wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2023 – 09:27 PM EDT

PDB ID	:	4K3N
Title	:	Phosphonic Arginine Mimetics as Inhibitors of the M17 Aminopeptidases from Plasmodium falciparum
Authors	:	McGowan, S.
Deposited on	:	2013-04-11
Resolution	:	2.00 Å(reported)

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

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

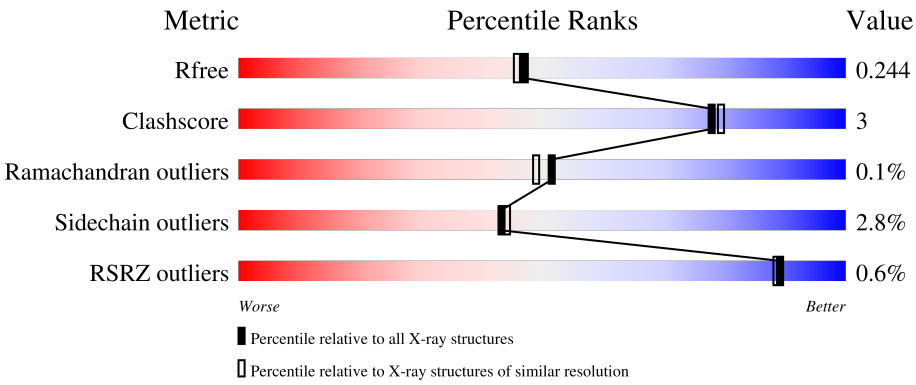
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	528	91% 8% •
1	B	528	% 88% 9% •
1	C	528	89% 9% •
1	D	528	% 89% 8% •
1	E	528	90% 6% •

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

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 49847 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	3995	2564	642	769	20	0	1	0
1	B	518	3939	2529	638	752	20	0	0	0
1	C	518	3960	2547	639	754	20	0	1	0
1	D	514	3947	2539	635	753	20	0	0	0
1	E	510	3905	2513	626	747	19	0	0	0
1	F	511	3849	2472	624	734	19	0	0	0
1	G	519	3993	2562	642	770	19	0	0	0
1	H	516	3914	2513	632	750	19	0	0	0
1	I	518	3964	2549	638	757	20	0	0	0
1	J	513	3939	2536	636	747	20	0	0	0
1	K	509	3906	2515	625	747	19	0	0	0
1	L	513	3885	2494	628	744	19	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

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

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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
			Total	Zn		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0
2	E	2	2	2	0	0
2	F	2	2	2	0	0
2	G	2	2	2	0	0
2	H	2	2	2	0	0
2	I	2	2	2	0	0
2	J	2	2	2	0	0

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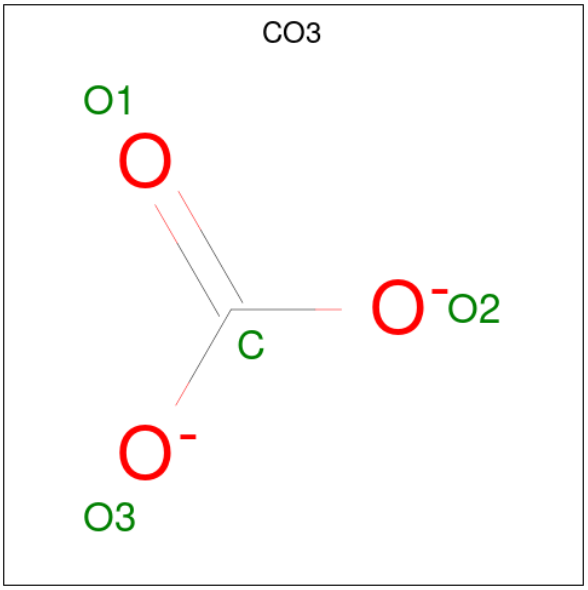
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	K	2	2	2	0	0
			Total	Zn		
2	L	2	2	2	0	0

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



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

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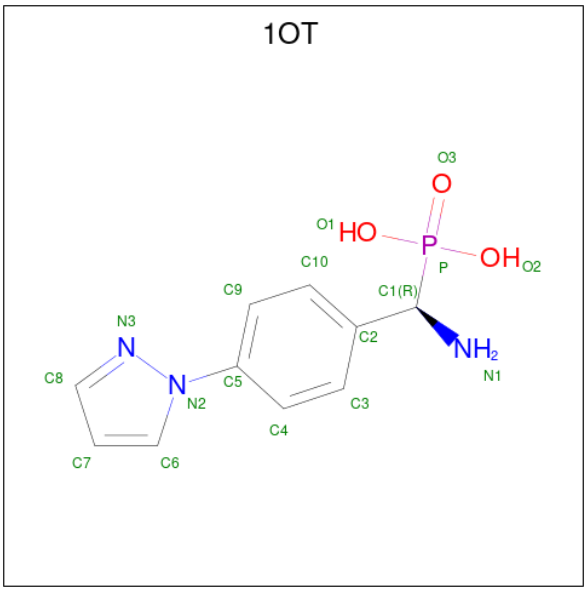
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	J	1	4	1	3		0	0
			Total	C	O			
3	K	1	4	1	3		0	0
			Total	C	O			
3	L	1	4	1	3		0	0

- Molecule 4 is {(R)-amino[4-(1H-pyrazol-1-yl)phenyl]methyl}phosphonic acid (three-letter code: 1OT) (formula: $C_{10}H_{12}N_3O_3P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	17	10	3	3	1	0	0
			Total	C	N	O	P		
4	B	1	17	10	3	3	1	0	0
			Total	C	N	O	P		
4	C	1	17	10	3	3	1	0	0
			Total	C	N	O	P		
4	D	1	17	10	3	3	1	0	0
			Total	C	N	O	P		
4	E	1	17	10	3	3	1	0	0
			Total	C	N	O	P		
4	F	1	17	10	3	3	1	0	0
			Total	C	N	O	P		
4	G	1	17	10	3	3	1	0	0
			Total	C	N	O	P		
4	H	1	17	10	3	3	1	0	0

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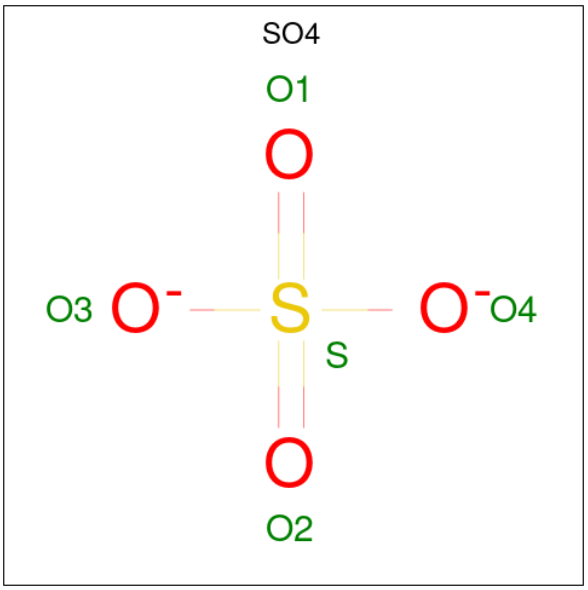
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	I	1	17	10	3	3	1	0	0
			Total	C	N	O	P		
4	J	1	17	10	3	3	1	0	0
			Total	C	N	O	P		
4	K	1	17	10	3	3	1	0	0
			Total	C	N	O	P		
4	L	1	17	10	3	3	1	0	0

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



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

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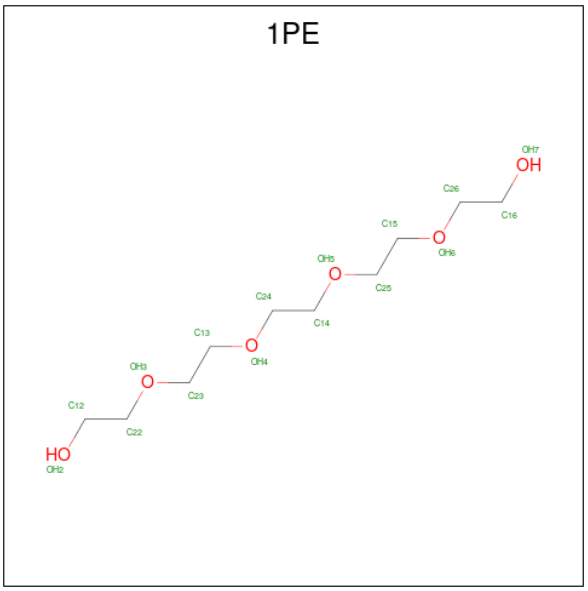
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	D	1	5	4	1	0	0
			Total	O	S		
5	E	1	5	4	1	0	0
			Total	O	S		
5	E	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0
			Total	O	S		
5	G	1	5	4	1	0	0
			Total	O	S		
5	G	1	5	4	1	0	0
			Total	O	S		
5	G	1	5	4	1	0	0
			Total	O	S		
5	H	1	5	4	1	0	0
			Total	O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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	A	1	9	6	3		0	0
			Total	C	O			
6	A	1	12	8	4		0	0
			Total	C	O			
6	C	1	13	9	4		0	0
			Total	C	O			
6	C	1	9	6	3		0	0
			Total	C	O			
6	C	1	7	5	2		0	0
			Total	C	O			
6	D	1	10	7	3		0	0
			Total	C	O			
6	D	1	9	6	3		0	0
			Total	C	O			
6	D	1	11	8	3		0	0
			Total	C	O			
6	E	1	12	8	4		0	0
			Total	C	O			
6	E	1	12	8	4		0	0
			Total	C	O			
6	E	1	8	5	3		0	0
			Total	C	O			
6	F	1	10	6	4		0	0
			Total	C	O			
6	F	1	10	6	4		0	0
			Total	C	O			
6	F	1	10	6	4		0	0

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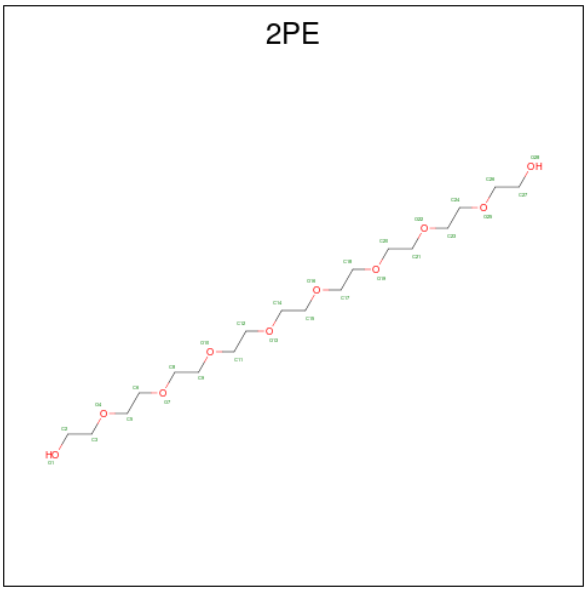
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	F	1	11	7	4	0	0
			Total	C	O		
6	G	1	9	6	3	0	0
			Total	C	O		
6	G	1	6	4	2	0	0
			Total	C	O		
6	G	1	6	4	2	0	0
			Total	C	O		
6	G	1	15	10	5	0	0
			Total	C	O		
6	I	1	15	10	5	0	0
			Total	C	O		
6	I	1	11	8	3	0	0
			Total	C	O		
6	I	1	5	3	2	0	0
			Total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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	26	17	9	0	0
			Total	C	O		
7	B	1	10	6	4	0	0
			Total	C	O		
7	C	1	9	6	3	0	0
			Total	C	O		
7	D	1	13	9	4	0	0
			Total	C	O		
7	D	1	5	3	2	0	0
			Total	C	O		
7	D	1	9	6	3	0	0
			Total	C	O		
7	E	1	9	6	3	0	0
			Total	C	O		
7	F	1	9	6	3	0	0
			Total	C	O		
7	H	1	25	16	9	0	0
			Total	C	O		
7	H	1	10	7	3	0	0
			Total	C	O		
7	I	1	8	5	3	0	0
			Total	C	O		
7	J	1	10	7	3	0	0

- Molecule 8 is water.

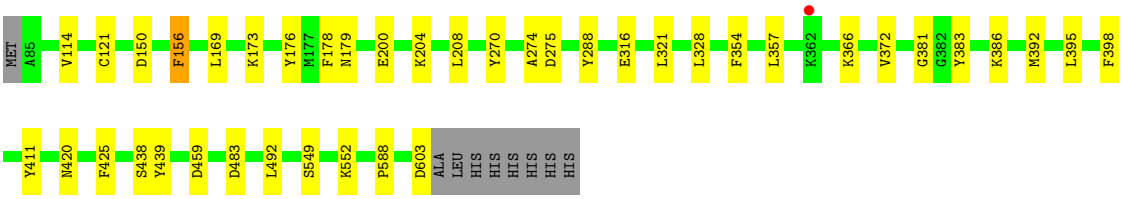
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	173	173	173	0	0
			Total	O		
8	B	125	125	125	0	0
			Total	O		
8	C	168	168	168	0	0
			Total	O		
8	D	150	150	150	0	0
			Total	O		
8	E	193	193	193	0	0
			Total	O		
8	F	117	117	117	0	0
			Total	O		
8	G	145	145	145	0	0
			Total	O		
8	H	129	129	129	0	0
			Total	O		
8	I	146	146	146	0	0
			Total	O		
8	J	137	137	137	0	0
			Total	O		
8	K	175	175	175	0	0
			Total	O		
8	L	126	126	126	0	0

3 Residue-property plots (i)

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

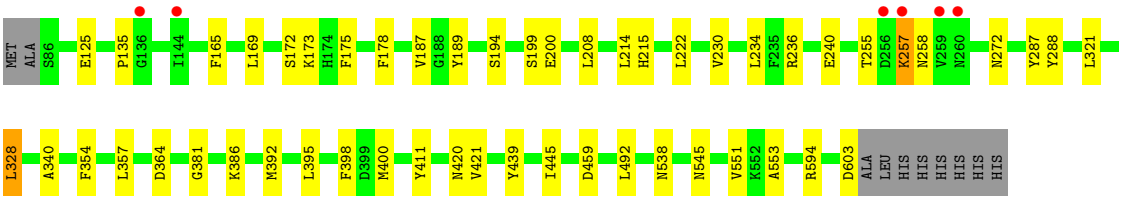
• Molecule 1: M17 leucyl aminopeptidase

Chain A:



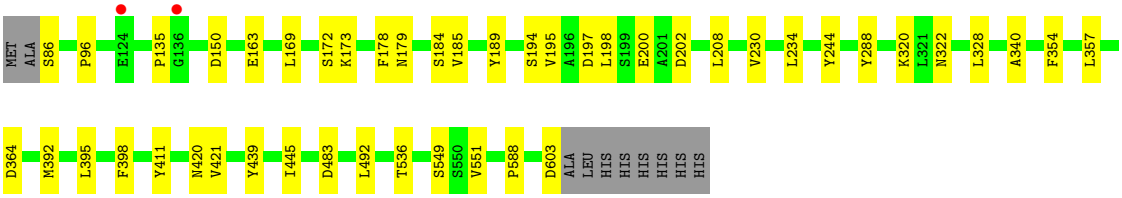
• Molecule 1: M17 leucyl aminopeptidase

Chain B:



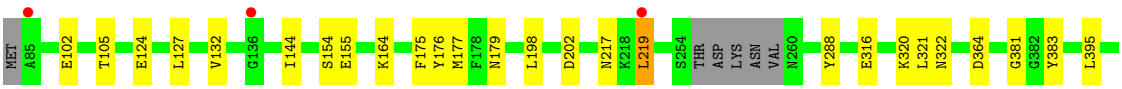
• Molecule 1: M17 leucyl aminopeptidase

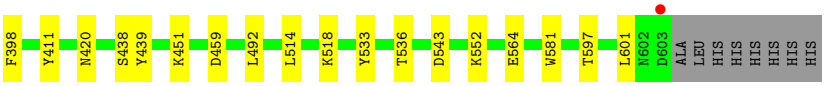
Chain C:



• Molecule 1: M17 leucyl aminopeptidase

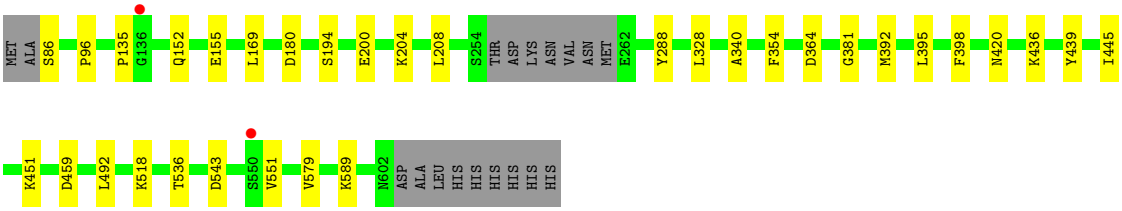
Chain D:





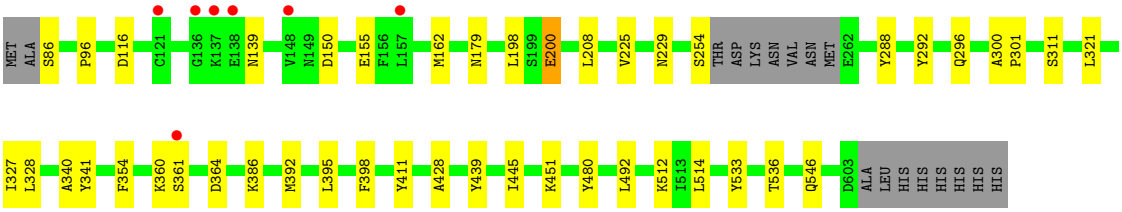
• Molecule 1: M17 leucyl aminopeptidase

Chain E:



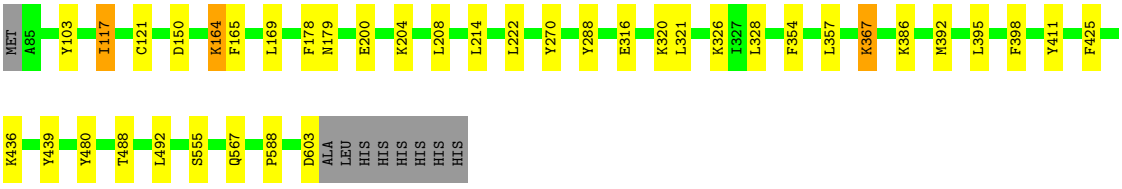
• Molecule 1: M17 leucyl aminopeptidase

Chain F:



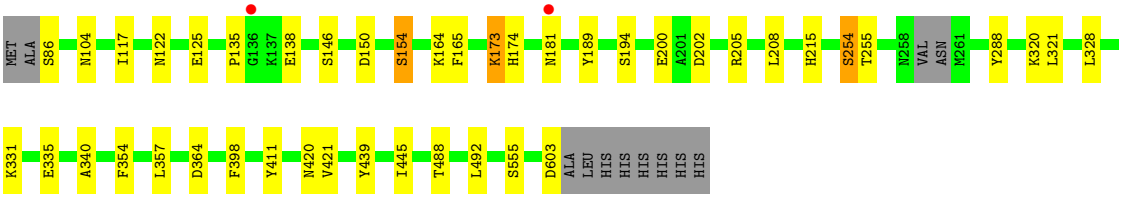
• Molecule 1: M17 leucyl aminopeptidase

Chain G:



• Molecule 1: M17 leucyl aminopeptidase

Chain H:

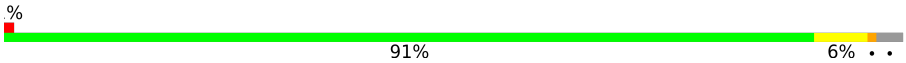


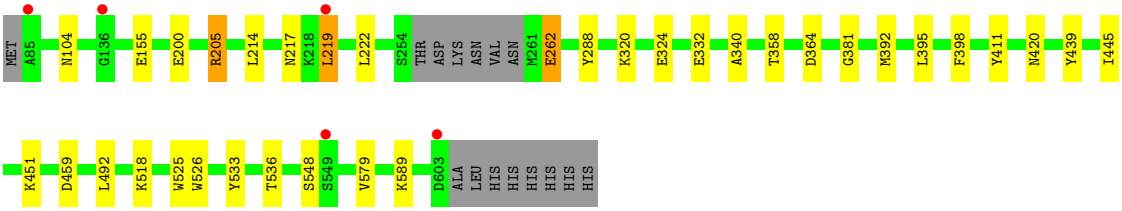
• Molecule 1: M17 leucyl aminopeptidase

Chain I:

• Molecule 1: M17 leucyl aminopeptidase

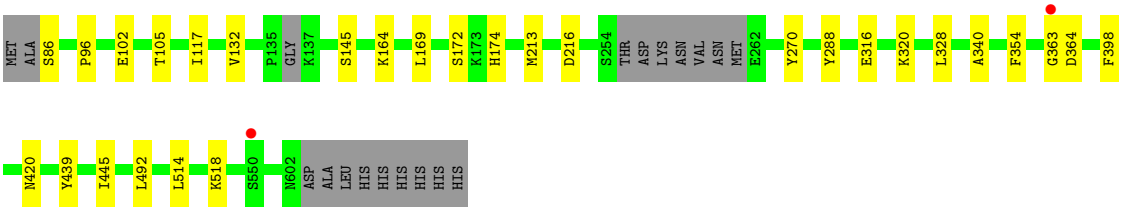
Chain J:





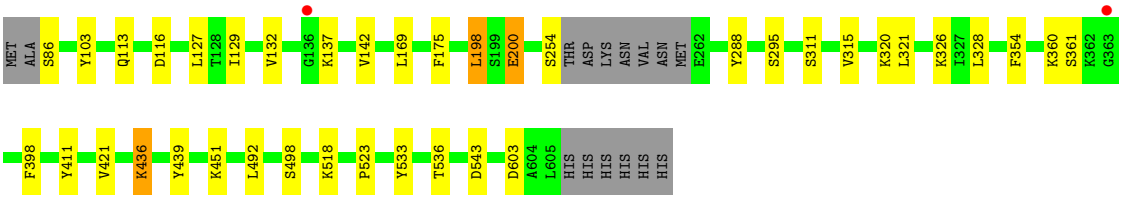
• Molecule 1: M17 leucyl aminopeptidase

Chain K:



• Molecule 1: M17 leucyl aminopeptidase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	173.72Å 177.08Å 229.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.11 – 2.00 62.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.11-2.00) 99.9 (62.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.196 , 0.240 0.205 , 0.244	Depositor DCC
R_{free} test set	23744 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49847	wwPDB-VP
Average B, all atoms (Å^2)	16.0	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 43.71 % 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 1.6963e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.37	0/4075	0.53	1/5525 (0.0%)
1	B	0.35	0/4017	0.53	0/5455
1	C	0.37	0/4041	0.53	0/5483
1	D	0.36	0/4024	0.53	0/5455
1	E	0.37	0/3982	0.53	0/5403
1	F	0.35	0/3925	0.53	1/5336 (0.0%)
1	G	0.39	0/4071	0.53	0/5521
1	H	0.35	0/3991	0.53	0/5422
1	I	0.36	0/4042	0.52	0/5484
1	J	0.36	0/4016	0.53	0/5443
1	K	0.37	0/3982	0.53	0/5400
1	L	0.37	0/3962	0.52	0/5384
All	All	0.37	0/48128	0.53	2/65311 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	156	PHE	CG-CD1-CE1	5.96	127.35	120.80
1	F	139	ASN	N-CA-C	5.81	126.68	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	257	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3995	0	3929	20	0
1	B	3939	0	3835	21	0
1	C	3960	0	3890	18	0
1	D	3947	0	3887	37	0
1	E	3905	0	3830	20	0
1	F	3849	0	3722	24	0
1	G	3993	0	3922	26	0
1	H	3914	0	3793	18	0
1	I	3964	0	3897	20	0
1	J	3939	0	3892	27	0
1	K	3906	0	3837	16	0
1	L	3885	0	3760	24	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	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	1	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
4	A	17	0	10	3	0
4	B	17	0	11	4	0
4	C	17	0	11	2	0
4	D	17	0	12	2	0
4	E	17	0	11	4	0
4	F	17	0	12	3	0
4	G	17	0	10	3	0
4	H	17	0	12	2	0
4	I	17	0	12	2	0
4	J	17	0	11	2	0
4	K	17	0	12	3	0
4	L	17	0	11	4	0
5	A	20	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
5	E	10	0	0	0	0
5	F	5	0	0	0	0
5	G	15	0	0	0	0
5	H	5	0	0	0	0
5	I	10	0	0	0	0
5	J	5	0	0	1	0
5	K	10	0	0	0	0
5	L	5	0	0	0	0
6	A	21	0	22	1	0
6	C	29	0	30	2	0
6	D	30	0	30	7	0
6	E	32	0	36	3	0
6	F	41	0	51	2	0
6	G	36	0	39	8	0
6	I	31	0	35	3	0
6	J	41	0	48	8	0
6	K	41	0	44	3	0
6	L	41	0	48	9	0
7	B	36	0	45	0	0
7	C	9	0	10	2	0
7	D	27	0	28	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	9	0	10	1	0
7	F	9	0	10	1	0
7	H	35	0	43	2	0
7	I	8	0	8	0	0
7	J	10	0	10	0	0
8	A	173	0	0	0	0
8	B	125	0	0	0	0
8	C	168	0	0	1	0
8	D	150	0	0	5	0
8	E	193	0	0	0	0
8	F	117	0	0	2	0
8	G	145	0	0	0	0
8	H	129	0	0	1	0
8	I	146	0	0	3	0
8	J	137	0	0	3	0
8	K	175	0	0	3	0
8	L	126	0	0	2	0
All	All	49847	0	46876	275	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 275 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:I:155:GLU:O	8:I:1103:HOH:O	1.97	0.82
1:I:161:ASN:ND2	8:I:1103:HOH:O	2.17	0.77
1:J:526:TRP:HB3	6:J:1009:1PE:H242	1.67	0.76
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.53	0.73
1:J:536:THR:OG1	8:J:1221:HOH:O	2.06	0.73

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/528 (98%)	507 (98%)	11 (2%)	0	100	100
1	B	516/528 (98%)	503 (98%)	11 (2%)	2 (0%)	34	30
1	C	517/528 (98%)	505 (98%)	12 (2%)	0	100	100
1	D	510/528 (97%)	498 (98%)	12 (2%)	0	100	100
1	E	506/528 (96%)	495 (98%)	11 (2%)	0	100	100
1	F	507/528 (96%)	497 (98%)	10 (2%)	0	100	100
1	G	517/528 (98%)	507 (98%)	10 (2%)	0	100	100
1	H	512/528 (97%)	502 (98%)	9 (2%)	1 (0%)	47	44
1	I	516/528 (98%)	505 (98%)	11 (2%)	0	100	100
1	J	509/528 (96%)	498 (98%)	11 (2%)	0	100	100
1	K	503/528 (95%)	494 (98%)	8 (2%)	1 (0%)	47	44
1	L	509/528 (96%)	500 (98%)	8 (2%)	1 (0%)	47	44
All	All	6140/6336 (97%)	6011 (98%)	124 (2%)	5 (0%)	51	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	138	GLU
1	L	137	LYS
1	B	257	LYS
1	B	258	ASN
1	K	363	GLY

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	429/455 (94%)	417 (97%)	12 (3%)	43	44
1	B	415/455 (91%)	399 (96%)	16 (4%)	32	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	421/455 (92%)	405 (96%)	16 (4%)	33	31
1	D	421/455 (92%)	414 (98%)	7 (2%)	60	65
1	E	416/455 (91%)	409 (98%)	7 (2%)	60	65
1	F	401/455 (88%)	389 (97%)	12 (3%)	41	41
1	G	428/455 (94%)	415 (97%)	13 (3%)	41	41
1	H	411/455 (90%)	395 (96%)	16 (4%)	32	30
1	I	423/455 (93%)	413 (98%)	10 (2%)	49	51
1	J	420/455 (92%)	412 (98%)	8 (2%)	57	61
1	K	417/455 (92%)	409 (98%)	8 (2%)	57	61
1	L	407/455 (90%)	393 (97%)	14 (3%)	37	36
All	All	5009/5460 (92%)	4870 (97%)	139 (3%)	43	44

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	439	TYR
1	K	145	SER
1	L	200	GLU
1	D	398	PHE
1	D	322	ASN

