



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 05:55 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 Full wwPDB X-ray Structure Validation 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

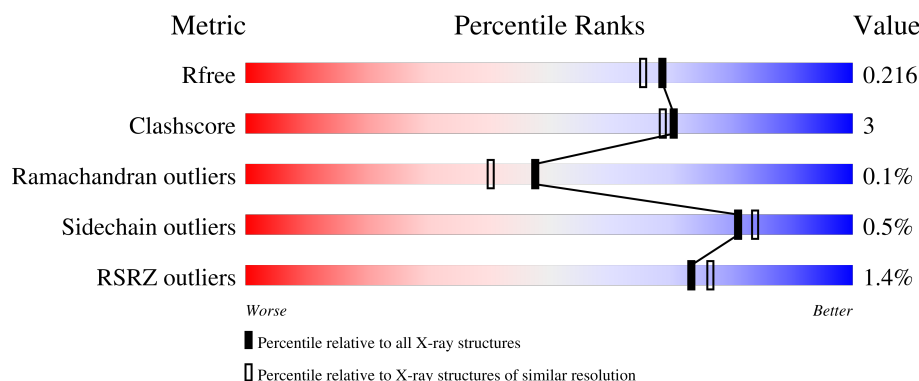
1 Overall quality at a glance

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.



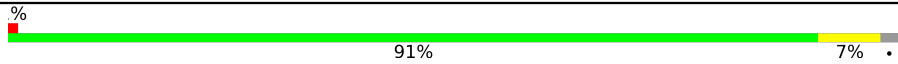
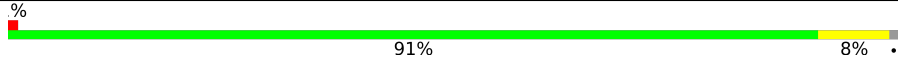
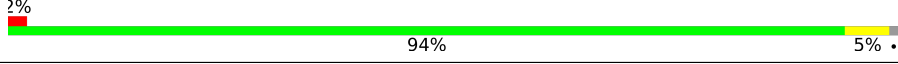
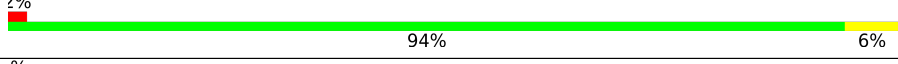
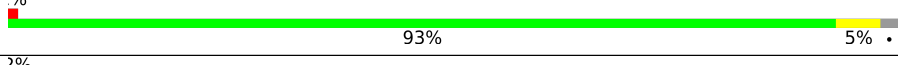
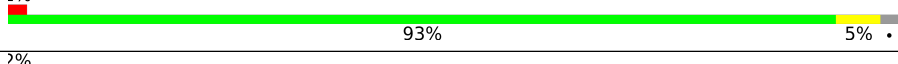
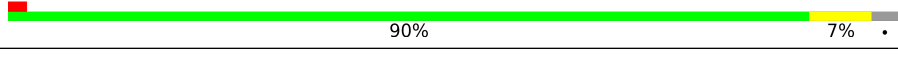
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

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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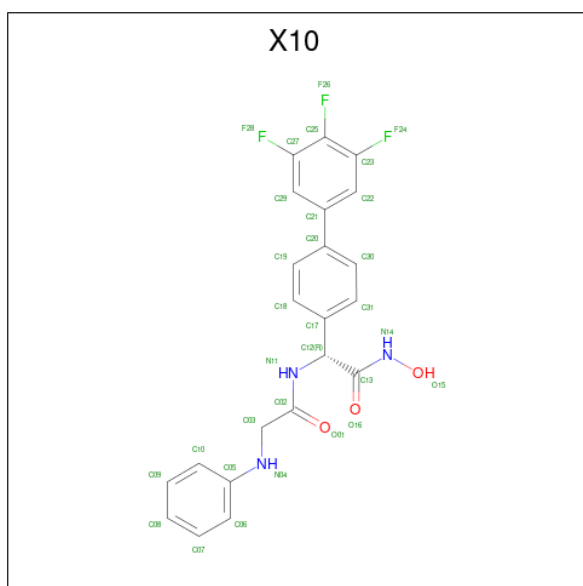
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	conflict	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP 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).



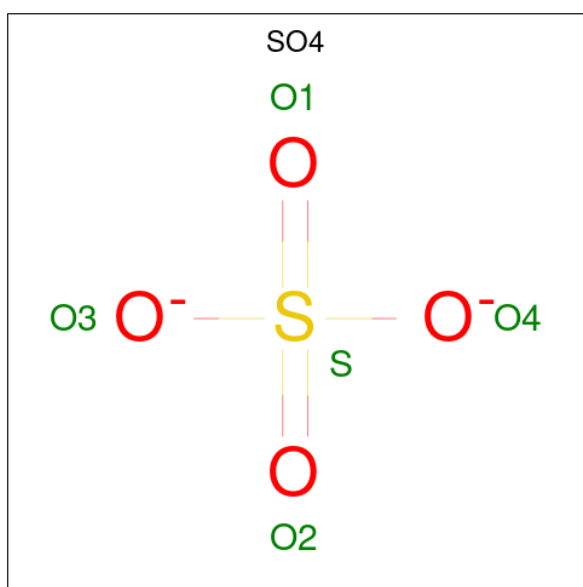
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			31	22	3	3	3		

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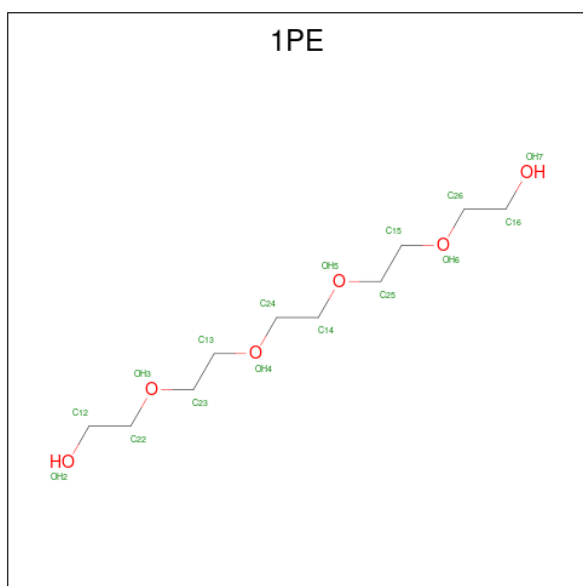
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			31	22	3	3	3		
2	C	1	Total	C	F	N	O	3	0
			31	22	3	3	3		
2	D	1	Total	C	F	N	O	1	0
			31	22	3	3	3		
2	E	1	Total	C	F	N	O	7	0
			31	22	3	3	3		
2	F	1	Total	C	F	N	O	2	0
			31	22	3	3	3		
2	G	1	Total	C	F	N	O	1	0
			31	22	3	3	3		
2	H	1	Total	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: $C_{10}H_{22}O_6$).



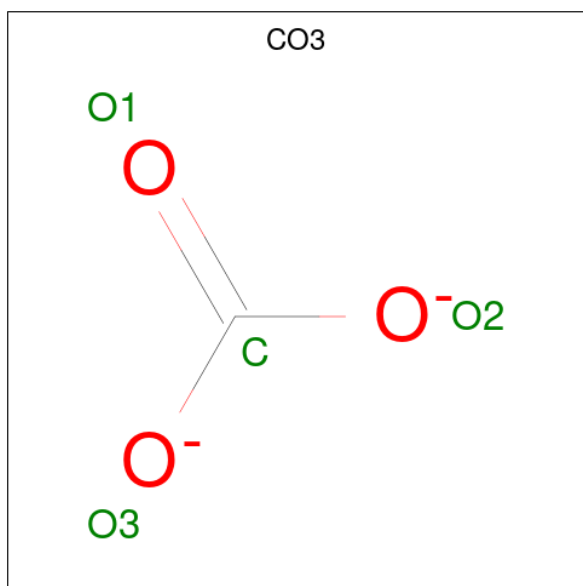
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	6	3		
4	A	1	Total	C	O	0	0
			12	8	4		
4	A	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			11	7	4		
4	C	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			8	5	3		
4	D	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			13	8	5		
4	D	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 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 (CCD ID: 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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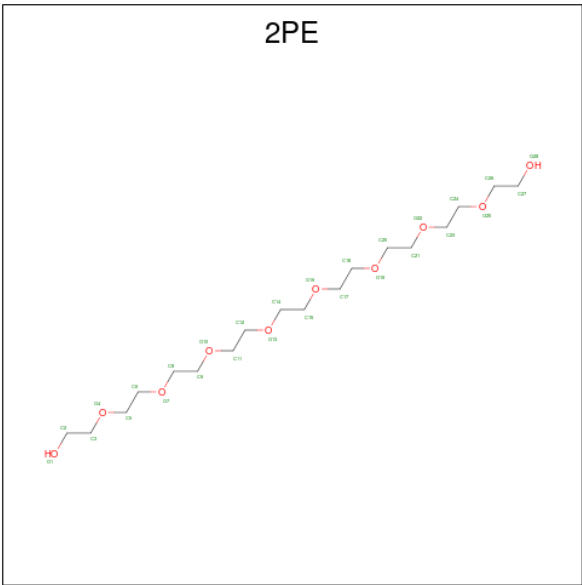
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	2	Total	Zn	0	0
			2	2		
6	L	2	Total	Zn	0	0
			2	2		

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

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

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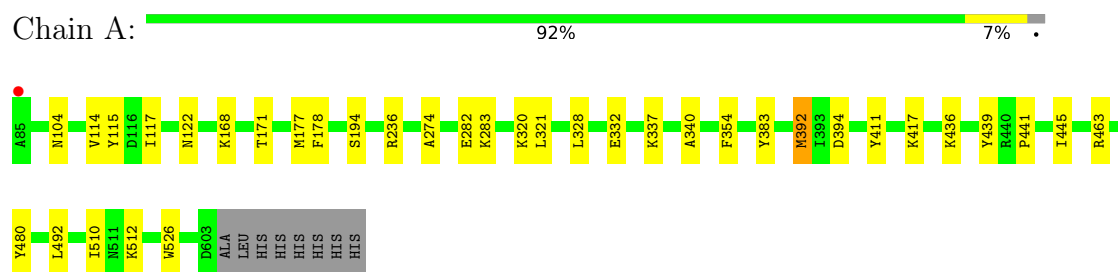
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	339	Total 339	O 339	0	0

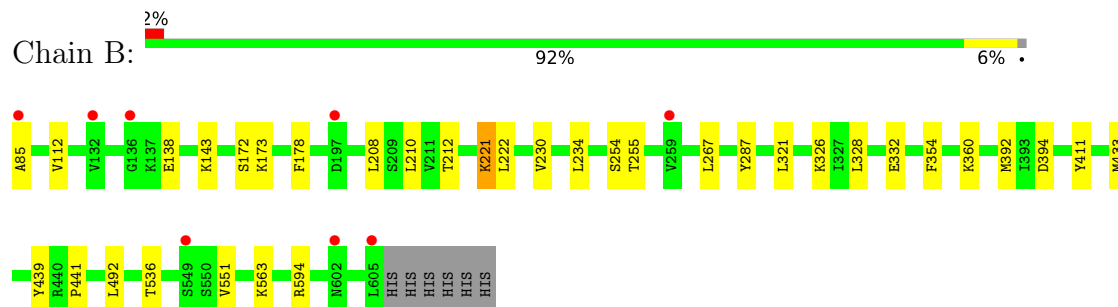
3 Residue-property plots [i](#)

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.

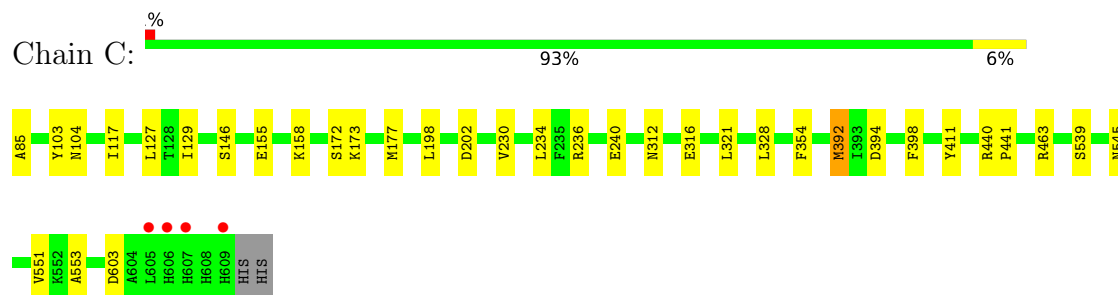
- Molecule 1: M17 leucyl aminopeptidase



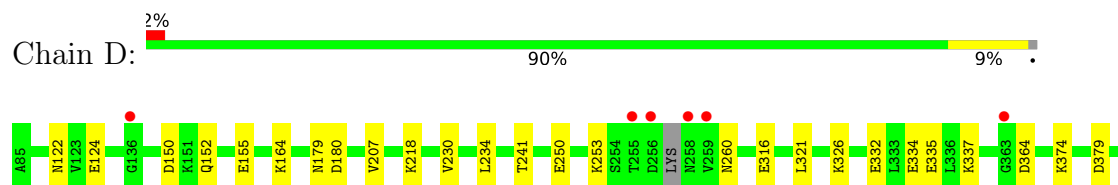
- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase

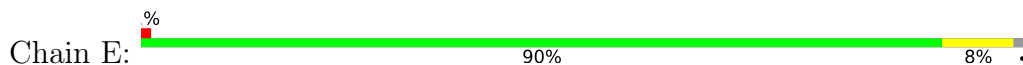


- Molecule 1: M17 leucyl aminopeptidase

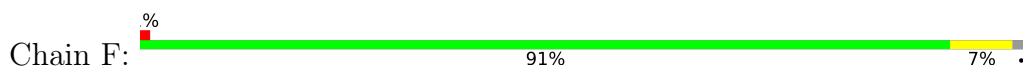




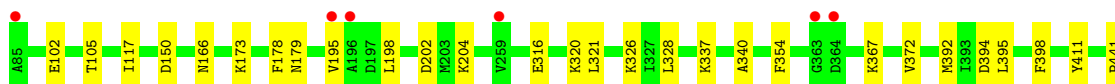
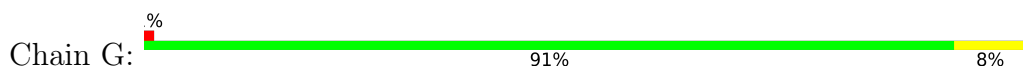
- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase

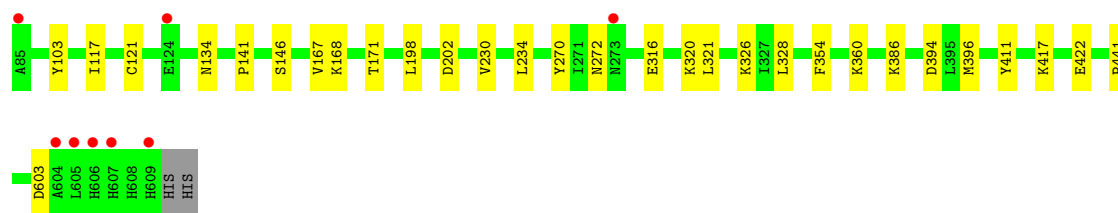


- Molecule 1: M17 leucyl aminopeptidase

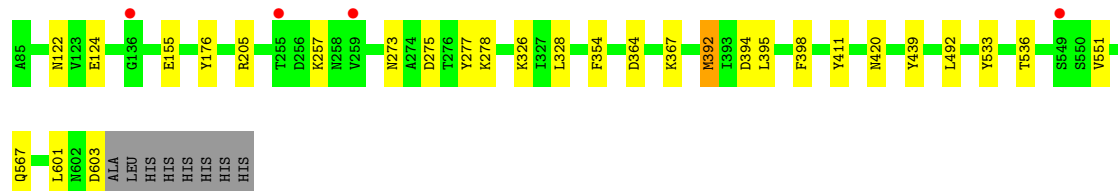
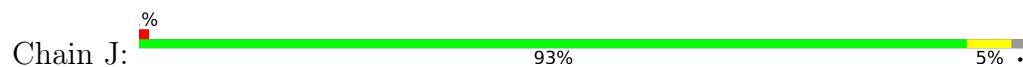


- Molecule 1: M17 leucyl aminopeptidase

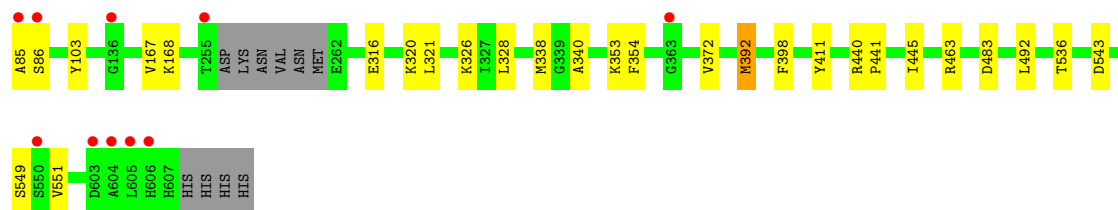




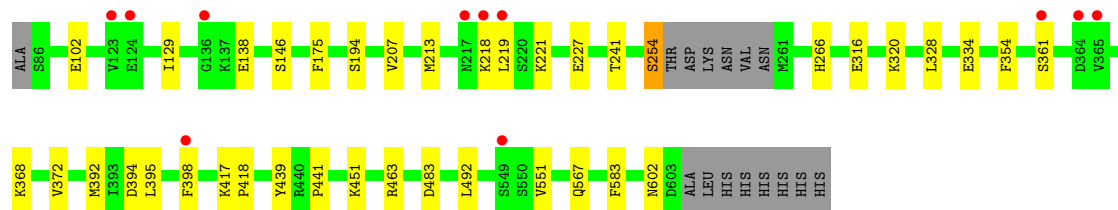
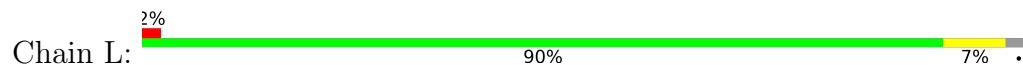
● Molecule 1: M17 leucyl aminopeptidase



