



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2026 – 05:46 PM UTC

PDB ID : 8EZ4 / pdb_00008ez4
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

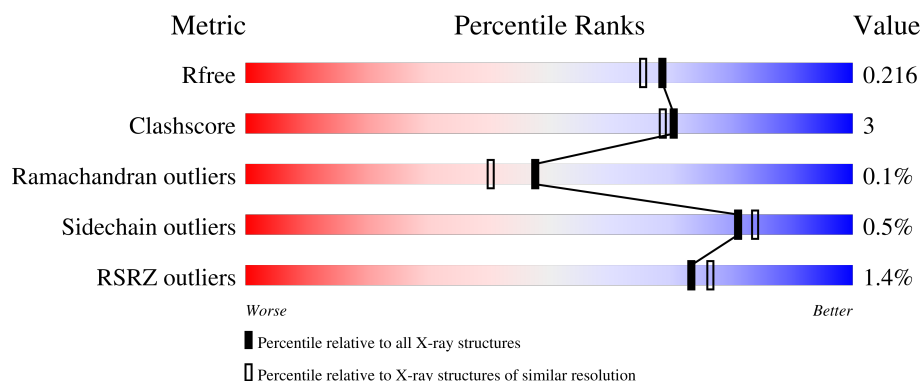
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

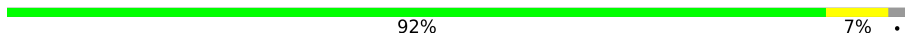
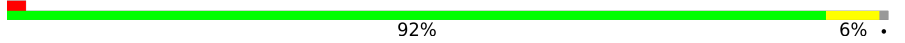
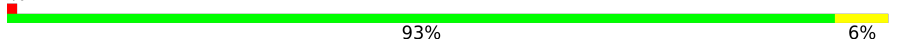
The reported resolution of this entry is 1.89 Å.

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.



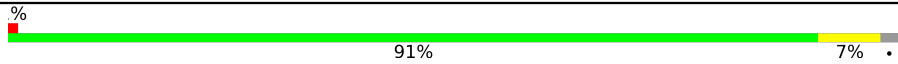
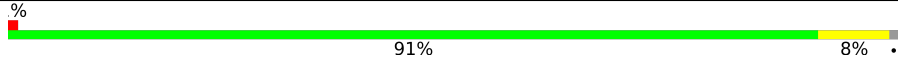
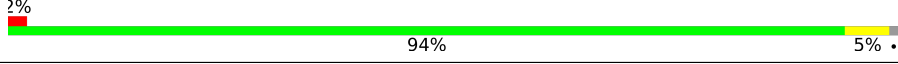
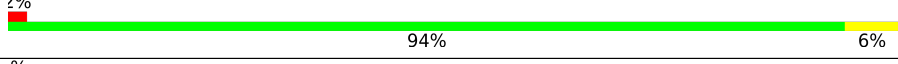
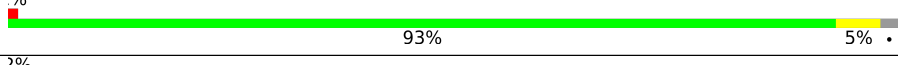
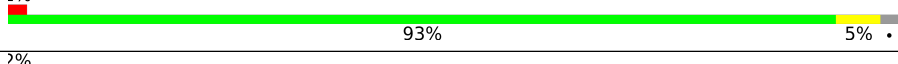
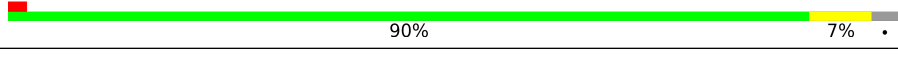
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	
1	B	527	
1	C	527	
1	D	527	
1	E	527	

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Mol	Chain	Length	Quality of chain
1	F	527	
1	G	527	
1	H	527	
1	I	527	
1	J	527	
1	K	527	
1	L	527	

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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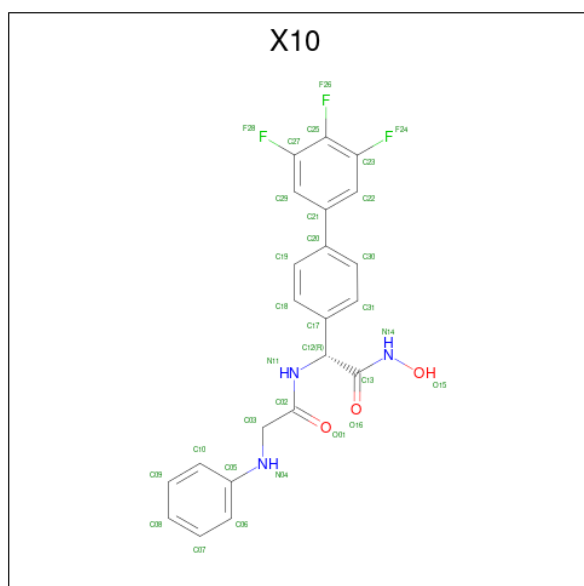
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	conflict	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP 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)ethyl]-N 2-phenylglycinamide (CCD ID: X10) (formula: C₂₂H₁₈F₃N₃O₃) (labeled as "Ligand of Interest" by depositor).



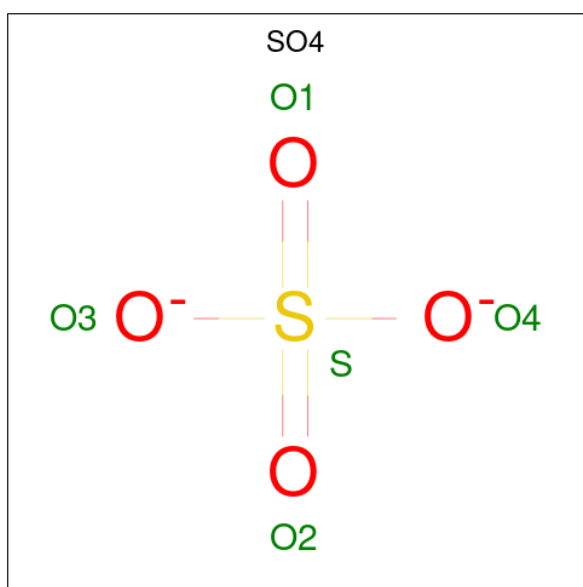
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			31	22	3	3	3		

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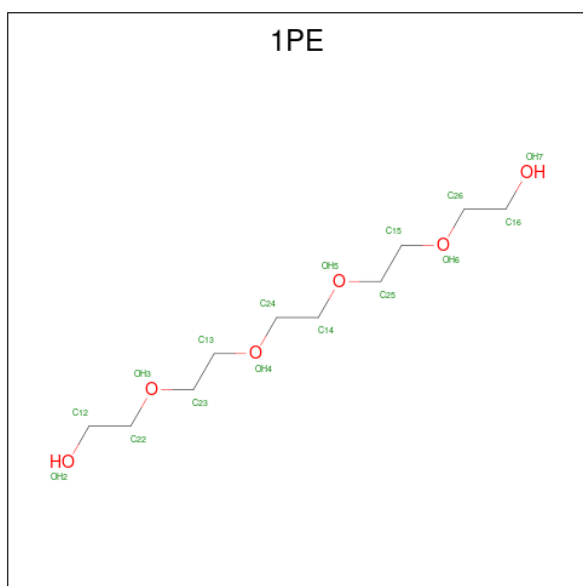
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			31	22	3	3	3		
2	C	1	Total	C	F	N	O	3	0
			31	22	3	3	3		
2	D	1	Total	C	F	N	O	1	0
			31	22	3	3	3		
2	E	1	Total	C	F	N	O	7	0
			31	22	3	3	3		
2	F	1	Total	C	F	N	O	2	0
			31	22	3	3	3		
2	G	1	Total	C	F	N	O	1	0
			31	22	3	3	3		
2	H	1	Total	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 (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



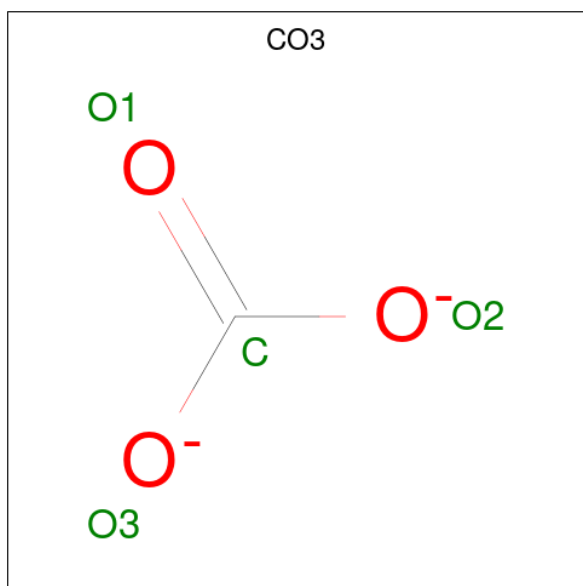
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	6	3		
4	A	1	Total	C	O	0	0
			12	8	4		
4	A	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			11	7	4		
4	C	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			8	5	3		
4	D	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			13	8	5		
4	D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

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

- Molecule 5 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



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

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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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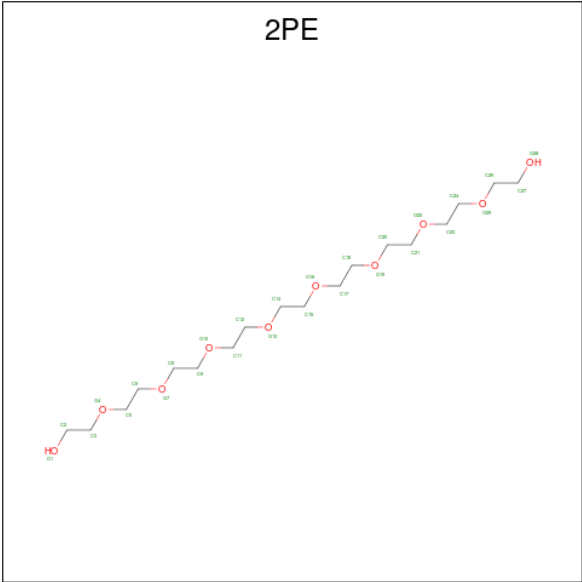
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	2	Total 2	Zn 2	0	0
6	L	2	Total 2	Zn 2	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 8 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: C₁₈H₃₈O₁₀).



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

- Molecule 9 is water.

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

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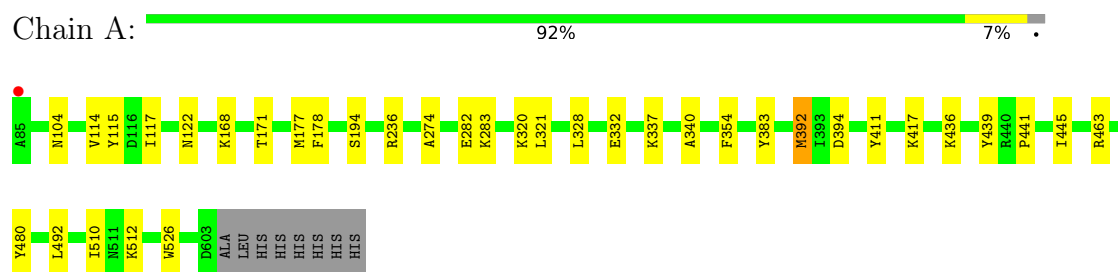
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	339	Total 339	O 339	0	0

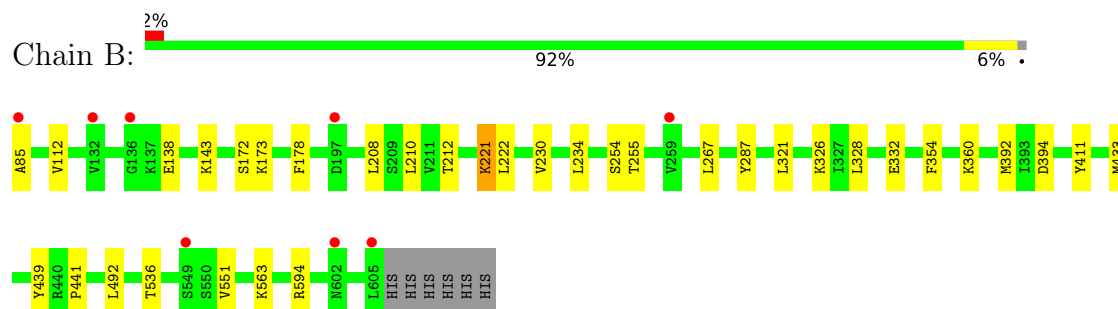
3 Residue-property plots [i](#)

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.

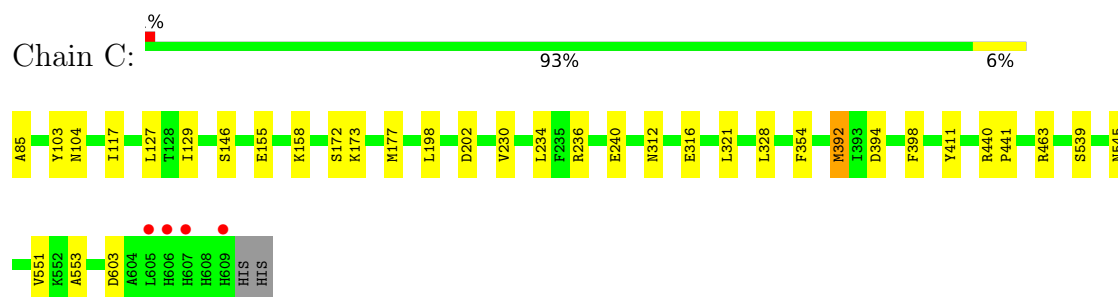
- Molecule 1: M17 leucyl aminopeptidase



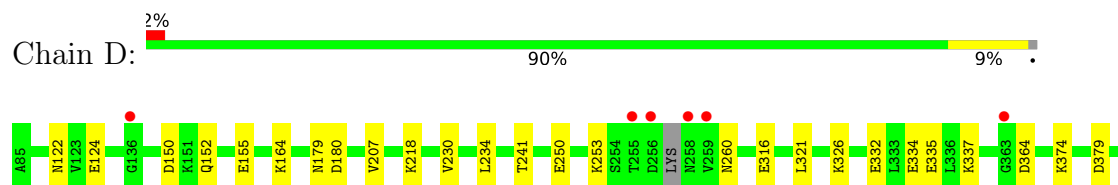
- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase

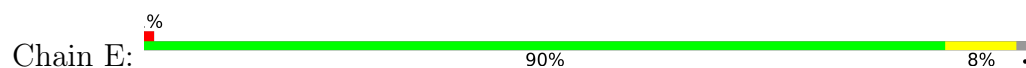


- Molecule 1: M17 leucyl aminopeptidase

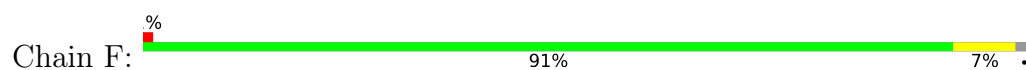




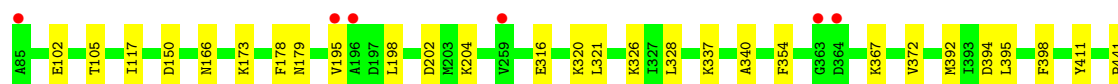
- Molecule 1: M17 leucyl aminopeptidase



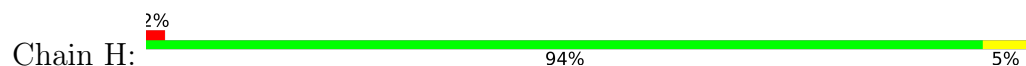
- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase

