Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 11:37 AM EST

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

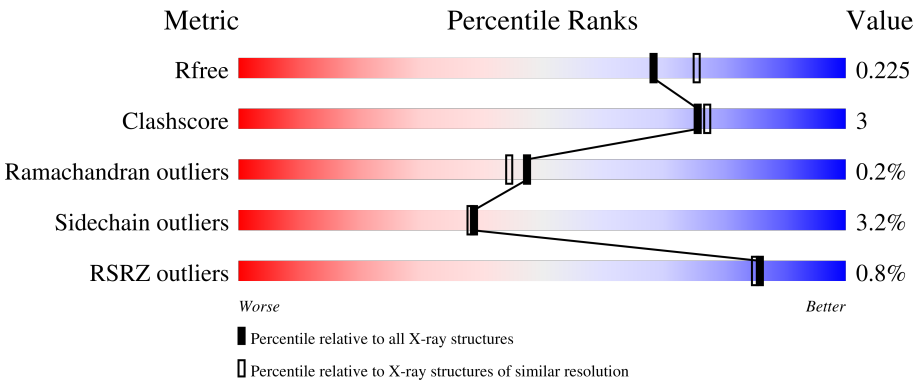
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	.% 93% 5% •
1	B	528	2% 90% 7% •
1	C	528	.% 91% 6% • •
1	D	528	.% 90% 7% •
1	E	528	90% 6% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	528	2% 87% 9%
1	G	528	% 91% 6%
1	H	528	% 90% 7%
1	I	528	92% 5%
1	J	528	% 89% 8%
1	K	528	89% 7%
1	L	528	% 88% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CO3	A	612	-	X	-	-
2	CO3	C	612	-	X	-	-
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	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	1PE	L	617	-	X	-	-
6	1PE	L	618	-	X	-	-
6	1PE	L	619	-	X	-	-
6	1PE	L	620	-	X	-	-

2 Entry composition (i)

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

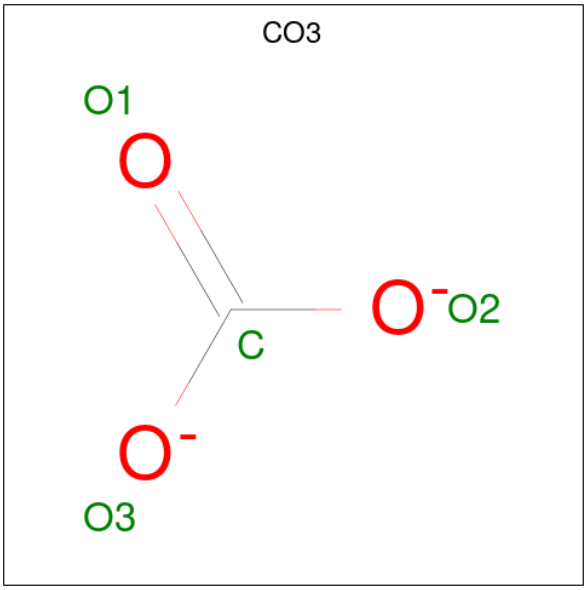
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression 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

Continued on next page...

Continued from previous page...

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: CO_3).



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

Continued on next page...

Continued from previous page...

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

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

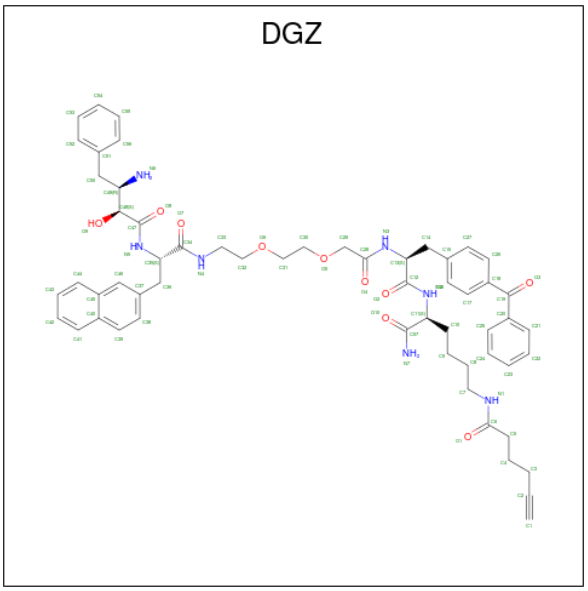
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	2	2	2	0	0
3	B	2	2	2	0	0
3	C	2	2	2	0	0
3	D	2	2	2	0	0
3	E	2	2	2	0	0
3	F	2	2	2	0	0
3	G	2	2	2	0	0
3	H	2	2	2	0	0
3	I	2	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	2	Total Zn 2 2	0	0
3	K	2	Total Zn 2 2	0	0
3	L	2	Total Zn 2 2	0	0

- 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-tetraazapentacosan-25-yl)hex-5-ynamide (three-letter code: DGZ) (formula: $C_{57}H_{67}N_7O_{10}$).



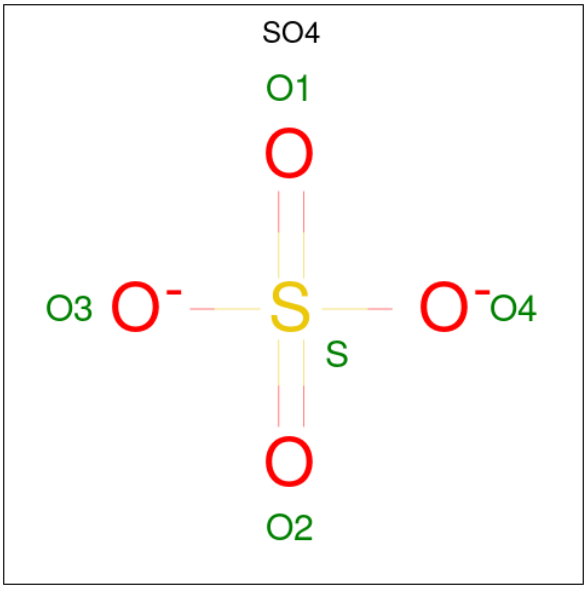
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 74 57 7 10	0	0
4	B	1	Total C N O 74 57 7 10	0	0
4	C	1	Total C N O 74 57 7 10	0	0
4	D	1	Total C N O 74 57 7 10	0	0
4	E	1	Total C N O 74 57 7 10	0	0
4	F	1	Total C N O 74 57 7 10	0	0
4	G	1	Total C N O 74 57 7 10	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

Continued on next page...

Continued from previous page...

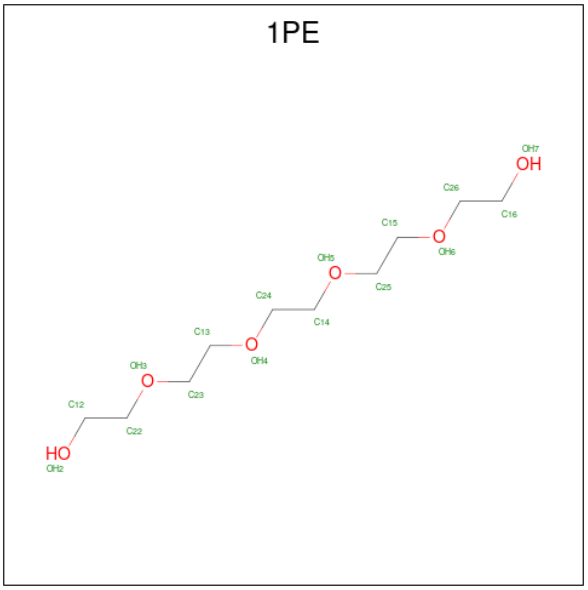
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	C	1	5	4	1	0	0
			Total	O	S		
5	D	1	5	4	1	0	0
			Total	O	S		
5	D	1	5	4	1	0	0
			Total	O	S		
5	E	1	5	4	1	0	0
			Total	O	S		
5	E	1	5	4	1	0	0
			Total	O	S		
5	E	1	5	4	1	0	0
			Total	O	S		
5	G	1	5	4	1	0	0
			Total	O	S		
5	G	1	5	4	1	0	0
			Total	O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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



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

Continued on next page...

Continued from previous page...

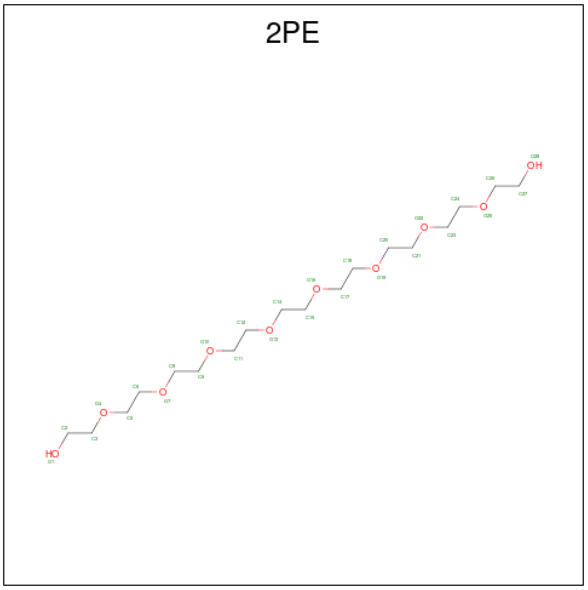
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	E	1	10	6	4		0	0
			Total	C	O			
6	E	1	8	5	3		0	0
			Total	C	O			
6	F	1	10	6	4		0	0
			Total	C	O			
6	F	1	10	6	4		0	0
			Total	C	O			
6	F	1	10	6	4		0	0
			Total	C	O			
6	G	1	9	6	3		0	0
			Total	C	O			
6	G	1	6	4	2		0	0
			Total	C	O			
6	G	1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

Continued on next page...

Continued from previous page...

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

- Molecule 7 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 26 17 9	0	0
7	H	1	Total C O 25 16 9	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	421	Total O 421 421	0	0
8	B	351	Total O 351 351	0	0
8	C	431	Total O 431 431	0	0
8	D	424	Total O 424 424	0	0

Continued on next page...

Continued from previous page...

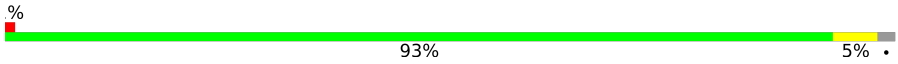
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	E	445	445	445	0	0
			Total	O		
8	F	364	364	364	0	0
			Total	O		
8	G	431	431	431	0	0
			Total	O		
8	H	334	334	334	0	0
			Total	O		
8	I	391	391	391	0	0
			Total	O		
8	J	406	406	406	0	0
			Total	O		
8	K	408	408	408	0	0
			Total	O		
8	L	389	389	389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

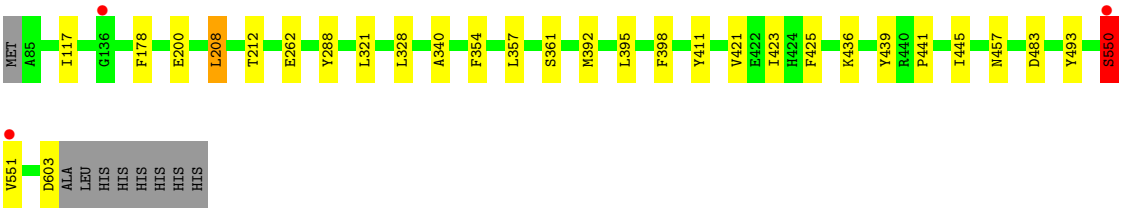
3 Residue-property plots (i)

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: M17 leucyl aminopeptidase

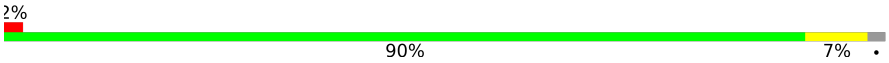
Chain A:

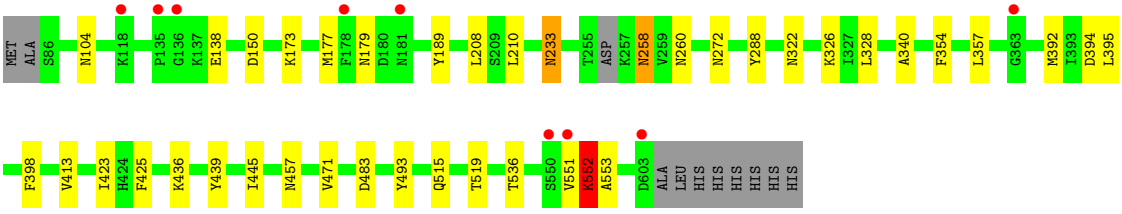




• Molecule 1: M17 leucyl aminopeptidase

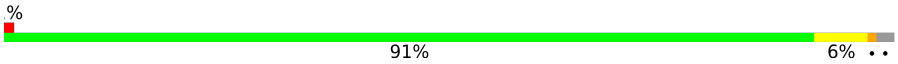
Chain B:

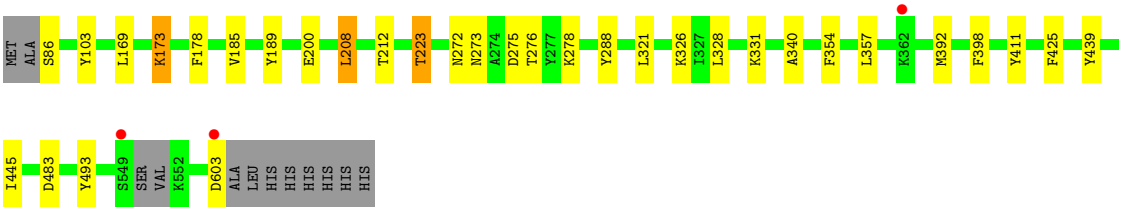




• Molecule 1: M17 leucyl aminopeptidase

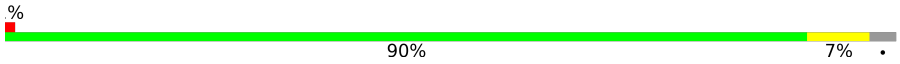
Chain C:

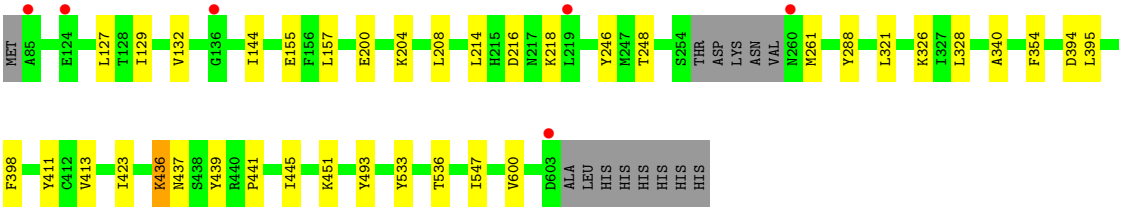




• Molecule 1: M17 leucyl aminopeptidase

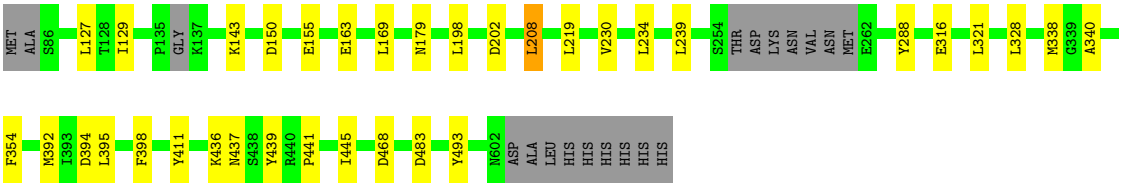
Chain D:





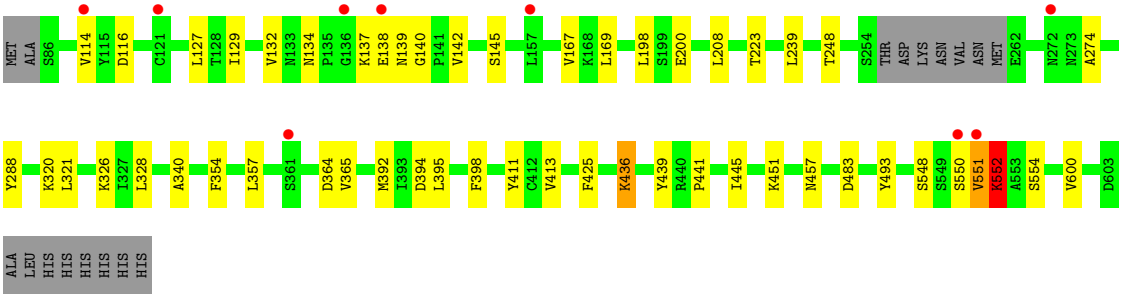
• Molecule 1: M17 leucyl aminopeptidase

Chain E:



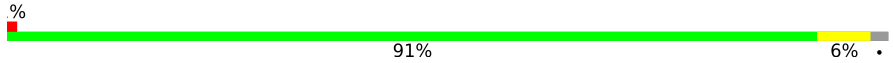
• Molecule 1: M17 leucyl aminopeptidase

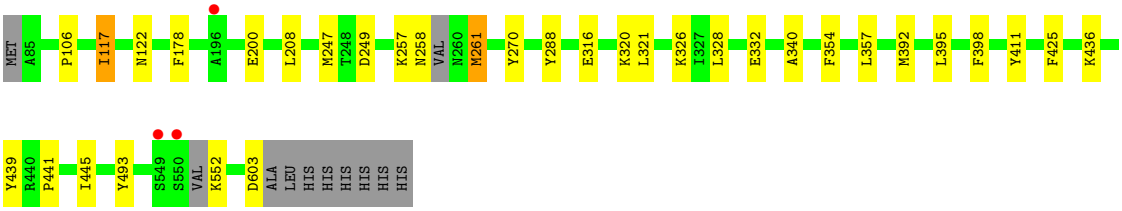
Chain F:



• Molecule 1: M17 leucyl aminopeptidase

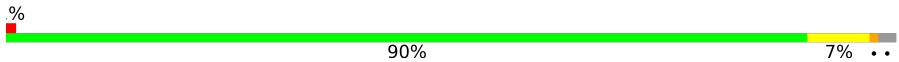
Chain G:

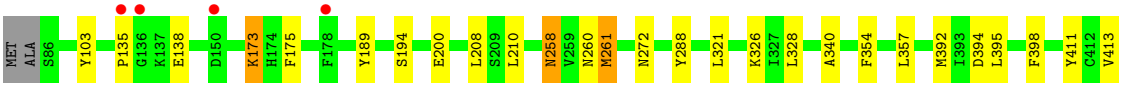


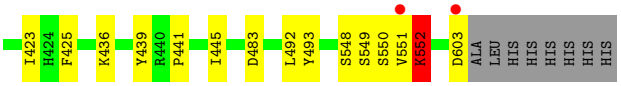


• Molecule 1: M17 leucyl aminopeptidase

Chain H:

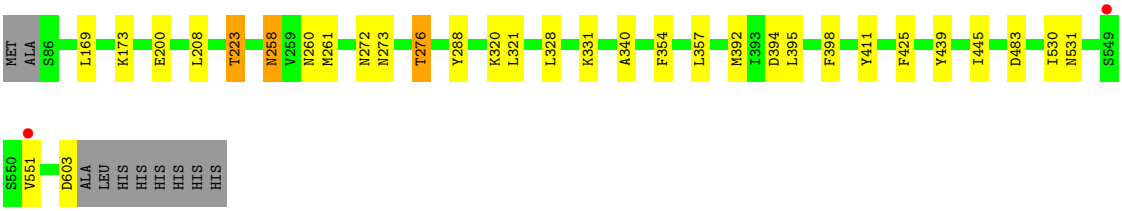






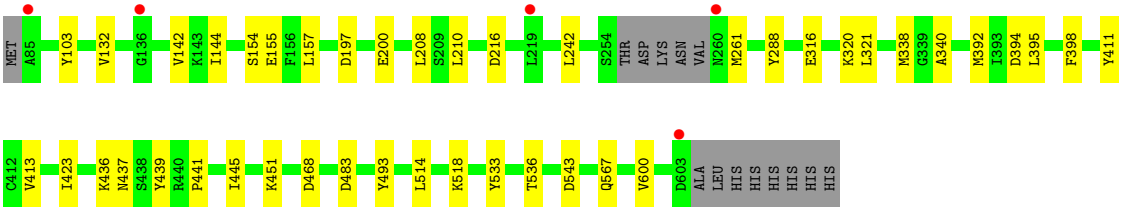
• Molecule 1: M17 leucyl aminopeptidase

Chain I:



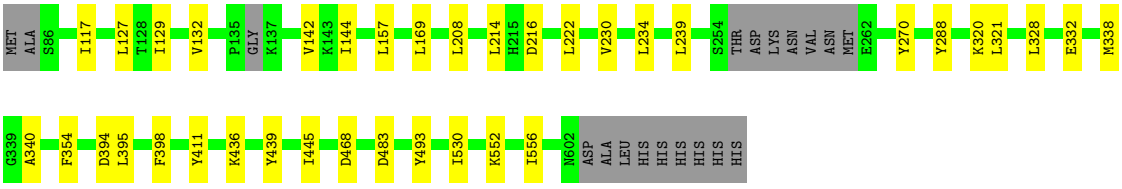
• Molecule 1: M17 leucyl aminopeptidase

Chain J:



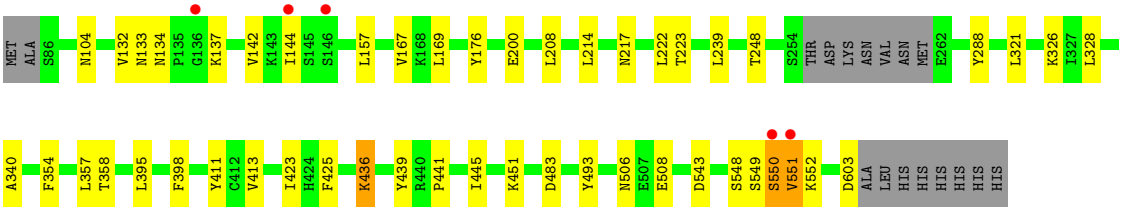
• Molecule 1: M17 leucyl aminopeptidase

Chain K:



• Molecule 1: M17 leucyl aminopeptidase

Chain L:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	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 $< |L| >$, $< L^2 >$ 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: 2PE, ZN, CO3, SO4, 1PE, 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(^{o})	Ideal(^{o})
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 (i)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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.