● 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

All (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
1	L	334	GLU	C-N-CA	-6.72	109.56	122.06
1	I	417	LYS	CA-CB-CG	-6.47	101.16	114.10
1	A	417	LYS	CA-CB-CG	6.45	127.00	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	417	LYS	CB-CG-CD	5.72	124.45	111.30
1	J	392	MET	CG-SD-CE	-5.54	88.72	100.90
1	B	563	LYS	CB-CG-CD	5.22	123.31	111.30
1	D	326	LYS	CA-CB-CG	5.21	124.52	114.10
1	A	417	LYS	CB-CA-C	-5.19	106.49	111.00
1	B	143	LYS	CB-CG-CD	5.10	123.03	111.30

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:A:436:LYS:NZ	9:A:801:HOH:O	1.94	0.91
5:H:704:CO3:O3	9:H:801:HOH:O	1.86	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:705:CO3:O3	9:J:801:HOH:O	1.87	0.90
5:C:706:CO3:O1	9:C:801:HOH:O	1.91	0.89
5:K:705:CO3:O2	9:K:801:HOH:O	1.91	0.88
1:B:360:LYS:NZ	9:B:1502:HOH:O	2.07	0.88
1:L:451:LYS:HZ3	4:L:705:1PE:H131	1.39	0.87
1:G:326:LYS:HE2	1:G:328:LEU:HD21	1.57	0.86
1:D:451:LYS:HG2	4:D:704:1PE:H232	1.60	0.82
1:L:316:GLU:HG3	4:L:704:1PE:H251	1.61	0.81
1:J:392:MET:HE1	2:J:701:X10:C23	2.10	0.81
1:E:451:LYS:HG2	4:E:704:1PE:H231	1.62	0.80
1:D:492:LEU:HD11	2:D:701:X10:F28	1.71	0.79
1:I:134:ASN:ND2	1:I:141:PRO:HD2	1.98	0.79
1:H:386:LYS:HE3	1:H:396:MET:HE2	1.63	0.79
1:L:602:ASN:OD1	9:L:801:HOH:O	2.01	0.78
1:F:392:MET:HE1	2:F:701:X10:C29	2.14	0.78
1:G:178:PHE:CZ	1:J:155:GLU:HG2	2.16	0.77
1:B:332:GLU:OE2	9:B:1501:HOH:O	2.03	0.77
1:K:392:MET:HE1	2:K:701:X10:C25	2.15	0.76
1:D:260:ASN:OD1	9:D:802:HOH:O	2.05	0.75
1:J:392:MET:HE1	2:J:701:X10:C25	2.16	0.75
1:L:392:MET:HE1	2:L:701:X10:C27	2.18	0.74
1:J:122:ASN:OD1	1:J:124:GLU:HG2	1.87	0.74
1:G:102:GLU:HG2	1:G:105:THR:HG22	1.70	0.74
5:G:706:CO3:O3	9:G:802:HOH:O	2.06	0.73
1:A:178:PHE:HZ	1:D:155:GLU:HG2	1.54	0.72
1:J:205:ARG:NH2	9:J:802:HOH:O	2.20	0.72
1:I:320:LYS:HB3	4:I:704:1PE:H142	1.71	0.72
2:G:701:X10:F26	9:G:961:HOH:O	1.96	0.72
1:F:102:GLU:OE1	9:F:802:HOH:O	2.10	0.70
1:J:278:LYS:NZ	9:J:803:HOH:O	2.25	0.70
1:F:102:GLU:OE2	9:F:801:HOH:O	2.09	0.70
1:A:337:LYS:NZ	9:A:804:HOH:O	2.23	0.70
4:I:703:1PE:H222	4:I:704:1PE:H141	1.73	0.69
1:I:360:LYS:HG2	1:I:422:GLU:HG3	1.75	0.68
1:G:395:LEU:HB3	1:G:398:PHE:CE2	2.29	0.68
1:E:543:ASP:HB3	4:E:704:1PE:H221	1.74	0.68
1:A:332[A]:GLU:HG3	9:A:1148:HOH:O	1.94	0.67
1:J:411:TYR:HE1	4:J:703:1PE:H132	1.60	0.66
1:D:510:ILE:O	9:D:804:HOH:O	2.14	0.66
1:D:549:SER:OG	9:D:803:HOH:O	2.14	0.65
1:L:395:LEU:O	1:L:398:PHE:HD1	1.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:708:CO3:O1	9:A:803:HOH:O	2.14	0.65
1:A:282:GLU:OE1	9:A:802:HOH:O	2.14	0.64
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.79	0.64
1:B:492:LEU:HD11	2:B:1401:X10:C25	2.27	0.64
1:L:361:SER:N	9:L:804:HOH:O	2.24	0.63
1:C:463:ARG:NE	5:C:706:CO3:O3	2.24	0.63
1:J:326:LYS:HD2	1:J:328:LEU:HD21	1.80	0.63
1:K:463:ARG:NE	5:K:705:CO3:O3	2.23	0.63
1:A:178:PHE:CZ	1:D:155:GLU:HG2	2.33	0.62
1:I:134:ASN:HD22	1:I:141:PRO:HD2	1.64	0.62
1:G:463:ARG:NH2	5:G:706:CO3:O2	2.26	0.62
1:A:492:LEU:HD11	2:A:701:X10:C25	2.30	0.62
1:I:316:GLU:HG3	4:I:703:1PE:H262	1.81	0.62
1:E:117:ILE:HG12	1:E:270:TYR:HB3	1.81	0.61
1:F:492:LEU:HD11	2:F:701:X10:C27	2.29	0.61
1:D:122:ASN:OD1	1:D:124:GLU:HG2	1.99	0.61
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.82	0.61
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.83	0.61
1:L:221:LYS:HG3	1:L:266:HIS:HB2	1.83	0.61
1:C:172:SER:O	1:C:173:LYS:HD3	2.00	0.60
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.83	0.60
1:D:583:PHE:CZ	2:D:701:X10:F26	2.44	0.60
1:L:129:ILE:HG13	1:L:213:MET:HE1	1.82	0.60
1:D:492:LEU:HD11	2:D:701:X10:C27	2.30	0.60
1:F:577:ALA:O	2:F:701:X10:C23	2.50	0.60
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.84	0.60
1:D:316:GLU:HG3	4:D:703:1PE:H221	1.83	0.60
1:A:392:MET:HE1	2:A:701:X10:C25	2.31	0.59
1:L:395:LEU:O	1:L:398:PHE:CD1	2.55	0.58
1:C:392:MET:HE1	2:C:701:X10:C29	2.33	0.58
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.84	0.58
1:L:320:LYS:HZ1	4:L:704:1PE:H252	1.67	0.58
1:K:85:ALA:N	1:K:353:LYS:HZ1	2.01	0.58
1:A:441:PRO:HB2	1:B:394:ASP:HA	1.84	0.58
1:C:155:GLU:O	1:C:158:LYS:HG2	2.03	0.58
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.86	0.57
1:D:441:PRO:HB2	1:E:394:ASP:HA	1.87	0.57
1:L:368:LYS:HD2	9:L:1080:HOH:O	2.03	0.57
1:D:230:VAL:HG23	1:D:234:LEU:HD23	1.87	0.57
1:K:316:GLU:HG3	4:K:703:1PE:H141	1.85	0.57
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:LEU:HD11	2:A:701:X10:C27	2.35	0.56
2:H:701:X10:O15	9:H:801:HOH:O	2.17	0.56
1:D:392:MET:HE1	2:D:701:X10:C29	2.35	0.56
1:E:441:PRO:HB2	1:F:394:ASP:HA	1.88	0.55
1:F:398:PHE:HZ	2:F:701:X10:C22	2.19	0.55
1:E:332:GLU:HG3	9:E:1054:HOH:O	2.06	0.55
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.89	0.55
1:E:100:PRO:O	1:E:101:ILE:HD13	2.07	0.55
1:G:567:GLN:NE2	1:G:567:GLN:HA	2.22	0.55
1:K:392:MET:CE	2:K:701:X10:C23	2.79	0.55
1:K:543:ASP:OD2	1:L:254:SER:HB2	2.07	0.55
1:J:533:TYR:O	1:J:536:THR:HG22	2.07	0.54
1:B:254:SER:OG	1:B:255:THR:N	2.40	0.54
1:I:103:TYR:HB2	3:I:702:SO4:O1	2.07	0.54
1:L:320:LYS:NZ	4:L:704:1PE:H252	2.23	0.54
1:F:417:LYS:NZ	9:F:806:HOH:O	2.37	0.54
1:E:195:VAL:HG22	9:E:823:HOH:O	2.08	0.54
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.90	0.54
1:D:332:GLU:HG3	9:D:1088:HOH:O	2.06	0.54
1:J:275:ASP:HA	1:J:278:LYS:HE2	1.90	0.54
1:E:536:THR:HG21	1:E:551:VAL:HG23	1.90	0.54
1:A:320:LYS:HE2	4:A:707:1PE:H131	1.91	0.53
1:A:320:LYS:HZ1	4:A:707:1PE:H142	1.73	0.53
1:E:567:GLN:NE2	4:E:704:1PE:H151	2.24	0.53
1:J:492:LEU:HD13	2:J:701:X10:C23	2.38	0.53
1:D:250:GLU:OE2	1:D:253:LYS:HG3	2.09	0.53
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.91	0.53
1:L:463:ARG:NE	5:L:706:CO3:O3	2.35	0.53
1:G:441:PRO:HB2	1:H:394:ASP:HA	1.91	0.52
1:C:539:SER:HB2	1:C:545:ASN:OD1	2.10	0.52
1:K:103:TYR:HB3	4:K:702:1PE:H142	1.91	0.52
1:B:492:LEU:HD11	2:B:1401:X10:C23	2.39	0.52
1:K:492:LEU:HD11	2:K:701:X10:C25	2.39	0.52
1:K:536:THR:HG21	1:K:551:VAL:HG23	1.91	0.52
1:F:567:GLN:CD	4:F:703:1PE:H121	2.35	0.52
1:J:567:GLN:HA	1:J:567:GLN:NE2	2.25	0.52
1:C:398:PHE:HZ	2:C:701:X10:C22	2.23	0.52
1:B:326:LYS:NZ	9:B:1508:HOH:O	2.42	0.51
1:D:583:PHE:HZ	2:D:701:X10:F26	1.82	0.51
1:F:114:VAL:HG12	1:F:274:ALA:HB1	1.93	0.51
1:E:576:ILE:HD12	1:E:580:SER:OG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:392:MET:HE1	2:F:701:X10:C27	2.40	0.51
1:L:583:PHE:CZ	2:L:701:X10:F26	2.53	0.51
1:H:379:ASP:HB3	1:H:396:MET:CE	2.41	0.51
1:D:506:ASN:O	1:D:510:ILE:HD12	2.11	0.51
2:K:701:X10:O15	9:K:801:HOH:O	2.18	0.51
1:L:463:ARG:HE	5:L:706:CO3:C	2.22	0.50
1:K:320:LYS:HB3	4:K:702:1PE:H232	1.93	0.50
1:C:117:ILE:HD11	1:C:146:SER:OG	2.11	0.50
1:C:551:VAL:HG12	1:C:553:ALA:H	1.76	0.50
1:A:122:ASN:HB2	4:A:706:1PE:H232	1.93	0.49
1:H:379:ASP:HB3	1:H:396:MET:HE3	1.94	0.49
1:L:320:LYS:HZ1	4:L:704:1PE:H242	1.77	0.49
1:D:164:LYS:HE2	9:D:918:HOH:O	2.11	0.49
1:A:480:TYR:OH	1:A:512:LYS:NZ	2.44	0.49
1:B:178:PHE:HZ	1:F:155:GLU:HG2	1.78	0.49
1:L:320:LYS:HD3	4:L:704:1PE:H122	1.94	0.49
1:E:369:ILE:HD11	1:E:604:ALA:HB1	1.94	0.48
1:I:198:LEU:HD22	1:I:202:ASP:HB3	1.96	0.48
1:A:463:ARG:HE	5:A:708:CO3:C	2.25	0.48
1:K:441:PRO:HB2	1:L:394:ASP:HA	1.95	0.48
1:L:361:SER:HB2	1:L:418:PRO:O	2.14	0.48
9:A:1131:HOH:O	1:F:551:VAL:HG13	2.13	0.48
1:G:579:VAL:O	1:G:589:LYS:HD2	2.13	0.48
2:C:701:X10:N14	9:C:801:HOH:O	2.35	0.48
1:B:321:LEU:HD11	1:B:411:TYR:HA	1.96	0.48
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.95	0.48
1:D:374:LYS:NZ	9:D:801:HOH:O	2.35	0.47
1:I:360:LYS:HE3	1:I:360:LYS:HB3	1.75	0.47
1:A:383:TYR:OH	1:B:433:MET:HE3	2.15	0.47
1:A:492:LEU:CD1	2:A:701:X10:C27	2.91	0.47
1:B:208:LEU:O	1:B:212:THR:HG23	2.14	0.47
1:H:320:LYS:NZ	8:H:705:2PE:H181	2.30	0.47
1:H:396:MET:HE1	9:H:946:HOH:O	2.14	0.47
1:J:364:ASP:O	1:J:420:ASN:HA	2.14	0.47
1:K:85:ALA:N	9:K:810:HOH:O	2.46	0.47
1:A:394:ASP:HA	1:C:441:PRO:HB2	1.97	0.47
1:E:104:ASN:HB3	9:E:1127:HOH:O	2.14	0.47
1:F:123:VAL:HG23	1:F:123:VAL:O	2.14	0.47
1:J:411:TYR:CE1	4:J:703:1PE:H132	2.45	0.47
1:A:392:MET:HE1	2:A:701:X10:C29	2.44	0.47
1:I:117:ILE:HD11	1:I:146:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:85:ALA:HA	1:K:353:LYS:HE3	1.96	0.47
1:K:492:LEU:HD11	2:K:701:X10:C23	2.45	0.47
1:F:326:LYS:HE3	9:F:965:HOH:O	2.15	0.47
1:B:230:VAL:HG12	1:B:234:LEU:HD23	1.96	0.47
1:C:103:TYR:HB2	3:C:702:SO4:O1	2.15	0.47
1:D:398:PHE:CD1	1:D:398:PHE:C	2.93	0.47
1:A:320:LYS:HZ1	4:A:707:1PE:C15	2.28	0.46
1:B:85:ALA:HB1	9:B:1832:HOH:O	2.15	0.46
1:D:321:LEU:HD11	1:D:411:TYR:HA	1.96	0.46
1:D:379:ASP:O	1:D:396:MET:HG3	2.15	0.46
1:K:326:LYS:HE2	1:K:328:LEU:HD21	1.98	0.46
1:B:178:PHE:CZ	1:F:155:GLU:HG2	2.49	0.46
1:D:152:GLN:HG2	1:D:180:ASP:OD1	2.15	0.46
1:F:156:PHE:CG	1:F:177:MET:HE1	2.51	0.46
1:A:236:ARG:HD2	1:A:283:LYS:HG2	1.98	0.46
1:G:367:LYS:HG2	1:G:603:ASP:OD2	2.16	0.46
4:C:703:1PE:H151	4:C:703:1PE:H142	1.70	0.46
1:E:451:LYS:NZ	4:E:704:1PE:H122	2.30	0.46
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.96	0.46
1:C:440:ARG:HE	1:C:440:ARG:HB2	1.67	0.46
1:L:583:PHE:HZ	2:L:701:X10:F26	1.89	0.46
1:A:321:LEU:HD11	1:A:411:TYR:HA	1.98	0.46
1:J:392:MET:CE	2:J:701:X10:C23	2.87	0.46
1:H:332:GLU:OE1	9:H:804:HOH:O	2.21	0.46
1:B:536:THR:HG21	1:B:551:VAL:HG23	1.98	0.45
1:E:198:LEU:HD22	1:E:202:ASP:HB3	1.98	0.45
1:H:441:PRO:HB2	1:I:394:ASP:HA	1.98	0.45
1:I:326:LYS:HG2	1:I:328:LEU:HD12	1.98	0.45
1:G:392:MET:HE1	2:G:701:X10:C29	2.46	0.45
1:H:320:LYS:HZ2	8:H:705:2PE:H181	1.81	0.45
1:K:398:PHE:CD1	1:K:398:PHE:C	2.94	0.45
1:D:334:GLU:O	1:D:337:LYS:HD3	2.16	0.45
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.97	0.45
1:G:372:VAL:O	1:G:483:ASP:HA	2.17	0.45
1:D:536:THR:HG21	1:D:551:VAL:HG23	1.99	0.45
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.99	0.45
1:E:321:LEU:HD11	1:E:411:TYR:HA	1.99	0.45
1:H:256:ASP:CG	1:H:256:ASP:O	2.60	0.45
1:A:115:TYR:CE1	4:A:706:1PE:H132	2.52	0.45
1:C:85:ALA:HB3	1:C:312:ASN:OD1	2.18	0.45
1:F:364:ASP:HB3	9:F:1043:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:230:VAL:HG12	1:I:234:LEU:HD23	2.00	0.44
1:L:567:GLN:NE2	4:L:705:1PE:H222	2.32	0.44
1:H:174:HIS:HB3	1:L:175:PHE:CD2	2.52	0.44
1:C:236:ARG:O	1:C:240:GLU:HG3	2.17	0.44
1:G:367:LYS:HE2	1:G:480:TYR:CE2	2.52	0.44
1:A:328:LEU:HD23	1:A:332[A]:GLU:HG2	1.99	0.44
1:J:328:LEU:HB2	1:J:354:PHE:HB3	2.00	0.44
1:A:114:VAL:HG12	1:A:274:ALA:HB1	2.00	0.44
1:E:451:LYS:HE3	1:E:564:GLU:O	2.17	0.44
1:L:567:GLN:NE2	1:L:567:GLN:HA	2.33	0.44
1:C:198:LEU:HD22	1:C:202:ASP:HB3	1.99	0.44
1:I:316:GLU:CD	4:I:703:1PE:H152	2.42	0.44
1:G:198:LEU:HD22	1:G:202:ASP:HB3	2.00	0.44
1:D:514:LEU:HG	9:D:804:HOH:O	2.18	0.44
1:J:273:ASN:O	1:J:277:TYR:HD1	2.01	0.44
1:K:440:ARG:HE	1:K:440:ARG:HB2	1.71	0.44
1:D:218:LYS:NZ	9:D:823:HOH:O	2.50	0.43
1:E:543:ASP:CG	4:E:704:1PE:H232	2.42	0.43
1:E:395:LEU:HB3	1:E:398:PHE:CE2	2.53	0.43
1:F:174:HIS:CE1	1:F:213:MET:HG2	2.52	0.43
1:E:214:LEU:HD11	1:E:222:LEU:HD22	2.00	0.43
1:G:394:ASP:HA	1:I:441:PRO:HB2	2.01	0.43
1:H:536:THR:HG21	1:H:551:VAL:HG23	2.00	0.43
1:C:177:MET:HE2	1:C:177:MET:HB3	1.93	0.43
1:I:321:LEU:HD11	1:I:411:TYR:HA	2.00	0.43
1:L:138:GLU:HA	1:L:194:SER:OG	2.19	0.43
1:E:203:MET:HE2	1:E:203:MET:HB2	1.92	0.43
1:E:156:PHE:CG	1:E:177:MET:HE1	2.54	0.43
4:E:703:1PE:H231	4:E:703:1PE:H122	1.74	0.43
1:L:129:ILE:CD1	1:L:213:MET:HE1	2.49	0.43
1:A:104:ASN:ND2	3:A:704:SO4:O4	2.40	0.43
1:C:316:GLU:CD	4:C:704:1PE:H231	2.44	0.43
1:C:398:PHE:CZ	2:C:701:X10:C22	3.02	0.43
1:C:85:ALA:HB1	9:C:1157:HOH:O	2.17	0.43
1:E:142:VAL:HG11	1:E:162:MET:HE3	2.00	0.43
1:F:475:LYS:NZ	9:F:821:HOH:O	2.48	0.43
8:H:705:2PE:H121	8:H:705:2PE:H92	1.63	0.43
1:B:287:TYR:CD2	1:B:594:ARG:HG2	2.54	0.42
1:B:326:LYS:HG2	1:B:328:LEU:CD1	2.49	0.42
1:C:127:LEU:HD11	1:C:129:ILE:HD11	2.00	0.42
1:D:150:ASP:OD2	1:D:179:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:VAL:HG11	1:D:241:THR:HG22	2.01	0.42
1:E:103:TYR:HB2	3:E:702:SO4:O2	2.19	0.42
1:A:510:ILE:HD13	1:A:526:TRP:NE1	2.34	0.42
1:G:337:LYS:HA	1:G:337:LYS:HD3	1.73	0.42
1:G:340:ALA:HA	1:G:445:ILE:HD12	2.02	0.42
1:K:338:MET:HE2	9:K:898:HOH:O	2.19	0.42
1:L:207:VAL:HG11	1:L:241:THR:HG22	2.01	0.42
1:L:372:VAL:O	1:L:483:ASP:HA	2.19	0.42
1:D:335:GLU:HG3	9:D:1048:HOH:O	2.20	0.42
1:D:583:PHE:CE2	2:D:701:X10:F26	2.62	0.42
1:G:150:ASP:OD2	1:G:179:ASN:HB2	2.19	0.42
1:G:204:LYS:HD3	9:G:1124:HOH:O	2.20	0.42
1:G:320:LYS:HZ1	4:G:705:1PE:C15	2.32	0.42
1:H:340:ALA:HA	1:H:445:ILE:HD12	2.01	0.42
1:A:436:LYS:HB3	1:A:436:LYS:HE2	1.78	0.42
1:D:579:VAL:O	1:D:589:LYS:HD2	2.20	0.42
1:B:172:SER:O	1:B:173:LYS:NZ	2.47	0.42
1:H:316:GLU:OE1	8:H:705:2PE:H242	2.19	0.42
1:A:320:LYS:HZ1	4:A:707:1PE:H152	1.84	0.42
1:C:230:VAL:HG12	1:C:234:LEU:HD23	2.02	0.42
1:J:601:LEU:HD23	1:J:601:LEU:HA	1.86	0.42
1:A:383:TYR:CZ	1:B:433:MET:HE3	2.55	0.42
1:A:463:ARG:NE	5:A:708:CO3:O3	2.47	0.42
1:H:321:LEU:HD11	1:H:411:TYR:HA	2.00	0.42
1:I:121:CYS:HA	1:I:270:TYR:CE2	2.55	0.42
1:E:369:ILE:HD11	1:E:604:ALA:CB	2.50	0.41
1:J:398:PHE:CD1	1:J:398:PHE:C	2.98	0.41
1:A:177:MET:HE2	1:A:177:MET:HB3	1.97	0.41
1:L:129:ILE:HD13	1:L:129:ILE:HA	1.90	0.41
1:L:492:LEU:HD21	2:L:701:X10:C27	2.49	0.41
9:G:1038:HOH:O	1:L:551:VAL:HG13	2.19	0.41
1:L:102:GLU:OE1	9:L:802:HOH:O	2.21	0.41
1:C:104[A]:ASN:ND2	9:C:823:HOH:O	2.53	0.41
1:F:210:LEU:HA	1:F:213:MET:HE2	2.03	0.41
1:L:146:SER:OG	1:L:227:GLU:OE2	2.26	0.41
1:K:372:VAL:O	1:K:483:ASP:HA	2.21	0.41
1:F:451:LYS:HG2	4:F:703:1PE:H132	2.01	0.41
1:G:602:ASN:ND2	9:G:801:HOH:O	2.05	0.41
9:I:1086:HOH:O	1:J:551:VAL:HG13	2.21	0.41
1:B:441:PRO:HB2	1:C:394:ASP:HA	2.03	0.41
1:E:442:GLY:O	1:F:301:PRO:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:481:ILE:O	1:E:571:TRP:HA	2.21	0.41
1:F:372:VAL:O	1:F:483:ASP:HA	2.20	0.41
1:B:112:VAL:HG22	1:B:267:LEU:HB3	2.03	0.41
1:B:221:LYS:HG3	1:B:222:LEU:N	2.36	0.41
1:D:364:ASP:O	1:D:420:ASN:HA	2.21	0.41
1:F:122:ASN:ND2	1:F:149:ASN:HD22	2.19	0.41
1:G:166:ASN:OD1	1:G:166:ASN:C	2.63	0.41
1:G:316:GLU:HG2	1:G:320:LYS:HE2	2.02	0.41
1:H:374:LYS:NZ	9:H:801:HOH:O	2.39	0.41
1:I:167:VAL:O	1:I:168:LYS:C	2.63	0.41
1:J:492:LEU:CD1	2:J:701:X10:C23	2.98	0.41
1:K:167:VAL:O	1:K:168:LYS:C	2.64	0.41
1:H:328:LEU:HD12	1:H:328:LEU:N	2.36	0.41
2:K:701:X10:N14	9:K:801:HOH:O	2.37	0.41
1:C:321:LEU:HD11	1:C:411:TYR:HA	2.03	0.40
1:D:497:THR:HA	1:D:578:GLY:O	2.21	0.40
1:F:214:LEU:HD21	1:F:222:LEU:HD22	2.04	0.40
1:I:386:LYS:HE3	1:I:396:MET:HE2	2.04	0.40
1:J:395:LEU:HB3	1:J:398:PHE:CE2	2.55	0.40
1:L:392:MET:HE1	2:L:701:X10:F28	2.12	0.40
1:K:321:LEU:HD11	1:K:411:TYR:HA	2.02	0.40
1:E:586:ARG:NH1	9:E:803:HOH:O	2.29	0.40
1:G:173:LYS:HD2	1:J:176:TYR:CE1	2.56	0.40
1:G:548:SER:HB2	1:G:557:VAL:HG11	2.02	0.40
1:I:171:THR:HG21	9:I:1037:HOH:O	2.20	0.40
1:A:168:LYS:O	1:A:171:THR:HG22	2.22	0.40
1:E:361:SER:OG	1:E:418:PRO:O	2.39	0.40
1:F:440:ARG:HE	1:F:440:ARG:HB2	1.77	0.40
1:J:367:LYS:HE2	1:J:367:LYS:HB2	1.85	0.40
1:A:122:ASN:HD22	4:A:706:1PE:H232	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

