



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:49 AM UTC

PDB ID : 3T8W / pdb_00003t8w
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

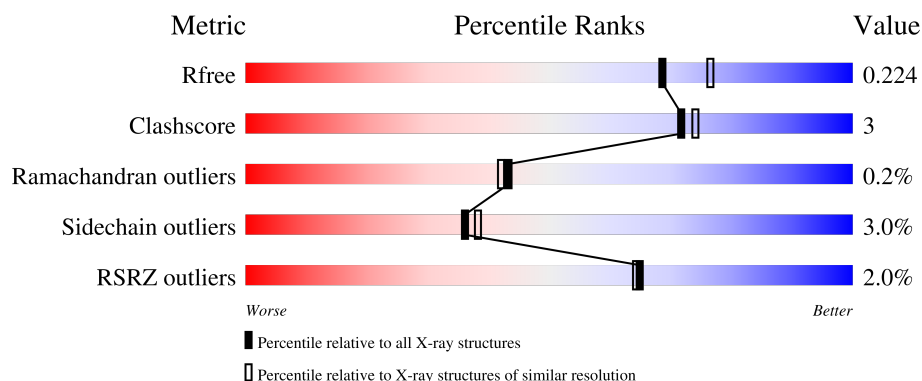
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	528	% 92% 6% .
1	B	528	4% 89% 8% ..
1	C	528	% 91% 6% ..
1	D	528	3% 88% 9% .
1	E	528	% 88% 8% .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CO3	A	612	-	X	-	-
2	CO3	C	612	-	X	-	-
2	CO3	D	612	-	X	-	-
2	CO3	E	612	-	X	-	-
2	CO3	H	612	-	X	-	-
2	CO3	J	612	-	X	-	-
2	CO3	L	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	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	1PE	J	622	-	X	-	-
6	1PE	K	617	-	X	-	-
6	1PE	K	618	-	X	-	-
6	1PE	K	619	-	X	-	-
6	1PE	K	620	-	X	-	-
6	1PE	L	617	-	X	-	-
6	1PE	L	618	-	X	-	-
6	1PE	L	619	-	X	-	-
6	1PE	L	620	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 53295 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called M17 leucyl aminopeptidase.

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

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP Q8IL11
A	515	GLN	ASN	engineered mutation	UNP Q8IL11
A	546	GLN	ASN	engineered mutation	UNP Q8IL11
A	606	HIS	-	expression tag	UNP Q8IL11
A	607	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	608	HIS	-	expression tag	UNP Q8IL11
A	609	HIS	-	expression tag	UNP Q8IL11
A	610	HIS	-	expression tag	UNP Q8IL11
A	611	HIS	-	expression tag	UNP Q8IL11
B	152	GLN	ASN	engineered mutation	UNP Q8IL11
B	515	GLN	ASN	engineered mutation	UNP Q8IL11
B	546	GLN	ASN	engineered mutation	UNP Q8IL11
B	606	HIS	-	expression tag	UNP Q8IL11
B	607	HIS	-	expression tag	UNP Q8IL11
B	608	HIS	-	expression tag	UNP Q8IL11
B	609	HIS	-	expression tag	UNP Q8IL11
B	610	HIS	-	expression tag	UNP Q8IL11
B	611	HIS	-	expression tag	UNP Q8IL11
C	152	GLN	ASN	engineered mutation	UNP Q8IL11
C	515	GLN	ASN	engineered mutation	UNP Q8IL11
C	546	GLN	ASN	engineered mutation	UNP Q8IL11
C	606	HIS	-	expression tag	UNP Q8IL11
C	607	HIS	-	expression tag	UNP Q8IL11
C	608	HIS	-	expression tag	UNP Q8IL11
C	609	HIS	-	expression tag	UNP Q8IL11
C	610	HIS	-	expression tag	UNP Q8IL11
C	611	HIS	-	expression tag	UNP Q8IL11
D	152	GLN	ASN	engineered mutation	UNP Q8IL11
D	515	GLN	ASN	engineered mutation	UNP Q8IL11
D	546	GLN	ASN	engineered mutation	UNP Q8IL11
D	606	HIS	-	expression tag	UNP Q8IL11
D	607	HIS	-	expression tag	UNP Q8IL11
D	608	HIS	-	expression tag	UNP Q8IL11
D	609	HIS	-	expression tag	UNP Q8IL11
D	610	HIS	-	expression tag	UNP Q8IL11
D	611	HIS	-	expression tag	UNP Q8IL11
E	152	GLN	ASN	engineered mutation	UNP Q8IL11
E	515	GLN	ASN	engineered mutation	UNP Q8IL11
E	546	GLN	ASN	engineered mutation	UNP Q8IL11
E	606	HIS	-	expression tag	UNP Q8IL11
E	607	HIS	-	expression tag	UNP Q8IL11
E	608	HIS	-	expression tag	UNP Q8IL11
E	609	HIS	-	expression tag	UNP Q8IL11
E	610	HIS	-	expression tag	UNP Q8IL11
E	611	HIS	-	expression tag	UNP Q8IL11
F	152	GLN	ASN	engineered mutation	UNP Q8IL11
F	515	GLN	ASN	engineered mutation	UNP Q8IL11

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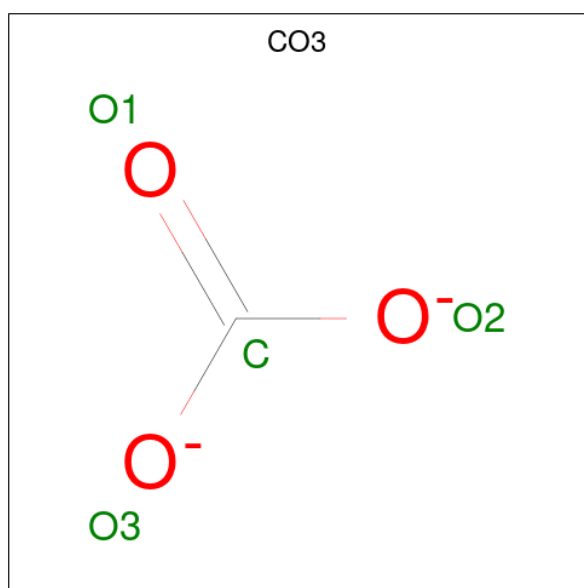
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP Q8IL11
G	152	GLN	ASN	engineered mutation	UNP Q8IL11
G	515	GLN	ASN	engineered mutation	UNP Q8IL11
G	546	GLN	ASN	engineered mutation	UNP Q8IL11
G	606	HIS	-	expression tag	UNP Q8IL11
G	607	HIS	-	expression tag	UNP Q8IL11
G	608	HIS	-	expression tag	UNP Q8IL11
G	609	HIS	-	expression tag	UNP Q8IL11
G	610	HIS	-	expression tag	UNP Q8IL11
G	611	HIS	-	expression tag	UNP Q8IL11
H	152	GLN	ASN	engineered mutation	UNP Q8IL11
H	515	GLN	ASN	engineered mutation	UNP Q8IL11
H	546	GLN	ASN	engineered mutation	UNP Q8IL11
H	606	HIS	-	expression tag	UNP Q8IL11
H	607	HIS	-	expression tag	UNP Q8IL11
H	608	HIS	-	expression tag	UNP Q8IL11
H	609	HIS	-	expression tag	UNP Q8IL11
H	610	HIS	-	expression tag	UNP Q8IL11
H	611	HIS	-	expression tag	UNP Q8IL11
I	152	GLN	ASN	engineered mutation	UNP Q8IL11
I	515	GLN	ASN	engineered mutation	UNP Q8IL11
I	546	GLN	ASN	engineered mutation	UNP Q8IL11
I	606	HIS	-	expression tag	UNP Q8IL11
I	607	HIS	-	expression tag	UNP Q8IL11
I	608	HIS	-	expression tag	UNP Q8IL11
I	609	HIS	-	expression tag	UNP Q8IL11
I	610	HIS	-	expression tag	UNP Q8IL11
I	611	HIS	-	expression tag	UNP Q8IL11
J	152	GLN	ASN	engineered mutation	UNP Q8IL11
J	515	GLN	ASN	engineered mutation	UNP Q8IL11
J	546	GLN	ASN	engineered mutation	UNP Q8IL11
J	606	HIS	-	expression tag	UNP Q8IL11
J	607	HIS	-	expression tag	UNP Q8IL11
J	608	HIS	-	expression tag	UNP Q8IL11
J	609	HIS	-	expression tag	UNP Q8IL11
J	610	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
J	611	HIS	-	expression tag	UNP Q8IL11
K	152	GLN	ASN	engineered mutation	UNP Q8IL11
K	515	GLN	ASN	engineered mutation	UNP Q8IL11
K	546	GLN	ASN	engineered mutation	UNP Q8IL11
K	606	HIS	-	expression tag	UNP Q8IL11
K	607	HIS	-	expression tag	UNP Q8IL11
K	608	HIS	-	expression tag	UNP Q8IL11
K	609	HIS	-	expression tag	UNP Q8IL11
K	610	HIS	-	expression tag	UNP Q8IL11
K	611	HIS	-	expression tag	UNP Q8IL11
L	152	GLN	ASN	engineered mutation	UNP Q8IL11
L	515	GLN	ASN	engineered mutation	UNP Q8IL11
L	546	GLN	ASN	engineered mutation	UNP Q8IL11
L	606	HIS	-	expression tag	UNP Q8IL11
L	607	HIS	-	expression tag	UNP Q8IL11
L	608	HIS	-	expression tag	UNP Q8IL11
L	609	HIS	-	expression tag	UNP Q8IL11
L	610	HIS	-	expression tag	UNP Q8IL11
L	611	HIS	-	expression tag	UNP Q8IL11

- Molecule 2 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



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

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

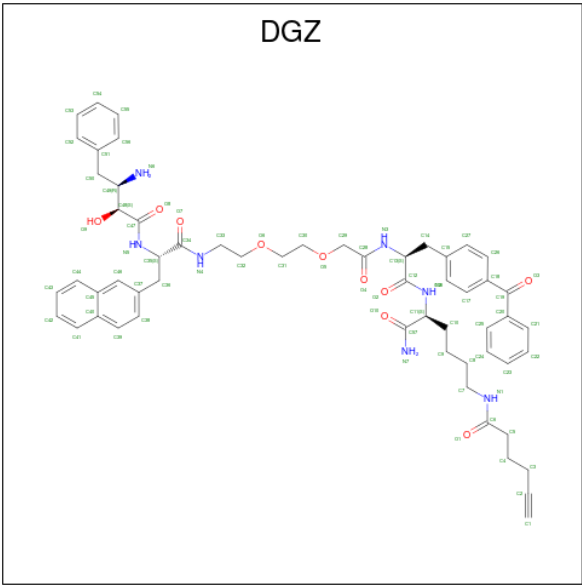
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	E	2	Total Zn 2 2	0	0
3	F	2	Total Zn 2 2	0	0
3	G	2	Total Zn 2 2	0	0
3	H	2	Total Zn 2 2	0	0
3	I	2	Total Zn 2 2	0	0

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

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



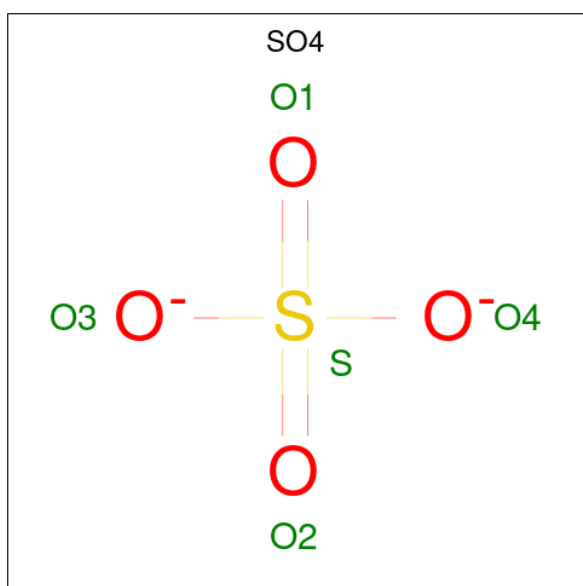
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			74	57	7	10		
4	B	1	Total	C	N	O	0	0
			74	57	7	10		
4	C	1	Total	C	N	O	0	0
			74	57	7	10		
4	D	1	Total	C	N	O	0	0
			74	57	7	10		
4	E	1	Total	C	N	O	0	0
			74	57	7	10		
4	F	1	Total	C	N	O	0	0
			74	57	7	10		
4	G	1	Total	C	N	O	0	0
			74	57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

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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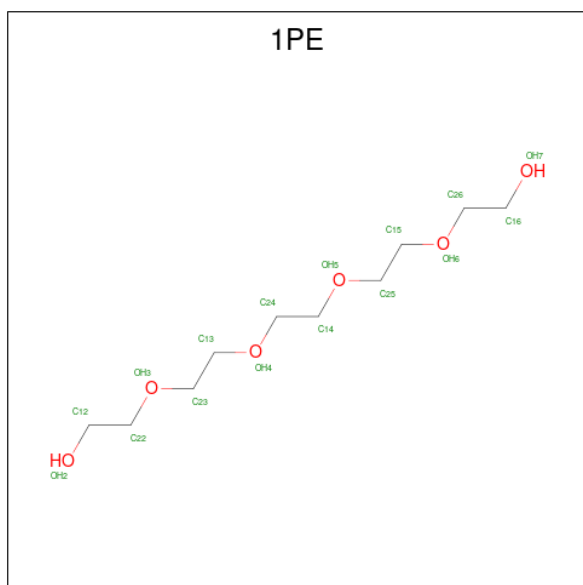
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total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

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

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



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

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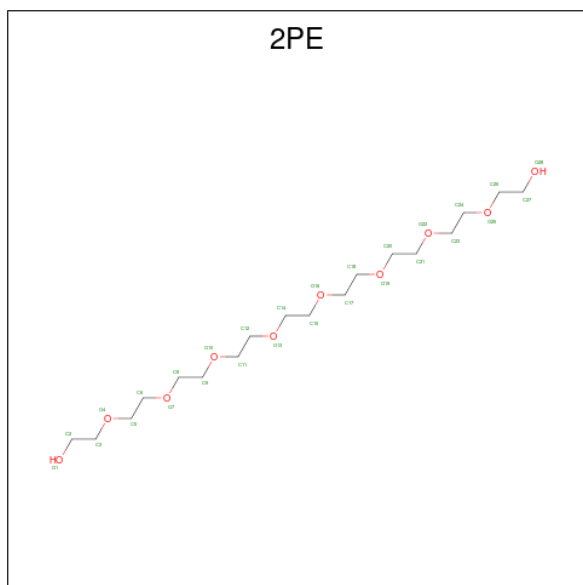
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			10	6	4		
6	E	1	Total	C	O	0	0
			8	5	3		
6	F	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			9	6	3		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1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

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

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



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

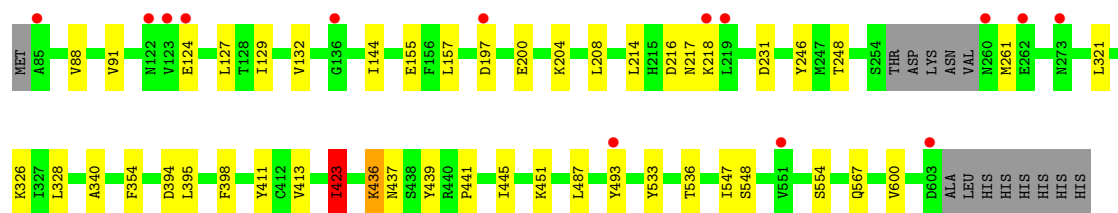
- Molecule 8 is water.

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

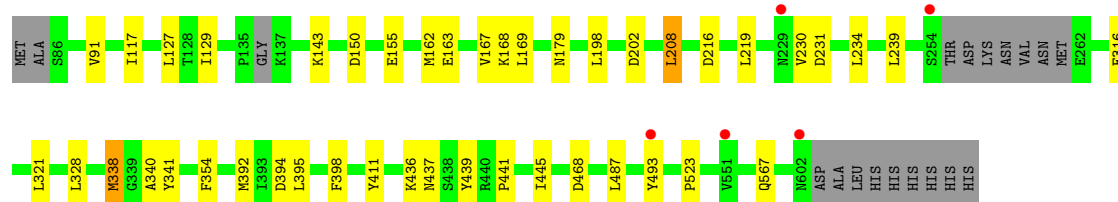
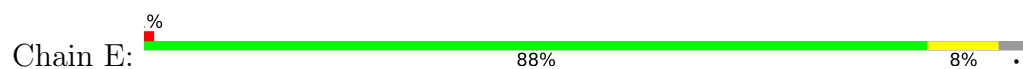
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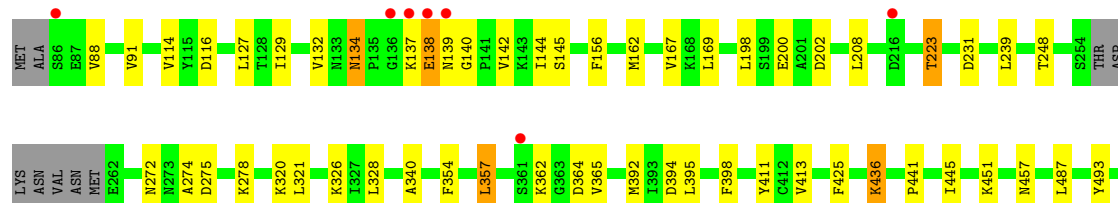
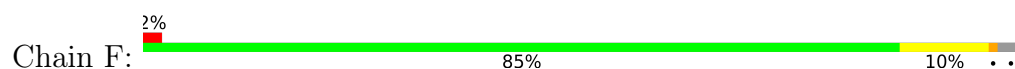
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	445	Total 445	O 445	0	0
8	F	364	Total 364	O 364	0	0
8	G	431	Total 431	O 431	0	0
8	H	334	Total 334	O 334	0	0
8	I	391	Total 391	O 391	0	0
8	J	406	Total 406	O 406	0	0
8	K	408	Total 408	O 408	0	0
8	L	389	Total 389	O 389	0	0



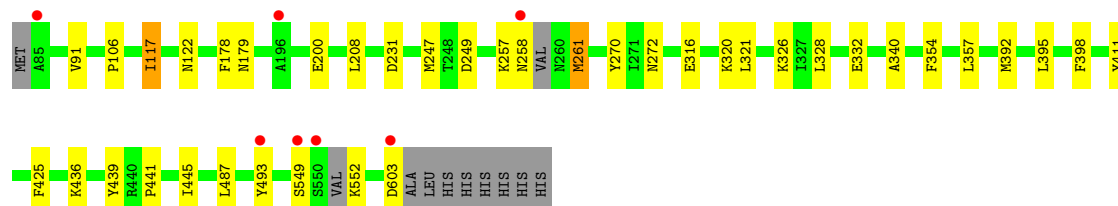
• Molecule 1: M17 leucyl aminopeptidase



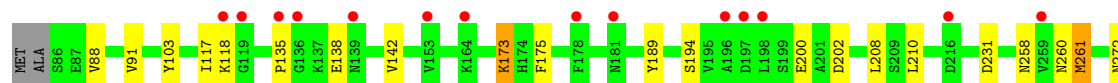
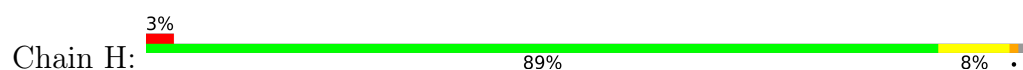
• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase

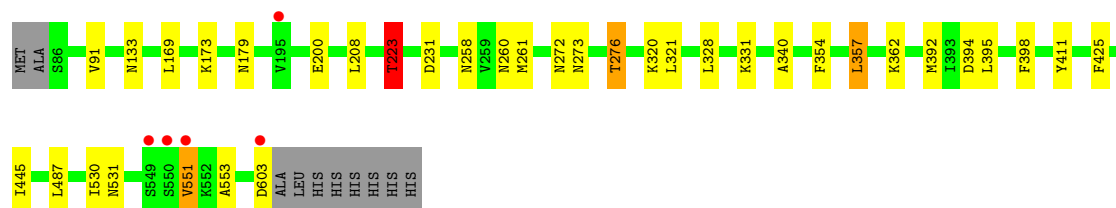


• Molecule 1: M17 leucyl aminopeptidase

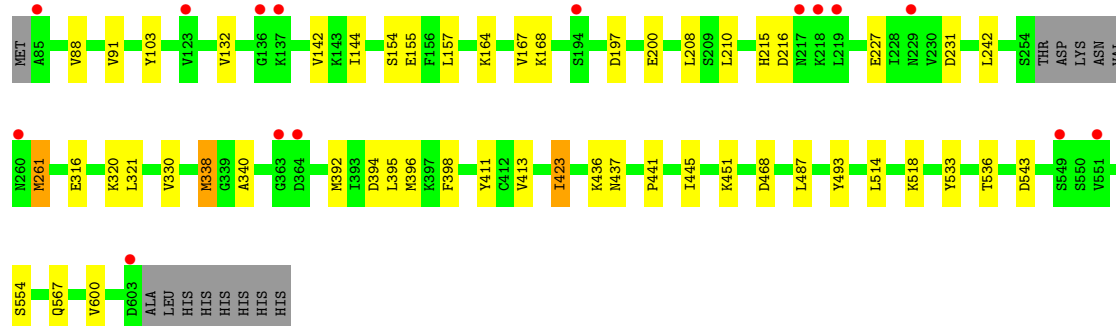
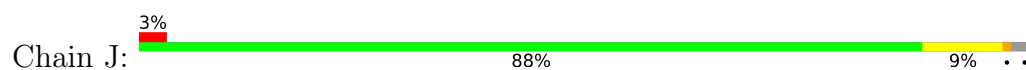




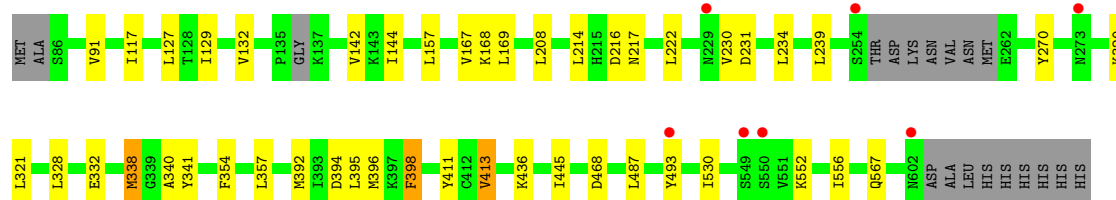
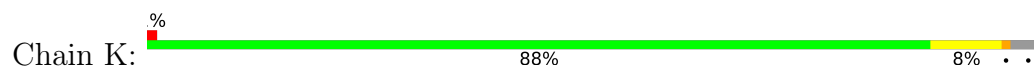
- Molecule 1: M17 leucyl aminopeptidase



