



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 05:38 pm BST

PDB ID : 6EE2  
Title : X-ray crystal structure of Pf-M17 in complex with inhibitor 6i and regulatory zinc ion  
Authors : Drinkwater, N.; McGowan, S.  
Deposited on : 2018-08-13  
Resolution : 2.10 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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

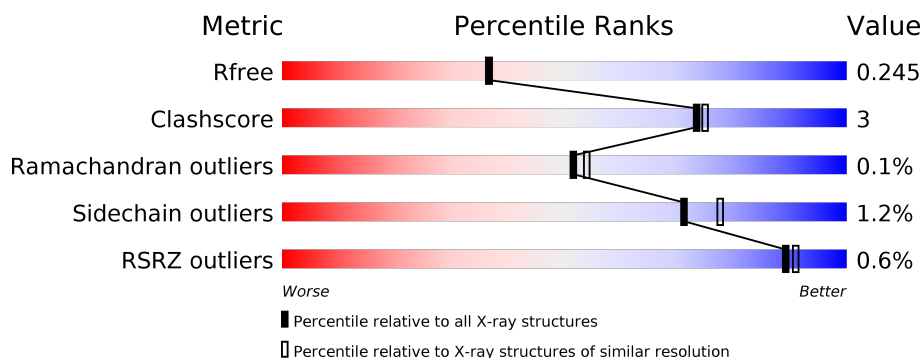
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	526	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>.</div> </div> </div>
1	B	526	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
1	C	526	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>.</div> </div> </div>
1	D	526	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>.</div> </div> </div>
1	E	526	<div> <div></div> <div> <div></div> <div>87%</div> <div>10%</div> <div>.</div> </div> </div>
1	F	526	<div> <div></div> <div> <div></div> <div>89%</div> <div>7%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	526	 90% 8% ..
1	H	526	 2% 91% 7% .
1	I	526	 % 94% 6% .
1	J	526	 90% 7% .
1	K	526	 87% 9% .
1	L	526	 90% 8% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	1PE	L	709	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 52312 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 Pf-M17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	1	0
			3994	2563	642	769	20			
1	B	518	Total	C	N	O	S	0	1	0
			3952	2541	642	749	20			
1	C	520	Total	C	N	O	S	0	1	0
			3994	2567	643	764	20			
1	D	516	Total	C	N	O	S	0	2	0
			3955	2549	639	746	21			
1	E	510	Total	C	N	O	S	0	0	0
			3912	2516	631	746	19			
1	F	510	Total	C	N	O	S	0	1	0
			3890	2502	627	742	19			
1	G	519	Total	C	N	O	S	0	1	0
			3993	2563	645	765	20			
1	H	520	Total	C	N	O	S	0	1	0
			3960	2548	640	752	20			
1	I	523	Total	C	N	O	S	0	0	0
			3992	2561	644	767	20			
1	J	512	Total	C	N	O	S	0	0	0
			3927	2528	636	743	20			
1	K	509	Total	C	N	O	S	0	0	0
			3900	2511	627	743	19			
1	L	513	Total	C	N	O	S	0	0	0
			3910	2511	632	748	19			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP W4I9J7
A	515	GLN	ASN	engineered mutation	UNP W4I9J7
A	546	GLN	ASN	engineered mutation	UNP W4I9J7
A	606	HIS	-	expression tag	UNP W4I9J7
A	607	HIS	-	expression tag	UNP W4I9J7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	608	HIS	-	expression tag	UNP W4I9J7
A	609	HIS	-	expression tag	UNP W4I9J7
A	610	HIS	-	expression tag	UNP W4I9J7
B	152	GLN	ASN	engineered mutation	UNP W4I9J7
B	515	GLN	ASN	engineered mutation	UNP W4I9J7
B	546	GLN	ASN	engineered mutation	UNP W4I9J7
B	606	HIS	-	expression tag	UNP W4I9J7
B	607	HIS	-	expression tag	UNP W4I9J7
B	608	HIS	-	expression tag	UNP W4I9J7
B	609	HIS	-	expression tag	UNP W4I9J7
B	610	HIS	-	expression tag	UNP W4I9J7
C	152	GLN	ASN	engineered mutation	UNP W4I9J7
C	515	GLN	ASN	engineered mutation	UNP W4I9J7
C	546	GLN	ASN	engineered mutation	UNP W4I9J7
C	606	HIS	-	expression tag	UNP W4I9J7
C	607	HIS	-	expression tag	UNP W4I9J7
C	608	HIS	-	expression tag	UNP W4I9J7
C	609	HIS	-	expression tag	UNP W4I9J7
C	610	HIS	-	expression tag	UNP W4I9J7
D	152	GLN	ASN	engineered mutation	UNP W4I9J7
D	515	GLN	ASN	engineered mutation	UNP W4I9J7
D	546	GLN	ASN	engineered mutation	UNP W4I9J7
D	606	HIS	-	expression tag	UNP W4I9J7
D	607	HIS	-	expression tag	UNP W4I9J7
D	608	HIS	-	expression tag	UNP W4I9J7
D	609	HIS	-	expression tag	UNP W4I9J7
D	610	HIS	-	expression tag	UNP W4I9J7
E	152	GLN	ASN	engineered mutation	UNP W4I9J7
E	515	GLN	ASN	engineered mutation	UNP W4I9J7
E	546	GLN	ASN	engineered mutation	UNP W4I9J7
E	606	HIS	-	expression tag	UNP W4I9J7
E	607	HIS	-	expression tag	UNP W4I9J7
E	608	HIS	-	expression tag	UNP W4I9J7
E	609	HIS	-	expression tag	UNP W4I9J7
E	610	HIS	-	expression tag	UNP W4I9J7
F	152	GLN	ASN	engineered mutation	UNP W4I9J7
F	515	GLN	ASN	engineered mutation	UNP W4I9J7
F	546	GLN	ASN	engineered mutation	UNP W4I9J7
F	606	HIS	-	expression tag	UNP W4I9J7
F	607	HIS	-	expression tag	UNP W4I9J7
F	608	HIS	-	expression tag	UNP W4I9J7
F	609	HIS	-	expression tag	UNP W4I9J7

