



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 02:03 am BST

PDB ID : 4R6T
Title : Structure of the m17 leucyl aminopeptidase from malaria complexed with a hydroxamic acid-based inhibitor
Authors : Drinkwater, N.; McGowan, S.
Deposited on : 2014-08-26
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

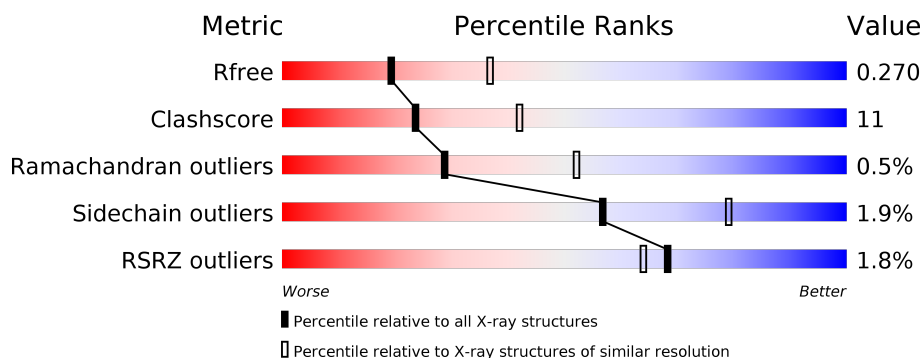
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	528	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> % 76% 20% .. </div> </div>
1	B	528	<div> <div style="width: 5%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> 5% 73% 23% .. </div> </div>
1	C	528	<div> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> 2% 73% 24% .. </div> </div>
1	D	528	<div> <div style="width: 0%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> 0% 71% 25% .. </div> </div>
1	E	528	<div> <div style="width: 0%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> 0% 75% 22% .. </div> </div>
1	F	528	<div> <div style="width: 3%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> 3% 73% 22% .. </div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	1004	-	-	X	-
6	1PE	C	1010	-	-	X	-
6	1PE	E	1006	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 49091 atoms, of which 6 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	514	Total	C	N	O	S	0	1	0
			3945	2537	632	757	19			
1	B	511	Total	C	N	O	S	0	0	0
			3869	2489	626	735	19			
1	C	518	Total	C	N	O	S	0	0	0
			3949	2541	637	752	19			
1	D	513	Total	C	N	O	S	0	0	0
			3918	2524	630	745	19			
1	E	513	Total	C	N	O	S	0	0	0
			3913	2521	626	746	20			
1	F	508	Total	C	N	O	S	0	0	0
			3785	2438	610	718	19			
1	G	514	Total	C	N	O	S	0	0	0
			3944	2537	630	758	19			
1	H	511	Total	C	N	O	S	0	0	0
			3878	2495	625	739	19			
1	I	516	Total	C	N	O	S	0	0	0
			3908	2516	629	744	19			
1	J	512	Total	C	N	O	S	0	0	0
			3910	2519	630	742	19			
1	K	509	Total	C	N	O	S	0	0	0
			3879	2500	622	738	19			
1	L	509	Total	C	N	O	S	0	0	0
			3823	2457	614	733	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 ZINC ION (three-letter code: ZN) (formula: Zn).

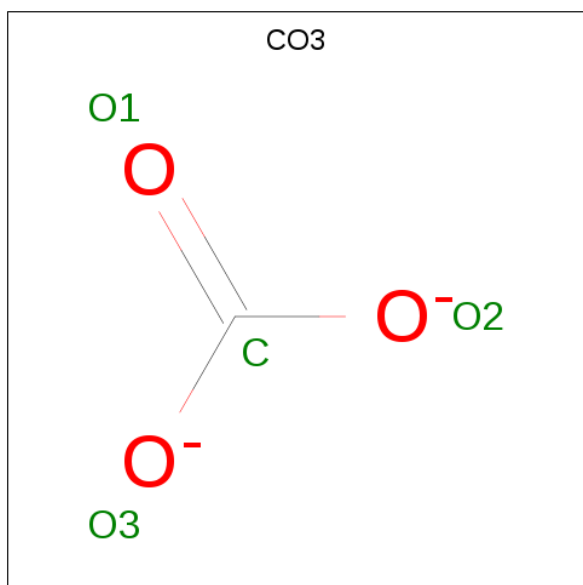
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	K	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0

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

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



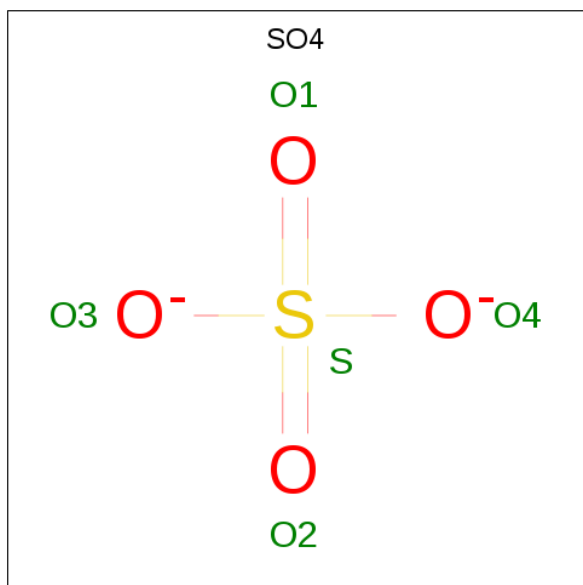
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 1	O 3	0	0
3	B	1	Total 4	C 1	O 3	0	0
3	C	1	Total 4	C 1	O 3	0	0
3	D	1	Total 4	C 1	O 3	0	0
3	E	1	Total 4	C 1	O 3	0	0
3	F	1	Total 4	C 1	O 3	0	0
3	G	1	Total 4	C 1	O 3	0	0
3	H	1	Total 4	C 1	O 3	0	0
3	I	1	Total 4	C 1	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	J	1	Total	C	O	0	0
			4	1	3		
3	K	1	Total	C	O	0	0
			4	1	3		
3	L	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



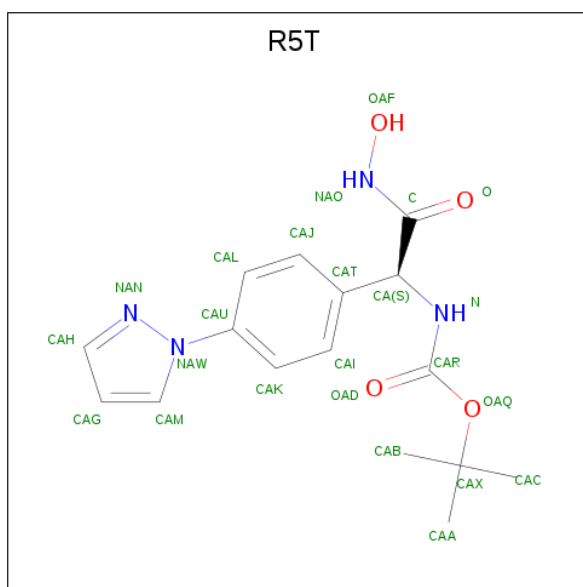
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is tert-butyl {(1S)-2-(hydroxyamino)-2-oxo-1-[4-(1H-pyrazol-1-yl)phenyl]ethyl}c arbamate (three-letter code: R5T) (formula: C₁₆H₂₀N₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			24	16	4	4		
5	B	1	Total	C	N	O	0	0
			24	16	4	4		
5	C	1	Total	C	N	O	0	0
			24	16	4	4		
5	D	1	Total	C	N	O	0	0
			24	16	4	4		
5	E	1	Total	C	N	O	0	0
			24	16	4	4		
5	F	1	Total	C	N	O	0	0
			24	16	4	4		
5	G	1	Total	C	N	O	0	0
			24	16	4	4		
5	H	1	Total	C	N	O	0	0
			24	16	4	4		
5	I	1	Total	C	N	O	0	0
			24	16	4	4		
5	J	1	Total	C	N	O	0	0
			24	16	4	4		
5	K	1	Total	C	N	O	0	0
			24	16	4	4		
5	L	1	Total	C	N	O	0	0
			21	13	4	4		

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



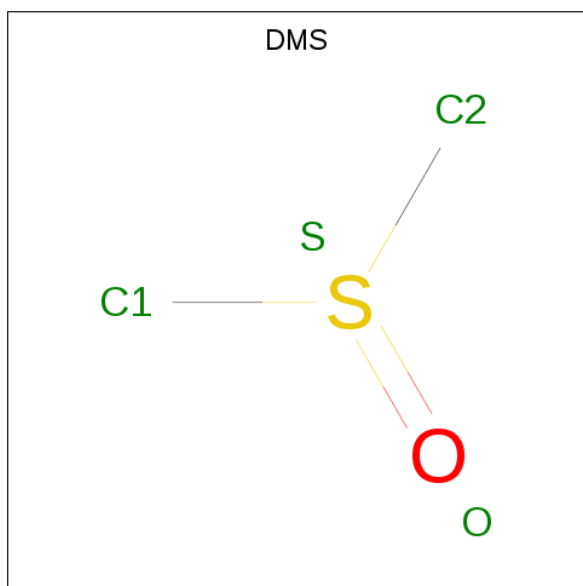
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	6	3		
6	B	1	Total	C	O	0	0
			14	9	5		
6	B	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			12	8	4		
6	C	1	Total	C	O	0	0
			9	6	3		
6	C	1	Total	C	O	0	0
			8	5	3		
6	D	1	Total	C	O	0	0
			9	6	3		
6	E	1	Total	C	O	0	0
			12	8	4		
6	E	1	Total	C	O	0	0
			13	9	4		
6	E	1	Total	C	O	0	0
			8	6	2		
6	F	1	Total	C	O	0	0
			8	6	2		
6	F	1	Total	C	O	0	0
			8	6	2		
6	G	1	Total	C	O	0	0
			7	5	2		
6	G	1	Total	C	O	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	C	O	0	0
			13	9	4		
6	I	1	Total	C	O	0	0
			8	5	3		
6	J	1	Total	C	O	0	0
			9	6	3		
6	J	1	Total	C	O	0	0
			12	8	4		
6	K	1	Total	C	O	0	0
			13	9	4		
6	L	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	G	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 8 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	160	Total	O	0	0
			160	160		
8	B	130	Total	O	0	0
			130	130		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	169	Total 169	O 169	0	0
8	D	151	Total 151	O 151	0	0
8	E	132	Total 132	O 132	0	0
8	F	94	Total 94	O 94	0	0
8	G	149	Total 149	O 149	0	0
8	H	117	Total 117	O 117	0	0
8	I	164	Total 164	O 164	0	0
8	J	154	Total 154	O 154	0	0
8	K	157	Total 157	O 157	0	0
8	L	114	Total 114	O 114	0	0

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Chain A: 