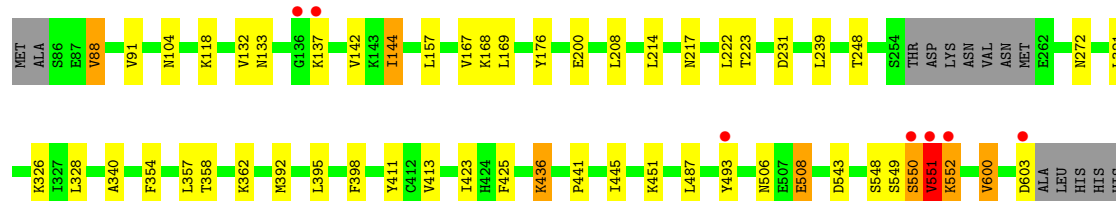
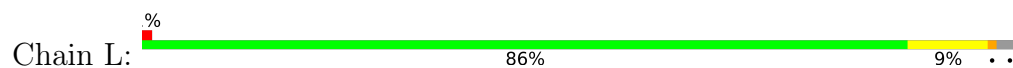
- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase



HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.75Å 177.06Å 231.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.32 – 2.00 81.32 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (81.32-2.00) 100.0 (81.32-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.164 , 0.200 0.184 , 0.224	Depositor DCC
R_{free} test set	23988 reflections (5.01%)	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 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	53295	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3495e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CO3, 1PE, 2PE, SO4, DGZ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.81	0/4051	1.14	9/5498 (0.2%)
1	B	0.81	1/3993 (0.0%)	1.20	17/5424 (0.3%)
1	C	0.81	0/4019	1.13	7/5453 (0.1%)
1	D	0.85	3/4005 (0.1%)	1.14	6/5431 (0.1%)
1	E	0.82	2/3976 (0.1%)	1.13	5/5391 (0.1%)
1	F	0.81	1/3924 (0.0%)	1.19	11/5336 (0.2%)
1	G	0.79	0/4054	1.13	7/5494 (0.1%)
1	H	0.82	3/4005 (0.1%)	1.17	9/5440 (0.2%)
1	I	0.81	0/4033	1.14	11/5473 (0.2%)
1	J	0.82	2/4002 (0.0%)	1.14	8/5428 (0.1%)
1	K	0.82	1/3973 (0.0%)	1.13	7/5389 (0.1%)
1	L	0.82	1/3921 (0.0%)	1.18	13/5332 (0.2%)
All	All	0.82	14/47956 (0.0%)	1.15	110/65089 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	547	ILE	C-N	-13.36	1.15	1.33
1	K	338	MET	SD-CE	-9.05	1.56	1.79
1	H	549	SER	C-N	8.75	1.45	1.33
1	E	338	MET	SD-CE	-8.49	1.58	1.79
1	J	338	MET	SD-CE	-7.54	1.60	1.79
1	B	423	ILE	CG1-CD1	-6.93	1.24	1.51
1	H	551	VAL	C-O	-6.52	1.16	1.24
1	H	423	ILE	CG1-CD1	-6.45	1.26	1.51
1	D	423	ILE	CG1-CD1	-6.33	1.27	1.51
1	J	423	ILE	CG1-CD1	-6.14	1.27	1.51
1	E	162	MET	SD-CE	-5.47	1.65	1.79
1	D	548	SER	C-N	5.34	1.41	1.33
1	F	138	GLU	CA-C	5.13	1.59	1.52
1	L	552	LYS	C-N	5.12	1.40	1.33

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	550	SER	CA-C-N	8.08	136.24	121.70
1	A	550	SER	C-N-CA	8.08	136.24	121.70
1	B	471	VAL	N-CA-CB	7.90	121.29	110.54
1	G	257	LYS	CA-C-N	7.61	135.40	121.70
1	G	257	LYS	C-N-CA	7.61	135.40	121.70
1	C	91	VAL	N-CA-C	-7.48	104.49	111.45
1	G	487	LEU	N-CA-C	7.25	120.25	111.40
1	I	91	VAL	N-CA-C	-7.24	104.72	111.45
1	F	552	LYS	N-CA-C	-7.22	95.41	110.80
1	C	362	LYS	N-CA-C	-6.89	98.81	109.76
1	L	508	GLU	CB-CG-CD	6.88	124.30	112.60
1	B	552	LYS	N-CA-C	-6.83	96.26	110.80
1	J	487	LEU	N-CA-C	6.75	119.64	111.40
1	D	487	LEU	N-CA-C	6.74	119.62	111.40
1	L	549	SER	CA-C-N	6.66	134.26	121.54
1	L	549	SER	C-N-CA	6.66	134.26	121.54
1	F	91	VAL	N-CA-C	-6.64	105.28	111.45
1	F	231	ASP	CA-CB-CG	6.56	119.16	112.60
1	L	551	VAL	CA-C-N	6.55	134.05	121.54
1	L	551	VAL	C-N-CA	6.55	134.05	121.54
1	D	91	VAL	N-CA-C	-6.41	105.49	111.45
1	I	362	LYS	N-CA-C	-6.38	99.62	109.76
1	K	487	LEU	N-CA-C	6.36	119.16	111.40
1	A	231	ASP	CA-CB-CG	6.36	118.96	112.60
1	B	254	SER	CA-C-N	6.34	133.11	121.70
1	B	254	SER	C-N-CA	6.34	133.11	121.70
1	K	217	ASN	CA-CB-CG	6.27	118.87	112.60
1	E	487	LEU	N-CA-C	6.21	118.97	111.40
1	I	487	LEU	N-CA-C	6.19	118.95	111.40
1	B	487	LEU	N-CA-C	6.18	118.94	111.40
1	K	396	MET	N-CA-C	6.18	120.29	112.87
1	A	91	VAL	N-CA-C	-6.17	105.71	111.45
1	K	413	VAL	N-CA-CB	6.09	119.72	110.58
1	L	91	VAL	N-CA-C	-6.07	105.80	111.45
1	E	91	VAL	N-CA-C	-6.06	105.81	111.45
1	J	91	VAL	N-CA-C	-6.06	105.81	111.45
1	A	487	LEU	N-CA-C	6.06	118.79	111.40
1	K	91	VAL	N-CA-C	-6.05	105.82	111.45
1	I	551	VAL	N-CA-C	6.05	121.92	109.34
1	H	91	VAL	N-CA-C	-6.03	105.84	111.45
1	I	553	ALA	CA-C-N	5.99	128.63	120.54
1	I	553	ALA	C-N-CA	5.99	128.63	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	290	GLY	CA-C-N	5.99	128.59	120.44
1	H	290	GLY	C-N-CA	5.99	128.59	120.44
1	C	487	LEU	N-CA-C	5.99	118.71	111.40
1	A	396	MET	N-CA-C	5.96	120.03	112.87
1	B	91	VAL	N-CA-C	-5.95	105.92	111.45
1	B	142	VAL	N-CA-CB	5.93	117.00	110.53
1	H	487	LEU	N-CA-C	5.90	118.60	111.40
1	L	487	LEU	N-CA-C	5.89	118.58	111.40
1	G	231	ASP	CA-CB-CG	5.82	118.42	112.60
1	B	231	ASP	CA-CB-CG	5.78	118.38	112.60
1	B	118	LYS	N-CA-C	-5.77	101.11	109.59
1	F	138	GLU	N-CA-C	5.76	121.21	113.72
1	B	118	LYS	CA-C-N	-5.69	116.71	123.08
1	B	118	LYS	C-N-CA	-5.69	116.71	123.08
1	J	396	MET	N-CA-C	5.65	119.64	112.87
1	C	396	MET	N-CA-C	5.61	119.60	112.87
1	F	487	LEU	N-CA-C	5.60	118.23	111.40
1	A	549	SER	CA-C-N	5.55	132.14	121.54
1	A	549	SER	C-N-CA	5.55	132.14	121.54
1	H	289	PHE	CA-CB-CG	-5.54	108.26	113.80
1	J	231	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	139	ASN	N-CA-C	-5.52	101.97	109.54
1	F	275	ASP	CA-C-N	5.52	128.22	120.28
1	F	275	ASP	C-N-CA	5.52	128.22	120.28
1	J	554	SER	N-CA-C	5.52	117.29	111.28
1	D	231	ASP	CA-CB-CG	5.50	118.10	112.60
1	D	124	GLU	N-CA-C	5.49	119.60	113.01
1	K	231	ASP	CA-CB-CG	5.48	118.08	112.60
1	L	362	LYS	N-CA-C	-5.48	102.17	110.28
1	G	91	VAL	N-CA-C	-5.44	106.39	111.45
1	F	362	LYS	N-CA-C	-5.43	102.44	110.48
1	H	231	ASP	CA-CB-CG	5.42	118.02	112.60
1	D	554	SER	N-CA-C	5.38	117.14	111.28
1	J	330	VAL	N-CA-C	5.38	116.01	110.36
1	E	231	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	133	ASN	CA-CB-CG	5.38	117.98	112.60
1	F	223	THR	CB-CA-C	5.36	119.51	109.71
1	B	232	LYS	CA-C-N	5.34	127.70	120.44
1	B	232	LYS	C-N-CA	5.34	127.70	120.44
1	C	231	ASP	CA-CB-CG	5.33	117.93	112.60
1	I	223	THR	CB-CA-C	5.33	119.45	109.71
1	I	179	ASN	CA-CB-CG	5.32	117.92	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	227	GLU	CA-C-N	5.31	130.23	122.69
1	J	227	GLU	C-N-CA	5.31	130.23	122.69
1	I	133	ASN	CA-CB-CG	5.30	117.90	112.60
1	H	118	LYS	N-CA-C	-5.28	101.83	109.59
1	H	202	ASP	CA-CB-CG	5.28	117.88	112.60
1	F	202	ASP	CA-CB-CG	5.27	117.87	112.60
1	E	523	PRO	N-CA-C	5.24	118.71	110.80
1	L	552	LYS	N-CA-C	5.23	121.95	110.80
1	H	142	VAL	N-CA-CB	5.22	116.41	110.72
1	E	216	ASP	CA-CB-CG	5.21	117.81	112.60
1	C	223	THR	CB-CA-C	5.18	119.20	109.71
1	L	231	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	199	SER	CA-C-N	5.17	127.47	120.38
1	B	199	SER	C-N-CA	5.17	127.47	120.38
1	B	133	ASN	CA-CB-CG	5.17	117.77	112.60
1	I	223	THR	N-CA-CB	5.16	119.35	110.68
1	G	549	SER	N-CA-C	-5.15	104.62	112.04
1	G	179	ASN	CA-CB-CG	5.12	117.72	112.60
1	A	133	ASN	CA-CB-CG	5.08	117.69	112.60
1	F	278	LYS	N-CA-C	5.08	117.48	111.33
1	L	118	LYS	N-CA-C	5.07	117.46	111.33
1	L	88	VAL	N-CA-CB	5.06	118.29	111.21
1	K	398	PHE	CA-CB-CG	5.05	118.85	113.80
1	D	217	ASN	CA-CB-CG	5.02	117.62	112.60
1	I	231	ASP	CA-CB-CG	5.01	117.61	112.60
1	L	600	VAL	N-CA-CB	5.00	118.09	110.58

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3973	0	3875	15	0
1	B	3916	0	3799	27	0
1	C	3942	0	3849	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3928	0	3856	27	0
1	E	3900	0	3831	24	0
1	F	3847	0	3710	35	0
1	G	3978	0	3903	19	0
1	H	3927	0	3812	27	0
1	I	3955	0	3877	17	0
1	J	3925	0	3848	33	0
1	K	3897	0	3817	20	0
1	L	3844	0	3687	30	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	11	0
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	8	0
4	G	74	0	66	5	0
4	H	74	0	66	7	0
4	I	74	0	66	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	74	0	66	5	0
4	K	74	0	66	5	0
4	L	74	0	66	7	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	3	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	13	0
6	K	37	0	38	1	0
6	L	40	0	48	9	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
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	311	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 (311) 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:E:338:MET:HE3	1:E:468:ASP:HB3	1.29	1.15
1:K:338:MET:HE3	1:K:468:ASP:HB3	1.31	1.05
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:F:320:LYS:HZ1	6:F:617:1PE:H152	1.32	0.91
1:H:550:SER:HG	1:H:552:LYS:HD2	1.09	0.86
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:CE	1:K:468:ASP:HB3	2.12	0.79
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:E:338:MET:CE	1:E:468:ASP:HB3	2.15	0.72
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:B:392:MET:HE3	4:B:615:DGZ:H54	1.73	0.69
1:J:320:LYS:HZ1	6:J:620:1PE:H152	1.58	0.68
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:F:551:VAL:C	1:F:552:LYS:O	2.36	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:J:338:MET:HE3	1:J:468:ASP:HB3	1.77	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:LYS:HZ2	1:E:437:ASN:HD22	1.47	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:G:392:MET:HE2	4:G:615:DGZ:H5	1.83	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: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
1:F:392:MET:HE2	4:F:615:DGZ:H5A	1.87	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:J:437:ASN:HD22	1:L:436:LYS:HZ1	1.52	0.56
1:F:320:LYS:NZ	6:F:617:1PE:H152	2.14	0.56
1:B:392:MET:HE2	4:B:615:DGZ:H5	1.86	0.56
1:C:326:LYS:HE3	1:C:328:LEU:HD11	1.87	0.56
1:J:316:GLU:CD	6:J:620:1PE:H251	2.31	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: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
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:L:392:MET:HE2	4:L:615:DGZ:H5A	1.89	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:E:338:MET:HE3	1:E:468:ASP:CB	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.90	0.54
1:I:392:MET:HE2	4:I:615:DGZ:H5	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:C:392:MET:HE2	4:C:615:DGZ:H5	1.89	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: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: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:392:MET:HE2	4:E:615:DGZ:H5	1.92	0.51
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.92	0.51
1:B:392:MET:CE	4:B:615:DGZ:H54	2.39	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: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:B:552:LYS:O	1:B:553:ALA:C	2.54	0.50
1:H:493:TYR:CE1	4:H:615:DGZ:H21	2.47	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:J:338:MET:CE	1:J:468:ASP:HB3	2.41	0.50
1:L:176:TYR:OH	1:L:217:ASN:ND2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:392:MET:HE2	4:K:615:DGZ:H5	1.93	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:B:551:VAL:C	1:B:552:LYS:O	2.55	0.49
1:F:156:PHE:O	1:F:162:MET:HE3	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: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:E:338:MET:HE2	1:E:341:TYR:HD2	1.78	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
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:D:451:LYS:HZ3	6:D:620:1PE:H142	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:215:HIS:HD2	1:J:261:MET:HE2	1.80	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:A:361:SER:HB3	8:A:728:HOH:O	2.16	0.46
1:B:233:ASN:HD21	1:B:519:THR:C	2.23	0.46
1:E:321:LEU:HD11	1:E:411:TYR:HA	1.97	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:E:338:MET:HE2	1:E:341:TYR:CD2	2.50	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: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
1:A:550:SER:HA	1:A:551:VAL:CB	2.47	0.45
1:A:321:LEU:HD11	1:A:411:TYR:HA	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:258:ASN:HD22	1:I:258:ASN:C	2.26	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:D:248:THR:HG23	8:D:969:HOH:O	2.17	0.43
1:F:134:ASN:C	1:F:134:ASN:HD22	2.26	0.43
1:L:451:LYS:HZ2	6:L:618:1PE:C12	2.32	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:L:550:SER:OG	1:L:551:VAL:N	2.50	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:167:VAL:O	1:K:168:LYS:C	2.62	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:L:167:VAL:O	1:L:168:LYS:C	2.62	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:H:551:VAL:O	1:H:552:LYS:C	2.61	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
1:E:167:VAL:O	1:E:168:LYS:C	2.62	0.41
1:G:320:LYS:HZ1	6:G:623:1PE:H152	1.85	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:J:320:LYS:HZ1	6:J:620:1PE:C15	2.31	0.41
1:H:103:TYR:O	7:H:619:2PE:H271	2.20	0.41
1:K:338:MET:HE2	1:K:341:TYR:HD2	1.85	0.41
4:B:615:DGZ:H17	4:B:615:DGZ:H7A	2.01	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:D:437:ASN:HD22	1:F:436:LYS:HZ2	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:167:VAL:O	1:J:168:LYS:C	2.64	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: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%)	43	42
1	B	513/528 (97%)	499 (97%)	12 (2%)	2 (0%)	30	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	512/528 (97%)	501 (98%)	11 (2%)	0	100	100
1	D	510/528 (97%)	502 (98%)	8 (2%)	0	100	100
1	E	503/528 (95%)	494 (98%)	9 (2%)	0	100	100
1	F	507/528 (96%)	494 (97%)	10 (2%)	3 (1%)	21	17
1	G	511/528 (97%)	501 (98%)	10 (2%)	0	100	100
1	H	516/528 (98%)	501 (97%)	13 (2%)	2 (0%)	30	27
1	I	516/528 (98%)	502 (97%)	13 (2%)	1 (0%)	43	42
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%)	21	17
All	All	6125/6336 (97%)	5985 (98%)	128 (2%)	12 (0%)	43	42

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 ⓘ

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%)	412 (98%)	9 (2%)	47	52
1	B	410/455 (90%)	398 (97%)	12 (3%)	37	40
1	C	417/455 (92%)	407 (98%)	10 (2%)	43	47
1	D	415/455 (91%)	401 (97%)	14 (3%)	32	33
1	E	415/455 (91%)	403 (97%)	12 (3%)	37	40
1	F	400/455 (88%)	380 (95%)	20 (5%)	22	20
1	G	426/455 (94%)	416 (98%)	10 (2%)	44	49
1	H	412/455 (90%)	398 (97%)	14 (3%)	32	33
1	I	420/455 (92%)	408 (97%)	12 (3%)	37	40
1	J	414/455 (91%)	402 (97%)	12 (3%)	37	40
1	K	414/455 (91%)	404 (98%)	10 (2%)	43	47
1	L	397/455 (87%)	383 (96%)	14 (4%)	32	32
All	All	4961/5460 (91%)	4812 (97%)	149 (3%)	36	38

All (149) 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	272	ASN
1	A	395	LEU
1	A	398	PHE
1	A	436	LYS
1	A	439	TYR
1	B	88	VAL
1	B	142	VAL
1	B	208	LEU
1	B	210	LEU
1	B	233	ASN
1	B	272	ASN
1	B	357	LEU
1	B	395	LEU
1	B	398	PHE
1	B	436	LYS
1	B	439	TYR
1	B	471	VAL
1	C	169	LEU

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Mol	Chain	Res	Type
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	276	THR
1	C	331	LYS
1	C	398	PHE
1	D	88	VAL
1	D	132	VAL
1	D	197	ASP
1	D	200	GLU
1	D	204	LYS
1	D	208	LEU
1	D	216	ASP
1	D	395	LEU
1	D	398	PHE
1	D	423	ILE
1	D	436	LYS
1	D	439	TYR
1	D	567	GLN
1	D	600	VAL
1	E	117	ILE
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	395	LEU
1	E	398	PHE
1	E	436	LYS
1	E	439	TYR
1	E	567	GLN
1	F	88	VAL
1	F	116	ASP
1	F	134	ASN
1	F	144	ILE
1	F	145	SER
1	F	167	VAL
1	F	169	LEU

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Mol	Chain	Res	Type
1	F	198	LEU
1	F	200	GLU
1	F	208	LEU
1	F	223	THR
1	F	239	LEU
1	F	272	ASN
1	F	357	LEU
1	F	364	ASP
1	F	395	LEU
1	F	398	PHE
1	F	436	LYS
1	F	554	SER
1	F	567	GLN
1	G	117	ILE
1	G	200	GLU
1	G	208	LEU
1	G	261	MET
1	G	272	ASN
1	G	395	LEU
1	G	398	PHE
1	G	436	LYS
1	G	439	TYR
1	G	603	ASP
1	H	88	VAL
1	H	117	ILE
1	H	173	LYS
1	H	200	GLU
1	H	208	LEU
1	H	210	LEU
1	H	261	MET
1	H	272	ASN
1	H	395	LEU
1	H	398	PHE
1	H	436	LYS
1	H	439	TYR
1	H	549	SER
1	H	552	LYS
1	I	169	LEU
1	I	173	LYS
1	I	200	GLU
1	I	208	LEU
1	I	223	THR

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Mol	Chain	Res	Type
1	I	272	ASN
1	I	276	THR
1	I	331	LYS
1	I	357	LEU
1	I	395	LEU
1	I	398	PHE
1	I	603	ASP
1	J	88	VAL
1	J	154	SER
1	J	164	LYS
1	J	197	ASP
1	J	200	GLU
1	J	208	LEU
1	J	216	ASP
1	J	261	MET
1	J	395	LEU
1	J	398	PHE
1	J	436	LYS
1	J	567	GLN
1	K	169	LEU
1	K	208	LEU
1	K	216	ASP
1	K	239	LEU
1	K	357	LEU
1	K	395	LEU
1	K	398	PHE
1	K	413	VAL
1	K	436	LYS
1	K	567	GLN
1	L	88	VAL
1	L	137	LYS
1	L	144	ILE
1	L	169	LEU
1	L	200	GLU
1	L	208	LEU
1	L	239	LEU
1	L	272	ASN
1	L	358	THR
1	L	395	LEU
1	L	398	PHE
1	L	436	LYS
1	L	600	VAL

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Mol	Chain	Res	Type
1	L	603	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	260	ASN
1	A	437	ASN
1	A	449	ASN
1	B	233	ASN
1	B	258	ASN
1	B	260	ASN
1	B	319	GLN
1	B	322	ASN
1	B	420	ASN
1	C	139	ASN
1	C	161	ASN
1	C	521	ASN
1	D	183	ASN
1	D	273	ASN
1	D	420	ASN
1	D	437	ASN
1	D	521	ASN
1	E	113	GLN
1	E	139	ASN
1	E	161	ASN
1	E	272	ASN
1	E	420	ASN
1	E	437	ASN
1	F	90	GLN
1	F	104	ASN
1	F	122	ASN
1	F	134	ASN
1	F	149	ASN
1	F	567	GLN
1	G	139	ASN
1	G	437	ASN
1	H	258	ASN
1	H	319	GLN
1	H	420	ASN
1	H	515	GLN
1	H	521	ASN