All (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:C26	6:G:623:1PE:C16	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:OH4	6:G:623:1PE:C13	1.63	1.47
1:H:550:SER:OG	1:H:552:LYS:CD	1.80	1.29
1:H:550:SER:OG	1:H:552:LYS:HD2	1.03	1.19
1:I:531:ASN:H	6:I:623:1PE:H142	1.31	0.93
1:J:316:GLU:HG3	6:J:620:1PE:H141	1.52	0.92
1:H:550:SER:HG	1:H:552:LYS:HD2	1.05	0.87
1:C:223:THR:HG23	8:C:864:HOH:O	1.79	0.83
1:L:506:ASN:OD1	1:L:508:GLU:HG2	1.79	0.81
1:F:451:LYS:HE2	6:F:618:1PE:H151	1.62	0.79
1:K:338:MET:HE3	1:K:468:ASP:HB3	1.65	0.79
1:K:338:MET:CE	1:K:468:ASP:HB3	2.12	0.79
1:E:338:MET:HE3	1:E:468:ASP:HB3	1.66	0.78
1:B:392:MET:HE3	4:B:615:DGZ:H54	1.66	0.75
1:E:338:MET:CE	1:E:468:ASP:HB3	2.15	0.75
1:I:223:THR:HG23	8:I:900:HOH:O	1.86	0.74
1:F:137:LYS:CB	1:F:140:GLY:H	2.01	0.73
1:K:332:GLU:HG2	8:K:946:HOH:O	1.87	0.73
1:F:493:TYR:CE1	4:F:615:DGZ:H21	2.24	0.72
1:L:133:ASN:HA	1:L:167:VAL:HG11	1.70	0.71
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.77	0.67
1:F:493:TYR:HE1	4:F:615:DGZ:C21	2.07	0.67
1:F:493:TYR:HE1	4:F:615:DGZ:H21	1.58	0.67
1:A:178:PHE:HZ	1:D:155:GLU:HG2	1.61	0.66
1:F:138:GLU:N	1:F:139:ASN:HA	2.10	0.66
1:C:86:SER:N	8:C:752:HOH:O	2.28	0.65
1:D:533:TYR:O	1:D:536:THR:HG22	1.97	0.64
1:H:258:ASN:HB3	1:H:261:MET:HG3	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:550:SER:OG	1:H:552:LYS:HD3	1.89	0.64
1:J:132:VAL:HG21	1:J:142:VAL:HG13	1.80	0.63
4:K:615:DGZ:H25	4:K:615:DGZ:H32	1.79	0.63
1:F:320:LYS:NZ	6:F:617:1PE:H152	2.14	0.63
1:J:451:LYS:HG2	6:J:621:1PE:H241	1.81	0.63
1:J:437:ASN:HD22	1:L:436:LYS:NZ	1.96	0.62
1:B:233:ASN:ND2	1:B:519:THR:O	2.32	0.62
1:F:320:LYS:HZ1	6:F:617:1PE:H152	1.64	0.62
1:F:551:VAL:C	1:F:552:LYS:O	2.36	0.62
8:G:657:HOH:O	6:L:619:1PE:H242	2.00	0.61
1:J:533:TYR:O	1:J:536:THR:HG22	2.00	0.61
1:D:437:ASN:HD22	1:F:436:LYS:NZ	1.99	0.61
1:H:552:LYS:HG2	8:H:951:HOH:O	1.99	0.61
1:L:451:LYS:HG2	6:L:618:1PE:H232	1.82	0.60
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.83	0.60
1:L:548:SER:OG	1:L:550:SER:HB3	2.03	0.59
1:D:436:LYS:NZ	1:E:437:ASN:HD22	2.00	0.59
4:G:615:DGZ:H25	4:G:615:DGZ:H32	1.82	0.59
1:H:413:VAL:HG11	1:H:423:ILE:HD13	1.83	0.59
1:H:493:TYR:HE1	4:H:615:DGZ:H21	1.68	0.59
1:K:132:VAL:HG21	1:K:142:VAL:HG13	1.84	0.59
1:J:543:ASP:HB3	6:J:621:1PE:H242	1.84	0.58
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.86	0.58
1:K:338:MET:HE2	1:K:468:ASP:HB3	1.86	0.58
1:A:493:TYR:HE1	4:A:615:DGZ:H21	1.68	0.58
1:B:413:VAL:HG11	1:B:423:ILE:HD13	1.85	0.57
4:L:615:DGZ:H32	8:L:787:HOH:O	2.04	0.57
4:C:615:DGZ:H32	4:C:615:DGZ:H25	1.86	0.57
1:C:411:TYR:CE1	6:C:622:1PE:H131	2.39	0.57
4:L:615:DGZ:HN3	4:L:615:DGZ:C27	2.18	0.57
1:G:332:GLU:HG3	8:G:844:HOH:O	2.05	0.56
1:C:326:LYS:HE3	1:C:328:LEU:HD11	1.87	0.56
1:J:413:VAL:HG11	1:J:423:ILE:HD13	1.87	0.56
1:D:248:THR:HG22	8:D:873:HOH:O	2.06	0.55
1:J:316:GLU:OE1	6:J:620:1PE:H251	2.06	0.55
1:A:493:TYR:HE1	4:A:615:DGZ:C21	2.19	0.55
6:F:618:1PE:C26	6:F:618:1PE:H162	2.18	0.55
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.89	0.55
1:G:392:MET:HE3	4:G:615:DGZ:H54	1.89	0.55
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.88	0.55
4:I:615:DGZ:H7A	4:I:615:DGZ:H17	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.89	0.54
1:A:493:TYR:CE1	4:A:615:DGZ:H21	2.41	0.54
1:D:436:LYS:HZ2	1:E:437:ASN:HD22	1.54	0.54
1:D:493:TYR:HE1	4:D:615:DGZ:C21	2.21	0.54
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.88	0.54
1:J:437:ASN:HD22	1:L:436:LYS:HZ1	1.55	0.54
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.90	0.54
1:C:392:MET:HE3	4:C:615:DGZ:H54	1.90	0.54
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.90	0.54
1:F:320:LYS:HE2	6:F:617:1PE:H142	1.89	0.54
1:L:248:THR:HG22	8:L:815:HOH:O	2.08	0.53
1:B:457:ASN:ND2	4:B:615:DGZ:H39	2.24	0.53
1:H:173:LYS:HB2	1:H:189:TYR:CE1	2.43	0.53
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.90	0.53
1:J:411:TYR:CE1	6:J:619:1PE:H152	2.44	0.53
1:B:258:ASN:HD22	1:B:260:ASN:H	1.55	0.53
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.91	0.52
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.91	0.52
2:F:612:CO3:O2	4:F:615:DGZ:H36A	2.10	0.52
1:H:258:ASN:HD22	1:H:260:ASN:H	1.56	0.52
1:K:320:LYS:HE2	6:K:617:1PE:H152	1.90	0.52
1:A:392:MET:HE3	4:A:615:DGZ:H54	1.90	0.52
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.92	0.52
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.91	0.52
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.92	0.52
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.91	0.52
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.91	0.52
1:D:326:LYS:HE3	1:D:328:LEU:HD11	1.91	0.52
1:L:326:LYS:HE3	1:L:328:LEU:HD11	1.91	0.52
1:B:392:MET:HE2	4:B:615:DGZ:H5	1.90	0.51
1:J:514:LEU:HD22	6:J:622:1PE:H242	1.92	0.51
1:J:518:LYS:NZ	6:J:622:1PE:H241	2.25	0.51
6:L:620:1PE:C26	6:L:620:1PE:H161	2.18	0.51
1:B:551:VAL:HG12	1:B:552:LYS:O	2.11	0.51
1:E:338:MET:HE2	1:E:468:ASP:HB3	1.93	0.51
1:J:316:GLU:CD	6:J:620:1PE:H251	2.31	0.51
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.92	0.51
1:I:392:MET:HE2	4:I:615:DGZ:H5	1.93	0.51
4:A:615:DGZ:H27	4:A:615:DGZ:H30A	1.93	0.51
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.91	0.51
1:J:338:MET:CE	1:J:468:ASP:HB3	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:551:VAL:O	1:H:552:LYS:O	2.28	0.50
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.93	0.50
4:G:615:DGZ:C27	1:L:493:TYR:HE2	2.24	0.50
1:H:493:TYR:CE1	4:H:615:DGZ:H21	2.47	0.50
1:B:392:MET:CE	4:B:615:DGZ:H54	2.39	0.50
6:G:623:1PE:C26	6:G:623:1PE:H161	2.19	0.50
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.94	0.50
1:L:176:TYR:OH	1:L:217:ASN:ND2	2.43	0.50
1:K:144:ILE:HG13	1:K:157:LEU:HD22	1.93	0.49
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.93	0.49
1:D:413:VAL:HG11	1:D:423:ILE:HD13	1.92	0.49
1:G:552:LYS:N	8:G:639:HOH:O	2.44	0.49
1:H:321:LEU:HD11	1:H:411:TYR:HA	1.94	0.49
1:H:493:TYR:HE1	4:H:615:DGZ:C21	2.25	0.49
1:L:133:ASN:HA	1:L:167:VAL:CG1	2.41	0.49
1:B:493:TYR:HE1	4:B:615:DGZ:C21	2.26	0.49
1:D:441:PRO:HB2	1:E:394:ASP:HA	1.95	0.49
1:F:413:VAL:CG2	1:F:600:VAL:HG21	2.42	0.49
1:B:104:ASN:HB2	8:B:834:HOH:O	2.12	0.49
1:F:457:ASN:ND2	4:F:615:DGZ:H39	2.27	0.49
1:I:530:ILE:HA	6:I:623:1PE:H141	1.94	0.49
4:G:615:DGZ:H16	4:L:615:DGZ:H16	1.95	0.49
1:H:392:MET:HE3	4:H:615:DGZ:H54	1.94	0.49
1:I:258:ASN:HD22	1:I:260:ASN:H	1.59	0.49
1:I:531:ASN:N	6:I:623:1PE:H142	2.14	0.49
1:F:326:LYS:HE3	1:F:328:LEU:HD11	1.95	0.48
1:J:144:ILE:HG13	1:J:157:LEU:HD22	1.95	0.48
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.78	0.48
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.94	0.48
4:L:615:DGZ:H8A	4:L:615:DGZ:C24	2.43	0.48
1:E:493:TYR:HE1	4:E:615:DGZ:H21	1.77	0.48
1:K:117:ILE:HG12	1:K:270:TYR:HB3	1.94	0.48
1:B:173:LYS:HB2	1:B:189:TYR:CE1	2.48	0.48
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.96	0.48
1:G:316:GLU:HG3	6:G:623:1PE:H232	1.95	0.48
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.96	0.48
1:H:326:LYS:HE3	1:H:328:LEU:HD11	1.96	0.48
1:B:515:GLN:HG3	8:B:732:HOH:O	2.13	0.48
1:E:493:TYR:CE1	4:E:615:DGZ:H21	2.48	0.47
1:F:451:LYS:HG2	6:F:618:1PE:H141	1.96	0.47
1:E:230:VAL:HG13	1:E:234:LEU:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:326:LYS:HE3	1:G:328:LEU:HD11	1.96	0.47
4:I:615:DGZ:C27	1:J:493:TYR:HE2	2.27	0.47
1:H:175:PHE:HD1	1:L:176:TYR:HB2	1.79	0.47
1:E:493:TYR:HE1	4:E:615:DGZ:C21	2.27	0.47
1:F:548:SER:HB3	1:F:551:VAL:HA	1.95	0.47
1:B:326:LYS:HE3	1:B:328:LEU:HD11	1.97	0.47
1:C:493:TYR:HE1	4:C:615:DGZ:H21	1.79	0.47
1:D:144:ILE:HG13	1:D:157:LEU:HD22	1.96	0.47
4:H:615:DGZ:H27	4:H:615:DGZ:H30	1.96	0.47
1:L:167:VAL:HG12	1:L:167:VAL:O	2.13	0.47
1:D:493:TYR:HE1	4:D:615:DGZ:H21	1.80	0.47
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.97	0.47
1:I:261:MET:HA	5:I:618:SO4:O4	2.15	0.47
1:D:493:TYR:CE1	4:D:615:DGZ:H21	2.50	0.46
1:K:493:TYR:HE1	4:K:615:DGZ:H21	1.79	0.46
1:B:536:THR:HG21	1:B:551:VAL:HG23	1.97	0.46
1:K:530:ILE:HD12	1:K:556:ILE:HD13	1.98	0.46
1:L:223:THR:HG23	8:L:808:HOH:O	2.15	0.46
1:D:451:LYS:NZ	6:D:620:1PE:H142	2.31	0.46
1:L:413:VAL:HG11	1:L:423:ILE:HD13	1.98	0.46
1:J:338:MET:HE2	1:J:468:ASP:HB3	1.97	0.46
1:A:361:SER:HB3	8:A:728:HOH:O	2.16	0.46
1:E:321:LEU:HD11	1:E:411:TYR:HA	1.97	0.46
1:J:320:LYS:HZ1	6:J:620:1PE:C26	2.28	0.46
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.81	0.46
1:L:214:LEU:HD21	1:L:222:LEU:HD22	1.97	0.46
4:A:615:DGZ:H30A	4:A:615:DGZ:C27	2.45	0.46
4:J:615:DGZ:C25	4:J:615:DGZ:H7A	2.46	0.46
4:A:615:DGZ:C27	4:A:615:DGZ:HN3	2.27	0.45
1:C:103:TYR:HB2	6:C:621:1PE:H251	1.98	0.45
1:F:248:THR:HG22	8:F:713:HOH:O	2.16	0.45
1:H:548:SER:OG	1:H:552:LYS:HE2	2.16	0.45
1:B:552:LYS:O	1:B:553:ALA:C	2.54	0.45
1:K:321:LEU:HD11	1:K:411:TYR:HA	1.98	0.45
1:L:321:LEU:HD11	1:L:411:TYR:HA	1.98	0.45
6:L:620:1PE:C26	6:L:620:1PE:H162	2.18	0.45
1:C:321:LEU:HD11	1:C:411:TYR:HA	1.98	0.45
1:L:104:ASN:ND2	6:L:617:1PE:H241	2.31	0.45
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.98	0.45
1:I:321:LEU:HD11	1:I:411:TYR:HA	1.98	0.45
1:F:248:THR:HG23	8:F:843:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:SER:HA	1:A:551:VAL:CB	2.47	0.45
1:G:320:LYS:HZ1	6:G:623:1PE:H152	1.81	0.45
1:A:321:LEU:HD11	1:A:411:TYR:HA	1.99	0.45
1:B:551:VAL:C	1:B:552:LYS:O	2.55	0.45
1:B:233:ASN:HD21	1:B:519:THR:HA	1.82	0.45
1:J:518:LYS:HZ2	6:J:622:1PE:H241	1.82	0.45
1:B:493:TYR:HE1	4:B:615:DGZ:H21	1.82	0.44
1:B:258:ASN:ND2	1:B:260:ASN:H	2.15	0.44
1:D:411:TYR:HE1	6:D:618:1PE:H232	1.83	0.44
1:K:230:VAL:HG13	1:K:234:LEU:HB3	2.00	0.44
1:L:144:ILE:HD13	1:L:157:LEU:HD22	1.98	0.44
1:A:208:LEU:O	1:A:212:THR:HG23	2.17	0.44
4:I:615:DGZ:H25	4:I:615:DGZ:H32	2.00	0.44
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.99	0.44
1:F:321:LEU:HD11	1:F:411:TYR:HA	1.99	0.44
1:F:413:VAL:HG22	1:F:600:VAL:HG21	2.00	0.44
1:G:493:TYR:HE2	4:L:615:DGZ:C27	2.31	0.44
6:G:623:1PE:C13	6:G:623:1PE:C24	2.85	0.44
2:J:612:CO3:O2	4:J:615:DGZ:H36A	2.17	0.44
1:B:493:TYR:CE1	4:B:615:DGZ:H21	2.53	0.44
1:C:273:ASN:O	1:C:276:THR:HG22	2.18	0.44
1:E:441:PRO:HB2	1:F:394:ASP:HA	1.99	0.44
1:F:392:MET:HE3	4:F:615:DGZ:H54	1.99	0.44
1:K:127:LEU:HD11	1:K:129:ILE:HD11	1.99	0.44
1:F:493:TYR:CE1	4:F:615:DGZ:C21	2.89	0.43
1:J:413:VAL:CG2	1:J:600:VAL:HG21	2.48	0.43
1:A:178:PHE:CZ	1:D:155:GLU:HG2	2.48	0.43
1:D:218:LYS:HG2	1:D:261:MET:HA	2.00	0.43
1:D:321:LEU:HD11	1:D:411:TYR:HA	1.98	0.43
1:E:127:LEU:HD11	1:E:129:ILE:HD11	2.00	0.43
1:K:214:LEU:HD11	1:K:222:LEU:HD22	2.00	0.43
1:L:550:SER:OG	1:L:551:VAL:N	2.50	0.43
1:D:248:THR:HG23	8:D:969:HOH:O	2.17	0.43
1:G:258:ASN:HB2	1:G:261:MET:H	1.83	0.43
1:C:275:ASP:HA	1:C:278:LYS:HD2	2.00	0.43
1:A:357:LEU:HB2	1:A:425:PHE:HB2	2.01	0.43
1:G:493:TYR:HE1	4:G:615:DGZ:H21	1.84	0.43
4:B:615:DGZ:H36	8:B:718:HOH:O	2.18	0.42
1:E:392:MET:HE3	4:E:615:DGZ:H54	2.01	0.42
7:H:619:2PE:H261	8:H:907:HOH:O	2.18	0.42
1:G:117:ILE:HG13	1:G:270:TYR:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:ASN:ND2	6:G:622:1PE:H151	2.34	0.42
1:D:127:LEU:HD11	1:D:129:ILE:HD11	2.01	0.42
6:G:623:1PE:C26	6:G:623:1PE:H162	2.19	0.42
1:L:543:ASP:OD2	6:L:618:1PE:H131	2.18	0.42
1:H:135:PRO:HA	1:H:194:SER:O	2.19	0.42
1:L:104:ASN:HD22	6:L:617:1PE:H241	1.84	0.42
1:C:208:LEU:O	1:C:212:THR:HG23	2.19	0.42
4:H:615:DGZ:H16	4:K:615:DGZ:H16	2.01	0.42
1:I:531:ASN:H	6:I:623:1PE:C14	2.17	0.42
4:K:615:DGZ:H32	4:K:615:DGZ:C25	2.47	0.42
1:E:198:LEU:HD22	1:E:202:ASP:HB3	2.01	0.42
4:E:615:DGZ:H30	4:E:615:DGZ:H32A	1.78	0.42
1:F:127:LEU:HD11	1:F:129:ILE:HD11	2.01	0.42
1:B:357:LEU:HB2	1:B:425:PHE:HB2	2.01	0.42
1:J:103:TYR:CD1	6:J:620:1PE:H161	2.55	0.42
4:A:615:DGZ:C27	1:F:493:TYR:HE2	2.32	0.42
1:C:493:TYR:HE1	4:C:615:DGZ:C21	2.32	0.42
1:F:357:LEU:HB2	1:F:425:PHE:HB2	2.02	0.41
1:I:320:LYS:HE2	6:I:621:1PE:H231	2.02	0.41
1:A:441:PRO:HB2	1:B:394:ASP:HA	2.02	0.41
1:B:150:ASP:OD1	1:B:179:ASN:HB2	2.21	0.41
4:A:615:DGZ:H31A	4:A:615:DGZ:H29A	1.88	0.41
1:G:357:LEU:HB2	1:G:425:PHE:HB2	2.02	0.41
1:I:273:ASN:O	1:I:276:THR:HG22	2.20	0.41
1:H:103:TYR:O	7:H:619:2PE:H271	2.20	0.41
4:B:615:DGZ:H17	4:B:615:DGZ:H7A	2.01	0.41
1:E:338:MET:HE2	1:E:338:MET:HB3	1.91	0.41
1:L:357:LEU:HB2	1:L:425:PHE:HB2	2.01	0.41
4:A:615:DGZ:H16	4:F:615:DGZ:H16	2.03	0.41
1:J:210:LEU:HD23	1:J:242:LEU:HD13	2.01	0.41
1:J:321:LEU:HD11	1:J:411:TYR:HA	2.01	0.41
1:J:441:PRO:HB2	1:K:394:ASP:HA	2.03	0.41
1:I:357:LEU:HB2	1:I:425:PHE:HB2	2.03	0.41
1:J:543:ASP:CB	6:J:621:1PE:H242	2.50	0.41
4:C:615:DGZ:C27	1:D:493:TYR:HE2	2.34	0.41
1:E:208:LEU:HD12	1:E:208:LEU:HA	1.96	0.41
1:G:249:ASP:HB2	5:G:619:SO4:O4	2.20	0.41
1:H:258:ASN:ND2	1:H:260:ASN:H	2.17	0.41
1:H:357:LEU:HB2	1:H:425:PHE:HB2	2.02	0.41
1:H:492:LEU:HD22	1:K:552:LYS:HE3	2.03	0.41
1:A:457:ASN:ND2	4:A:615:DGZ:H39	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:LEU:HB2	1:C:425:PHE:HB2	2.03	0.41
1:F:365:VAL:HG22	8:F:851:HOH:O	2.20	0.41
4:H:615:DGZ:H30A	8:H:890:HOH:O	2.21	0.41
1:I:258:ASN:ND2	1:I:260:ASN:H	2.18	0.41
1:E:150:ASP:OD1	1:E:179:ASN:HB2	2.21	0.40
1:H:441:PRO:HB2	1:I:394:ASP:HA	2.03	0.40
4:A:615:DGZ:H38	4:A:615:DGZ:H35	1.98	0.40
1:J:493:TYR:HE1	4:J:615:DGZ:C21	2.34	0.40
4:J:615:DGZ:H7A	4:J:615:DGZ:C24	2.51	0.40
1:B:233:ASN:ND2	1:B:519:THR:HA	2.36	0.40
1:E:316:GLU:HG3	6:E:619:1PE:H252	2.03	0.40
1:G:441:PRO:HB2	1:H:394:ASP:HA	2.03	0.40
4:H:615:DGZ:H32	8:H:890:HOH:O	2.21	0.40
1:A:421:VAL:CG2	1:A:423:ILE:HD11	2.52	0.40
1:D:214:LEU:HB3	1:D:246:TYR:CE1	2.56	0.40
1:F:392:MET:HE2	4:F:615:DGZ:H5A	2.03	0.40
1:G:106:PRO:HD2	1:G:247:MET:SD	2.62	0.40
1:J:392:MET:CE	4:J:615:DGZ:H54	2.51	0.40
4:L:615:DGZ:H8A	4:L:615:DGZ:C25	2.51	0.40
1:C:173:LYS:HB2	1:C:189:TYR:CE1	2.56	0.40
1:F:114:VAL:HG12	1:F:274:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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
1	F	552	LYS
1	H	138	GLU
1	L	551	VAL
1	B	138	GLU
1	F	551	VAL
1	L	552	LYS
1	A	550	SER

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	421/455 (92%)	410 (97%)	11 (3%)	46	48
1	B	410/455 (90%)	396 (97%)	14 (3%)	37	36

Continued on next page...

Continued from previous page...

