.54	1.38
2	H	117[B]	E13	CAW-CBJ	7.13	1.54	1.38
2	I	117[A]	E13	CAV-CBJ	7.13	1.54	1.38
2	C	117[A]	E13	CAV-CBJ	7.13	1.54	1.38
2	L	117	E13	CAT-CAX	7.13	1.53	1.38
2	H	117[B]	E13	CAR-CAV	7.08	1.53	1.38
2	I	117[A]	E13	CAR-CAV	7.04	1.53	1.38
2	H	117[A]	E13	CAR-CAV	7.00	1.53	1.38
2	L	117	E13	CAR-CAV	6.99	1.53	1.38
2	H	117[A]	E13	CAS-CAW	6.99	1.53	1.38
2	B	117	E13	CAW-CBJ	6.94	1.53	1.38
2	C	117[A]	E13	CAS-CAW	6.93	1.53	1.38
2	C	117[A]	E13	CAR-CAV	6.83	1.53	1.38
2	H	117[A]	E13	CAT-CAQ	6.71	1.55	1.38
2	I	117[A]	E13	CAU-CAQ	6.63	1.55	1.38
2	L	117	E13	CAW-CBJ	6.63	1.53	1.38
2	B	117	E13	CAT-CAQ	6.59	1.55	1.38
2	B	117	E13	CAV-CBJ	6.57	1.53	1.38
2	I	117[A]	E13	CAR-CAP	6.52	1.55	1.38
2	C	117[B]	E13	CAT-CAQ	6.51	1.55	1.38
2	C	117[B]	E13	CAU-CAQ	6.51	1.55	1.38
2	C	117[A]	E13	CAT-CAQ	6.49	1.55	1.38
2	H	117[A]	E13	CAU-CAQ	6.48	1.55	1.38
2	C	117[B]	E13	CAR-CAP	6.47	1.55	1.38
2	B	117	E13	CAU-CAQ	6.47	1.55	1.38
2	E	117	E13	CAS-CAP	6.47	1.55	1.38
2	E	117	E13	CAV-CBJ	6.46	1.52	1.38
2	L	117	E13	CAT-CAQ	6.44	1.55	1.38
2	C	117[A]	E13	CAU-CAQ	6.38	1.54	1.38
2	L	117	E13	CAU-CAQ	6.37	1.54	1.38
2	H	117[B]	E13	CAR-CAP	6.36	1.54	1.38
2	E	117	E13	CAR-CAP	6.34	1.54	1.38
2	I	117[A]	E13	CAS-CAP	6.33	1.54	1.38
2	H	117[B]	E13	CAT-CAQ	6.33	1.54	1.38
2	I	117[B]	E13	CAT-CAQ	6.30	1.54	1.38
2	H	117[B]	E13	CAS-CAP	6.29	1.54	1.38
2	C	117[B]	E13	CAS-CAP	6.28	1.54	1.38
2	B	117	E13	CAR-CAP	6.27	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	117[B]	E13	CAS-CAP	6.27	1.54	1.38
2	E	117	E13	CAT-CAQ	6.27	1.54	1.38
2	I	117[B]	E13	CAR-CAP	6.26	1.54	1.38
2	C	117[A]	E13	CAS-CAP	6.26	1.54	1.38
2	H	117[B]	E13	CAU-CAQ	6.25	1.54	1.38
2	I	117[B]	E13	CAU-CAQ	6.24	1.54	1.38
2	L	117	E13	CAV-CBJ	6.23	1.52	1.38
2	H	117[A]	E13	CAS-CAP	6.21	1.54	1.38
2	H	117[B]	E13	CBH-NBB	6.20	1.47	1.33
2	I	117[A]	E13	CAT-CAQ	6.20	1.54	1.38
2	E	117	E13	CAU-CAQ	6.19	1.54	1.38
2	H	117[A]	E13	CAR-CAP	6.19	1.54	1.38
2	B	117	E13	CAS-CAP	6.18	1.54	1.38
2	L	117	E13	CAR-CAP	6.11	1.54	1.38
2	H	117[A]	E13	CBH-NBB	6.08	1.46	1.33
2	C	117[A]	E13	CAR-CAP	6.07	1.54	1.38
2	E	117	E13	CBH-NBB	6.06	1.46	1.33
2	L	117	E13	CAS-CAP	6.02	1.54	1.38
2	C	117[A]	E13	CBH-NBB	5.98	1.46	1.33
2	I	117[B]	E13	CAZ-SBE	-5.91	1.69	1.83
2	L	117	E13	CAZ-SBE	-5.90	1.69	1.83
2	B	117	E13	CBH-NBB	5.87	1.46	1.33
2	C	117[B]	E13	CBH-NBB	5.86	1.46	1.33
2	I	117[A]	E13	CBH-NBB	5.80	1.46	1.33
2	E	117	E13	CBF-N	5.77	1.46	1.34
2	H	117[A]	E13	CBF-N	5.76	1.46	1.34
2	C	117[A]	E13	CAZ-SBE	-5.76	1.69	1.83
2	B	117	E13	CAZ-SBE	-5.73	1.69	1.83
2	I	117[A]	E13	CAZ-SBE	-5.69	1.69	1.83
2	I	117[B]	E13	CBH-NBB	5.65	1.46	1.33
2	H	117[A]	E13	CAZ-SBE	-5.65	1.69	1.83
2	L	117	E13	CBF-N	5.55	1.46	1.34
2	H	117[B]	E13	CAZ-SBE	-5.53	1.69	1.83
2	C	117[B]	E13	CAZ-SBE	-5.52	1.69	1.83
2	B	117	E13	CBF-N	5.49	1.46	1.34
2	C	117[A]	E13	CBF-N	5.46	1.46	1.34
2	C	117[A]	E13	C-NBC	5.42	1.46	1.34
2	H	117[B]	E13	CBF-N	5.36	1.45	1.34
2	B	117	E13	CB1-NAJ	5.35	1.47	1.34
2	I	117[A]	E13	CBF-N	5.32	1.45	1.34
2	E	117	E13	CB1-NAJ	5.31	1.47	1.34
2	E	117	E13	CAZ-SBE	-5.28	1.70	1.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	117[B]	E13	C-NBC	5.24	1.45	1.34
2	I	117[A]	E13	CBI-NBR	5.23	1.46	1.34
2	L	117	E13	CBH-NBB	5.23	1.45	1.33
2	H	117[A]	E13	C-NBC	5.21	1.45	1.34
2	C	117[B]	E13	CBF-N	5.21	1.45	1.34
2	I	117[B]	E13	CBI-NAJ	5.14	1.47	1.34
2	I	117[A]	E13	C-NBC	5.14	1.45	1.34
2	I	117[B]	E13	C-NBC	5.05	1.45	1.34
2	L	117	E13	CBI-NAJ	5.04	1.47	1.34
2	C	117[B]	E13	CBI-NBR	5.03	1.46	1.34
2	E	117	E13	C-NBC	5.02	1.45	1.34
2	C	117[A]	E13	CBI-NBR	5.02	1.46	1.34
2	H	117[A]	E13	CBI-NBR	5.00	1.46	1.34
2	I	117[A]	E13	CBI-NAJ	4.96	1.46	1.34
2	H	117[B]	E13	CBI-NAJ	4.96	1.46	1.34
2	C	117[B]	E13	C-NBC	4.92	1.44	1.34
2	I	117[B]	E13	CBI-NBR	4.79	1.45	1.34
2	L	117	E13	C-NBC	4.79	1.44	1.34
2	C	117[B]	E13	CBI-NAJ	4.78	1.46	1.34
2	H	117[B]	E13	CBI-NBR	4.78	1.45	1.34
2	B	117	E13	C-NBC	4.75	1.44	1.34
2	I	117[B]	E13	CBF-N	4.72	1.44	1.34
2	E	117	E13	CBI-NBR	4.69	1.45	1.34
2	E	117	E13	CAZ-NBR	4.65	1.54	1.46
2	H	117[B]	E13	CAZ-NBR	4.64	1.54	1.46
2	B	117	E13	CBI-NBR	4.57	1.45	1.34
2	H	117[A]	E13	CBI-NAJ	4.52	1.45	1.34
2	C	117[B]	E13	CAZ-NBR	4.48	1.54	1.46
2	C	117[A]	E13	CBI-NAJ	4.42	1.45	1.34
2	C	117[A]	E13	CAZ-NBR	4.23	1.53	1.46
2	E	117	E13	CBU-SBE	-4.23	1.76	1.85
2	H	117[A]	E13	CAZ-NBR	4.17	1.53	1.46
2	C	117[B]	E13	CBU-SBE	-4.16	1.76	1.85
2	L	117	E13	CAZ-NBR	4.15	1.53	1.46
2	B	117	E13	CAZ-NBR	4.14	1.53	1.46
2	I	117[A]	E13	CAZ-NBR	4.09	1.53	1.46
2	H	117[A]	E13	CBU-SBE	-4.05	1.77	1.85
2	I	117[B]	E13	CAZ-NBR	4.04	1.53	1.46
2	I	117[A]	E13	CBU-SBE	-4.01	1.77	1.85
2	B	117	E13	CBU-SBE	-3.97	1.77	1.85
2	I	117[B]	E13	CBU-SBE	-3.96	1.77	1.85
2	C	117[A]	E13	CBU-SBE	-3.91	1.77	1.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	117	E13	CBI-NBR	3.83	1.43	1.34
2	B	117	E13	OA2-CB2	3.67	1.53	1.45
2	L	117	E13	CBU-SBE	-3.62	1.77	1.85
2	E	117	E13	OA2-CB2	3.57	1.53	1.45
2	C	117[B]	E13	OA2-CB2	3.42	1.53	1.45
2	I	117[A]	E13	OA2-CB2	3.40	1.53	1.45
2	L	117	E13	OA2-CB2	3.40	1.53	1.45
2	C	117[B]	E13	OAN-CBI	-3.35	1.16	1.22
2	I	117[B]	E13	OA2-CB2	3.32	1.53	1.45
2	H	117[B]	E13	OA2-CB2	3.32	1.53	1.45
2	H	117[A]	E13	OA2-CB2	3.23	1.52	1.45
2	H	117[B]	E13	CBU-SBE	-3.14	1.78	1.85
2	C	117[A]	E13	OA2-CB2	3.13	1.52	1.45
2	L	117	E13	O-C	-2.74	1.17	1.23
2	I	117[A]	E13	OAN-CBI	-2.65	1.17	1.22
2	H	117[A]	E13	OAN-CBI	-2.53	1.17	1.22
2	E	117	E13	O-C	-2.42	1.18	1.23
2	E	117	E13	OAN-CBI	-2.37	1.18	1.22
2	B	117	E13	CBK-CBM	2.32	1.56	1.52
2	I	117[A]	E13	OAM-CBH	-2.29	1.18	1.23
2	L	117	E13	OAN-CBI	-2.27	1.18	1.22
2	I	117[B]	E13	O-C	-2.24	1.18	1.23
2	I	117[B]	E13	OAN-CBI	-2.13	1.18	1.22
2	E	117	E13	CBK-CBM	2.13	1.56	1.52
2	H	117[A]	E13	OAM-CBH	-2.10	1.19	1.23
2	E	117	E13	CA-N	-2.05	1.42	1.45
2	H	117[B]	E13	OAN-CBI	-2.02	1.18	1.22
2	B	117	E13	OAN-CBI	-2.01	1.18	1.22