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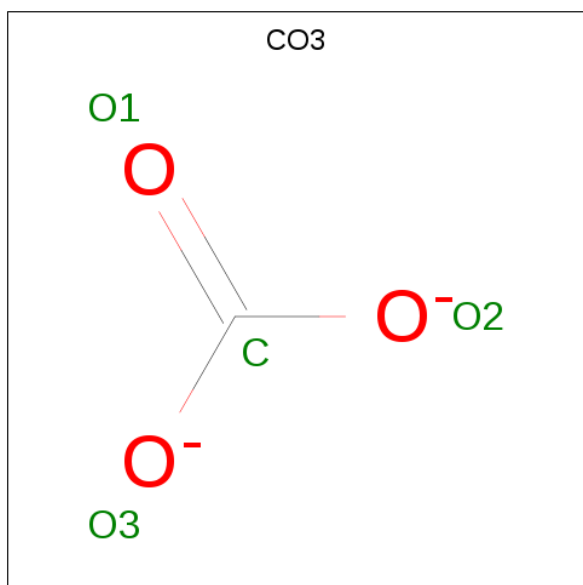
Chain	Residue	Modelled	Actual	Comment	Reference
F	610	HIS	-	expression tag	UNP W4I9J7
G	152	GLN	ASN	engineered mutation	UNP W4I9J7
G	515	GLN	ASN	engineered mutation	UNP W4I9J7
G	546	GLN	ASN	engineered mutation	UNP W4I9J7
G	606	HIS	-	expression tag	UNP W4I9J7
G	607	HIS	-	expression tag	UNP W4I9J7
G	608	HIS	-	expression tag	UNP W4I9J7
G	609	HIS	-	expression tag	UNP W4I9J7
G	610	HIS	-	expression tag	UNP W4I9J7
H	152	GLN	ASN	engineered mutation	UNP W4I9J7
H	515	GLN	ASN	engineered mutation	UNP W4I9J7
H	546	GLN	ASN	engineered mutation	UNP W4I9J7
H	606	HIS	-	expression tag	UNP W4I9J7
H	607	HIS	-	expression tag	UNP W4I9J7
H	608	HIS	-	expression tag	UNP W4I9J7
H	609	HIS	-	expression tag	UNP W4I9J7
H	610	HIS	-	expression tag	UNP W4I9J7
I	152	GLN	ASN	engineered mutation	UNP W4I9J7
I	515	GLN	ASN	engineered mutation	UNP W4I9J7
I	546	GLN	ASN	engineered mutation	UNP W4I9J7
I	606	HIS	-	expression tag	UNP W4I9J7
I	607	HIS	-	expression tag	UNP W4I9J7
I	608	HIS	-	expression tag	UNP W4I9J7
I	609	HIS	-	expression tag	UNP W4I9J7
I	610	HIS	-	expression tag	UNP W4I9J7
J	152	GLN	ASN	engineered mutation	UNP W4I9J7
J	515	GLN	ASN	engineered mutation	UNP W4I9J7
J	546	GLN	ASN	engineered mutation	UNP W4I9J7
J	606	HIS	-	expression tag	UNP W4I9J7
J	607	HIS	-	expression tag	UNP W4I9J7
J	608	HIS	-	expression tag	UNP W4I9J7
J	609	HIS	-	expression tag	UNP W4I9J7
J	610	HIS	-	expression tag	UNP W4I9J7
K	152	GLN	ASN	engineered mutation	UNP W4I9J7
K	515	GLN	ASN	engineered mutation	UNP W4I9J7
K	546	GLN	ASN	engineered mutation	UNP W4I9J7
K	606	HIS	-	expression tag	UNP W4I9J7
K	607	HIS	-	expression tag	UNP W4I9J7
K	608	HIS	-	expression tag	UNP W4I9J7
K	609	HIS	-	expression tag	UNP W4I9J7
K	610	HIS	-	expression tag	UNP W4I9J7
L	152	GLN	ASN	engineered mutation	UNP W4I9J7

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Chain	Residue	Modelled	Actual	Comment	Reference
L	515	GLN	ASN	engineered mutation	UNP W4I9J7
L	546	GLN	ASN	engineered mutation	UNP W4I9J7
L	606	HIS	-	expression tag	UNP W4I9J7
L	607	HIS	-	expression tag	UNP W4I9J7
L	608	HIS	-	expression tag	UNP W4I9J7
L	609	HIS	-	expression tag	UNP W4I9J7
L	610	HIS	-	expression tag	UNP W4I9J7

- Molecule 2 is CARBONATE ION (three-letter code: 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		
2	C	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		
2	E	1	Total	C	O	0	0
			4	1	3		
2	F	1	Total	C	O	0	0
			4	1	3		
2	G	1	Total	C	O	0	0
			4	1	3		
2	H	1	Total	C	O	0	0
			4	1	3		

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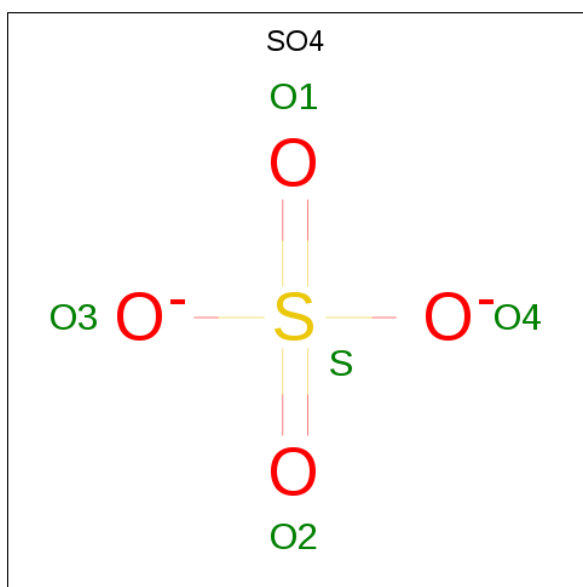
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	C	O	0	0
			4	1	3		
2	J	1	Total	C	O	0	0
			4	1	3		
2	K	1	Total	C	O	0	0
			4	1	3		
2	L	1	Total	C	O	0	0
			4	1	3		

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

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

- Molecule 4 is N-[(1R)-2-(hydroxyamino)-2-oxo-1-(3',4',5'-trifluoro[1,1'-biphenyl]-4-yl)ethyl]cyclohexanecarboxamide (three-letter code: J1V) (formula: C<sub>21</sub>H<sub>21</sub>F<sub>3</sub>N<sub>2</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by author).