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

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ILE
1	A	200	GLU
1	A	208	LEU
1	A	262	GLU
1	A	288	TYR
1	A	395	LEU
1	A	398	PHE
1	A	436	LYS
1	A	439	TYR
1	A	483	ASP
1	A	603	ASP
1	B	177	MET
1	B	208	LEU
1	B	210	LEU
1	B	233	ASN
1	B	258	ASN
1	B	272	ASN
1	B	288	TYR
1	B	322	ASN
1	B	395	LEU
1	B	398	PHE
1	B	436	LYS
1	B	439	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	471	VAL
1	B	483	ASP
1	C	169	LEU
1	C	173	LYS
1	C	185	VAL
1	C	200	GLU
1	C	208	LEU
1	C	223	THR
1	C	272	ASN
1	C	288	TYR
1	C	331	LYS
1	C	398	PHE
1	C	439	TYR
1	C	483	ASP
1	C	603	ASP
1	D	132	VAL
1	D	200	GLU
1	D	204	LYS
1	D	208	LEU
1	D	216	ASP
1	D	288	TYR
1	D	395	LEU
1	D	398	PHE
1	D	436	LYS
1	D	439	TYR
1	D	600	VAL
1	E	143	LYS
1	E	163	GLU
1	E	169	LEU
1	E	208	LEU
1	E	219	LEU
1	E	239	LEU
1	E	288	TYR
1	E	395	LEU
1	E	398	PHE
1	E	436	LYS
1	E	439	TYR
1	E	483	ASP
1	F	116	ASP
1	F	134	ASN
1	F	145	SER
1	F	167	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	169	LEU
1	F	198	LEU
1	F	200	GLU
1	F	208	LEU
1	F	223	THR
1	F	239	LEU
1	F	288	TYR
1	F	364	ASP
1	F	395	LEU
1	F	398	PHE
1	F	436	LYS
1	F	439	TYR
1	F	483	ASP
1	F	554	SER
1	G	117	ILE
1	G	200	GLU
1	G	208	LEU
1	G	261	MET
1	G	288	TYR
1	G	395	LEU
1	G	398	PHE
1	G	436	LYS
1	G	439	TYR
1	G	603	ASP
1	H	173	LYS
1	H	200	GLU
1	H	208	LEU
1	H	210	LEU
1	H	258	ASN
1	H	261	MET
1	H	272	ASN
1	H	288	TYR
1	H	395	LEU
1	H	398	PHE
1	H	436	LYS
1	H	439	TYR
1	H	483	ASP
1	H	549	SER
1	H	552	LYS
1	H	603	ASP
1	I	169	LEU
1	I	173	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	200	GLU
1	I	208	LEU
1	I	223	THR
1	I	258	ASN
1	I	272	ASN
1	I	276	THR
1	I	288	TYR
1	I	331	LYS
1	I	395	LEU
1	I	398	PHE
1	I	439	TYR
1	I	483	ASP
1	I	603	ASP
1	J	154	SER
1	J	197	ASP
1	J	200	GLU
1	J	208	LEU
1	J	216	ASP
1	J	261	MET
1	J	288	TYR
1	J	395	LEU
1	J	398	PHE
1	J	436	LYS
1	J	439	TYR
1	J	483	ASP
1	J	567	GLN
1	K	169	LEU
1	K	208	LEU
1	K	216	ASP
1	K	239	LEU
1	K	288	TYR
1	K	395	LEU
1	K	398	PHE
1	K	436	LYS
1	K	439	TYR
1	K	483	ASP
1	L	134	ASN
1	L	137	LYS
1	L	169	LEU
1	L	200	GLU
1	L	208	LEU
1	L	239	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	288	TYR
1	L	358	THR
1	L	395	LEU
1	L	398	PHE
1	L	436	LYS
1	L	439	TYR
1	L	483	ASP
1	L	603	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	ASN
1	A	449	ASN
1	B	233	ASN
1	B	258	ASN
1	B	319	GLN
1	B	322	ASN
1	B	521	ASN
1	C	161	ASN
1	D	437	ASN
1	E	181	ASN
1	E	273	ASN
1	E	437	ASN
1	F	104	ASN
1	F	134	ASN
1	F	567	GLN
1	G	515	GLN
1	H	258	ASN
1	H	319	GLN
1	I	161	ASN
1	I	258	ASN
1	J	437	ASN
1	K	161	ASN
1	L	104	ASN
1	L	134	ASN
1	L	217	ASN
1	L	602	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 monosaccharides 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	E	621	-	7,7,15	2.22	3 (42%)	6,6,14	2.76	4 (66%)
5	SO4	G	619	-	4,4,4	0.82	0	6,6,6	0.28	0
6	1PE	L	620	-	10,10,15	3.12	5 (50%)	9,9,14	2.75	5 (55%)
2	CO3	D	612	-	2,3,3	1.63	1 (50%)	2,3,3	5.64	1 (50%)
5	SO4	H	616	-	4,4,4	0.09	0	6,6,6	0.34	0
2	CO3	I	612	-	2,3,3	1.05	0	2,3,3	5.73	1 (50%)
5	SO4	I	620	-	4,4,4	0.92	0	6,6,6	0.32	0
2	CO3	A	612	-	2,3,3	2.11	2 (100%)	2,3,3	8.40	2 (100%)
4	DGZ	C	615	3	78,78,78	0.89	1 (1%)	99,101,101	2.36	3 (3%)
5	SO4	L	616	-	4,4,4	0.65	0	6,6,6	0.36	0
2	CO3	C	612	-	2,3,3	2.06	1 (50%)	2,3,3	6.60	2 (100%)
6	1PE	I	623	-	4,4,15	1.69	1 (25%)	3,3,14	0.97	0
6	1PE	L	617	-	9,9,15	2.26	4 (44%)	8,8,14	1.86	3 (37%)
6	1PE	K	617	-	7,7,15	2.39	3 (42%)	6,6,14	2.63	3 (50%)
5	SO4	D	617	-	4,4,4	0.43	0	6,6,6	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	SO4	A	616	-	4,4,4	0.22	0	6,6,6	0.20	0
5	SO4	G	618	-	4,4,4	0.15	0	6,6,6	0.21	0
4	DGZ	E	615	3	78,78,78	0.88	1 (1%)	99,101,101	2.34	3 (3%)
4	DGZ	I	615	3	78,78,78	0.90	1 (1%)	99,101,101	2.37	3 (3%)
5	SO4	A	617	-	4,4,4	0.54	0	6,6,6	0.25	0
5	SO4	E	617	-	4,4,4	0.37	0	6,6,6	0.10	0
7	2PE	H	619	-	24,24,27	0.74	0	23,23,26	0.67	0
4	DGZ	J	615	3	78,78,78	0.89	1 (1%)	99,101,101	2.34	4 (4%)
5	SO4	C	617	-	4,4,4	0.23	0	6,6,6	0.07	0
4	DGZ	G	615	3	78,78,78	0.88	1 (1%)	99,101,101	2.33	3 (3%)
5	SO4	C	616	-	4,4,4	0.28	0	6,6,6	0.57	0
6	1PE	A	618	-	8,8,15	2.05	2 (25%)	7,7,14	3.10	3 (42%)
6	1PE	L	618	-	11,11,15	2.20	4 (36%)	10,10,14	3.33	6 (60%)
5	SO4	K	616	-	4,4,4	0.32	0	6,6,6	0.15	0
6	1PE	K	619	-	10,10,15	2.68	5 (50%)	9,9,14	2.61	5 (55%)
5	SO4	J	617	-	4,4,4	0.21	0	6,6,6	0.17	0
2	CO3	G	612	-	2,3,3	1.18	0	2,3,3	5.62	2 (100%)
4	DGZ	A	615	3	78,78,78	0.91	1 (1%)	99,101,101	2.33	3 (3%)
5	SO4	I	616	-	4,4,4	0.37	0	6,6,6	0.12	0
4	DGZ	D	615	3	78,78,78	0.89	1 (1%)	99,101,101	2.38	3 (3%)
5	SO4	J	616	-	4,4,4	0.83	0	6,6,6	0.28	0
5	SO4	I	617	-	4,4,4	0.77	0	6,6,6	0.39	0
6	1PE	C	621	-	11,11,15	2.26	4 (36%)	10,10,14	3.07	5 (50%)
6	1PE	F	616	-	9,9,15	2.56	5 (55%)	8,8,14	2.96	4 (50%)
5	SO4	J	618	-	4,4,4	0.40	0	6,6,6	0.21	0
6	1PE	A	619	-	6,6,15	1.67	1 (16%)	5,5,14	2.37	2 (40%)
6	1PE	K	620	-	5,5,15	2.07	1 (20%)	4,4,14	1.89	2 (50%)
2	CO3	F	612	-	2,3,3	1.34	0	2,3,3	5.15	1 (50%)
6	1PE	G	622	-	5,5,15	1.62	1 (20%)	4,4,14	3.09	2 (50%)
5	SO4	E	616	-	4,4,4	0.16	0	6,6,6	0.16	0
6	1PE	F	617	-	9,9,15	2.60	4 (44%)	8,8,14	2.99	5 (62%)
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
6	1PE	G	620	-	8,8,15	2.17	4 (50%)	7,7,14	2.54	4 (57%)
6	1PE	I	621	-	11,11,15	2.37	4 (36%)	10,10,14	3.02	5 (50%)
5	SO4	G	617	-	4,4,4	0.81	0	6,6,6	0.42	0
6	1PE	D	620	-	10,10,15	2.18	5 (50%)	9,9,14	2.84	5 (55%)
6	1PE	E	620	-	9,9,15	2.22	4 (44%)	8,8,14	3.01	6 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	G	616	-	4,4,4	0.19	0	6,6,6	0.17	0
5	SO4	C	619	-	4,4,4	0.79	0	6,6,6	0.32	0
4	DGZ	H	615	3	78,78,78	0.91	2 (2%)	99,101,101	2.26	2 (2%)
5	SO4	D	616	-	4,4,4	0.20	0	6,6,6	0.09	0
5	SO4	E	618	-	4,4,4	0.77	0	6,6,6	0.41	0
6	1PE	I	622	-	9,9,15	2.29	4 (44%)	8,8,14	2.26	3 (37%)
6	1PE	G	623	-	14,14,15	3.18	7 (50%)	13,13,14	3.42	7 (53%)
6	1PE	D	621	-	4,4,15	2.86	4 (100%)	3,3,14	1.91	1 (33%)
2	CO3	E	612	-	2,3,3	0.38	0	2,3,3	6.56	2 (100%)
2	CO3	J	612	-	2,3,3	1.53	0	2,3,3	6.66	2 (100%)
5	SO4	C	618	-	4,4,4	0.18	0	6,6,6	0.18	0
2	CO3	L	612	-	2,3,3	1.44	1 (50%)	2,3,3	4.68	1 (50%)
7	2PE	B	616	-	25,25,27	0.94	0	24,24,26	0.57	0
2	CO3	K	612	-	2,3,3	0.91	0	2,3,3	12.44	2 (100%)
6	1PE	J	620	-	9,9,15	2.79	5 (55%)	8,8,14	3.14	4 (50%)
5	SO4	H	618	-	4,4,4	0.93	0	6,6,6	0.38	0
6	1PE	J	619	-	10,10,15	2.54	5 (50%)	9,9,14	2.13	5 (55%)
2	CO3	B	612	-	2,3,3	1.82	0	2,3,3	8.21	2 (100%)
4	DGZ	B	615	3	78,78,78	0.89	1 (1%)	99,101,101	2.36	2 (2%)
6	1PE	F	618	-	9,9,15	3.07	5 (55%)	8,8,14	3.27	4 (50%)
6	1PE	E	619	-	11,11,15	2.43	4 (36%)	10,10,14	3.11	6 (60%)
5	SO4	H	617	-	4,4,4	0.21	0	6,6,6	0.14	0
6	1PE	D	618	-	9,9,15	2.22	3 (33%)	8,8,14	3.07	4 (50%)
6	1PE	G	621	-	5,5,15	1.63	1 (20%)	4,4,14	2.96	2 (50%)
6	1PE	C	622	-	8,8,15	2.42	3 (37%)	7,7,14	3.16	3 (42%)
2	CO3	H	612	-	2,3,3	1.40	0	2,3,3	5.86	2 (100%)
6	1PE	J	621	-	10,10,15	2.21	4 (40%)	9,9,14	2.71	3 (33%)
6	1PE	J	622	-	8,8,15	2.36	3 (37%)	7,7,14	2.95	3 (42%)
5	SO4	I	619	-	4,4,4	0.25	0	6,6,6	0.12	0
6	1PE	K	618	-	11,11,15	2.14	4 (36%)	10,10,14	3.06	4 (40%)
6	1PE	L	619	-	6,6,15	1.87	1 (16%)	5,5,14	2.26	2 (40%)
4	DGZ	K	615	3	78,78,78	0.89	1 (1%)	99,101,101	2.37	3 (3%)
4	DGZ	L	615	3	78,78,78	0.90	1 (1%)	99,101,101	2.35	3 (3%)
6	1PE	D	619	-	7,7,15	2.26	2 (28%)	6,6,14	2.29	3 (50%)
5	SO4	C	620	-	4,4,4	0.41	0	6,6,6	0.17	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	E	621	-	-	2/5/5/13	-
6	1PE	D	618	-	-	5/7/7/13	-
6	1PE	F	617	-	-	4/7/7/13	-
4	DGZ	F	615	3	-	20/75/76/76	0/5/5/5
6	1PE	G	620	-	-	4/6/6/13	-
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	I	621	-	-	4/9/9/13	-
6	1PE	D	620	-	-	4/8/8/13	-
7	2PE	H	619	-	-	13/22/22/25	-
4	DGZ	J	615	3	-	14/75/76/76	0/5/5/5
6	1PE	E	620	-	-	2/7/7/13	-
4	DGZ	G	615	3	-	21/75/76/76	0/5/5/5
4	DGZ	H	615	3	-	19/75/76/76	0/5/5/5
6	1PE	A	618	-	-	0/6/6/13	-
6	1PE	J	621	-	-	4/8/8/13	-
4	DGZ	C	615	3	-	20/75/76/76	0/5/5/5
6	1PE	I	622	-	-	2/7/7/13	-
6	1PE	J	622	-	-	5/6/6/13	-
6	1PE	G	623	-	-	7/12/12/13	-
6	1PE	K	618	-	-	6/9/9/13	-
6	1PE	K	619	-	-	3/8/8/13	-
6	1PE	L	618	-	-	5/9/9/13	-
6	1PE	D	621	-	-	2/2/2/13	-
7	2PE	B	616	-	-	9/23/23/25	-
4	DGZ	A	615	3	-	24/75/76/76	0/5/5/5
4	DGZ	D	615	3	-	11/75/76/76	0/5/5/5
6	1PE	J	620	-	-	6/7/7/13	-
6	1PE	I	623	-	-	1/2/2/13	-
6	1PE	L	617	-	-	4/7/7/13	-
6	1PE	J	619	-	-	6/8/8/13	-
4	DGZ	K	615	3	-	20/75/76/76	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	L	619	-	-	3/4/4/13	-
6	1PE	C	621	-	-	5/9/9/13	-
6	1PE	F	616	-	-	6/7/7/13	-
6	1PE	K	617	-	-	3/5/5/13	-
4	DGZ	L	615	3	-	17/75/76/76	0/5/5/5
6	1PE	D	619	-	-	1/5/5/13	-
6	1PE	A	619	-	-	1/4/4/13	-
4	DGZ	E	615	3	-	20/75/76/76	0/5/5/5
6	1PE	K	620	-	-	3/3/3/13	-
4	DGZ	I	615	3	-	20/75/76/76	0/5/5/5
4	DGZ	B	615	3	-	13/75/76/76	0/5/5/5
6	1PE	G	622	-	-	3/3/3/13	-
6	1PE	F	618	-	-	4/7/7/13	-
6	1PE	E	619	-	-	5/9/9/13	-

All (133) 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
6	L	620	1PE	C26-C16	4.88	1.75	1.49
4	A	615	DGZ	C2-C1	4.88	1.32	1.18
4	L	615	DGZ	C2-C1	4.87	1.32	1.18
4	D	615	DGZ	C2-C1	4.86	1.32	1.18
4	E	615	DGZ	C2-C1	4.85	1.32	1.18
4	G	615	DGZ	C2-C1	4.85	1.32	1.18
4	F	615	DGZ	C2-C1	4.85	1.32	1.18
4	B	615	DGZ	C2-C1	4.84	1.32	1.18
4	I	615	DGZ	C2-C1	4.80	1.32	1.18
6	G	623	1PE	OH6-C26	4.77	1.62	1.42
6	F	618	1PE	C26-C16	4.76	1.74	1.49
4	C	615	DGZ	C2-C1	4.76	1.32	1.18
6	F	618	1PE	OH6-C26	4.65	1.62	1.42
6	J	622	1PE	OH4-C13	4.62	1.62	1.42
6	D	618	1PE	OH4-C13	4.55	1.61	1.42
6	L	620	1PE	OH6-C26	4.54	1.61	1.42
6	C	622	1PE	OH4-C13	4.54	1.61	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	619	1PE	OH4-C13	4.45	1.61	1.42
6	I	621	1PE	OH4-C13	4.41	1.61	1.42
6	I	622	1PE	OH4-C13	4.40	1.61	1.42
6	E	619	1PE	OH4-C13	4.34	1.60	1.42
6	J	620	1PE	C26-C16	4.33	1.72	1.49
6	F	617	1PE	C26-C16	4.15	1.71	1.49
6	K	619	1PE	OH6-C26	4.09	1.62	1.42
6	E	621	1PE	OH4-C13	4.04	1.59	1.42
6	J	619	1PE	OH4-C13	4.04	1.62	1.42
6	C	621	1PE	OH4-C13	4.04	1.59	1.42
6	E	620	1PE	OH4-C13	4.04	1.59	1.42
6	F	616	1PE	OH6-C26	4.03	1.59	1.42
6	A	618	1PE	OH4-C13	4.01	1.59	1.42
6	L	620	1PE	OH4-C13	4.01	1.62	1.42
6	D	619	1PE	OH6-C26	4.00	1.62	1.42
6	G	620	1PE	OH4-C13	3.99	1.59	1.42
6	F	617	1PE	OH6-C26	3.98	1.59	1.42
6	F	616	1PE	C26-C16	3.98	1.70	1.49
6	J	620	1PE	OH6-C26	3.97	1.59	1.42
6	K	620	1PE	OH4-C13	3.89	1.61	1.42
6	G	623	1PE	OH6-C15	3.86	1.58	1.42
6	K	618	1PE	OH4-C13	3.84	1.58	1.42
6	F	618	1PE	OH7-C16	3.84	1.61	1.42
6	G	623	1PE	OH7-C16	3.79	1.61	1.42
6	K	617	1PE	OH4-C13	3.78	1.61	1.42
6	D	620	1PE	OH6-C15	3.78	1.58	1.42
6	J	619	1PE	OH6-C26	3.78	1.58	1.42
6	F	618	1PE	OH6-C15	3.76	1.58	1.42
6	G	623	1PE	C23-C13	3.73	1.68	1.49
6	L	617	1PE	C26-C16	3.68	1.69	1.49
6	D	621	1PE	OH6-C15	3.66	1.60	1.42
6	L	620	1PE	OH7-C16	3.58	1.60	1.42
6	J	619	1PE	OH7-C16	3.56	1.60	1.42
6	J	619	1PE	C26-C16	3.54	1.68	1.49
6	G	623	1PE	OH3-C23	3.53	1.57	1.42
6	J	621	1PE	OH6-C15	3.51	1.57	1.42
6	L	618	1PE	OH4-C13	3.44	1.57	1.42
6	J	620	1PE	OH7-C16	3.38	1.59	1.42
6	D	620	1PE	C16-C26	3.37	1.73	1.46
6	F	617	1PE	OH7-C16	3.35	1.59	1.42
6	I	621	1PE	OH3-C23	3.34	1.56	1.42
6	J	621	1PE	C16-C26	3.34	1.73	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	619	1PE	OH6-C15	3.33	1.59	1.42
6	L	619	1PE	OH6-C15	3.32	1.59	1.42
6	L	617	1PE	OH6-C26	3.26	1.56	1.42
6	C	621	1PE	C23-C13	3.26	1.65	1.49
6	F	616	1PE	OH7-C16	3.25	1.58	1.42
6	C	622	1PE	OH3-C23	3.23	1.56	1.42
6	G	621	1PE	OH6-C15	3.22	1.58	1.42
6	L	618	1PE	OH6-C15	3.22	1.58	1.42
6	L	620	1PE	OH6-C15	3.22	1.56	1.42
6	E	621	1PE	C13-C23	3.14	1.66	1.49
6	E	619	1PE	OH3-C23	3.13	1.55	1.42
6	K	617	1PE	OH6-C15	3.11	1.58	1.42
6	L	617	1PE	OH7-C16	3.10	1.58	1.42
6	E	619	1PE	C23-C13	3.10	1.65	1.49
6	C	621	1PE	OH6-C15	3.06	1.57	1.42
6	I	621	1PE	OH6-C15	3.01	1.57	1.42
6	K	618	1PE	OH3-C23	3.00	1.55	1.42
6	A	619	1PE	OH6-C15	3.00	1.57	1.42
6	I	621	1PE	C23-C13	2.99	1.64	1.49
6	G	620	1PE	C23-C13	2.98	1.64	1.49
6	J	620	1PE	OH6-C15	2.96	1.54	1.42
6	C	622	1PE	C23-C13	2.96	1.64	1.49
6	F	617	1PE	OH6-C15	2.93	1.54	1.42
6	E	620	1PE	OH3-C23	2.93	1.57	1.42
6	D	619	1PE	OH6-C15	2.92	1.57	1.40
6	I	622	1PE	C23-C13	2.91	1.64	1.49
6	K	619	1PE	OH6-C15	2.90	1.57	1.40
6	D	618	1PE	OH3-C23	2.87	1.54	1.42
6	K	619	1PE	C13-C23	2.85	1.64	1.49
6	G	622	1PE	OH6-C15	2.84	1.56	1.42
6	L	618	1PE	C23-C13	2.83	1.63	1.49
6	A	618	1PE	C23-C13	2.83	1.63	1.49
6	D	618	1PE	C23-C13	2.82	1.63	1.49
6	L	618	1PE	OH3-C23	2.80	1.54	1.42
6	C	621	1PE	OH3-C23	2.80	1.54	1.42
6	K	618	1PE	C23-C13	2.77	1.63	1.49
6	E	620	1PE	C13-C23	2.76	1.64	1.49
6	J	621	1PE	C23-C13	2.69	1.67	1.46
6	D	621	1PE	C26-C16	2.69	1.63	1.49
6	J	622	1PE	C13-C23	2.62	1.63	1.49
6	F	616	1PE	OH6-C15	2.60	1.53	1.42
6	D	621	1PE	OH7-C16	2.57	1.55	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	622	1PE	OH3-C23	2.55	1.55	1.40
6	K	618	1PE	OH6-C15	2.55	1.55	1.42
6	K	619	1PE	OH3-C23	2.51	1.55	1.42
2	C	612	CO3	O3-C	-2.50	1.11	1.33
6	J	620	1PE	OH5-C14	2.46	1.52	1.42
6	E	620	1PE	OH6-C15	2.43	1.54	1.42
6	L	617	1PE	OH6-C15	2.37	1.52	1.42
6	J	621	1PE	OH4-C13	2.36	1.62	1.42
6	D	621	1PE	OH6-C26	2.36	1.54	1.40
6	G	620	1PE	OH3-C23	2.36	1.54	1.40
6	J	622	1PE	OH3-C23	2.34	1.54	1.42
6	I	622	1PE	OH3-C22	2.31	1.53	1.42
6	D	620	1PE	C23-C13	2.29	1.64	1.46
6	I	623	1PE	OH4-C24	2.23	1.53	1.42
6	J	619	1PE	OH6-C15	2.22	1.51	1.42
2	D	612	CO3	O3-C	-2.20	1.14	1.33
6	K	617	1PE	OH5-C25	2.18	1.51	1.42
6	E	621	1PE	OH3-C23	2.16	1.53	1.42
6	D	620	1PE	OH4-C13	2.16	1.61	1.42
2	A	612	CO3	O2-C	2.16	1.52	1.33
6	F	618	1PE	C25-C15	2.15	1.60	1.49
6	G	620	1PE	OH3-C22	2.09	1.52	1.42
2	A	612	CO3	O3-C	-2.07	1.15	1.33
2	L	612	CO3	O3-C	-2.04	1.16	1.33
6	D	620	1PE	OH6-C26	2.02	1.59	1.42
6	F	616	1PE	OH4-C24	2.02	1.52	1.42
4	H	615	DGZ	C3-C2	2.01	1.51	1.47