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Mol	Chain	Res	Type
1	I	139	ASN
1	I	161	ASN
1	I	183	ASN
1	I	258	ASN
1	I	420	ASN
1	J	183	ASN
1	J	420	ASN
1	J	437	ASN
1	K	139	ASN
1	K	161	ASN
1	K	273	ASN
1	K	420	ASN
1	L	104	ASN
1	L	134	ASN
1	L	139	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 oligosaccharides 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
2	CO3	C	612	-	3,3,3	4.20	2 (66%)	2,3,3	6.64	2 (100%)
6	1PE	K	617	-	7,7,15	2.43	3 (42%)	6,6,14	2.63	3 (50%)
5	SO4	J	616	-	4,4,4	0.86	0	6,6,6	0.27	0
2	CO3	J	612	-	3,3,3	5.05	1 (33%)	2,3,3	6.71	2 (100%)
4	DGZ	C	615	3	78,78,78	0.91	1 (1%)	98,101,101	2.00	3 (3%)
2	CO3	H	612	-	3,3,3	1.80	1 (33%)	2,3,3	5.94	2 (100%)
4	DGZ	E	615	3	78,78,78	0.89	1 (1%)	98,101,101	1.99	2 (2%)
2	CO3	I	612	-	3,3,3	4.48	1 (33%)	2,3,3	5.78	1 (50%)
5	SO4	I	617	-	4,4,4	0.84	0	6,6,6	0.28	0
6	1PE	E	620	-	9,9,15	2.23	4 (44%)	8,8,14	2.98	6 (75%)
6	1PE	J	622	-	8,8,15	2.38	3 (37%)	7,7,14	2.94	3 (42%)
6	1PE	L	617	-	9,9,15	2.27	4 (44%)	8,8,14	1.84	3 (37%)
6	1PE	G	621	-	5,5,15	1.65	1 (20%)	4,4,14	2.98	2 (50%)
2	CO3	B	612	-	3,3,3	1.53	0	2,3,3	8.34	2 (100%)
7	2PE	B	616	-	25,25,27	0.95	0	24,24,26	0.56	0
6	1PE	J	621	-	10,10,15	2.30	5 (50%)	9,9,14	2.69	3 (33%)
5	SO4	C	619	-	4,4,4	0.79	0	6,6,6	0.32	0
2	CO3	D	612	-	3,3,3	3.92	2 (66%)	2,3,3	5.69	1 (50%)
6	1PE	C	621	-	11,11,15	2.28	4 (36%)	10,10,14	3.05	5 (50%)
5	SO4	H	617	-	4,4,4	0.32	0	6,6,6	0.13	0
6	1PE	L	618	-	11,11,15	2.22	4 (36%)	10,10,14	3.31	6 (60%)
6	1PE	I	623	-	4,4,15	1.72	1 (25%)	3,3,14	1.00	0
2	CO3	F	612	-	3,3,3	3.96	1 (33%)	2,3,3	5.19	1 (50%)
5	SO4	G	616	-	4,4,4	0.29	0	6,6,6	0.19	0
6	1PE	K	619	-	10,10,15	2.71	5 (50%)	9,9,14	2.60	5 (55%)
5	SO4	E	616	-	4,4,4	0.22	0	6,6,6	0.17	0
4	DGZ	F	615	3	78,78,78	0.94	1 (1%)	98,101,101	2.03	2 (2%)
5	SO4	J	618	-	4,4,4	0.42	0	6,6,6	0.22	0
5	SO4	C	620	-	4,4,4	0.48	0	6,6,6	0.16	0
5	SO4	G	617	-	4,4,4	0.83	0	6,6,6	0.43	0
6	1PE	K	620	-	5,5,15	2.13	1 (20%)	4,4,14	1.96	2 (50%)
5	SO4	I	618	-	4,4,4	0.78	0	6,6,6	0.27	0
6	1PE	I	622	-	9,9,15	2.32	4 (44%)	8,8,14	2.29	3 (37%)
6	1PE	J	620	-	9,9,15	2.80	5 (55%)	8,8,14	3.11	4 (50%)
5	SO4	L	616	-	4,4,4	0.69	0	6,6,6	0.36	0
2	CO3	L	612	-	3,3,3	4.39	2 (66%)	2,3,3	4.71	1 (50%)
6	1PE	F	618	-	9,9,15	3.08	5 (55%)	8,8,14	3.23	4 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	1PE	E	621	-	7,7,15	2.23	3 (42%)	6,6,14	2.74	4 (66%)
6	1PE	D	618	-	9,9,15	2.25	3 (33%)	8,8,14	3.06	4 (50%)
5	SO4	A	616	-	4,4,4	0.31	0	6,6,6	0.20	0
6	1PE	A	618	-	8,8,15	2.07	2 (25%)	7,7,14	3.08	3 (42%)
5	SO4	G	619	-	4,4,4	0.88	0	6,6,6	0.25	0
5	SO4	D	617	-	4,4,4	0.49	0	6,6,6	0.38	0
6	1PE	F	617	-	9,9,15	2.62	4 (44%)	8,8,14	2.96	5 (62%)
6	1PE	L	620	-	10,10,15	3.15	5 (50%)	9,9,14	2.73	5 (55%)
5	SO4	C	616	-	4,4,4	0.36	0	6,6,6	0.57	0
5	SO4	J	617	-	4,4,4	0.18	0	6,6,6	0.19	0
6	1PE	G	622	-	5,5,15	1.63	1 (20%)	4,4,14	3.09	2 (50%)
2	CO3	A	612	-	3,3,3	1.88	2 (66%)	2,3,3	8.54	2 (100%)
2	CO3	G	612	-	3,3,3	1.46	0	2,3,3	5.69	2 (100%)
4	DGZ	D	615	3	78,78,78	0.90	1 (1%)	98,101,101	2.04	3 (3%)
4	DGZ	H	615	3	78,78,78	0.92	1 (1%)	98,101,101	1.91	2 (2%)
4	DGZ	B	615	3	78,78,78	0.90	1 (1%)	98,101,101	2.03	2 (2%)
5	SO4	D	616	-	4,4,4	0.19	0	6,6,6	0.07	0
5	SO4	I	616	-	4,4,4	0.46	0	6,6,6	0.13	0
4	DGZ	K	615	3	78,78,78	0.91	1 (1%)	98,101,101	2.04	2 (2%)
4	DGZ	A	615	3	78,78,78	0.92	1 (1%)	98,101,101	1.99	3 (3%)
4	DGZ	G	615	3	78,78,78	0.88	1 (1%)	98,101,101	1.99	3 (3%)
4	DGZ	J	615	3	78,78,78	0.91	1 (1%)	98,101,101	2.01	4 (4%)
6	1PE	G	620	-	8,8,15	2.20	4 (50%)	7,7,14	2.58	4 (57%)
6	1PE	D	621	-	4,4,15	2.92	4 (100%)	3,3,14	1.89	1 (33%)
6	1PE	G	623	-	14,14,15	3.20	7 (50%)	13,13,14	3.39	7 (53%)
6	1PE	D	619	-	7,7,15	2.31	2 (28%)	6,6,14	2.30	3 (50%)
5	SO4	I	620	-	4,4,4	0.97	0	6,6,6	0.31	0
5	SO4	H	618	-	4,4,4	0.99	0	6,6,6	0.32	0
5	SO4	I	619	-	4,4,4	0.35	0	6,6,6	0.12	0
6	1PE	F	616	-	9,9,15	2.57	5 (55%)	8,8,14	2.93	4 (50%)
5	SO4	C	618	-	4,4,4	0.20	0	6,6,6	0.17	0
6	1PE	E	619	-	11,11,15	2.45	4 (36%)	10,10,14	3.09	6 (60%)
6	1PE	L	619	-	6,6,15	1.88	1 (16%)	5,5,14	2.23	2 (40%)
5	SO4	E	617	-	4,4,4	0.47	0	6,6,6	0.13	0
5	SO4	G	618	-	4,4,4	0.24	0	6,6,6	0.21	0
6	1PE	D	620	-	10,10,15	2.27	5 (50%)	9,9,14	2.84	4 (44%)
6	1PE	A	619	-	6,6,15	1.68	1 (16%)	5,5,14	2.34	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	H	616	-	4,4,4	0.17	0	6,6,6	0.35	0
6	1PE	C	622	-	8,8,15	2.44	3 (37%)	7,7,14	3.14	3 (42%)
5	SO4	E	618	-	4,4,4	0.84	0	6,6,6	0.32	0
4	DGZ	I	615	3	78,78,78	0.92	1 (1%)	98,101,101	2.03	3 (3%)
6	1PE	I	621	-	11,11,15	2.39	4 (36%)	10,10,14	2.99	5 (50%)
5	SO4	A	617	-	4,4,4	0.61	0	6,6,6	0.21	0
6	1PE	J	619	-	10,10,15	2.57	5 (50%)	9,9,14	2.14	5 (55%)
5	SO4	C	617	-	4,4,4	0.34	0	6,6,6	0.09	0
4	DGZ	L	615	3	78,78,78	0.91	1 (1%)	98,101,101	2.01	3 (3%)
7	2PE	H	619	-	24,24,27	0.75	0	23,23,26	0.67	0
5	SO4	K	616	-	4,4,4	0.33	0	6,6,6	0.18	0
6	1PE	K	618	-	11,11,15	2.16	4 (36%)	10,10,14	3.04	4 (40%)
2	CO3	K	612	-	3,3,3	0.79	0	2,3,3	12.63	2 (100%)
2	CO3	E	612	-	3,3,3	1.70	1 (33%)	2,3,3	6.65	2 (100%)

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
4	DGZ	J	615	3	-	14/75/76/76	0/5/5/5
6	1PE	K	619	-	-	3/8/8/13	-
6	1PE	G	620	-	-	3/6/6/13	-
4	DGZ	F	615	3	-	20/75/76/76	0/5/5/5
6	1PE	F	617	-	-	4/7/7/13	-
6	1PE	K	617	-	-	3/5/5/13	-
6	1PE	D	621	-	-	2/2/2/13	-
6	1PE	G	623	-	-	7/12/12/13	-
6	1PE	E	621	-	-	2/5/5/13	-
6	1PE	D	619	-	-	1/5/5/13	-
6	1PE	L	620	-	-	5/8/8/13	-
4	DGZ	C	615	3	-	20/75/76/76	0/5/5/5
4	DGZ	E	615	3	-	21/75/76/76	0/5/5/5
6	1PE	F	616	-	-	6/7/7/13	-
6	1PE	K	620	-	-	3/3/3/13	-
6	1PE	E	619	-	-	5/9/9/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	L	619	-	-	3/4/4/13	-
4	DGZ	G	615	3	-	21/75/76/76	0/5/5/5
6	1PE	E	620	-	-	2/7/7/13	-
6	1PE	G	622	-	-	3/3/3/13	-
6	1PE	K	618	-	-	6/9/9/13	-
6	1PE	J	622	-	-	5/6/6/13	-
6	1PE	D	620	-	-	4/8/8/13	-
6	1PE	G	621	-	-	1/3/3/13	-
6	1PE	L	617	-	-	4/7/7/13	-
4	DGZ	D	615	3	-	11/75/76/76	0/5/5/5
6	1PE	A	619	-	-	1/4/4/13	-
4	DGZ	H	615	3	-	19/75/76/76	0/5/5/5
6	1PE	I	622	-	-	2/7/7/13	-
7	2PE	B	616	-	-	9/23/23/25	-
6	1PE	C	622	-	-	4/6/6/13	-
6	1PE	J	621	-	-	4/8/8/13	-
6	1PE	J	620	-	-	6/7/7/13	-
4	DGZ	I	615	3	-	19/75/76/76	0/5/5/5
6	1PE	I	621	-	-	4/9/9/13	-
6	1PE	J	619	-	-	6/8/8/13	-
4	DGZ	B	615	3	-	14/75/76/76	0/5/5/5
4	DGZ	L	615	3	-	17/75/76/76	0/5/5/5
7	2PE	H	619	-	-	13/22/22/25	-
6	1PE	C	621	-	-	5/9/9/13	-
4	DGZ	K	615	3	-	21/75/76/76	0/5/5/5
4	DGZ	A	615	3	-	25/75/76/76	0/5/5/5
6	1PE	F	618	-	-	4/7/7/13	-
6	1PE	D	618	-	-	4/7/7/13	-
6	1PE	L	618	-	-	5/9/9/13	-
6	1PE	I	623	-	-	1/2/2/13	-
6	1PE	A	618	-	-	0/6/6/13	-

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	612	CO3	O1-C	8.48	1.54	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	612	CO3	O1-C	7.61	1.51	1.25
2	L	612	CO3	O1-C	7.33	1.51	1.25
2	C	612	CO3	O1-C	6.66	1.48	1.25
2	F	612	CO3	O1-C	6.59	1.48	1.25
2	D	612	CO3	O1-C	6.39	1.47	1.25
6	G	623	1PE	C26-C16	5.08	1.76	1.49
4	K	615	DGZ	C2-C1	5.02	1.32	1.18
4	J	615	DGZ	C2-C1	4.99	1.32	1.18
4	H	615	DGZ	C2-C1	4.97	1.32	1.18
4	A	615	DGZ	C2-C1	4.97	1.32	1.18
6	G	623	1PE	OH4-C13	4.96	1.63	1.42
4	L	615	DGZ	C2-C1	4.96	1.32	1.18
4	D	615	DGZ	C2-C1	4.95	1.32	1.18
4	E	615	DGZ	C2-C1	4.94	1.32	1.18
4	G	615	DGZ	C2-C1	4.94	1.32	1.18
4	F	615	DGZ	C2-C1	4.94	1.32	1.18
4	B	615	DGZ	C2-C1	4.92	1.32	1.18
6	L	620	1PE	C26-C16	4.91	1.75	1.49
4	I	615	DGZ	C2-C1	4.89	1.32	1.18
4	C	615	DGZ	C2-C1	4.85	1.32	1.18
6	F	618	1PE	C26-C16	4.79	1.74	1.49
6	G	623	1PE	OH6-C26	4.77	1.62	1.42
6	F	618	1PE	OH6-C26	4.66	1.62	1.42
6	J	622	1PE	OH4-C13	4.63	1.62	1.42
6	D	618	1PE	OH4-C13	4.56	1.61	1.42
6	L	620	1PE	OH6-C26	4.55	1.61	1.42
6	C	622	1PE	OH4-C13	4.54	1.61	1.42
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	J	620	1PE	C26-C16	4.36	1.72	1.49
6	E	619	1PE	OH4-C13	4.34	1.60	1.42
6	K	619	1PE	OH6-C26	4.21	1.62	1.42
6	F	617	1PE	C26-C16	4.18	1.71	1.49
6	J	619	1PE	OH4-C13	4.16	1.62	1.42
6	L	620	1PE	OH4-C13	4.13	1.62	1.42
6	D	619	1PE	OH6-C26	4.12	1.62	1.42
6	E	621	1PE	OH4-C13	4.04	1.59	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	616	1PE	C26-C16	4.01	1.70	1.49
6	K	620	1PE	OH4-C13	4.00	1.61	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	J	620	1PE	OH6-C26	3.98	1.59	1.42
6	F	618	1PE	OH7-C16	3.89	1.61	1.42
6	K	617	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	G	623	1PE	OH7-C16	3.84	1.61	1.42
6	G	623	1PE	C23-C13	3.82	1.68	1.49
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	D	621	1PE	OH6-C15	3.77	1.60	1.42
6	F	618	1PE	OH6-C15	3.76	1.58	1.42
6	L	617	1PE	C26-C16	3.71	1.69	1.49
6	D	620	1PE	C16-C26	3.67	1.73	1.47
6	J	621	1PE	C16-C26	3.63	1.73	1.47
6	L	620	1PE	OH7-C16	3.63	1.60	1.42
6	J	619	1PE	OH7-C16	3.60	1.60	1.42
6	J	619	1PE	C26-C16	3.57	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	3.43	1.57	1.42
6	J	620	1PE	OH7-C16	3.42	1.59	1.42
6	F	617	1PE	OH7-C16	3.39	1.59	1.42
6	E	619	1PE	OH6-C15	3.37	1.59	1.42
6	L	619	1PE	OH6-C15	3.36	1.59	1.42
6	I	621	1PE	OH3-C23	3.34	1.56	1.42
6	C	621	1PE	C23-C13	3.33	1.65	1.49
6	F	616	1PE	OH7-C16	3.29	1.58	1.42
6	L	617	1PE	OH6-C26	3.26	1.56	1.42
6	G	621	1PE	OH6-C15	3.26	1.58	1.42
6	L	618	1PE	OH6-C15	3.26	1.58	1.42
6	C	622	1PE	OH3-C23	3.22	1.56	1.42
6	L	620	1PE	OH6-C15	3.22	1.56	1.42
6	E	619	1PE	C23-C13	3.18	1.65	1.49
6	E	621	1PE	C13-C23	3.17	1.66	1.49
6	K	617	1PE	OH6-C15	3.15	1.58	1.42
6	L	617	1PE	OH7-C16	3.14	1.58	1.42
6	E	619	1PE	OH3-C23	3.13	1.55	1.42
6	C	621	1PE	OH6-C15	3.10	1.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	621	1PE	C23-C13	3.07	1.64	1.49
6	G	620	1PE	C23-C13	3.05	1.64	1.49
6	I	621	1PE	OH6-C15	3.04	1.57	1.42
6	A	619	1PE	OH6-C15	3.03	1.57	1.42
6	C	622	1PE	C23-C13	3.03	1.64	1.49
6	K	618	1PE	OH3-C23	3.00	1.55	1.42
6	D	619	1PE	OH6-C15	3.00	1.57	1.40
6	I	622	1PE	C23-C13	2.98	1.64	1.49
6	K	619	1PE	OH6-C15	2.98	1.57	1.40
6	E	620	1PE	OH3-C23	2.96	1.57	1.42
6	J	620	1PE	OH6-C15	2.96	1.54	1.42
6	F	617	1PE	OH6-C15	2.93	1.54	1.42
6	J	621	1PE	C23-C13	2.91	1.67	1.47
6	L	618	1PE	C23-C13	2.90	1.63	1.49
6	A	618	1PE	C23-C13	2.90	1.63	1.49
6	D	618	1PE	C23-C13	2.89	1.63	1.49
2	E	612	CO3	O1-C	2.88	1.35	1.25
6	K	619	1PE	C13-C23	2.87	1.64	1.49
6	G	622	1PE	OH6-C15	2.87	1.56	1.42
6	D	618	1PE	OH3-C23	2.87	1.54	1.42
6	K	618	1PE	C23-C13	2.84	1.63	1.49
6	L	618	1PE	OH3-C23	2.80	1.54	1.42
6	C	621	1PE	OH3-C23	2.79	1.54	1.42
6	E	620	1PE	C13-C23	2.79	1.64	1.49
6	D	621	1PE	C26-C16	2.71	1.63	1.49
6	J	622	1PE	C13-C23	2.64	1.63	1.49
6	I	622	1PE	OH3-C23	2.62	1.55	1.40
6	D	621	1PE	OH7-C16	2.60	1.55	1.42
6	F	616	1PE	OH6-C15	2.59	1.53	1.42
6	K	618	1PE	OH6-C15	2.58	1.55	1.42
6	K	619	1PE	OH3-C23	2.54	1.55	1.42
2	C	612	CO3	O3-C	-2.53	1.11	1.33
6	J	621	1PE	OH4-C13	2.48	1.62	1.42
6	E	620	1PE	OH6-C15	2.46	1.54	1.42
6	D	620	1PE	C23-C13	2.46	1.64	1.47
6	J	620	1PE	OH5-C14	2.45	1.52	1.42
6	D	621	1PE	OH6-C26	2.42	1.54	1.40
6	G	620	1PE	OH3-C23	2.42	1.54	1.40
6	I	622	1PE	OH3-C22	2.38	1.53	1.42
6	L	617	1PE	OH6-C15	2.37	1.52	1.42
6	J	622	1PE	OH3-C23	2.37	1.54	1.42
2	H	612	CO3	O1-C	2.34	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	612	CO3	O2-C	2.26	1.52	1.33
6	D	620	1PE	OH4-C13	2.26	1.61	1.42
6	I	623	1PE	OH4-C24	2.25	1.53	1.42
6	J	619	1PE	OH6-C15	2.21	1.51	1.42
2	D	612	CO3	O3-C	-2.21	1.14	1.33
6	F	618	1PE	C25-C15	2.20	1.60	1.49
6	E	621	1PE	OH3-C23	2.19	1.53	1.42
6	K	617	1PE	OH5-C25	2.18	1.51	1.42
6	G	620	1PE	OH3-C22	2.14	1.52	1.42
6	D	620	1PE	OH6-C26	2.12	1.59	1.42
2	A	612	CO3	O3-C	-2.08	1.15	1.33
6	J	621	1PE	OH6-C26	2.07	1.59	1.42
2	L	612	CO3	O3-C	-2.05	1.16	1.33
6	F	616	1PE	OH4-C24	2.04	1.52	1.42

