wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 07:37 AM EDT

PDB ID	:	8EZ4
Title	:	Plasmodium falciparum M17 in complex with inhibitor 9aa
Authors	:	Calic, P.P.S.; McGowan, S.; Webb, C.T.
Deposited on	:	2022-10-31
Resolution	:	1.89 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:

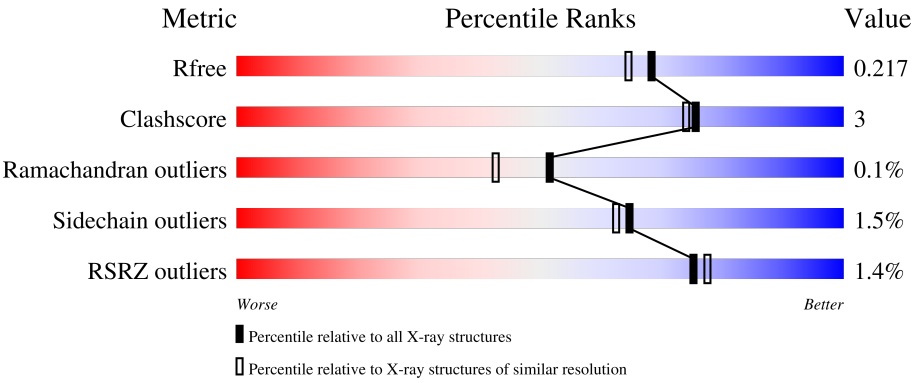
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	527	91% 7%
1	B	527	92% 6%
1	C	527	93% 7%
1	D	527	89% 9%
1	E	527	90% 7%

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Mol	Chain	Length	Quality of chain
1	F	527	91% 6%
1	G	527	91% 8%
1	H	527	94% 5%
1	I	527	94% 6%
1	J	527	92% 6%
1	K	527	93% 5%
1	L	527	89% 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
5	CO3	A	708	-	-	X	-
5	CO3	C	706	-	-	X	-
5	CO3	G	706	-	-	X	-
5	CO3	K	705	-	-	X	-
5	CO3	L	706	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 53046 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	1	0
			3993	2563	642	768	20			
1	B	521	Total	C	N	O	S	0	0	0
			3952	2542	641	749	20			
1	C	525	Total	C	N	O	S	0	2	0
			4007	2575	652	760	20			
1	D	522	Total	C	N	O	S	0	1	0
			3983	2556	647	760	20			
1	E	514	Total	C	N	O	S	0	1	0
			3917	2519	630	749	19			
1	F	515	Total	C	N	O	S	0	1	0
			3895	2502	626	748	19			
1	G	521	Total	C	N	O	S	0	1	0
			4002	2569	644	769	20			
1	H	522	Total	C	N	O	S	0	0	0
			3933	2525	639	749	20			
1	I	525	Total	C	N	O	S	0	1	0
			4017	2578	653	766	20			
1	J	519	Total	C	N	O	S	0	0	0
			3962	2545	643	754	20			
1	K	517	Total	C	N	O	S	0	0	0
			3944	2536	639	750	19			
1	L	512	Total	C	N	O	S	0	0	0
			3866	2483	622	742	19			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	conflict	UNP Q8IL11
A	515	GLN	ASN	conflict	UNP Q8IL11
A	546	GLN	ASN	conflict	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	conflict	UNP Q8IL11
B	515	GLN	ASN	conflict	UNP Q8IL11
B	546	GLN	ASN	conflict	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	conflict	UNP Q8IL11
C	515	GLN	ASN	conflict	UNP Q8IL11
C	546	GLN	ASN	conflict	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	conflict	UNP Q8IL11
D	515	GLN	ASN	conflict	UNP Q8IL11
D	546	GLN	ASN	conflict	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	conflict	UNP Q8IL11
E	515	GLN	ASN	conflict	UNP Q8IL11
E	546	GLN	ASN	conflict	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	conflict	UNP Q8IL11
F	515	GLN	ASN	conflict	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	conflict	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	conflict	UNP Q8IL11
G	515	GLN	ASN	conflict	UNP Q8IL11
G	546	GLN	ASN	conflict	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	conflict	UNP Q8IL11
H	515	GLN	ASN	conflict	UNP Q8IL11
H	546	GLN	ASN	conflict	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	conflict	UNP Q8IL11
I	515	GLN	ASN	conflict	UNP Q8IL11
I	546	GLN	ASN	conflict	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	conflict	UNP Q8IL11
J	515	GLN	ASN	conflict	UNP Q8IL11
J	546	GLN	ASN	conflict	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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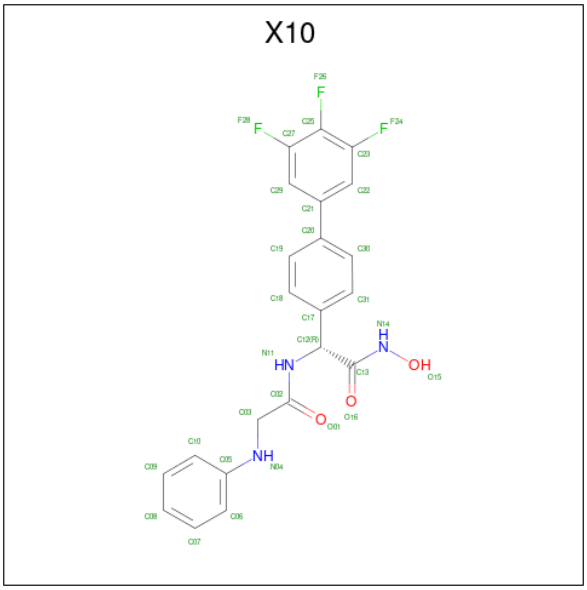
Chain	Residue	Modelled	Actual	Comment	Reference
J	611	HIS	-	expression tag	UNP Q8IL11
K	152	GLN	ASN	conflict	UNP Q8IL11
K	515	GLN	ASN	conflict	UNP Q8IL11
K	546	GLN	ASN	conflict	UNP Q8IL11
K	606	HIS	-	expression tag	UNP Q8IL11
K	607	HIS	-	expression tag	UNP Q8IL11
K	608	HIS	-	expression tag	UNP Q8IL11
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	conflict	UNP Q8IL11
L	515	GLN	ASN	conflict	UNP Q8IL11
L	546	GLN	ASN	conflict	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 N-[(1R)-2-(hydroxyamino)-2-oxo-1-(3',4',5'-trifluoro[1,1'-biphenyl]-4-yl)eth yl]-N 2 -phenylglycinamide (three-letter code: X10) (formula: $C_{22}H_{18}F_3N_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			31	22	3	3	3		

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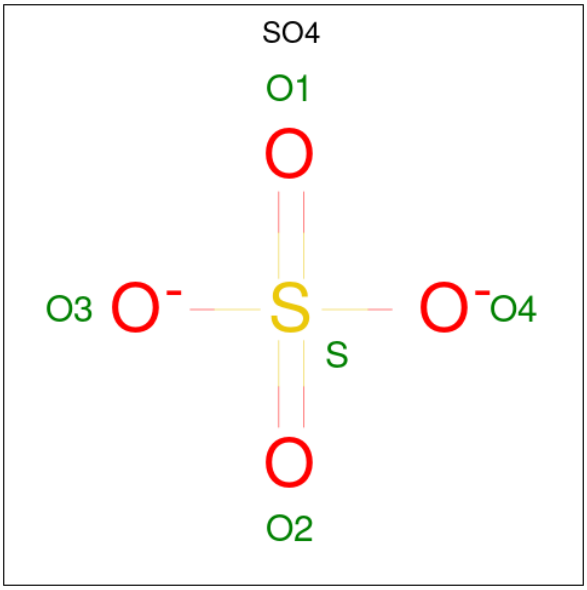
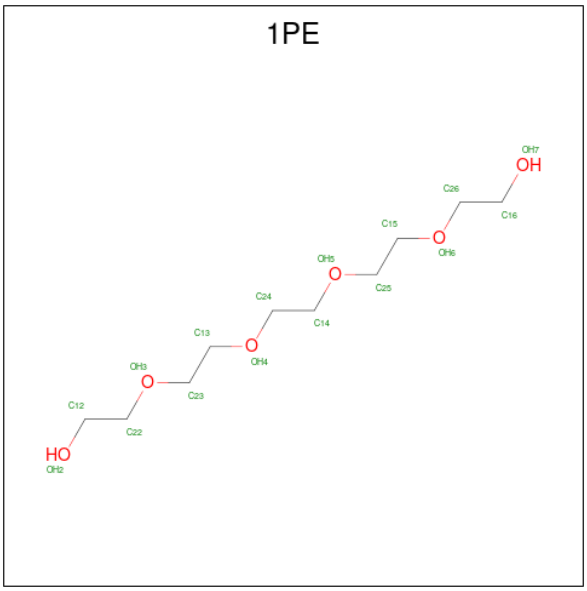
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			31	22	3	3	3		
2	C	1	Total	C	F	N	O	3	0
			31	22	3	3	3		
2	D	1	Total	C	F	N	O	1	0
			31	22	3	3	3		
2	E	1	Total	C	F	N	O	7	0
			31	22	3	3	3		
2	F	1	Total	C	F	N	O	2	0
			31	22	3	3	3		
2	G	1	Total	C	F	N	O	1	0
			31	22	3	3	3		
2	H	1	Total	C	F	N	O	5	0
			31	22	3	3	3		
2	I	1	Total	C	F	N	O	4	0
			31	22	3	3	3		
2	J	1	Total	C	F	N	O	1	0
			31	22	3	3	3		
2	K	1	Total	C	F	N	O	1	0
			31	22	3	3	3		
2	L	1	Total	C	F	N	O	1	0
			31	22	3	3	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 9 6 3	0	0
4	A	1	Total C O 12 8 4	0	0
4	A	1	Total C O 13 8 5	0	0
4	C	1	Total C O 11 7 4	0	0
4	C	1	Total C O 13 8 5	0	0
4	C	1	Total C O 8 5 3	0	0
4	D	1	Total C O 10 6 4	0	0
4	D	1	Total C O 13 8 5	0	0
4	D	1	Total C O 7 4 3	0	0
4	E	1	Total C O 11 7 4	0	0
4	E	1	Total C O 13 8 5	0	0
4	E	1	Total C O 12 8 4	0	0
4	F	1	Total C O 13 8 5	0	0
4	F	1	Total C O 10 6 4	0	0
4	F	1	Total C O 7 4 3	0	0
4	F	1	Total C O 10 6 4	0	0
4	G	1	Total C O 11 7 4	0	0
4	G	1	Total C O 7 4 3	0	0
4	H	1	Total C O 7 4 3	0	0
4	I	1	Total C O 15 10 5	0	0
4	I	1	Total C O 13 8 5	0	0
4	I	1	Total C O 8 5 3	0	0

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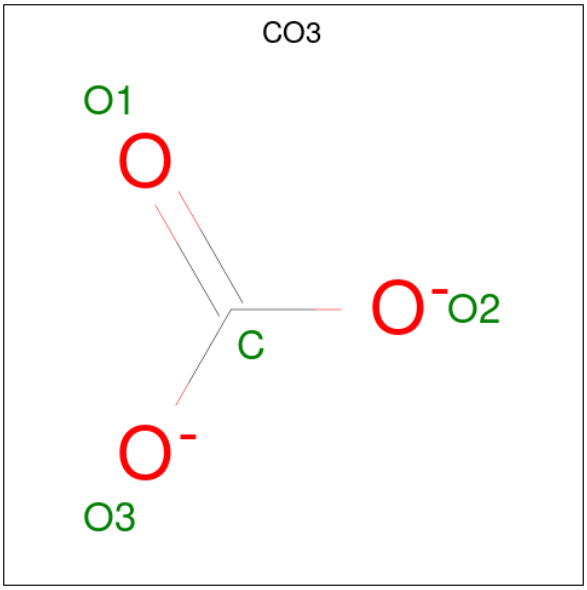
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total C O 9 6 3	0	0
4	J	1	Total C O 13 8 5	0	0
4	K	1	Total C O 13 8 5	0	0
4	K	1	Total C O 11 7 4	0	0
4	K	1	Total C O 13 8 5	0	0
4	L	1	Total C O 9 6 3	0	0
4	L	1	Total C O 13 8 5	0	0
4	L	1	Total C O 16 10 6	0	0

- Molecule 5 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



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

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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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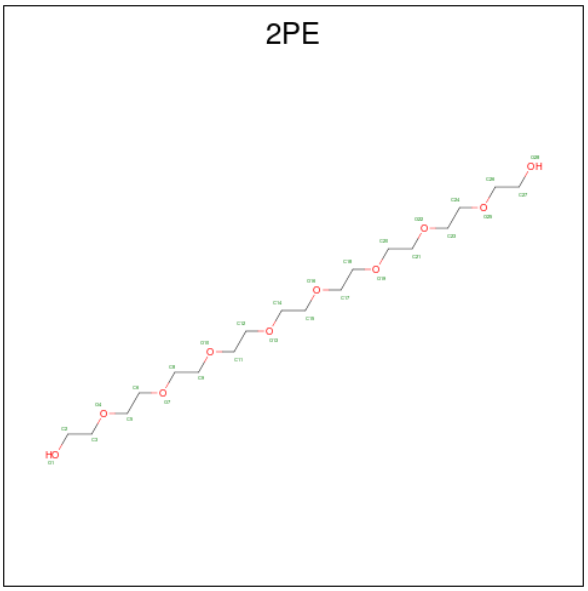
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	K	2	Total Zn 2 2	0	0
6	L	2	Total Zn 2 2	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	B	1	Total Na 1 1	0	0
7	D	1	Total Na 1 1	0	0
7	F	1	Total Na 1 1	0	0
7	G	1	Total Na 1 1	0	0
7	H	1	Total Na 1 1	0	0
7	I	1	Total Na 1 1	0	0
7	J	1	Total Na 1 1	0	0
7	K	1	Total Na 1 1	0	0

- Molecule 8 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total C O 26 17 9	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	430	Total O 430 430	0	0
9	B	349	Total O 349 349	0	0
9	C	406	Total O 406 406	0	0
9	D	386	Total O 386 386	0	0
9	E	382	Total O 382 382	0	0
9	F	371	Total O 371 371	0	0
9	G	421	Total O 421 421	0	0
9	H	360	Total O 360 360	0	0
9	I	408	Total O 408 408	0	0
9	J	413	Total O 413 413	0	0
9	K	436	Total O 436 436	0	0

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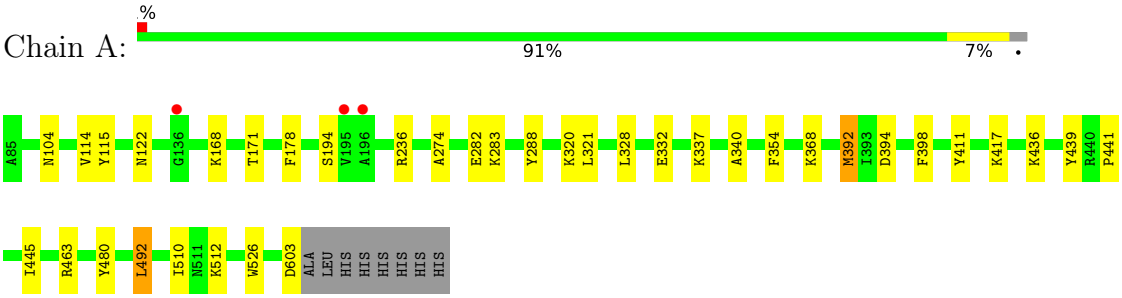
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	339	Total 339	O 339	0	0

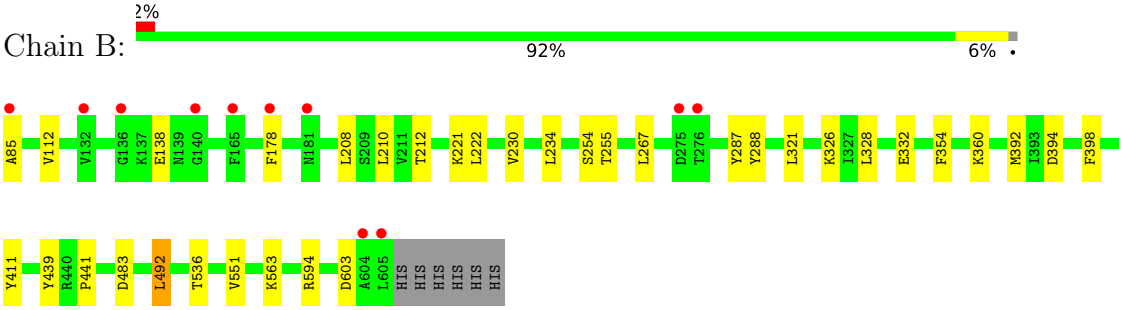
3 Residue-property plots (i)

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.

