



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 03:44 am BST

PDB ID : 3T8W
Title : A bestatin-based chemical biology strategy reveals distinct roles for malaria M1- and M17-family aminopeptidases
Authors : McGowan, S.; Klemba, M.; Greebaum, D.C.
Deposited on : 2011-08-01
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

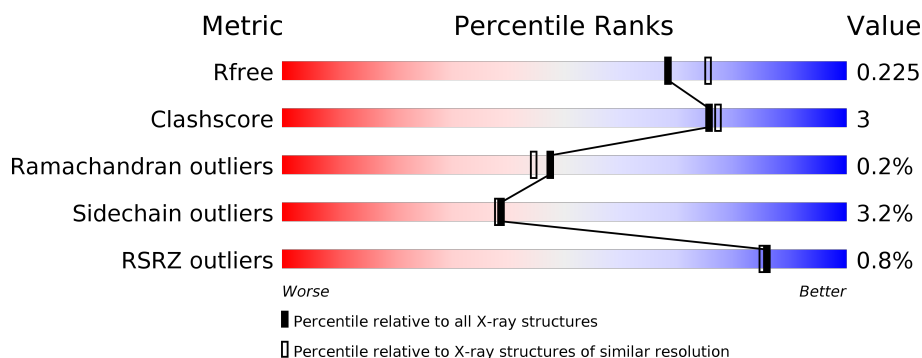
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	528	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>5%</div> <div>•</div> </div> </div>
1	B	528	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>•</div> </div> </div>
1	C	528	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>••</div> </div> </div>
1	D	528	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>•</div> </div> </div>
1	E	528	<div> <div></div> <div> <div></div> <div>90%</div> <div>6%</div> <div>•</div> </div> </div>
1	F	528	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	528	
1	H	528	
1	I	528	
1	J	528	
1	K	528	
1	L	528	

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
6	1PE	C	621	-	X	-	-
6	1PE	C	622	-	X	-	-
6	1PE	D	618	-	X	-	-
6	1PE	D	620	-	X	-	-
6	1PE	D	621	-	X	-	-
6	1PE	E	619	-	X	-	-
6	1PE	E	620	-	X	-	-
6	1PE	E	621	-	X	-	-
6	1PE	F	616	-	X	-	-
6	1PE	F	617	-	X	-	-
6	1PE	F	618	-	X	-	-
6	1PE	G	620	-	X	-	-
6	1PE	G	622	-	X	-	-
6	1PE	G	623	-	X	X	-
6	1PE	I	621	-	X	-	-
6	1PE	J	619	-	X	-	-
6	1PE	J	620	-	X	-	-
6	1PE	J	621	-	X	-	-
6	1PE	J	622	-	X	-	-
6	1PE	K	617	-	X	-	-
6	1PE	K	618	-	X	-	-
6	1PE	K	619	-	X	-	-
6	1PE	K	620	-	X	-	-
6	1PE	L	617	-	X	-	-
6	1PE	L	618	-	X	-	-
6	1PE	L	619	-	X	-	-
6	1PE	L	620	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 53295 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 M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3973	2550	638	766	19			
1	B	517	Total	C	N	O	S	0	0	0
			3916	2515	636	746	19			
1	C	516	Total	C	N	O	S	0	0	0
			3942	2533	635	755	19			
1	D	514	Total	C	N	O	S	0	0	0
			3928	2529	633	746	20			
1	E	509	Total	C	N	O	S	0	0	0
			3900	2512	625	744	19			
1	F	511	Total	C	N	O	S	0	0	0
			3847	2473	621	734	19			
1	G	517	Total	C	N	O	S	0	0	0
			3978	2553	638	767	20			
1	H	518	Total	C	N	O	S	0	0	0
			3927	2521	636	750	20			
1	I	518	Total	C	N	O	S	0	0	0
			3955	2543	637	755	20			
1	J	514	Total	C	N	O	S	0	0	0
			3925	2527	632	746	20			
1	K	509	Total	C	N	O	S	0	0	0
			3897	2509	624	745	19			
1	L	511	Total	C	N	O	S	0	0	0
			3844	2469	621	735	19			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
A	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
A	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
A	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	607	HIS	-	EXPRESSION TAG	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
A	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
B	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
B	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
B	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
B	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
C	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
C	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
C	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
C	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
D	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
D	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
D	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
D	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
E	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
E	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
E	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
E	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
F	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11

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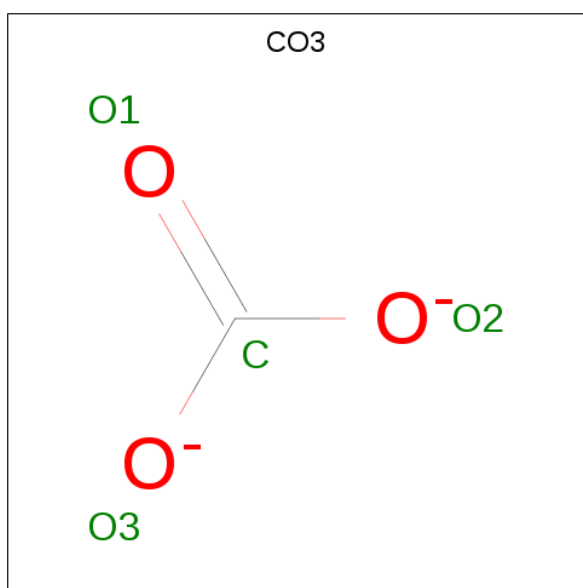
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
F	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
F	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
G	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
G	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
G	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
G	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
H	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
H	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
H	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
H	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
I	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
I	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
I	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
I	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
J	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
J	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
J	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
J	610	HIS	-	EXPRESSION TAG	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
J	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
K	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
K	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
K	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
K	611	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	152	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
L	515	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
L	546	GLN	ASN	ENGINEERED MUTATION	UNP Q8IL11
L	606	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	607	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	608	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	609	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	610	HIS	-	EXPRESSION TAG	UNP Q8IL11
L	611	HIS	-	EXPRESSION TAG	UNP Q8IL11

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 1 3	0	0
2	D	1	Total C O 4 1 3	0	0
2	E	1	Total C O 4 1 3	0	0
2	F	1	Total C O 4 1 3	0	0
2	G	1	Total C O 4 1 3	0	0
2	H	1	Total C O 4 1 3	0	0
2	I	1	Total C O 4 1 3	0	0
2	J	1	Total C O 4 1 3	0	0
2	K	1	Total C O 4 1 3	0	0
2	L	1	Total C O 4 1 3	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

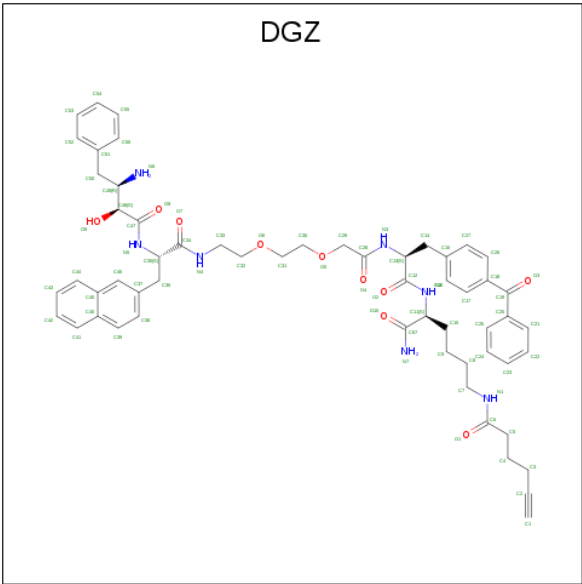
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Zn 2 2	0	0
3	J	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	K	2	Total Zn 2 2	0	0
3	E	2	Total Zn 2 2	0	0
3	H	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	I	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	L	2	Total	Zn	0	0
			2	2		
3	F	2	Total	Zn	0	0
			2	2		

- Molecule 4 is N-((2R,3S,6S,18S,21S)-2-amino-18-(4-benzoylbenzyl)-21-carbamoyl-3-hydroxy-6-(naphthalen-2-ylmethyl)-4,7,16,19-tetraoxo-1-phenyl-11,14-dioxa-5,8,17,20-tetraazapenta cosan-25-yl)hex-5-ynamide (three-letter code: DGZ) (formula: C₅₇H₆₇N₇O₁₀).



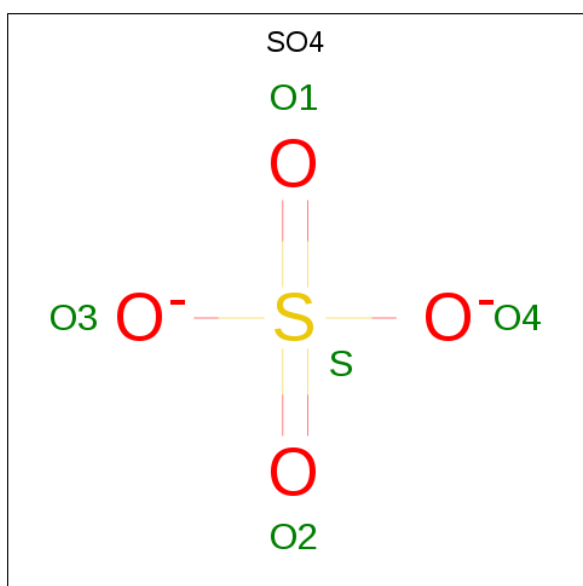
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			74	57	7	10		
4	B	1	Total	C	N	O	0	0
			74	57	7	10		
4	C	1	Total	C	N	O	0	0
			74	57	7	10		
4	D	1	Total	C	N	O	0	0
			74	57	7	10		
4	E	1	Total	C	N	O	0	0
			74	57	7	10		
4	F	1	Total	C	N	O	0	0
			74	57	7	10		
4	G	1	Total	C	N	O	0	0
			74	57	7	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			74	57	7	10		
4	I	1	Total	C	N	O	0	0
			74	57	7	10		
4	J	1	Total	C	N	O	0	0
			74	57	7	10		
4	K	1	Total	C	N	O	0	0
			74	57	7	10		
4	L	1	Total	C	N	O	0	0
			74	57	7	10		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O S	0	0
			5	4 1		
5	A	1	Total	O S	0	0
			5	4 1		
5	C	1	Total	O S	0	0
			5	4 1		
5	C	1	Total	O S	0	0
			5	4 1		
5	C	1	Total	O S	0	0
			5	4 1		

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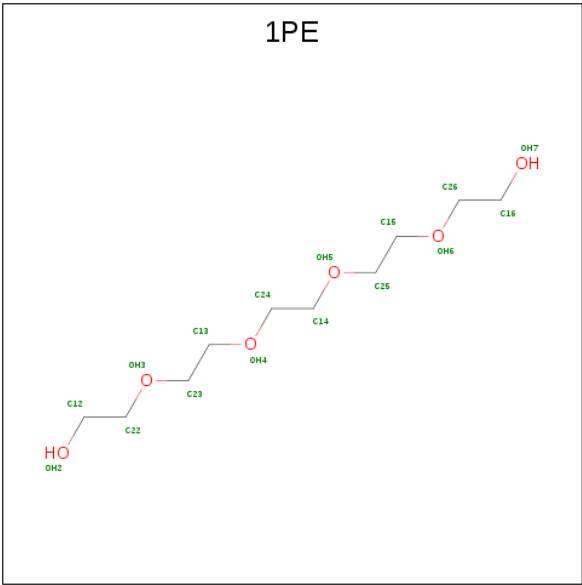
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	6	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			12	8	4		
6	C	1	Total	C	O	0	0
			9	6	3		
6	D	1	Total	C	O	0	0
			10	7	3		
6	D	1	Total	C	O	0	0
			8	5	3		
6	D	1	Total	C	O	0	0
			11	8	3		
6	D	1	Total	C	O	0	0
			5	3	2		
6	E	1	Total	C	O	0	0
			12	8	4		

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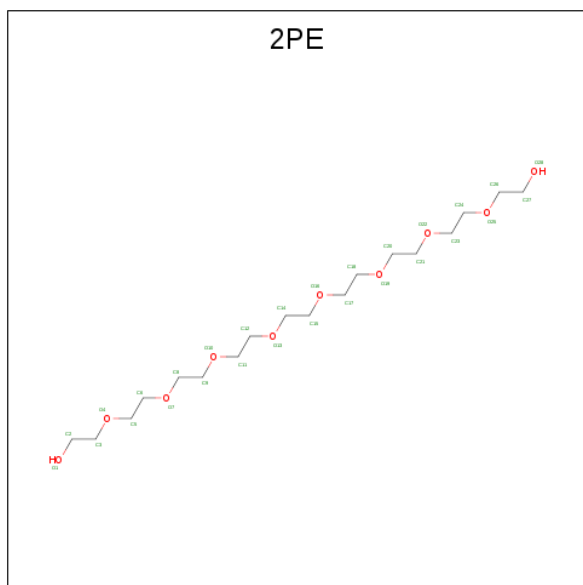
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			10	6	4		
6	E	1	Total	C	O	0	0
			8	5	3		
6	F	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			9	6	3		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			15	10	5		
6	I	1	Total	C	O	0	0
			12	8	4		
6	I	1	Total	C	O	0	0
			10	7	3		
6	I	1	Total	C	O	0	0
			5	3	2		
6	J	1	Total	C	O	0	0
			11	7	4		
6	J	1	Total	C	O	0	0
			10	6	4		
6	J	1	Total	C	O	0	0
			11	8	3		
6	J	1	Total	C	O	0	0
			9	6	3		
6	K	1	Total	C	O	0	0
			8	5	3		
6	K	1	Total	C	O	0	0
			12	8	4		
6	K	1	Total	C	O	0	0
			11	7	4		
6	K	1	Total	C	O	0	0
			6	4	2		
6	L	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			12	8	4		
6	L	1	Total	C	O	0	0
			7	4	3		
6	L	1	Total	C	O	0	0
			11	7	4		

- Molecule 7 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C₁₈H₃₈O₁₀).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	445	Total 445	O 445	0	0
8	F	364	Total 364	O 364	0	0
8	G	431	Total 431	O 431	0	0
8	H	334	Total 334	O 334	0	0
8	I	391	Total 391	O 391	0	0
8	J	406	Total 406	O 406	0	0
8	K	408	Total 408	O 408	0	0
8	L	389	Total 389	O 389	0	0

- Molecule 1: M17 leucyl aminopeptidase





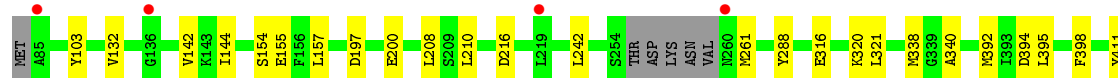
- Molecule 1: M17 leucyl aminopeptidase

Chain I: 92% 5% ..



- Molecule 1: M17 leucyl aminopeptidase

Chain J: 89% 8% .



- Molecule 1: M17 leucyl aminopeptidase

Chain K: 89% 7% .