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	117[A]	E13	CBJ-CBA-CBO	-12.23	92.10	113.33
2	I	117[B]	E13	CBM-NAJ-CB1	-10.25	103.93	120.99
2	C	117[B]	E13	CBM-NAJ-CB1	-9.16	105.75	120.99
2	C	117[A]	E13	CBM-NAJ-CB1	-9.01	105.99	120.99
2	I	117[A]	E13	CBM-NAJ-CB1	-8.43	106.96	120.99
2	H	117[B]	E13	CBM-NAJ-CB1	-8.33	107.12	120.99
2	H	117[A]	E13	CBM-NAJ-CB1	-6.87	109.56	120.99
2	I	117[B]	E13	CBN-CBO-NBC	-6.83	97.17	110.03
2	E	117	E13	CBA-CBO-NBC	6.51	119.57	110.07
2	I	117[A]	E13	CBN-CBO-NBC	-6.46	97.88	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	117[A]	E13	CB2-OA2-CB1	-6.33	108.19	115.66
2	I	117[B]	E13	OA2-CB1-NAJ	5.98	121.29	110.80
2	C	117[A]	E13	CBJ-CBA-CBO	-5.81	103.25	113.33
2	B	117	E13	OA2-CB1-NAJ	5.75	120.89	110.80
2	E	117	E13	CBM-NAJ-CB1	-5.74	111.43	120.99
2	H	117[B]	E13	CB2-OA2-CB1	-5.64	109.01	115.66
2	E	117	E13	OA2-CB1-NAJ	5.51	120.48	110.80
2	C	117[A]	E13	CB2-OA2-CB1	-5.45	109.23	115.66
2	I	117[B]	E13	CB2-OA2-CB1	-5.35	109.35	115.66
2	L	117	E13	CB2-OA2-CB1	-5.27	109.44	115.66
2	I	117[B]	E13	CBK-CBM-NAJ	-5.19	99.42	112.89
2	I	117[A]	E13	OA2-CB1-NAJ	5.18	119.89	110.80
2	B	117	E13	CBJ-CBA-CBO	-5.12	104.44	113.33
2	L	117	E13	OA2-CB1-NAJ	5.03	119.64	110.80
2	B	117	E13	CBM-NAJ-CB1	-5.02	112.64	120.99
2	H	117[A]	E13	OA2-CB1-NAJ	5.00	119.58	110.80
2	E	117	E13	CBL-NBB-CBH	-4.99	114.91	122.79
2	H	117[A]	E13	CBJ-CBA-CBO	-4.93	104.77	113.33
2	C	117[B]	E13	CBN-CBO-NBC	-4.93	100.76	110.03
2	B	117	E13	CB2-OA2-CB1	-4.90	109.87	115.66
2	C	117[B]	E13	OA2-CB1-NAJ	4.83	119.28	110.80
2	E	117	E13	CBN-CBO-NBC	-4.78	101.03	110.03
2	H	117[A]	E13	CBN-CBO-NBC	-4.78	101.03	110.03
2	L	117	E13	CBN-CBO-NBC	-4.76	101.08	110.03
2	H	117[B]	E13	CBN-CBO-NBC	-4.72	101.16	110.03
2	H	117[B]	E13	OA2-CB1-NAJ	4.66	118.98	110.80
2	C	117[B]	E13	CBJ-CBA-CBO	-4.57	105.39	113.33
2	I	117[B]	E13	CB-CA-C	-4.52	108.56	112.81
2	L	117	E13	CBJ-CBA-CBO	-4.47	105.58	113.33
2	H	117[B]	E13	CB-CA-N	-4.44	106.28	111.84
2	C	117[A]	E13	CBK-CBM-NAJ	-4.44	101.38	112.89
2	H	117[B]	E13	CBJ-CBA-CBO	-4.43	105.64	113.33
2	B	117	E13	CBN-CBO-NBC	-4.31	101.92	110.03
2	C	117[A]	E13	OA2-CB1-NAJ	4.20	118.17	110.80
2	I	117[A]	E13	CB-CA-N	-4.18	106.61	111.84
2	C	117[A]	E13	CB-CA-N	-4.17	106.62	111.84
2	I	117[B]	E13	OA2-CB1-OA1	-3.94	118.79	124.58
2	C	117[A]	E13	CBN-CBO-NBC	-3.77	102.94	110.03
2	B	117	E13	OA2-CB1-OA1	-3.75	119.07	124.58
2	E	117	E13	OA2-CB1-OA1	-3.73	119.10	124.58
2	E	117	E13	CB2-OA2-CB1	-3.65	111.35	115.66
2	C	117[B]	E13	CBK-CBM-NAJ	-3.65	103.43	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	117[A]	E13	CBL-NBB-CBH	-3.62	117.07	122.79
2	H	117[A]	E13	CBS-CBL-NBB	-3.56	108.31	113.90
2	H	117[A]	E13	CB-CA-N	-3.53	107.41	111.84
2	I	117[B]	E13	CB-CA-N	-3.42	107.55	111.84
2	C	117[B]	E13	CB-CA-C	-3.42	109.59	112.81
2	L	117	E13	CBL-NBB-CBH	-3.41	117.40	122.79
2	I	117[A]	E13	CBQ-CBH-NBB	3.40	121.11	115.28
2	L	117	E13	OA2-CB1-OA1	-3.37	119.62	124.58
2	C	117[A]	E13	CBS-CBL-NBB	-3.26	108.78	113.90
2	L	117	E13	CBQ-CBH-NBB	3.24	120.84	115.28
2	H	117[B]	E13	CBL-NBB-CBH	-3.19	117.75	122.79
2	H	117[B]	E13	OA2-CB1-OA1	-3.18	119.90	124.58
2	C	117[B]	E13	CB2-OA2-CB1	-3.17	111.92	115.66
2	I	117[A]	E13	CB2-OA2-CB1	-3.12	111.98	115.66
2	H	117[B]	E13	CBA-CBO-NBC	3.12	114.61	110.07
2	H	117[B]	E13	CA-N-CBF	-3.11	115.62	122.05
2	I	117[A]	E13	OA2-CB1-OA1	-3.10	120.03	124.58
2	E	117	E13	CB-CA-C	3.09	115.70	112.81
2	L	117	E13	CBS-CBL-NBB	-3.08	109.06	113.90
2	E	117	E13	CBS-CBL-NBB	-3.03	109.15	113.90
2	I	117[B]	E13	OA1-CB1-NAJ	-3.01	119.92	124.85
2	L	117	E13	O-C-CA	3.01	125.79	120.89
2	B	117	E13	OA1-CB1-NAJ	-2.94	120.04	124.85
2	C	117[A]	E13	CAW-CBJ-CAV	2.92	122.75	118.17
2	H	117[B]	E13	CBK-CBM-NAJ	-2.92	105.32	112.89
2	I	117[A]	E13	OA1-CB1-NAJ	-2.91	120.08	124.85
2	H	117[A]	E13	OA2-CB1-OA1	-2.91	120.30	124.58
2	H	117[A]	E13	OA1-CB1-NAJ	-2.89	120.11	124.85
2	E	117	E13	CBA-CBO-CBN	2.89	119.21	111.38
2	H	117[B]	E13	OAO-CBN-CBI	2.88	112.90	108.54
2	I	117[B]	E13	OAO-CBN-CBI	2.88	112.89	108.54
2	C	117[B]	E13	OA2-CB1-OA1	-2.85	120.39	124.58
2	B	117	E13	CBL-NBB-CBH	-2.82	118.34	122.79
2	C	117[A]	E13	OA1-CB1-NAJ	-2.81	120.25	124.85
2	H	117[B]	E13	CAH-CBU-SBE	2.78	113.88	109.22
2	I	117[B]	E13	CBQ-CBH-NBB	2.77	120.03	115.28
2	C	117[B]	E13	OA1-CB1-NAJ	-2.75	120.33	124.85
2	I	117[B]	E13	OAK-CBF-CBM	2.75	125.41	120.64
2	E	117	E13	CAW-CBJ-CAV	2.70	122.42	118.17
2	H	117[B]	E13	CBS-CBL-NBB	-2.70	109.66	113.90
2	E	117	E13	OA1-CB1-NAJ	-2.70	120.42	124.85
2	H	117[A]	E13	OAO-CBN-CBI	2.69	112.60	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	117[A]	E13	CB-CA-C	-2.64	110.33	112.81
2	H	117[A]	E13	CAW-CBJ-CAV	2.63	122.30	118.17
2	E	117	E13	OAO-CBN-CBI	2.62	112.51	108.54
2	C	117[A]	E13	CA-N-CBF	-2.60	116.68	122.05
2	C	117[B]	E13	CA-N-CBF	-2.60	116.68	122.05
2	E	117	E13	O-C-CA	2.59	125.11	120.89
2	C	117[A]	E13	CAR-CAV-CBJ	-2.56	116.71	120.63
2	I	117[A]	E13	CBK-CBM-NAJ	-2.51	106.37	112.89
2	B	117	E13	OAO-CBN-CBO	2.51	115.65	108.54
2	L	117	E13	OA1-CB1-NAJ	-2.51	120.74	124.85
2	B	117	E13	CA-N-CBF	-2.50	116.89	122.05
2	B	117	E13	O-C-CA	2.49	124.95	120.89
2	H	117[B]	E13	CAW-CBJ-CAV	2.49	122.08	118.17
2	C	117[A]	E13	CBA-CBO-NBC	2.44	113.63	110.07
2	B	117	E13	CBK-CBM-NAJ	-2.41	106.63	112.89
2	C	117[B]	E13	CAY-CBK-CAX	2.38	121.27	118.29
2	B	117	E13	CBA-CBO-CBN	2.38	117.83	111.38
2	H	117[B]	E13	CBQ-CBH-NBB	2.36	119.32	115.28
2	C	117[B]	E13	CBO-NBC-C	-2.32	118.97	123.07
2	E	117	E13	SBE-CAZ-NBR	2.32	108.56	105.37
2	I	117[B]	E13	OAK-CBF-N	-2.30	118.68	122.93
2	E	117	E13	CAI-CBU-CAH	-2.28	107.06	110.78
2	L	117	E13	CA-C-NBC	-2.28	112.16	116.26
2	H	117[B]	E13	OA1-CB1-NAJ	-2.28	121.11	124.85
2	C	117[B]	E13	CBS-CBL-NBB	-2.28	110.33	113.90
2	C	117[B]	E13	CB-CA-N	-2.27	108.99	111.84
2	H	117[A]	E13	CA-N-CBF	-2.25	117.39	122.05
2	C	117[B]	E13	CAI-CBU-CBQ	-2.22	106.64	111.57
2	C	117[A]	E13	CAP-CAS-CAW	-2.22	116.81	120.19
2	E	117	E13	CA-C-NBC	-2.20	112.32	116.26
2	I	117[A]	E13	O-C-CA	2.17	124.43	120.89
2	E	117	E13	CG2-CB-CAG	-2.16	104.61	108.80
2	L	117	E13	CAD-CBS-CBL	-2.15	103.08	109.42
2	I	117[A]	E13	CAW-CBJ-CAV	2.13	121.52	118.17
2	E	117	E13	CB-CA-N	-2.13	109.17	111.84
2	I	117[B]	E13	CA-N-CBF	-2.10	117.70	122.05
2	H	117[B]	E13	CAI-CBU-SBE	2.10	112.73	109.22
2	L	117	E13	OAM-CBH-NBB	-2.10	118.49	122.99
2	B	117	E13	CBF-CBM-NAJ	2.09	114.84	108.44
2	B	117	E13	CA-C-NBC	-2.08	112.53	116.26
2	I	117[B]	E13	CBJ-CBA-CBO	-2.06	109.75	113.33
2	H	117[A]	E13	CBQ-CBH-NBB	2.05	118.81	115.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	117	E13	OAN-CBI-CBN	2.04	123.19	119.12
2	C	117[A]	E13	OA2-CB1-OA1	-2.04	121.58	124.58
2	L	117	E13	CBK-CBM-NAJ	-2.03	107.62	112.89
2	C	117[A]	E13	CBO-NBC-C	-2.01	119.52	123.07