bits

Position

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200

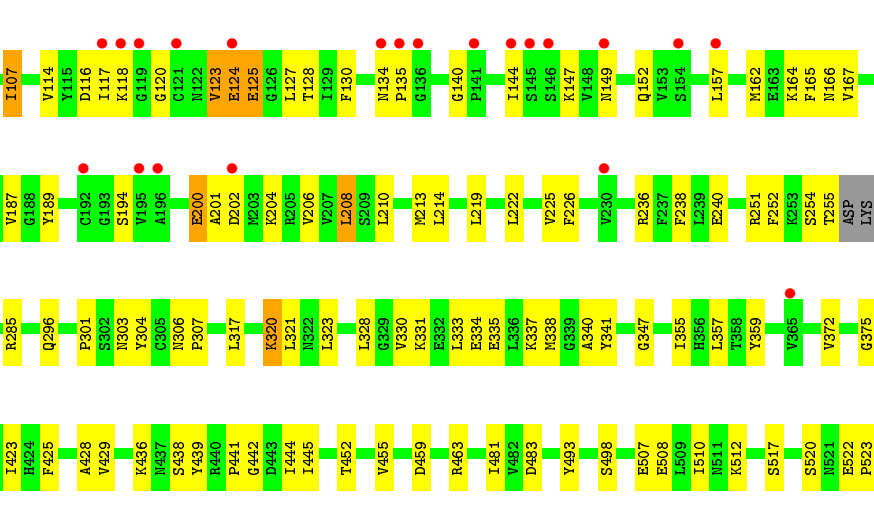
100%

76%

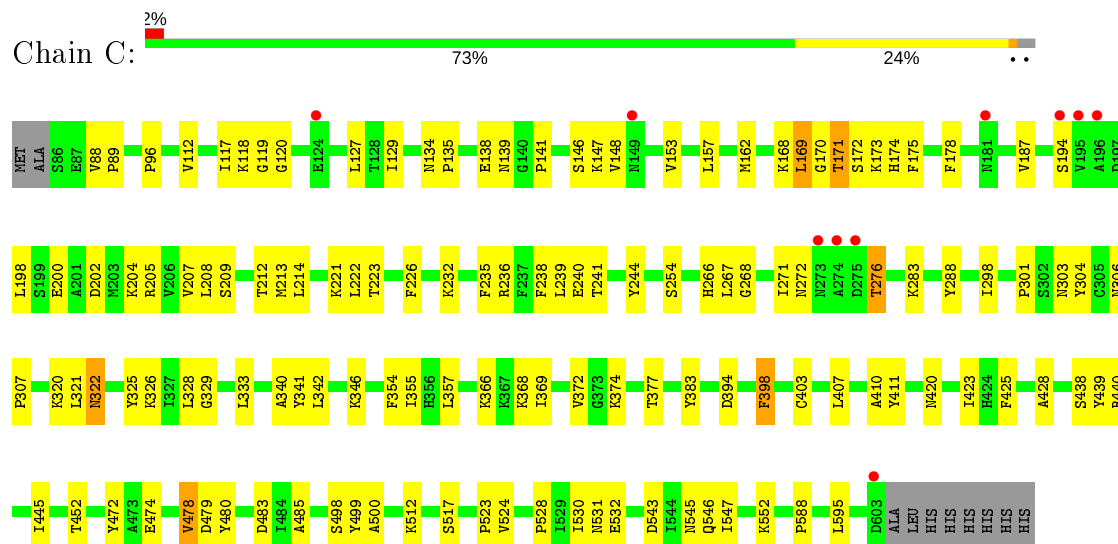
20%

• •

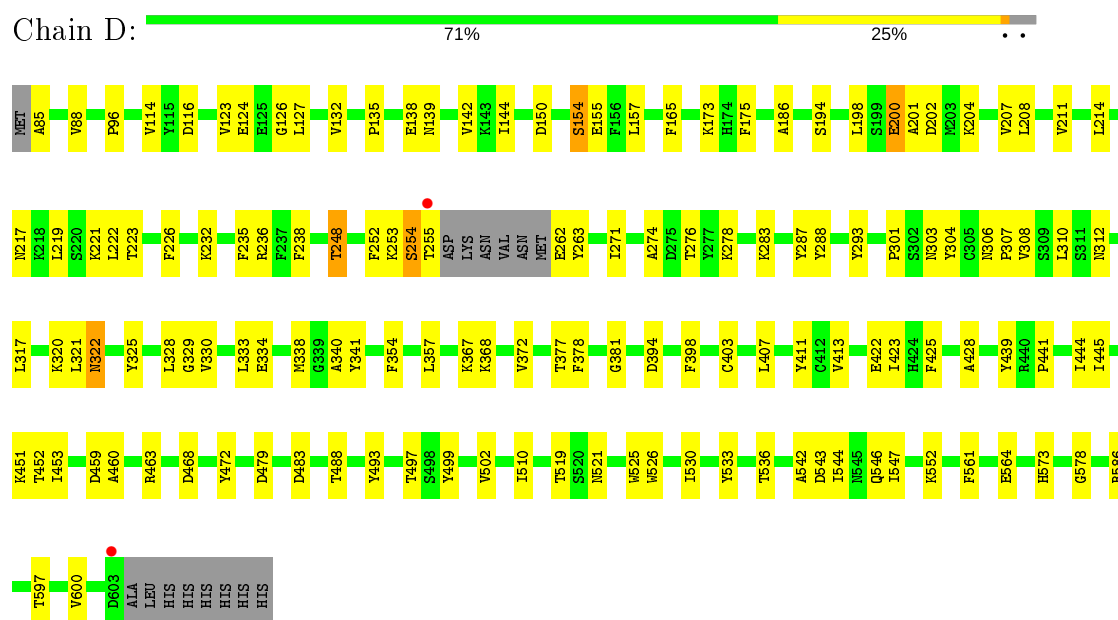
Sequence logo for Chain A showing information content (bits) across 200 positions. The y-axis is labeled 'bits' and ranges from 0 to 1. The x-axis is labeled 'Position' and ranges from 1 to 200. The logo shows a high concentration of 'A' at position 1 (approx. 0.8 bits) and 'G' at position 2 (approx. 0.7 bits). Other positions show lower information content, mostly below 0.2 bits.

- Chain B:
- 
- 5% 73% 23%
- Chain B:
- Y411 C412 V413 V421 E422 I423 F425 A428 V429 K436 N437 S438 Y439 R440 P441 G442 I444 I445 T452 V455 D459 R463 I461 V462 D463 Y463 S468 E507 E508 L509 I510 N511 K512 S517 S520 E522 P523 W526 T536 L537 N543
- A274 T275 E282 R285 Q296 P301 N302 Y304 N306 P307 C311 S312 K320 L321 N322 L323 L328 G329 V330 K331 E332 L333 E334 E335 K337 N338 G339 A340 Y341 G347 I355 H356 L357 T358 Y359 V365 V372 G375 I376 T377 G381 F398
- N181 K182 N183 S184 Y185 A186 G188 Y189 C192 G193 S194 Y195 A196 E200 A201 M203 K204 R205 V206 V207 L208 S209 L210 M213 L214 L219 L222 V225 F226 V230 R236 F237 F238 L239 E240 R251 F252 K253 S254 T255 ASP LYS ASN VAL M261 Y270 N179 F178 F190

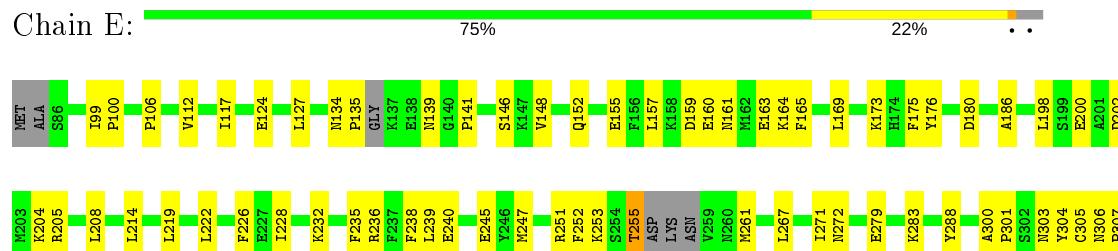
- Molecule 1: M17 leucyl aminopeptidase

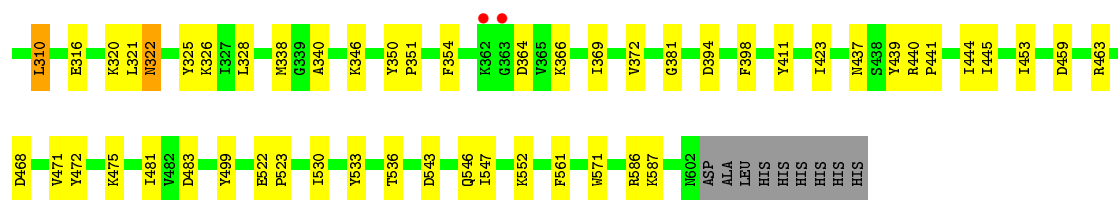


- Molecule 1: M17 leucyl aminopeptidase

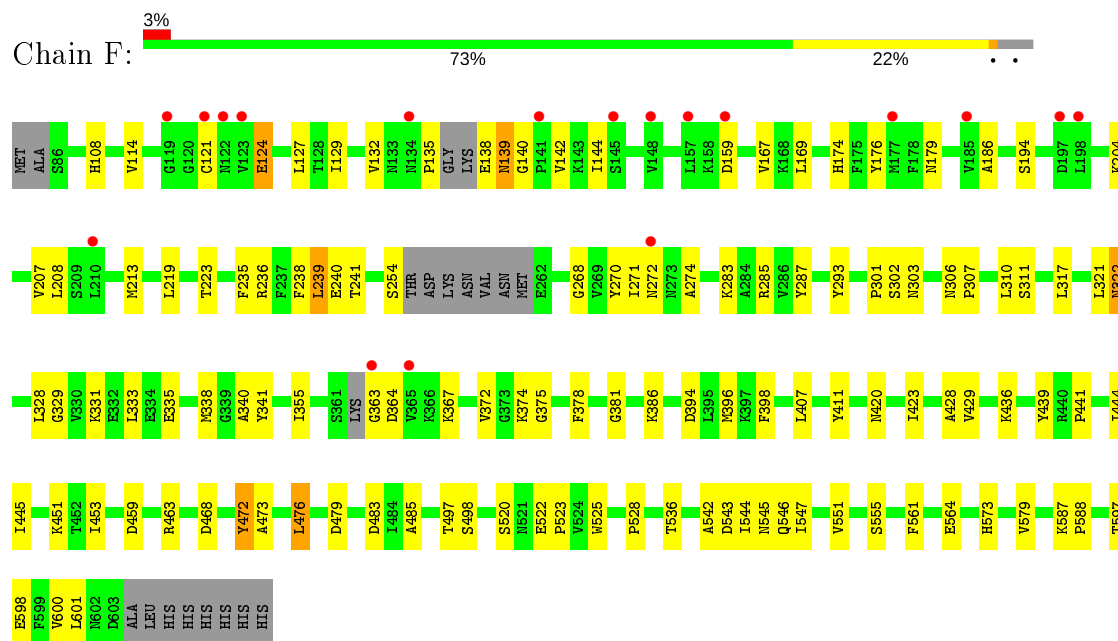


- Molecule 1: M17 leucyl aminopeptidase

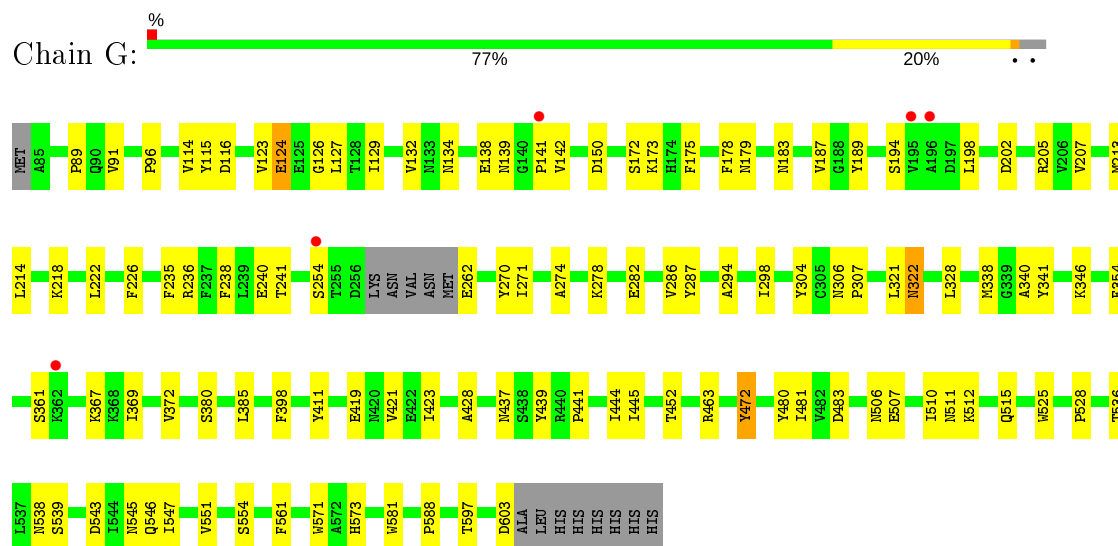




• Molecule 1: M17 leucyl aminopeptidase

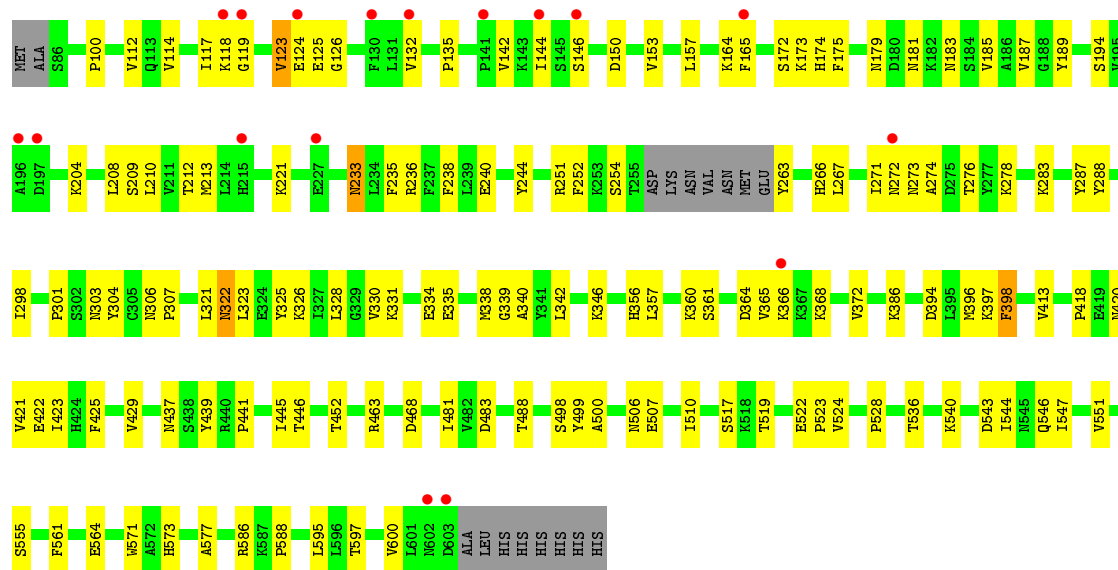


• Molecule 1: M17 leucyl aminopeptidase

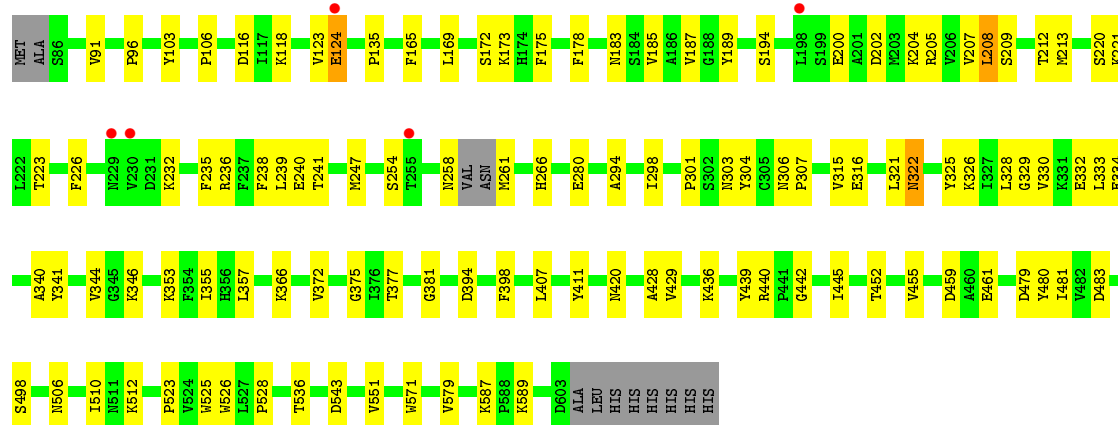
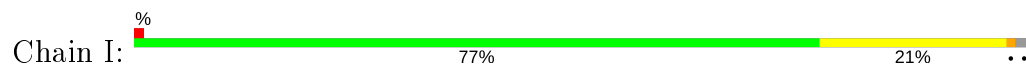


