wwPDB X-ray Structure Validation Summary Report (i)

Sep 13, 2023 – 06:20 AM EDT

PDB ID	:	4R7M
Title	:	Structure of the m17 leucyl aminopeptidase from malaria complexed with a hydroxamic acid-based inhibitor
Authors	:	Drinkwater, N.; Mcgowan, S.
Deposited on	:	2014-08-28
Resolution	:	2.85 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 (i) symbol.

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

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

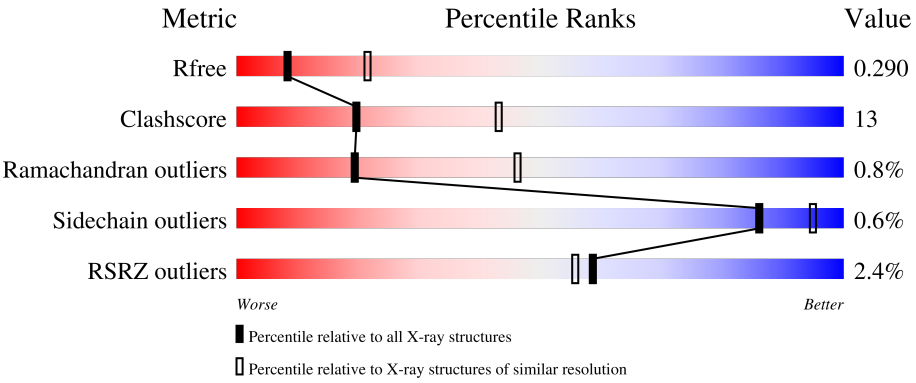
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	528	2% 69% 28%
1	B	528	4% 71% 26%
1	C	528	2% 70% 27%
1	D	528	2% 72% 24%
1	E	528	% 71% 25%

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Mol	Chain	Length	Quality of chain
1	F	528	3% 72% 24%
1	G	528	2% 71% 26%
1	H	528	4% 73% 24%
1	I	528	2% 71% 26%
1	J	528	% 67% 30%
1	K	528	2% 72% 24%
1	L	528	3% 74% 21%

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	1PE	C	1006	-	-	X	-
4	1PE	G	1007	-	-	X	-
6	SO4	B	1004	-	-	X	-
6	SO4	G	1004	-	-	X	-
6	SO4	L	1004	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 47476 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	516	Total	C	N	O	S	0	0	0
			3948	2538	633	758	19			
1	B	512	Total	C	N	O	S	0	0	0
			3860	2484	625	732	19			
1	C	518	Total	C	N	O	S	0	1	0
			3960	2546	640	755	19			
1	D	514	Total	C	N	O	S	0	0	0
			3935	2534	633	748	20			
1	E	510	Total	C	N	O	S	0	0	0
			3898	2510	625	744	19			
1	F	510	Total	C	N	O	S	0	0	0
			3792	2443	612	718	19			
1	G	513	Total	C	N	O	S	0	0	0
			3943	2535	632	757	19			
1	H	511	Total	C	N	O	S	0	0	0
			3872	2489	625	739	19			
1	I	516	Total	C	N	O	S	0	0	0
			3908	2516	629	744	19			
1	J	511	Total	C	N	O	S	0	0	0
			3898	2511	629	739	19			
1	K	509	Total	C	N	O	S	0	0	0
			3884	2505	623	737	19			
1	L	509	Total	C	N	O	S	0	0	0
			3819	2453	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	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0

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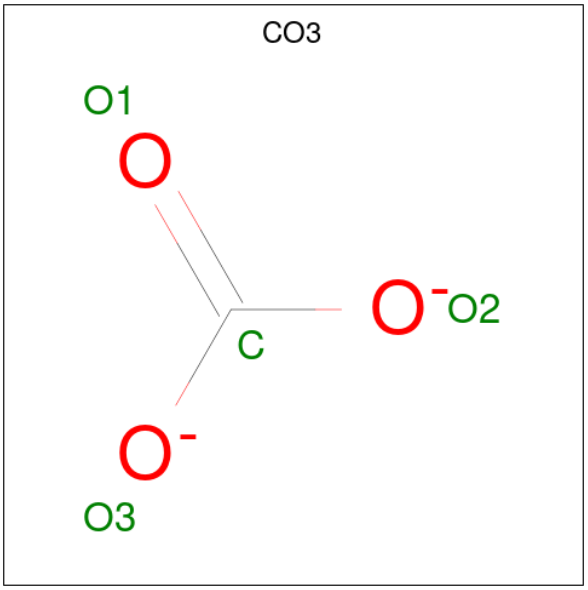
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	2	Total Zn 2 2	0	0
2	L	2	Total Zn 2 2	0	0

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



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

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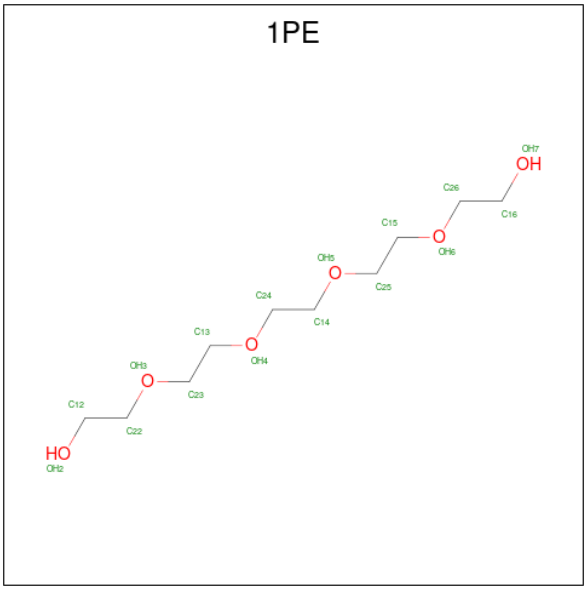
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total C O 4 1 3	0	0
3	K	1	Total C O 4 1 3	0	0
3	L	1	Total C O 4 1 3	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



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

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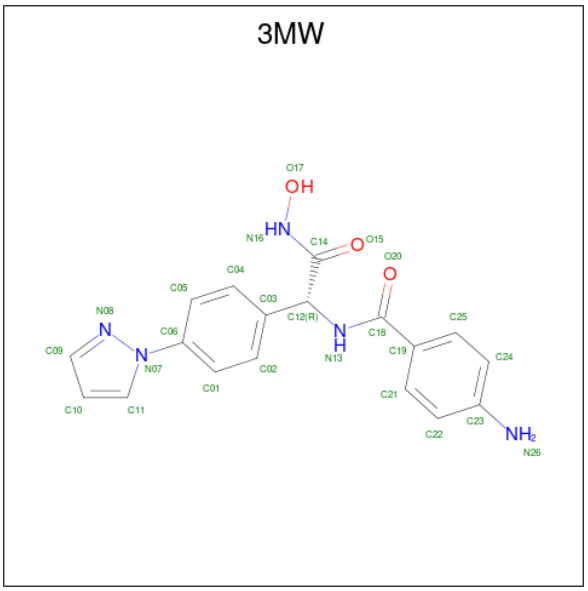
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C O 13 8 5	0	0
4	H	1	Total C O 10 6 4	0	0
4	K	1	Total C O 12 8 4	0	0

- Molecule 5 is 4-amino-N-{(1R)-2-(hydroxyamino)-2-oxo-1-[4-(1H-pyrazol-1-yl)phenyl]ethyl} benzamide (three-letter code: 3MW) (formula: $C_{18}H_{17}N_5O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 26 18 5 3	0	0
5	B	1	Total C N O 26 18 5 3	0	0
5	C	1	Total C N O 26 18 5 3	0	0
5	D	1	Total C N O 26 18 5 3	0	0
5	E	1	Total C N O 26 18 5 3	0	0
5	F	1	Total C N O 26 18 5 3	0	0
5	G	1	Total C N O 26 18 5 3	0	0
5	H	1	Total C N O 26 18 5 3	0	0

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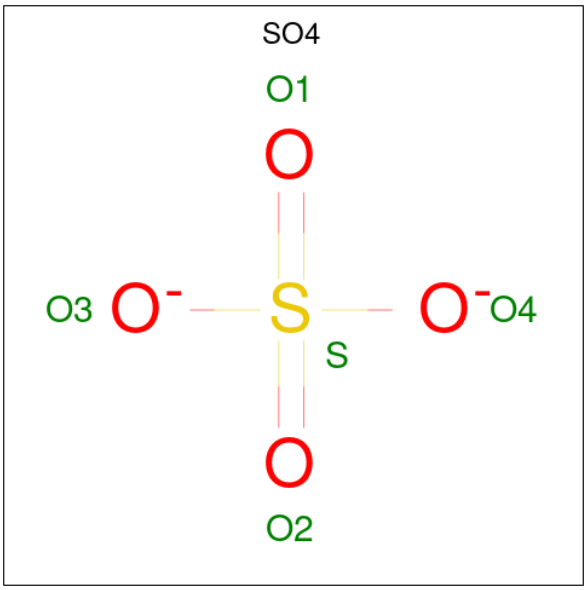
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total C N O 26 18 5 3	0	0
5	J	1	Total C N O 26 18 5 3	0	0
5	K	1	Total C N O 26 18 5 3	0	0
5	L	1	Total C N O 26 18 5 3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0
6	J	1	Total O S 5 4 1	0	0
6	K	1	Total O S 5 4 1	0	0

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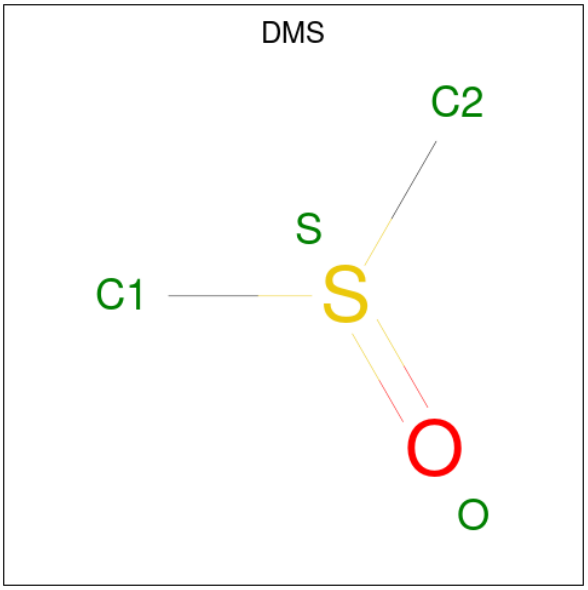
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total O S 5 4 1	0	0

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	26	Total O 26 26	0	0
8	B	22	Total O 22 22	0	0
8	C	17	Total O 17 17	0	0
8	D	28	Total O 28 28	0	0
8	E	23	Total O 23 23	0	0
8	F	24	Total O 24 24	0	0
8	G	17	Total O 17 17	0	0

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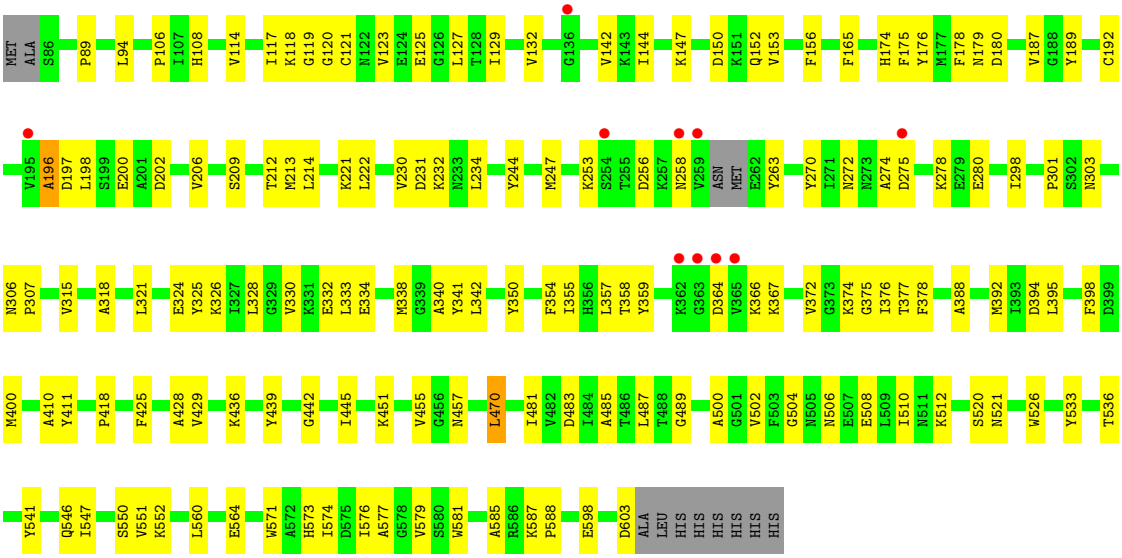
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	13	Total O 13 13	0	0
8	I	11	Total O 11 11	0	0
8	J	14	Total O 14 14	0	0
8	K	13	Total O 13 13	0	0
8	L	10	Total O 10 10	0	0

3 Residue-property plots (i)

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

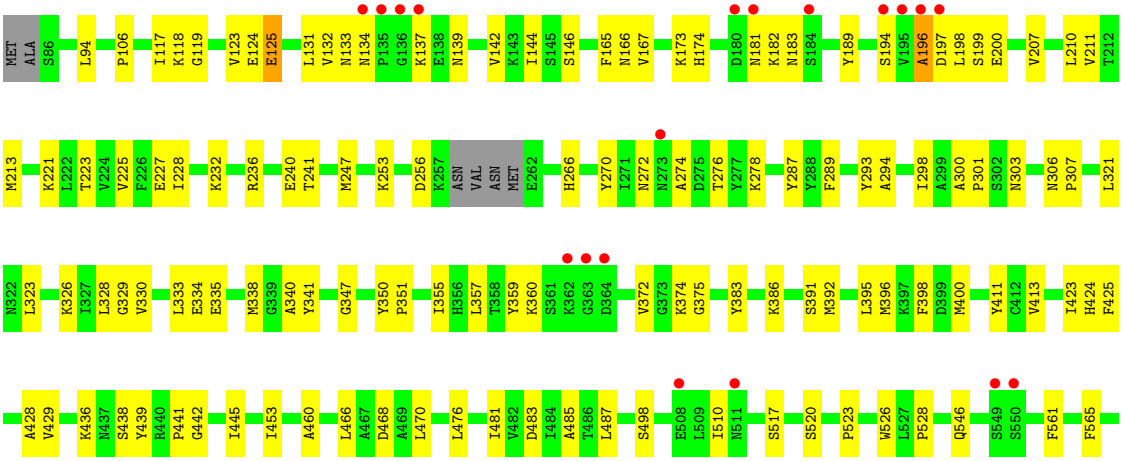
• Molecule 1: M17 leucyl aminopeptidase

Chain A:



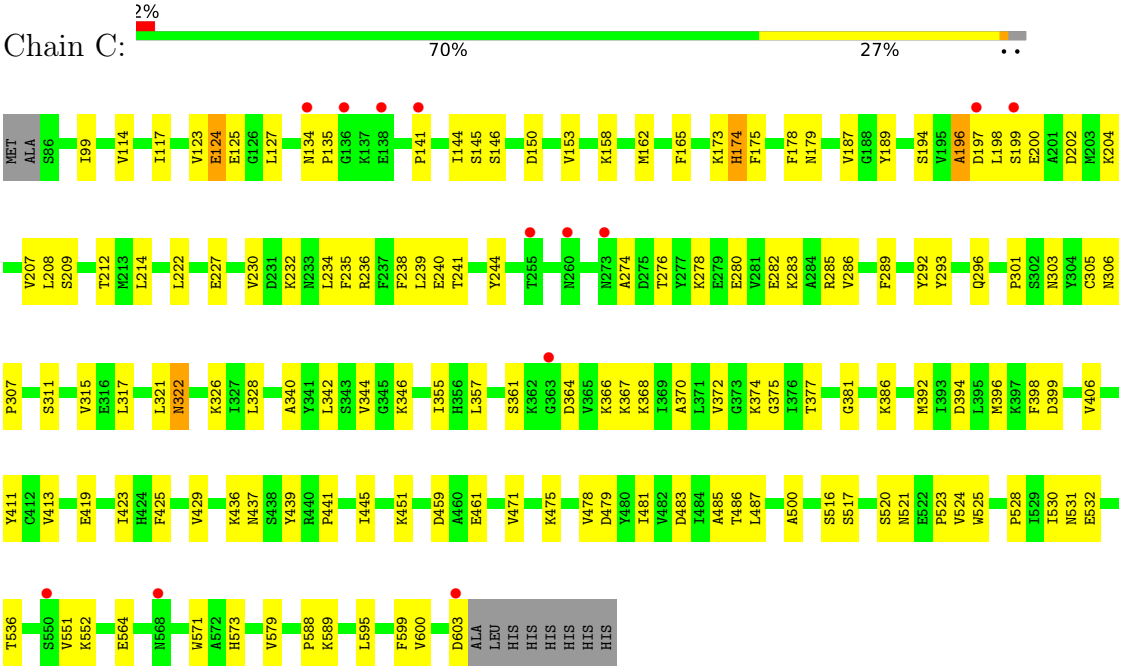
• Molecule 1: M17 leucyl aminopeptidase

Chain B:



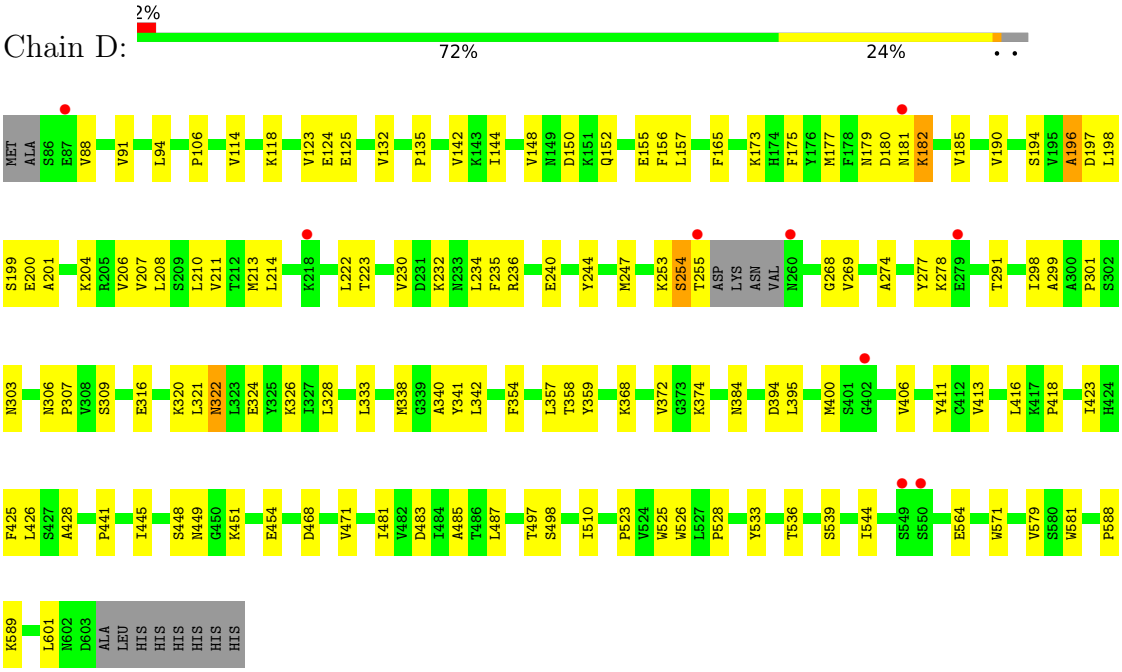
• Molecule 1: M17 leucyl aminopeptidase

Chain C:



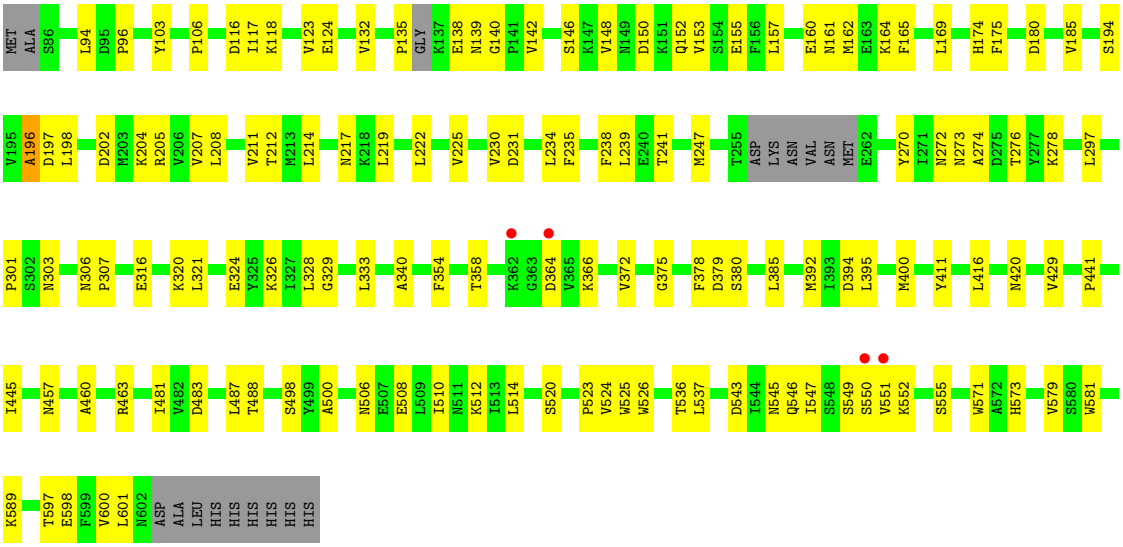
• Molecule 1: M17 leucyl aminopeptidase

Chain D:



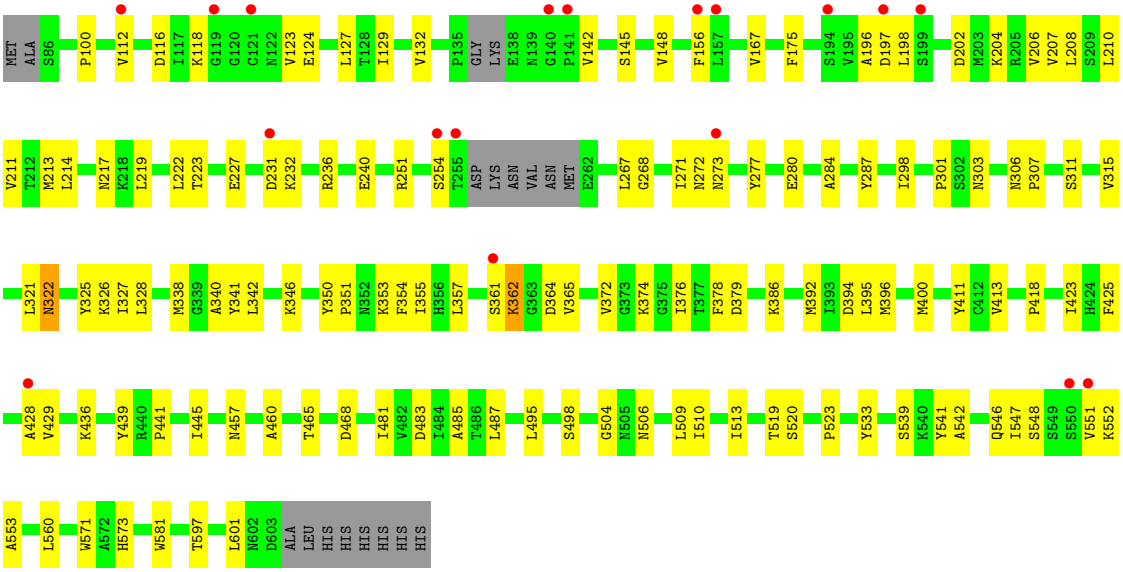
• Molecule 1: M17 leucyl aminopeptidase

Chain E:



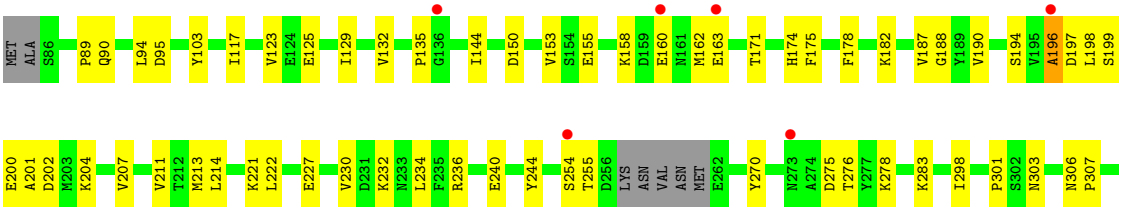
• Molecule 1: M17 leucyl aminopeptidase

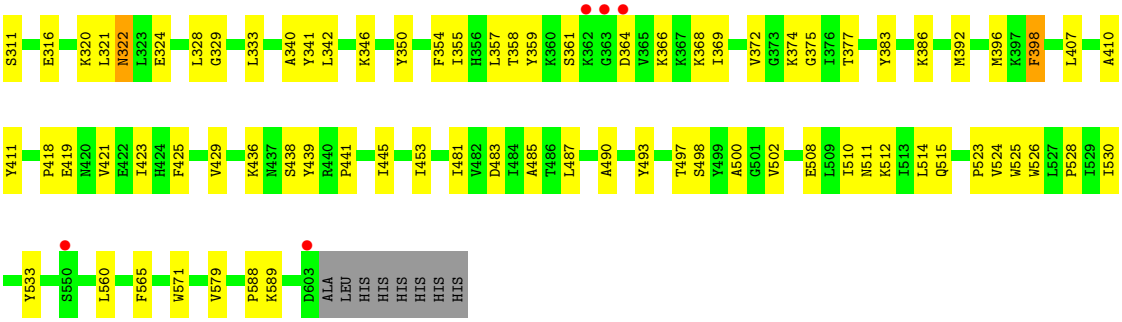
Chain F:



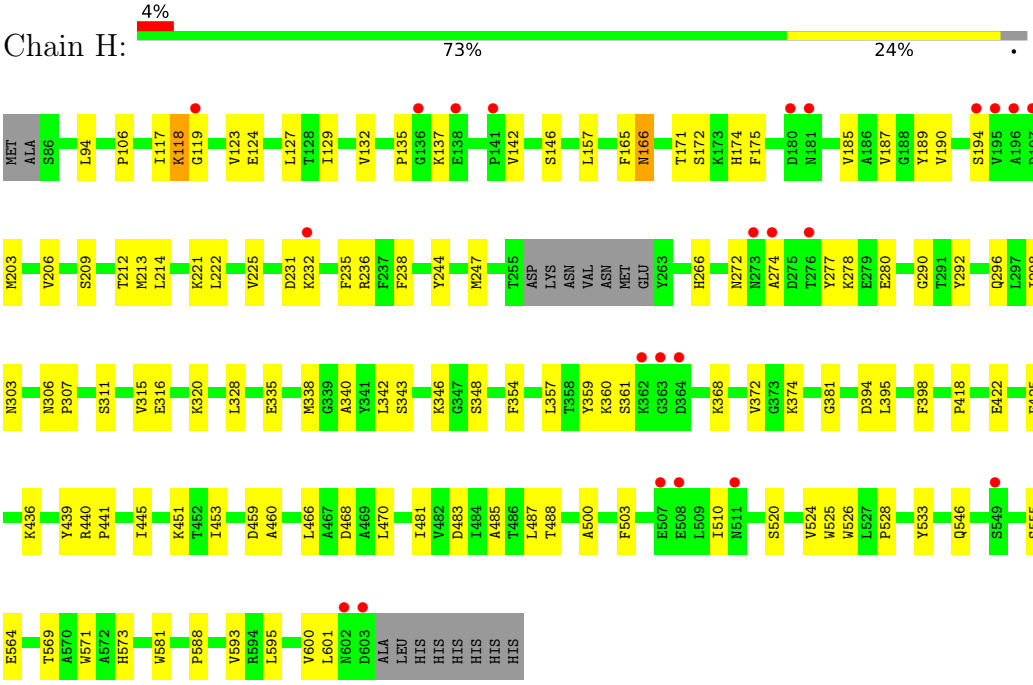
• Molecule 1: M17 leucyl aminopeptidase

Chain G:

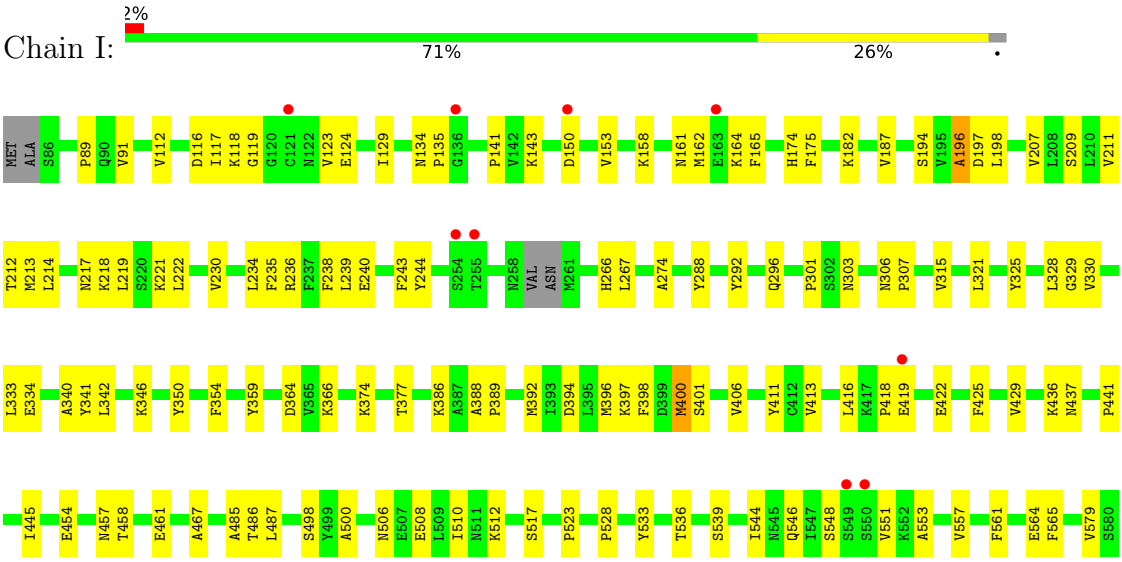


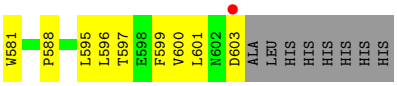


- Molecule 1: M17 leucyl aminopeptidase



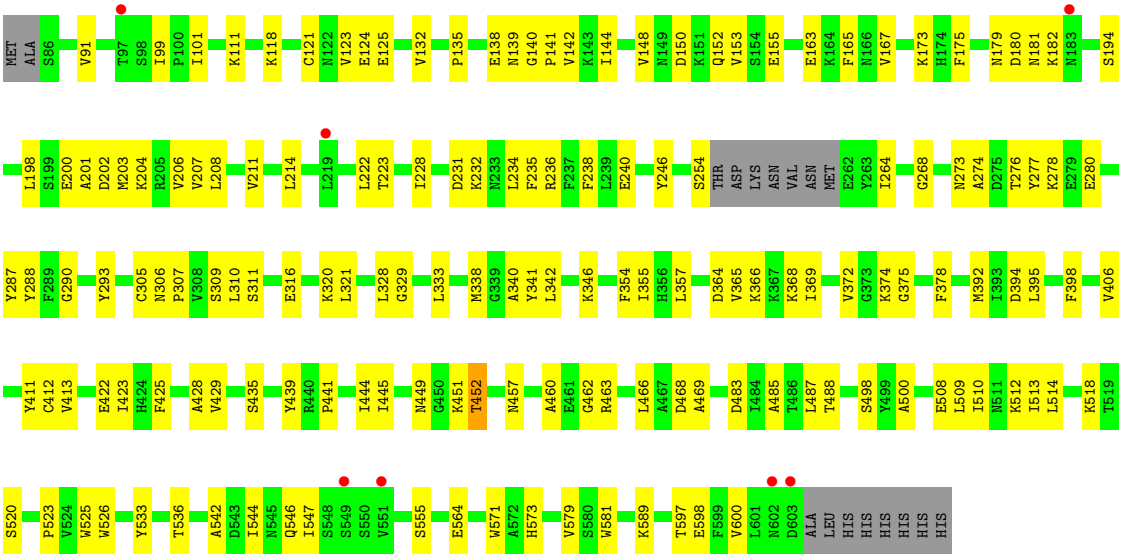
- Molecule 1: M17 leucyl aminopeptidase





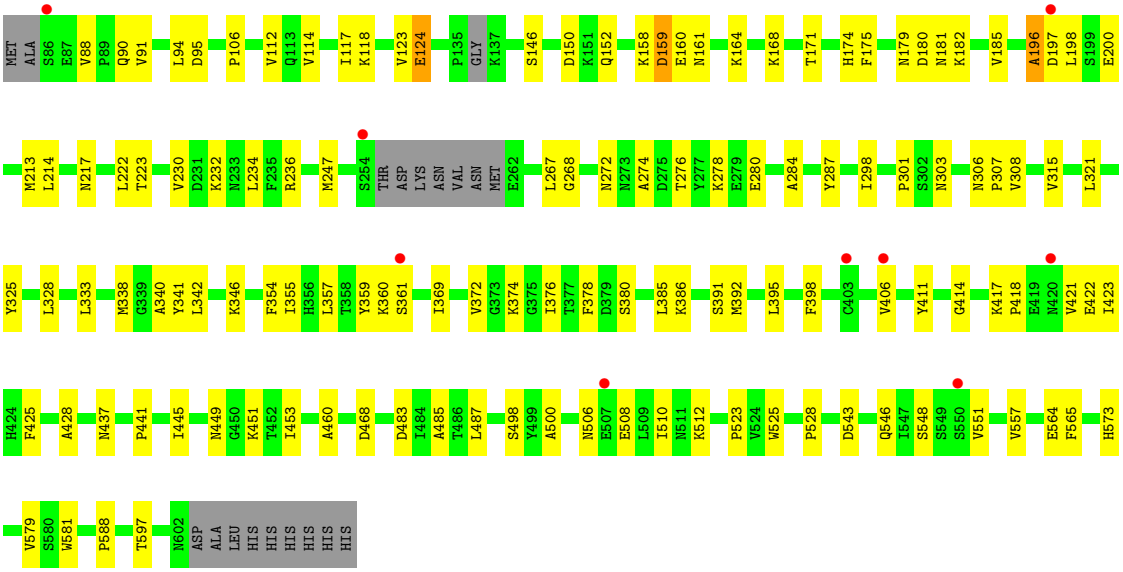
• Molecule 1: M17 leucyl aminopeptidase

Chain J:



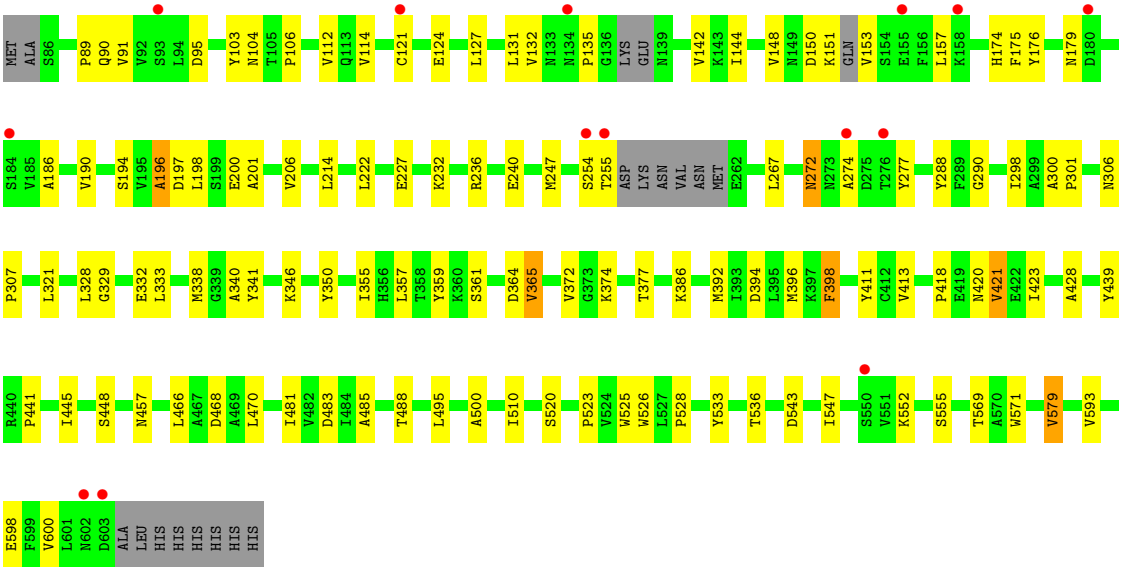
• Molecule 1: M17 leucyl aminopeptidase

Chain K:



• Molecule 1: M17 leucyl aminopeptidase

Chain L:


MET ALA S86
P89 Q90 V91 V92 S93 L94 D95
Y103 N104 T105 P106
V112 Q113 V114
C121
E124
L127
L131 V132 N133 N134 P135 G136 LYS GLU N139
V142 K143 I144
V148 N149 D150 K151 GLN V153 S154 E155 F156 L157 K158
H174 F175 Y176
N179 D180
S184 V185 A186
V190
S194 V195 A196 D197 L198 S199 E200 A201
V206
L214
L222
E227
K232
R236
E240
M247
S254 T255 ASP LYS ASN VAL ASN MET E262
L267
N272 N273 A274 D275 T276 Y277
Y288 F289 G290
I298 A299 A300 P301
N306
P307
L321
L328 G329
E332 L333
M338 G339 A340 Y341
K346
Y350
I355 H356 L357 T358 Y359 K360 S361
D364 V365
V372 G373 K374
T377
K386
M392 I393 D394 L395 M396 K397 F398
Y411 C412 V413
P418 E419 N420 V421 E422 I423
A428
Y439
R440 P441
I445
S448
N457
L466 A467 D468 A469 L470
I481 V482 D483 I484 A485
T488
L495
A500
I510
S520
P523 V524 W525 W526 L527 P528
Y533
T536
D543
I547
S550 V551 K552
S555
T569 A570 W571
V579
V593
E598 F599 V600 L601 N602 D603 ALA LEU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	172.56Å 175.59Å 225.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.01 – 2.85 36.01 – 2.85	Depositor EDS
% Data completeness (in resolution range)	90.2 (36.01-2.85) 90.3 (36.01-2.85)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.237 , 0.291 0.242 , 0.290	Depositor DCC
R_{free} test set	7254 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.904	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	47476	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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 37.56 % 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 4.2130e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, 1PE, SO4, 3MW, ZN, DMS

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	0.23	0/4025	0.42	0/5461
1	B	0.22	0/3935	0.42	0/5348
1	C	0.23	0/4041	0.41	0/5484
1	D	0.23	0/4012	0.42	0/5440
1	E	0.23	0/3974	0.41	0/5392
1	F	0.23	0/3868	0.43	0/5267
1	G	0.23	0/4020	0.41	0/5451
1	H	0.23	0/3947	0.42	0/5362
1	I	0.23	0/3985	0.41	0/5410
1	J	0.22	0/3975	0.41	0/5393
1	K	0.22	0/3960	0.40	0/5372
1	L	0.22	0/3893	0.40	0/5293
All	All	0.23	0/47635	0.41	0/64673

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	3948	0	3861	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3860	0	3733	92	0
1	C	3960	0	3887	115	1
1	D	3935	0	3867	101	0
1	E	3898	0	3824	102	1
1	F	3792	0	3601	96	0
1	G	3943	0	3877	112	0
1	H	3872	0	3758	102	0
1	I	3908	0	3800	97	0
1	J	3898	0	3822	120	0
1	K	3884	0	3813	99	0
1	L	3819	0	3653	96	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	1	0
3	D	4	0	0	0	0
3	E	4	0	0	1	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	1	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	23	4	0
4	C	17	0	18	13	0
4	E	18	0	21	2	0
4	F	7	0	6	0	0
4	G	23	0	27	9	0
4	H	10	0	12	0	0
4	K	12	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	26	0	16	4	0
5	B	26	0	16	4	0
5	C	26	0	16	3	0
5	D	26	0	16	1	0
5	E	26	0	16	5	0
5	F	26	0	16	6	0
5	G	26	0	16	3	0
5	H	26	0	16	3	0
5	I	26	0	16	3	0
5	J	26	0	16	4	0
5	K	26	0	16	4	0
5	L	26	0	16	3	0
6	B	5	0	0	3	0
6	C	5	0	0	0	0
6	E	5	0	0	1	0
6	G	10	0	0	3	0
6	J	5	0	0	1	0
6	K	5	0	0	0	0
6	L	5	0	0	2	0
7	K	4	6	6	0	0
8	A	26	0	0	2	0
8	B	22	0	0	1	0
8	C	17	0	0	1	0
8	D	28	0	0	0	0
8	E	23	0	0	0	0
8	F	24	0	0	1	0
8	G	17	0	0	0	0
8	H	13	0	0	0	0
8	I	11	0	0	1	0
8	J	14	0	0	0	0
8	K	13	0	0	0	0
8	L	10	0	0	2	0
All	All	47470	6	45815	1181	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 1181 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:J:124:GLU:HG3	1:J:125:GLU:H	1.22	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:LEU:HD21	1:F:213:MET:HE2	1.44	0.97
1:L:423:ILE:HD11	1:L:600:VAL:HG11	1.51	0.90
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.56	0.87
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.56	0.87

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:ASP:OD1	1:E:366:LYS:NZ[4_455]	2.17	0.03

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	512/528 (97%)	489 (96%)	19 (4%)	4 (1%)	19	46
1	B	508/528 (96%)	481 (95%)	21 (4%)	6 (1%)	13	35
1	C	517/528 (98%)	498 (96%)	15 (3%)	4 (1%)	19	46
1	D	510/528 (97%)	485 (95%)	19 (4%)	6 (1%)	13	35
1	E	504/528 (96%)	482 (96%)	19 (4%)	3 (1%)	25	53
1	F	504/528 (96%)	479 (95%)	18 (4%)	7 (1%)	11	31
1	G	509/528 (96%)	486 (96%)	19 (4%)	4 (1%)	19	46
1	H	507/528 (96%)	489 (96%)	17 (3%)	1 (0%)	47	75
1	I	512/528 (97%)	491 (96%)	16 (3%)	5 (1%)	15	40
1	J	507/528 (96%)	486 (96%)	18 (4%)	3 (1%)	25	53
1	K	503/528 (95%)	483 (96%)	16 (3%)	4 (1%)	19	46
1	L	501/528 (95%)	481 (96%)	16 (3%)	4 (1%)	19	46
All	All	6094/6336 (96%)	5830 (96%)	213 (4%)	51 (1%)	19	46

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	ASP
1	A	258	ASN
1	B	125	GLU
1	B	197	ASP
1	C	196	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	419/455 (92%)	416 (99%)	3 (1%)	84 94
1	B	399/455 (88%)	398 (100%)	1 (0%)	92 97
1	C	421/455 (92%)	417 (99%)	4 (1%)	76 91
1	D	417/455 (92%)	415 (100%)	2 (0%)	88 96
1	E	415/455 (91%)	415 (100%)	0	100 100
1	F	382/455 (84%)	380 (100%)	2 (0%)	88 96
1	G	422/455 (93%)	420 (100%)	2 (0%)	88 96
1	H	405/455 (89%)	403 (100%)	2 (0%)	88 96
1	I	408/455 (90%)	406 (100%)	2 (0%)	88 96
1	J	411/455 (90%)	407 (99%)	4 (1%)	76 91
1	K	411/455 (90%)	410 (100%)	1 (0%)	93 98
1	L	393/455 (86%)	387 (98%)	6 (2%)	65 86
All	All	4903/5460 (90%)	4874 (99%)	29 (1%)	86 95

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	166	ASN
1	L	439	TYR
1	I	419	GLU
1	L	288	TYR