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	615	DGZ	C3-C2-C1	-18.24	119.55	177.02
4	F	615	DGZ	C3-C2-C1	-18.21	119.64	177.02
4	D	615	DGZ	C3-C2-C1	-18.15	119.86	177.02
4	I	615	DGZ	C3-C2-C1	-18.09	120.03	177.02
4	E	615	DGZ	C3-C2-C1	-18.07	120.11	177.02
4	B	615	DGZ	C3-C2-C1	-17.95	120.48	177.02
4	L	615	DGZ	C3-C2-C1	-17.93	120.53	177.02
4	A	615	DGZ	C3-C2-C1	-17.86	120.77	177.02
4	J	615	DGZ	C3-C2-C1	-17.85	120.78	177.02
4	K	615	DGZ	C3-C2-C1	-17.85	120.80	177.02
4	G	615	DGZ	C3-C2-C1	-17.83	120.87	177.02
4	H	615	DGZ	C3-C2-C1	-17.77	121.05	177.02
2	K	612	CO3	O2-C-O1	-15.93	78.93	119.68
2	A	612	CO3	O3-C-O1	-11.44	90.42	119.68
2	B	612	CO3	O3-C-O1	-10.47	92.90	119.68
2	J	612	CO3	O3-C-O1	9.07	142.87	119.68
2	I	612	CO3	O2-C-O1	8.13	140.48	119.68
2	K	612	CO3	O3-C-O1	8.08	140.33	119.68
2	D	612	CO3	O3-C-O1	8.00	140.13	119.68
2	C	612	CO3	O3-C-O1	7.65	139.24	119.68
6	G	623	1PE	OH3-C23-C13	7.60	144.99	110.35
6	D	618	1PE	OH3-C23-C13	7.34	143.79	110.35
2	F	612	CO3	O3-C-O1	7.24	138.19	119.68
2	E	612	CO3	O3-C-O1	7.05	137.71	119.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	622	1PE	OH3-C23-C13	7.02	142.35	110.35
6	I	621	1PE	OH3-C23-C13	6.94	141.99	110.35
2	L	612	CO3	O3-C-O1	6.63	136.64	119.68
6	K	618	1PE	OH3-C23-C13	6.54	140.15	110.35
2	H	612	CO3	O2-C-O1	6.47	136.23	119.68
2	G	612	CO3	O2-C-O1	6.47	136.22	119.68
2	E	612	CO3	O2-C-O1	-6.21	103.78	119.68
6	L	618	1PE	OH3-C23-C13	6.12	138.25	110.35
6	F	618	1PE	OH6-C15-C25	6.09	138.12	110.35
6	E	619	1PE	OH3-C23-C13	5.87	137.09	110.35
6	C	621	1PE	OH3-C23-C13	5.83	136.91	110.35
6	J	621	1PE	OH6-C15-C25	5.62	135.95	110.35
6	A	618	1PE	OH3-C23-C13	5.59	135.81	110.35
6	G	623	1PE	OH6-C15-C25	5.50	135.44	110.35
2	C	612	CO3	O2-C-O1	5.46	133.63	119.68
2	B	612	CO3	O2-C-O1	5.43	133.58	119.68
2	H	612	CO3	O3-C-O1	-5.35	105.98	119.68
6	J	620	1PE	OH6-C15-C25	5.28	134.40	110.35
6	F	616	1PE	OH6-C15-C25	5.26	134.34	110.35
6	D	620	1PE	C13-OH4-C24	5.20	131.31	113.06
6	K	619	1PE	OH3-C23-C13	5.18	142.32	111.82
6	G	621	1PE	C14-OH5-C25	5.14	131.08	113.06
6	J	622	1PE	C25-OH5-C14	5.06	130.80	113.06
6	F	617	1PE	OH6-C15-C25	5.05	133.37	110.35
6	E	620	1PE	C24-OH4-C13	4.95	134.91	113.26
2	G	612	CO3	O3-C-O1	-4.79	107.42	119.68
6	J	622	1PE	OH3-C23-C13	4.78	139.98	111.82
6	D	620	1PE	OH6-C15-C25	4.62	131.39	110.35
6	L	618	1PE	C24-OH4-C13	4.57	133.27	113.26
6	J	621	1PE	C25-OH5-C14	4.44	132.68	113.26
6	L	619	1PE	OH6-C15-C25	4.43	137.90	111.82
6	G	622	1PE	OH6-C15-C25	4.37	137.57	111.82
6	E	621	1PE	OH3-C23-C13	4.36	137.47	111.82
6	E	619	1PE	C24-OH4-C13	4.34	132.27	113.26
6	G	623	1PE	C24-OH4-C13	4.33	132.20	113.26
6	J	620	1PE	C25-OH5-C14	4.27	131.95	113.26
6	G	623	1PE	OH7-C16-C26	4.21	136.59	111.82
6	G	622	1PE	C14-OH5-C25	4.18	127.73	113.06
4	J	615	DGZ	O9-C48-C49	4.10	118.08	109.64
6	I	622	1PE	C25-OH5-C14	4.08	127.38	113.06
6	A	618	1PE	C24-OH4-C13	4.07	131.06	113.26
6	E	620	1PE	OH3-C23-C13	4.05	135.65	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	617	1PE	OH6-C26-C16	4.03	127.89	110.11
6	D	619	1PE	C25-OH5-C14	4.01	130.80	113.26
6	L	620	1PE	OH7-C16-C26	4.00	135.36	111.82
6	L	618	1PE	OH6-C15-C25	3.99	135.30	111.82
4	K	615	DGZ	O9-C48-C49	3.98	117.83	109.64
6	G	620	1PE	OH3-C23-C13	3.97	140.05	111.00
6	C	621	1PE	C25-OH5-C14	3.95	130.55	113.26
6	K	618	1PE	C24-OH4-C13	3.94	130.51	113.26
6	L	620	1PE	C25-OH5-C14	3.94	130.50	113.26
4	D	615	DGZ	O9-C48-C49	3.93	117.73	109.64
6	F	616	1PE	C25-OH5-C14	3.91	130.37	113.26
6	K	617	1PE	OH6-C15-C25	3.87	134.62	111.82
6	L	620	1PE	OH6-C15-C25	3.86	127.96	110.35
2	A	612	CO3	O2-C-O1	3.86	129.55	119.68
6	C	621	1PE	C24-OH4-C13	3.84	130.07	113.26
6	F	618	1PE	OH7-C16-C26	3.84	134.42	111.82
6	J	620	1PE	OH7-C16-C26	3.82	134.31	111.82
6	A	619	1PE	OH6-C15-C25	3.73	133.75	111.82
6	K	617	1PE	C25-OH5-C14	3.71	129.50	113.26
6	E	621	1PE	C24-OH4-C13	3.68	129.38	113.26
6	I	622	1PE	OH3-C23-C13	3.66	137.78	111.00
6	F	618	1PE	C25-OH5-C14	3.64	129.21	113.26
6	I	621	1PE	C24-OH4-C13	3.61	129.07	113.26
6	I	621	1PE	OH6-C15-C25	3.57	132.85	111.82
6	F	618	1PE	OH6-C26-C16	3.56	125.80	110.11
6	E	619	1PE	C25-OH5-C14	3.53	128.71	113.26
4	I	615	DGZ	O9-C48-C49	3.50	116.85	109.64
6	K	618	1PE	OH6-C15-C25	3.46	132.21	111.82
6	L	617	1PE	OH6-C15-C25	3.46	126.13	110.35
6	J	619	1PE	OH6-C15-C25	3.41	125.92	110.35
6	A	618	1PE	OH4-C24-C14	-3.39	95.17	110.11
6	C	621	1PE	C22-OH3-C23	3.38	124.92	113.06
6	D	620	1PE	C25-OH5-C14	3.37	128.03	113.26
6	G	620	1PE	OH4-C24-C14	-3.35	95.08	110.35
4	F	615	DGZ	O9-C48-C49	3.34	116.52	109.64
4	B	615	DGZ	O9-C48-C47	-3.33	103.67	110.63
6	F	617	1PE	C25-OH5-C14	3.32	127.80	113.26
4	G	615	DGZ	O9-C48-C49	3.32	116.46	109.64
6	J	622	1PE	C24-OH4-C13	3.29	127.66	113.26
6	J	621	1PE	C13-OH4-C24	3.28	124.57	113.06
4	C	615	DGZ	O9-C48-C49	3.27	116.38	109.64
6	A	619	1PE	C25-OH5-C14	3.24	127.45	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	619	1PE	C24-OH4-C13	3.24	127.42	113.26
6	L	618	1PE	OH4-C24-C14	-3.18	95.88	110.35
6	L	618	1PE	C22-OH3-C23	3.17	124.18	113.06
6	G	620	1PE	C24-OH4-C13	3.17	127.12	113.26
6	G	623	1PE	C25-OH5-C14	3.16	127.09	113.26
6	D	619	1PE	OH6-C15-C25	3.16	134.10	111.00
6	F	616	1PE	OH7-C16-C26	3.15	130.35	111.82
6	J	620	1PE	OH6-C26-C16	3.14	123.94	110.11
6	K	619	1PE	C25-OH5-C14	3.13	126.98	113.26
4	L	615	DGZ	O9-C48-C49	3.13	116.08	109.64
6	K	620	1PE	C25-OH5-C14	3.12	131.72	112.90
6	C	621	1PE	OH6-C15-C25	3.09	129.99	111.82
6	C	622	1PE	C24-OH4-C13	3.06	126.64	113.26
6	I	622	1PE	C24-OH4-C13	2.99	126.36	113.26
6	F	617	1PE	OH7-C16-C26	2.99	129.40	111.82
6	E	619	1PE	OH6-C15-C25	2.98	129.38	111.82
6	D	621	1PE	OH7-C16-C26	2.98	129.34	111.82
6	E	620	1PE	OH4-C24-C14	-2.95	96.89	110.35
6	K	619	1PE	OH6-C15-C25	2.93	132.42	111.00
6	K	618	1PE	C25-OH5-C14	2.91	126.00	113.26
6	F	616	1PE	OH6-C26-C16	2.89	122.87	110.11
6	K	617	1PE	C13-OH4-C24	2.87	130.22	112.90
6	J	619	1PE	OH4-C24-C14	-2.82	90.33	111.00
6	G	620	1PE	C25-OH5-C14	2.81	129.83	112.90
2	J	612	CO3	O2-C-O1	2.79	126.80	119.68
6	E	619	1PE	OH4-C24-C14	-2.78	97.68	110.35
6	J	619	1PE	OH7-C16-C26	2.73	127.89	111.82
4	A	615	DGZ	O9-C48-C49	2.71	115.22	109.64
6	L	618	1PE	C25-OH5-C14	2.69	125.03	113.26
4	D	615	DGZ	C12-C13-N3	2.67	118.32	111.11
6	L	617	1PE	OH7-C16-C26	2.66	127.47	111.82
6	D	618	1PE	OH4-C24-C14	-2.64	98.31	110.35
6	C	622	1PE	OH4-C24-C14	-2.63	98.54	110.11
6	E	620	1PE	C25-OH5-C14	2.62	124.71	113.26
6	G	621	1PE	OH6-C15-C25	2.58	127.02	111.82
4	H	615	DGZ	O9-C48-C49	2.58	114.95	109.64
6	L	620	1PE	OH6-C26-C16	2.58	121.46	110.11
4	J	615	DGZ	O9-C48-C47	-2.56	105.28	110.63
6	J	619	1PE	C26-OH6-C15	2.54	124.40	113.26
6	I	621	1PE	OH5-C14-C24	2.53	121.89	110.35
6	E	619	1PE	C22-OH3-C23	2.48	121.77	113.06
6	E	620	1PE	OH6-C15-C25	2.39	125.87	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	621	1PE	C25-OH5-C14	2.38	127.25	112.90
4	L	615	DGZ	C13-N3-C28	2.38	127.64	121.68
6	J	619	1PE	C13-OH4-C24	2.37	127.21	112.90
6	E	621	1PE	OH4-C24-C14	-2.35	99.63	110.35
4	I	615	DGZ	C37-C36-C35	-2.34	107.13	113.36
6	L	620	1PE	C13-OH4-C24	2.33	126.97	112.90
4	A	615	DGZ	O9-C48-C47	-2.33	105.76	110.63
6	G	623	1PE	OH4-C24-C14	-2.30	99.88	110.35
6	G	623	1PE	OH6-C26-C16	2.29	120.22	110.11
6	D	618	1PE	C24-OH4-C13	2.26	123.15	113.26
6	K	620	1PE	C13-OH4-C24	2.23	126.33	112.90
4	E	615	DGZ	O9-C48-C49	2.22	114.21	109.64
6	L	619	1PE	C25-OH5-C14	2.21	122.94	113.26
6	E	620	1PE	OH4-C13-C23	-2.18	100.49	110.11
6	I	621	1PE	C25-OH5-C14	2.18	122.82	113.26
6	K	619	1PE	OH4-C24-C14	-2.18	100.41	110.35
6	D	618	1PE	C25-OH5-C14	2.13	125.75	112.90
6	D	620	1PE	C26-OH6-C15	2.12	120.50	113.06
6	F	617	1PE	OH4-C24-C14	-2.11	99.40	111.82
6	L	617	1PE	C25-OH5-C14	2.11	122.49	113.26
4	C	615	DGZ	C37-C36-C35	-2.05	107.91	113.36
6	D	619	1PE	OH4-C24-C14	-2.05	99.78	111.82
4	G	615	DGZ	C37-C36-C35	-2.02	107.97	113.36
4	J	615	DGZ	C57-C11-N2	2.02	115.25	110.30

There are no chirality outliers.

All (362) 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

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Mol	Chain	Res	Type	Atoms
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
4	I	615	DGZ	C2-C3-C4-C5
4	F	615	DGZ	C9-C10-C11-N2
4	L	615	DGZ	C9-C10-C11-N2
4	H	615	DGZ	N1-C7-C8-C9
6	L	620	1PE	OH5-C14-C24-OH4
7	B	616	2PE	O13-C14-C15-O16
6	F	616	1PE	C16-C26-OH6-C15
4	F	615	DGZ	C9-C10-C11-C57
6	L	618	1PE	C15-C25-OH5-C14
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	I	615	DGZ	N1-C7-C8-C9
6	D	621	1PE	OH7-C16-C26-OH6
6	F	617	1PE	OH7-C16-C26-OH6

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

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Mol	Chain	Res	Type	Atoms
6	D	618	1PE	C24-C14-OH5-C25
6	K	620	1PE	OH5-C14-C24-OH4
6	C	622	1PE	C12-C22-OH3-C23
4	K	615	DGZ	C17-C18-C19-C20
6	J	622	1PE	C15-C25-OH5-C14
6	L	618	1PE	OH5-C14-C24-OH4
6	L	618	1PE	C12-C22-OH3-C23
6	F	616	1PE	OH7-C16-C26-OH6
6	L	619	1PE	OH6-C15-C25-OH5
6	I	621	1PE	OH4-C13-C23-OH3
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	L	617	1PE	OH6-C15-C25-OH5
4	I	615	DGZ	C9-C10-C11-C57
6	G	620	1PE	C24-C14-OH5-C25
4	A	615	DGZ	N3-C28-C29-O5
4	B	615	DGZ	N3-C28-C29-O5
4	I	615	DGZ	N3-C28-C29-O5
4	J	615	DGZ	N3-C28-C29-O5
4	K	615	DGZ	N3-C28-C29-O5
4	A	615	DGZ	C11-C10-C9-C8
4	K	615	DGZ	C26-C18-C19-C20
6	C	622	1PE	OH5-C14-C24-OH4
6	F	616	1PE	OH5-C14-C24-OH4
4	A	615	DGZ	O4-C28-C29-O5
4	H	615	DGZ	O4-C28-C29-O5
4	I	615	DGZ	O5-C30-C31-O6
7	B	616	2PE	O4-C5-C6-O7
4	J	615	DGZ	O4-C28-C29-O5
6	L	617	1PE	OH5-C14-C24-OH4
4	E	615	DGZ	C2-C3-C4-C5
4	B	615	DGZ	O4-C28-C29-O5
4	K	615	DGZ	O4-C28-C29-O5
4	C	615	DGZ	N6-C49-C50-C51
4	D	615	DGZ	N6-C49-C50-C51
4	E	615	DGZ	N6-C49-C50-C51

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Mol	Chain	Res	Type	Atoms
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	H	615	DGZ	N3-C28-C29-O5
6	C	621	1PE	OH5-C14-C24-OH4
6	L	620	1PE	OH6-C15-C25-OH5
4	C	615	DGZ	N3-C28-C29-O5
4	G	615	DGZ	N3-C28-C29-O5
6	J	622	1PE	OH5-C14-C24-OH4
6	J	621	1PE	OH6-C15-C25-OH5
4	F	615	DGZ	O4-C28-C29-O5
4	I	615	DGZ	O4-C28-C29-O5
4	A	615	DGZ	C17-C18-C19-O3
6	J	619	1PE	OH6-C15-C25-OH5
4	H	615	DGZ	C11-C10-C9-C8
6	I	621	1PE	OH5-C14-C24-OH4
6	G	620	1PE	C23-C13-OH4-C24
4	I	615	DGZ	C9-C10-C11-N2
4	C	615	DGZ	O4-C28-C29-O5
4	G	615	DGZ	O4-C28-C29-O5
4	I	615	DGZ	C3-C4-C5-C6
4	A	615	DGZ	C17-C18-C19-C20
6	F	618	1PE	OH6-C15-C25-OH5
4	F	615	DGZ	N3-C28-C29-O5
6	D	620	1PE	OH6-C15-C25-OH5
4	A	615	DGZ	C26-C18-C19-O3
7	B	616	2PE	O10-C11-C12-O13
6	E	619	1PE	C12-C22-OH3-C23
6	G	622	1PE	OH6-C15-C25-OH5
4	A	615	DGZ	O6-C32-C33-N4
4	A	615	DGZ	C26-C18-C19-C20
4	J	615	DGZ	C11-C10-C9-C8
6	J	621	1PE	C23-C13-OH4-C24
6	I	622	1PE	OH4-C13-C23-OH3
6	L	619	1PE	OH5-C14-C24-OH4
4	J	615	DGZ	O5-C30-C31-O6
4	H	615	DGZ	C26-C18-C19-O3
4	E	615	DGZ	C11-C10-C9-C8
6	J	621	1PE	C16-C26-OH6-C15
6	L	620	1PE	C14-C24-OH4-C13

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Mol	Chain	Res	Type	Atoms
6	D	621	1PE	C16-C26-OH6-C15
6	K	619	1PE	C25-C15-OH6-C26
6	E	619	1PE	OH6-C15-C25-OH5
4	H	615	DGZ	C2-C3-C4-C5
4	H	615	DGZ	C26-C18-C19-C20
6	K	617	1PE	C15-C25-OH5-C14
6	E	620	1PE	OH4-C13-C23-OH3
6	D	618	1PE	C13-C23-OH3-C22
4	I	615	DGZ	C30-C31-O6-C32
6	G	622	1PE	C15-C25-OH5-C14
4	F	615	DGZ	O5-C30-C31-O6
6	L	617	1PE	C16-C26-OH6-C15
4	D	615	DGZ	C30-C31-O6-C32
7	H	619	2PE	C9-C8-O7-C6
6	F	618	1PE	C15-C25-OH5-C14
7	H	619	2PE	C18-C17-O16-C15
4	G	615	DGZ	C26-C18-C19-O3
6	E	620	1PE	C23-C13-OH4-C24
6	J	620	1PE	C16-C26-OH6-C15
6	J	622	1PE	C24-C14-OH5-C25
7	H	619	2PE	C24-C23-O22-C21
4	H	615	DGZ	C31-C30-O5-C29
7	H	619	2PE	C15-C14-O13-C12
6	F	616	1PE	C24-C14-OH5-C25
6	J	619	1PE	C24-C14-OH5-C25
6	E	619	1PE	C24-C14-OH5-C25
6	K	618	1PE	C23-C13-OH4-C24
4	C	615	DGZ	C30-C31-O6-C32
4	A	615	DGZ	N6-C49-C50-C51
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-O3
6	G	621	1PE	OH6-C15-C25-OH5
6	L	617	1PE	OH7-C16-C26-OH6
4	G	615	DGZ	C30-C31-O6-C32
4	L	615	DGZ	C33-C32-O6-C31
7	B	616	2PE	C14-C15-O16-C17
4	G	615	DGZ	C33-C32-O6-C31
4	C	615	DGZ	C26-C18-C19-O3
7	H	619	2PE	C12-C11-O10-C9
4	A	615	DGZ	C33-C32-O6-C31

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Mol	Chain	Res	Type	Atoms
4	C	615	DGZ	C33-C32-O6-C31
4	F	615	DGZ	C48-C49-C50-C51
4	K	615	DGZ	C48-C49-C50-C51
4	D	615	DGZ	C35-C36-C37-C38
4	L	615	DGZ	C11-C10-C9-C8
6	F	618	1PE	C25-C15-OH6-C26
4	H	615	DGZ	C17-C18-C19-C20
4	L	615	DGZ	C30-C31-O6-C32
4	G	615	DGZ	C26-C18-C19-C20
6	L	620	1PE	C24-C14-OH5-C25
4	E	615	DGZ	C33-C32-O6-C31
4	C	615	DGZ	C26-C18-C19-C20
6	C	621	1PE	OH6-C15-C25-OH5
6	J	622	1PE	OH4-C13-C23-OH3
6	G	623	1PE	C23-C13-OH4-C24
6	J	619	1PE	C25-C15-OH6-C26
4	D	615	DGZ	C33-C32-O6-C31
4	I	615	DGZ	C33-C32-O6-C31
6	F	617	1PE	C24-C14-OH5-C25
4	A	615	DGZ	C47-C48-C49-C50
4	B	615	DGZ	C47-C48-C49-C50
4	C	615	DGZ	C47-C48-C49-C50
4	E	615	DGZ	C47-C48-C49-C50
4	F	615	DGZ	C47-C48-C49-C50
4	G	615	DGZ	C47-C48-C49-C50
4	H	615	DGZ	C47-C48-C49-C50
4	J	615	DGZ	C47-C48-C49-C50
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	F	615	DGZ	C26-C18-C19-O3
6	E	621	1PE	C23-C13-OH4-C24
4	F	615	DGZ	C26-C18-C19-C20
4	K	615	DGZ	C33-C32-O6-C31
6	J	619	1PE	C14-C24-OH4-C13
4	I	615	DGZ	C35-C36-C37-C38
6	J	620	1PE	C24-C14-OH5-C25
4	K	615	DGZ	C30-C31-O6-C32
6	K	620	1PE	C24-C14-OH5-C25
4	D	615	DGZ	C35-C36-C37-C46
6	K	620	1PE	C14-C24-OH4-C13
6	L	618	1PE	C14-C24-OH4-C13

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Mol	Chain	Res	Type	Atoms
4	E	615	DGZ	C26-C18-C19-C20
4	E	615	DGZ	C26-C18-C19-O3
4	A	615	DGZ	C30-C31-O6-C32
6	G	623	1PE	C15-C25-OH5-C14
6	G	622	1PE	C24-C14-OH5-C25
4	F	615	DGZ	C31-C30-O5-C29
6	J	620	1PE	C15-C25-OH5-C14
7	B	616	2PE	C18-C17-O16-C15
4	C	615	DGZ	C17-C18-C19-O3
4	G	615	DGZ	C17-C18-C19-O3
6	K	618	1PE	C12-C22-OH3-C23
6	A	619	1PE	OH6-C15-C25-OH5
4	F	615	DGZ	C17-C18-C19-O3
6	F	616	1PE	C15-C25-OH5-C14
6	C	621	1PE	C23-C13-OH4-C24
4	C	615	DGZ	C17-C18-C19-C20
6	I	623	1PE	C24-C14-OH5-C25
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	C	621	1PE	C12-C22-OH3-C23
4	F	615	DGZ	C17-C18-C19-C20
4	A	615	DGZ	C31-C30-O5-C29
4	D	615	DGZ	C28-C29-O5-C30
4	K	615	DGZ	C28-C29-O5-C30
4	H	615	DGZ	C3-C4-C5-C6
6	C	621	1PE	C24-C14-OH5-C25
4	G	615	DGZ	C17-C18-C19-C20
4	J	615	DGZ	N1-C7-C8-C9
7	H	619	2PE	C14-C15-O16-C17
7	B	616	2PE	C2-C3-O4-C5
4	H	615	DGZ	C33-C32-O6-C31
6	D	620	1PE	C15-C25-OH5-C14
6	D	618	1PE	C12-C22-OH3-C23
4	D	615	DGZ	C2-C3-C4-C5
6	E	619	1PE	C23-C13-OH4-C24
6	E	619	1PE	C13-C23-OH3-C22
4	C	615	DGZ	C11-C10-C9-C8
6	F	617	1PE	C25-C15-OH6-C26

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Mol	Chain	Res	Type	Atoms
4	C	615	DGZ	C35-C36-C37-C38
4	E	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-O3
4	E	615	DGZ	C17-C18-C19-C20
4	E	615	DGZ	C28-C29-O5-C30
4	K	615	DGZ	C11-C10-C9-C8
4	K	615	DGZ	C2-C3-C4-C5
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	F	615	DGZ	C33-C32-O6-C31
6	D	620	1PE	C23-C13-OH4-C24
4	L	615	DGZ	C26-C18-C19-O3
4	L	615	DGZ	C26-C18-C19-C20
4	A	615	DGZ	C35-C36-C37-C46
4	E	615	DGZ	C31-C30-O5-C29
4	A	615	DGZ	C7-C8-C9-C10
4	I	615	DGZ	C26-C18-C19-C20
6	D	618	1PE	OH5-C14-C24-OH4
4	J	615	DGZ	C33-C32-O6-C31
6	D	619	1PE	C15-C25-OH5-C14
6	F	617	1PE	OH6-C15-C25-OH5
4	K	615	DGZ	C35-C36-C37-C38
6	K	618	1PE	C15-C25-OH5-C14
4	D	615	DGZ	C48-C49-C50-C51
4	I	615	DGZ	C48-C49-C50-C51
6	I	621	1PE	C14-C24-OH4-C13
6	I	622	1PE	C23-C13-OH4-C24
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	G	615	DGZ	C11-C10-C9-C8
7	B	616	2PE	C11-C12-O13-C14
4	K	615	DGZ	C9-C10-C11-C57
6	J	621	1PE	OH5-C14-C24-OH4
4	I	615	DGZ	C11-C10-C9-C8
4	B	615	DGZ	C2-C3-C4-C5
4	A	615	DGZ	O5-C30-C31-O6
4	L	615	DGZ	C35-C36-C37-C46
4	B	615	DGZ	C26-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
7	H	619	2PE	C21-C20-O19-C18
7	H	619	2PE	C11-C12-O13-C14
4	L	615	DGZ	C2-C3-C4-C5
4	B	615	DGZ	C35-C36-C37-C38
4	C	615	DGZ	C35-C36-C37-C46
7	H	619	2PE	O13-C14-C15-O16
6	K	619	1PE	OH6-C15-C25-OH5
4	I	615	DGZ	C12-C13-C14-C15
7	B	616	2PE	C17-C18-O19-C20
4	G	615	DGZ	C35-C36-C37-C46
4	E	615	DGZ	O9-C48-C49-C50
4	K	615	DGZ	O9-C48-C49-C50
7	H	619	2PE	O19-C20-C21-O22

There are no ring outliers.