- Molecule 1: M17 leucyl aminopeptidase

Chain L: 88% 9% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.75Å 177.06Å 231.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.32 – 2.00 81.32 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (81.32-2.00) 99.7 (81.32-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.164 , 0.200 0.185 , 0.225	Depositor DCC
R_{free} test set	23988 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53295	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.29 % 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 1.3495e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: CO3, ZN, 1PE, 2PE, SO4, DGZ

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	0.49	0/4051	0.63	1/5498 (0.0%)
1	B	0.48	0/3993	0.66	1/5424 (0.0%)
1	C	0.50	0/4019	0.63	0/5453
1	D	0.52	1/4005 (0.0%)	0.64	0/5431
1	E	0.50	0/3976	0.63	0/5391
1	F	0.49	0/3924	0.66	1/5336 (0.0%)
1	G	0.49	0/4054	0.62	1/5494 (0.0%)
1	H	0.49	0/4005	0.64	0/5440
1	I	0.49	0/4033	0.64	0/5473
1	J	0.49	0/4002	0.63	0/5428
1	K	0.50	0/3973	0.63	0/5389
1	L	0.50	0/3921	0.66	1/5332 (0.0%)
All	All	0.50	1/47956 (0.0%)	0.64	5/65089 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	547	ILE	C-N	-8.24	1.15	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	550	SER	C-N-CA	5.82	136.24	121.70
1	F	552	LYS	N-CA-C	-5.77	95.41	111.00
1	G	257	LYS	C-N-CA	5.48	135.40	121.70
1	B	552	LYS	N-CA-C	-5.46	96.26	111.00
1	L	549	SER	C-N-CA	5.02	134.26	121.70

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	3973	0	3875	16	0
1	B	3916	0	3799	26	0
1	C	3942	0	3849	17	0
1	D	3928	0	3856	25	0
1	E	3900	0	3831	22	0
1	F	3847	0	3710	33	0
1	G	3978	0	3903	19	0
1	H	3927	0	3812	27	0
1	I	3955	0	3877	16	0
1	J	3925	0	3848	30	0
1	K	3897	0	3817	18	0
1	L	3844	0	3687	27	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	1	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	1	0
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	74	0	66	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	74	0	66	9	0
4	C	74	0	66	5	0
4	D	74	0	66	3	0
4	E	74	0	66	5	0
4	F	74	0	66	9	0
4	G	74	0	66	5	0
4	H	74	0	66	8	0
4	I	74	0	66	4	0
4	J	74	0	66	5	0
4	K	74	0	66	4	0
4	L	74	0	66	6	0
5	A	10	0	0	0	0
5	C	25	0	0	0	0
5	D	10	0	0	0	0
5	E	15	0	0	0	0
5	G	20	0	0	1	0
5	H	15	0	0	0	0
5	I	25	0	0	1	0
5	J	15	0	0	0	0
5	K	5	0	0	0	0
5	L	5	0	0	0	0
6	A	16	0	18	0	0
6	C	21	0	24	2	0
6	D	34	0	35	2	0
6	E	30	0	34	1	0
6	F	30	0	39	7	0
6	G	36	0	39	8	0
6	I	27	0	28	5	0
6	J	41	0	48	12	0
6	K	37	0	38	1	0
6	L	40	0	48	8	0
7	B	26	0	33	0	0
7	H	25	0	33	2	0
8	A	421	0	0	1	0
8	B	351	0	0	3	0
8	C	431	0	0	2	0
8	D	424	0	0	2	0
8	E	445	0	0	0	0
8	F	364	0	0	3	0
8	G	431	0	0	3	0
8	H	334	0	0	4	0
8	I	391	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	406	0	0	0	0
8	K	408	0	0	1	0
8	L	389	0	0	3	0
All	All	53295	0	47073	297	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 3.

The worst 5 of 297 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)
6:G:623:1PE:C16	6:G:623:1PE:C26	1.76	1.64
6:F:618:1PE:C26	6:F:618:1PE:C16	1.74	1.60
6:L:620:1PE:C16	6:L:620:1PE:C26	1.75	1.55
6:G:623:1PE:C13	6:G:623:1PE:OH4	1.63	1.47
1:H:550:SER:OG	1:H:552:LYS:CD	1.80	1.29

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	517/528 (98%)	501 (97%)	15 (3%)	1 (0%)	47	44
1	B	513/528 (97%)	499 (97%)	12 (2%)	2 (0%)	34	30
1	C	512/528 (97%)	501 (98%)	11 (2%)	0	100	100
1	D	510/528 (97%)	502 (98%)	8 (2%)	0	100	100
1	E	503/528 (95%)	494 (98%)	9 (2%)	0	100	100
1	F	507/528 (96%)	494 (97%)	10 (2%)	3 (1%)	25	19
1	G	511/528 (97%)	501 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	516/528 (98%)	501 (97%)	13 (2%)	2 (0%)	34	30
1	I	516/528 (98%)	502 (97%)	13 (2%)	1 (0%)	47	44
1	J	510/528 (97%)	501 (98%)	9 (2%)	0	100	100
1	K	503/528 (95%)	495 (98%)	8 (2%)	0	100	100
1	L	507/528 (96%)	494 (97%)	10 (2%)	3 (1%)	25	19
All	All	6125/6336 (97%)	5985 (98%)	128 (2%)	12 (0%)	47	44

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	552	LYS
1	H	552	LYS
1	I	551	VAL
1	L	550	SER
1	F	550	SER

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	421/455 (92%)	410 (97%)	11 (3%)	46	48
1	B	410/455 (90%)	396 (97%)	14 (3%)	37	36
1	C	417/455 (92%)	404 (97%)	13 (3%)	40	40
1	D	415/455 (91%)	404 (97%)	11 (3%)	44	46
1	E	415/455 (91%)	403 (97%)	12 (3%)	42	43
1	F	400/455 (88%)	382 (96%)	18 (4%)	27	24
1	G	426/455 (94%)	416 (98%)	10 (2%)	50	53
1	H	412/455 (90%)	396 (96%)	16 (4%)	32	30
1	I	420/455 (92%)	405 (96%)	15 (4%)	35	34
1	J	414/455 (91%)	401 (97%)	13 (3%)	40	40
1	K	414/455 (91%)	404 (98%)	10 (2%)	49	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	397/455 (87%)	383 (96%)	14 (4%)	36	35
All	All	4961/5460 (91%)	4804 (97%)	157 (3%)	39	38

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	288	TYR
1	G	439	TYR
1	L	169	LEU
1	F	395	LEU
1	G	117	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	437	ASN
1	F	567	GLN
1	L	217	ASN
1	F	104	ASN
1	F	134	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 112 ligands modelled in this entry, 24 are monoatomic - leaving 88 for Mogul analysis.

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	$\# Z > 2$
6	1PE	G	620	-	8,8,15	2.17	4 (50%)	7,7,14	2.54	4 (57%)
6	1PE	D	620	-	10,10,15	2.18	5 (50%)	9,9,14	2.84	5 (55%)
4	DGZ	H	615	3	78,78,78	0.91	2 (2%)	99,101,101	2.26	2 (2%)
5	SO4	L	616	-	4,4,4	0.65	0	6,6,6	0.36	0
6	1PE	I	622	-	9,9,15	2.29	4 (44%)	8,8,14	2.26	3 (37%)
5	SO4	I	617	-	4,4,4	0.77	0	6,6,6	0.39	0
5	SO4	E	616	-	4,4,4	0.16	0	6,6,6	0.16	0
4	DGZ	J	615	3	78,78,78	0.89	1 (1%)	99,101,101	2.34	4 (4%)
4	DGZ	L	615	3	78,78,78	0.90	1 (1%)	99,101,101	2.35	3 (3%)
6	1PE	I	621	-	11,11,15	2.37	4 (36%)	10,10,14	3.02	5 (50%)
5	SO4	C	617	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	H	616	-	4,4,4	0.09	0	6,6,6	0.34	0
6	1PE	L	617	-	9,9,15	2.26	4 (44%)	8,8,14	1.86	3 (37%)
6	1PE	A	619	-	6,6,15	1.67	1 (16%)	5,5,14	2.37	2 (40%)
5	SO4	H	618	-	4,4,4	0.93	0	6,6,6	0.38	0
5	SO4	C	620	-	4,4,4	0.41	0	6,6,6	0.17	0
2	CO3	K	612	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	L	619	-	6,6,15	1.87	1 (16%)	5,5,14	2.26	2 (40%)
5	SO4	I	620	-	4,4,4	0.92	0	6,6,6	0.32	0
6	1PE	K	620	-	5,5,15	2.07	1 (20%)	4,4,14	1.89	2 (50%)
4	DGZ	I	615	3	78,78,78	0.90	1 (1%)	99,101,101	2.37	3 (3%)
4	DGZ	K	615	3	78,78,78	0.89	1 (1%)	99,101,101	2.37	3 (3%)
5	SO4	G	619	-	4,4,4	0.82	0	6,6,6	0.28	0
6	1PE	K	618	-	11,11,15	2.14	4 (36%)	10,10,14	3.06	4 (40%)
5	SO4	J	616	-	4,4,4	0.83	0	6,6,6	0.28	0
5	SO4	D	617	-	4,4,4	0.43	0	6,6,6	0.37	0
6	1PE	J	620	-	9,9,15	2.79	5 (55%)	8,8,14	3.14	4 (50%)
6	1PE	K	617	-	7,7,15	2.39	3 (42%)	6,6,14	2.63	3 (50%)
5	SO4	C	616	-	4,4,4	0.28	0	6,6,6	0.57	0
6	1PE	F	616	-	9,9,15	2.56	5 (55%)	8,8,14	2.96	4 (50%)
6	1PE	E	620	-	9,9,15	2.22	4 (44%)	8,8,14	3.01	6 (75%)
2	CO3	F	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	E	615	3	78,78,78	0.88	1 (1%)	99,101,101	2.34	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CO3	A	612	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	J	621	-	10,10,15	2.21	4 (40%)	9,9,14	2.71	3 (33%)
6	1PE	D	619	-	7,7,15	2.26	2 (28%)	6,6,14	2.29	3 (50%)
5	SO4	K	616	-	4,4,4	0.32	0	6,6,6	0.15	0
5	SO4	J	618	-	4,4,4	0.40	0	6,6,6	0.21	0
5	SO4	A	616	-	4,4,4	0.22	0	6,6,6	0.20	0
2	CO3	H	612	-	0,3,3	0.00	-	0,3,3	0.00	-
7	2PE	H	619	-	24,24,27	0.74	0	23,23,26	0.67	0
2	CO3	G	612	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	B	612	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	G	616	-	4,4,4	0.19	0	6,6,6	0.17	0
6	1PE	F	618	-	9,9,15	3.07	5 (55%)	8,8,14	3.27	4 (50%)
5	SO4	C	618	-	4,4,4	0.18	0	6,6,6	0.18	0
6	1PE	D	621	-	4,4,15	2.86	4 (100%)	3,3,14	1.91	1 (33%)
5	SO4	I	616	-	4,4,4	0.37	0	6,6,6	0.12	0
2	CO3	I	612	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	A	618	-	8,8,15	2.05	2 (25%)	7,7,14	3.10	3 (42%)
5	SO4	D	616	-	4,4,4	0.20	0	6,6,6	0.09	0
6	1PE	G	621	-	5,5,15	1.63	1 (20%)	4,4,14	2.96	2 (50%)
6	1PE	L	620	-	10,10,15	3.12	5 (50%)	9,9,14	2.75	5 (55%)
5	SO4	G	618	-	4,4,4	0.15	0	6,6,6	0.21	0
6	1PE	C	622	-	8,8,15	2.42	3 (37%)	7,7,14	3.16	3 (42%)
5	SO4	H	617	-	4,4,4	0.21	0	6,6,6	0.14	0
6	1PE	G	623	-	14,14,15	3.18	7 (50%)	13,13,14	3.42	7 (53%)
5	SO4	I	619	-	4,4,4	0.25	0	6,6,6	0.12	0
6	1PE	L	618	-	11,11,15	2.20	4 (36%)	10,10,14	3.33	6 (60%)
2	CO3	E	612	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	E	618	-	4,4,4	0.77	0	6,6,6	0.41	0
6	1PE	C	621	-	11,11,15	2.26	4 (36%)	10,10,14	3.07	5 (50%)
6	1PE	J	622	-	8,8,15	2.36	3 (37%)	7,7,14	2.95	3 (42%)
6	1PE	E	619	-	11,11,15	2.43	4 (36%)	10,10,14	3.11	6 (60%)
2	CO3	D	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	C	615	3	78,78,78	0.89	1 (1%)	99,101,101	2.36	3 (3%)
4	DGZ	B	615	3	78,78,78	0.89	1 (1%)	99,101,101	2.36	2 (2%)
6	1PE	G	622	-	5,5,15	1.62	1 (20%)	4,4,14	3.09	2 (50%)
4	DGZ	D	615	3	78,78,78	0.89	1 (1%)	99,101,101	2.38	3 (3%)
5	SO4	C	619	-	4,4,4	0.79	0	6,6,6	0.32	0
6	1PE	I	623	-	4,4,15	1.69	1 (25%)	3,3,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DGZ	F	615	3	78,78,78	0.92	1 (1%)	99,101,101	2.38	2 (2%)
5	SO4	I	618	-	4,4,4	0.71	0	6,6,6	0.25	0
2	CO3	J	612	-	0,3,3	0.00	-	0,3,3	0.00	-
4	DGZ	G	615	3	78,78,78	0.88	1 (1%)	99,101,101	2.33	3 (3%)
6	1PE	D	618	-	9,9,15	2.22	3 (33%)	8,8,14	3.07	4 (50%)
6	1PE	J	619	-	10,10,15	2.54	5 (50%)	9,9,14	2.13	5 (55%)
6	1PE	E	621	-	7,7,15	2.22	3 (42%)	6,6,14	2.76	4 (66%)
4	DGZ	A	615	3	78,78,78	0.91	1 (1%)	99,101,101	2.33	3 (3%)
5	SO4	E	617	-	4,4,4	0.37	0	6,6,6	0.10	0
2	CO3	L	612	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	J	617	-	4,4,4	0.21	0	6,6,6	0.17	0
6	1PE	K	619	-	10,10,15	2.68	5 (50%)	9,9,14	2.61	5 (55%)
6	1PE	F	617	-	9,9,15	2.60	4 (44%)	8,8,14	2.99	5 (62%)
5	SO4	G	617	-	4,4,4	0.81	0	6,6,6	0.42	0
2	CO3	C	612	-	0,3,3	0.00	-	0,3,3	0.00	-
7	2PE	B	616	-	25,25,27	0.94	0	24,24,26	0.57	0
5	SO4	A	617	-	4,4,4	0.54	0	6,6,6	0.25	0

