wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 04:39 am GMT

PDB ID	:	5CBM
Title	:	Crystal structure of PfA-M17 with virtual ligand inhibitor
Authors	:	Ruggeri, C.; Drinkwater, N.; McGowan, S.
Deposited on	:	2015-07-01
Resolution	:	2.30 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:

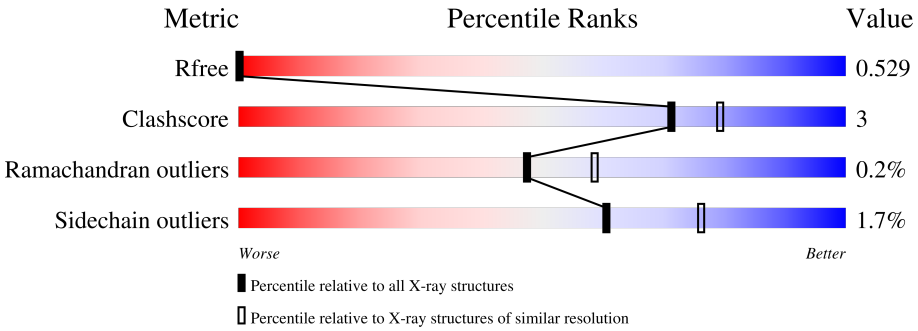
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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%

Mol	Chain	Length	Quality of chain
1	A	519	92% 8%
1	B	519	89% 10% .
1	C	519	91% 9%
1	D	519	89% 10% .
1	E	519	90% 8% .
1	F	519	90% 8% .
1	G	519	90% 10%

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Mol	Chain	Length	Quality of chain
1	H	519	90% 9%
1	I	519	92% 7%
1	J	519	87% 11%
1	K	519	92% 6%
1	L	519	90% 8%

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
7	SO4	A	712	-	-	X	-
7	SO4	G	711	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 50850 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 family aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	1	0
			3971	2547	639	766	19			
1	B	516	Total	C	N	O	S	0	0	0
			3902	2509	633	740	20			
1	C	517	Total	C	N	O	S	0	0	0
			3941	2532	637	753	19			
1	D	514	Total	C	N	O	S	0	0	0
			3920	2526	633	741	20			
1	E	509	Total	C	N	O	S	0	0	0
			3893	2509	624	741	19			
1	F	511	Total	C	N	O	S	0	0	0
			3851	2477	622	733	19			
1	G	519	Total	C	N	O	S	0	0	0
			3974	2554	640	760	20			
1	H	517	Total	C	N	O	S	1	0	0
			3902	2508	632	743	19			
1	I	517	Total	C	N	O	S	0	0	0
			3951	2540	637	754	20			
1	J	514	Total	C	N	O	S	0	0	0
			3926	2529	633	744	20			
1	K	509	Total	C	N	O	S	0	0	0
			3884	2504	623	738	19			
1	L	511	Total	C	N	O	S	0	0	0
			3848	2475	622	732	19			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	515	GLN	ASN	engineered mutation	UNP A0A024V0B1

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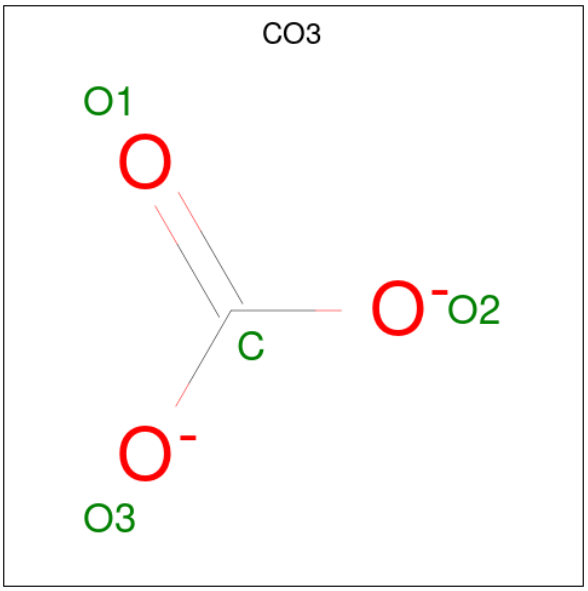
Chain	Residue	Modelled	Actual	Comment	Reference
B	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	546	GLN	ASN	engineered mutation	UNP A0A024V0B1

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).

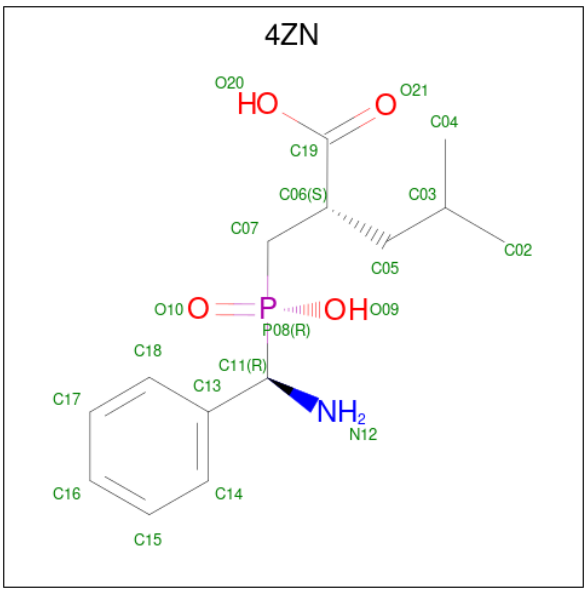


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 1 3	0	0
2	B	1	Total C O 4 1 3	0	0
2	C	1	Total C O 4 1 3	0	0
2	D	1	Total C O 4 1 3	0	0
2	E	1	Total C O 4 1 3	0	0
2	F	1	Total C O 4 1 3	0	0
2	G	1	Total C O 4 1 3	0	0
2	H	1	Total C O 4 1 3	0	0
2	I	1	Total C O 4 1 3	0	0
2	J	1	Total C O 4 1 3	0	0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

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

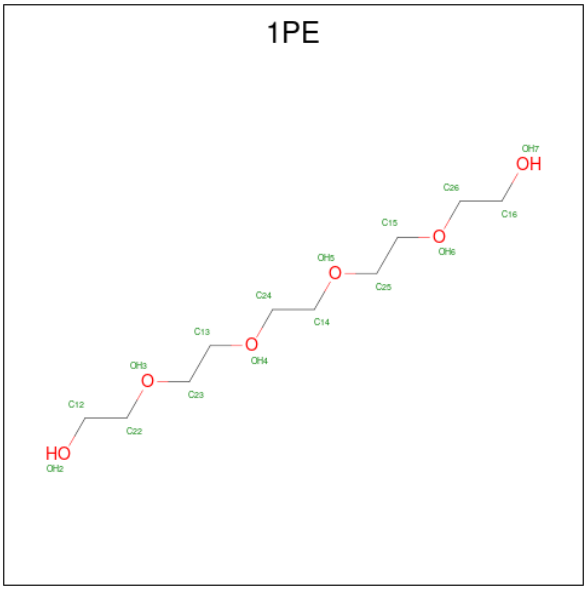
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	E	2	Total Zn 2 2	0	0
3	F	2	Total Zn 2 2	0	0
3	G	2	Total Zn 2 2	0	0
3	H	2	Total Zn 2 2	0	0
3	I	2	Total Zn 2 2	0	0
3	J	2	Total Zn 2 2	0	0
3	K	2	Total Zn 2 2	0	0
3	L	2	Total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

- Molecule 4 is (2S)-2-{[(R)-[(R)-amino(phenyl)methyl](hydroxy)phosphoryl]methyl}-4-methylpentanoic acid (three-letter code: 4ZN) (formula: $C_{14}H_{22}NO_4P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	B	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	C	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	D	1	Total	C	N	O	P	0	0
			20	14	1	4	1		
4	E	1	Total	C	N	O	P	0	0
			20	14	1	4	1		
4	F	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	G	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	H	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	I	1	Total	C	N	O	P	0	0
			12	8	1	2	1		
4	J	1	Total	C	N	O	P	0	0
			16	10	1	4	1		
4	K	1	Total	C	N	O	P	0	0
			14	10	1	2	1		
4	L	1	Total	C	N	O	P	0	0
			16	10	1	4	1		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



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

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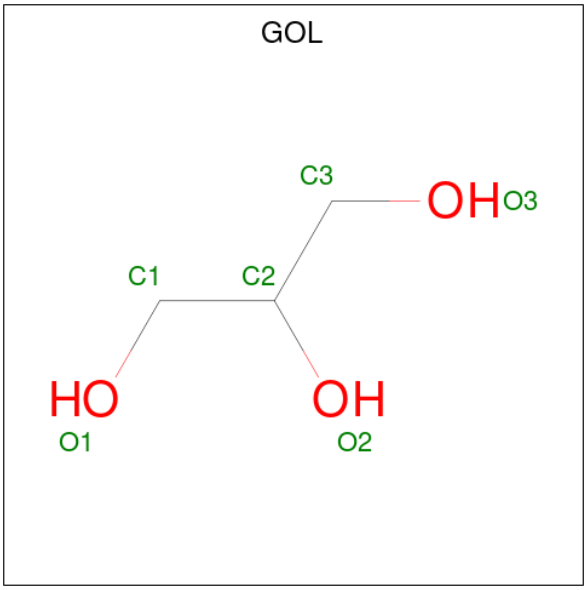
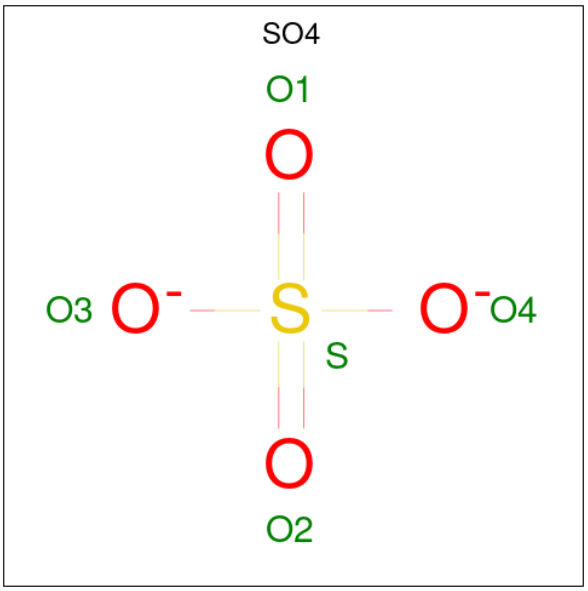
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	1	Total C O 12 8 4	0	0
5	L	1	Total C O 7 4 3	0	0
5	L	1	Total C O 10 6 4	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	265	Total O 265 265	0	0
8	B	246	Total O 246 246	0	0
8	C	277	Total O 277 277	0	0
8	D	283	Total O 283 283	0	0
8	E	322	Total O 322 322	0	0

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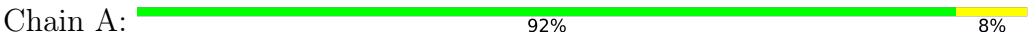
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	245	Total O 245 245	0	0
8	G	281	Total O 281 281	0	0
8	H	220	Total O 220 220	0	0
8	I	272	Total O 272 272	0	0
8	J	287	Total O 287 287	0	0
8	K	283	Total O 283 283	0	0
8	L	240	Total O 240 240	0	0

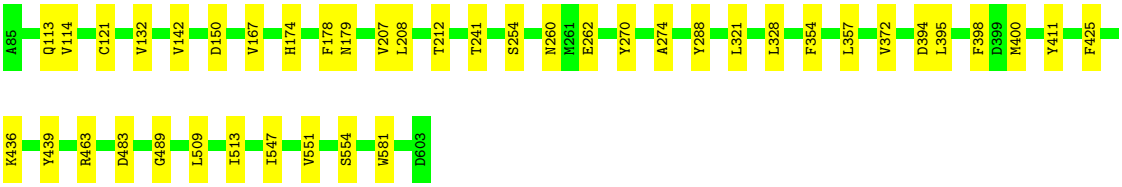
3 Residue-property plots (i)

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. 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. 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 family aminopeptidase

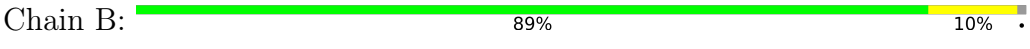
Chain A:

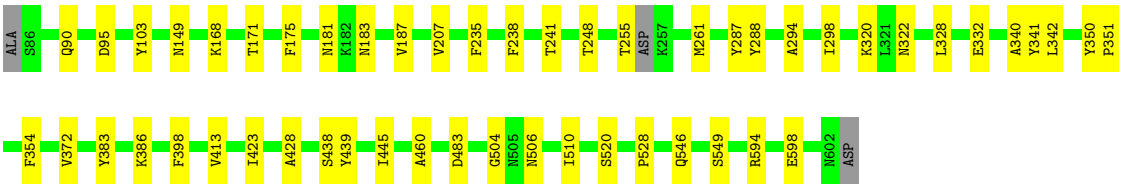




• Molecule 1: M17 family aminopeptidase

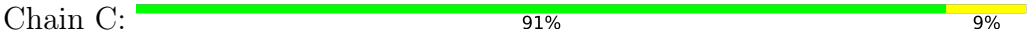
Chain B:

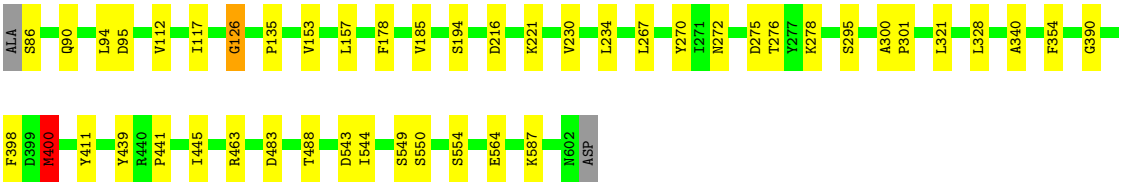




• Molecule 1: M17 family aminopeptidase

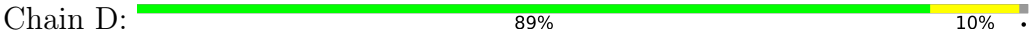
Chain C:

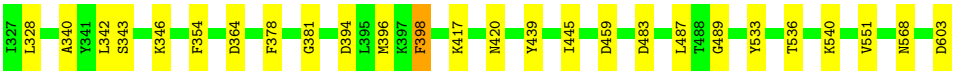




• Molecule 1: M17 family aminopeptidase

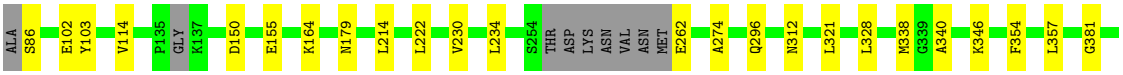
Chain D:

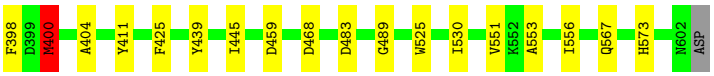




• Molecule 1: M17 family aminopeptidase

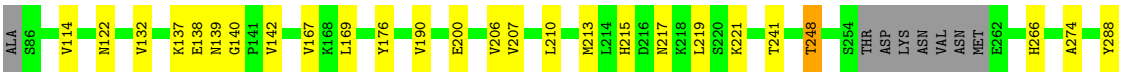
Chain E:

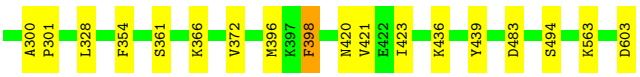




• Molecule 1: M17 family aminopeptidase

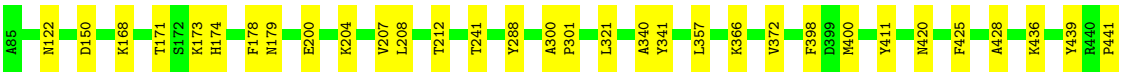
Chain F:





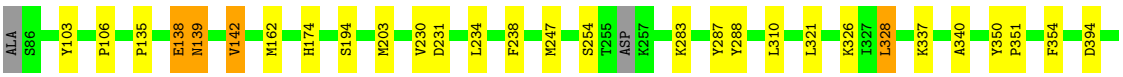
• Molecule 1: M17 family aminopeptidase

Chain G:



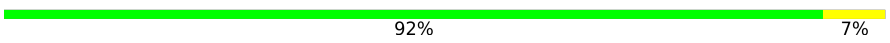
• Molecule 1: M17 family aminopeptidase

Chain H:



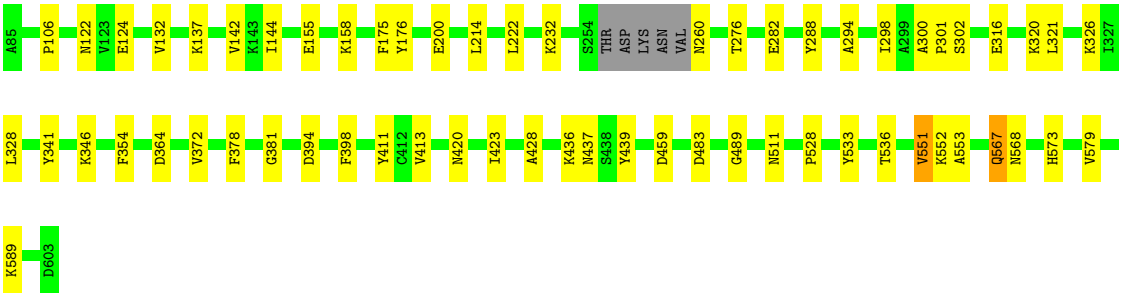
• Molecule 1: M17 family aminopeptidase

Chain I:



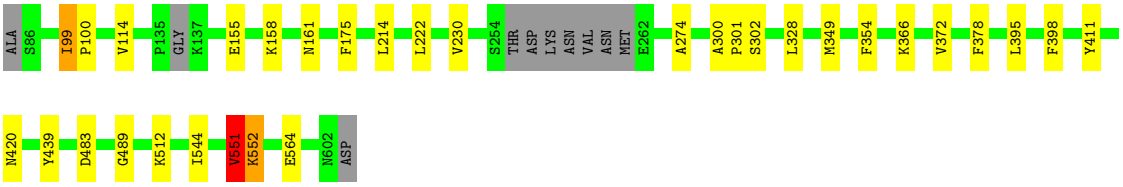
• Molecule 1: M17 family aminopeptidase

Chain J:



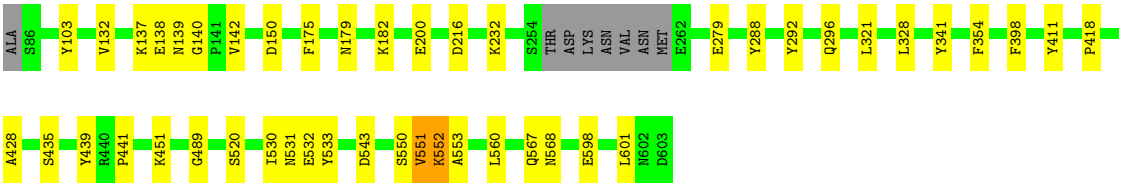
• Molecule 1: M17 family aminopeptidase

Chain K:



• Molecule 1: M17 family 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	174.09Å 177.73Å 230.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 2.30 48.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.98-2.30) 99.9 (48.98-2.30)	Depositor EDS
R_{merge}	0.48	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.182 , 0.235 0.518 , 0.529	Depositor DCC
R_{free} test set	15699 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	64.1	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 24.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	50850	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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 52.83 % 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 4.6001e-05. 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: ZN, 1PE, SO4, GOL, CO3, 4ZN

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	0.43	0/4052	0.55	0/5502
1	B	0.40	0/3979	0.52	0/5405
1	C	0.43	0/4019	0.55	1/5456 (0.0%)
1	D	0.44	0/3997	0.54	0/5422
1	E	0.43	0/3969	0.56	1/5384 (0.0%)
1	F	0.40	0/3928	0.53	0/5342
1	G	0.42	0/4052	0.53	0/5497
1	H	0.39	0/3979	0.52	0/5407
1	I	0.41	0/4029	0.54	1/5466 (0.0%)
1	J	0.43	0/4003	0.54	0/5430
1	K	0.42	0/3960	0.58	1/5372 (0.0%)
1	L	0.41	0/3925	0.54	0/5338
All	All	0.42	0/47892	0.54	4/65021 (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	K	0	2
1	L	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	99	ILE	C-N-CD	-13.20	91.55	120.60
1	I	400	MET	CA-CB-CG	-7.64	100.31	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	400	MET	CA-CB-CG	-6.05	103.01	113.30
1	C	400	MET	CA-CB-CG	-5.85	103.35	113.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	551	VAL	Peptide
1	K	99	ILE	Peptide
1	L	551	VAL	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	3971	0	3875	26	0
1	B	3902	0	3787	29	0
1	C	3941	0	3855	25	0
1	D	3920	0	3851	31	0
1	E	3893	0	3820	26	0
1	F	3851	0	3726	21	0
1	G	3974	0	3899	31	0
1	H	3902	0	3774	31	0
1	I	3951	0	3877	22	0
1	J	3926	0	3854	45	0
1	K	3884	0	3805	18	0
1	L	3848	0	3716	32	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	16	0	9	2	0
4	B	16	0	9	3	0
4	C	16	0	9	1	0
4	D	20	0	20	3	0
4	E	20	0	19	2	0
4	F	16	0	9	0	0
4	G	16	0	9	0	0
4	H	16	0	9	1	0
4	I	12	0	7	0	0
4	J	16	0	9	2	0
4	K	14	0	9	1	0
4	L	16	0	9	1	0
5	A	21	0	22	0	0
5	B	20	0	20	3	0
5	C	22	0	24	1	0
5	D	20	0	20	2	0
5	E	24	0	28	2	0
5	F	10	0	13	0	0
5	G	21	0	20	4	0
5	H	20	0	20	1	0
5	I	23	0	26	2	0
5	J	32	0	39	12	0
5	K	24	0	28	2	0
5	L	17	0	21	6	0
6	A	6	0	8	0	0
7	A	25	0	0	2	0
7	B	5	0	0	0	0
7	C	25	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	5	0	0	1	0
7	E	15	0	0	1	0
7	F	10	0	0	0	0
7	G	20	0	0	2	0
7	I	10	0	0	0	0
7	J	10	0	0	0	0
7	K	10	0	0	0	0
7	L	5	0	0	0	0
8	A	265	0	0	3	0
8	B	246	0	0	3	0
8	C	277	0	0	2	0
8	D	283	0	0	5	0
8	E	322	0	0	5	0
8	F	245	0	0	4	0
8	G	281	0	0	0	0
8	H	220	0	0	2	0
8	I	272	0	0	3	0
8	J	287	0	0	5	0
8	K	283	0	0	1	0
8	L	240	0	0	4	0
All	All	50850	0	46255	326	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 326 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:320:LYS:HZ1	5:J:706:1PE:H151	1.30	0.96
1:J:489:GLY:N	4:J:704:4ZN:O20	2.06	0.88
1:L:532:GLU:HB2	5:L:705:1PE:H142	1.55	0.87
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.65	0.78
1:B:320:LYS:HZ1	5:B:706:1PE:H241	1.50	0.77

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	518/519 (100%)	501 (97%)	16 (3%)	1 (0%)	47	58
1	B	512/519 (99%)	495 (97%)	16 (3%)	1 (0%)	47	58
1	C	515/519 (99%)	499 (97%)	15 (3%)	1 (0%)	47	58
1	D	510/519 (98%)	496 (97%)	13 (2%)	1 (0%)	47	58
1	E	503/519 (97%)	493 (98%)	10 (2%)	0	100	100
1	F	507/519 (98%)	490 (97%)	17 (3%)	0	100	100
1	G	517/519 (100%)	503 (97%)	14 (3%)	0	100	100
1	H	513/519 (99%)	500 (98%)	11 (2%)	2 (0%)	34	42
1	I	515/519 (99%)	505 (98%)	8 (2%)	2 (0%)	34	42
1	J	510/519 (98%)	496 (97%)	12 (2%)	2 (0%)	34	42
1	K	503/519 (97%)	490 (97%)	10 (2%)	3 (1%)	25	31
1	L	507/519 (98%)	491 (97%)	14 (3%)	2 (0%)	34	42
All	All	6130/6228 (98%)	5959 (97%)	156 (2%)	15 (0%)	47	58

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	551	VAL
1	H	138	GLU
1	K	100	PRO
1	K	551	VAL
1	K	552	LYS

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	423/447 (95%)	417 (99%)	6 (1%)	67	81
1	B	407/447 (91%)	403 (99%)	4 (1%)	76	87
1	C	418/447 (94%)	406 (97%)	12 (3%)	42	58
1	D	413/447 (92%)	405 (98%)	8 (2%)	57	73
1	E	413/447 (92%)	410 (99%)	3 (1%)	84	92
1	F	402/447 (90%)	391 (97%)	11 (3%)	44	61
1	G	422/447 (94%)	415 (98%)	7 (2%)	60	76
1	H	406/447 (91%)	397 (98%)	9 (2%)	52	69
1	I	420/447 (94%)	414 (99%)	6 (1%)	67	81
1	J	414/447 (93%)	408 (99%)	6 (1%)	67	81
1	K	410/447 (92%)	406 (99%)	4 (1%)	76	87
1	L	400/447 (90%)	394 (98%)	6 (2%)	65	79
All	All	4948/5364 (92%)	4866 (98%)	82 (2%)	60	76

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	483	ASP
1	J	567	GLN
1	H	554	SER
1	I	483	ASP
1	K	439	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	149	ASN
1	H	139	ASN
1	J	181	ASN
1	B	181	ASN
1	A	260	ASN