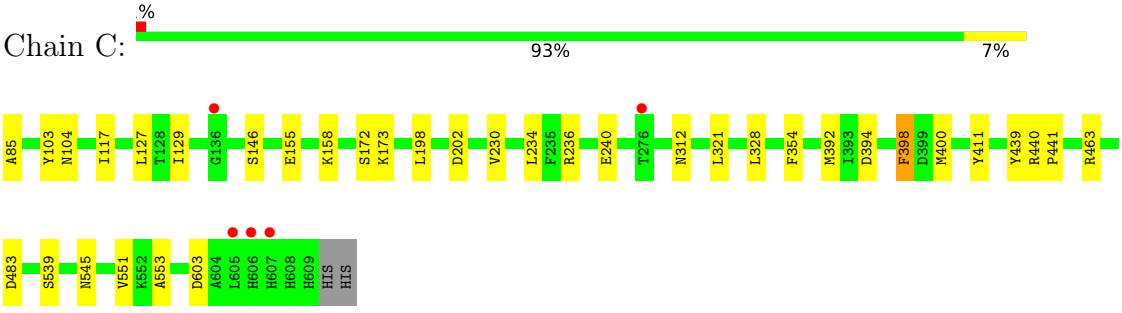
• Molecule 1: M17 leucyl aminopeptidase



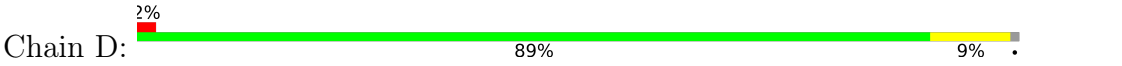
• Molecule 1: M17 leucyl aminopeptidase

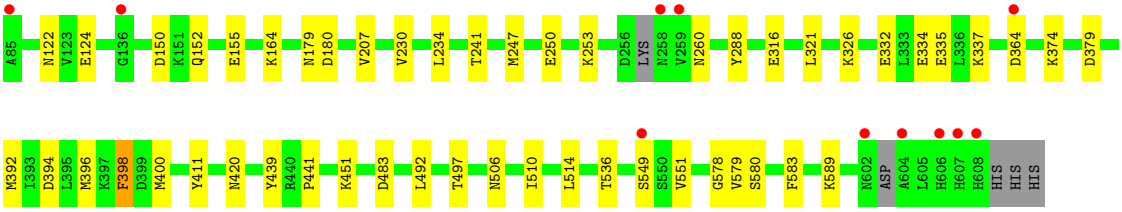


• Molecule 1: M17 leucyl aminopeptidase

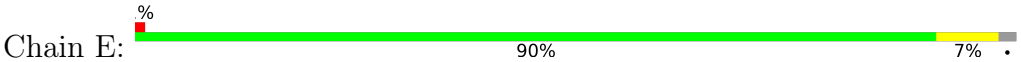


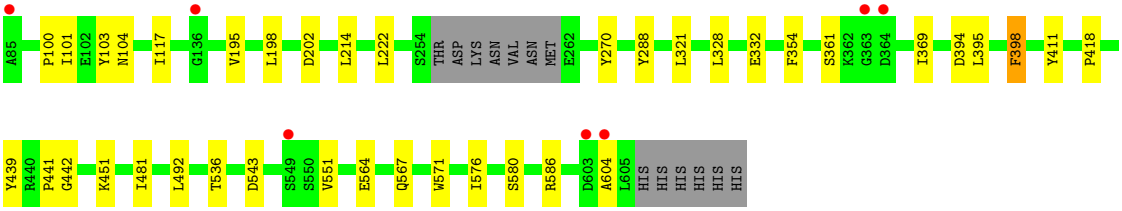
• Molecule 1: M17 leucyl aminopeptidase



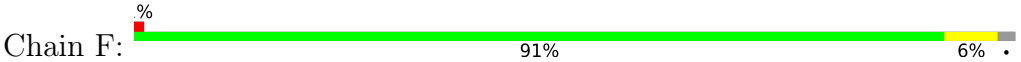


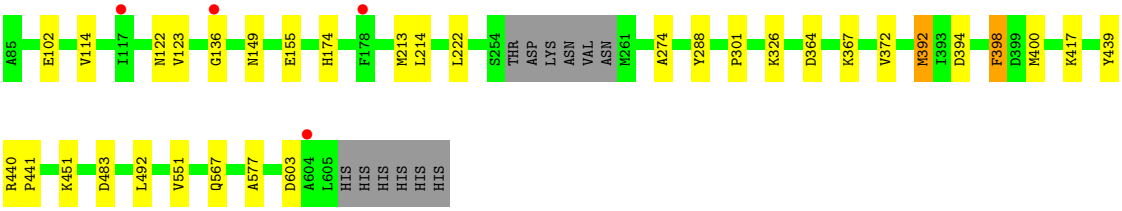
• Molecule 1: M17 leucyl aminopeptidase



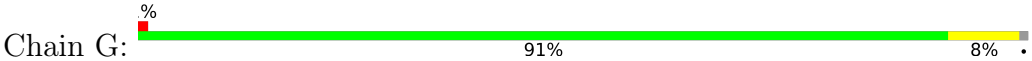


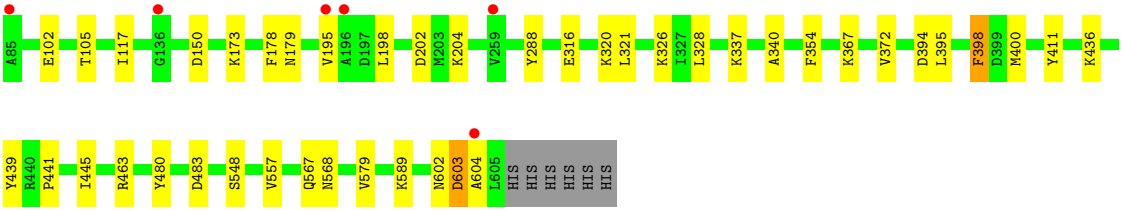
• Molecule 1: M17 leucyl aminopeptidase



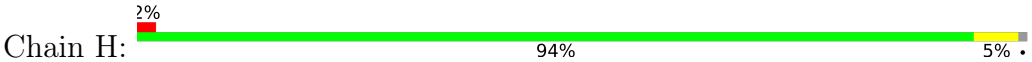


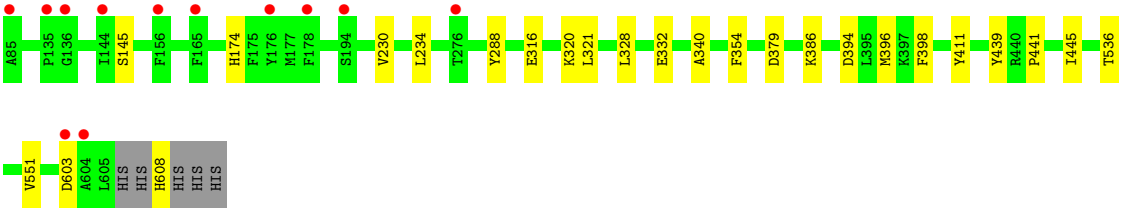
• Molecule 1: M17 leucyl aminopeptidase





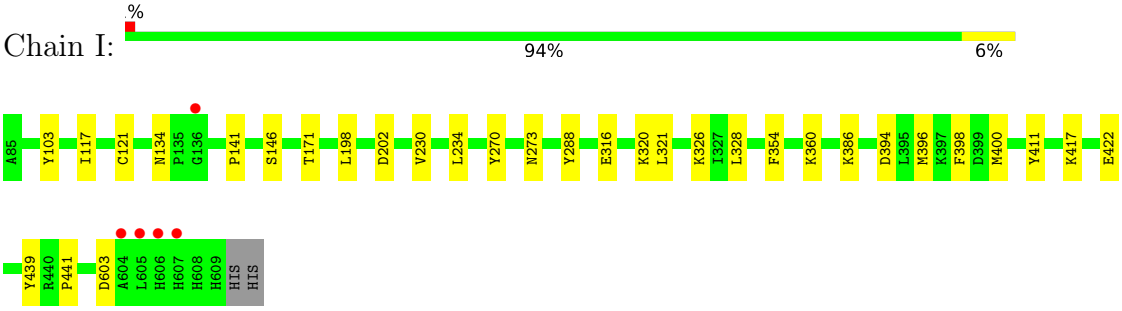
• Molecule 1: M17 leucyl aminopeptidase





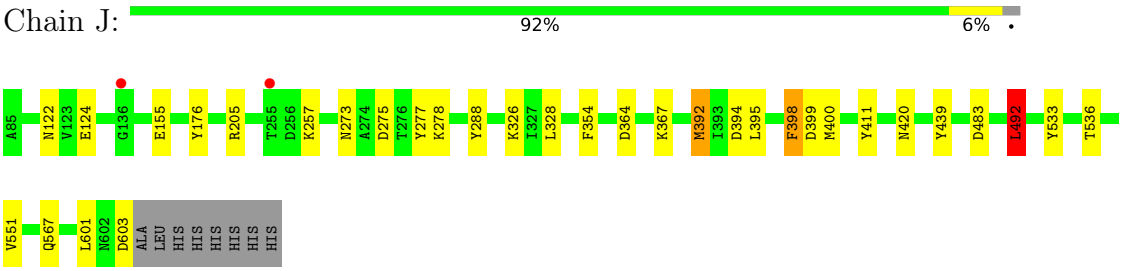
• Molecule 1: M17 leucyl aminopeptidase

Chain I:



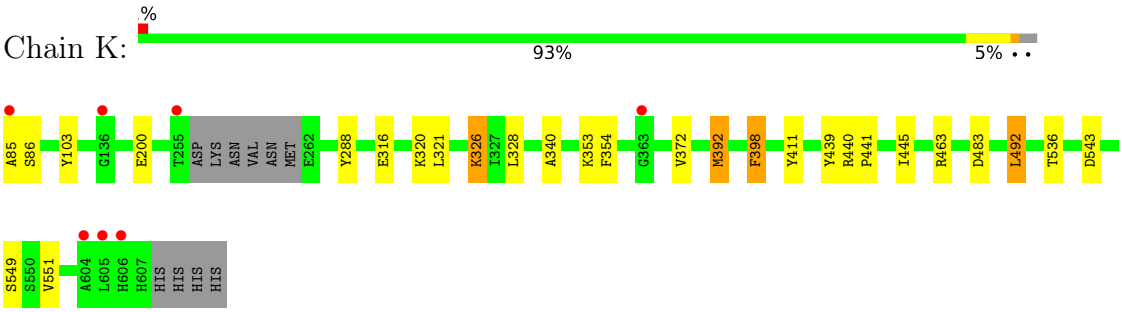
• Molecule 1: M17 leucyl aminopeptidase

Chain J:



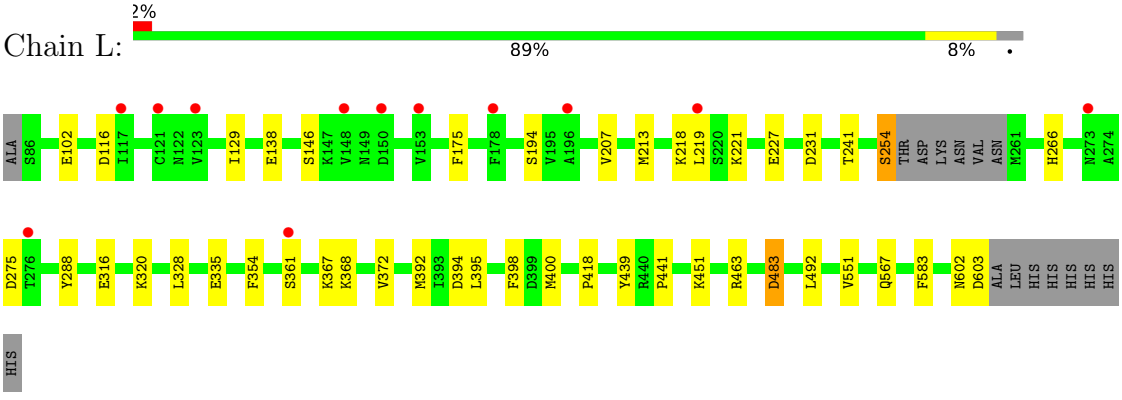
• Molecule 1: M17 leucyl aminopeptidase

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	173.94Å 176.60Å 230.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 1.89 48.47 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.47-1.89) 99.4 (48.47-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 1.90Å)	Xtriage
Refinement program	PHENIX v1.20.1-4487	Depositor
R, R_{free}	0.177 , 0.216 0.177 , 0.217	Depositor DCC
R_{free} test set	27706 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	53046	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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 41.55 % 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 2.3219e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CO3, 2PE, ZN, 1PE, SO4, X10

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	0.46	0/4074	0.64	3/5525 (0.1%)
1	B	0.46	0/4030	0.64	2/5472 (0.0%)
1	C	0.46	0/4095	0.62	1/5563 (0.0%)
1	D	0.46	0/4063	0.64	2/5513 (0.0%)
1	E	0.48	0/3997	0.63	1/5428 (0.0%)
1	F	0.45	0/3975	0.61	1/5404 (0.0%)
1	G	0.45	0/4083	0.60	0/5538
1	H	0.44	0/4011	0.59	0/5452
1	I	0.47	0/4101	0.62	2/5567 (0.0%)
1	J	0.48	0/4040	0.63	2/5480 (0.0%)
1	K	0.47	0/4023	0.64	2/5461 (0.0%)
1	L	0.46	1/3943 (0.0%)	0.60	2/5362 (0.0%)
All	All	0.46	1/48435 (0.0%)	0.62	18/65765 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	335	GLU	CB-CG	-5.76	1.41	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	392	MET	CG-SD-CE	-12.53	80.15	100.20
1	C	392	MET	CG-SD-CE	-10.36	83.62	100.20
1	A	392	MET	CG-SD-CE	-9.36	85.22	100.20
1	A	492	LEU	CB-CG-CD1	-8.57	96.43	111.00
1	E	492	LEU	CB-CG-CD1	-8.13	97.18	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3993	0	3925	36	0
1	B	3952	0	3867	21	0
1	C	4007	0	3911	21	0
1	D	3983	0	3889	34	0
1	E	3917	0	3824	26	0
1	F	3895	0	3770	24	0
1	G	4002	0	3938	25	0
1	H	3933	0	3799	16	0
1	I	4017	0	3932	18	0
1	J	3962	0	3891	24	0
1	K	3944	0	3862	22	0
1	L	3866	0	3738	37	0
2	A	31	0	0	7	0
2	B	31	0	0	2	0
2	C	31	0	0	3	0
2	D	31	0	0	5	0
2	E	31	0	0	0	0
2	F	31	0	0	4	0
2	G	31	0	0	1	0
2	H	31	0	0	1	0
2	I	31	0	0	0	0
2	J	31	0	0	4	0
2	K	31	0	0	7	0
2	L	31	0	0	3	0
3	A	15	0	0	1	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
3	E	5	0	0	1	0
3	F	5	0	0	0	0
3	G	10	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	1	0
3	J	5	0	0	0	0
3	L	5	0	0	0	0
4	A	34	0	40	7	0
4	C	32	0	38	1	0
4	D	30	0	38	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	36	0	45	5	0
4	F	40	0	52	2	0
4	G	18	0	20	0	0
4	H	7	0	9	0	0
4	I	36	0	45	3	0
4	J	22	0	25	2	0
4	K	37	0	47	3	0
4	L	38	0	47	10	0
5	A	4	0	0	3	0
5	B	4	0	0	0	0
5	C	4	0	0	2	0
5	D	4	0	0	1	0
5	E	4	0	0	0	0
5	F	4	0	0	0	0
5	G	4	0	0	2	0
5	H	4	0	0	1	0
5	I	4	0	0	0	0
5	J	4	0	0	1	0
5	K	4	0	0	2	0
5	L	4	0	0	2	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0
6	I	2	0	0	0	0
6	J	2	0	0	0	0
6	K	2	0	0	0	0
6	L	2	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
8	H	26	0	33	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	430	0	0	7	0
9	B	349	0	0	4	0
9	C	406	0	0	4	0
9	D	386	0	0	9	0
9	E	382	0	0	4	0
9	F	371	0	0	5	0
9	G	421	0	0	6	0
9	H	360	0	0	3	0
9	I	408	0	0	2	0
9	J	413	0	0	3	0
9	K	436	0	0	4	0
9	L	339	0	0	4	0
All	All	53046	0	46785	299	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 299 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:G:178:PHE:HZ	1:J:155:GLU:HG2	1.24	1.03
1:A:122:ASN:HD21	4:A:706:1PE:H251	1.28	0.97
5:D:705:CO3:O2	9:D:801:HOH:O	1.88	0.92
1:A:436:LYS:NZ	9:A:801:HOH:O	1.94	0.91
1:H:379:ASP:HB3	1:H:396:MET:HE2	1.51	0.91

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	518/527 (98%)	508 (98%)	10 (2%)	0	100	100
1	B	519/527 (98%)	506 (98%)	12 (2%)	1 (0%)	47	38
1	C	525/527 (100%)	515 (98%)	10 (2%)	0	100	100
1	D	517/527 (98%)	510 (99%)	7 (1%)	0	100	100
1	E	511/527 (97%)	504 (99%)	7 (1%)	0	100	100
1	F	512/527 (97%)	502 (98%)	9 (2%)	1 (0%)	47	38
1	G	520/527 (99%)	509 (98%)	10 (2%)	1 (0%)	47	38
1	H	519/527 (98%)	509 (98%)	10 (2%)	0	100	100
1	I	524/527 (99%)	516 (98%)	8 (2%)	0	100	100
1	J	517/527 (98%)	506 (98%)	10 (2%)	1 (0%)	47	38
1	K	513/527 (97%)	502 (98%)	10 (2%)	1 (0%)	47	38
1	L	508/527 (96%)	498 (98%)	8 (2%)	2 (0%)	34	24
All	All	6203/6324 (98%)	6085 (98%)	111 (2%)	7 (0%)	51	42

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	138	GLU
1	L	218	LYS
1	K	86	SER
1	G	604	ALA
1	J	257	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	428/454 (94%)	423 (99%)	5 (1%)	71	70
1	B	415/454 (91%)	409 (99%)	6 (1%)	67	65
1	C	424/454 (93%)	419 (99%)	5 (1%)	71	70
1	D	422/454 (93%)	415 (98%)	7 (2%)	60	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	414/454 (91%)	411 (99%)	3 (1%)	84	84
1	F	409/454 (90%)	403 (98%)	6 (2%)	65	62
1	G	429/454 (94%)	421 (98%)	8 (2%)	57	53
1	H	409/454 (90%)	403 (98%)	6 (2%)	65	62
1	I	428/454 (94%)	422 (99%)	6 (1%)	67	65
1	J	421/454 (93%)	413 (98%)	8 (2%)	57	53
1	K	418/454 (92%)	412 (99%)	6 (1%)	67	65
1	L	407/454 (90%)	398 (98%)	9 (2%)	52	47
All	All	5024/5448 (92%)	4949 (98%)	75 (2%)	65	62

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	483	ASP
1	L	400	MET
1	J	603	ASP
1	K	549	SER
1	E	398	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	272	ASN
1	G	567	GLN
1	L	567	GLN
1	J	531	ASN
1	J	567	GLN