All (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
1	L	219	LEU
1	F	136	GLY

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ILE
1	A	194	SER
1	A	439	TYR
1	B	210	LEU
1	B	221	LYS
1	B	392	MET
1	B	439	TYR
1	C	603	ASP
1	E	398	PHE
1	F	439	TYR
1	F	549	SER
1	F	550	SER
1	G	117	ILE
1	G	195	VAL
1	H	145	SER
1	H	439	TYR
1	H	608	HIS
1	I	272	ASN
1	I	603	ASP
1	J	439	TYR
1	J	603	ASP
1	K	549	SER

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Mol	Chain	Res	Type
1	L	254	SER
1	L	439	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	149	ASN
1	A	567	GLN
1	A	568	ASN
1	B	567	GLN
1	C	420	ASN
1	C	607	HIS
1	D	104	ASN
1	D	183	ASN
1	D	266	HIS
1	D	567	GLN
1	E	113	GLN
1	E	181	ASN
1	E	420	ASN
1	E	567	GLN
1	F	122	ASN
1	G	229	ASN
1	G	567	GLN
1	H	139	ASN
1	H	161	ASN
1	H	272	ASN
1	H	567	GLN
1	I	215	HIS
1	I	266	HIS
1	I	272	ASN
1	I	273	ASN
1	I	322	ASN
1	I	567	GLN
1	J	420	ASN
1	J	531	ASN
1	J	567	GLN
1	K	602	ASN
1	L	567	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

All (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
2	F	701	X10	C02-N11	5.39	1.45	1.34
2	B	1401	X10	C02-N11	5.35	1.45	1.34
2	H	701	X10	C02-N11	5.26	1.45	1.34
2	E	701	X10	C02-N11	5.13	1.44	1.34
2	I	701	X10	C02-N11	4.96	1.44	1.34
2	L	701	X10	C02-N11	4.80	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	701	X10	C02-N11	4.75	1.44	1.34
2	D	701	X10	C02-N11	4.53	1.43	1.34
2	D	701	X10	O16-C13	-4.05	1.15	1.23
2	L	701	X10	O16-C13	-3.71	1.16	1.23
2	D	701	X10	O01-C02	-3.10	1.17	1.23
2	A	701	X10	O16-C13	-2.73	1.18	1.23
5	I	706	CO3	O1-C	2.73	1.35	1.25
2	A	701	X10	C05-N04	2.71	1.46	1.38
2	B	1401	X10	C05-N04	2.70	1.46	1.38
2	L	701	X10	O01-C02	-2.65	1.18	1.23
2	B	1401	X10	O16-C13	-2.65	1.18	1.23
2	H	701	X10	C05-N04	2.65	1.46	1.38
2	K	701	X10	C05-N04	2.63	1.46	1.38
2	C	701	X10	O16-C13	-2.60	1.18	1.23
2	C	701	X10	C05-N04	2.60	1.46	1.38
2	I	701	X10	O16-C13	-2.56	1.18	1.23
2	J	701	X10	O01-C02	-2.52	1.18	1.23
2	L	701	X10	C22-C21	-2.52	1.35	1.39
2	L	701	X10	C05-N04	2.47	1.45	1.38
2	H	701	X10	O01-C02	-2.47	1.18	1.23
2	I	701	X10	C05-N04	2.44	1.45	1.38
2	J	701	X10	O16-C13	-2.41	1.18	1.23
2	F	701	X10	C05-N04	2.35	1.45	1.38
2	G	701	X10	C05-N04	2.27	1.45	1.38
2	D	701	X10	C22-C21	-2.27	1.35	1.39
2	F	701	X10	O16-C13	-2.26	1.19	1.23
2	K	701	X10	O16-C13	-2.25	1.19	1.23
2	C	701	X10	O01-C02	-2.25	1.18	1.23
2	E	701	X10	O01-C02	-2.15	1.19	1.23
2	D	701	X10	C29-C21	-2.14	1.36	1.39
2	E	701	X10	C05-N04	2.13	1.44	1.38
2	G	701	X10	O16-C13	-2.12	1.19	1.23
2	B	1401	X10	O01-C02	-2.11	1.19	1.23
2	J	701	X10	C05-N04	2.06	1.44	1.38
2	K	701	X10	O01-C02	-2.05	1.19	1.23
2	F	701	X10	O01-C02	-2.02	1.19	1.23
2	E	701	X10	O16-C13	-2.00	1.19	1.23
2	H	701	X10	O16-C13	-2.00	1.19	1.23

All (127) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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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
2	A	701	X10	C29-C21-C20	-5.05	112.38	120.84
2	J	701	X10	C22-C21-C20	-5.01	112.44	120.84
2	C	701	X10	C22-C21-C20	4.51	128.39	120.84
2	K	701	X10	C29-C21-C20	4.40	128.21	120.84
4	A	706	1PE	C24-OH4-C13	-4.02	95.68	113.26
2	B	1401	X10	C19-C18-C17	-3.90	117.29	121.18
2	K	701	X10	C31-C17-C18	3.75	122.95	118.30
2	B	1401	X10	C29-C21-C20	3.74	127.10	120.84
2	F	701	X10	C19-C20-C21	-3.62	115.01	121.25
2	I	701	X10	C19-C18-C17	-3.51	117.67	121.18
2	A	701	X10	C30-C20-C21	-3.49	115.23	121.25
2	H	701	X10	C19-C20-C21	-3.47	115.27	121.25
2	B	1401	X10	C31-C17-C18	3.46	122.59	118.30
2	I	701	X10	C17-C12-C13	3.45	116.54	108.42
2	C	701	X10	C19-C20-C21	-3.41	115.37	121.25
2	K	701	X10	C19-C20-C21	-3.38	115.42	121.25
2	J	701	X10	C29-C21-C20	3.36	126.46	120.84
2	A	701	X10	C17-C12-C13	3.33	116.27	108.42
2	B	1401	X10	F24-C23-C25	3.27	122.76	118.32
2	F	701	X10	C18-C17-C12	-3.24	115.59	120.78
2	F	701	X10	C21-C29-C27	3.24	122.17	119.61
2	B	1401	X10	C31-C30-C20	-3.23	116.98	121.12
2	J	701	X10	C30-C31-C17	-3.21	117.98	121.18
2	A	701	X10	C22-C21-C20	3.20	126.20	120.84
2	E	701	X10	C31-C17-C18	3.19	122.26	118.30
2	C	701	X10	F28-C27-C25	3.17	122.62	118.32
2	J	701	X10	C31-C17-C18	3.16	122.22	118.30
2	B	1401	X10	C19-C20-C21	-3.15	115.81	121.25
2	G	701	X10	C03-N04-C05	-3.14	116.34	122.42
2	E	701	X10	C19-C20-C21	-3.10	115.90	121.25
2	K	701	X10	C19-C18-C17	-3.10	118.09	121.18
2	C	701	X10	C31-C17-C18	2.98	122.00	118.30
2	I	701	X10	C02-C03-N04	-2.98	104.53	112.26
2	E	701	X10	C30-C31-C17	-2.95	118.24	121.18
2	E	701	X10	C17-C12-C13	2.94	115.36	108.42
2	A	701	X10	C31-C17-C18	2.94	121.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	701	X10	C31-C17-C18	2.94	121.94	118.30
2	B	1401	X10	C02-C03-N04	-2.93	104.64	112.26
2	B	1401	X10	C17-C12-C13	2.90	115.25	108.42
2	D	701	X10	C31-C17-C18	2.84	121.83	118.30
2	I	701	X10	C31-C17-C18	2.83	121.81	118.30
2	E	701	X10	C22-C21-C20	2.81	125.55	120.84
2	E	701	X10	C03-N04-C05	-2.81	116.97	122.42
2	D	701	X10	C21-C29-C27	2.78	121.81	119.61
2	G	701	X10	C31-C17-C12	-2.76	116.35	120.78
2	B	1401	X10	C30-C20-C19	2.73	122.56	117.68
2	K	701	X10	C30-C31-C17	-2.68	118.51	121.18
2	K	701	X10	C30-C20-C19	2.67	122.46	117.68
2	F	701	X10	C31-C17-C18	2.67	121.62	118.30
2	B	1401	X10	C18-C17-C12	-2.66	116.51	120.78
2	C	701	X10	C13-C12-N11	2.66	116.74	108.55
2	I	701	X10	C19-C20-C21	-2.64	116.70	121.25
2	L	701	X10	C30-C20-C19	2.64	122.40	117.68
2	L	701	X10	C30-C20-C21	-2.61	116.74	121.25
2	F	701	X10	C29-C27-C25	-2.61	118.10	121.61
2	E	701	X10	C30-C20-C19	2.60	122.33	117.68
2	G	701	X10	C19-C18-C17	-2.58	118.60	121.18
2	I	701	X10	C22-C21-C20	-2.58	116.52	120.84
2	B	1401	X10	C21-C29-C27	-2.58	117.57	119.61
2	D	701	X10	O01-C02-N11	-2.56	118.62	122.95
2	E	701	X10	F28-C27-C25	2.56	121.78	118.32
2	G	701	X10	C30-C20-C21	-2.55	116.85	121.25
2	E	701	X10	C29-C21-C22	2.54	122.07	118.35
2	B	1401	X10	C22-C23-C25	-2.49	118.27	121.61
2	J	701	X10	C17-C12-C13	2.46	114.22	108.42
5	F	707	CO3	O2-C-O1	-2.46	113.39	119.68
2	A	701	X10	C31-C17-C12	-2.44	116.87	120.78
2	B	1401	X10	C27-C25-C23	2.44	120.91	118.71
2	A	701	X10	C30-C20-C19	2.43	122.03	117.68
2	E	701	X10	C18-C17-C12	-2.43	116.89	120.78
2	C	701	X10	C30-C20-C19	2.43	122.02	117.68
2	J	701	X10	C19-C20-C21	-2.36	117.19	121.25
2	F	701	X10	C19-C18-C17	-2.34	118.85	121.18
2	D	701	X10	C30-C20-C19	2.34	121.87	117.68
2	F	701	X10	C17-C12-C13	2.34	113.93	108.42
2	E	701	X10	C02-C03-N04	-2.32	106.23	112.26
2	K	701	X10	C18-C17-C12	-2.31	117.07	120.78
2	K	701	X10	F24-C23-C25	2.31	121.45	118.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	701	X10	O01-C02-N11	-2.31	119.05	122.95
2	C	701	X10	C19-C18-C17	-2.29	118.90	121.18
2	A	701	X10	C19-C18-C17	-2.27	118.92	121.18
2	C	701	X10	C30-C31-C17	-2.26	118.92	121.18
2	B	1401	X10	C29-C21-C22	2.26	121.66	118.35
2	F	701	X10	O01-C02-N11	-2.26	119.12	122.95
2	J	701	X10	C30-C20-C19	2.22	121.66	117.68
2	H	701	X10	C27-C25-C23	2.22	120.71	118.71
2	I	701	X10	F26-C25-C27	2.22	123.71	119.18
2	C	701	X10	C02-C03-N04	-2.22	106.51	112.26
2	I	701	X10	F24-C23-C25	-2.20	115.34	118.32
5	B	1402	CO3	O2-C-O1	-2.20	114.05	119.68
2	D	701	X10	C19-C18-C17	-2.19	118.99	121.18
2	C	701	X10	C18-C17-C12	-2.19	117.28	120.78
2	A	701	X10	C30-C31-C17	-2.17	119.02	121.18
2	K	701	X10	C03-N04-C05	-2.16	118.23	122.42
2	J	701	X10	C02-C03-N04	-2.16	106.66	112.26
5	H	704	CO3	O3-C-O1	-2.16	114.16	119.68
2	L	701	X10	C30-C31-C17	-2.13	119.05	121.18
2	L	701	X10	C18-C19-C20	-2.13	118.38	121.12
2	G	701	X10	C31-C17-C18	2.13	120.94	118.30
2	D	701	X10	C31-C17-C12	-2.13	117.37	120.78
2	E	701	X10	C21-C22-C23	-2.11	117.94	119.61
2	K	701	X10	O16-C13-C12	-2.11	117.06	120.58
2	G	701	X10	C17-C12-N11	2.11	118.07	112.75
2	A	701	X10	C13-C12-N11	2.10	115.02	108.55
2	K	701	X10	C29-C21-C22	2.10	121.41	118.35
2	D	701	X10	C03-N04-C05	-2.09	118.37	122.42
2	F	701	X10	F26-C25-C27	2.08	123.43	119.18
2	H	701	X10	C30-C20-C19	2.08	121.40	117.68
2	D	701	X10	C30-C20-C21	-2.08	117.67	121.25
2	L	701	X10	C19-C18-C17	-2.07	119.12	121.18
2	J	701	X10	C06-C05-C10	2.07	121.79	119.04
2	D	701	X10	C17-C12-C13	2.07	113.29	108.42
2	K	701	X10	O01-C02-N11	-2.05	119.47	122.95
2	F	701	X10	C30-C31-C17	-2.05	119.13	121.18
2	J	701	X10	C19-C18-C17	-2.04	119.14	121.18
2	C	701	X10	C03-C02-N11	2.04	121.02	116.16
2	G	701	X10	C22-C21-C20	-2.04	117.42	120.84
2	E	701	X10	C06-C05-C10	2.03	121.73	119.04
2	D	701	X10	C30-C31-C17	-2.02	119.17	121.18
2	H	701	X10	C31-C30-C20	-2.01	118.54	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	701	X10	C31-C30-C20	-2.01	118.54	121.12
2	G	701	X10	C06-C05-C10	2.00	121.70	119.04