37 monomers are involved in 124 short contacts:

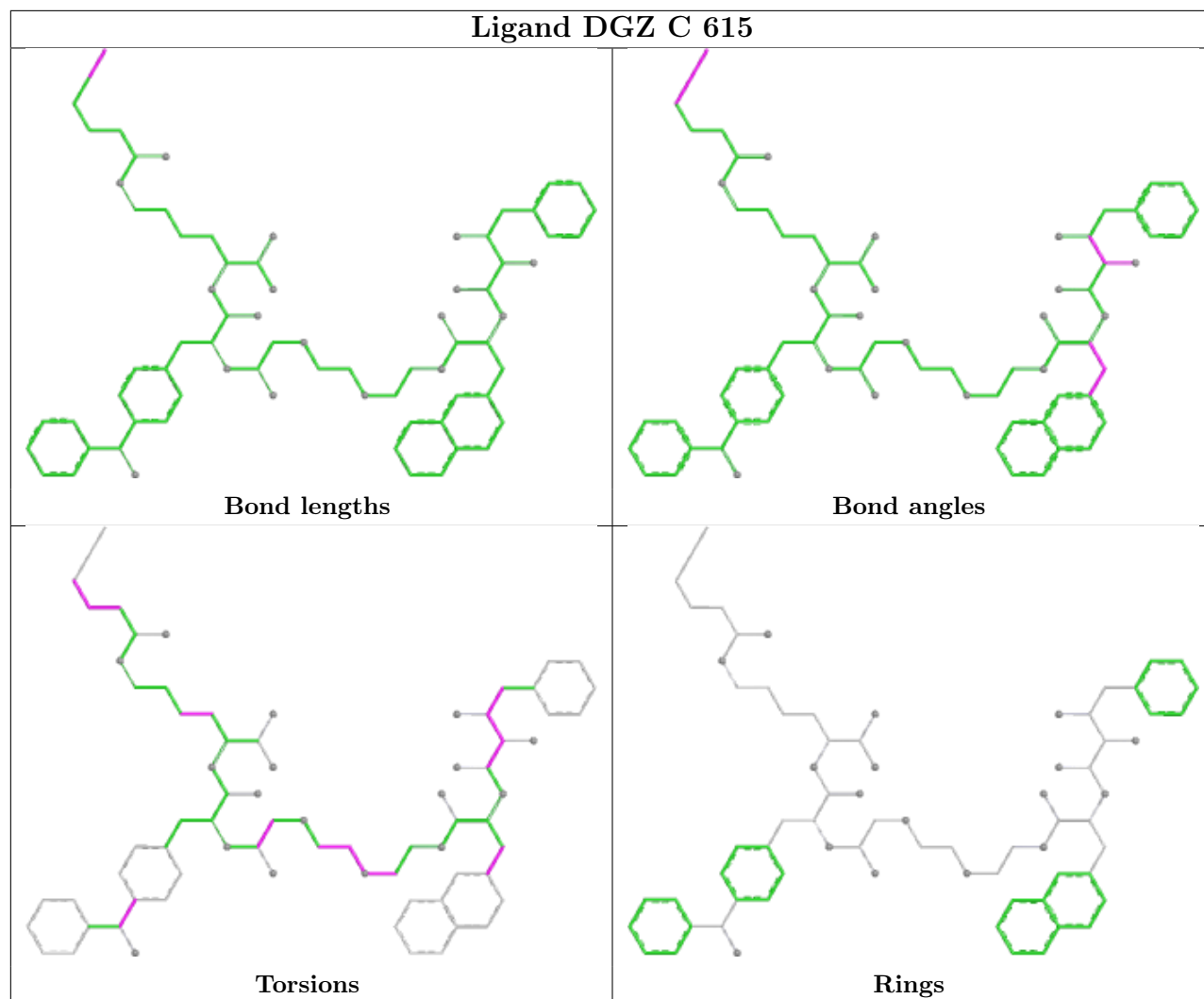
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	617	1PE	1	0
2	J	612	CO3	1	0
4	C	615	DGZ	5	0
4	E	615	DGZ	5	0
6	J	622	1PE	3	0
6	L	617	1PE	2	0
6	J	621	1PE	3	0
6	C	621	1PE	1	0
6	L	618	1PE	3	0
6	I	623	1PE	4	0
2	F	612	CO3	1	0
4	F	615	DGZ	8	0
5	I	618	SO4	1	0
6	J	620	1PE	6	0
6	F	618	1PE	4	0
6	D	618	1PE	1	0
5	G	619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

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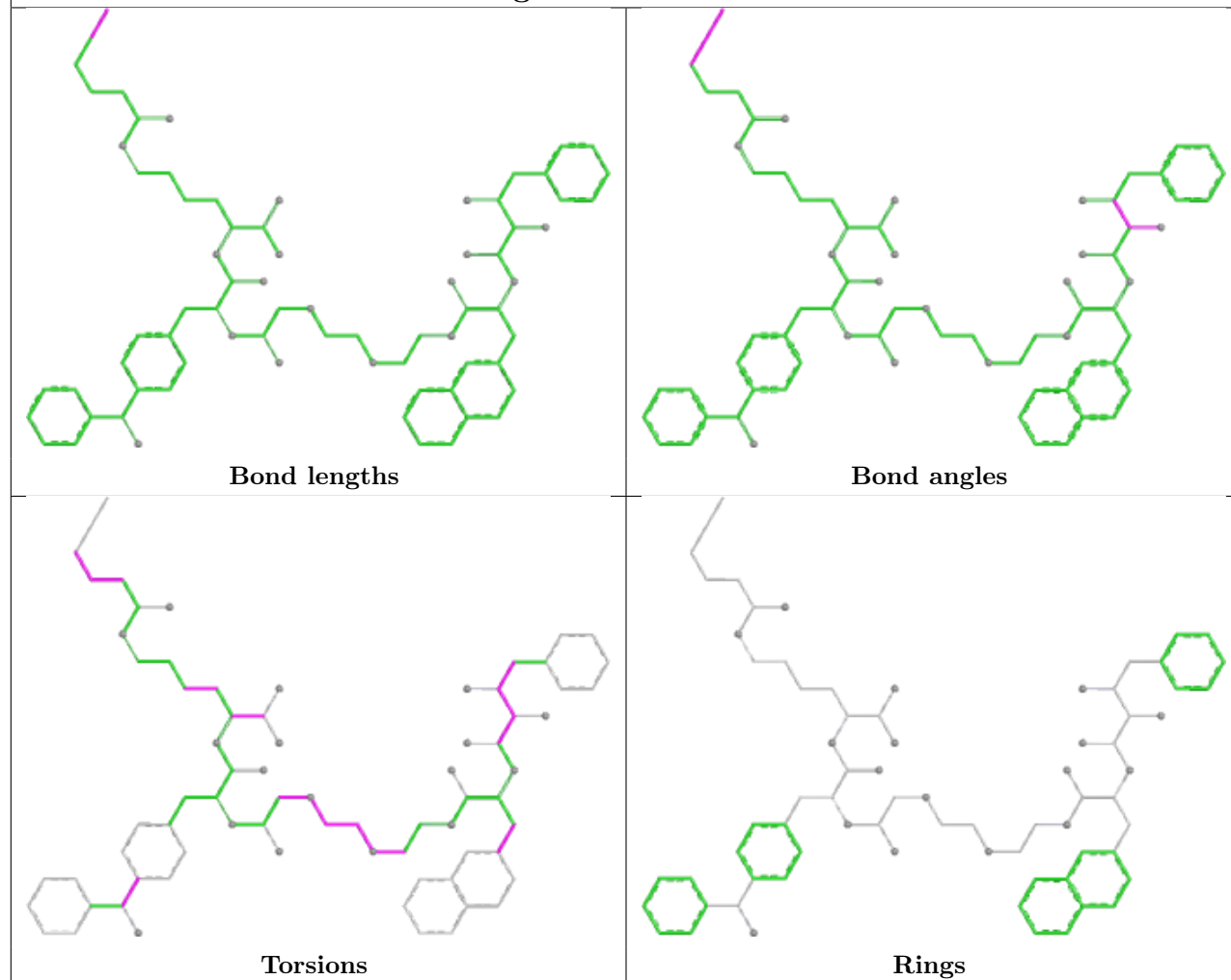
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	615	DGZ	11	0
4	G	615	DGZ	5	0
4	J	615	DGZ	5	0
6	G	623	1PE	7	0
6	E	619	1PE	1	0
6	L	619	1PE	1	0
6	D	620	1PE	2	0
6	C	622	1PE	1	0
4	I	615	DGZ	4	0
6	I	621	1PE	1	0
6	J	619	1PE	1	0
4	L	615	DGZ	7	0
7	H	619	2PE	2	0

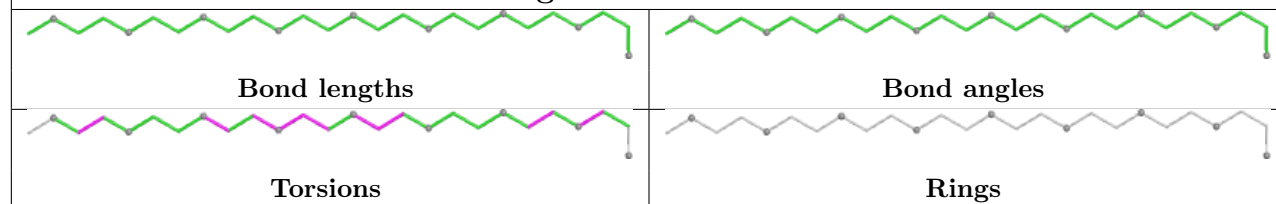
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