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 101 ligands modelled in this entry, 33 are monoatomic - leaving 68 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	D	706	-	4,4,4	0.16	0	6,6,6	0.32	0
5	CO3	D	705	-	2,3,3	0.36	0	2,3,3	0.63	0
5	CO3	J	705	-	2,3,3	0.72	0	2,3,3	0.91	0
3	SO4	H	702	-	4,4,4	0.19	0	6,6,6	0.30	0
4	1PE	G	705	-	6,6,15	0.13	0	5,5,14	0.10	0
4	1PE	L	705	-	15,15,15	0.16	0	14,14,14	0.47	0
3	SO4	E	702	-	4,4,4	0.13	0	6,6,6	0.16	0
5	CO3	L	706	-	2,3,3	0.82	0	2,3,3	0.73	0
5	CO3	A	708	-	2,3,3	0.67	0	2,3,3	0.67	0
2	X10	G	701	6	33,33,33	1.92	4 (12%)	42,45,45	1.42	6 (14%)
2	X10	I	701	6	33,33,33	1.85	4 (12%)	42,45,45	1.51	7 (16%)
4	1PE	E	703	-	10,10,15	0.15	0	9,9,14	0.31	0
4	1PE	G	704	-	10,10,15	0.17	0	9,9,14	0.13	0
4	1PE	I	704	-	12,12,15	0.13	0	11,11,14	0.16	0
4	1PE	L	704	-	12,12,15	0.24	0	11,11,14	0.35	0
4	1PE	D	702	-	9,9,15	0.08	0	8,8,14	0.28	0
2	X10	F	701	6	33,33,33	1.86	4 (12%)	42,45,45	1.65	11 (26%)
4	1PE	E	705	-	11,11,15	0.21	0	10,10,14	0.14	0
4	1PE	F	703	-	12,12,15	0.24	0	11,11,14	0.20	0
4	1PE	J	703	-	8,8,15	0.26	0	7,7,14	0.18	0
4	1PE	A	706	-	11,11,15	11.03	1 (9%)	10,10,14	2.37	2 (20%)
3	SO4	A	702	-	4,4,4	0.21	0	6,6,6	0.16	0
4	1PE	C	703	-	10,10,15	0.23	0	9,9,14	0.37	0
5	CO3	C	706	-	2,3,3	0.91	0	2,3,3	0.56	0
3	SO4	I	702	-	4,4,4	0.22	0	6,6,6	0.14	0
4	1PE	I	705	-	6,6,15	0.17	0	5,5,14	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	CO3	E	706	-	2,3,3	0.66	0	2,3,3	1.60	0
5	CO3	F	707	-	2,3,3	0.59	0	2,3,3	1.92	1 (50%)
3	SO4	L	702	-	4,4,4	0.32	0	6,6,6	0.22	0
4	1PE	K	703	-	10,10,15	0.26	0	9,9,14	0.17	0
2	X10	D	701	6	33,33,33	1.78	6 (18%)	42,45,45	1.52	11 (26%)
2	X10	J	701	6	33,33,33	1.96	4 (12%)	42,45,45	1.71	9 (21%)
4	1PE	J	704	-	12,12,15	0.13	0	11,11,14	0.18	0
4	1PE	D	703	-	12,12,15	0.15	0	11,11,14	0.15	0
5	CO3	B	1402	-	2,3,3	0.33	0	2,3,3	1.54	1 (50%)
4	1PE	F	705	-	6,6,15	0.23	0	5,5,14	0.14	0
3	SO4	A	703	-	4,4,4	0.16	0	6,6,6	0.38	0
4	1PE	A	707	-	12,12,15	0.22	0	11,11,14	0.17	0
3	SO4	J	702	-	4,4,4	0.16	0	6,6,6	0.23	0
4	1PE	H	703	-	6,6,15	0.20	0	5,5,14	0.16	0
4	1PE	K	702	-	12,12,15	0.19	0	11,11,14	0.44	0
5	CO3	H	704	-	2,3,3	0.65	0	2,3,3	1.64	1 (50%)
2	X10	B	1401	6	33,33,33	1.96	5 (15%)	42,45,45	2.04	14 (33%)
5	CO3	G	706	-	2,3,3	0.51	0	2,3,3	0.97	0
2	X10	E	701	6	33,33,33	1.81	4 (12%)	42,45,45	1.86	11 (26%)
4	1PE	C	704	-	12,12,15	0.17	0	11,11,14	0.18	0
3	SO4	C	702	-	4,4,4	0.23	0	6,6,6	0.34	0
8	2PE	H	705	-	25,25,27	0.21	0	24,24,26	0.16	0
4	1PE	K	704	-	12,12,15	0.22	0	11,11,14	0.24	0
2	X10	L	701	6	33,33,33	1.92	6 (18%)	42,45,45	1.32	6 (14%)
3	SO4	G	702	-	4,4,4	0.18	0	6,6,6	0.41	0
4	1PE	I	703	-	14,14,15	0.22	0	13,13,14	0.23	0
4	1PE	F	704	-	9,9,15	0.06	0	8,8,14	0.28	0
2	X10	C	701	6	33,33,33	1.99	5 (15%)	42,45,45	1.87	13 (30%)
3	SO4	F	702	-	4,4,4	0.19	0	6,6,6	0.15	0
4	1PE	L	703	-	8,8,15	0.24	0	7,7,14	0.13	0
5	CO3	K	705	-	2,3,3	0.89	0	2,3,3	0.76	0
2	X10	K	701	6	33,33,33	1.97	5 (15%)	42,45,45	1.99	14 (33%)
4	1PE	F	706	-	9,9,15	0.18	0	8,8,14	0.10	0
4	1PE	C	705	-	6,6,15	0.19	0	5,5,14	0.13	0
3	SO4	G	703	-	4,4,4	0.20	0	6,6,6	0.16	0
3	SO4	A	704	-	4,4,4	0.19	0	6,6,6	0.17	0
2	X10	H	701	6	33,33,33	1.79	4 (12%)	42,45,45	1.29	3 (7%)
4	1PE	D	704	-	6,6,15	0.29	0	5,5,14	0.19	0
5	CO3	I	706	-	2,3,3	0.64	0	2,3,3	1.59	0
2	X10	A	701	6	33,33,33	1.91	4 (12%)	42,45,45	1.74	11 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	1PE	A	705	-	8,8,15	0.26	0	7,7,14	0.14	0
4	1PE	E	704	-	12,12,15	0.20	0	11,11,14	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1PE	G	705	-	-	3/4/4/13	-
4	1PE	L	705	-	-	7/13/13/13	-
2	X10	G	701	6	-	4/23/23/23	0/3/3/3
2	X10	I	701	6	-	4/23/23/23	0/3/3/3
4	1PE	E	703	-	-	5/8/8/13	-
4	1PE	G	704	-	-	2/8/8/13	-
4	1PE	I	704	-	-	2/10/10/13	-
4	1PE	L	704	-	-	9/10/10/13	-
4	1PE	D	702	-	-	1/7/7/13	-
2	X10	F	701	6	-	4/23/23/23	0/3/3/3
4	1PE	E	705	-	-	2/9/9/13	-
4	1PE	F	703	-	-	5/10/10/13	-
4	1PE	J	703	-	-	5/6/6/13	-
4	1PE	A	706	-	-	6/9/9/13	-
4	1PE	C	703	-	-	4/8/8/13	-
4	1PE	I	705	-	-	0/4/4/13	-
4	1PE	K	703	-	-	3/8/8/13	-
2	X10	D	701	6	-	4/23/23/23	0/3/3/3
2	X10	J	701	6	-	5/23/23/23	0/3/3/3
4	1PE	J	704	-	-	5/10/10/13	-
4	1PE	D	703	-	-	3/10/10/13	-
4	1PE	F	705	-	-	0/4/4/13	-
4	1PE	A	707	-	-	5/10/10/13	-
4	1PE	H	703	-	-	2/4/4/13	-
4	1PE	K	702	-	-	3/10/10/13	-
2	X10	B	1401	6	-	4/23/23/23	0/3/3/3
2	X10	E	701	6	-	4/23/23/23	0/3/3/3
4	1PE	C	704	-	-	2/10/10/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2PE	H	705	-	-	13/23/23/25	-
4	1PE	K	704	-	-	2/10/10/13	-
2	X10	L	701	6	-	0/23/23/23	0/3/3/3
4	1PE	I	703	-	-	2/12/12/13	-
4	1PE	F	704	-	-	1/7/7/13	-
2	X10	C	701	6	-	4/23/23/23	0/3/3/3
4	1PE	L	703	-	-	5/6/6/13	-
2	X10	K	701	6	-	0/23/23/23	0/3/3/3
4	1PE	F	706	-	-	3/7/7/13	-
4	1PE	C	705	-	-	2/4/4/13	-
2	X10	H	701	6	-	4/23/23/23	0/3/3/3
4	1PE	D	704	-	-	4/4/4/13	-
2	X10	A	701	6	-	0/23/23/23	0/3/3/3
4	1PE	A	705	-	-	6/6/6/13	-
4	1PE	E	704	-	-	8/10/10/13	-

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	706	1PE	OH4-C13	36.59	3.00	1.42
2	G	701	X10	C13-N14	8.57	1.45	1.33
2	C	701	X10	C13-N14	8.47	1.45	1.33
2	K	701	X10	C13-N14	8.27	1.44	1.33
2	J	701	X10	C13-N14	8.24	1.44	1.33

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	701	X10	C22-C21-C20	-6.51	110.09	120.86
4	A	706	1PE	OH4-C13-C23	6.28	138.71	110.39
2	B	1401	X10	C22-C21-C20	-6.09	110.80	120.86
2	C	701	X10	C29-C21-C20	-5.54	111.70	120.86
2	E	701	X10	C29-C21-C20	-5.27	112.15	120.86

There are no chirality outliers.

5 of 157 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	705	1PE	C14-C24-OH4-C13

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Mol	Chain	Res	Type	Atoms
8	H	705	2PE	C21-C20-O19-C18
2	H	701	X10	C19-C20-C21-C29
4	D	704	1PE	OH4-C13-C23-OH3
2	H	701	X10	C19-C20-C21-C22

There are no ring outliers.

38 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	705	CO3	1	0
5	J	705	CO3	1	0
4	L	705	1PE	6	0
3	E	702	SO4	1	0
5	L	706	CO3	2	0
5	A	708	CO3	3	0
2	G	701	X10	1	0
4	E	703	1PE	1	0
4	I	704	1PE	2	0
4	L	704	1PE	4	0
2	F	701	X10	4	0
4	F	703	1PE	2	0
4	J	703	1PE	2	0
4	A	706	1PE	4	0
4	C	703	1PE	1	0
5	C	706	CO3	2	0
3	I	702	SO4	1	0
4	K	703	1PE	1	0
2	D	701	X10	5	0
2	J	701	X10	4	0
4	D	703	1PE	1	0
4	A	707	1PE	3	0
4	K	702	1PE	2	0
5	H	704	CO3	1	0
2	B	1401	X10	2	0
5	G	706	CO3	2	0
3	C	702	SO4	1	0
8	H	705	2PE	4	0
2	L	701	X10	3	0
4	I	703	1PE	2	0
2	C	701	X10	3	0
5	K	705	CO3	2	0
2	K	701	X10	7	0

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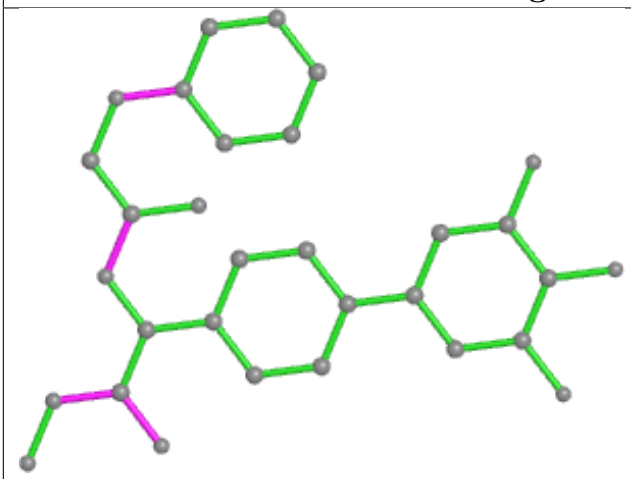
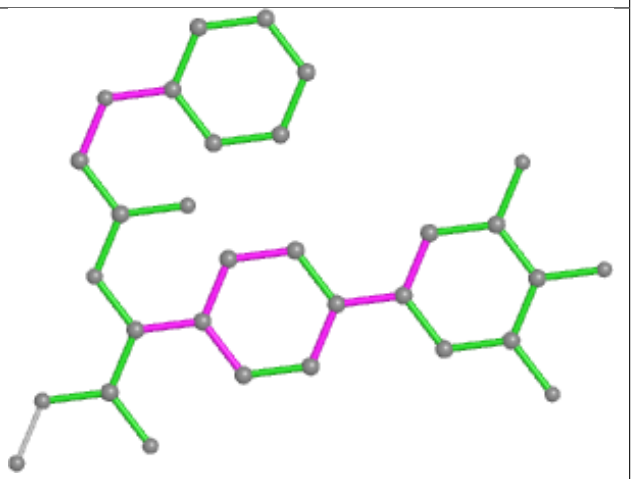
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	704	SO4	1	0
2	H	701	X10	1	0
4	D	704	1PE	1	0
2	A	701	X10	7	0
4	E	704	1PE	4	0

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.

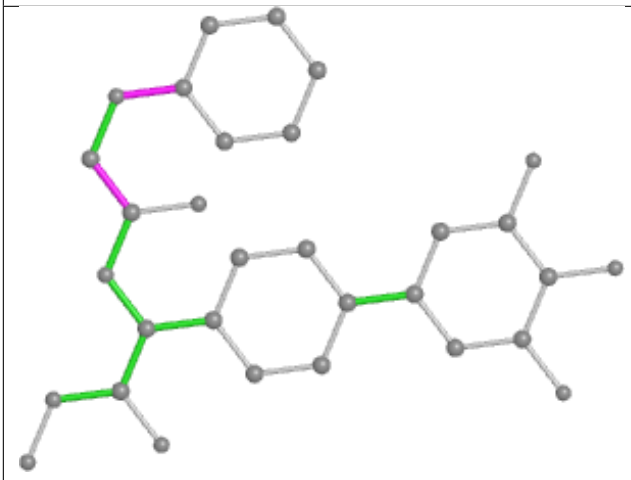
Ligand X10 G 701



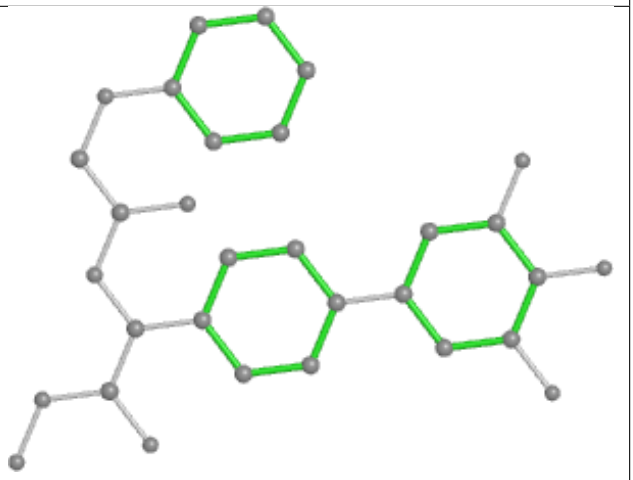
Bond lengths



Bond angles

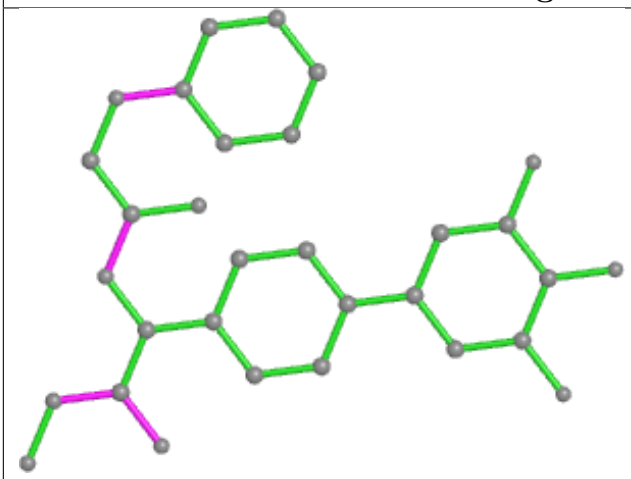


Torsions



Rings

Ligand X10 I 701



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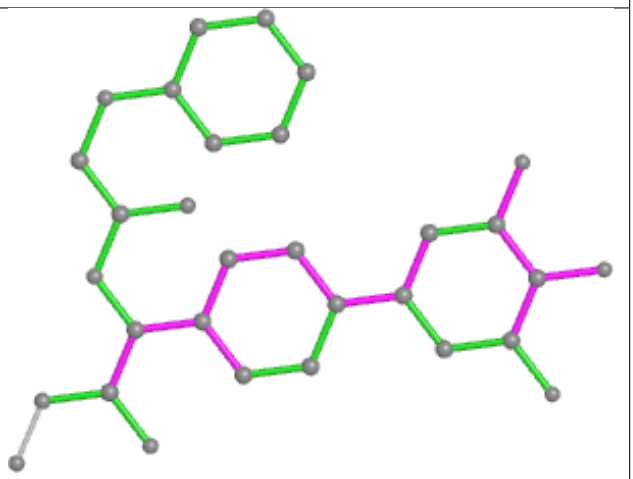

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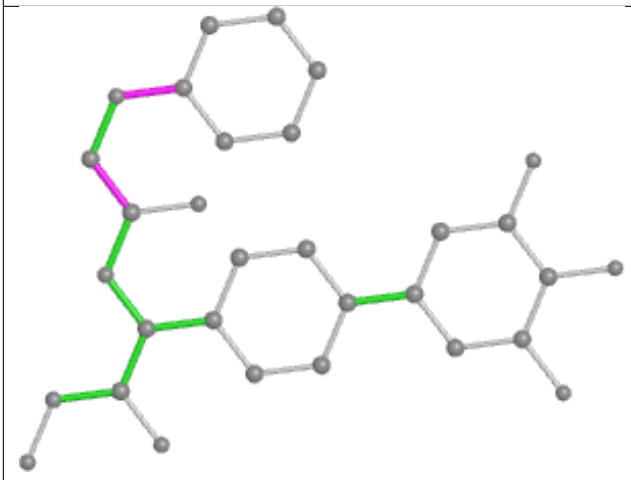