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	117	E13	OA1-CB1-OA2-CB2
2	B	117	E13	NAJ-CB1-OA2-CB2
2	B	117	E13	O-C-CA-CB
2	B	117	E13	NBC-C-CA-CB
2	C	117[A]	E13	OA1-CB1-OA2-CB2
2	C	117[A]	E13	NAJ-CB1-OA2-CB2
2	C	117[A]	E13	NBC-C-CA-CB
2	E	117	E13	OA1-CB1-OA2-CB2
2	E	117	E13	NAJ-CB1-OA2-CB2
2	E	117	E13	O-C-CA-CB
2	E	117	E13	NBC-C-CA-CB
2	H	117[A]	E13	OA1-CB1-OA2-CB2
2	H	117[A]	E13	NAJ-CB1-OA2-CB2
2	H	117[A]	E13	O-C-CA-CB
2	H	117[A]	E13	NBC-C-CA-CB
2	H	117[B]	E13	OA1-CB1-OA2-CB2
2	H	117[B]	E13	NAJ-CB1-OA2-CB2
2	I	117[A]	E13	OA1-CB1-OA2-CB2
2	I	117[A]	E13	NAJ-CB1-OA2-CB2
2	I	117[A]	E13	NBC-C-CA-CB
2	I	117[A]	E13	OA1-CB1-OA2-CB2
2	I	117[B]	E13	OA1-CB1-OA2-CB2
2	I	117[B]	E13	NAJ-CB1-OA2-CB2
2	L	117	E13	OA1-CB1-OA2-CB2
2	L	117	E13	NAJ-CB1-OA2-CB2
2	L	117	E13	O-C-CA-CB
2	L	117	E13	NBC-C-CA-CB
2	H	117[B]	E13	C-CA-CB-CG2
2	H	117[B]	E13	C-CA-CB-CAG
2	H	117[B]	E13	C-CA-CB-CG1
2	I	117[B]	E13	CAY-CBK-CBM-CBF
2	H	117[B]	E13	N-CA-CB-CG1
2	E	117	E13	CBI-CBN-CBO-NBC

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Mol	Chain	Res	Type	Atoms
2	C	117[B]	E13	CAX-CBK-CBM-CBF
2	C	117[B]	E13	CAY-CBK-CBM-CBF
2	E	117	E13	CAX-CBK-CBM-CBF
2	I	117[B]	E13	CAX-CBK-CBM-CBF
2	H	117[B]	E13	N-CA-CB-CG2
2	B	117	E13	O-C-CA-N
2	C	117[A]	E13	O-C-CA-N
2	C	117[B]	E13	O-C-CA-N
2	E	117	E13	O-C-CA-N
2	H	117[B]	E13	O-C-CA-N
2	I	117[A]	E13	O-C-CA-N
2	I	117[B]	E13	O-C-CA-N
2	L	117	E13	O-C-CA-N
2	B	117	E13	NBC-C-CA-N
2	C	117[A]	E13	NBC-C-CA-N
2	C	117[B]	E13	NBC-C-CA-N
2	E	117	E13	NBC-C-CA-N
2	H	117[B]	E13	NBC-C-CA-N
2	I	117[A]	E13	NBC-C-CA-N
2	I	117[B]	E13	NBC-C-CA-N
2	L	117	E13	NBC-C-CA-N
2	B	117	E13	CAY-CBK-CBM-CBF
2	H	117[A]	E13	CAY-CBK-CBM-CBF
2	I	117[A]	E13	CAX-CBK-CBM-CBF
2	L	117	E13	CAX-CBK-CBM-CBF
2	L	117	E13	CAY-CBK-CBM-CBF
2	L	117	E13	OAO-CBN-CBO-CBA
2	H	117[B]	E13	N-CA-CB-CAG
2	I	117[B]	E13	N-CA-CB-CG2
2	C	117[A]	E13	O-C-CA-CB
2	C	117[B]	E13	O-C-CA-CB
2	H	117[B]	E13	O-C-CA-CB
2	I	117[A]	E13	O-C-CA-CB
2	I	117[B]	E13	O-C-CA-CB
2	I	117[A]	E13	CBI-CBN-CBO-CBA
2	B	117	E13	CAX-CBK-CBM-CBF
2	C	117[A]	E13	CAX-CBK-CBM-CBF
2	E	117	E13	CAY-CBK-CBM-CBF
2	H	117[A]	E13	CAX-CBK-CBM-CBF
2	H	117[B]	E13	CAX-CBK-CBM-CBF
2	I	117[A]	E13	CAY-CBK-CBM-CBF
2	C	117[B]	E13	NBC-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	H	117[B]	E13	NBC-C-CA-CB
2	I	117[B]	E13	NBC-C-CA-CB
2	E	117	E13	CBF-CBM-NAJ-CB1
2	I	117[B]	E13	CBF-CBM-NAJ-CB1
2	B	117	E13	CBI-CBN-CBO-NBC
2	C	117[B]	E13	CBI-CBN-CBO-NBC
2	H	117[A]	E13	CBI-CBN-CBO-NBC
2	H	117[B]	E13	CBI-CBN-CBO-NBC
2	I	117[A]	E13	CBI-CBN-CBO-NBC
2	L	117	E13	CBI-CBN-CBO-NBC
2	I	117[B]	E13	N-CA-CB-CG1
2	H	117[A]	E13	OA1-CB1-NAJ-CBM
2	H	117[A]	E13	OA2-CB1-NAJ-CBM
2	C	117[A]	E13	CAY-CBK-CBM-CBF
2	H	117[B]	E13	CAY-CBK-CBM-CBF
2	C	117[B]	E13	CBF-CBM-NAJ-CB1
2	I	117[B]	E13	CBI-CBN-CBO-NBC
2	B	117	E13	OA0-CBN-CBO-CBA
2	C	117[B]	E13	OA0-CBN-CBO-CBA
2	H	117[A]	E13	OA0-CBN-CBO-CBA
2	H	117[B]	E13	OA0-CBN-CBO-CBA
2	E	117	E13	C-CA-CB-CAG
2	I	117[B]	E13	N-CA-CB-CAG

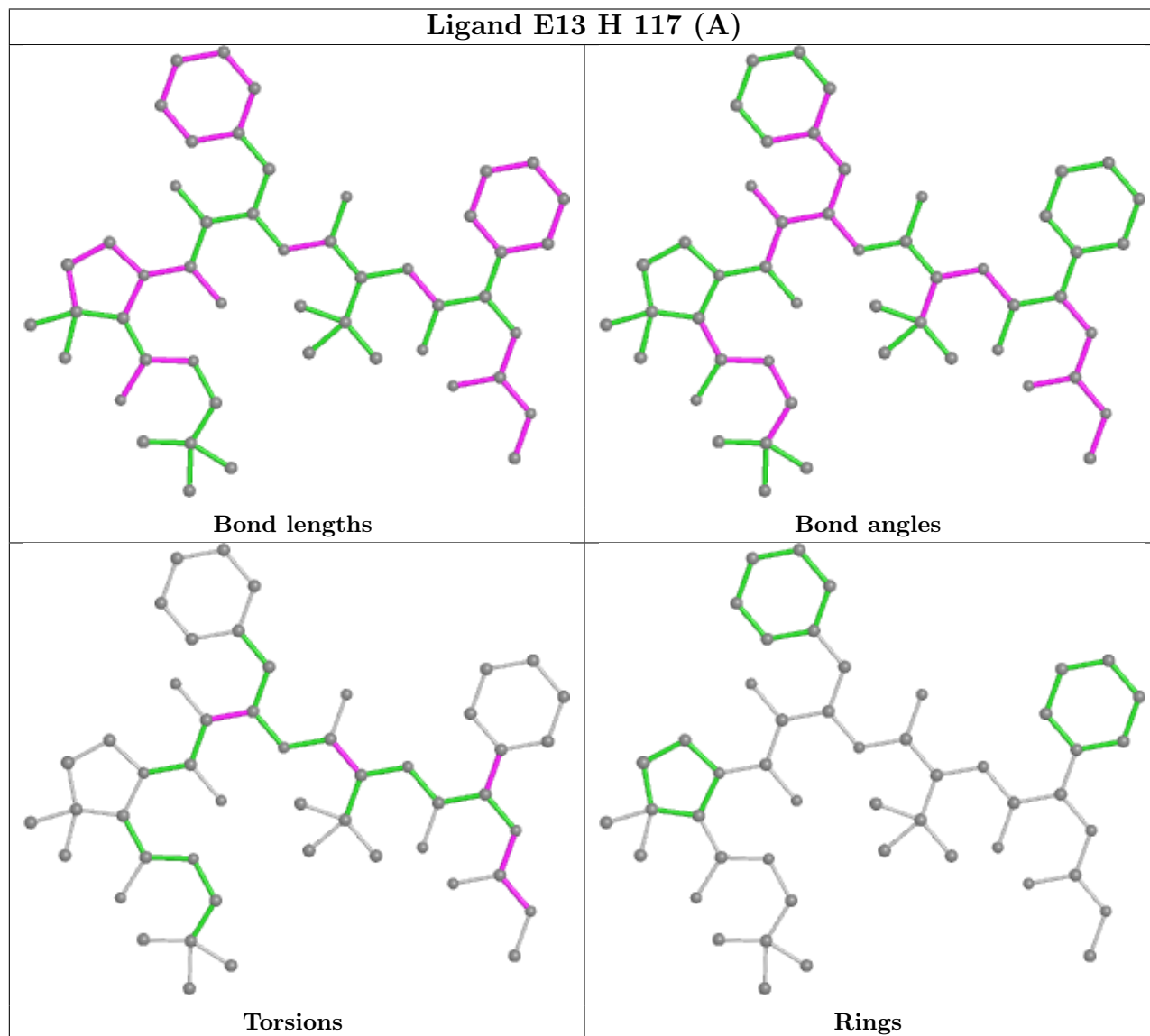
There are no ring outliers.