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
6	1PE	G	620	-	-	4/6/6/13	-
6	1PE	D	620	-	-	4/8/8/13	-
6	1PE	J	620	-	-	6/7/7/13	-
6	1PE	A	618	-	-	0/6/6/13	-
4	DGZ	H	615	3	-	19/75/76/76	0/5/5/5
6	1PE	G	621	-	-	1/3/3/13	-
6	1PE	L	620	-	-	5/8/8/13	-
6	1PE	C	622	-	-	4/6/6/13	-
6	1PE	K	617	-	-	3/5/5/13	-
6	1PE	I	622	-	-	2/7/7/13	-
6	1PE	G	623	-	-	7/12/12/13	-
6	1PE	I	623	-	-	1/2/2/13	-
6	1PE	C	621	-	-	5/9/9/13	-
6	1PE	F	616	-	-	6/7/7/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	E	620	-	-	2/7/7/13	-
4	DGZ	F	615	3	-	20/75/76/76	0/5/5/5
4	DGZ	J	615	3	-	14/75/76/76	0/5/5/5
4	DGZ	L	615	3	-	17/75/76/76	0/5/5/5
6	1PE	I	621	-	-	4/9/9/13	-
4	DGZ	E	615	3	-	20/75/76/76	0/5/5/5
4	DGZ	G	615	3	-	21/75/76/76	0/5/5/5
6	1PE	D	618	-	-	5/7/7/13	-
6	1PE	L	617	-	-	4/7/7/13	-
6	1PE	J	621	-	-	4/8/8/13	-
6	1PE	A	619	-	-	1/4/4/13	-
6	1PE	D	619	-	-	1/5/5/13	-
6	1PE	J	619	-	-	6/8/8/13	-
6	1PE	L	619	-	-	3/4/4/13	-
4	DGZ	A	615	3	-	24/75/76/76	0/5/5/5
6	1PE	J	622	-	-	5/6/6/13	-
6	1PE	L	618	-	-	5/9/9/13	-
6	1PE	E	621	-	-	2/5/5/13	-
6	1PE	E	619	-	-	5/9/9/13	-
6	1PE	K	619	-	-	3/8/8/13	-
6	1PE	K	620	-	-	3/3/3/13	-
4	DGZ	I	615	3	-	20/75/76/76	0/5/5/5
7	2PE	H	619	-	-	13/22/22/25	-
4	DGZ	K	615	3	-	20/75/76/76	0/5/5/5
6	1PE	F	617	-	-	4/7/7/13	-
6	1PE	K	618	-	-	6/9/9/13	-
4	DGZ	C	615	3	-	20/75/76/76	0/5/5/5
4	DGZ	B	615	3	-	13/75/76/76	0/5/5/5
7	2PE	B	616	-	-	9/23/23/25	-
6	1PE	G	622	-	-	3/3/3/13	-
4	DGZ	D	615	3	-	11/75/76/76	0/5/5/5
6	1PE	F	618	-	-	4/7/7/13	-
6	1PE	D	621	-	-	2/2/2/13	-

The worst 5 of 128 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	623	1PE	C26-C16	5.05	1.76	1.49
6	G	623	1PE	OH4-C13	4.96	1.63	1.42
4	K	615	DGZ	C2-C1	4.93	1.32	1.18
4	J	615	DGZ	C2-C1	4.90	1.32	1.18
4	H	615	DGZ	C2-C1	4.88	1.32	1.18

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	615	DGZ	C3-C2-C1	-22.10	119.55	177.14
4	F	615	DGZ	C3-C2-C1	-22.07	119.64	177.14
4	D	615	DGZ	C3-C2-C1	-21.99	119.86	177.14
4	I	615	DGZ	C3-C2-C1	-21.92	120.03	177.14
4	E	615	DGZ	C3-C2-C1	-21.89	120.11	177.14

There are no chirality outliers.

5 of 361 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	615	DGZ	N5-C47-C48-O9
4	H	615	DGZ	O9-C48-C49-C50
4	H	615	DGZ	C47-C48-C49-N6
4	H	615	DGZ	C48-C49-C50-C51
4	J	615	DGZ	N5-C47-C48-O9

There are no ring outliers.

37 monomers are involved in 122 short contacts:

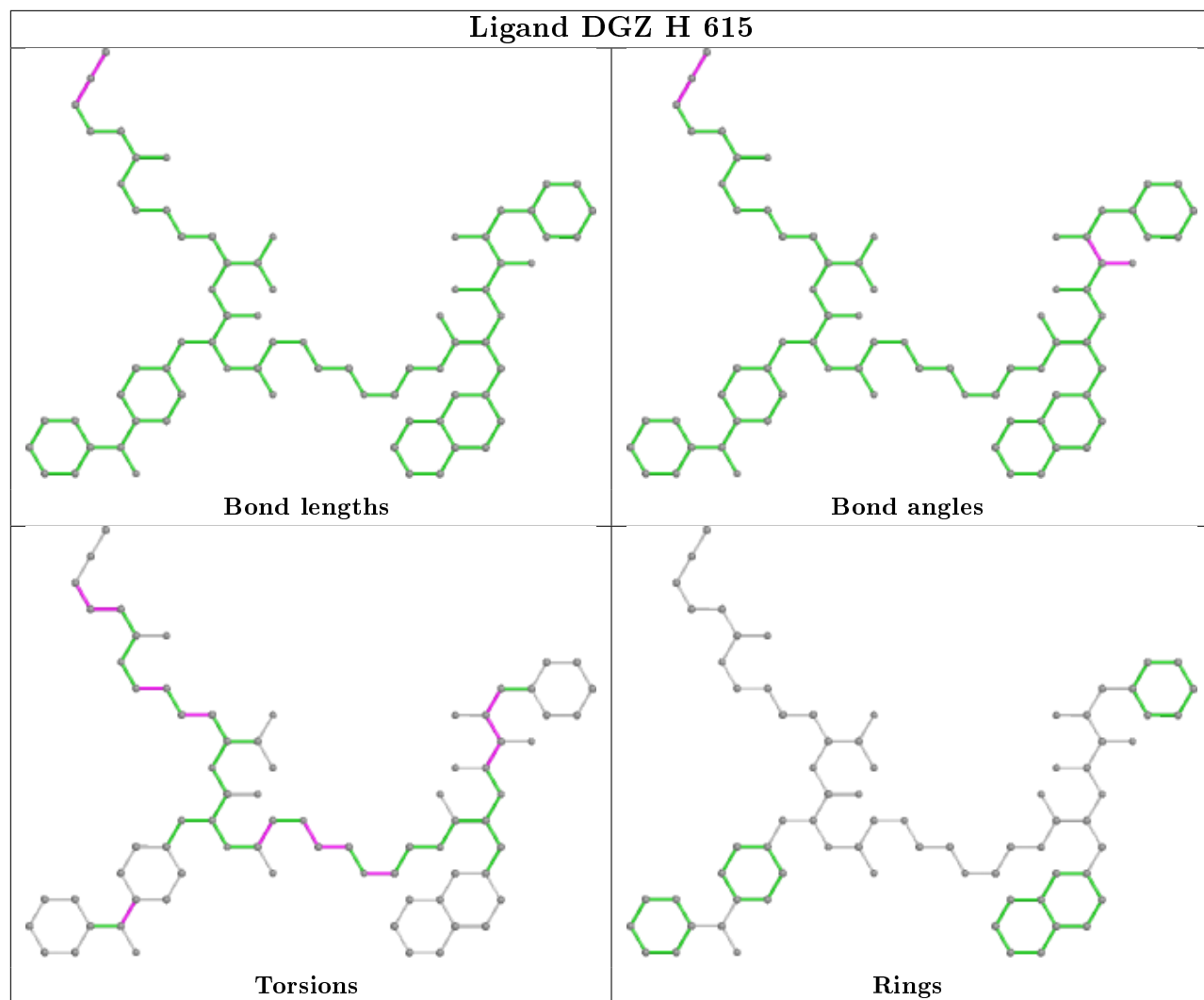
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	620	1PE	1	0
4	H	615	DGZ	8	0
4	J	615	DGZ	5	0
4	L	615	DGZ	6	0
6	I	621	1PE	1	0
6	L	617	1PE	2	0
6	L	619	1PE	1	0
4	I	615	DGZ	4	0
4	K	615	DGZ	4	0
5	G	619	SO4	1	0
6	J	620	1PE	5	0
6	K	617	1PE	1	0
2	F	612	CO3	1	0

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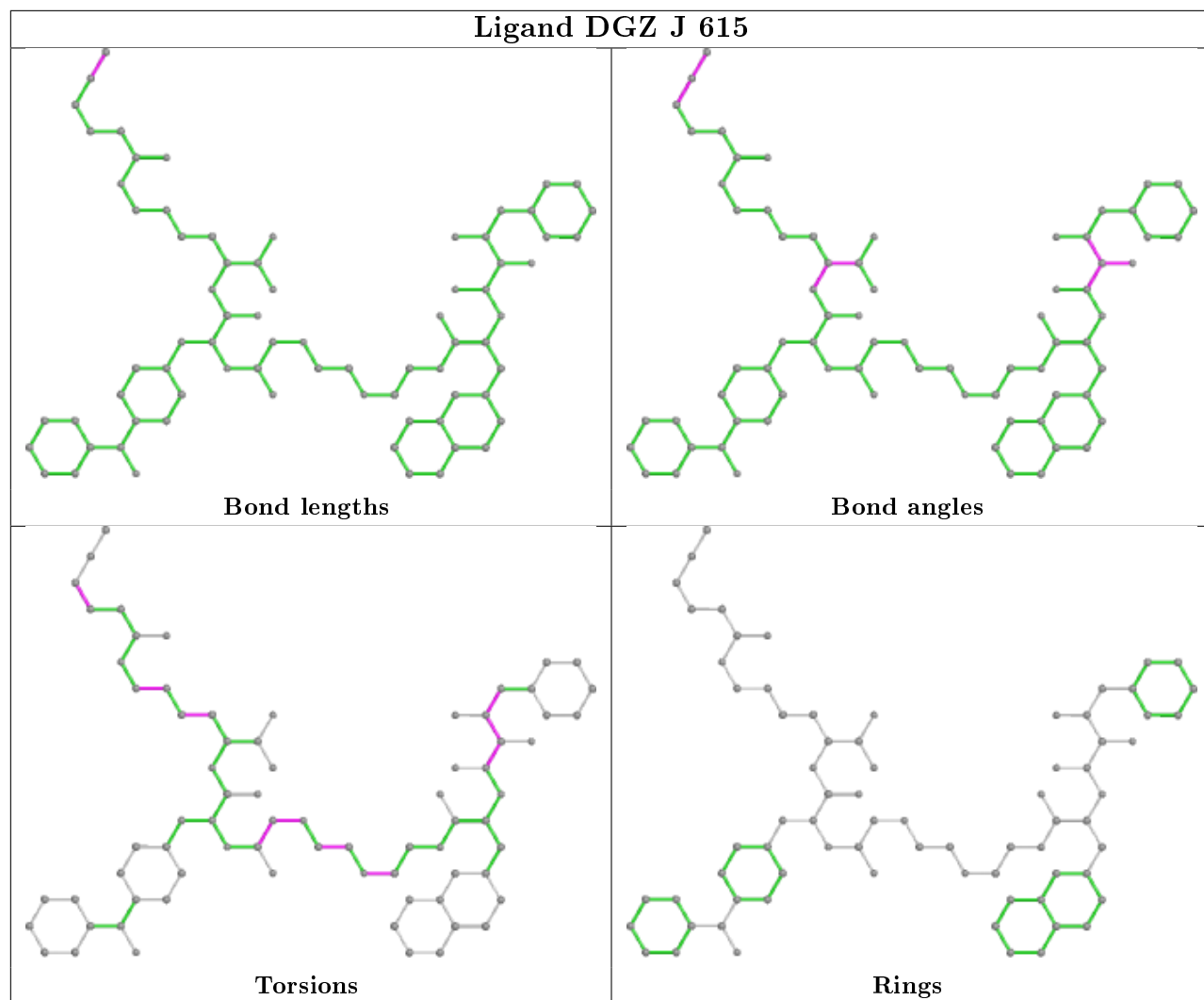
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	615	DGZ	5	0
6	J	621	1PE	3	0
7	H	619	2PE	2	0
6	F	618	1PE	4	0
6	L	620	1PE	3	0
6	C	622	1PE	1	0
6	G	623	1PE	7	0
6	L	618	1PE	2	0
6	C	621	1PE	1	0
6	J	622	1PE	3	0
6	E	619	1PE	1	0
4	C	615	DGZ	5	0
4	B	615	DGZ	9	0
6	G	622	1PE	1	0
4	D	615	DGZ	3	0
6	I	623	1PE	4	0
4	F	615	DGZ	9	0
5	I	618	SO4	1	0
2	J	612	CO3	1	0
4	G	615	DGZ	5	0
6	D	618	1PE	1	0
6	J	619	1PE	1	0
4	A	615	DGZ	12	0
6	F	617	1PE	3	0

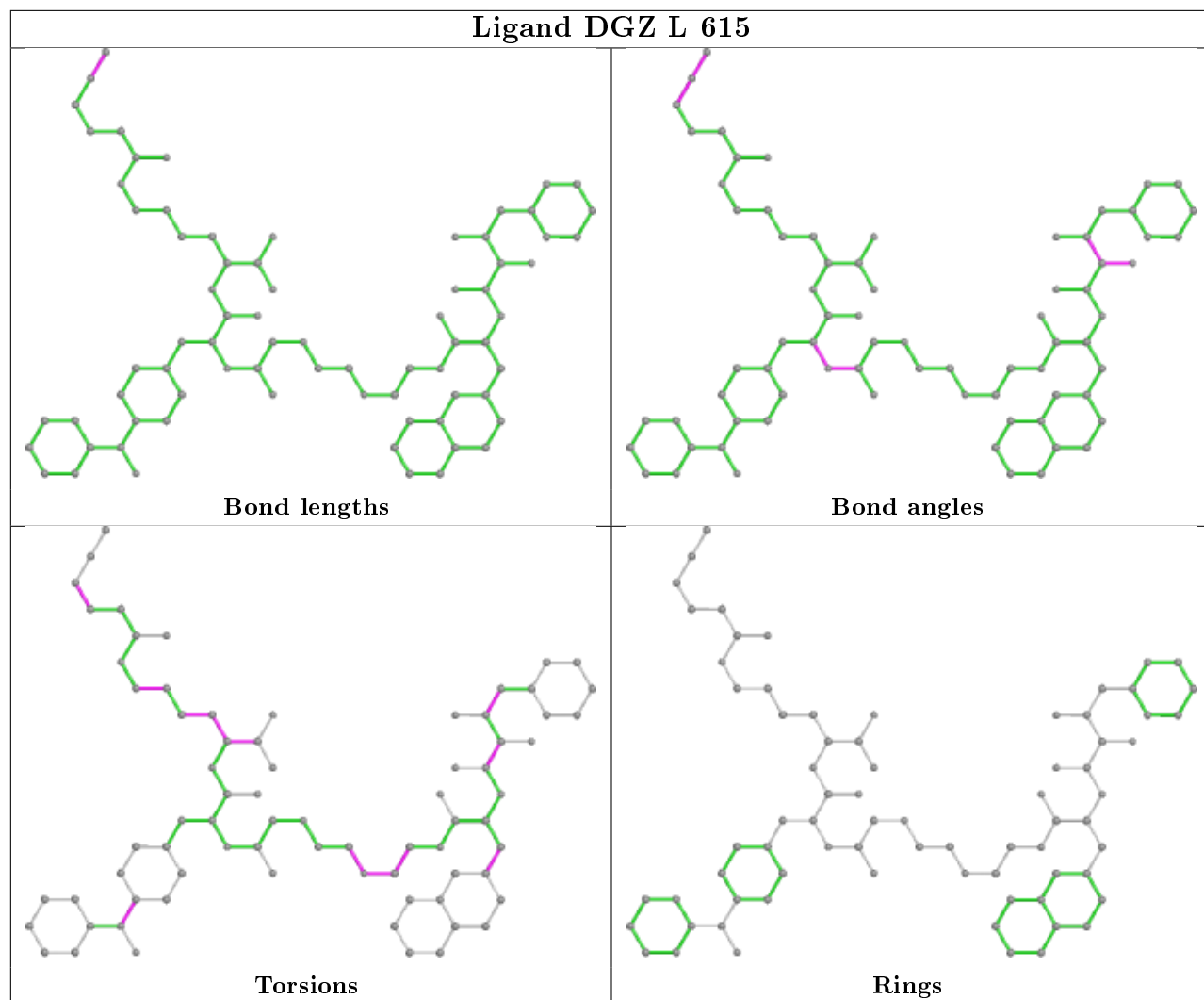
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



