



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 11:45 AM UTC

PDB ID : 8SVM / pdb\_00008svm  
Title : Plasmodium falciparum M17 aminopeptidase bound to MMV1557817  
Authors : McGowan, S.; Drinkwater, N.  
Deposited on : 2023-05-17  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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)  
Xtrriage (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

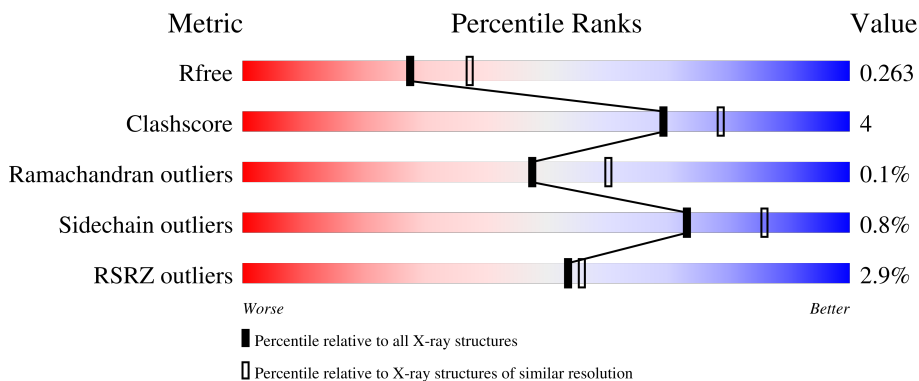
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



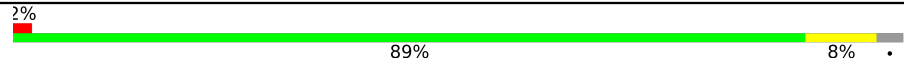
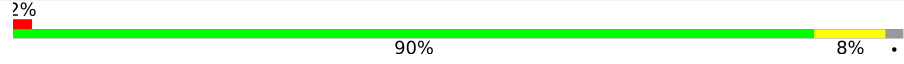
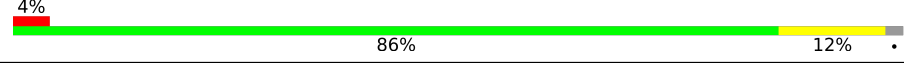

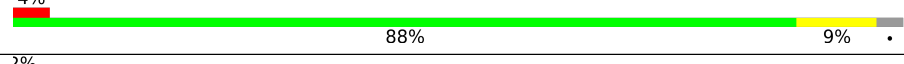


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	528	 2% 87% 11% .
1	B	528	 6% 88% 10% .
1	C	528	 3% 88% 9% ..
1	D	528	 2% 89% 8% .
1	E	528	 % 90% 7% .

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Mol	Chain	Length	Quality of chain
1	F	528	 2% 89% 8% .
1	G	528	 2% 90% 8% .
1	H	528	 4% 86% 12% .
1	I	528	 2% 87% 11% .
1	J	528	 4% 88% 9% .
1	K	528	 2% 87% 9% .
1	L	528	 4% 90% 7% . .

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 50860 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 Leucine aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	3962	2544	637	761	20	0	1	0
1	B	517	3913	2511	636	746	20	0	1	0
1	C	516	3961	2543	639	758	21	0	1	0
1	D	514	3917	2521	634	742	20	0	0	0
1	E	509	3904	2509	631	745	19	0	0	0
1	F	512	3869	2487	622	740	20	0	1	0
1	G	519	3971	2549	640	762	20	0	1	0
1	H	517	3910	2513	635	742	20	0	1	0
1	I	518	3964	2548	638	756	22	0	2	0
1	J	514	3945	2537	637	751	20	0	0	0
1	K	509	3894	2508	626	741	19	0	0	0
1	L	512	3861	2479	624	739	19	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	608	HIS	-	expression tag	UNP Q8IL11
A	609	HIS	-	expression tag	UNP Q8IL11
A	610	HIS	-	expression tag	UNP Q8IL11
A	611	HIS	-	expression tag	UNP Q8IL11
B	152	GLN	ASN	engineered mutation	UNP Q8IL11
B	515	GLN	ASN	engineered mutation	UNP Q8IL11
B	546	GLN	ASN	engineered mutation	UNP Q8IL11
B	606	HIS	-	expression tag	UNP Q8IL11
B	607	HIS	-	expression tag	UNP Q8IL11
B	608	HIS	-	expression tag	UNP Q8IL11
B	609	HIS	-	expression tag	UNP Q8IL11
B	610	HIS	-	expression tag	UNP Q8IL11
B	611	HIS	-	expression tag	UNP Q8IL11
C	152	GLN	ASN	engineered mutation	UNP Q8IL11
C	515	GLN	ASN	engineered mutation	UNP Q8IL11
C	546	GLN	ASN	engineered mutation	UNP Q8IL11
C	606	HIS	-	expression tag	UNP Q8IL11
C	607	HIS	-	expression tag	UNP Q8IL11
C	608	HIS	-	expression tag	UNP Q8IL11
C	609	HIS	-	expression tag	UNP Q8IL11
C	610	HIS	-	expression tag	UNP Q8IL11
C	611	HIS	-	expression tag	UNP Q8IL11
D	152	GLN	ASN	engineered mutation	UNP Q8IL11
D	515	GLN	ASN	engineered mutation	UNP Q8IL11
D	546	GLN	ASN	engineered mutation	UNP Q8IL11
D	606	HIS	-	expression tag	UNP Q8IL11
D	607	HIS	-	expression tag	UNP Q8IL11
D	608	HIS	-	expression tag	UNP Q8IL11
D	609	HIS	-	expression tag	UNP Q8IL11
D	610	HIS	-	expression tag	UNP Q8IL11
D	611	HIS	-	expression tag	UNP Q8IL11
E	152	GLN	ASN	engineered mutation	UNP Q8IL11
E	515	GLN	ASN	engineered mutation	UNP Q8IL11
E	546	GLN	ASN	engineered mutation	UNP Q8IL11
E	606	HIS	-	expression tag	UNP Q8IL11
E	607	HIS	-	expression tag	UNP Q8IL11
E	608	HIS	-	expression tag	UNP Q8IL11
E	609	HIS	-	expression tag	UNP Q8IL11
E	610	HIS	-	expression tag	UNP Q8IL11
E	611	HIS	-	expression tag	UNP Q8IL11
F	152	GLN	ASN	engineered mutation	UNP Q8IL11
F	515	GLN	ASN	engineered mutation	UNP Q8IL11

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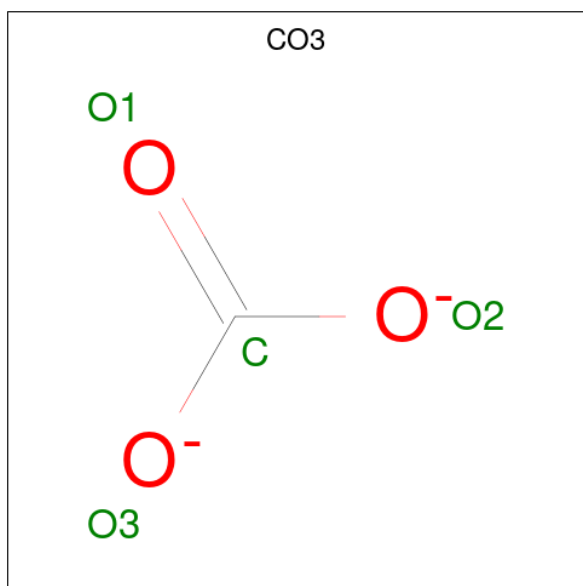
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP Q8IL11
G	152	GLN	ASN	engineered mutation	UNP Q8IL11
G	515	GLN	ASN	engineered mutation	UNP Q8IL11
G	546	GLN	ASN	engineered mutation	UNP Q8IL11
G	606	HIS	-	expression tag	UNP Q8IL11
G	607	HIS	-	expression tag	UNP Q8IL11
G	608	HIS	-	expression tag	UNP Q8IL11
G	609	HIS	-	expression tag	UNP Q8IL11
G	610	HIS	-	expression tag	UNP Q8IL11
G	611	HIS	-	expression tag	UNP Q8IL11
H	152	GLN	ASN	engineered mutation	UNP Q8IL11
H	515	GLN	ASN	engineered mutation	UNP Q8IL11
H	546	GLN	ASN	engineered mutation	UNP Q8IL11
H	606	HIS	-	expression tag	UNP Q8IL11
H	607	HIS	-	expression tag	UNP Q8IL11
H	608	HIS	-	expression tag	UNP Q8IL11
H	609	HIS	-	expression tag	UNP Q8IL11
H	610	HIS	-	expression tag	UNP Q8IL11
H	611	HIS	-	expression tag	UNP Q8IL11
I	152	GLN	ASN	engineered mutation	UNP Q8IL11
I	515	GLN	ASN	engineered mutation	UNP Q8IL11
I	546	GLN	ASN	engineered mutation	UNP Q8IL11
I	606	HIS	-	expression tag	UNP Q8IL11
I	607	HIS	-	expression tag	UNP Q8IL11
I	608	HIS	-	expression tag	UNP Q8IL11
I	609	HIS	-	expression tag	UNP Q8IL11
I	610	HIS	-	expression tag	UNP Q8IL11
I	611	HIS	-	expression tag	UNP Q8IL11
J	152	GLN	ASN	engineered mutation	UNP Q8IL11
J	515	GLN	ASN	engineered mutation	UNP Q8IL11
J	546	GLN	ASN	engineered mutation	UNP Q8IL11
J	606	HIS	-	expression tag	UNP Q8IL11
J	607	HIS	-	expression tag	UNP Q8IL11
J	608	HIS	-	expression tag	UNP Q8IL11
J	609	HIS	-	expression tag	UNP Q8IL11
J	610	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
J	611	HIS	-	expression tag	UNP Q8IL11
K	152	GLN	ASN	engineered mutation	UNP Q8IL11
K	515	GLN	ASN	engineered mutation	UNP Q8IL11
K	546	GLN	ASN	engineered mutation	UNP Q8IL11
K	606	HIS	-	expression tag	UNP Q8IL11
K	607	HIS	-	expression tag	UNP Q8IL11
K	608	HIS	-	expression tag	UNP Q8IL11
K	609	HIS	-	expression tag	UNP Q8IL11
K	610	HIS	-	expression tag	UNP Q8IL11
K	611	HIS	-	expression tag	UNP Q8IL11
L	152	GLN	ASN	engineered mutation	UNP Q8IL11
L	515	GLN	ASN	engineered mutation	UNP Q8IL11
L	546	GLN	ASN	engineered mutation	UNP Q8IL11
L	606	HIS	-	expression tag	UNP Q8IL11
L	607	HIS	-	expression tag	UNP Q8IL11
L	608	HIS	-	expression tag	UNP Q8IL11
L	609	HIS	-	expression tag	UNP Q8IL11
L	610	HIS	-	expression tag	UNP Q8IL11
L	611	HIS	-	expression tag	UNP Q8IL11

- Molecule 2 is CARBONATE ION (CCD ID: CO3) (formula: CO<sub>3</sub>).



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

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

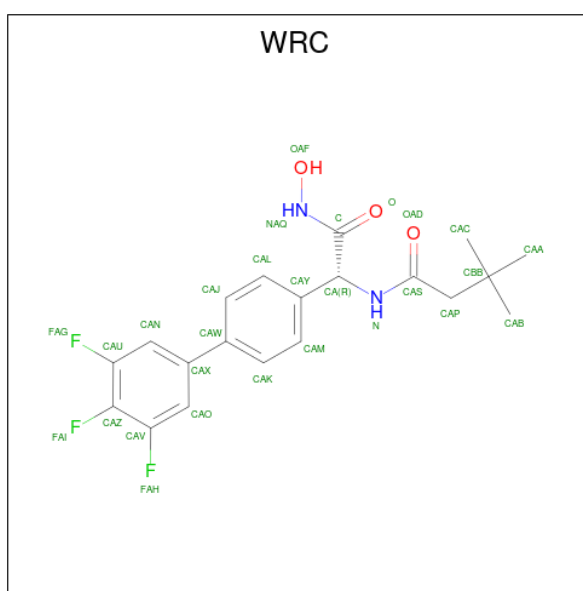
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	E	2	Total Zn 2 2	0	0
3	F	2	Total Zn 2 2	0	0
3	G	2	Total Zn 2 2	0	0
3	H	2	Total Zn 2 2	0	0
3	I	2	Total Zn 2 2	0	0

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

- Molecule 4 is N-[(1R)-2-(hydroxyamino)-2-oxo-1-(3',4',5'-trifluoro[1,1'-biphenyl]-4-yl)ethyl]-3,3-dimethylbutanamide (CCD ID: WRC) (formula: C<sub>20</sub>H<sub>21</sub>F<sub>3</sub>N<sub>2</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



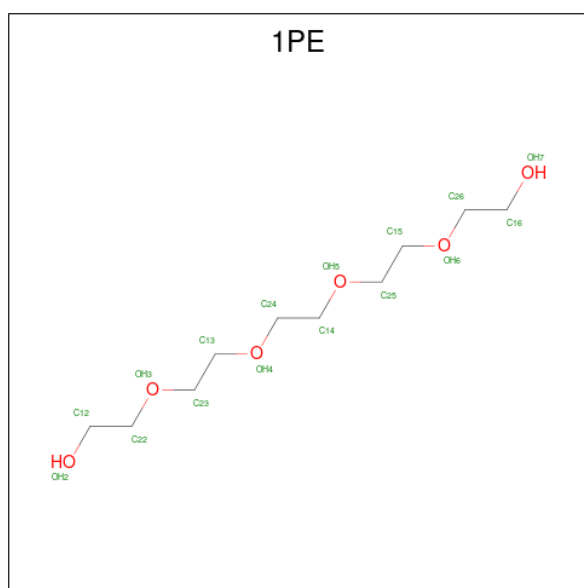
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	F	N	O	0	0
			28	20	3	2	3		
4	B	1	Total	C	F	N	O	0	0
			28	20	3	2	3		
4	C	1	Total	C	F	N	O	0	0
			28	20	3	2	3		
4	D	1	Total	C	F	N	O	0	0
			28	20	3	2	3		
4	E	1	Total	C	F	N	O	0	0
			28	20	3	2	3		
4	F	1	Total	C	F	N	O	0	0
			28	20	3	2	3		
4	G	1	Total	C	F	N	O	0	0
			28	20	3	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	H	1	Total	C	F	N	O	0	0
			28	20	3	2	3		
4	I	1	Total	C	F	N	O	0	0
			28	20	3	2	3		
4	J	1	Total	C	F	N	O	0	0
			28	20	3	2	3		
4	K	1	Total	C	F	N	O	0	0
			28	20	3	2	3		
4	L	1	Total	C	F	N	O	0	0
			28	20	3	2	3		

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			9	6 3		
5	A	1	Total	C O	0	0
			6	4 2		
5	A	1	Total	C O	0	0
			15	10 5		
5	B	1	Total	C O	0	0
			10	7 3		
5	B	1	Total	C O	0	0
			10	7 3		
5	C	1	Total	C O	0	0
			15	10 5		