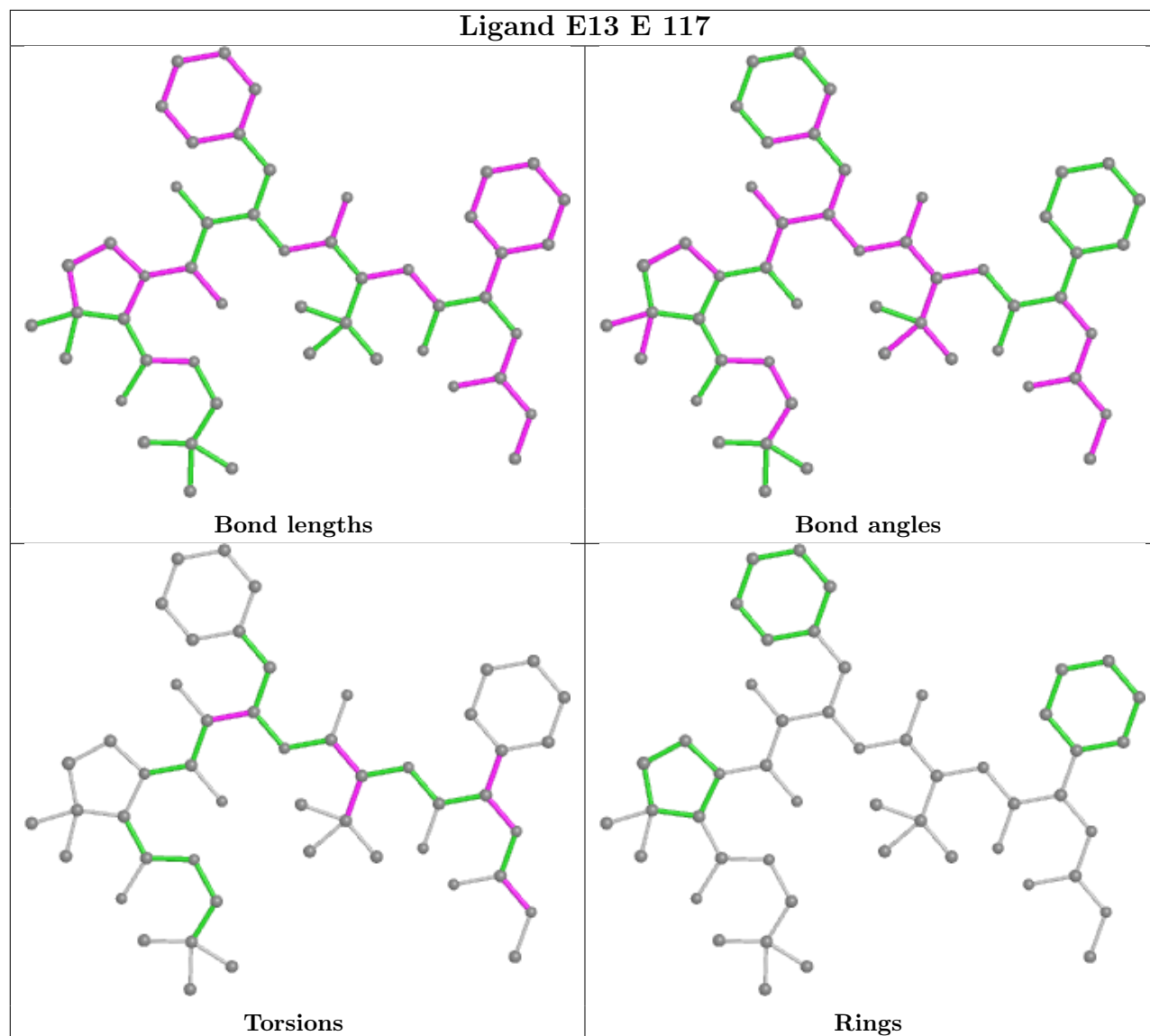
9 monomers are involved in 66 short contacts:

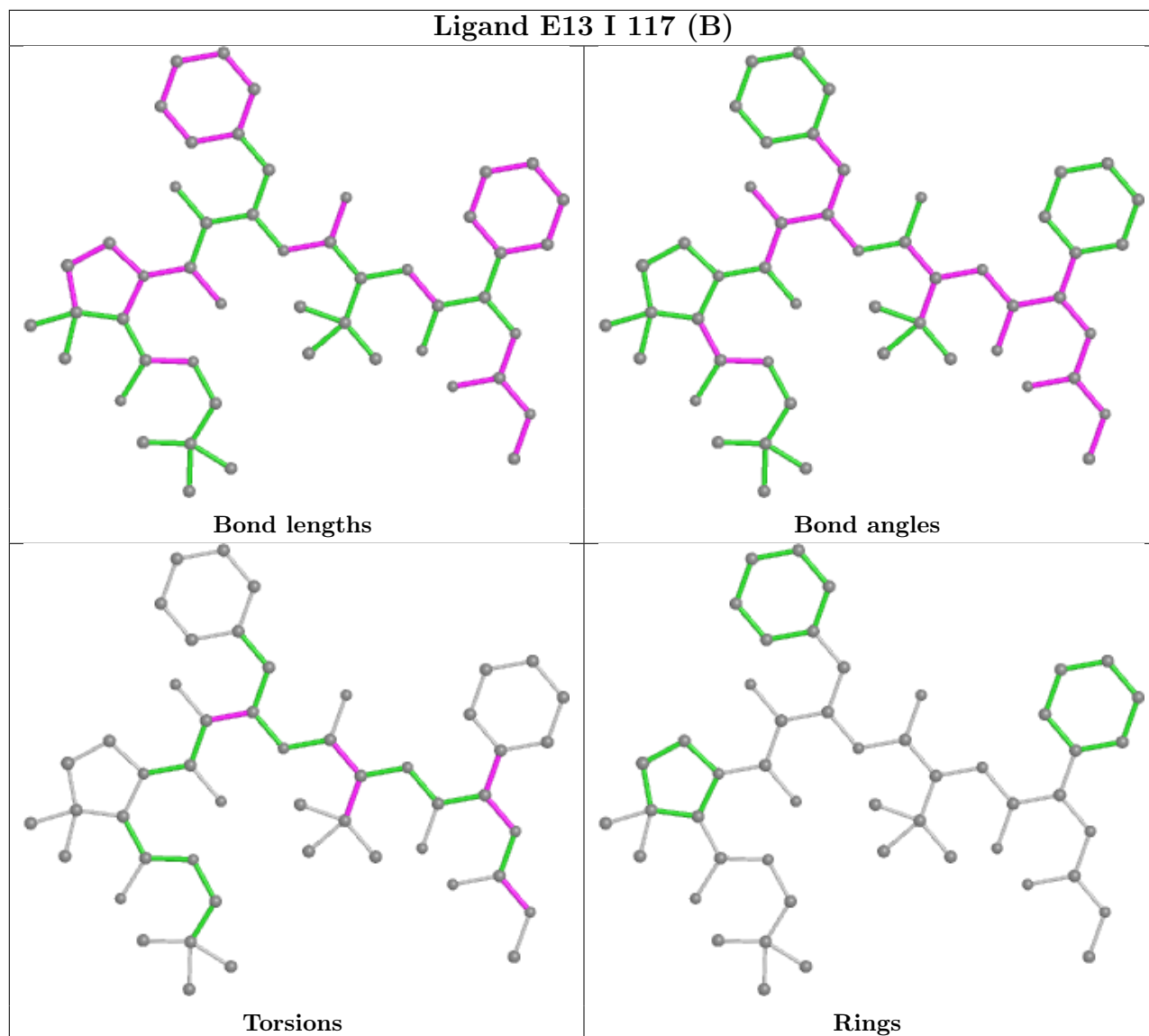
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	117[A]	E13	10	0
2	E	117	E13	2	0
2	I	117[B]	E13	1	0
2	L	117	E13	1	0
2	I	117[A]	E13	20	0
2	C	117[B]	E13	10	0
2	C	117[A]	E13	14	0
2	B	117	E13	2	0
2	H	117[B]	E13	6	0

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

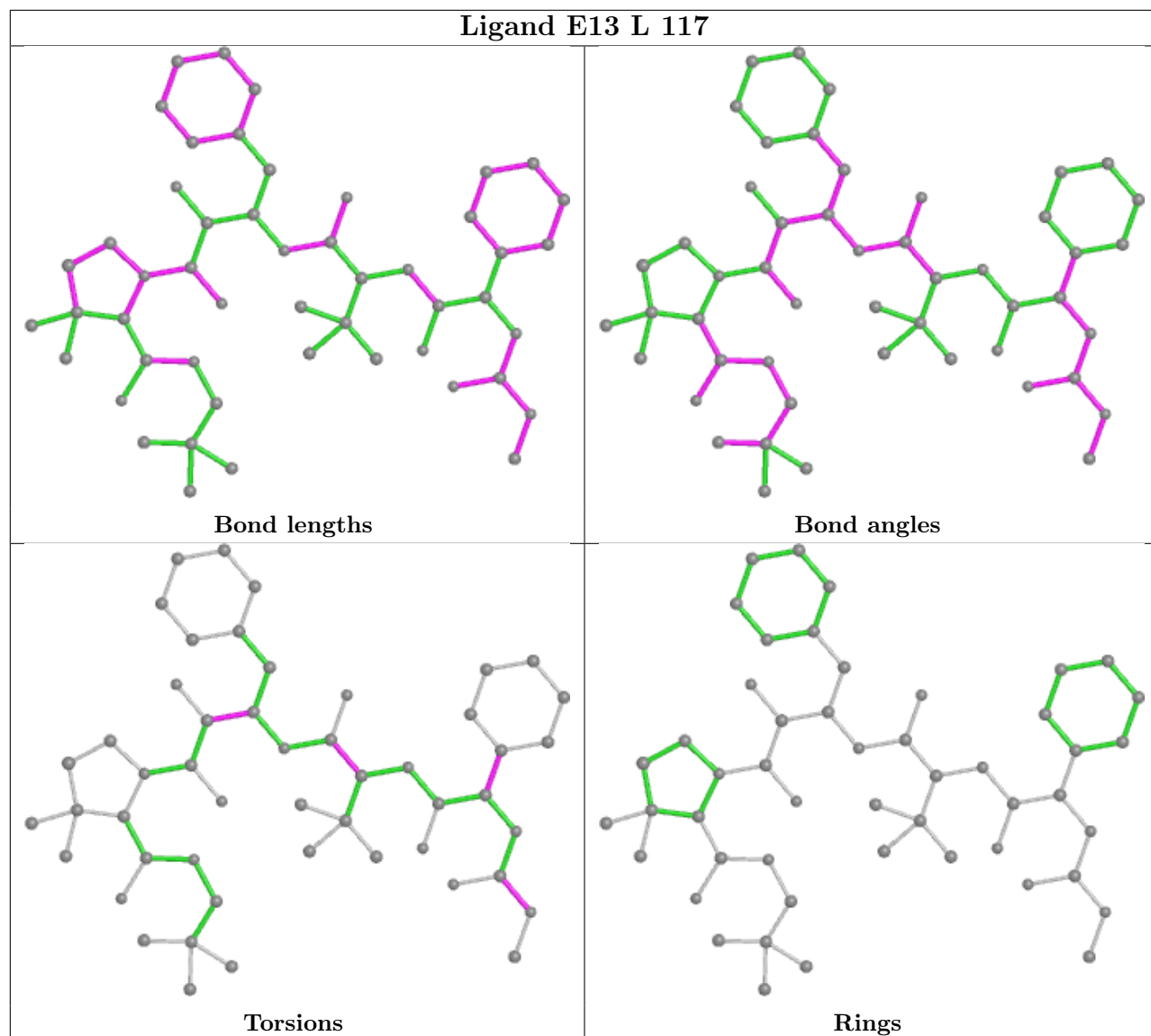
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