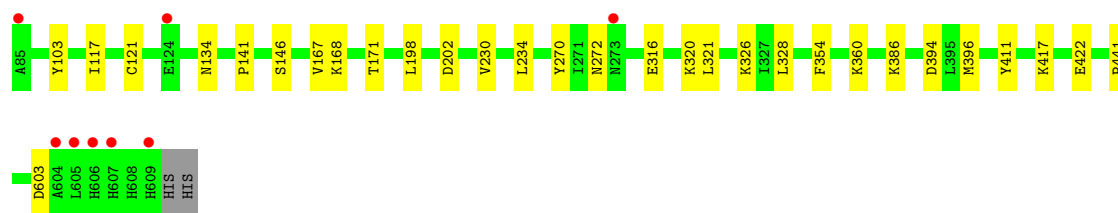


- Molecule 1: M17 leucyl aminopeptidase

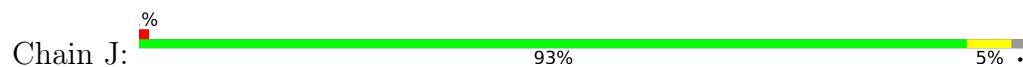


- Molecule 1: M17 leucyl aminopeptidase

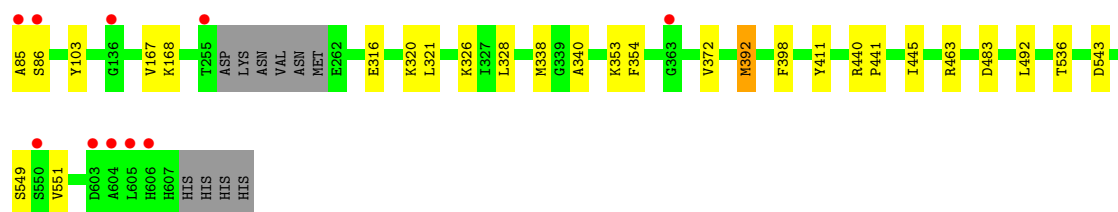




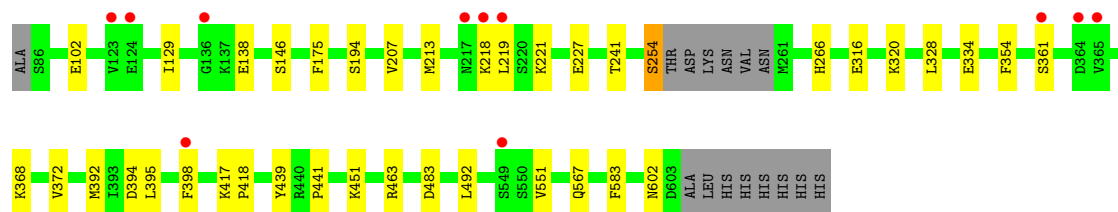
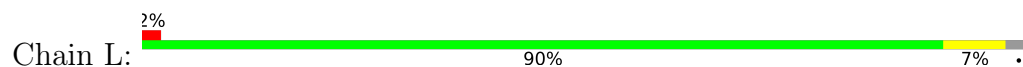
● Molecule 1: M17 leucyl aminopeptidase



● Molecule 1: M17 leucyl aminopeptidase



● Molecule 1: M17 leucyl aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.94Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.90Å)	Xtriage
Refinement program	PHENIX v1.20.1-4487	Depositor
R, R_{free}	0.177 , 0.216 0.177 , 0.216	Depositor DCC
R_{free} test set	27740 reflections (4.96%)	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 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	0/4074	0.61	3/5525 (0.1%)
1	B	0.41	0/4030	0.63	3/5472 (0.1%)
1	C	0.41	0/4095	0.59	1/5563 (0.0%)
1	D	0.39	0/4063	0.61	1/5513 (0.0%)
1	E	0.41	0/3997	0.59	0/5428
1	F	0.39	0/3975	0.59	0/5404
1	G	0.38	0/4083	0.56	0/5538
1	H	0.38	0/4011	0.55	0/5452
1	I	0.41	0/4101	0.59	2/5567 (0.0%)
1	J	0.41	0/4040	0.59	1/5480 (0.0%)
1	K	0.41	0/4023	0.61	1/5461 (0.0%)
1	L	0.41	1/3943 (0.0%)	0.59	2/5362 (0.0%)
All	All	0.40	1/48435 (0.0%)	0.59	14/65765 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	417	LYS	C-O	7.33	1.27	1.23

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	392	MET	CG-SD-CE	-9.43	80.15	100.90
1	C	392	MET	CG-SD-CE	-7.85	83.62	100.90
1	B	563	LYS	CA-CB-CG	7.84	129.78	114.10
1	A	392	MET	CG-SD-CE	-7.12	85.22	100.90
1	L	334	GLU	CA-C-N	-6.72	109.56	122.06

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3993	0	3925	38	0
1	B	3952	0	3867	23	0
1	C	4007	0	3911	24	0
1	D	3983	0	3889	36	0
1	E	3917	0	3824	30	0
1	F	3895	0	3770	28	0
1	G	4002	0	3938	27	0
1	H	3933	0	3799	19	0
1	I	4017	0	3932	20	0
1	J	3962	0	3891	26	0
1	K	3944	0	3862	24	0
1	L	3866	0	3738	36	0
2	A	31	0	0	6	0
2	B	31	0	0	2	0
2	C	31	0	0	4	0
2	D	31	0	0	6	0
2	E	31	0	0	0	0
2	F	31	0	0	5	0
2	G	31	0	0	2	0
2	H	31	0	0	1	0
2	I	31	0	0	0	0
2	J	31	0	0	5	0
2	K	31	0	0	7	0
2	L	31	0	0	5	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	8	0
4	C	32	0	38	2	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	6	0
4	F	40	0	52	2	0
4	G	18	0	20	1	0
4	H	7	0	9	0	0
4	I	36	0	45	4	0
4	J	22	0	25	2	0
4	K	37	0	47	3	0
4	L	38	0	47	7	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	6	0
9	B	349	0	0	4	0
9	C	406	0	0	4	0
9	D	386	0	0	10	0
9	E	382	0	0	4	0
9	F	371	0	0	6	0
9	G	421	0	0	5	0
9	H	360	0	0	5	0
9	I	408	0	0	2	0
9	J	413	0	0	3	0
9	K	436	0	0	5	0
9	L	339	0	0	4	0
All	All	53046	0	46785	324	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 324 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:392:MET:HE1	2:A:701:X10:C27	1.93	0.98
1:A:122:ASN:HD21	4:A:706:1PE:H251	1.28	0.97
1:K:392:MET:HE1	2:K:701:X10:C23	1.95	0.96
5:D:705:CO3:O2	9:D:801:HOH:O	1.88	0.92

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%)	43	36
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%)	43	36
1	G	520/527 (99%)	509 (98%)	10 (2%)	1 (0%)	43	36
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%)	43	36
1	K	513/527 (97%)	502 (98%)	10 (2%)	1 (0%)	43	36
1	L	508/527 (96%)	498 (98%)	8 (2%)	2 (0%)	30	22
All	All	6203/6324 (98%)	6085 (98%)	111 (2%)	7 (0%)	48	40

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 ⓘ

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%)	425 (99%)	3 (1%)	76	78
1	B	415/454 (91%)	411 (99%)	4 (1%)	68	70
1	C	424/454 (93%)	423 (100%)	1 (0%)	87	90
1	D	422/454 (93%)	422 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	414/454 (91%)	413 (100%)	1 (0%)	87	90
1	F	409/454 (90%)	406 (99%)	3 (1%)	76	78
1	G	429/454 (94%)	427 (100%)	2 (0%)	81	84
1	H	409/454 (90%)	406 (99%)	3 (1%)	76	78
1	I	428/454 (94%)	426 (100%)	2 (0%)	81	84
1	J	421/454 (93%)	419 (100%)	2 (0%)	81	84
1	K	418/454 (92%)	417 (100%)	1 (0%)	87	90
1	L	407/454 (90%)	405 (100%)	2 (0%)	81	84
All	All	5024/5448 (92%)	5000 (100%)	24 (0%)	81	84

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	145	SER
1	I	272	ASN
1	H	608	HIS
1	I	603	ASP
1	B	439	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	420	ASN
1	J	531	ASN
1	L	567	GLN
1	E	181	ASN
1	E	113	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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$
4	1PE	A	705	-	8,8,15	0.26	0	7,7,14	0.14	0
3	SO4	D	706	-	4,4,4	0.23	0	6,6,6	0.28	0
4	1PE	E	703	-	10,10,15	0.15	0	9,9,14	0.31	0
3	SO4	E	702	-	4,4,4	0.17	0	6,6,6	0.18	0
4	1PE	D	704	-	6,6,15	0.29	0	5,5,14	0.18	0
4	1PE	K	702	-	12,12,15	0.20	0	11,11,14	0.44	0
4	1PE	E	705	-	11,11,15	0.20	0	10,10,14	0.14	0
4	1PE	D	703	-	12,12,15	0.15	0	11,11,14	0.15	0
3	SO4	A	702	-	4,4,4	0.23	0	6,6,6	0.11	0
4	1PE	F	705	-	6,6,15	0.23	0	5,5,14	0.14	0
3	SO4	G	703	-	4,4,4	0.29	0	6,6,6	0.11	0
4	1PE	F	706	-	9,9,15	0.18	0	8,8,14	0.10	0
2	X10	I	701	6	32,33,33	1.30	3 (9%)	42,45,45	1.58	9 (21%)
4	1PE	F	703	-	12,12,15	0.24	0	11,11,14	0.20	0
5	CO3	I	706	-	3,3,3	1.65	1 (33%)	2,3,3	1.56	0
4	1PE	A	707	-	12,12,15	0.22	0	11,11,14	0.17	0
3	SO4	A	703	-	4,4,4	0.28	0	6,6,6	0.39	0
4	1PE	C	704	-	12,12,15	0.17	0	11,11,14	0.19	0
3	SO4	F	702	-	4,4,4	0.28	0	6,6,6	0.17	0
3	SO4	G	702	-	4,4,4	0.29	0	6,6,6	0.40	0
4	1PE	H	703	-	6,6,15	0.21	0	5,5,14	0.16	0
2	X10	B	1401	6	32,33,33	1.40	4 (12%)	42,45,45	2.10	15 (35%)
4	1PE	F	704	-	9,9,15	0.06	0	8,8,14	0.27	0
2	X10	D	701	6	32,33,33	1.53	5 (15%)	42,45,45	1.44	10 (23%)
2	X10	G	701	6	32,33,33	1.26	3 (9%)	42,45,45	1.46	8 (19%)
4	1PE	L	704	-	12,12,15	0.24	0	11,11,14	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CO3	K	705	-	3,3,3	0.88	0	2,3,3	0.72	0
4	1PE	D	702	-	9,9,15	0.08	0	8,8,14	0.28	0
5	CO3	J	705	-	3,3,3	1.00	0	2,3,3	0.88	0
3	SO4	H	702	-	4,4,4	0.24	0	6,6,6	0.26	0
5	CO3	C	706	-	3,3,3	1.03	0	2,3,3	0.55	0
3	SO4	I	702	-	4,4,4	0.26	0	6,6,6	0.11	0
4	1PE	J	704	-	12,12,15	0.13	0	11,11,14	0.18	0
4	1PE	K	704	-	12,12,15	0.22	0	11,11,14	0.24	0
4	1PE	I	705	-	6,6,15	0.17	0	5,5,14	0.13	0
4	1PE	L	705	-	15,15,15	0.16	0	14,14,14	0.47	0
2	X10	H	701	6	32,33,33	1.33	4 (12%)	42,45,45	1.30	5 (11%)
5	CO3	L	706	-	3,3,3	0.89	0	2,3,3	0.69	0
2	X10	L	701	6	32,33,33	1.53	5 (15%)	42,45,45	1.30	6 (14%)
4	1PE	C	703	-	10,10,15	0.23	0	9,9,14	0.36	0
5	CO3	D	705	-	3,3,3	0.47	0	2,3,3	0.68	0
5	CO3	B	1402	-	3,3,3	0.25	0	2,3,3	1.59	1 (50%)
2	X10	A	701	6	32,33,33	1.38	3 (9%)	42,45,45	1.70	10 (23%)
4	1PE	E	704	-	12,12,15	0.19	0	11,11,14	0.26	0
3	SO4	C	702	-	4,4,4	0.30	0	6,6,6	0.33	0
2	X10	K	701	6	32,33,33	1.40	4 (12%)	42,45,45	2.00	13 (30%)
2	X10	J	701	6	32,33,33	1.37	4 (12%)	42,45,45	1.73	10 (23%)
5	CO3	F	707	-	3,3,3	0.87	0	2,3,3	1.97	1 (50%)
8	2PE	H	705	-	25,25,27	0.21	0	24,24,26	0.16	0
3	SO4	A	704	-	4,4,4	0.26	0	6,6,6	0.18	0
4	1PE	L	703	-	8,8,15	0.24	0	7,7,14	0.14	0
5	CO3	E	706	-	3,3,3	1.05	0	2,3,3	1.62	0
4	1PE	I	703	-	14,14,15	0.21	0	13,13,14	0.23	0
4	1PE	I	704	-	12,12,15	0.13	0	11,11,14	0.16	0
4	1PE	G	705	-	6,6,15	0.13	0	5,5,14	0.10	0
5	CO3	A	708	-	3,3,3	0.52	0	2,3,3	0.70	0
4	1PE	C	705	-	6,6,15	0.19	0	5,5,14	0.13	0
2	X10	E	701	6	32,33,33	1.30	4 (12%)	42,45,45	1.92	14 (33%)
4	1PE	A	706	-	11,11,15	11.06	1 (9%)	10,10,14	2.35	2 (20%)
5	CO3	H	704	-	3,3,3	0.65	0	2,3,3	1.68	1 (50%)
4	1PE	J	703	-	8,8,15	0.25	0	7,7,14	0.18	0
2	X10	F	701	6	32,33,33	1.33	4 (12%)	42,45,45	1.66	10 (23%)
4	1PE	K	703	-	10,10,15	0.26	0	9,9,14	0.17	0
2	X10	C	701	6	32,33,33	1.38	4 (12%)	42,45,45	1.86	12 (28%)
4	1PE	G	704	-	10,10,15	0.17	0	9,9,14	0.12	0
3	SO4	J	702	-	4,4,4	0.15	0	6,6,6	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	L	702	-	4,4,4	0.42	0	6,6,6	0.23	0
5	CO3	G	706	-	3,3,3	0.55	0	2,3,3	0.99	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	A	705	-	-	6/6/6/13	-
4	1PE	E	703	-	-	5/8/8/13	-
4	1PE	D	704	-	-	4/4/4/13	-
4	1PE	K	702	-	-	3/10/10/13	-
4	1PE	E	705	-	-	2/9/9/13	-
4	1PE	D	703	-	-	3/10/10/13	-
4	1PE	F	705	-	-	0/4/4/13	-
4	1PE	F	706	-	-	3/7/7/13	-
2	X10	I	701	6	-	4/23/23/23	0/3/3/3
4	1PE	F	703	-	-	5/10/10/13	-
4	1PE	C	704	-	-	2/10/10/13	-
4	1PE	H	703	-	-	2/4/4/13	-
2	X10	B	1401	6	-	4/23/23/23	0/3/3/3
4	1PE	F	704	-	-	1/7/7/13	-
2	X10	D	701	6	-	4/23/23/23	0/3/3/3
2	X10	G	701	6	-	4/23/23/23	0/3/3/3
4	1PE	L	704	-	-	9/10/10/13	-
4	1PE	D	702	-	-	1/7/7/13	-
4	1PE	J	704	-	-	5/10/10/13	-
4	1PE	K	704	-	-	2/10/10/13	-
4	1PE	I	705	-	-	0/4/4/13	-
4	1PE	L	705	-	-	7/13/13/13	-
2	X10	H	701	6	-	4/23/23/23	0/3/3/3
2	X10	L	701	6	-	0/23/23/23	0/3/3/3
4	1PE	C	703	-	-	4/8/8/13	-
2	X10	A	701	6	-	1/23/23/23	0/3/3/3
4	1PE	E	704	-	-	8/10/10/13	-
2	X10	K	701	6	-	0/23/23/23	0/3/3/3
2	X10	J	701	6	-	5/23/23/23	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2PE	H	705	-	-	12/23/23/25	-
4	1PE	L	703	-	-	5/6/6/13	-
4	1PE	I	703	-	-	2/12/12/13	-
4	1PE	I	704	-	-	3/10/10/13	-
4	1PE	G	705	-	-	3/4/4/13	-
4	1PE	C	705	-	-	2/4/4/13	-
2	X10	E	701	6	-	4/23/23/23	0/3/3/3
4	1PE	A	706	-	-	6/9/9/13	-
4	1PE	J	703	-	-	5/6/6/13	-
2	X10	F	701	6	-	4/23/23/23	0/3/3/3
4	1PE	K	703	-	-	3/8/8/13	-
2	X10	C	701	6	-	4/23/23/23	0/3/3/3
4	1PE	G	704	-	-	2/8/8/13	-
4	1PE	A	707	-	-	5/10/10/13	-