There are no chirality outliers.

All (158) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	705	1PE	C14-C24-OH4-C13
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
2	H	701	X10	C30-C20-C21-C29
2	H	701	X10	C30-C20-C21-C22
2	J	701	X10	C10-C05-N04-C03
2	J	701	X10	C06-C05-N04-C03
4	E	704	1PE	OH4-C13-C23-OH3
4	L	704	1PE	OH4-C13-C23-OH3
2	C	701	X10	C10-C05-N04-C03
2	C	701	X10	C06-C05-N04-C03
2	F	701	X10	C06-C05-N04-C03
4	A	707	1PE	OH4-C13-C23-OH3
4	C	703	1PE	OH4-C13-C23-OH3
4	L	703	1PE	OH5-C14-C24-OH4
4	D	704	1PE	OH4-C13-C23-OH3
4	A	706	1PE	OH4-C13-C23-OH3
4	E	703	1PE	OH4-C13-C23-OH3
2	D	701	X10	C10-C05-N04-C03
4	J	703	1PE	OH4-C13-C23-OH3
4	E	704	1PE	C24-C14-OH5-C25
4	A	705	1PE	OH4-C13-C23-OH3
4	F	706	1PE	OH6-C15-C25-OH5
8	H	705	2PE	O10-C11-C12-O13
2	D	701	X10	C06-C05-N04-C03
4	A	705	1PE	OH5-C14-C24-OH4
4	J	704	1PE	OH5-C14-C24-OH4
4	K	703	1PE	OH6-C15-C25-OH5
2	E	701	X10	C10-C05-N04-C03
2	G	701	X10	C10-C05-N04-C03
4	H	703	1PE	OH4-C13-C23-OH3
4	K	703	1PE	OH5-C14-C24-OH4
4	L	703	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
8	H	705	2PE	O4-C5-C6-O7
4	E	703	1PE	OH2-C12-C22-OH3
8	H	705	2PE	O19-C20-C21-O22
4	E	704	1PE	OH5-C14-C24-OH4
4	F	703	1PE	OH2-C12-C22-OH3
4	G	705	1PE	OH5-C14-C24-OH4
2	E	701	X10	C06-C05-N04-C03
2	G	701	X10	C06-C05-N04-C03
4	G	704	1PE	OH4-C13-C23-OH3
2	B	1401	X10	O01-C02-C03-N04
2	J	701	X10	O01-C02-C03-N04
4	L	704	1PE	OH5-C14-C24-OH4
4	C	703	1PE	OH6-C15-C25-OH5
4	F	706	1PE	OH5-C14-C24-OH4
4	F	706	1PE	OH7-C16-C26-OH6
2	B	1401	X10	N11-C02-C03-N04
2	E	701	X10	N11-C02-C03-N04
2	J	701	X10	N11-C02-C03-N04
8	H	705	2PE	C9-C8-O7-C6
2	B	1401	X10	C06-C05-N04-C03
2	G	701	X10	N11-C02-C03-N04
4	I	704	1PE	OH6-C15-C25-OH5
4	J	703	1PE	OH5-C14-C24-OH4
4	K	702	1PE	OH4-C13-C23-OH3
4	A	706	1PE	C24-C14-OH5-C25
4	A	706	1PE	OH5-C14-C24-OH4
8	H	705	2PE	C12-C11-O10-C9
4	A	707	1PE	OH6-C15-C25-OH5
4	L	704	1PE	OH2-C12-C22-OH3
2	C	701	X10	O01-C02-C03-N04
2	G	701	X10	O01-C02-C03-N04
2	I	701	X10	N11-C02-C03-N04
2	I	701	X10	C10-C05-N04-C03
2	B	1401	X10	C10-C05-N04-C03
2	F	701	X10	O01-C02-C03-N04
4	E	705	1PE	OH5-C14-C24-OH4
4	E	704	1PE	OH2-C12-C22-OH3
2	E	701	X10	O01-C02-C03-N04
2	I	701	X10	O01-C02-C03-N04
2	C	701	X10	N11-C02-C03-N04
2	F	701	X10	N11-C02-C03-N04
4	D	703	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
2	I	701	X10	C06-C05-N04-C03
4	I	703	1PE	OH7-C16-C26-OH6
4	J	704	1PE	OH4-C13-C23-OH3
4	K	702	1PE	OH5-C14-C24-OH4
4	K	703	1PE	C14-C24-OH4-C13
2	D	701	X10	O01-C02-C03-N04
2	D	701	X10	N11-C02-C03-N04
4	I	703	1PE	OH5-C14-C24-OH4
4	L	705	1PE	OH2-C12-C22-OH3
4	A	705	1PE	C23-C13-OH4-C24
4	F	704	1PE	C12-C22-OH3-C23
4	A	706	1PE	C13-C23-OH3-C22
4	A	707	1PE	C14-C24-OH4-C13
4	I	704	1PE	C24-C14-OH5-C25
4	L	705	1PE	C16-C26-OH6-C15
4	G	705	1PE	C15-C25-OH5-C14
4	J	703	1PE	C24-C14-OH5-C25
4	L	703	1PE	C24-C14-OH5-C25
4	E	703	1PE	C23-C13-OH4-C24
4	L	704	1PE	C15-C25-OH5-C14
4	C	704	1PE	OH2-C12-C22-OH3
4	D	702	1PE	OH4-C13-C23-OH3
4	F	703	1PE	C13-C23-OH3-C22
8	H	705	2PE	O16-C17-C18-O19
4	K	702	1PE	C15-C25-OH5-C14
4	L	703	1PE	C23-C13-OH4-C24
4	H	703	1PE	C13-C23-OH3-C22
8	H	705	2PE	C23-C24-O25-C26
4	F	703	1PE	C12-C22-OH3-C23
4	E	705	1PE	OH4-C13-C23-OH3
4	L	704	1PE	C24-C14-OH5-C25
4	L	705	1PE	C15-C25-OH5-C14
4	E	704	1PE	OH6-C15-C25-OH5
4	F	703	1PE	OH6-C15-C25-OH5
4	J	704	1PE	OH2-C12-C22-OH3
4	D	704	1PE	C12-C22-OH3-C23
4	D	704	1PE	OH2-C12-C22-OH3
4	A	707	1PE	C12-C22-OH3-C23
4	L	703	1PE	C13-C23-OH3-C22
4	F	703	1PE	OH4-C13-C23-OH3
4	C	705	1PE	OH2-C12-C22-OH3
4	E	704	1PE	C23-C13-OH4-C24

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Mol	Chain	Res	Type	Atoms
4	A	705	1PE	C24-C14-OH5-C25
4	L	705	1PE	C24-C14-OH5-C25
4	K	704	1PE	OH4-C13-C23-OH3
4	A	706	1PE	C23-C13-OH4-C24
4	J	704	1PE	C14-C24-OH4-C13
4	D	703	1PE	C13-C23-OH3-C22
4	A	706	1PE	C14-C24-OH4-C13
4	E	703	1PE	C12-C22-OH3-C23
8	H	705	2PE	C17-C18-O19-C20
4	L	704	1PE	OH6-C15-C25-OH5
4	A	705	1PE	C14-C24-OH4-C13
2	J	701	X10	C17-C12-N11-C02
4	C	703	1PE	C15-C25-OH5-C14
4	A	705	1PE	C13-C23-OH3-C22
4	L	704	1PE	C13-C23-OH3-C22
4	D	704	1PE	C13-C23-OH3-C22
4	J	704	1PE	C13-C23-OH3-C22
4	L	705	1PE	C13-C23-OH3-C22
4	G	705	1PE	OH6-C15-C25-OH5
4	K	704	1PE	C12-C22-OH3-C23
4	J	703	1PE	C14-C24-OH4-C13
4	L	704	1PE	C23-C13-OH4-C24
4	C	704	1PE	OH4-C13-C23-OH3
4	E	704	1PE	C12-C22-OH3-C23
4	E	703	1PE	C14-C24-OH4-C13
8	H	705	2PE	C24-C23-O22-C21
4	G	704	1PE	C13-C23-OH3-C22
4	E	704	1PE	C15-C25-OH5-C14
8	H	705	2PE	C6-C5-O4-C3
4	C	705	1PE	C13-C23-OH3-C22
8	H	705	2PE	O13-C14-C15-O16
4	A	707	1PE	OH5-C14-C24-OH4
4	D	703	1PE	C24-C14-OH5-C25
4	L	704	1PE	C12-C22-OH3-C23
4	C	703	1PE	OH5-C14-C24-OH4
4	J	703	1PE	C13-C23-OH3-C22
2	A	701	X10	C02-C03-N04-C05
4	L	705	1PE	OH4-C13-C23-OH3
4	I	704	1PE	C14-C24-OH4-C13

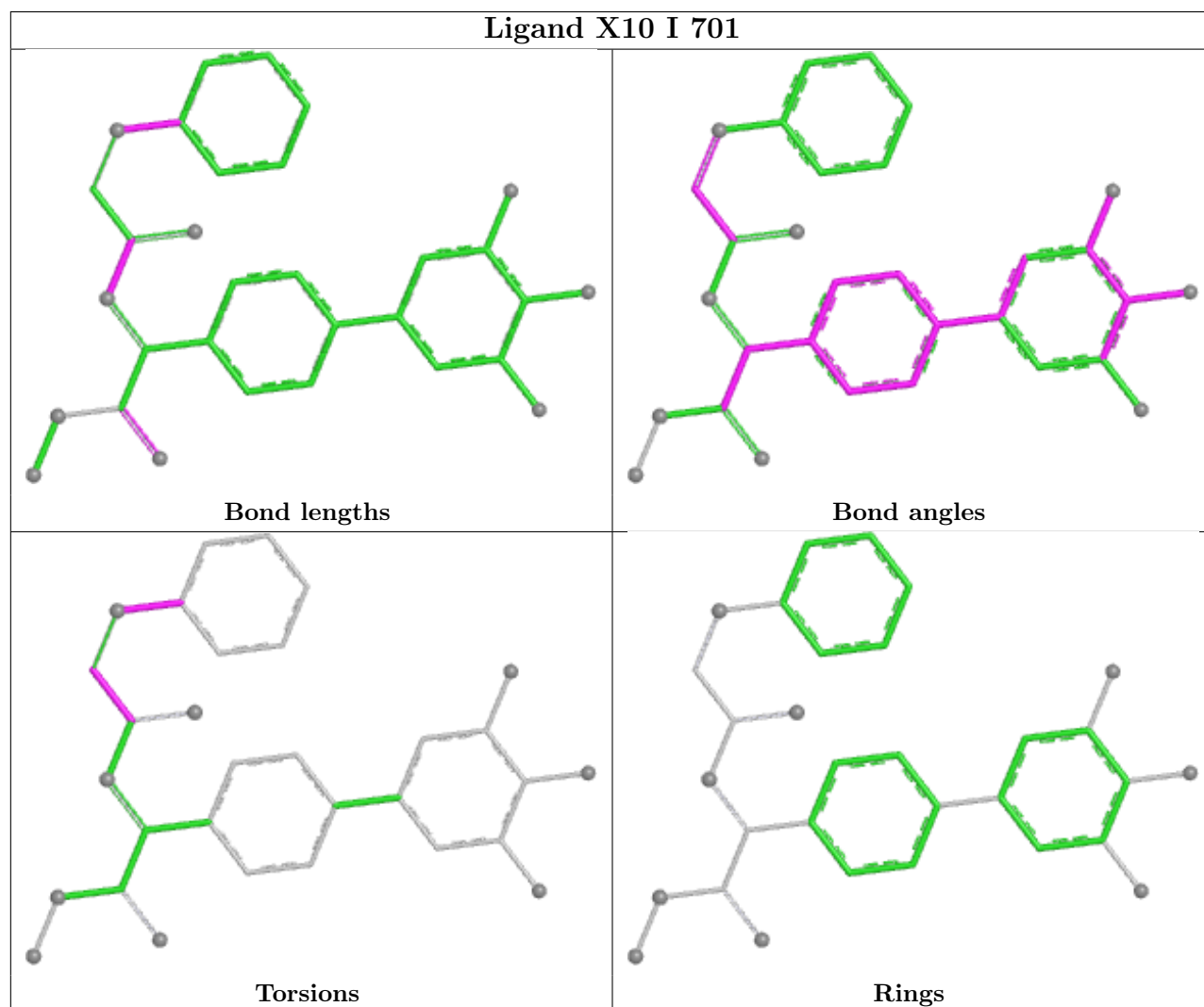
There are no ring outliers.

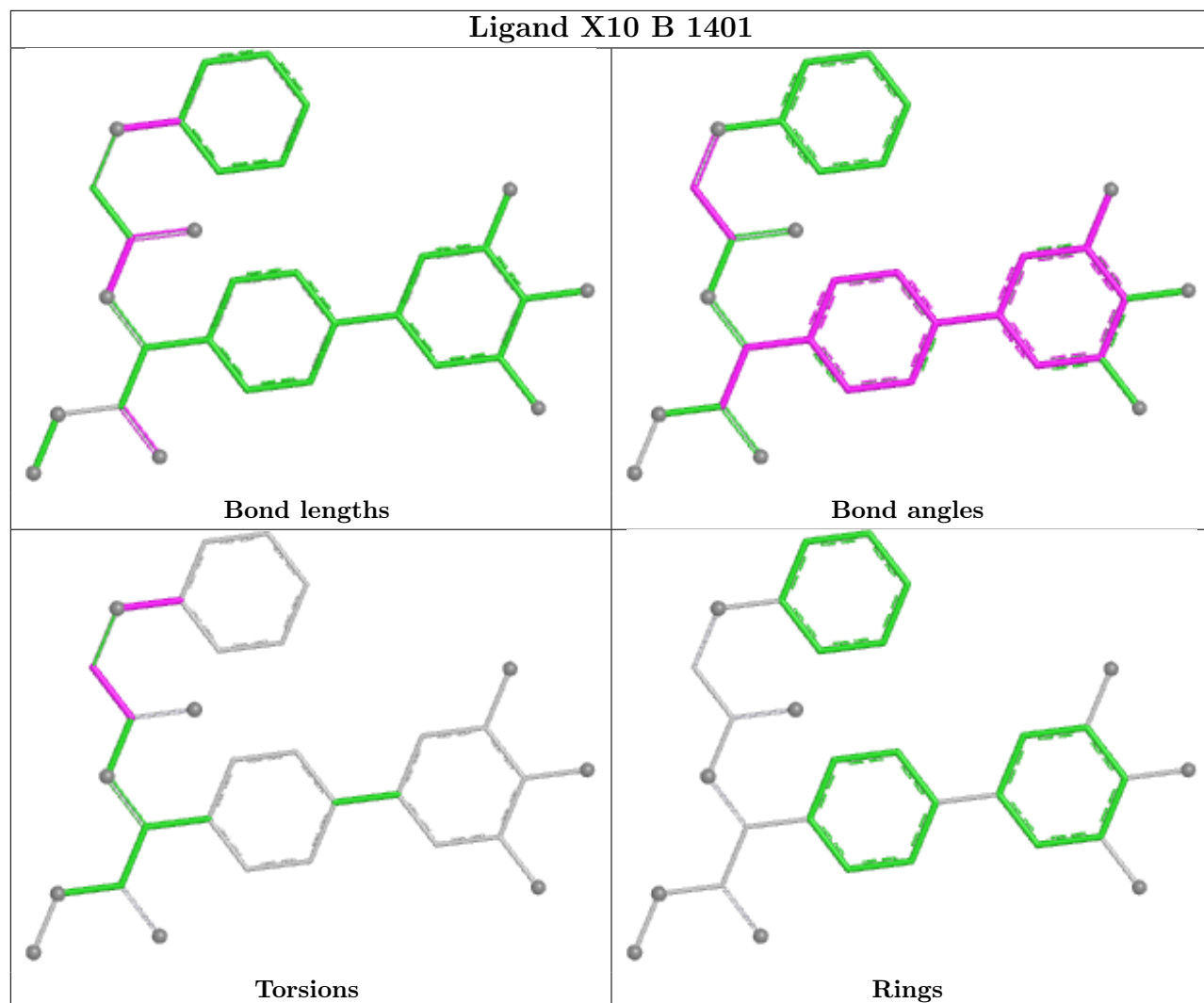
40 monomers are involved in 102 short contacts:

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
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

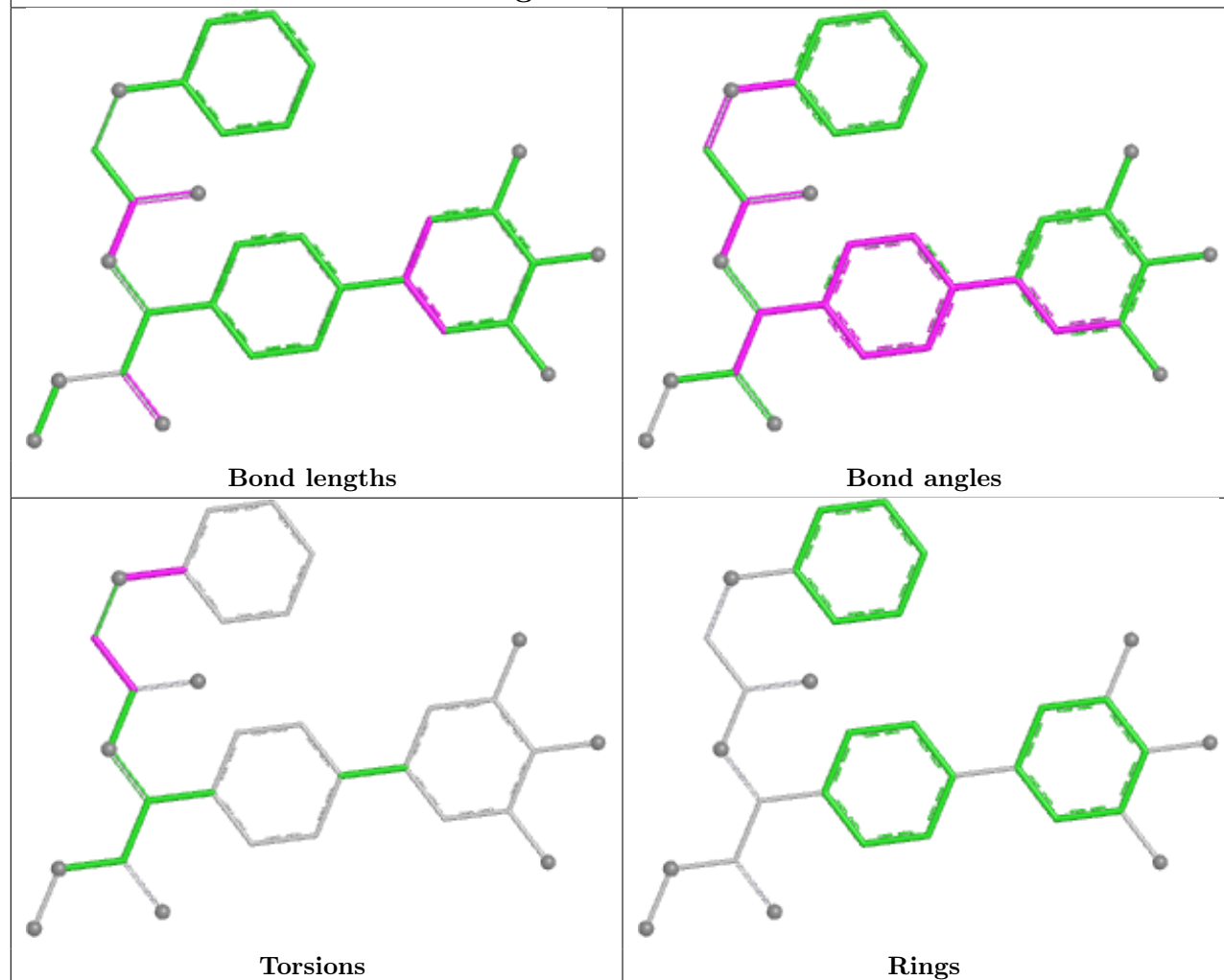
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