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

Mol	Chain	Res	Type
1	J	531	ASN
1	K	229	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 115 ligands modelled in this entry, 24 are monoatomic - leaving 91 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	$\#\|Z\| > 2$
7	2PE	B	1007	-	9,9,27	0.06	0	8,8,26	0.23	0
4	1OT	C	1004	2	16,18,18	2.63	5 (31%)	22,26,26	2.71	9 (40%)
7	2PE	H	1006	-	24,24,27	0.21	0	23,23,26	0.15	0
7	2PE	D	1010	-	12,12,27	0.20	0	11,11,26	0.15	0
5	SO4	B	1005	-	4,4,4	0.15	0	6,6,6	0.05	0
6	1PE	J	1008	-	10,10,15	0.55	0	9,9,14	0.27	0
6	1PE	L	1008	-	7,7,15	0.46	0	6,6,14	0.39	0
7	2PE	C	1009	-	8,8,27	0.16	0	7,7,26	0.24	0
6	1PE	F	1009	-	10,10,15	0.47	0	9,9,14	0.22	0
4	1OT	J	1004	2	16,18,18	2.66	5 (31%)	22,26,26	2.77	8 (36%)
5	SO4	K	1006	-	4,4,4	0.18	0	6,6,6	0.09	0
6	1PE	C	1008	-	6,6,15	0.50	0	5,5,14	0.26	0
3	CO3	I	1002	-	2,3,3	0.37	0	2,3,3	0.31	0
4	1OT	D	1004	2	16,18,18	2.79	5 (31%)	22,26,26	3.14	10 (45%)
3	CO3	L	1002	-	2,3,3	0.42	0	2,3,3	0.26	0
5	SO4	E	1005	-	4,4,4	0.13	0	6,6,6	0.15	0
6	1PE	K	1008	-	11,11,15	0.46	0	10,10,14	0.20	0
4	1OT	L	1004	2	16,18,18	2.66	5 (31%)	22,26,26	2.86	10 (45%)
7	2PE	I	1010	-	7,7,27	0.15	0	6,6,26	0.12	0
3	CO3	G	1002	-	2,3,3	0.43	0	2,3,3	0.35	0
3	CO3	B	1002	-	2,3,3	0.38	0	2,3,3	0.29	0
4	1OT	B	1004	2	16,18,18	2.72	5 (31%)	22,26,26	2.79	8 (36%)
6	1PE	E	1007	-	11,11,15	0.48	0	10,10,14	0.32	0
7	2PE	D	1012	-	8,8,27	0.18	0	7,7,26	0.17	0
7	2PE	H	1007	-	9,9,27	0.21	0	8,8,26	0.08	0
6	1PE	K	1007	-	11,11,15	0.52	0	10,10,14	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	1PE	E	1008	-	11,11,15	0.49	0	10,10,14	0.31	0
3	CO3	D	1002	-	2,3,3	0.42	0	2,3,3	0.33	0
3	CO3	E	1002	-	2,3,3	0.40	0	2,3,3	0.09	0
4	1OT	A	1004	2	16,18,18	2.70	5 (31%)	22,26,26	2.96	9 (40%)
5	SO4	D	1005	-	4,4,4	0.29	0	6,6,6	0.13	0
5	SO4	H	1005	-	4,4,4	0.12	0	6,6,6	0.17	0
5	SO4	E	1006	-	4,4,4	0.17	0	6,6,6	0.23	0
7	2PE	F	1010	-	8,8,27	0.21	0	7,7,26	0.22	0
7	2PE	B	1006	-	25,25,27	0.18	0	24,24,26	0.17	0
3	CO3	C	1002	-	2,3,3	0.41	0	2,3,3	0.19	0
5	SO4	D	1006	-	4,4,4	0.13	0	6,6,6	0.05	0
6	1PE	F	1008	-	9,9,15	0.47	0	8,8,14	0.18	0
7	2PE	D	1011	-	4,4,27	0.25	0	3,3,26	0.37	0
7	2PE	E	1010	-	8,8,27	0.14	0	7,7,26	0.19	0
5	SO4	C	1005	-	4,4,4	0.14	0	6,6,6	0.17	0
5	SO4	J	1005	-	4,4,4	0.13	0	6,6,6	0.08	0
5	SO4	G	1006	-	4,4,4	0.17	0	6,6,6	0.24	0
6	1PE	J	1006	-	10,10,15	0.43	0	9,9,14	0.44	0
6	1PE	F	1007	-	9,9,15	0.48	0	8,8,14	0.15	0
4	1OT	F	1004	2	16,18,18	2.68	5 (31%)	22,26,26	2.75	9 (40%)
5	SO4	L	1005	-	4,4,4	0.11	0	6,6,6	0.11	0
6	1PE	A	1010	-	11,11,15	0.51	0	10,10,14	0.15	0
6	1PE	G	1010	-	5,5,15	0.49	0	4,4,14	0.37	0
6	1PE	I	1007	-	14,14,15	0.39	0	13,13,14	0.49	0
6	1PE	G	1011	-	14,14,15	0.41	0	13,13,14	0.57	0
5	SO4	G	1005	-	4,4,4	0.19	0	6,6,6	0.25	0
6	1PE	L	1006	-	9,9,15	0.36	0	8,8,14	0.69	0
3	CO3	A	1002	-	2,3,3	0.41	0	2,3,3	0.29	0
6	1PE	D	1008	-	8,8,15	0.50	0	7,7,14	0.22	0
6	1PE	D	1007	-	9,9,15	0.44	0	8,8,14	0.43	0
6	1PE	L	1009	-	10,10,15	0.50	0	9,9,14	0.49	0
5	SO4	K	1005	-	4,4,4	0.24	0	6,6,6	0.16	0
6	1PE	K	1010	-	5,5,15	0.47	0	4,4,14	0.16	0
5	SO4	A	1005	-	4,4,4	0.09	0	6,6,6	0.27	0
6	1PE	L	1007	-	11,11,15	0.52	0	10,10,14	0.20	0
6	1PE	K	1009	-	10,10,15	0.47	0	9,9,14	0.15	0
5	SO4	A	1008	-	4,4,4	0.17	0	6,6,6	0.26	0
4	1OT	I	1004	2	16,18,18	2.57	5 (31%)	22,26,26	2.83	12 (54%)
6	1PE	D	1009	-	10,10,15	0.53	0	9,9,14	0.39	0
6	1PE	J	1009	-	8,8,15	0.54	0	7,7,14	0.38	0
3	CO3	J	1002	-	2,3,3	0.44	0	2,3,3	0.35	0
5	SO4	I	1006	-	4,4,4	0.20	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	2PE	J	1010	-	9,9,27	0.21	0	8,8,26	0.11	0
3	CO3	F	1002	-	2,3,3	0.45	0	2,3,3	0.21	0
5	SO4	A	1007	-	4,4,4	0.16	0	6,6,6	0.28	0
4	1OT	E	1004	2	16,18,18	2.72	5 (31%)	22,26,26	2.91	10 (45%)
6	1PE	I	1008	-	10,10,15	0.46	0	9,9,14	0.33	0
5	SO4	F	1005	-	4,4,4	0.12	0	6,6,6	0.07	0
5	SO4	A	1006	-	4,4,4	0.13	0	6,6,6	0.17	0
3	CO3	H	1002	-	2,3,3	0.43	0	2,3,3	0.46	0
6	1PE	C	1006	-	12,12,15	0.55	0	11,11,14	0.20	0
5	SO4	I	1005	-	4,4,4	0.16	0	6,6,6	0.07	0
6	1PE	C	1007	-	8,8,15	0.43	0	7,7,14	0.22	0
6	1PE	E	1009	-	7,7,15	0.43	0	6,6,14	0.36	0
6	1PE	F	1006	-	9,9,15	0.43	0	8,8,14	0.24	0
4	1OT	G	1004	2	16,18,18	2.66	5 (31%)	22,26,26	2.65	9 (40%)
6	1PE	I	1009	-	4,4,15	0.39	0	3,3,14	0.34	0
6	1PE	G	1008	-	8,8,15	0.41	0	7,7,14	0.36	0
4	1OT	H	1004	2	16,18,18	2.73	5 (31%)	22,26,26	2.63	7 (31%)
3	CO3	K	1002	-	2,3,3	0.34	0	2,3,3	0.12	0
6	1PE	G	1009	-	5,5,15	0.45	0	4,4,14	0.49	0
6	1PE	A	1009	-	8,8,15	0.43	0	7,7,14	0.27	0
4	1OT	K	1004	2	16,18,18	2.58	5 (31%)	22,26,26	2.73	10 (45%)
6	1PE	J	1007	-	9,9,15	0.52	0	8,8,14	0.32	0
5	SO4	G	1007	-	4,4,4	0.14	0	6,6,6	0.18	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
7	2PE	B	1007	-	-	4/7/7/25	-
4	1OT	C	1004	2	-	5/13/14/14	0/2/2/2
6	1PE	L	1006	-	-	3/7/7/13	-
4	1OT	E	1004	2	-	4/13/14/14	0/2/2/2
6	1PE	I	1008	-	-	3/8/8/13	-
7	2PE	H	1006	-	-	7/22/22/25	-
4	1OT	A	1004	2	-	5/13/14/14	0/2/2/2
6	1PE	C	1006	-	-	1/10/10/13	-
6	1PE	D	1008	-	-	3/6/6/13	-
7	2PE	D	1010	-	-	7/10/10/25	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	C	1007	-	-	4/6/6/13	-
6	1PE	D	1007	-	-	4/7/7/13	-
6	1PE	E	1009	-	-	3/5/5/13	-
6	1PE	F	1006	-	-	1/7/7/13	-
6	1PE	J	1008	-	-	3/8/8/13	-
6	1PE	L	1008	-	-	3/5/5/13	-
6	1PE	L	1009	-	-	4/8/8/13	-
7	2PE	C	1009	-	-	3/6/6/25	-
4	1OT	G	1004	2	-	4/13/14/14	0/2/2/2
6	1PE	K	1010	-	-	2/3/3/13	-
7	2PE	H	1007	-	-	3/7/7/25	-
6	1PE	L	1007	-	-	6/9/9/13	-
6	1PE	F	1009	-	-	2/8/8/13	-
6	1PE	K	1009	-	-	1/8/8/13	-
6	1PE	I	1009	-	-	1/2/2/13	-
4	1OT	I	1004	2	-	5/13/14/14	0/2/2/2
7	2PE	F	1010	-	-	4/6/6/25	-
7	2PE	B	1006	-	-	9/23/23/25	-
6	1PE	D	1009	-	-	7/8/8/13	-
6	1PE	J	1009	-	-	3/6/6/13	-
4	1OT	J	1004	2	-	4/13/14/14	0/2/2/2
6	1PE	G	1008	-	-	5/6/6/13	-
6	1PE	F	1008	-	-	2/7/7/13	-
4	1OT	H	1004	2	-	5/13/14/14	0/2/2/2
6	1PE	G	1009	-	-	1/3/3/13	-
6	1PE	C	1008	-	-	2/4/4/13	-
6	1PE	A	1009	-	-	0/6/6/13	-
4	1OT	K	1004	2	-	5/13/14/14	0/2/2/2
7	2PE	D	1011	-	-	2/2/2/25	-
7	2PE	E	1010	-	-	3/6/6/25	-
4	1OT	D	1004	2	-	4/13/14/14	0/2/2/2
6	1PE	J	1007	-	-	0/7/7/13	-
6	1PE	K	1008	-	-	2/9/9/13	-
4	1OT	L	1004	2	-	4/13/14/14	0/2/2/2
7	2PE	I	1010	-	-	1/5/5/25	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	J	1006	-	-	6/8/8/13	-
7	2PE	J	1010	-	-	5/7/7/25	-
6	1PE	F	1007	-	-	4/7/7/13	-
4	1OT	B	1004	2	-	5/13/14/14	0/2/2/2
6	1PE	E	1007	-	-	4/9/9/13	-
4	1OT	F	1004	2	-	4/13/14/14	0/2/2/2
7	2PE	D	1012	-	-	3/6/6/25	-
6	1PE	A	1010	-	-	5/9/9/13	-
6	1PE	G	1010	-	-	3/3/3/13	-
6	1PE	I	1007	-	-	5/12/12/13	-
6	1PE	G	1011	-	-	6/12/12/13	-
6	1PE	K	1007	-	-	3/9/9/13	-
6	1PE	E	1008	-	-	3/9/9/13	-

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1004	1OT	P-O3	7.79	1.62	1.49
4	F	1004	1OT	P-O3	7.60	1.62	1.49
4	J	1004	1OT	P-O3	7.58	1.62	1.49
4	H	1004	1OT	P-O3	7.57	1.62	1.49
4	E	1004	1OT	P-O3	7.55	1.62	1.49

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1004	1OT	C4-C5-N2	7.13	125.38	119.15
4	A	1004	1OT	C4-C5-N2	6.15	124.53	119.15
4	L	1004	1OT	C6-N2-N3	6.10	116.06	111.94
4	E	1004	1OT	C6-N2-N3	6.01	115.99	111.94
4	L	1004	1OT	C7-C6-N2	-5.84	102.63	107.08

There are no chirality outliers.

5 of 210 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1004	1OT	P-C1-C2-C10
4	D	1004	1OT	P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	E	1004	1OT	P-C1-C2-C10
4	F	1004	1OT	P-C1-C2-C10
4	F	1004	1OT	P-C1-C2-C3

There are no ring outliers.

44 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1004	1OT	2	0
7	H	1006	2PE	1	0
7	D	1010	2PE	4	0
6	J	1008	1PE	2	0
6	L	1008	1PE	2	0
7	C	1009	2PE	2	0
6	F	1009	1PE	1	0
4	J	1004	1OT	2	0
4	D	1004	1OT	2	0
3	L	1002	CO3	1	0
4	L	1004	1OT	4	0
4	B	1004	1OT	4	0
7	D	1012	2PE	1	0
7	H	1007	2PE	1	0
6	K	1007	1PE	2	0
3	D	1002	CO3	1	0
4	A	1004	1OT	3	0
7	F	1010	2PE	1	0
6	F	1008	1PE	1	0
7	E	1010	2PE	1	0
5	J	1005	SO4	1	0
6	J	1006	1PE	3	0
4	F	1004	1OT	3	0
6	A	1010	1PE	1	0
6	I	1007	1PE	1	0
6	G	1011	1PE	6	0
6	D	1007	1PE	2	0
6	L	1009	1PE	4	0
6	K	1010	1PE	1	0
6	L	1007	1PE	3	0
4	I	1004	1OT	2	0
6	D	1009	1PE	5	0
6	J	1009	1PE	2	0
4	E	1004	1OT	4	0

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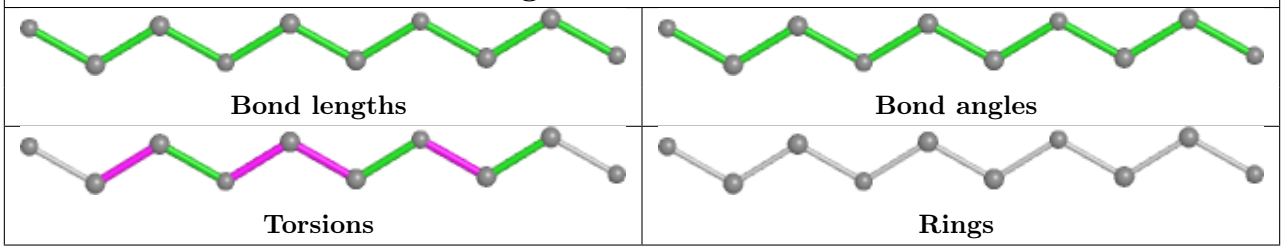
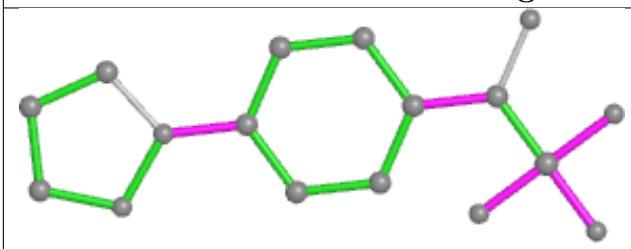
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1008	1PE	1	0
6	C	1006	1PE	1	0
6	C	1007	1PE	1	0
6	E	1009	1PE	3	0
4	G	1004	1OT	3	0
6	I	1009	1PE	1	0
6	G	1008	1PE	2	0
4	H	1004	1OT	2	0
4	K	1004	1OT	3	0
6	J	1007	1PE	1	0

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.