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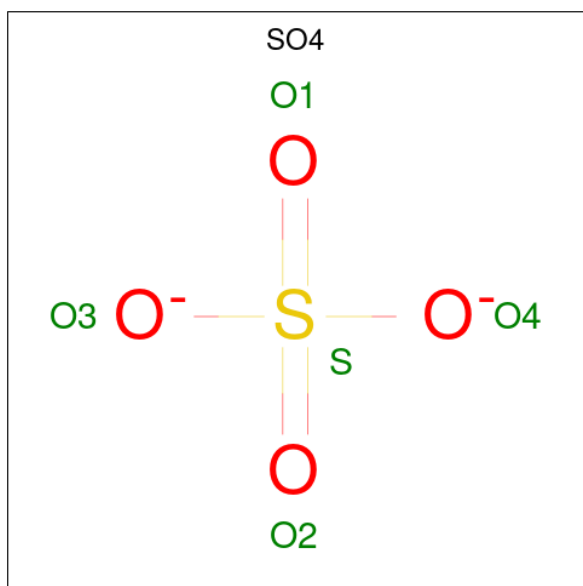
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			11	8	3		
5	C	1	Total	C	O	0	0
			7	5	2		
5	D	1	Total	C	O	0	0
			11	7	4		
5	D	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			12	8	4		
5	E	1	Total	C	O	0	0
			6	4	2		
5	F	1	Total	C	O	0	0
			10	6	4		
5	F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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	L	1	10	6	4	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	A	1	5	4	1	0	0
6	A	1	5	4	1	0	0
6	C	1	5	4	1	0	0
6	C	1	5	4	1	0	0
6	D	1	5	4	1	0	0
6	F	1	5	4	1	0	0
6	G	1	5	4	1	0	0
6	G	1	5	4	1	0	0
6	G	1	5	4	1	0	0
6	J	1	5	4	1	0	0

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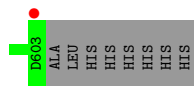
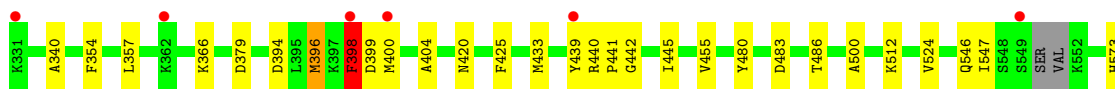
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	K	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		

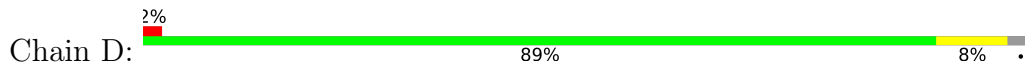
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	282	Total	O	0	0
			282	282		
7	B	229	Total	O	0	0
			229	229		
7	C	254	Total	O	0	0
			254	254		
7	D	246	Total	O	0	0
			246	246		
7	E	281	Total	O	0	0
			281	281		
7	F	225	Total	O	0	0
			225	225		
7	G	270	Total	O	0	0
			270	270		
7	H	219	Total	O	0	0
			219	219		
7	I	281	Total	O	0	0
			281	281		
7	J	271	Total	O	0	0
			271	271		
7	K	254	Total	O	0	0
			254	254		
7	L	221	Total	O	0	0
			221	221		

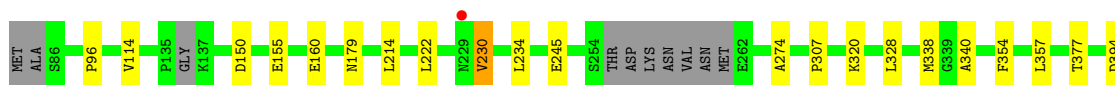
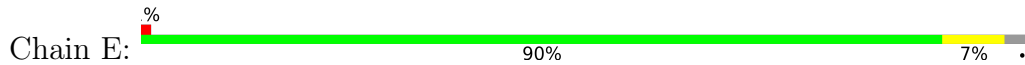




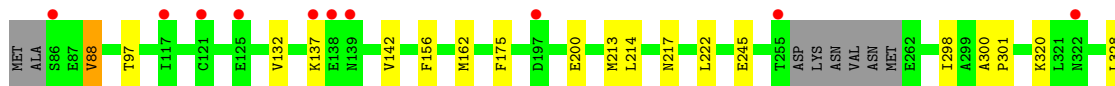
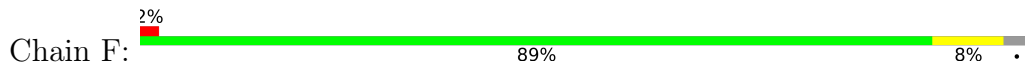
• Molecule 1: Leucine aminopeptidase



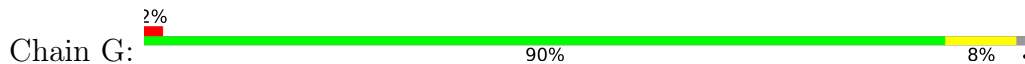
• Molecule 1: Leucine aminopeptidase



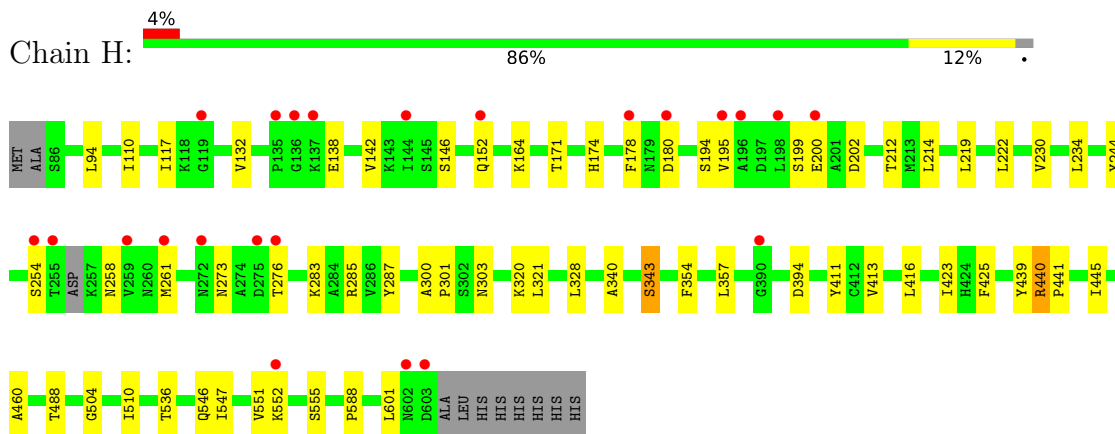
• Molecule 1: Leucine aminopeptidase



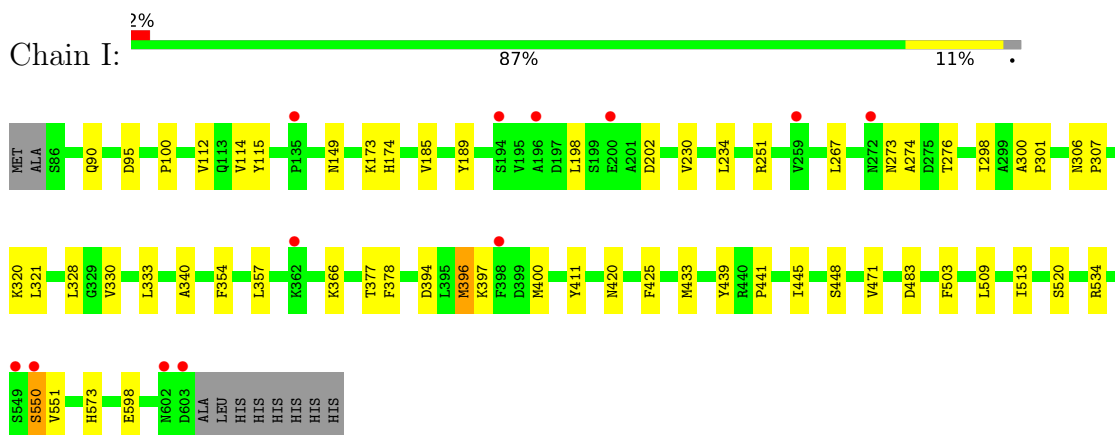
• Molecule 1: Leucine aminopeptidase



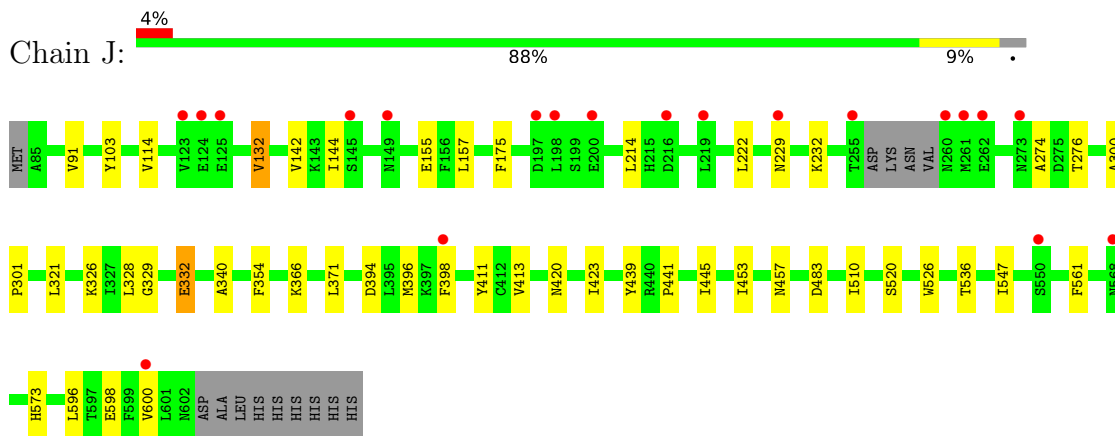
- Molecule 1: Leucine aminopeptidase



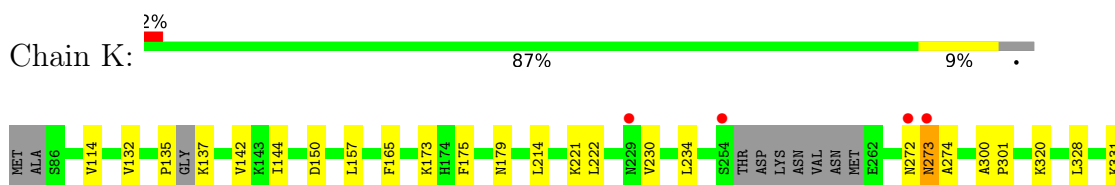
- Molecule 1: Leucine aminopeptidase

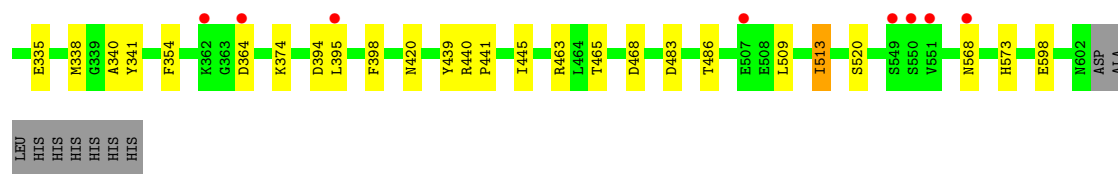


- Molecule 1: Leucine aminopeptidase

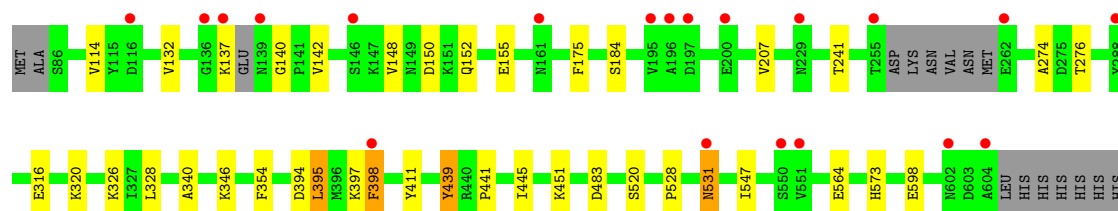
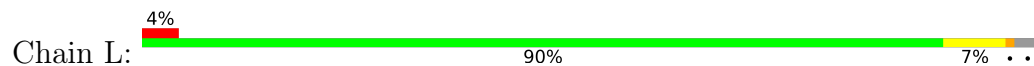


- Molecule 1: Leucine aminopeptidase





● Molecule 1: Leucine aminopeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.20Å 177.93Å 229.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.30 49.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.6 (49.00-2.30) 97.4 (49.00-2.30)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.204 , 0.252 0.218 , 0.263	Depositor DCC
$R_{free}$ test set	15216 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtrriage
Anisotropy	0.762	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	50860	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9207e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SO4, CO3, WRC, ZN, 1PE

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	0.29	1/4043 (0.0%)	0.70	0/5490
1	B	0.29	1/3993 (0.0%)	0.72	2/5426 (0.0%)
1	C	0.32	1/4041 (0.0%)	0.72	2/5480 (0.0%)
1	D	0.30	0/3994	0.71	0/5419
1	E	0.28	1/3980 (0.0%)	0.69	0/5398
1	F	0.31	1/3949 (0.0%)	0.72	1/5369 (0.0%)
1	G	0.29	0/4052	0.71	0/5498
1	H	0.42	5/3990 (0.1%)	0.73	1/5421 (0.0%)
1	I	0.33	1/4048 (0.0%)	0.71	2/5492 (0.0%)
1	J	0.28	1/4022 (0.0%)	0.70	0/5453
1	K	0.28	1/3970 (0.0%)	0.70	0/5385
1	L	0.43	3/3937 (0.1%)	0.75	1/5354 (0.0%)
All	All	0.32	16/48019 (0.0%)	0.71	9/65185 (0.0%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	440	ARG	C-O	-6.90	1.17	1.24
1	H	440	ARG	C-N	6.62	1.41	1.33
1	L	439	TYR	C-O	-6.57	1.15	1.23
1	I	439	TYR	C-O	-6.42	1.16	1.23
1	H	343	SER	C-O	-5.68	1.17	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	396[A]	MET	CA-C-O	8.32	130.02	119.12
1	C	396[B]	MET	CA-C-O	8.32	130.02	119.12
1	I	396[A]	MET	CA-C-O	7.49	128.94	119.12
1	I	396[B]	MET	CA-C-O	7.49	128.94	119.12
1	B	138	GLU	CA-C-N	-7.28	113.16	123.20

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	3962	0	3865	38	0
1	B	3913	0	3789	28	0
1	C	3961	0	3893	33	0
1	D	3917	0	3840	23	0
1	E	3904	0	3836	21	0
1	F	3869	0	3733	25	0
1	G	3971	0	3881	29	0
1	H	3910	0	3791	36	0
1	I	3964	0	3888	38	0
1	J	3945	0	3893	29	0
1	K	3894	0	3828	31	0
1	L	3861	0	3721	25	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	0	0
2	K	4	0	0	1	0
2	L	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	28	0	0	0	0
4	B	28	0	0	0	0
4	C	28	0	0	0	0
4	D	28	0	0	0	0
4	E	28	0	0	0	0
4	F	28	0	0	1	0
4	G	28	0	0	0	0
4	H	28	0	0	0	0
4	I	28	0	0	0	0
4	J	28	0	0	0	0
4	K	28	0	0	0	0
4	L	28	0	0	0	0
5	A	30	0	33	2	0
5	B	20	0	20	0	0
5	C	33	0	37	1	0
5	D	21	0	26	1	0
5	E	28	0	30	2	0
5	F	22	0	27	3	0
5	G	21	0	22	3	0
5	H	20	0	20	2	0
5	I	31	0	34	4	0
5	J	20	0	20	1	0
5	K	12	0	14	1	0
5	L	30	0	39	3	0
6	A	10	0	0	1	0
6	C	10	0	0	1	0
6	D	5	0	0	0	0
6	F	5	0	0	0	0
6	G	15	0	0	1	0
6	J	5	0	0	0	0
6	K	5	0	0	0	0
6	L	5	0	0	0	0
7	A	282	0	0	4	0
7	B	229	0	0	5	0
7	C	254	0	0	2	0
7	D	246	0	0	2	0
7	E	281	0	0	1	0
7	F	225	0	0	1	0
7	G	270	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	219	0	0	0	0
7	I	281	0	0	1	0
7	J	271	0	0	2	0
7	K	254	0	0	2	0
7	L	221	0	0	0	0
All	All	50860	0	46280	329	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 4.