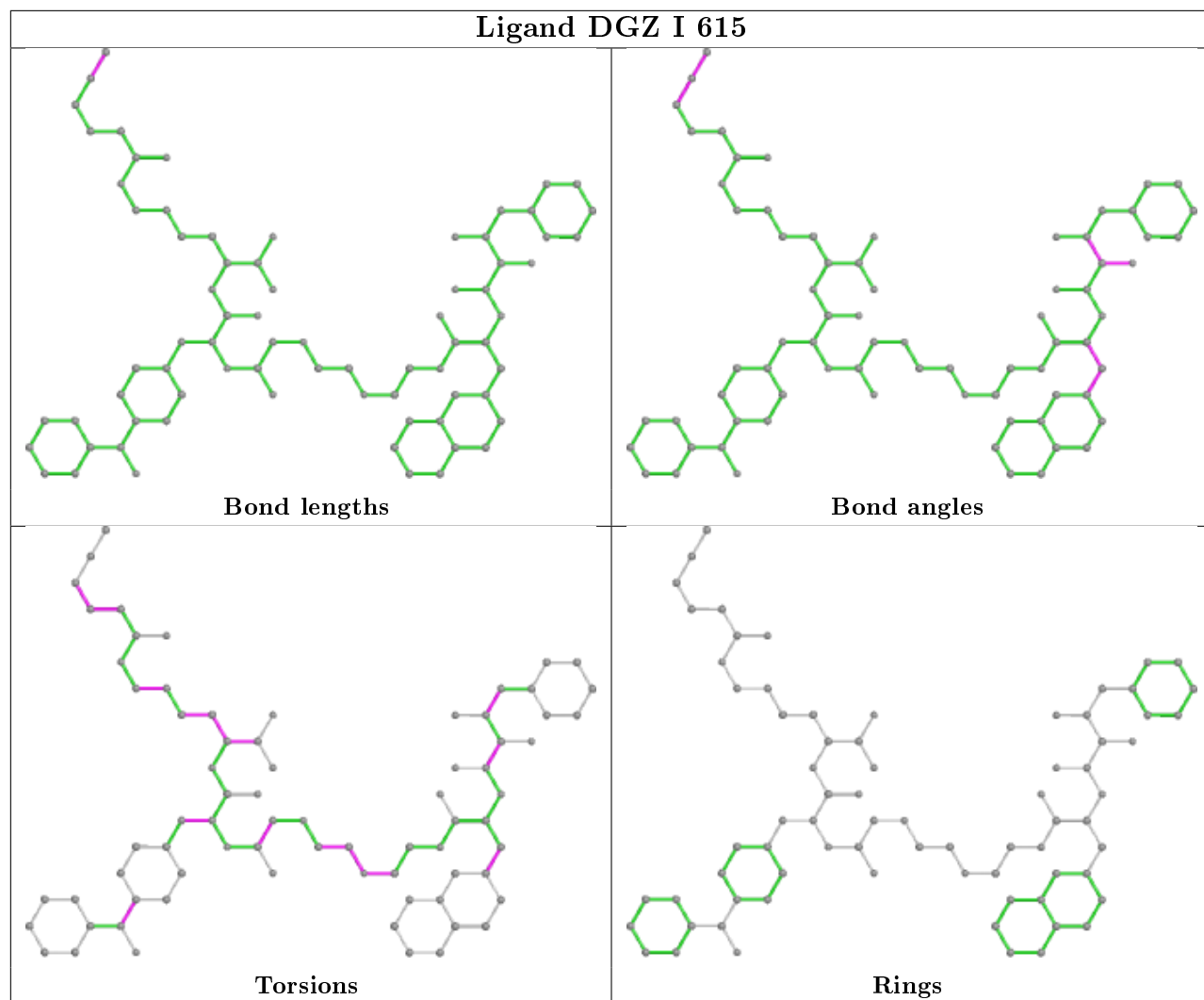
Ligand DGZ J 615

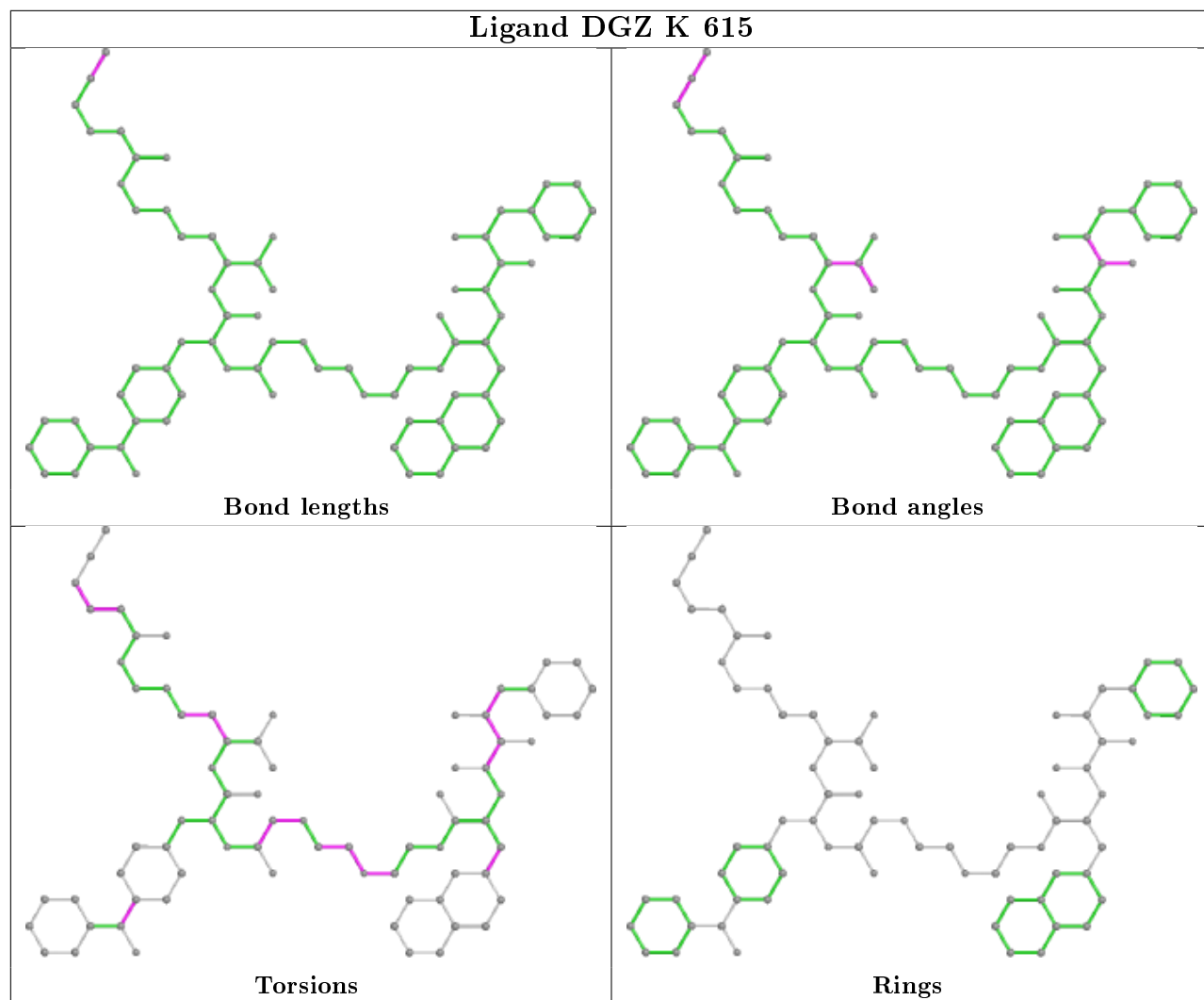


Ligand DGZ L 615

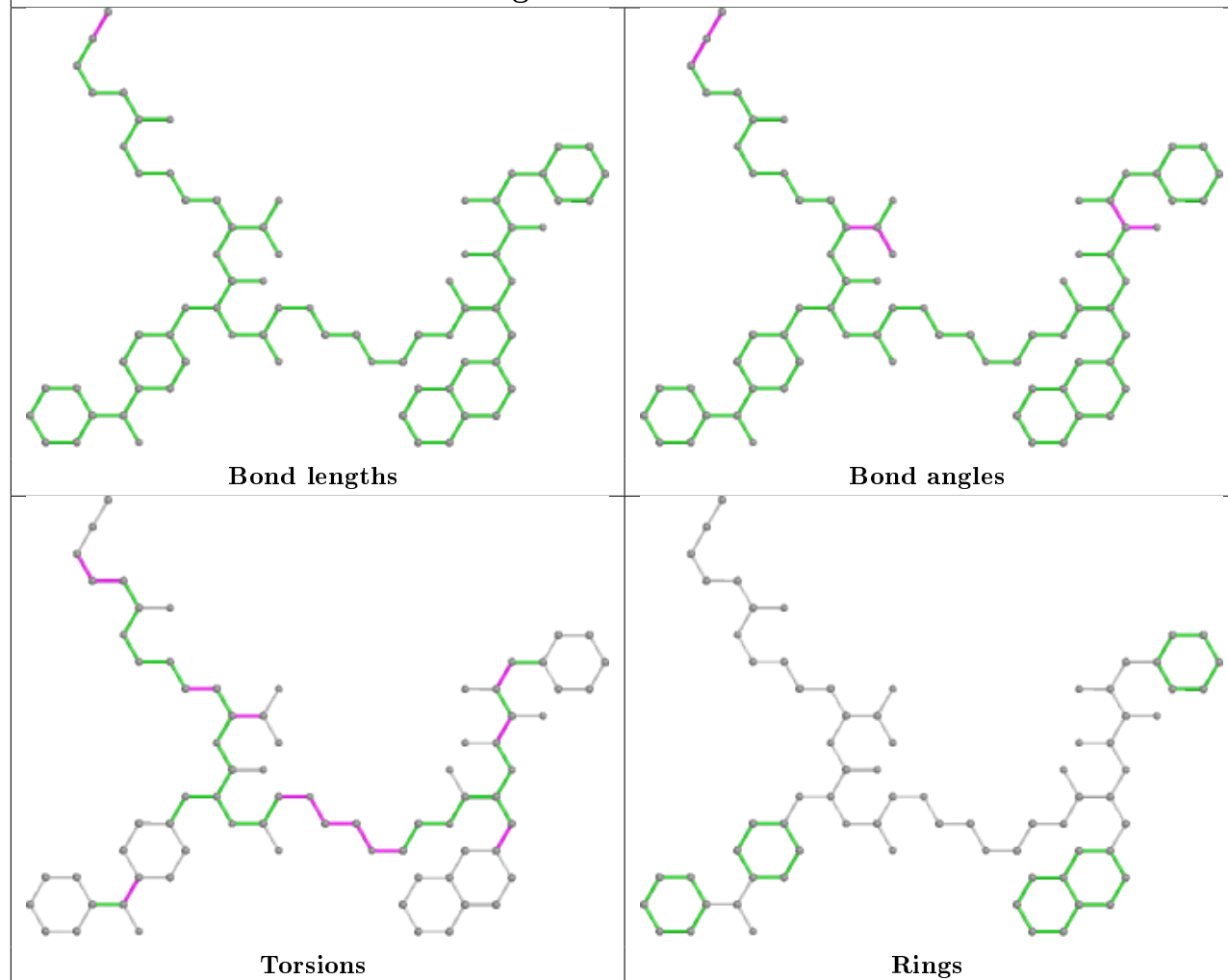


Ligand DGZ I 615

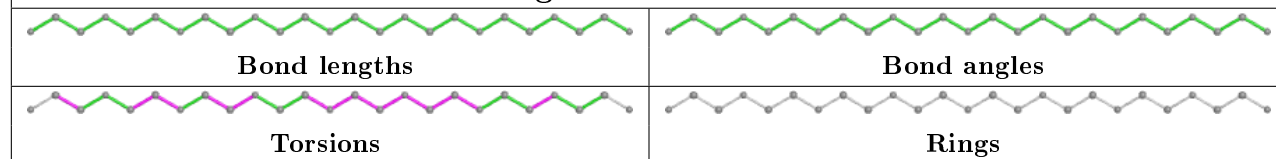


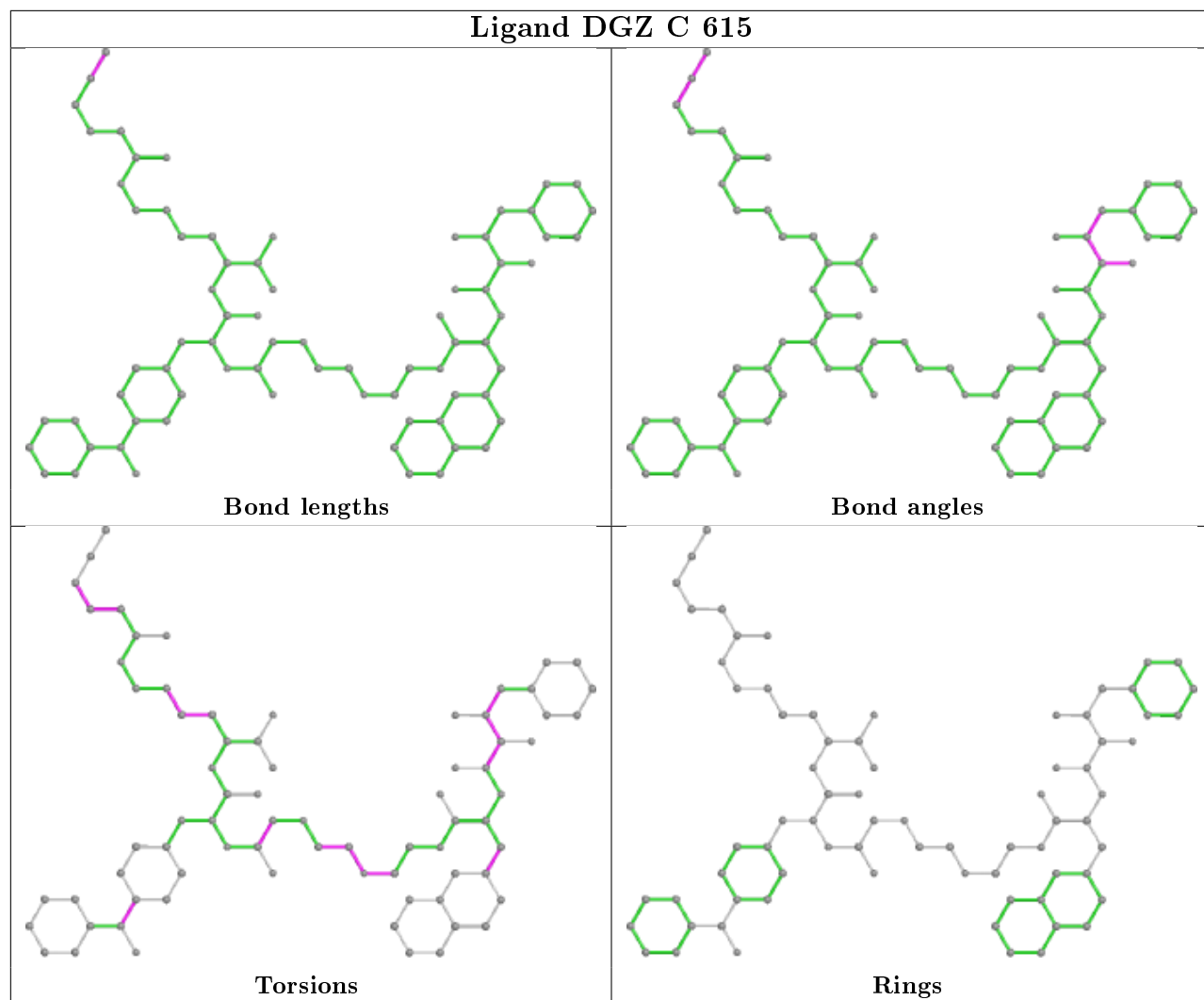


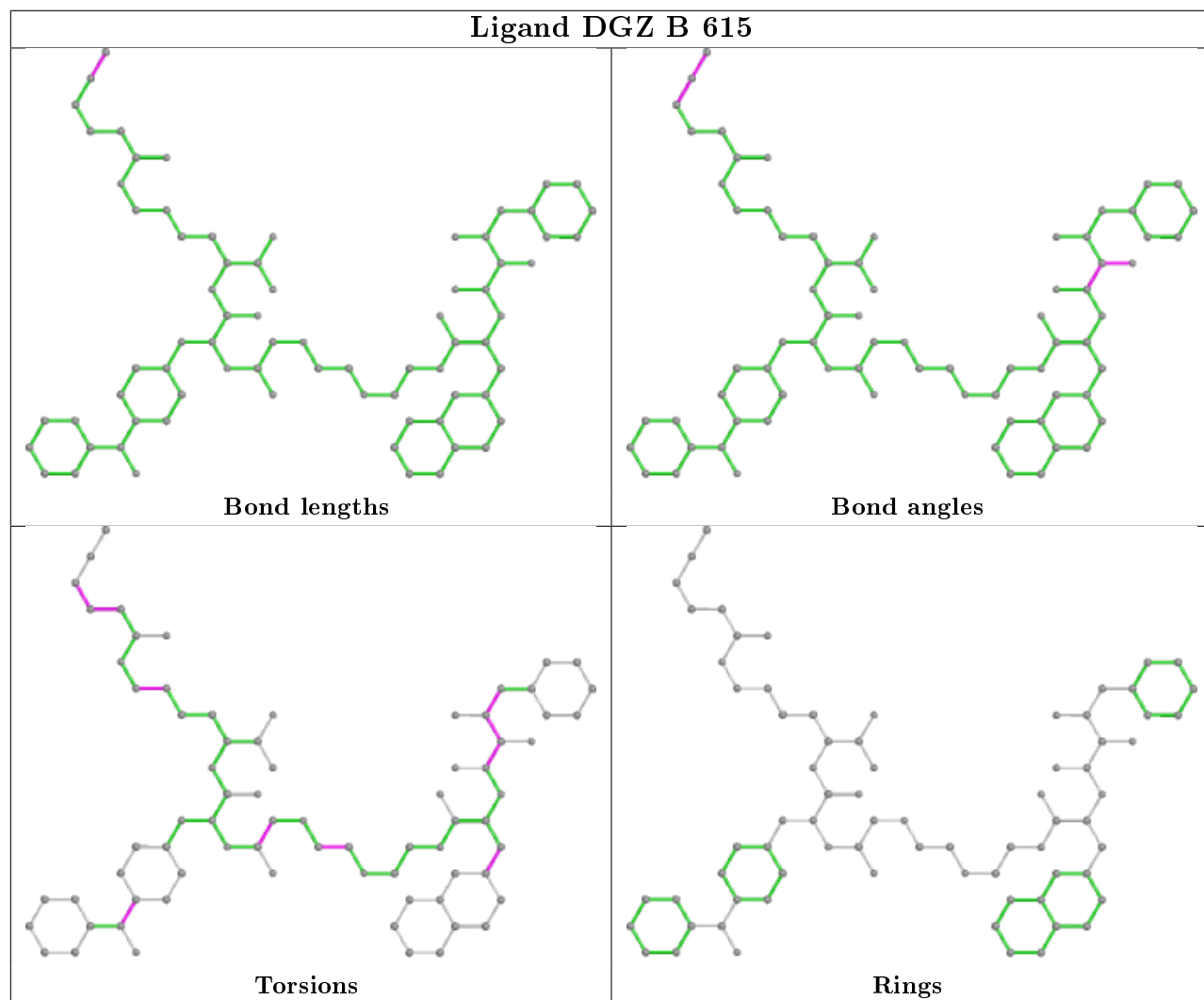
Ligand DGZ E 615

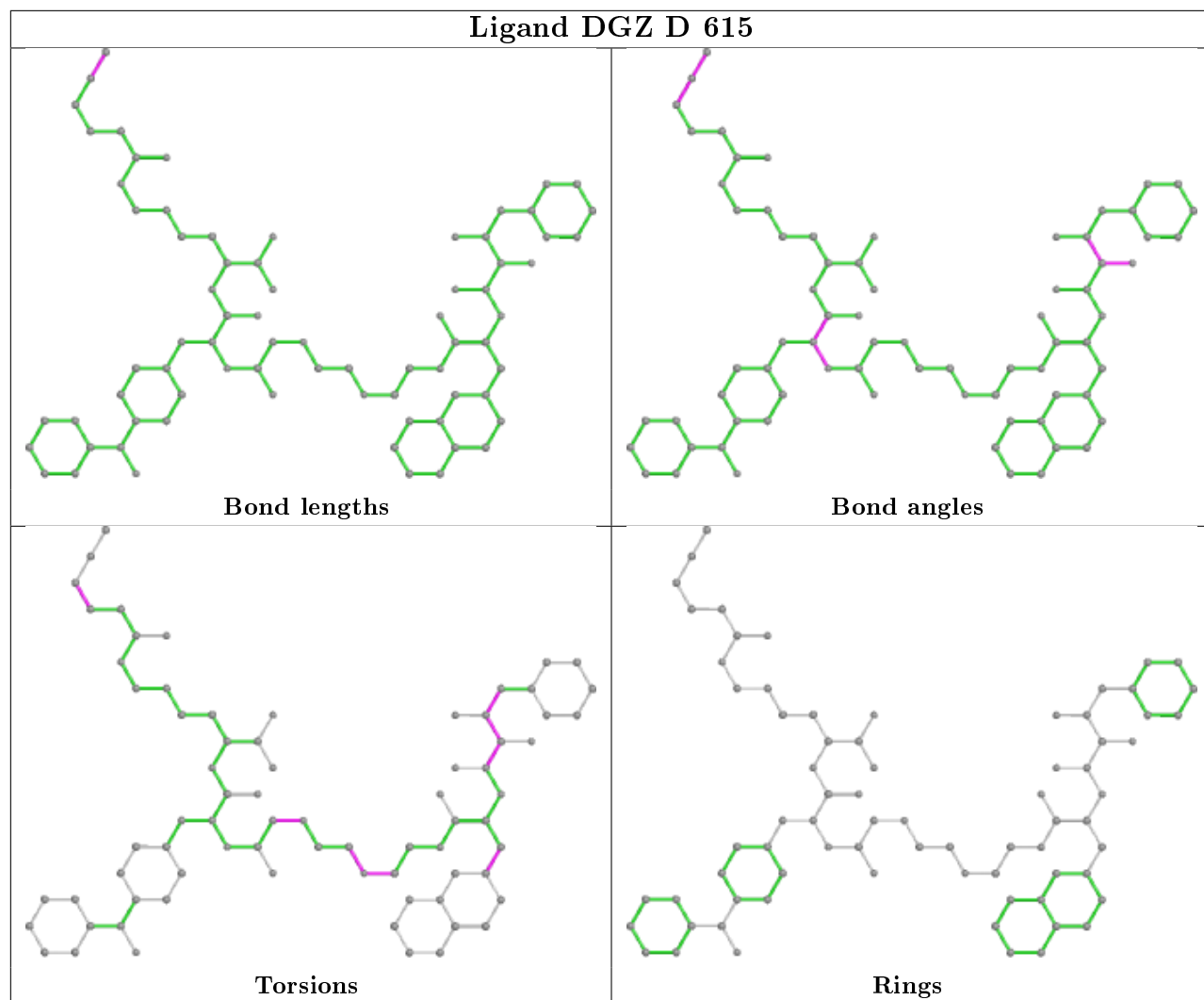


Ligand 2PE H 619

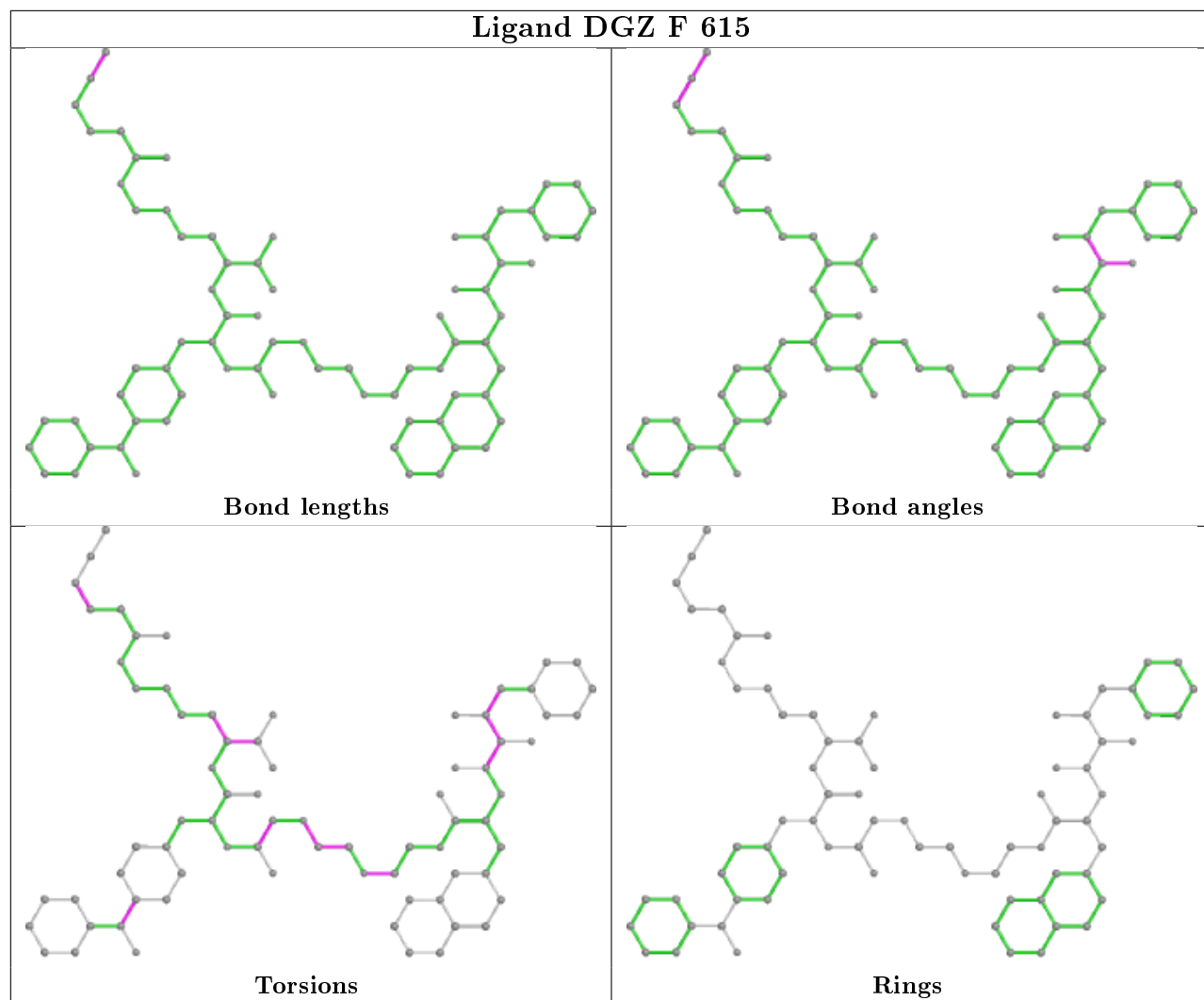


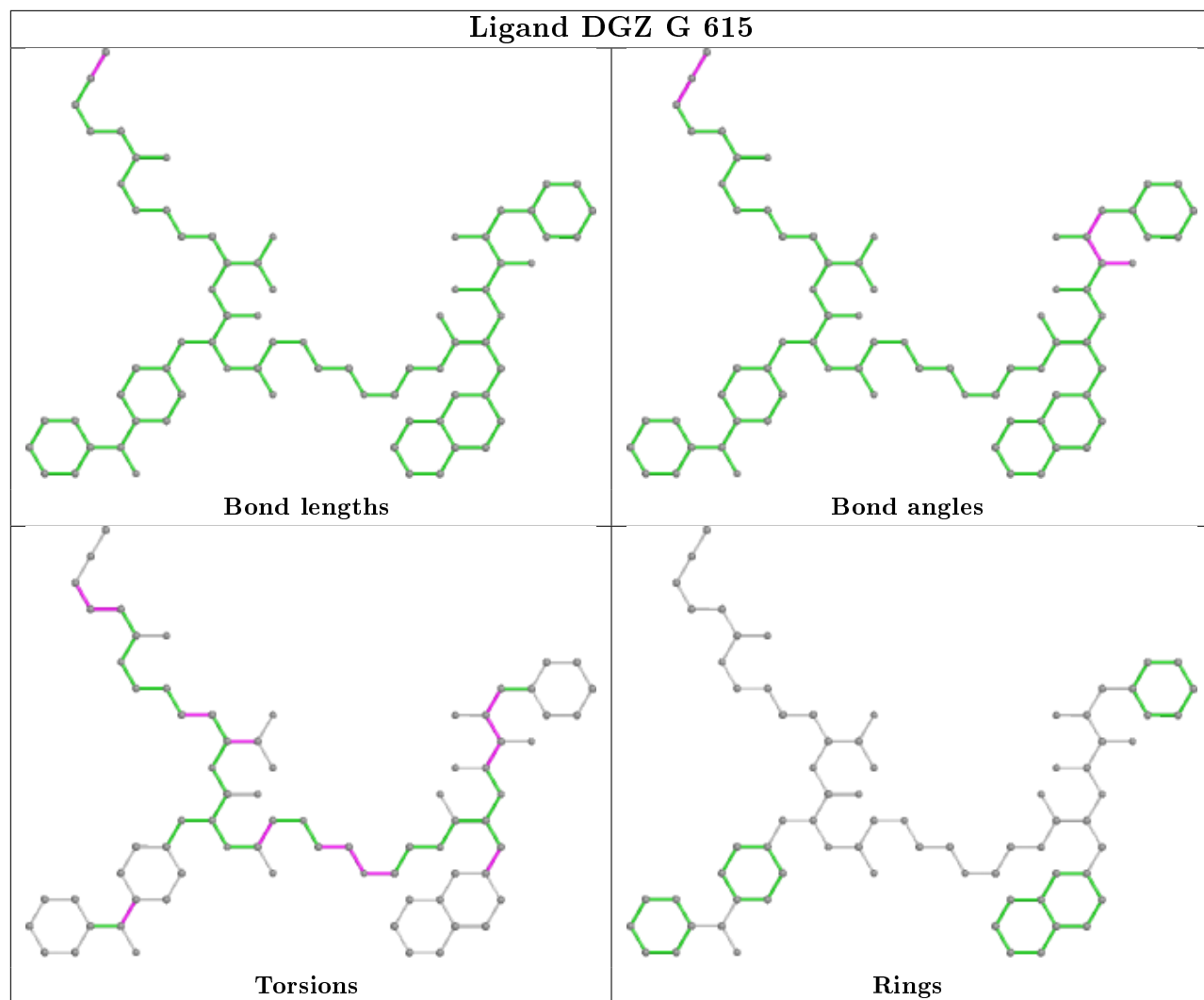


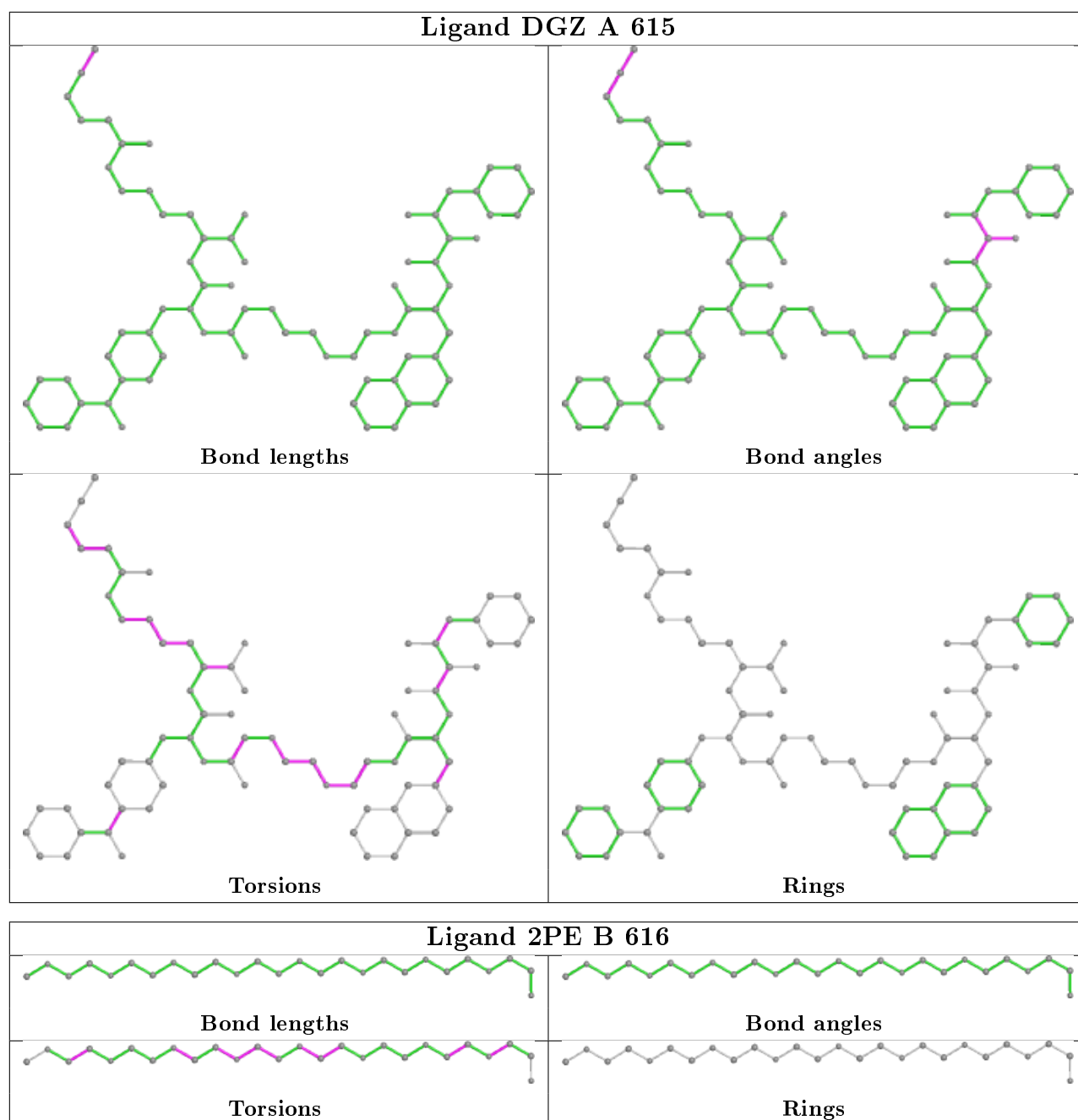




Ligand DGZ F 615







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	547:ILE	C	548:SER	N	1.15

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	519/528 (98%)	-0.43	3 (0%) 89 88	5, 15, 35, 70	0
1	B	517/528 (97%)	-0.33	9 (1%) 70 68	5, 17, 46, 73	1 (0%)
1	C	516/528 (97%)	-0.43	3 (0%) 89 88	5, 15, 39, 76	0
1	D	514/528 (97%)	-0.47	6 (1%) 79 78	6, 14, 35, 80	0
1	E	509/528 (96%)	-0.55	0 100 100	7, 14, 30, 48	0
1	F	511/528 (96%)	-0.22	9 (1%) 68 66	6, 18, 40, 71	0
1	G	517/528 (97%)	-0.42	3 (0%) 89 88	6, 14, 36, 61	0
1	H	518/528 (98%)	-0.32	6 (1%) 79 78	6, 18, 46, 68	1 (0%)
1	I	518/528 (98%)	-0.43	2 (0%) 92 92	5, 16, 39, 81	0
1	J	514/528 (97%)	-0.44	5 (0%) 82 81	7, 15, 37, 82	0
1	K	509/528 (96%)	-0.54	0 100 100	7, 15, 32, 47	0
1	L	511/528 (96%)	-0.33	5 (0%) 82 81	6, 16, 37, 64	0
All	All	6173/6336 (97%)	-0.41	51 (0%) 86 85	5, 15, 39, 82	2 (0%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	138	GLU	6.0
1	F	551	VAL	5.4
1	L	136	GLY	5.3
1	L	550	SER	4.5
1	J	260	ASN	4.4

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(Å ²)	Q<0.9