5.3.3 RNA

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 102 ligands modelled in this entry, 24 are monoatomic - leaving 78 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	SO4	E	708	-	4,4,4	0.16	0	6,6,6	0.23	0
7	SO4	G	710	-	4,4,4	0.19	0	6,6,6	0.16	0
4	4ZN	C	704	3	13,16,20	1.41	1 (7%)	15,22,28	1.01	1 (6%)
7	SO4	C	711	-	4,4,4	0.24	0	6,6,6	0.39	0
7	SO4	I	707	-	4,4,4	0.13	0	6,6,6	0.18	0
4	4ZN	J	704	3	13,16,20	1.43	1 (7%)	15,22,28	1.05	1 (6%)
5	1PE	C	706	-	8,8,15	0.78	0	7,7,14	0.30	0
5	1PE	G	707	-	5,5,15	0.68	0	4,4,14	0.43	0
7	SO4	C	708	-	4,4,4	0.16	0	6,6,6	0.27	0
2	CO3	A	701	-	2,3,3	0.20	0	2,3,3	0.65	0
2	CO3	B	701	-	2,3,3	0.44	0	2,3,3	0.80	0
7	SO4	L	707	-	4,4,4	0.15	0	6,6,6	0.17	0
7	SO4	A	712	-	4,4,4	0.20	0	6,6,6	0.59	0
5	1PE	E	705	-	11,11,15	0.83	0	10,10,14	0.39	0
5	1PE	G	705	-	8,8,15	0.70	0	7,7,14	0.34	0
2	CO3	J	701	-	2,3,3	0.44	0	2,3,3	0.57	0
5	1PE	H	706	-	9,9,15	0.74	0	8,8,14	0.20	0
5	1PE	K	706	-	11,11,15	0.74	0	10,10,14	0.45	0
7	SO4	A	709	-	4,4,4	0.18	0	6,6,6	0.10	0
7	SO4	F	706	-	4,4,4	0.20	0	6,6,6	0.16	0
7	SO4	C	709	-	4,4,4	0.26	0	6,6,6	0.32	0
5	1PE	E	706	-	11,11,15	0.70	0	10,10,14	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CO3	K	701	-	2,3,3	0.28	0	2,3,3	0.12	0
7	SO4	E	709	-	4,4,4	0.23	0	6,6,6	0.11	0
7	SO4	J	709	-	4,4,4	0.18	0	6,6,6	0.12	0
4	4ZN	I	704	3	8,12,20	1.55	1 (12%)	11,17,28	1.68	1 (9%)
5	1PE	B	705	-	9,9,15	0.70	0	8,8,14	0.38	0
7	SO4	K	707	-	4,4,4	0.19	0	6,6,6	0.12	0
5	1PE	I	705	-	11,11,15	0.76	0	10,10,14	0.40	0
6	GOL	A	707	-	5,5,5	0.45	0	5,5,5	0.21	0
7	SO4	I	708	-	4,4,4	0.14	0	6,6,6	0.10	0
5	1PE	J	706	-	10,10,15	0.72	0	9,9,14	0.48	0
2	CO3	E	701	-	2,3,3	0.41	0	2,3,3	0.48	0
5	1PE	A	705	-	8,8,15	0.75	0	7,7,14	0.34	0
7	SO4	G	709	-	4,4,4	0.12	0	6,6,6	0.21	0
4	4ZN	B	704	3	13,16,20	0.87	0	15,22,28	2.75	5 (33%)
4	4ZN	L	704	3	13,16,20	0.65	0	15,22,28	1.15	1 (6%)
7	SO4	K	708	-	4,4,4	0.11	0	6,6,6	0.26	0
7	SO4	C	707	-	4,4,4	0.11	0	6,6,6	0.10	0
5	1PE	B	706	-	9,9,15	0.72	0	8,8,14	0.47	0
5	1PE	D	705	-	9,9,15	0.82	0	8,8,14	0.49	0
4	4ZN	K	704	3	11,14,20	0.79	1 (9%)	13,19,28	1.39	2 (15%)
7	SO4	F	707	-	4,4,4	0.21	0	6,6,6	0.13	0
5	1PE	C	705	-	12,12,15	0.80	0	11,11,14	0.56	0
4	4ZN	A	704	3	13,16,20	0.61	0	15,22,28	1.73	3 (20%)
5	1PE	K	705	-	11,11,15	0.72	0	10,10,14	0.25	0
5	1PE	L	705	-	6,6,15	0.70	0	5,5,14	0.38	0
2	CO3	H	701	-	2,3,3	0.40	0	2,3,3	0.42	0
5	1PE	L	706	-	9,9,15	0.62	0	8,8,14	0.41	0
5	1PE	G	706	-	5,5,15	0.60	0	4,4,14	0.58	0
7	SO4	J	708	-	4,4,4	0.13	0	6,6,6	0.31	0
5	1PE	D	706	-	9,9,15	0.75	0	8,8,14	0.34	0
5	1PE	J	707	-	9,9,15	0.61	0	8,8,14	0.32	0
5	1PE	I	706	-	10,10,15	0.71	0	9,9,14	0.46	0
4	4ZN	F	704	3	13,16,20	0.67	0	15,22,28	1.43	2 (13%)
7	SO4	A	710	-	4,4,4	0.18	0	6,6,6	0.35	0
2	CO3	L	701	-	2,3,3	0.39	0	2,3,3	0.19	0
7	SO4	C	710	-	4,4,4	0.26	0	6,6,6	0.24	0
4	4ZN	H	704	3	13,16,20	1.64	2 (15%)	15,22,28	1.10	2 (13%)
2	CO3	G	701	-	2,3,3	0.28	0	2,3,3	0.27	0
7	SO4	E	707	-	4,4,4	0.15	0	6,6,6	0.16	0
7	SO4	D	707	-	4,4,4	0.21	0	6,6,6	0.25	0
5	1PE	J	705	-	10,10,15	0.69	0	9,9,14	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CO3	F	701	-	2,3,3	0.40	0	2,3,3	0.30	0
2	CO3	D	701	-	2,3,3	0.40	0	2,3,3	0.61	0
7	SO4	B	707	-	4,4,4	0.13	0	6,6,6	0.26	0
2	CO3	I	701	-	2,3,3	0.35	0	2,3,3	0.14	0
2	CO3	C	701	-	2,3,3	0.28	0	2,3,3	0.78	0
5	1PE	H	705	-	9,9,15	0.76	0	8,8,14	0.27	0
7	SO4	G	708	-	4,4,4	0.18	0	6,6,6	0.13	0
5	1PE	A	706	-	11,11,15	0.78	0	10,10,14	0.34	0
5	1PE	F	705	-	9,9,15	0.68	0	8,8,14	0.38	0
7	SO4	A	708	-	4,4,4	0.16	0	6,6,6	0.24	0
7	SO4	G	711	-	4,4,4	0.11	0	6,6,6	0.53	0
4	4ZN	E	704	3	16,20,20	0.82	1 (6%)	18,28,28	1.62	2 (11%)
7	SO4	A	711	-	4,4,4	0.19	0	6,6,6	0.20	0
4	4ZN	D	704	3	16,20,20	1.41	2 (12%)	18,28,28	1.58	4 (22%)
4	4ZN	G	704	3	13,16,20	0.67	0	15,22,28	1.60	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4ZN	F	704	3	-	6/11/16/23	0/1/1/1
4	4ZN	C	704	3	-	8/11/16/23	0/1/1/1
4	4ZN	I	704	3	-	3/5/10/23	0/1/1/1
5	1PE	B	705	-	-	4/7/7/13	-
5	1PE	B	706	-	-	6/7/7/13	-
4	4ZN	J	704	3	-	8/11/16/23	0/1/1/1
5	1PE	D	705	-	-	6/7/7/13	-
4	4ZN	K	704	3	-	6/9/14/23	0/1/1/1
4	4ZN	H	704	3	-	9/11/16/23	0/1/1/1
5	1PE	C	706	-	-	4/6/6/13	-
5	1PE	C	705	-	-	4/10/10/13	-
5	1PE	G	707	-	-	2/3/3/13	-
5	1PE	J	705	-	-	4/8/8/13	-
5	1PE	I	705	-	-	6/9/9/13	-
4	4ZN	A	704	3	-	9/11/16/23	0/1/1/1
5	1PE	E	705	-	-	3/9/9/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	E	706	-	-	5/9/9/13	-
6	GOL	A	707	-	-	2/4/4/4	-
5	1PE	J	706	-	-	5/8/8/13	-
5	1PE	K	705	-	-	3/9/9/13	-
5	1PE	G	705	-	-	4/6/6/13	-
5	1PE	H	705	-	-	4/7/7/13	-
5	1PE	L	705	-	-	2/4/4/13	-
5	1PE	L	706	-	-	5/7/7/13	-
5	1PE	A	706	-	-	3/9/9/13	-
5	1PE	A	705	-	-	3/6/6/13	-
5	1PE	F	705	-	-	6/7/7/13	-
5	1PE	H	706	-	-	4/7/7/13	-
5	1PE	I	706	-	-	4/8/8/13	-
5	1PE	K	706	-	-	4/9/9/13	-
5	1PE	G	706	-	-	2/3/3/13	-
5	1PE	D	706	-	-	6/7/7/13	-
4	4ZN	E	704	3	-	9/17/23/23	0/1/1/1
4	4ZN	D	704	3	-	5/17/23/23	0/1/1/1
4	4ZN	B	704	3	-	8/11/16/23	0/1/1/1
5	1PE	J	707	-	-	4/7/7/13	-
4	4ZN	G	704	3	-	6/11/16/23	0/1/1/1
4	4ZN	L	704	3	-	7/11/16/23	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	704	4ZN	P08-O10	4.78	1.58	1.49
4	J	704	4ZN	P08-O10	4.55	1.58	1.49
4	C	704	4ZN	P08-O10	4.39	1.58	1.49
4	D	704	4ZN	P08-O10	4.26	1.57	1.49
4	I	704	4ZN	P08-O10	4.02	1.57	1.50

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	704	4ZN	C07-P08-C11	7.03	123.35	106.82
4	B	704	4ZN	C07-C06-C19	5.58	122.13	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	704	4ZN	O09-P08-O10	-5.14	107.35	114.23
4	A	704	4ZN	C07-C06-C19	-4.23	106.93	113.49
4	E	704	4ZN	C06-C05-C03	4.21	125.35	115.68

There are no chirality outliers.

5 of 189 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	704	4ZN	C19-C06-C07-P08
4	A	704	4ZN	C06-C07-P08-O09
4	A	704	4ZN	C06-C07-P08-O10
4	A	704	4ZN	C06-C07-P08-C11
4	B	704	4ZN	C06-C07-P08-O09

There are no ring outliers.

32 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	704	4ZN	1	0
7	C	711	SO4	1	0
4	J	704	4ZN	2	0
5	C	706	1PE	1	0
5	G	707	1PE	1	0
7	C	708	SO4	1	0
7	A	712	SO4	2	0
5	E	705	1PE	1	0
5	G	705	1PE	1	0
5	K	706	1PE	2	0
5	E	706	1PE	1	0
5	I	705	1PE	1	0
5	J	706	1PE	5	0
4	B	704	4ZN	3	0
4	L	704	4ZN	1	0
5	B	706	1PE	3	0
5	D	705	1PE	2	0
4	K	704	4ZN	1	0
4	A	704	4ZN	2	0
5	L	705	1PE	5	0
5	L	706	1PE	1	0
5	G	706	1PE	2	0
5	J	707	1PE	3	0

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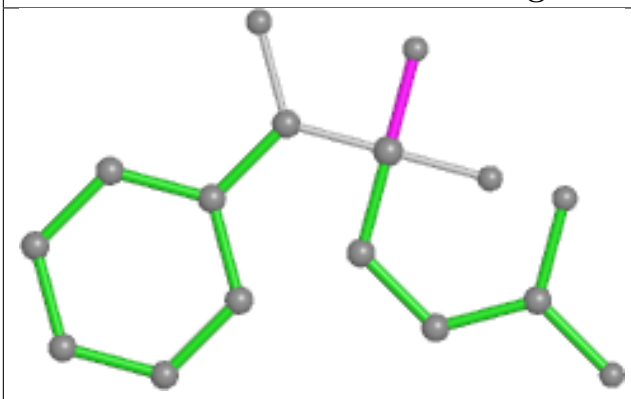
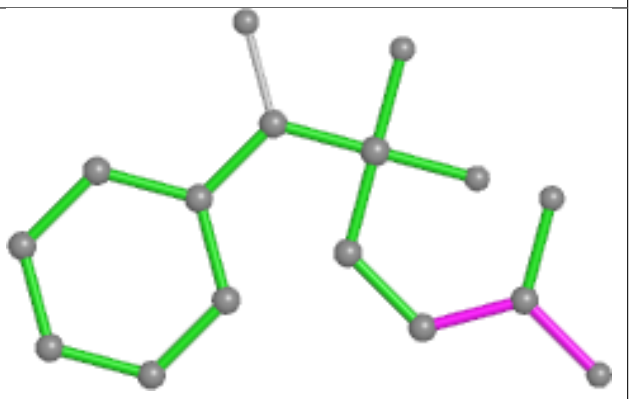
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	706	1PE	1	0
4	H	704	4ZN	1	0
7	E	707	SO4	1	0
7	D	707	SO4	1	0
5	J	705	1PE	4	0
5	H	705	1PE	1	0
7	G	711	SO4	2	0
4	E	704	4ZN	2	0
4	D	704	4ZN	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

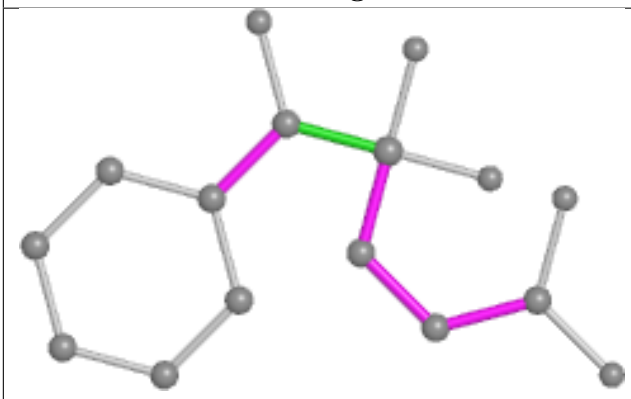
Ligand 4ZN C 704



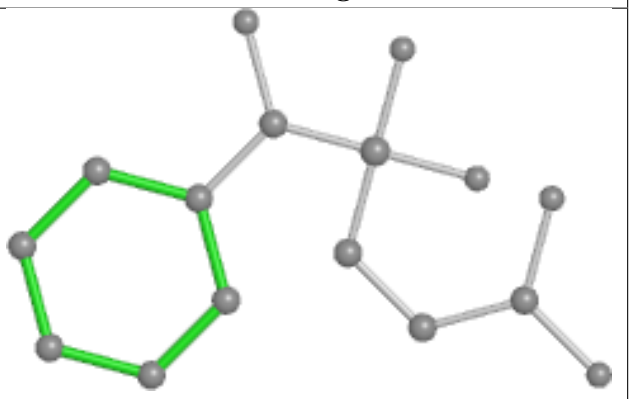
Bond lengths



Bond angles

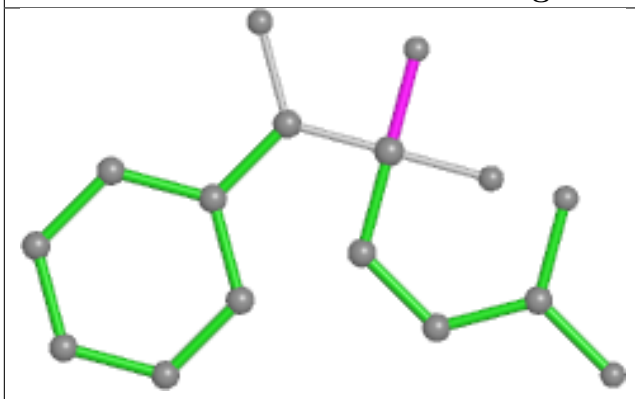


Torsions



Rings

Ligand 4ZN J 704



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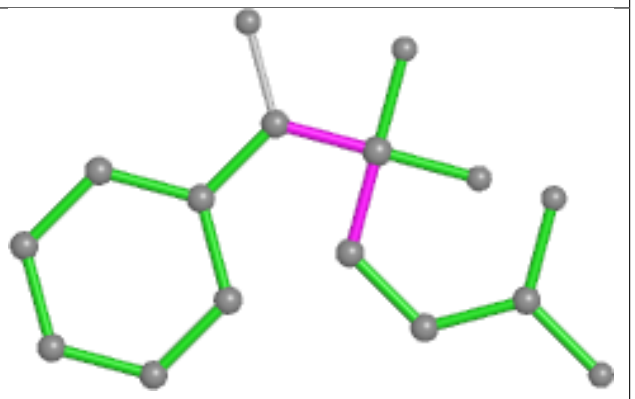