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	706	1PE	OH4-C13	36.69	3.00	1.42
2	J	701	X10	C02-N11	5.65	1.46	1.34
2	C	701	X10	C02-N11	5.60	1.45	1.34
2	A	701	X10	C02-N11	5.55	1.45	1.34
2	K	701	X10	C02-N11	5.40	1.45	1.34

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	701	X10	C22-C21-C20	-6.41	110.09	120.84
4	A	706	1PE	OH4-C13-C23	6.22	138.71	110.35
2	B	1401	X10	C22-C21-C20	-5.99	110.80	120.84
2	C	701	X10	C29-C21-C20	-5.45	111.70	120.84
2	E	701	X10	C29-C21-C20	-5.18	112.15	120.84

There are no chirality outliers.

5 of 158 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
2	H	701	X10	C19-C20-C21-C29
2	F	701	X10	C10-C05-N04-C03
8	H	705	2PE	C21-C20-O19-C18
2	H	701	X10	C19-C20-C21-C22

There are no ring outliers.

40 monomers are involved in 102 short contacts:

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

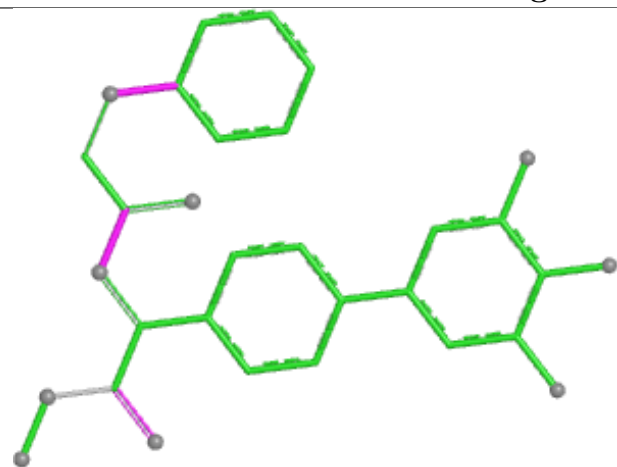
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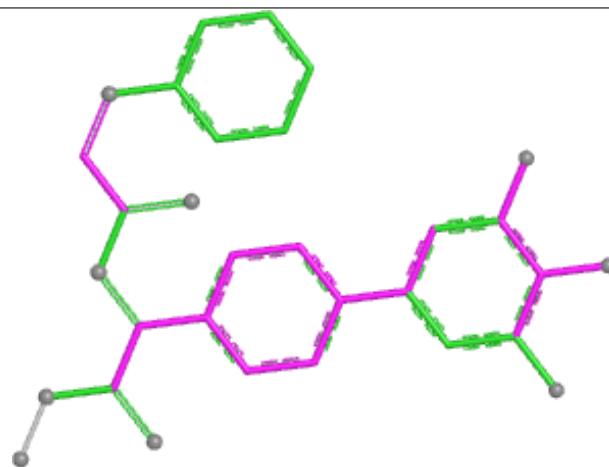
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	706	1PE	4	0
5	H	704	CO3	1	0
4	J	703	1PE	2	0
2	F	701	X10	5	0
4	K	703	1PE	1	0
2	C	701	X10	4	0
5	G	706	CO3	2	0