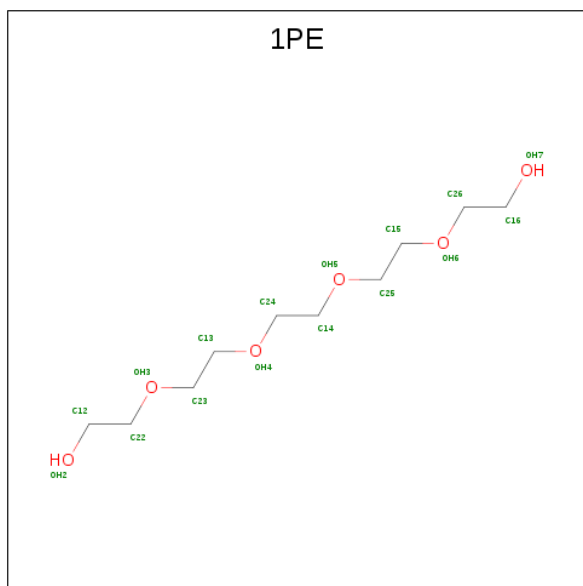
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total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

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

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	6	3		
6	A	1	Total	C	O	0	0
			12	8	4		

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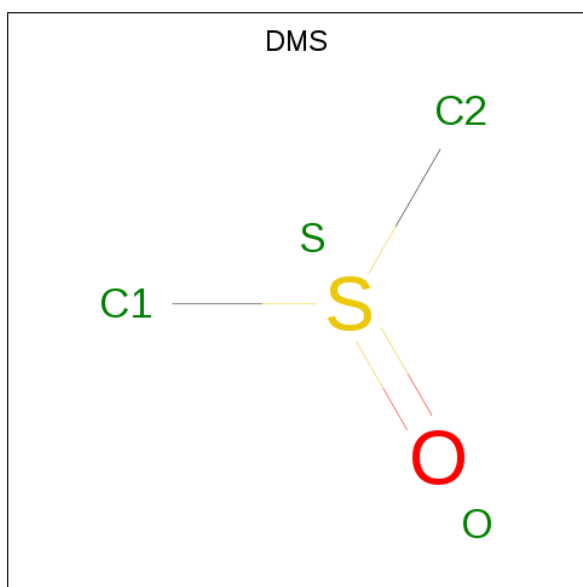
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	7	3		
6	B	1	Total	C	O	0	0
			10	7	3		
6	C	1	Total	C	O	0	0
			13	9	4		
6	C	1	Total	C	O	0	0
			9	6	3		
6	D	1	Total	C	O	0	0
			10	7	3		
6	D	1	Total	C	O	0	0
			11	8	3		
6	D	1	Total	C	O	0	0
			10	7	3		
6	D	1	Total	C	O	0	0
			7	5	2		
6	E	1	Total	C	O	0	0
			12	8	4		
6	E	1	Total	C	O	0	0
			12	8	4		
6	E	1	Total	C	O	0	0
			8	5	3		
6	F	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			9	6	3		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			6	4	2		
6	G	1	Total	C	O	0	0
			12	8	4		
6	H	1	Total	C	O	0	0
			10	7	3		
6	H	1	Total	C	O	0	0
			10	7	3		
6	I	1	Total	C	O	0	0
			15	10	5		

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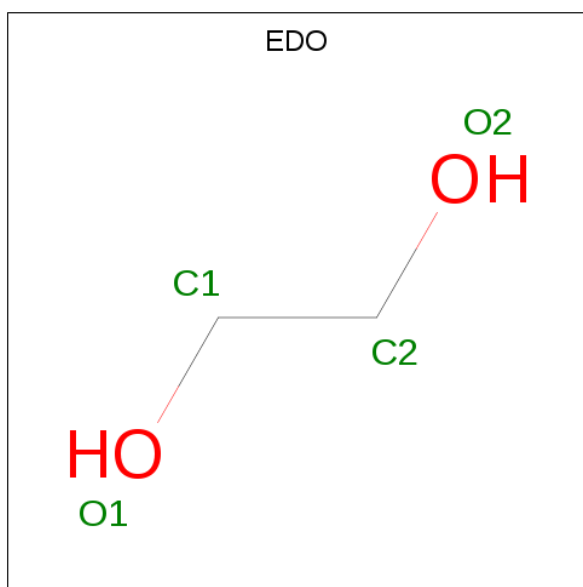
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	1	Total	C	O	0	0
			11	8	3		
6	I	1	Total	C	O	0	0
			7	5	2		
6	J	1	Total	C	O	0	0
			6	4	2		
6	J	1	Total	C	O	0	0
			9	6	3		
6	J	1	Total	C	O	0	0
			9	6	3		
6	K	1	Total	C	O	0	0
			12	8	4		
6	K	1	Total	C	O	0	0
			12	8	4		
6	K	1	Total	C	O	0	0
			11	7	4		
6	K	1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

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	A	1	Total	C	O	S	0	0
			4	2	1	1		
7	B	1	Total	C	O	S	0	0
			4	2	1	1		
7	C	1	Total	C	O	S	0	0
			4	2	1	1		
7	D	1	Total	C	O	S	0	0
			4	2	1	1		
7	E	1	Total	C	O	S	0	0
			4	2	1	1		
7	G	1	Total	C	O	S	0	0
			4	2	1	1		
7	J	1	Total	C	O	S	0	0
			4	2	1	1		
7	K	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	I	1	Total	C	O	0	0
			4	2	2		
8	I	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	330	Total	O	0	0
			330	330		
9	B	326	Total	O	0	0
			326	326		
9	C	356	Total	O	0	0
			356	356		
9	D	318	Total	O	0	0
			318	318		
9	E	363	Total	O	0	0
			363	363		
9	F	318	Total	O	0	0
			318	318		
9	G	351	Total	O	0	0
			351	351		
9	H	283	Total	O	0	0
			283	283		
9	I	350	Total	O	0	0
			350	350		
9	J	331	Total	O	0	0
			331	331		