• Molecule 1: M17 leucyl aminopeptidase

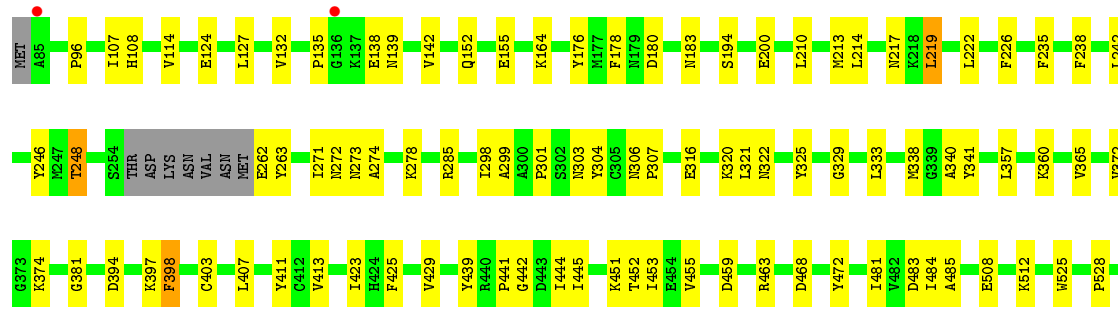
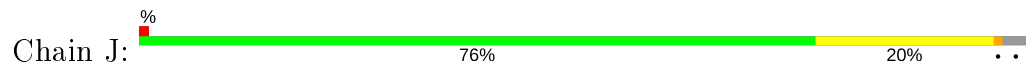




• Molecule 1: M17 leucyl aminopeptidase

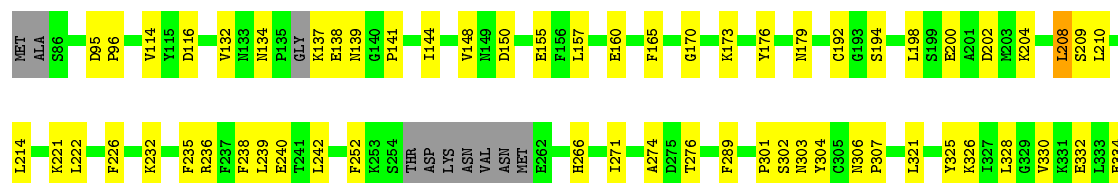


• Molecule 1: M17 leucyl aminopeptidase

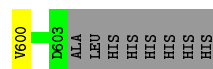
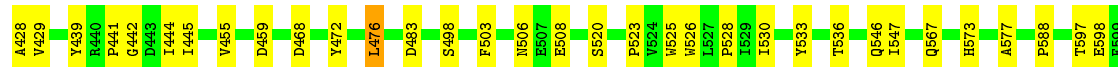
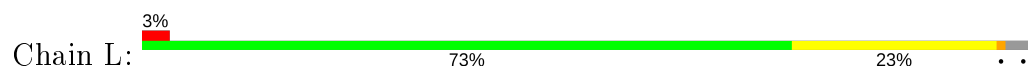




• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.90Å 175.93Å 231.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.70 – 2.60 46.70 – 2.60	Depositor EDS
% Data completeness (in resolution range)	87.1 (46.70-2.60) 77.7 (46.70-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, R_{free}	0.211 , 0.269 0.211 , 0.270	Depositor DCC
R_{free} test set	9435 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	49091	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 45.60 % 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 1.2912e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CO3, 1PE, DMS, SO4, R5T

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	0.22	0/4025	0.38	0/5459
1	B	0.23	0/3946	0.41	0/5361
1	C	0.21	0/4027	0.39	0/5465
1	D	0.22	0/3995	0.39	0/5420
1	E	0.23	0/3989	0.39	0/5412
1	F	0.21	0/3860	0.39	0/5254
1	G	0.21	0/4021	0.38	0/5453
1	H	0.21	0/3955	0.39	0/5373
1	I	0.21	0/3985	0.39	0/5410
1	J	0.22	0/3987	0.38	0/5409
1	K	0.21	0/3955	0.38	0/5368
1	L	0.22	0/3897	0.41	0/5298
All	All	0.22	0/47642	0.39	0/64682

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3945	0	3876	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3869	0	3760	106	0
1	C	3949	0	3873	100	1
1	D	3918	0	3847	107	0
1	E	3913	0	3830	85	2
1	F	3785	0	3598	102	0
1	G	3944	0	3875	85	0
1	H	3878	0	3776	112	0
1	I	3908	0	3800	84	1
1	J	3910	0	3840	84	0
1	K	3879	0	3795	78	1
1	L	3823	0	3664	98	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	4	0	0	1	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
3	I	4	0	0	0	0
3	J	4	0	0	0	0
3	K	4	0	0	0	0
3	L	4	0	0	0	0
4	A	20	0	0	0	0
4	B	10	0	0	2	0
4	C	15	0	0	0	0
4	E	5	0	0	0	0
4	F	10	0	0	1	0
4	G	10	0	0	0	0
4	H	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	10	0	0	0	0
4	K	15	0	0	1	0
4	L	15	0	0	1	0
5	A	24	0	20	0	0
5	B	24	0	19	0	0
5	C	24	0	20	0	0
5	D	24	0	19	1	0
5	E	24	0	19	0	0
5	F	24	0	19	1	0
5	G	24	0	19	1	0
5	H	24	0	19	1	0
5	I	24	0	20	0	0
5	J	24	0	19	0	0
5	K	24	0	19	0	0
5	L	21	0	10	1	0
6	A	9	0	10	2	0
6	B	21	0	26	6	0
6	C	29	0	32	13	0
6	D	9	0	10	1	0
6	E	33	0	36	10	0
6	F	16	0	16	2	0
6	G	17	0	16	2	0
6	I	21	0	22	3	0
6	J	21	0	22	3	0
6	K	13	0	14	1	0
6	L	8	0	8	0	0
7	G	4	6	6	2	0
8	A	160	0	0	5	0
8	B	130	0	0	1	0
8	C	169	0	0	1	0
8	D	151	0	0	5	0
8	E	132	0	0	4	0
8	F	94	0	0	1	0
8	G	149	0	0	9	1
8	H	117	0	0	5	0
8	I	164	0	0	7	0
8	J	154	0	0	3	0
8	K	157	0	0	3	0
8	L	114	0	0	5	0
All	All	49085	6	45974	1047	3

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 11.

The worst 5 of 1047 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:157:LEU:HA	1:L:162:MET:HE3	1.42	0.99
1:G:545:ASN:ND2	8:G:1180:HOH:O	1.98	0.97
1:I:366:LYS:HE2	1:I:420:ASN:HB3	1.47	0.94
1:F:174:HIS:HB3	1:F:213:MET:HE1	1.48	0.94
1:L:360:LYS:HD2	1:L:422:GLU:HG3	1.52	0.90

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:479:ASP:OD1	1:K:366:LYS:NZ[4_456]	2.18	0.02
1:C:479:ASP:OD1	1:E:366:LYS:NZ[4_455]	2.19	0.01
1:E:124:GLU:OE1	8:G:1223:HOH:O[3_645]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	511/528 (97%)	495 (97%)	12 (2%)	4 (1%)	19	39
1	B	507/528 (96%)	487 (96%)	18 (4%)	2 (0%)	34	57
1	C	516/528 (98%)	500 (97%)	13 (2%)	3 (1%)	25	47
1	D	509/528 (96%)	493 (97%)	13 (3%)	3 (1%)	25	47
1	E	507/528 (96%)	492 (97%)	13 (3%)	2 (0%)	34	57
1	F	500/528 (95%)	483 (97%)	14 (3%)	3 (1%)	25	47
1	G	510/528 (97%)	494 (97%)	13 (2%)	3 (1%)	25	47
1	H	507/528 (96%)	488 (96%)	16 (3%)	3 (1%)	25	47
1	I	512/528 (97%)	497 (97%)	13 (2%)	2 (0%)	34	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	508/528 (96%)	494 (97%)	12 (2%)	2 (0%)	34	57
1	K	503/528 (95%)	488 (97%)	14 (3%)	1 (0%)	47	71
1	L	501/528 (95%)	488 (97%)	13 (3%)	0	100	100
All	All	6091/6336 (96%)	5899 (97%)	164 (3%)	28 (0%)	29	52

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	ASN
1	B	124	GLU
1	D	254	SER
1	D	322	ASN
1	E	139	ASN

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%)	417 (99%)	4 (1%)	76	90
1	B	405/455 (89%)	394 (97%)	11 (3%)	44	71
1	C	418/455 (92%)	407 (97%)	11 (3%)	46	72
1	D	414/455 (91%)	405 (98%)	9 (2%)	52	76
1	E	414/455 (91%)	406 (98%)	8 (2%)	57	79
1	F	383/455 (84%)	375 (98%)	8 (2%)	53	77
1	G	421/455 (92%)	418 (99%)	3 (1%)	84	94
1	H	408/455 (90%)	400 (98%)	8 (2%)	55	78
1	I	408/455 (90%)	402 (98%)	6 (2%)	65	83
1	J	413/455 (91%)	405 (98%)	8 (2%)	57	79
1	K	410/455 (90%)	404 (98%)	6 (2%)	65	83
1	L	394/455 (87%)	384 (98%)	10 (2%)	47	73
All	All	4909/5460 (90%)	4817 (98%)	92 (2%)	57	79

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	439	TYR
1	G	398	PHE
1	L	225	VAL
1	E	472	TYR
1	F	398	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	174	HIS
1	L	266	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 24 are monoatomic - leaving 68 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	$\# Z > 2$
4	SO4	C	1006	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	K	1005	-	4,4,4	0.15	0	6,6,6	0.04	0
3	CO3	J	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	L	1008	-	4,4,4	0.13	0	6,6,6	0.05	0
6	1PE	J	1005	-	8,8,15	0.47	0	7,7,14	0.30	0
6	1PE	B	1007	-	13,13,15	0.45	0	12,12,14	0.40	0
4	SO4	K	1004	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	L	1004	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	E	1008	-	4,4,4	0.14	0	6,6,6	0.05	0
5	R5T	E	1004	2	24,25,25	2.56	6 (25%)	33,35,35	2.70	9 (27%)
4	SO4	G	1005	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	A	1009	-	4,4,4	0.14	0	6,6,6	0.05	0
6	1PE	G	1008	-	9,9,15	0.45	0	8,8,14	0.49	0
5	R5T	G	1006	2	24,25,25	2.52	6 (25%)	33,35,35	2.69	6 (18%)
4	SO4	J	1008	-	4,4,4	0.14	0	6,6,6	0.05	0
5	R5T	J	1004	2	24,25,25	2.52	5 (20%)	33,35,35	2.75	7 (21%)
5	R5T	I	1004	2	24,25,25	2.49	6 (25%)	33,35,35	2.67	6 (18%)
4	SO4	K	1006	-	4,4,4	0.14	0	6,6,6	0.05	0
3	CO3	A	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	I	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	E	1006	-	12,12,15	0.47	0	11,11,14	0.33	0
6	1PE	F	1007	-	7,7,15	0.50	0	6,6,14	0.25	0
6	1PE	G	1007	-	6,6,15	0.49	0	5,5,14	0.27	0
4	SO4	G	1004	-	4,4,4	0.14	0	6,6,6	0.05	0
6	1PE	B	1008	-	6,6,15	0.43	0	5,5,14	0.31	0
4	SO4	L	1005	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	F	1004	-	4,4,4	0.14	0	6,6,6	0.06	0
6	1PE	C	1008	-	11,11,15	0.46	0	10,10,14	0.27	0
3	CO3	D	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	B	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	A	1006	-	4,4,4	0.14	0	6,6,6	0.05	0
6	1PE	A	1008	-	8,8,15	0.47	0	7,7,14	0.26	0
4	SO4	J	1007	-	4,4,4	0.13	0	6,6,6	0.05	0
6	1PE	I	1006	-	7,7,15	0.43	0	6,6,14	0.27	0
4	SO4	B	1005	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	F	1008	-	4,4,4	0.14	0	6,6,6	0.05	0
5	R5T	K	1007	2	24,25,25	2.54	5 (20%)	33,35,35	2.82	7 (21%)
6	1PE	J	1006	-	11,11,15	0.47	0	10,10,14	0.24	0
3	CO3	K	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	SO4	A	1004	-	4,4,4	0.15	0	6,6,6	0.05	0
6	1PE	C	1010	-	7,7,15	0.42	0	6,6,14	0.26	0
4	SO4	A	1005	-	4,4,4	0.14	0	6,6,6	0.05	0
5	R5T	C	1007	2	24,25,25	2.52	6 (25%)	33,35,35	2.68	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	1PE	F	1006	-	7,7,15	0.48	0	6,6,14	0.33	0
5	R5T	L	1006	2	21,22,25	2.65	5 (23%)	27,29,35	2.96	8 (29%)
5	R5T	H	1005	2	24,25,25	2.43	6 (25%)	33,35,35	2.66	8 (24%)
6	1PE	K	1008	-	12,12,15	0.46	0	11,11,14	0.26	0
3	CO3	H	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	F	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	E	1005	-	11,11,15	0.45	0	10,10,14	0.26	0
6	1PE	D	1005	-	8,8,15	0.48	0	7,7,14	0.26	0
4	SO4	H	1004	-	4,4,4	0.14	0	6,6,6	0.04	0
3	CO3	L	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
3	CO3	C	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
5	R5T	B	1006	2	24,25,25	2.51	5 (20%)	33,35,35	2.70	7 (21%)
3	CO3	G	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	L	1007	-	7,7,15	0.53	0	6,6,14	0.24	0
4	SO4	C	1004	-	4,4,4	0.14	0	6,6,6	0.04	0
5	R5T	D	1004	2	24,25,25	2.46	5 (20%)	33,35,35	2.76	10 (30%)
4	SO4	B	1004	-	4,4,4	0.15	0	6,6,6	0.04	0
3	CO3	E	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
7	DMS	G	1009	-	3,3,3	0.65	0	3,3,3	0.47	0
5	R5T	A	1007	2	24,25,25	2.54	5 (20%)	33,35,35	2.65	6 (18%)
4	SO4	C	1005	-	4,4,4	0.14	0	6,6,6	0.05	0
6	1PE	C	1009	-	8,8,15	0.47	0	7,7,14	0.28	0
6	1PE	E	1007	-	7,7,15	0.47	0	6,6,14	0.45	0
5	R5T	F	1005	2	24,25,25	2.61	6 (25%)	33,35,35	2.53	7 (21%)
6	1PE	I	1005	-	12,12,15	0.47	0	11,11,14	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	I	1005	-	-	0/10/10/13	-
6	1PE	J	1005	-	-	2/6/6/13	-
5	R5T	G	1006	2	-	6/23/23/23	0/2/2/2
5	R5T	J	1004	2	-	9/23/23/23	0/2/2/2
5	R5T	I	1004	2	-	8/23/23/23	0/2/2/2
6	1PE	E	1006	-	-	5/10/10/13	-
6	1PE	A	1008	-	-	0/6/6/13	-
6	1PE	G	1007	-	-	1/4/4/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	F	1007	-	-	0/5/5/13	-
6	1PE	B	1008	-	-	0/4/4/13	-
6	1PE	C	1008	-	-	1/9/9/13	-
5	R5T	B	1006	2	-	4/23/23/23	0/2/2/2
5	R5T	K	1007	2	-	11/23/23/23	0/2/2/2
6	1PE	J	1006	-	-	0/9/9/13	-
5	R5T	H	1005	2	-	9/23/23/23	0/2/2/2
6	1PE	G	1008	-	-	6/7/7/13	-
6	1PE	C	1010	-	-	1/5/5/13	-
5	R5T	C	1007	2	-	7/23/23/23	0/2/2/2
5	R5T	L	1006	2	-	4/20/20/23	0/2/2/2
6	1PE	C	1009	-	-	0/6/6/13	-
6	1PE	K	1008	-	-	0/10/10/13	-
6	1PE	I	1006	-	-	0/5/5/13	-
6	1PE	E	1005	-	-	0/9/9/13	-
6	1PE	D	1005	-	-	0/6/6/13	-
6	1PE	L	1007	-	-	1/5/5/13	-
6	1PE	B	1007	-	-	3/11/11/13	-
5	R5T	D	1004	2	-	8/23/23/23	0/2/2/2
5	R5T	E	1004	2	-	9/23/23/23	0/2/2/2
5	R5T	A	1007	2	-	5/23/23/23	0/2/2/2
6	1PE	F	1006	-	-	0/5/5/13	-
6	1PE	E	1007	-	-	3/5/5/13	-
5	R5T	F	1005	2	-	6/23/23/23	0/2/2/2