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Mol	Chain	Res	Type
1	I	400	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	183	ASN
1	B	233	ASN
1	B	521	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 68 ligands modelled in this entry, 24 are monoatomic - leaving 44 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	$\#\|Z\| > 2$
3	CO3	G	1002	-	2,3,3	0.40	0	2,3,3	0.12	0
3	CO3	I	1002	-	2,3,3	0.40	0	2,3,3	0.22	0
3	CO3	F	1002	-	2,3,3	0.40	0	2,3,3	0.29	0
5	3MW	F	1005	2	27,28,28	2.52	6 (22%)	35,38,38	2.61	8 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SO4	L	1004	-	4,4,4	0.15	0	6,6,6	0.06	0
3	CO3	C	1002	-	2,3,3	0.42	0	2,3,3	0.26	0
5	3MW	E	1007	2	27,28,28	2.56	5 (18%)	35,38,38	2.38	5 (14%)
4	1PE	A	1005	-	7,7,15	0.43	0	6,6,14	0.45	0
7	DMS	K	1007	-	3,3,3	0.66	0	3,3,3	0.49	0
4	1PE	C	1006	-	7,7,15	0.44	0	6,6,14	0.25	0
6	SO4	K	1004	-	4,4,4	0.15	0	6,6,6	0.04	0
5	3MW	K	1006	2	27,28,28	2.42	5 (18%)	35,38,38	2.28	9 (25%)
3	CO3	D	1002	-	2,3,3	0.41	0	2,3,3	0.27	0
5	3MW	J	1005	2	27,28,28	2.52	5 (18%)	35,38,38	2.19	6 (17%)
5	3MW	C	1007	2	27,28,28	2.49	6 (22%)	35,38,38	2.47	6 (17%)
6	SO4	J	1004	-	4,4,4	0.14	0	6,6,6	0.06	0
4	1PE	F	1004	-	6,6,15	0.46	0	5,5,14	0.25	0
4	1PE	C	1005	-	8,8,15	0.47	0	7,7,14	0.26	0
5	3MW	B	1005	2	27,28,28	2.52	5 (18%)	35,38,38	2.45	6 (17%)
3	CO3	E	1002	-	2,3,3	0.40	0	2,3,3	0.16	0
5	3MW	A	1006	2	27,28,28	2.43	5 (18%)	35,38,38	2.27	9 (25%)
6	SO4	G	1004	-	4,4,4	0.14	0	6,6,6	0.08	0
6	SO4	C	1004	-	4,4,4	0.14	0	6,6,6	0.05	0
4	1PE	E	1005	-	11,11,15	0.46	0	10,10,14	0.26	0
6	SO4	E	1004	-	4,4,4	0.13	0	6,6,6	0.06	0
5	3MW	G	1008	2	27,28,28	2.52	5 (18%)	35,38,38	2.44	8 (22%)
6	SO4	G	1005	-	4,4,4	0.13	0	6,6,6	0.09	0
4	1PE	G	1006	-	9,9,15	0.46	0	8,8,14	0.25	0
5	3MW	H	1005	2	27,28,28	2.37	5 (18%)	35,38,38	2.31	8 (22%)
3	CO3	B	1002	-	2,3,3	0.41	0	2,3,3	0.23	0
3	CO3	L	1002	-	2,3,3	0.41	0	2,3,3	0.22	0
5	3MW	L	1005	2	27,28,28	2.46	5 (18%)	35,38,38	2.25	7 (20%)
5	3MW	I	1004	2	27,28,28	2.50	6 (22%)	35,38,38	2.27	6 (17%)
4	1PE	H	1004	-	9,9,15	0.44	0	8,8,14	0.30	0
4	1PE	G	1007	-	12,12,15	0.46	0	11,11,14	0.38	0
4	1PE	K	1005	-	11,11,15	0.45	0	10,10,14	0.36	0
4	1PE	A	1004	-	11,11,15	0.45	0	10,10,14	0.34	0
3	CO3	J	1002	-	2,3,3	0.41	0	2,3,3	0.23	0
4	1PE	E	1006	-	5,5,15	0.50	0	4,4,14	0.27	0
3	CO3	H	1002	-	2,3,3	0.41	0	2,3,3	0.15	0
3	CO3	K	1002	-	2,3,3	0.38	0	2,3,3	0.14	0
5	3MW	D	1004	2	27,28,28	2.50	5 (18%)	35,38,38	2.58	8 (22%)
6	SO4	B	1004	-	4,4,4	0.15	0	6,6,6	0.15	0
3	CO3	A	1002	-	2,3,3	0.39	0	2,3,3	0.22	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
5	3MW	F	1005	2	-	4/22/22/22	0/3/3/3
5	3MW	E	1007	2	-	4/22/22/22	0/3/3/3
4	1PE	A	1005	-	-	4/5/5/13	-
4	1PE	C	1006	-	-	2/5/5/13	-
5	3MW	K	1006	2	-	4/22/22/22	0/3/3/3
5	3MW	J	1005	2	-	6/22/22/22	0/3/3/3
5	3MW	C	1007	2	-	5/22/22/22	0/3/3/3
4	1PE	F	1004	-	-	0/4/4/13	-
4	1PE	C	1005	-	-	0/6/6/13	-
5	3MW	B	1005	2	-	4/22/22/22	0/3/3/3
5	3MW	A	1006	2	-	6/22/22/22	0/3/3/3
4	1PE	E	1005	-	-	0/9/9/13	-
5	3MW	G	1008	2	-	2/22/22/22	0/3/3/3
5	3MW	H	1005	2	-	3/22/22/22	0/3/3/3
4	1PE	G	1006	-	-	0/7/7/13	-
5	3MW	L	1005	2	-	6/22/22/22	0/3/3/3
5	3MW	I	1004	2	-	6/22/22/22	0/3/3/3
4	1PE	H	1004	-	-	3/7/7/13	-
4	1PE	G	1007	-	-	4/10/10/13	-
4	1PE	K	1005	-	-	1/9/9/13	-
4	1PE	A	1004	-	-	4/9/9/13	-
4	1PE	E	1006	-	-	0/3/3/13	-
5	3MW	D	1004	2	-	2/22/22/22	0/3/3/3

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	1005	3MW	C03-C12	-8.00	1.39	1.52
5	L	1005	3MW	C03-C12	-7.97	1.39	1.52
5	I	1004	3MW	C03-C12	-7.88	1.39	1.52
5	E	1007	3MW	N08-N07	-7.87	1.19	1.38
5	G	1008	3MW	C03-C12	-7.87	1.39	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1005	3MW	C06-N07-N08	10.16	127.82	118.80
5	D	1004	3MW	C06-N07-N08	9.73	127.44	118.80
5	B	1005	3MW	C06-N07-N08	9.47	127.20	118.80
5	C	1007	3MW	C06-N07-N08	9.38	127.12	118.80
5	I	1004	3MW	C09-N08-N07	9.08	110.31	103.70

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1007	3MW	C03-C12-C14-O15
5	E	1007	3MW	C03-C12-C14-N16
5	F	1005	3MW	C03-C12-C14-O15
5	F	1005	3MW	C03-C12-C14-N16
5	I	1004	3MW	C14-C12-N13-C18

There are no ring outliers.

28 monomers are involved in 83 short contacts:

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

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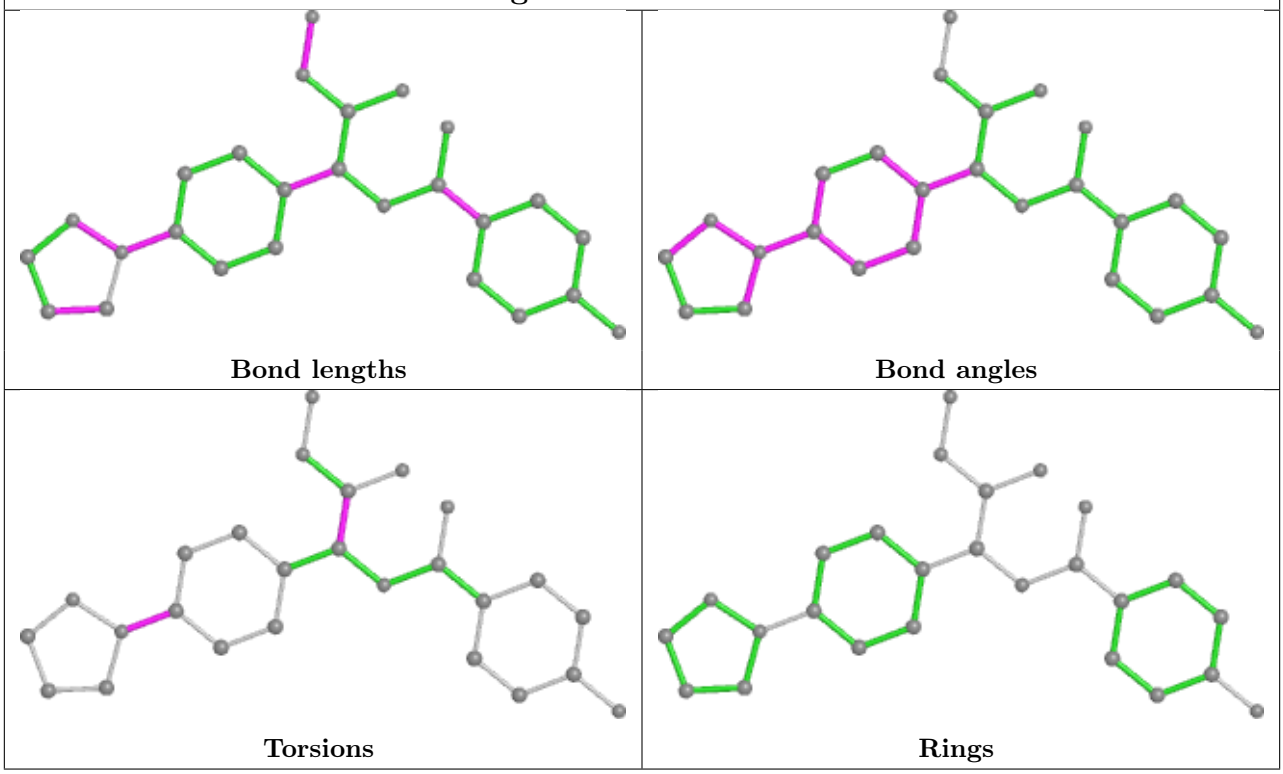
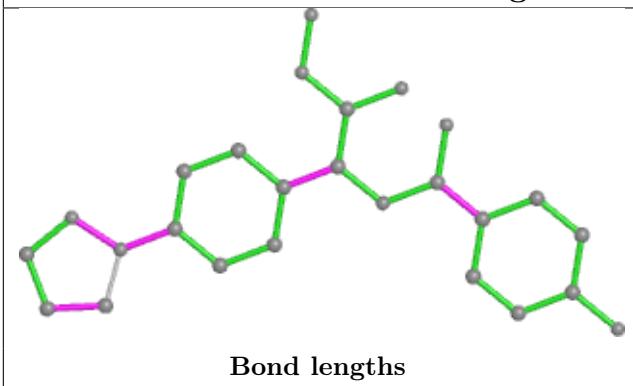
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	1PE	2	0
4	E	1006	1PE	2	0
3	H	1002	CO3	1	0
5	D	1004	3MW	1	0
6	B	1004	SO4	3	0
3	A	1002	CO3	1	0