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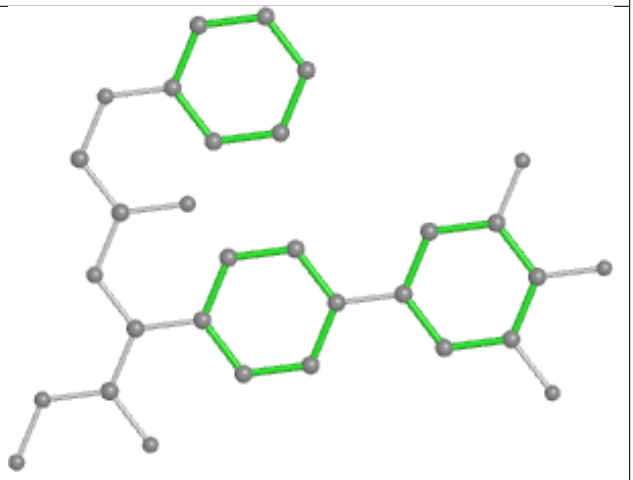
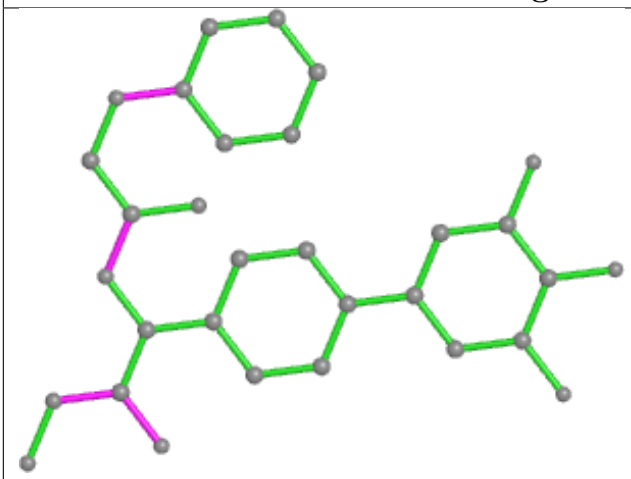
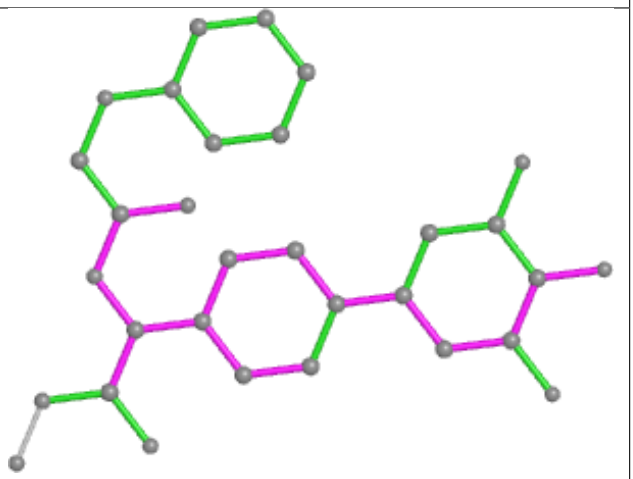


Rings

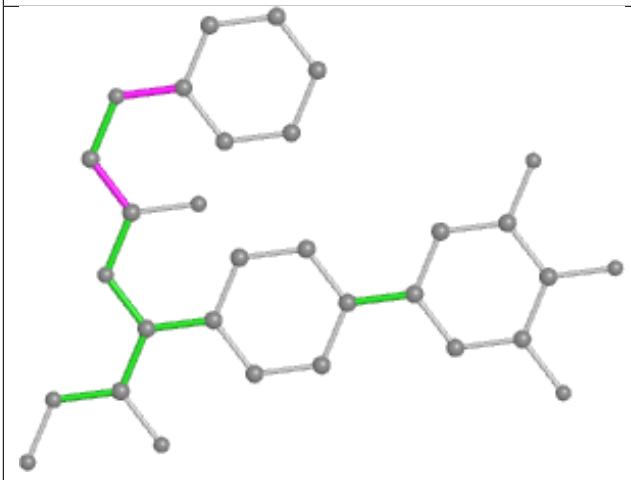
Ligand X10 F 701



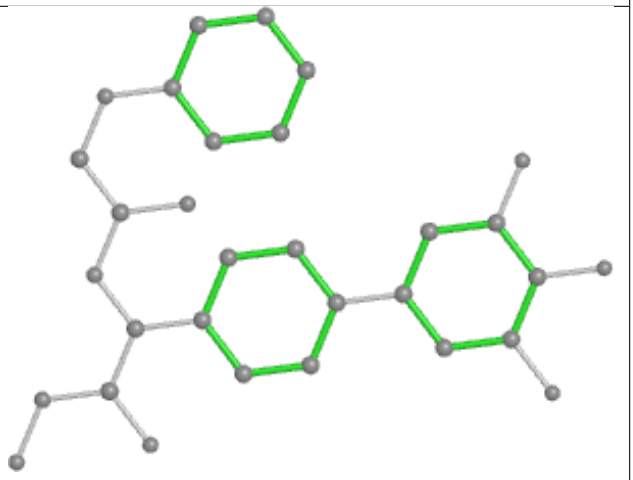
Bond lengths



Bond angles

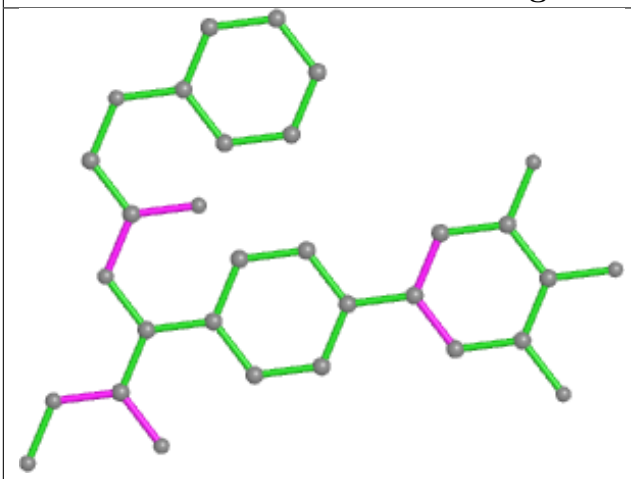


Torsions

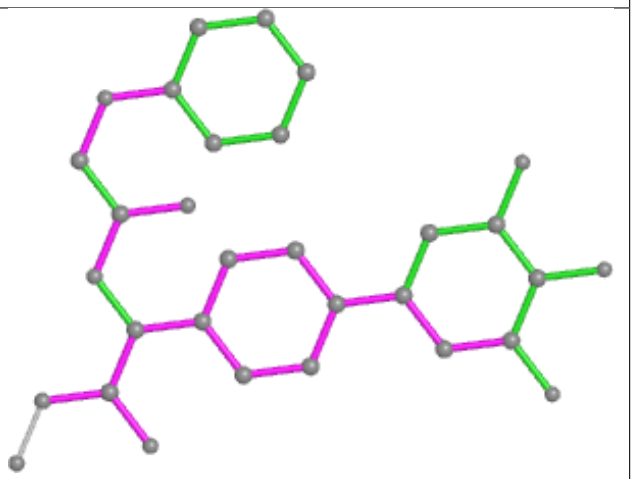


Rings

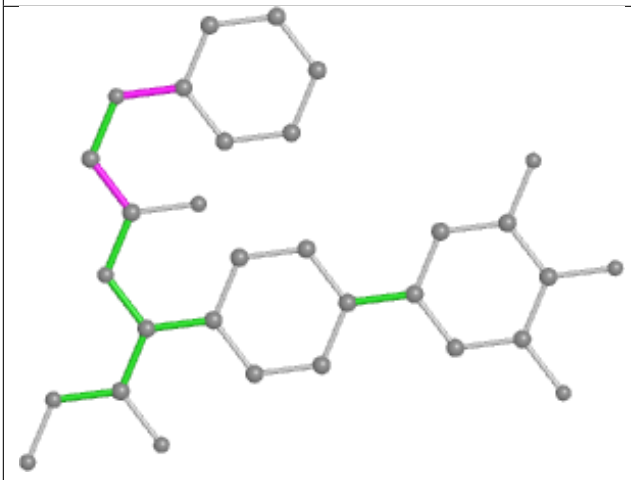
Ligand X10 D 701



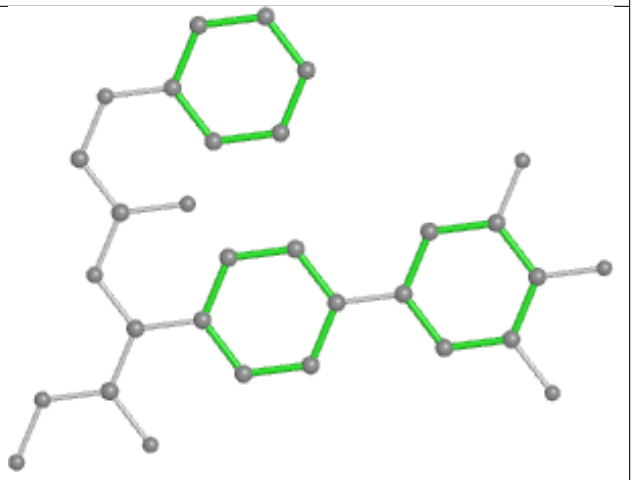
Bond lengths



Bond angles

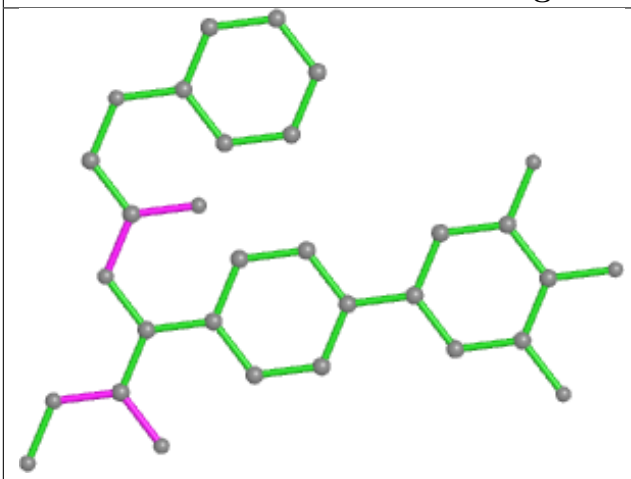


Torsions



Rings

Ligand X10 J 701



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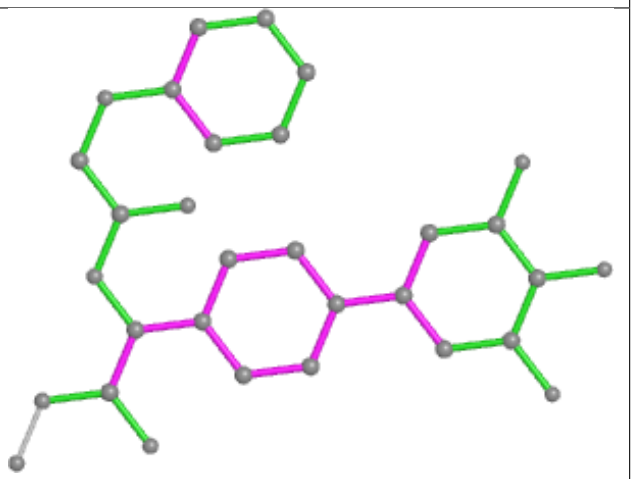
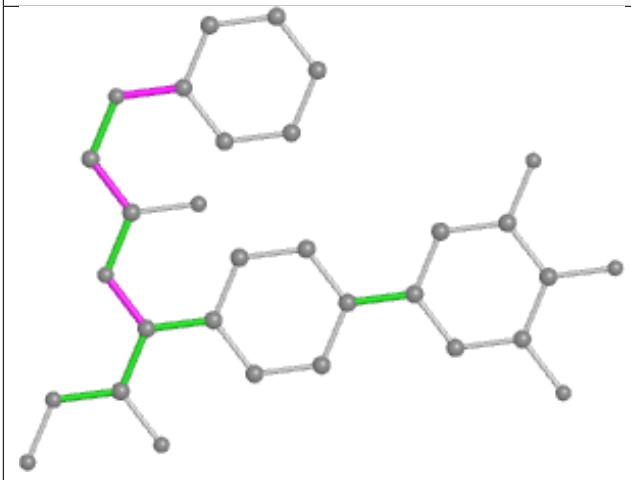


Bond angles



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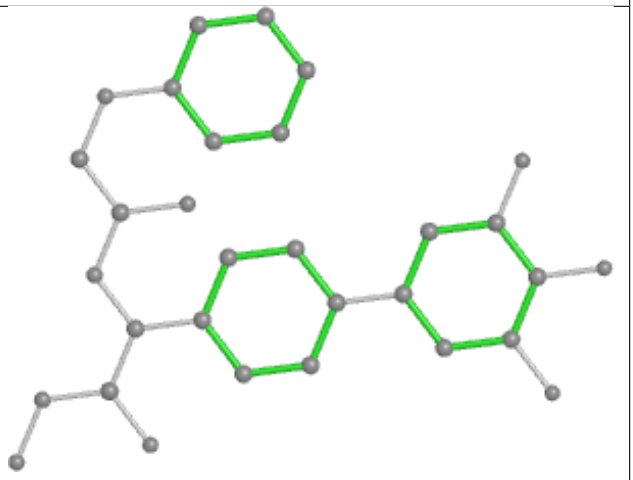
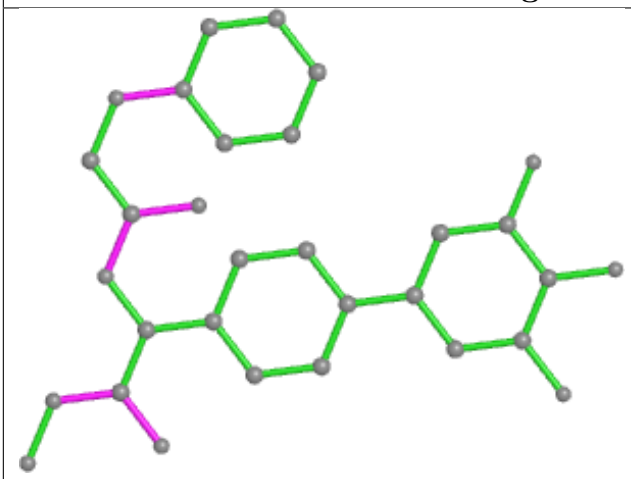
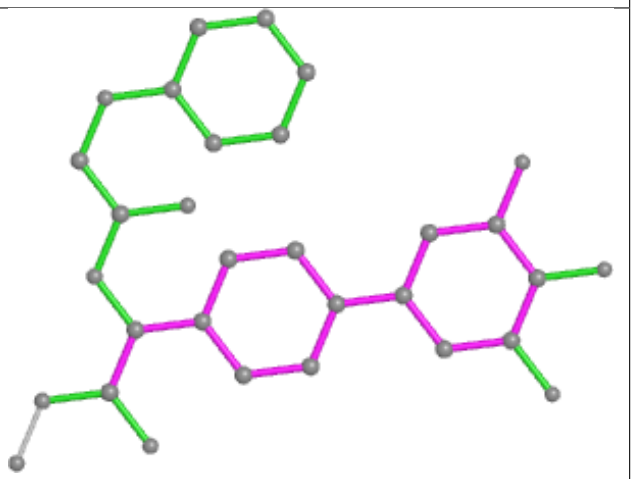


Rings

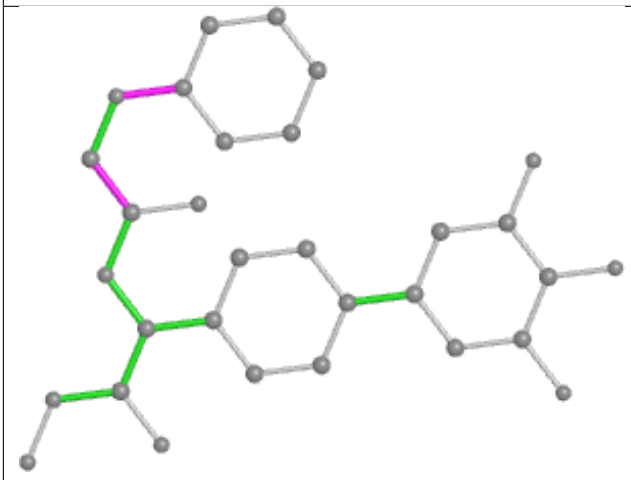
Ligand X10 B 1401



Bond lengths



Bond angles



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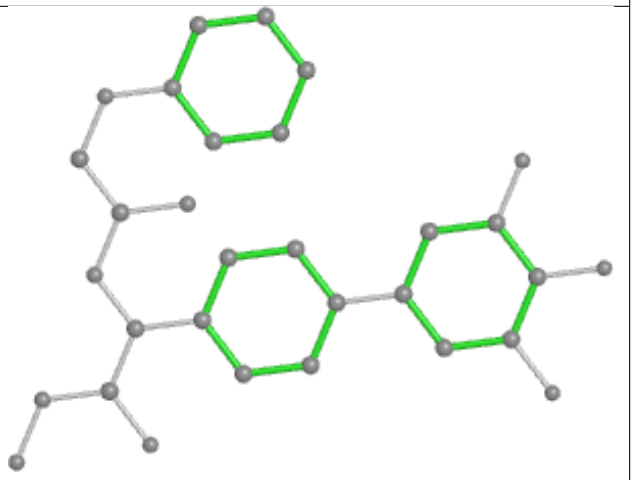
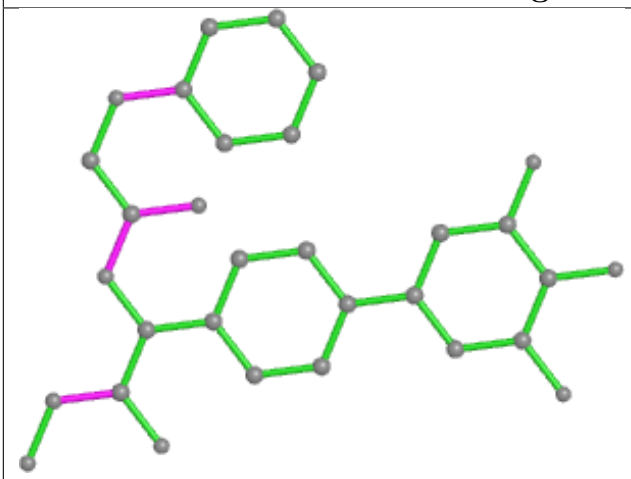
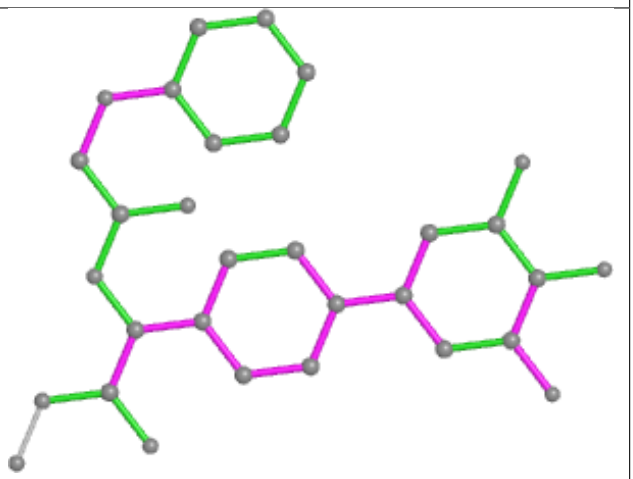