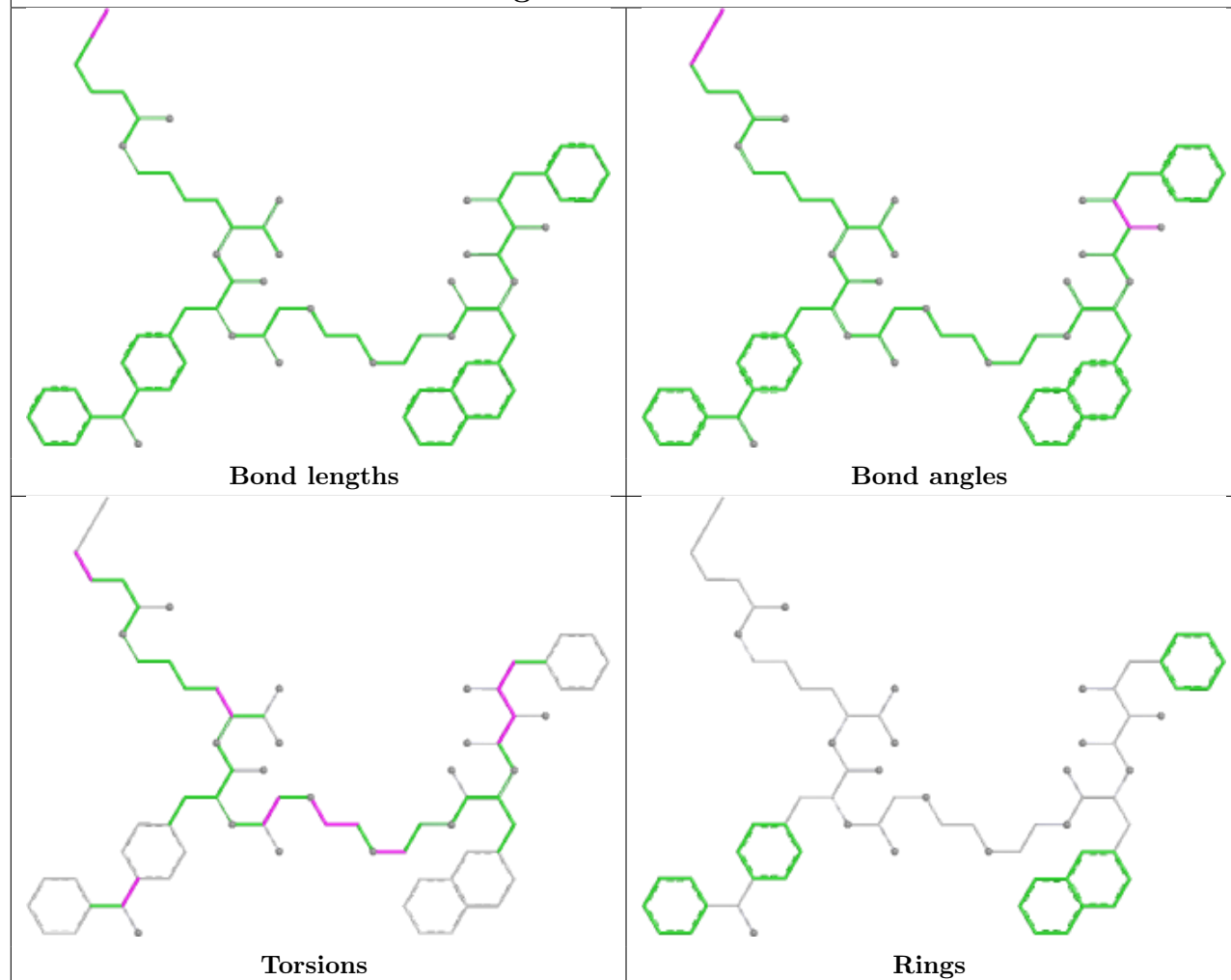
Ligand DGZ E 615

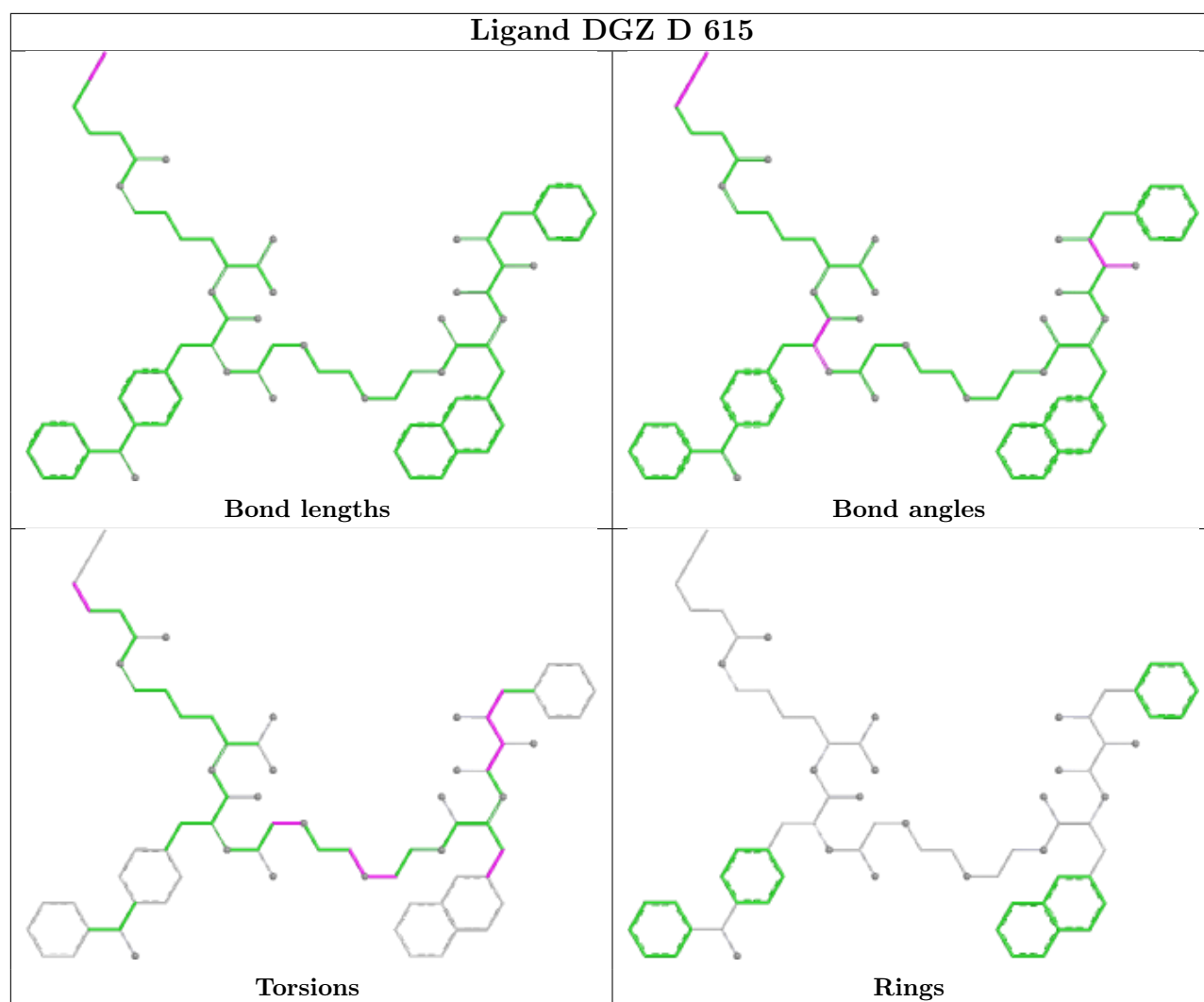


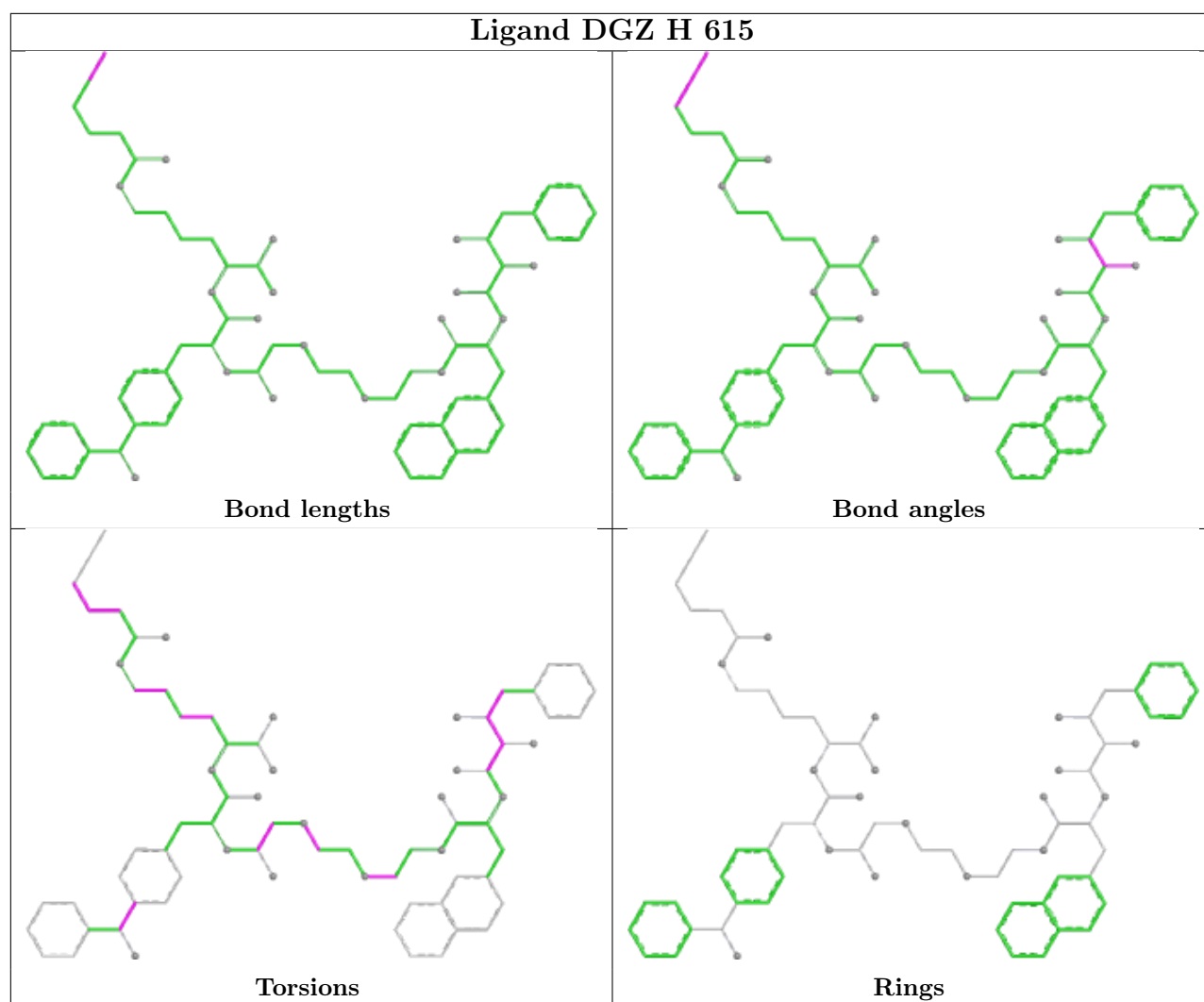
Ligand 2PE B 616



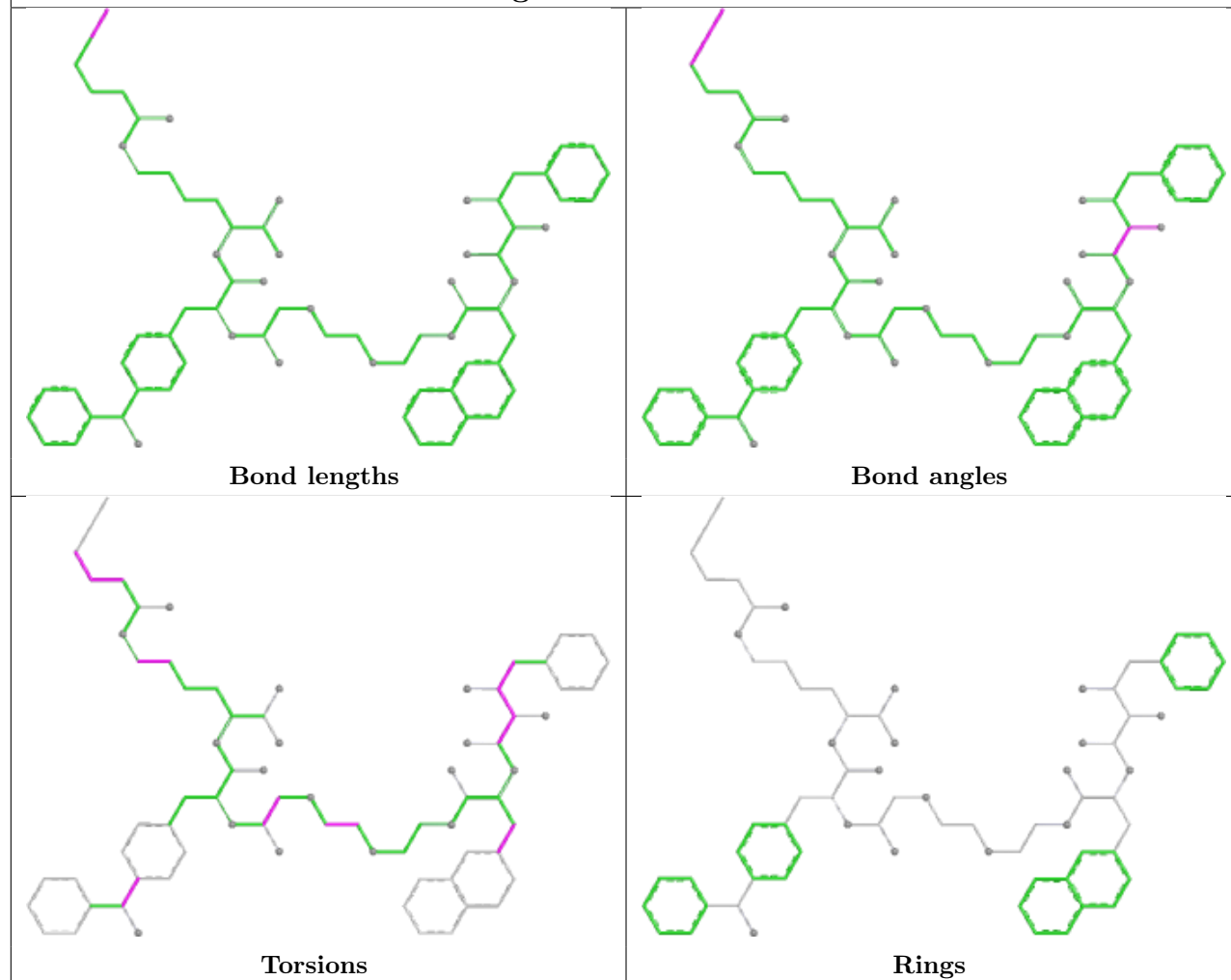
Ligand DGZ F 615

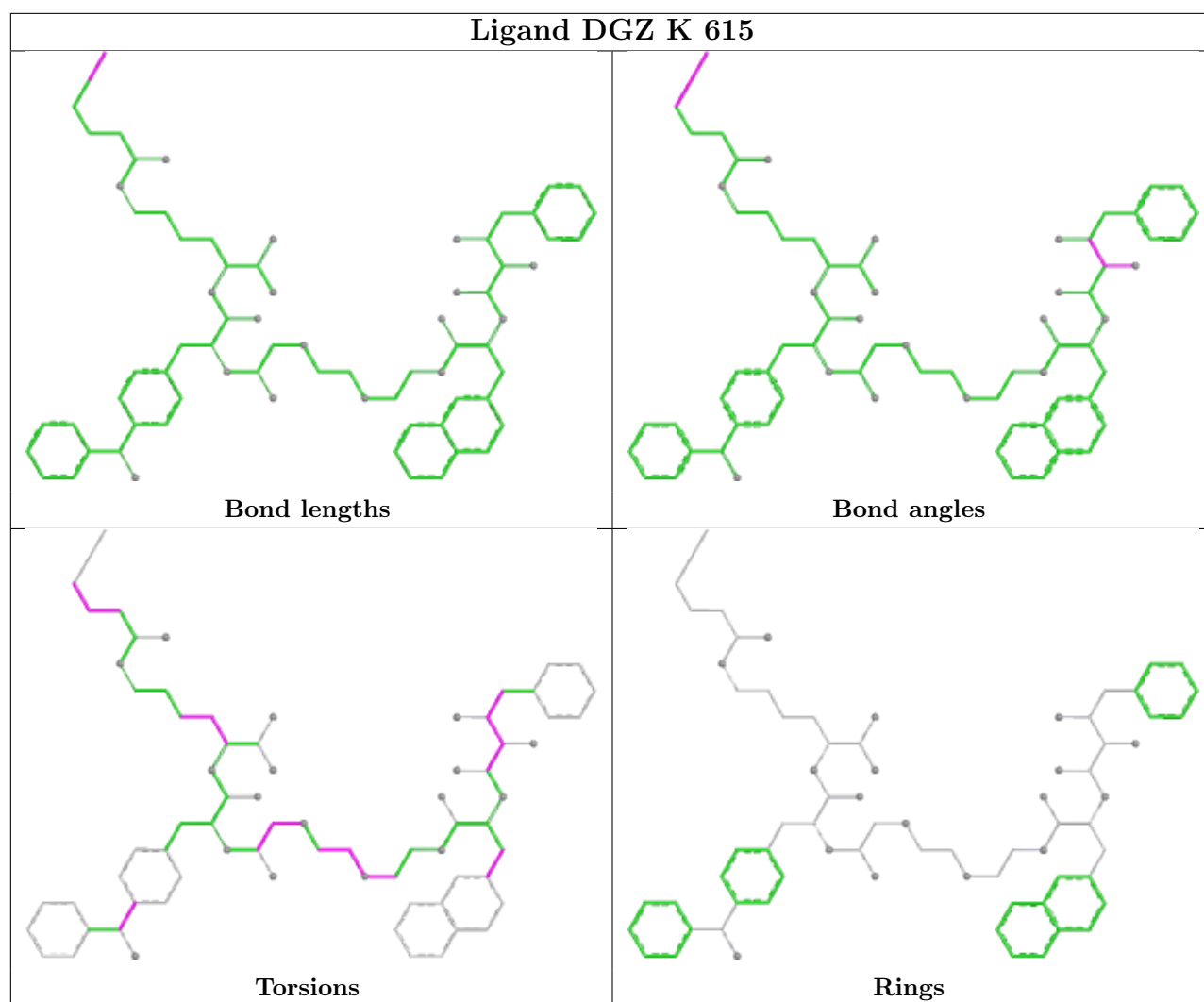


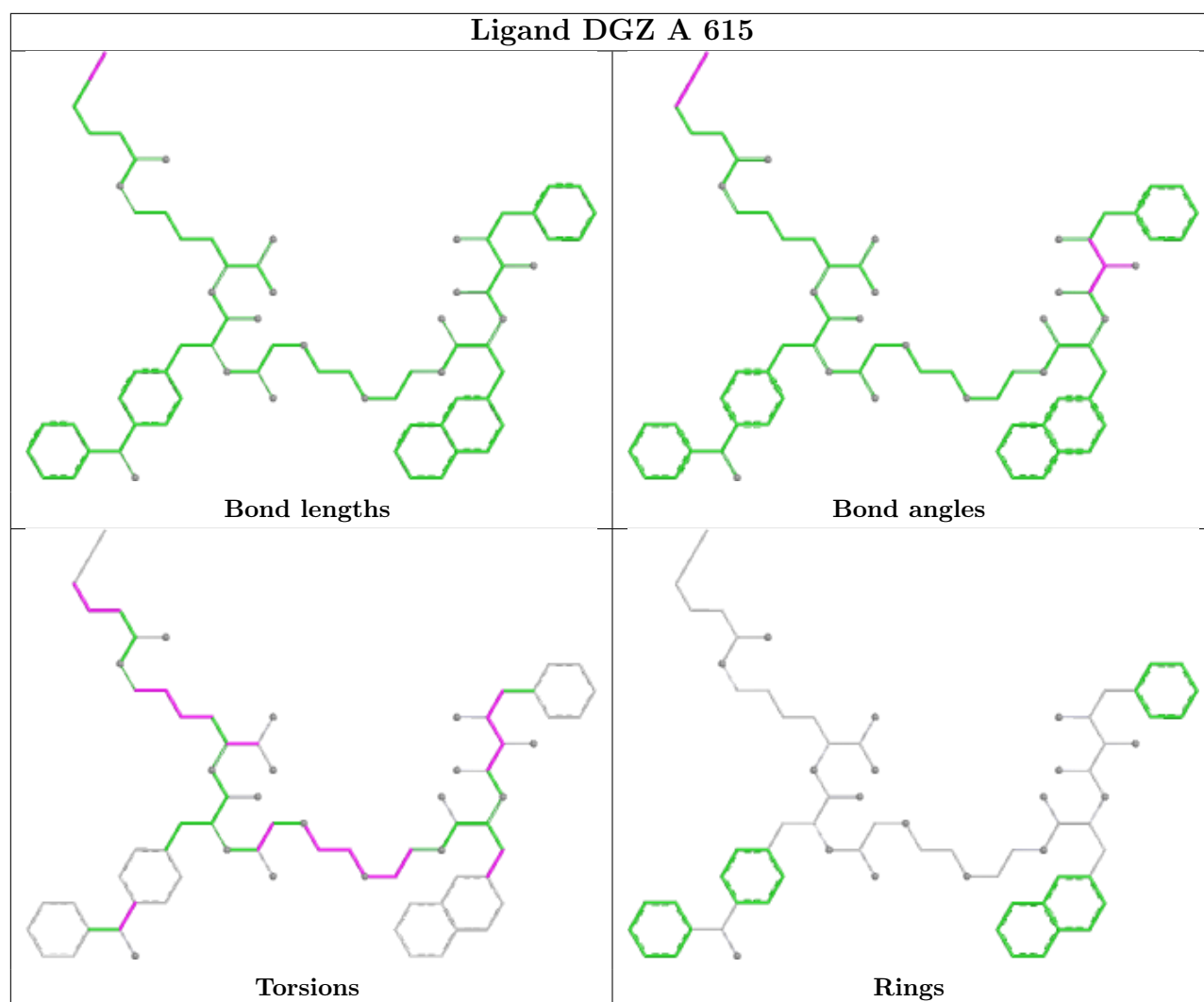


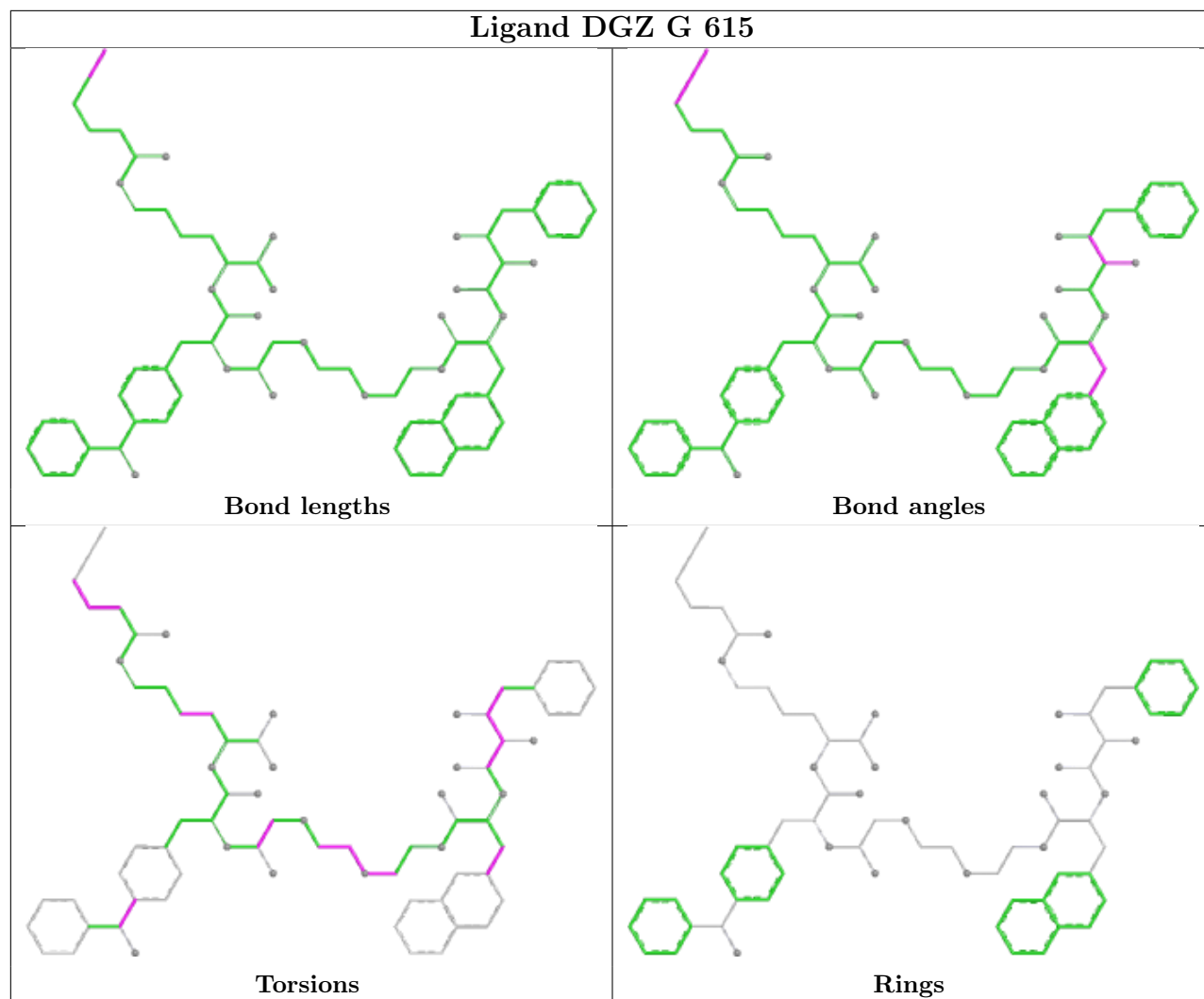


Ligand DGZ B 615

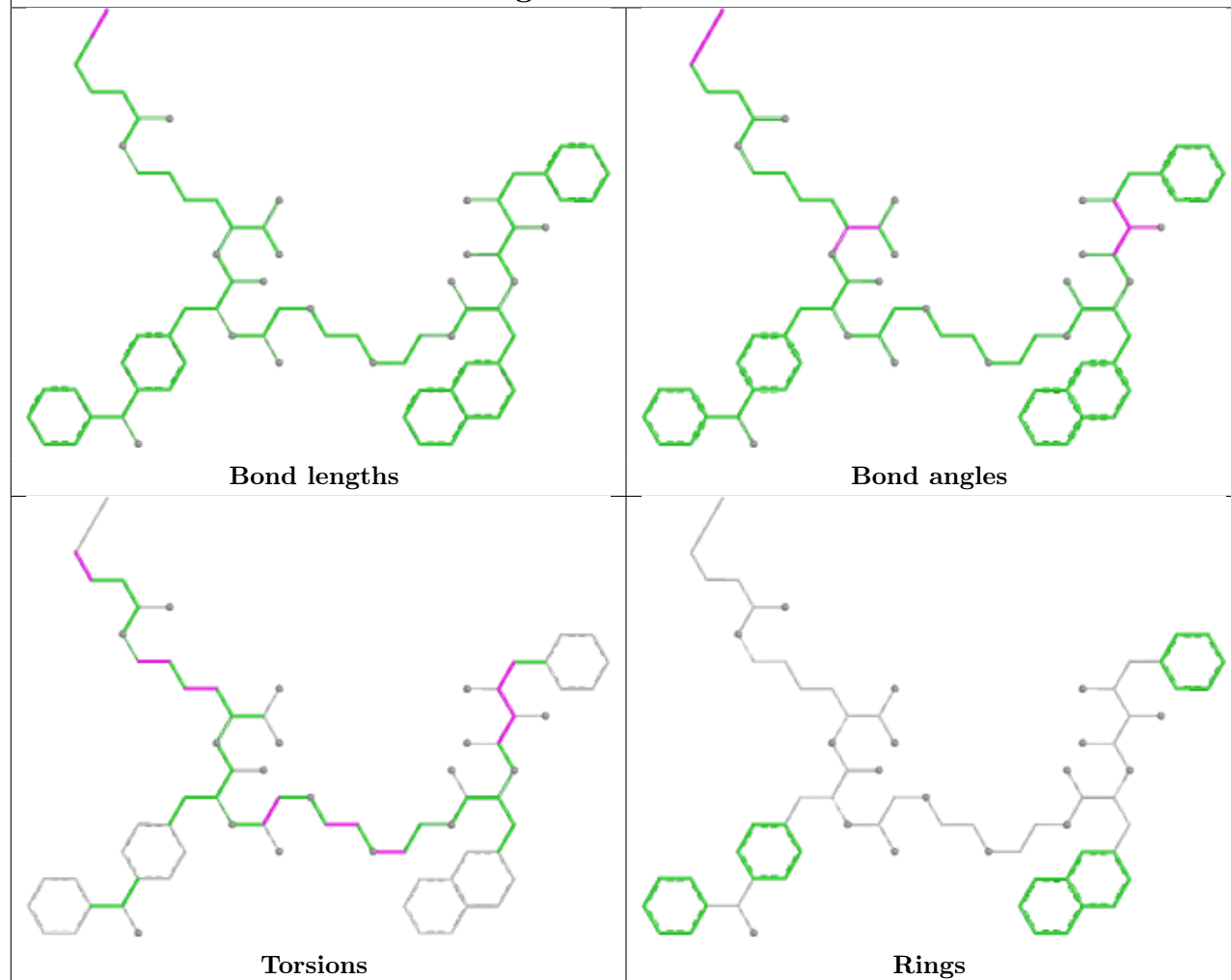




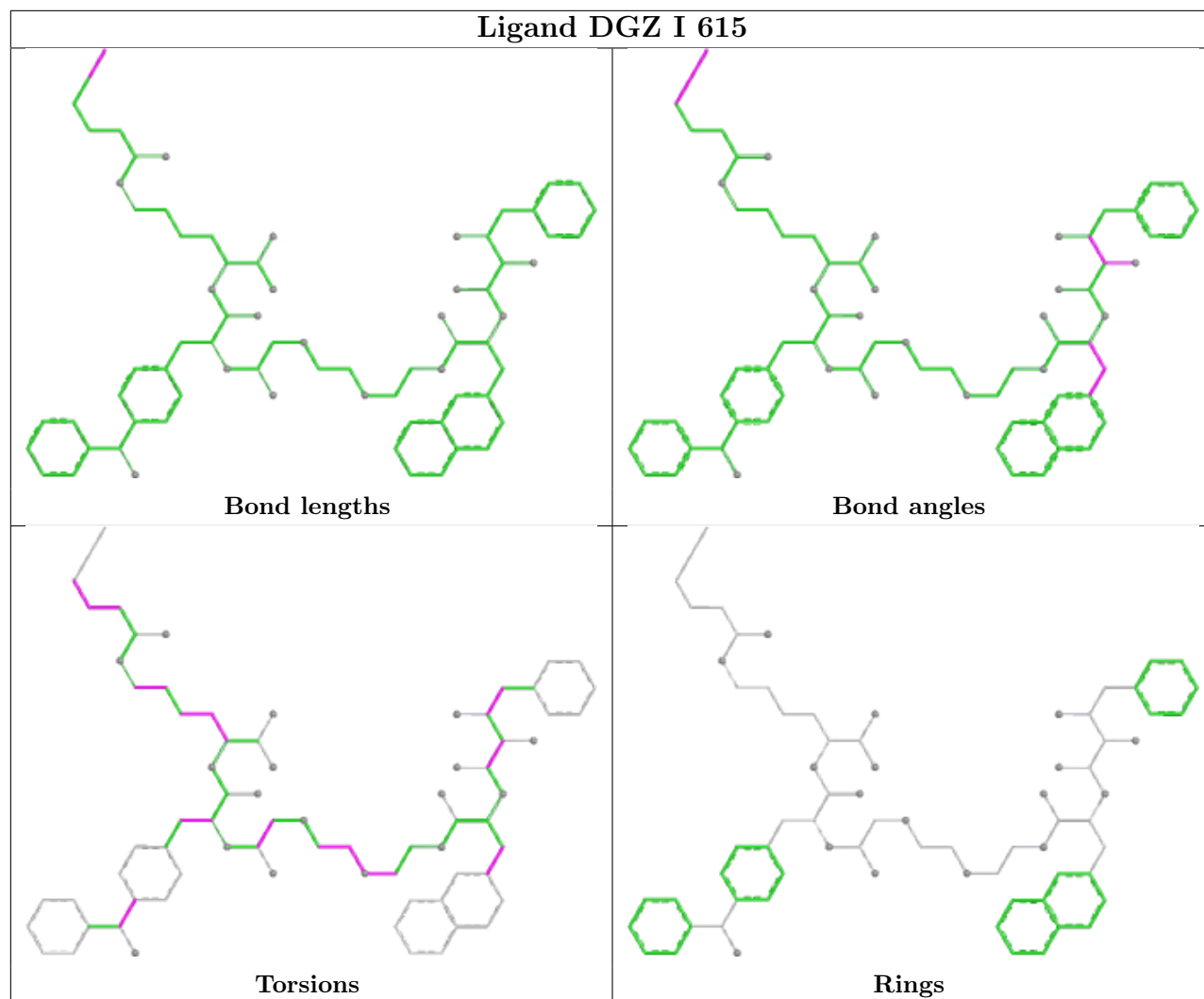


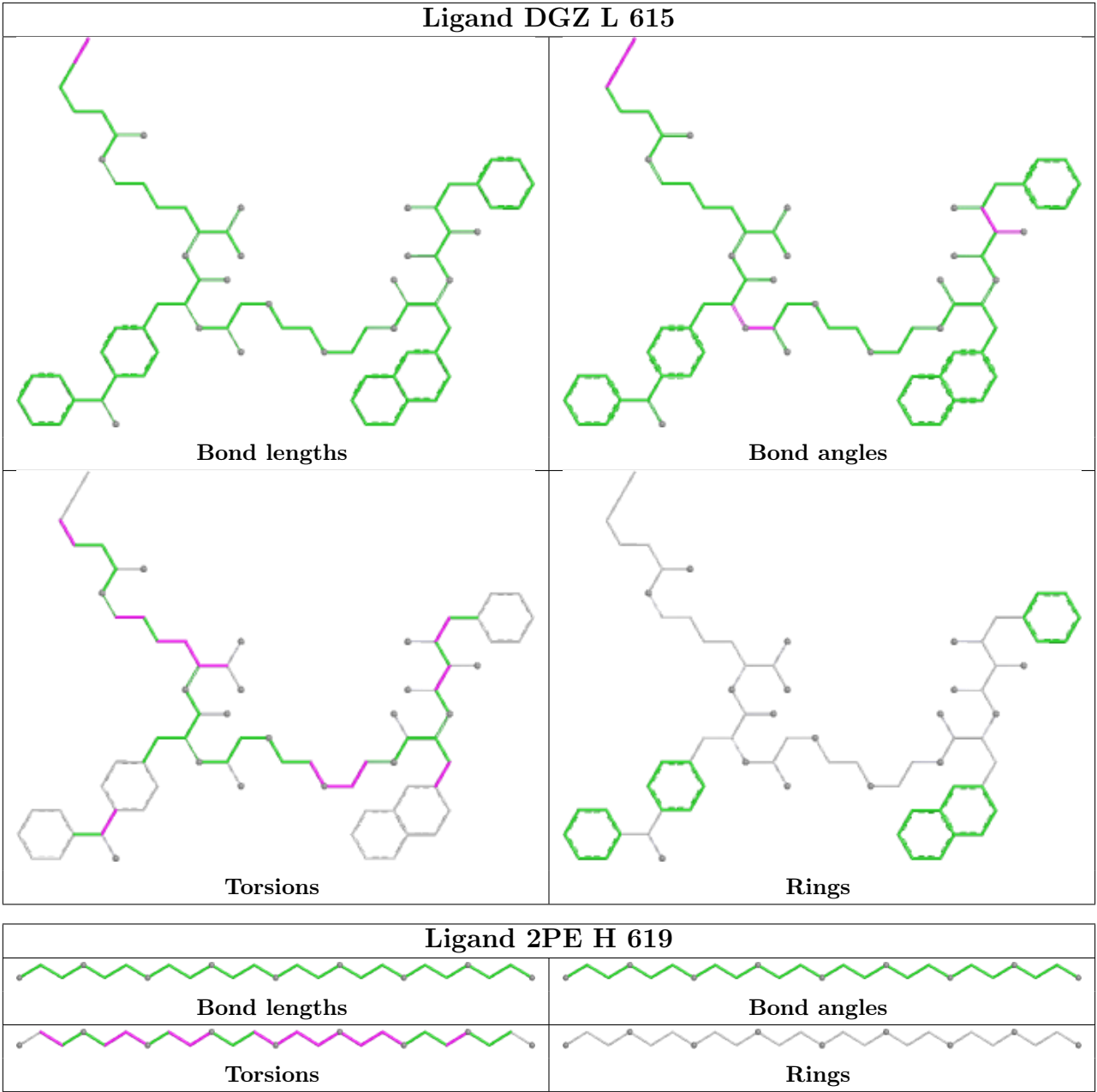


Ligand DGZ J 615



Ligand DGZ I 615





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

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

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	519/528 (98%)	-0.46	7 (1%) 75 74	5, 15, 35, 70	0
1	B	517/528 (97%)	-0.20	19 (3%) 45 44	5, 17, 46, 73	1 (0%)
1	C	516/528 (97%)	-0.44	5 (0%) 79 79	5, 15, 39, 76	0
1	D	514/528 (97%)	-0.46	14 (2%) 56 55	6, 14, 35, 80	0
1	E	509/528 (96%)	-0.57	5 (0%) 79 79	7, 14, 30, 48	0
1	F	511/528 (96%)	-0.29	12 (2%) 61 60	6, 18, 40, 71	0
1	G	517/528 (97%)	-0.50	7 (1%) 73 73	6, 14, 36, 61	0
1	H	518/528 (98%)	-0.20	18 (3%) 47 46	6, 18, 46, 68	1 (0%)
1	I	518/528 (98%)	-0.42	5 (0%) 79 79	5, 16, 39, 81	0
1	J	514/528 (97%)	-0.44	15 (2%) 53 52	7, 15, 37, 82	0
1	K	509/528 (96%)	-0.54	7 (1%) 73 73	7, 14, 32, 47	0
1	L	511/528 (96%)	-0.42	7 (1%) 73 73	6, 16, 37, 64	0
All	All	6173/6336 (97%)	-0.41	121 (1%) 65 64	5, 15, 39, 82	2 (0%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	551	VAL	6.9
1	D	603	ASP	6.8
1	F	551	VAL	6.6
1	L	550	SER	6.5
1	F	138	GLU	5.8
1	L	551	VAL	5.6
1	A	551	VAL	5.6
1	B	603	ASP	5.2
1	I	551	VAL	5.2
1	F	603	ASP	5.2
1	I	603	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	J	603	ASP	4.7
1	J	260	ASN	4.6
1	C	603	ASP	4.5
1	B	118	LYS	4.4
1	G	603	ASP	4.3
1	B	550	SER	4.2
1	L	136	GLY	4.1
1	H	118	LYS	4.1
1	H	603	ASP	4.0
1	E	602	ASN	3.9
1	A	603	ASP	3.9
1	B	551	VAL	3.8
1	H	549	SER	3.6
1	J	136	GLY	3.6
1	D	124	GLU	3.5
1	J	219	LEU	3.5
1	D	219	LEU	3.5
1	B	549	SER	3.4
1	B	171	THR	3.4
1	E	551	VAL	3.4
1	H	216	ASP	3.3
1	A	550	SER	3.3
1	F	361	SER	3.3
1	H	119	GLY	3.3
1	D	260	ASN	3.3
1	B	135	PRO	3.2
1	C	549	SER	3.2
1	H	198	LEU	3.1
1	B	363	GLY	3.1
1	G	550	SER	3.1
1	D	218	LYS	3.0
1	G	258	ASN	3.0
1	H	135	PRO	3.0
1	L	552	LYS	3.0
1	J	85	ALA	2.9
1	D	85	ALA	2.8
1	D	122	ASN	2.7
1	B	119	GLY	2.7
1	B	136	GLY	2.7
1	D	136	GLY	2.7
1	H	136	GLY	2.7
1	A	85	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	551	VAL	2.6
1	F	139	ASN	2.6
1	A	552	LYS	2.6
1	F	216	ASP	2.6
1	F	549	SER	2.6
1	H	181	ASN	2.6
1	L	137	LYS	2.6
1	G	85	ALA	2.6
1	I	549	SER	2.6
1	G	196	ALA	2.5
1	G	549	SER	2.5
1	C	204	LYS	2.5
1	D	551	VAL	2.5
1	H	259	VAL	2.4
1	F	550	SER	2.4
1	K	254	SER	2.4
1	J	364	ASP	2.4
1	H	197	ASP	2.4
1	B	121	CYS	2.4
1	B	196	ALA	2.3
1	K	602	ASN	2.3
1	F	136	GLY	2.3
1	F	137	LYS	2.3
1	B	602	ASN	2.3
1	A	362	LYS	2.3
1	B	552	LYS	2.3
1	J	218	LYS	2.3
1	L	603	ASP	2.3
1	C	362	LYS	2.3
1	J	137	LYS	2.3
1	J	549	SER	2.2
1	E	229	ASN	2.2
1	E	493	TYR	2.2
1	E	254	SER	2.2
1	J	194	SER	2.2
1	B	181	ASN	2.2
1	H	164	LYS	2.2
1	I	195	VAL	2.2
1	D	197	ASP	2.2
1	H	196	ALA	2.2
1	D	493	TYR	2.2
1	K	550	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	139	ASN	2.2
1	H	602	ASN	2.2
1	H	178	PHE	2.1
1	B	183	ASN	2.1
1	G	493	TYR	2.1
1	J	217	ASN	2.1
1	K	273	ASN	2.1
1	J	123	VAL	2.1
1	D	273	ASN	2.1
1	J	229	ASN	2.1
1	B	178	PHE	2.1
1	F	552	LYS	2.1
1	B	198	LEU	2.1
1	K	493	TYR	2.1
1	A	363	GLY	2.1
1	C	552	LYS	2.1
1	H	153	VAL	2.1
1	F	86	SER	2.1
1	I	550	SER	2.1
1	K	549	SER	2.1
1	L	493	TYR	2.0
1	D	123	VAL	2.0
1	D	262	GLU	2.0
1	B	273	ASN	2.0
1	K	229	ASN	2.0
1	J	363	GLY	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	SO4	C	617	5/5	0.63	0.21	95,99,100,101	0
6	1PE	D	621	5/16	0.63	0.28	26,28,34,37	0
6	1PE	J	622	9/16	0.66	0.25	45,50,55,55	0
5	SO4	I	618	5/5	0.72	0.22	57,61,62,63	0
5	SO4	K	616	5/5	0.74	0.18	72,76,78,79	0
6	1PE	D	619	8/16	0.75	0.21	52,53,54,55	0
5	SO4	G	618	5/5	0.76	0.20	74,77,80,80	0
6	1PE	G	623	15/16	0.77	0.20	42,48,57,58	0
2	CO3	F	612	4/4	0.77	0.18	9,11,13,15	0
2	CO3	I	612	4/4	0.78	0.18	10,11,12,14	0
6	1PE	J	621	11/16	0.78	0.18	38,38,41,43	0
5	SO4	A	617	5/5	0.78	0.17	54,55,59,59	0
2	CO3	G	612	4/4	0.79	0.17	4,9,10,12	0
2	CO3	L	612	4/4	0.79	0.15	9,10,12,14	0
7	2PE	B	616	26/28	0.79	0.18	42,48,56,57	0
5	SO4	I	616	5/5	0.80	0.18	75,80,80,80	0