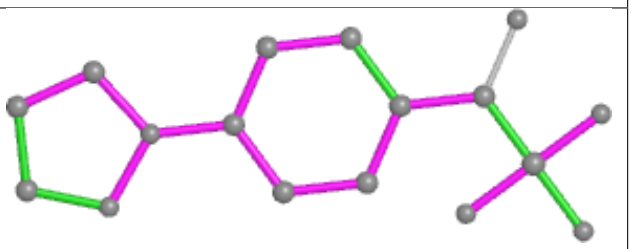
Ligand 2PE B 1007



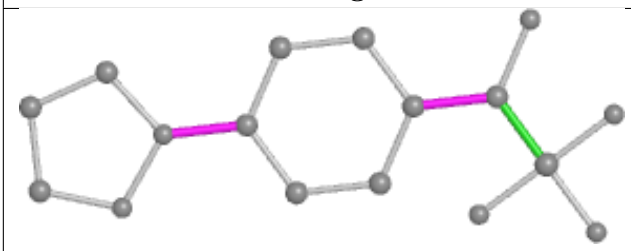
Ligand 1OT C 1004



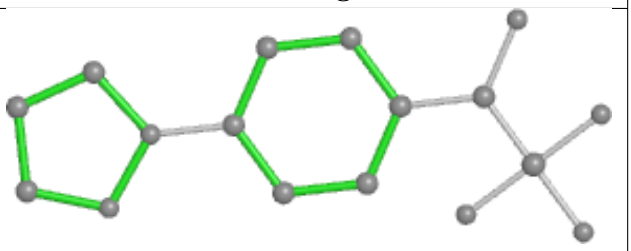
Bond lengths



Bond angles



Torsions



Rings

Ligand 2PE H 1006

Bond lengths

Bond angles

Torsions

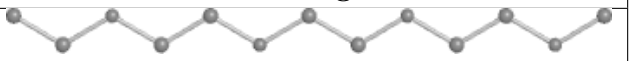
Rings

Ligand 2PE D 1010

Bond lengths

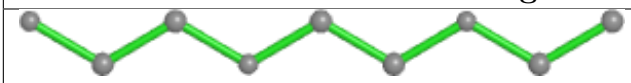
Bond angles

Torsions

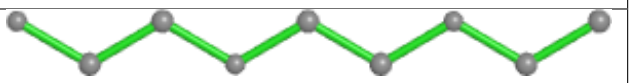


Rings

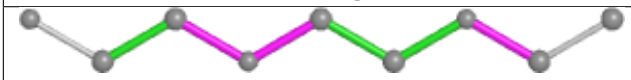
Ligand 2PE C 1009



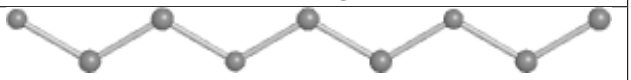
Bond lengths



Bond angles

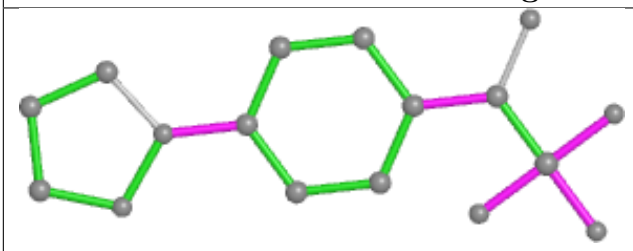


Torsions

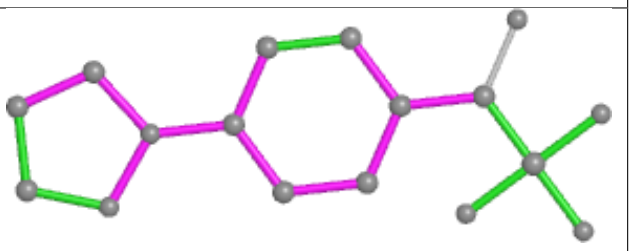


Rings

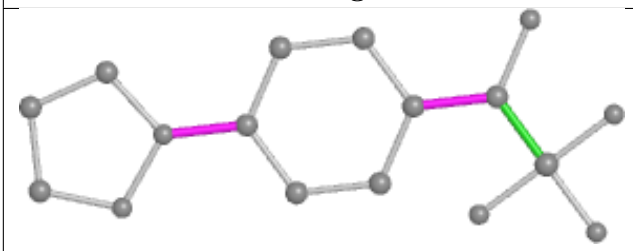
Ligand 1OT J 1004



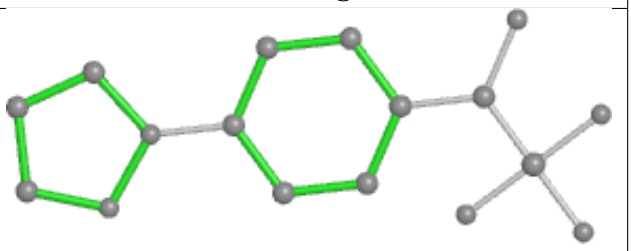
Bond lengths



Bond angles

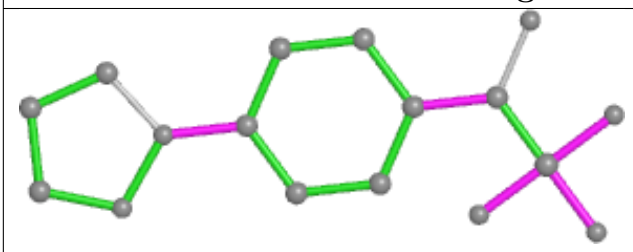


Torsions

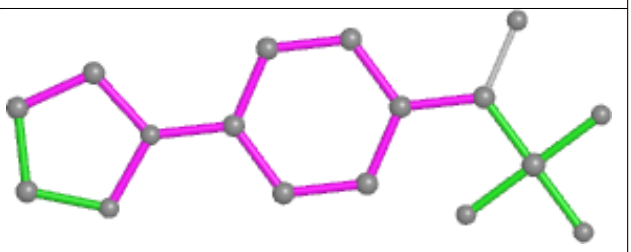


Rings

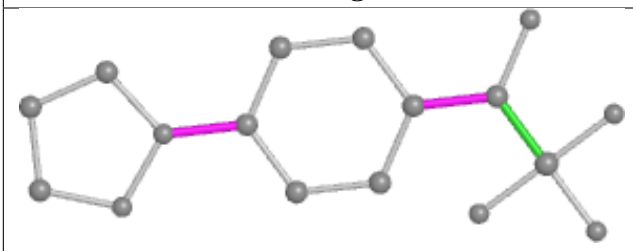
Ligand 1OT D 1004



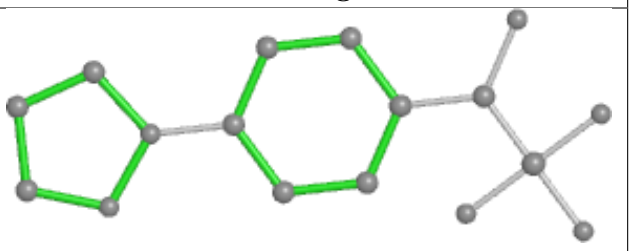
Bond lengths



Bond angles

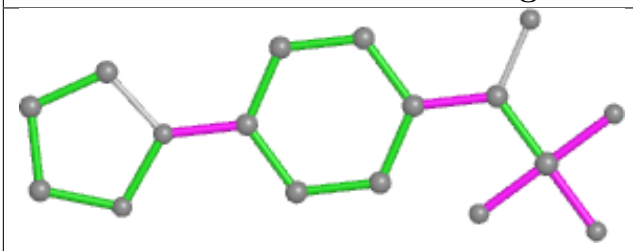


Torsions

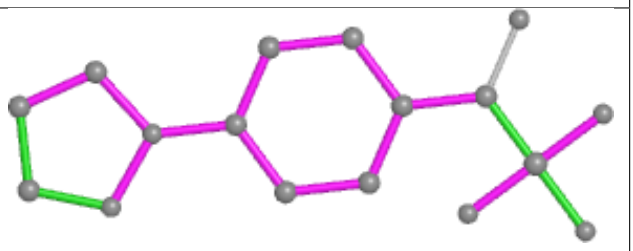


Rings

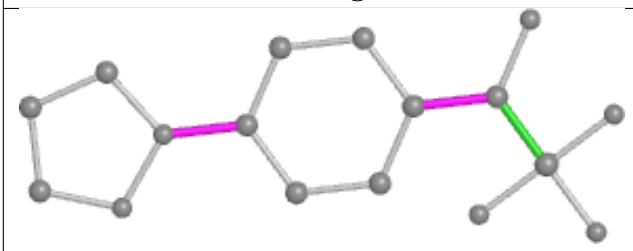
Ligand 1OT L 1004



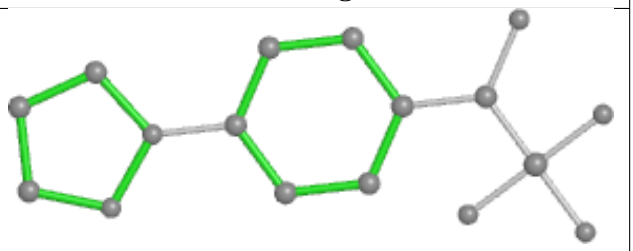
Bond lengths



Bond angles

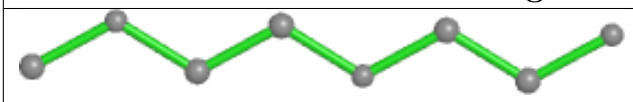


Torsions



Rings

Ligand 2PE I 1010



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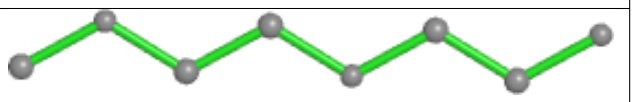
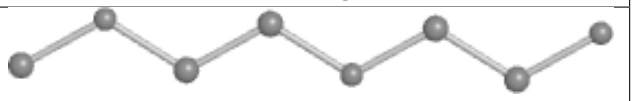


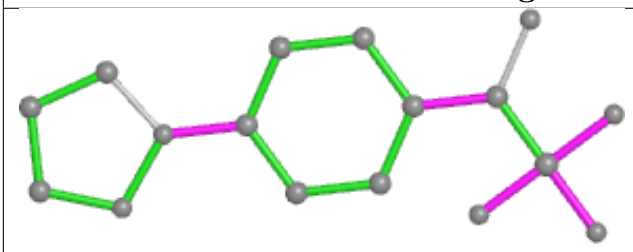
Bond angles

Torsions



Rings

Ligand 1OT B 1004



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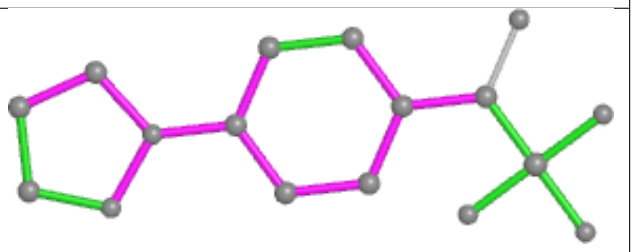
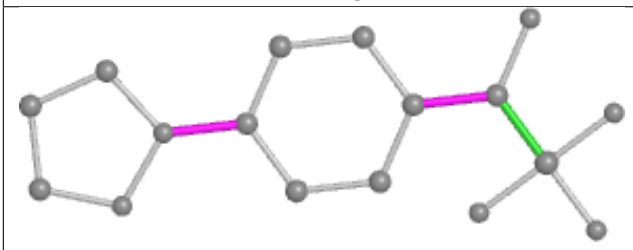
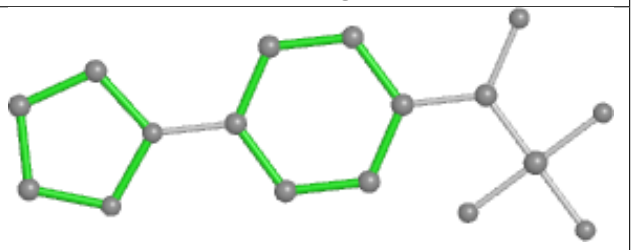


Bond angles

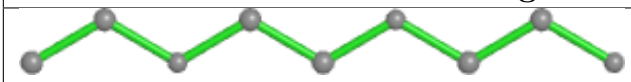


Torsions

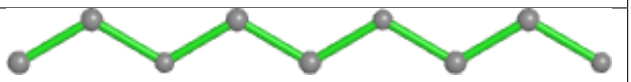


Rings

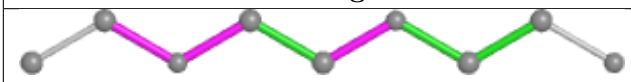
Ligand 2PE D 1012



Bond lengths



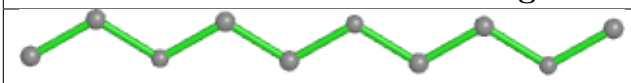
Bond angles



Torsions

Rings

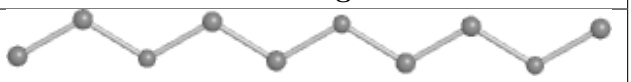
Ligand 2PE H 1007



Bond lengths

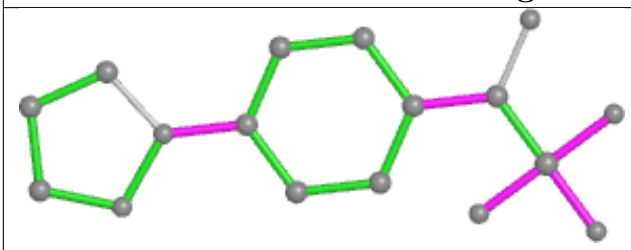
Bond angles

Torsions

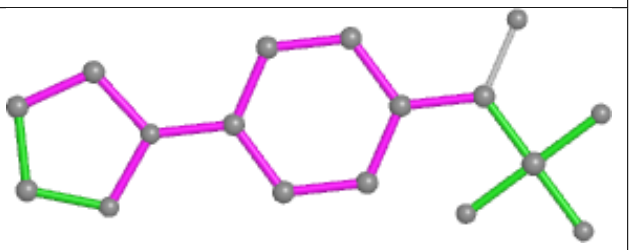


Rings

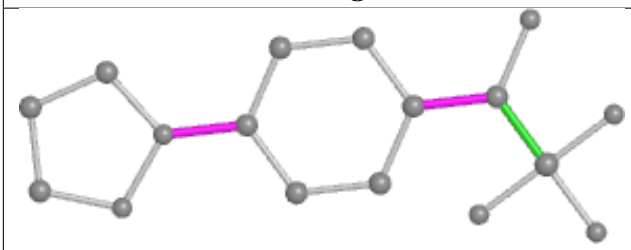
Ligand 1OT A 1004



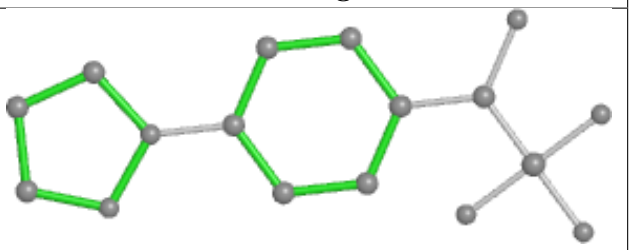
Bond lengths



Bond angles

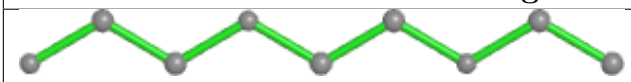


Torsions



Rings

Ligand 2PE F 1010



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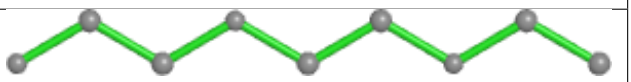
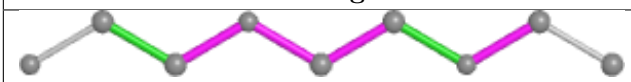


Bond angles

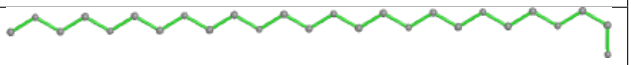


Torsions

Rings

Ligand 2PE B 1006

Bond lengths

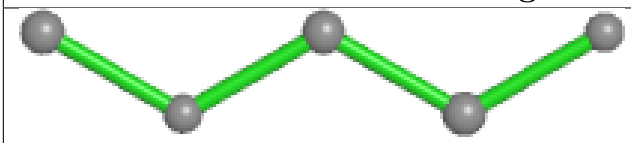


Bond angles

Torsions

Rings

Ligand 2PE D 1011



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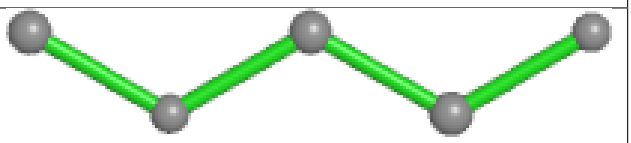
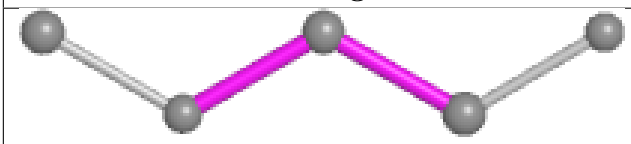
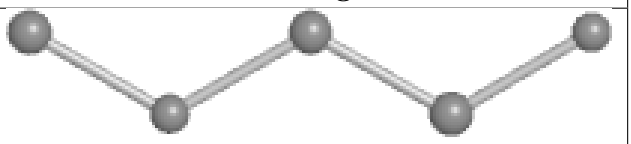


Bond angles

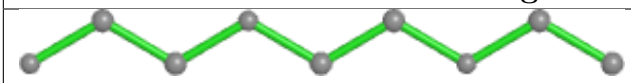


Torsions



Rings

Ligand 2PE E 1010



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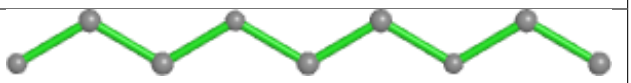
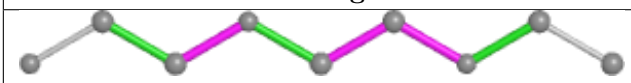


Bond angles



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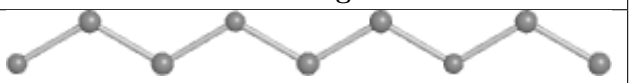
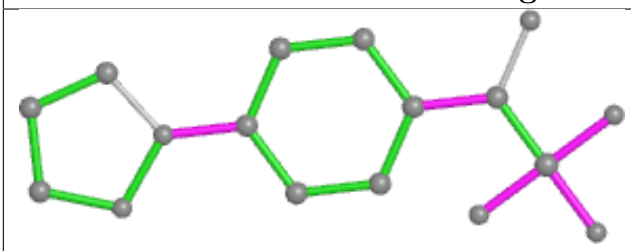


Rings

Ligand 1OT F 1004



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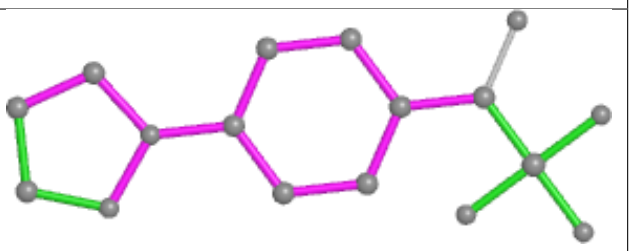
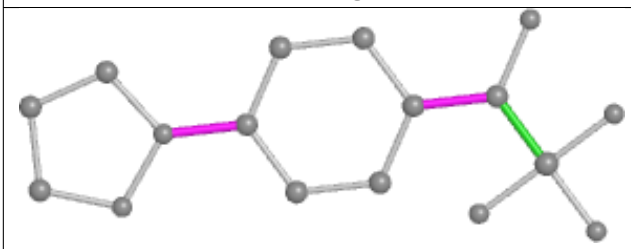
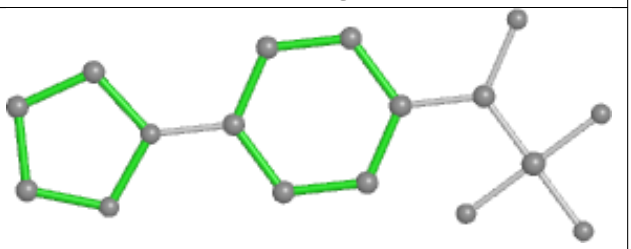