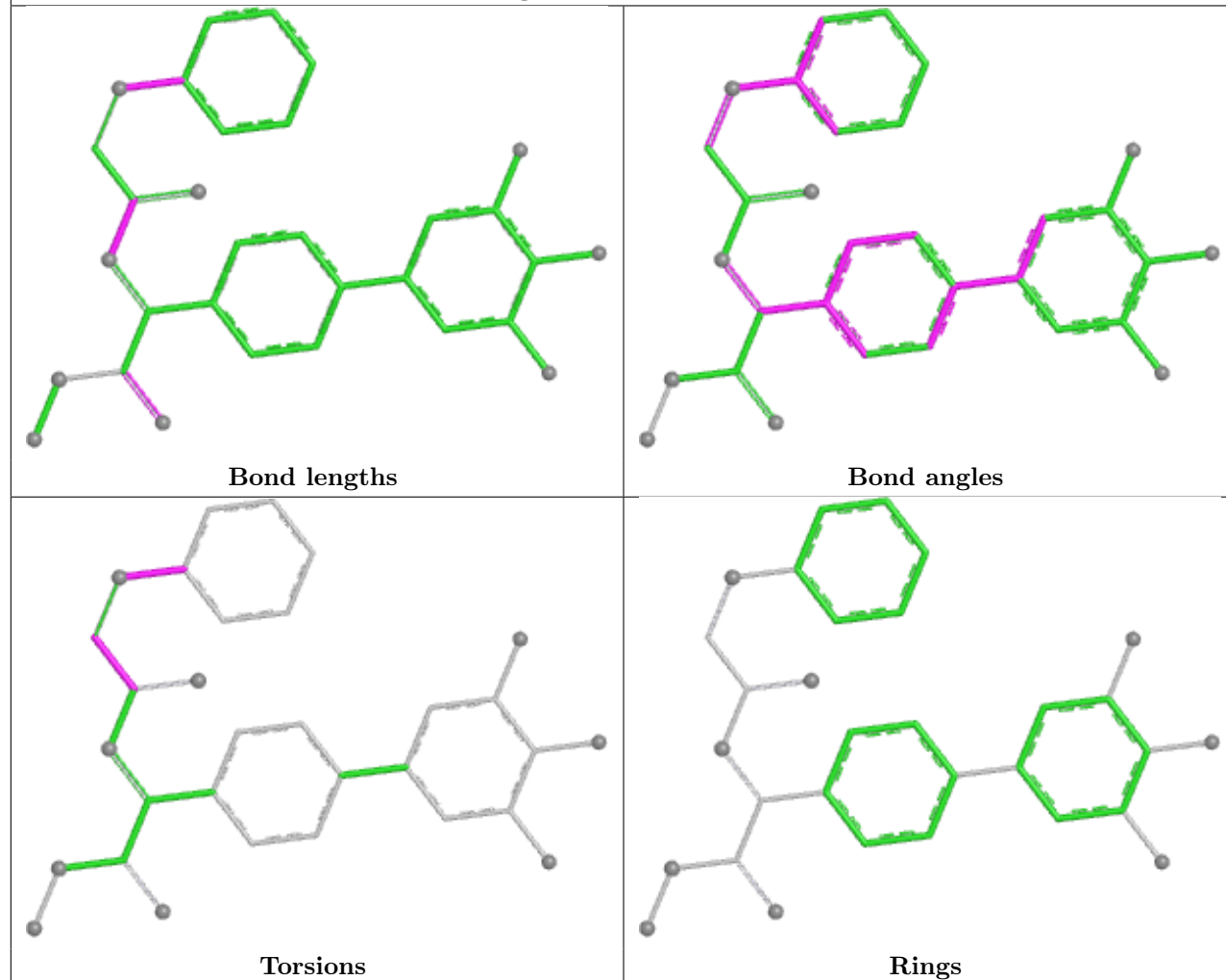




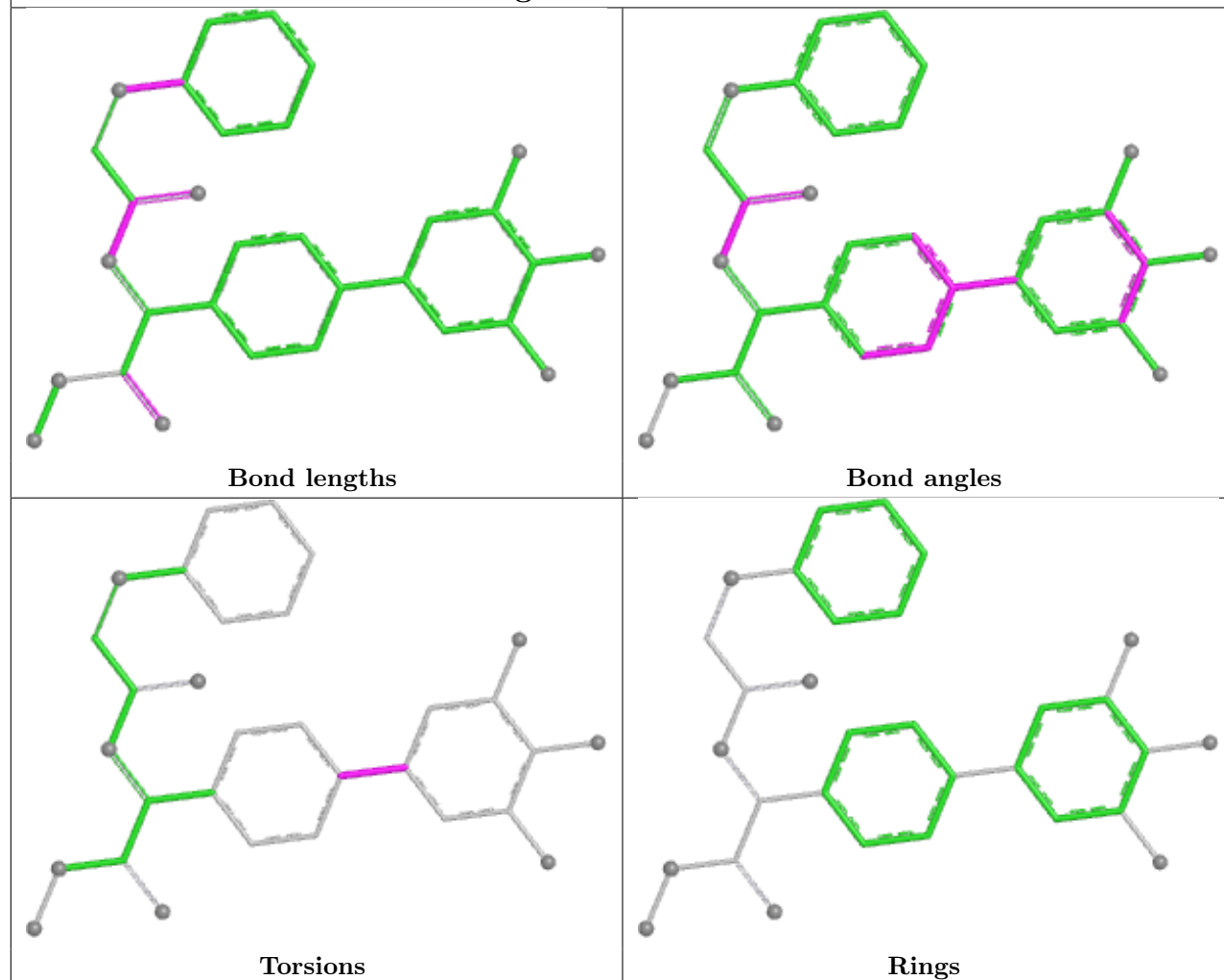
Ligand X10 D 701



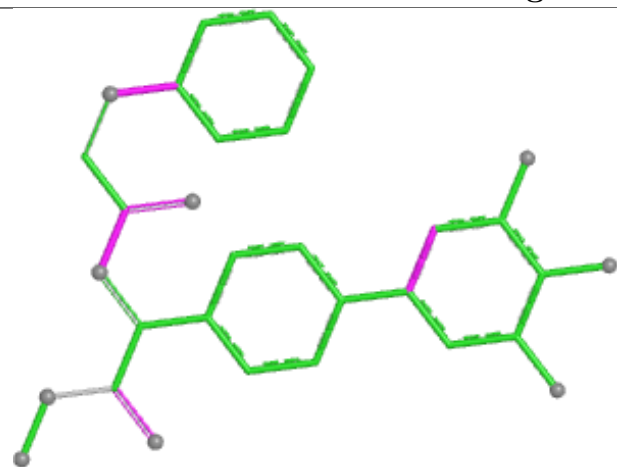
Ligand X10 G 701



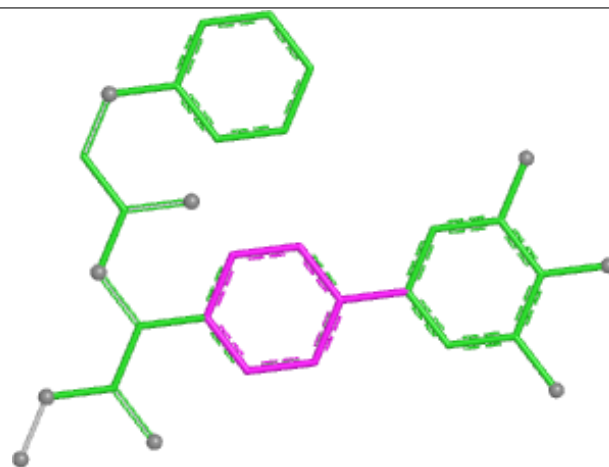
Ligand X10 H 701



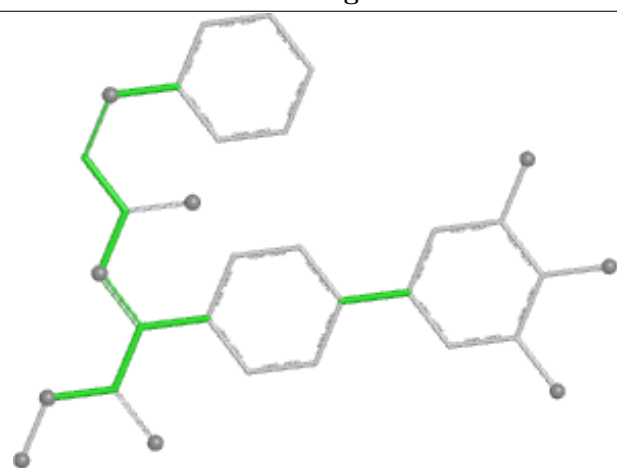
Ligand X10 L 701



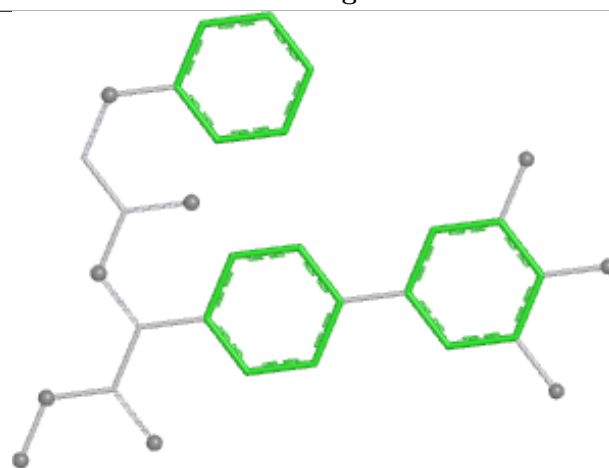
Bond lengths



Bond angles

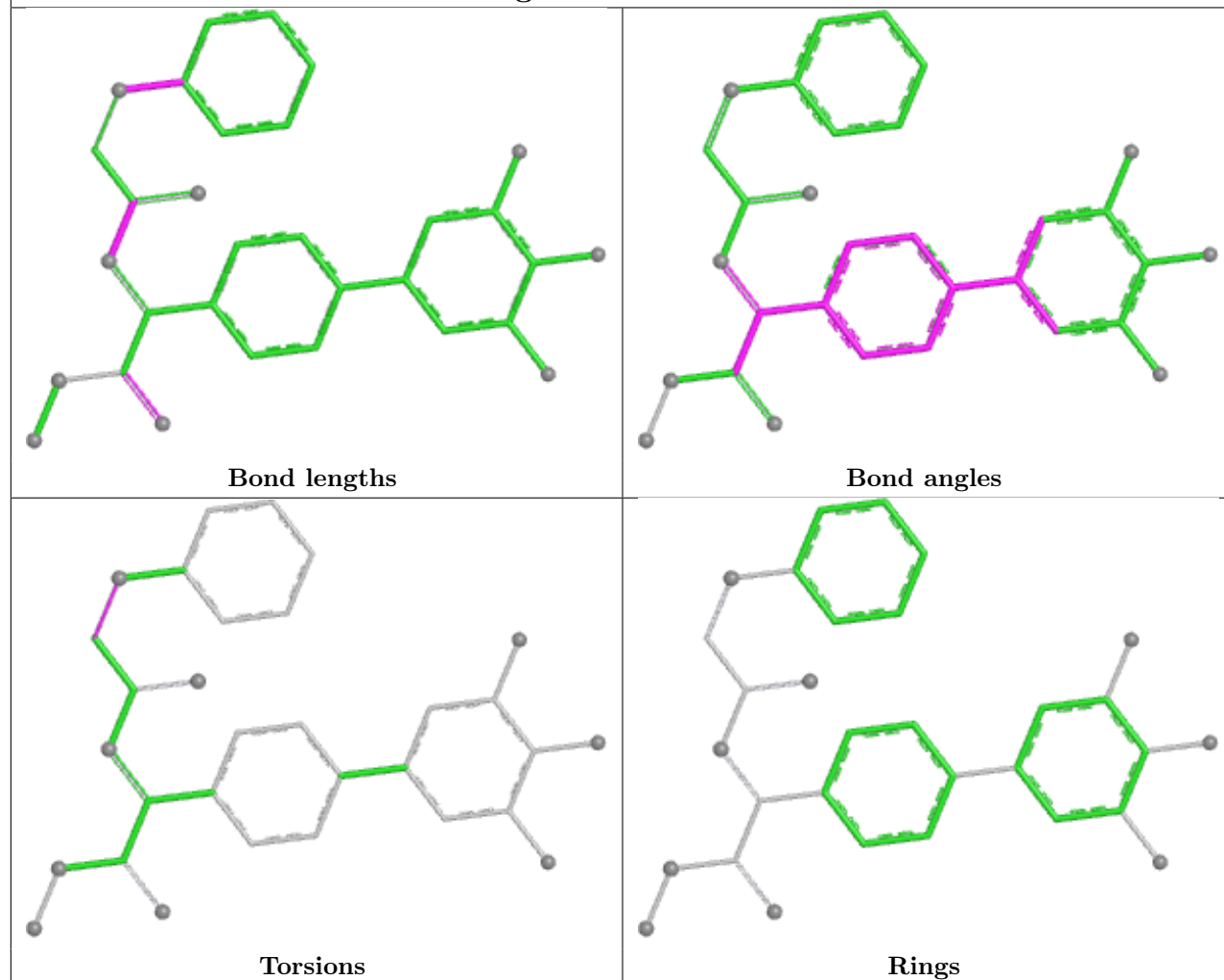


Torsions

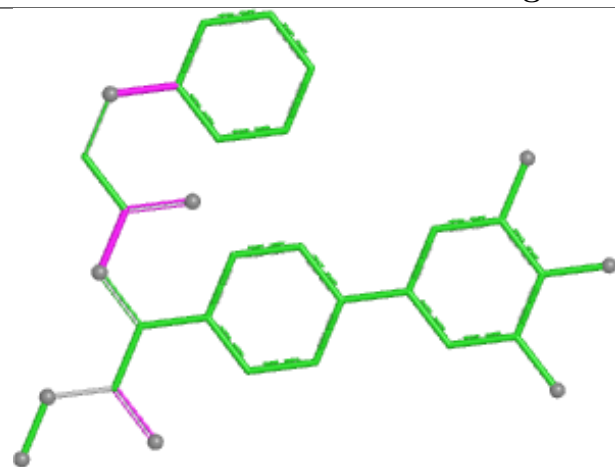


Rings

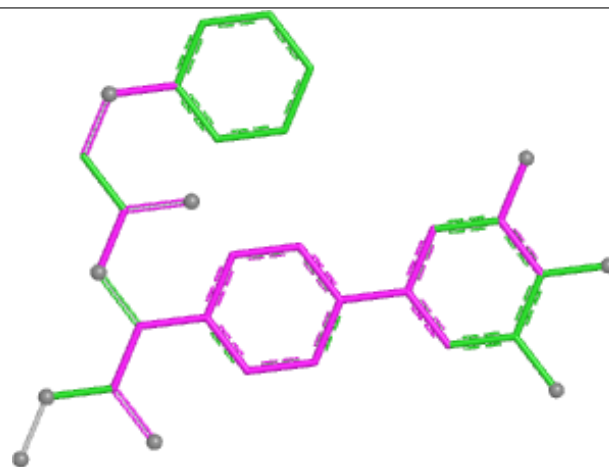
Ligand X10 A 701



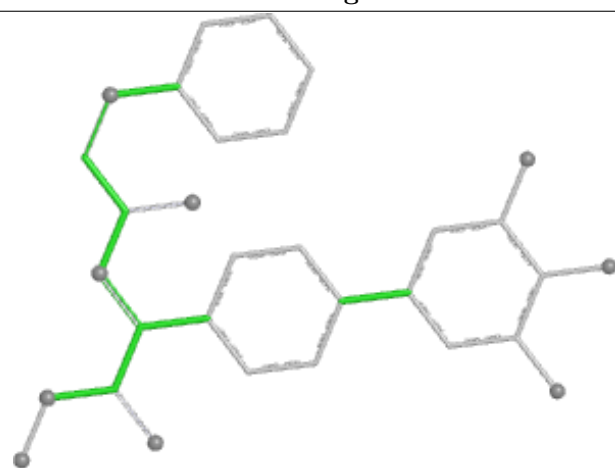
Ligand X10 K 701



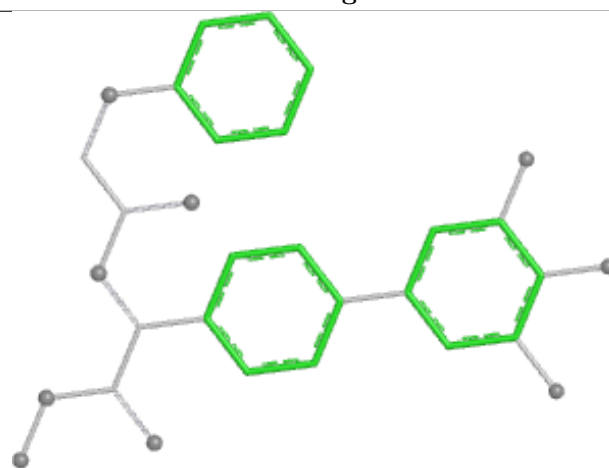
Bond lengths



Bond angles

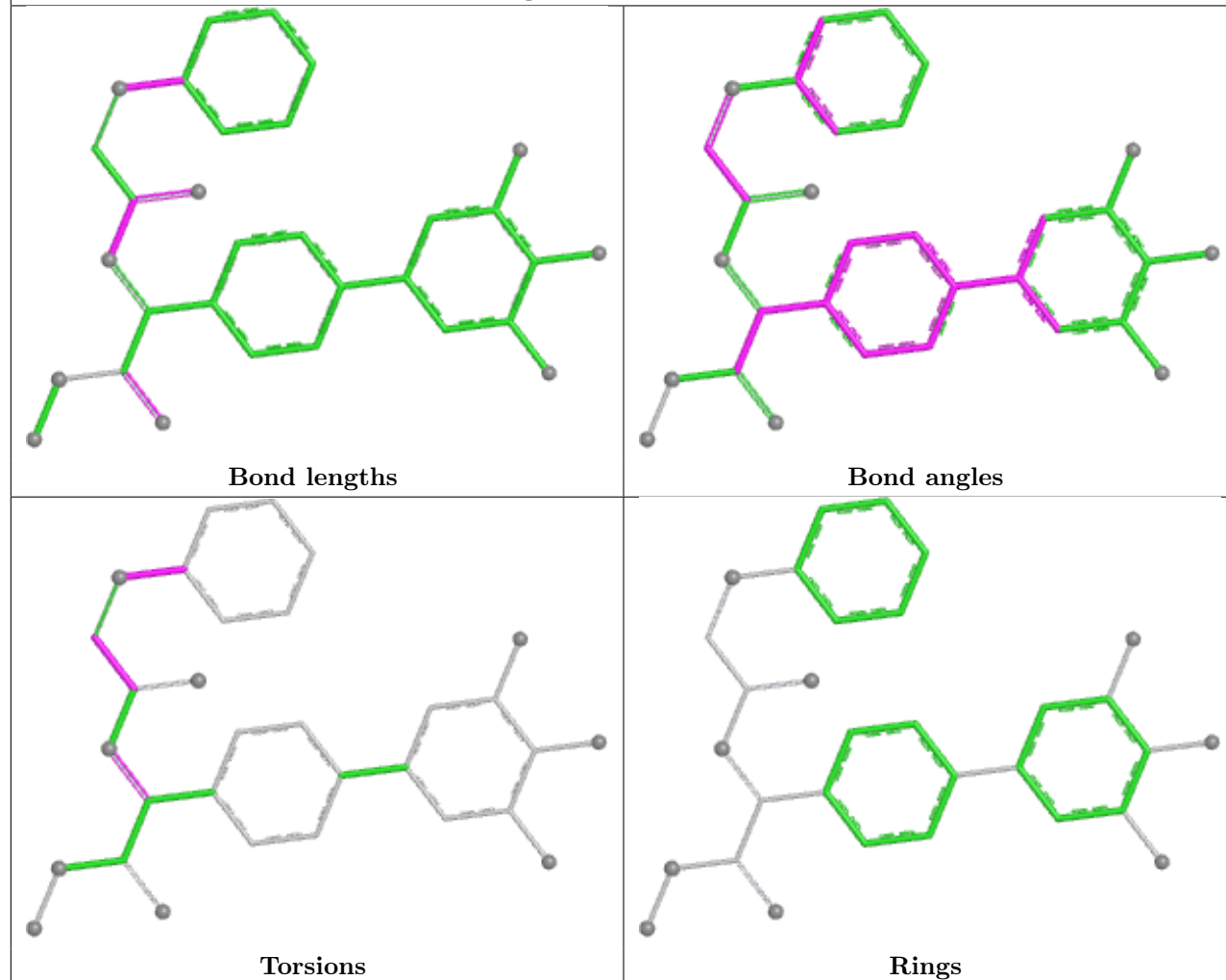


Torsions

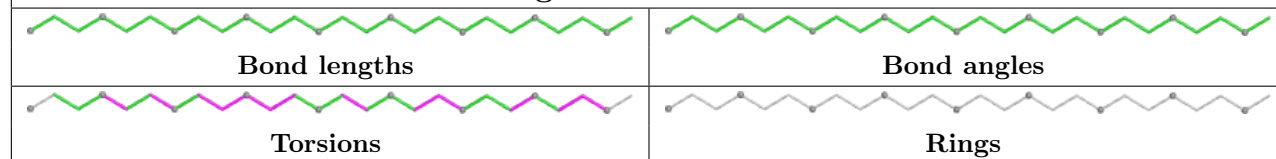


Rings

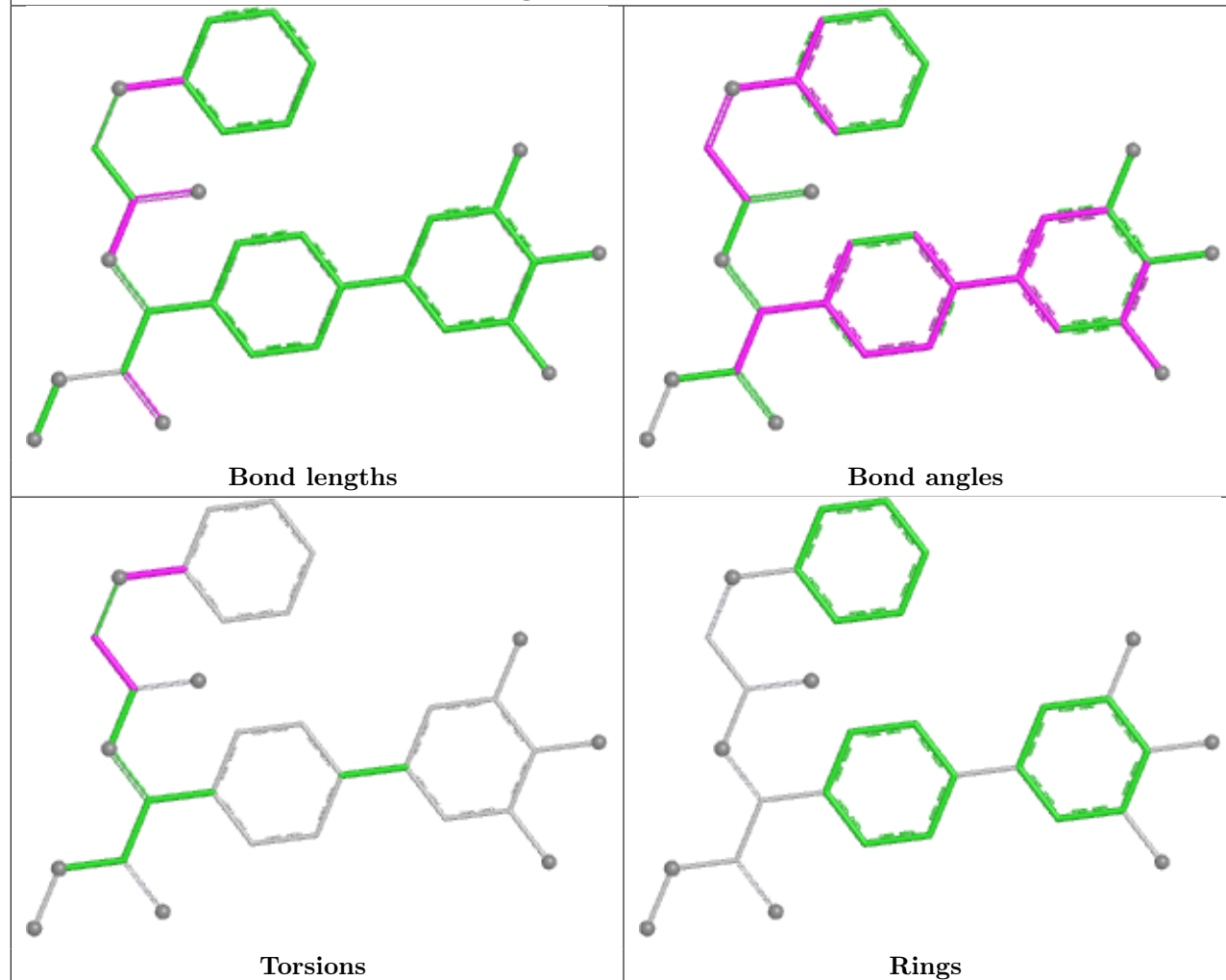
Ligand X10 J 701



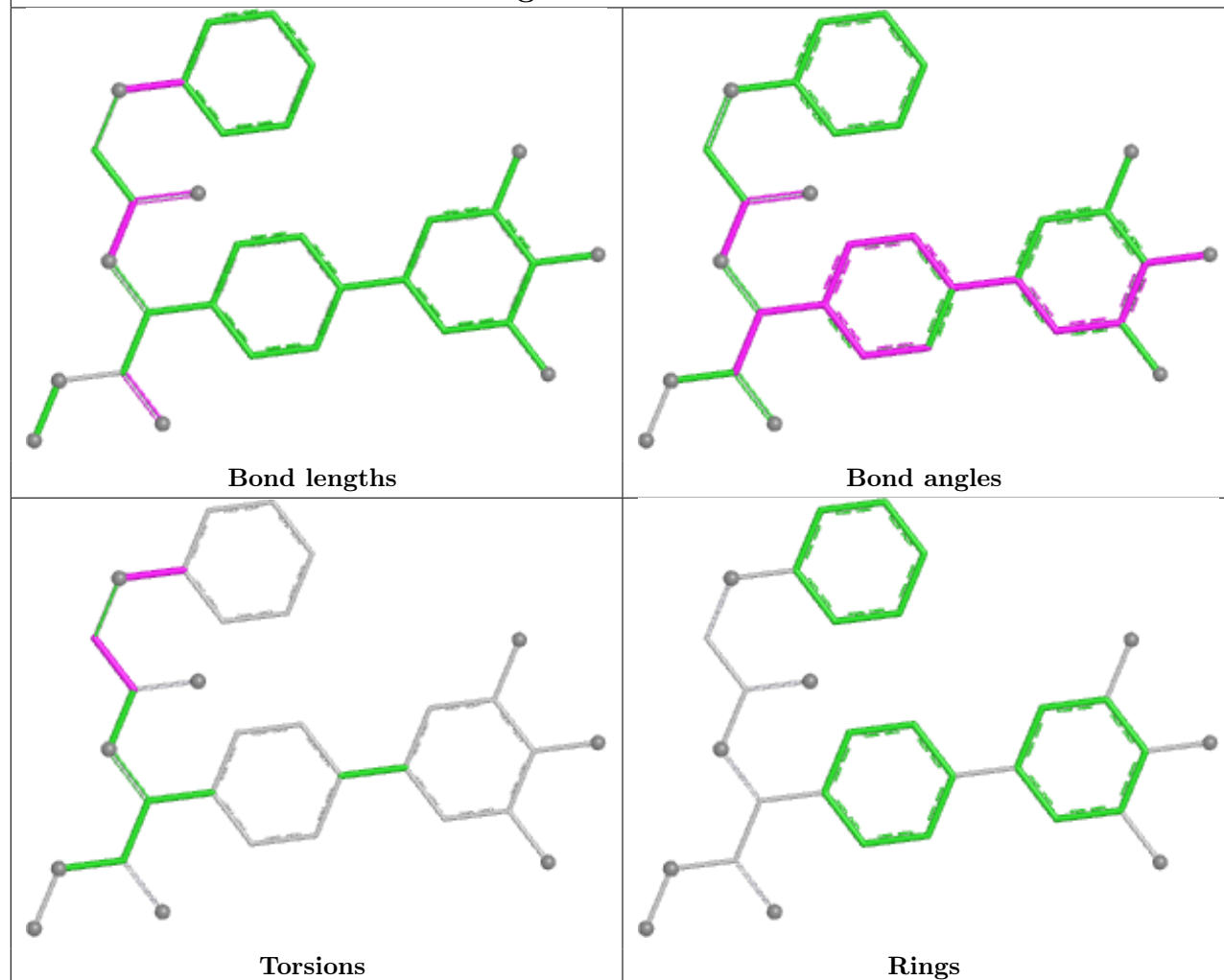
Ligand 2PE H 705

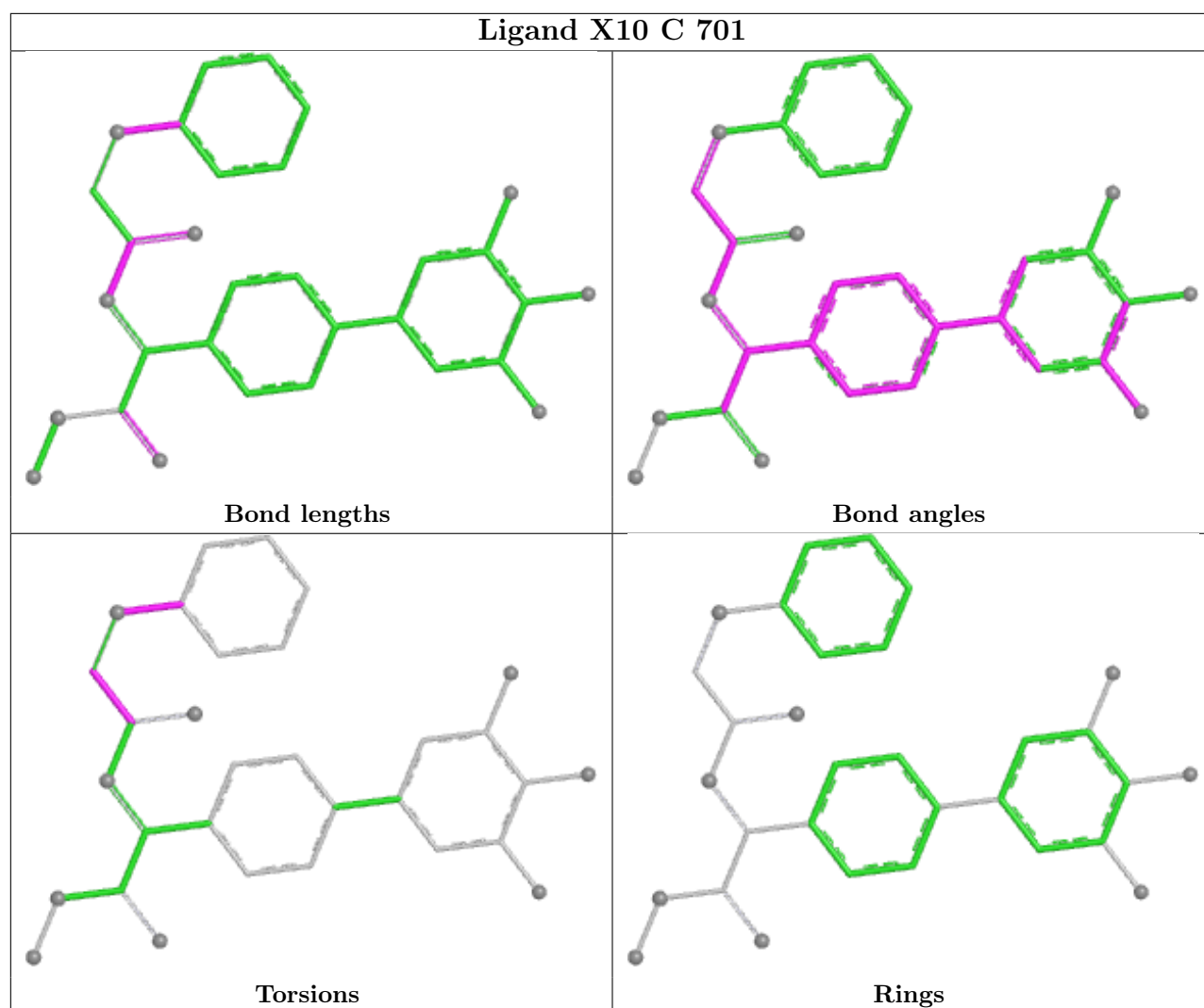


Ligand X10 E 701



Ligand X10 F 701





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%)