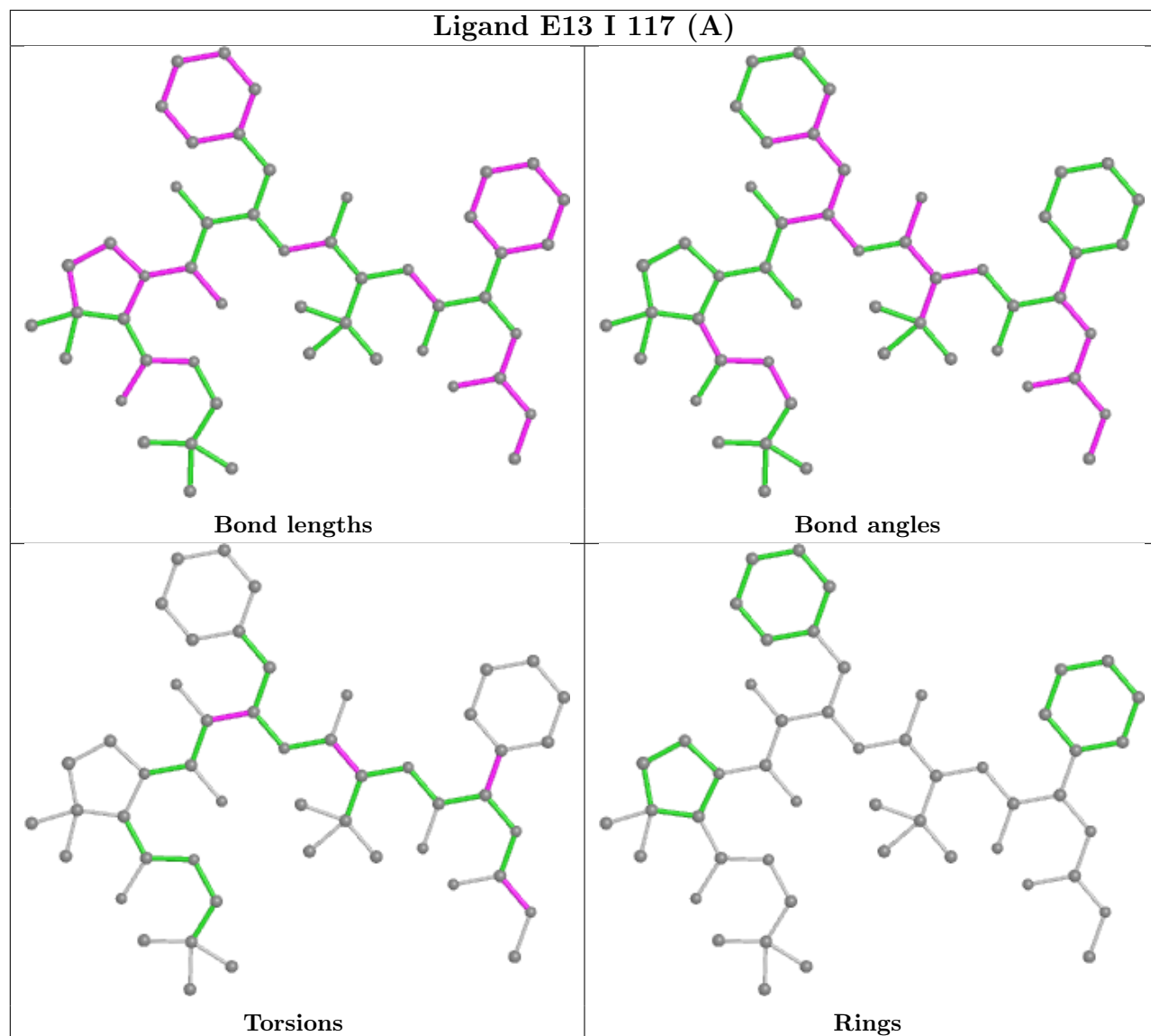


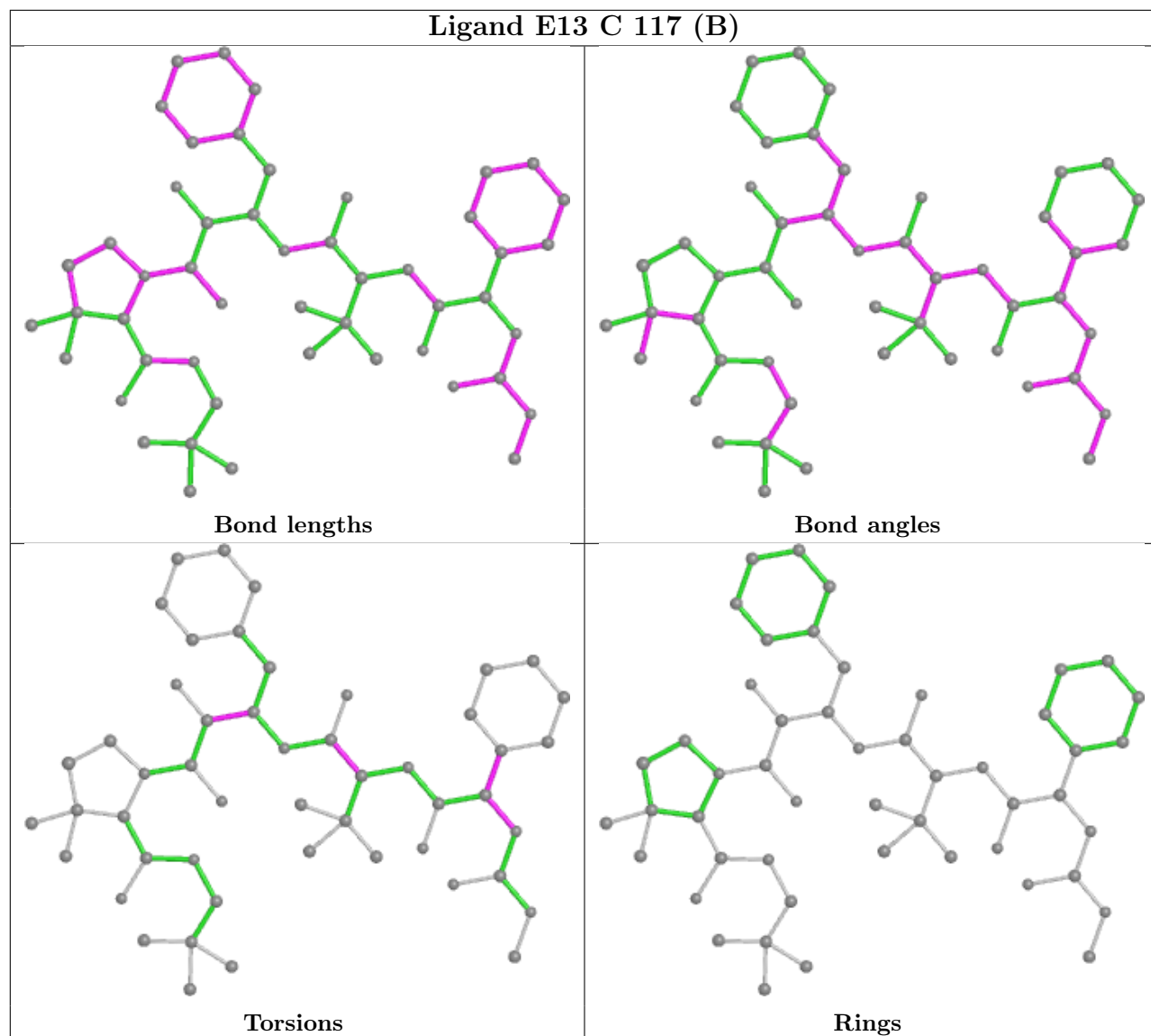


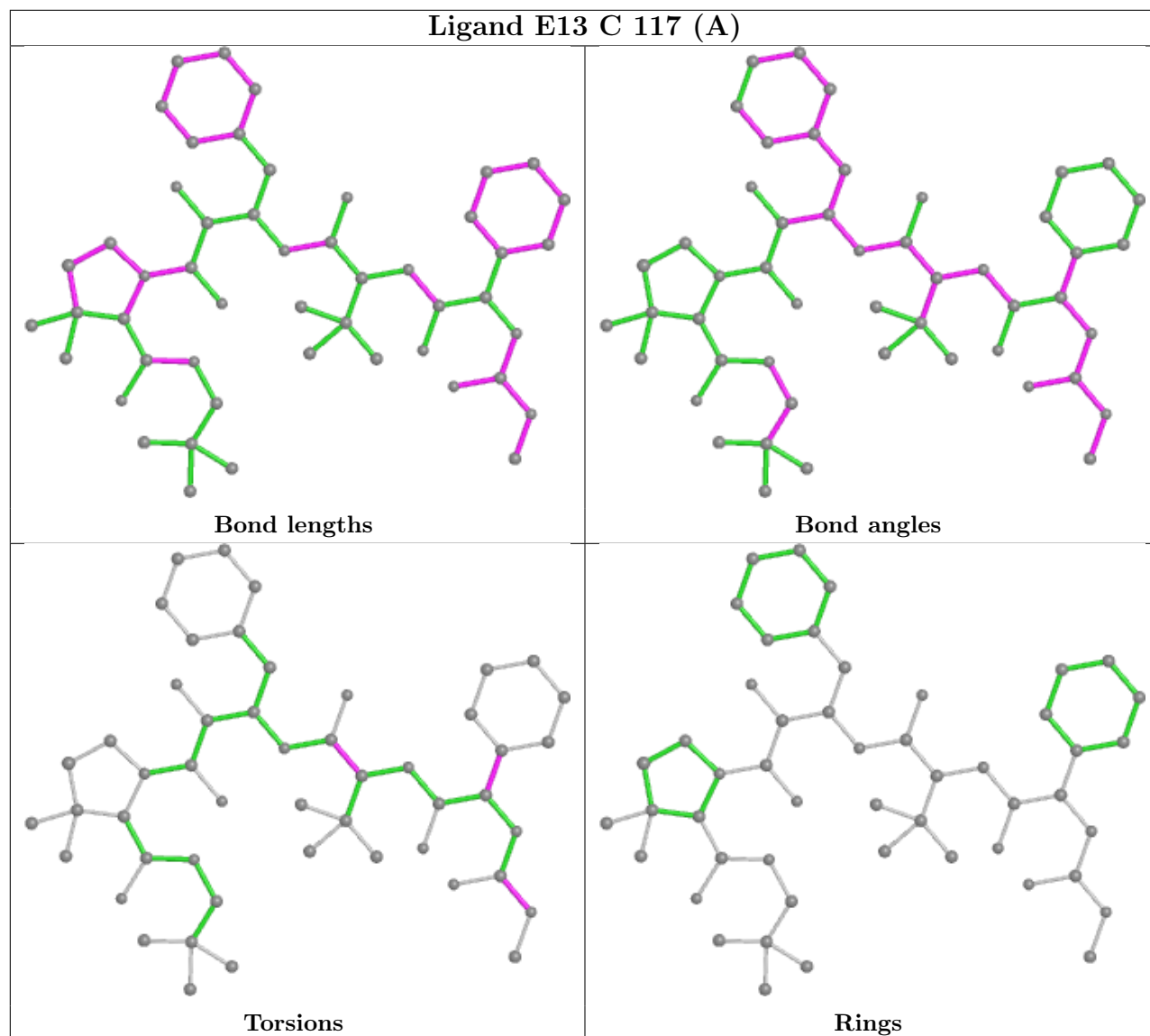


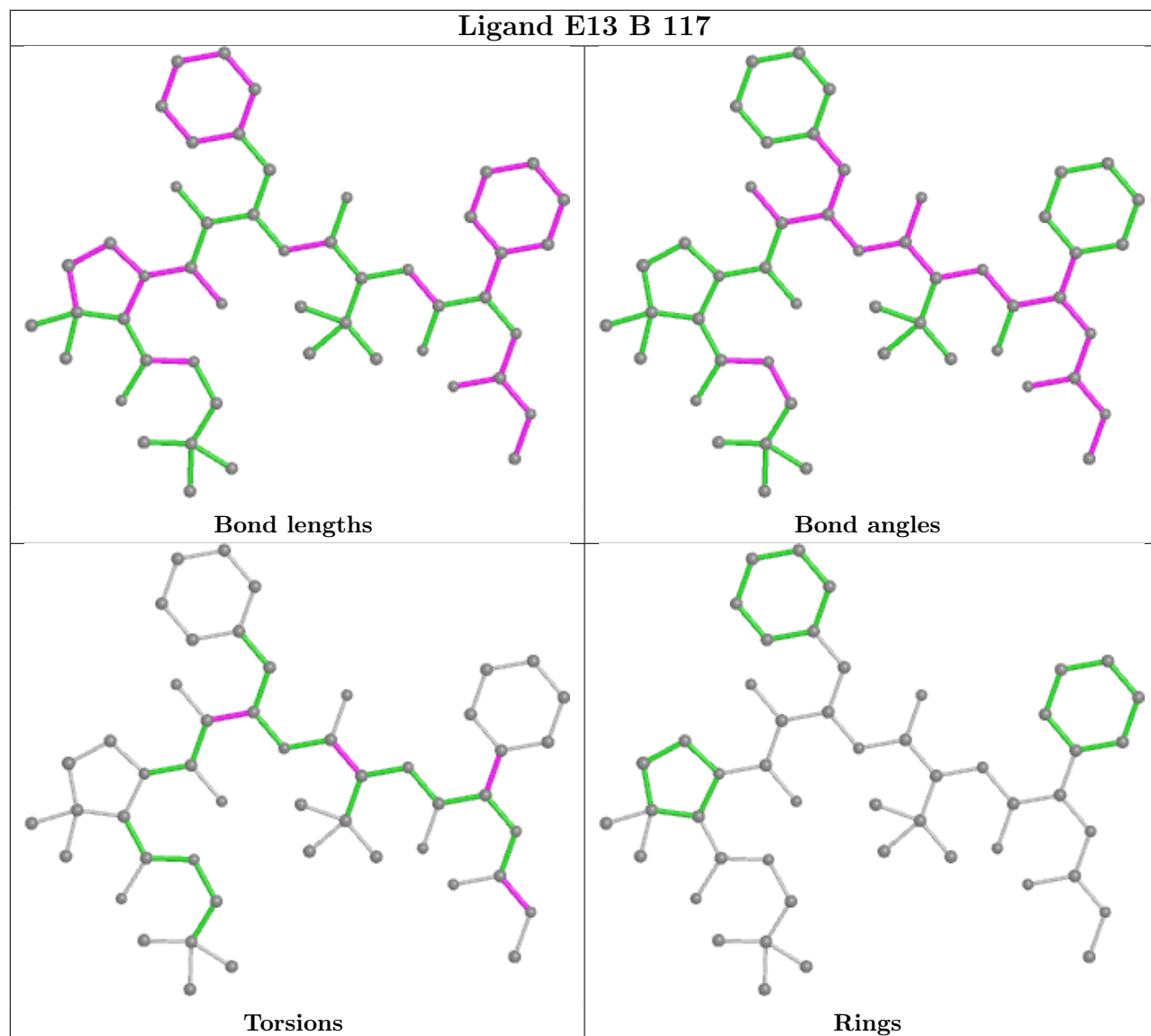


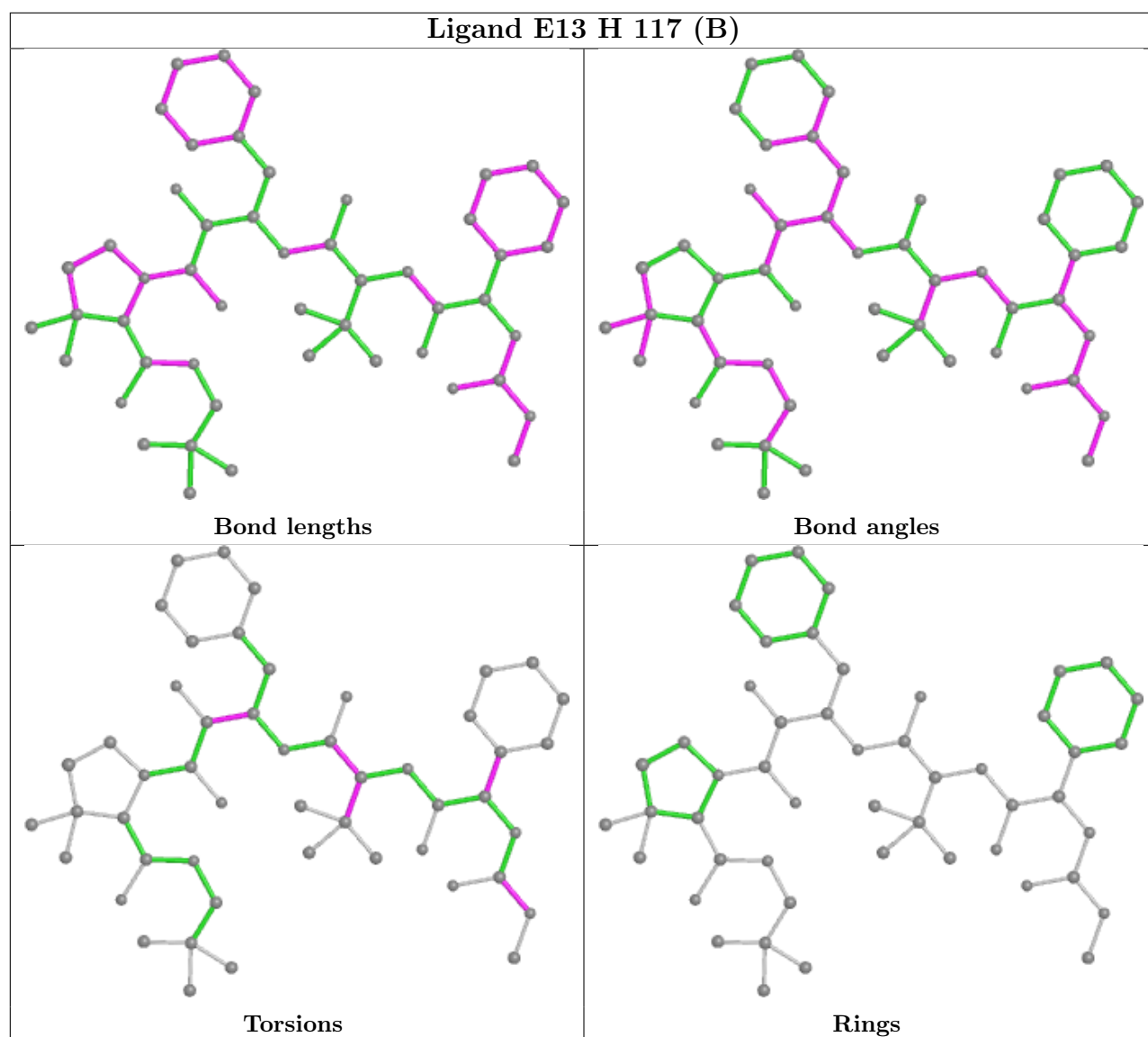












## 5.7 Other polymers [\(i\)](#)

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 i

### 6.1 Protein, DNA and RNA chains i

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	116/116 (100%)	0.37	5 (4%) 35 45	23, 41, 69, 94	0
1	B	116/116 (100%)	0.41	9 (7%) 13 20	20, 36, 66, 92	0
1	C	116/116 (100%)	0.37	5 (4%) 35 45	22, 38, 64, 92	0
1	D	116/116 (100%)	0.31	2 (1%) 70 77	20, 34, 63, 92	0
1	E	116/116 (100%)	0.24	6 (5%) 27 37	19, 32, 61, 89	0
1	F	116/116 (100%)	0.33	7 (6%) 21 30	22, 39, 64, 94	0
1	G	116/116 (100%)	0.37	6 (5%) 27 37	22, 38, 64, 92	0
1	H	116/116 (100%)	0.28	5 (4%) 35 45	20, 34, 62, 92	0
1	I	116/116 (100%)	0.31	5 (4%) 35 45	19, 33, 62, 90	0
1	J	116/116 (100%)	0.52	12 (10%) 6 10	21, 37, 64, 93	0
1	K	116/116 (100%)	0.36	6 (5%) 27 37	22, 38, 70, 90	0
1	L	116/116 (100%)	0.33	6 (5%) 27 37	21, 36, 69, 92	0