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
4	B	615	DGZ	C3-C2-C1	-21.75	120.48	177.14
4	L	615	DGZ	C3-C2-C1	-21.73	120.53	177.14
4	A	615	DGZ	C3-C2-C1	-21.64	120.77	177.14
4	J	615	DGZ	C3-C2-C1	-21.63	120.78	177.14
4	K	615	DGZ	C3-C2-C1	-21.63	120.80	177.14
4	G	615	DGZ	C3-C2-C1	-21.60	120.87	177.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	615	DGZ	C3-C2-C1	-21.53	121.05	177.14
2	K	612	CO3	O2-C-O1	-15.66	78.93	119.55
2	A	612	CO3	O3-C-O1	-11.23	90.42	119.55
2	B	612	CO3	O3-C-O1	-10.27	92.90	119.55
2	J	612	CO3	O3-C-O1	8.99	142.87	119.55
2	I	612	CO3	O2-C-O1	8.07	140.48	119.55
2	K	612	CO3	O3-C-O1	8.01	140.33	119.55
2	D	612	CO3	O3-C-O1	7.94	140.13	119.55
6	G	623	1PE	OH3-C23-C13	7.67	144.99	110.39
2	C	612	CO3	O3-C-O1	7.59	139.24	119.55
6	D	618	1PE	OH3-C23-C13	7.41	143.79	110.39
2	F	612	CO3	O3-C-O1	7.19	138.19	119.55
6	C	622	1PE	OH3-C23-C13	7.09	142.35	110.39
6	I	621	1PE	OH3-C23-C13	7.01	141.99	110.39
2	E	612	CO3	O3-C-O1	7.00	137.71	119.55
6	K	618	1PE	OH3-C23-C13	6.60	140.15	110.39
2	L	612	CO3	O3-C-O1	6.59	136.64	119.55
2	H	612	CO3	O2-C-O1	6.43	136.23	119.55
2	G	612	CO3	O2-C-O1	6.43	136.22	119.55
6	L	618	1PE	OH3-C23-C13	6.18	138.25	110.39
6	F	618	1PE	OH6-C15-C25	6.15	138.12	110.39
2	E	612	CO3	O2-C-O1	-6.08	103.78	119.55
6	E	619	1PE	OH3-C23-C13	5.92	137.09	110.39
6	C	621	1PE	OH3-C23-C13	5.88	136.91	110.39
6	J	621	1PE	OH6-C15-C25	5.67	135.95	110.39
6	A	618	1PE	OH3-C23-C13	5.64	135.81	110.39
6	G	623	1PE	OH6-C15-C25	5.56	135.44	110.39
2	C	612	CO3	O2-C-O1	5.43	133.63	119.55
2	B	612	CO3	O2-C-O1	5.41	133.58	119.55
6	J	620	1PE	OH6-C15-C25	5.32	134.40	110.39
6	F	616	1PE	OH6-C15-C25	5.31	134.34	110.39
6	K	619	1PE	OH3-C23-C13	5.26	142.32	111.81
2	H	612	CO3	O3-C-O1	-5.23	105.98	119.55
6	D	620	1PE	C13-OH4-C24	5.14	131.31	112.90
6	F	617	1PE	OH6-C15-C25	5.10	133.37	110.39
6	G	621	1PE	C14-OH5-C25	5.07	131.08	112.90
6	J	622	1PE	C25-OH5-C14	5.00	130.80	112.90
6	E	620	1PE	C24-OH4-C13	4.99	134.91	113.29
6	J	622	1PE	OH3-C23-C13	4.86	139.98	111.81
2	G	612	CO3	O3-C-O1	-4.67	107.42	119.55
6	D	620	1PE	OH6-C15-C25	4.66	131.39	110.39
6	L	618	1PE	C24-OH4-C13	4.61	133.27	113.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	619	1PE	OH6-C15-C25	4.50	137.90	111.81
6	J	621	1PE	C25-OH5-C14	4.47	132.68	113.29
6	G	622	1PE	OH6-C15-C25	4.44	137.57	111.81
6	E	621	1PE	OH3-C23-C13	4.42	137.47	111.81
6	E	619	1PE	C24-OH4-C13	4.38	132.27	113.29
6	G	623	1PE	C24-OH4-C13	4.36	132.20	113.29
6	J	620	1PE	C25-OH5-C14	4.31	131.95	113.29
6	G	623	1PE	OH7-C16-C26	4.27	136.59	111.81
6	G	622	1PE	C14-OH5-C25	4.14	127.73	112.90
6	E	620	1PE	OH3-C23-C13	4.11	135.65	111.81
6	A	618	1PE	C24-OH4-C13	4.10	131.06	113.29
6	L	620	1PE	OH7-C16-C26	4.06	135.36	111.81
6	F	617	1PE	OH6-C26-C16	4.06	127.89	110.07
6	L	618	1PE	OH6-C15-C25	4.05	135.30	111.81
6	I	622	1PE	C25-OH5-C14	4.04	127.38	112.90
6	D	619	1PE	C25-OH5-C14	4.04	130.80	113.29
4	J	615	DGZ	O9-C48-C49	4.02	118.08	109.64
6	C	621	1PE	C25-OH5-C14	3.98	130.55	113.29
6	K	618	1PE	C24-OH4-C13	3.97	130.51	113.29
6	L	620	1PE	C25-OH5-C14	3.97	130.50	113.29
6	F	616	1PE	C25-OH5-C14	3.94	130.37	113.29
6	K	617	1PE	OH6-C15-C25	3.93	134.62	111.81
4	K	615	DGZ	O9-C48-C49	3.91	117.83	109.64
6	F	618	1PE	OH7-C16-C26	3.90	134.42	111.81
6	L	620	1PE	OH6-C15-C25	3.89	127.96	110.39
6	J	620	1PE	OH7-C16-C26	3.88	134.31	111.81
6	C	621	1PE	C24-OH4-C13	3.87	130.07	113.29
4	D	615	DGZ	O9-C48-C49	3.86	117.73	109.64
2	A	612	CO3	O2-C-O1	3.86	129.55	119.55
6	G	620	1PE	OH3-C23-C13	3.80	140.05	111.07
6	A	619	1PE	OH6-C15-C25	3.78	133.75	111.81
6	K	617	1PE	C25-OH5-C14	3.74	129.50	113.29
6	E	621	1PE	C24-OH4-C13	3.71	129.38	113.29
6	F	618	1PE	C25-OH5-C14	3.68	129.21	113.29
6	I	621	1PE	C24-OH4-C13	3.64	129.07	113.29
6	I	621	1PE	OH6-C15-C25	3.63	132.85	111.81
6	F	618	1PE	OH6-C26-C16	3.58	125.80	110.07
6	E	619	1PE	C25-OH5-C14	3.56	128.71	113.29
6	K	618	1PE	OH6-C15-C25	3.52	132.21	111.81
6	I	622	1PE	OH3-C23-C13	3.50	137.78	111.07
6	L	617	1PE	OH6-C15-C25	3.49	126.13	110.39
6	J	619	1PE	OH6-C15-C25	3.44	125.92	110.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	615	DGZ	O9-C48-C49	3.44	116.85	109.64
6	D	620	1PE	C25-OH5-C14	3.40	128.03	113.29
6	G	620	1PE	OH4-C24-C14	-3.40	95.08	110.39
6	A	618	1PE	OH4-C24-C14	-3.39	95.17	110.07
6	C	621	1PE	C22-OH3-C23	3.36	124.92	112.90
6	F	617	1PE	C25-OH5-C14	3.35	127.80	113.29
6	J	622	1PE	C24-OH4-C13	3.32	127.66	113.29
4	F	615	DGZ	O9-C48-C49	3.28	116.52	109.64
6	A	619	1PE	C25-OH5-C14	3.27	127.45	113.29
6	K	619	1PE	C24-OH4-C13	3.26	127.42	113.29
6	J	621	1PE	C13-OH4-C24	3.26	124.57	112.90
4	G	615	DGZ	O9-C48-C49	3.25	116.46	109.64
4	B	615	DGZ	O9-C48-C47	-3.23	103.67	110.63
6	L	618	1PE	OH4-C24-C14	-3.22	95.88	110.39
4	C	615	DGZ	O9-C48-C49	3.21	116.38	109.64
6	F	616	1PE	OH7-C16-C26	3.20	130.35	111.81
6	G	620	1PE	C24-OH4-C13	3.19	127.12	113.29
6	G	623	1PE	C25-OH5-C14	3.19	127.09	113.29
6	K	619	1PE	C25-OH5-C14	3.16	126.98	113.29
6	J	620	1PE	OH6-C26-C16	3.16	123.94	110.07
6	L	618	1PE	C22-OH3-C23	3.15	124.18	112.90
6	C	621	1PE	OH6-C15-C25	3.13	129.99	111.81
6	C	622	1PE	C24-OH4-C13	3.08	126.64	113.29
4	L	615	DGZ	O9-C48-C49	3.07	116.08	109.64
6	F	617	1PE	OH7-C16-C26	3.03	129.40	111.81
6	E	619	1PE	OH6-C15-C25	3.03	129.38	111.81
6	D	621	1PE	OH7-C16-C26	3.02	129.34	111.81
6	D	619	1PE	OH6-C15-C25	3.02	134.10	111.07
6	I	622	1PE	C24-OH4-C13	3.02	126.36	113.29
6	K	620	1PE	C25-OH5-C14	3.02	131.72	112.96
6	E	620	1PE	OH4-C24-C14	-2.99	96.89	110.39
6	K	618	1PE	C25-OH5-C14	2.93	126.00	113.29
6	F	616	1PE	OH6-C26-C16	2.91	122.87	110.07
6	E	619	1PE	OH4-C24-C14	-2.82	97.68	110.39
6	K	619	1PE	OH6-C15-C25	2.80	132.42	111.07
2	J	612	CO3	O2-C-O1	2.80	126.80	119.55
6	K	617	1PE	C13-OH4-C24	2.77	130.22	112.96
6	J	619	1PE	OH7-C16-C26	2.77	127.89	111.81
6	J	619	1PE	OH4-C24-C14	-2.72	90.33	111.07
6	G	620	1PE	C25-OH5-C14	2.71	129.83	112.96
6	L	618	1PE	C25-OH5-C14	2.71	125.03	113.29
6	L	617	1PE	OH7-C16-C26	2.70	127.47	111.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	618	1PE	OH4-C24-C14	-2.68	98.31	110.39
4	A	615	DGZ	O9-C48-C49	2.66	115.22	109.64
6	E	620	1PE	C25-OH5-C14	2.64	124.71	113.29
4	D	615	DGZ	C12-C13-N3	2.63	118.32	111.16
6	C	622	1PE	OH4-C24-C14	-2.62	98.54	110.07
6	G	621	1PE	OH6-C15-C25	2.62	127.02	111.81
6	L	620	1PE	OH6-C26-C16	2.59	121.46	110.07
6	J	619	1PE	C26-OH6-C15	2.56	124.40	113.29
6	I	621	1PE	OH5-C14-C24	2.55	121.89	110.39
4	H	615	DGZ	O9-C48-C49	2.53	114.95	109.64
4	J	615	DGZ	O9-C48-C47	-2.48	105.28	110.63
6	E	619	1PE	C22-OH3-C23	2.48	121.77	112.90
6	E	620	1PE	OH6-C15-C25	2.42	125.87	111.81
6	E	621	1PE	OH4-C24-C14	-2.39	99.63	110.39
6	G	623	1PE	OH4-C24-C14	-2.33	99.88	110.39
4	L	615	DGZ	C13-N3-C28	2.33	127.64	121.65
6	G	623	1PE	OH6-C26-C16	2.31	120.22	110.07
6	E	621	1PE	C25-OH5-C14	2.30	127.25	112.96
6	J	619	1PE	C13-OH4-C24	2.29	127.21	112.96
6	D	618	1PE	C24-OH4-C13	2.28	123.15	113.29
4	I	615	DGZ	C37-C36-C35	-2.27	107.13	113.39
4	A	615	DGZ	O9-C48-C47	-2.26	105.76	110.63
6	L	620	1PE	C13-OH4-C24	2.25	126.97	112.96
4	G	615	DGZ	C50-C49-C48	-2.25	105.27	111.38
6	L	619	1PE	C25-OH5-C14	2.23	122.94	113.29
6	K	619	1PE	OH4-C24-C14	-2.21	100.41	110.39
6	I	621	1PE	C25-OH5-C14	2.20	122.82	113.29
6	E	620	1PE	OH4-C13-C23	-2.18	100.49	110.07
4	E	615	DGZ	O9-C48-C49	2.18	114.21	109.64
4	C	615	DGZ	C50-C49-C48	-2.16	105.51	111.38
6	K	620	1PE	C13-OH4-C24	2.15	126.33	112.96
6	F	617	1PE	OH4-C24-C14	-2.14	99.40	111.81
6	L	617	1PE	C25-OH5-C14	2.12	122.49	113.29
6	D	620	1PE	C26-OH6-C15	2.12	120.50	112.90
4	J	615	DGZ	C57-C11-N2	2.09	115.25	110.18
6	D	619	1PE	OH4-C24-C14	-2.07	99.78	111.81
6	D	618	1PE	C25-OH5-C14	2.05	125.75	112.96
4	E	615	DGZ	C11-C57-N7	2.03	120.16	116.69
4	K	615	DGZ	C11-C57-N7	2.03	120.16	116.69
6	D	620	1PE	OH4-C24-C14	-2.00	101.37	110.39

There are no chirality outliers.

All (361) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	615	DGZ	N5-C47-C48-O9
4	A	615	DGZ	C48-C49-C50-C51
4	B	615	DGZ	N5-C47-C48-O9
4	B	615	DGZ	C47-C48-C49-N6
4	B	615	DGZ	C48-C49-C50-C51
4	C	615	DGZ	N5-C47-C48-O9
4	C	615	DGZ	O8-C47-C48-O9
4	C	615	DGZ	C48-C49-C50-C51
4	D	615	DGZ	N5-C47-C48-O9
4	D	615	DGZ	O8-C47-C48-O9
4	E	615	DGZ	N5-C47-C48-O9
4	F	615	DGZ	N5-C47-C48-O9
4	F	615	DGZ	O9-C48-C49-N6
4	F	615	DGZ	O9-C48-C49-C50
4	F	615	DGZ	C47-C48-C49-N6
4	G	615	DGZ	N5-C47-C48-O9
4	G	615	DGZ	O8-C47-C48-O9
4	G	615	DGZ	O9-C48-C49-C50
4	G	615	DGZ	C48-C49-C50-C51
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	I	615	DGZ	N5-C47-C48-O9
4	J	615	DGZ	N5-C47-C48-O9
4	J	615	DGZ	C48-C49-C50-C51
4	K	615	DGZ	N5-C47-C48-O9
4	K	615	DGZ	O8-C47-C48-O9
4	L	615	DGZ	C9-C10-C11-C57
4	L	615	DGZ	N5-C47-C48-O9
4	A	615	DGZ	C3-C4-C5-C6
4	B	615	DGZ	C3-C4-C5-C6
4	C	615	DGZ	C3-C4-C5-C6
4	G	615	DGZ	C3-C4-C5-C6
4	K	615	DGZ	C3-C4-C5-C6
6	J	622	1PE	C14-C24-OH4-C13
6	L	619	1PE	C24-C14-OH5-C25
6	G	623	1PE	C16-C26-OH6-C15
6	C	622	1PE	C23-C13-OH4-C24
6	D	621	1PE	OH7-C16-C26-OH6
6	F	617	1PE	OH7-C16-C26-OH6
4	F	615	DGZ	C9-C10-C11-N2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	L	615	DGZ	C9-C10-C11-N2
4	I	615	DGZ	C2-C3-C4-C5
6	F	616	1PE	C16-C26-OH6-C15
6	L	618	1PE	C15-C25-OH5-C14
6	L	620	1PE	OH5-C14-C24-OH4
7	B	616	2PE	O13-C14-C15-O16
4	K	615	DGZ	O5-C30-C31-O6
6	F	616	1PE	OH6-C15-C25-OH5
4	A	615	DGZ	N1-C7-C8-C9
4	B	615	DGZ	N1-C7-C8-C9
4	H	615	DGZ	N1-C7-C8-C9
4	I	615	DGZ	N1-C7-C8-C9
4	F	615	DGZ	C9-C10-C11-C57
4	B	615	DGZ	O5-C30-C31-O6
6	C	622	1PE	OH4-C13-C23-OH3
6	E	621	1PE	OH5-C14-C24-OH4
7	B	616	2PE	O22-C23-C24-O25
6	K	618	1PE	OH4-C13-C23-OH3
6	D	620	1PE	OH5-C14-C24-OH4
4	L	615	DGZ	O6-C32-C33-N4
4	A	615	DGZ	C2-C3-C4-C5
4	C	615	DGZ	C2-C3-C4-C5
4	C	615	DGZ	O5-C30-C31-O6
6	K	618	1PE	C13-C23-OH3-C22
4	L	615	DGZ	N1-C7-C8-C9
6	G	623	1PE	OH4-C13-C23-OH3
6	G	623	1PE	OH5-C14-C24-OH4
4	E	615	DGZ	C3-C4-C5-C6
4	K	615	DGZ	C17-C18-C19-O3
7	H	619	2PE	O10-C11-C12-O13
6	G	623	1PE	OH6-C15-C25-OH5
7	H	619	2PE	O22-C23-C24-O25
4	G	615	DGZ	O5-C30-C31-O6
6	K	617	1PE	OH5-C14-C24-OH4
4	K	615	DGZ	C26-C18-C19-O3
6	J	620	1PE	OH6-C15-C25-OH5
6	F	618	1PE	OH7-C16-C26-OH6
6	G	623	1PE	OH7-C16-C26-OH6
6	J	620	1PE	OH5-C14-C24-OH4
6	K	617	1PE	OH6-C15-C25-OH5
6	L	620	1PE	OH7-C16-C26-OH6
7	H	619	2PE	O25-C26-C27-O28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	615	DGZ	C30-C31-O6-C32
6	G	620	1PE	OH4-C13-C23-OH3
6	L	618	1PE	OH4-C13-C23-OH3
4	I	615	DGZ	C9-C10-C11-C57
6	J	619	1PE	OH5-C14-C24-OH4
4	E	615	DGZ	O5-C30-C31-O6
6	K	620	1PE	OH5-C14-C24-OH4
6	D	618	1PE	C24-C14-OH5-C25
4	A	615	DGZ	C11-C10-C9-C8
6	I	621	1PE	C12-C22-OH3-C23
4	K	615	DGZ	C17-C18-C19-C20
6	I	621	1PE	OH4-C13-C23-OH3
6	L	618	1PE	OH5-C14-C24-OH4
6	F	616	1PE	OH7-C16-C26-OH6
6	J	619	1PE	OH7-C16-C26-OH6
6	J	620	1PE	OH7-C16-C26-OH6
6	K	618	1PE	OH6-C15-C25-OH5
6	K	619	1PE	OH4-C13-C23-OH3
6	L	619	1PE	OH6-C15-C25-OH5
4	K	615	DGZ	C26-C18-C19-C20
6	C	622	1PE	C12-C22-OH3-C23
6	J	622	1PE	C15-C25-OH5-C14
4	F	615	DGZ	C2-C3-C4-C5
4	G	615	DGZ	C2-C3-C4-C5
4	J	615	DGZ	C2-C3-C4-C5
6	L	618	1PE	C12-C22-OH3-C23
6	L	617	1PE	OH6-C15-C25-OH5
4	A	615	DGZ	O8-C47-C48-O9
4	B	615	DGZ	O8-C47-C48-O9
4	E	615	DGZ	O8-C47-C48-O9
4	F	615	DGZ	O8-C47-C48-O9
4	H	615	DGZ	O8-C47-C48-O9
4	I	615	DGZ	O8-C47-C48-O9
4	J	615	DGZ	O8-C47-C48-O9
4	L	615	DGZ	O8-C47-C48-O9
6	G	620	1PE	C24-C14-OH5-C25
6	L	617	1PE	OH5-C14-C24-OH4
4	I	615	DGZ	O5-C30-C31-O6
4	E	615	DGZ	C11-C10-C9-C8
4	A	615	DGZ	N3-C28-C29-O5
4	B	615	DGZ	N3-C28-C29-O5
4	I	615	DGZ	N3-C28-C29-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	J	615	DGZ	N3-C28-C29-O5
4	K	615	DGZ	N3-C28-C29-O5
4	H	615	DGZ	C11-C10-C9-C8
6	C	622	1PE	OH5-C14-C24-OH4
6	F	616	1PE	OH5-C14-C24-OH4
7	B	616	2PE	O4-C5-C6-O7
4	A	615	DGZ	O4-C28-C29-O5
4	H	615	DGZ	O4-C28-C29-O5
6	J	622	1PE	OH5-C14-C24-OH4
4	I	615	DGZ	C9-C10-C11-N2
6	C	621	1PE	OH5-C14-C24-OH4
4	C	615	DGZ	N6-C49-C50-C51
4	D	615	DGZ	N6-C49-C50-C51
4	E	615	DGZ	N6-C49-C50-C51
4	G	615	DGZ	N6-C49-C50-C51
4	H	615	DGZ	N6-C49-C50-C51
4	I	615	DGZ	N6-C49-C50-C51
4	J	615	DGZ	N6-C49-C50-C51
4	L	615	DGZ	N6-C49-C50-C51
4	J	615	DGZ	O4-C28-C29-O5
6	G	620	1PE	C23-C13-OH4-C24
6	L	620	1PE	OH6-C15-C25-OH5
4	J	615	DGZ	C11-C10-C9-C8
4	A	615	DGZ	C17-C18-C19-O3
6	J	621	1PE	OH6-C15-C25-OH5
4	B	615	DGZ	O4-C28-C29-O5
4	K	615	DGZ	O4-C28-C29-O5
4	H	615	DGZ	N3-C28-C29-O5
4	A	615	DGZ	C26-C18-C19-O3
6	J	619	1PE	OH6-C15-C25-OH5
4	I	615	DGZ	C3-C4-C5-C6
6	I	621	1PE	OH5-C14-C24-OH4
4	E	615	DGZ	C2-C3-C4-C5
4	C	615	DGZ	N3-C28-C29-O5
4	G	615	DGZ	N3-C28-C29-O5
4	A	615	DGZ	C17-C18-C19-C20
6	D	620	1PE	OH6-C15-C25-OH5
4	A	615	DGZ	C26-C18-C19-C20
4	F	615	DGZ	O4-C28-C29-O5
4	I	615	DGZ	O4-C28-C29-O5
6	F	618	1PE	OH6-C15-C25-OH5
7	B	616	2PE	O10-C11-C12-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	615	DGZ	O4-C28-C29-O5
4	G	615	DGZ	O4-C28-C29-O5
4	A	615	DGZ	O6-C32-C33-N4
4	J	615	DGZ	O5-C30-C31-O6
4	F	615	DGZ	N3-C28-C29-O5
6	G	622	1PE	OH6-C15-C25-OH5
6	L	619	1PE	OH5-C14-C24-OH4
4	L	615	DGZ	C11-C10-C9-C8
4	H	615	DGZ	C26-C18-C19-O3
6	E	619	1PE	C12-C22-OH3-C23
6	I	622	1PE	OH4-C13-C23-OH3
6	J	621	1PE	C23-C13-OH4-C24
4	H	615	DGZ	C2-C3-C4-C5
6	L	620	1PE	C14-C24-OH4-C13
6	J	621	1PE	C16-C26-OH6-C15
4	H	615	DGZ	C26-C18-C19-C20
6	D	621	1PE	C16-C26-OH6-C15
4	F	615	DGZ	O5-C30-C31-O6
6	K	619	1PE	C25-C15-OH6-C26
6	E	619	1PE	OH6-C15-C25-OH5
6	E	620	1PE	OH4-C13-C23-OH3
4	G	615	DGZ	C26-C18-C19-O3
4	H	615	DGZ	C17-C18-C19-O3
4	C	615	DGZ	C26-C18-C19-O3
6	G	622	1PE	C15-C25-OH5-C14
6	G	621	1PE	OH6-C15-C25-OH5
6	L	617	1PE	OH7-C16-C26-OH6
4	I	615	DGZ	C30-C31-O6-C32
6	K	617	1PE	C15-C25-OH5-C14
6	D	618	1PE	C13-C23-OH3-C22
4	D	615	DGZ	C30-C31-O6-C32
4	D	615	DGZ	C35-C36-C37-C38
4	L	615	DGZ	C30-C31-O6-C32
7	H	619	2PE	C9-C8-O7-C6
6	E	620	1PE	C23-C13-OH4-C24
6	L	617	1PE	C16-C26-OH6-C15
6	J	622	1PE	C24-C14-OH5-C25
4	L	615	DGZ	C33-C32-O6-C31
6	F	618	1PE	C15-C25-OH5-C14
7	H	619	2PE	C18-C17-O16-C15
4	G	615	DGZ	C26-C18-C19-C20
4	A	615	DGZ	N6-C49-C50-C51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	615	DGZ	N6-C49-C50-C51
4	F	615	DGZ	N6-C49-C50-C51
4	K	615	DGZ	N6-C49-C50-C51
4	H	615	DGZ	C17-C18-C19-C20
6	J	620	1PE	C16-C26-OH6-C15
7	H	619	2PE	C15-C14-O13-C12
7	H	619	2PE	C24-C23-O22-C21
6	J	619	1PE	C24-C14-OH5-C25
4	C	615	DGZ	C26-C18-C19-C20
4	C	615	DGZ	C30-C31-O6-C32
4	H	615	DGZ	C31-C30-O5-C29
6	E	619	1PE	C24-C14-OH5-C25
6	F	616	1PE	C24-C14-OH5-C25
4	G	615	DGZ	C30-C31-O6-C32
6	K	618	1PE	C23-C13-OH4-C24
7	B	616	2PE	C14-C15-O16-C17
4	G	615	DGZ	C33-C32-O6-C31
4	A	615	DGZ	C33-C32-O6-C31
4	C	615	DGZ	C33-C32-O6-C31
6	F	618	1PE	C25-C15-OH6-C26
7	H	619	2PE	C12-C11-O10-C9
6	L	620	1PE	C24-C14-OH5-C25
4	F	615	DGZ	C26-C18-C19-C20
4	E	615	DGZ	C33-C32-O6-C31
6	C	621	1PE	OH6-C15-C25-OH5
6	J	622	1PE	OH4-C13-C23-OH3
4	D	615	DGZ	C33-C32-O6-C31
6	G	623	1PE	C23-C13-OH4-C24
6	J	619	1PE	C25-C15-OH6-C26
4	I	615	DGZ	C33-C32-O6-C31
4	F	615	DGZ	C26-C18-C19-O3
4	I	615	DGZ	C35-C36-C37-C38
4	D	615	DGZ	C35-C36-C37-C46
4	F	615	DGZ	C48-C49-C50-C51
4	K	615	DGZ	C48-C49-C50-C51
4	E	615	DGZ	C26-C18-C19-C20
6	F	617	1PE	C24-C14-OH5-C25
4	C	615	DGZ	O9-C48-C49-C50
4	D	615	DGZ	O9-C48-C49-C50
4	J	615	DGZ	O9-C48-C49-C50
4	K	615	DGZ	C33-C32-O6-C31
4	E	615	DGZ	C26-C18-C19-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	615	DGZ	N2-C11-C57-N7
4	A	615	DGZ	N2-C11-C57-O10
4	E	615	DGZ	N2-C11-C57-N7
4	E	615	DGZ	N2-C11-C57-O10
4	L	615	DGZ	N2-C11-C57-N7
4	L	615	DGZ	N2-C11-C57-O10
6	K	620	1PE	C24-C14-OH5-C25
6	J	620	1PE	C24-C14-OH5-C25
6	E	621	1PE	C23-C13-OH4-C24
6	J	619	1PE	C14-C24-OH4-C13
4	K	615	DGZ	C30-C31-O6-C32
6	L	618	1PE	C14-C24-OH4-C13
6	J	620	1PE	C15-C25-OH5-C14
6	K	618	1PE	C12-C22-OH3-C23
4	A	615	DGZ	C30-C31-O6-C32
7	B	616	2PE	C18-C17-O16-C15
6	G	623	1PE	C15-C25-OH5-C14
4	C	615	DGZ	C11-C10-C9-C8
4	C	615	DGZ	C17-C18-C19-O3
4	G	615	DGZ	C17-C18-C19-O3
6	K	620	1PE	C14-C24-OH4-C13
4	F	615	DGZ	C31-C30-O5-C29
6	G	622	1PE	C24-C14-OH5-C25
4	F	615	DGZ	C17-C18-C19-O3
4	K	615	DGZ	C11-C10-C9-C8
6	C	621	1PE	C23-C13-OH4-C24
6	F	616	1PE	C15-C25-OH5-C14
4	A	615	DGZ	C31-C30-O5-C29
4	C	615	DGZ	C17-C18-C19-C20
4	H	615	DGZ	C3-C4-C5-C6
4	J	615	DGZ	N1-C7-C8-C9
4	F	615	DGZ	C17-C18-C19-C20
6	A	619	1PE	OH6-C15-C25-OH5
4	G	615	DGZ	C17-C18-C19-C20
6	C	621	1PE	C24-C14-OH5-C25
6	I	623	1PE	C24-C14-OH5-C25
6	C	621	1PE	C12-C22-OH3-C23
4	D	615	DGZ	C2-C3-C4-C5
6	D	620	1PE	C15-C25-OH5-C14
4	F	615	DGZ	N2-C11-C57-O10
4	G	615	DGZ	N2-C11-C57-O10
4	I	615	DGZ	N2-C11-C57-O10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	H	615	DGZ	C33-C32-O6-C31
7	H	619	2PE	C14-C15-O16-C17
7	B	616	2PE	C2-C3-O4-C5
6	D	618	1PE	C12-C22-OH3-C23
4	G	615	DGZ	C11-C10-C9-C8
6	E	619	1PE	C23-C13-OH4-C24
4	E	615	DGZ	C35-C36-C37-C38
4	C	615	DGZ	C35-C36-C37-C38
4	L	615	DGZ	C35-C36-C37-C38
4	I	615	DGZ	C35-C36-C37-C46
4	E	615	DGZ	C17-C18-C19-C20
4	K	615	DGZ	C2-C3-C4-C5
6	E	619	1PE	C13-C23-OH3-C22
4	A	615	DGZ	C35-C36-C37-C38
4	E	615	DGZ	C35-C36-C37-C46
4	G	615	DGZ	C35-C36-C37-C38
4	E	615	DGZ	C17-C18-C19-O3
4	I	615	DGZ	C11-C10-C9-C8
4	D	615	DGZ	C28-C29-O5-C30
4	K	615	DGZ	C28-C29-O5-C30
4	A	615	DGZ	C35-C36-C37-C46
6	F	617	1PE	C25-C15-OH6-C26
4	A	615	DGZ	C7-C8-C9-C10
4	L	615	DGZ	C26-C18-C19-O3
6	D	618	1PE	OH5-C14-C24-OH4
4	L	615	DGZ	C26-C18-C19-C20
4	F	615	DGZ	C33-C32-O6-C31
6	F	617	1PE	OH6-C15-C25-OH5
4	E	615	DGZ	C31-C30-O5-C29
4	K	615	DGZ	C35-C36-C37-C38
4	I	615	DGZ	C26-C18-C19-C20
4	J	615	DGZ	C33-C32-O6-C31
6	J	621	1PE	OH5-C14-C24-OH4
6	D	619	1PE	C15-C25-OH5-C14
6	D	620	1PE	C23-C13-OH4-C24
4	A	615	DGZ	O5-C30-C31-O6
4	K	615	DGZ	C9-C10-C11-C57
6	I	621	1PE	C14-C24-OH4-C13
4	L	615	DGZ	C35-C36-C37-C46
4	B	615	DGZ	C2-C3-C4-C5
6	I	622	1PE	C23-C13-OH4-C24
7	H	619	2PE	C21-C20-O19-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	615	DGZ	C35-C36-C37-C38
6	K	618	1PE	C15-C25-OH5-C14
4	L	615	DGZ	C2-C3-C4-C5
7	H	619	2PE	O13-C14-C15-O16
4	C	615	DGZ	C35-C36-C37-C46
4	G	615	DGZ	C47-C48-C49-N6
4	J	615	DGZ	C47-C48-C49-N6
4	K	615	DGZ	C47-C48-C49-N6
4	B	615	DGZ	C26-C18-C19-C20
4	E	615	DGZ	C28-C29-O5-C30
4	J	615	DGZ	C28-C29-O5-C30
7	B	616	2PE	C11-C12-O13-C14
6	K	619	1PE	OH6-C15-C25-OH5
7	H	619	2PE	C11-C12-O13-C14
4	G	615	DGZ	C35-C36-C37-C46
4	I	615	DGZ	C12-C13-C14-C15
7	H	619	2PE	O19-C20-C21-O22
4	H	615	DGZ	O5-C30-C31-O6
7	B	616	2PE	C17-C18-O19-C20
6	G	620	1PE	OH5-C14-C24-OH4
4	D	615	DGZ	C48-C49-C50-C51
4	E	615	DGZ	C48-C49-C50-C51
4	I	615	DGZ	C48-C49-C50-C51
6	D	618	1PE	OH4-C13-C23-OH3
4	C	615	DGZ	C7-C8-C9-C10