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

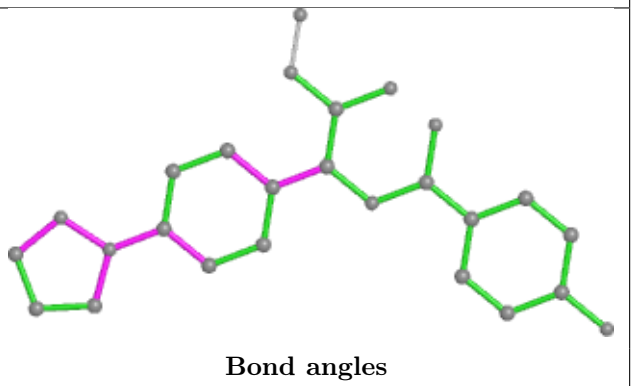
Ligand 3MW F 1005



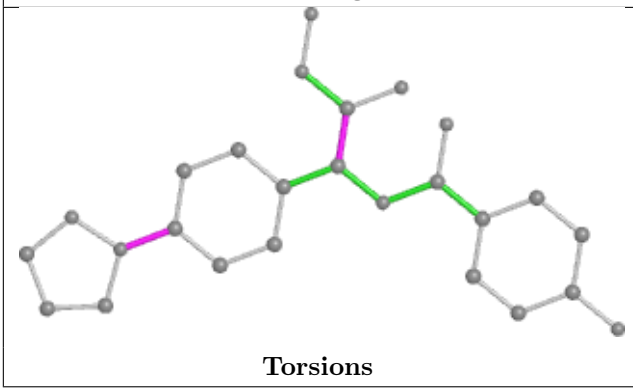
Ligand 3MW E 1007



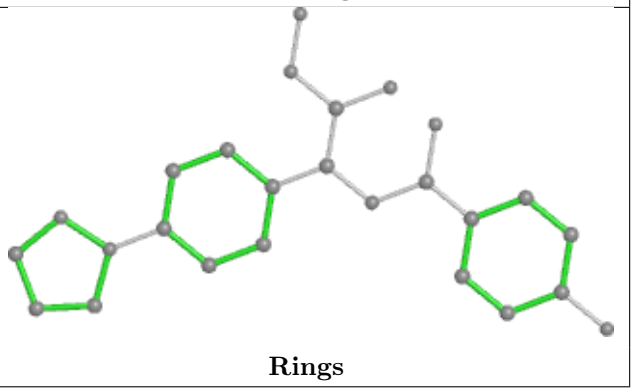
Bond lengths



Bond angles

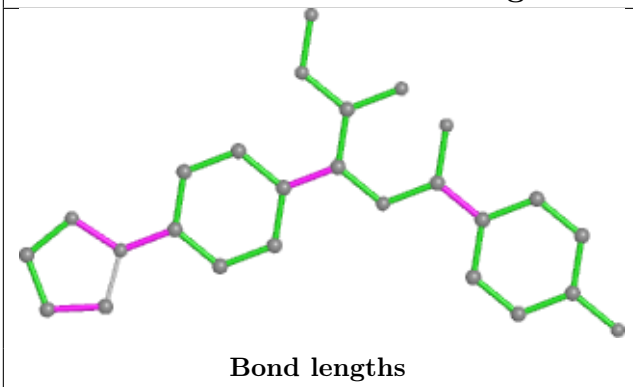


Torsions

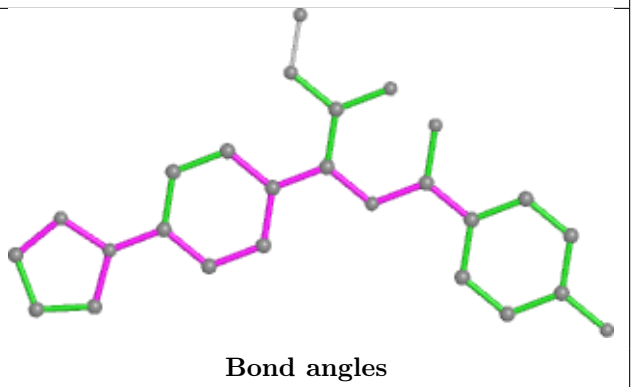


Rings

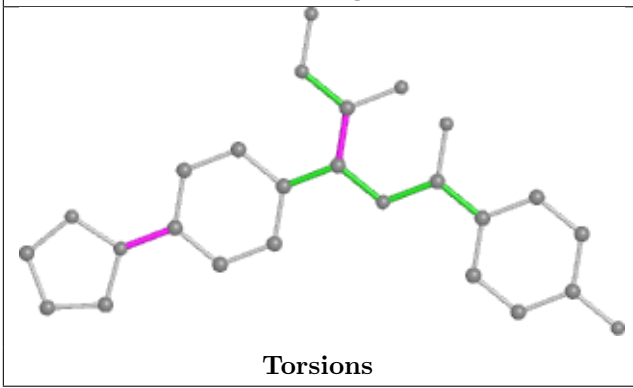
Ligand 3MW K 1006



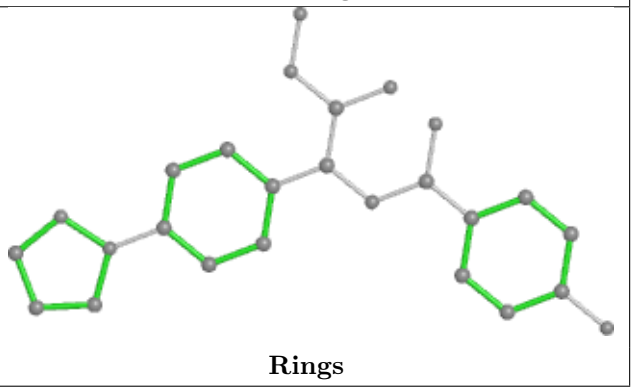
Bond lengths



Bond angles

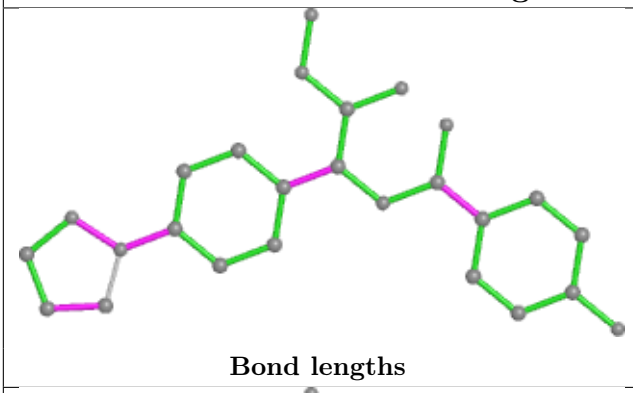


Torsions

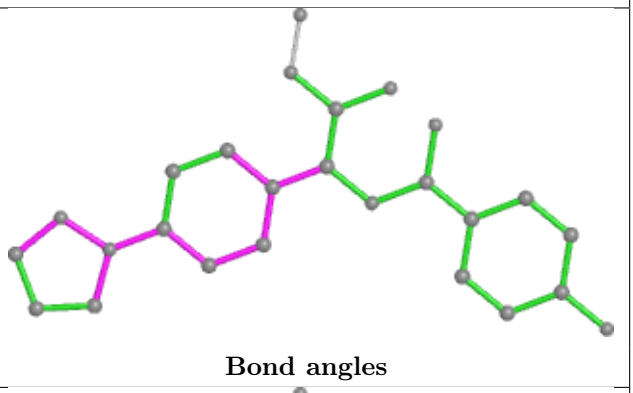


Rings

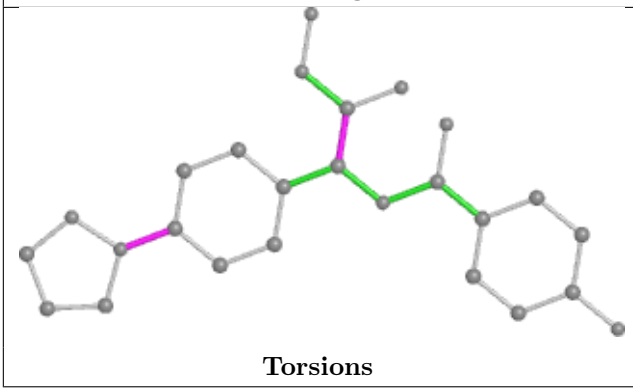
Ligand 3MW J 1005



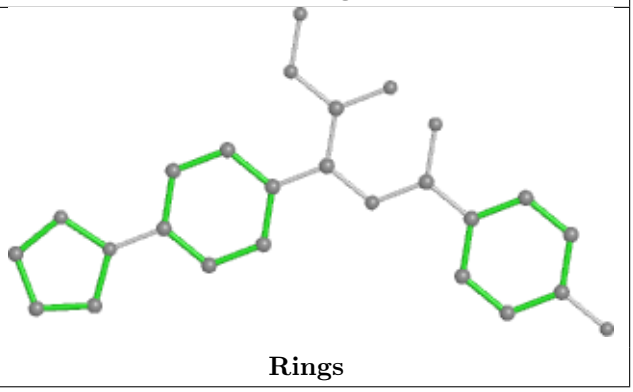
Bond lengths



Bond angles

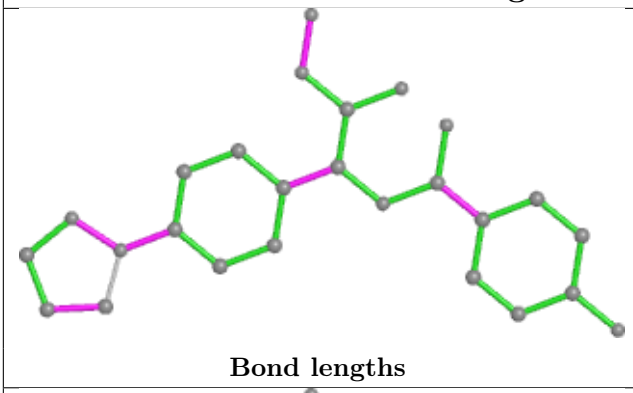


Torsions



Rings

Ligand 3MW C 1007



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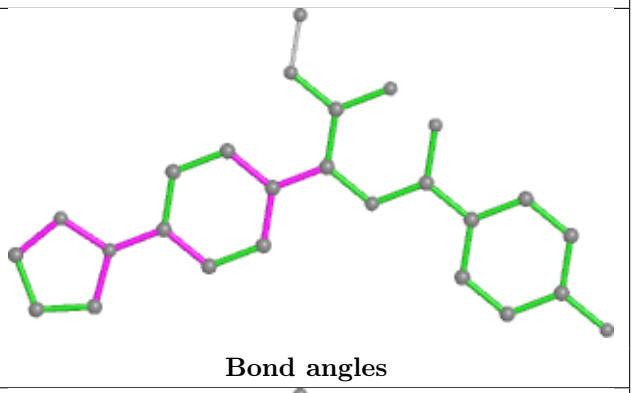
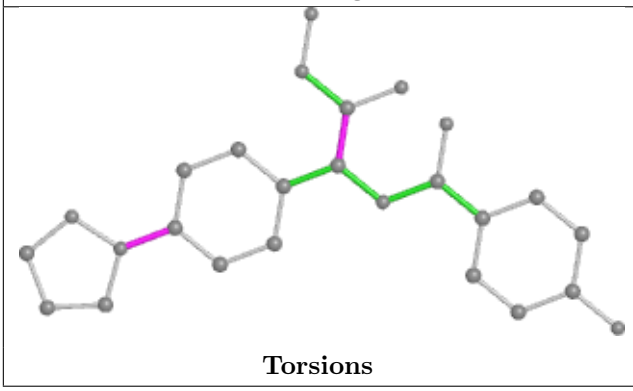


Bond angles



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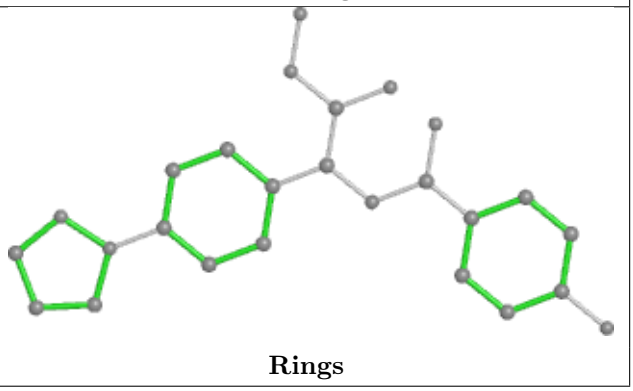

Rings

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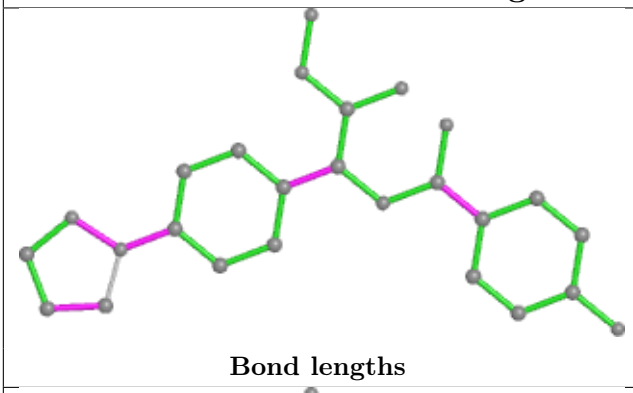

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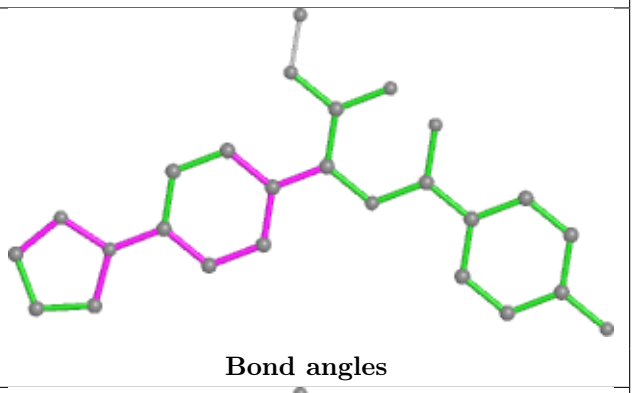
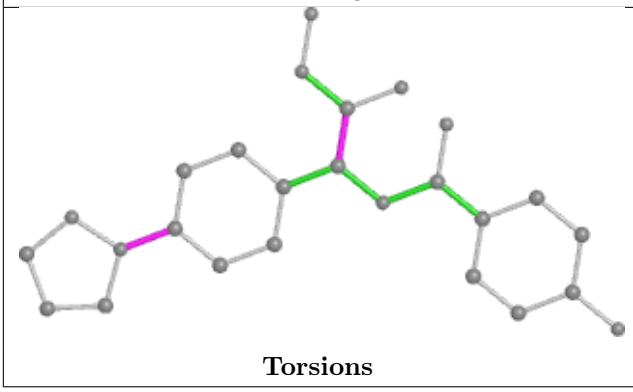


Bond angles



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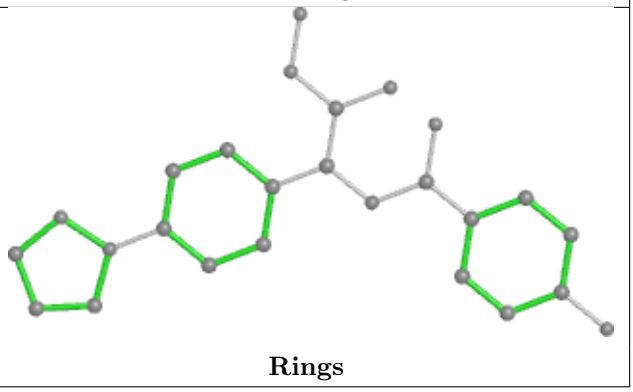
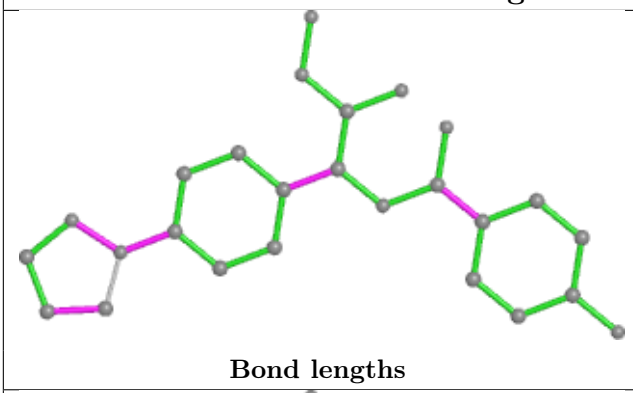


Rings

Ligand 3MW A 1006



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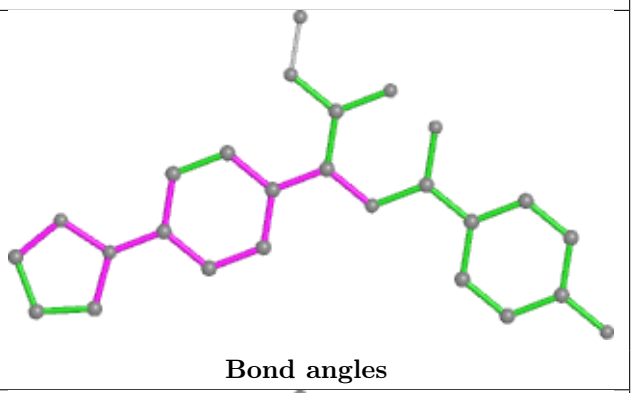
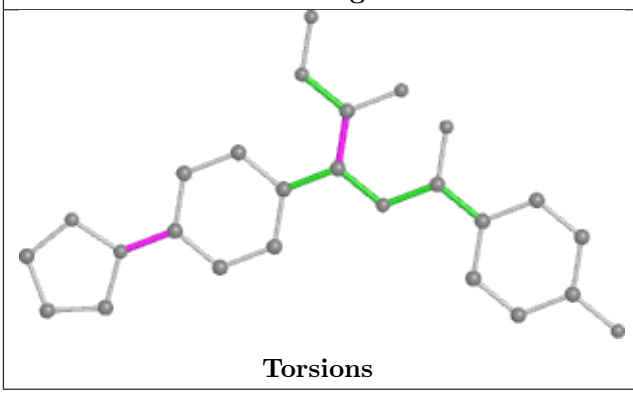


Bond angles



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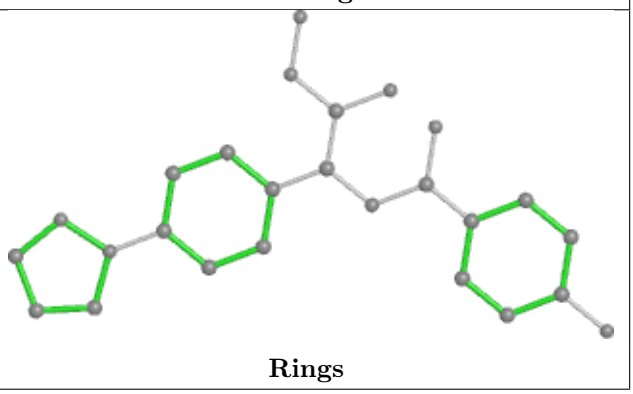
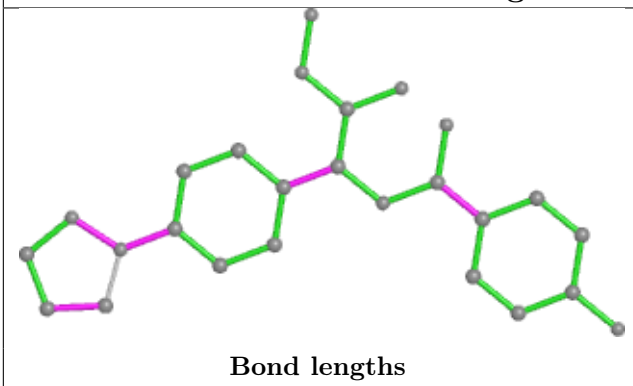


Rings

Ligand 3MW G 1008



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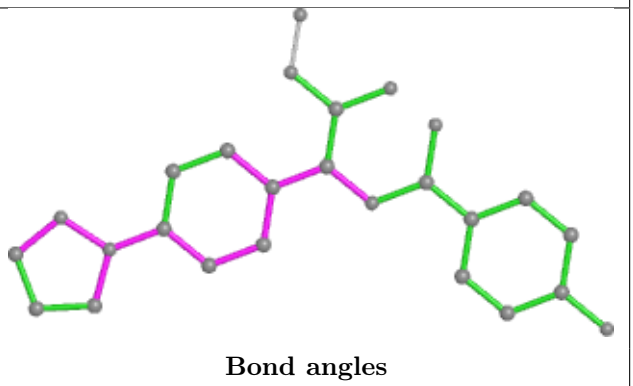
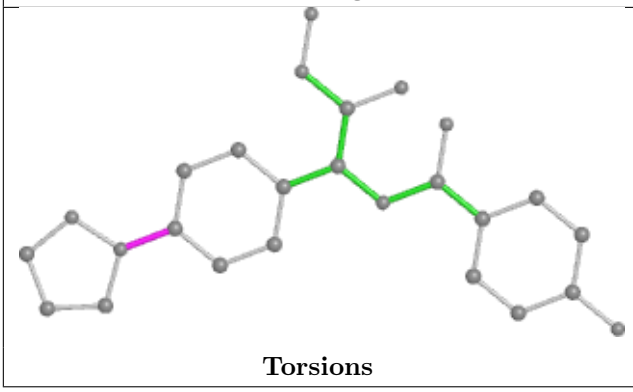