6	1PE	D	621	5/16	0.68	0.30	26,28,34,37	0
6	1PE	J	622	9/16	0.68	0.26	45,50,55,55	0
5	SO4	C	618	5/5	0.69	0.33	100,104,104,106	0
6	1PE	D	619	8/16	0.71	0.21	52,53,54,55	0
5	SO4	C	617	5/5	0.75	0.27	95,99,100,101	0
6	1PE	G	623	15/16	0.76	0.21	42,48,57,58	0
5	SO4	G	618	5/5	0.78	0.23	74,77,80,80	0
6	1PE	J	621	11/16	0.79	0.21	38,38,41,43	0
7	2PE	B	616	26/28	0.79	0.27	42,48,56,57	0
5	SO4	C	619	5/5	0.80	0.35	48,51,54,54	0
7	2PE	H	619	25/28	0.80	0.22	40,44,55,57	0
2	CO3	I	612	4/4	0.81	0.26	10,11,12,14	0
6	1PE	L	618	12/16	0.82	0.18	25,35,48,48	0
6	1PE	D	620	11/16	0.82	0.20	35,39,46,48	0
6	1PE	E	619	12/16	0.83	0.20	40,42,46,47	0
2	CO3	G	612	4/4	0.83	0.23	4,9,10,12	0
5	SO4	I	618	5/5	0.83	0.29	57,61,62,63	0
5	SO4	E	616	5/5	0.83	0.34	90,94,95,96	0
2	CO3	F	612	4/4	0.84	0.24	9,11,13,15	0
6	1PE	L	620	11/16	0.84	0.20	39,42,45,45	0
2	CO3	H	612	4/4	0.85	0.21	5,11,12,14	0
2	CO3	J	612	4/4	0.85	0.20	11,11,13,14	0
6	1PE	A	619	7/16	0.85	0.23	43,44,48,51	0
6	1PE	F	618	10/16	0.85	0.16	36,40,44,44	0
5	SO4	K	616	5/5	0.85	0.36	72,76,78,79	0
5	SO4	A	617	5/5	0.85	0.19	54,55,59,59	0
6	1PE	C	621	12/16	0.86	0.18	42,44,47,48	0
5	SO4	I	619	5/5	0.86	0.17	90,94,95,96	0
5	SO4	H	618	5/5	0.86	0.23	45,47,50,52	0
2	CO3	L	612	4/4	0.87	0.20	9,10,12,14	0
6	1PE	F	616	10/16	0.87	0.14	29,32,40,41	0
6	1PE	K	619	11/16	0.87	0.14	25,39,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	H	617	5/5	0.87	0.27	80,84,86,86	0
2	CO3	D	612	4/4	0.87	0.23	10,12,15,15	0
6	1PE	F	617	10/16	0.88	0.22	46,50,52,52	0
6	1PE	C	622	9/16	0.88	0.15	27,29,35,40	0