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1004	R5T	CAT-CA	-8.29	1.39	1.52
5	F	1005	R5T	CAT-CA	-8.28	1.39	1.52
5	K	1007	R5T	CAT-CA	-8.15	1.39	1.52
5	J	1004	R5T	CAT-CA	-7.95	1.39	1.52
5	L	1006	R5T	CAT-CA	-7.93	1.39	1.52

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1005	R5T	CAH-NAN-NAW	9.16	110.36	103.70
5	I	1004	R5T	CAH-NAN-NAW	9.14	110.35	103.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	1006	R5T	CAU-NAW-NAN	8.95	126.74	118.80
5	L	1006	R5T	CAH-NAN-NAW	8.90	110.18	103.70
5	D	1004	R5T	CAH-NAN-NAW	8.87	110.15	103.70

There are no chirality outliers.

5 of 109 torsion outliers are listed below:

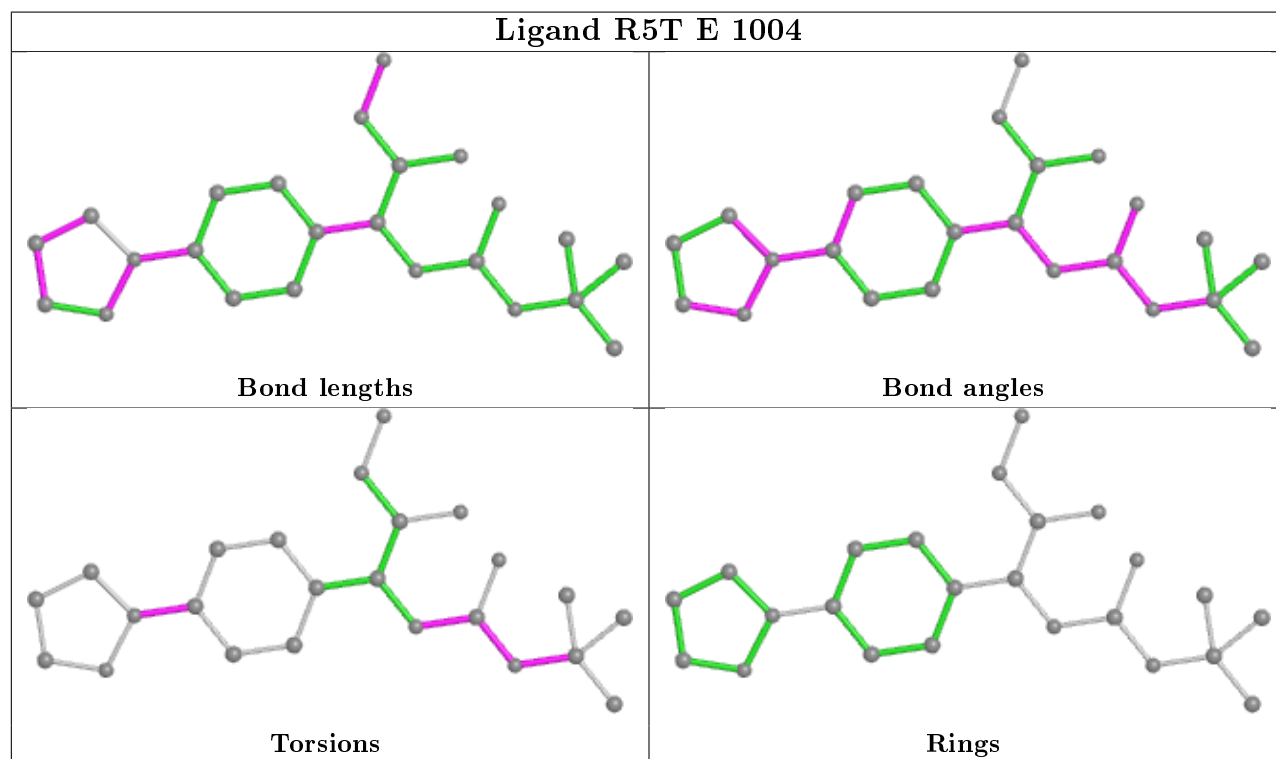
Mol	Chain	Res	Type	Atoms
5	I	1004	R5T	N-CAR-OAQ-CAX
5	K	1007	R5T	N-CAR-OAQ-CAX
5	K	1007	R5T	C-CA-N-CAR
5	K	1007	R5T	CAT-CA-N-CAR
5	C	1007	R5T	O-C-CA-N

There are no ring outliers.

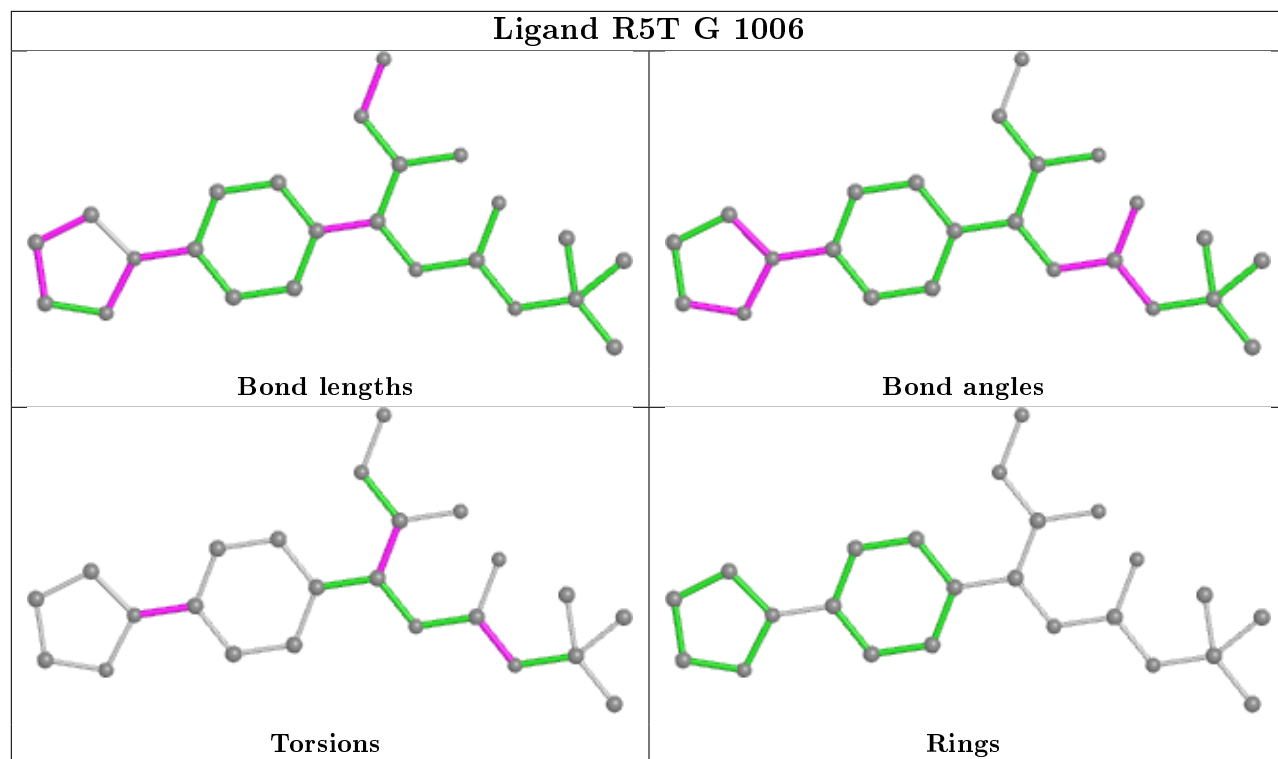
24 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1005	SO4	1	0
4	L	1008	SO4	1	0
6	B	1007	1PE	6	0
6	G	1008	1PE	2	0
5	G	1006	R5T	1	0
3	A	1002	CO3	1	0
6	E	1006	1PE	8	0
4	F	1004	SO4	1	0
6	C	1008	1PE	2	0
6	A	1008	1PE	2	0
6	J	1006	1PE	3	0
6	C	1010	1PE	11	0
6	F	1006	1PE	2	0
5	L	1006	R5T	1	0
5	H	1005	R5T	1	0
6	K	1008	1PE	1	0
6	E	1005	1PE	3	0
6	D	1005	1PE	1	0
4	H	1004	SO4	1	0
5	D	1004	R5T	1	0
4	B	1004	SO4	2	0
7	G	1009	DMS	2	0
5	F	1005	R5T	1	0
6	I	1005	1PE	3	0

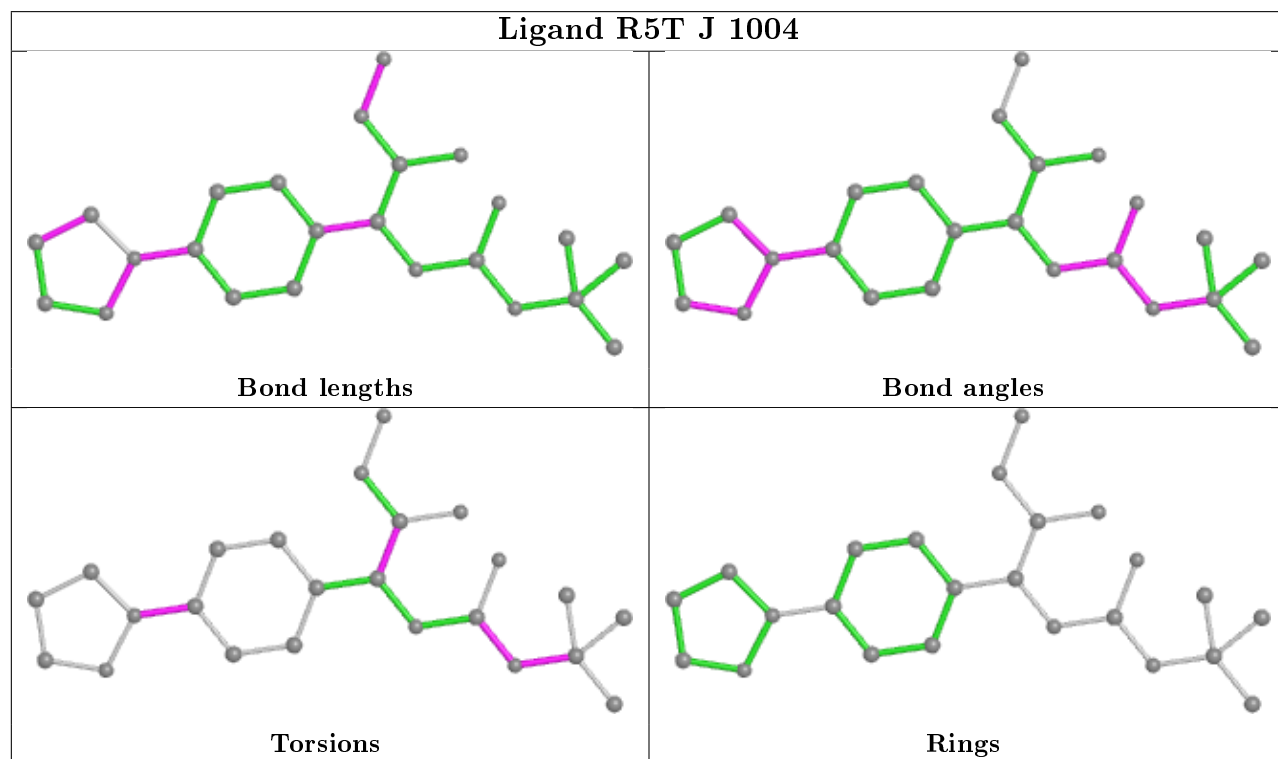
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