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

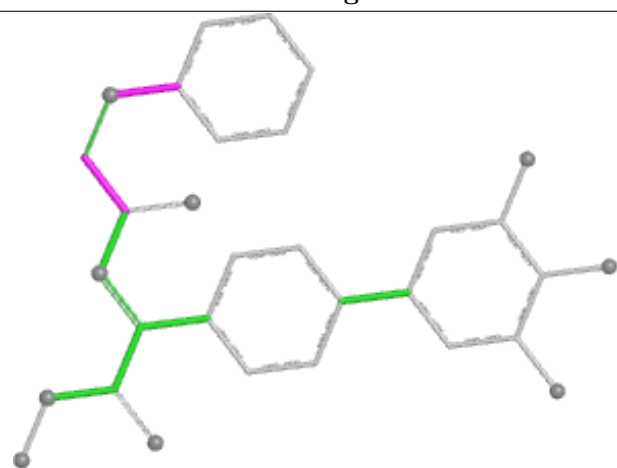
Ligand X10 I 701



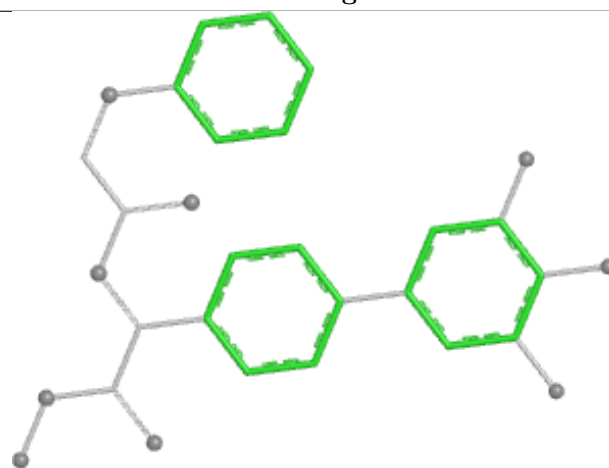
Bond lengths



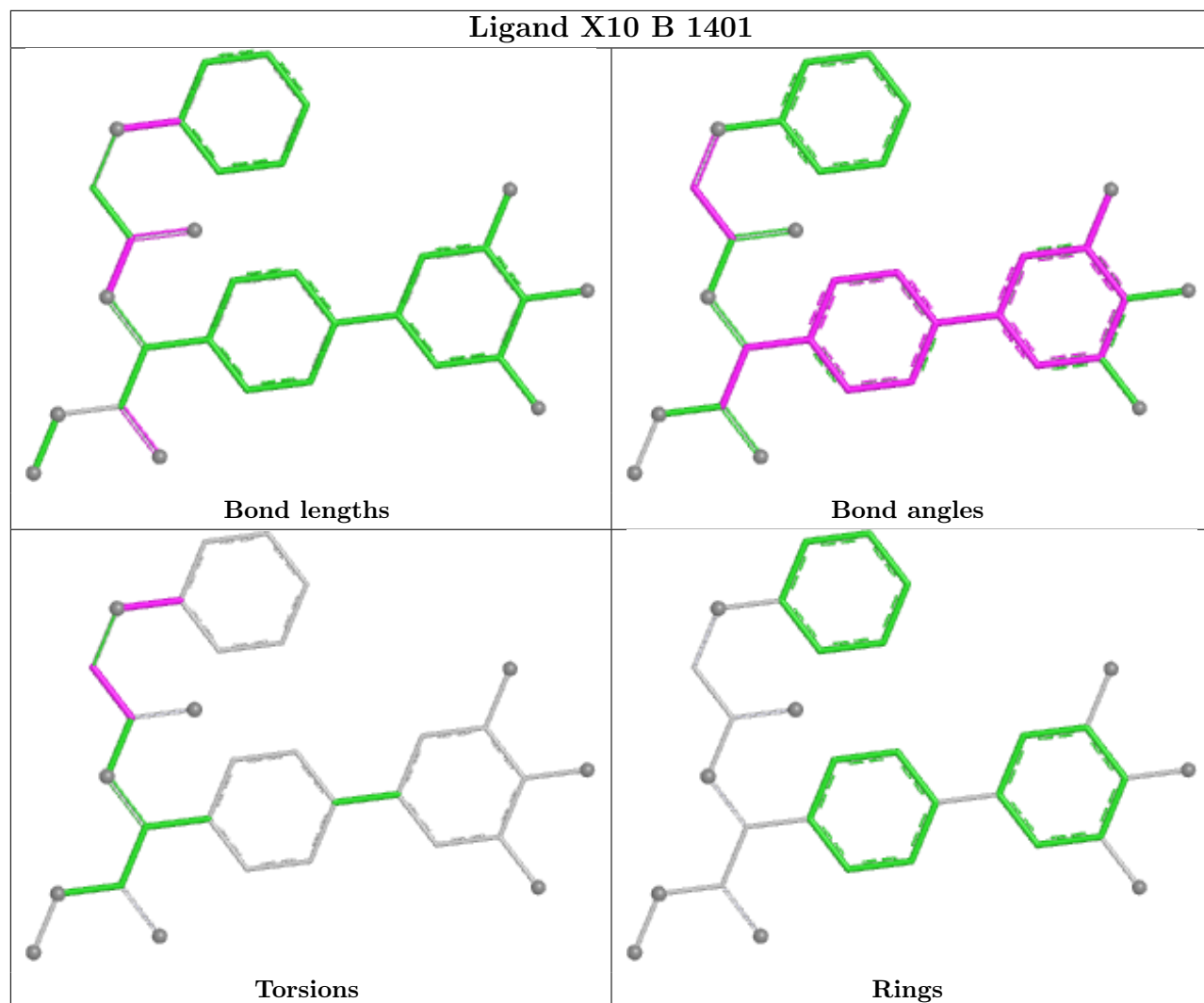
Bond angles



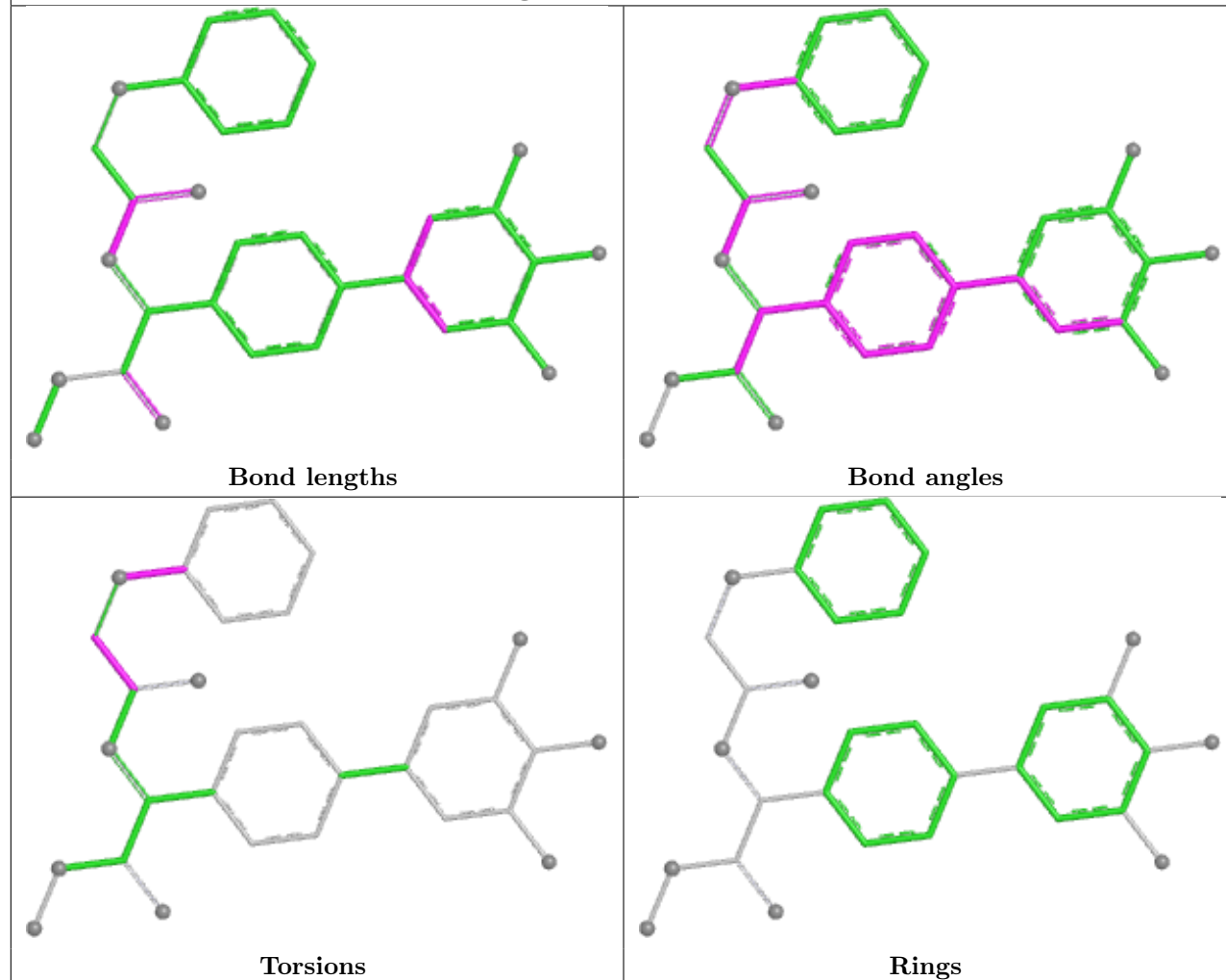
Torsions



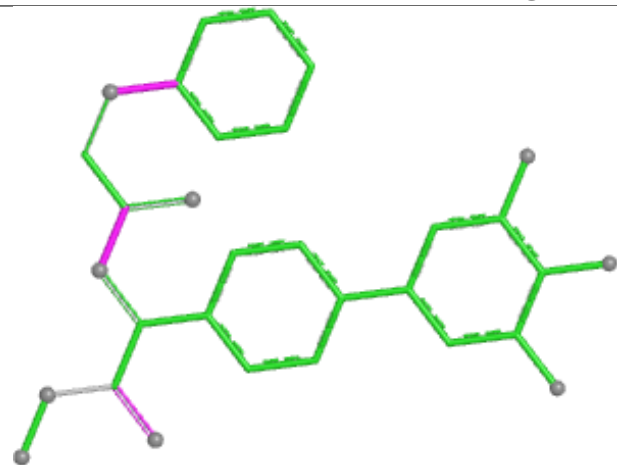
Rings



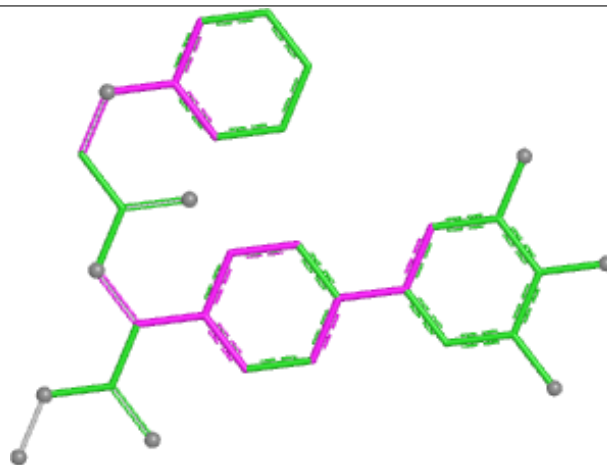
Ligand X10 D 701



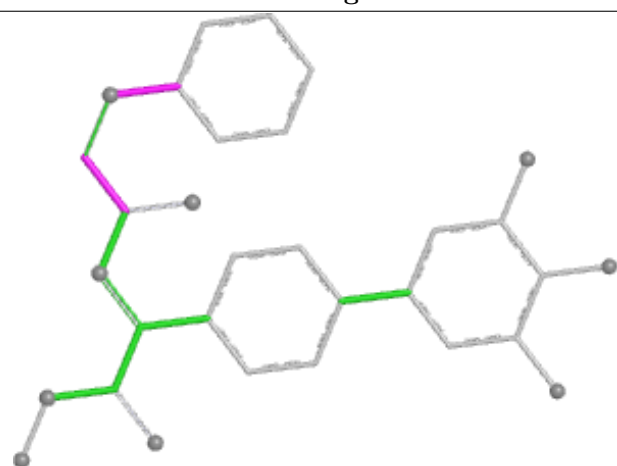
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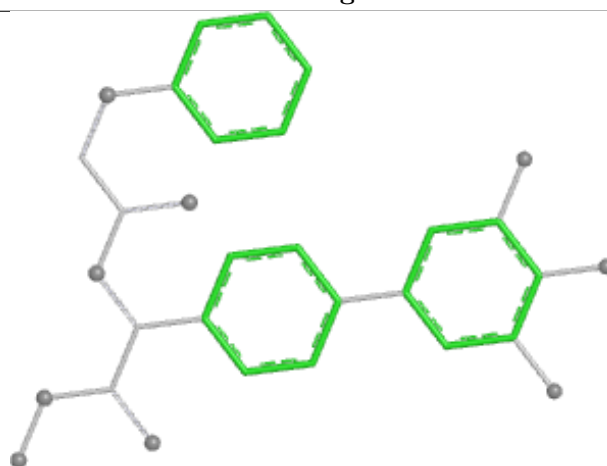
Bond lengths