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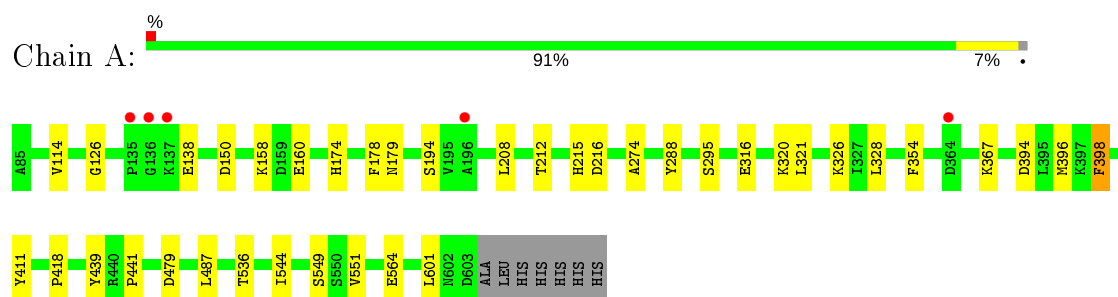
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	K	367	Total	O	0	0
			367	367		
9	L	307	Total	O	0	0
			307	307		

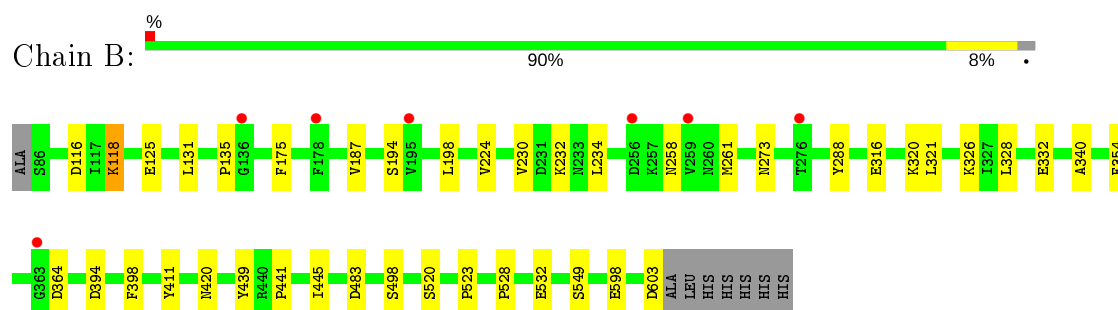
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

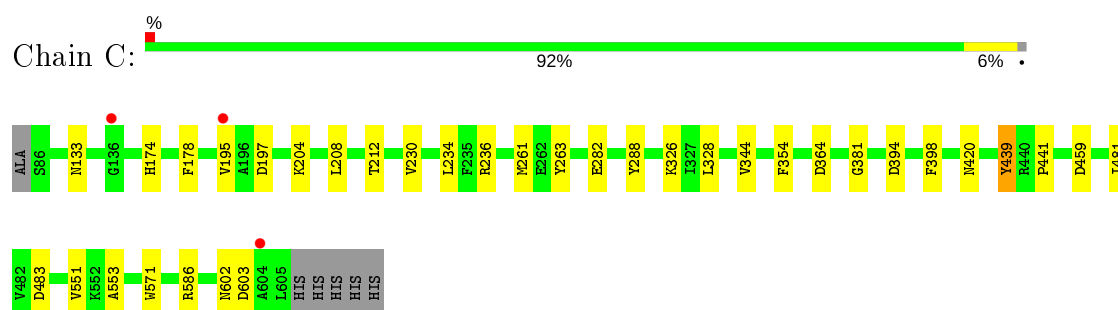
#### • Molecule 1: Pf-M17



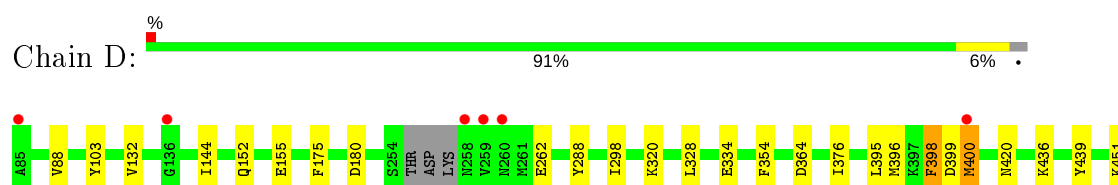
#### • Molecule 1: Pf-M17



#### • Molecule 1: Pf-M17



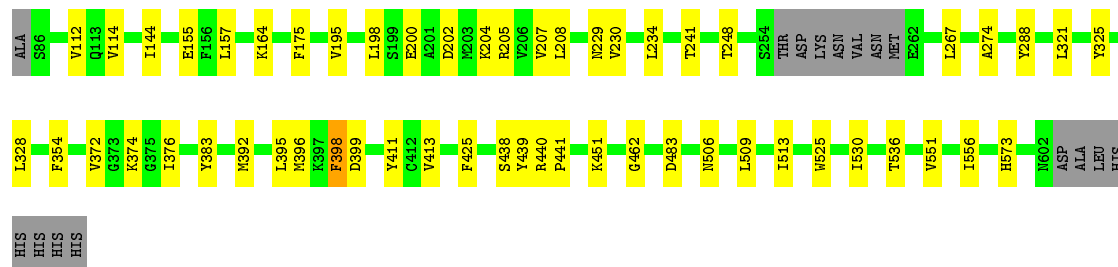
#### • Molecule 1: Pf-M17





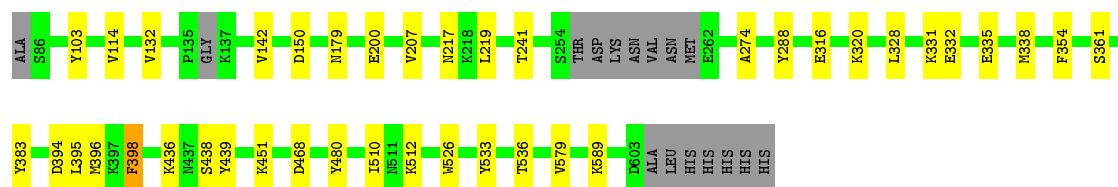
• Molecule 1: Pf-M17

Chain E: 87% 10% .