There are no ring outliers.

37 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	619	SO4	1	0
6	L	620	1PE	3	0
4	C	615	DGZ	5	0
6	I	623	1PE	4	0
6	L	617	1PE	2	0
6	K	617	1PE	1	0
4	E	615	DGZ	5	0
4	I	615	DGZ	4	0
7	H	619	2PE	2	0
4	J	615	DGZ	5	0
4	G	615	DGZ	5	0
6	L	618	1PE	2	0

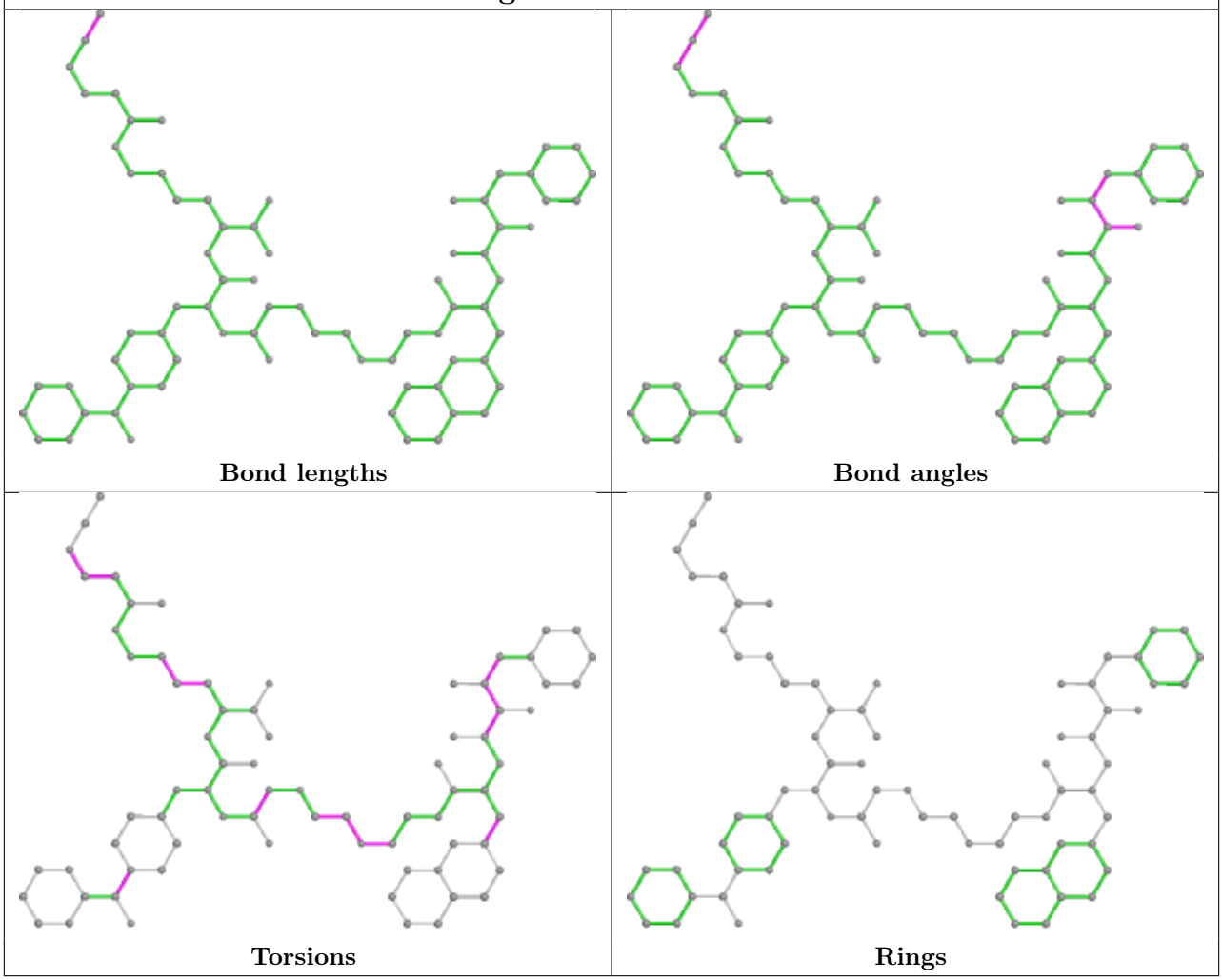
Continued on next page...

Continued from previous page...

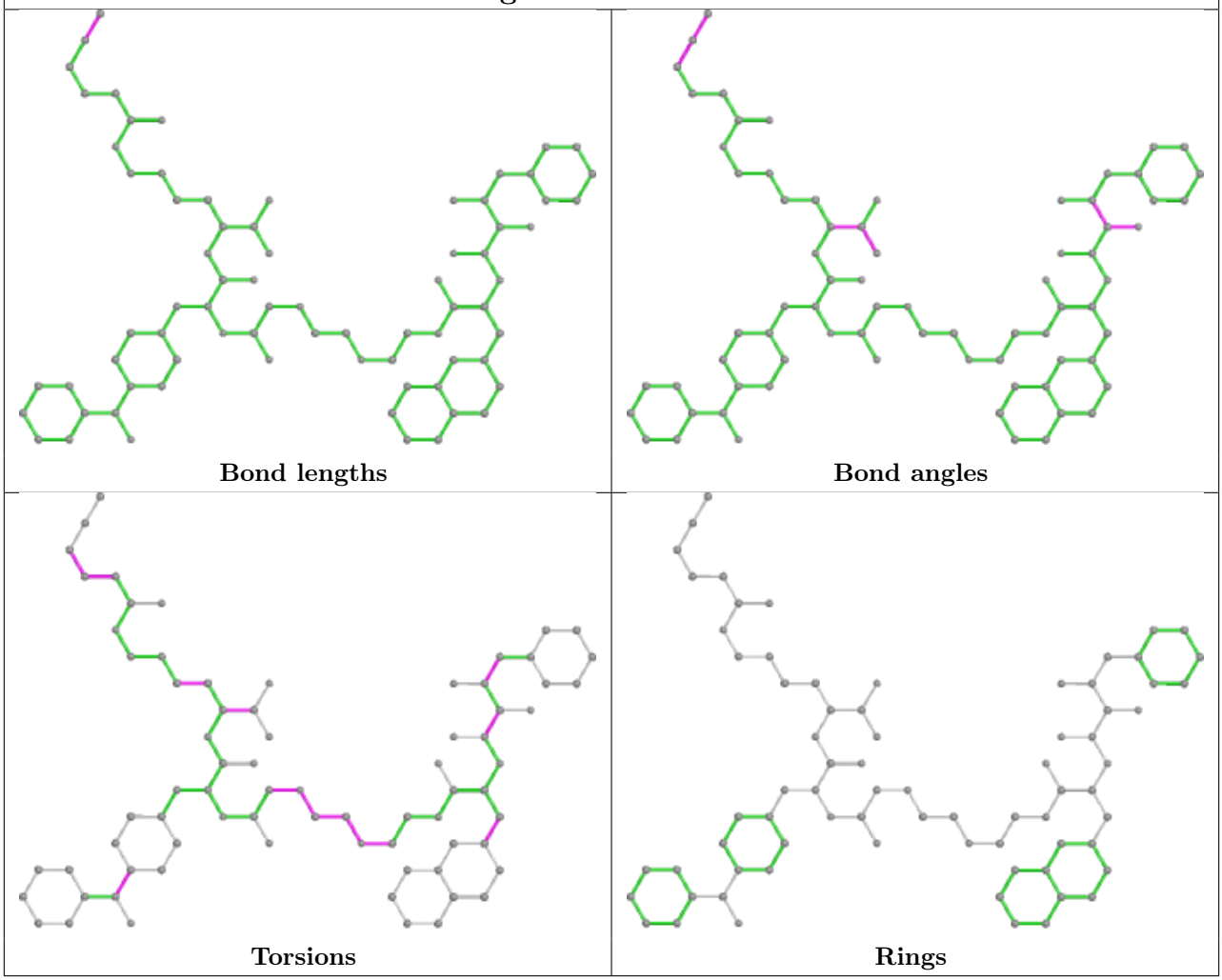
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	615	DGZ	12	0
4	D	615	DGZ	3	0
6	C	621	1PE	1	0
2	F	612	CO3	1	0
6	G	622	1PE	1	0
6	F	617	1PE	3	0
4	F	615	DGZ	9	0
5	I	618	SO4	1	0
6	I	621	1PE	1	0
6	D	620	1PE	1	0
4	H	615	DGZ	8	0
6	G	623	1PE	7	0
2	J	612	CO3	1	0
6	J	620	1PE	5	0
6	J	619	1PE	1	0
4	B	615	DGZ	9	0
6	F	618	1PE	4	0
6	E	619	1PE	1	0
6	D	618	1PE	1	0
6	C	622	1PE	1	0
6	J	621	1PE	3	0
6	J	622	1PE	3	0
6	L	619	1PE	1	0
4	K	615	DGZ	4	0
4	L	615	DGZ	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 then 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.