All	All	1392/1392 (100%)	0.35	74 (5%) 26 35	19, 36, 67, 94	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	80	PHE	6.6
1	F	48	ASN	6.3
1	J	48	ASN	5.5
1	K	80	PHE	5.3
1	G	80	PHE	4.7
1	F	82	THR	4.6
1	G	48	ASN	4.3
1	J	61	GLY	4.2
1	J	82	THR	4.1
1	G	83	THR	4.0
1	B	50	PRO	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	80	PHE	4.0
1	E	82	THR	4.0
1	B	48	ASN	3.8
1	B	49	THR	3.7
1	C	48	ASN	3.6
1	F	98	TRP	3.5
1	L	50	PRO	3.5
1	F	50	PRO	3.4
1	C	57[A]	LEU	3.4
1	G	59	ALA	3.4
1	B	47	SER	3.3
1	J	60	GLY	3.2
1	I	80	PHE	3.2
1	C	81	ARG	3.2
1	I	98	TRP	3.1
1	I	48	ASN	3.1
1	J	80	PHE	3.1
1	I	96	ASN	3.0
1	A	1	PRO	3.0
1	K	96	ASN	2.9
1	B	61	GLY	2.9
1	L	47	SER	2.9
1	A	62	GLN	2.8
1	B	82	THR	2.8
1	J	49	THR	2.8
1	L	49	THR	2.8
1	L	63	THR	2.8
1	J	46	SER	2.8
1	J	59	ALA	2.7
1	K	48	ASN	2.7
1	L	98	TRP	2.7
1	J	50	PRO	2.7
1	H	48	ASN	2.7
1	K	62	GLN	2.6
1	H	47	SER	2.6
1	I	23	HIS	2.6
1	J	81	ARG	2.5
1	H	46	SER	2.5
1	F	81	ARG	2.4
1	C	82	THR	2.4
1	D	48	ASN	2.4
1	H	98	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	97	ASN	2.4
1	A	69	LEU	2.3
1	K	81	ARG	2.3
1	G	98	TRP	2.2
1	E	49	THR	2.2
1	J	23	HIS	2.2
1	H	80	PHE	2.2
1	E	83	THR	2.1
1	D	60	GLY	2.1