Bond angles

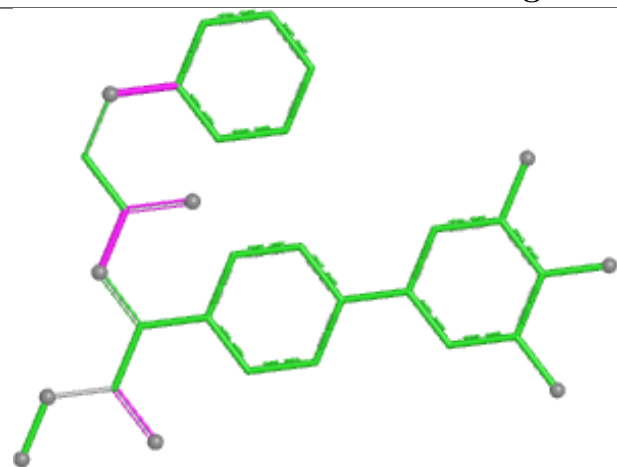


Torsions

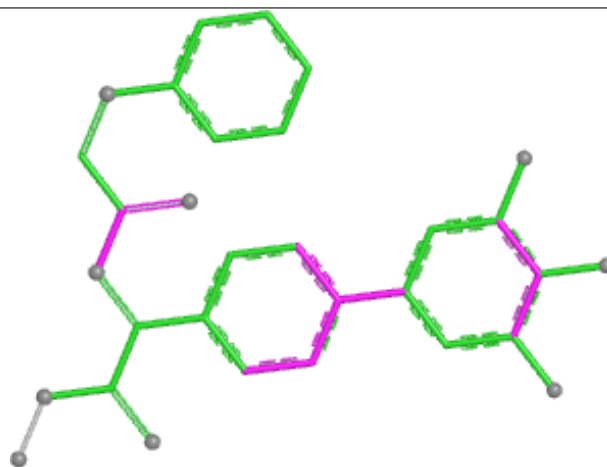


Rings

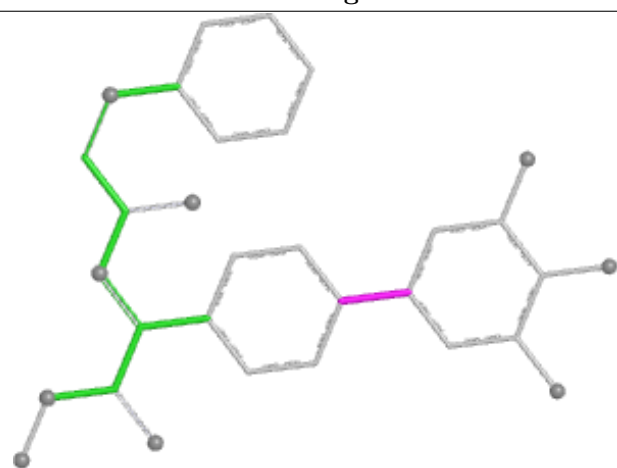
Ligand X10 H 701



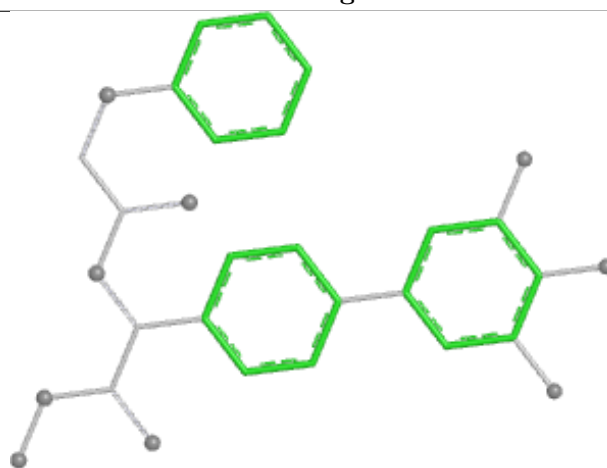
Bond lengths



Bond angles

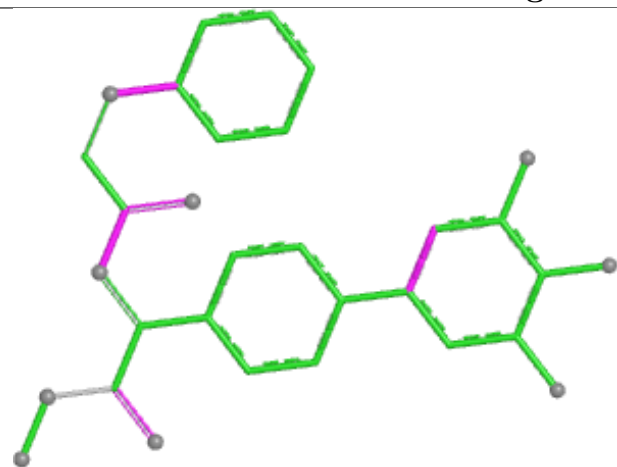


Torsions

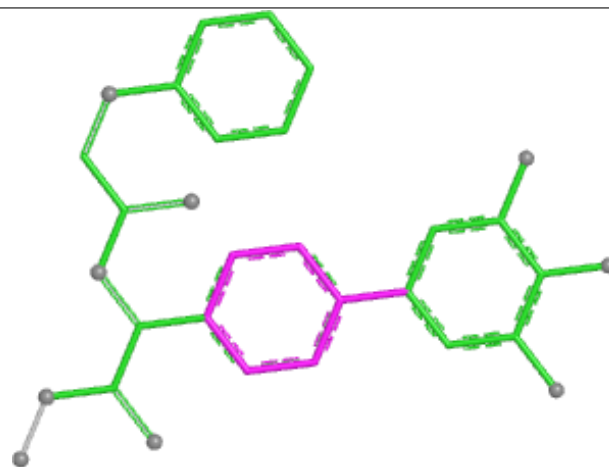


Rings

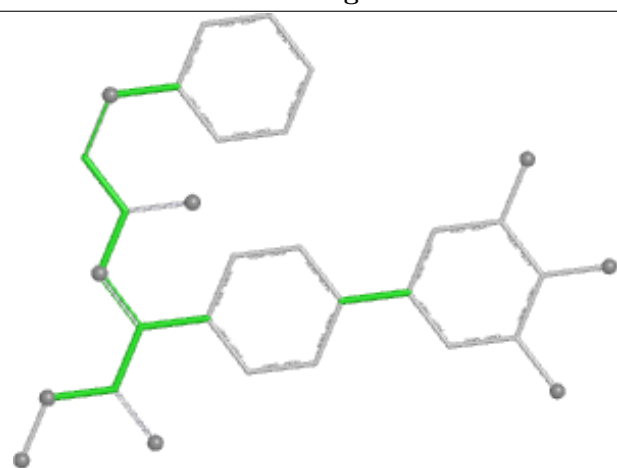
Ligand X10 L 701



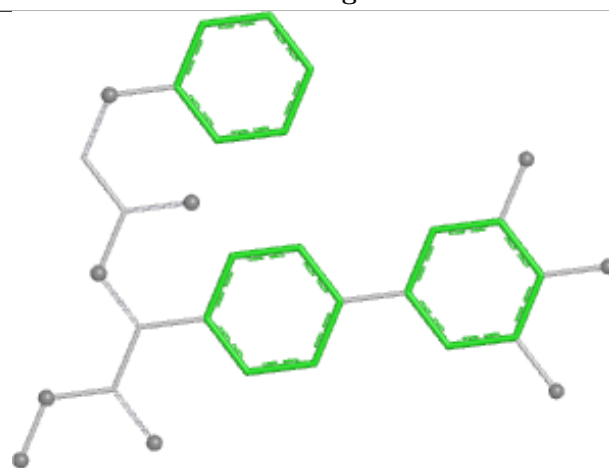
Bond lengths



Bond angles

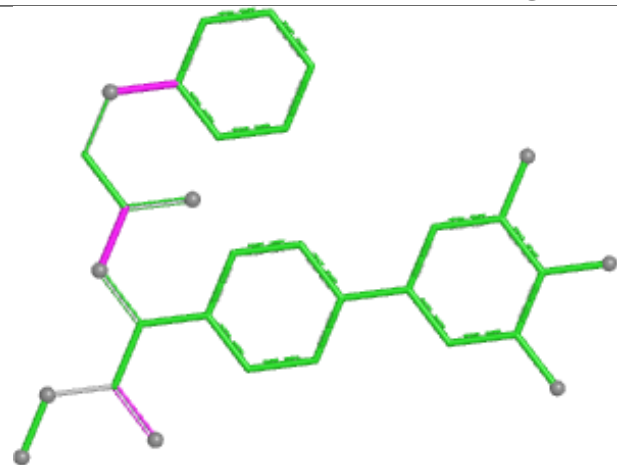


Torsions

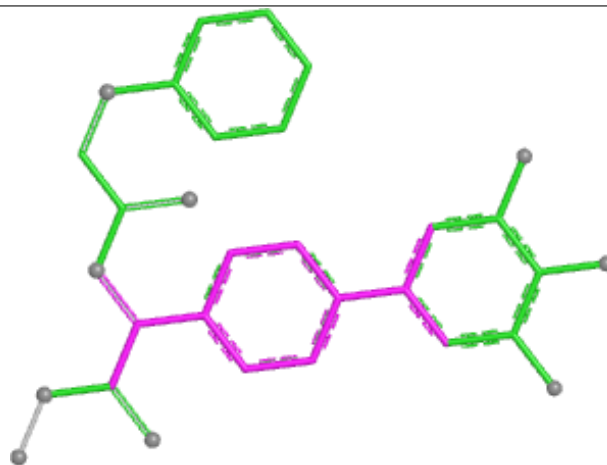


Rings

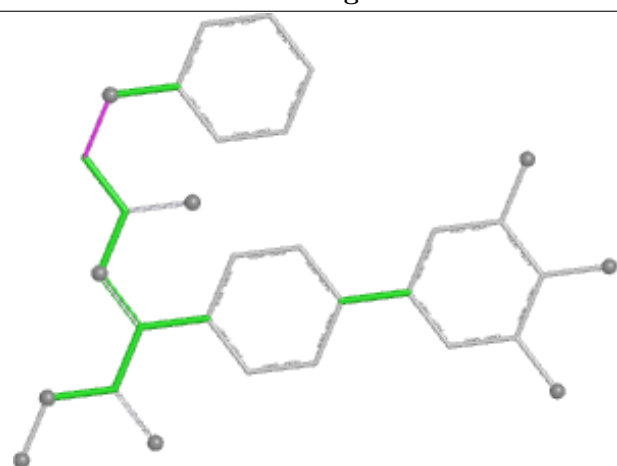
Ligand X10 A 701



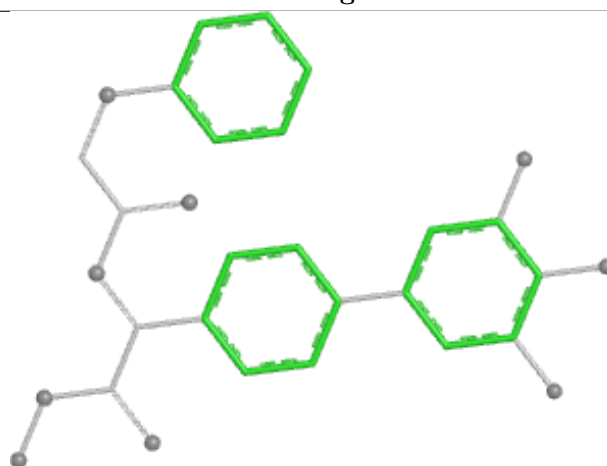
Bond lengths



Bond angles

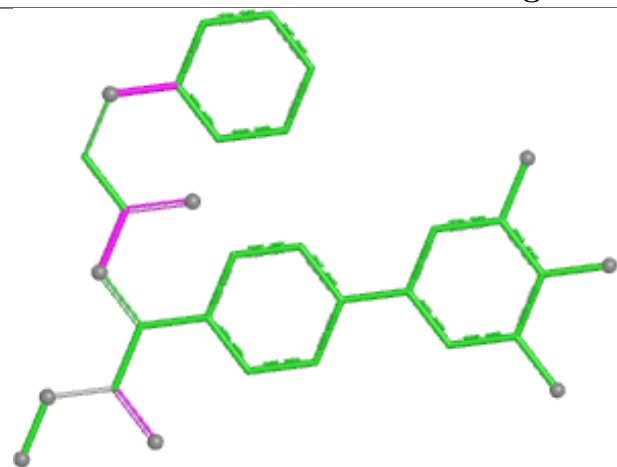


Torsions

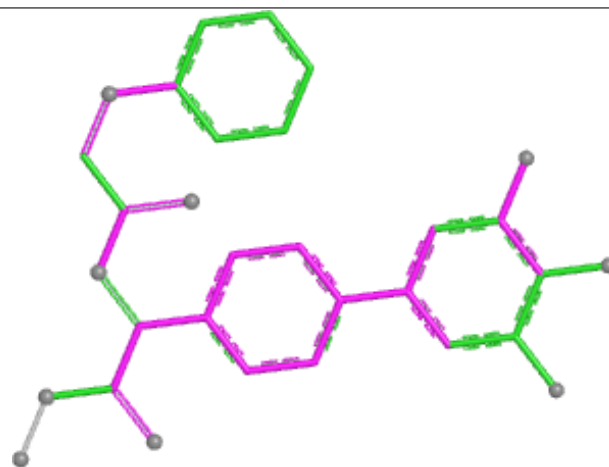


Rings

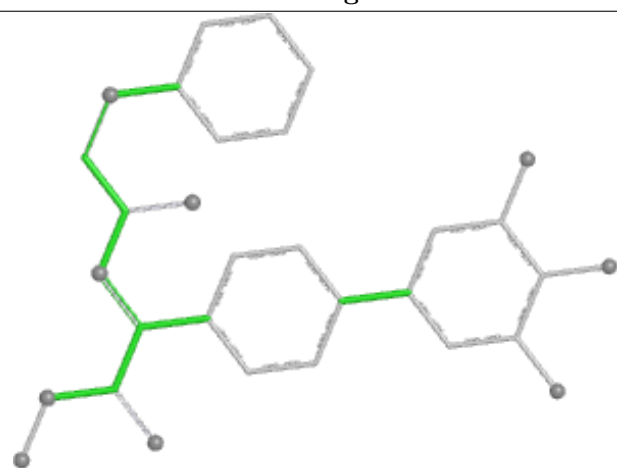
Ligand X10 K 701



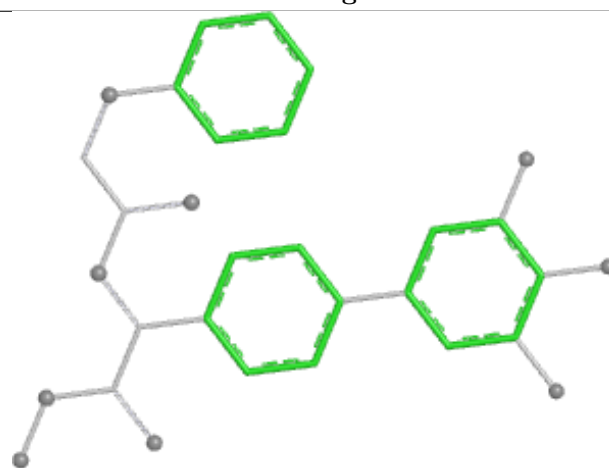
Bond lengths



Bond angles

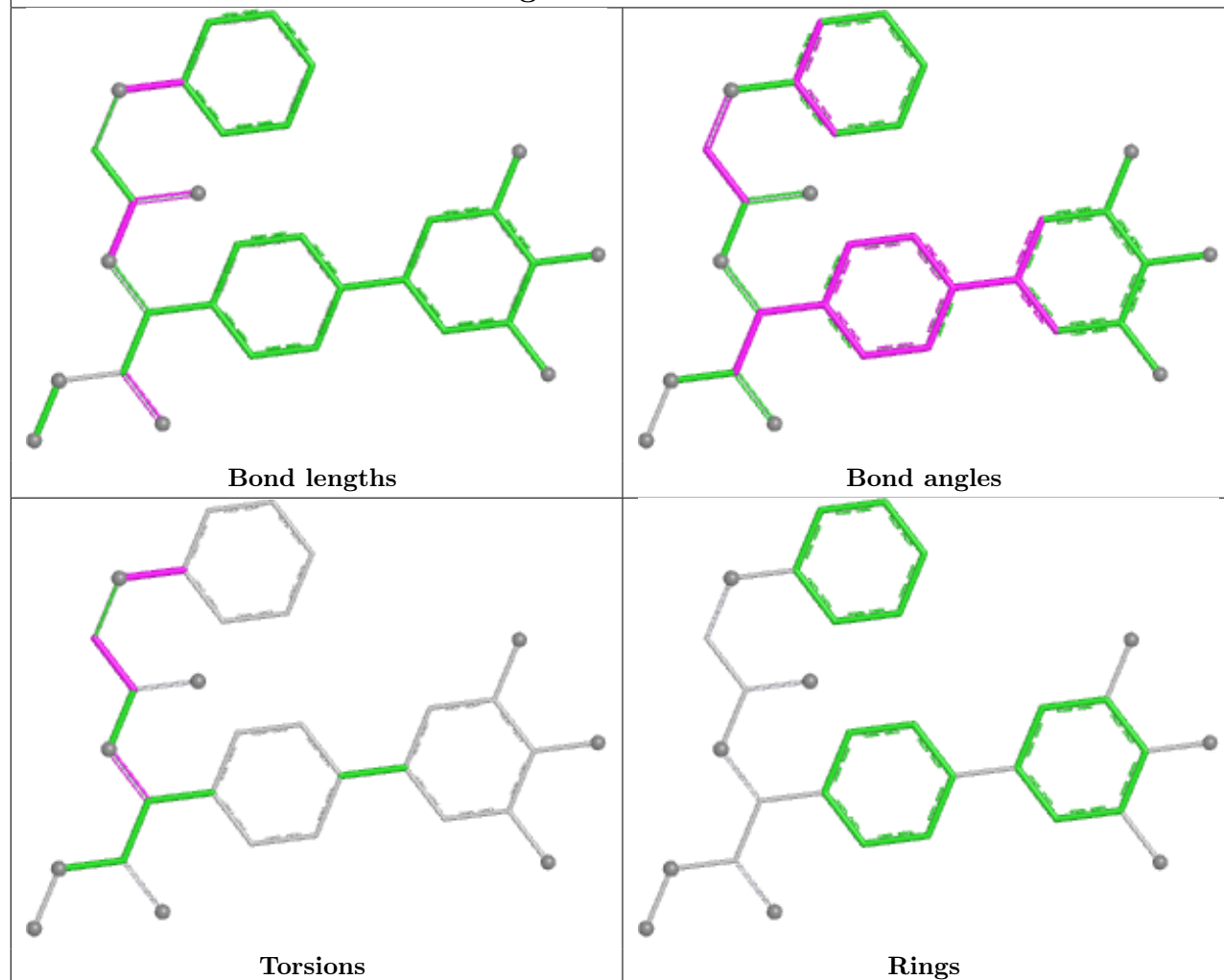


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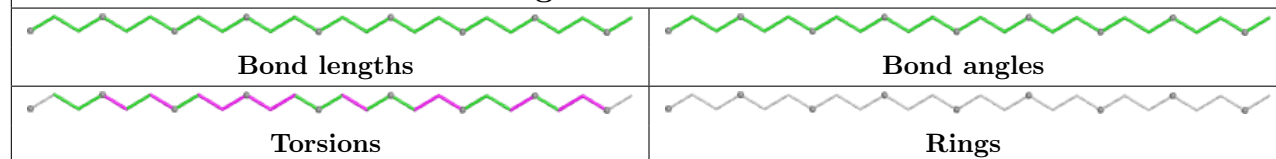


Rings

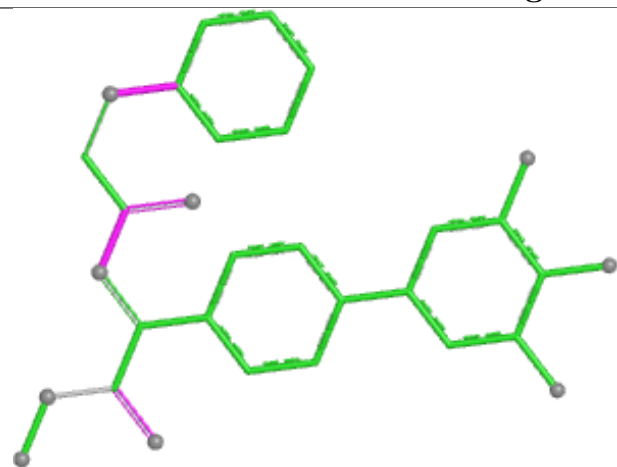
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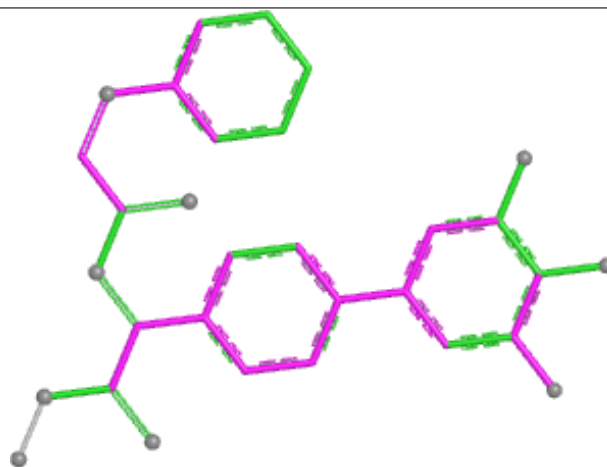
Ligand 2PE H 705