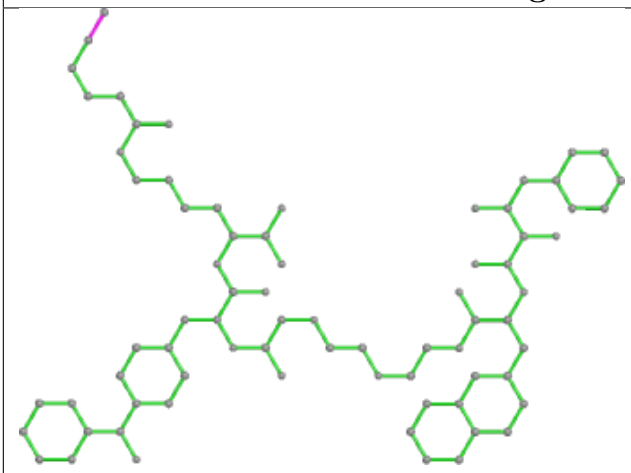
Ligand DGZ C 615



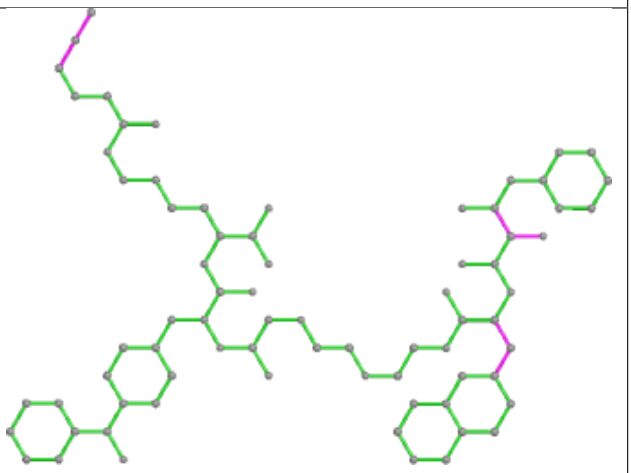
Ligand DGZ E 615



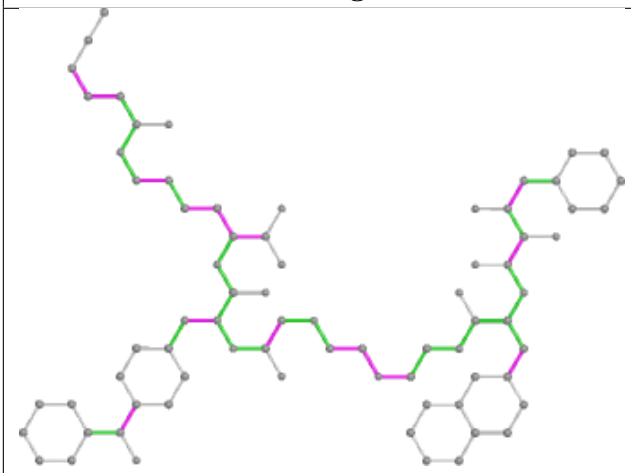
Ligand DGZ I 615



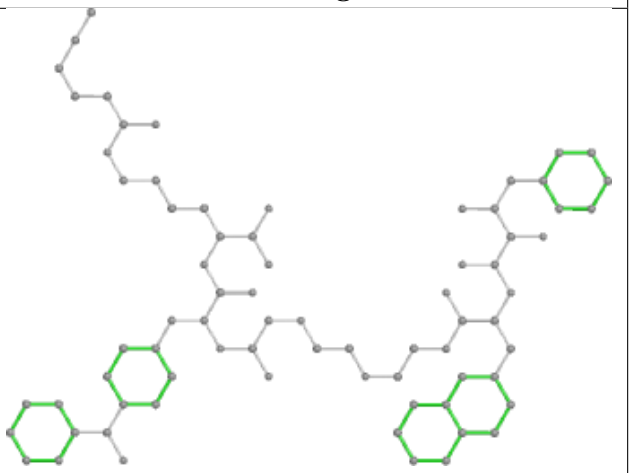
Bond lengths



Bond angles



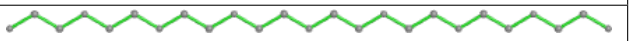
Torsions



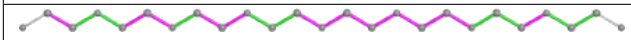
Rings

Ligand 2PE H 619

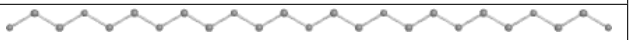
Bond lengths



Bond angles

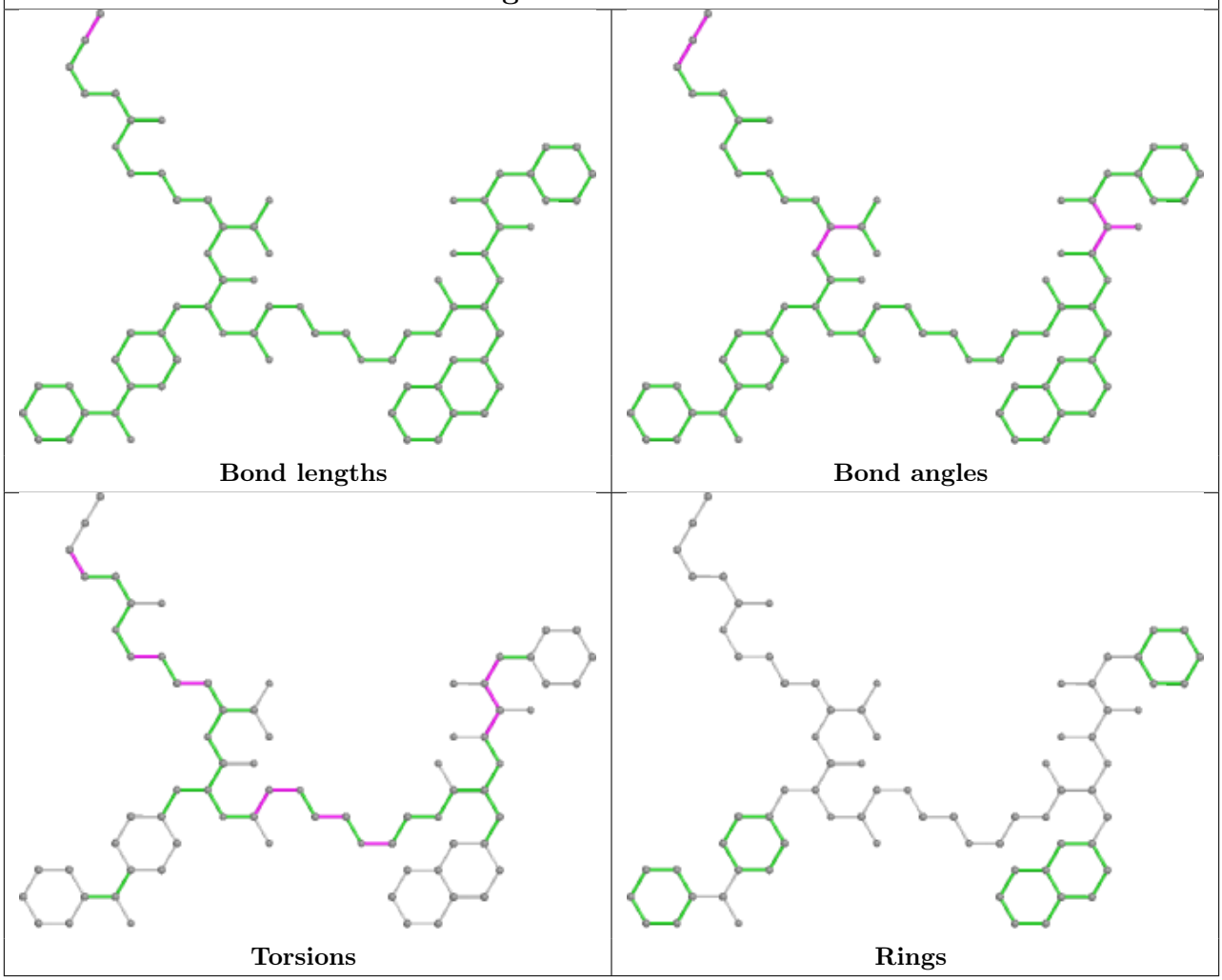


Torsions

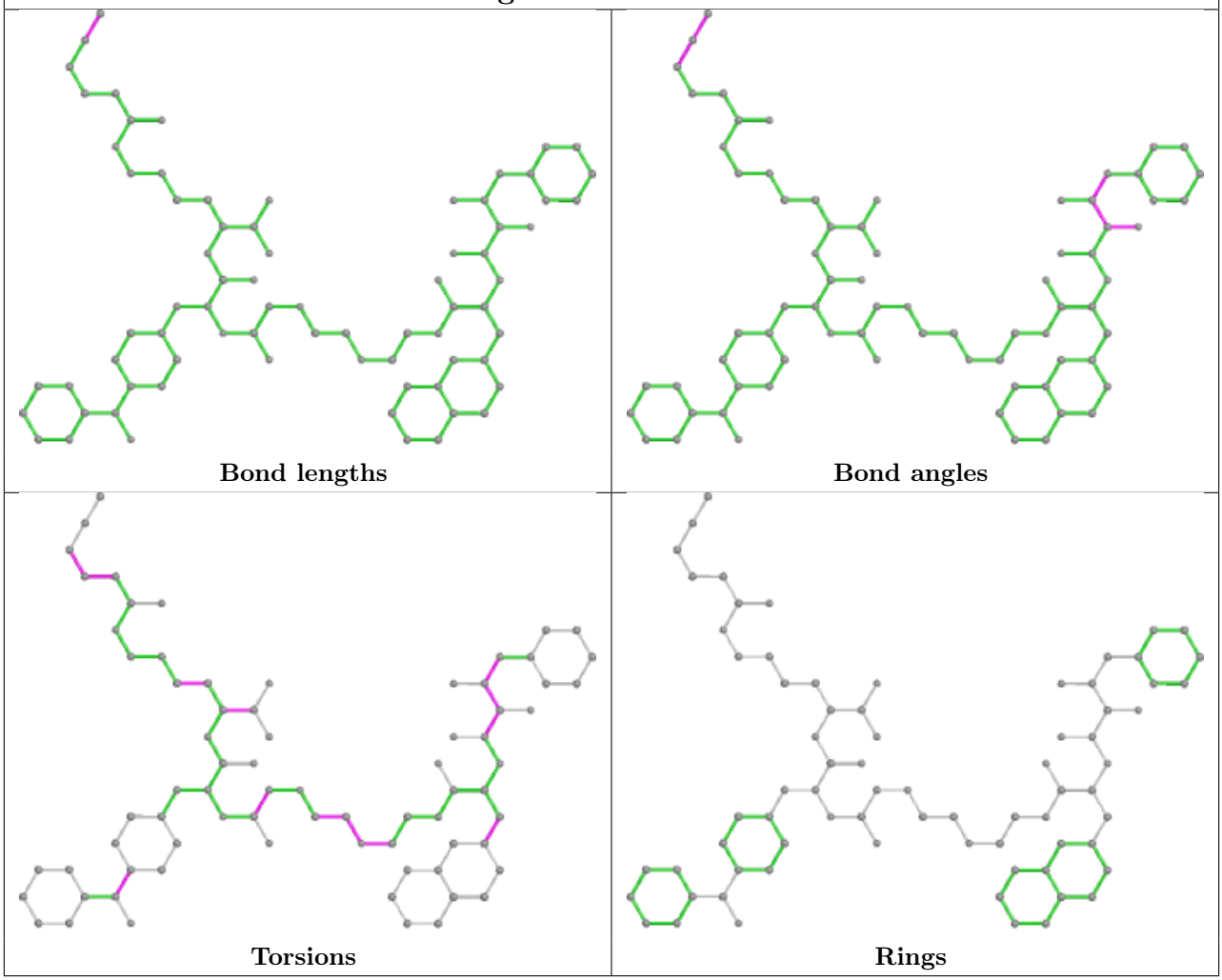


Rings

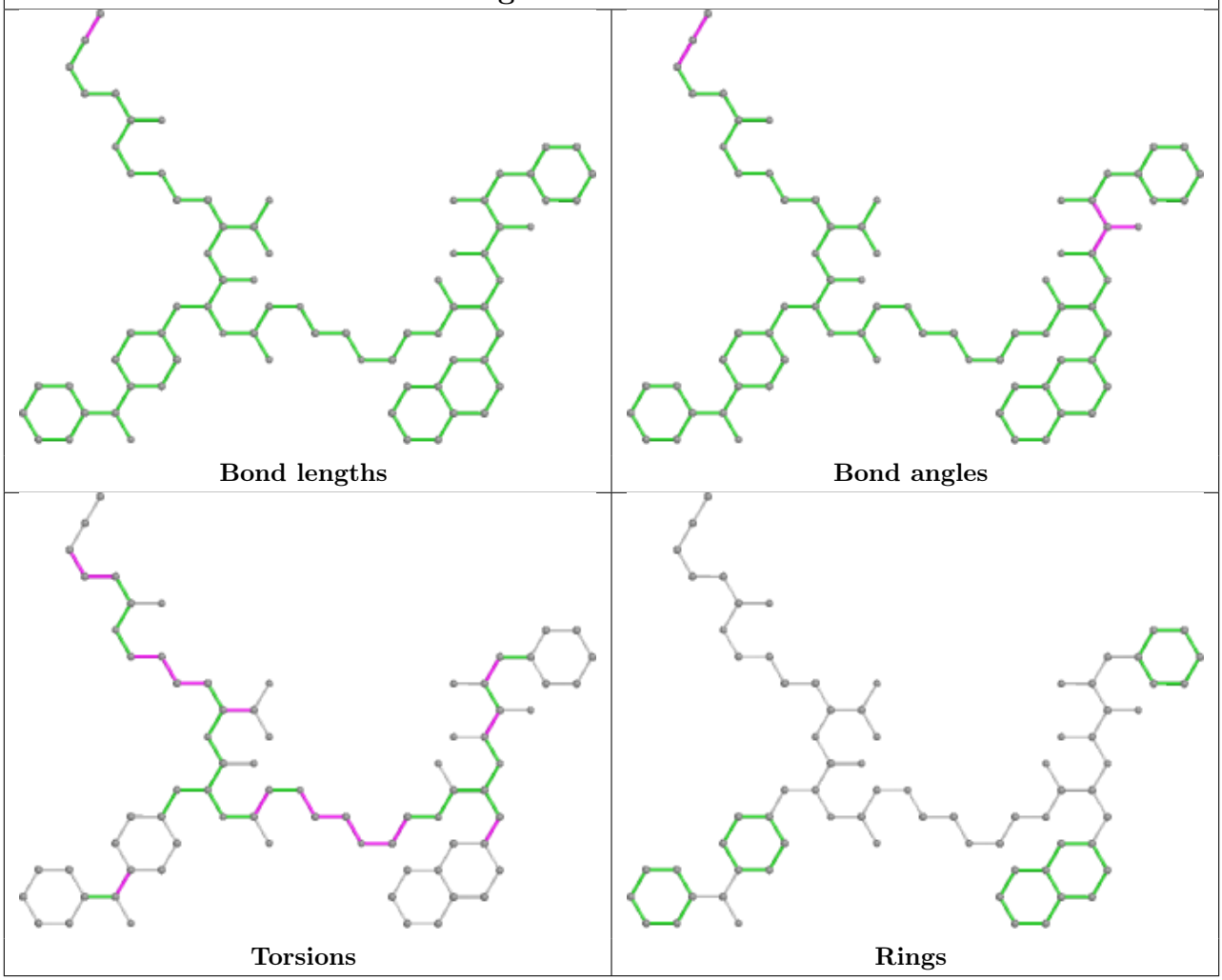
Ligand DGZ J 615



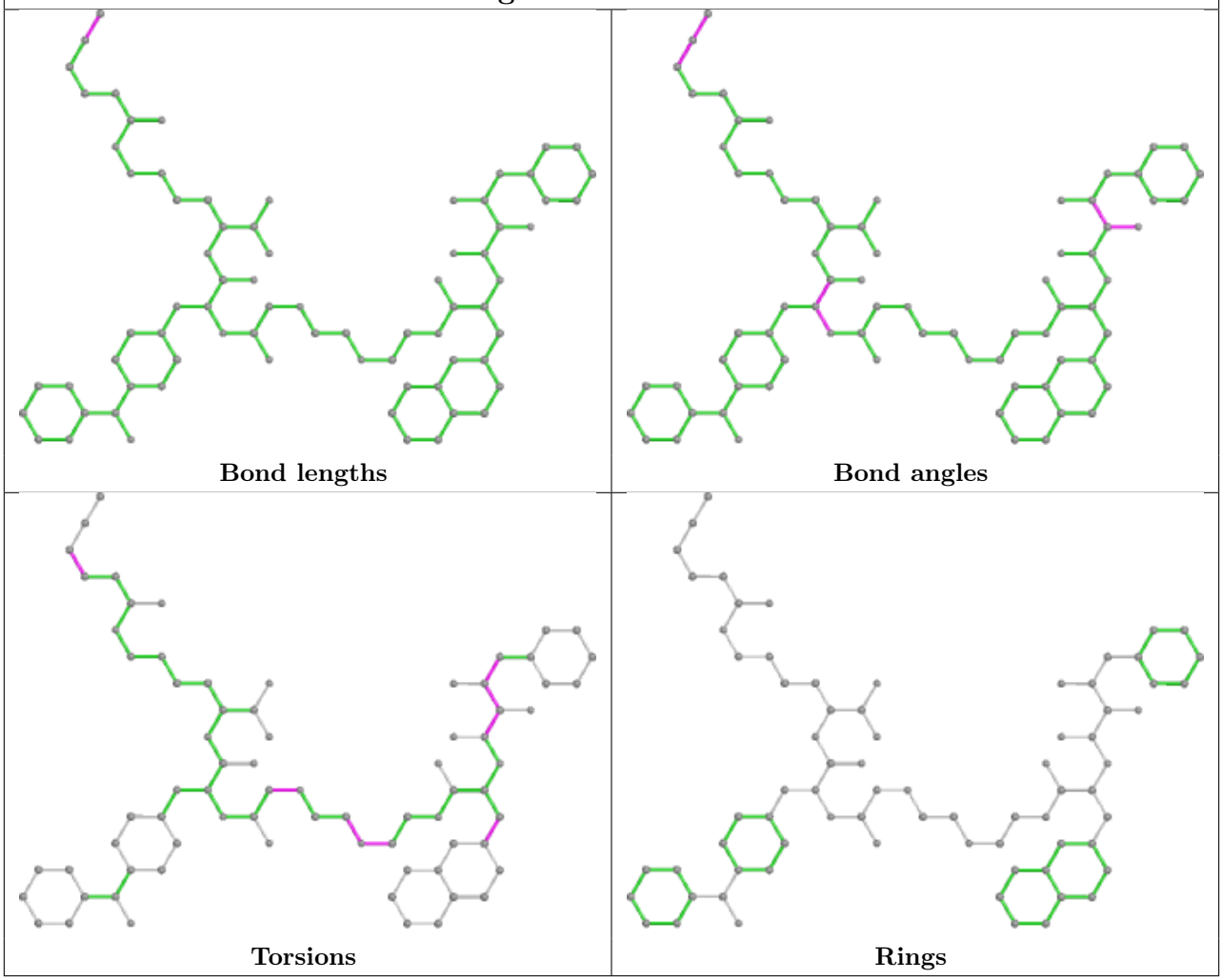
Ligand DGZ G 615



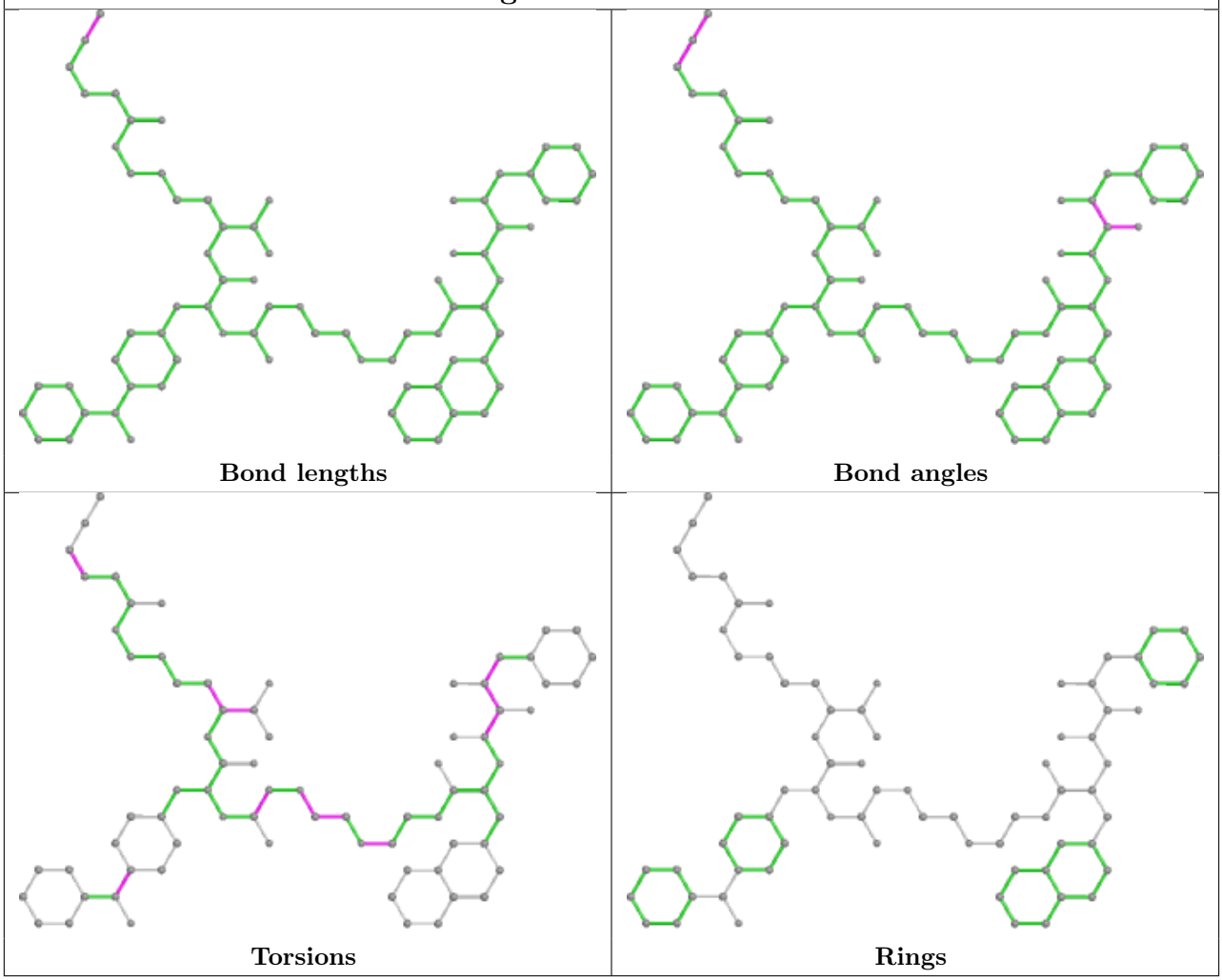
Ligand DGZ A 615



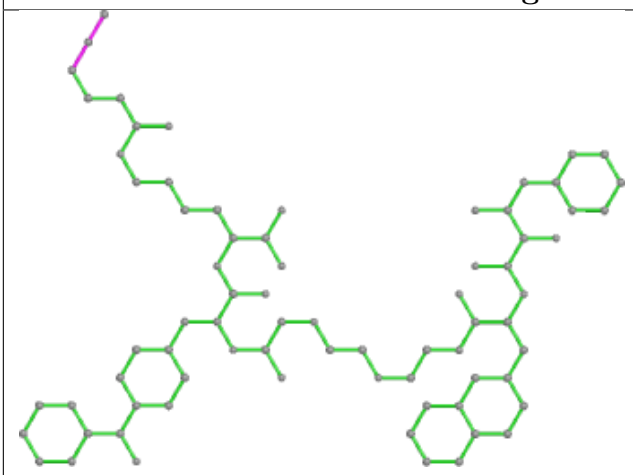
Ligand DGZ D 615



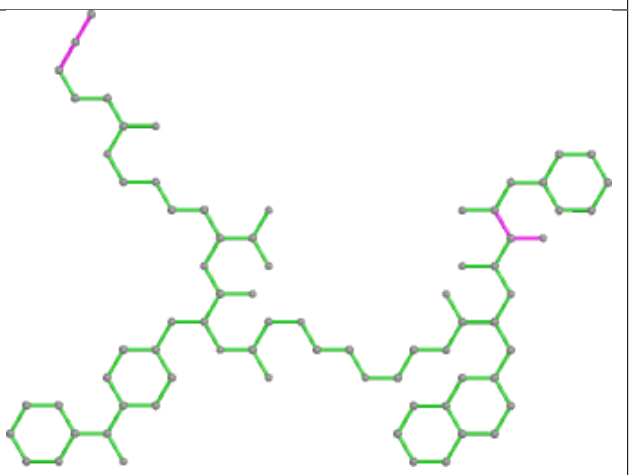
Ligand DGZ F 615



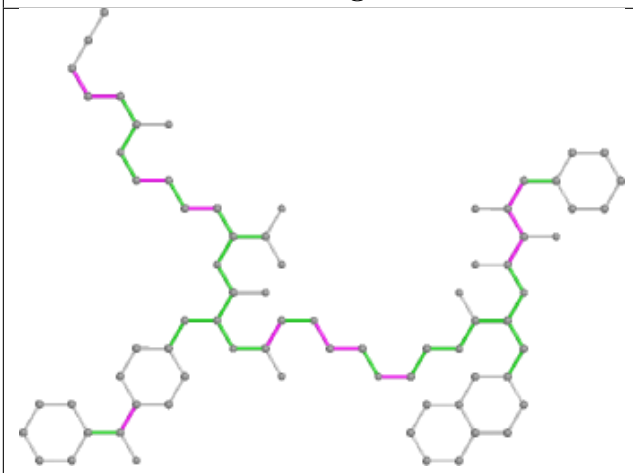
Ligand DGZ H 615



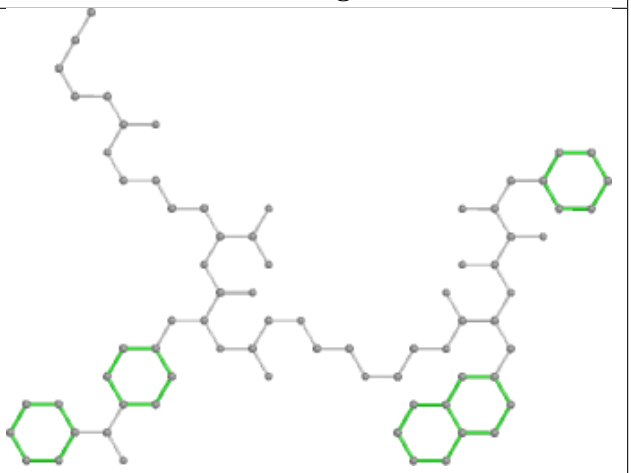
Bond lengths



Bond angles



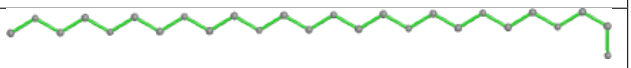
Torsions



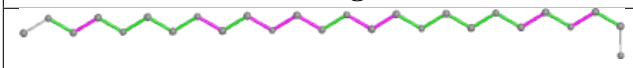
Rings

Ligand 2PE B 616

Bond lengths



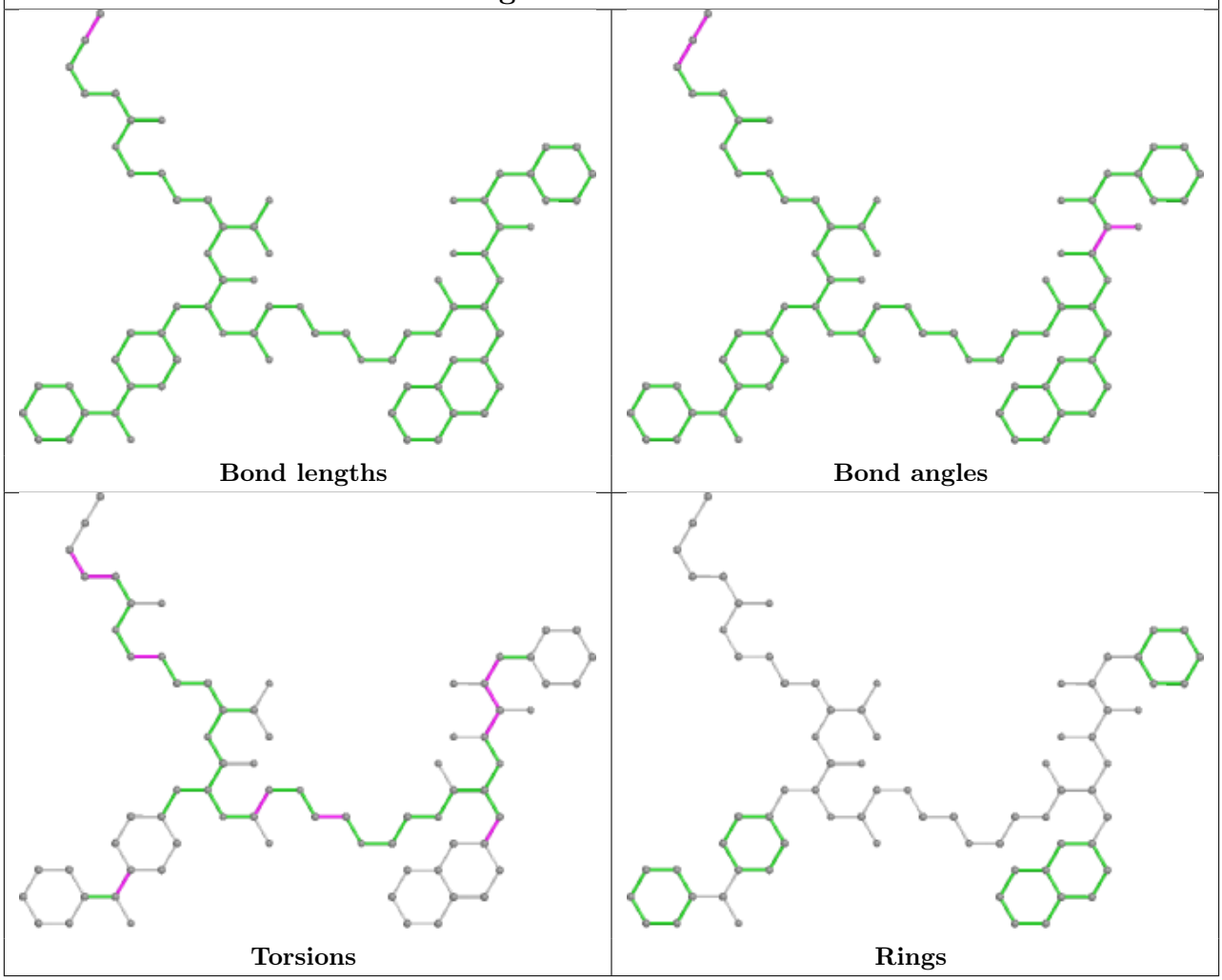
Bond angles



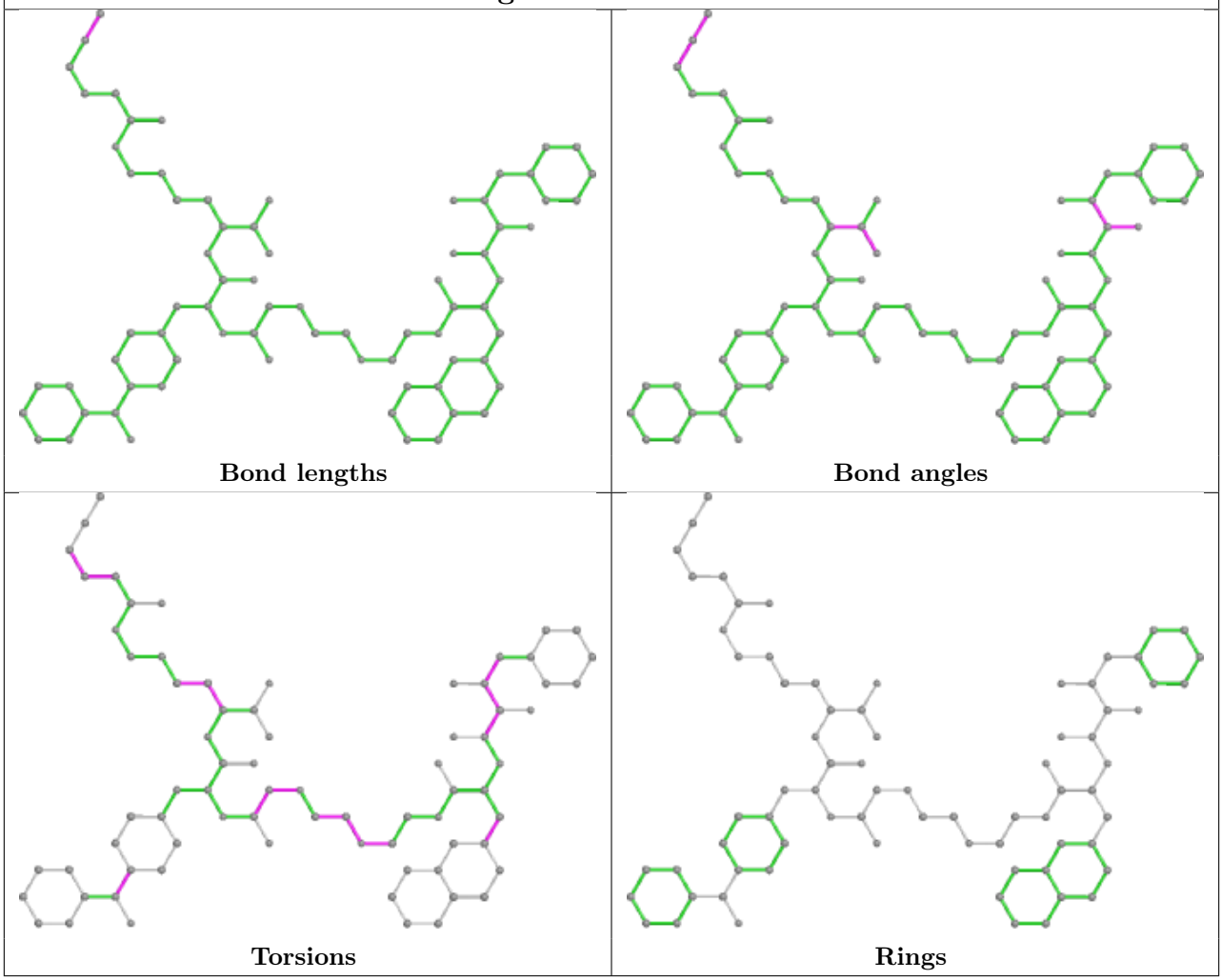
Torsions

Rings

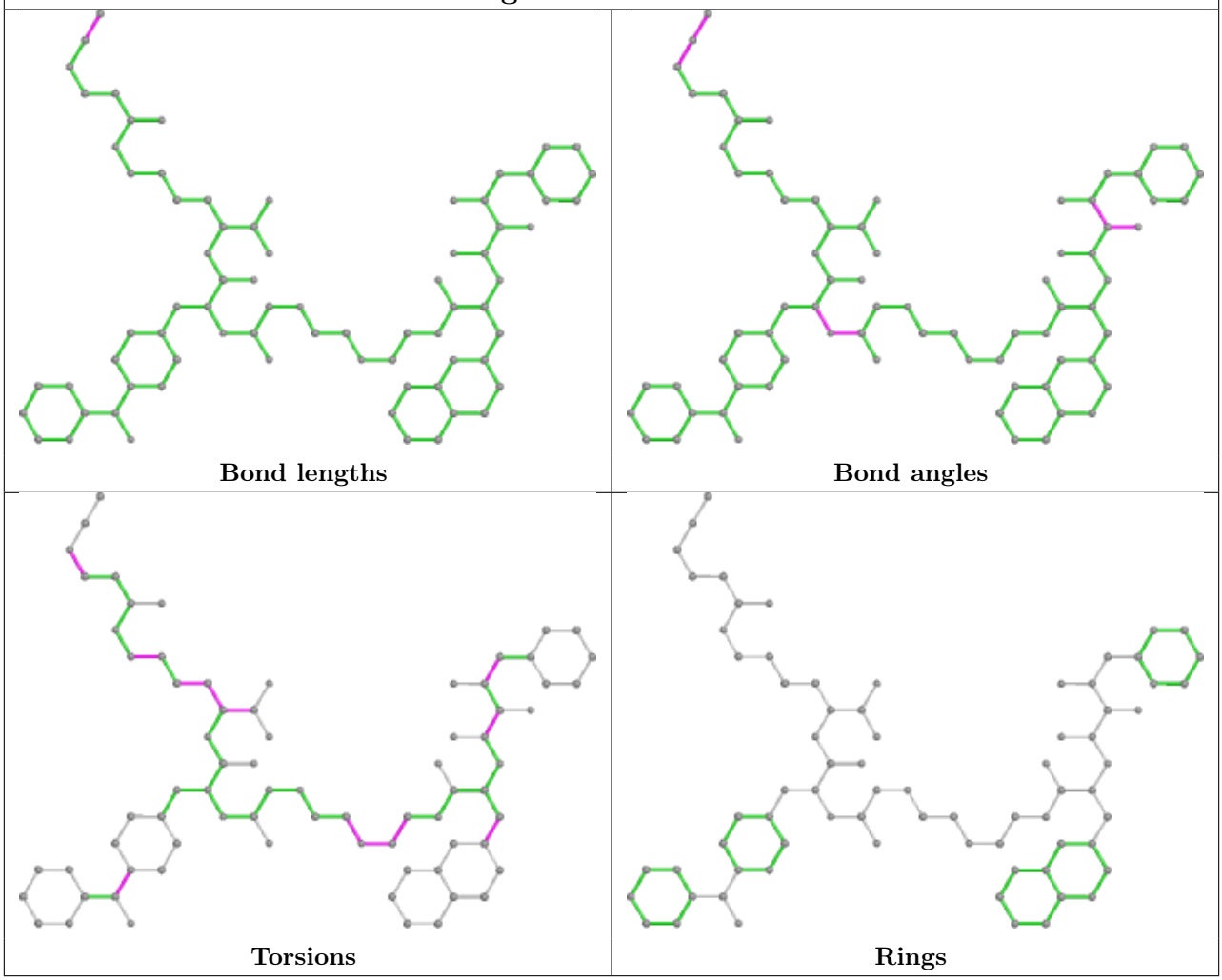
Ligand DGZ B 615



Ligand DGZ K 615



Ligand DGZ L 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 (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, 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, 14, 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%)

All (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
1	A	551	VAL	4.4
1	H	136	GLY	4.2
1	H	551	VAL	4.1
1	B	550	SER	4.0
1	B	363	GLY	3.9
1	J	136	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	136	GLY	3.7
1	L	551	VAL	3.7
1	C	603	ASP	3.6
1	D	603	ASP	3.6
1	H	178	PHE	3.4
1	B	551	VAL	3.3
1	I	551	VAL	3.1
1	J	85	ALA	2.9
1	F	121	CYS	2.9
1	G	550	SER	2.9
1	B	181	ASN	2.8
1	F	136	GLY	2.7
1	D	219	LEU	2.7
1	D	136	GLY	2.7
1	I	549	SER	2.6
1	J	219	LEU	2.5
1	D	85	ALA	2.5
1	H	603	ASP	2.4
1	L	146	SER	2.4
1	F	361	SER	2.4
1	B	603	ASP	2.4
1	B	135	PRO	2.4
1	B	178	PHE	2.3
1	F	157	LEU	2.3
1	B	118	LYS	2.3
1	C	362	LYS	2.3
1	H	135	PRO	2.2
1	J	603	ASP	2.2
1	A	136	GLY	2.2
1	A	550	SER	2.1
1	G	196	ALA	2.1
1	F	272	ASN	2.1
1	C	549	SER	2.1
1	G	549	SER	2.1
1	F	550	SER	2.0
1	D	260	ASN	2.0
1	D	124	GLU	2.0
1	F	114	VAL	2.0
1	L	144	ILE	2.0
1	H	150	ASP	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, 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	D	620	11/16	0.82	0.20	35,39,46,48	0
6	1PE	L	618	12/16	0.82	0.18	25,35,48,48	0
5	SO4	I	618	5/5	0.83	0.29	57,61,62,63	0
6	1PE	E	619	12/16	0.83	0.20	40,42,46,47	0
5	SO4	E	616	5/5	0.83	0.34	90,94,95,96	0
2	CO3	G	612	4/4	0.83	0.23	4,9,10,12	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
5	SO4	A	617	5/5	0.85	0.19	54,55,59,59	0
5	SO4	K	616	5/5	0.85	0.36	72,76,78,79	0
6	1PE	F	618	10/16	0.85	0.16	36,40,44,44	0
6	1PE	A	619	7/16	0.85	0.23	43,44,48,51	0
5	SO4	H	618	5/5	0.86	0.23	45,47,50,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	I	619	5/5	0.86	0.17	90,94,95,96	0
6	1PE	C	621	12/16	0.86	0.18	42,44,47,48	0
6	1PE	K	619	11/16	0.87	0.14	25,39,44,44	0
2	CO3	L	612	4/4	0.87	0.20	9,10,12,14	0
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	616	10/16	0.87	0.14	29,32,40,41	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	F	617	10/16	0.88	0.22	46,50,52,52	0
6	1PE	J	620	10/16	0.89	0.19	27,35,41,41	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	I	621	12/16	0.89	0.21	35,37,40,43	0