1	K	23	HIS	2.1
1	L	60	GLY	2.1
1	B	98	TRP	2.1
1	B	83	THR	2.1
1	F	59	ALA	2.1
1	F	61	GLY	2.1
1	A	63	THR	2.1
1	B	80	PHE	2.1
1	A	80	PHE	2.0
1	E	2	VAL	2.0
1	G	96	ASN	2.0
1	J	47	SER	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.

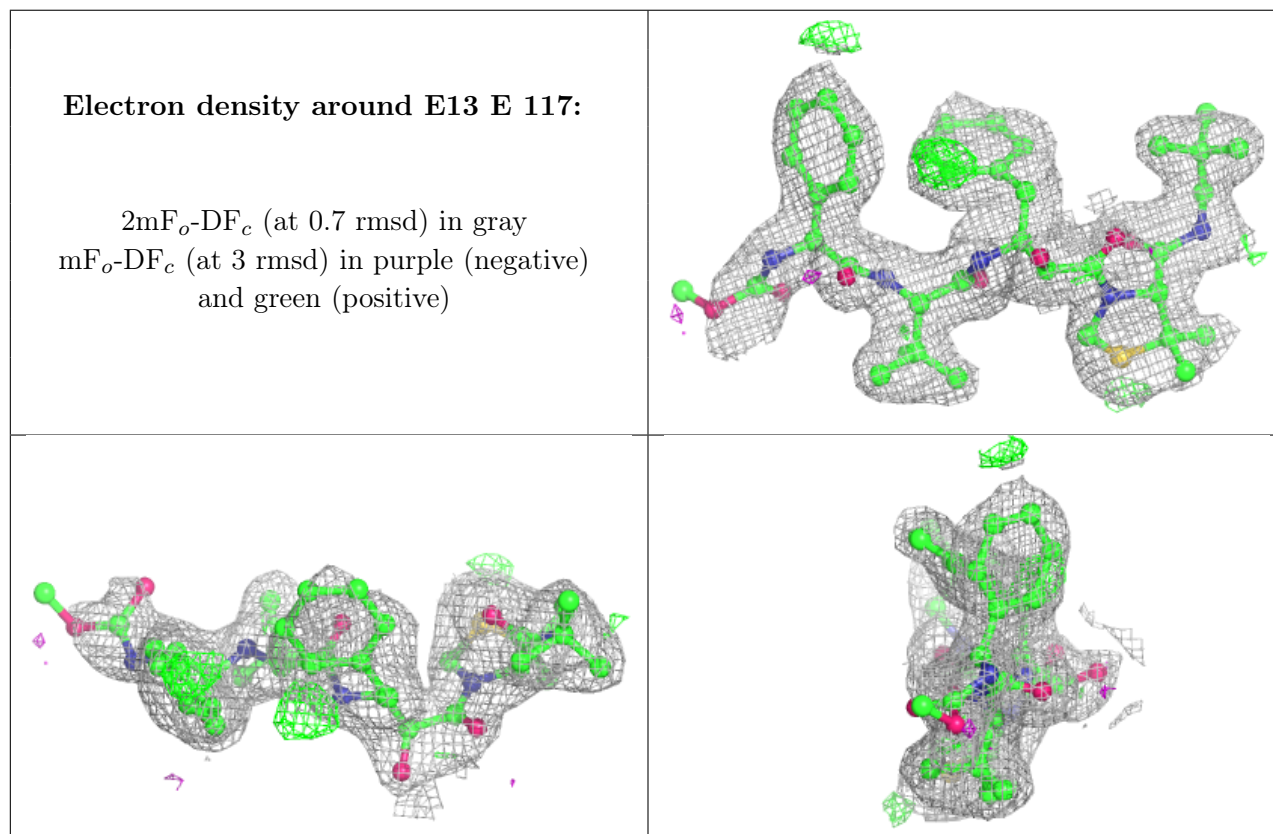
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	E13	E	117	50/50	0.93	0.15	23,38,71,84	0
2	E13	I	117[A]	50/50	0.93	0.21	14,33,46,64	50

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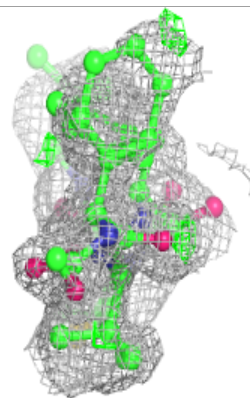
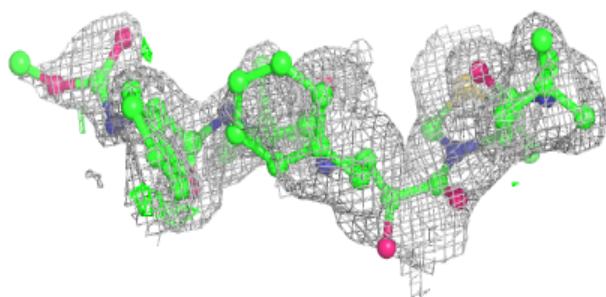
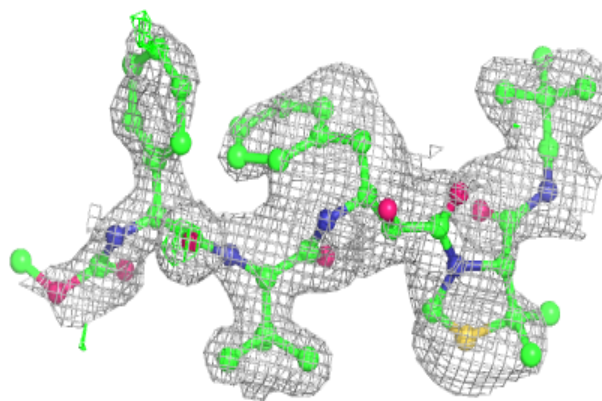
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	E13	I	117[B]	50/50	0.93	0.21	12,24,48,56	50
2	E13	H	117[B]	50/50	0.94	0.19	14,29,45,66	50
2	E13	B	117	50/50	0.94	0.15	22,37,64,85	0
2	E13	H	117[A]	50/50	0.94	0.19	14,31,44,48	50
2	E13	L	117	50/50	0.94	0.13	20,34,63,92	0
2	E13	C	117[A]	50/50	0.95	0.17	15,31,45,54	50
2	E13	C	117[B]	50/50	0.95	0.17	8,23,42,56	50

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.

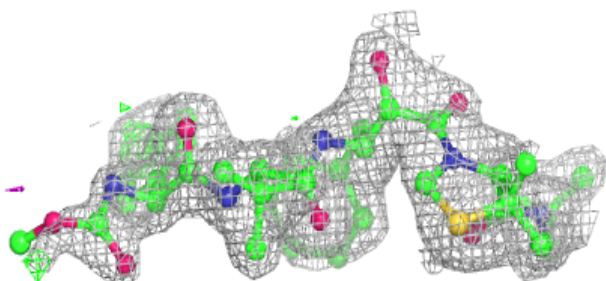
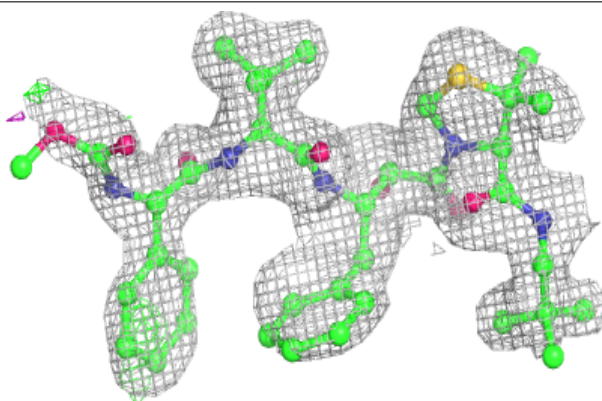