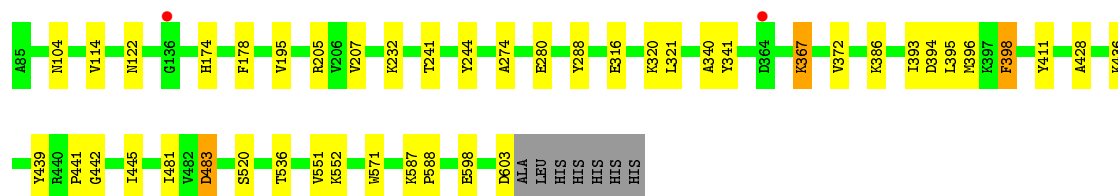
• Molecule 1: Pf-M17

Chain F: 89% 7% .



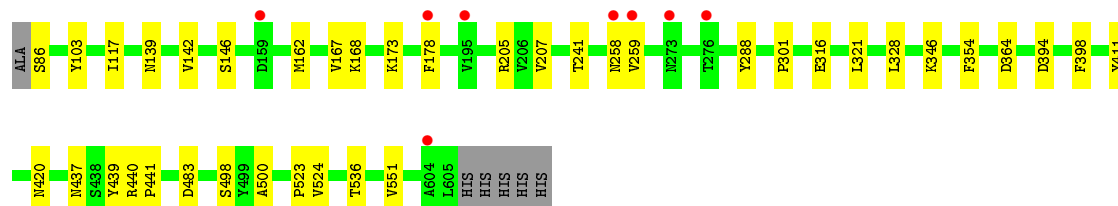
• Molecule 1: Pf-M17

Chain G: 90% 8% ..



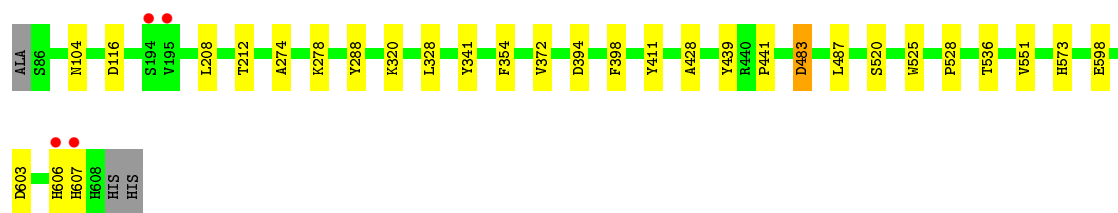
• Molecule 1: Pf-M17

Chain H: 91% 7% .



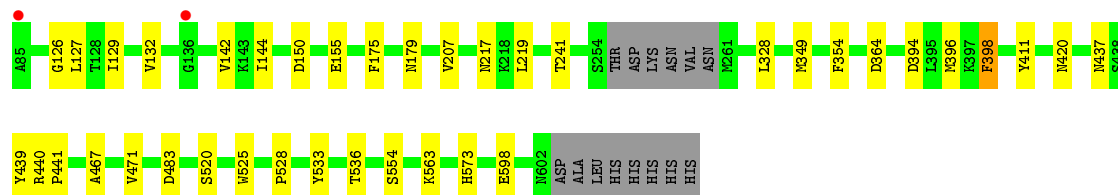
• Molecule 1: Pf-M17

Chain I: 94% 6% .



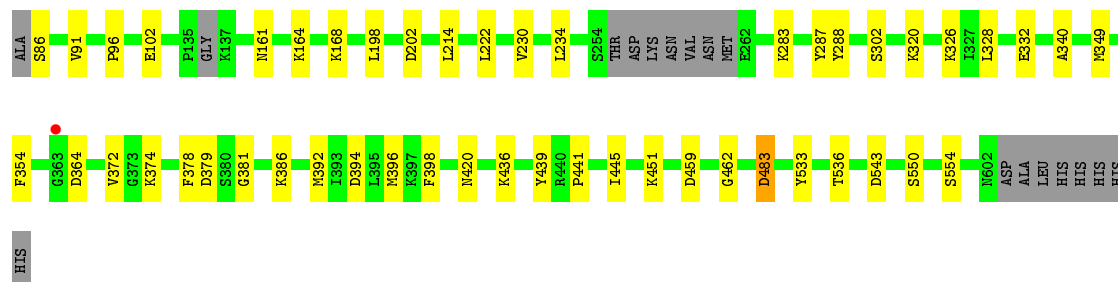
• Molecule 1: Pf-M17

Chain J: 90% 7% .



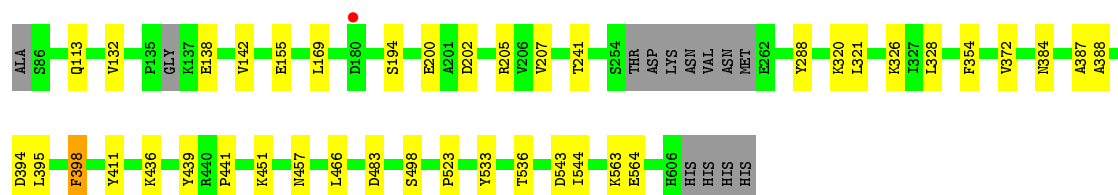
• Molecule 1: Pf-M17

Chain K: 87% 9% .