Bond angles



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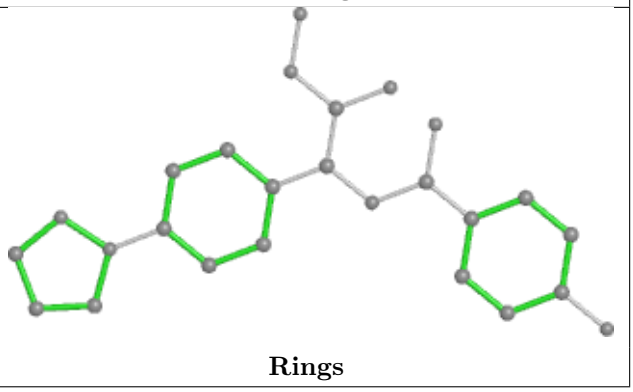
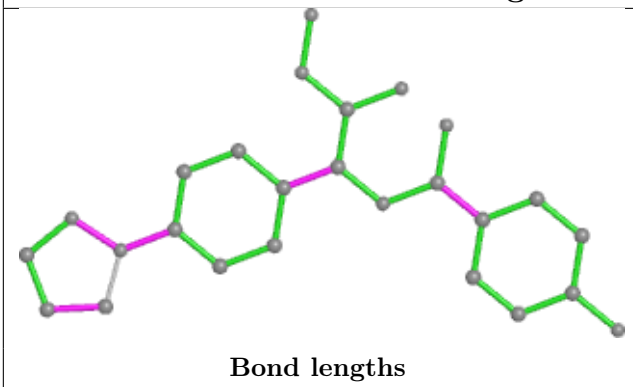
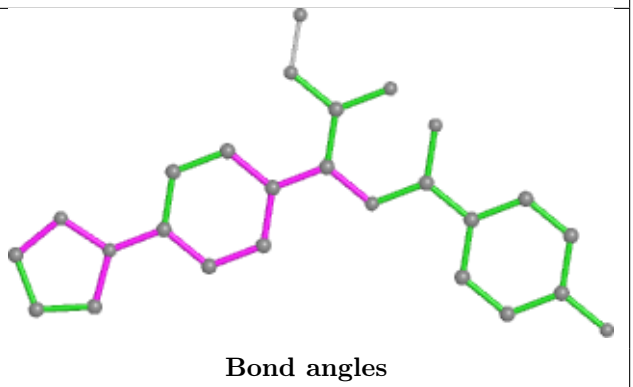


Rings

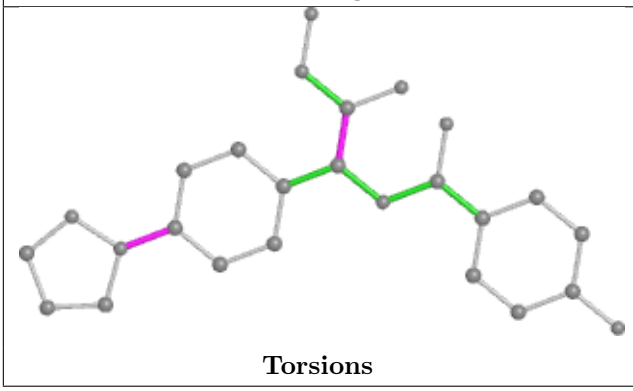
Ligand 3MW H 1005



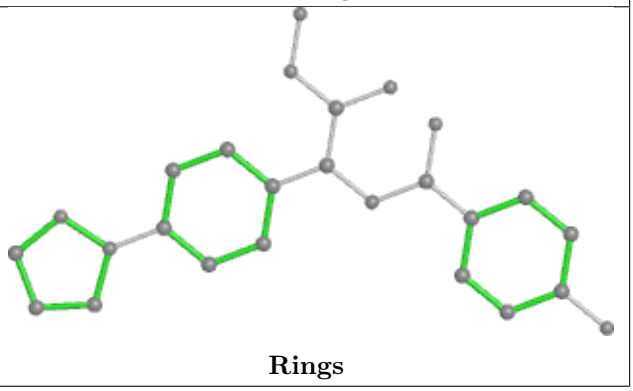
Bond lengths



Bond angles

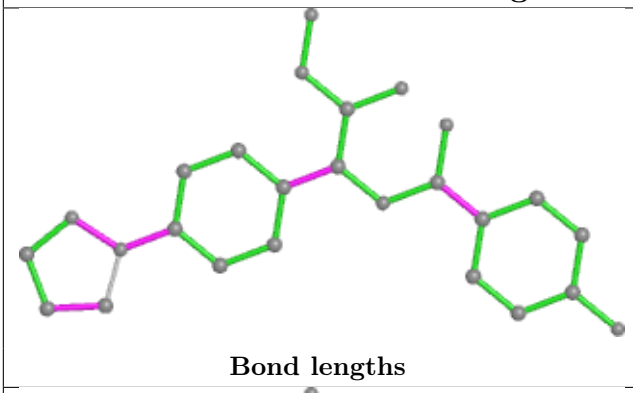


Torsions

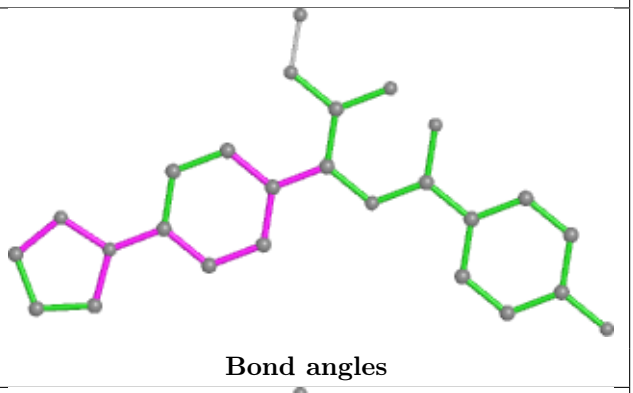


Rings

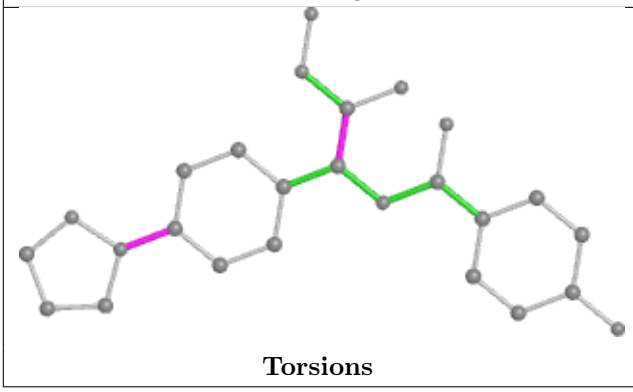
Ligand 3MW L 1005



Bond lengths



Bond angles



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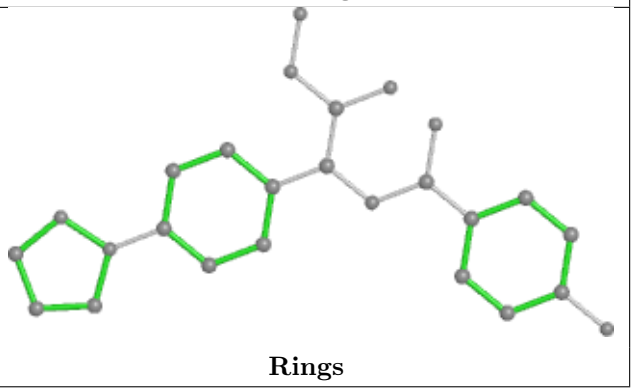
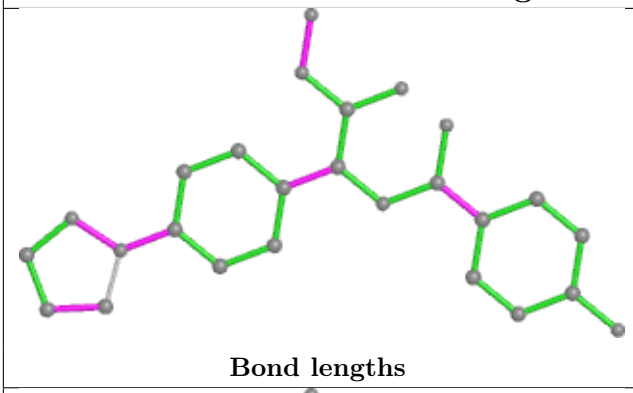
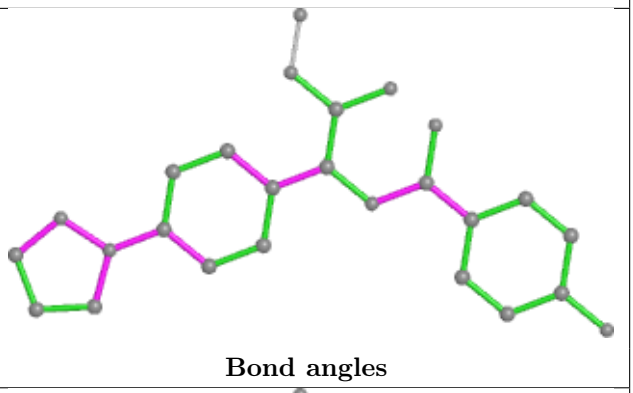


Rings

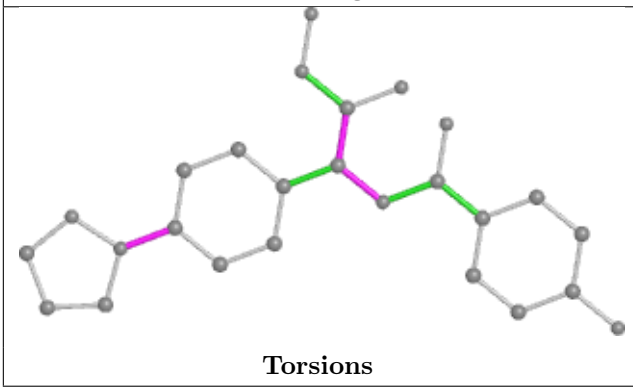
Ligand 3MW I 1004



Bond lengths



Bond angles



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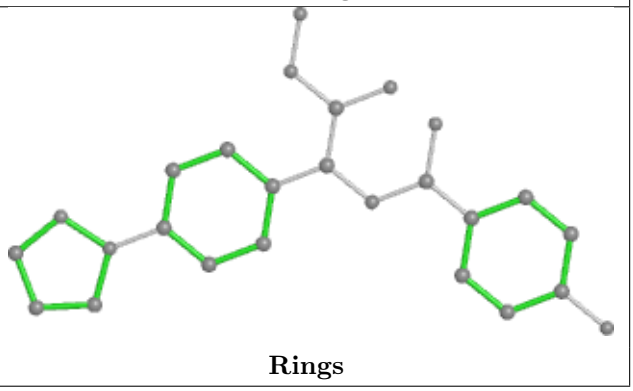
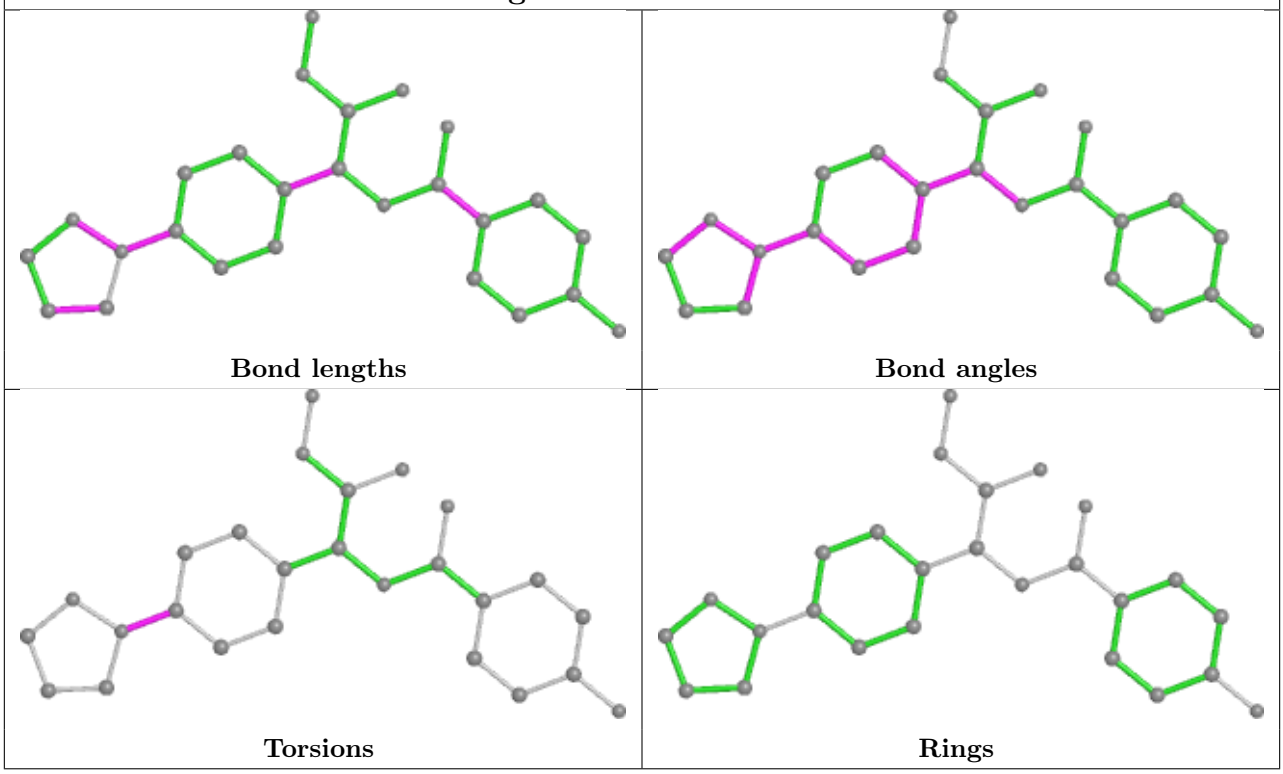


Rings

Ligand 3MW D 1004



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	516/528 (97%)	-0.11	10 (1%)	66	64	6, 21, 50, 64	0
1	B	512/528 (96%)	0.05	19 (3%)	41	36	8, 26, 56, 71	0
1	C	518/528 (98%)	-0.08	13 (2%)	57	54	9, 23, 51, 73	0
1	D	514/528 (97%)	-0.15	9 (1%)	68	66	11, 23, 49, 77	0
1	E	510/528 (96%)	-0.07	4 (0%)	86	85	14, 24, 46, 69	0
1	F	510/528 (96%)	0.11	18 (3%)	44	38	10, 29, 56, 71	0
1	G	513/528 (97%)	0.04	11 (2%)	63	60	16, 28, 51, 78	0
1	H	511/528 (96%)	0.16	23 (4%)	33	28	14, 29, 63, 86	0
1	I	516/528 (97%)	0.01	10 (1%)	66	64	13, 27, 53, 85	0
1	J	511/528 (96%)	0.04	7 (1%)	75	74	21, 30, 49, 70	0
1	K	509/528 (96%)	0.10	9 (1%)	68	66	18, 29, 49, 68	0
1	L	509/528 (96%)	0.26	14 (2%)	53	48	26, 34, 56, 85	0
All	All	6149/6336 (97%)	0.03	147 (2%)	59	56	6, 28, 53, 86	0