Bond angles

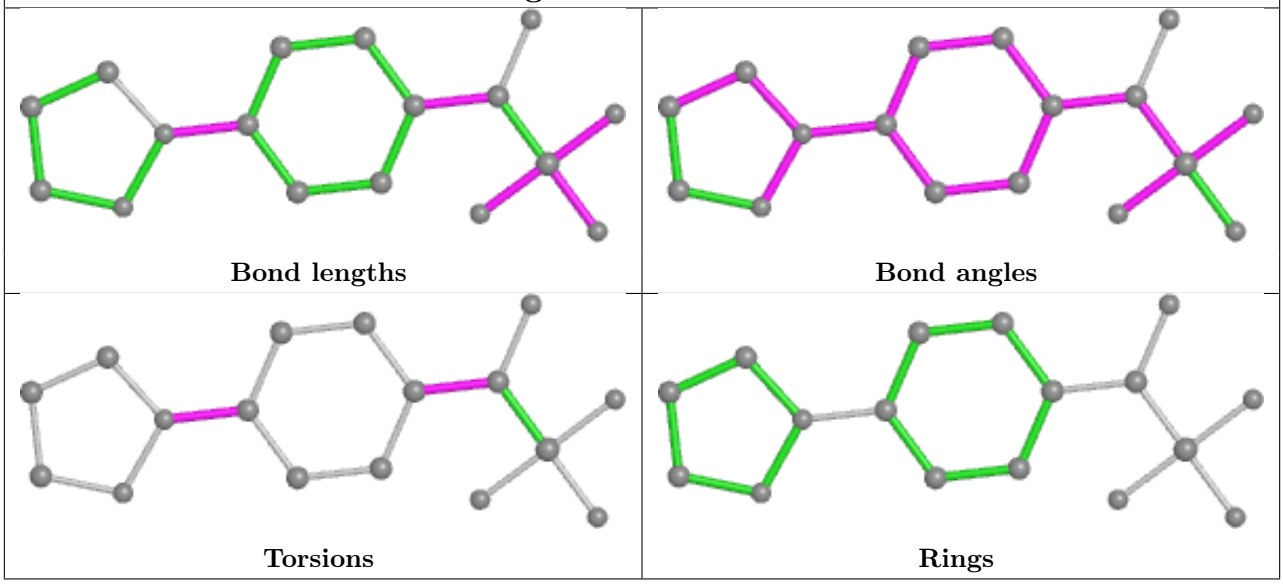


Torsions

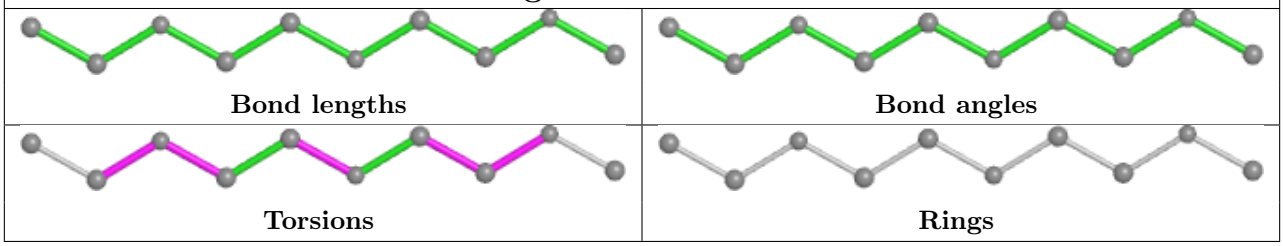


Rings

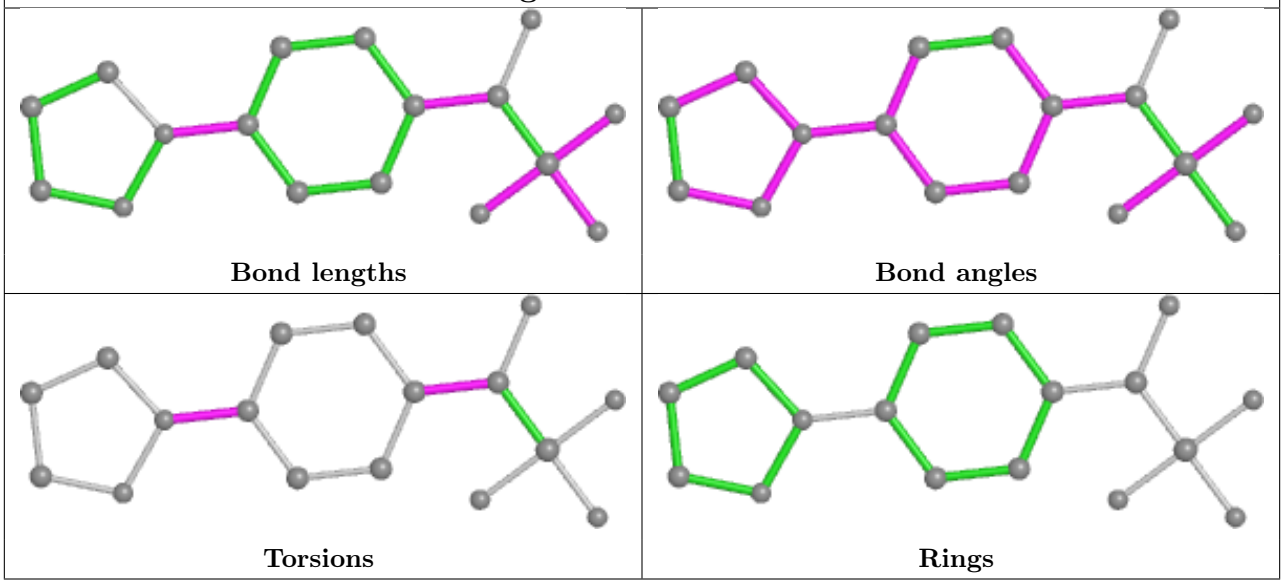
Ligand 1OT I 1004



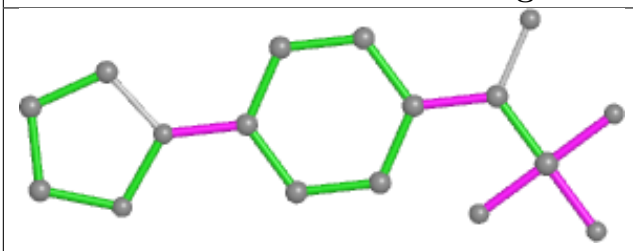
Ligand 2PE J 1010



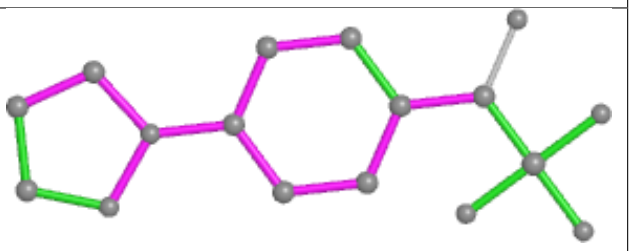
Ligand 1OT E 1004



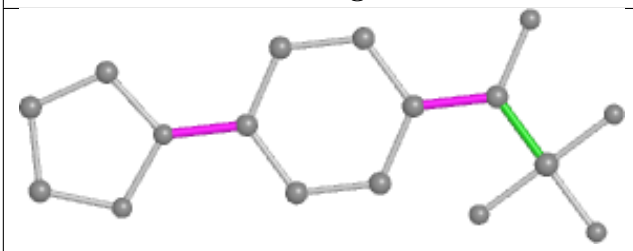
Ligand 1OT G 1004



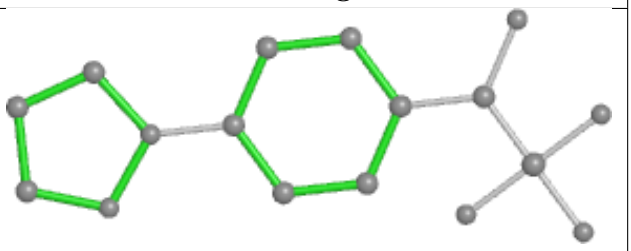
Bond lengths



Bond angles

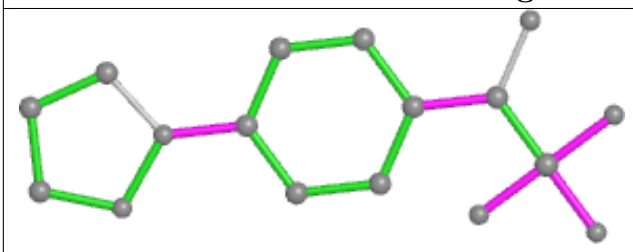


Torsions

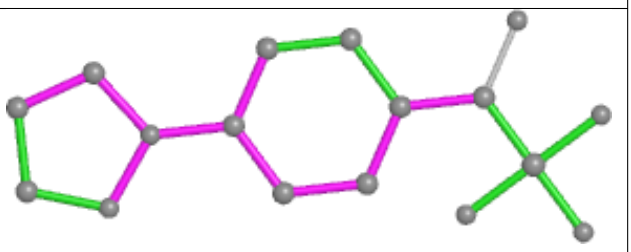


Rings

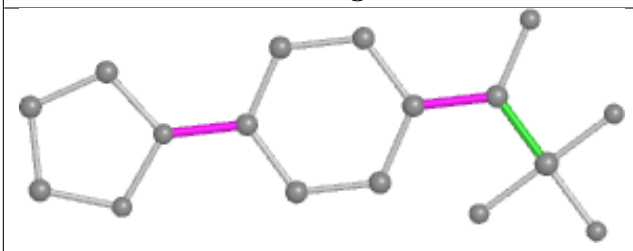
Ligand 1OT H 1004



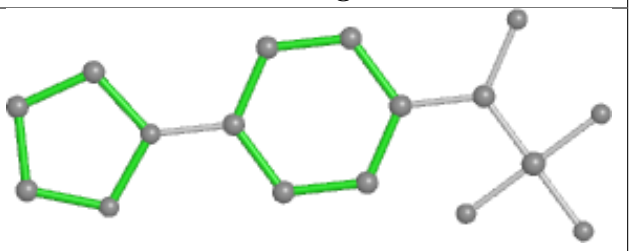
Bond lengths



Bond angles

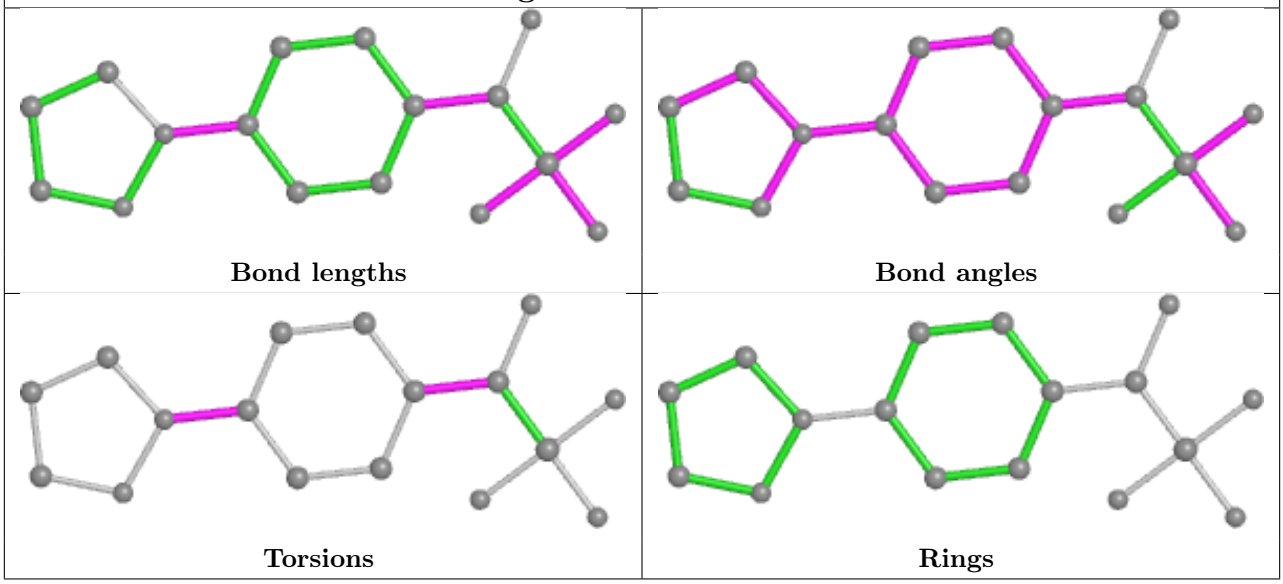


Torsions



Rings

Ligand 1OT K 1004



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	519/528 (98%)	-0.34	1 (0%)	95	94	6, 13, 30, 50	0
1	B	518/528 (98%)	-0.21	6 (1%)	79	78	5, 14, 43, 65	1 (0%)
1	C	518/528 (98%)	-0.33	2 (0%)	92	92	4, 12, 33, 48	0
1	D	514/528 (97%)	-0.39	4 (0%)	86	85	5, 12, 31, 54	0
1	E	510/528 (96%)	-0.47	2 (0%)	92	92	4, 11, 25, 50	0
1	F	511/528 (96%)	-0.20	7 (1%)	75	74	6, 16, 37, 69	0
1	G	519/528 (98%)	-0.34	0	100	100	5, 12, 31, 52	0
1	H	516/528 (97%)	-0.26	2 (0%)	92	92	5, 14, 41, 63	1 (0%)
1	I	518/528 (98%)	-0.34	1 (0%)	95	94	4, 13, 33, 56	0
1	J	513/528 (97%)	-0.40	5 (0%)	82	81	4, 13, 32, 57	0
1	K	509/528 (96%)	-0.47	2 (0%)	92	92	5, 12, 26, 52	0
1	L	513/528 (97%)	-0.27	2 (0%)	92	92	5, 14, 35, 52	0
All	All	6178/6336 (97%)	-0.33	34 (0%)	89	88	4, 13, 34, 69	2 (0%)

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	VAL	5.9
1	H	136	GLY	4.0
1	B	257	LYS	3.8
1	J	136	GLY	3.7
1	J	85	ALA	3.5

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	1PE	L	1008	8/16	0.67	0.20	48,51,53,53	0
6	1PE	J	1009	9/16	0.73	0.25	26,32,38,39	0
6	1PE	J	1008	11/16	0.75	0.23	26,32,42,42	0
6	1PE	A	1010	12/16	0.75	0.23	32,38,46,48	0
6	1PE	D	1008	9/16	0.75	0.22	46,49,60,60	0
6	1PE	L	1009	11/16	0.76	0.20	36,39,43,45	0
6	1PE	C	1008	7/16	0.77	0.35	42,43,44,45	0
6	1PE	K	1010	6/16	0.77	0.18	23,28,37,39	0
6	1PE	L	1007	12/16	0.78	0.18	28,35,39,41	0
6	1PE	J	1007	10/16	0.80	0.22	28,32,39,41	0
6	1PE	F	1009	11/16	0.81	0.29	46,51,55,56	0
6	1PE	G	1011	15/16	0.81	0.22	26,38,47,51	0
6	1PE	E	1009	8/16	0.81	0.22	29,42,43,43	0
7	2PE	H	1007	10/28	0.81	0.19	36,45,53,53	0
7	2PE	J	1010	10/28	0.81	0.22	18,47,48,48	0
6	1PE	F	1007	10/16	0.82	0.18	40,42,49,51	0
7	2PE	I	1010	8/28	0.82	0.18	32,39,48,49	0
6	1PE	D	1009	11/16	0.82	0.19	23,35,40,43	0
6	1PE	E	1007	12/16	0.83	0.15	29,32,34,34	0
7	2PE	E	1010	9/28	0.84	0.19	36,39,42,46	0
7	2PE	D	1010	13/28	0.84	0.20	28,38,49,51	0
7	2PE	H	1006	25/28	0.85	0.15	21,31,39,44	0
6	1PE	C	1006	13/16	0.85	0.17	12,34,44,45	0
6	1PE	K	1007	12/16	0.85	0.17	31,37,40,41	0
6	1PE	K	1009	11/16	0.85	0.17	30,33,36,38	0
7	2PE	D	1012	9/28	0.86	0.21	36,42,45,47	0
7	2PE	B	1006	26/28	0.86	0.18	17,43,51,51	0
6	1PE	I	1007	15/16	0.86	0.21	20,31,40,40	0
7	2PE	B	1007	10/28	0.87	0.17	45,49,53,55	0
6	1PE	F	1008	10/16	0.87	0.17	26,32,35,36	0
6	1PE	G	1008	9/16	0.88	0.15	17,25,29,30	0
5	SO4	A	1008	5/5	0.88	0.18	26,35,41,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	2PE	C	1009	9/28	0.88	0.15	29,32,38,39	0
7	2PE	F	1010	9/28	0.88	0.14	35,38,39,42	0
6	1PE	C	1007	9/16	0.90	0.13	13,22,29,31	0
6	1PE	E	1008	12/16	0.90	0.16	19,23,39,39	0
5	SO4	E	1006	5/5	0.90	0.27	46,53,54,62	0
6	1PE	I	1008	11/16	0.90	0.14	18,24,31,33	0
6	1PE	G	1010	6/16	0.91	0.14	30,32,32,33	0
7	2PE	D	1011	5/28	0.91	0.25	21,21,28,28	0
5	SO4	C	1005	5/5	0.91	0.26	41,47,51,54	0
4	1OT	F	1004	17/17	0.92	0.15	10,24,32,32	0
4	1OT	H	1004	17/17	0.92	0.15	10,24,37,37	0
6	1PE	L	1006	10/16	0.92	0.15	19,25,29,35	0
6	1PE	I	1009	5/16	0.92	0.15	14,20,20,21	0
6	1PE	J	1006	11/16	0.92	0.16	20,25,35,37	0
4	1OT	L	1004	17/17	0.92	0.15	7,25,34,34	0
5	SO4	G	1007	5/5	0.92	0.16	43,48,51,56	0
6	1PE	D	1007	10/16	0.92	0.12	17,24,28,32	0
6	1PE	F	1006	10/16	0.92	0.13	29,32,36,37	0
4	1OT	J	1004	17/17	0.93	0.17	15,21,43,44	0
6	1PE	A	1009	9/16	0.93	0.09	18,21,25,34	0
5	SO4	B	1005	5/5	0.93	0.18	67,68,68,69	0
4	1OT	I	1004	17/17	0.93	0.14	9,24,37,37	0
5	SO4	A	1007	5/5	0.93	0.19	38,42,45,49	0
5	SO4	G	1006	5/5	0.94	0.21	40,41,45,49	0
4	1OT	K	1004	17/17	0.94	0.15	12,20,40,40	0
5	SO4	I	1006	5/5	0.94	0.24	53,55,56,60	0
5	SO4	J	1005	5/5	0.94	0.28	51,51,55,56	0
5	SO4	L	1005	5/5	0.94	0.17	33,40,45,48	0
4	1OT	E	1004	17/17	0.94	0.15	14,20,41,42	0
2	ZN	J	1003	1/1	0.94	0.16	53,53,53,53	0
6	1PE	K	1008	12/16	0.94	0.14	16,25,38,39	0
4	1OT	G	1004	17/17	0.94	0.13	8,20,32,35	0
4	1OT	A	1004	17/17	0.94	0.12	5,20,33,34	0
4	1OT	B	1004	17/17	0.94	0.12	9,18,39,41	0
5	SO4	D	1006	5/5	0.94	0.23	44,51,54,55	0
4	1OT	C	1004	17/17	0.94	0.13	9,18,36,37	0
4	1OT	D	1004	17/17	0.95	0.13	12,21,39,39	0
5	SO4	G	1005	5/5	0.95	0.18	32,32,33,40	0
5	SO4	I	1005	5/5	0.95	0.30	50,51,54,55	0
2	ZN	C	1003	1/1	0.96	0.13	41,41,41,41	0
5	SO4	E	1005	5/5	0.96	0.22	42,45,49,50	0
5	SO4	A	1006	5/5	0.96	0.20	45,46,50,50	0