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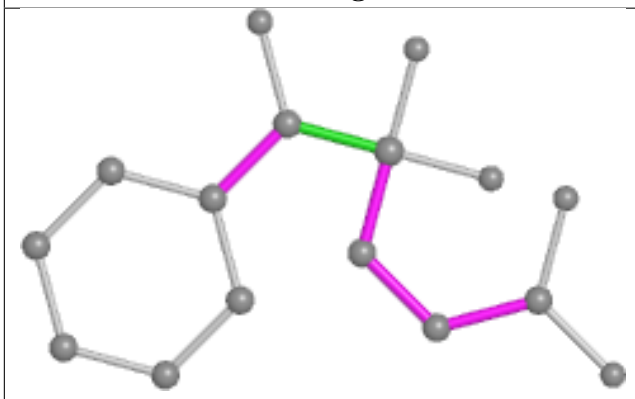

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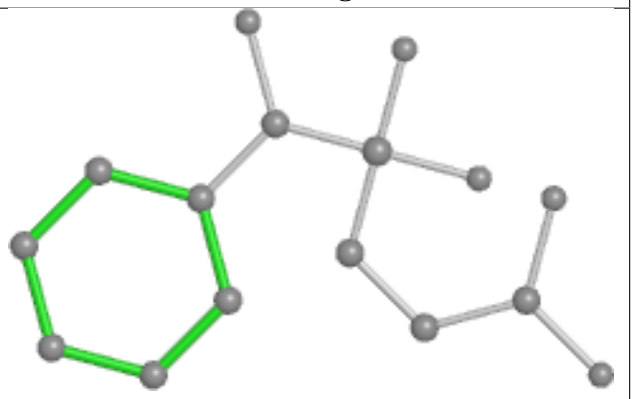
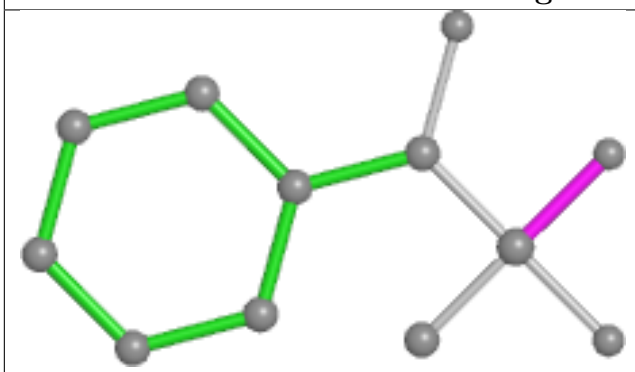


Rings

Ligand 4ZN I 704



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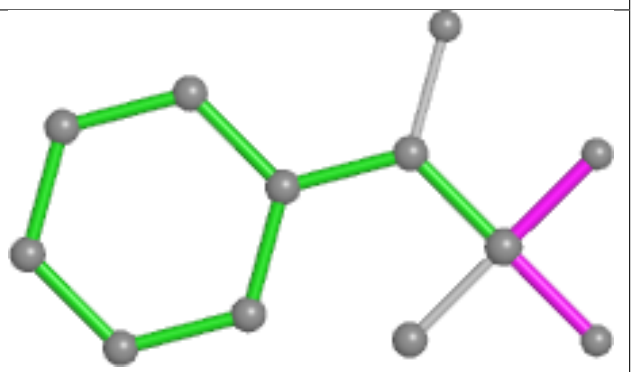
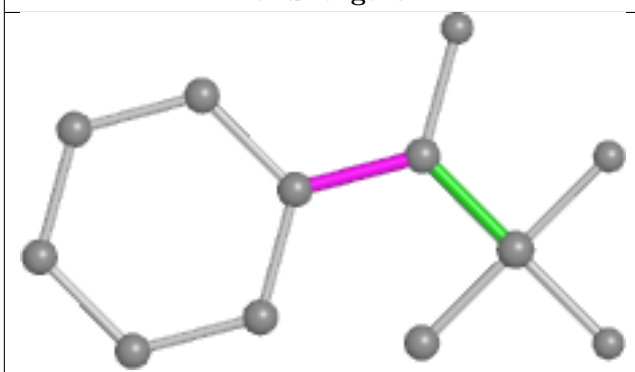
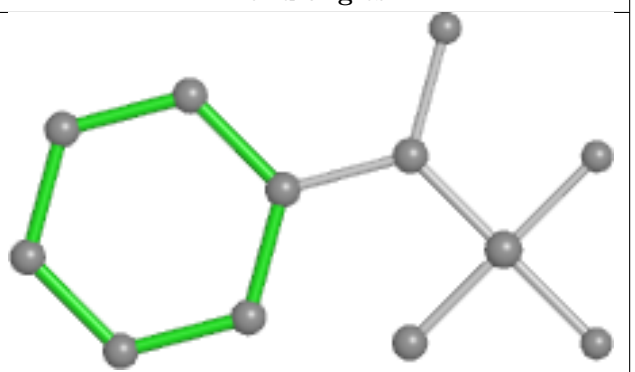


Bond angles

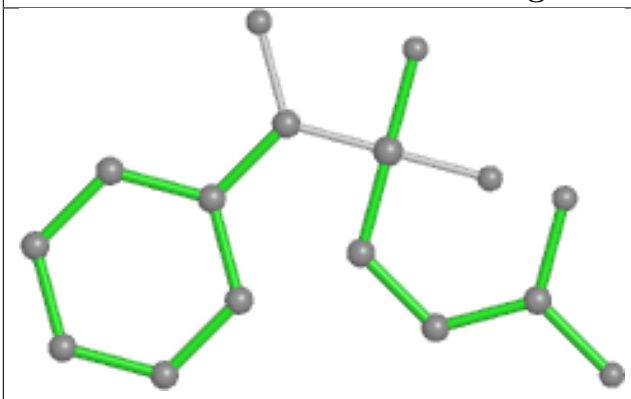


Torsions



Rings

Ligand 4ZN B 704



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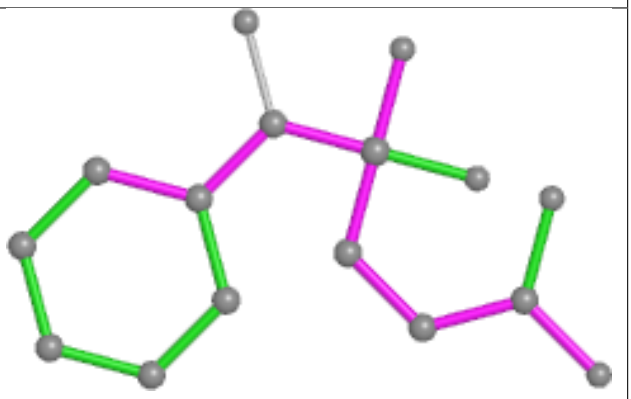
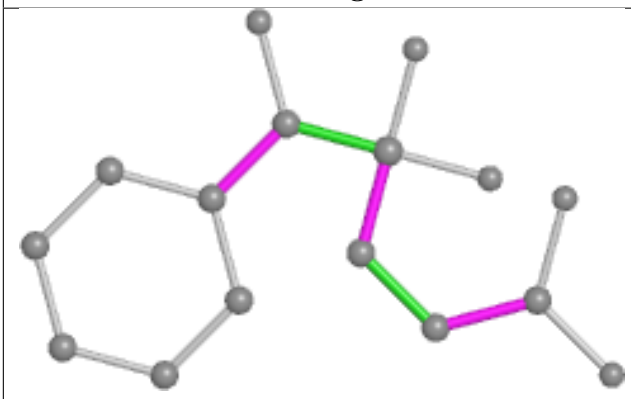


Bond angles



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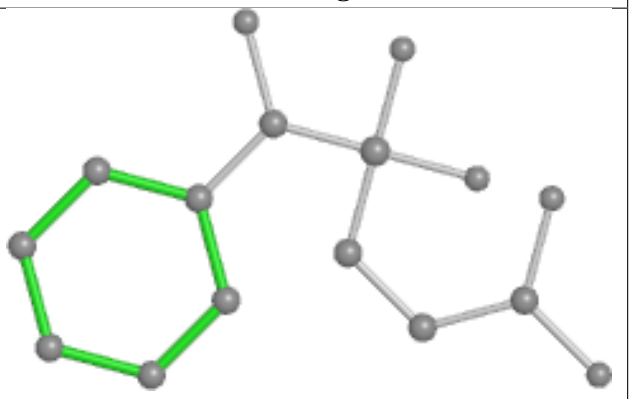
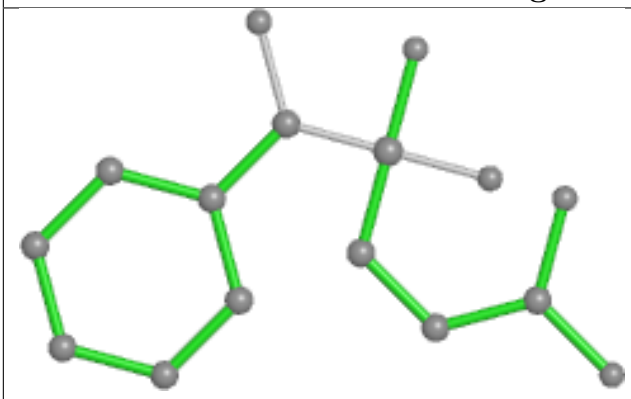


Rings

Ligand 4ZN L 704



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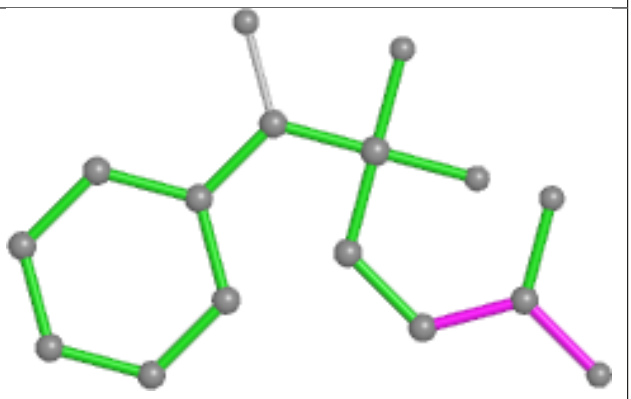

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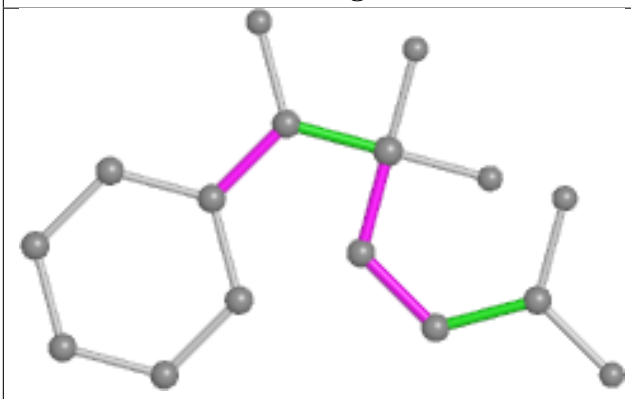

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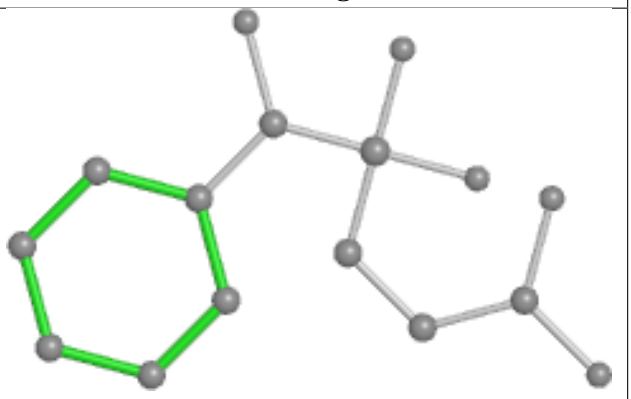
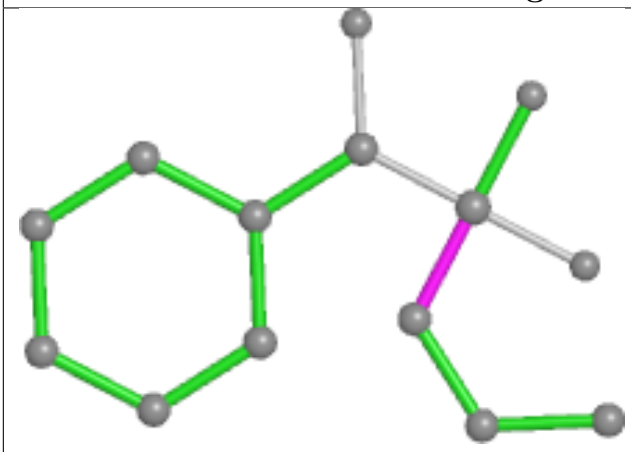


Rings

Ligand 4ZN K 704



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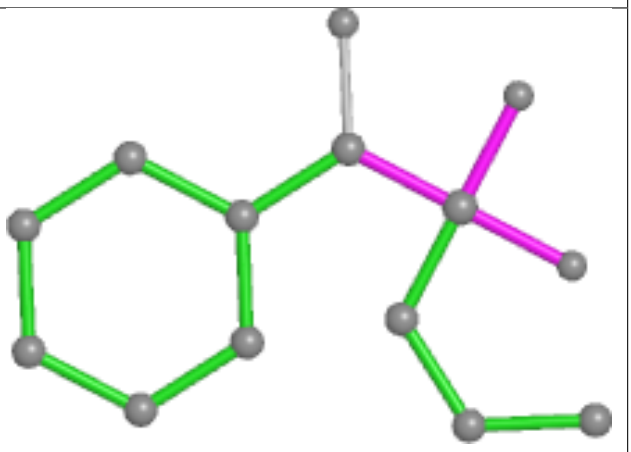