6	1PE	F	617	10/16	0.80	0.17	46,50,52,52	0
6	1PE	L	618	12/16	0.80	0.15	25,35,48,48	0
5	SO4	C	619	5/5	0.80	0.31	48,51,54,54	0
6	1PE	D	620	11/16	0.81	0.17	35,39,46,48	0
7	2PE	H	619	25/28	0.81	0.16	40,44,55,57	0
6	1PE	E	619	12/16	0.82	0.16	40,42,46,47	0
5	SO4	E	617	5/5	0.82	0.15	73,78,79,79	0
5	SO4	I	619	5/5	0.82	0.18	90,94,95,96	0
5	SO4	J	617	5/5	0.82	0.16	77,81,82,83	0
5	SO4	C	618	5/5	0.82	0.19	100,104,104,106	0
5	SO4	H	617	5/5	0.82	0.17	80,84,86,86	0
5	SO4	H	618	5/5	0.82	0.24	45,47,50,52	0
2	CO3	D	612	4/4	0.82	0.17	10,12,15,15	0
6	1PE	F	616	10/16	0.83	0.14	29,32,40,41	0
2	CO3	J	612	4/4	0.83	0.13	11,11,13,14	0
6	1PE	C	621	12/16	0.83	0.14	42,44,47,48	0
2	CO3	H	612	4/4	0.83	0.16	5,11,12,14	0
5	SO4	D	616	5/5	0.84	0.16	73,78,78,80	0
6	1PE	K	619	11/16	0.84	0.15	25,39,44,44	0
5	SO4	G	616	5/5	0.84	0.17	75,79,81,81	0
5	SO4	E	616	5/5	0.84	0.18	90,94,95,96	0
5	SO4	G	619	5/5	0.84	0.30	45,49,50,52	0
2	CO3	E	612	4/4	0.85	0.17	6,13,14,16	0
6	1PE	A	619	7/16	0.85	0.14	43,44,48,51	0
6	1PE	L	620	11/16	0.85	0.13	39,42,45,45	0
5	SO4	C	620	5/5	0.85	0.14	52,56,58,58	0
5	SO4	J	618	5/5	0.85	0.14	57,60,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	1PE	C	622	9/16	0.86	0.14	27,29,35,40	0
5	SO4	G	617	5/5	0.86	0.22	36,40,41,42	0
6	1PE	I	621	12/16	0.86	0.12	35,37,40,43	0
6	1PE	K	620	6/16	0.86	0.14	30,31,32,33	0
6	1PE	G	620	9/16	0.87	0.13	24,26,31,31	0
5	SO4	E	618	5/5	0.87	0.17	52,55,59,59	0
6	1PE	K	617	8/16	0.87	0.12	32,37,42,43	0
6	1PE	K	618	12/16	0.87	0.13	25,31,40,40	0
6	1PE	F	618	10/16	0.87	0.13	36,40,44,44	0
5	SO4	A	616	5/5	0.88	0.13	62,67,67,67	0
6	1PE	J	620	10/16	0.88	0.11	27,35,41,41	0
2	CO3	A	612	4/4	0.89	0.12	12,12,14,15	0
2	CO3	K	612	4/4	0.89	0.13	10,10,10,11	0
6	1PE	L	619	7/16	0.89	0.12	30,32,35,35	0
4	DGZ	B	615	74/74	0.90	0.16	9,37,133,171	0
6	1PE	A	618	9/16	0.90	0.11	23,24,26,29	0
6	1PE	D	618	10/16	0.90	0.13	30,34,40,40	0
6	1PE	G	622	6/16	0.90	0.14	30,30,30,32	0
6	1PE	E	620	10/16	0.90	0.11	26,27,35,41	0
2	CO3	B	612	4/4	0.90	0.10	14,14,15,15	0
5	SO4	L	616	5/5	0.91	0.26	41,43,48,48	0
4	DGZ	I	615	74/74	0.91	0.17	5,42,189,216	0
4	DGZ	K	615	74/74	0.91	0.17	7,41,147,213	0
4	DGZ	A	615	74/74	0.91	0.16	5,38,181,208	0
5	SO4	I	617	5/5	0.91	0.21	43,46,49,49	0
2	CO3	C	612	4/4	0.91	0.12	12,12,13,15	0
4	DGZ	C	615	74/74	0.91	0.16	10,38,182,231	0
4	DGZ	E	615	74/74	0.91	0.17	10,41,146,207	0
4	DGZ	G	615	74/74	0.91	0.17	6,36,151,232	0
4	DGZ	H	615	74/74	0.91	0.17	4,38,142,180	0
6	1PE	L	617	10/16	0.92	0.10	17,27,36,40	0
6	1PE	E	621	8/16	0.92	0.11	31,34,36,37	0
4	DGZ	J	615	74/74	0.92	0.17	8,34,179,236	0
5	SO4	I	620	5/5	0.92	0.20	39,41,44,47	0
4	DGZ	F	615	74/74	0.92	0.14	8,35,127,202	0
4	DGZ	D	615	74/74	0.92	0.15	7,34,121,208	0
6	1PE	J	619	11/16	0.93	0.10	19,23,34,38	0
6	1PE	G	621	6/16	0.93	0.09	25,25,27,32	0
4	DGZ	L	615	74/74	0.94	0.14	7,33,109,190	0
6	1PE	I	623	5/16	0.94	0.08	14,14,16,18	0
6	1PE	I	622	10/16	0.95	0.07	21,23,34,35	0
3	ZN	C	614	1/1	0.99	0.07	25,25,25,25	0

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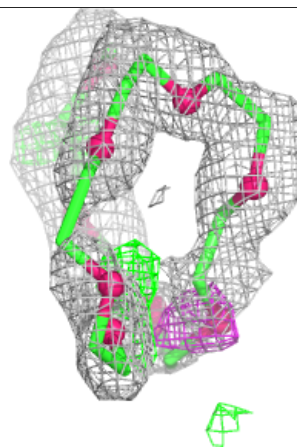
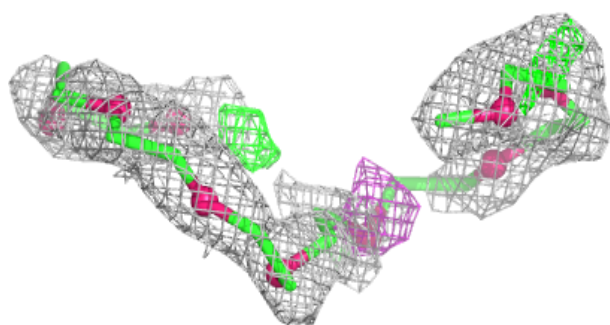
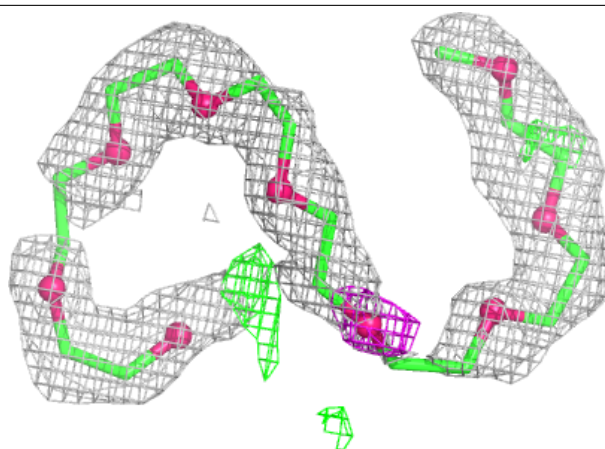
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	F	614	1/1	0.99	0.06	27,27,27,27	0
3	ZN	I	614	1/1	0.99	0.08	27,27,27,27	0
3	ZN	K	614	1/1	0.99	0.09	29,29,29,29	0
5	SO4	D	617	5/5	0.99	0.04	12,13,14,17	0
5	SO4	J	616	5/5	0.99	0.04	14,14,17,17	0
5	SO4	H	616	5/5	0.99	0.04	12,12,14,14	0
5	SO4	C	616	5/5	0.99	0.03	9,9,10,12	0
3	ZN	L	613	1/1	0.99	0.07	27,27,27,27	0
3	ZN	A	613	1/1	1.00	0.08	26,26,26,26	0
3	ZN	D	613	1/1	1.00	0.01	16,16,16,16	0
3	ZN	D	614	1/1	1.00	0.07	29,29,29,29	0
3	ZN	E	613	1/1	1.00	0.01	18,18,18,18	0
3	ZN	E	614	1/1	1.00	0.10	28,28,28,28	0
3	ZN	F	613	1/1	1.00	0.01	17,17,17,17	0
3	ZN	A	614	1/1	1.00	0.02	17,17,17,17	0
3	ZN	G	613	1/1	1.00	0.01	16,16,16,16	0
3	ZN	G	614	1/1	1.00	0.06	27,27,27,27	0
3	ZN	H	613	1/1	1.00	0.01	19,19,19,19	0
3	ZN	H	614	1/1	1.00	0.07	29,29,29,29	0
3	ZN	I	613	1/1	1.00	0.02	17,17,17,17	0
3	ZN	B	613	1/1	1.00	0.08	26,26,26,26	0
3	ZN	J	613	1/1	1.00	0.02	19,19,19,19	0
3	ZN	J	614	1/1	1.00	0.09	24,24,24,24	0
3	ZN	K	613	1/1	1.00	0.01	18,18,18,18	0
3	ZN	B	614	1/1	1.00	0.02	16,16,16,16	0
3	ZN	C	613	1/1	1.00	0.01	17,17,17,17	0
3	ZN	L	614	1/1	1.00	0.01	17,17,17,17	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.