**Electron density around E13 I 117 (A):**

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

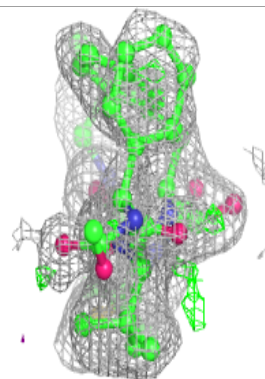
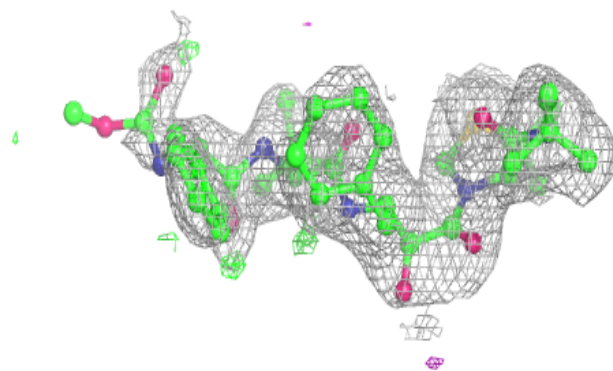
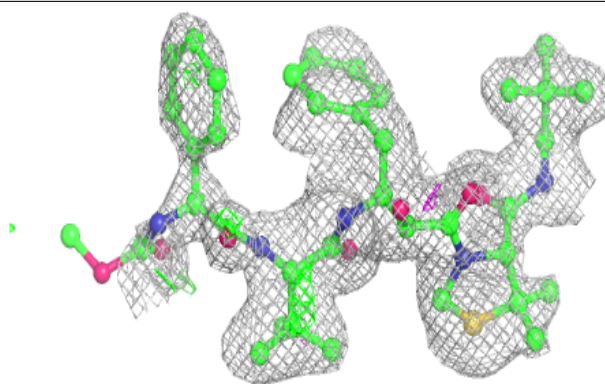
**Electron density around E13 I 117 (B):**

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

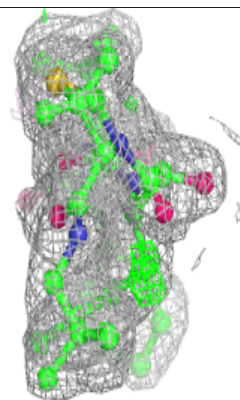
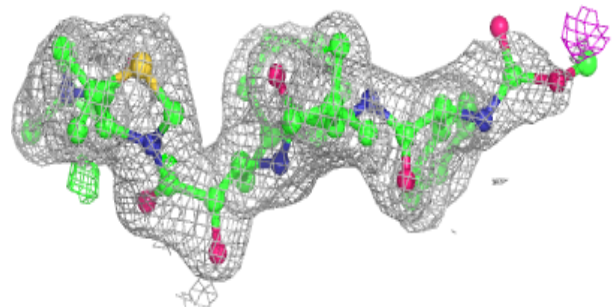
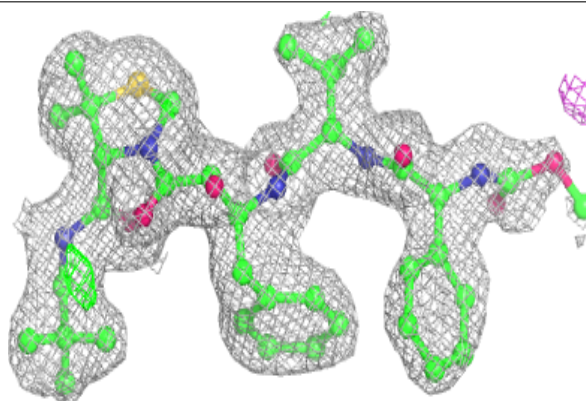


**Electron density around E13 H 117 (B):**

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

**Electron density around E13 B 117:**

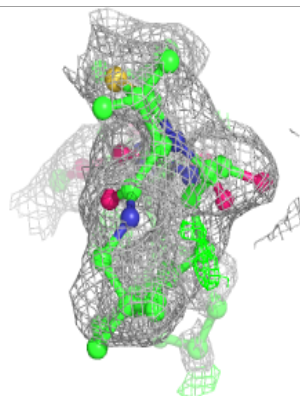
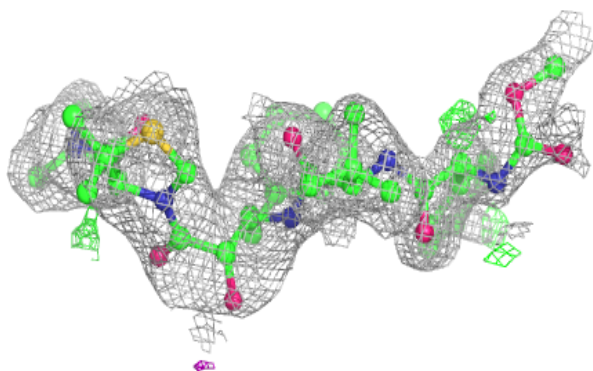
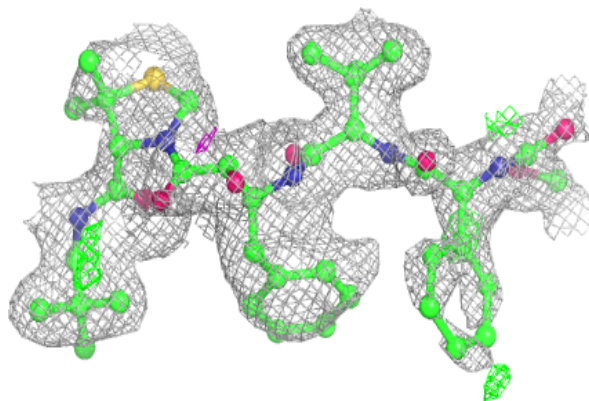
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



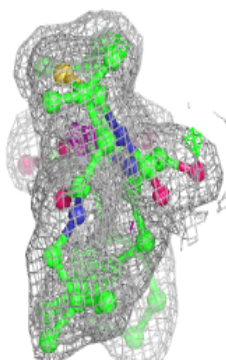
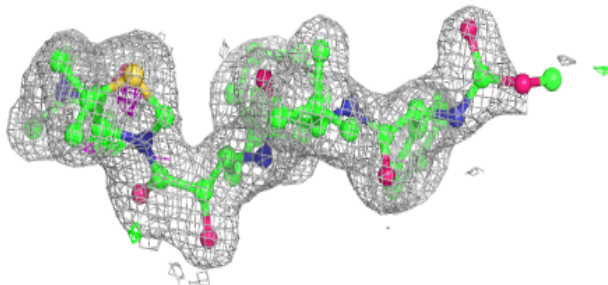
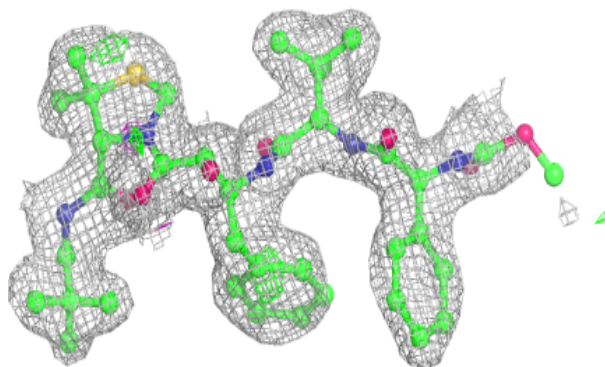


**Electron density around E13 H 117 (A):**

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

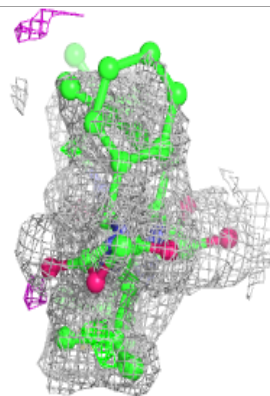
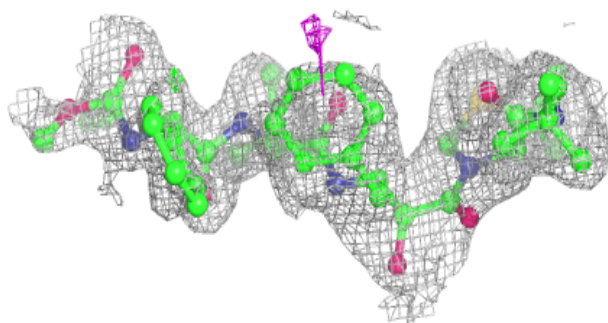
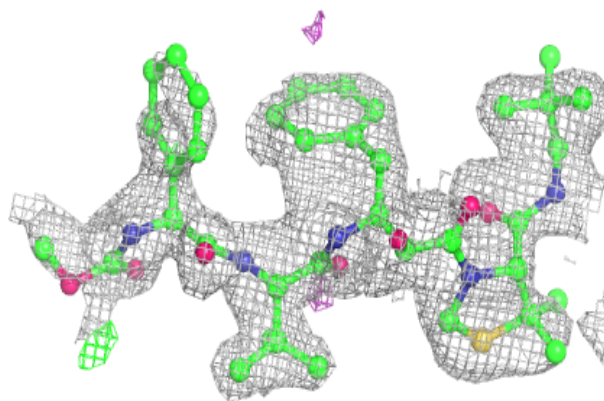
**Electron density around E13 L 117:**

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

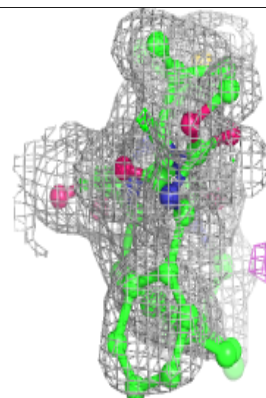
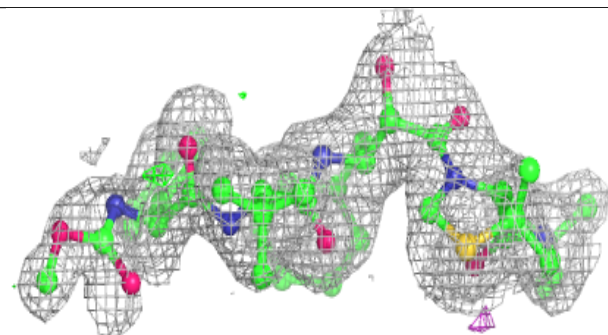
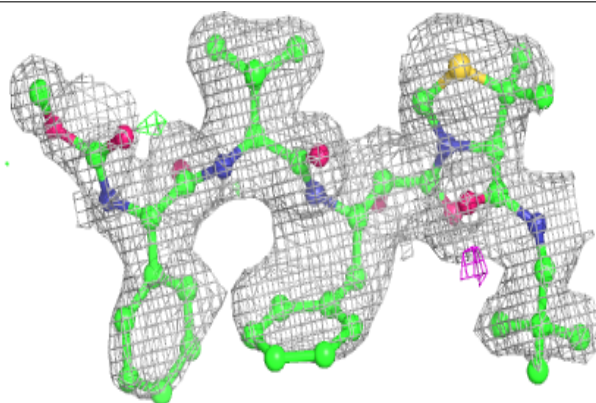


**Electron density around E13 C 117 (A):**

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

**Electron density around E13 C 117 (B):**

$2mF_o-DF_c$  (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.