2	CO3	E	612	4/4	0.88	0.23	6,13,14,16	0
6	1PE	I	621	12/16	0.89	0.21	35,37,40,43	0
5	SO4	L	616	5/5	0.89	0.32	41,43,48,48	0
5	SO4	G	619	5/5	0.89	0.33	45,49,50,52	0
6	1PE	J	620	10/16	0.89	0.19	27,35,41,41	0
6	1PE	D	618	10/16	0.90	0.16	30,34,40,40	0
5	SO4	E	617	5/5	0.90	0.35	73,78,79,79	0
5	SO4	D	616	5/5	0.90	0.39	73,78,78,80	0
6	1PE	K	617	8/16	0.90	0.14	32,37,42,43	0
5	SO4	J	618	5/5	0.90	0.27	57,60,62,62	0
6	1PE	K	618	12/16	0.90	0.17	25,31,40,40	0
5	SO4	E	618	5/5	0.90	0.26	52,55,59,59	0
6	1PE	L	619	7/16	0.90	0.17	30,32,35,35	0
5	SO4	C	620	5/5	0.91	0.25	52,56,58,58	0
2	CO3	K	612	4/4	0.91	0.17	10,10,10,11	0
6	1PE	G	620	9/16	0.91	0.14	24,26,31,31	0
6	1PE	E	621	8/16	0.92	0.23	31,34,36,37	0
5	SO4	I	620	5/5	0.92	0.28	39,41,44,47	0
6	1PE	K	620	6/16	0.92	0.11	30,31,32,33	0
4	DGZ	H	615	74/74	0.92	0.16	4,38,142,180	0
5	SO4	J	617	5/5	0.92	0.40	77,81,82,83	0
5	SO4	I	616	5/5	0.92	0.41	75,80,80,80	0
4	DGZ	F	615	74/74	0.92	0.16	8,35,127,202	0
5	SO4	G	617	5/5	0.92	0.24	36,40,41,42	0
5	SO4	G	616	5/5	0.92	0.31	75,79,81,81	0
6	1PE	A	618	9/16	0.92	0.12	23,24,26,29	0
4	DGZ	A	615	74/74	0.93	0.16	5,38,181,208	0
6	1PE	G	621	6/16	0.93	0.21	25,25,27,32	0
6	1PE	G	622	6/16	0.93	0.10	30,30,30,32	0
4	DGZ	I	615	74/74	0.93	0.16	5,42,189,216	0
2	CO3	A	612	4/4	0.93	0.16	12,12,14,15	0
4	DGZ	G	615	74/74	0.94	0.15	6,36,151,232	0
4	DGZ	L	615	74/74	0.94	0.14	7,33,109,190	0
5	SO4	A	616	5/5	0.94	0.31	62,67,67,67	0
4	DGZ	E	615	74/74	0.94	0.15	10,41,146,207	0
4	DGZ	C	615	74/74	0.94	0.15	10,38,182,231	0
4	DGZ	B	615	74/74	0.94	0.15	9,37,133,171	0
5	SO4	I	617	5/5	0.94	0.25	43,46,49,49	0