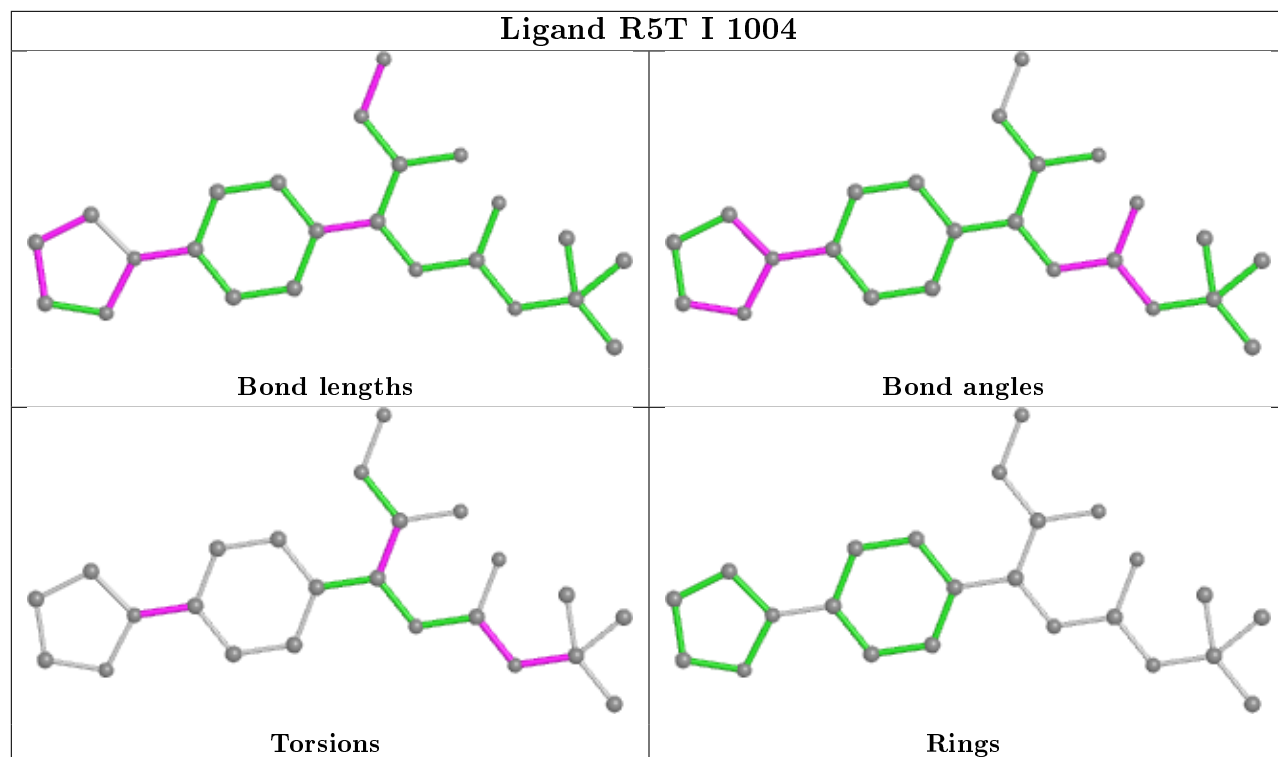
Ligand R5T G 1006



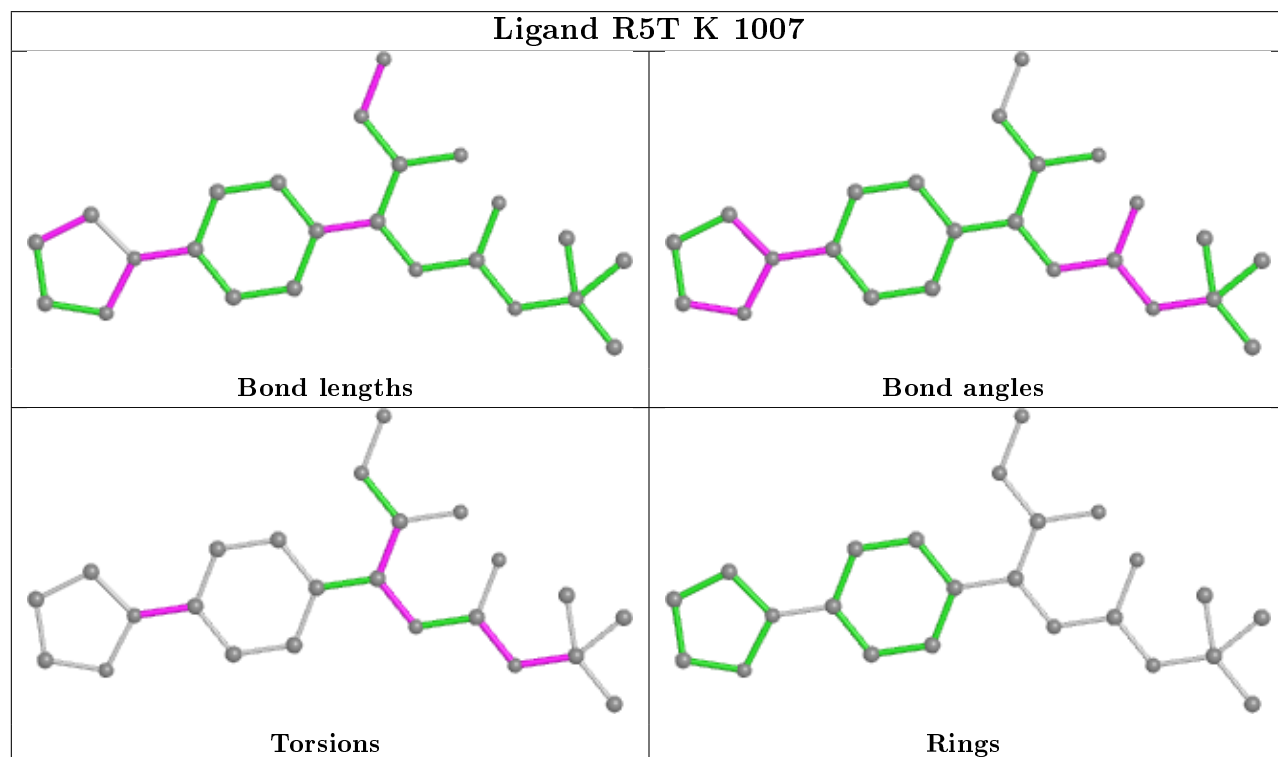
Ligand R5T J 1004



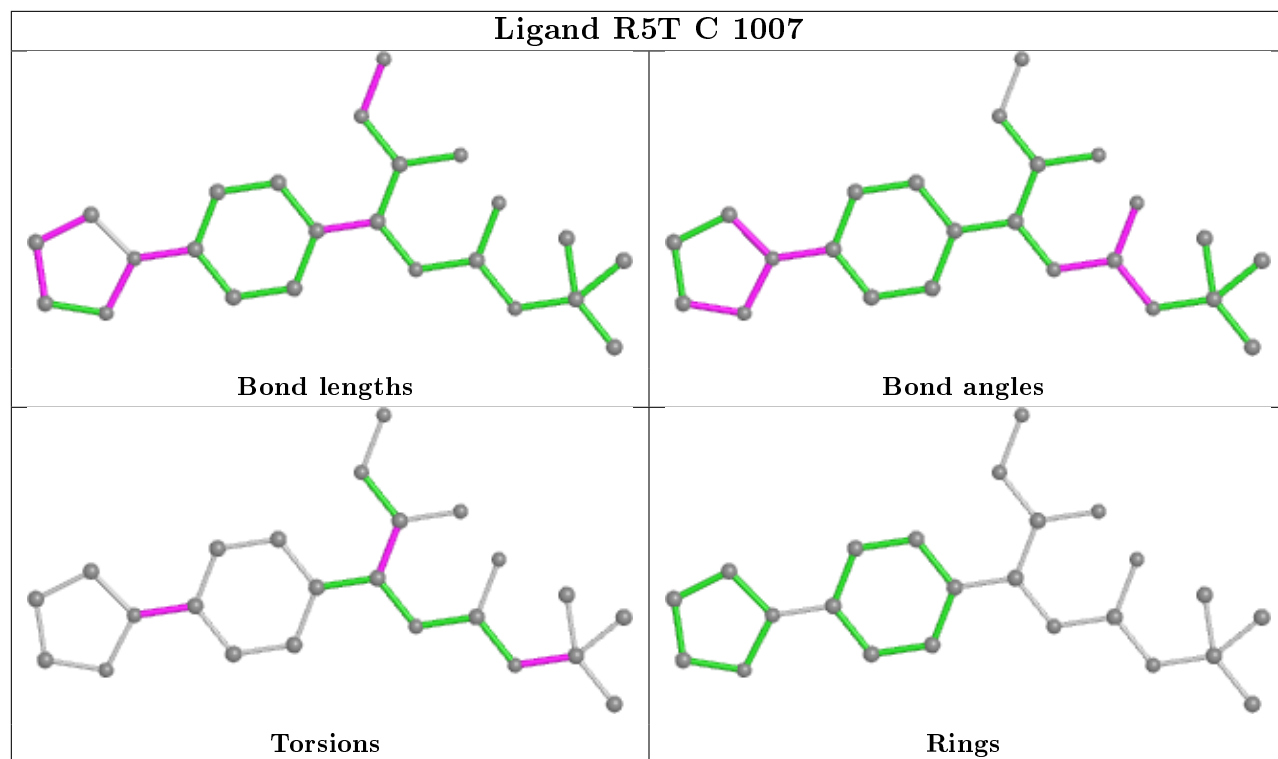
Ligand R5T I 1004



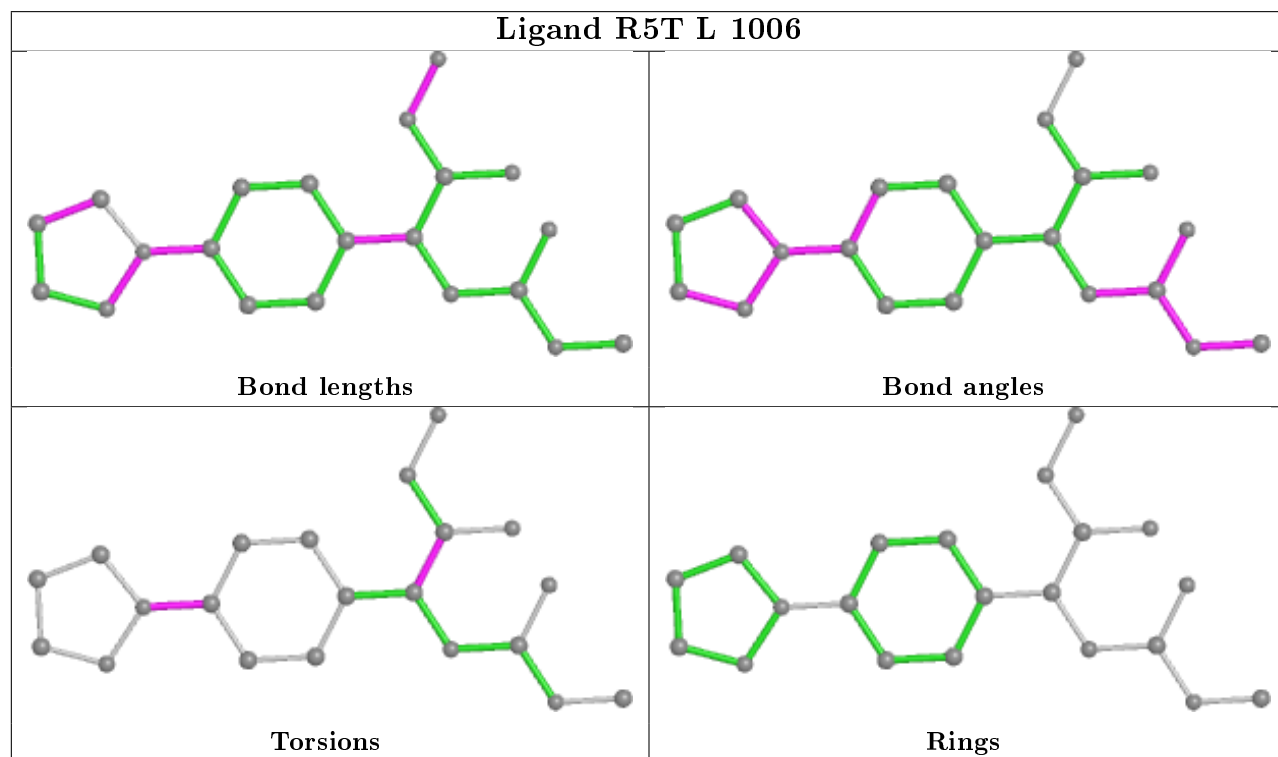
Ligand R5T K 1007



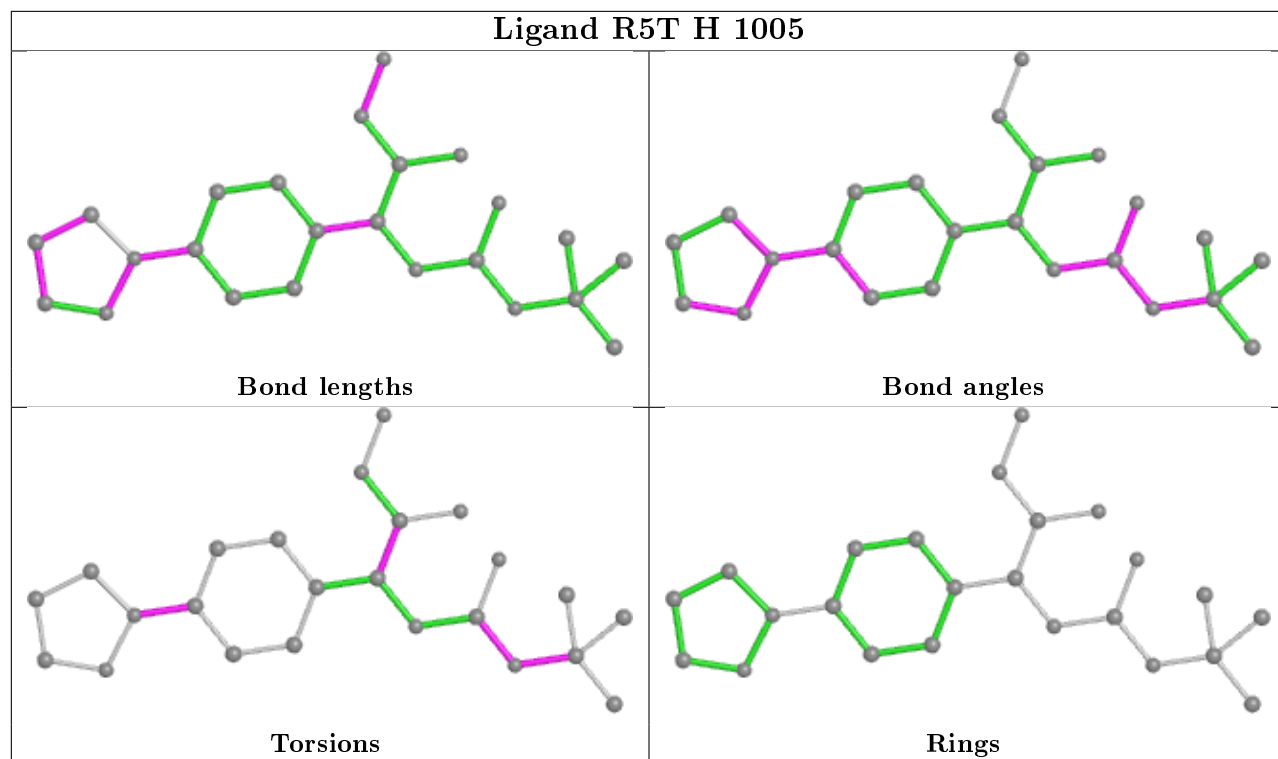
Ligand R5T C 1007



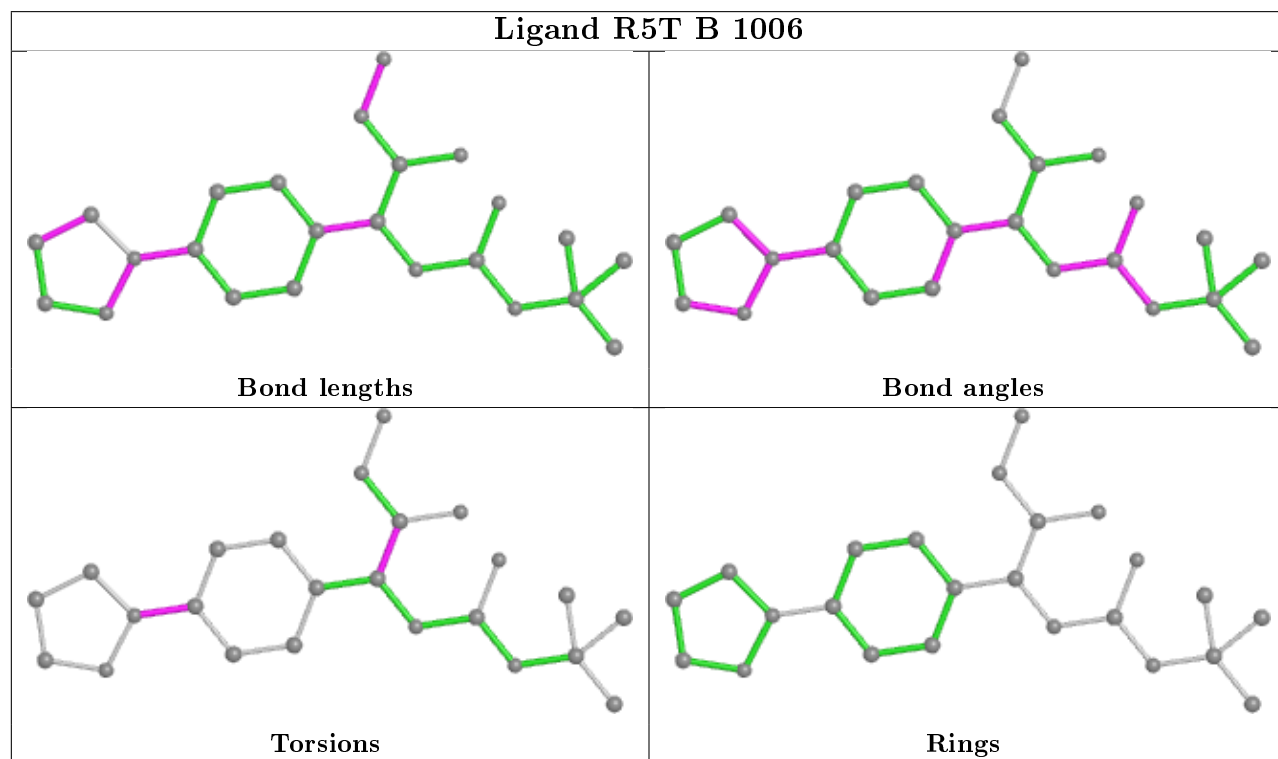
Ligand R5T L 1006



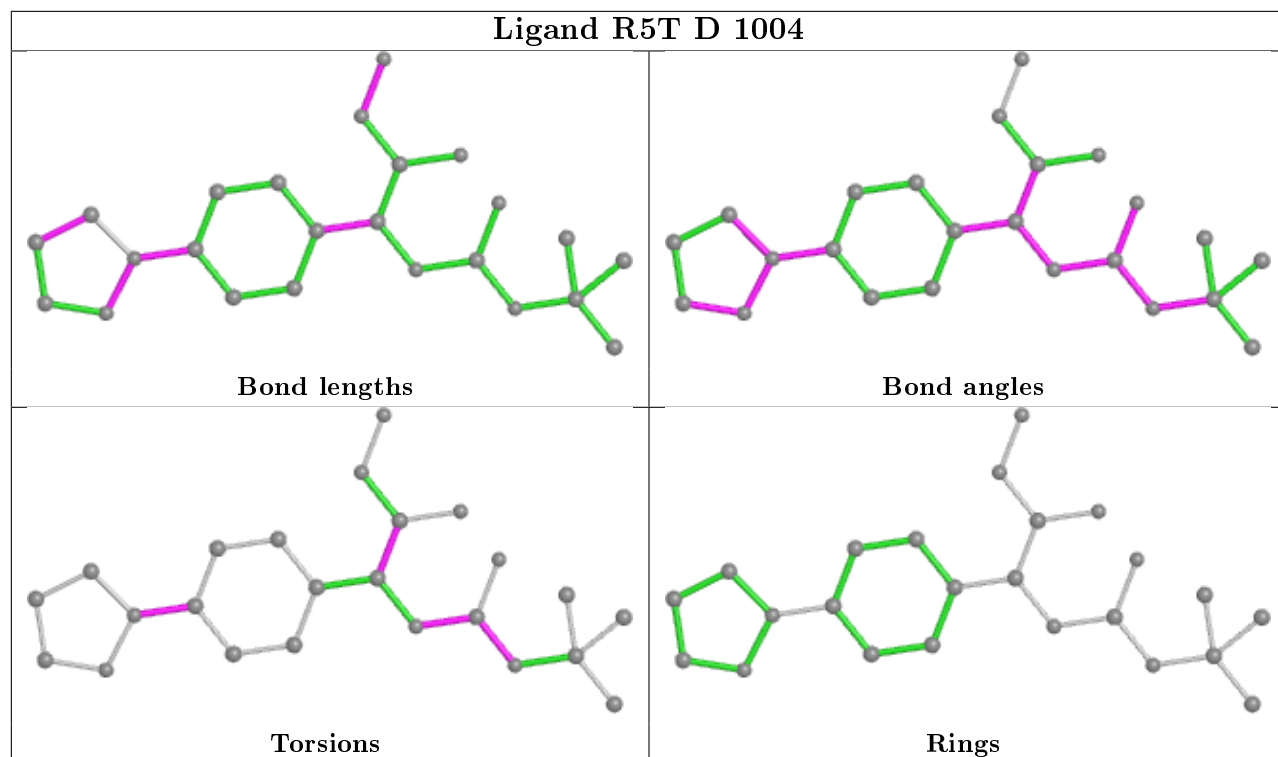
Ligand R5T H 1005



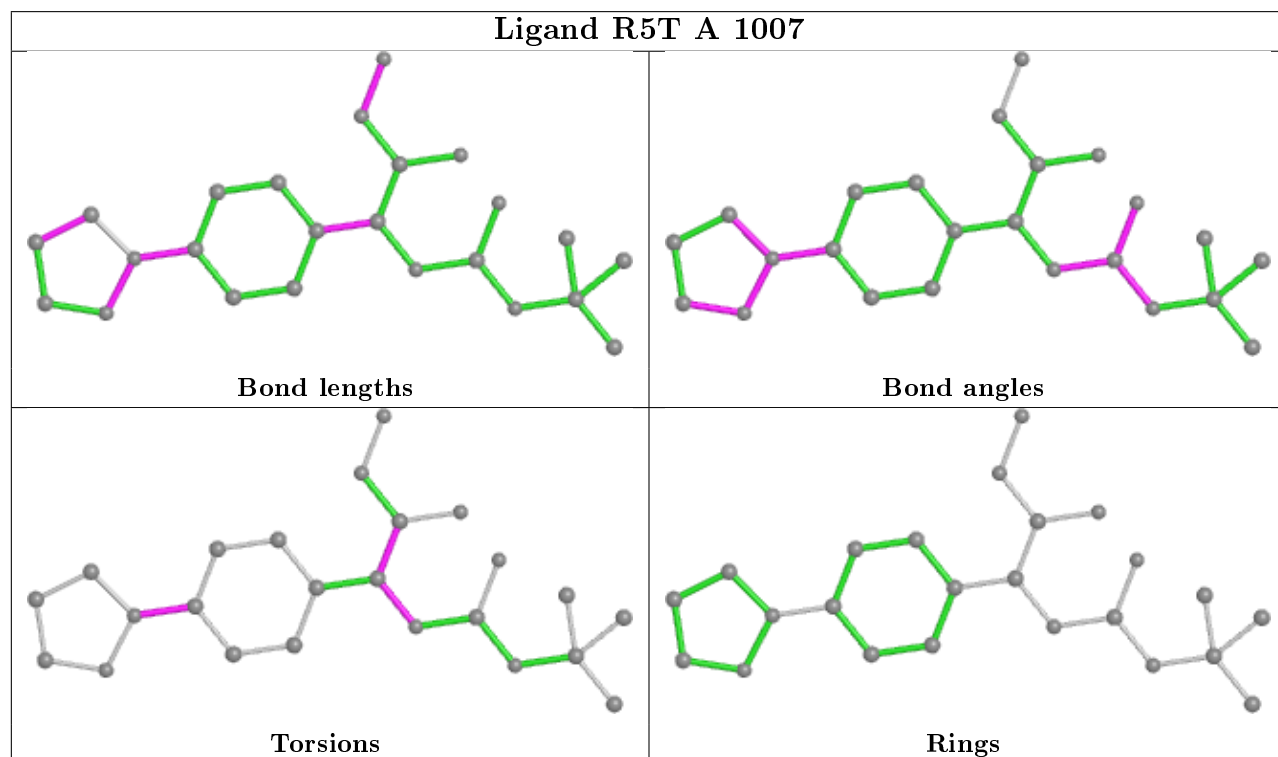
Ligand R5T B 1006

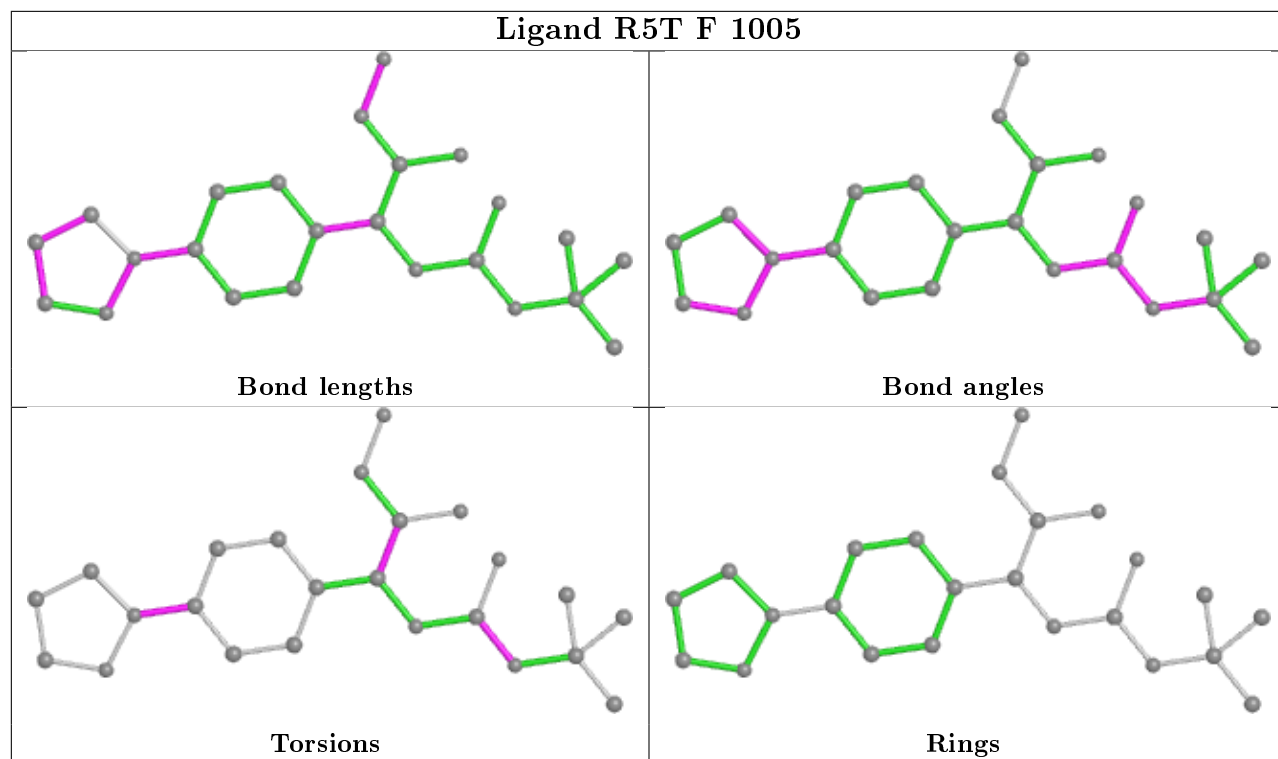


Ligand R5T D 1004



Ligand R5T A 1007





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	514/528 (97%)	-0.22	6 (1%) 79 76	27, 41, 65, 95	0