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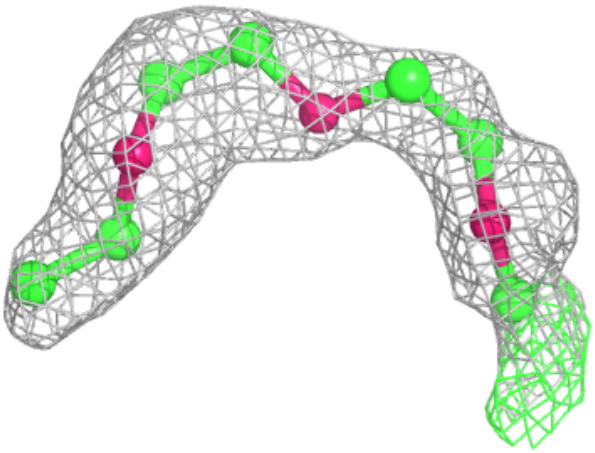
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	F	1005	5/5	0.96	0.21	44,46,49,51	0
2	ZN	H	1003	1/1	0.96	0.15	46,46,46,46	0
6	1PE	G	1009	6/16	0.96	0.19	21,22,26,33	0
5	SO4	K	1006	5/5	0.96	0.22	42,45,47,53	0
3	CO3	J	1002	4/4	0.97	0.11	5,6,11,15	0
2	ZN	F	1001	1/1	0.97	0.11	39,39,39,39	0
3	CO3	C	1002	4/4	0.98	0.12	8,10,12,17	0
3	CO3	D	1002	4/4	0.98	0.09	6,7,10,12	0
3	CO3	E	1002	4/4	0.98	0.11	8,10,11,17	0
3	CO3	F	1002	4/4	0.98	0.12	7,12,14,15	0
3	CO3	G	1002	4/4	0.98	0.10	7,8,8,17	0
3	CO3	H	1002	4/4	0.98	0.10	4,10,10,12	0
3	CO3	I	1002	4/4	0.98	0.11	7,8,8,15	0
2	ZN	B	1001	1/1	0.98	0.08	36,36,36,36	0
3	CO3	K	1002	4/4	0.98	0.07	8,12,13,18	0
3	CO3	L	1002	4/4	0.98	0.12	6,8,10,12	0
2	ZN	F	1003	1/1	0.98	0.12	51,51,51,51	0
2	ZN	H	1001	1/1	0.98	0.10	36,36,36,36	0
2	ZN	B	1003	1/1	0.98	0.14	38,38,38,38	0
2	ZN	A	1003	1/1	0.98	0.10	46,46,46,46	0
2	ZN	K	1003	1/1	0.98	0.19	46,46,46,46	0
2	ZN	L	1003	1/1	0.98	0.13	45,45,45,45	0
3	CO3	B	1002	4/4	0.98	0.12	5,6,7,11	0
2	ZN	G	1001	1/1	0.99	0.06	39,39,39,39	0
2	ZN	G	1003	1/1	0.99	0.11	39,39,39,39	0
2	ZN	D	1001	1/1	0.99	0.09	36,36,36,36	0
5	SO4	D	1005	5/5	0.99	0.08	9,9,11,12	0
2	ZN	D	1003	1/1	0.99	0.14	45,45,45,45	0
2	ZN	I	1001	1/1	0.99	0.12	40,40,40,40	0
2	ZN	E	1001	1/1	0.99	0.10	36,36,36,36	0
2	ZN	K	1001	1/1	0.99	0.12	35,35,35,35	0
2	ZN	E	1003	1/1	0.99	0.17	49,49,49,49	0
2	ZN	L	1001	1/1	0.99	0.09	41,41,41,41	0
2	ZN	C	1001	1/1	0.99	0.13	41,41,41,41	0
5	SO4	H	1005	5/5	0.99	0.09	7,8,10,11	0
5	SO4	A	1005	5/5	0.99	0.07	6,7,11,13	0
3	CO3	A	1002	4/4	0.99	0.09	7,10,12,18	0
2	ZN	A	1001	1/1	0.99	0.07	37,37,37,37	0
5	SO4	K	1005	5/5	0.99	0.08	9,11,11,12	0
2	ZN	I	1003	1/1	1.00	0.15	42,42,42,42	0
2	ZN	J	1001	1/1	1.00	0.07	36,36,36,36	0

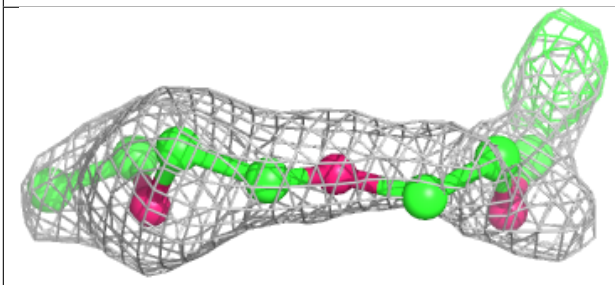
The following is a graphical depiction of the model fit to experimental electron density of all

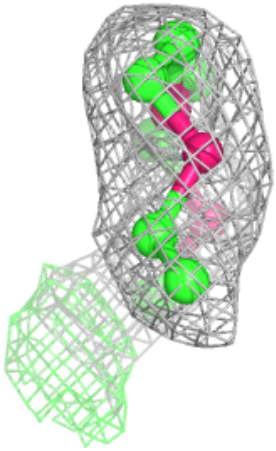
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 2PE H 1007:

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

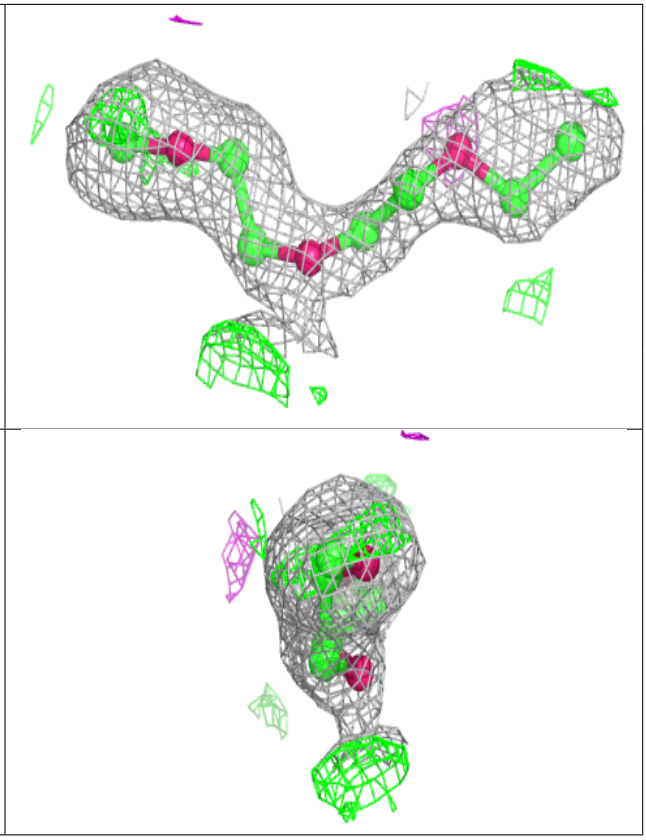






Electron density around 2PE J 1010:

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



Electron density around 2PE I 1010:

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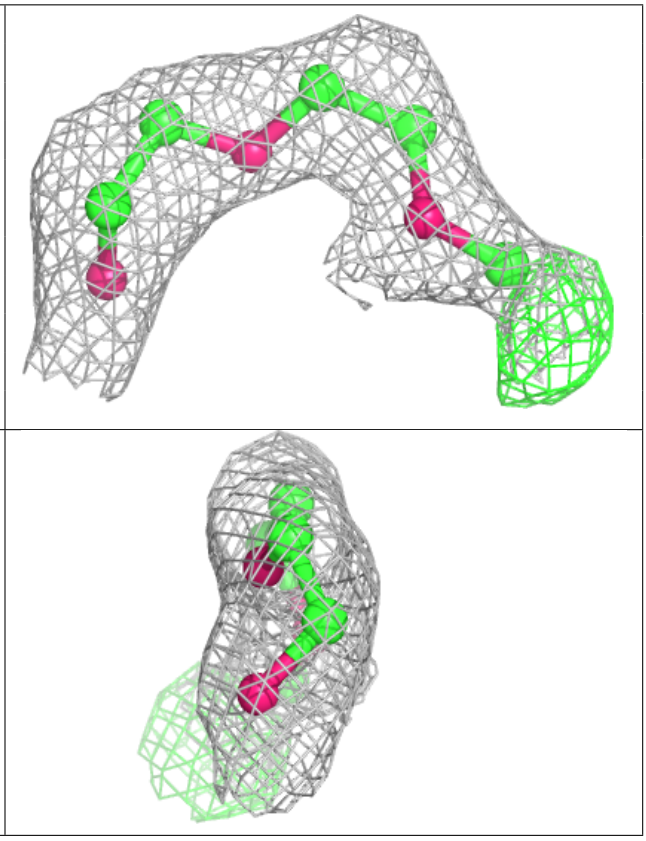
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 2PE E 1010:

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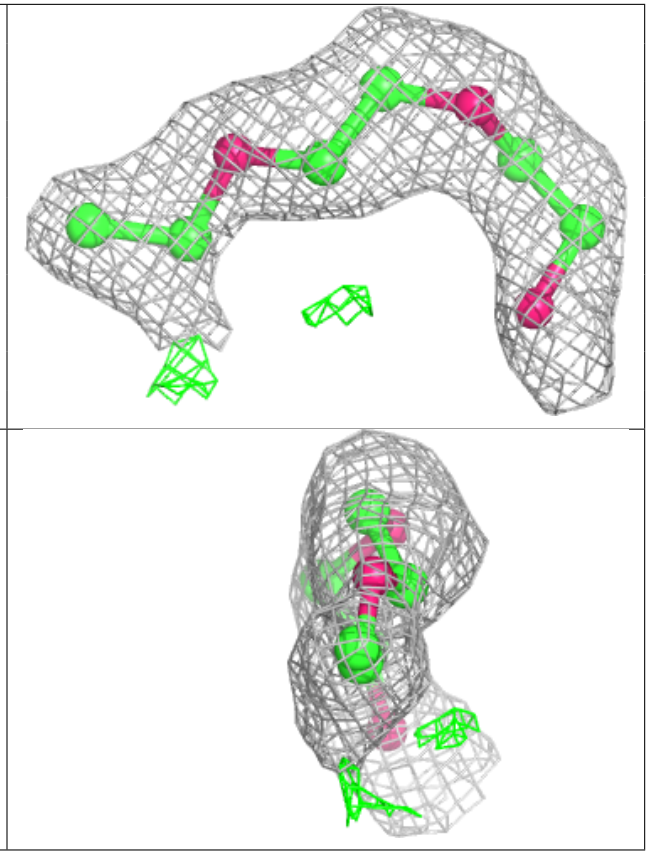
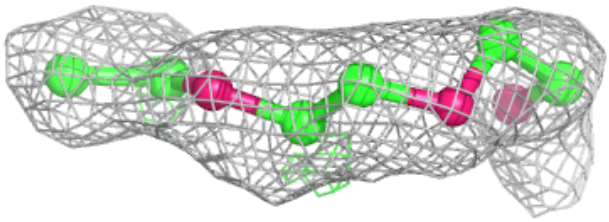
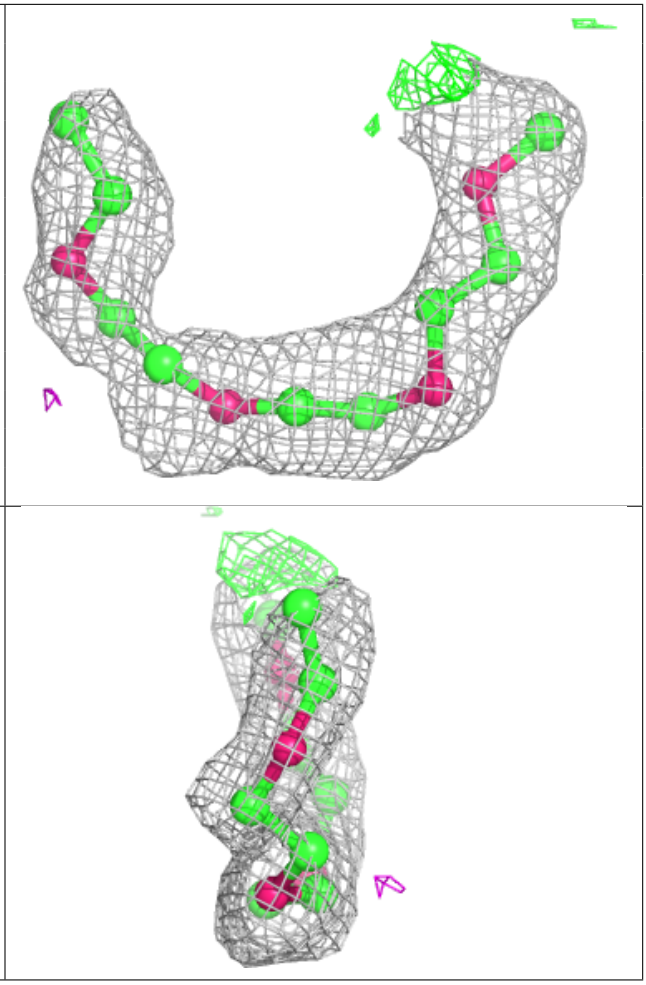
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





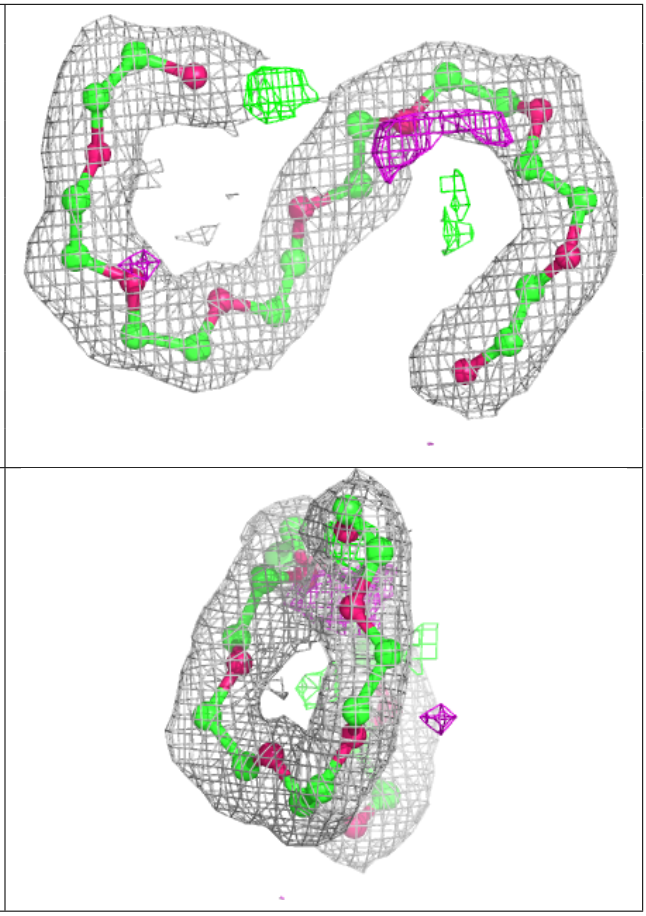
Electron density around 2PE D 1010:

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



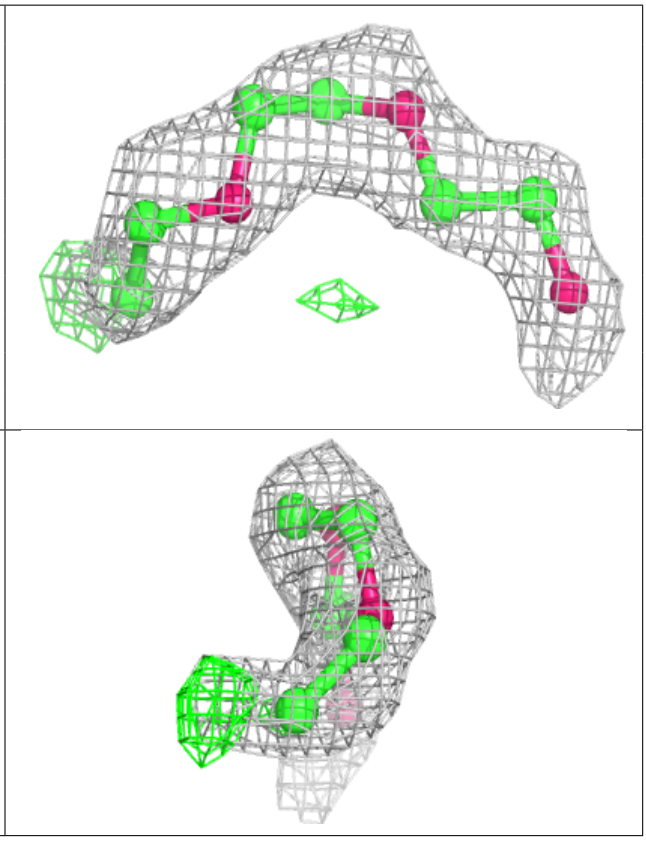
Electron density around 2PE H 1006:

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



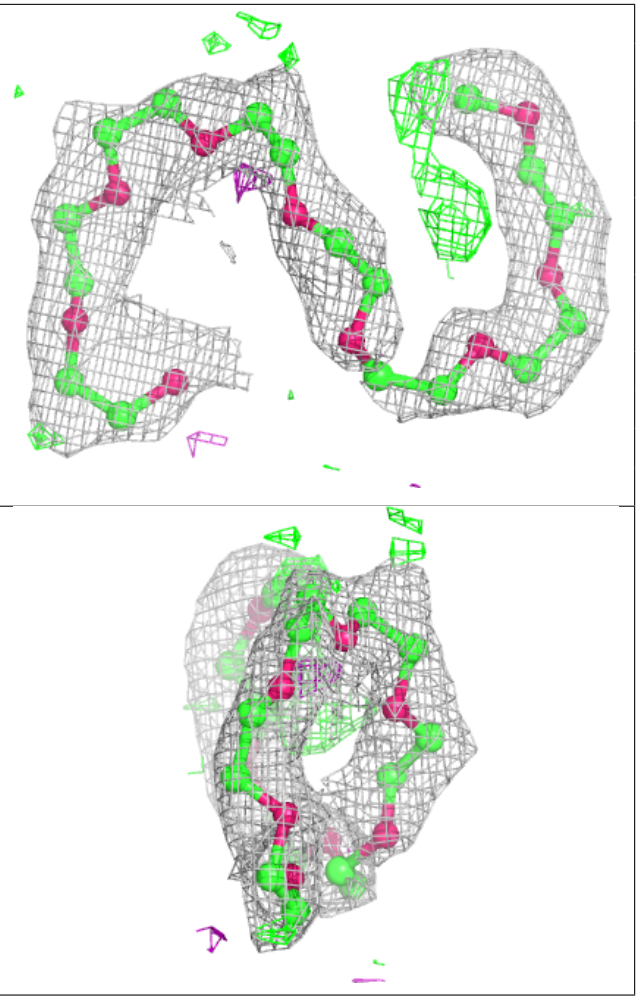
Electron density around 2PE D 1012:

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



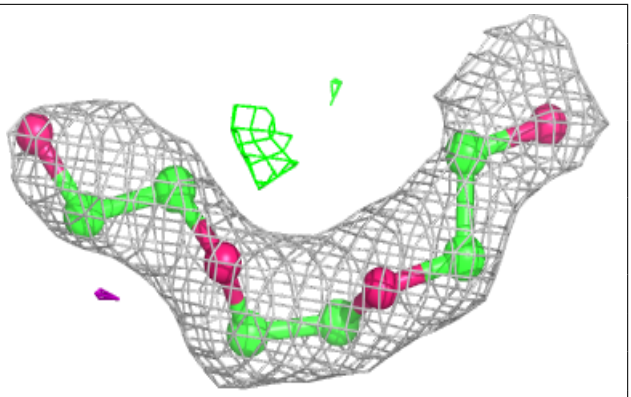
Electron density around 2PE B 1006:

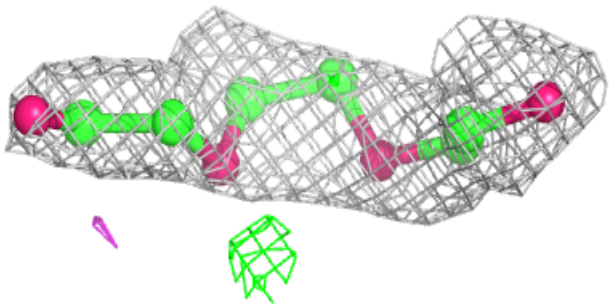
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

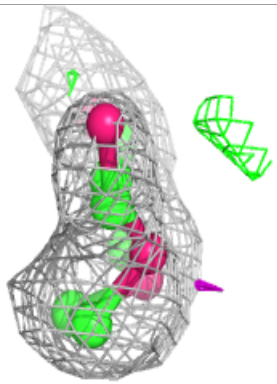


Electron density around 2PE B 1007:

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

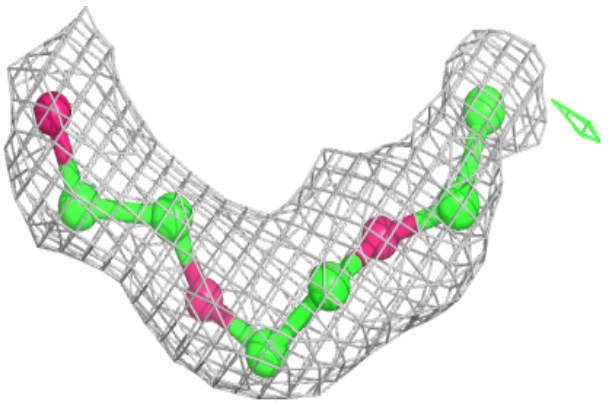


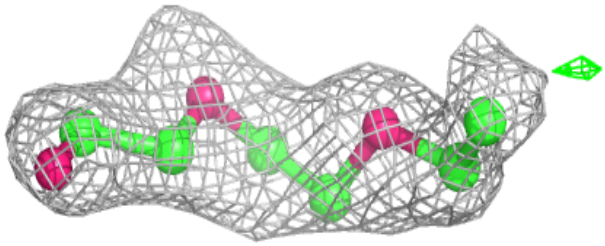


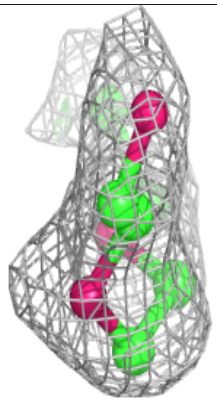


Electron density around 2PE C 1009:

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

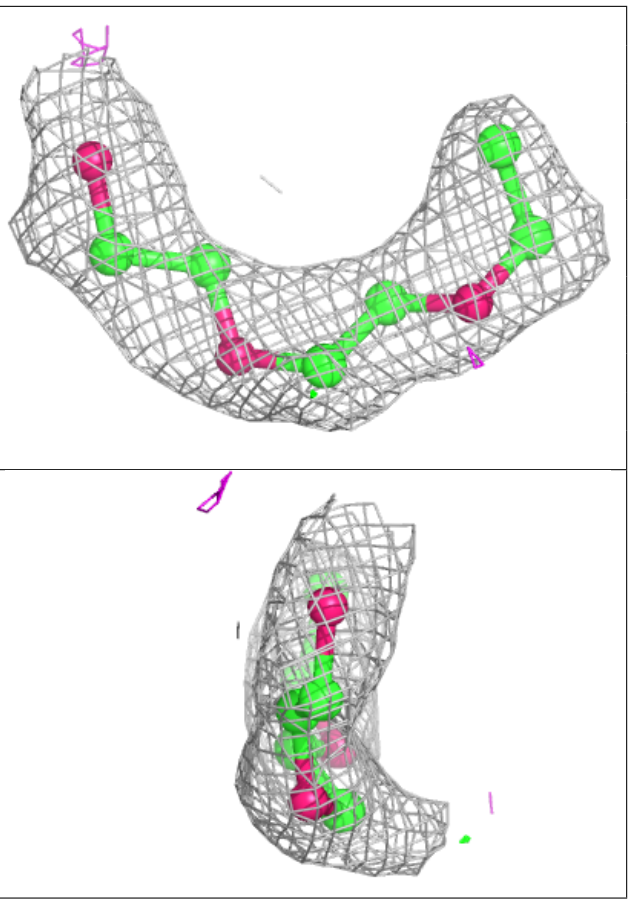


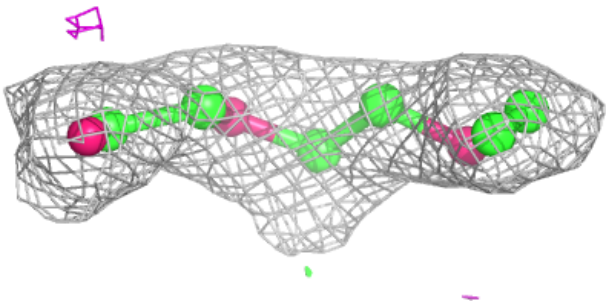




Electron density around 2PE F 1010:

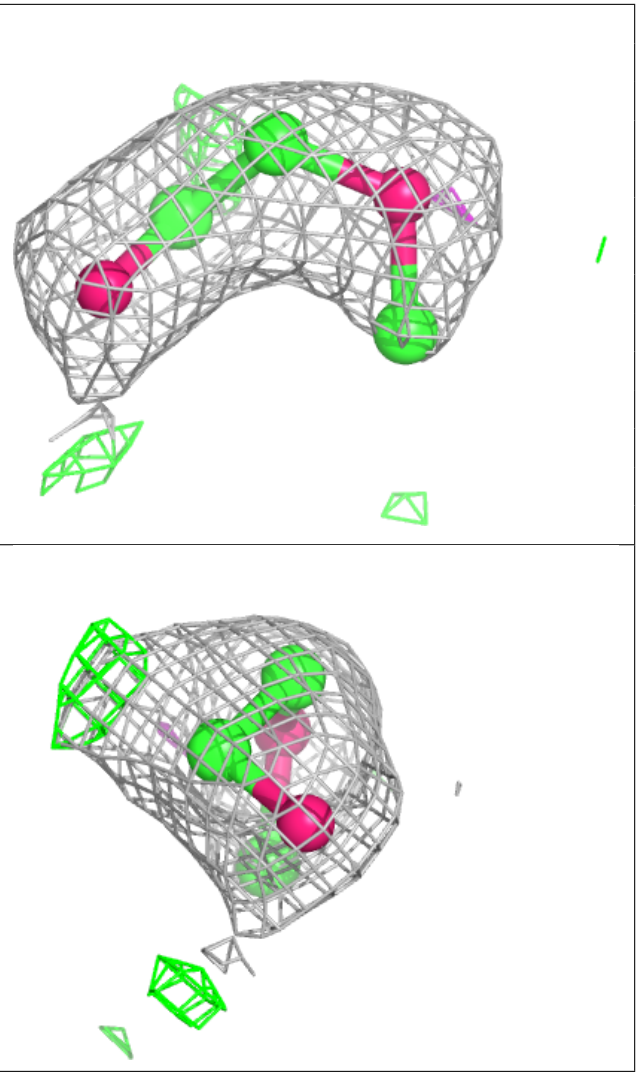
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





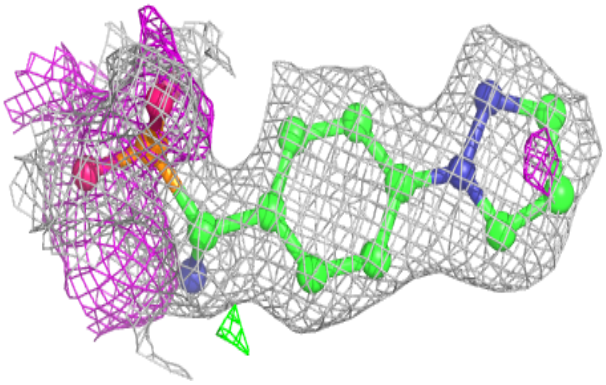
Electron density around 2PE D 1011:

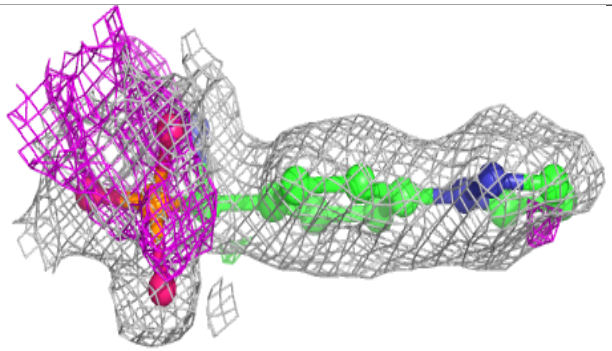
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

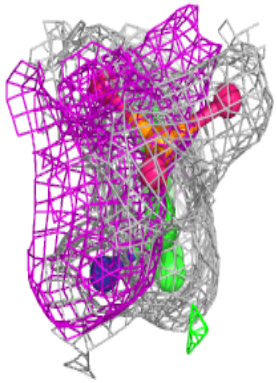


Electron density around 1OT F 1004:

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

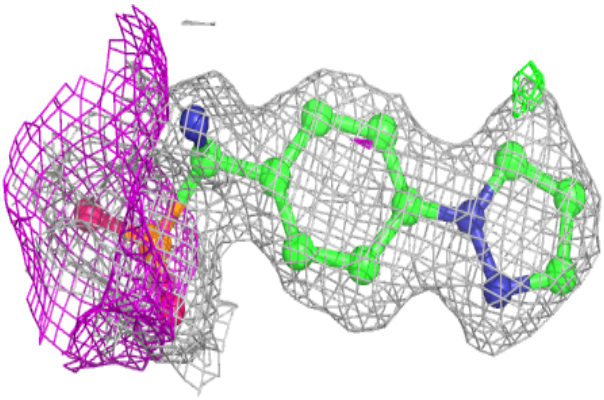


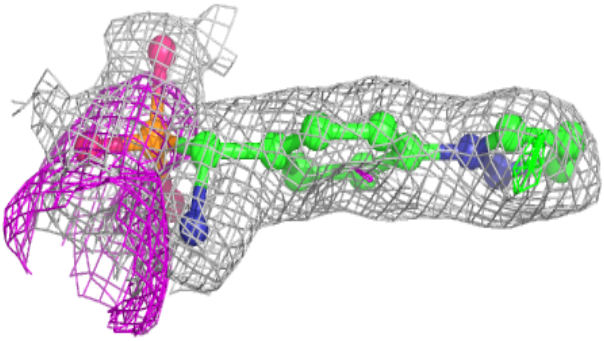


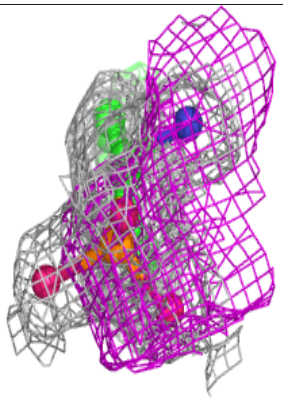


Electron density around 1OT H 1004:

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

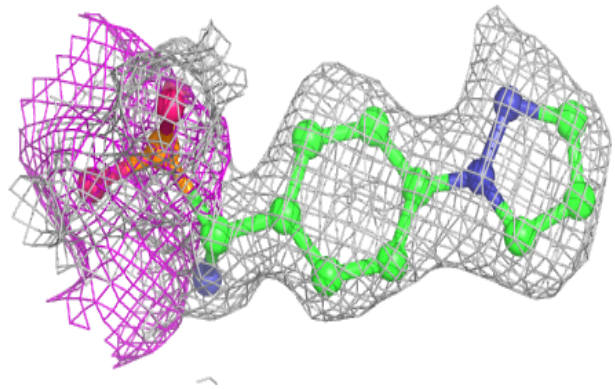


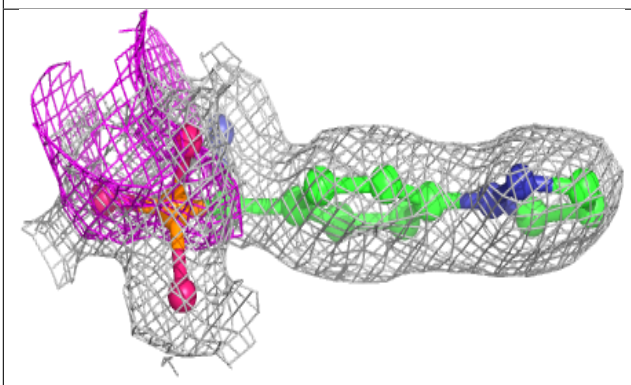


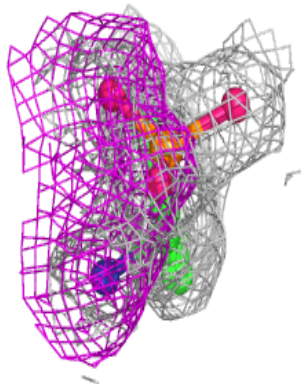


Electron density around 1OT L 1004:

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

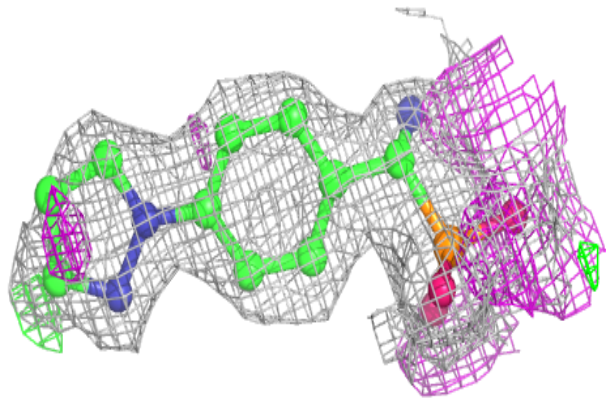


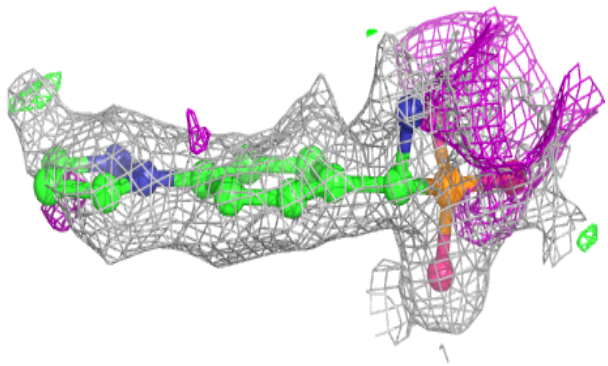


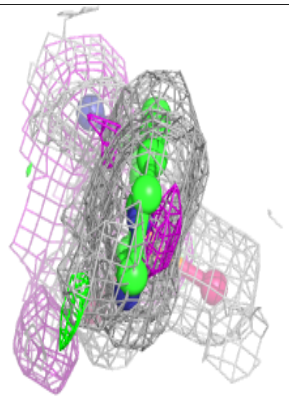


Electron density around 1OT J 1004:

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

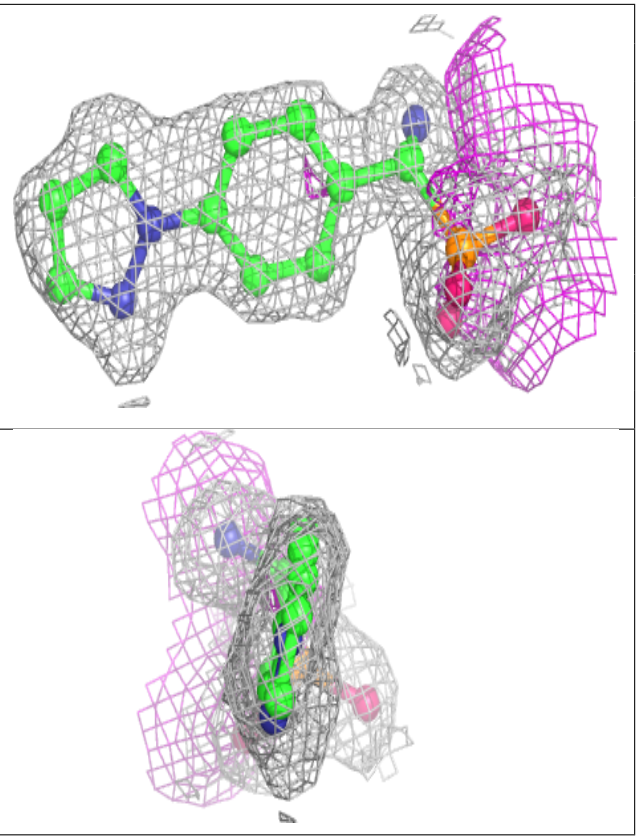






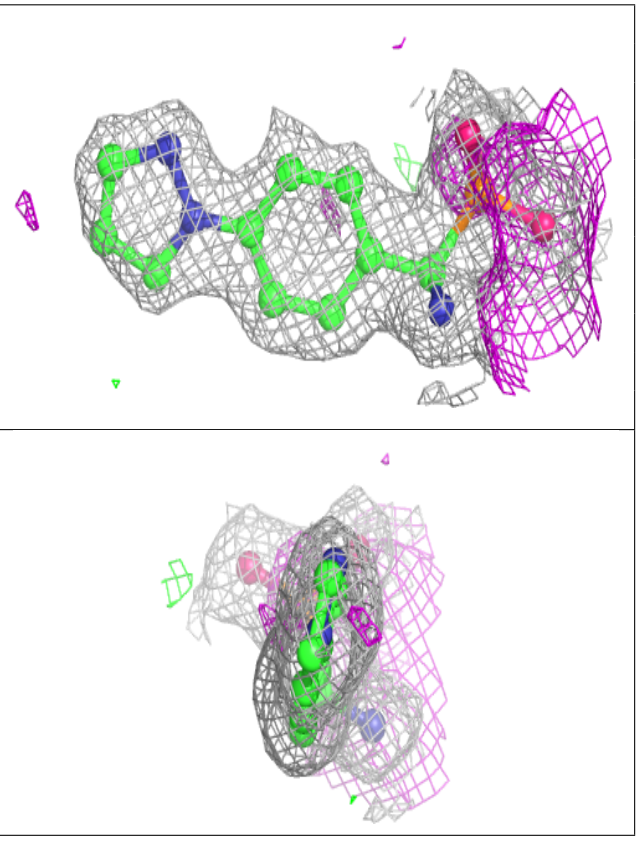
Electron density around 1OT I 1004:

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



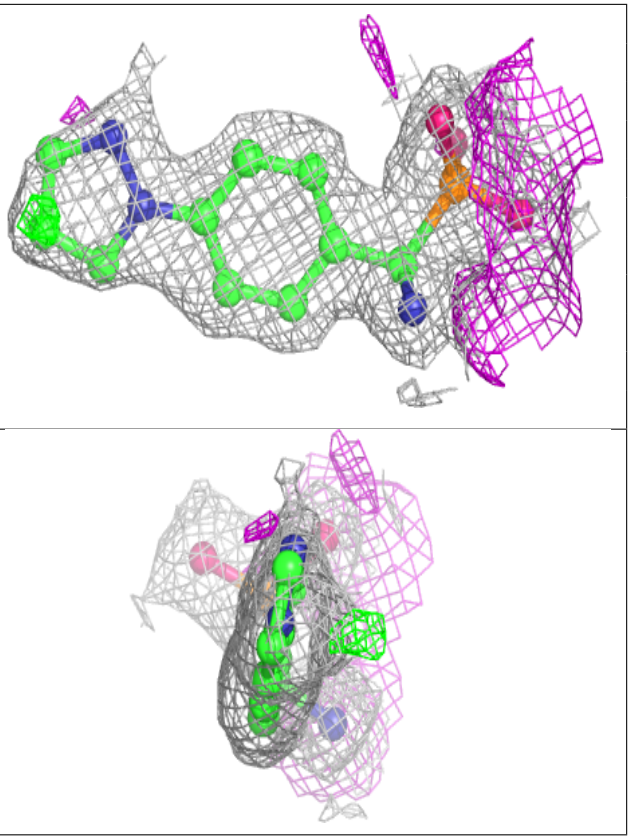
Electron density around 1OT K 1004:

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



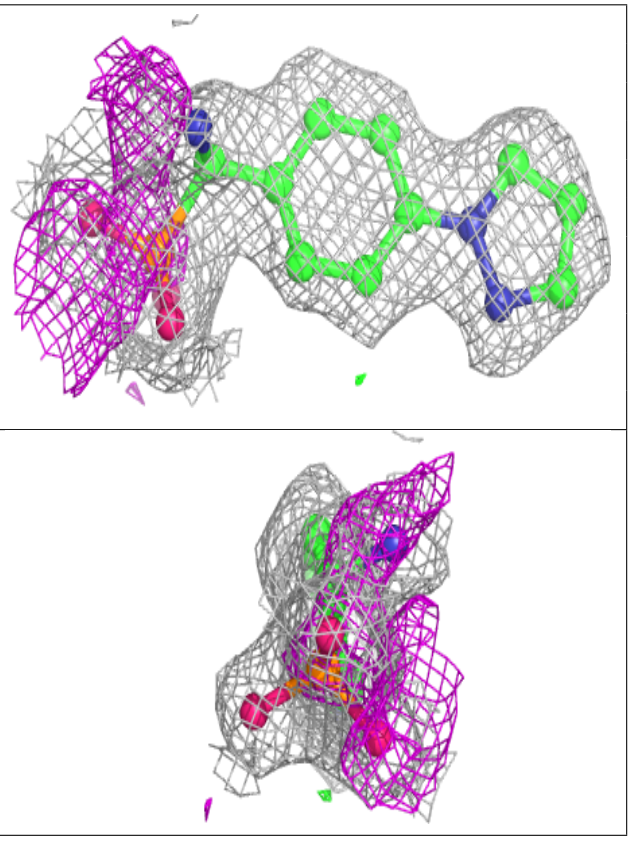
Electron density around 1OT E 1004:

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



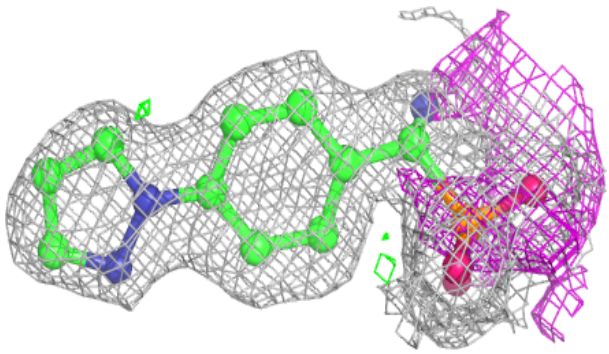
Electron density around 1OT G 1004:

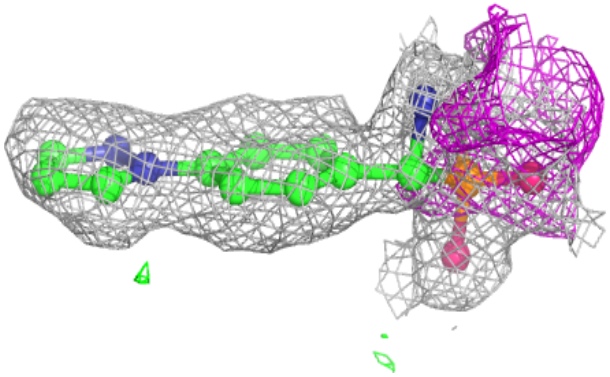
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

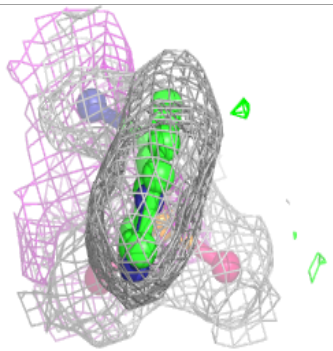


Electron density around 1OT A 1004:

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

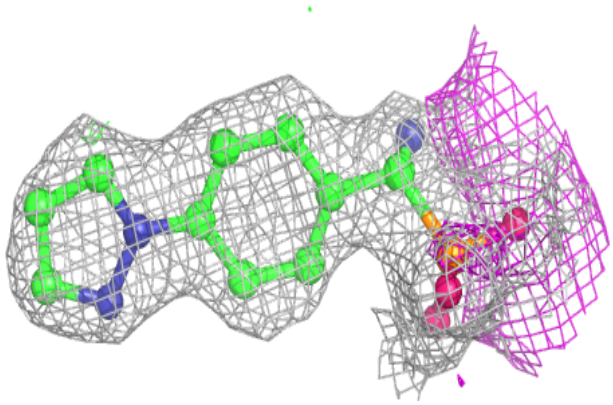


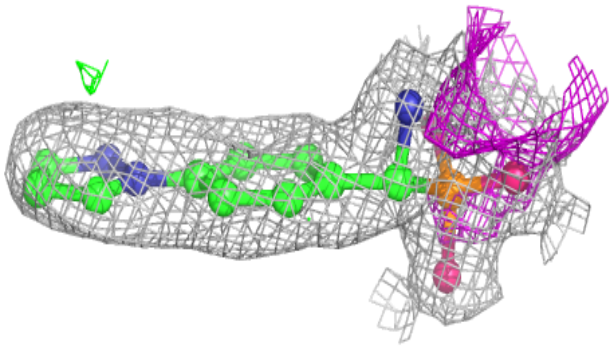


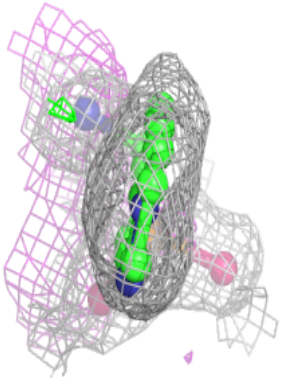


Electron density around 1OT B 1004:

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

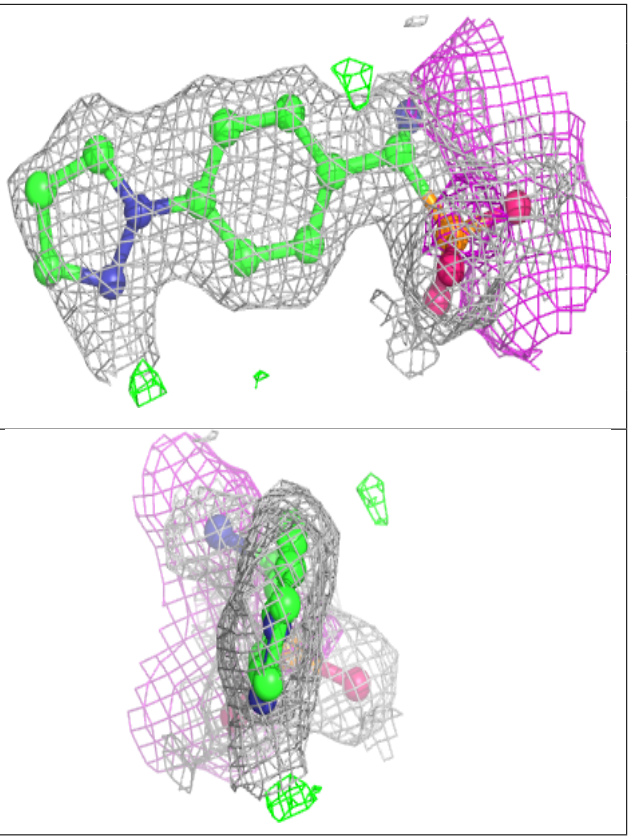






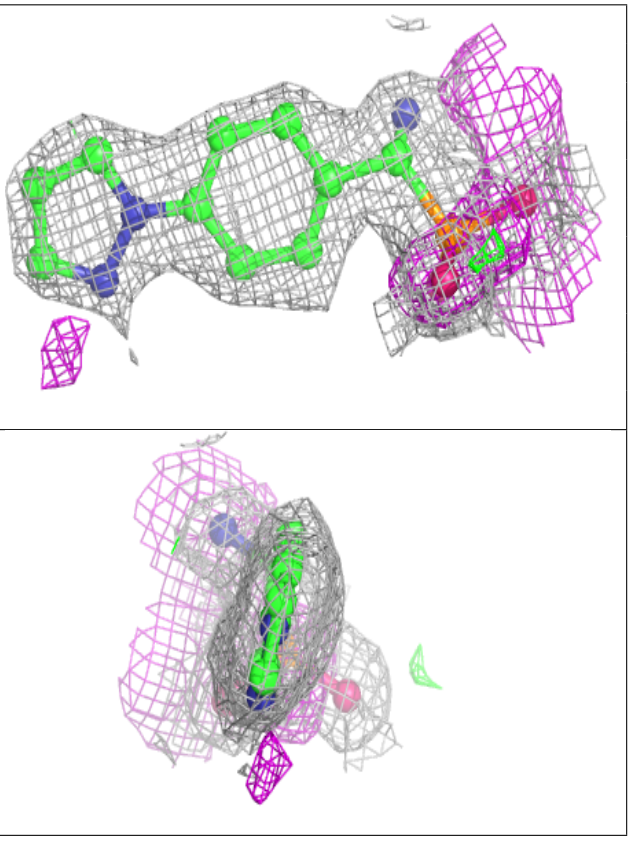
Electron density around 1OT C 1004:

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



Electron density around 1OT 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)



6.5 Other polymers (i)

There are no such residues in this entry.