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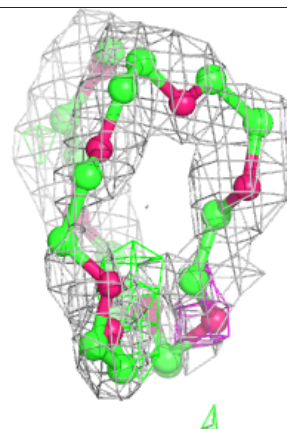
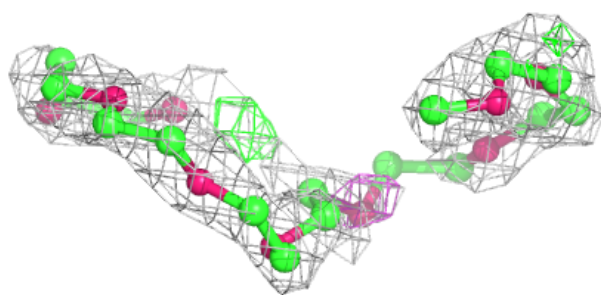
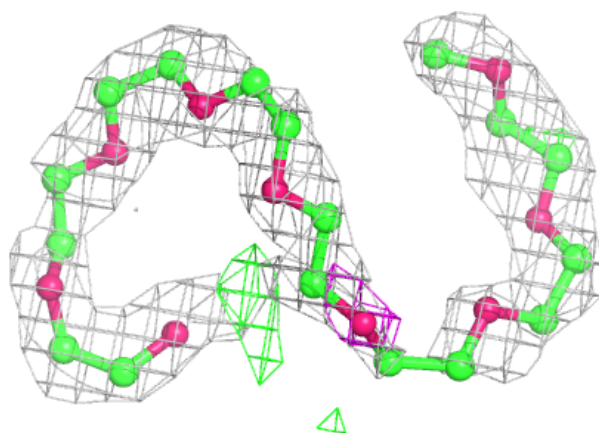
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DGZ	D	615	74/74	0.94	0.15	7,34,121,208	0
4	DGZ	K	615	74/74	0.94	0.15	7,41,147,213	0
2	CO3	B	612	4/4	0.94	0.13	14,14,15,15	0
6	1PE	E	620	10/16	0.94	0.15	26,27,35,41	0
2	CO3	C	612	4/4	0.94	0.16	12,12,13,15	0
4	DGZ	J	615	74/74	0.94	0.16	8,34,179,236	0
6	1PE	I	623	5/16	0.94	0.16	14,14,16,18	0
6	1PE	I	622	10/16	0.95	0.15	21,23,34,35	0
6	1PE	L	617	10/16	0.95	0.12	17,27,36,40	0
6	1PE	J	619	11/16	0.95	0.15	19,23,34,38	0
5	SO4	D	617	5/5	0.99	0.09	12,13,14,17	0
3	ZN	K	614	1/1	0.99	0.06	29,29,29,29	0
3	ZN	F	614	1/1	0.99	0.05	27,27,27,27	0
3	ZN	E	614	1/1	0.99	0.07	28,28,28,28	0
3	ZN	D	614	1/1	0.99	0.05	29,29,29,29	0
3	ZN	C	614	1/1	0.99	0.05	25,25,25,25	0
5	SO4	H	616	5/5	0.99	0.09	12,12,14,14	0
5	SO4	C	616	5/5	0.99	0.07	9,9,10,12	0
3	ZN	I	614	1/1	0.99	0.06	27,27,27,27	0
5	SO4	J	616	5/5	0.99	0.09	14,14,17,17	0
3	ZN	G	614	1/1	1.00	0.05	27,27,27,27	0
3	ZN	C	613	1/1	1.00	0.04	17,17,17,17	0
3	ZN	L	614	1/1	1.00	0.05	17,17,17,17	0
3	ZN	L	613	1/1	1.00	0.05	27,27,27,27	0
3	ZN	J	613	1/1	1.00	0.07	19,19,19,19	0
3	ZN	B	614	1/1	1.00	0.04	16,16,16,16	0
3	ZN	H	613	1/1	1.00	0.04	19,19,19,19	0
3	ZN	K	613	1/1	1.00	0.04	18,18,18,18	0
3	ZN	J	614	1/1	1.00	0.07	24,24,24,24	0
3	ZN	A	614	1/1	1.00	0.06	17,17,17,17	0
3	ZN	H	614	1/1	1.00	0.05	29,29,29,29	0
3	ZN	D	613	1/1	1.00	0.05	16,16,16,16	0
3	ZN	E	613	1/1	1.00	0.04	18,18,18,18	0
3	ZN	I	613	1/1	1.00	0.05	17,17,17,17	0
3	ZN	B	613	1/1	1.00	0.05	26,26,26,26	0
3	ZN	F	613	1/1	1.00	0.05	17,17,17,17	0
3	ZN	G	613	1/1	1.00	0.05	16,16,16,16	0
3	ZN	A	613	1/1	1.00	0.07	26,26,26,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

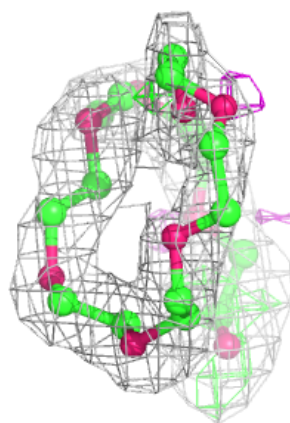
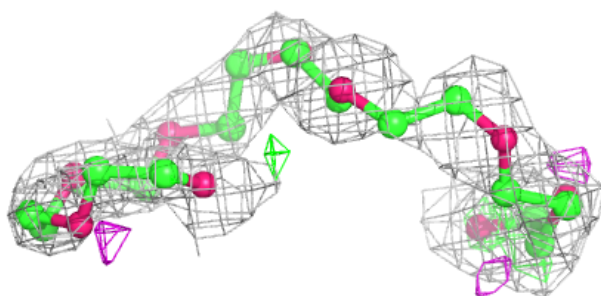
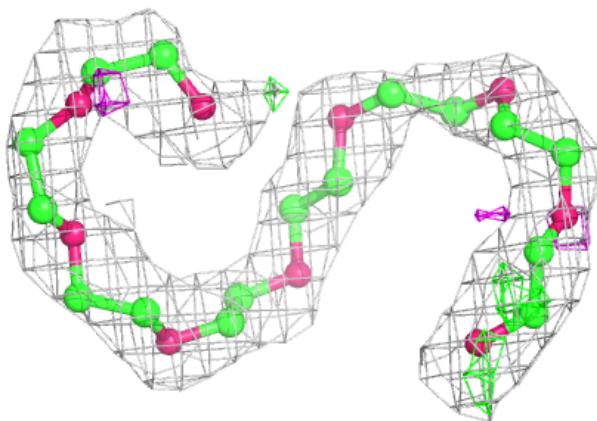
Electron density around 2PE B 616:

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



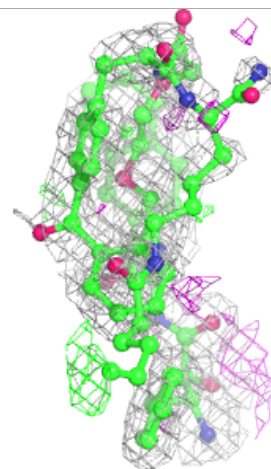
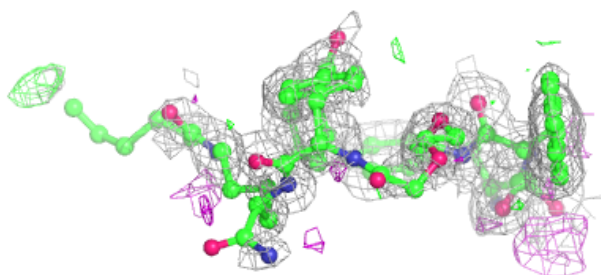
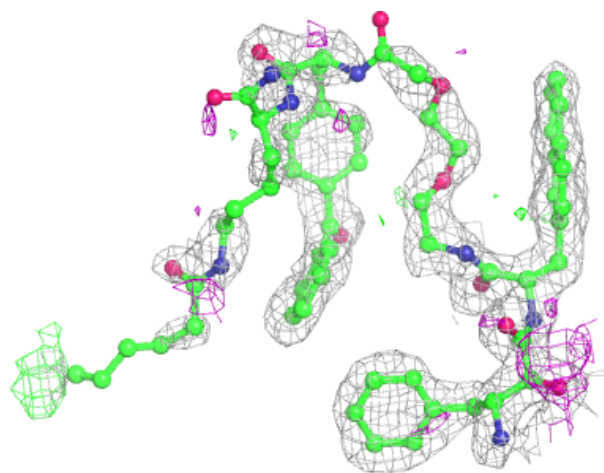
Electron density around 2PE H 619:

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



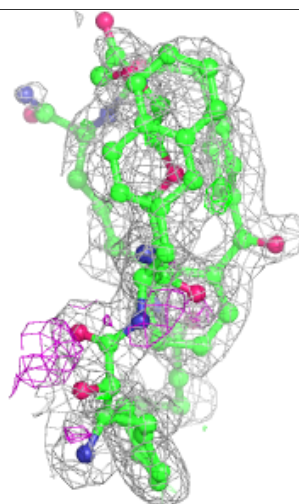
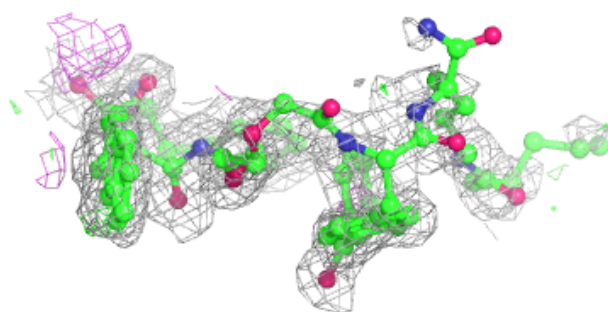
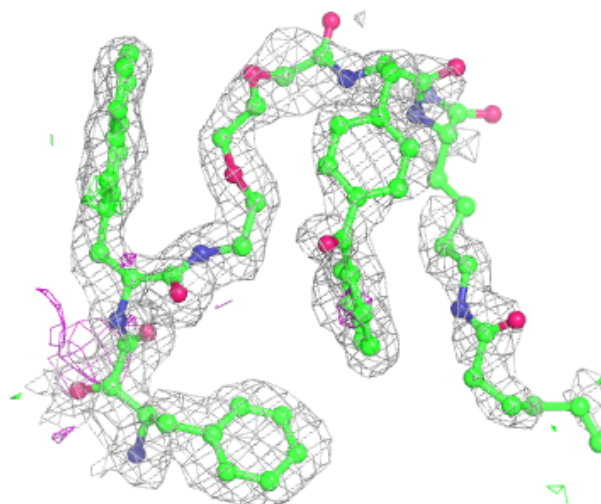
Electron density around DGZ H 615:

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



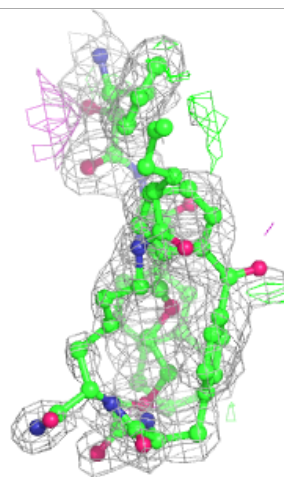
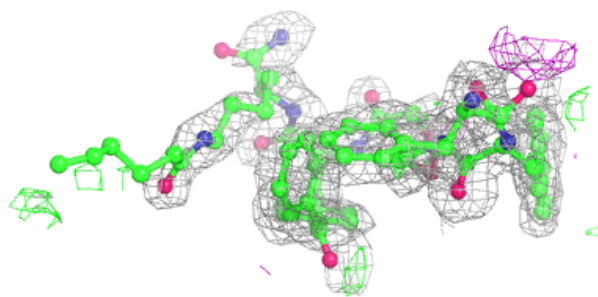
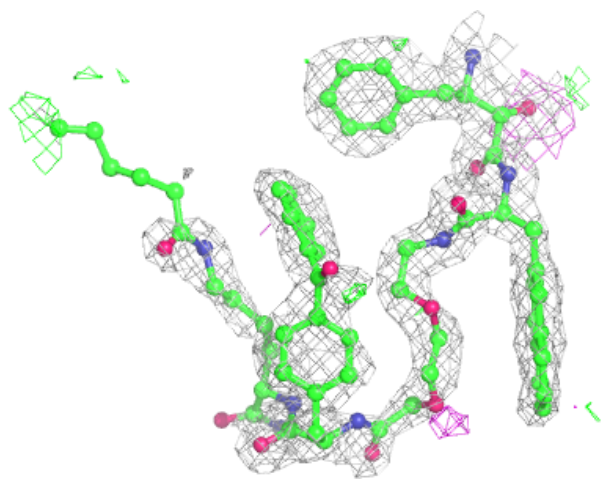
Electron density around DGZ F 615:

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



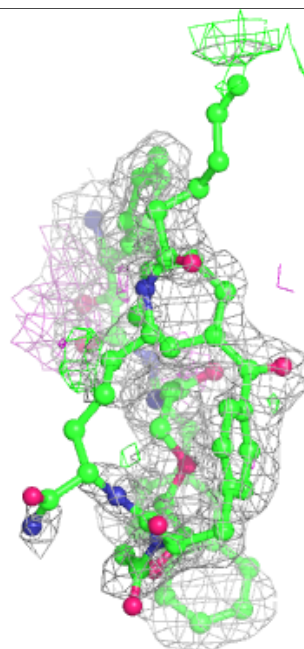
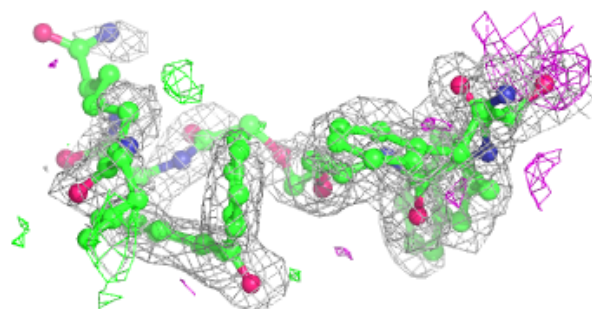
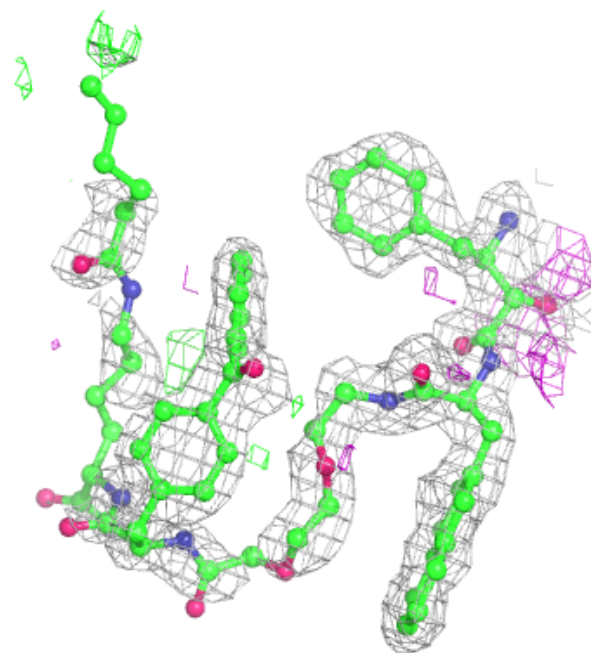
Electron density around DGZ A 615:

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and green (positive)



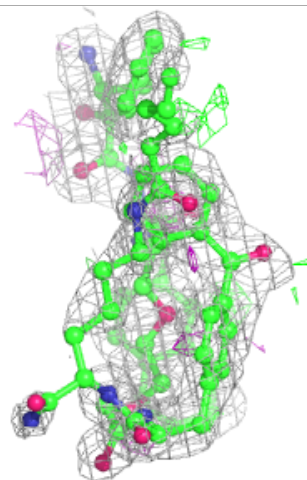
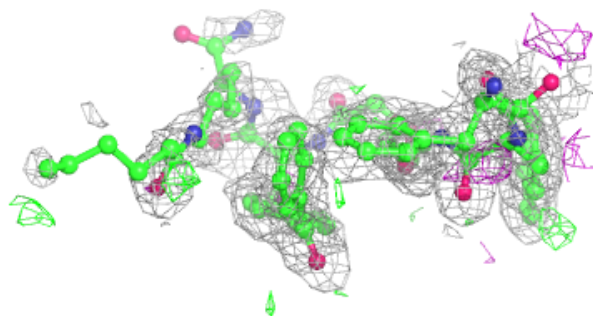
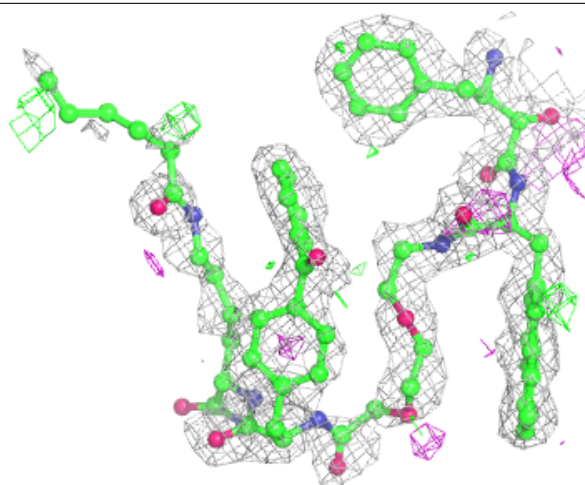
Electron density around DGZ I 615:

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



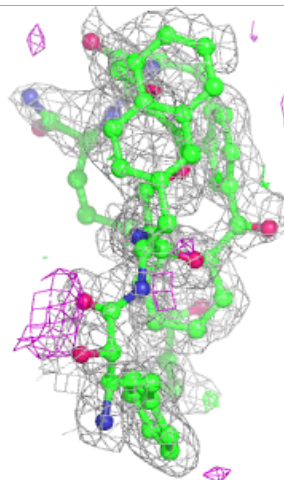
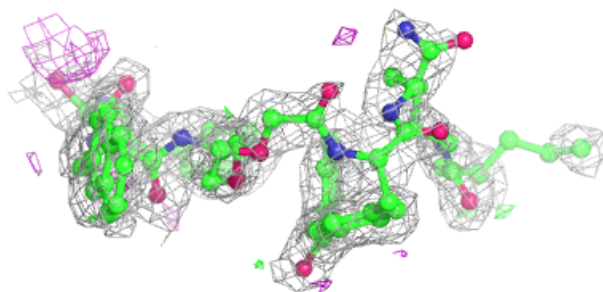
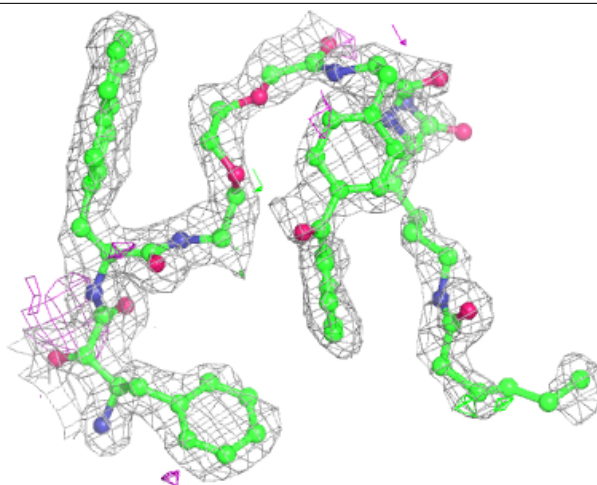
Electron density around DGZ G 615:

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



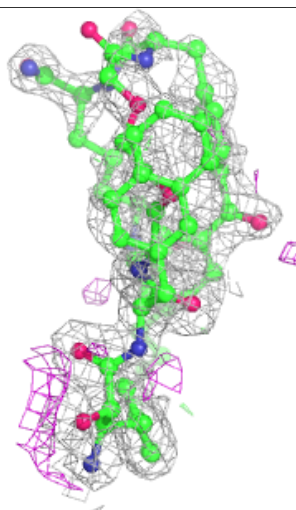
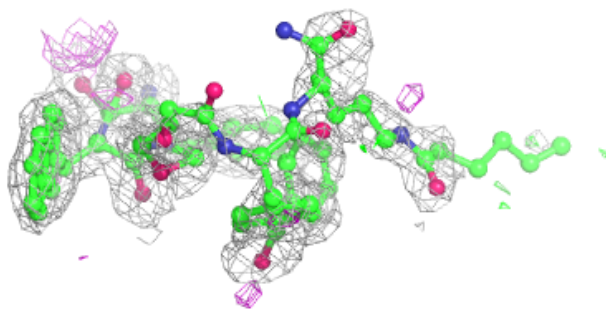
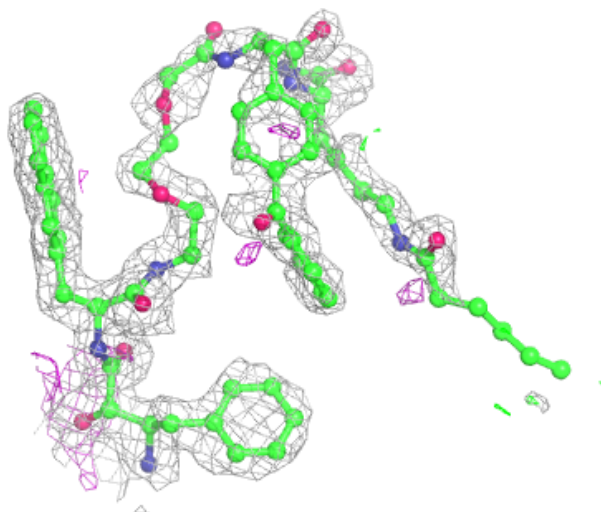
Electron density around DGZ L 615:

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and green (positive)



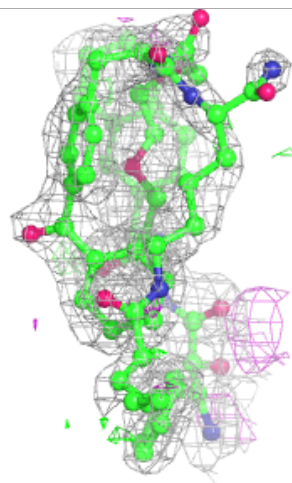
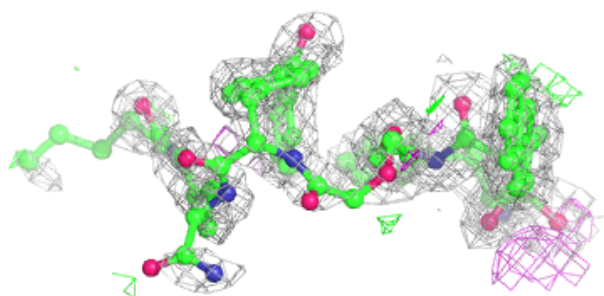
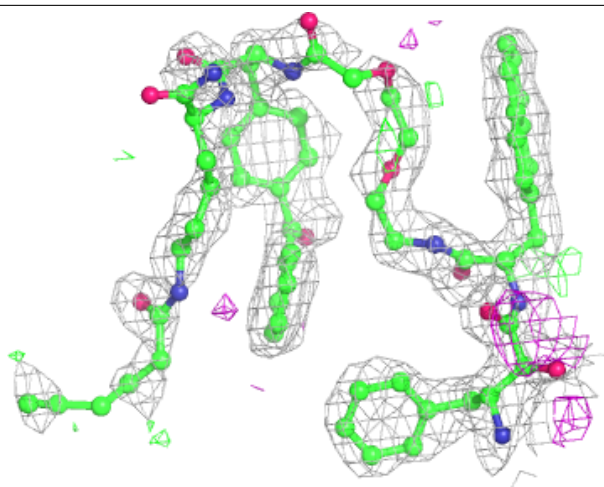
Electron density around DGZ E 615:

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



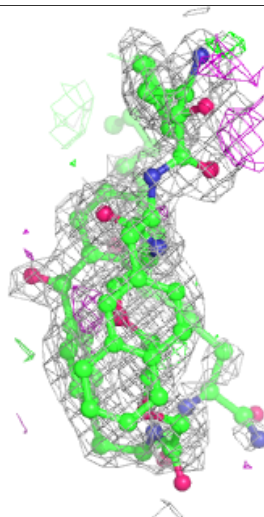
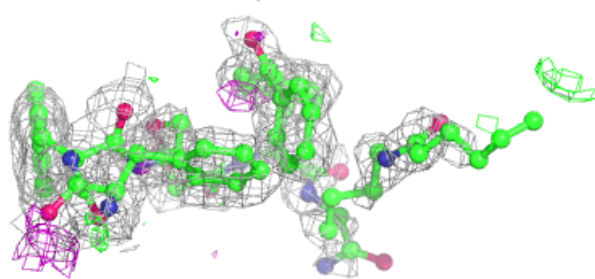
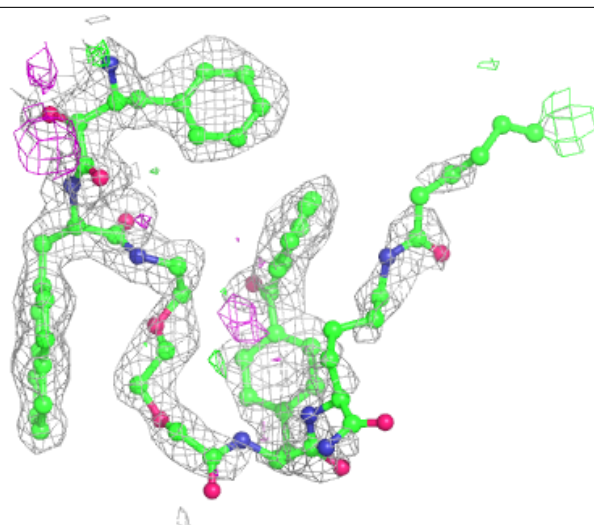
Electron density around DGZ C 615:

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and green (positive)



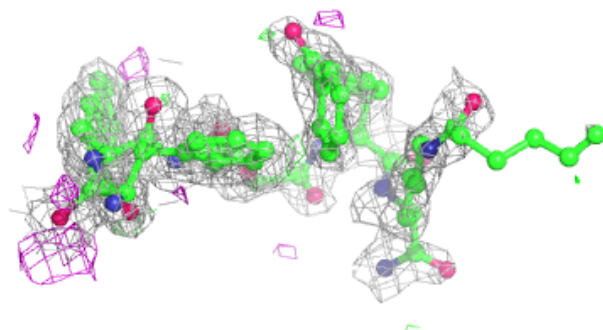
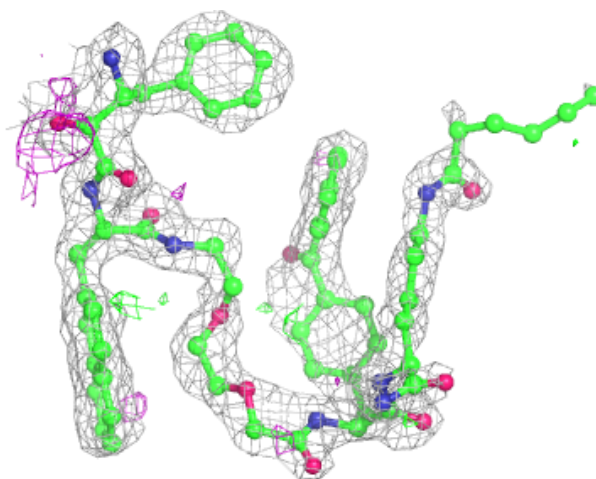
Electron density around DGZ B 615:

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



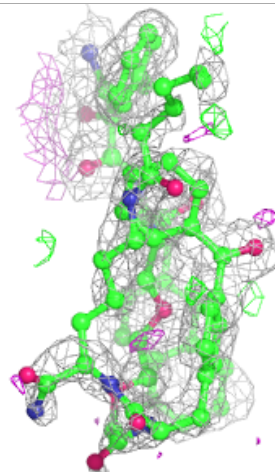
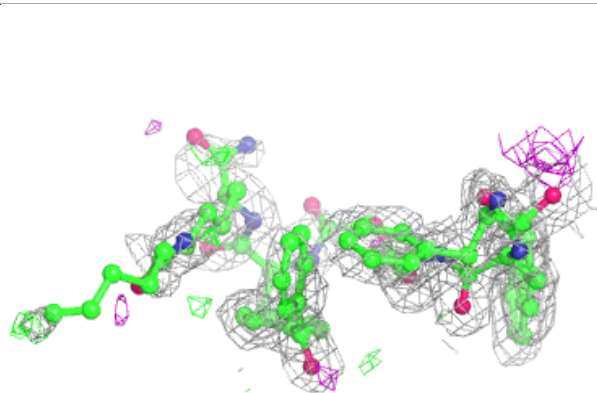
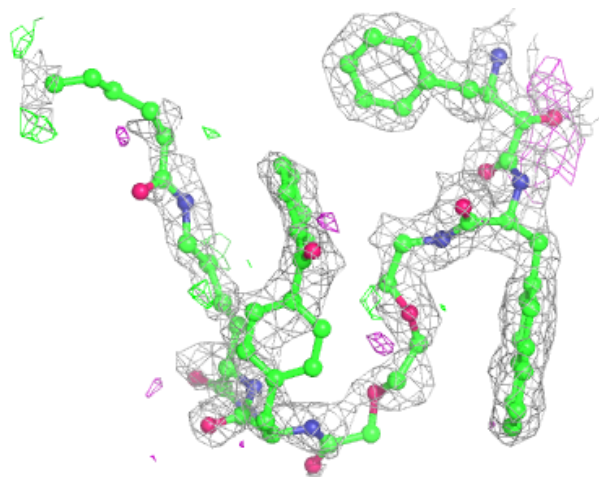
Electron density around DGZ D 615:

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and green (positive)



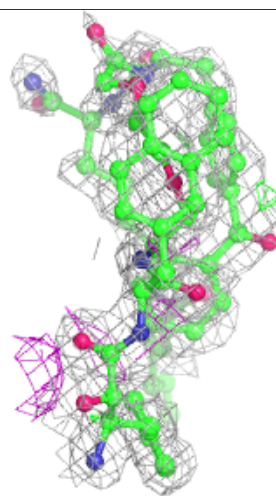
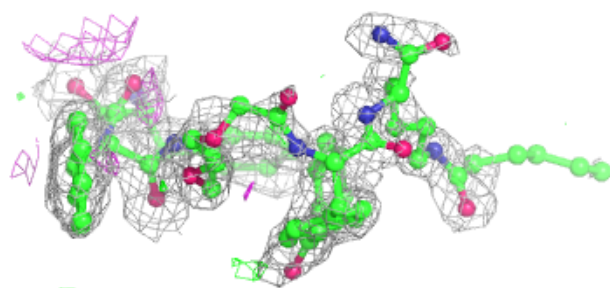
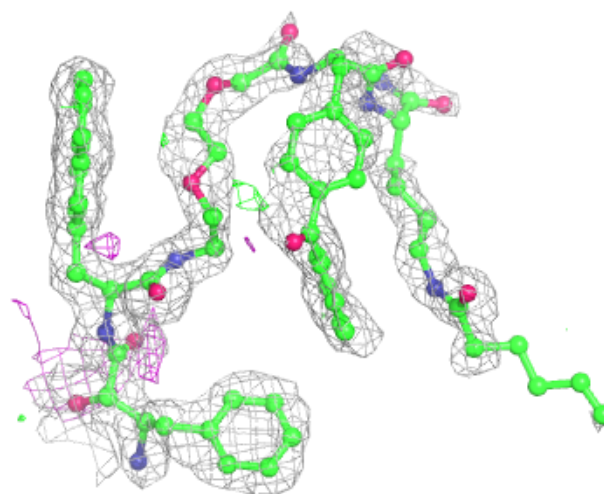
Electron density around DGZ K 615:

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



Electron density around DGZ J 615:

$2mF_o-DF_c$ (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.