• Molecule 1: Pf-M17

Chain L: 90% 8% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.18Å 177.87Å 229.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.77 – 2.10 44.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.77-2.10) 99.4 (44.77-2.10)	Depositor EDS
$R_{merge}$	0.51	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.193 , 0.240 0.200 , 0.245	Depositor DCC
$R_{free}$ test set	20510 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	52312	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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 46.70 % 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 1.1034e-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: CO3, ZN, EDO, DMS, SO4, J1V, 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	0.40	0/4075	0.54	0/5526
1	B	0.39	0/4030	0.55	0/5471
1	C	0.40	0/4076	0.54	0/5530
1	D	0.40	0/4039	0.54	0/5476
1	E	0.40	0/3989	0.55	0/5411
1	F	0.38	0/3970	0.54	0/5393
1	G	0.40	0/4074	0.54	0/5524
1	H	0.40	0/4042	0.55	0/5488
1	I	0.40	0/4070	0.55	0/5524
1	J	0.40	0/4004	0.55	0/5427
1	K	0.42	0/3976	0.56	0/5393
1	L	0.40	0/3986	0.54	0/5412
All	All	0.40	0/48331	0.55	0/65575

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3994	0	3928	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3952	0	3869	29	0
1	C	3994	0	3930	20	0
1	D	3955	0	3903	26	0
1	E	3912	0	3848	40	0
1	F	3890	0	3792	26	0
1	G	3993	0	3936	30	0
1	H	3960	0	3873	21	0
1	I	3992	0	3903	21	0
1	J	3927	0	3888	29	0
1	K	3900	0	3833	33	0
1	L	3910	0	3818	30	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	0	0
2	L	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	29	0	0	0	0
4	B	29	0	0	1	0
4	C	29	0	0	0	0
4	D	29	0	0	2	0
4	E	29	0	0	1	0
4	F	29	0	0	0	0
4	G	29	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	29	0	0	0	0
4	I	29	0	0	0	0
4	J	29	0	0	0	0
4	K	29	0	0	1	0
4	L	29	0	0	0	0
5	A	25	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	1	0
5	E	10	0	0	1	0
5	F	5	0	0	0	0
5	G	15	0	0	1	0
5	I	10	0	0	0	0
5	K	15	0	0	0	0
5	L	15	0	0	0	0
6	A	21	0	22	2	0
6	B	20	0	20	2	0
6	C	22	0	24	1	0
6	D	38	0	38	3	0
6	E	32	0	36	1	0
6	F	30	0	39	6	0
6	G	33	0	34	3	0
6	H	20	0	20	2	0
6	I	33	0	37	6	0
6	J	24	0	20	1	0
6	K	41	0	44	4	0
6	L	52	0	63	12	0
7	A	8	0	12	5	0
7	B	4	0	6	0	0
7	C	4	0	6	0	0
7	D	4	0	6	1	0
7	E	4	0	6	1	0
7	G	4	0	6	2	0
7	J	4	0	6	0	0
7	K	4	0	6	0	0
8	I	8	0	12	0	0
9	A	330	0	0	0	0
9	B	326	0	0	3	0
9	C	356	0	0	6	0
9	D	318	0	0	2	0
9	E	363	0	0	9	0
9	F	318	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	351	0	0	4	0
9	H	283	0	0	2	0
9	I	350	0	0	3	0
9	J	331	0	0	4	0
9	K	367	0	0	5	0
9	L	307	0	0	1	0
All	All	52312	0	46984	311	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 311 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)
4:D:703:J1V:NAR	4:D:703:J1V:OAC	1.58	1.31
1:B:116:ASP:OD2	1:B:118:LYS:HE2	1.69	0.91
1:L:457:ASN:HD21	6:L:709:1PE:H162	1.36	0.90
9:I:855:HOH:O	1:K:164:LYS:HE3	1.72	0.88
1:B:131:LEU:HD21	1:B:224:VAL:HG13	1.60	0.83

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	518/526 (98%)	504 (97%)	14 (3%)	0	100	100
1	B	517/526 (98%)	505 (98%)	12 (2%)	0	100	100
1	C	519/526 (99%)	510 (98%)	9 (2%)	0	100	100
1	D	514/526 (98%)	504 (98%)	10 (2%)	0	100	100
1	E	506/526 (96%)	495 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	505/526 (96%)	495 (98%)	10 (2%)	0	100	100
1	G	518/526 (98%)	507 (98%)	11 (2%)	0	100	100
1	H	519/526 (99%)	504 (97%)	13 (2%)	2 (0%)	34	32
1	I	521/526 (99%)	511 (98%)	8 (2%)	2 (0%)	34	32
1	J	508/526 (97%)	497 (98%)	11 (2%)	0	100	100
1	K	503/526 (96%)	495 (98%)	8 (2%)	0	100	100
1	L	507/526 (96%)	492 (97%)	15 (3%)	0	100	100
All	All	6155/6312 (98%)	6019 (98%)	132 (2%)	4 (0%)	51	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	258	ASN
1	I	606	HIS
1	I	607	HIS
1	H	259	VAL

### 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	429/453 (95%)	424 (99%)	5 (1%)	71	77
1	B	417/453 (92%)	409 (98%)	8 (2%)	57	63
1	C	428/453 (94%)	421 (98%)	7 (2%)	62	69
1	D	420/453 (93%)	414 (99%)	6 (1%)	67	73
1	E	418/453 (92%)	415 (99%)	3 (1%)	84	88
1	F	413/453 (91%)	406 (98%)	7 (2%)	60	67
1	G	429/453 (95%)	424 (99%)	5 (1%)	71	77
1	H	418/453 (92%)	412 (99%)	6 (1%)	67	73
1	I	425/453 (94%)	420 (99%)	5 (1%)	71	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	420/453 (93%)	418 (100%)	2 (0%)	88	92
1	K	416/453 (92%)	410 (99%)	6 (1%)	67	73
1	L	416/453 (92%)	411 (99%)	5 (1%)	71	77
All	All	5049/5436 (93%)	4984 (99%)	65 (1%)	71	75