6	1PE	K	617	8/16	0.90	0.14	32,37,42,43	0
6	1PE	K	618	12/16	0.90	0.17	25,31,40,40	0
5	SO4	J	618	5/5	0.90	0.27	57,60,62,62	0
5	SO4	D	616	5/5	0.90	0.39	73,78,78,80	0
6	1PE	L	619	7/16	0.90	0.17	30,32,35,35	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	E	618	5/5	0.90	0.26	52,55,59,59	0
5	SO4	C	620	5/5	0.91	0.25	52,56,58,58	0
6	1PE	G	620	9/16	0.91	0.14	24,26,31,31	0
2	CO3	K	612	4/4	0.91	0.17	10,10,10,11	0
6	1PE	E	621	8/16	0.92	0.23	31,34,36,37	0
4	DGZ	H	615	74/74	0.92	0.16	4,38,142,180	0
4	DGZ	F	615	74/74	0.92	0.16	8,35,127,202	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
5	SO4	J	617	5/5	0.92	0.40	77,81,82,83	0
5	SO4	G	616	5/5	0.92	0.31	75,79,81,81	0
5	SO4	G	617	5/5	0.92	0.24	36,40,41,42	0
5	SO4	I	616	5/5	0.92	0.41	75,80,80,80	0
6	1PE	A	618	9/16	0.92	0.12	23,24,26,29	0
6	1PE	G	622	6/16	0.93	0.10	30,30,30,32	0
4	DGZ	A	615	74/74	0.93	0.16	5,38,181,208	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
6	1PE	G	621	6/16	0.93	0.21	25,25,27,32	0
2	CO3	C	612	4/4	0.94	0.16	12,12,13,15	0
6	1PE	I	623	5/16	0.94	0.16	14,14,16,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DGZ	B	615	74/74	0.94	0.15	9,37,133,171	0
4	DGZ	J	615	74/74	0.94	0.16	8,34,179,236	0
4	DGZ	K	615	74/74	0.94	0.15	7,41,147,213	0
6	1PE	E	620	10/16	0.94	0.15	26,27,35,41	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	C	615	74/74	0.94	0.15	10,38,182,231	0
4	DGZ	D	615	74/74	0.94	0.15	7,34,121,208	0
4	DGZ	E	615	74/74	0.94	0.15	10,41,146,207	0
2	CO3	B	612	4/4	0.94	0.13	14,14,15,15	0
4	DGZ	G	615	74/74	0.94	0.15	6,36,151,232	0
5	SO4	I	617	5/5	0.94	0.25	43,46,49,49	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
6	1PE	I	622	10/16	0.95	0.15	21,23,34,35	0
5	SO4	J	616	5/5	0.99	0.09	14,14,17,17	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	D	617	5/5	0.99	0.09	12,13,14,17	0
3	ZN	D	614	1/1	0.99	0.05	29,29,29,29	0
5	SO4	C	616	5/5	0.99	0.07	9,9,10,12	0
3	ZN	E	614	1/1	0.99	0.07	28,28,28,28	0
3	ZN	F	614	1/1	0.99	0.05	27,27,27,27	0
3	ZN	I	614	1/1	0.99	0.06	27,27,27,27	0
3	ZN	K	614	1/1	0.99	0.06	29,29,29,29	0
3	ZN	F	613	1/1	1.00	0.05	17,17,17,17	0
3	ZN	B	614	1/1	1.00	0.04	16,16,16,16	0
3	ZN	G	613	1/1	1.00	0.05	16,16,16,16	0
3	ZN	G	614	1/1	1.00	0.05	27,27,27,27	0
3	ZN	H	613	1/1	1.00	0.04	19,19,19,19	0
3	ZN	H	614	1/1	1.00	0.05	29,29,29,29	0
3	ZN	I	613	1/1	1.00	0.05	17,17,17,17	0
3	ZN	C	613	1/1	1.00	0.04	17,17,17,17	0
3	ZN	J	613	1/1	1.00	0.07	19,19,19,19	0
3	ZN	J	614	1/1	1.00	0.07	24,24,24,24	0
3	ZN	K	613	1/1	1.00	0.04	18,18,18,18	0
3	ZN	A	613	1/1	1.00	0.07	26,26,26,26	0
3	ZN	L	613	1/1	1.00	0.05	27,27,27,27	0
3	ZN	L	614	1/1	1.00	0.05	17,17,17,17	0
3	ZN	D	613	1/1	1.00	0.05	16,16,16,16	0
3	ZN	A	614	1/1	1.00	0.06	17,17,17,17	0
3	ZN	E	613	1/1	1.00	0.04	18,18,18,18	0

Continued on next page...

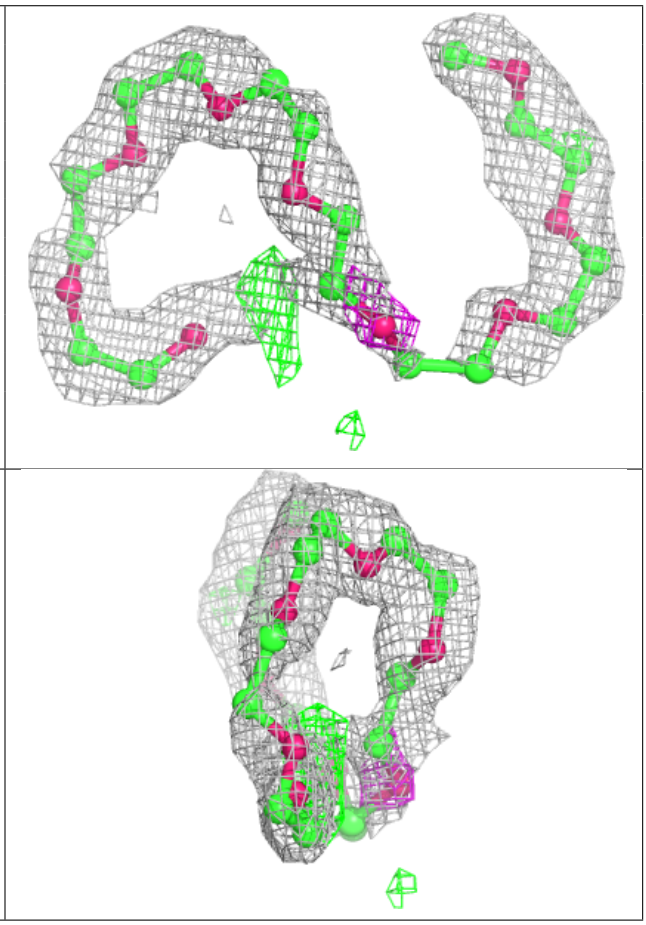
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	B	613	1/1	1.00	0.05	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.

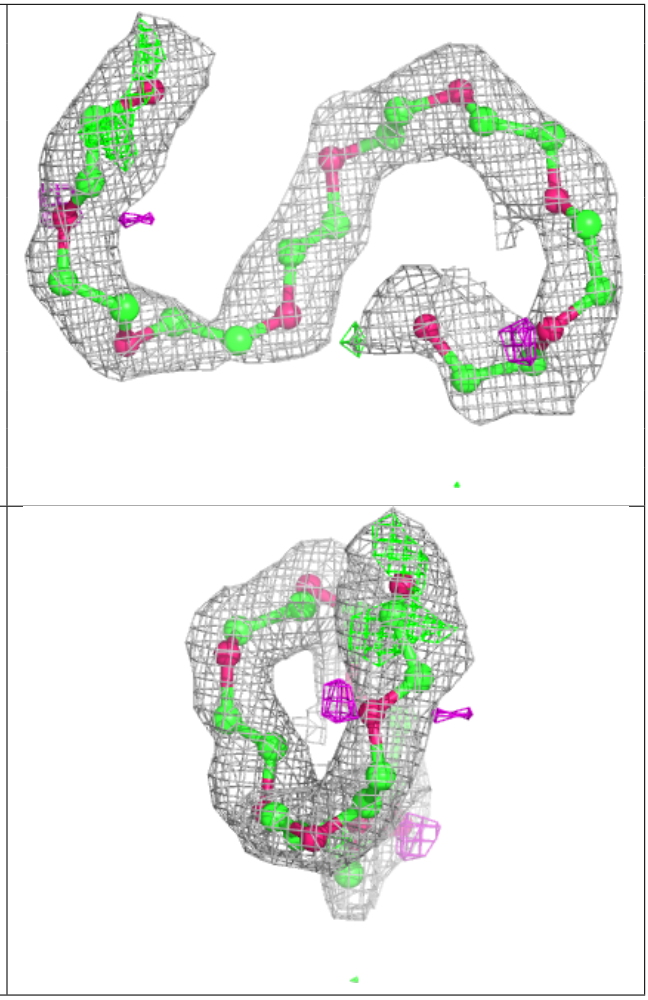
Electron density around 2PE B 616:

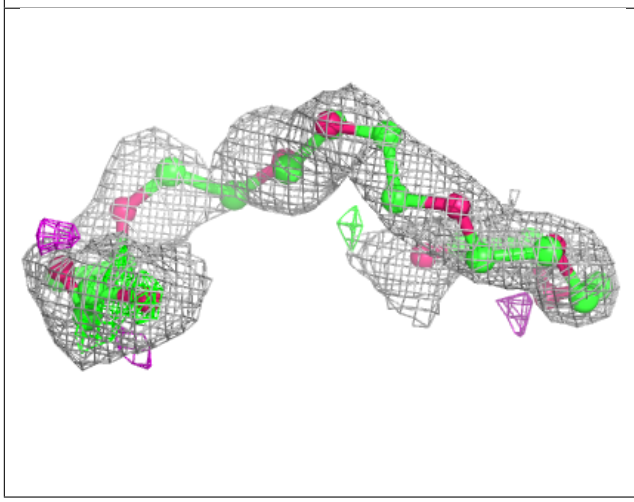
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 2PE H 619:

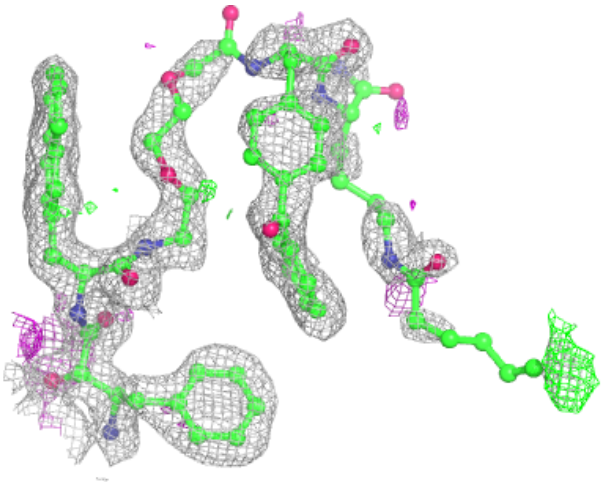
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

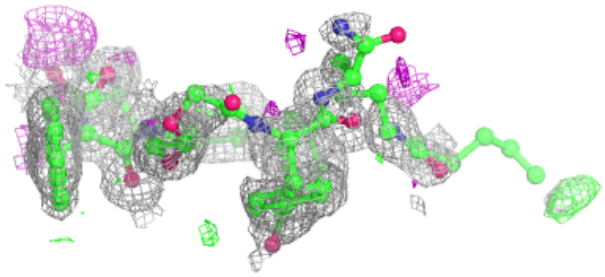


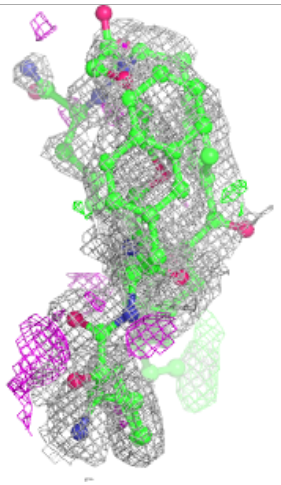


Electron density around DGZ H 615:

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

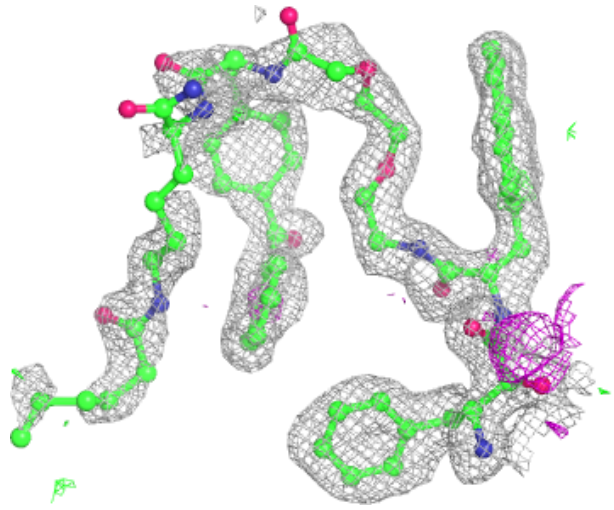


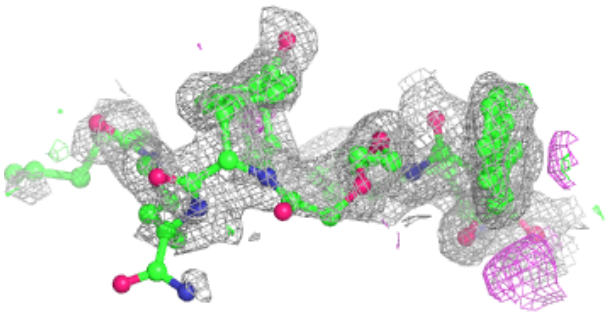


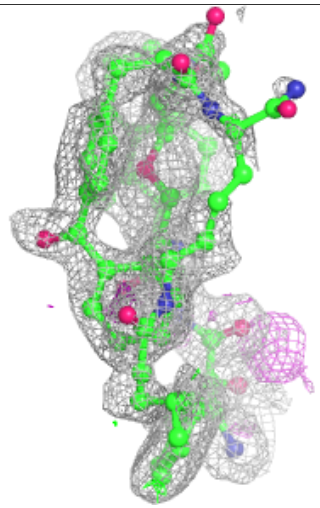


Electron density around DGZ F 615:

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

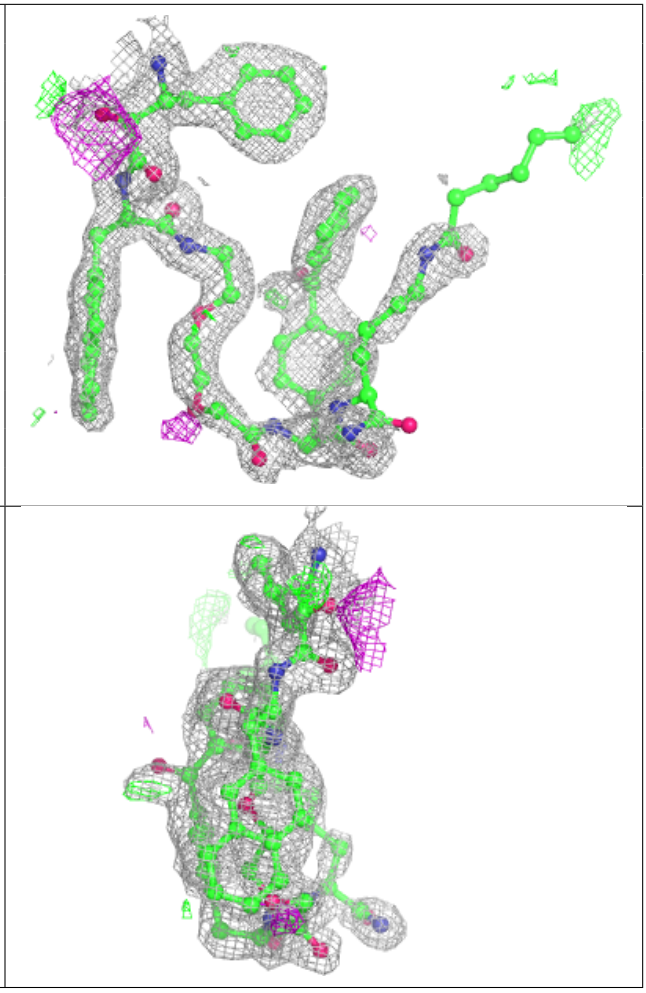






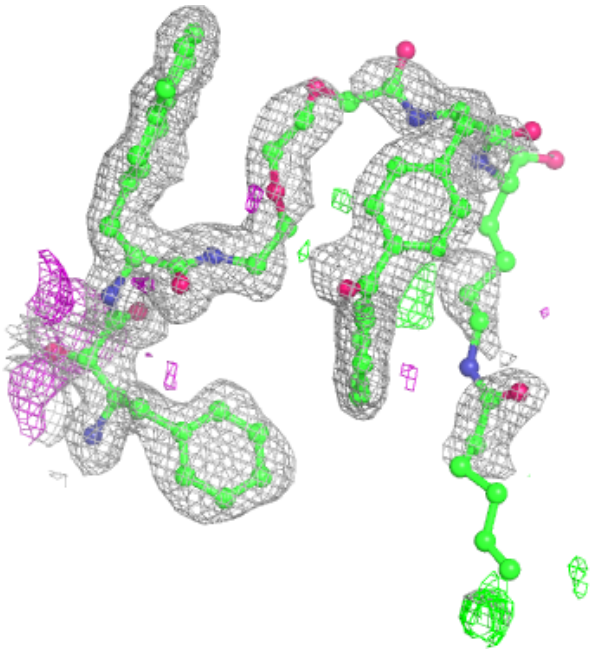
Electron density around DGZ A 615:

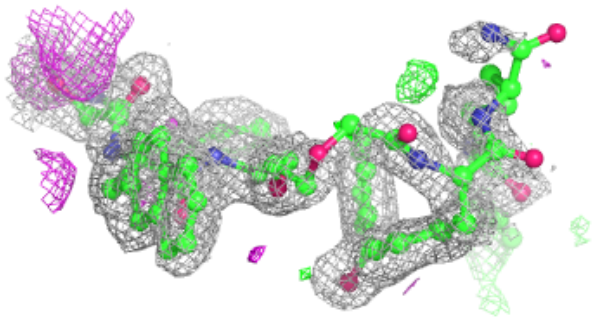
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

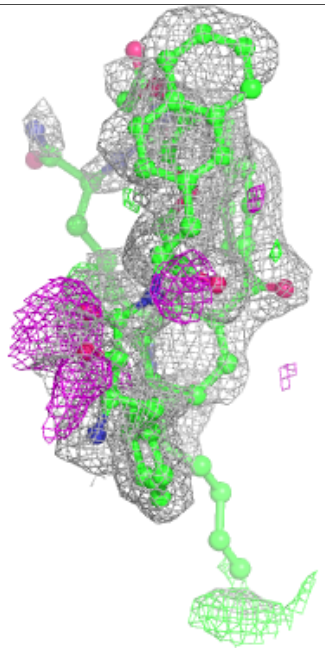


Electron density around DGZ I 615:

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

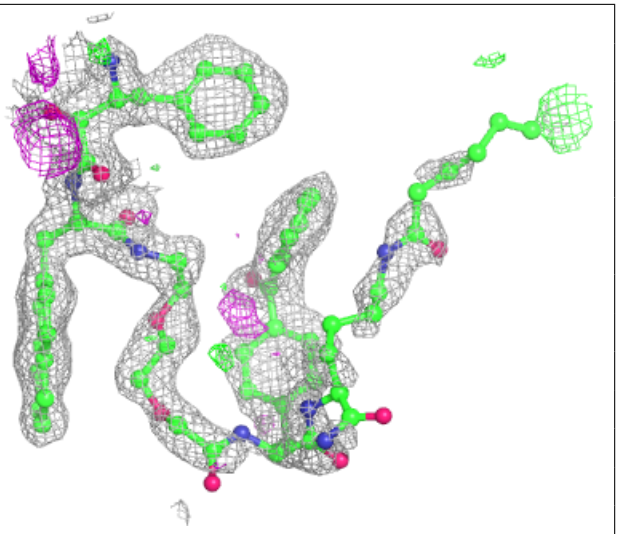


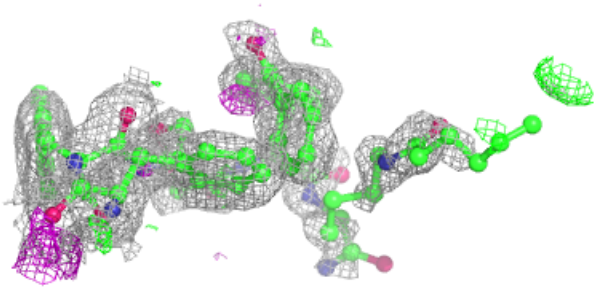


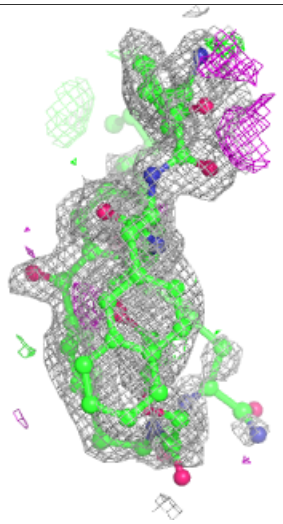


Electron density around DGZ B 615:

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

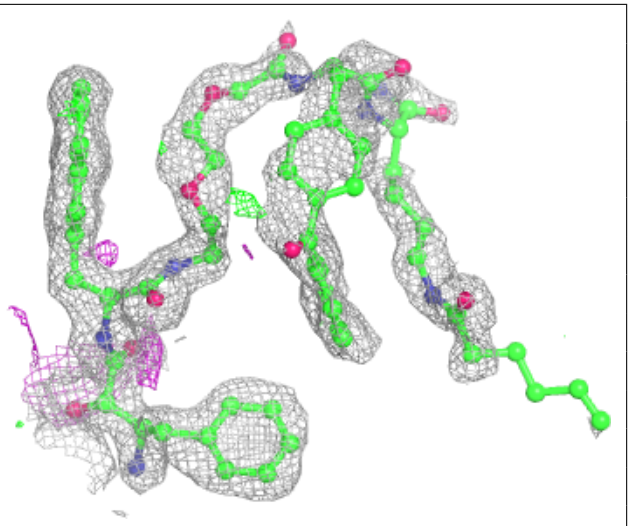


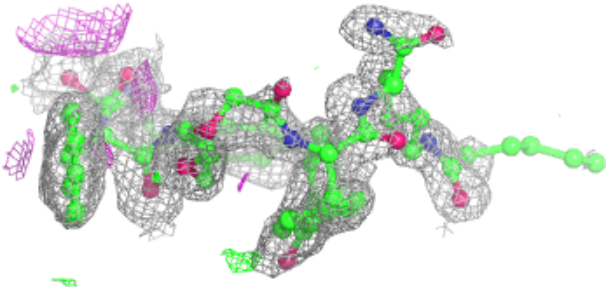


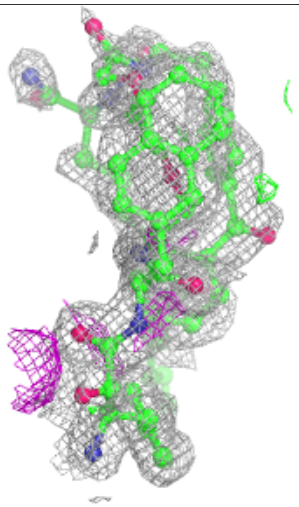


Electron density around DGZ J 615:

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

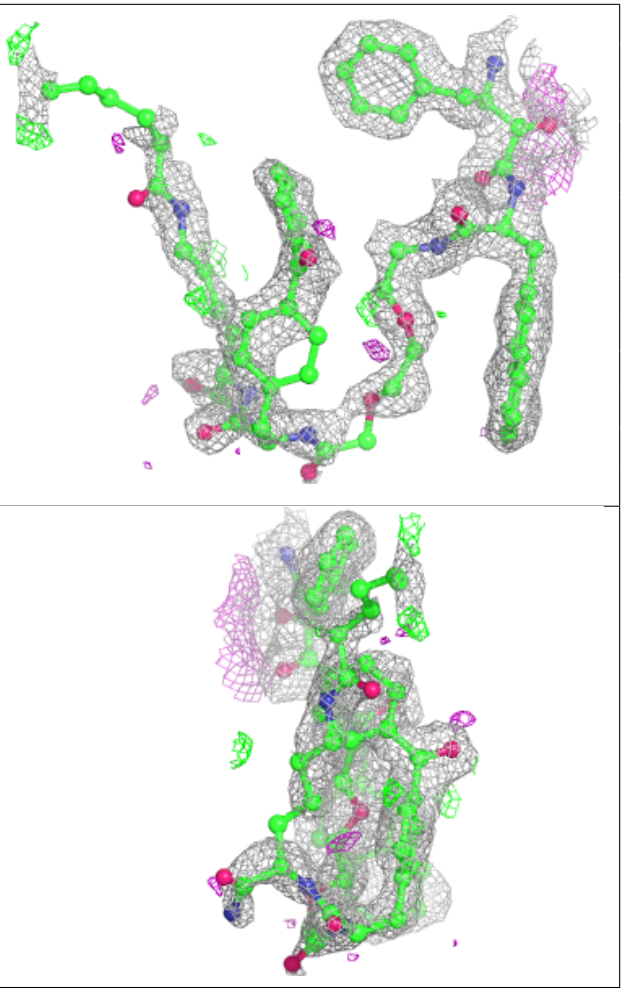






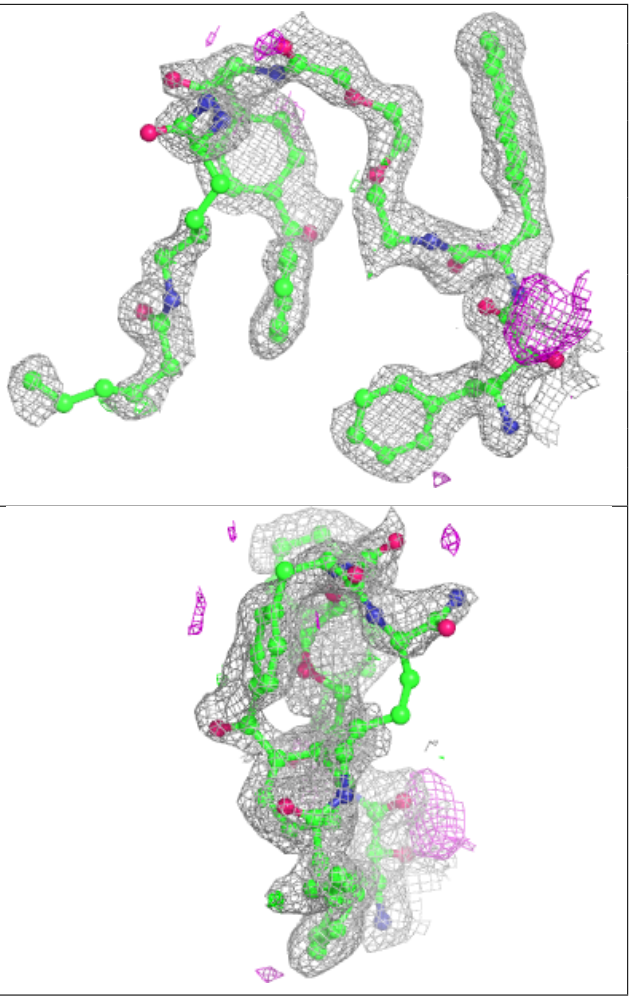
Electron density around DGZ K 615:

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



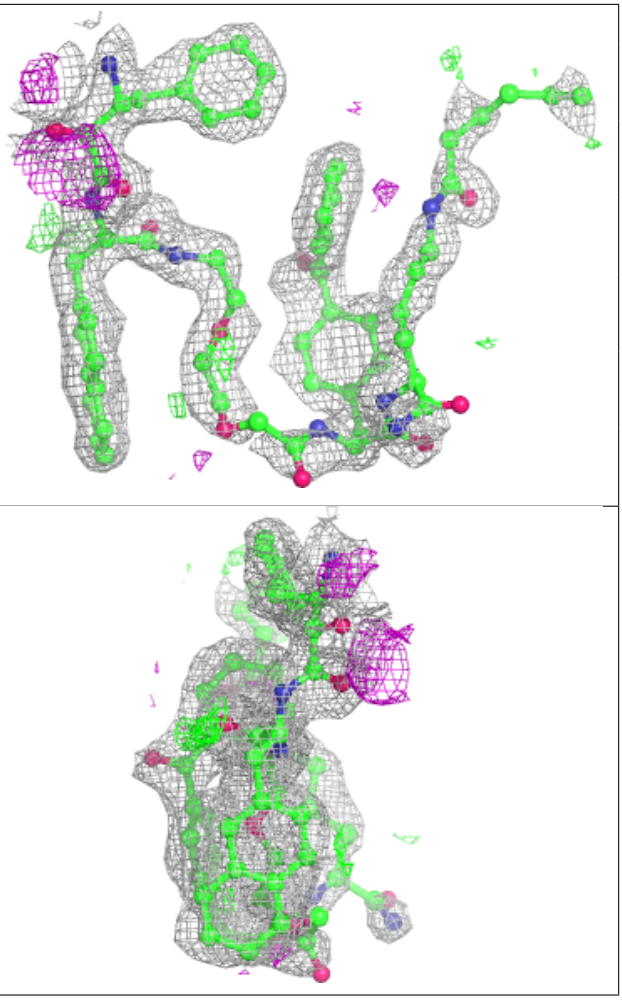
Electron density around DGZ L 615:

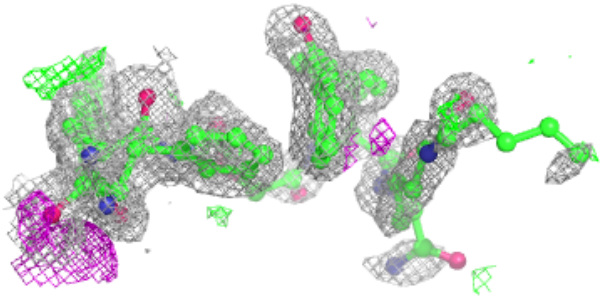
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DGZ C 615:

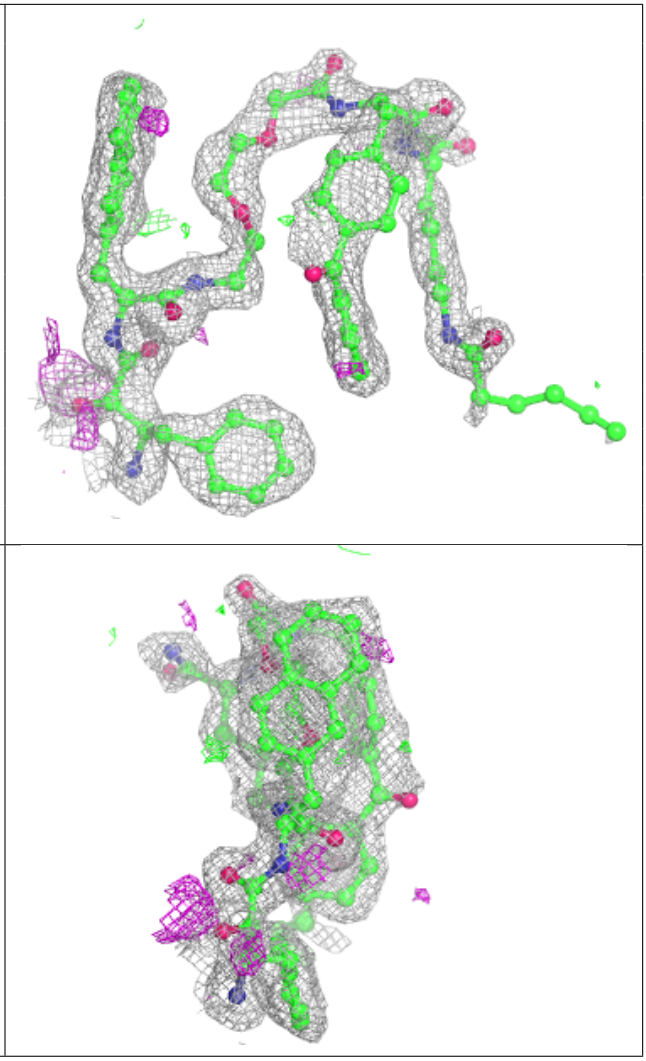
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

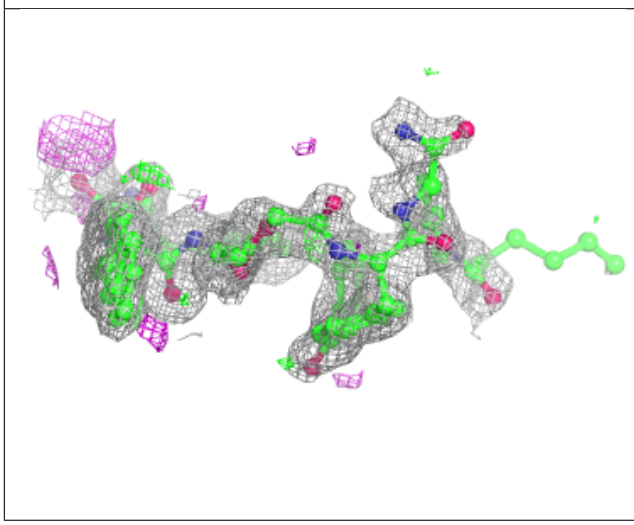




Electron density around DGZ D 615:

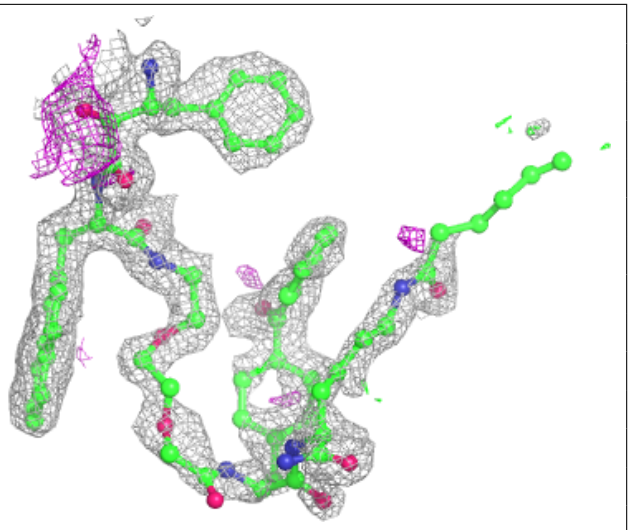
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

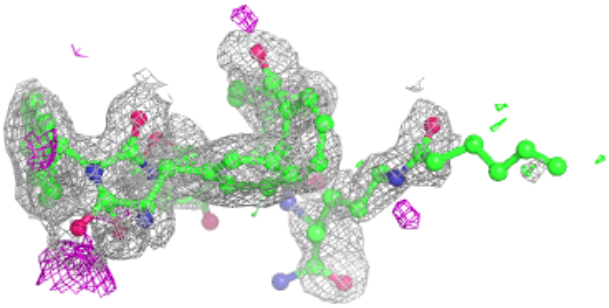




Electron density around DGZ E 615:

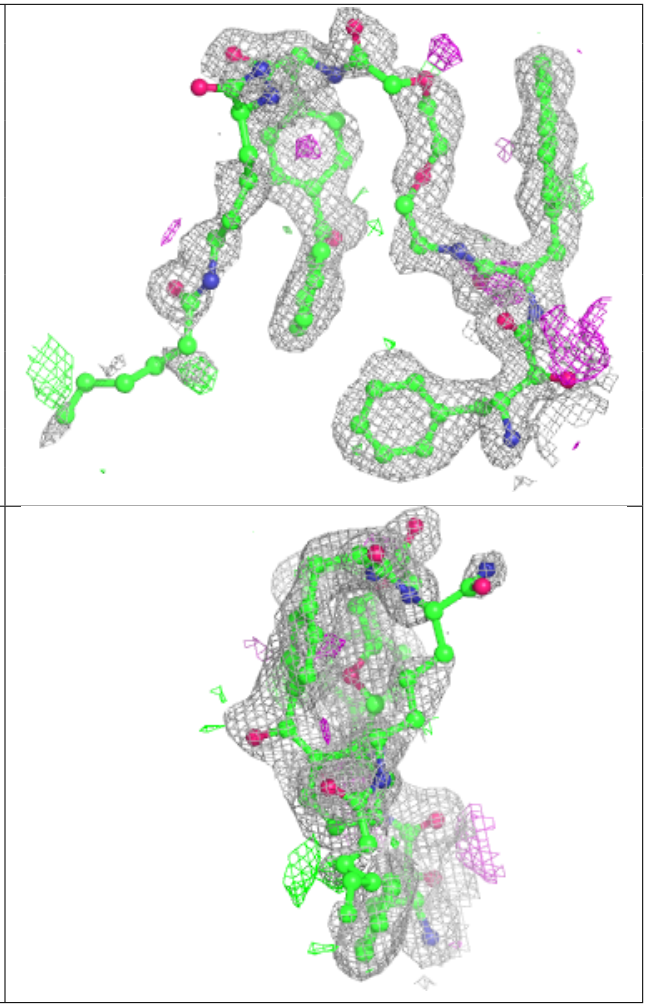
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around DGZ G 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.