1	B	511/528 (96%)	0.15	26 (5%) 28 22	29, 48, 80, 113	1 (0%)
1	C	518/528 (98%)	-0.14	10 (1%) 66 62	27, 43, 72, 111	0
1	D	513/528 (97%)	-0.25	2 (0%) 92 91	28, 40, 63, 100	0
1	E	513/528 (97%)	-0.23	2 (0%) 92 91	31, 43, 64, 97	0
1	F	508/528 (96%)	0.04	18 (3%) 44 36	30, 48, 82, 101	0
1	G	514/528 (97%)	-0.22	5 (0%) 82 80	30, 42, 68, 103	0
1	H	511/528 (96%)	0.03	17 (3%) 46 39	29, 46, 79, 102	1 (0%)
1	I	516/528 (97%)	-0.20	5 (0%) 82 80	27, 42, 72, 127	0
1	J	512/528 (96%)	-0.19	3 (0%) 89 88	31, 43, 66, 95	0
1	K	509/528 (96%)	-0.23	1 (0%) 95 95	32, 44, 63, 89	0
1	L	509/528 (96%)	-0.01	15 (2%) 51 45	34, 49, 79, 144	0
All	All	6148/6336 (97%)	-0.12	110 (1%) 68 64	27, 44, 73, 144	2 (0%)