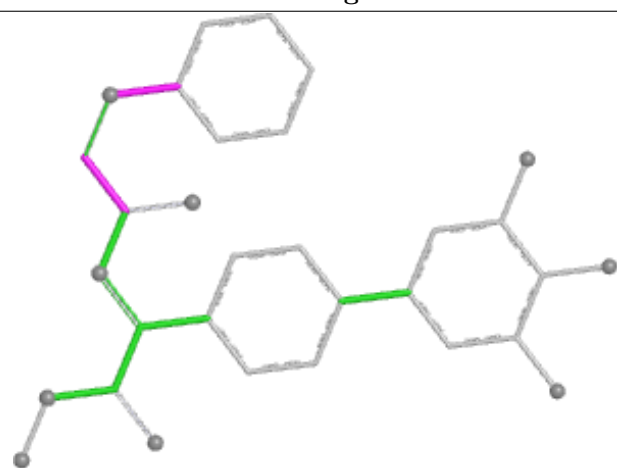
Ligand X10 E 701



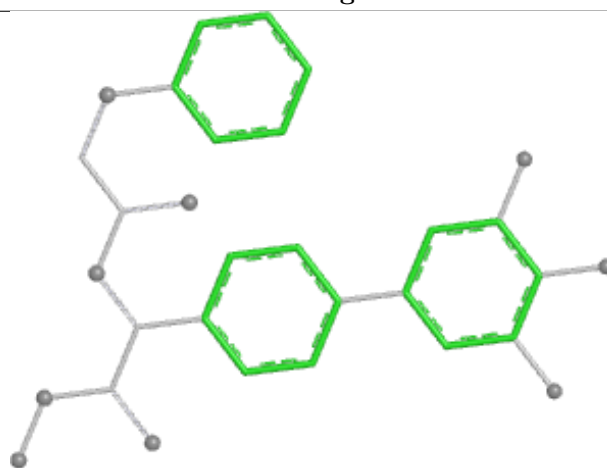
Bond lengths



Bond angles

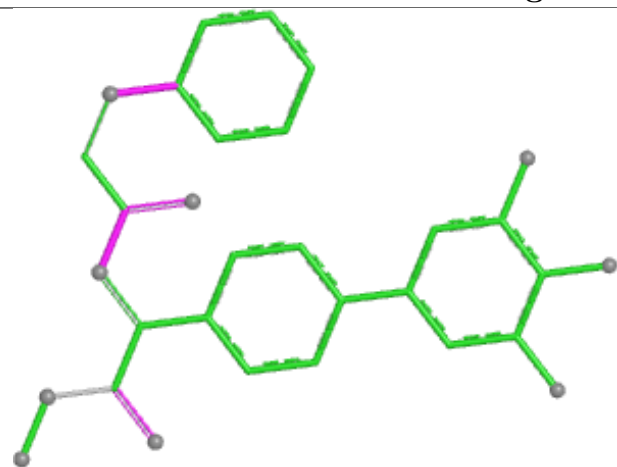


Torsions

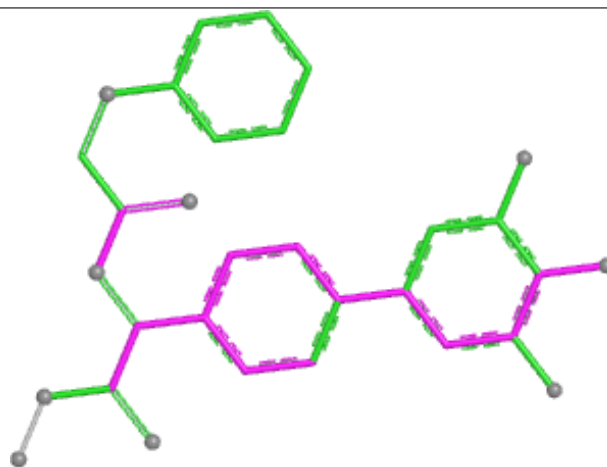


Rings

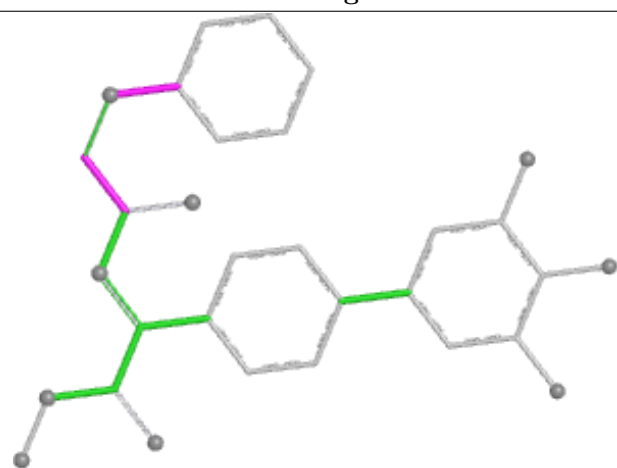
Ligand X10 F 701



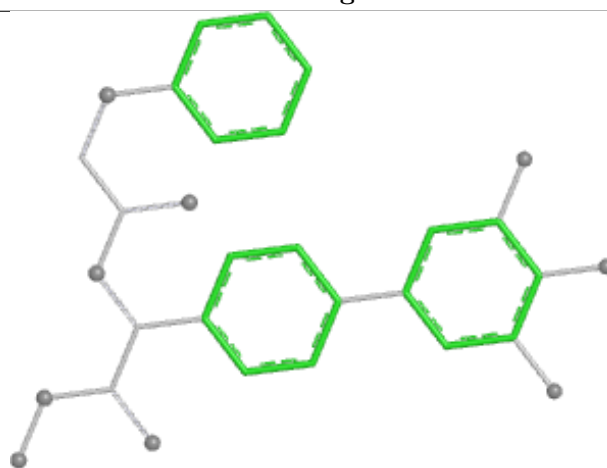
Bond lengths



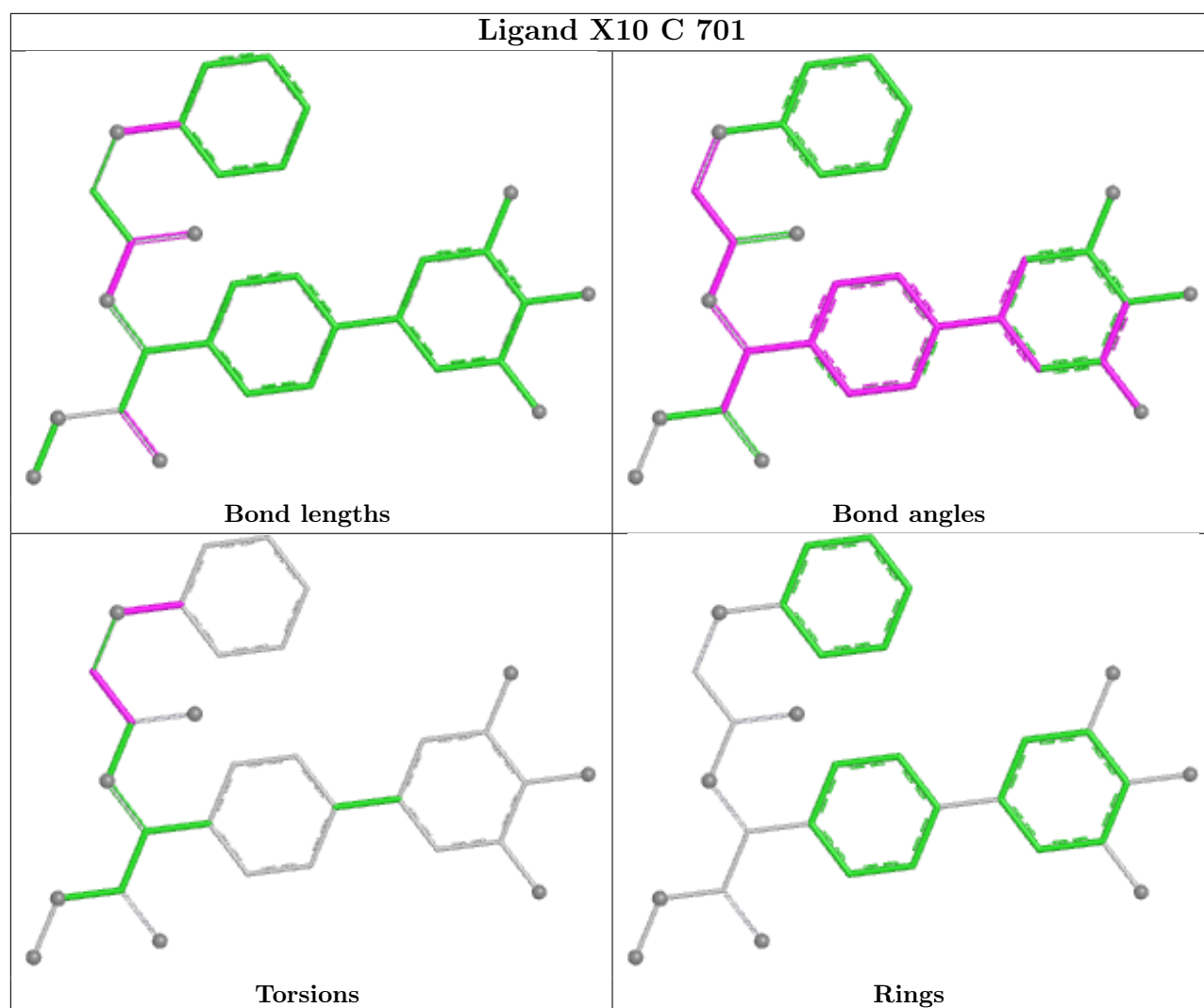
Bond angles



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	519/527 (98%)	-0.37	1 (0%) 91 92	15, 24, 40, 61	1 (0%)
1	B	521/527 (98%)	-0.18	8 (1%) 72 75	18, 26, 48, 72	1 (0%)
1	C	525/527 (99%)	-0.33	4 (0%) 82 85	18, 24, 41, 71	2 (0%)
1	D	522/527 (99%)	-0.34	12 (2%) 61 65	17, 24, 41, 86	1 (0%)
1	E	514/527 (97%)	-0.38	7 (1%) 73 76	17, 23, 36, 69	1 (0%)
1	F	515/527 (97%)	-0.22	7 (1%) 73 76	19, 25, 49, 74	1 (0%)
1	G	521/527 (98%)	-0.32	7 (1%) 75 78	17, 24, 40, 67	1 (0%)
1	H	522/527 (99%)	-0.16	10 (1%) 66 70	19, 26, 48, 69	0
1	I	525/527 (99%)	-0.31	8 (1%) 72 75	18, 24, 42, 84	1 (0%)
1	J	519/527 (98%)	-0.43	4 (0%) 82 85	17, 23, 38, 79	1 (0%)
1	K	517/527 (98%)	-0.41	10 (1%) 66 70	17, 23, 37, 78	0
1	L	512/527 (97%)	-0.15	11 (2%) 63 67	18, 27, 50, 86	0
All	All	6232/6324 (98%)	-0.30	89 (1%) 73 76	15, 24, 45, 86	10 (0%)

The worst 5 of 89 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	255	THR	6.6
1	E	603	ASP	4.4
1	H	259	VAL	4.3
1	D	604	ALA	4.2
1	K	85	ALA	4.2

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ZN	F	708	1/1	0.72	0.12	26,26,26,26	1
6	ZN	A	709	1/1	0.73	0.14	22,22,22,22	1
6	ZN	E	707	1/1	0.77	0.12	28,28,28,28	1
2	X10	L	701	31/31	0.77	0.17	30,45,58,62	3
4	1PE	A	707	13/16	0.81	0.13	40,54,60,64	0
6	ZN	I	707	1/1	0.82	0.12	22,22,22,22	1
2	X10	C	701	31/31	0.83	0.15	28,39,53,59	9
4	1PE	A	705	9/16	0.83	0.14	31,36,47,51	0
2	X10	D	701	31/31	0.83	0.14	28,39,50,51	3
4	1PE	I	705	8/16	0.83	0.13	33,46,50,50	0
4	1PE	F	705	7/16	0.84	0.12	37,46,49,52	0
2	X10	B	1401	31/31	0.84	0.14	28,43,69,82	0
2	X10	E	701	31/31	0.85	0.13	27,38,41,44	9
4	1PE	F	706	10/16	0.85	0.12	41,51,58,63	0
4	1PE	G	705	7/16	0.85	0.12	45,48,51,52	0
4	1PE	C	705	8/16	0.85	0.14	34,41,48,54	0
5	CO3	A	708	4/4	0.86	0.22	19,31,35,43	4
2	X10	F	701	31/31	0.86	0.14	28,40,58,60	7
4	1PE	D	704	7/16	0.86	0.11	31,43,49,56	0
6	ZN	E	708	1/1	0.86	0.08	21,21,21,21	1
4	1PE	K	703	11/16	0.86	0.11	28,36,50,53	0
6	ZN	F	709	1/1	0.86	0.07	21,21,21,21	1
4	1PE	K	704	13/16	0.86	0.11	38,43,54,56	0
6	ZN	I	708	1/1	0.86	0.08	19,19,19,19	1
4	1PE	J	704	13/16	0.87	0.11	36,45,54,60	0
2	X10	J	701	31/31	0.87	0.12	31,38,48,60	3
2	X10	H	701	31/31	0.87	0.12	25,38,52,53	5
4	1PE	L	705	16/16	0.87	0.13	38,46,64,67	0
2	X10	I	701	31/31	0.87	0.13	23,37,47,54	5
4	1PE	F	703	13/16	0.87	0.11	31,41,49,49	0
8	2PE	H	705	26/28	0.87	0.12	33,52,62,71	0
4	1PE	E	705	12/16	0.88	0.10	38,44,46,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	X10	G	701	31/31	0.88	0.13	26,34,53,54	7
5	CO3	F	707	4/4	0.88	0.18	18,30,35,44	0
5	CO3	L	706	4/4	0.88	0.26	16,34,43,48	0
4	1PE	E	704	13/16	0.88	0.10	29,44,51,52	0
4	1PE	L	704	13/16	0.88	0.11	38,46,56,60	0
3	SO4	G	702	5/5	0.89	0.09	34,43,59,61	0
3	SO4	G	703	5/5	0.89	0.11	55,59,70,77	0
3	SO4	I	702	5/5	0.89	0.12	45,52,64,69	0
2	X10	K	701	31/31	0.89	0.12	23,40,51,62	3
4	1PE	A	706	12/16	0.89	0.12	28,40,45,47	0
2	X10	A	701	31/31	0.89	0.13	27,45,54,56	4
3	SO4	F	702	5/5	0.89	0.10	53,60,65,76	0
4	1PE	I	703	15/16	0.89	0.11	32,42,49,50	0
5	CO3	K	705	4/4	0.89	0.17	17,36,40,43	0
4	1PE	D	703	13/16	0.90	0.09	31,46,54,58	0
3	SO4	A	703	5/5	0.90	0.09	33,40,58,61	0
5	CO3	I	706	4/4	0.90	0.14	18,24,27,41	0
4	1PE	L	703	9/16	0.90	0.11	28,36,49,52	0
4	1PE	J	703	9/16	0.90	0.10	21,32,41,42	0
4	1PE	E	703	11/16	0.90	0.11	22,33,48,48	0
6	ZN	B	1404	1/1	0.90	0.26	74,74,74,74	0
5	CO3	B	1402	4/4	0.91	0.12	18,27,32,36	0
4	1PE	I	704	13/16	0.91	0.10	24,34,51,53	0
4	1PE	C	704	13/16	0.91	0.10	36,41,46,48	0
6	ZN	A	710	1/1	0.91	0.08	18,18,18,18	1
5	CO3	D	705	4/4	0.92	0.13	17,17,30,39	4
5	CO3	E	706	4/4	0.92	0.15	18,29,39,48	0
4	1PE	G	704	11/16	0.92	0.09	30,37,51,58	0
5	CO3	G	706	4/4	0.92	0.20	18,18,50,53	0
4	1PE	C	703	11/16	0.92	0.10	29,33,47,53	0
5	CO3	J	705	4/4	0.92	0.18	17,17,44,48	4
4	1PE	K	702	13/16	0.93	0.09	26,32,55,57	0
4	1PE	H	703	7/16	0.93	0.10	34,39,47,47	0
5	CO3	C	706	4/4	0.93	0.14	17,26,37,41	0
5	CO3	H	704	4/4	0.94	0.11	18,23,34,45	0
3	SO4	J	702	5/5	0.95	0.12	27,34,36,38	5
6	ZN	B	1403	1/1	0.95	0.27	58,58,58,58	0
4	1PE	D	702	10/16	0.95	0.07	27,31,44,49	0
4	1PE	F	704	10/16	0.95	0.07	26,35,45,47	0
3	SO4	C	702	5/5	0.95	0.14	21,32,39,42	5
3	SO4	A	704	5/5	0.96	0.10	25,35,37,39	5
6	ZN	D	707	1/1	0.96	0.04	21,21,21,21	1

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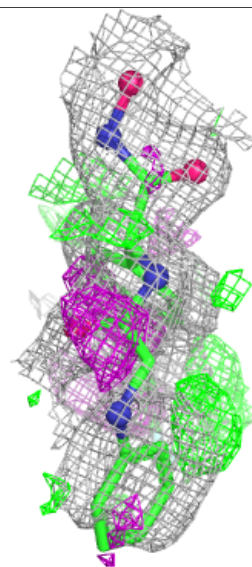
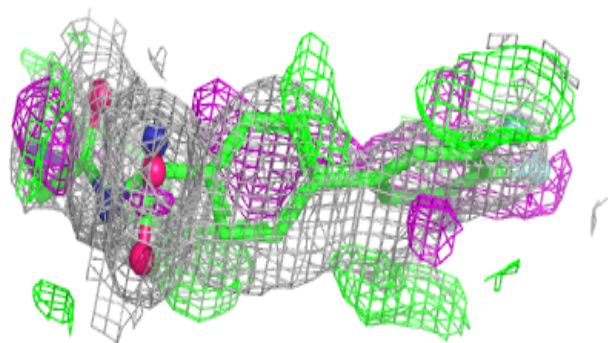
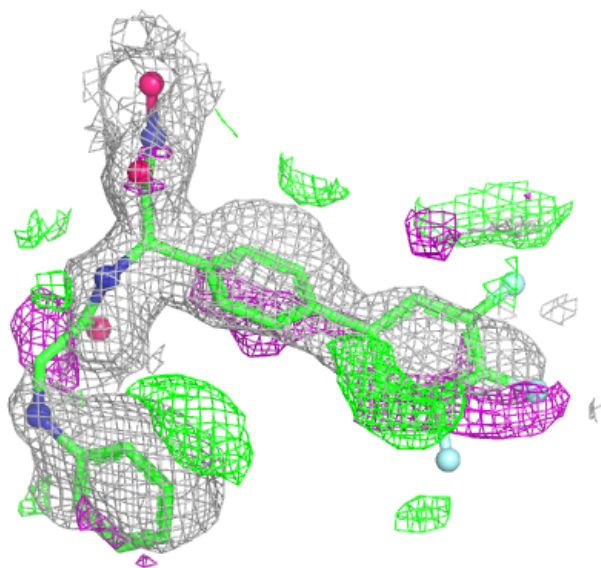
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	E	702	5/5	0.96	0.10	28,29,40,41	5
6	ZN	C	707	1/1	0.97	0.06	22,22,22,22	1
6	ZN	D	708	1/1	0.97	0.03	19,19,19,19	1
6	ZN	K	707	1/1	0.97	0.04	19,19,19,19	1
7	NA	G	709	1/1	0.97	0.04	22,22,22,22	0
7	NA	J	708	1/1	0.97	0.04	21,21,21,21	0
6	ZN	H	706	1/1	0.97	0.03	22,22,22,22	1
6	ZN	G	708	1/1	0.98	0.03	20,20,20,20	1
6	ZN	L	707	1/1	0.98	0.04	27,27,27,27	1
6	ZN	L	708	1/1	0.98	0.04	19,19,19,19	1
6	ZN	C	708	1/1	0.98	0.02	18,18,18,18	1
6	ZN	J	706	1/1	0.98	0.03	23,23,23,23	1
6	ZN	K	706	1/1	0.98	0.05	19,19,19,19	1
3	SO4	D	706	5/5	0.99	0.04	19,20,21,25	0
3	SO4	L	702	5/5	0.99	0.04	17,19,20,22	0
6	ZN	H	707	1/1	0.99	0.06	19,19,19,19	1
3	SO4	H	702	5/5	0.99	0.03	19,19,19,21	0
7	NA	A	711	1/1	0.99	0.03	25,25,25,25	0
7	NA	B	1405	1/1	0.99	0.02	23,23,23,23	0
7	NA	D	709	1/1	0.99	0.03	22,22,22,22	0
7	NA	F	710	1/1	0.99	0.03	23,23,23,23	0
3	SO4	A	702	5/5	0.99	0.03	18,18,21,22	0
7	NA	H	708	1/1	0.99	0.04	23,23,23,23	0
7	NA	I	709	1/1	0.99	0.04	20,20,20,20	0
6	ZN	G	707	1/1	0.99	0.03	25,25,25,25	1
7	NA	K	708	1/1	0.99	0.03	21,21,21,21	0
6	ZN	J	707	1/1	0.99	0.02	21,21,21,21	1

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.