The worst 5 of 329 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:K:272:ASN:C	1:K:273:ASN:HD22	1.81	0.87
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.63	0.78
1:I:298:ILE:HA	1:I:400[B]:MET:HE1	1.66	0.77
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.68	0.76
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.68	0.75

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/528 (98%)	501 (97%)	17 (3%)	0	100	100
1	B	514/528 (97%)	497 (97%)	17 (3%)	0	100	100
1	C	513/528 (97%)	495 (96%)	18 (4%)	0	100	100
1	D	510/528 (97%)	495 (97%)	14 (3%)	1 (0%)	43	55
1	E	503/528 (95%)	487 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	509/528 (96%)	489 (96%)	19 (4%)	1 (0%)	43	55
1	G	518/528 (98%)	502 (97%)	16 (3%)	0	100	100
1	H	514/528 (97%)	496 (96%)	16 (3%)	2 (0%)	30	38
1	I	518/528 (98%)	501 (97%)	16 (3%)	1 (0%)	43	55
1	J	510/528 (97%)	497 (98%)	13 (2%)	0	100	100
1	K	503/528 (95%)	489 (97%)	14 (3%)	0	100	100
1	L	506/528 (96%)	491 (97%)	14 (3%)	1 (0%)	43	55
All	All	6136/6336 (97%)	5940 (97%)	190 (3%)	6 (0%)	48	60

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	392	MET
1	H	552	LYS
1	I	550	SER
1	L	531	ASN
1	H	254	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	420/455 (92%)	417 (99%)	3 (1%)	76	87
1	B	410/455 (90%)	405 (99%)	5 (1%)	63	79
1	C	425/455 (93%)	421 (99%)	4 (1%)	70	84
1	D	413/455 (91%)	409 (99%)	4 (1%)	68	82
1	E	418/455 (92%)	417 (100%)	1 (0%)	87	94
1	F	404/455 (89%)	402 (100%)	2 (0%)	81	90
1	G	421/455 (92%)	416 (99%)	5 (1%)	63	79
1	H	408/455 (90%)	402 (98%)	6 (2%)	57	75
1	I	422/455 (93%)	421 (100%)	1 (0%)	87	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	422/455 (93%)	418 (99%)	4 (1%)	70	84
1	K	415/455 (91%)	412 (99%)	3 (1%)	76	87
1	L	403/455 (89%)	397 (98%)	6 (2%)	57	75
All	All	4981/5460 (91%)	4937 (99%)	44 (1%)	73	84

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	219	LEU
1	K	273	ASN
1	H	343	SER
1	J	332	GLU
1	K	568	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	602	ASN
1	L	521	ASN
1	K	149	ASN
1	K	272	ASN
1	F	181	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 88 ligands modelled in this entry, 24 are monoatomic - leaving 64 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
2	CO3	B	701	-	3,3,3	0.75	0	2,3,3	0.07	0
5	1PE	E	706	-	11,11,15	0.68	0	10,10,14	0.22	0
5	1PE	K	705	-	11,11,15	0.68	0	10,10,14	0.23	0
5	1PE	B	705	-	9,9,15	0.66	0	8,8,14	0.23	0
2	CO3	D	701	-	3,3,3	0.83	0	2,3,3	0.17	0
5	1PE	C	706	-	10,10,15	0.72	0	9,9,14	0.18	0
5	1PE	I	707	-	8,8,15	0.68	0	7,7,14	0.26	0
2	CO3	L	701	-	3,3,3	0.84	0	2,3,3	0.22	0
5	1PE	E	705	-	9,9,15	0.70	0	8,8,14	0.22	0
4	WRC	B	704	3	28,29,29	1.87	3 (10%)	38,42,42	0.83	0
5	1PE	D	705	-	10,10,15	0.64	0	9,9,14	0.23	0
6	SO4	D	707	-	4,4,4	0.23	0	6,6,6	0.08	0
4	WRC	G	704	3	28,29,29	1.91	3 (10%)	38,42,42	0.85	0
6	SO4	G	709	-	4,4,4	0.23	0	6,6,6	0.06	0
6	SO4	K	706	-	4,4,4	0.24	0	6,6,6	0.06	0
5	1PE	D	706	-	9,9,15	0.64	0	8,8,14	0.23	0
5	1PE	H	706	-	9,9,15	0.68	0	8,8,14	0.17	0
4	WRC	A	704	3	28,29,29	1.92	3 (10%)	38,42,42	0.88	0
5	1PE	A	707	-	14,14,15	0.67	0	13,13,14	0.17	0
5	1PE	E	707	-	5,5,15	0.63	0	4,4,14	0.19	0
5	1PE	C	707	-	6,6,15	0.71	0	5,5,14	0.19	0
5	1PE	G	705	-	8,8,15	0.69	0	7,7,14	0.23	0
2	CO3	A	701	-	3,3,3	0.86	0	2,3,3	0.19	0
5	1PE	I	706	-	8,8,15	0.69	0	7,7,14	0.21	0
6	SO4	F	707	-	4,4,4	0.23	0	6,6,6	0.10	0
5	1PE	J	706	-	9,9,15	0.68	0	8,8,14	0.19	0
5	1PE	A	705	-	8,8,15	0.67	0	7,7,14	0.17	0
6	SO4	J	707	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	C	708	-	4,4,4	0.23	0	6,6,6	0.09	0
5	1PE	I	705	-	12,12,15	0.69	0	11,11,14	0.18	0
5	1PE	A	706	-	5,5,15	0.64	0	4,4,14	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CO3	K	701	-	3,3,3	0.85	0	2,3,3	0.22	0
4	WRC	H	704	3	28,29,29	1.88	2 (7%)	38,42,42	0.81	0
5	1PE	L	707	-	9,9,15	0.64	0	8,8,14	0.24	0
4	WRC	F	704	3	28,29,29	1.98	2 (7%)	38,42,42	1.00	2 (5%)
6	SO4	G	707	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	L	708	-	4,4,4	0.23	0	6,6,6	0.09	0
4	WRC	J	704	3	28,29,29	1.93	3 (10%)	38,42,42	0.88	0
2	CO3	C	701	-	3,3,3	0.87	0	2,3,3	0.18	0
5	1PE	H	705	-	9,9,15	0.67	0	8,8,14	0.21	0
2	CO3	E	701	-	3,3,3	0.83	0	2,3,3	0.18	0
2	CO3	H	701	-	3,3,3	0.77	0	2,3,3	0.07	0
5	1PE	L	705	-	9,9,15	0.63	0	8,8,14	0.28	0
2	CO3	F	701	-	3,3,3	0.82	0	2,3,3	0.15	0
4	WRC	I	704	3	28,29,29	1.94	2 (7%)	38,42,42	0.87	0
5	1PE	C	705	-	14,14,15	0.67	0	13,13,14	0.22	0
4	WRC	E	704	3	28,29,29	1.86	2 (7%)	38,42,42	0.81	0
5	1PE	J	705	-	9,9,15	0.67	0	8,8,14	0.18	0
6	SO4	A	709	-	4,4,4	0.23	0	6,6,6	0.09	0
4	WRC	L	704	3	28,29,29	1.92	2 (7%)	38,42,42	0.82	0
4	WRC	K	704	3	28,29,29	1.96	3 (10%)	38,42,42	0.90	0
6	SO4	A	708	-	4,4,4	0.24	0	6,6,6	0.08	0
2	CO3	J	701	-	3,3,3	0.79	0	2,3,3	0.09	0
4	WRC	C	704	3	28,29,29	1.84	2 (7%)	38,42,42	0.86	0
4	WRC	D	704	3	28,29,29	1.93	2 (7%)	38,42,42	0.86	0
2	CO3	I	701	-	3,3,3	0.89	0	2,3,3	0.26	0
5	1PE	B	706	-	9,9,15	0.67	0	8,8,14	0.19	0
5	1PE	F	705	-	9,9,15	0.64	0	8,8,14	0.25	0
5	1PE	G	706	-	11,11,15	0.68	0	10,10,14	0.17	0
6	SO4	G	708	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	C	709	-	4,4,4	0.23	0	6,6,6	0.07	0
5	1PE	F	706	-	11,11,15	0.69	0	10,10,14	0.22	0
2	CO3	G	701	-	3,3,3	0.78	0	2,3,3	0.09	0
5	1PE	L	706	-	9,9,15	0.66	0	8,8,14	0.30	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	E	706	-	-	1/9/9/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	K	705	-	-	4/9/9/13	-
5	1PE	B	705	-	-	4/7/7/13	-
5	1PE	C	706	-	-	5/8/8/13	-
5	1PE	I	707	-	-	3/6/6/13	-
5	1PE	E	705	-	-	4/7/7/13	-
4	WRC	B	704	3	-	0/23/23/23	0/2/2/2
5	1PE	D	705	-	-	7/8/8/13	-
4	WRC	G	704	3	-	0/23/23/23	0/2/2/2
5	1PE	D	706	-	-	4/7/7/13	-
5	1PE	H	706	-	-	6/7/7/13	-
4	WRC	A	704	3	-	0/23/23/23	0/2/2/2
5	1PE	A	707	-	-	3/12/12/13	-
5	1PE	E	707	-	-	1/3/3/13	-
5	1PE	C	707	-	-	2/4/4/13	-
5	1PE	G	705	-	-	2/6/6/13	-
5	1PE	I	706	-	-	5/6/6/13	-
5	1PE	J	706	-	-	3/7/7/13	-
5	1PE	A	705	-	-	3/6/6/13	-
5	1PE	I	705	-	-	7/10/10/13	-
5	1PE	A	706	-	-	3/3/3/13	-
4	WRC	H	704	3	-	0/23/23/23	0/2/2/2
5	1PE	L	707	-	-	4/7/7/13	-
4	WRC	F	704	3	-	0/23/23/23	0/2/2/2
4	WRC	J	704	3	-	1/23/23/23	0/2/2/2
5	1PE	H	705	-	-	3/7/7/13	-
5	1PE	L	705	-	-	5/7/7/13	-
4	WRC	I	704	3	-	0/23/23/23	0/2/2/2
5	1PE	C	705	-	-	6/12/12/13	-
4	WRC	E	704	3	-	0/23/23/23	0/2/2/2
5	1PE	J	705	-	-	4/7/7/13	-
4	WRC	L	704	3	-	0/23/23/23	0/2/2/2
4	WRC	K	704	3	-	0/23/23/23	0/2/2/2
4	WRC	C	704	3	-	0/23/23/23	0/2/2/2
4	WRC	D	704	3	-	0/23/23/23	0/2/2/2
5	1PE	B	706	-	-	2/7/7/13	-
5	1PE	F	705	-	-	4/7/7/13	-
5	1PE	G	706	-	-	5/9/9/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	F	706	-	-	5/9/9/13	-
5	1PE	L	706	-	-	3/7/7/13	-

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	704	WRC	CAY-CA	-9.08	1.38	1.52
4	K	704	WRC	CAY-CA	-8.77	1.39	1.52
4	L	704	WRC	CAY-CA	-8.66	1.39	1.52
4	D	704	WRC	CAY-CA	-8.64	1.39	1.52
4	I	704	WRC	CAY-CA	-8.60	1.39	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	704	WRC	CAJ-CAL-CAY	-2.13	119.05	121.18
4	F	704	WRC	CAL-CAY-CAM	2.01	120.80	118.30

There are no chirality outliers.

5 of 109 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	705	1PE	C16-C26-OH6-C15
5	C	706	1PE	OH4-C13-C23-OH3
5	A	705	1PE	OH4-C13-C23-OH3
5	G	706	1PE	OH4-C13-C23-OH3
5	L	707	1PE	OH7-C16-C26-OH6

There are no ring outliers.

24 monomers are involved in 28 short contacts:

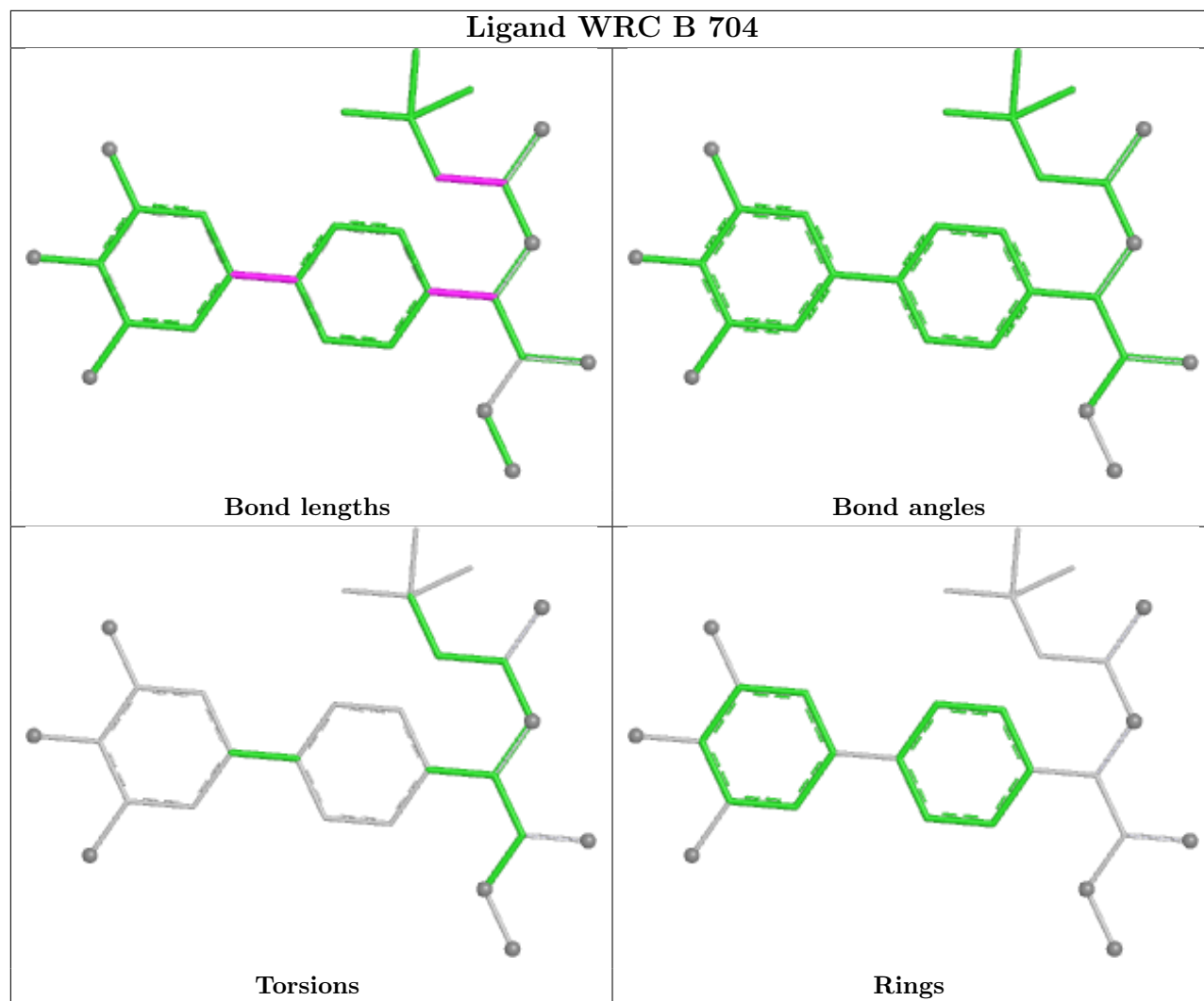
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	705	1PE	1	0
5	I	707	1PE	2	0
5	E	705	1PE	1	0
5	D	706	1PE	1	0
5	H	706	1PE	2	0
5	A	707	1PE	2	0
5	E	707	1PE	1	0
5	G	705	1PE	1	0