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	363	GLY	9.5
1	F	157	LEU	4.8
1	H	124	GLU	4.6
1	J	85	ALA	4.6
1	E	363	GLY	4.5

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	1PE	B	1007	14/16	0.80	0.26	54,69,82,82	0
6	1PE	E	1007	8/16	0.81	0.23	47,64,68,71	0
4	SO4	C	1006	5/5	0.81	0.19	115,118,121,124	0
6	1PE	J	1006	12/16	0.82	0.25	49,73,83,87	0
4	SO4	J	1007	5/5	0.83	0.33	126,131,132,133	0
6	1PE	C	1009	9/16	0.85	0.23	48,62,78,79	0
4	SO4	J	1008	5/5	0.86	0.28	118,119,124,127	0
4	SO4	L	1008	5/5	0.88	0.41	104,105,109,109	0
6	1PE	G	1007	7/16	0.89	0.22	56,58,68,72	0
6	1PE	C	1008	12/16	0.89	0.20	47,55,73,75	0
6	1PE	E	1005	12/16	0.89	0.18	42,60,68,70	0
5	R5T	I	1004	24/24	0.90	0.21	31,47,65,73	0
5	R5T	F	1005	24/24	0.90	0.22	41,60,74,85	0
6	1PE	E	1006	13/16	0.90	0.15	43,52,59,60	0
5	R5T	L	1006	21/24	0.90	0.19	34,49,58,61	0
3	CO3	C	1002	4/4	0.91	0.21	42,46,48,51	0
6	1PE	I	1005	13/16	0.91	0.22	51,59,62,64	0
4	SO4	A	1004	5/5	0.91	0.23	65,78,82,83	0
4	SO4	B	1005	5/5	0.91	0.16	85,86,92,93	0
4	SO4	L	1005	5/5	0.91	0.21	69,72,76,79	0
3	CO3	G	1002	4/4	0.91	0.20	30,34,44,54	0
6	1PE	F	1006	8/16	0.92	0.15	40,50,55,59	0
6	1PE	C	1010	8/16	0.92	0.27	40,47,58,60	0
6	1PE	K	1008	13/16	0.92	0.20	34,52,64,67	0
4	SO4	G	1004	5/5	0.92	0.20	83,90,90,95	0
6	1PE	I	1006	8/16	0.92	0.18	47,50,51,58	0
3	CO3	A	1002	4/4	0.93	0.15	27,37,37,40	0
5	R5T	A	1007	24/24	0.93	0.20	30,49,63,64	0
5	R5T	B	1006	24/24	0.93	0.19	28,52,65,66	0
5	R5T	K	1007	24/24	0.93	0.20	32,49,58,73	0
4	SO4	E	1008	5/5	0.93	0.20	86,87,90,91	0
3	CO3	D	1002	4/4	0.93	0.19	44,55,58,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	B	1003	1/1	0.93	0.05	41,41,41,41	0
5	R5T	G	1006	24/24	0.94	0.17	32,48,59,64	0
6	1PE	D	1005	9/16	0.94	0.17	49,50,54,58	0
5	R5T	D	1004	24/24	0.94	0.19	26,44,55,67	0
4	SO4	A	1006	5/5	0.94	0.12	71,74,79,83	0
5	R5T	H	1005	24/24	0.94	0.16	29,49,63,79	0
7	DMS	G	1009	4/4	0.94	0.25	39,53,74,76	0
4	SO4	A	1009	5/5	0.94	0.19	79,83,85,89	0
4	SO4	C	1005	5/5	0.94	0.29	84,85,89,105	0
5	R5T	J	1004	24/24	0.94	0.18	33,52,85,89	0
6	1PE	F	1007	8/16	0.94	0.19	32,44,49,56	0
3	CO3	F	1002	4/4	0.95	0.20	35,45,48,51	0
5	R5T	E	1004	24/24	0.95	0.17	31,62,70,75	0
4	SO4	F	1008	5/5	0.95	0.24	103,105,107,110	0
6	1PE	B	1008	7/16	0.95	0.17	42,49,51,57	0
5	R5T	C	1007	24/24	0.95	0.17	31,47,55,57	0
4	SO4	K	1005	5/5	0.95	0.14	70,72,77,89	0
4	SO4	G	1005	5/5	0.95	0.34	76,82,82,88	0
6	1PE	A	1008	9/16	0.95	0.18	41,45,51,53	0
4	SO4	C	1004	5/5	0.95	0.22	69,77,79,83	0
3	CO3	J	1002	4/4	0.96	0.17	30,36,40,40	0
6	1PE	L	1007	8/16	0.96	0.13	38,58,60,62	0
6	1PE	G	1008	10/16	0.96	0.15	39,48,61,65	0
4	SO4	K	1006	5/5	0.96	0.17	62,64,69,77	0
3	CO3	I	1002	4/4	0.96	0.16	26,31,31,45	0
3	CO3	K	1002	4/4	0.96	0.15	33,48,58,60	0
4	SO4	L	1004	5/5	0.96	0.14	86,86,91,92	0
6	1PE	J	1005	9/16	0.96	0.15	36,39,52,57	0
4	SO4	A	1005	5/5	0.97	0.15	60,66,68,83	0
3	CO3	E	1002	4/4	0.97	0.20	30,33,36,39	0
3	CO3	B	1002	4/4	0.97	0.15	28,28,29,34	0
2	ZN	D	1003	1/1	0.97	0.06	49,49,49,49	0
2	ZN	C	1001	1/1	0.97	0.07	42,42,42,42	0
2	ZN	B	1001	1/1	0.97	0.06	48,48,48,48	0
2	ZN	J	1001	1/1	0.97	0.07	52,52,52,52	0
2	ZN	H	1003	1/1	0.98	0.03	44,44,44,44	0
2	ZN	A	1003	1/1	0.98	0.08	56,56,56,56	0
2	ZN	G	1001	1/1	0.98	0.07	42,42,42,42	0
2	ZN	D	1001	1/1	0.98	0.06	43,43,43,43	0
2	ZN	K	1001	1/1	0.98	0.07	37,37,37,37	0
2	ZN	L	1003	1/1	0.98	0.08	52,52,52,52	0
2	ZN	G	1003	1/1	0.98	0.06	44,44,44,44	0

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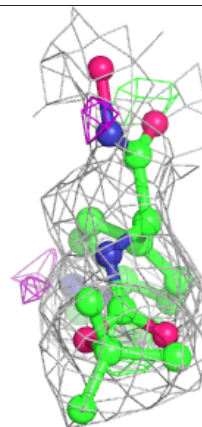
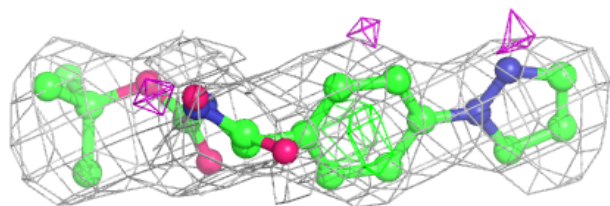
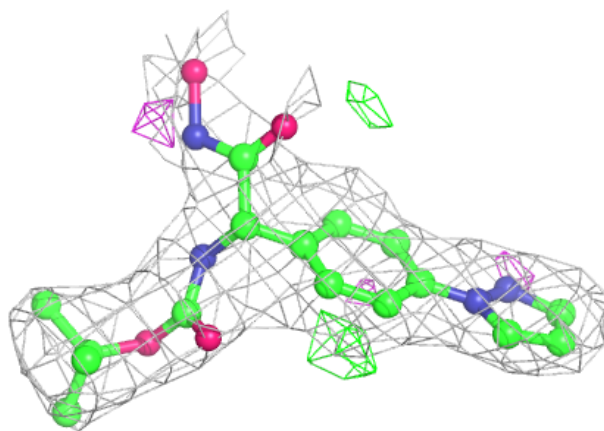
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	H	1004	5/5	0.98	0.13	26,26,40,49	0
4	SO4	B	1004	5/5	0.98	0.13	31,32,36,39	0
2	ZN	C	1003	1/1	0.98	0.08	43,43,43,43	0
3	CO3	L	1002	4/4	0.99	0.13	33,37,39,47	0
2	ZN	E	1003	1/1	0.99	0.07	48,48,48,48	0
2	ZN	L	1001	1/1	0.99	0.06	42,42,42,42	0
4	SO4	K	1004	5/5	0.99	0.15	34,34,44,44	0
2	ZN	K	1003	1/1	0.99	0.07	48,48,48,48	0
2	ZN	F	1003	1/1	0.99	0.07	50,50,50,50	0
2	ZN	E	1001	1/1	0.99	0.09	40,40,40,40	0
3	CO3	H	1002	4/4	0.99	0.20	28,39,44,53	0
2	ZN	I	1003	1/1	0.99	0.07	46,46,46,46	0
2	ZN	F	1001	1/1	0.99	0.09	48,48,48,48	0
2	ZN	H	1001	1/1	0.99	0.03	44,44,44,44	0
4	SO4	F	1004	5/5	0.99	0.12	29,30,37,43	0
2	ZN	J	1003	1/1	0.99	0.04	47,47,47,47	0
2	ZN	I	1001	1/1	0.99	0.09	45,45,45,45	0
2	ZN	A	1001	1/1	1.00	0.07	40,40,40,40	0

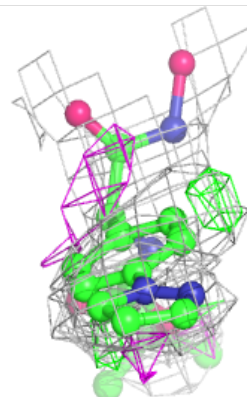
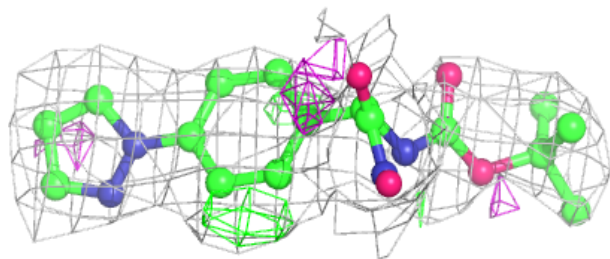
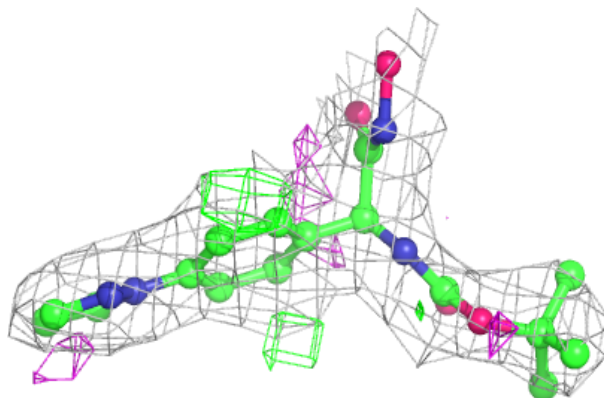
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around R5T I 1004:

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

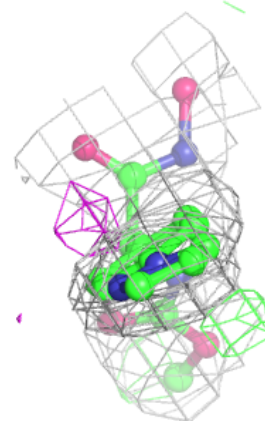
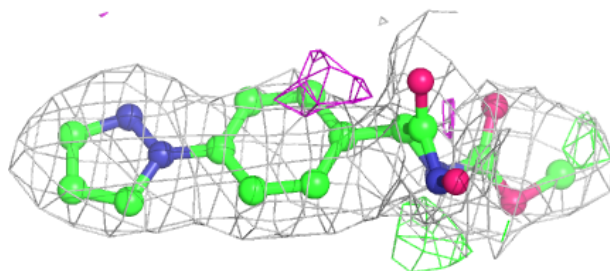
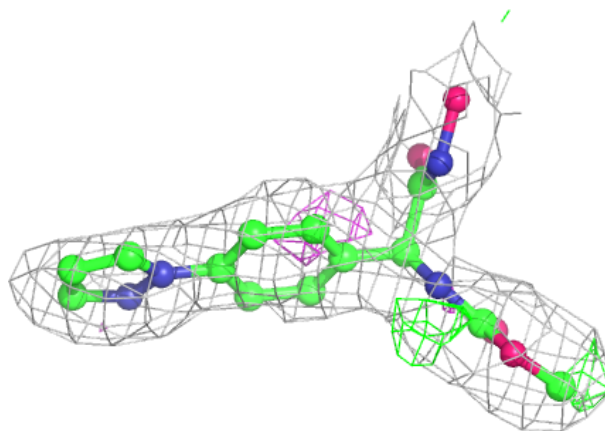
**Electron density around R5T F 1005:**