Rings

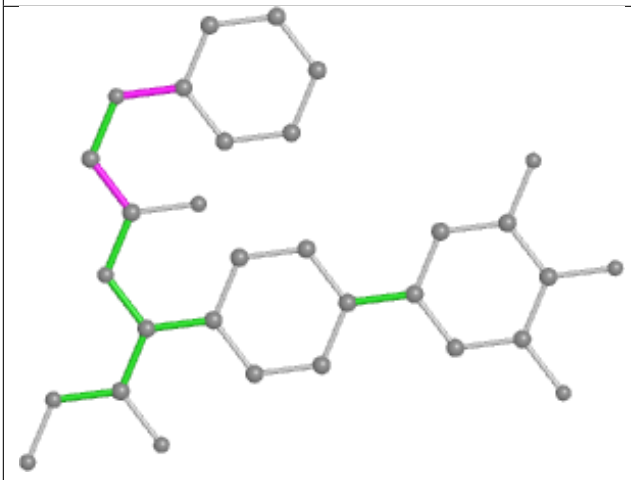
Ligand X10 E 701



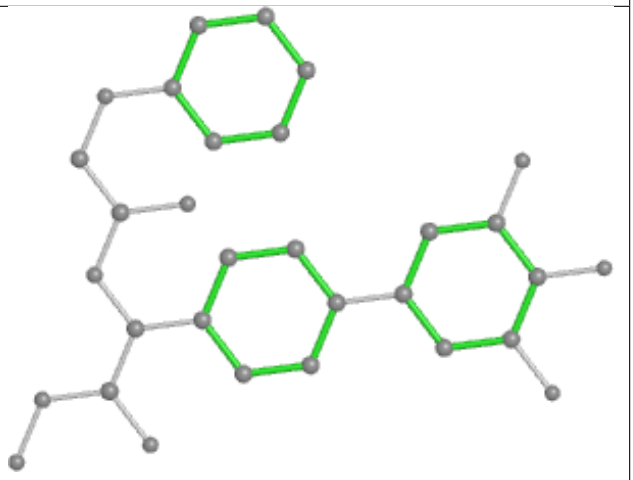
Bond lengths



Bond angles

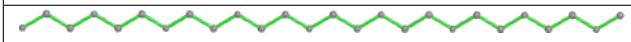


Torsions

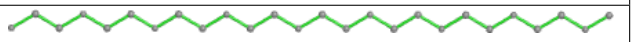


Rings

Ligand 2PE H 705



Bond lengths

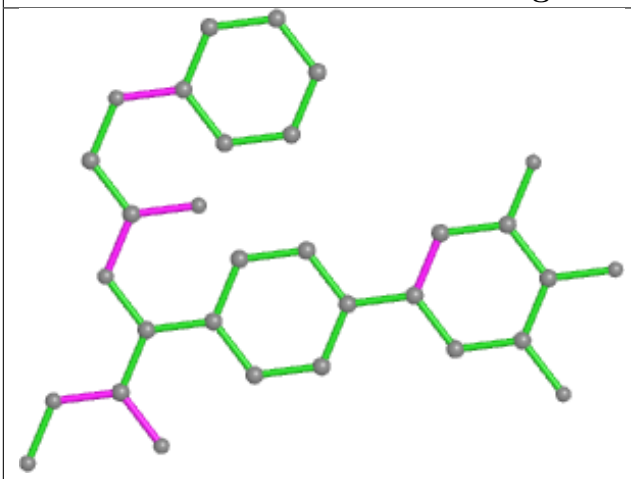


Bond angles

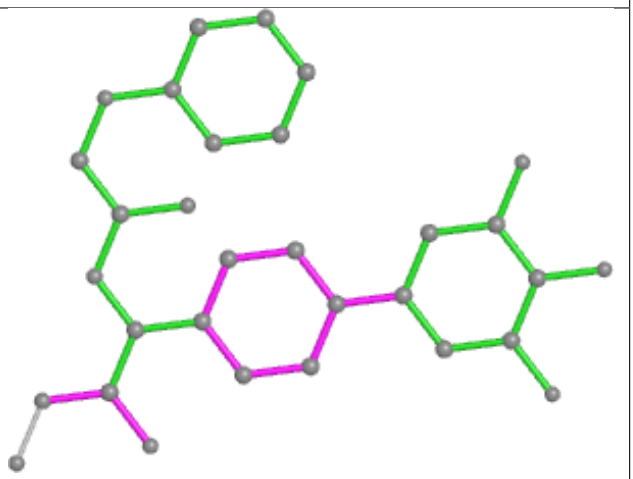
Torsions

Rings

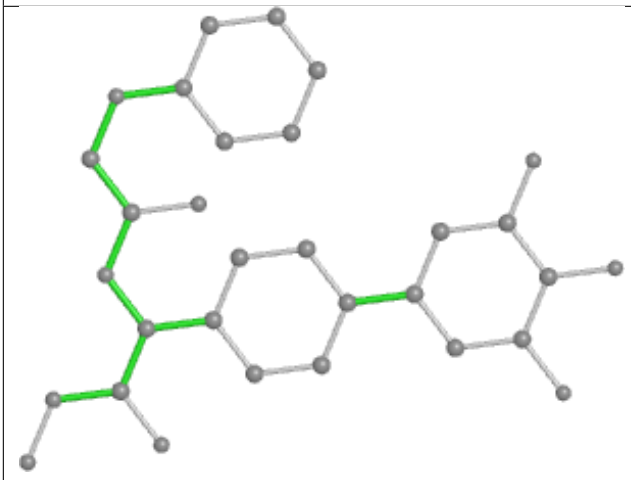
Ligand X10 L 701



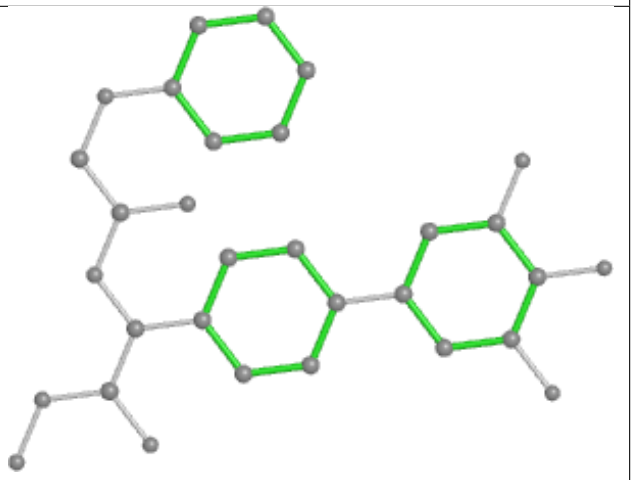
Bond lengths



Bond angles

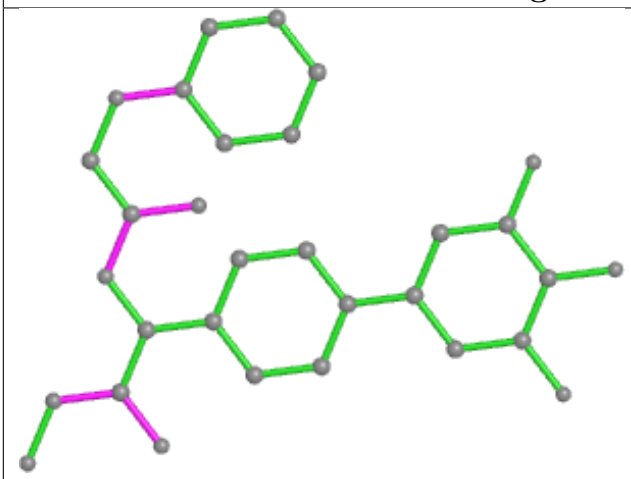


Torsions

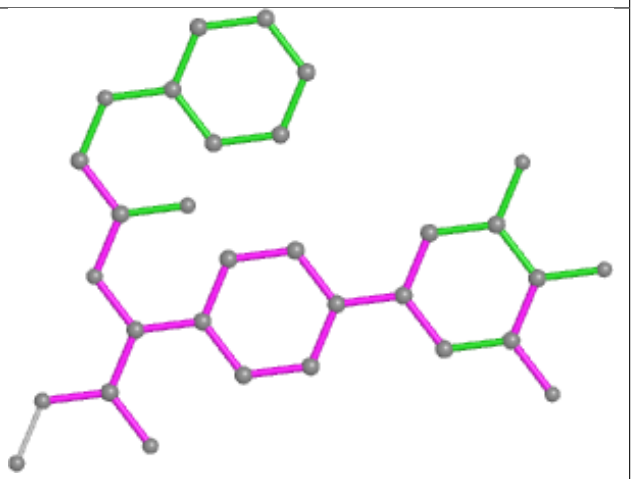


Rings

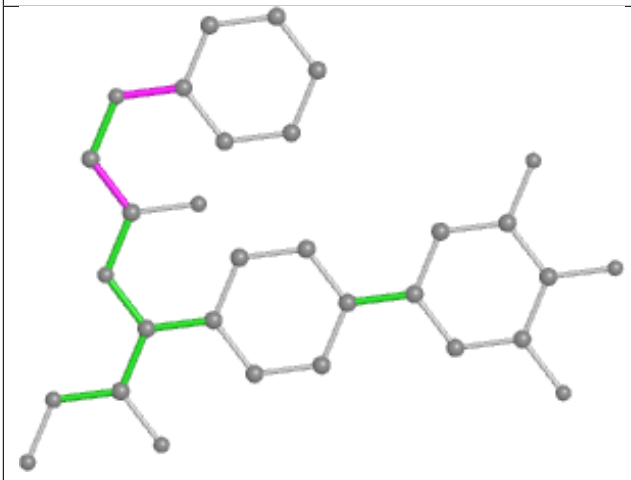
Ligand X10 C 701



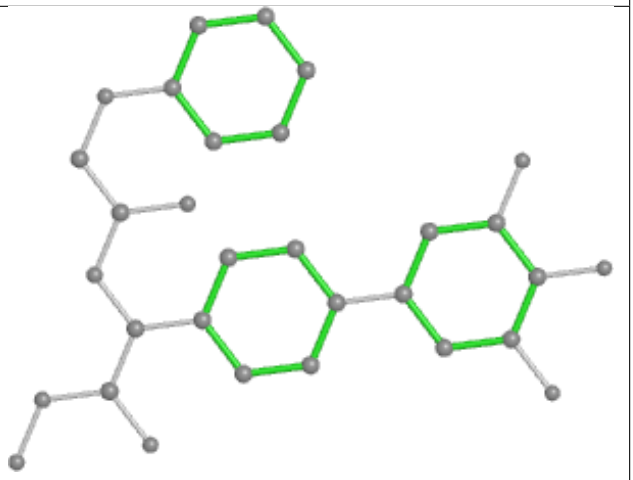
Bond lengths



Bond angles

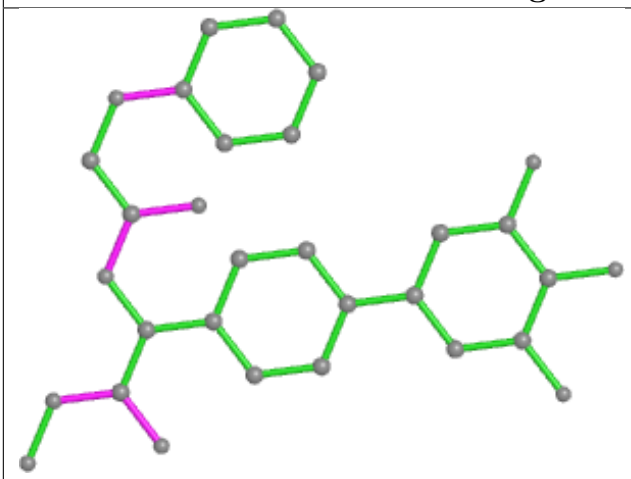


Torsions

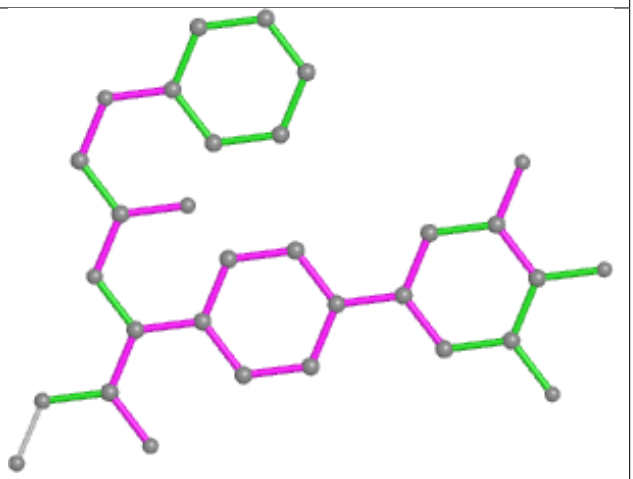


Rings

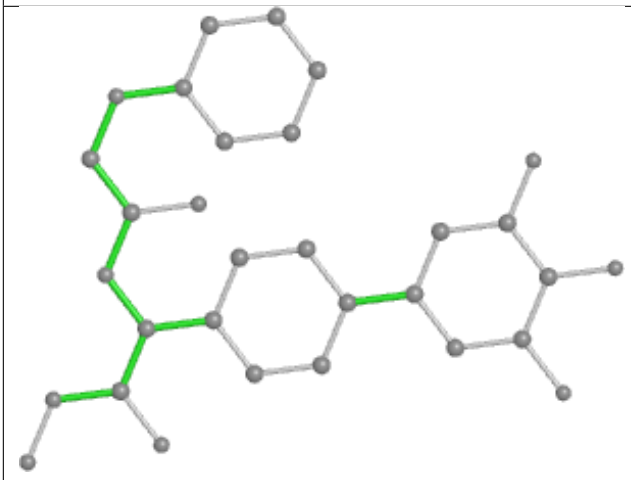
Ligand X10 K 701



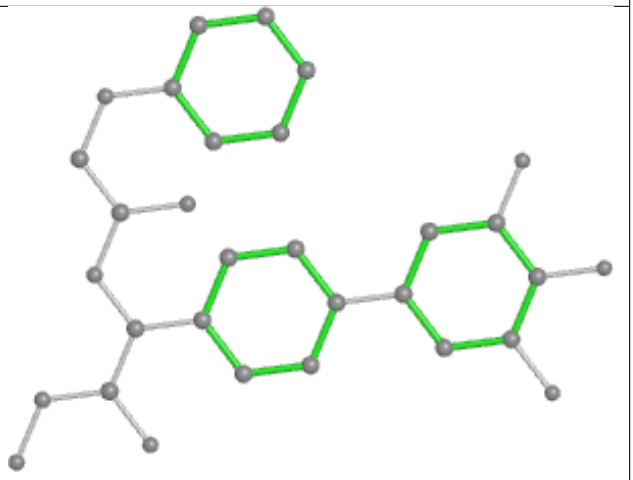
Bond lengths



Bond angles

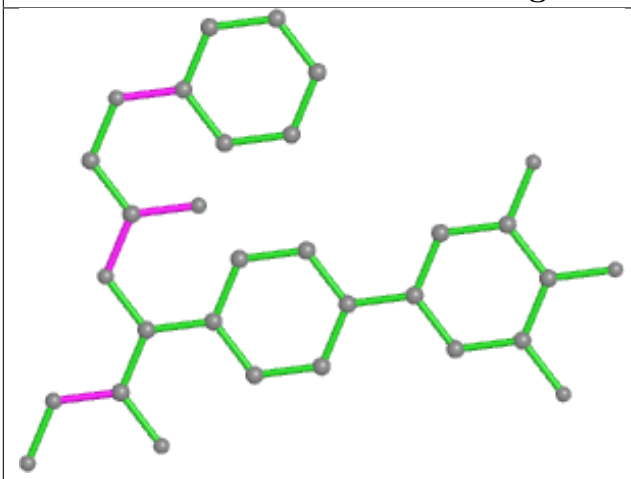


Torsions

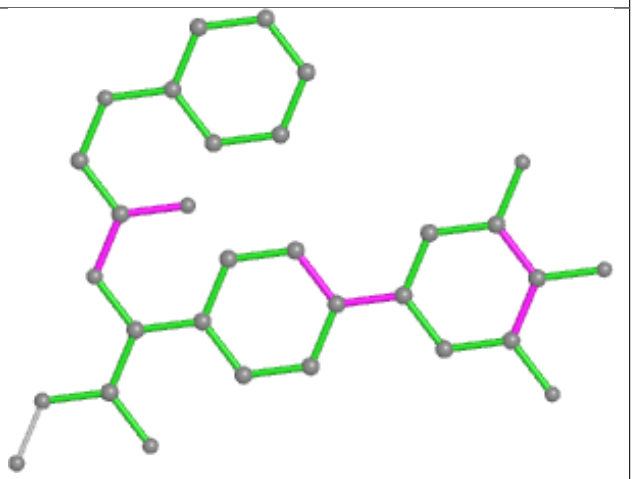


Rings

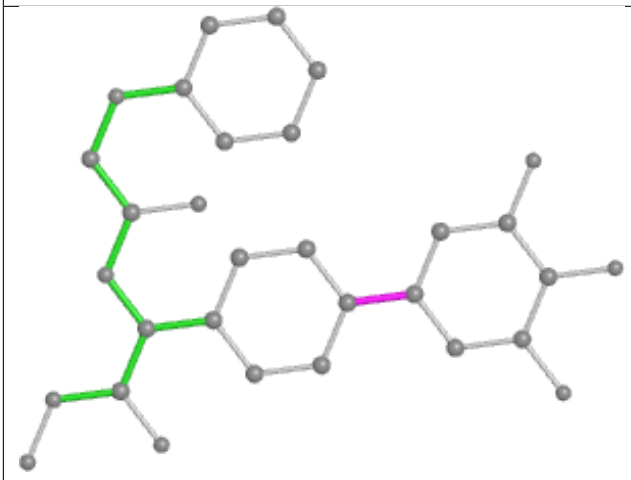
Ligand X10 H 701



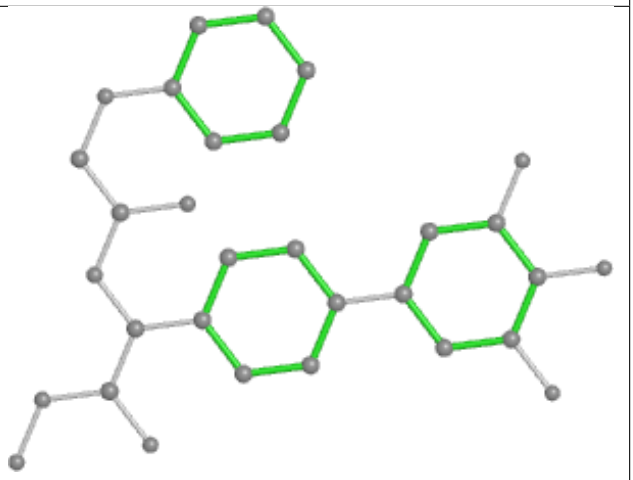
Bond lengths



Bond angles

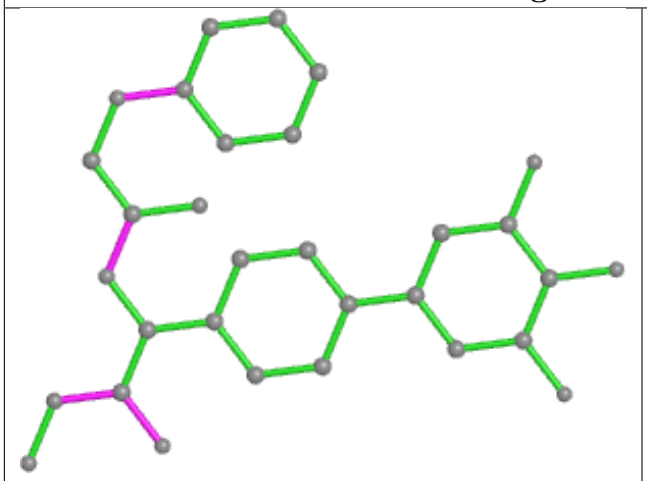


Torsions

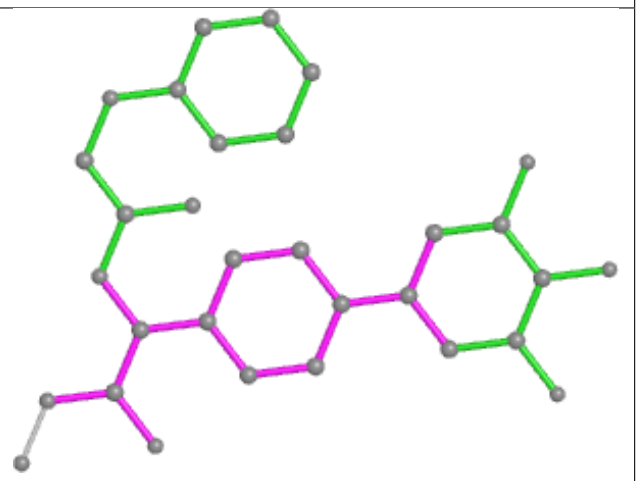


Rings

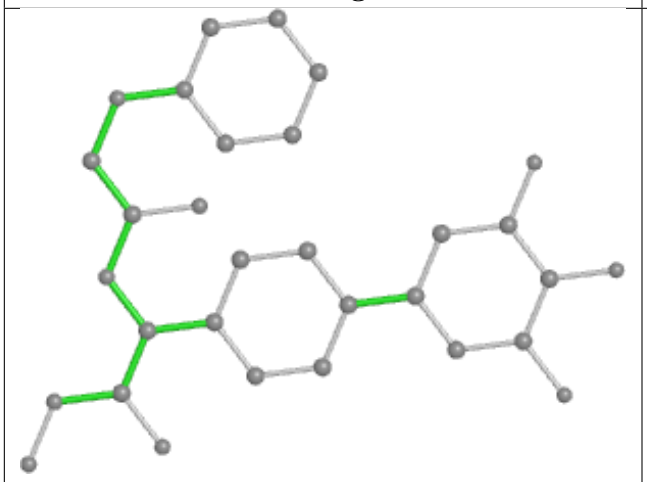
Ligand X10 A 701



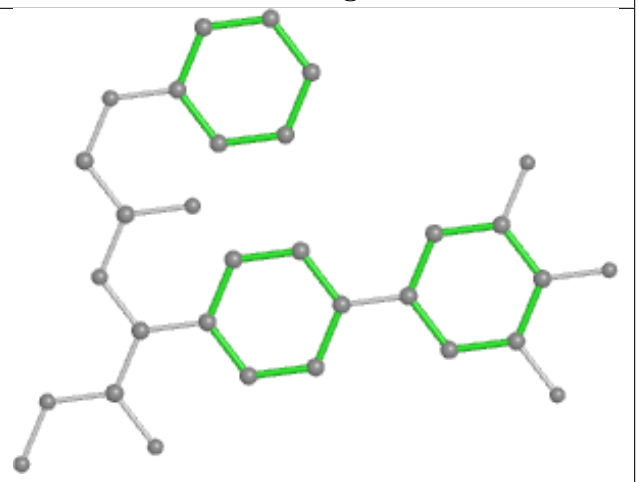
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	519/527 (98%)	-0.20	3 (0%)	89	90	18, 24, 40, 61	0
1	B	521/527 (98%)	-0.15	11 (2%)	63	66	18, 26, 48, 72	1 (0%)
1	C	525/527 (99%)	-0.27	5 (0%)	82	84	18, 24, 41, 71	0
1	D	522/527 (99%)	-0.37	11 (2%)	63	66	18, 24, 41, 86	0
1	E	514/527 (97%)	-0.34	7 (1%)	75	77	18, 23, 36, 69	0
1	F	515/527 (97%)	-0.26	4 (0%)	86	87	19, 25, 49, 74	0
1	G	521/527 (98%)	-0.16	6 (1%)	79	81	18, 24, 40, 67	0
1	H	522/527 (99%)	-0.10	12 (2%)	60	63	19, 26, 48, 69	0
1	I	525/527 (99%)	-0.23	5 (0%)	82	84	18, 24, 42, 84	0
1	J	519/527 (98%)	-0.42	2 (0%)	92	93	17, 23, 38, 79	1 (0%)
1	K	517/527 (98%)	-0.35	7 (1%)	75	77	17, 23, 37, 78	0
1	L	512/527 (97%)	-0.19	12 (2%)	60	63	18, 27, 50, 86	0
All	All	6232/6324 (98%)	-0.25	85 (1%)	75	77	17, 24, 45, 86	2 (0%)

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	604	ALA	5.8
1	K	255	THR	5.7
1	J	136	GLY	4.8
1	E	136	GLY	4.7
1	G	136	GLY	4.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ZN	A	709	1/1	0.69	0.19	22,22,22,22	1
6	ZN	E	708	1/1	0.70	0.12	21,21,21,21	1
4	1PE	F	706	10/16	0.77	0.18	41,51,58,63	0
6	ZN	E	707	1/1	0.80	0.19	28,28,28,28	1
4	1PE	L	704	13/16	0.80	0.16	38,46,56,60	0
2	X10	L	701	31/31	0.81	0.24	30,45,58,62	3
6	ZN	I	707	1/1	0.81	0.20	22,22,22,22	1
4	1PE	A	707	13/16	0.82	0.18	40,54,60,64	0
4	1PE	C	705	8/16	0.82	0.23	34,41,48,54	0
4	1PE	D	704	7/16	0.83	0.21	31,43,49,56	0
4	1PE	G	705	7/16	0.84	0.19	45,48,51,52	0
4	1PE	I	705	8/16	0.85	0.20	33,46,50,50	0
2	X10	D	701	31/31	0.85	0.22	28,39,50,51	3
4	1PE	F	705	7/16	0.85	0.12	37,46,49,52	0
5	CO3	F	707	4/4	0.86	0.24	18,30,35,44	0
2	X10	C	701	31/31	0.86	0.20	28,39,53,59	9
4	1PE	A	705	9/16	0.86	0.14	31,36,47,51	0
4	1PE	F	703	13/16	0.86	0.13	31,41,49,49	0
6	ZN	F	709	1/1	0.86	0.13	21,21,21,21	1
2	X10	B	1401	31/31	0.86	0.24	28,43,69,82	0
8	2PE	H	705	26/28	0.86	0.16	33,52,62,71	0
6	ZN	F	708	1/1	0.87	0.21	26,26,26,26	1
4	1PE	K	703	11/16	0.87	0.12	28,36,50,53	0
4	1PE	L	705	16/16	0.88	0.18	38,46,64,67	0