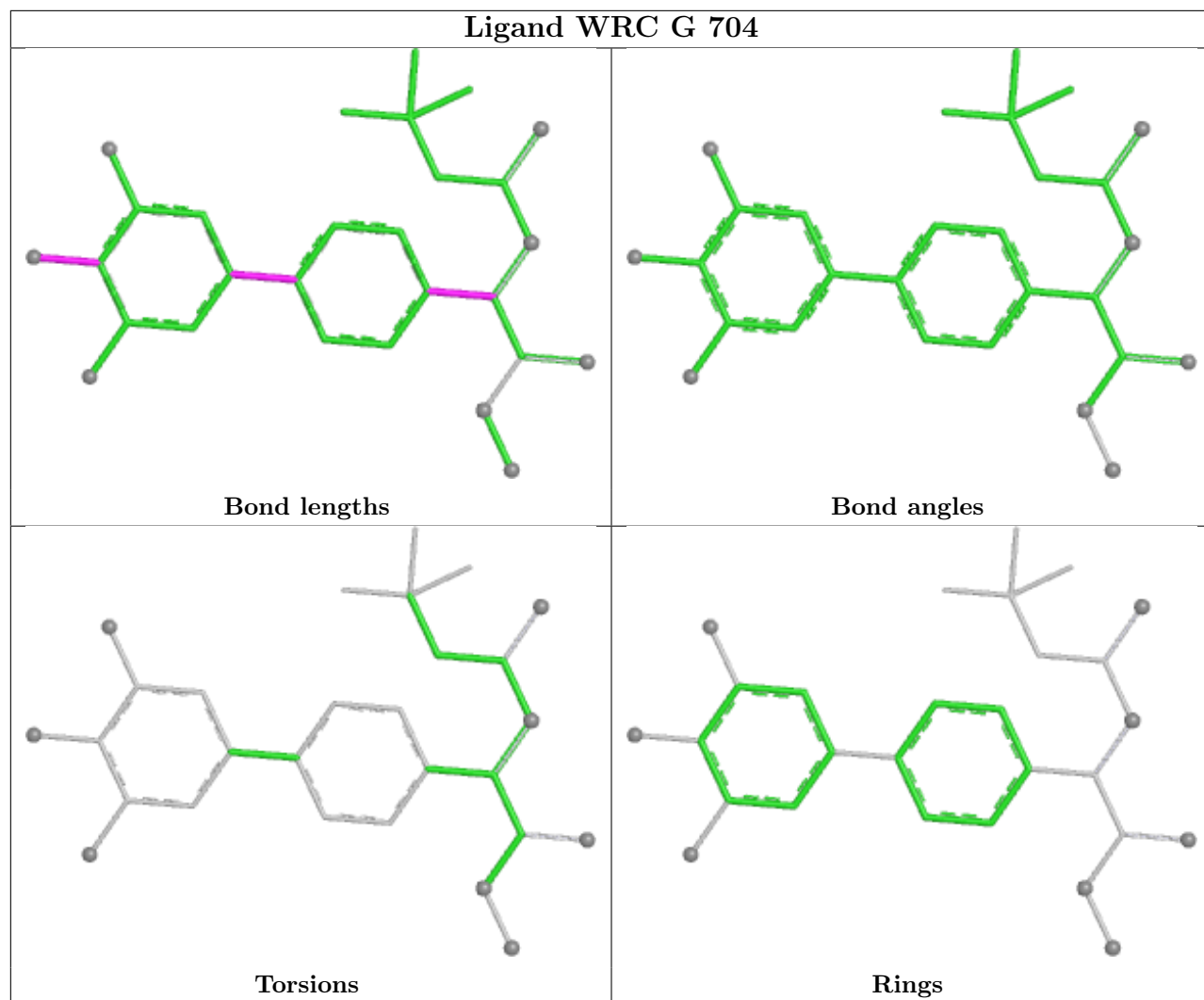
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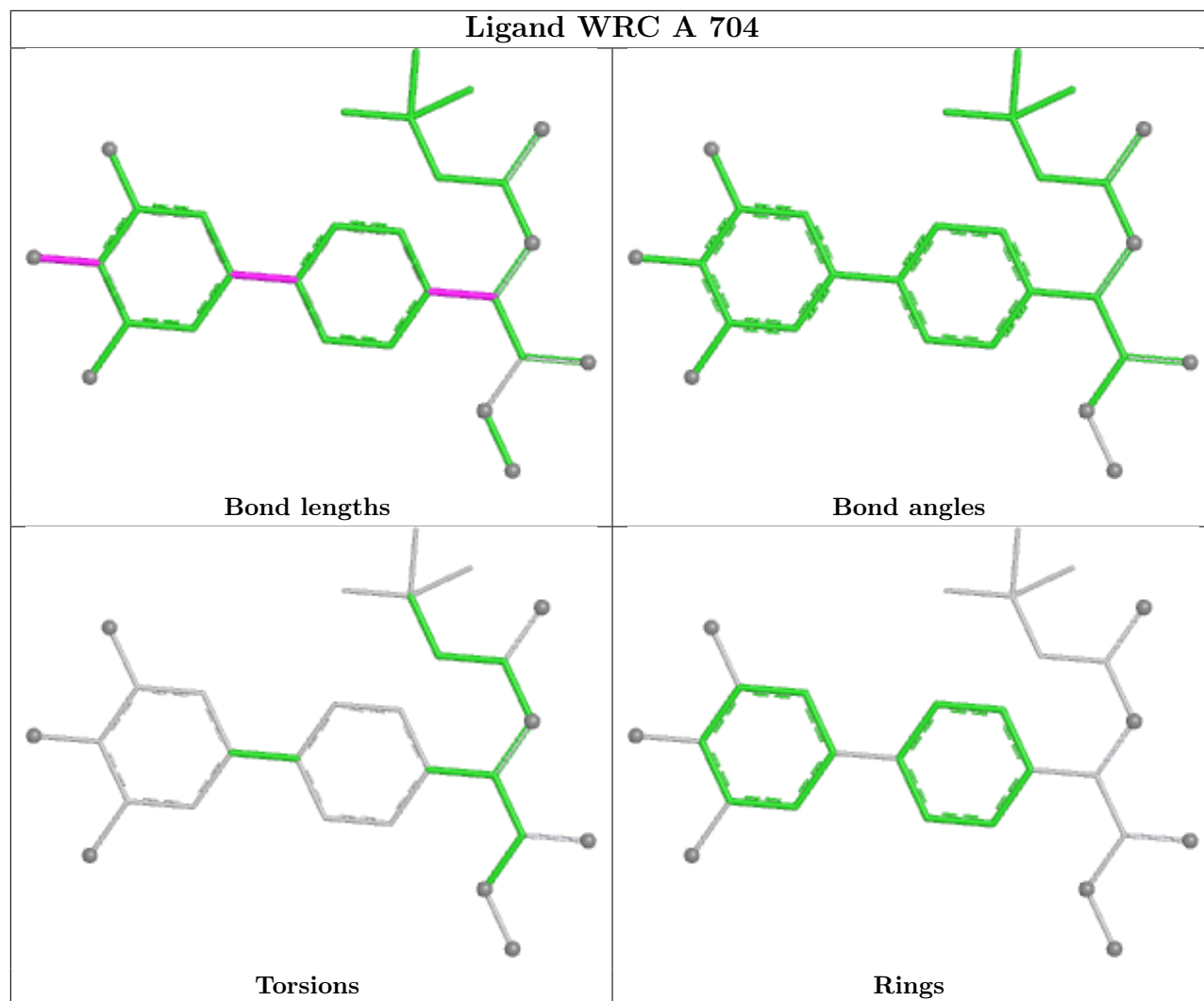
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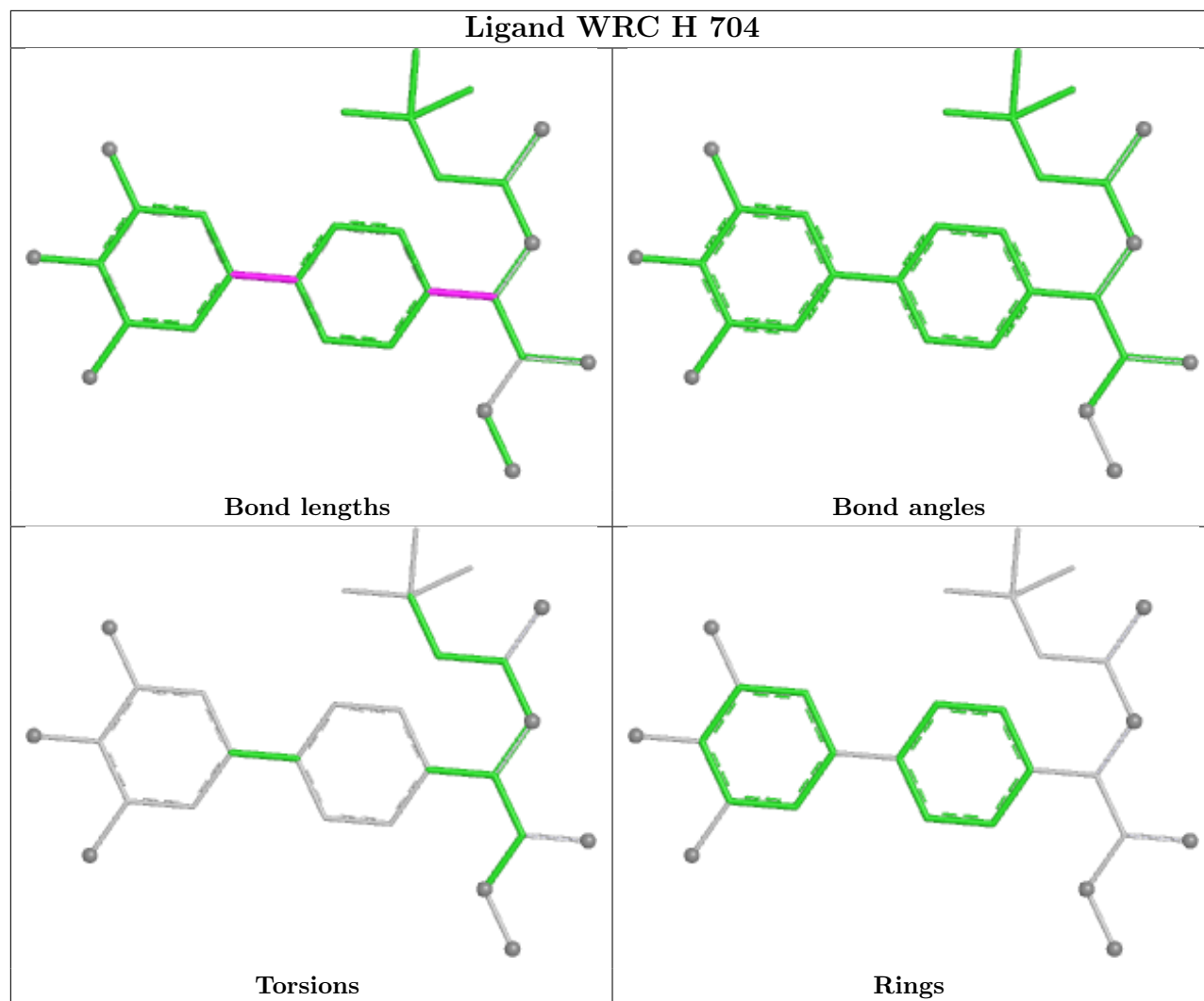
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	706	1PE	1	0
5	A	705	1PE	1	0
6	C	708	SO4	1	0
5	I	705	1PE	1	0
2	K	701	CO3	1	0
5	L	707	1PE	1	0
4	F	704	WRC	1	0
6	G	707	SO4	1	0
5	L	705	1PE	1	0
5	C	705	1PE	1	0
5	J	705	1PE	1	0
6	A	708	SO4	1	0
5	F	705	1PE	1	0
5	G	706	1PE	2	0
5	F	706	1PE	2	0
5	L	706	1PE	1	0