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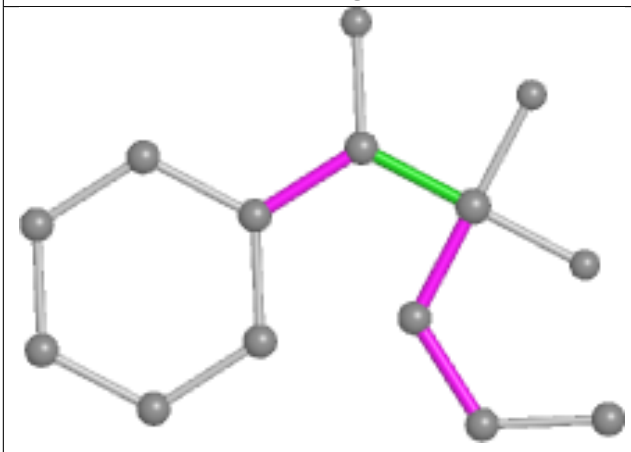

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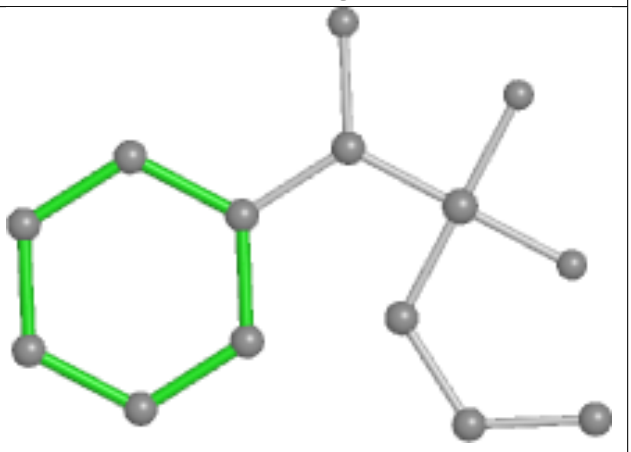
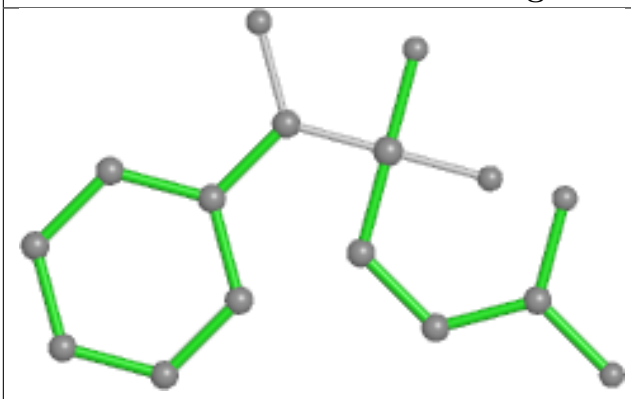


Rings

Ligand 4ZN A 704



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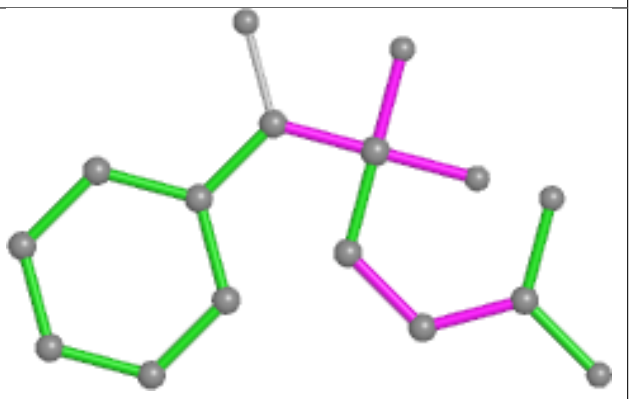

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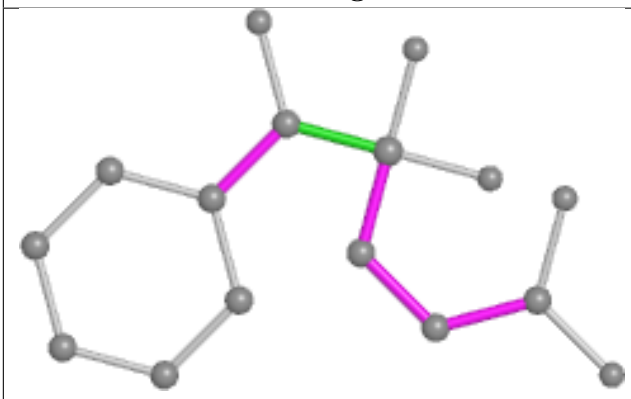

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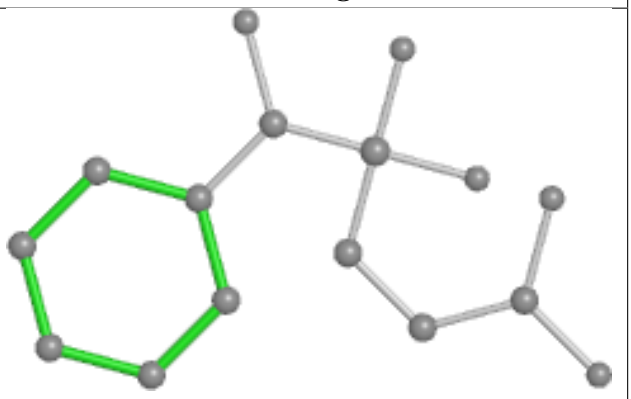
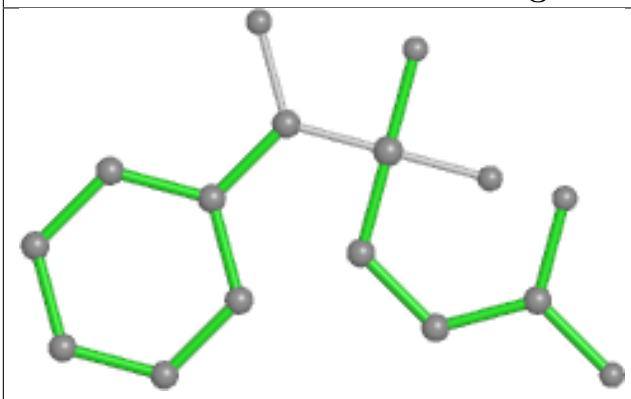


Rings

Ligand 4ZN F 704



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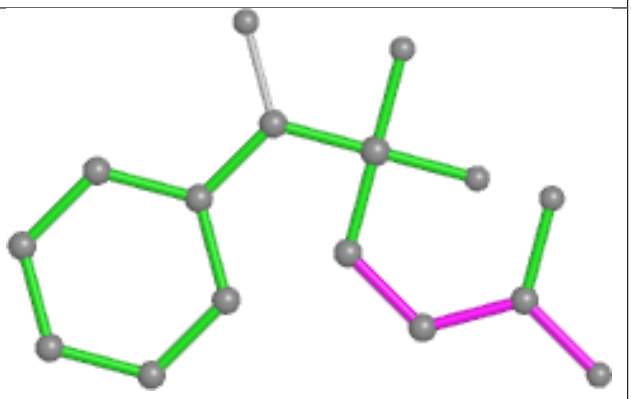
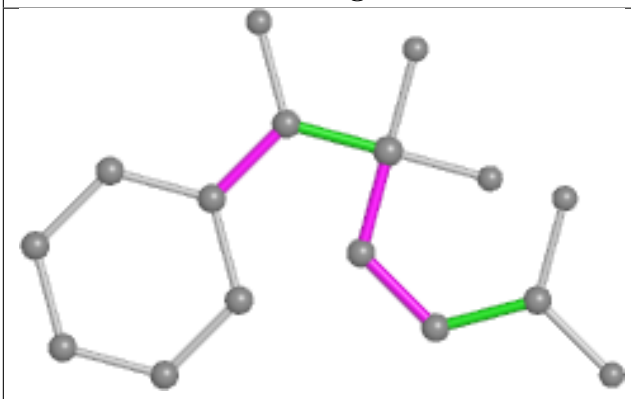


Bond angles



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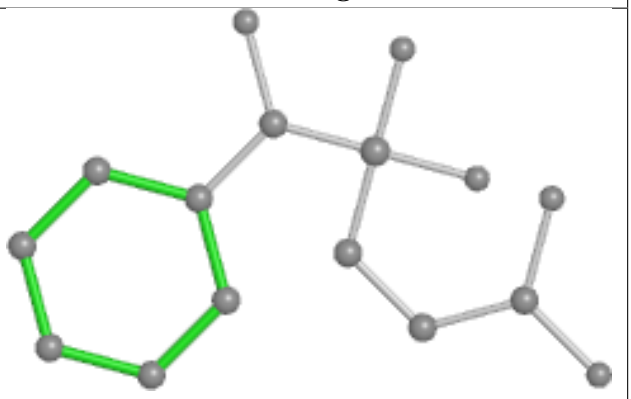
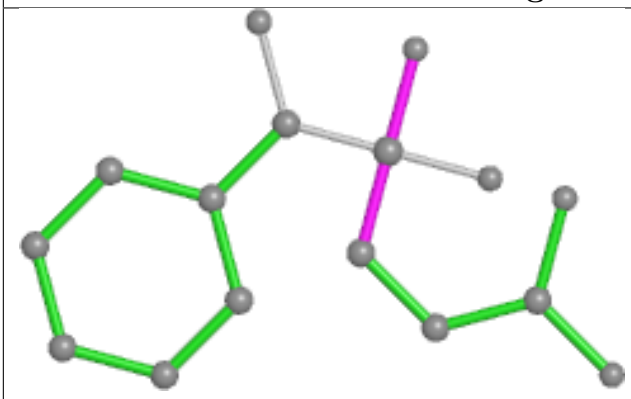
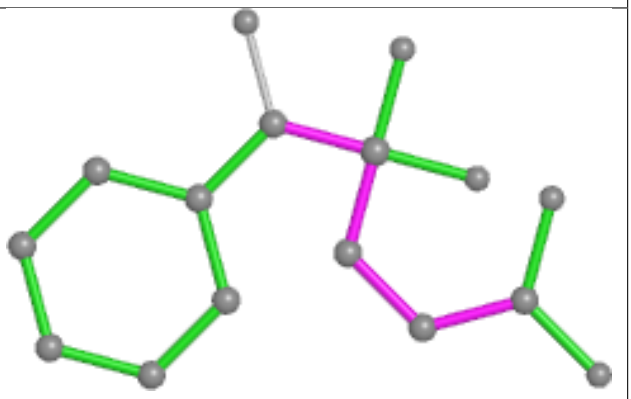