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	364	ASP	4.9
1	F	255	THR	4.3
1	H	197	ASP	4.3
1	A	136	GLY	3.9
1	C	550	SER	3.9

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	1PE	A	1004	12/16	0.82	0.24	35,42,50,52	0
4	1PE	G	1007	13/16	0.88	0.23	29,39,44,44	0
4	1PE	G	1006	10/16	0.91	0.19	32,39,43,44	0
4	1PE	C	1005	9/16	0.91	0.23	13,14,17,23	0
4	1PE	K	1005	12/16	0.91	0.30	31,38,45,49	0
3	CO3	K	1002	4/4	0.92	0.24	25,26,26,26	0
4	1PE	E	1006	6/16	0.92	0.28	22,28,33,35	0
4	1PE	F	1004	7/16	0.92	0.35	25,26,33,33	0
5	3MW	F	1005	26/26	0.92	0.20	22,30,38,42	0
6	SO4	C	1004	5/5	0.92	0.21	51,53,59,65	0
7	DMS	K	1007	4/4	0.92	0.24	28,35,48,53	0
4	1PE	H	1004	10/16	0.93	0.17	17,18,30,32	0
4	1PE	A	1005	8/16	0.94	0.17	25,28,33,33	0
3	CO3	J	1002	4/4	0.94	0.22	25,28,30,36	0
4	1PE	E	1005	12/16	0.94	0.25	23,24,35,35	0
5	3MW	A	1006	26/26	0.94	0.17	14,25,32,36	0
5	3MW	C	1007	26/26	0.94	0.17	11,12,18,24	0
2	ZN	D	1003	1/1	0.94	0.05	41,41,41,41	0
5	3MW	G	1008	26/26	0.94	0.16	21,23,31,34	0
5	3MW	I	1004	26/26	0.94	0.17	17,19,27,29	0
5	3MW	J	1005	26/26	0.94	0.19	23,25,32,35	0
5	3MW	L	1005	26/26	0.94	0.17	26,27,37,39	0
3	CO3	L	1002	4/4	0.94	0.25	29,29,32,39	0
6	SO4	L	1004	5/5	0.94	0.20	70,71,73,76	0
3	CO3	E	1002	4/4	0.94	0.21	25,26,29,35	0
5	3MW	K	1006	26/26	0.95	0.16	23,25,28,30	0
4	1PE	C	1006	8/16	0.95	0.19	19,25,32,36	0
5	3MW	H	1005	26/26	0.95	0.16	19,22,32,33	0
5	3MW	D	1004	26/26	0.95	0.18	13,16,32,41	0
5	3MW	B	1005	26/26	0.95	0.16	12,25,33,39	0
3	CO3	H	1002	4/4	0.96	0.20	17,18,18,18	0
6	SO4	B	1004	5/5	0.96	0.16	8,12,21,26	0

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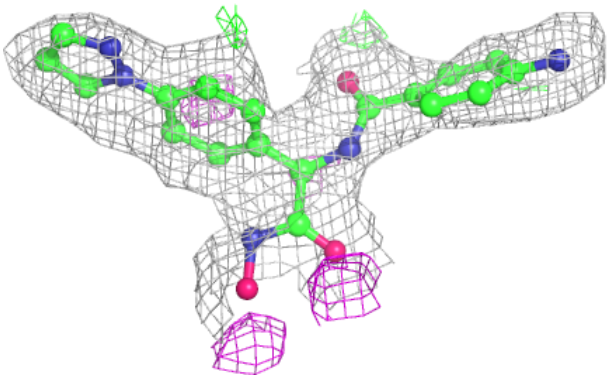
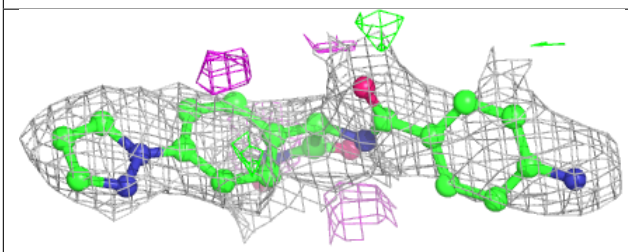
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	3MW	E	1007	26/26	0.96	0.17	13,18,28,53	0
6	SO4	G	1005	5/5	0.96	0.29	50,51,59,60	0
3	CO3	C	1002	4/4	0.96	0.17	10,10,13,27	0
3	CO3	G	1002	4/4	0.96	0.17	22,24,26,28	0
3	CO3	F	1002	4/4	0.97	0.15	12,15,16,17	0
2	ZN	F	1003	1/1	0.97	0.04	28,28,28,28	0
3	CO3	A	1002	4/4	0.97	0.14	7,7,13,18	0
3	CO3	I	1002	4/4	0.97	0.17	17,18,18,18	0
3	CO3	B	1002	4/4	0.97	0.19	11,11,11,18	0
6	SO4	K	1004	5/5	0.97	0.35	49,51,57,59	0
2	ZN	B	1001	1/1	0.97	0.07	15,15,15,15	0
2	ZN	E	1003	1/1	0.97	0.04	36,36,36,36	0
2	ZN	I	1001	1/1	0.98	0.14	47,47,47,47	0
2	ZN	I	1003	1/1	0.98	0.12	38,38,38,38	0
2	ZN	J	1001	1/1	0.98	0.06	26,26,26,26	0
2	ZN	J	1003	1/1	0.98	0.06	32,32,32,32	0
2	ZN	B	1003	1/1	0.98	0.08	34,34,34,34	0
6	SO4	E	1004	5/5	0.98	0.09	23,23,30,34	0
6	SO4	G	1004	5/5	0.98	0.11	16,16,22,26	0
2	ZN	A	1003	1/1	0.98	0.05	31,31,31,31	0
6	SO4	J	1004	5/5	0.98	0.10	30,30,31,31	0
2	ZN	H	1001	1/1	0.98	0.03	18,18,18,18	0
3	CO3	D	1002	4/4	0.98	0.22	14,15,15,15	0
2	ZN	H	1003	1/1	0.98	0.08	40,40,40,40	0
2	ZN	C	1003	1/1	0.99	0.10	33,33,33,33	0
2	ZN	G	1003	1/1	0.99	0.05	27,27,27,27	0
2	ZN	K	1001	1/1	0.99	0.06	26,26,26,26	0
2	ZN	K	1003	1/1	0.99	0.02	26,26,26,26	0
2	ZN	L	1001	1/1	0.99	0.05	29,29,29,29	0
2	ZN	L	1003	1/1	0.99	0.02	29,29,29,29	0
2	ZN	D	1001	1/1	0.99	0.04	31,31,31,31	0
2	ZN	A	1001	1/1	0.99	0.03	27,27,27,27	0
2	ZN	C	1001	1/1	0.99	0.04	18,18,18,18	0
2	ZN	F	1001	1/1	0.99	0.04	24,24,24,24	0
2	ZN	G	1001	1/1	1.00	0.08	31,31,31,31	0
2	ZN	E	1001	1/1	1.00	0.02	15,15,15,15	0

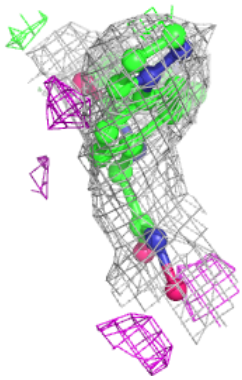
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3MW 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)

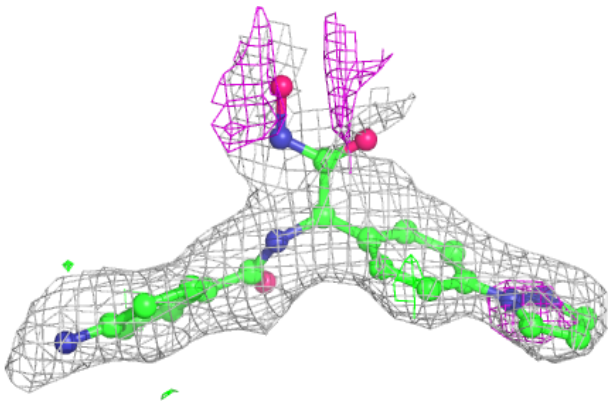


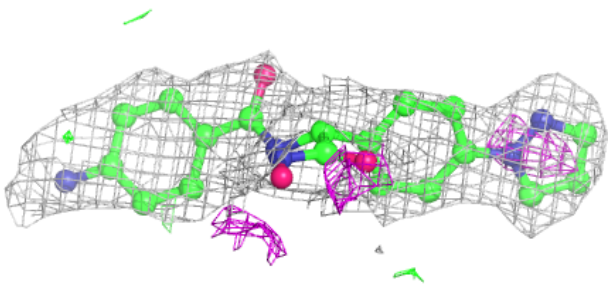


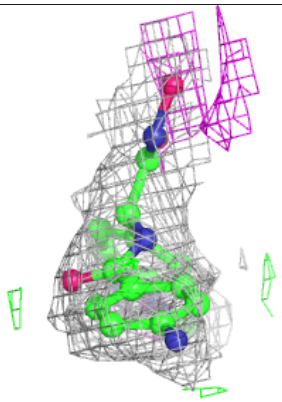


Electron density around 3MW A 1006:

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

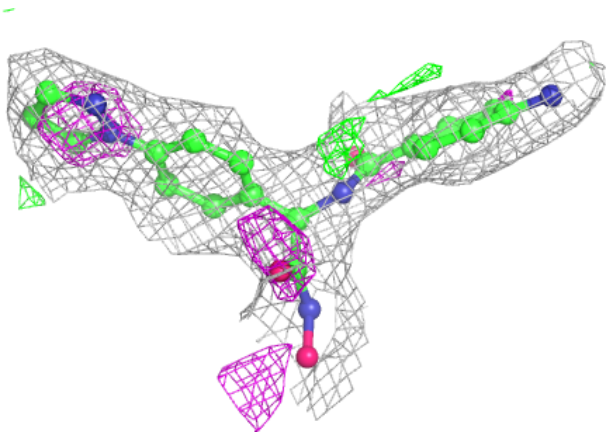


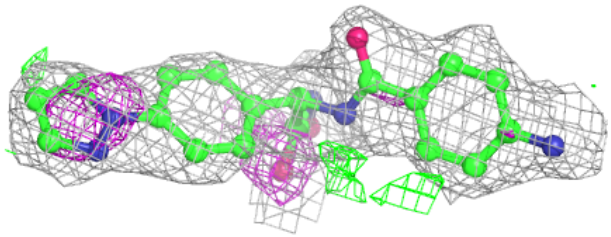


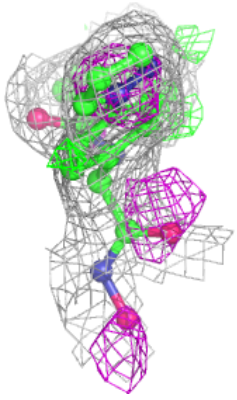


Electron density around 3MW C 1007:

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

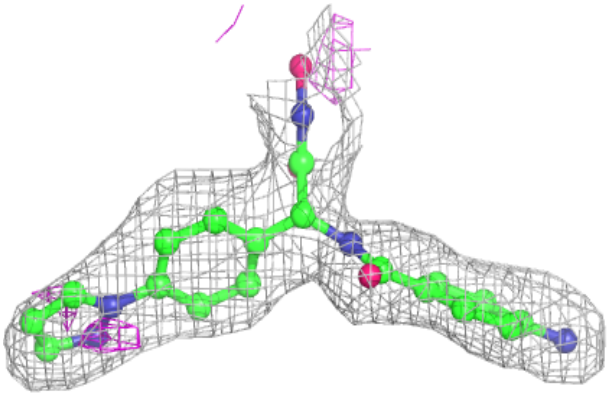


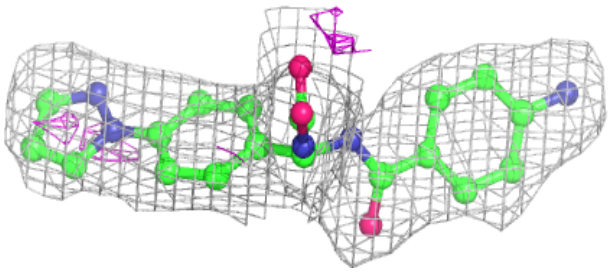


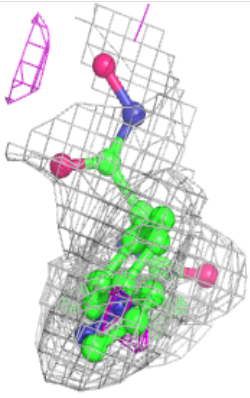


Electron density around 3MW G 1008:

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

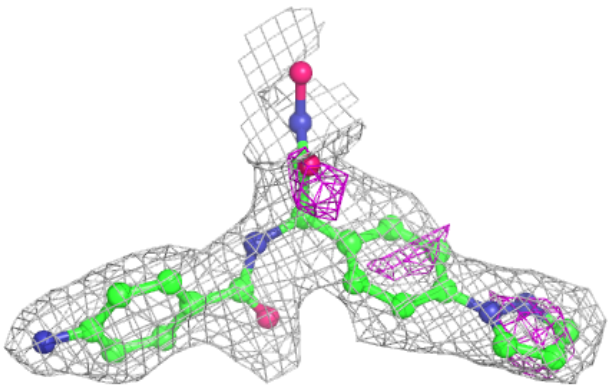


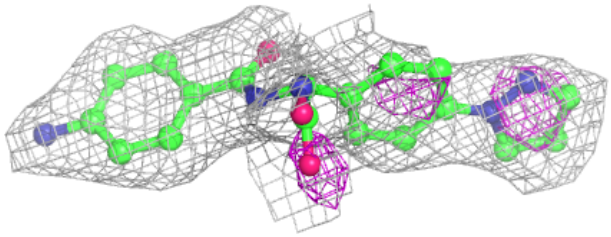


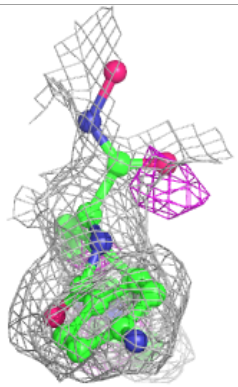


Electron density around 3MW I 1004:

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

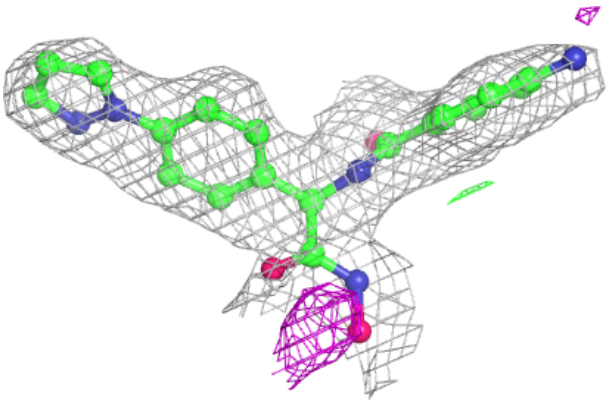


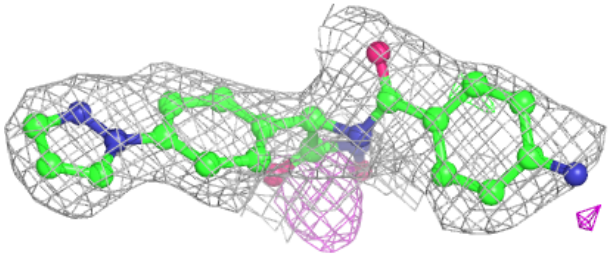


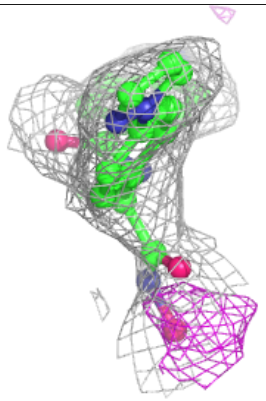


Electron density around 3MW J 1005:

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

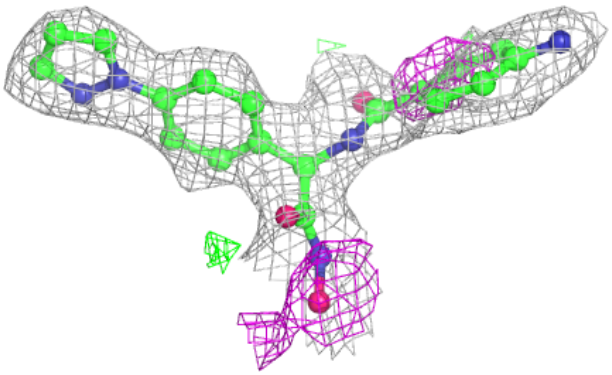


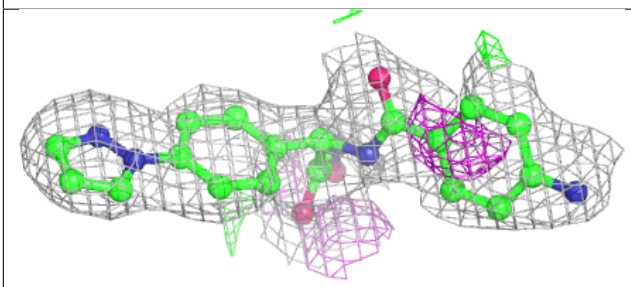


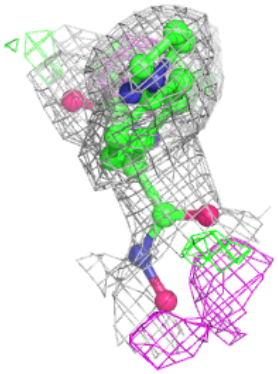


Electron density around 3MW L 1005:

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

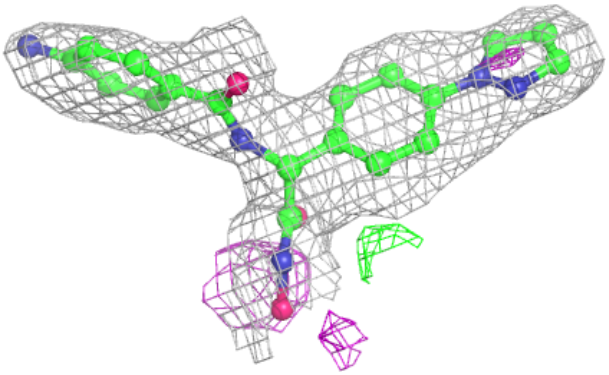


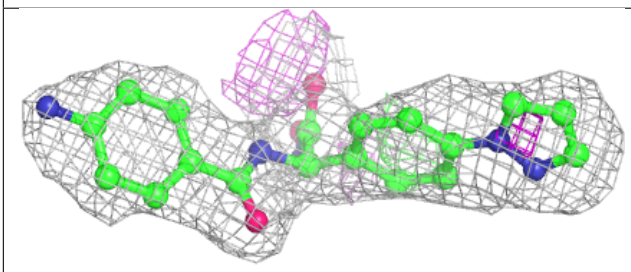


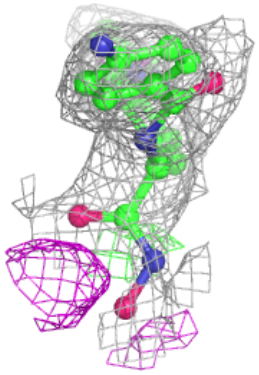


Electron density around 3MW K 1006:

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

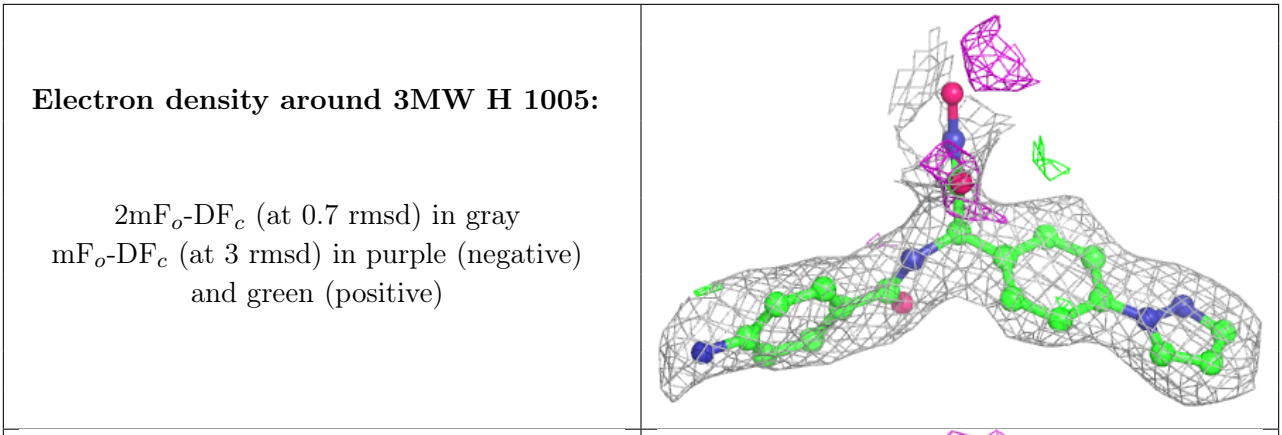






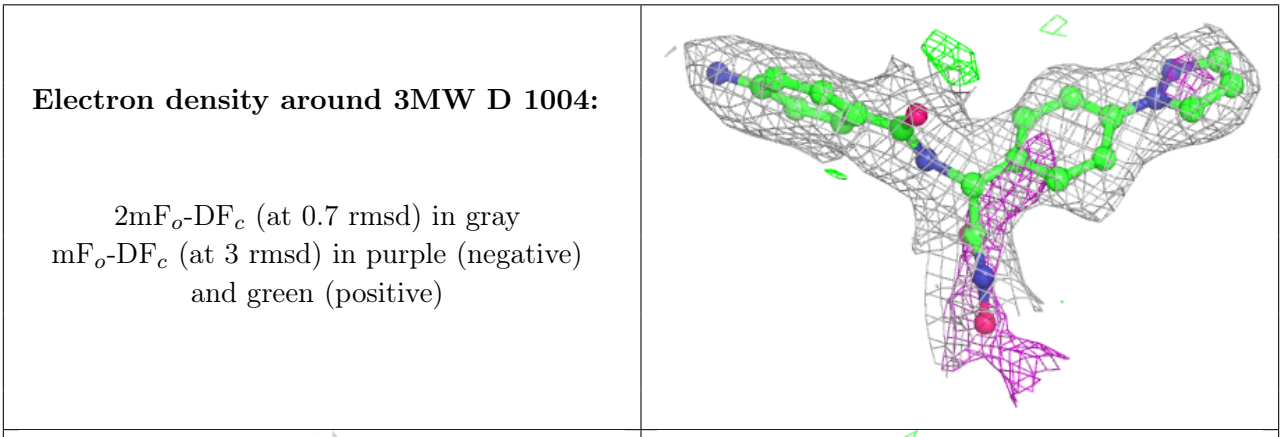
Electron density around 3MW H 1005:

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



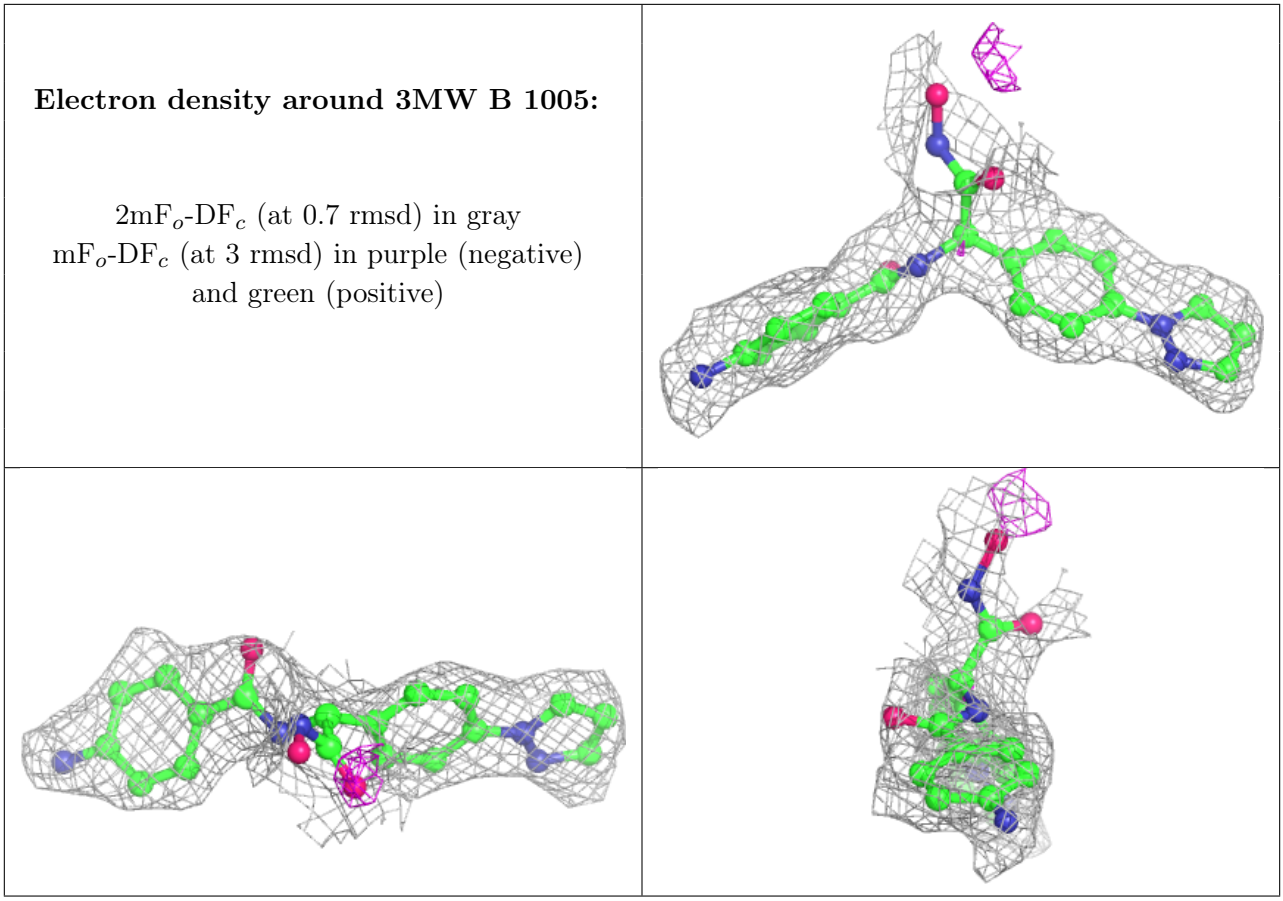
Electron density around 3MW D 1004:

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



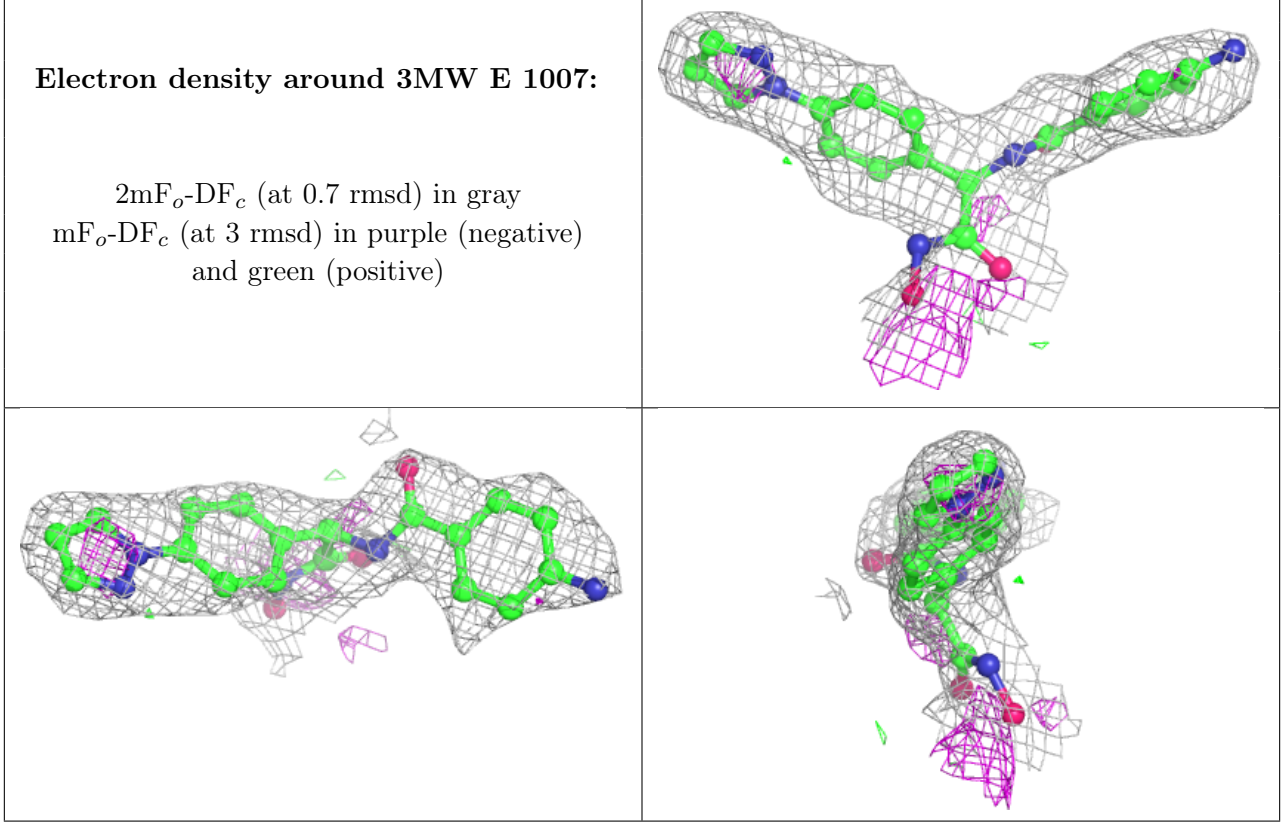
Electron density around 3MW B 1005:

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



Electron density around 3MW E 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.