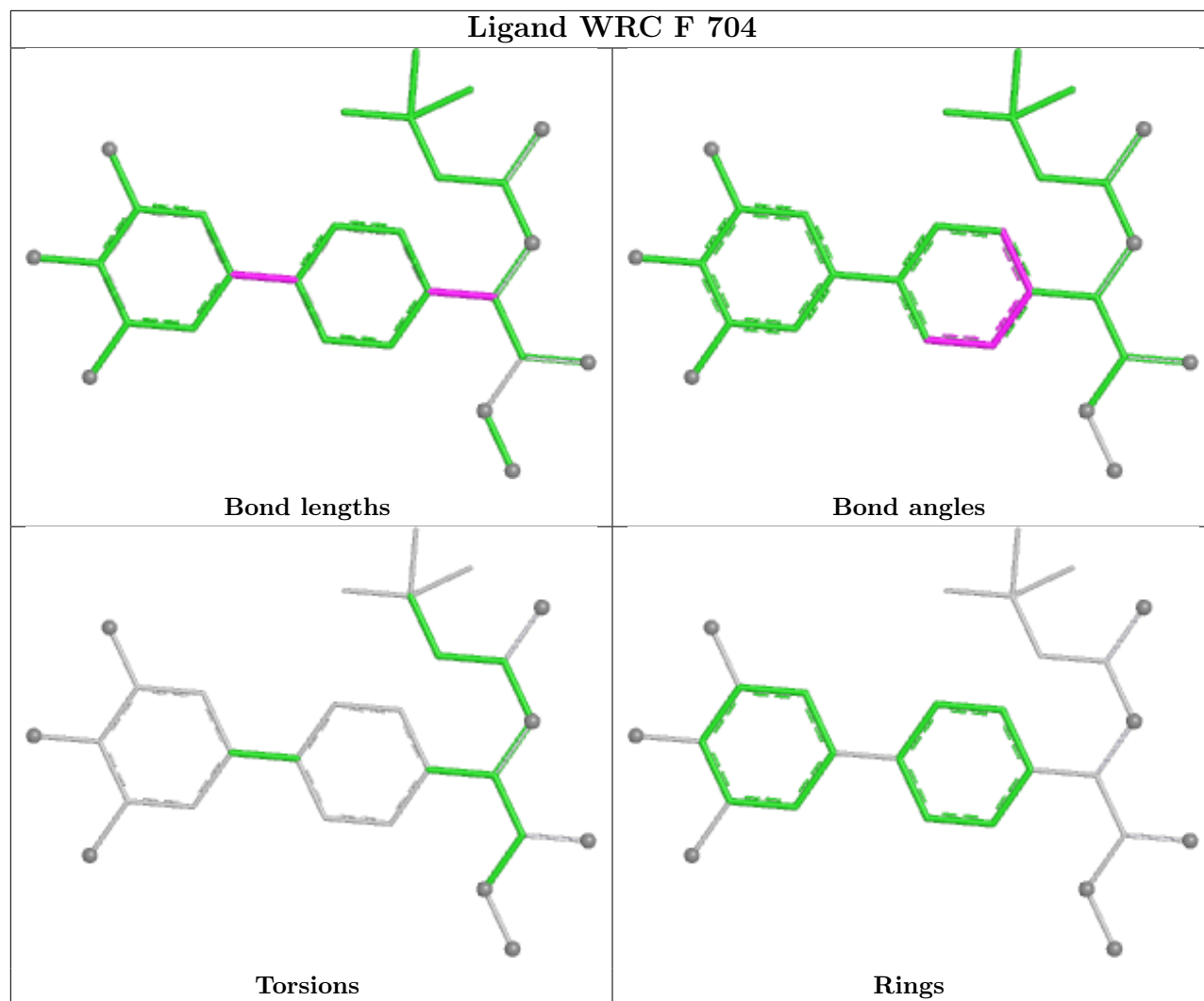
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