All (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
1	E	549	SER	4.1
1	L	549	SER	4.0
1	B	259	VAL	3.9
1	L	123	VAL	3.9
1	K	603	ASP	3.8
1	I	85	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	219	LEU	3.6
1	H	605	LEU	3.5
1	I	604	ALA	3.5
1	L	218	LYS	3.5
1	K	604	ALA	3.4
1	C	605	LEU	3.4
1	B	85	ALA	3.3
1	D	607	HIS	3.3
1	D	549	SER	3.3
1	E	136	GLY	3.3
1	D	605	LEU	3.2
1	L	136	GLY	3.2
1	L	219	LEU	3.2
1	D	258	ASN	3.1
1	I	605	LEU	3.1
1	B	197	ASP	3.1
1	C	609	HIS	3.1
1	J	136	GLY	3.1
1	L	361	SER	3.1
1	E	363	GLY	3.1
1	J	255	THR	3.0
1	D	602	ASN	3.0
1	H	196	ALA	3.0
1	D	259	VAL	3.0
1	D	136	GLY	3.0
1	F	195	VAL	2.9
1	E	604	ALA	2.9
1	D	606	HIS	2.9
1	E	605	LEU	2.8
1	I	607	HIS	2.8
1	F	136	GLY	2.8
1	I	124	GLU	2.8
1	E	85	ALA	2.7
1	K	605	LEU	2.7
1	J	549	SER	2.7
1	C	607	HIS	2.7
1	I	606	HIS	2.6
1	L	398	PHE	2.6
1	H	604	ALA	2.6
1	I	273	ASN	2.6
1	I	609	HIS	2.5
1	A	85	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	196	ALA	2.5
1	G	195	VAL	2.5
1	L	365	VAL	2.5
1	K	606	HIS	2.4
1	J	259	VAL	2.4
1	F	605	LEU	2.4
1	L	364	ASP	2.4
1	F	604	ALA	2.4
1	C	606	HIS	2.4
1	F	123	VAL	2.4
1	G	259	VAL	2.4
1	B	136	GLY	2.3
1	D	363	GLY	2.3
1	G	605	LEU	2.3
1	H	135	PRO	2.3
1	G	364	ASP	2.2
1	H	195	VAL	2.2
1	G	85	ALA	2.2
1	D	255	THR	2.2
1	D	256	ASP	2.2
1	K	363	GLY	2.2
1	K	550	SER	2.2
1	B	132	VAL	2.2
1	F	549	SER	2.2
1	H	276	THR	2.1
1	G	363	GLY	2.1
1	H	136	GLY	2.1
1	K	136	GLY	2.1
1	B	605	LEU	2.1
1	L	124	GLU	2.1
1	H	398	PHE	2.1
1	K	86	SER	2.1
1	L	217	ASN	2.1
1	H	85	ALA	2.0
1	B	549	SER	2.0
1	B	602	ASN	2.0

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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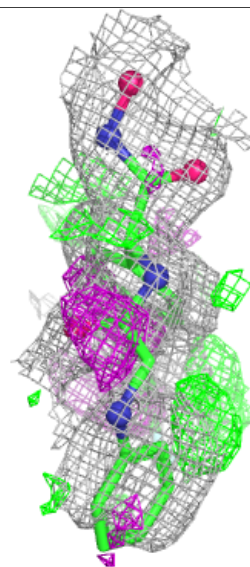
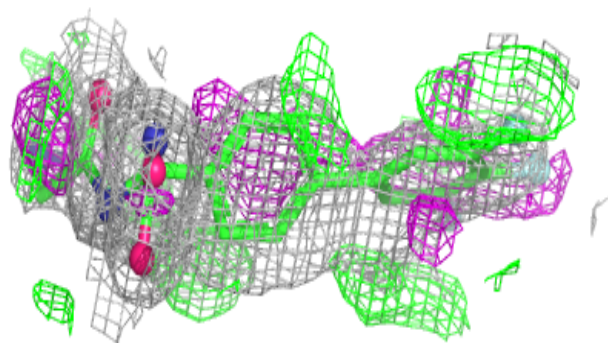
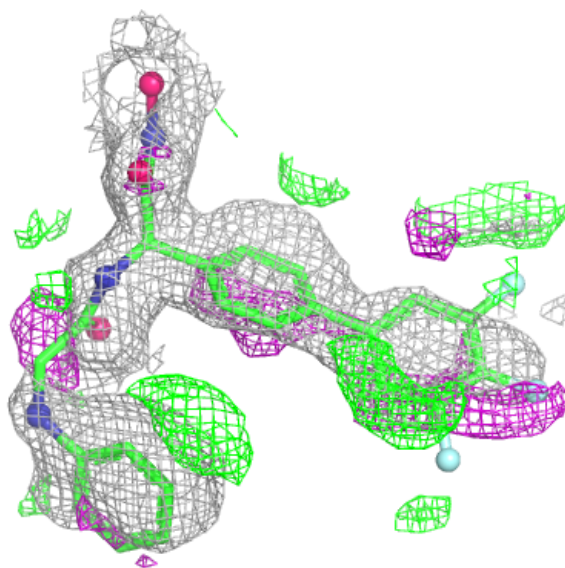
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	E	702	5/5	0.96	0.10	28,29,40,41	5
6	ZN	C	707	1/1	0.97	0.06	22,22,22,22	1
6	ZN	D	708	1/1	0.97	0.03	19,19,19,19	1
6	ZN	K	707	1/1	0.97	0.04	19,19,19,19	1
7	NA	G	709	1/1	0.97	0.04	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.

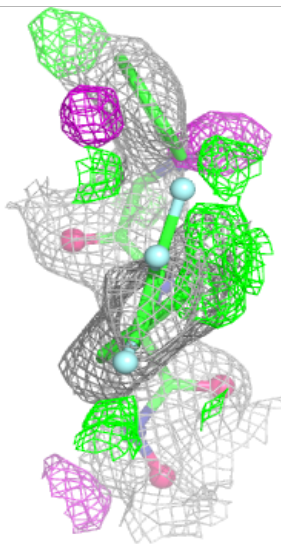
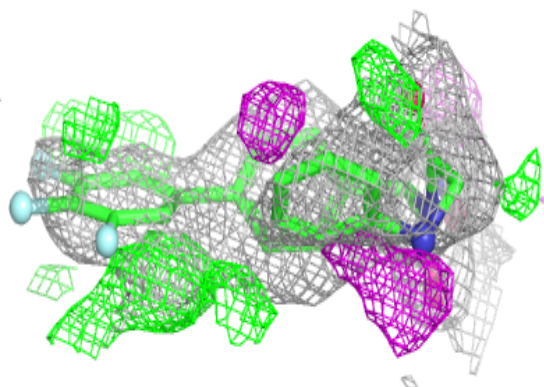
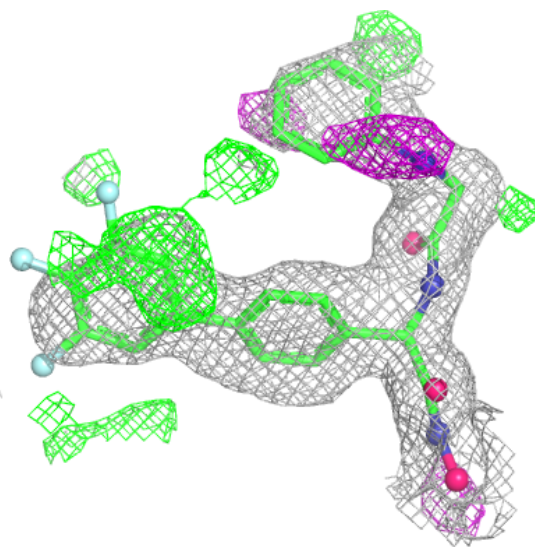
Electron density around X10 L 701:

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



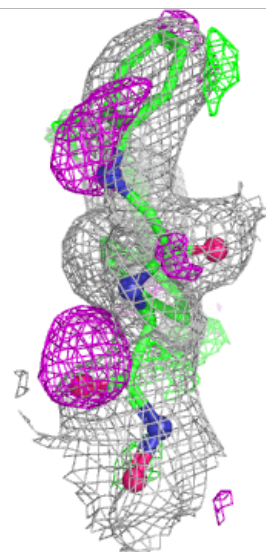
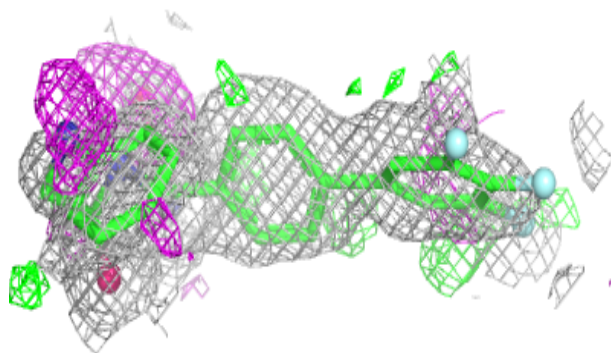
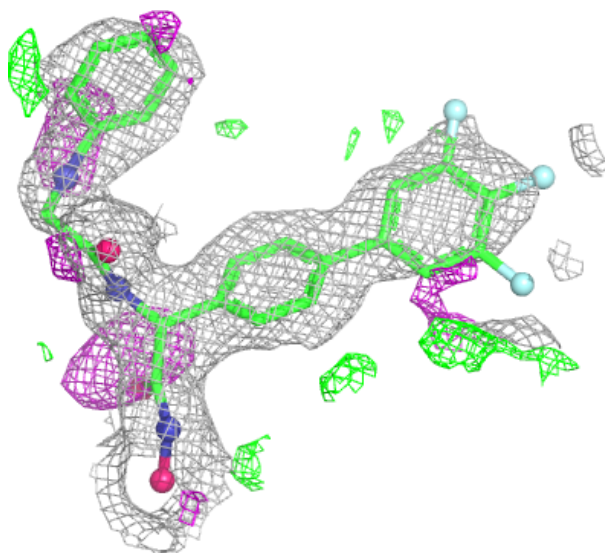
Electron density around X10 C 701:

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



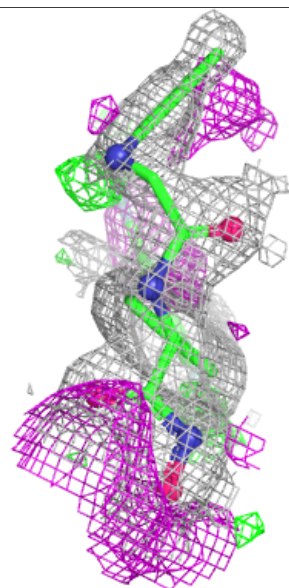
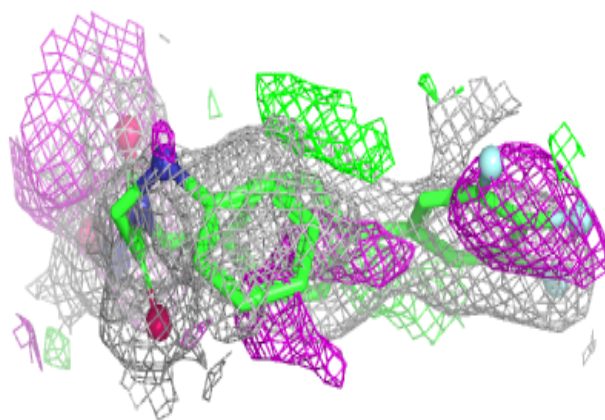
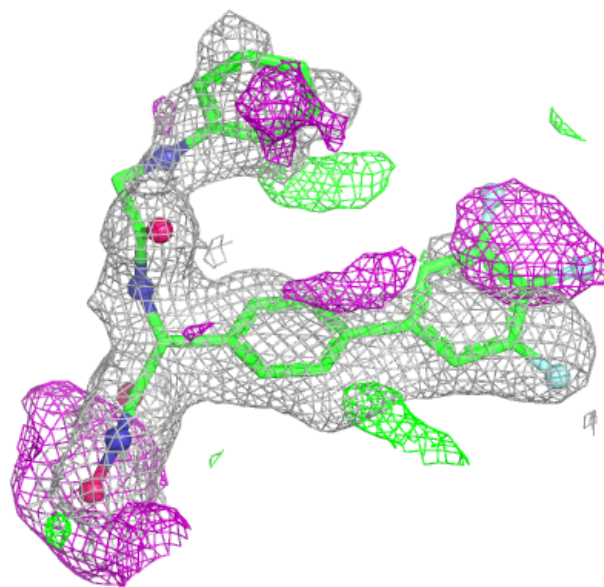
Electron density around X10 D 701:

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



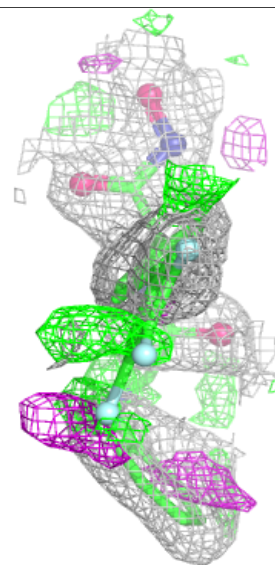
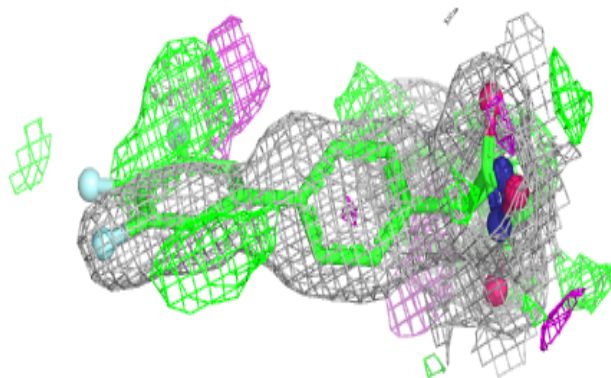
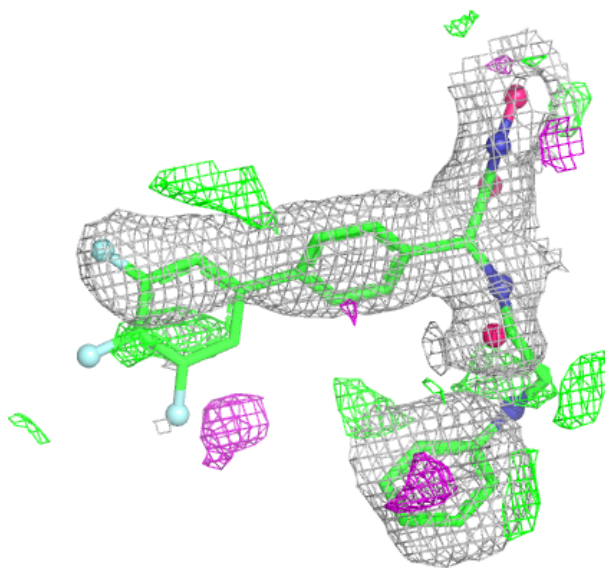
Electron density around X10 B 1401:

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



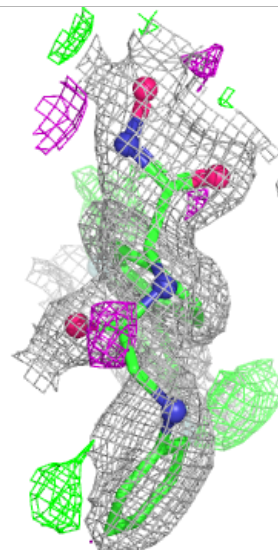
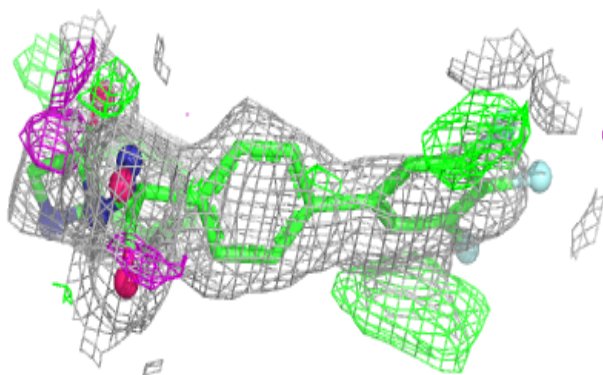
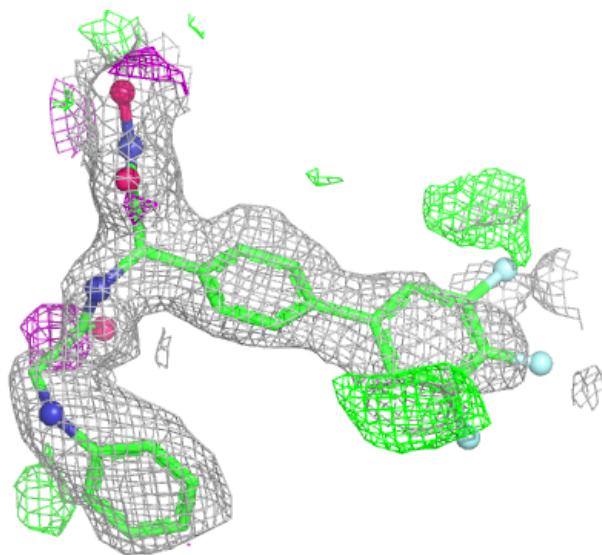
Electron density around X10 E 701:

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



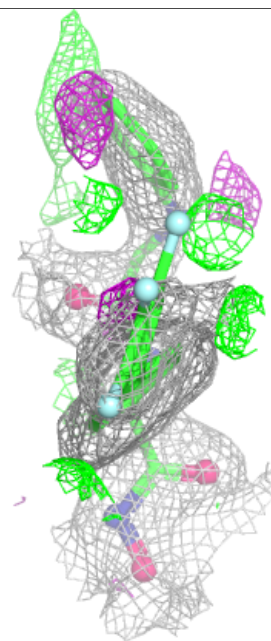
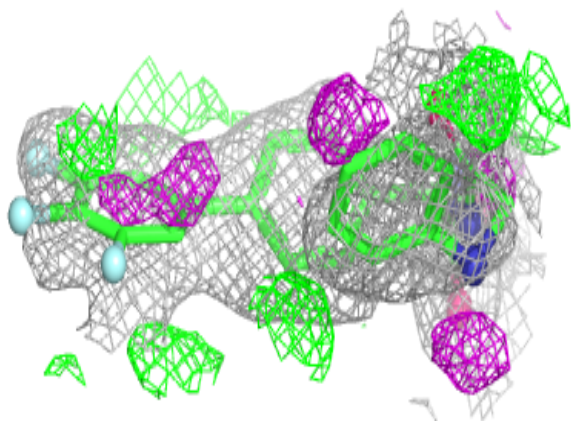
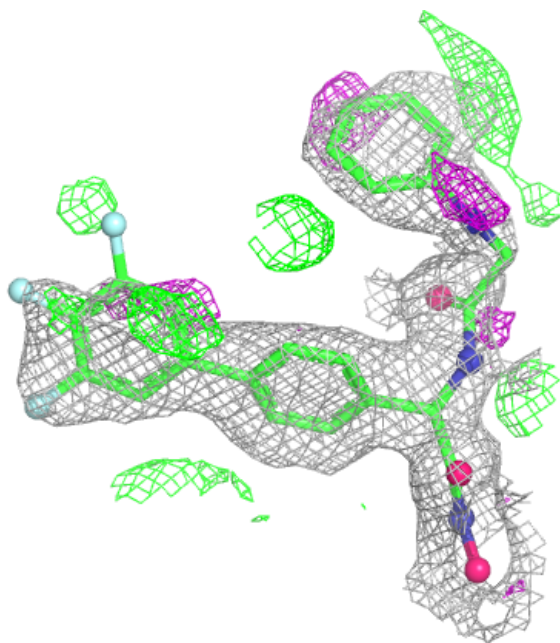
Electron density around X10 F 701:

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



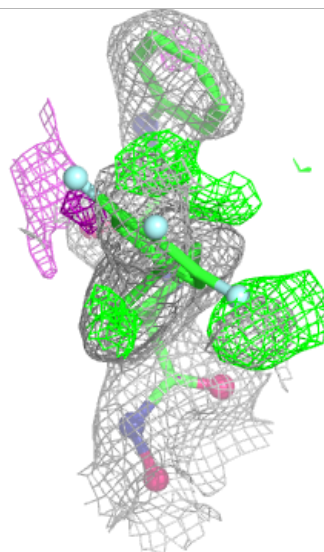
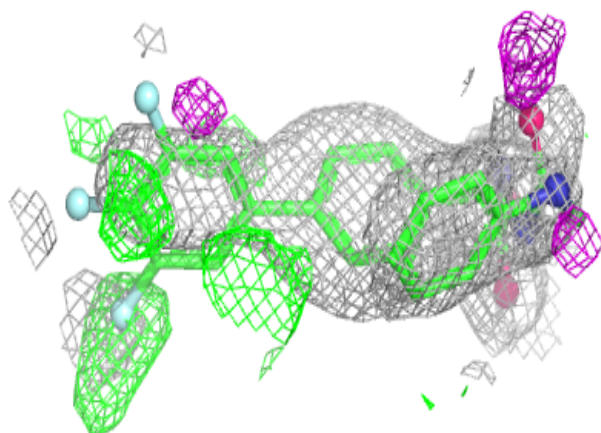
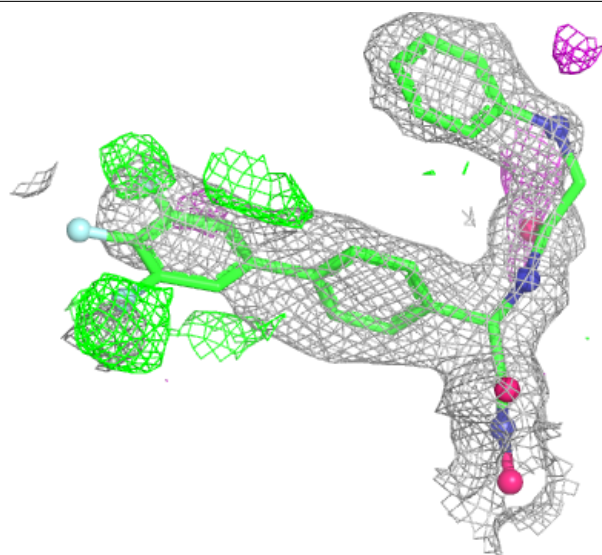
Electron density around X10 J 701:

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



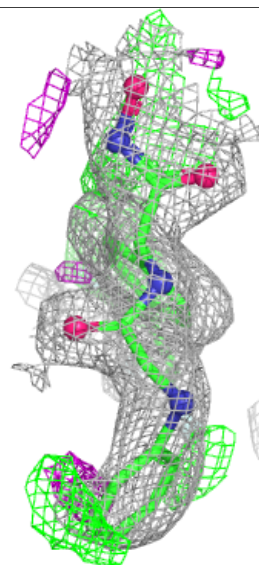
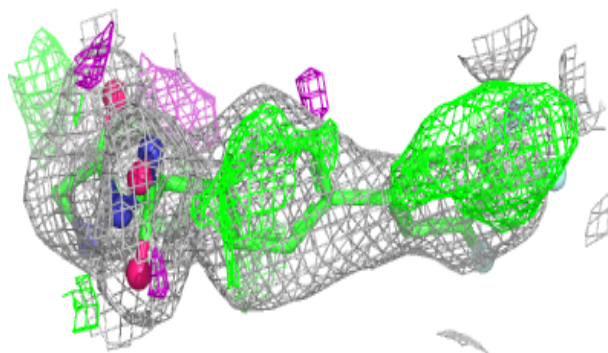
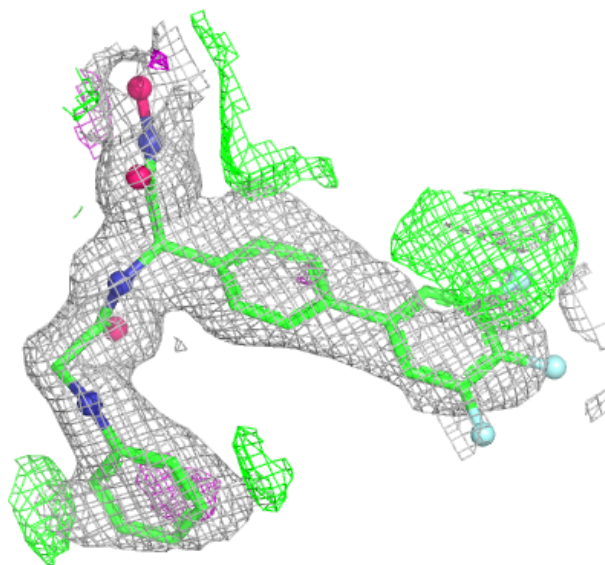
Electron density around X10 H 701:

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



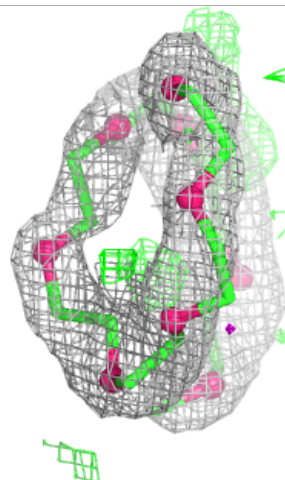
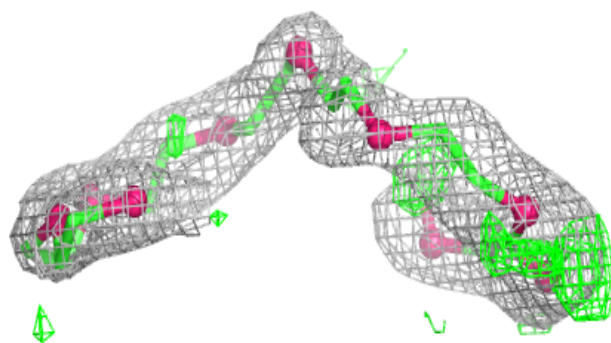
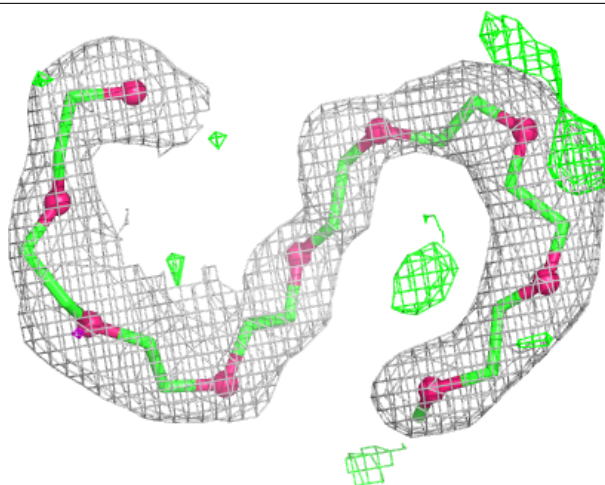
Electron density around X10 I 701:

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



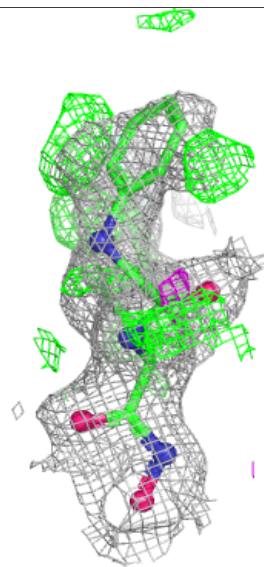
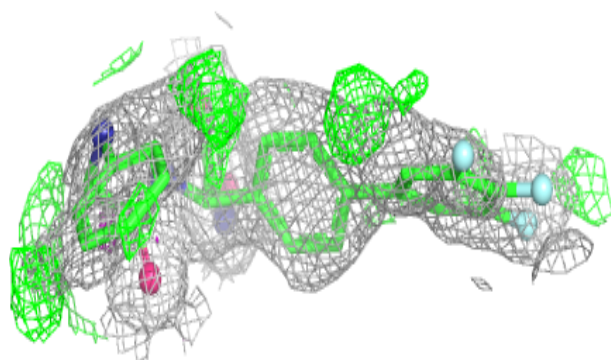
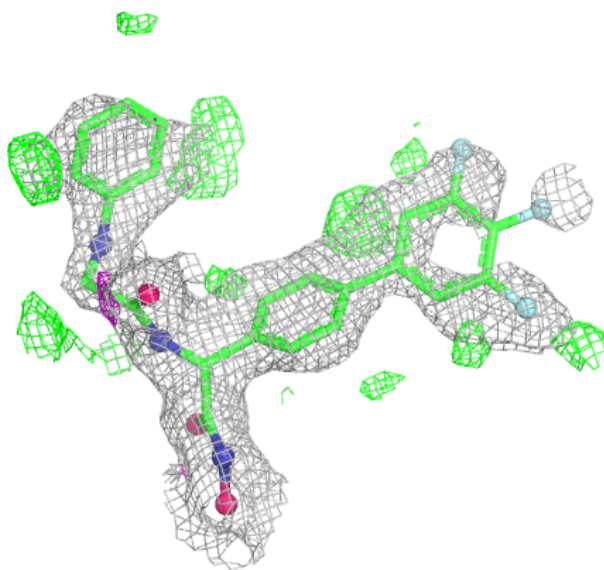
Electron density around 2PE H 705:

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



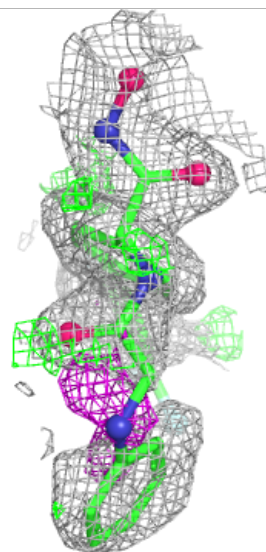
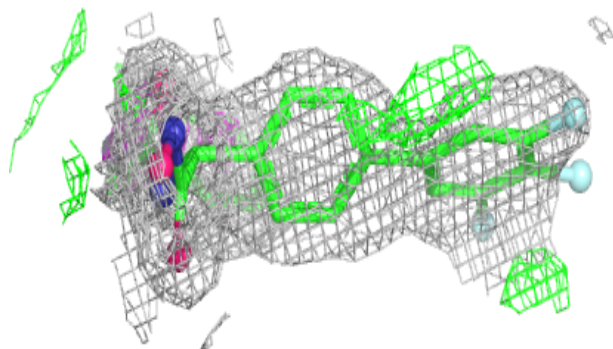
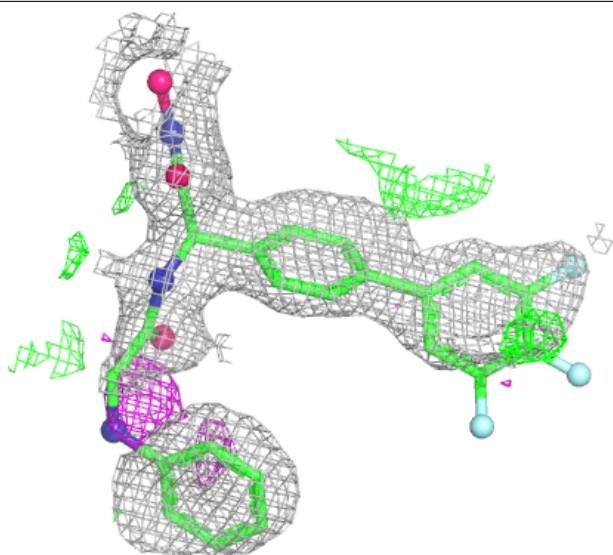
Electron density around X10 G 701:

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



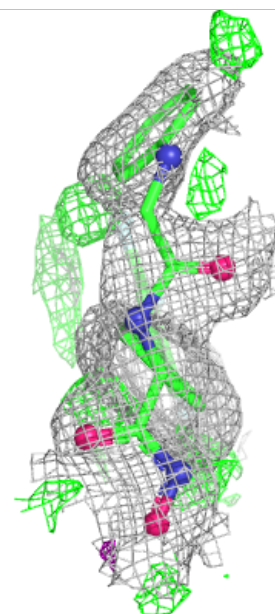
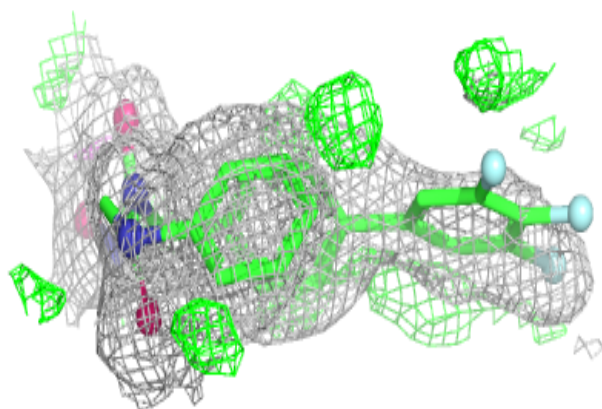
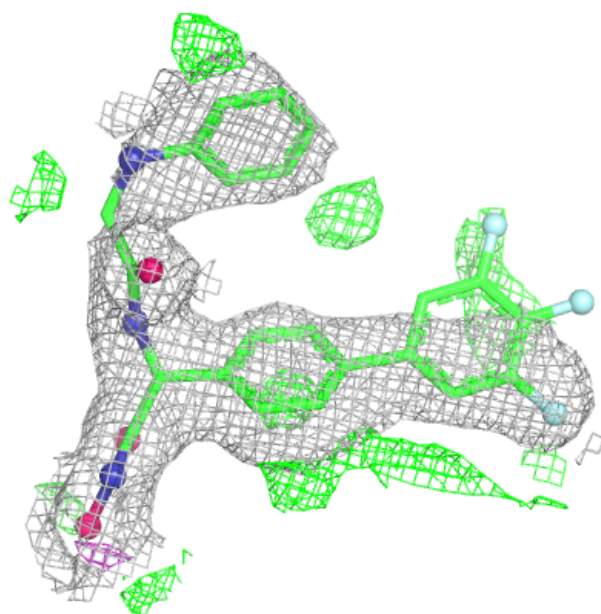
Electron density around X10 K 701:

$2mF_o-DF_c$ (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.