2	X10	E	701	31/31	0.88	0.16	27,38,41,44	9
6	ZN	I	708	1/1	0.88	0.11	19,19,19,19	1
2	X10	I	701	31/31	0.88	0.15	23,37,47,54	5
2	X10	H	701	31/31	0.89	0.18	25,38,52,53	5
4	1PE	K	704	13/16	0.89	0.21	38,43,54,56	0
2	X10	J	701	31/31	0.89	0.19	31,38,48,60	3
4	1PE	E	704	13/16	0.89	0.23	29,44,51,52	0
4	1PE	I	703	15/16	0.89	0.16	32,42,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	X10	K	701	31/31	0.89	0.18	23,40,51,62	3
6	ZN	A	710	1/1	0.89	0.13	18,18,18,18	1
4	1PE	J	704	13/16	0.90	0.15	36,45,54,60	0
2	X10	F	701	31/31	0.90	0.16	28,40,58,60	7
2	X10	G	701	31/31	0.90	0.17	26,34,53,54	7
5	CO3	I	706	4/4	0.91	0.17	18,24,27,41	0
4	1PE	L	703	9/16	0.91	0.10	28,36,49,52	0
2	X10	A	701	31/31	0.91	0.16	27,45,54,56	4
4	1PE	I	704	13/16	0.91	0.12	24,34,51,53	0
4	1PE	D	703	13/16	0.91	0.19	31,46,54,58	0
5	CO3	E	706	4/4	0.92	0.18	18,29,39,48	0
4	1PE	H	703	7/16	0.92	0.18	34,39,47,47	0
4	1PE	A	706	12/16	0.92	0.13	28,40,45,47	0
4	1PE	K	702	13/16	0.92	0.14	26,32,55,57	0
4	1PE	E	705	12/16	0.92	0.15	38,44,46,48	0
5	CO3	A	708	4/4	0.92	0.26	19,31,35,43	4
4	1PE	E	703	11/16	0.93	0.12	22,33,48,48	0
5	CO3	K	705	4/4	0.93	0.21	17,36,40,43	0
5	CO3	B	1402	4/4	0.93	0.16	18,27,32,36	0
4	1PE	J	703	9/16	0.93	0.11	21,32,41,42	0
6	ZN	B	1404	1/1	0.93	0.23	74,74,74,74	0
4	1PE	G	704	11/16	0.93	0.11	30,37,51,58	0
4	1PE	C	704	13/16	0.94	0.13	36,41,46,48	0
5	CO3	C	706	4/4	0.94	0.16	17,26,37,41	0
3	SO4	G	702	5/5	0.95	0.09	34,43,59,61	0
6	ZN	D	707	1/1	0.95	0.07	21,21,21,21	1
3	SO4	G	703	5/5	0.95	0.22	55,59,70,77	0
4	1PE	C	703	11/16	0.95	0.11	29,33,47,53	0
5	CO3	J	705	4/4	0.95	0.24	17,17,44,48	4
3	SO4	I	702	5/5	0.95	0.37	45,52,64,69	0
5	CO3	L	706	4/4	0.95	0.36	16,34,43,48	0
3	SO4	C	702	5/5	0.95	0.23	21,32,39,42	5
6	ZN	L	707	1/1	0.95	0.06	27,27,27,27	1
5	CO3	D	705	4/4	0.95	0.19	17,17,30,39	4
3	SO4	J	702	5/5	0.96	0.17	27,34,36,38	5
4	1PE	F	704	10/16	0.96	0.08	26,35,45,47	0
3	SO4	E	702	5/5	0.96	0.15	28,29,40,41	5
5	CO3	H	704	4/4	0.96	0.14	18,23,34,45	0
6	ZN	B	1403	1/1	0.97	0.28	58,58,58,58	0
5	CO3	G	706	4/4	0.97	0.26	18,18,50,53	0
6	ZN	G	708	1/1	0.97	0.07	20,20,20,20	1
6	ZN	C	707	1/1	0.97	0.09	22,22,22,22	1

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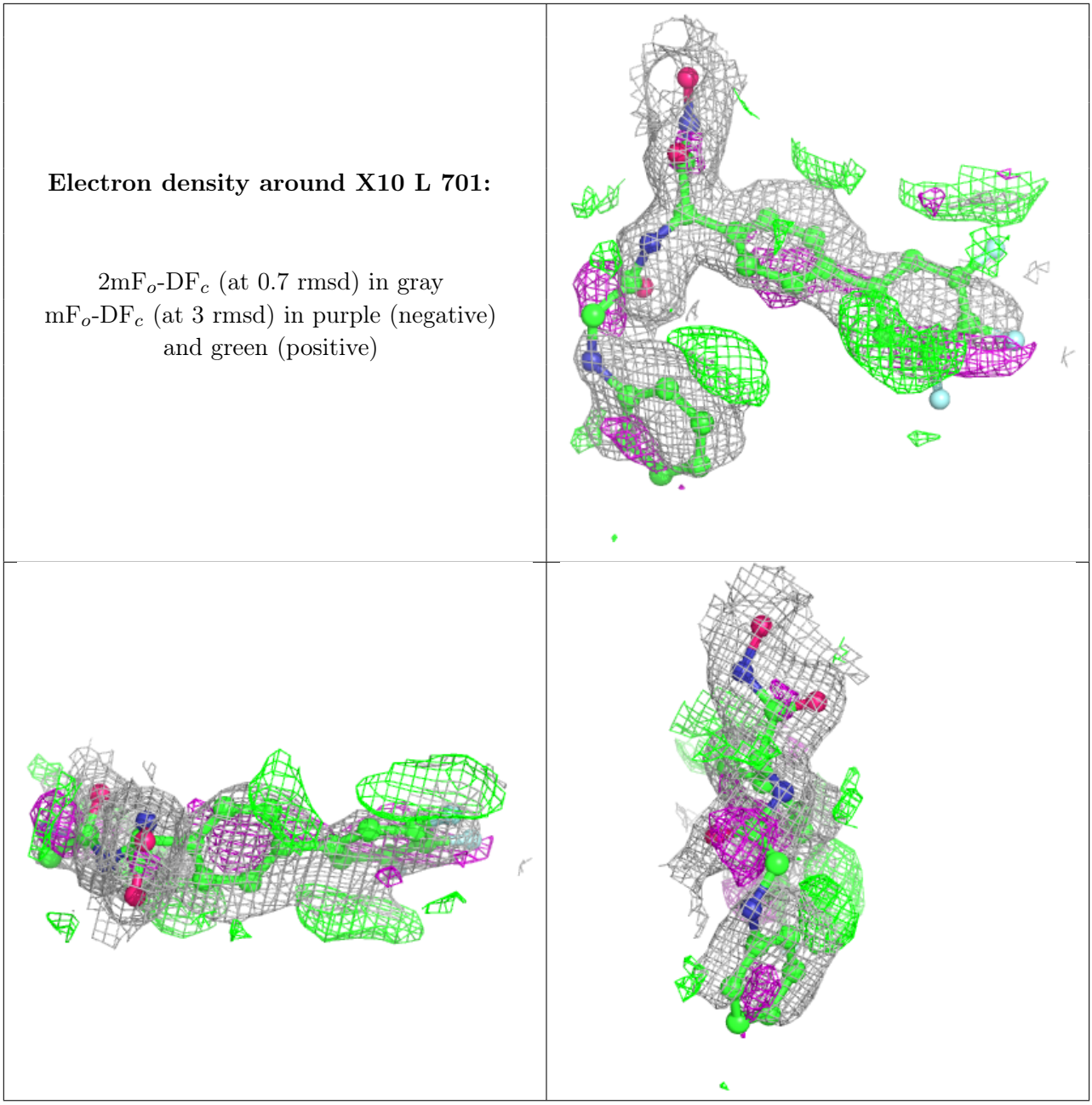
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	1PE	D	702	10/16	0.97	0.08	27,31,44,49	0
6	ZN	J	706	1/1	0.97	0.06	23,23,23,23	1
6	ZN	K	706	1/1	0.97	0.10	19,19,19,19	1
6	ZN	K	707	1/1	0.97	0.08	19,19,19,19	1
3	SO4	A	703	5/5	0.97	0.07	33,40,58,61	0
3	SO4	F	702	5/5	0.97	0.26	53,60,65,76	0
6	ZN	G	707	1/1	0.98	0.08	25,25,25,25	1
3	SO4	A	704	5/5	0.98	0.16	25,35,37,39	5
6	ZN	H	706	1/1	0.98	0.04	22,22,22,22	1
6	ZN	D	708	1/1	0.98	0.04	19,19,19,19	1
7	NA	F	710	1/1	0.98	0.07	23,23,23,23	0
7	NA	G	709	1/1	0.98	0.10	22,22,22,22	0
6	ZN	C	708	1/1	0.98	0.06	18,18,18,18	1
3	SO4	H	702	5/5	0.99	0.07	19,19,19,21	0
6	ZN	H	707	1/1	0.99	0.06	19,19,19,19	1
3	SO4	A	702	5/5	0.99	0.08	18,18,21,22	0
6	ZN	L	708	1/1	0.99	0.09	19,19,19,19	1
7	NA	A	711	1/1	0.99	0.07	25,25,25,25	0
7	NA	D	709	1/1	0.99	0.08	22,22,22,22	0
3	SO4	D	706	5/5	0.99	0.09	19,20,21,25	0
3	SO4	L	702	5/5	0.99	0.07	17,19,20,22	0
7	NA	H	708	1/1	0.99	0.05	23,23,23,23	0
7	NA	I	709	1/1	0.99	0.06	20,20,20,20	0
7	NA	J	708	1/1	0.99	0.08	21,21,21,21	0
7	NA	K	708	1/1	0.99	0.09	21,21,21,21	0
6	ZN	J	707	1/1	0.99	0.03	21,21,21,21	1
7	NA	B	1405	1/1	1.00	0.04	23,23,23,23	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.