Rings

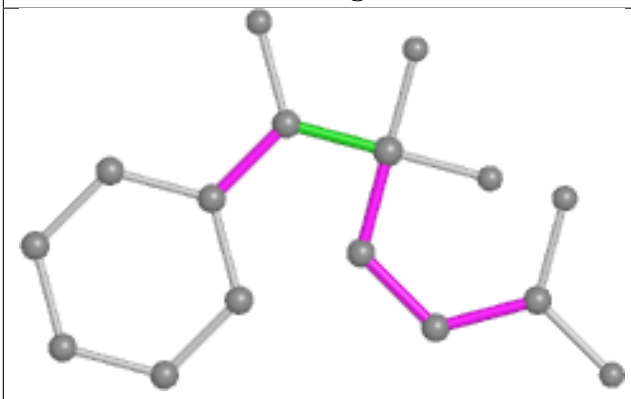
Ligand 4ZN H 704



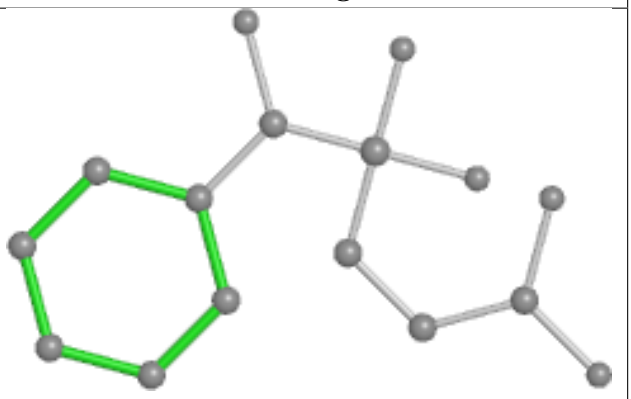
Bond lengths



Bond angles

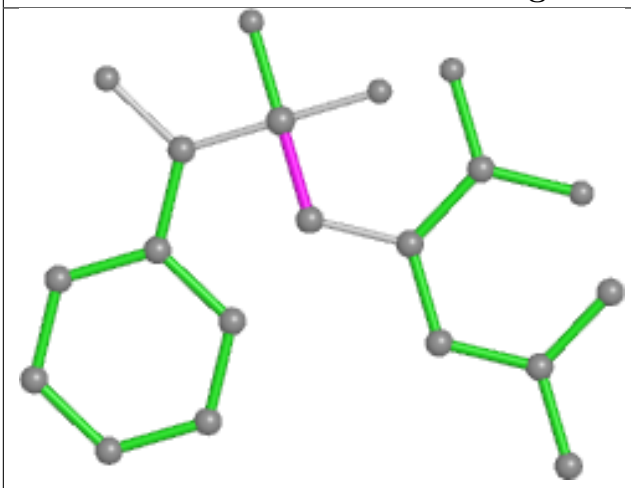


Torsions

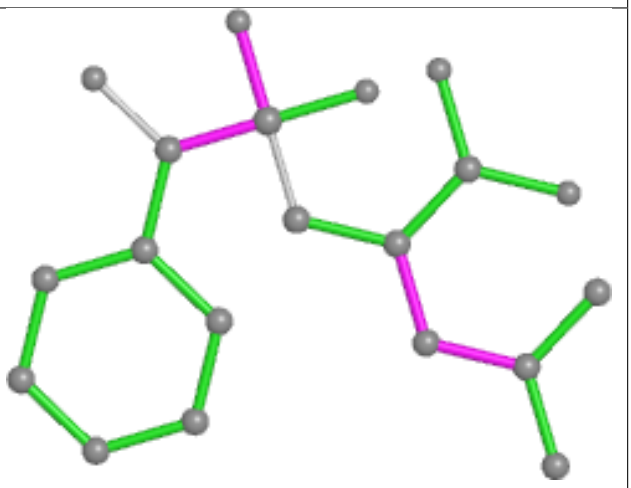


Rings

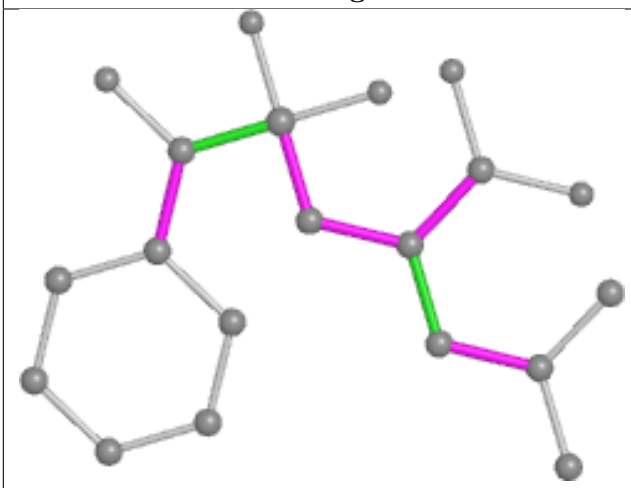
Ligand 4ZN E 704



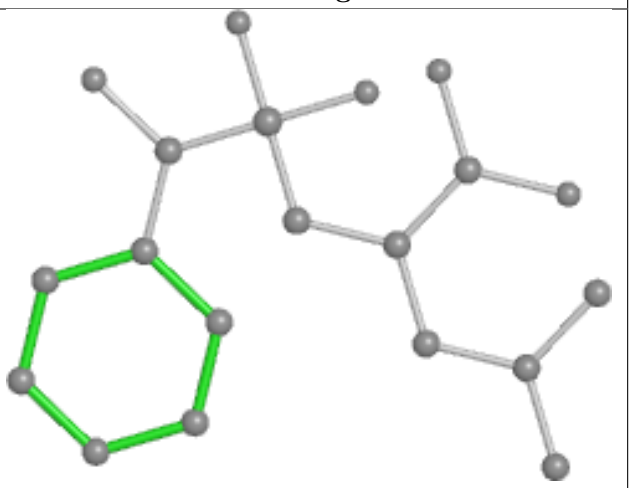
Bond lengths



Bond angles

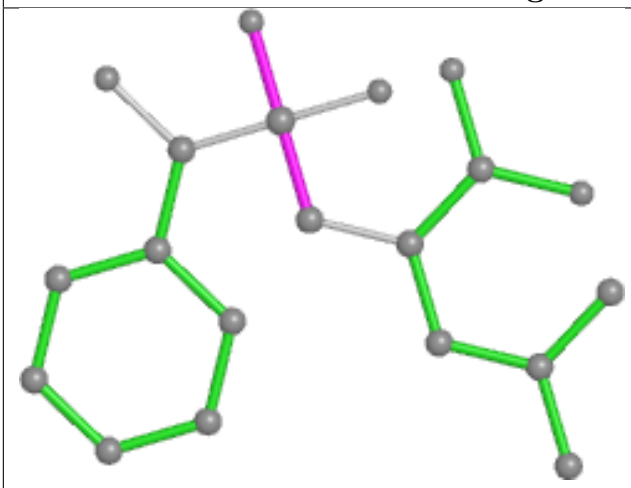


Torsions

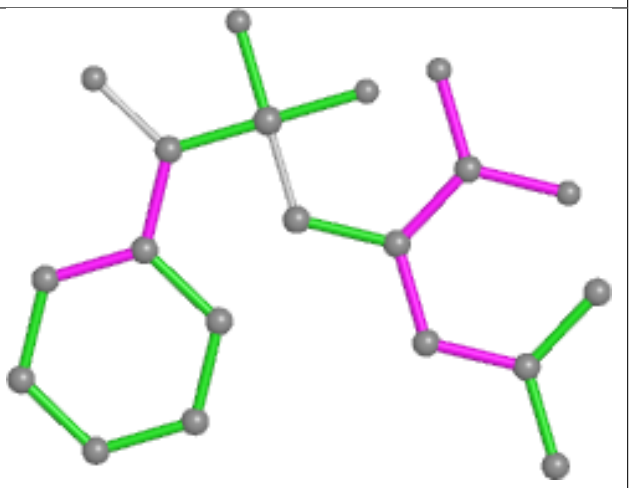


Rings

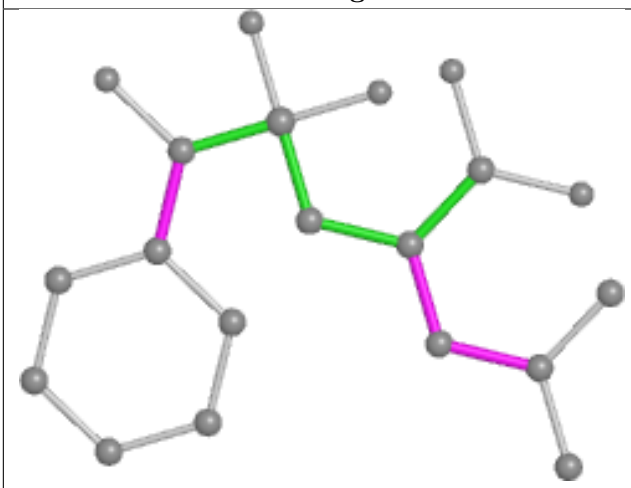
Ligand 4ZN D 704



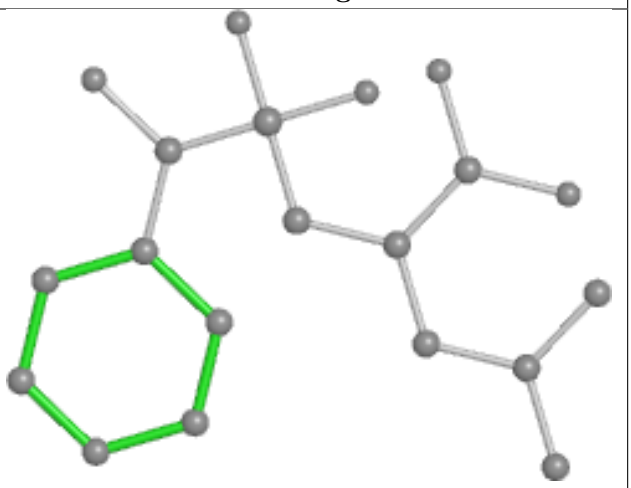
Bond lengths



Bond angles

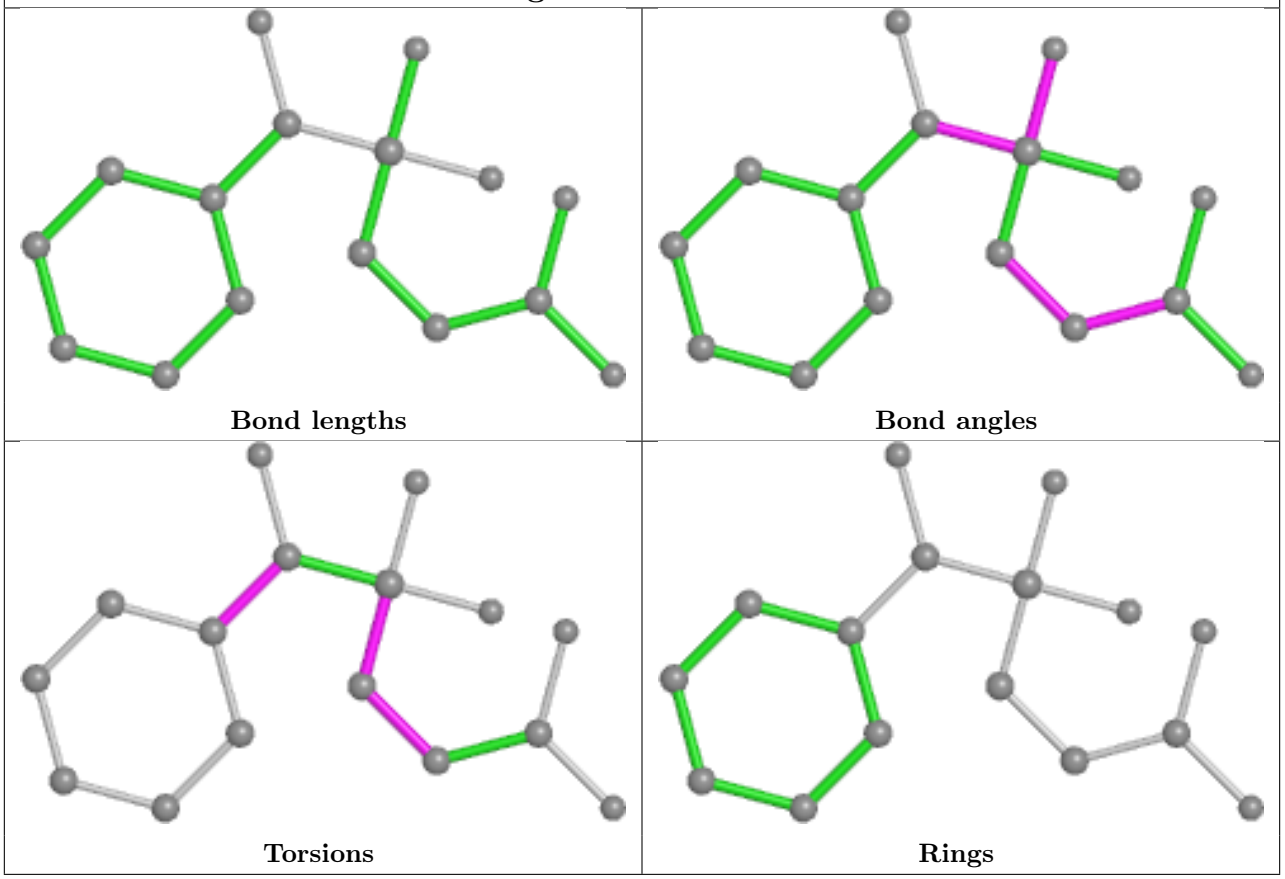


Torsions



Rings

Ligand 4ZN G 704



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

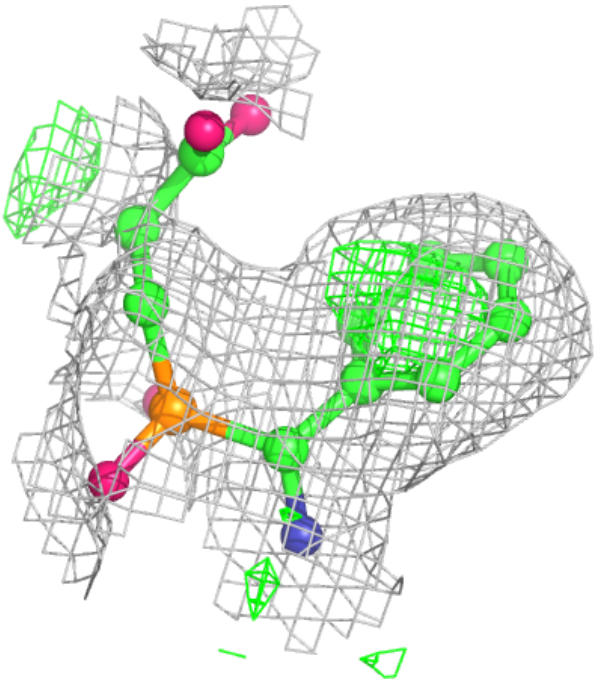
6.4 Ligands

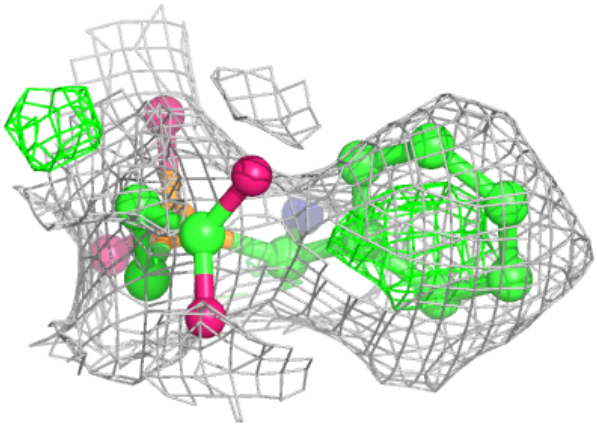
Unable to reproduce the depositors R factor - this section is therefore empty.