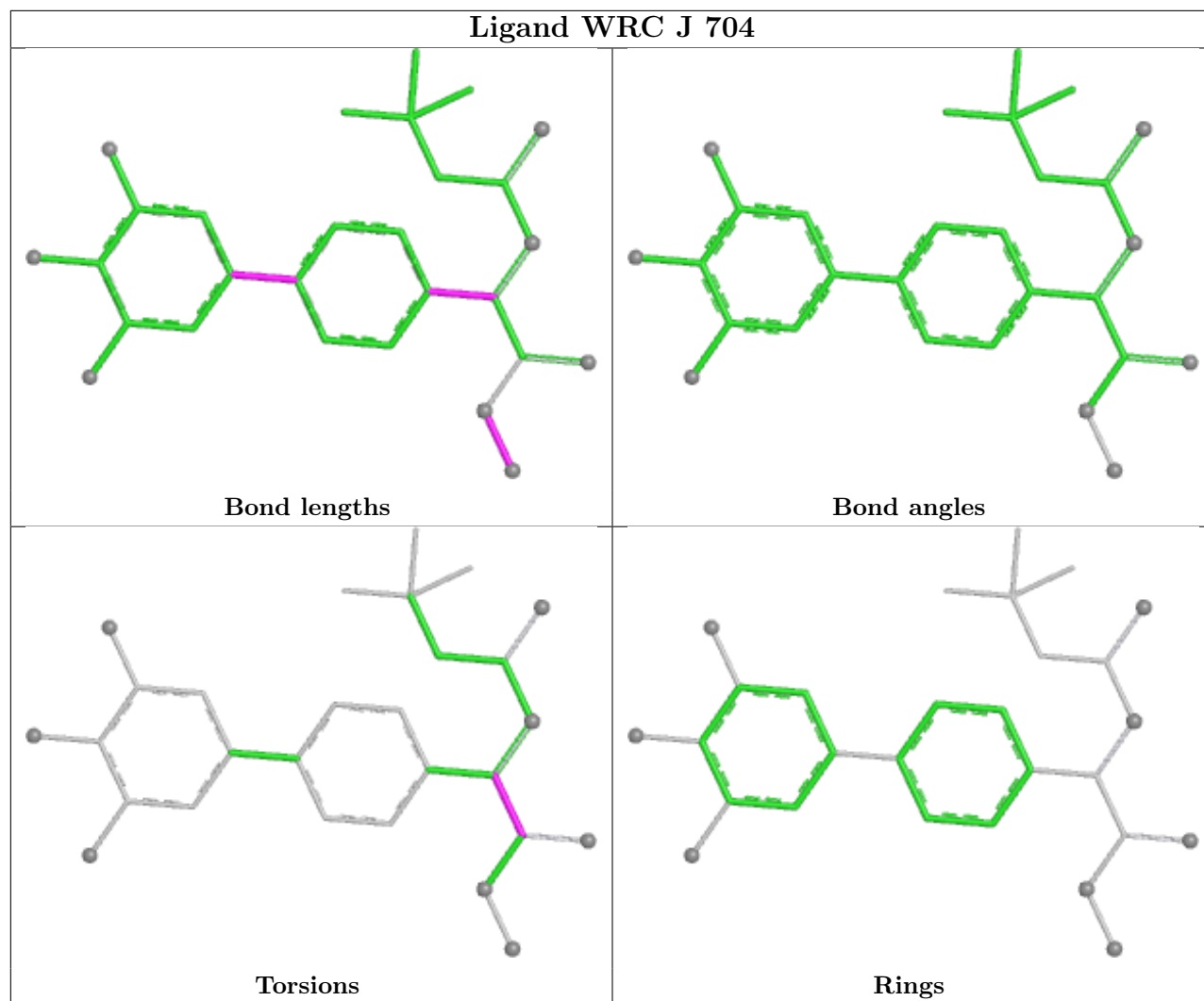


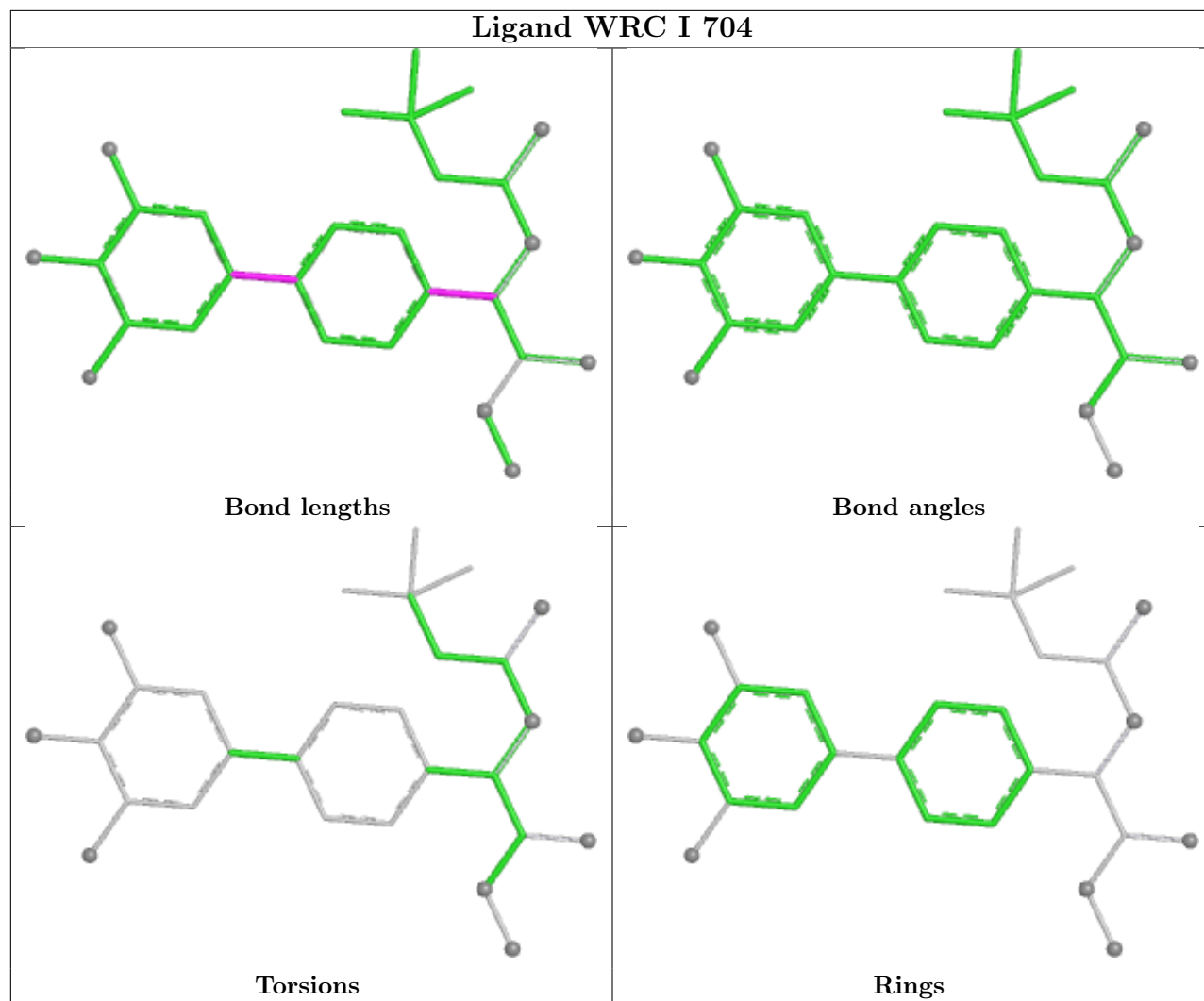


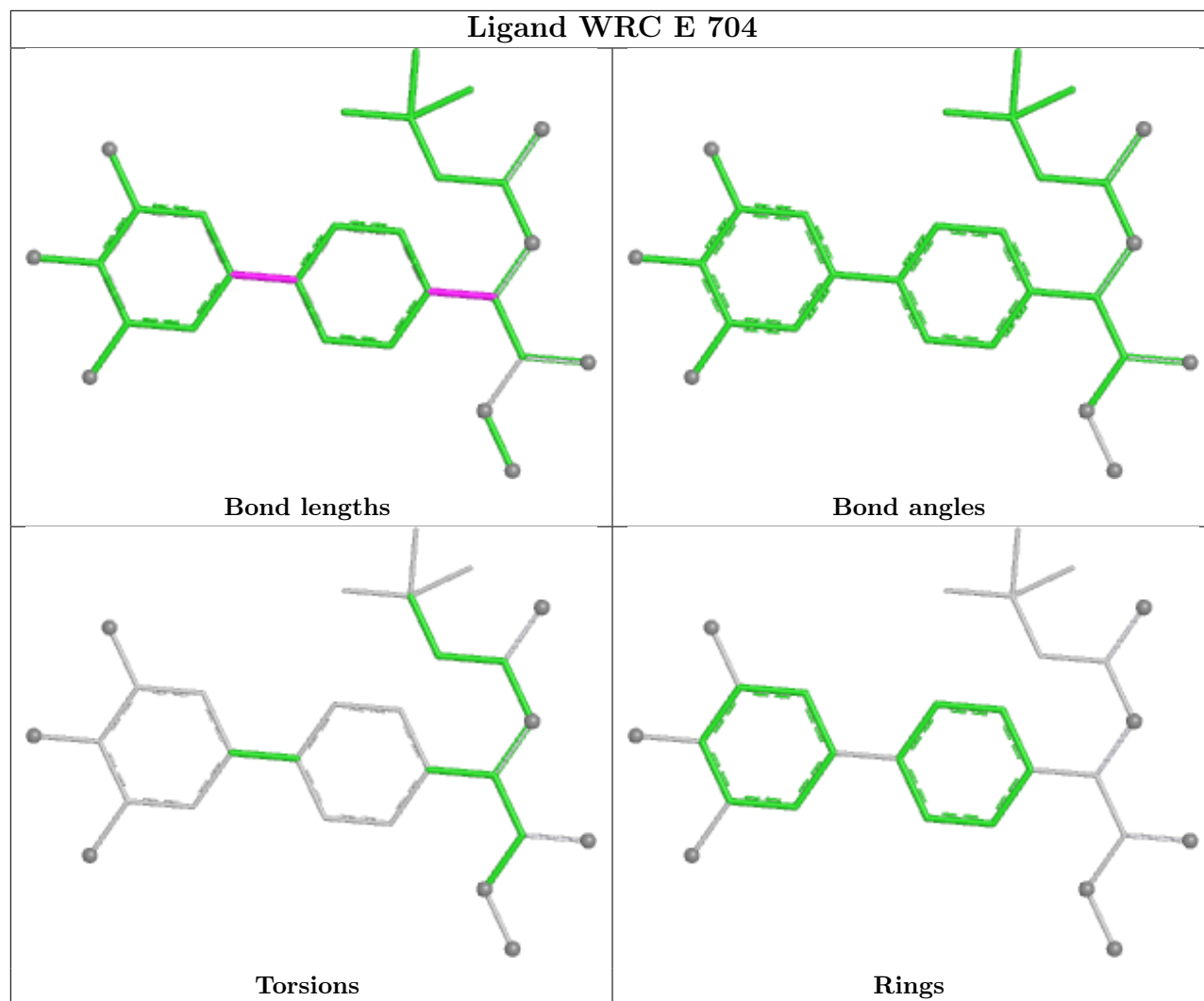


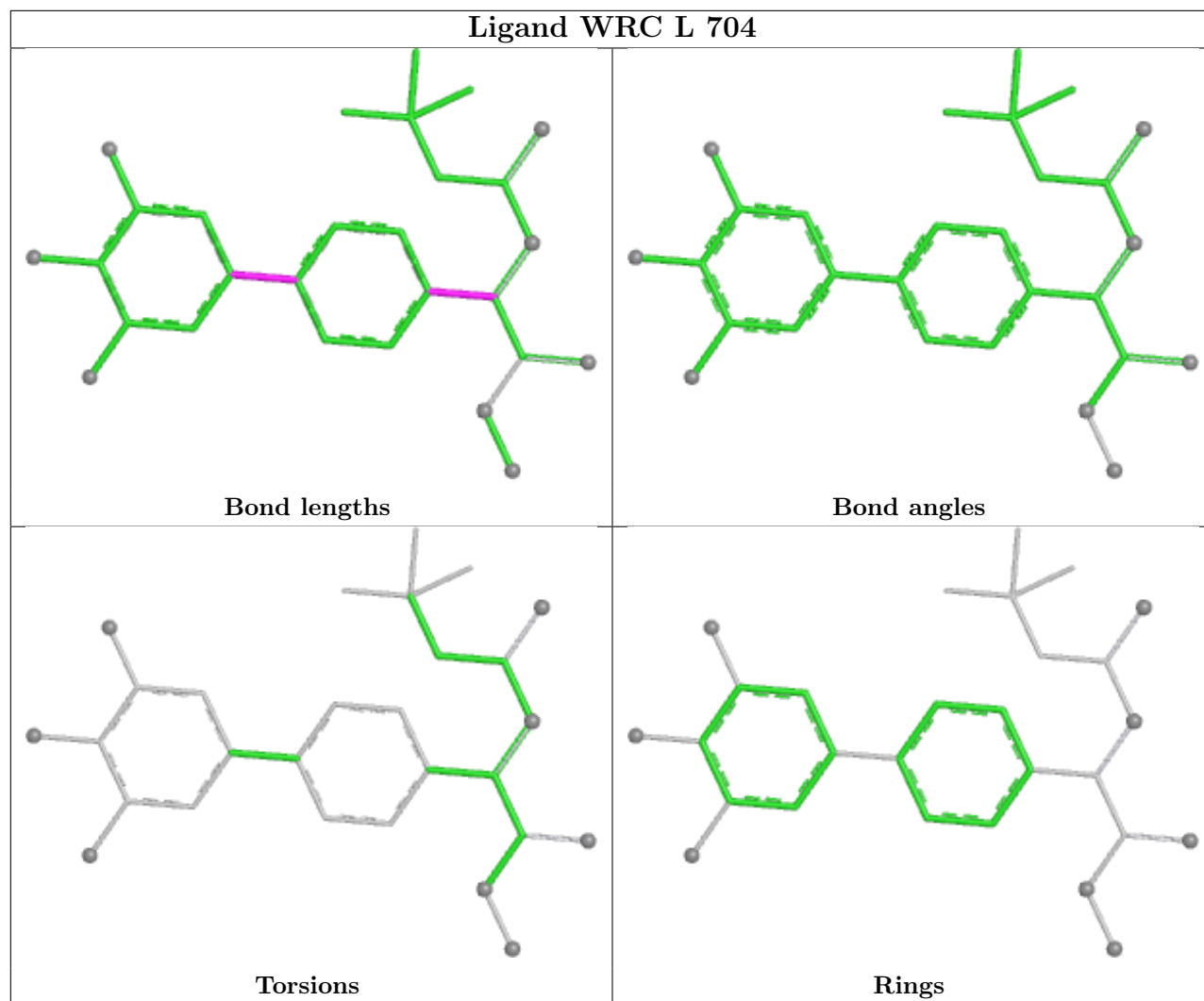


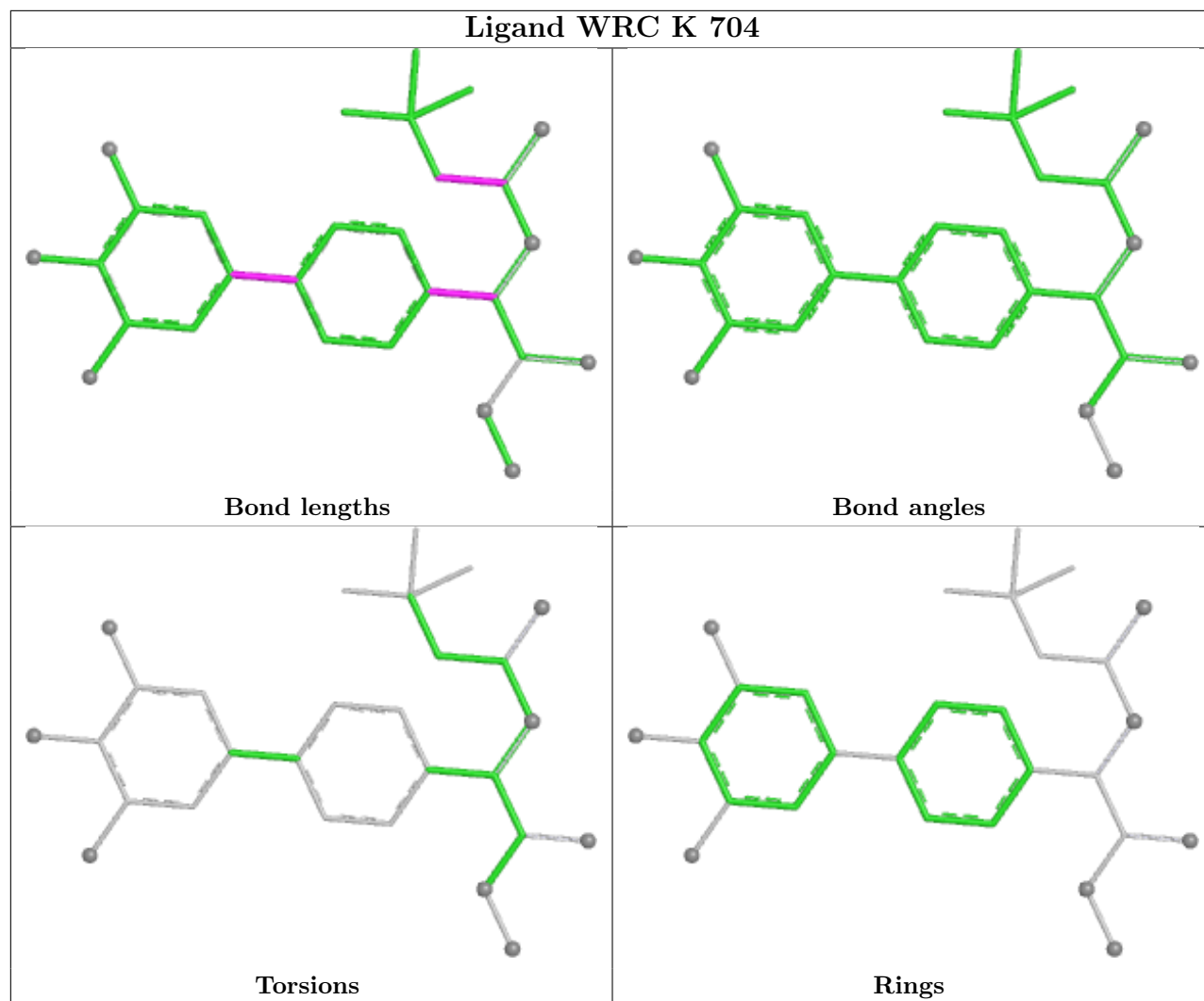


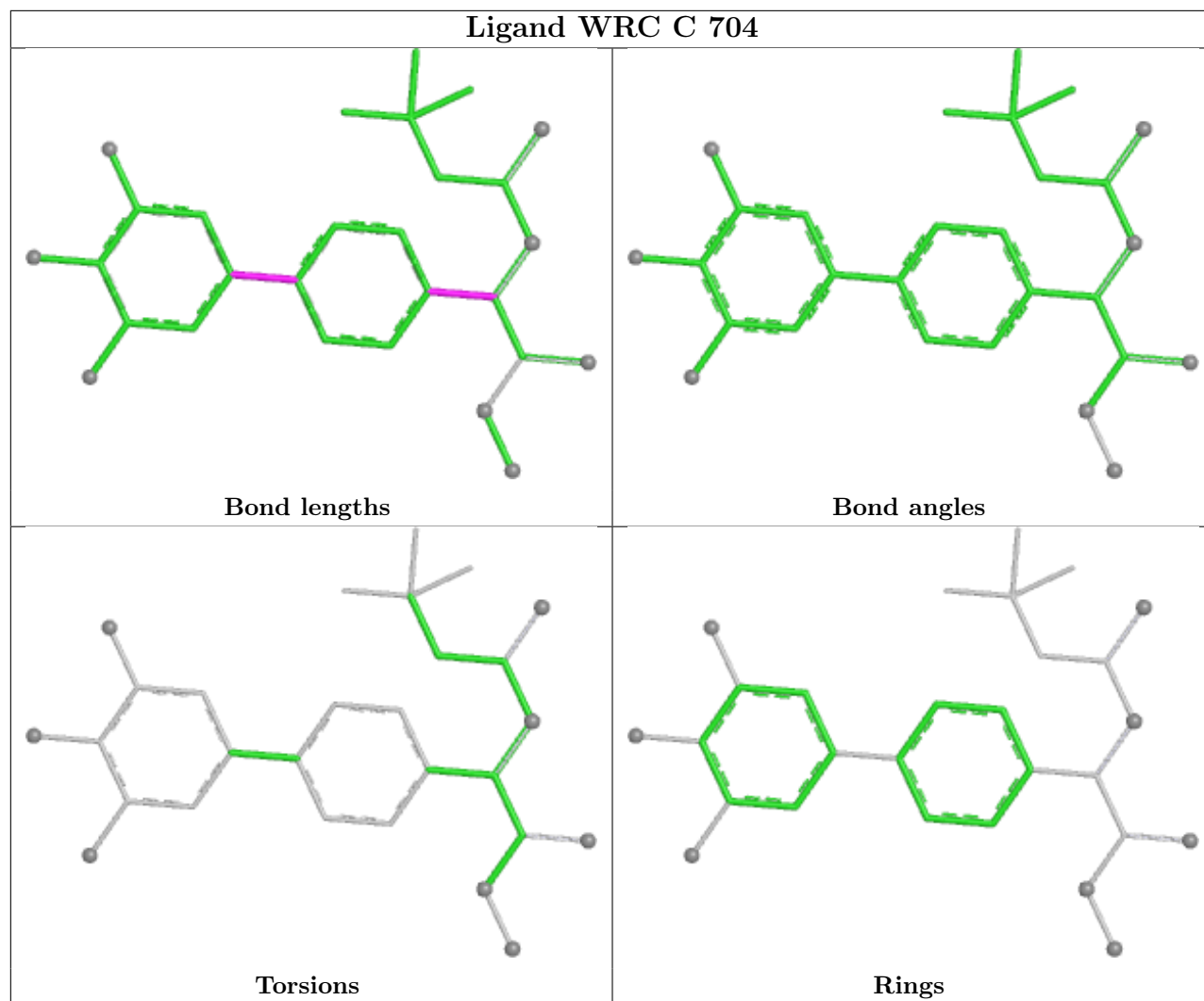


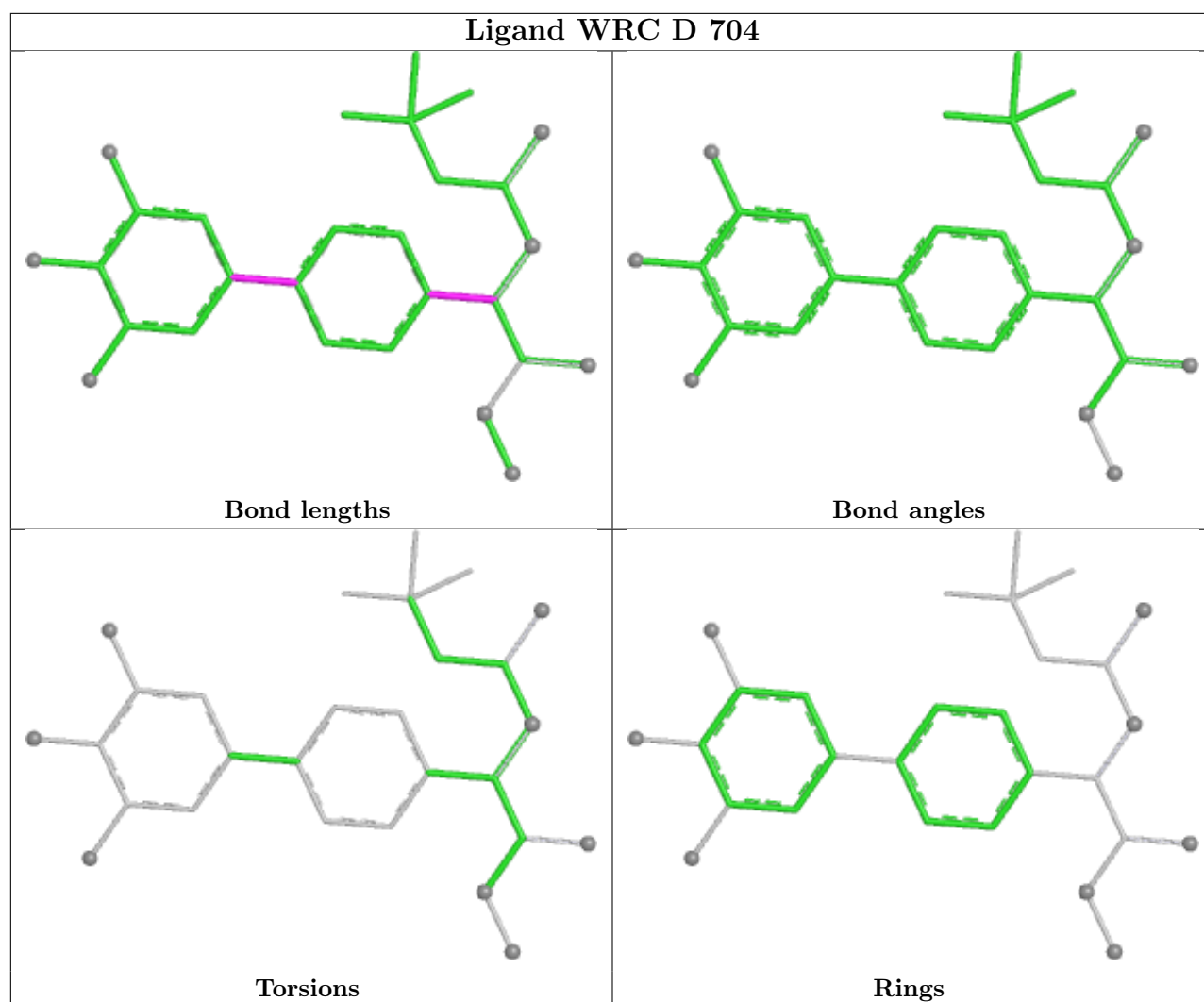












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	519/528 (98%)	0.10	9 (1%) 69 70	12, 23, 42, 68	5 (0%)
1	B	517/528 (97%)	0.36	33 (6%) 25 27	13, 26, 56, 84	14 (2%)
1	C	516/528 (97%)	0.22	14 (2%) 56 58	10, 23, 47, 76	6 (1%)
1	D	514/528 (97%)	0.15	10 (1%) 66 68	9, 23, 43, 87	5 (0%)
1	E	509/528 (96%)	0.05	4 (0%) 82 83	11, 22, 38, 76	7 (1%)
1	F	512/528 (96%)	0.28	13 (2%) 58 60	11, 25, 50, 72	10 (1%)
1	G	519/528 (98%)	0.11	12 (2%) 61 63	11, 23, 41, 74	9 (1%)
1	H	517/528 (97%)	0.34	23 (4%) 39 41	12, 26, 58, 85	6 (1%)
1	I	518/528 (98%)	0.20	12 (2%) 61 63	11, 23, 46, 93	12 (2%)
1	J	514/528 (97%)	0.16	20 (3%) 43 45	10, 22, 44, 79	11 (2%)
1	K	509/528 (96%)	0.08	12 (2%) 59 62	12, 22, 38, 65	8 (1%)
1	L	512/528 (96%)	0.28	20 (3%) 43 45	12, 24, 49, 75	6 (1%)
All	All	6176/6336 (97%)	0.19	182 (2%) 53 56	9, 23, 49, 93	99 (1%)

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	603	ASP	7.1
1	J	260	ASN	6.4
1	D	260	ASN	5.5
1	I	549	SER	5.1
1	G	398	PHE	5.0