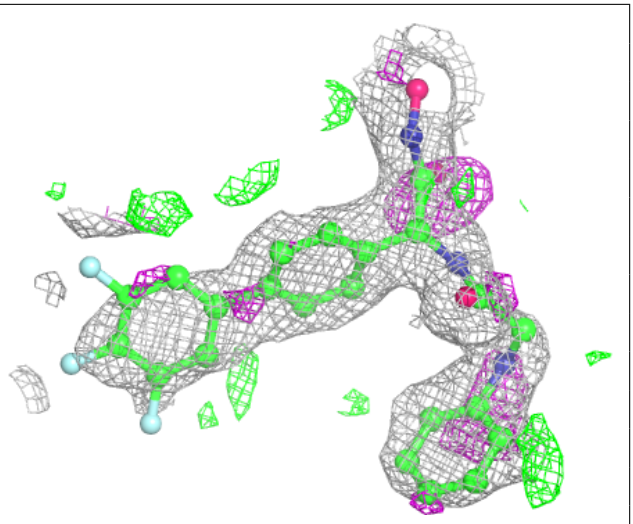
Electron density around X10 L 701:

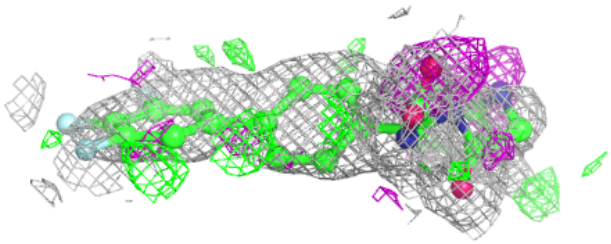
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

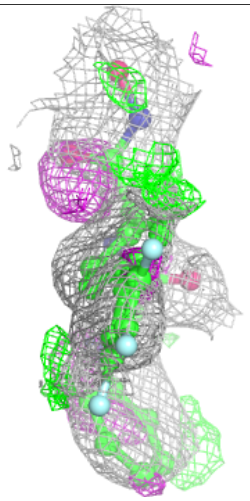


Electron density around X10 D 701:

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

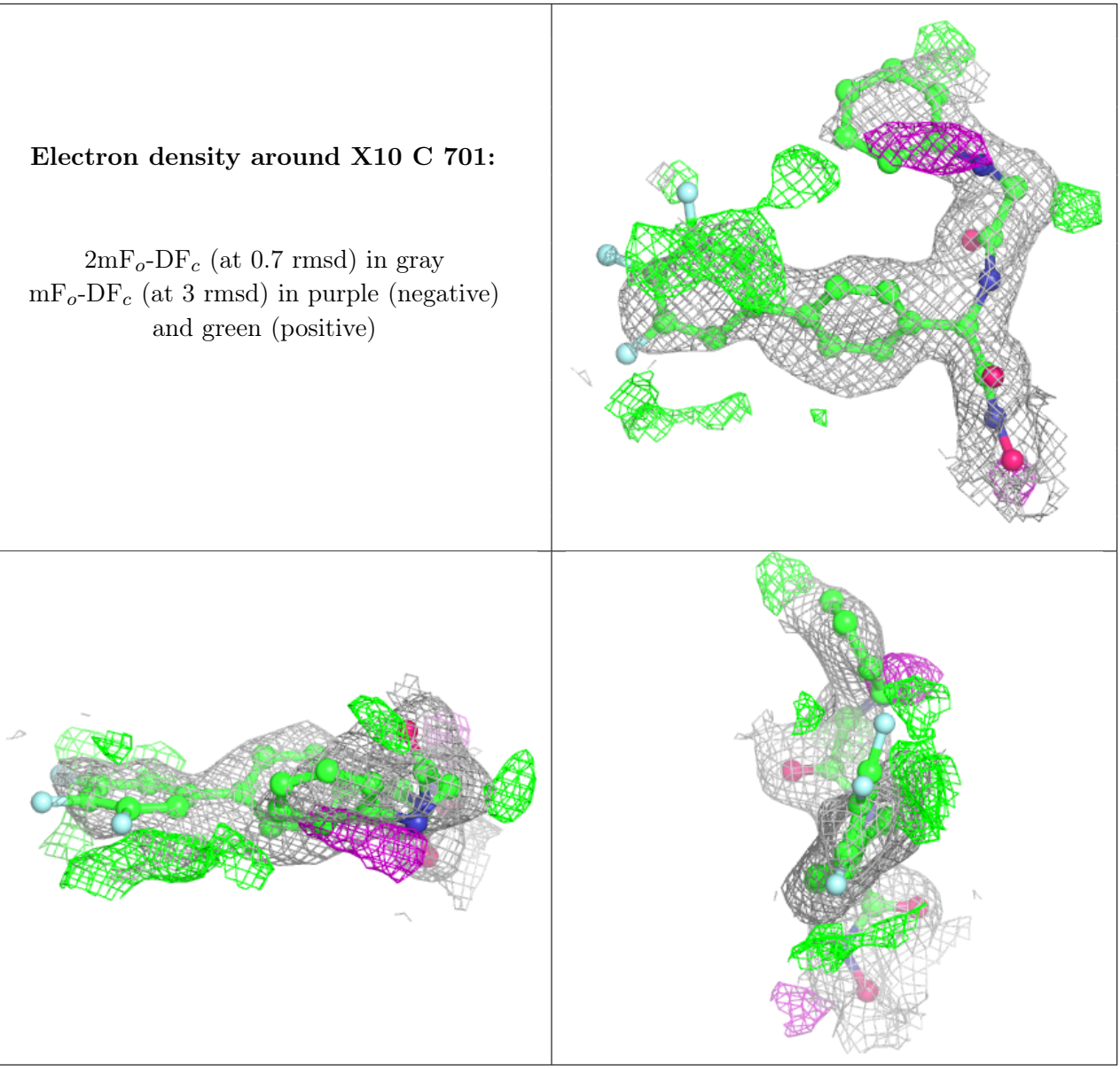






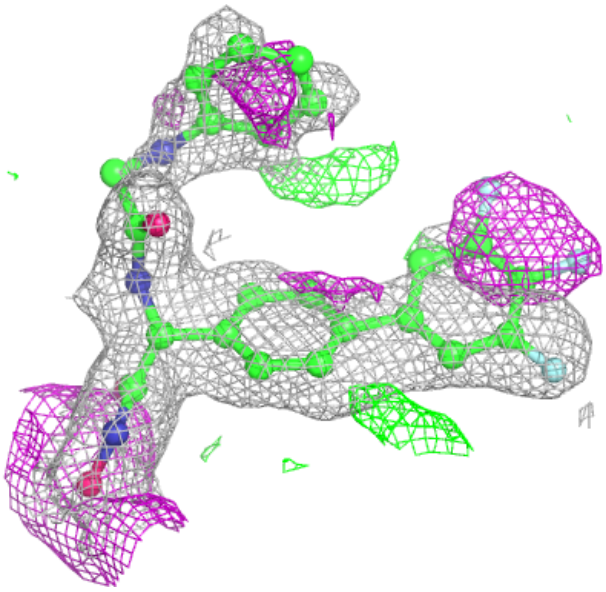
Electron density around X10 C 701:

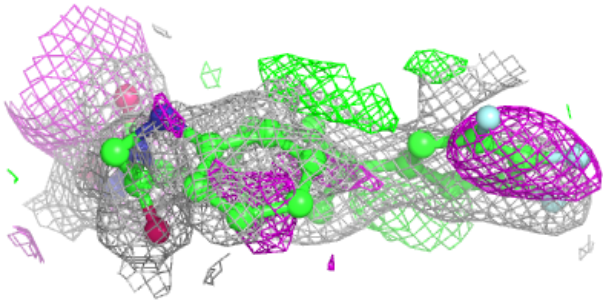
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

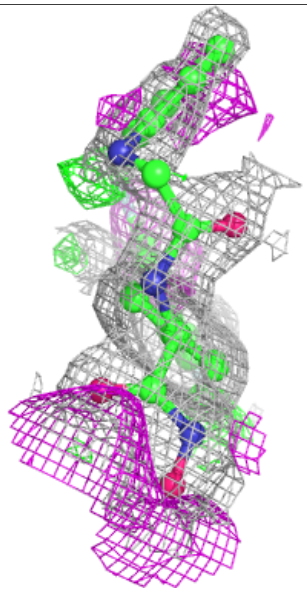


Electron density around X10 B 1401:

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

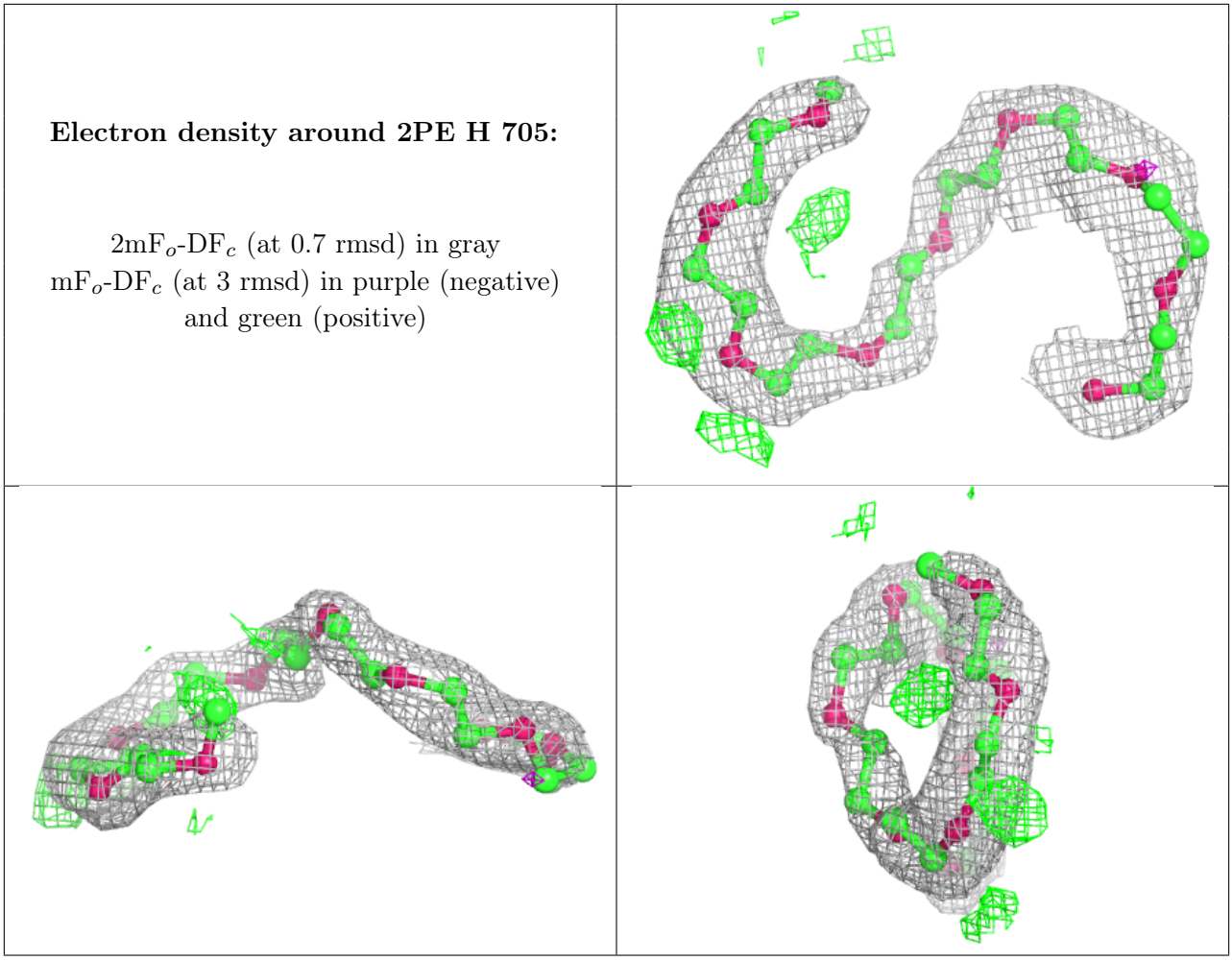






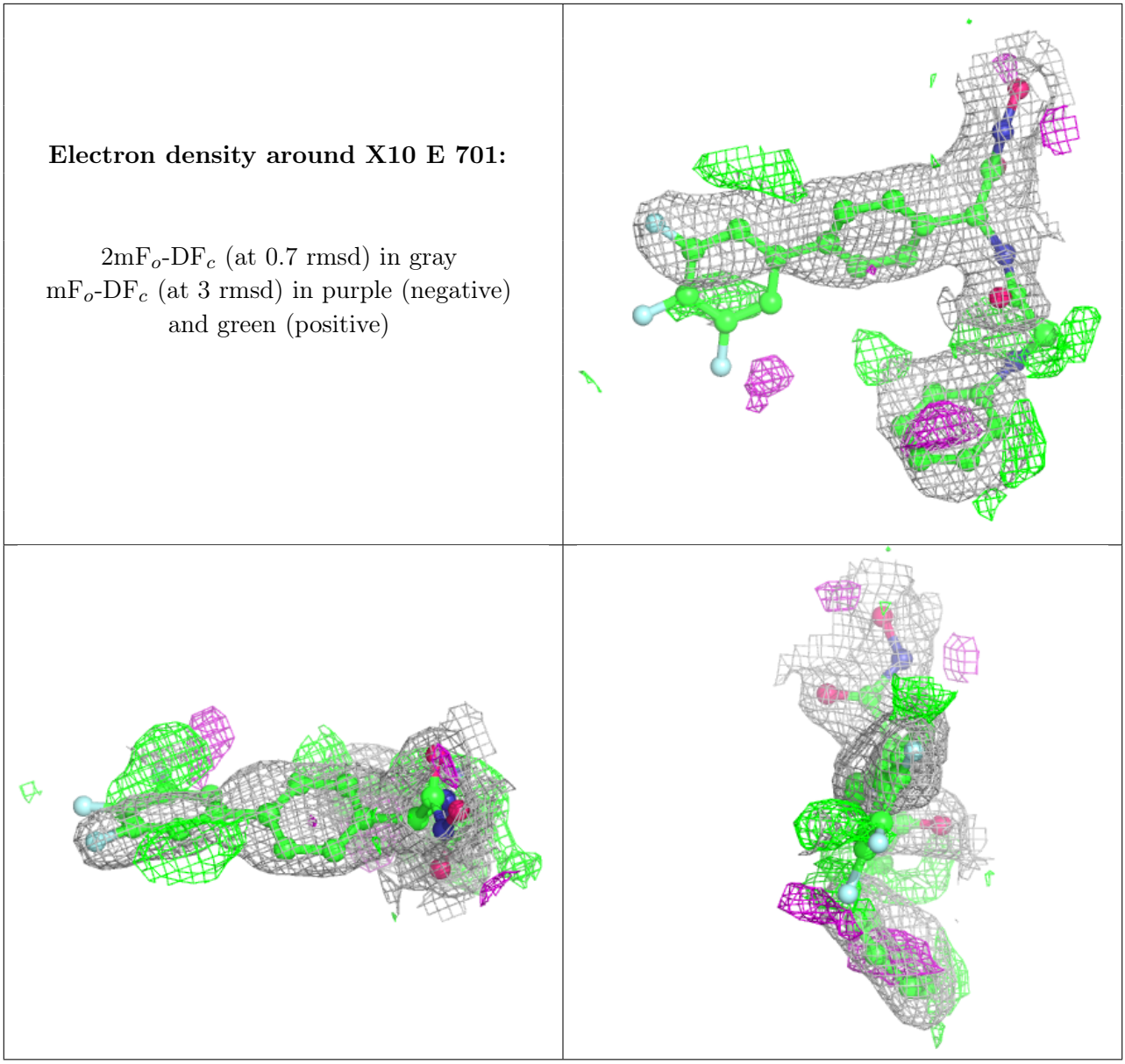
Electron density around 2PE H 705:

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



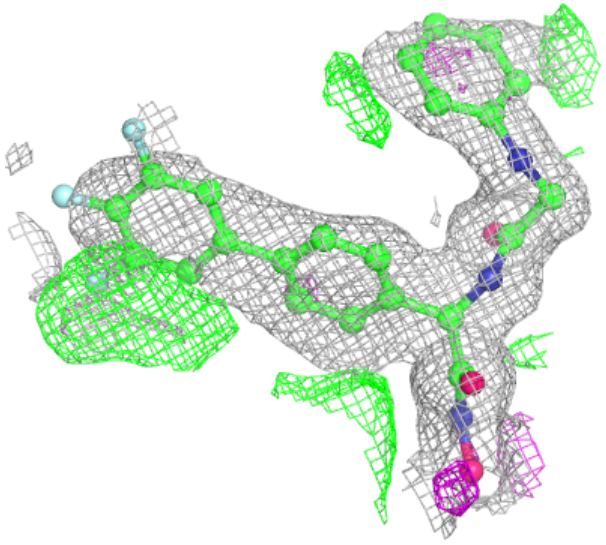
Electron density around X10 E 701:

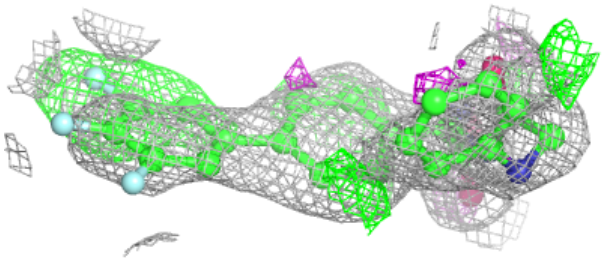
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

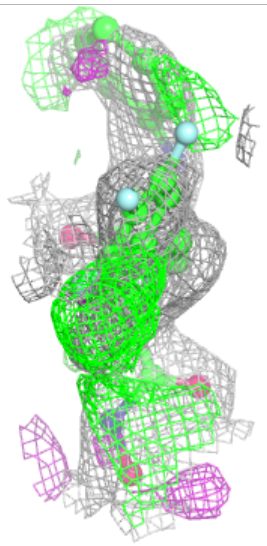


Electron density around X10 I 701:

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

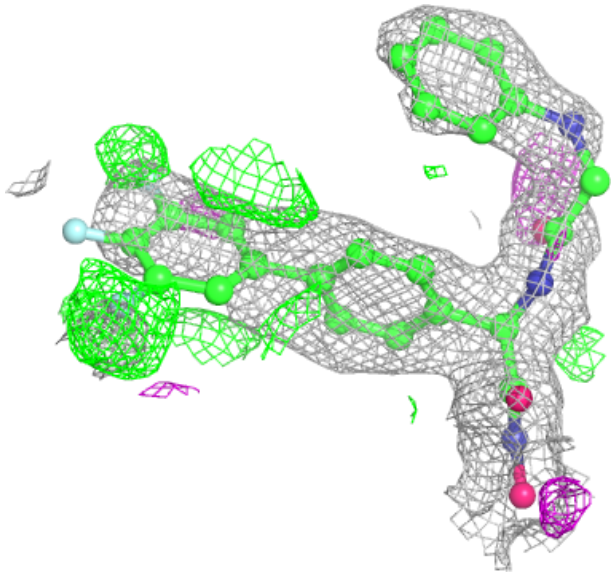


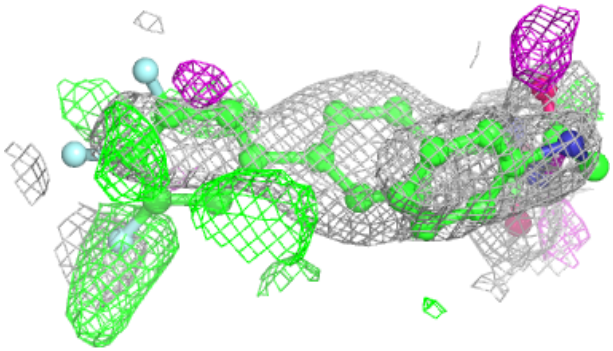


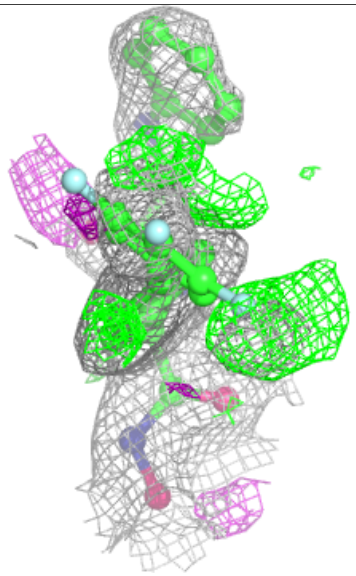


Electron density around X10 H 701:

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

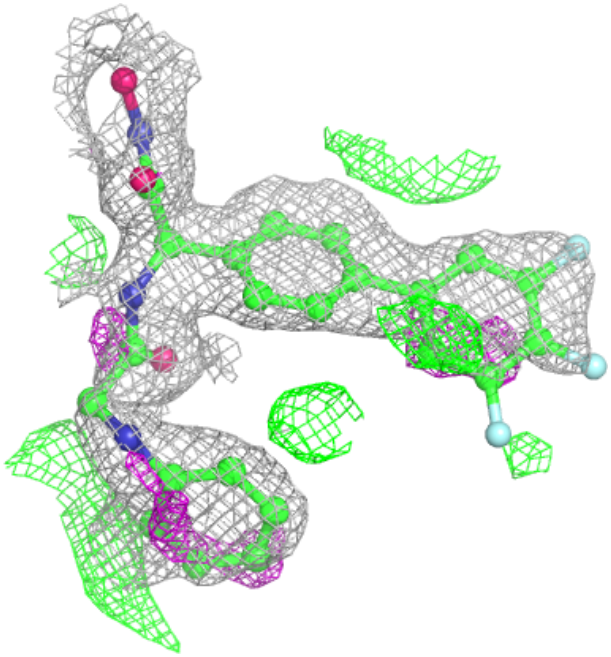


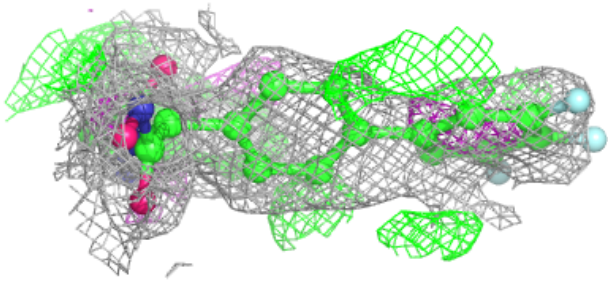


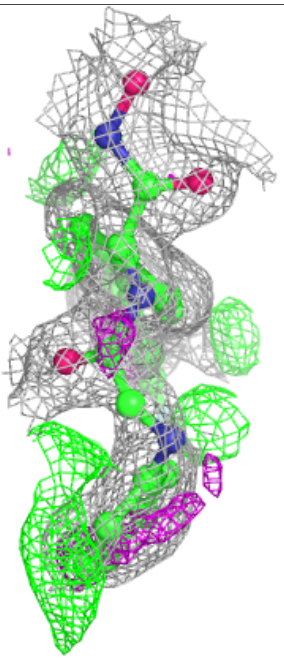


Electron density around X10 J 701:

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

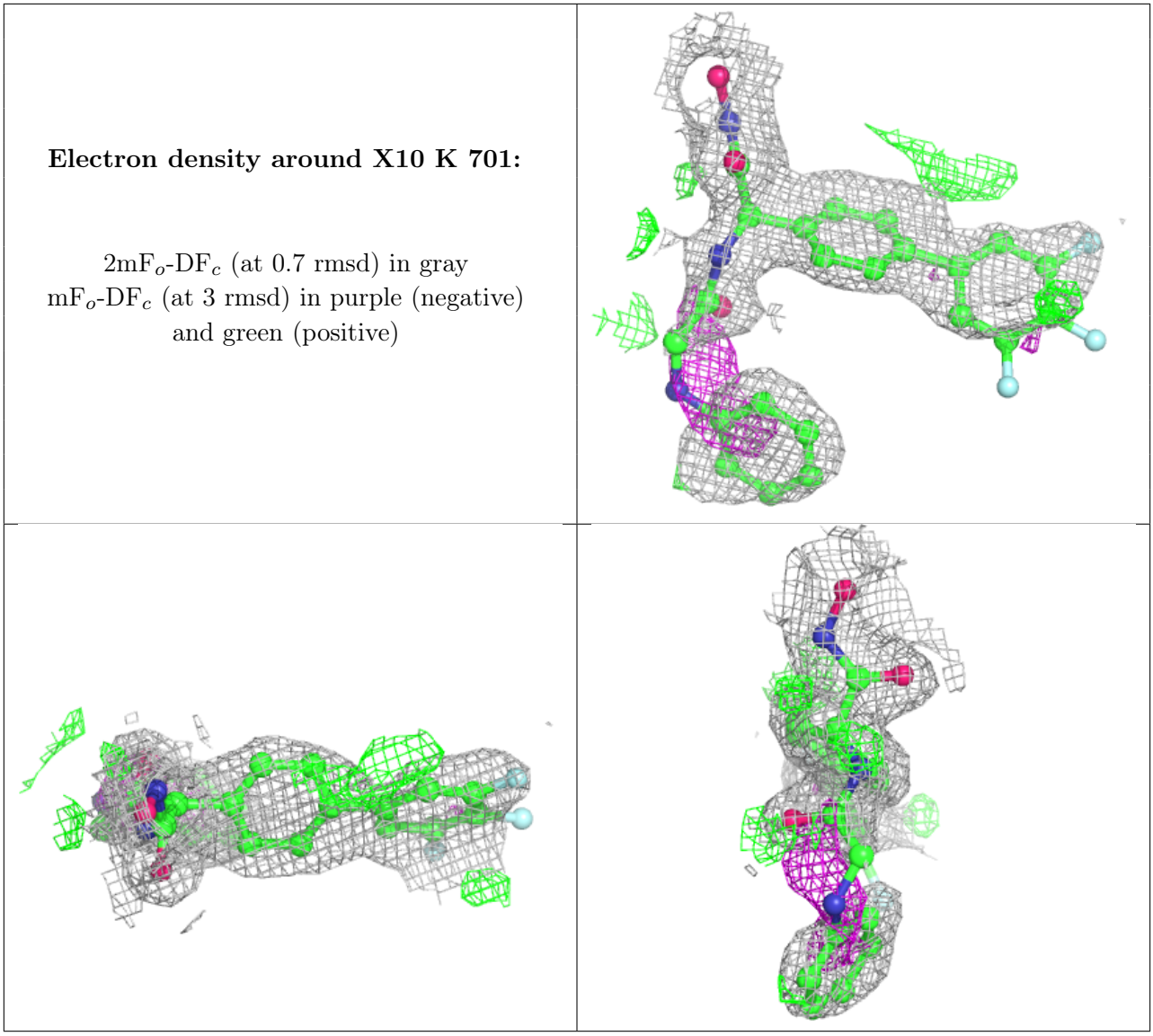






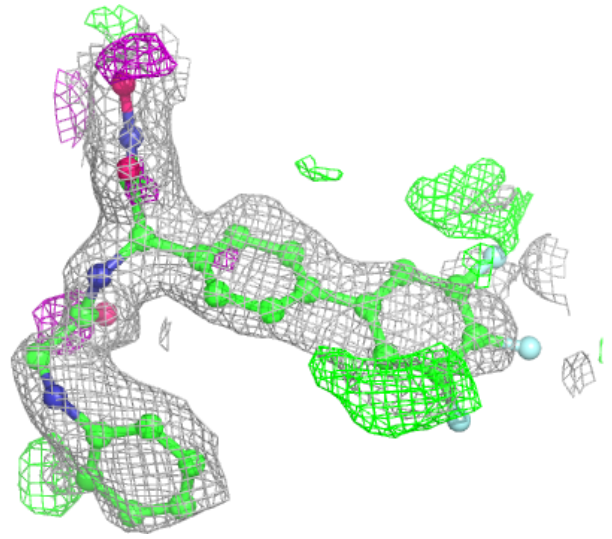
Electron density around X10 K 701:

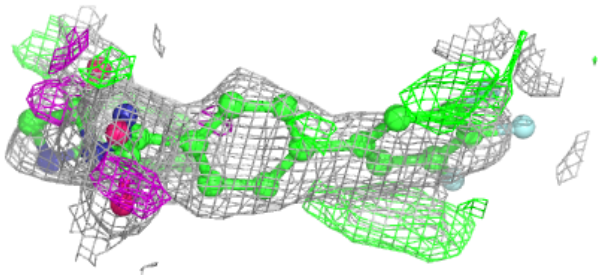
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

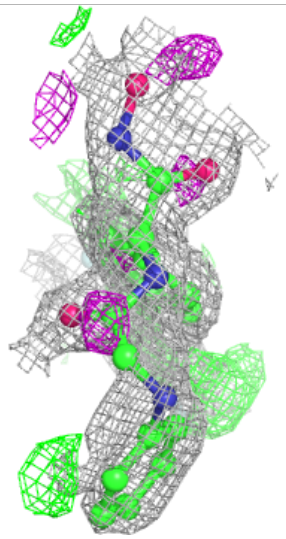


Electron density around X10 F 701:

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

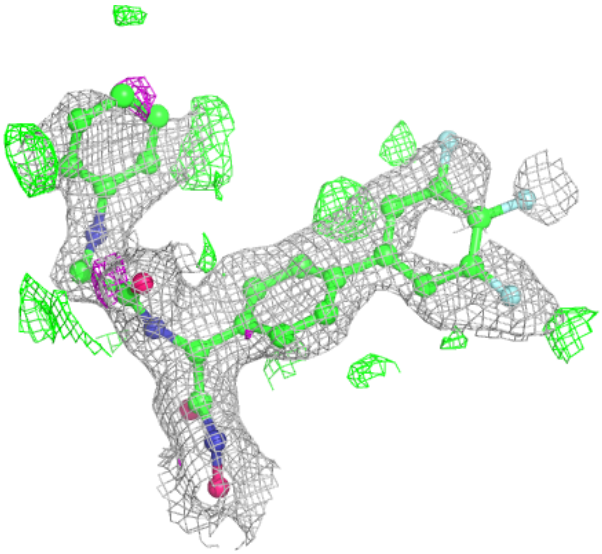


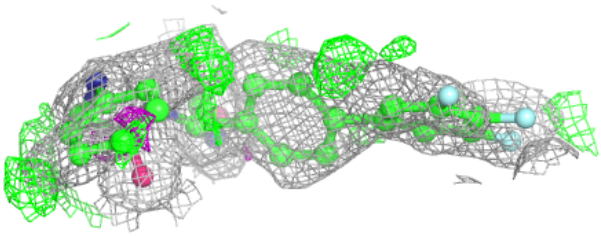


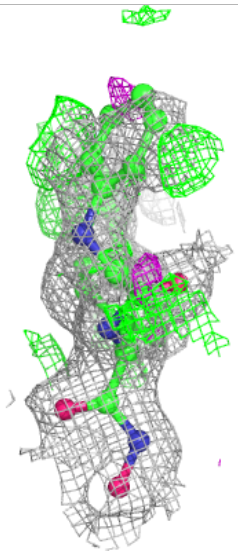


Electron density around X10 G 701:

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

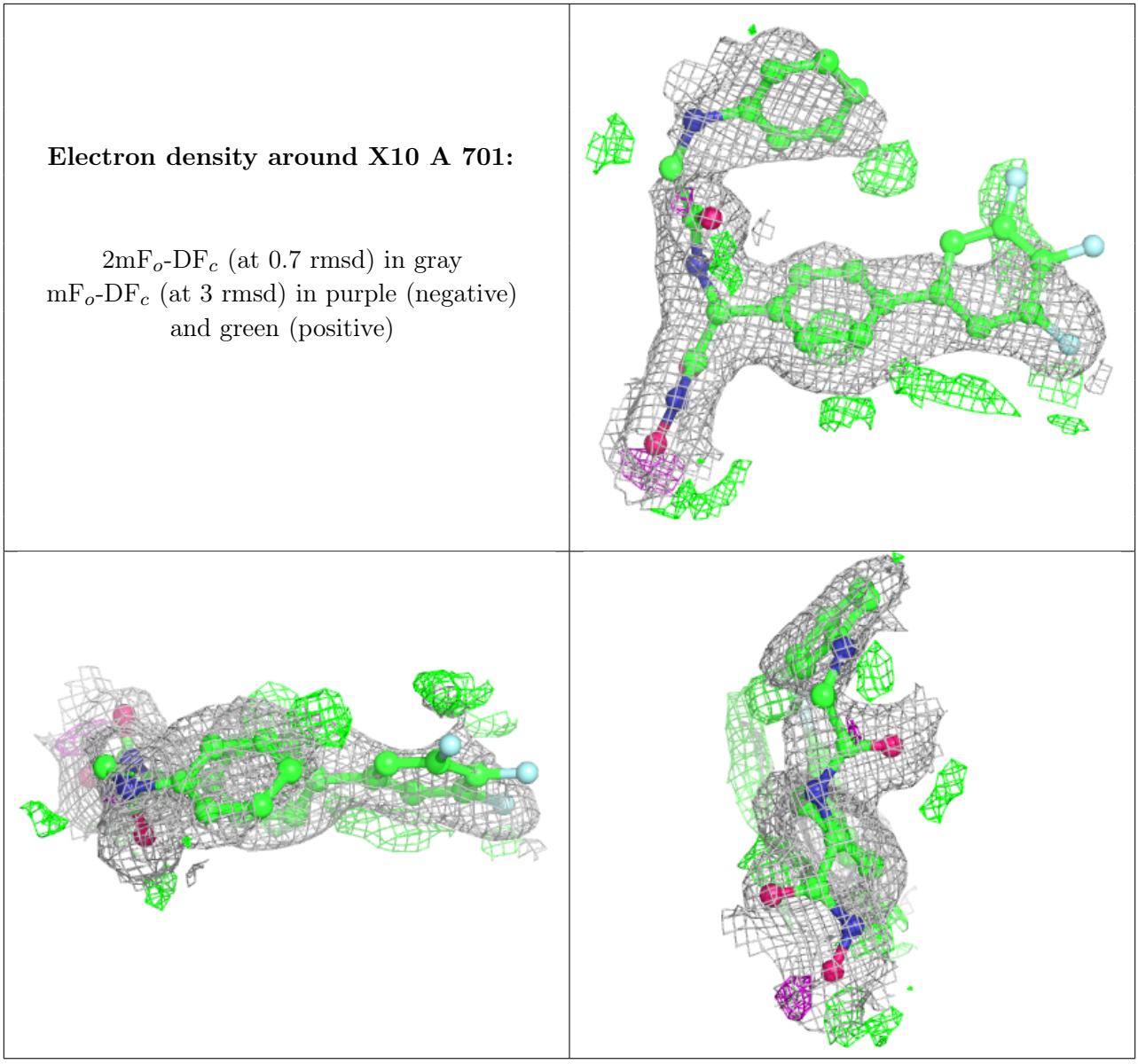






Electron density around X10 A 701:

$2mF_o$-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

There are no such residues in this entry.