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	200	GLU
1	G	288	TYR
1	L	113	GLN
1	F	288	TYR
1	F	439[A]	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 107 ligands modelled in this entry, 12 are monoatomic - leaving 95 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	$\# Z  > 2$
5	SO4	G	705	-	4,4,4	0.13	0	6,6,6	0.17	0
4	J1V	G	703	3	31,31,31	2.10	5 (16%)	42,43,43	1.75	9 (21%)
4	J1V	I	703	3	31,31,31	1.73	3 (9%)	42,43,43	1.47	7 (16%)
7	DMS	J	707	-	3,3,3	0.59	0	3,3,3	0.68	0
6	1PE	H	705	-	9,9,15	0.78	0	8,8,14	0.39	0
6	1PE	K	707	-	10,10,15	0.78	0	9,9,14	0.32	0
4	J1V	C	703	3	31,31,31	1.75	6 (19%)	42,43,43	1.31	5 (11%)
6	1PE	L	709	-	11,11,15	0.78	0	10,10,14	0.66	0
5	SO4	F	704	-	4,4,4	0.11	0	6,6,6	0.18	0
7	DMS	G	710	-	3,3,3	0.67	0	3,3,3	0.66	0
6	1PE	L	707	-	11,11,15	0.74	0	10,10,14	0.32	0
5	SO4	A	712	-	4,4,4	0.13	0	6,6,6	0.09	0
5	SO4	D	705	-	4,4,4	0.17	0	6,6,6	0.17	0
7	DMS	E	707	-	3,3,3	0.58	0	3,3,3	0.97	0
2	CO3	K	701	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	C	704	-	12,12,15	0.73	0	11,11,14	0.33	0
2	CO3	D	701	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	J	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	J1V	E	703	3	31,31,31	2.02	5 (16%)	42,43,43	1.39	7 (16%)
4	J1V	D	703	3	31,31,31	2.08	5 (16%)	42,43,43	1.44	7 (16%)
6	1PE	I	706	-	6,6,15	0.73	0	5,5,14	0.25	0
5	SO4	E	709	-	4,4,4	0.20	0	6,6,6	0.15	0
8	EDO	I	707	-	3,3,3	0.52	0	2,2,2	0.45	0
5	SO4	A	708	-	4,4,4	0.20	0	6,6,6	0.17	0
7	DMS	C	706	-	3,3,3	0.76	0	3,3,3	0.55	0
2	CO3	B	701	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	B	707	-	4,4,4	0.15	0	6,6,6	0.09	0
6	1PE	I	705	-	10,10,15	0.69	0	9,9,14	0.34	0
7	DMS	A	710	-	3,3,3	0.65	0	3,3,3	0.79	0
6	1PE	F	705	-	9,9,15	0.64	0	8,8,14	0.36	0
8	EDO	I	708	-	3,3,3	0.46	0	2,2,2	0.48	0
7	DMS	K	709	-	3,3,3	0.58	0	3,3,3	0.67	0
4	J1V	B	703	3	31,31,31	1.73	3 (9%)	42,43,43	1.46	7 (16%)
6	1PE	K	706	-	11,11,15	0.71	0	10,10,14	0.42	0
6	1PE	E	705	-	11,11,15	0.69	0	10,10,14	0.27	0
6	1PE	K	708	-	5,5,15	0.77	0	4,4,14	0.35	0
5	SO4	A	711	-	4,4,4	0.14	0	6,6,6	0.10	0
6	1PE	K	705	-	11,11,15	0.73	0	10,10,14	0.43	0
6	1PE	E	704	-	11,11,15	0.72	0	10,10,14	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	DMS	D	710	-	3,3,3	0.73	0	3,3,3	0.64	0
6	1PE	A	707	-	11,11,15	0.74	0	10,10,14	0.28	0
2	CO3	L	702	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	G	706	-	8,8,15	0.68	0	7,7,14	0.24	0
5	SO4	L	711	-	4,4,4	0.13	0	6,6,6	0.13	0
6	1PE	H	704	-	9,9,15	0.68	0	8,8,14	0.39	0
2	CO3	A	701	-	0,3,3	0.00	-	0,3,3	0.00	-
2	CO3	C	701	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	E	708	-	4,4,4	0.21	0	6,6,6	0.14	0
5	SO4	A	704	-	4,4,4	0.12	0	6,6,6	0.12	0
4	J1V	J	703	3	31,31,31	1.96	5 (16%)	42,43,43	1.37	6 (14%)
6	1PE	B	704	-	9,9,15	0.72	0	8,8,14	0.28	0
5	SO4	K	704	-	4,4,4	0.13	0	6,6,6	0.14	0
5	SO4	G	704	-	4,4,4	0.15	0	6,6,6	0.33	0
6	1PE	D	706	-	9,9,15	0.69	0	8,8,14	0.24	0
6	1PE	C	705	-	8,8,15	0.68	0	7,7,14	0.33	0
6	1PE	F	707	-	9,9,15	0.70	0	8,8,14	0.27	0
6	1PE	D	707	-	10,10,15	0.82	0	9,9,14	0.52	0
6	1PE	L	706	-	9,9,15	0.58	0	8,8,14	0.17	0
4	J1V	F	703	3	31,31,31	1.94	4 (12%)	42,43,43	1.52	8 (19%)
5	SO4	I	710	-	4,4,4	0.30	0	6,6,6	0.36	0
4	J1V	H	703	3	31,31,31	1.82	3 (9%)	42,43,43	1.67	8 (19%)
5	SO4	D	704	-	4,4,4	0.17	0	6,6,6	0.05	0
5	SO4	I	709	-	4,4,4	0.14	0	6,6,6	0.26	0
7	DMS	B	706	-	3,3,3	0.64	0	3,3,3	0.77	0
7	DMS	A	709	-	3,3,3	0.79	0	3,3,3	0.78	0
5	SO4	L	705	-	4,4,4	0.16	0	6,6,6	0.18	0
6	1PE	D	709	-	6,6,15	0.78	0	5,5,14	0.32	0
5	SO4	G	711	-	4,4,4	0.12	0	6,6,6	0.08	0
6	1PE	G	709	-	11,11,15	0.73	0	10,10,14	0.28	0
6	1PE	I	704	-	14,14,15	0.46	0	13,13,14	0.49	0
4	J1V	A	703	3	31,31,31	2.05	4 (12%)	42,43,43	1.76	9 (21%)
4	J1V	L	704	3	31,31,31	1.90	5 (16%)	42,43,43	1.66	9 (21%)
5	SO4	A	705	-	4,4,4	0.18	0	6,6,6	0.12	0
2	CO3	I	702	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	B	705	-	9,9,15	0.75	0	8,8,14	0.53	0
6	1PE	J	704	-	5,5,15	0.69	0	4,4,14	0.32	0
5	SO4	L	710	-	4,4,4	0.12	0	6,6,6	0.21	0
6	1PE	G	707	-	5,5,15	0.61	0	4,4,14	0.48	0
6	1PE	J	705	-	8,8,15	0.68	0	7,7,14	0.30	0
6	1PE	G	708	-	5,5,15	0.70	0	4,4,14	0.35	0
6	1PE	D	708	-	9,9,15	0.77	0	8,8,14	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CO3	G	701	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	L	708	-	10,10,15	0.69	0	9,9,14	0.24	0
5	SO4	K	711	-	4,4,4	0.12	0	6,6,6	0.32	0
2	CO3	H	701	-	0,3,3	0.00	-	0,3,3	0.00	-
4	J1V	K	703	3	31,31,31	2.02	4 (12%)	42,43,43	1.64	9 (21%)
2	CO3	E	701	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	K	710	-	4,4,4	0.18	0	6,6,6	0.23	0
6	1PE	A	706	-	8,8,15	0.68	0	7,7,14	0.25	0
6	1PE	F	706	-	9,9,15	0.67	0	8,8,14	0.23	0
6	1PE	E	706	-	7,7,15	0.69	0	6,6,14	0.43	0
2	CO3	F	701	-	0,3,3	0.00	-	0,3,3	0.00	-
6	1PE	L	701	-	6,6,15	0.72	0	5,5,14	0.32	0
5	SO4	C	707	-	4,4,4	0.09	0	6,6,6	0.35	0
6	1PE	J	706	-	8,8,15	0.74	0	7,7,14	0.44	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	J1V	J	703	3	-	4/22/30/30	0/3/3/3
8	EDO	I	707	-	-	1/1/1/1	-
6	1PE	B	704	-	-	1/7/7/13	-
6	1PE	B	705	-	-	4/7/7/13	-
6	1PE	J	704	-	-	1/3/3/13	-
6	1PE	G	707	-	-	2/3/3/13	-
6	1PE	L	701	-	-	3/4/4/13	-
6	1PE	J	705	-	-	4/6/6/13	-
6	1PE	D	706	-	-	6/7/7/13	-
4	J1V	G	703	3	-	3/22/30/30	0/3/3/3
6	1PE	D	708	-	-	2/7/7/13	-
4	J1V	I	703	3	-	4/22/30/30	0/3/3/3
6	1PE	C	705	-	-	5/6/6/13	-
6	1PE	F	707	-	-	2/7/7/13	-
6	1PE	D	707	-	-	3/8/8/13	-
6	1PE	L	706	-	-	4/7/7/13	-
6	1PE	I	705	-	-	5/8/8/13	-
4	J1V	F	703	3	-	4/22/30/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	F	705	-	-	2/7/7/13	-
6	1PE	H	705	-	-	1/7/7/13	-
6	1PE	K	707	-	-	4/8/8/13	-
8	EDO	I	708	-	-	0/1/1/1	-
4	J1V	C	703	3	-	3/22/30/30	0/3/3/3
4	J1V	B	703	3	-	4/22/30/30	0/3/3/3
6	1PE	K	706	-	-	4/9/9/13	-
4	J1V	H	703	3	-	3/22/30/30	0/3/3/3
4	J1V	K	703	3	-	3/22/30/30	0/3/3/3
6	1PE	E	705	-	-	3/9/9/13	-
6	1PE	K	708	-	-	3/3/3/13	-
6	1PE	L	708	-	-	4/8/8/13	-
6	1PE	K	705	-	-	2/9/9/13	-
6	1PE	E	704	-	-	3/9/9/13	-
6	1PE	L	707	-	-	7/9/9/13	-
6	1PE	A	707	-	-	4/9/9/13	-
4	J1V	L	704	3	-	5/22/30/30	0/3/3/3
6	1PE	A	706	-	-	2/6/6/13	-
6	1PE	G	706	-	-	5/6/6/13	-
6	1PE	F	706	-	-	3/7/7/13	-
6	1PE	E	706	-	-	3/5/5/13	-
6	1PE	D	709	-	-	4/4/4/13	-
6	1PE	C	704	-	-	5/10/10/13	-
6	1PE	G	709	-	-	5/9/9/13	-
6	1PE	I	704	-	-	6/12/12/13	-
6	1PE	H	704	-	-	0/7/7/13	-
6	1PE	G	708	-	-	2/3/3/13	-
4	J1V	A	703	3	-	3/22/30/30	0/3/3/3
6	1PE	L	709	-	-	5/9/9/13	-
4	J1V	E	703	3	-	4/22/30/30	0/3/3/3
4	J1V	D	703	3	-	4/22/30/30	0/3/3/3
6	1PE	J	706	-	-	5/6/6/13	-
6	1PE	I	706	-	-	3/4/4/13	-