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	1PE	L	706	10/16	0.33	0.37	82,95,103,104	0
5	1PE	L	705	10/16	0.72	0.38	86,89,93,93	0
5	1PE	F	706	12/16	0.72	0.23	28,76,81,81	0
5	1PE	H	706	10/16	0.74	0.23	57,61,71,72	0
5	1PE	C	707	7/16	0.74	0.18	42,46,48,48	0
5	1PE	G	706	12/16	0.74	0.21	58,60,67,69	0
5	1PE	L	707	10/16	0.74	0.21	44,59,68,68	0
5	1PE	J	706	10/16	0.76	0.21	45,49,65,66	0
5	1PE	C	705	15/16	0.76	0.21	45,56,67,67	0
5	1PE	I	705	13/16	0.77	0.22	47,54,58,59	0
5	1PE	J	705	10/16	0.78	0.19	42,46,52,53	0
5	1PE	I	707	9/16	0.79	0.15	47,50,51,52	0
5	1PE	B	706	10/16	0.79	0.15	36,46,48,49	0
5	1PE	E	705	10/16	0.80	0.19	41,48,53,54	0
5	1PE	H	705	10/16	0.81	0.20	52,59,66,67	0
5	1PE	I	706	9/16	0.81	0.17	32,42,50,51	0
5	1PE	D	705	11/16	0.82	0.18	44,50,58,59	0
5	1PE	B	705	10/16	0.82	0.16	38,42,52,52	0
6	SO4	L	708	5/5	0.82	0.17	83,83,84,87	0
5	1PE	E	707	6/16	0.83	0.14	32,37,40,42	0
6	SO4	C	708	5/5	0.83	0.16	86,86,87,87	0
5	1PE	D	706	10/16	0.83	0.15	51,53,55,57	0
5	1PE	A	706	6/16	0.84	0.19	38,39,42,43	0
5	1PE	C	706	11/16	0.84	0.15	30,40,45,46	0
5	1PE	A	707	15/16	0.84	0.16	46,56,64,65	0
2	CO3	E	701	4/4	0.85	0.15	23,25,28,32	0
2	CO3	K	701	4/4	0.85	0.19	29,32,34,34	0
3	ZN	B	703	1/1	0.85	0.16	82,82,82,82	1
5	1PE	A	705	9/16	0.85	0.13	36,39,43,43	0
5	1PE	K	705	12/16	0.85	0.15	44,49,57,60	0
5	1PE	E	706	12/16	0.86	0.16	34,44,62,62	0
6	SO4	C	709	5/5	0.86	0.19	73,74,76,76	0

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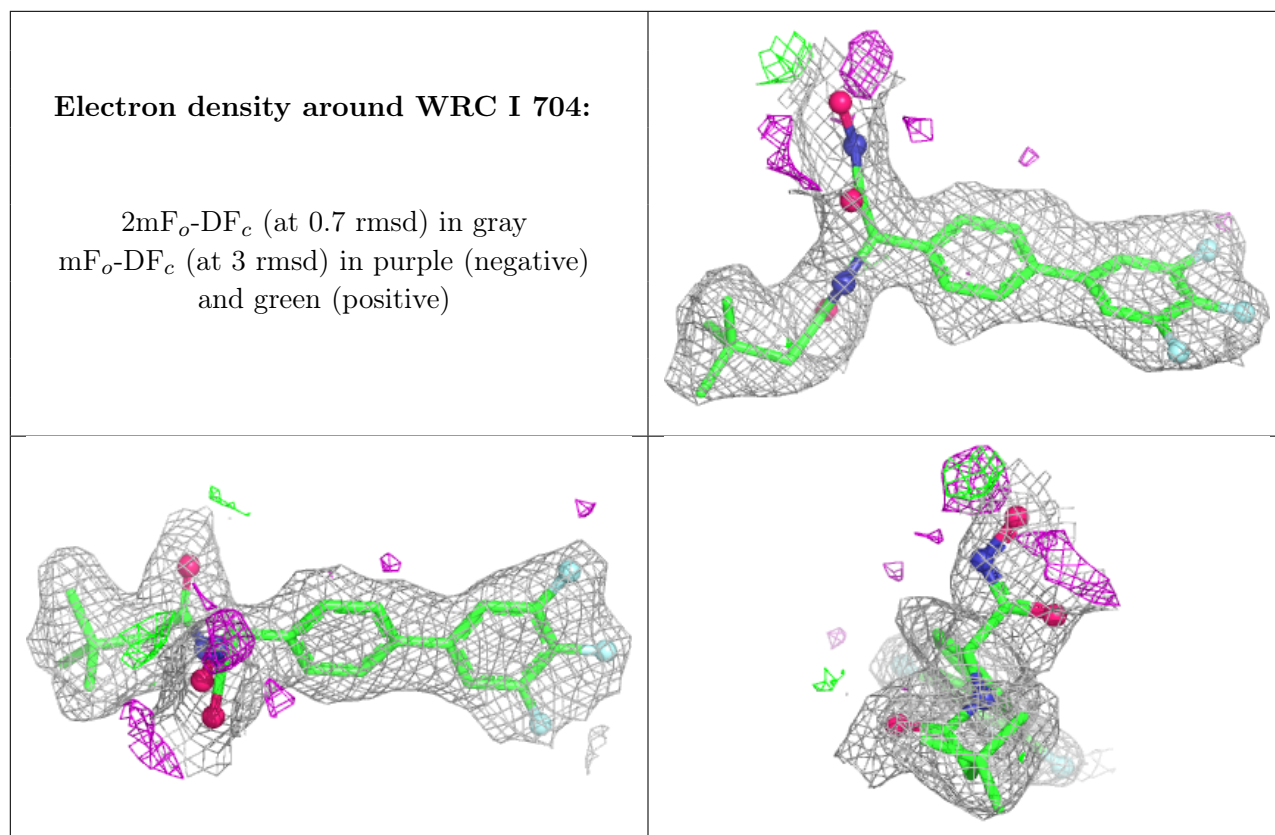
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	A	708	5/5	0.86	0.15	86,86,87,87	0
2	CO3	C	701	4/4	0.87	0.19	23,30,32,34	0
5	1PE	F	705	10/16	0.87	0.15	36,43,48,49	0
2	CO3	B	701	4/4	0.87	0.20	14,22,24,35	0
5	1PE	G	705	9/16	0.87	0.12	29,34,36,36	0
6	SO4	K	706	5/5	0.88	0.13	87,87,89,89	0
2	CO3	H	701	4/4	0.89	0.16	28,31,33,35	0
6	SO4	G	707	5/5	0.89	0.19	69,69,70,72	0
4	WRC	I	704	28/28	0.90	0.12	27,35,52,56	0
4	WRC	J	704	28/28	0.90	0.12	19,33,44,45	0
2	CO3	F	701	4/4	0.90	0.12	31,32,32,37	0
6	SO4	D	707	5/5	0.90	0.17	58,58,59,60	0
2	CO3	L	701	4/4	0.90	0.14	16,26,31,32	0
2	CO3	I	701	4/4	0.90	0.14	18,19,19,25	0
4	WRC	F	704	28/28	0.90	0.12	22,32,56,60	0
4	WRC	E	704	28/28	0.91	0.11	19,29,49,54	0
2	CO3	J	701	4/4	0.91	0.10	17,25,29,31	0
4	WRC	G	704	28/28	0.91	0.12	22,26,51,62	0
2	CO3	A	701	4/4	0.91	0.14	25,28,29,33	0
4	WRC	C	704	28/28	0.91	0.11	14,27,53,58	0
2	CO3	G	701	4/4	0.92	0.12	21,22,23,30	0
4	WRC	H	704	28/28	0.92	0.09	19,28,48,54	0
4	WRC	A	704	28/28	0.92	0.12	16,28,51,56	0
6	SO4	G	708	5/5	0.92	0.16	60,60,61,62	0
4	WRC	B	704	28/28	0.92	0.10	17,27,49,55	0
4	WRC	L	704	28/28	0.92	0.10	19,27,50,53	0
3	ZN	C	702	1/1	0.93	0.08	44,44,44,44	1
3	ZN	H	702	1/1	0.93	0.11	62,62,62,62	1
4	WRC	D	704	28/28	0.93	0.12	13,28,53,59	0
3	ZN	L	703	1/1	0.93	0.11	68,68,68,68	0
4	WRC	K	704	28/28	0.93	0.09	19,27,46,48	0
2	CO3	D	701	4/4	0.93	0.14	19,26,31,35	0
3	ZN	E	703	1/1	0.94	0.09	36,36,36,36	1
3	ZN	I	702	1/1	0.95	0.12	56,56,56,56	1
3	ZN	E	702	1/1	0.95	0.13	70,70,70,70	0
3	ZN	A	703	1/1	0.95	0.09	57,57,57,57	1
3	ZN	G	702	1/1	0.95	0.10	61,61,61,61	1
3	ZN	C	703	1/1	0.95	0.07	35,35,35,35	1
3	ZN	K	702	1/1	0.96	0.15	70,70,70,70	0
3	ZN	L	702	1/1	0.97	0.08	44,44,44,44	0
3	ZN	I	703	1/1	0.97	0.09	50,50,50,50	0
3	ZN	J	703	1/1	0.97	0.08	42,42,42,42	0

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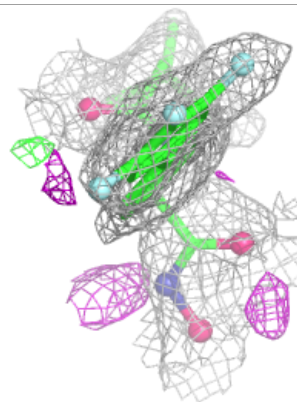
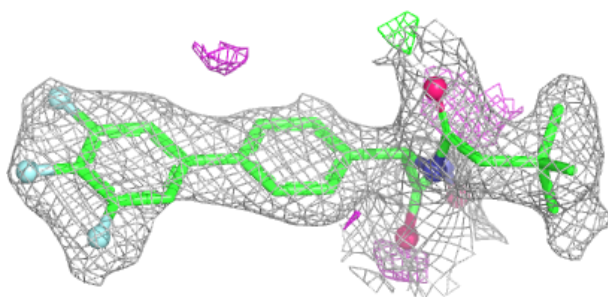
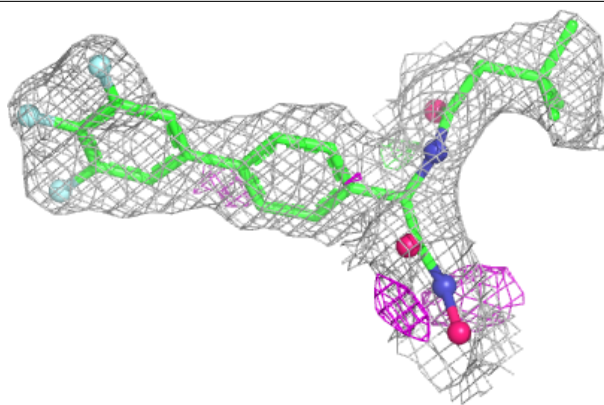
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	D	702	1/1	0.97	0.08	48,48,48,48	1
3	ZN	K	703	1/1	0.97	0.07	45,45,45,45	0
3	ZN	B	702	1/1	0.98	0.06	39,39,39,39	0
3	ZN	F	702	1/1	0.98	0.10	65,65,65,65	0
3	ZN	J	702	1/1	0.98	0.07	56,56,56,56	0
3	ZN	F	703	1/1	0.98	0.04	45,45,45,45	0
6	SO4	F	707	5/5	0.98	0.06	23,24,26,26	0
3	ZN	D	703	1/1	0.98	0.06	32,32,32,32	1
3	ZN	G	703	1/1	0.98	0.04	38,38,38,38	0
6	SO4	J	707	5/5	0.98	0.07	21,25,25,26	0
3	ZN	A	702	1/1	0.98	0.05	37,37,37,37	0
3	ZN	H	703	1/1	0.98	0.04	42,42,42,42	0
6	SO4	G	709	5/5	0.99	0.05	14,21,24,24	0
6	SO4	A	709	5/5	0.99	0.07	19,19,25,26	0

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

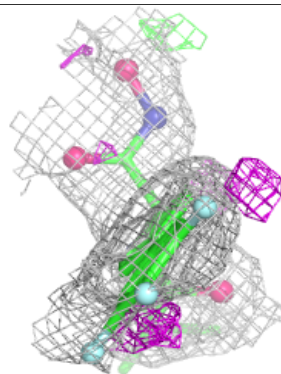
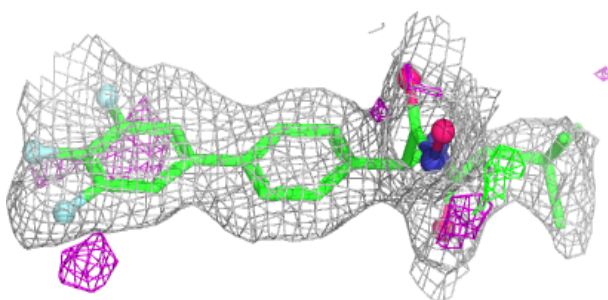
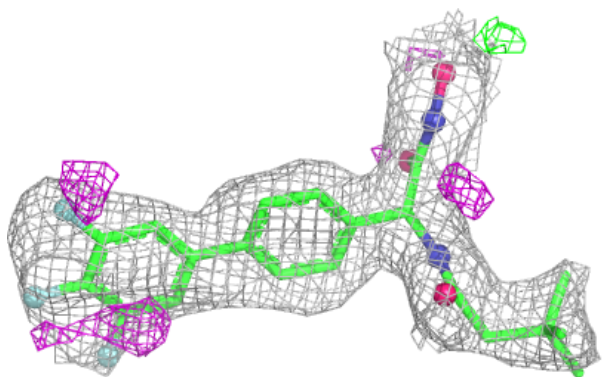


**Electron density around WRC J 704:**

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

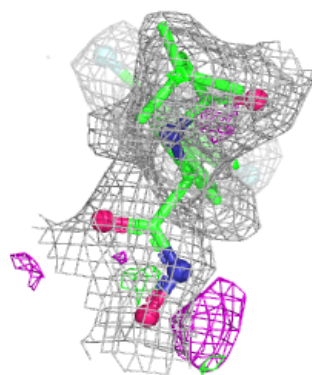
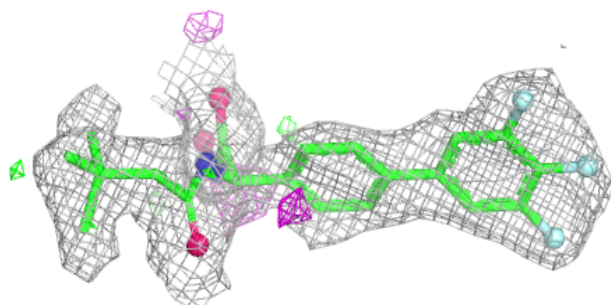
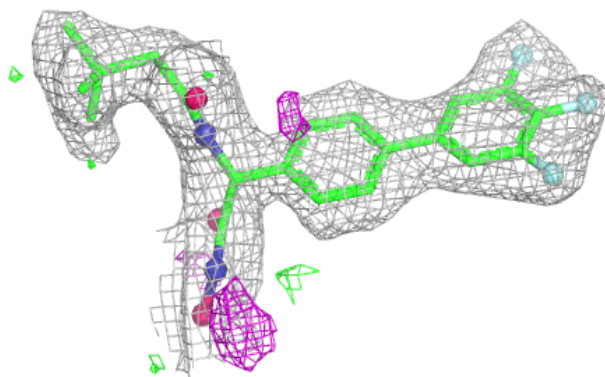
**Electron density around WRC F 704:**