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

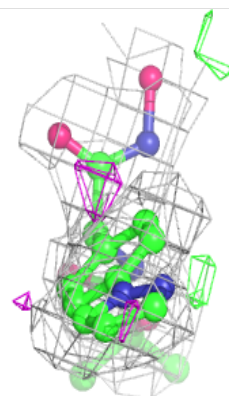
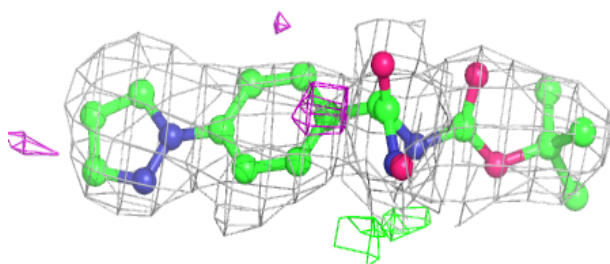
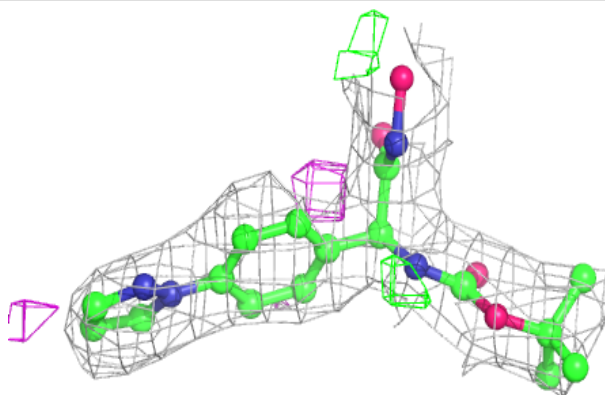


Electron density around R5T L 1006:

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

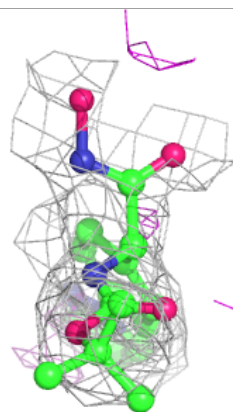
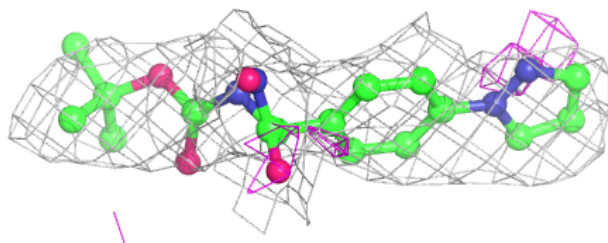
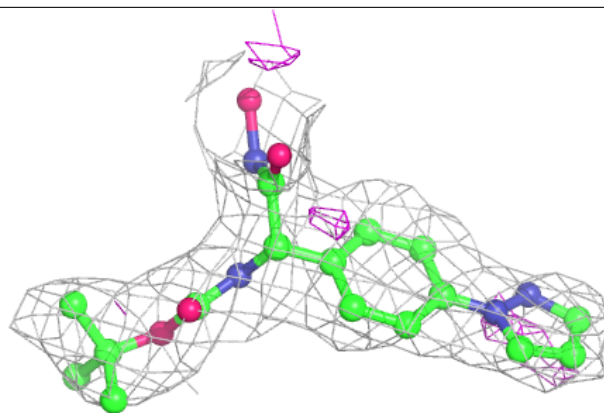
**Electron density around R5T A 1007:**

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



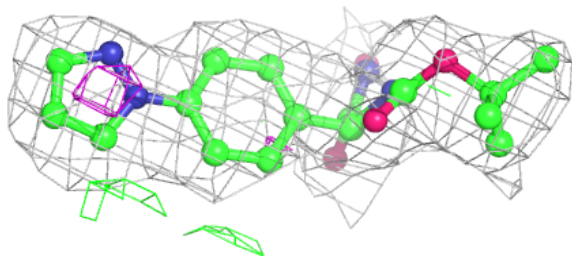
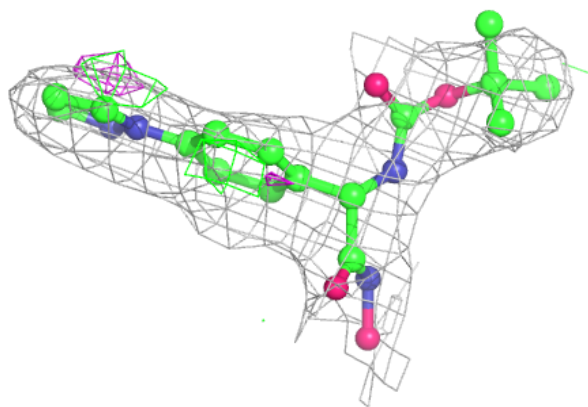
Electron density around R5T B 1006:

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



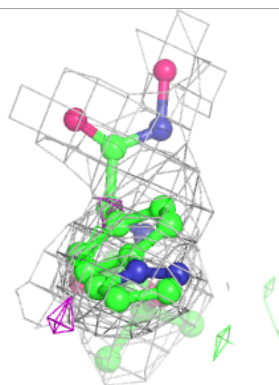
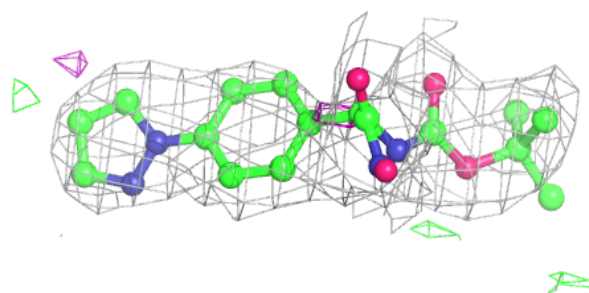
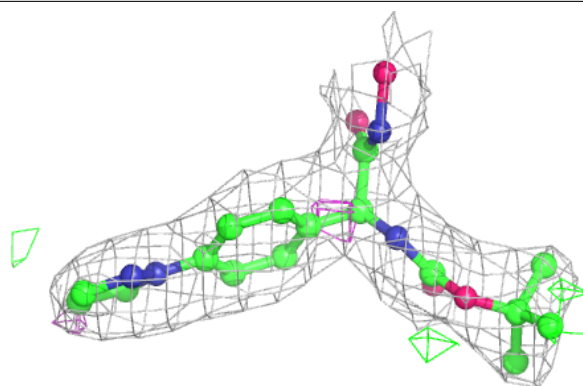
Electron density around R5T K 1007:

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

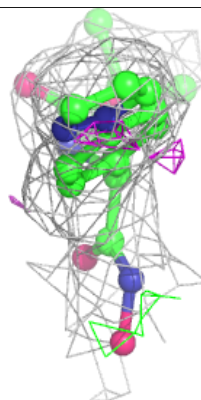
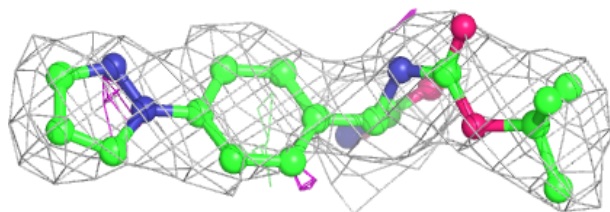
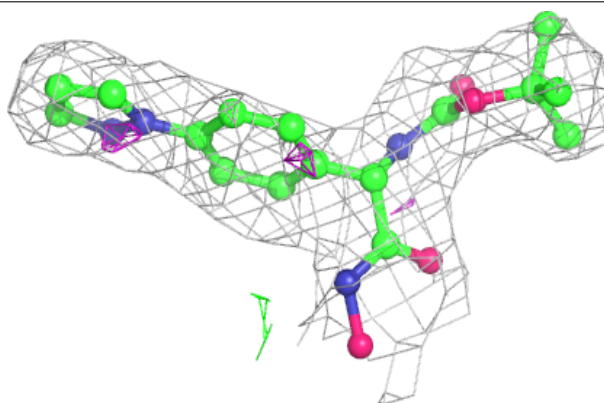


Electron density around R5T G 1006:

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

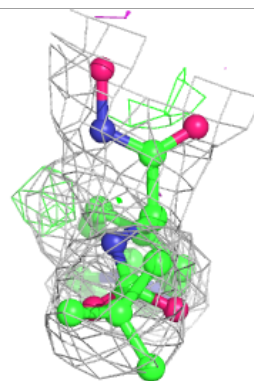
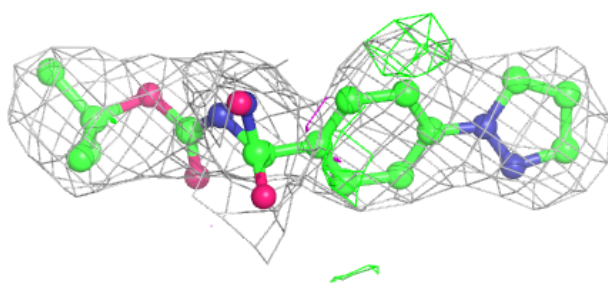
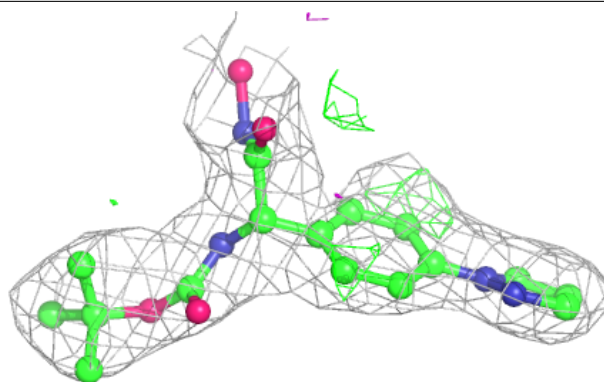
**Electron density around R5T D 1004:**

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

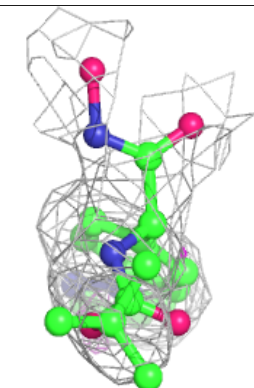
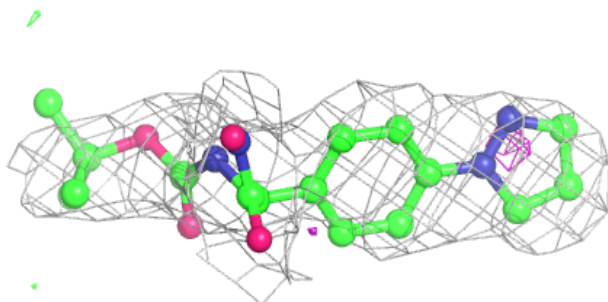
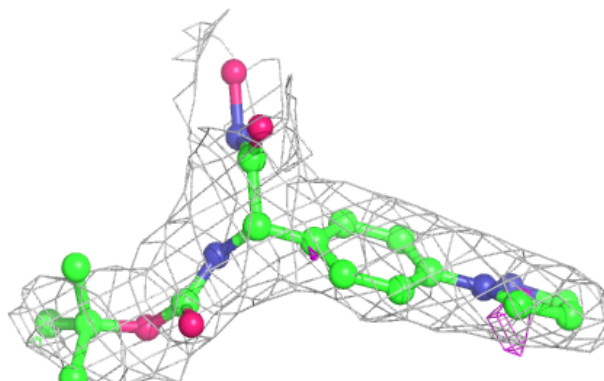


Electron density around R5T H 1005:

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

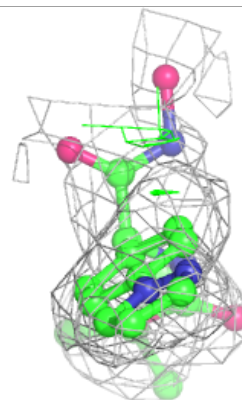
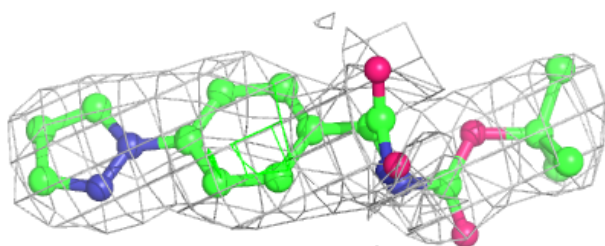
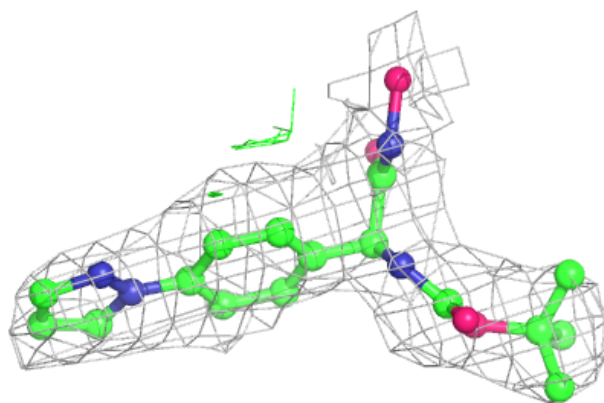
**Electron density around R5T J 1004:**

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

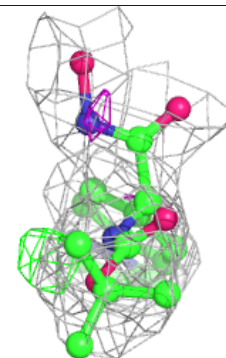
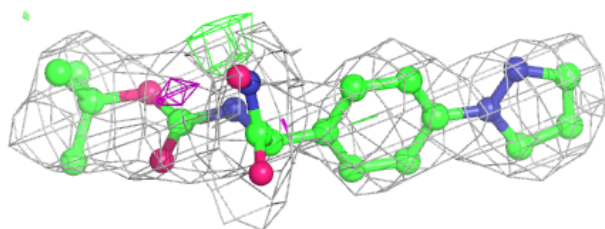
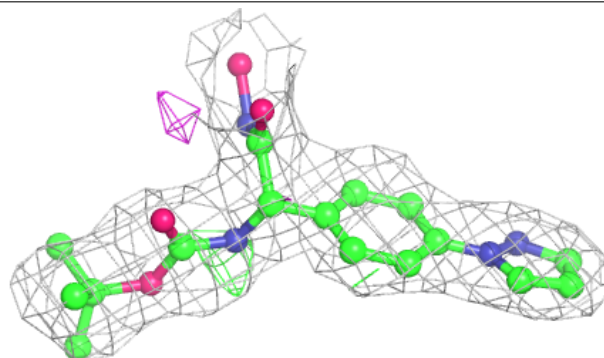


Electron density around R5T E 1004:

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

**Electron density around R5T C 1007:**

$2mF_o-DF_c$ (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.