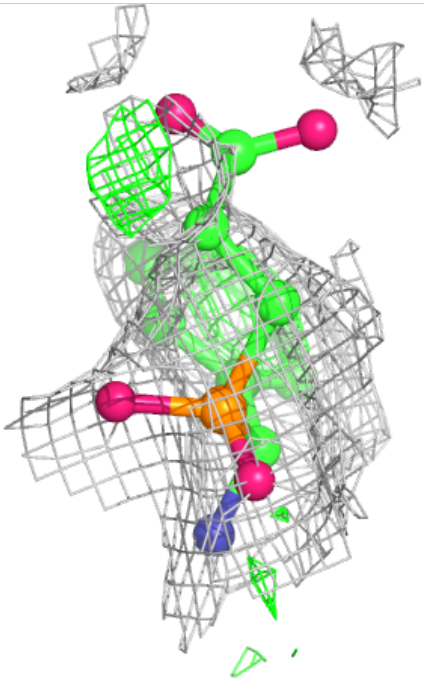
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4ZN A 704:

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

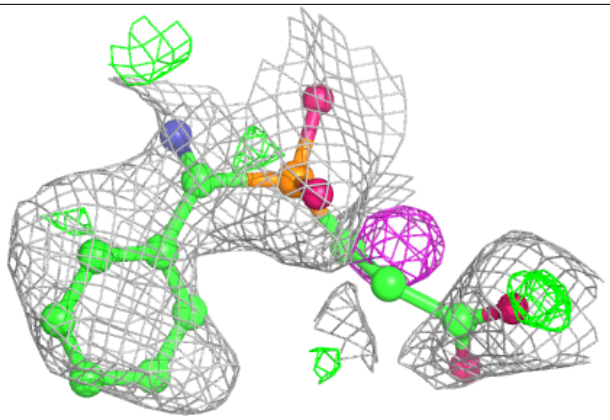


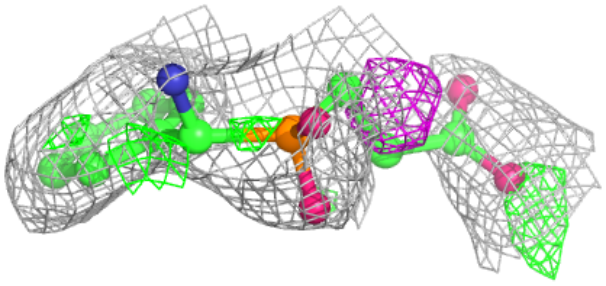


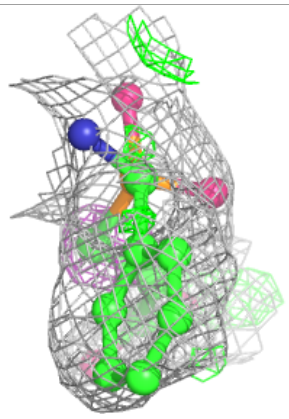


Electron density around 4ZN B 704:

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

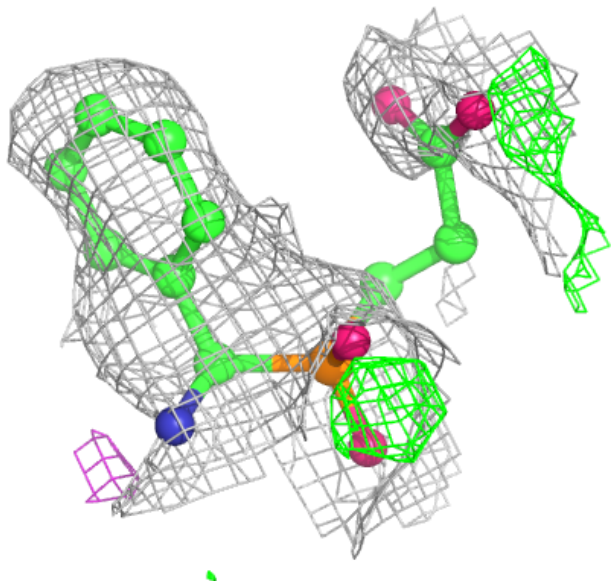


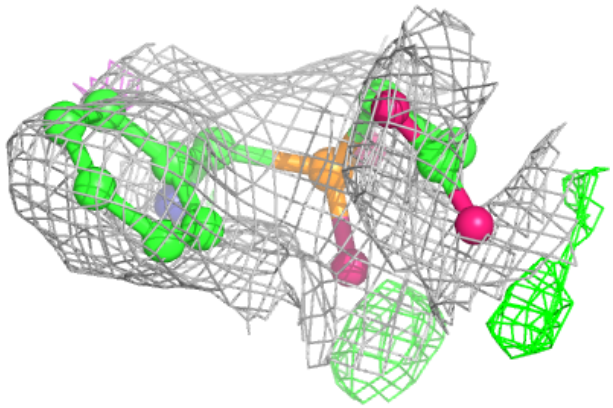


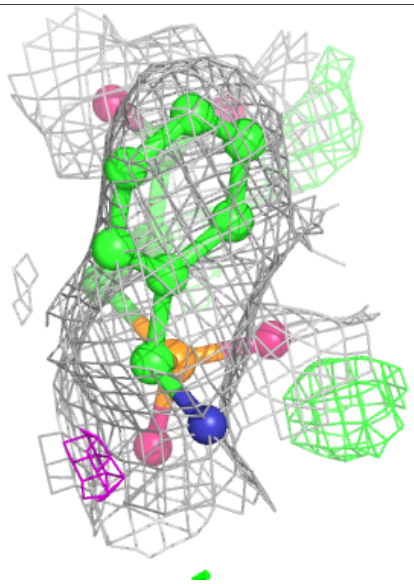


Electron density around 4ZN C 704:

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

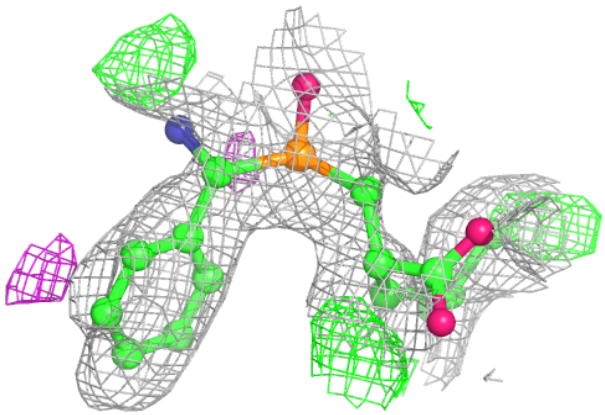


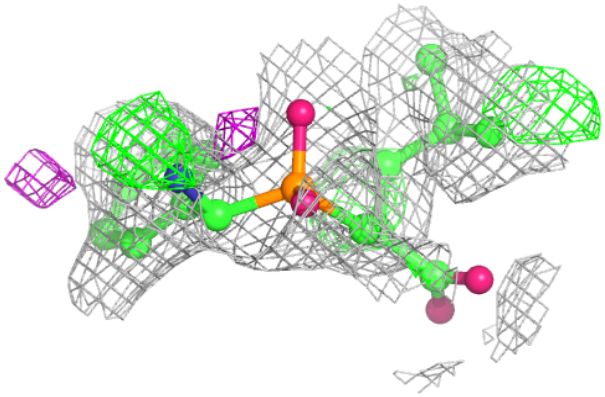


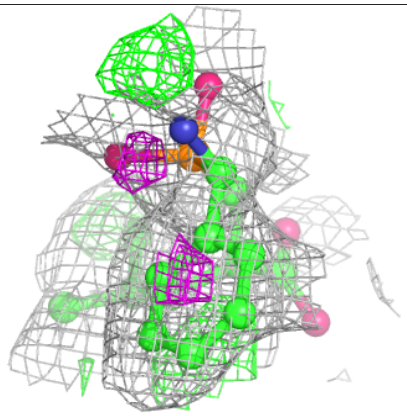


Electron density around 4ZN D 704:

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

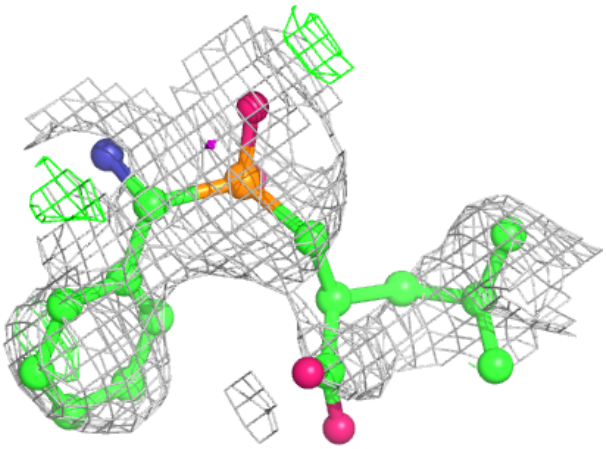


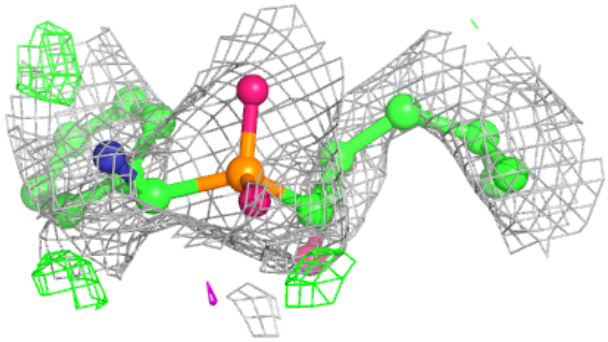




Electron density around 4ZN E 704:

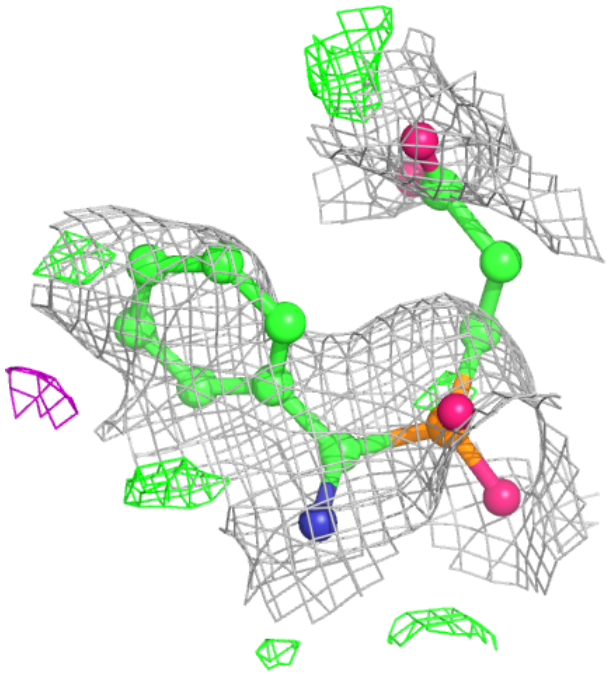
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

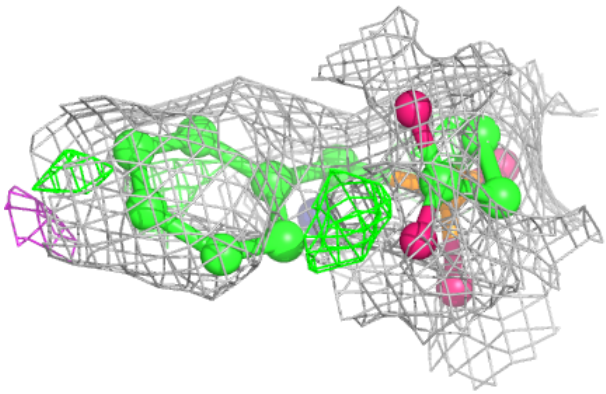


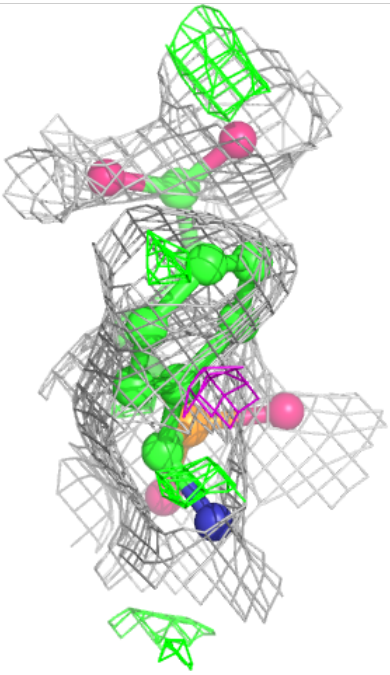


Electron density around 4ZN F 704:

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

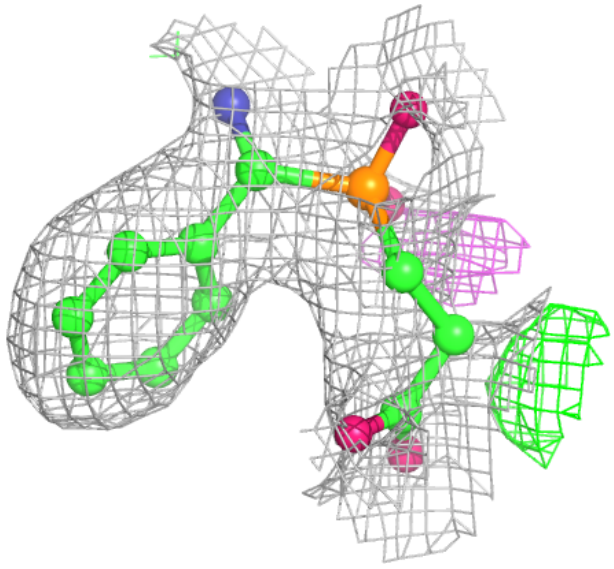


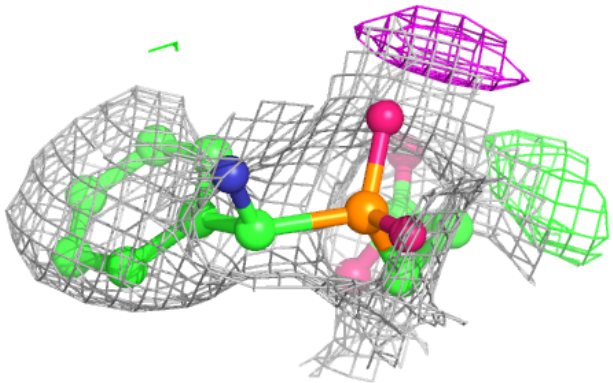


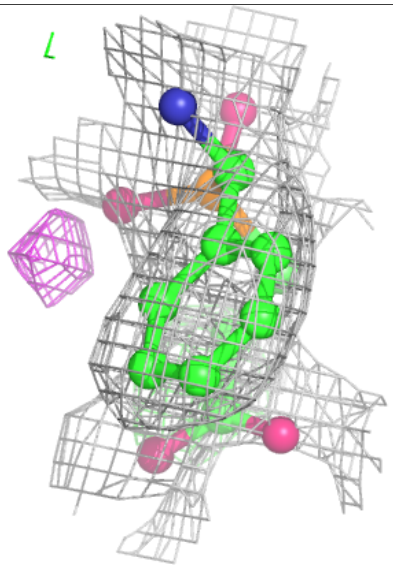


Electron density around 4ZN G 704:

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

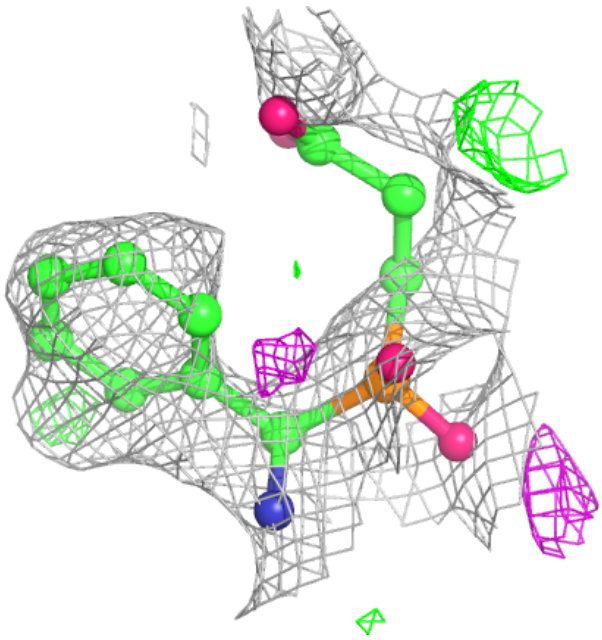


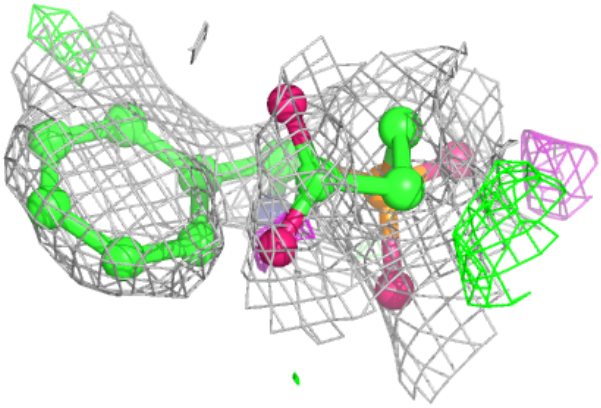


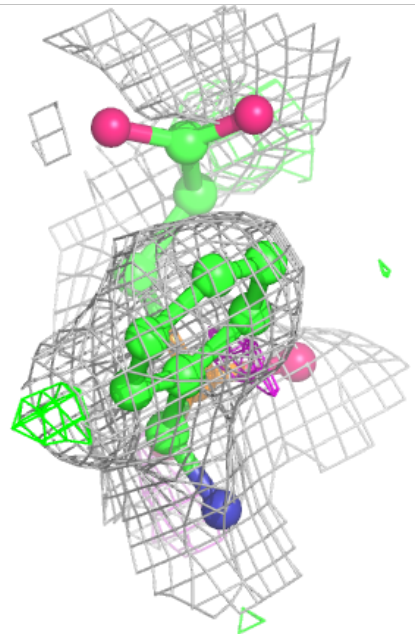


Electron density around 4ZN H 704:

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

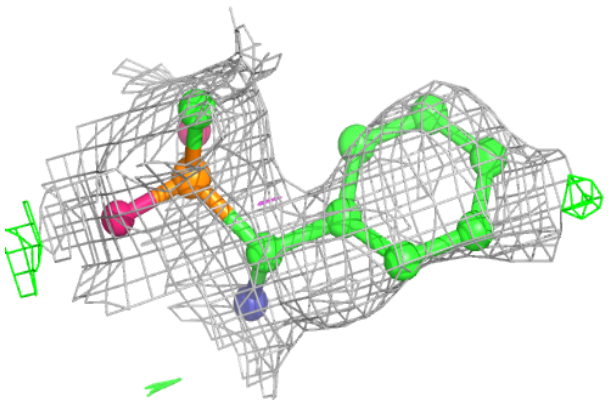


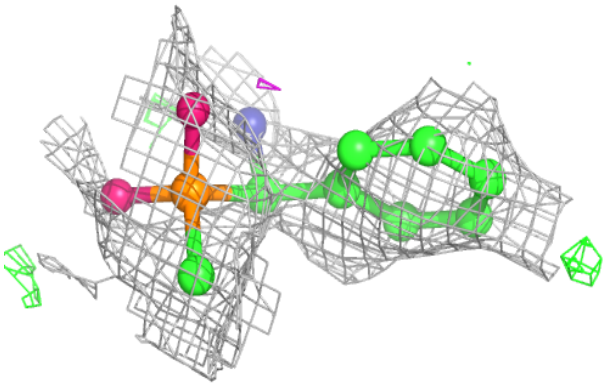


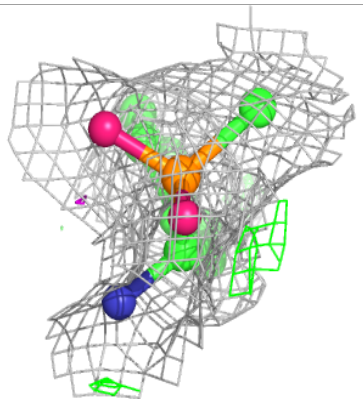


Electron density around 4ZN I 704:

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

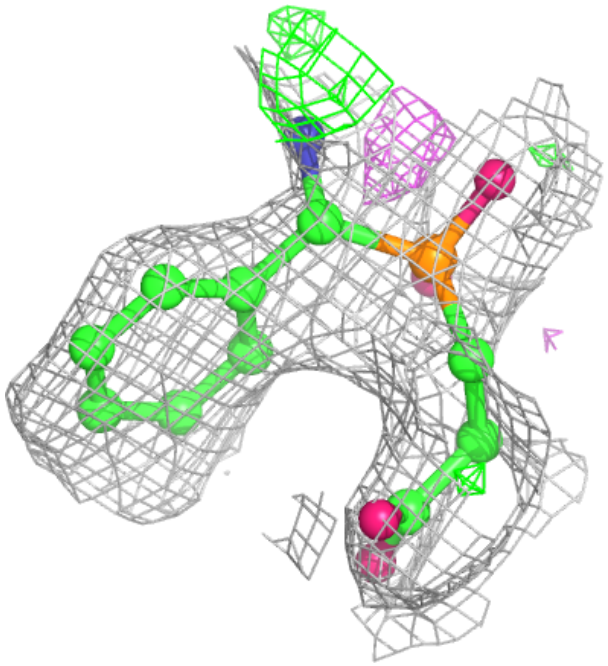


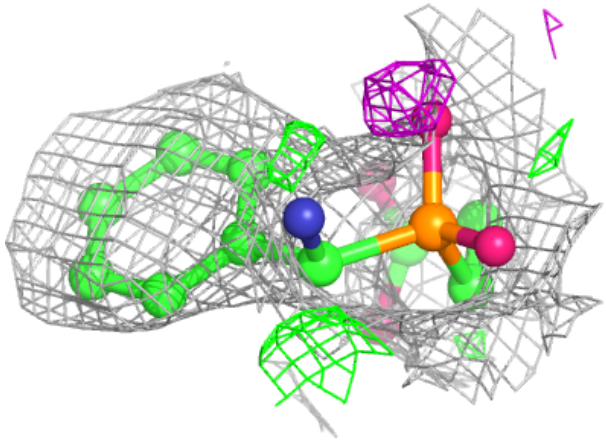


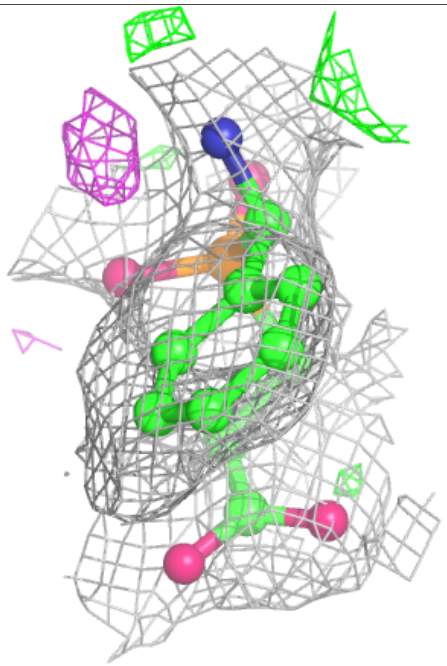


Electron density around 4ZN J 704:

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

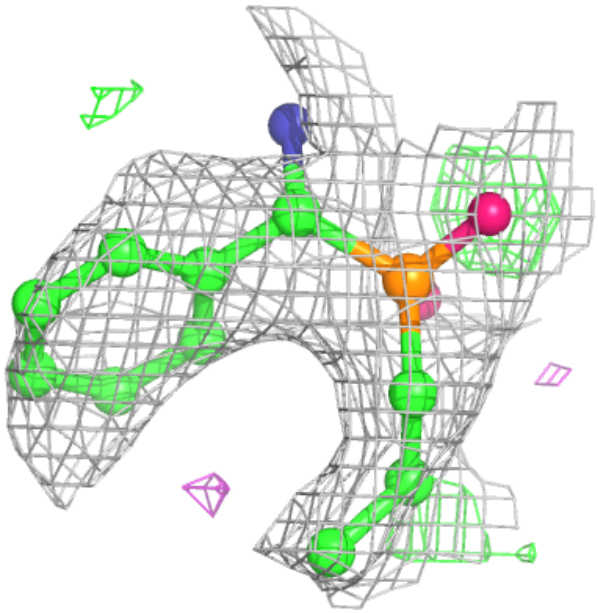


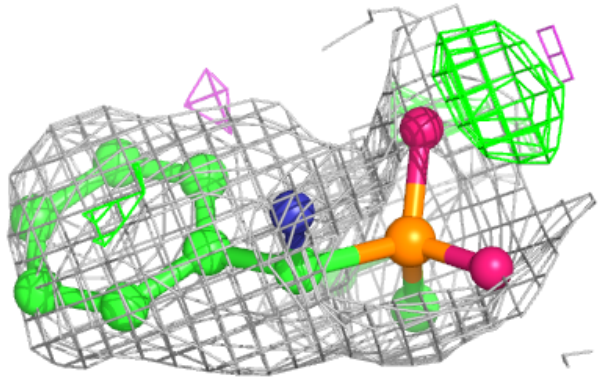


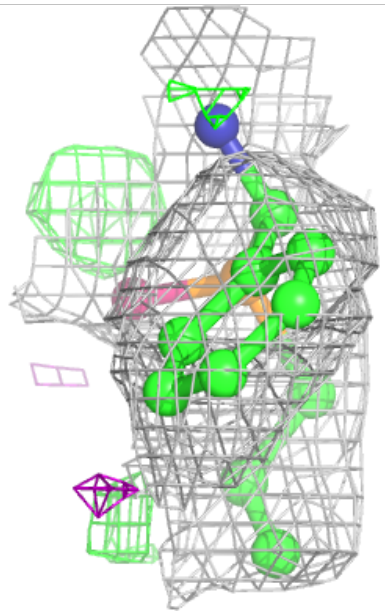


Electron density around 4ZN K 704:

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

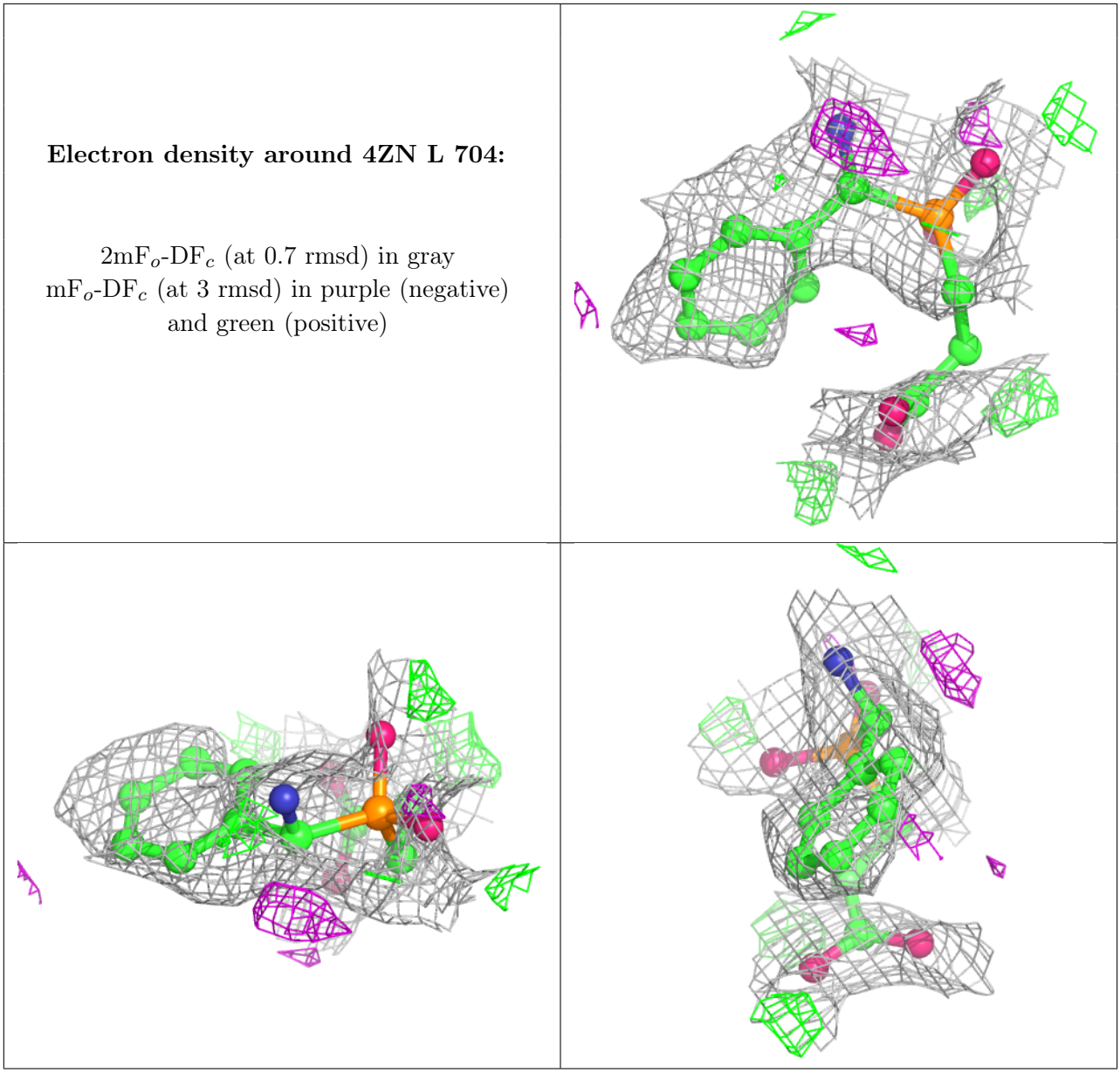






Electron density around 4ZN L 704:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.