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

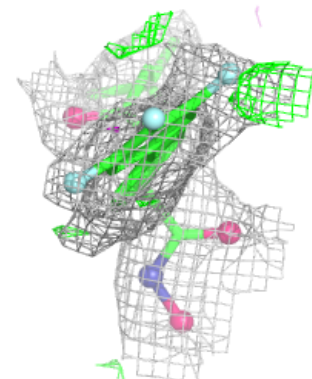
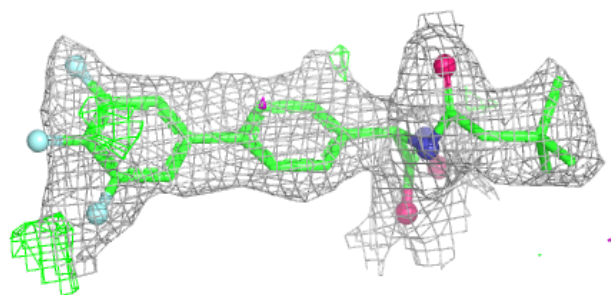


**Electron density around WRC E 704:**

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

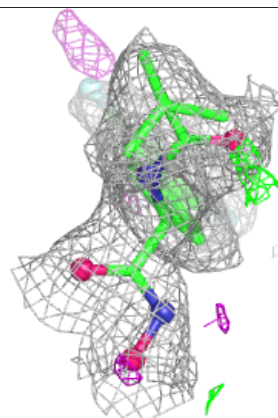
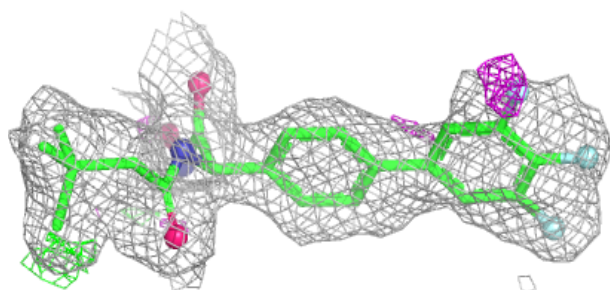
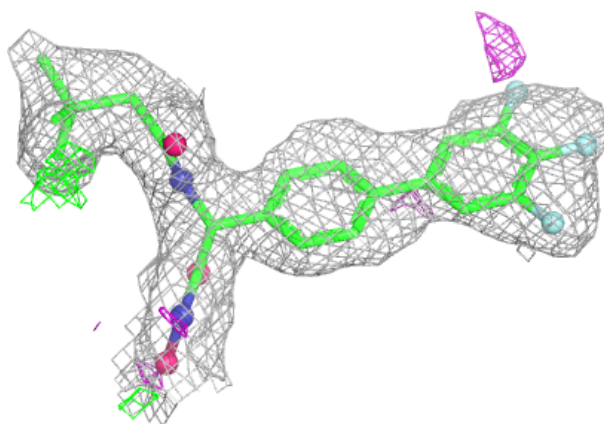
**Electron density around WRC G 704:**

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

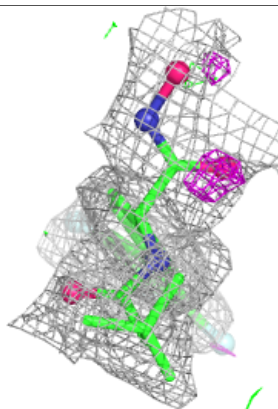
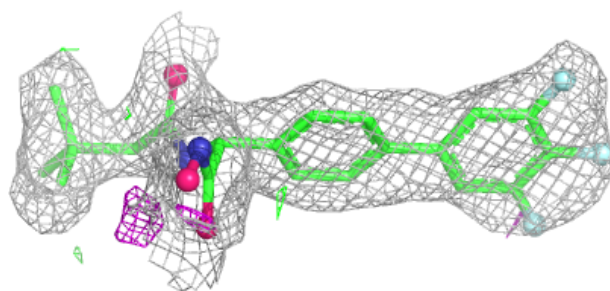
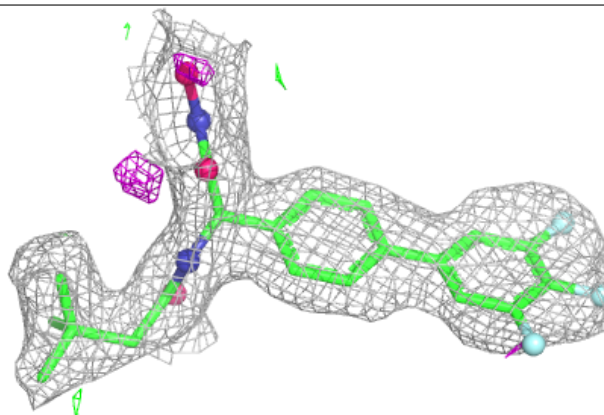


**Electron density around WRC C 704:**

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

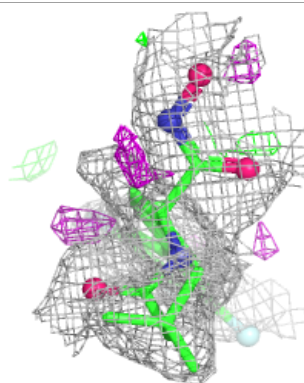
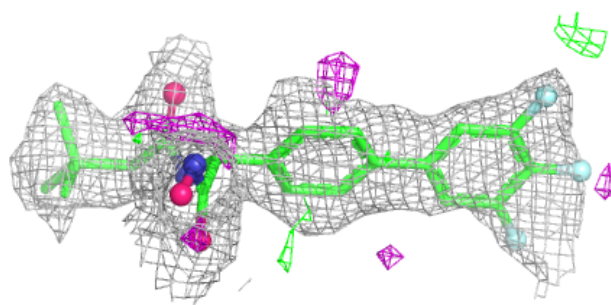
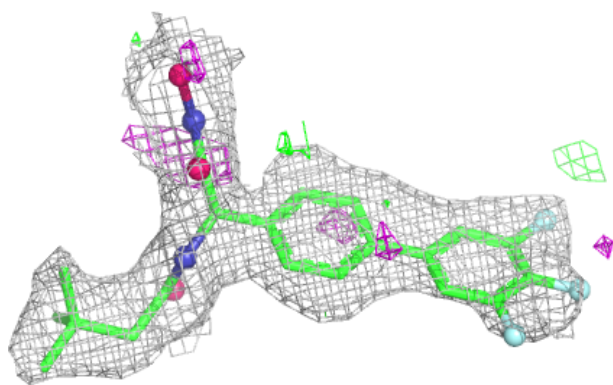
**Electron density around WRC H 704:**

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

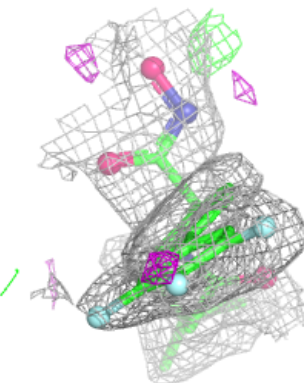
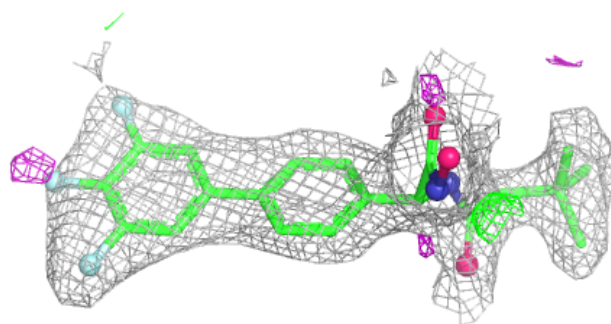
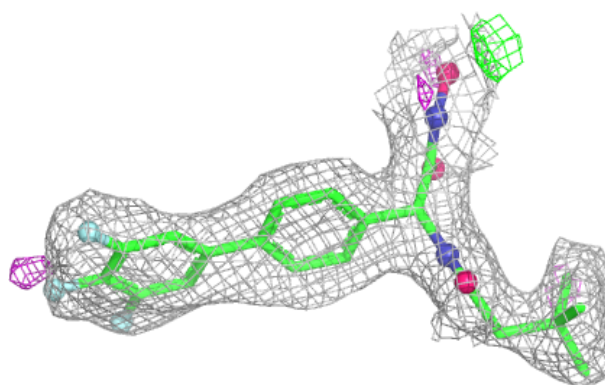


**Electron density around WRC A 704:**

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

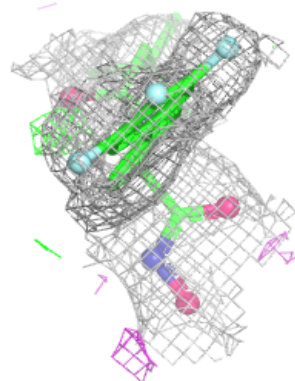
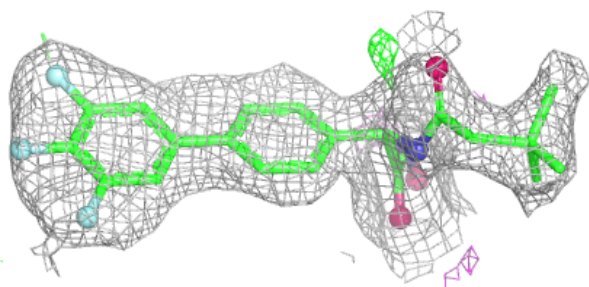
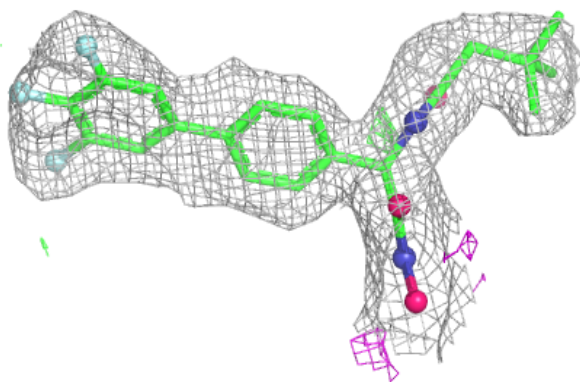
**Electron density around WRC B 704:**

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

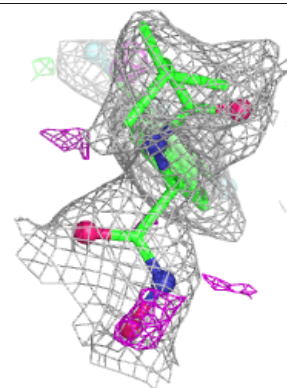
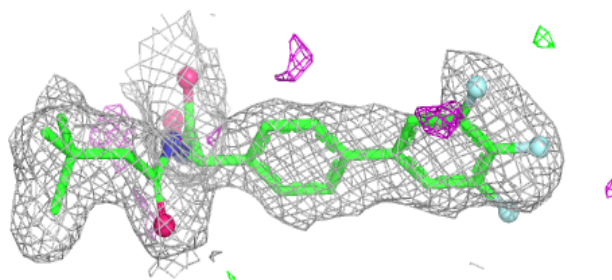
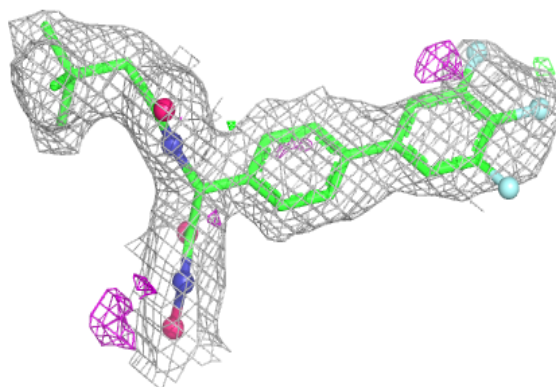


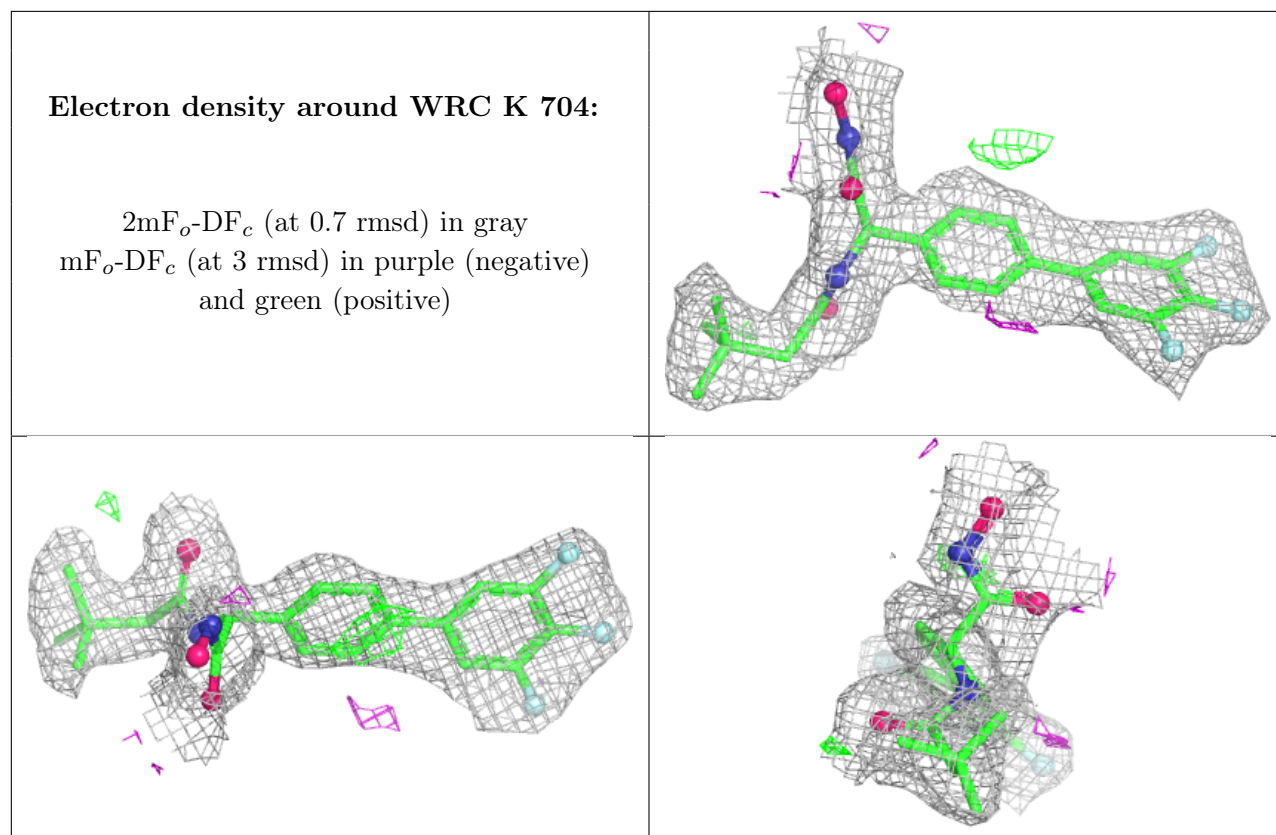
**Electron density around WRC L 704:**

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

**Electron density around WRC D 704:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.