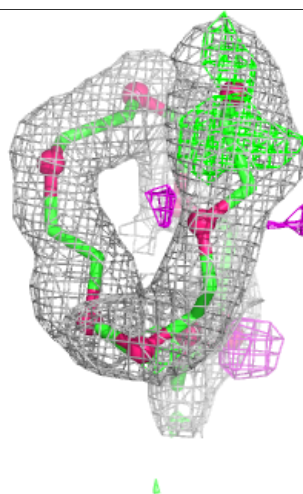
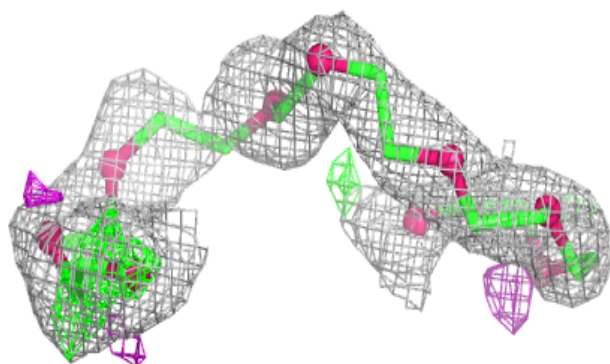
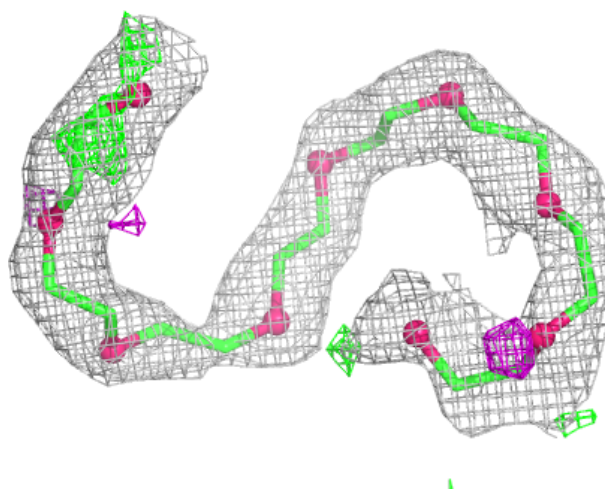
Electron density around 2PE B 616:

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



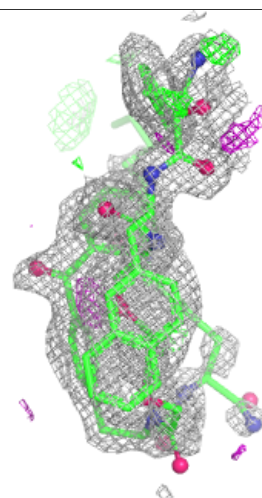
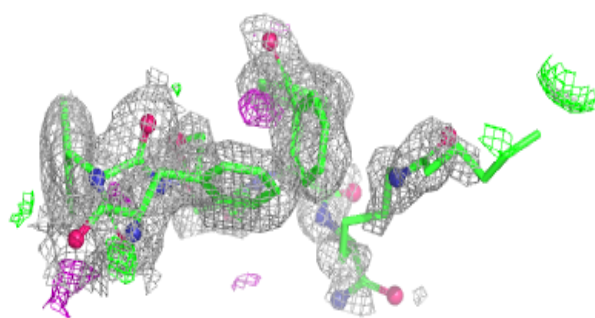
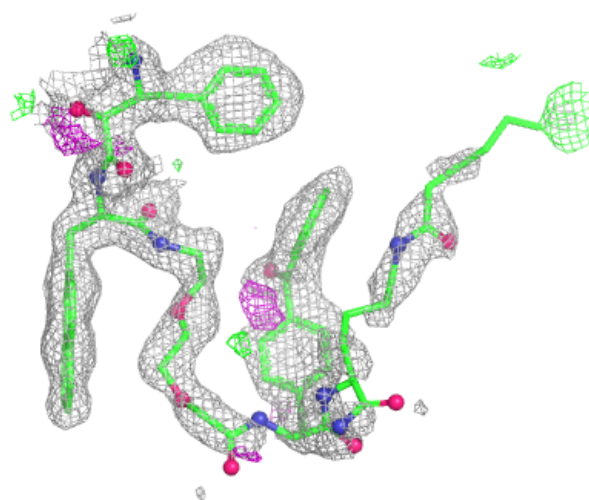
Electron density around 2PE H 619:

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and green (positive)



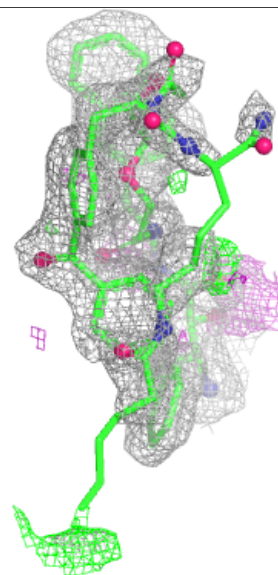
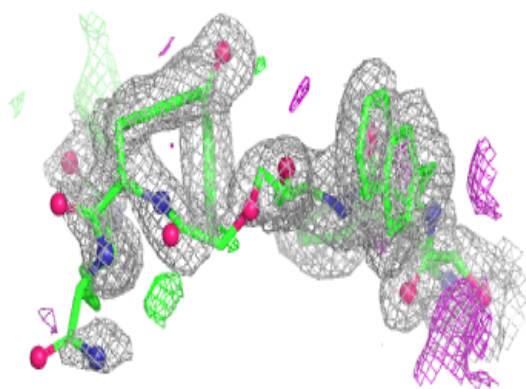
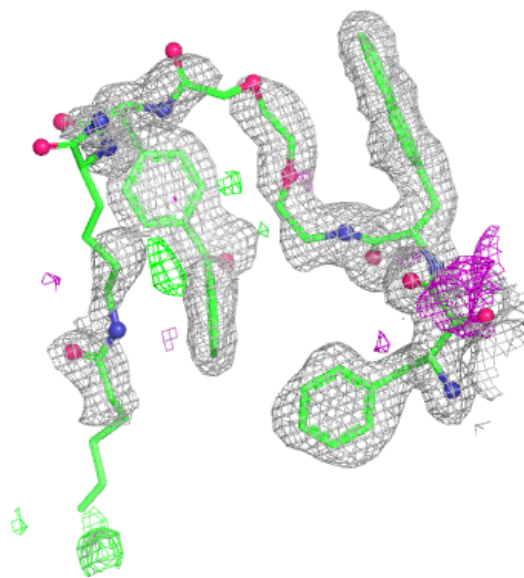
Electron density around DGZ B 615:

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



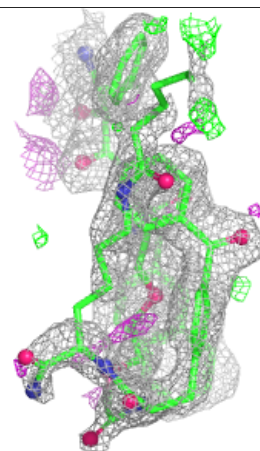
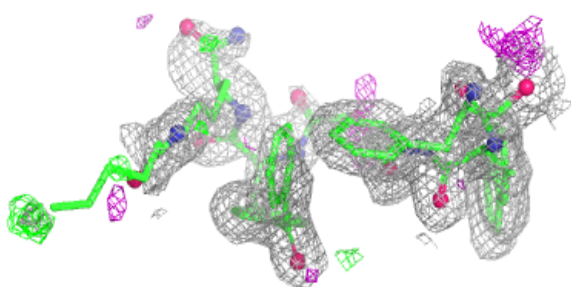
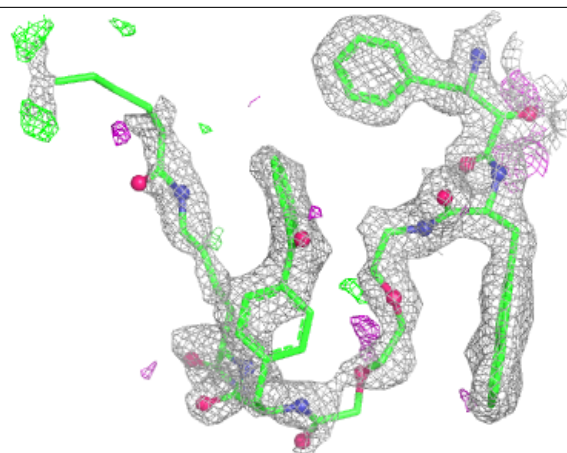
Electron density around DGZ I 615:

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and green (positive)



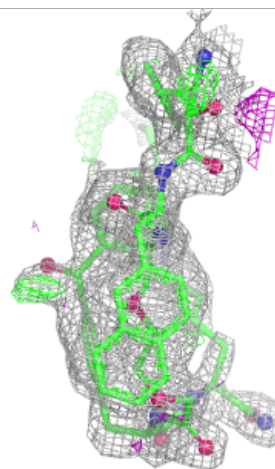
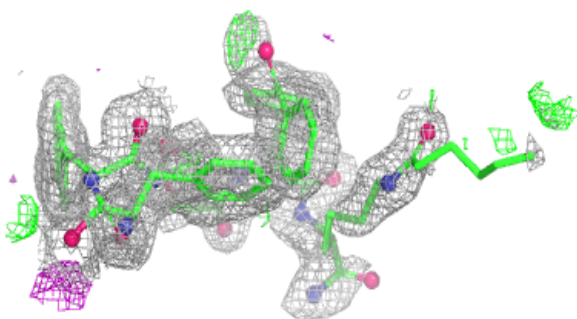
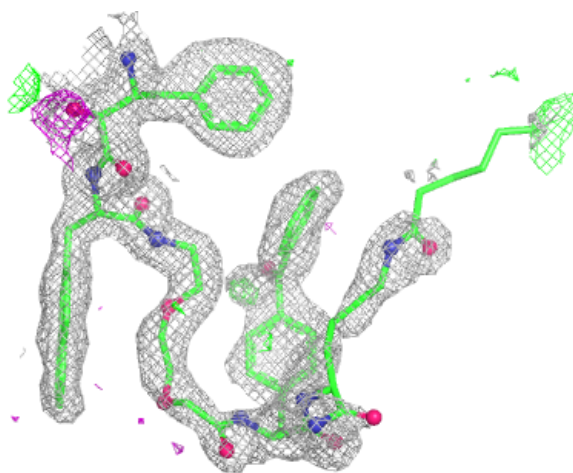
Electron density around DGZ K 615:

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and green (positive)



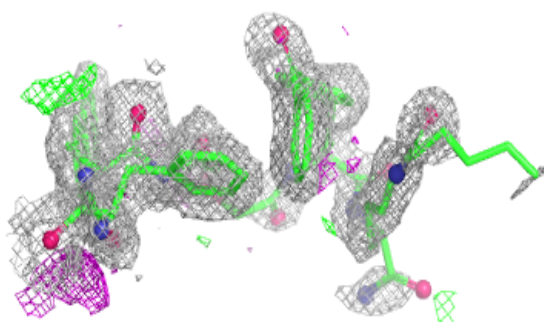
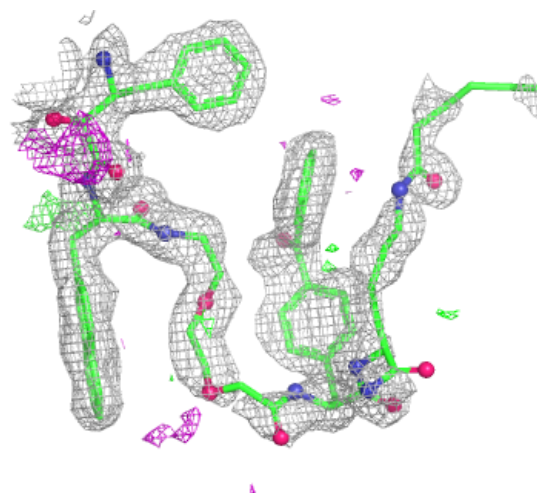
Electron density around DGZ A 615:

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and green (positive)



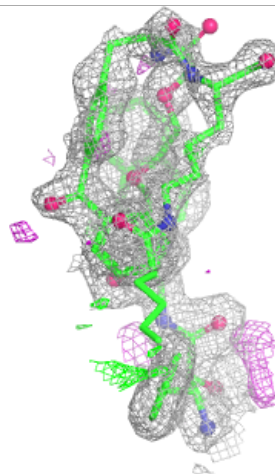
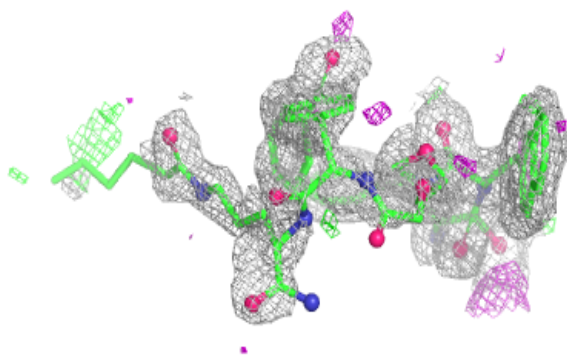
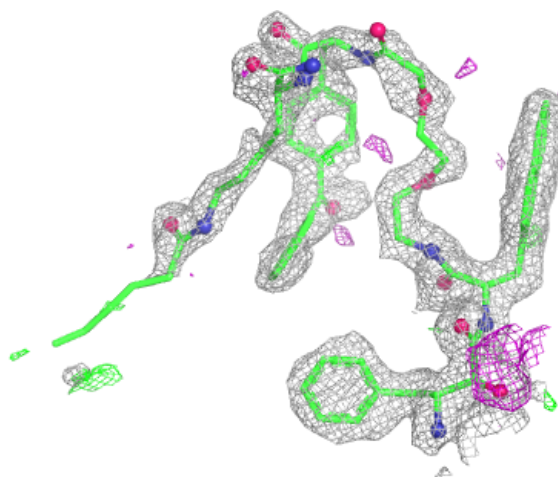
Electron density around DGZ C 615:

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



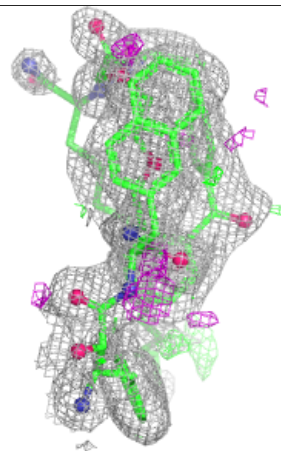
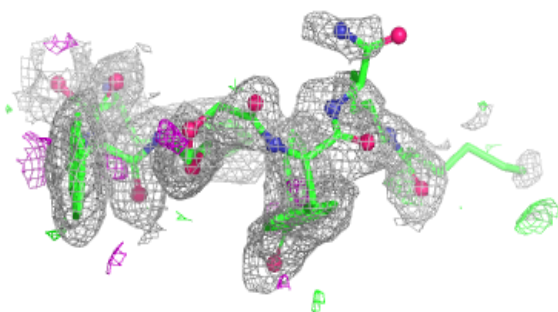
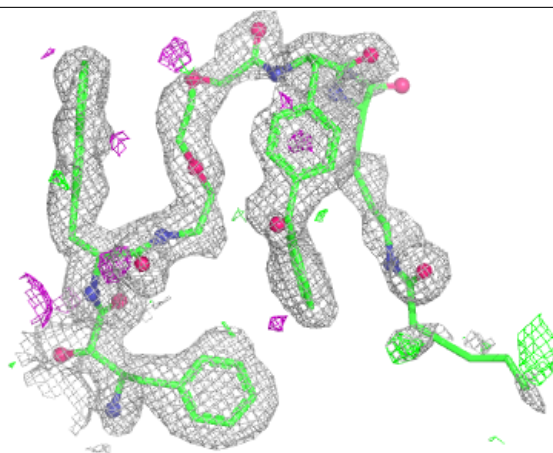
Electron density around DGZ E 615:

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and green (positive)



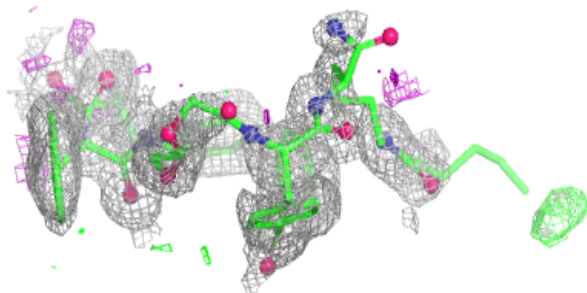
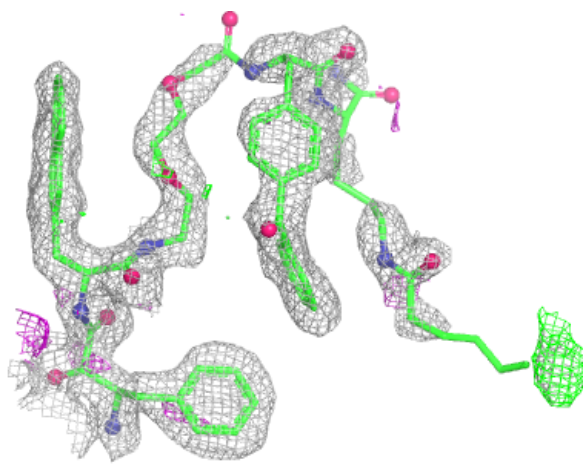
Electron density around DGZ G 615:

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and green (positive)



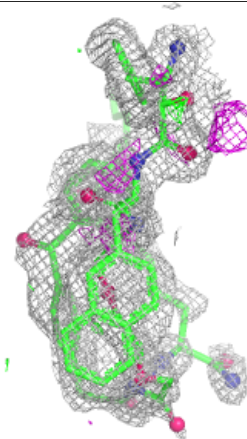
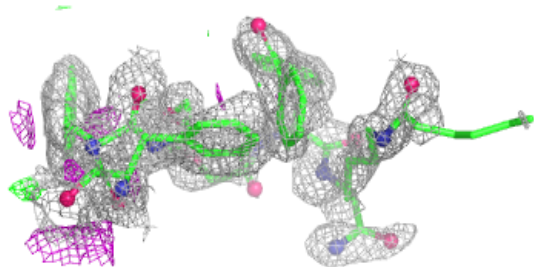
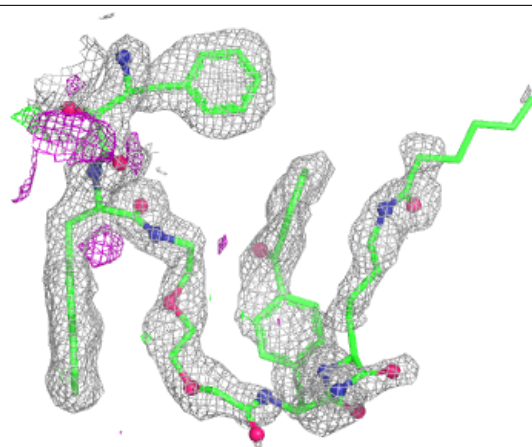
Electron density around DGZ H 615:

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



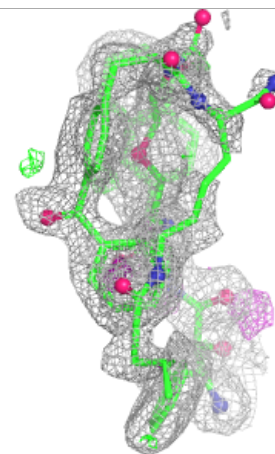
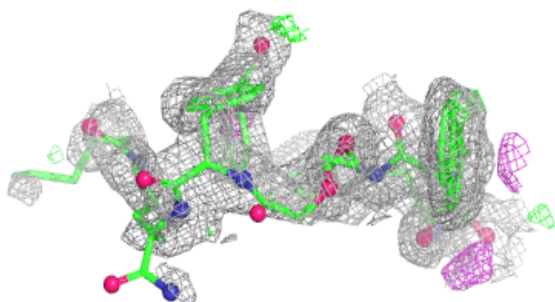
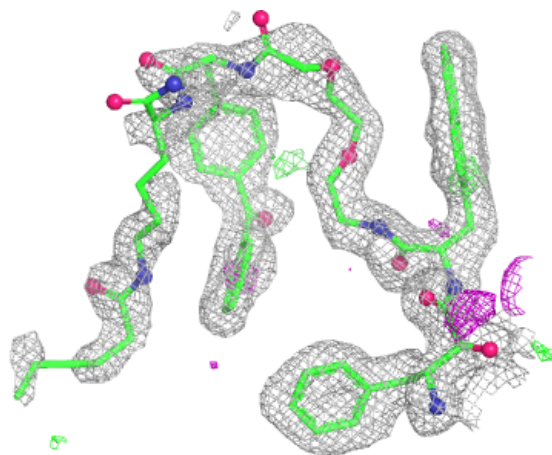
Electron density around DGZ J 615:

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



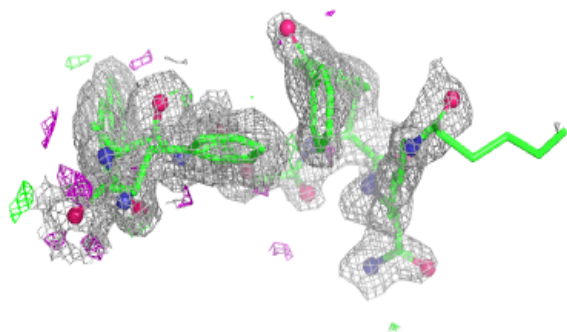
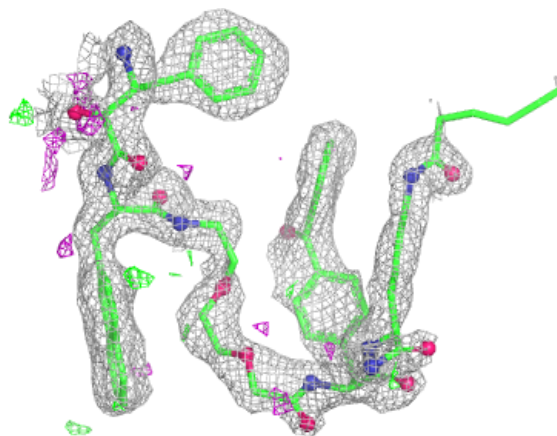
Electron density around DGZ F 615:

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



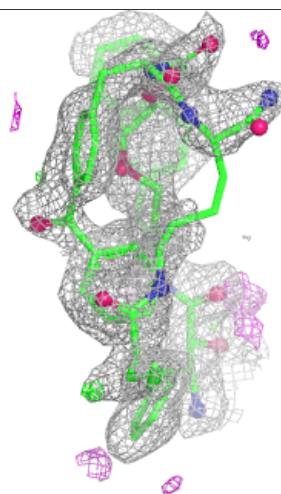
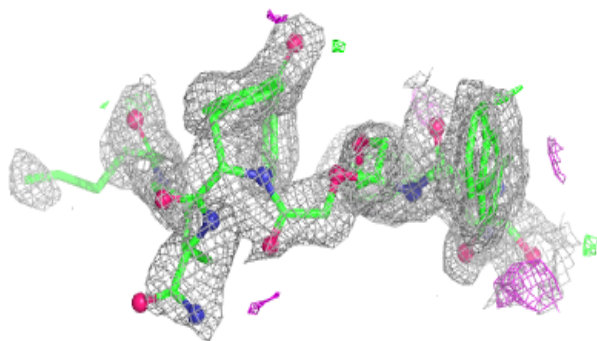
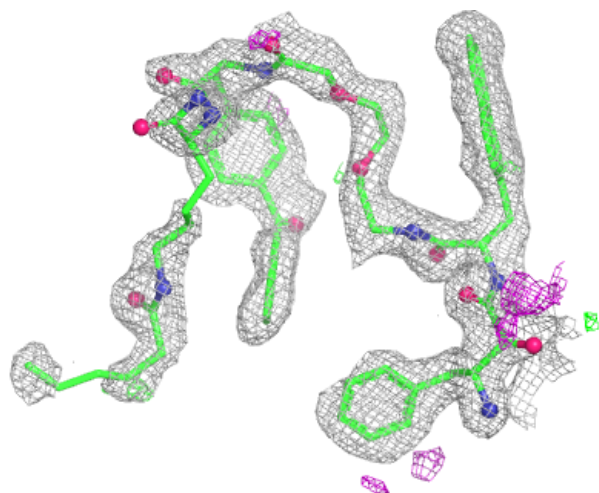
Electron density around DGZ D 615:

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



Electron density around DGZ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.