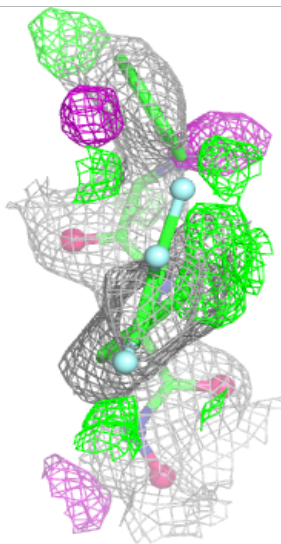
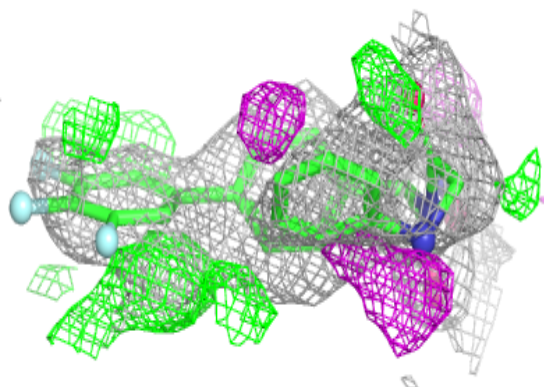
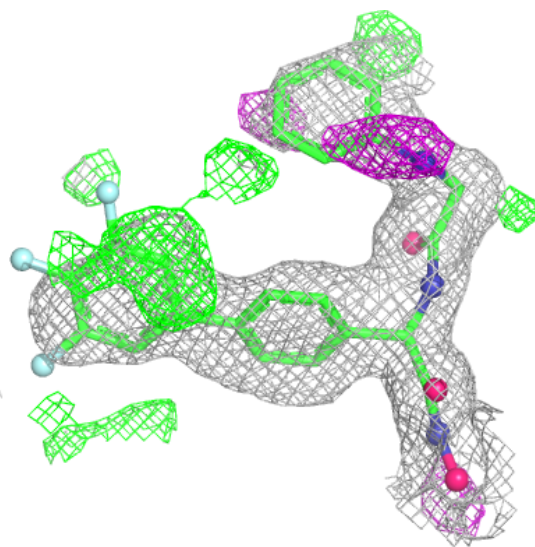
Electron density around X10 L 701:

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



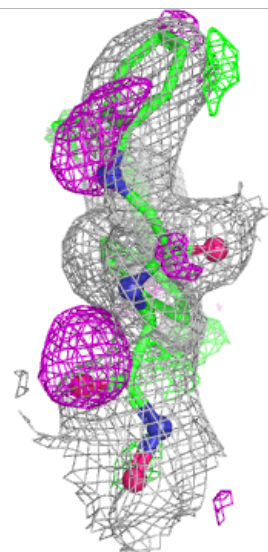
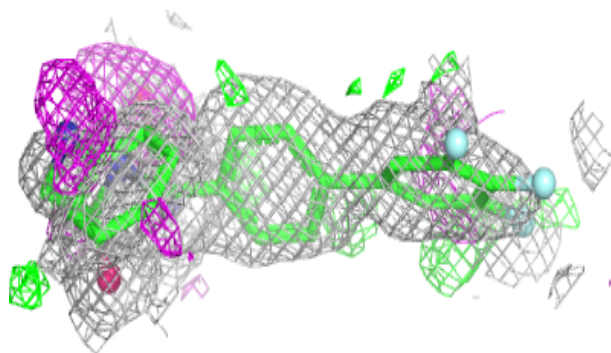
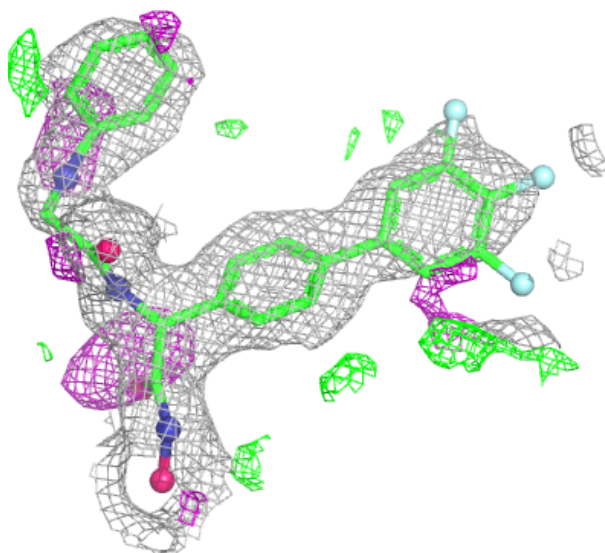
Electron density around X10 C 701:

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



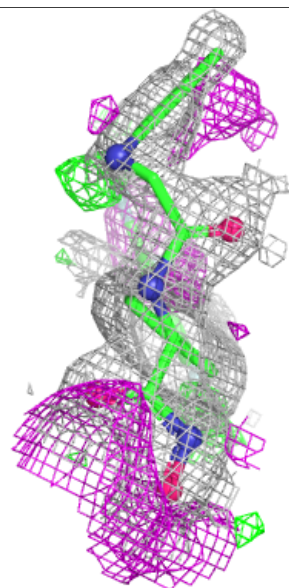
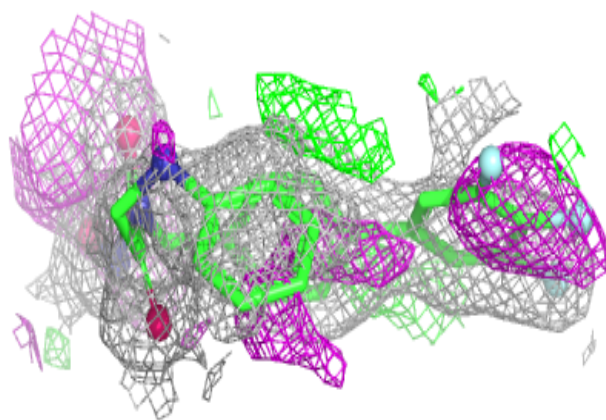
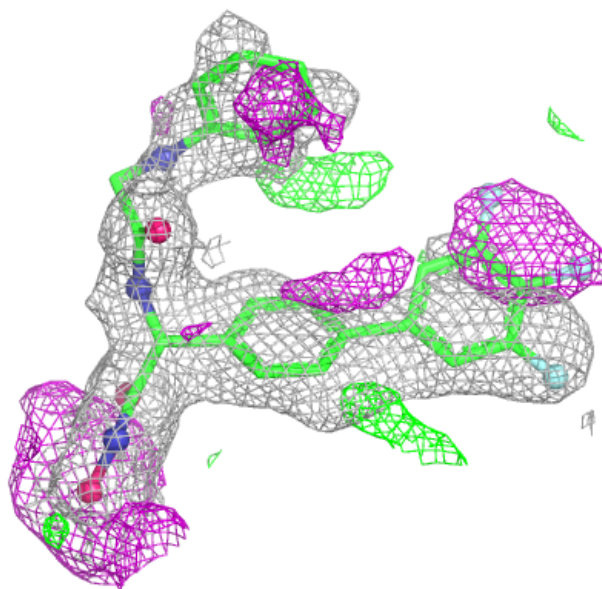
Electron density around X10 D 701:

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



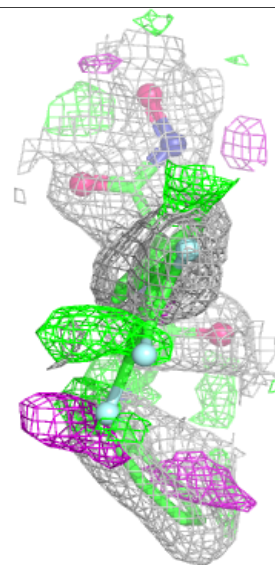
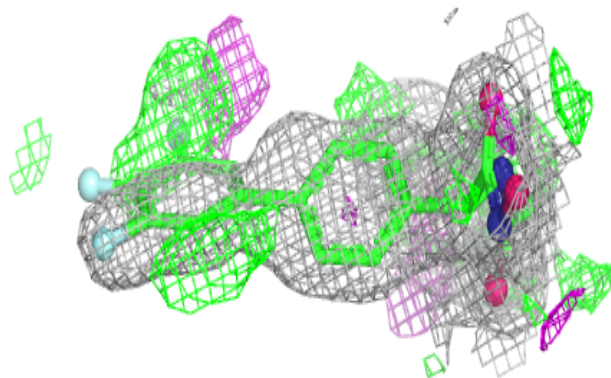
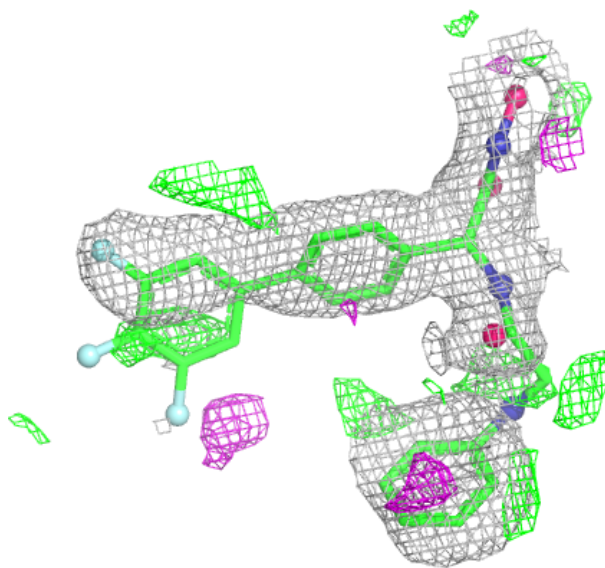
Electron density around X10 B 1401:

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



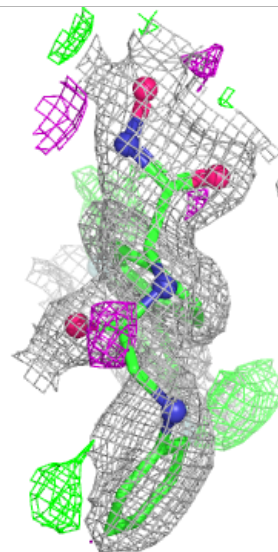
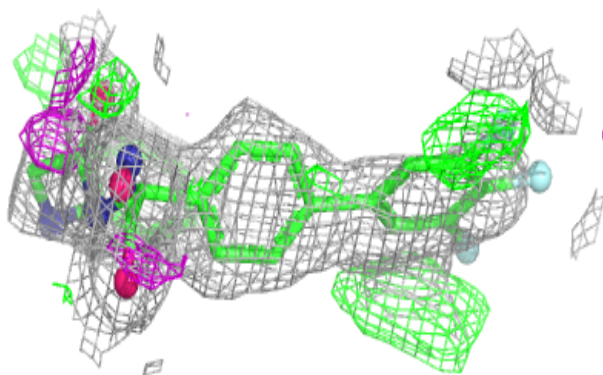
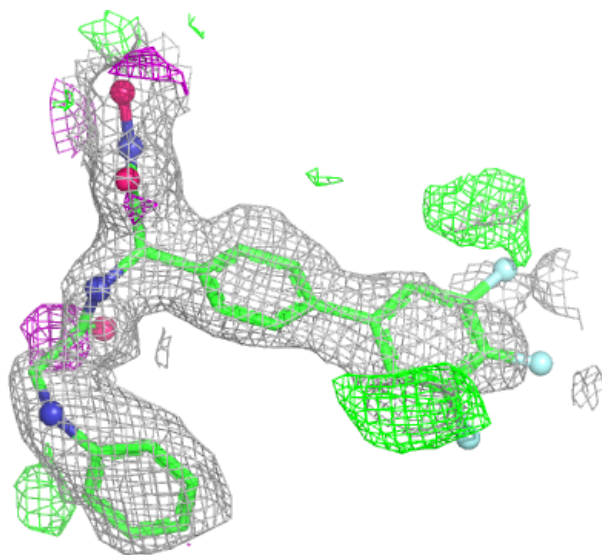
Electron density around X10 E 701:

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



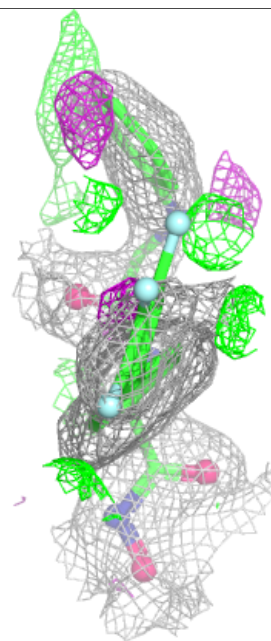
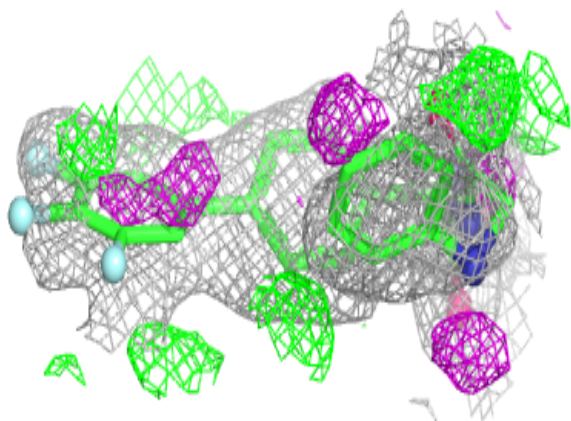
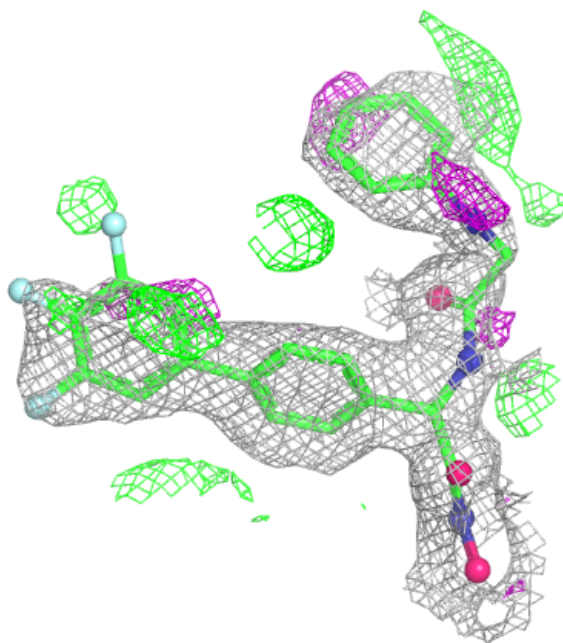
Electron density around X10 F 701:

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



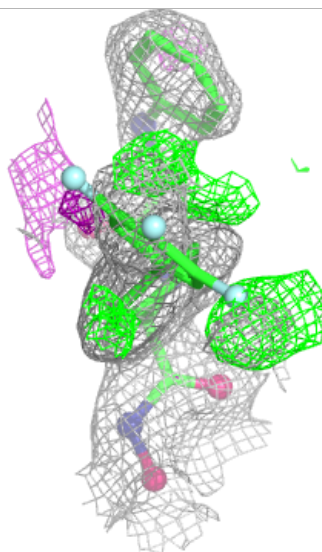
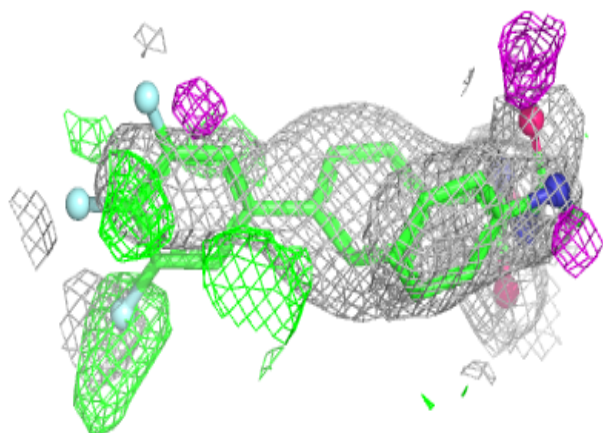
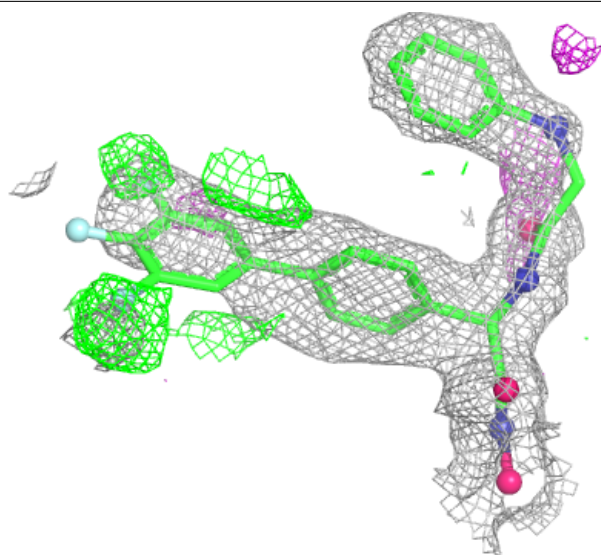
Electron density around X10 J 701:

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



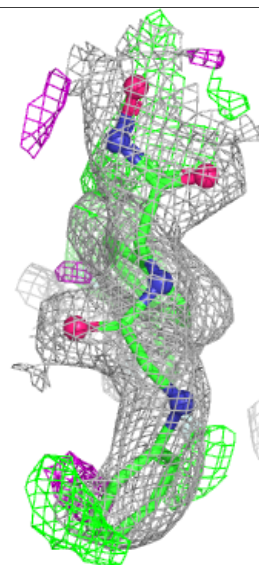
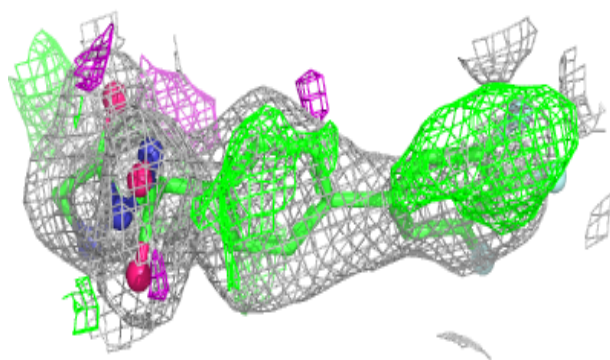
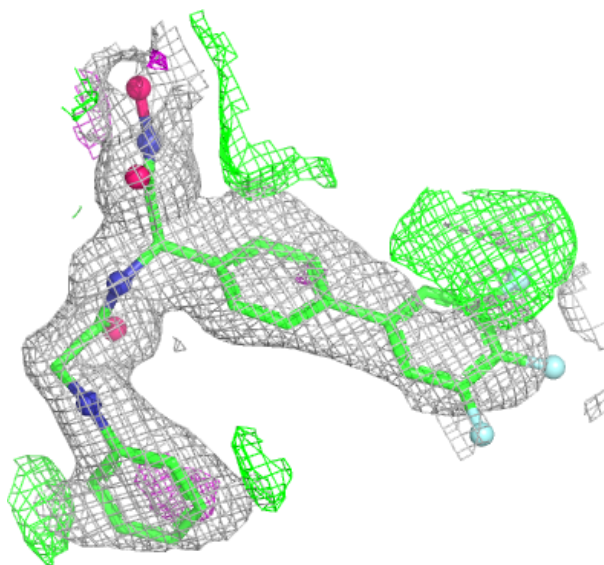
Electron density around X10 H 701:

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



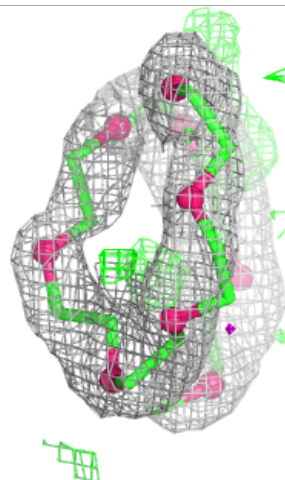
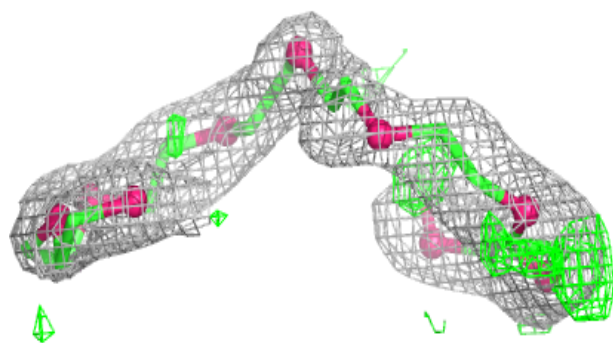
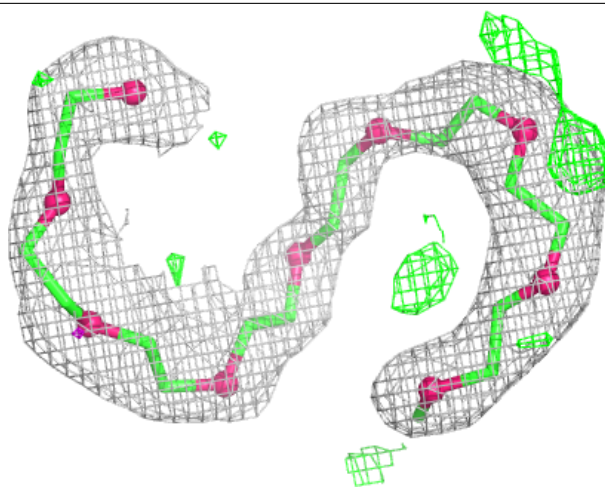
Electron density around X10 I 701:

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



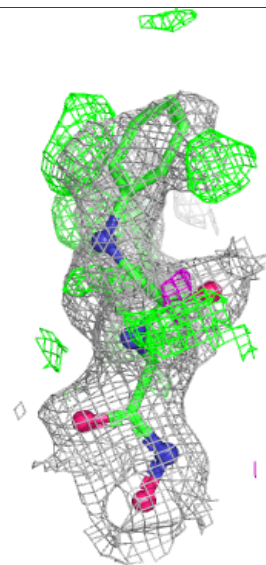
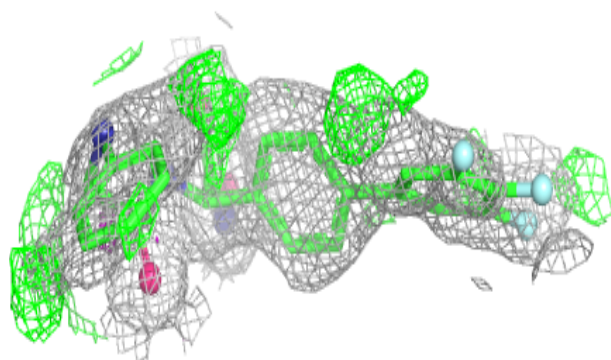
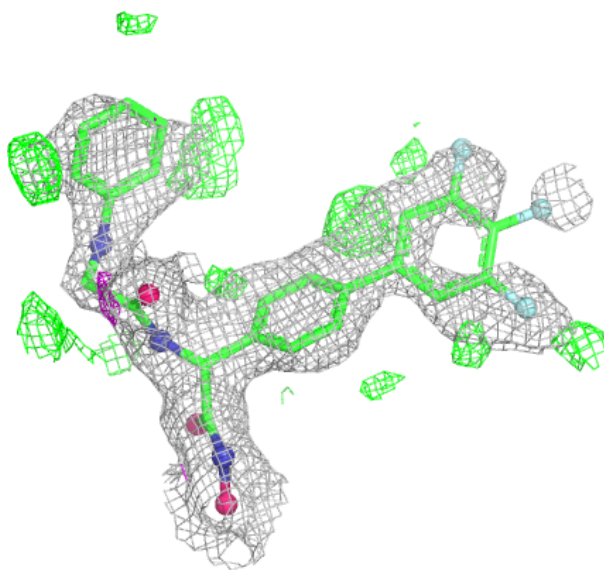
Electron density around 2PE H 705:

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



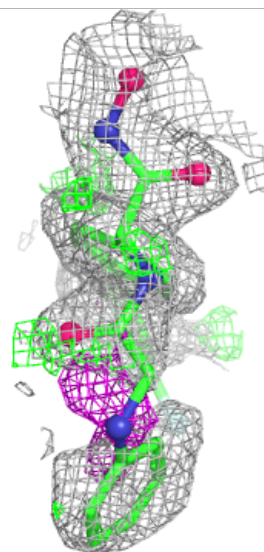
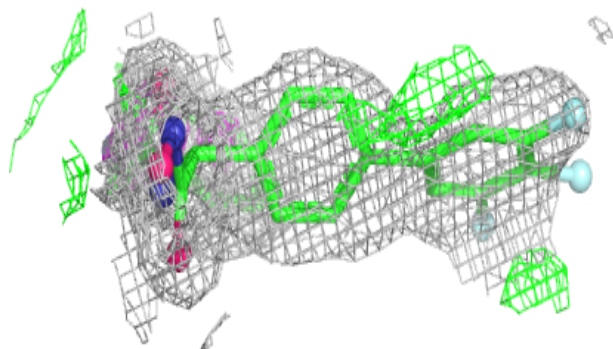
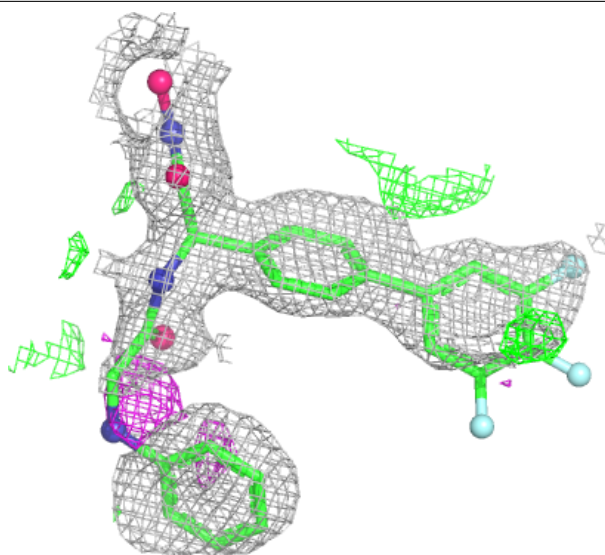
Electron density around X10 G 701:

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



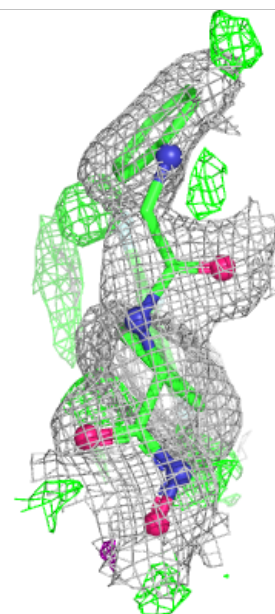
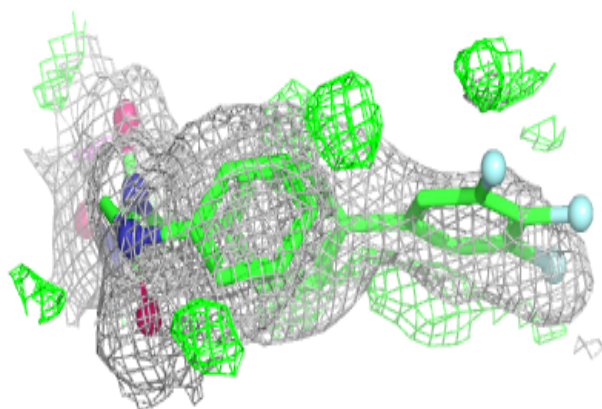
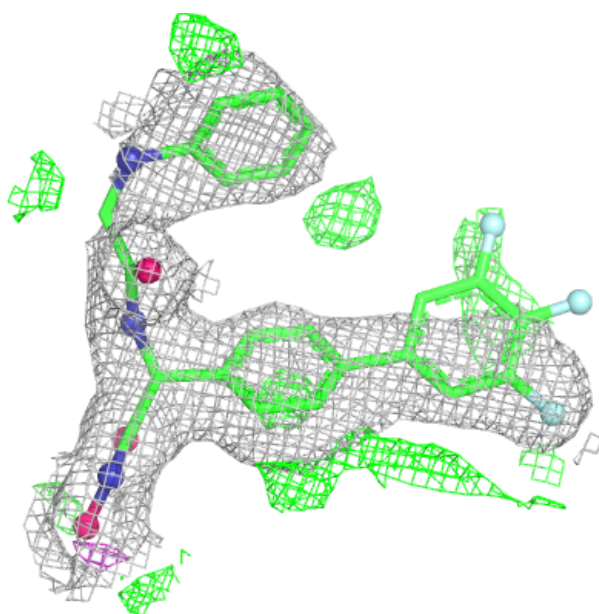
Electron density around X10 K 701:

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



Electron density around X10 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.