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	703	J1V	CAZ-CA	-8.67	1.38	1.52
4	H	703	J1V	CAZ-CA	-8.40	1.39	1.52
4	G	703	J1V	CAZ-CA	-8.26	1.39	1.52
4	E	703	J1V	CAZ-CA	-8.11	1.39	1.52
4	F	703	J1V	CAZ-CA	-8.11	1.39	1.52

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	703	J1V	CAJ-CAZ-CA	-3.95	114.31	120.80
4	H	703	J1V	CAG-CAI-CAZ	-3.92	117.25	121.20
4	L	704	J1V	CAJ-CAZ-CA	-3.92	114.36	120.80
4	A	703	J1V	O-C-NAR	3.82	128.21	123.27
4	K	703	J1V	CAN-CAP-CBB	-3.63	104.45	111.33

There are no chirality outliers.

5 of 172 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	J1V	N-CAU-CBB-CAP
6	L	709	1PE	C25-C15-OH6-C26
6	L	709	1PE	OH6-C15-C25-OH5
6	L	706	1PE	OH6-C15-C25-OH5
6	L	709	1PE	C15-C25-OH5-C14

There are no ring outliers.

34 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	705	SO4	1	0
4	G	703	J1V	1	0
6	H	705	1PE	2	0
6	K	707	1PE	2	0
6	L	709	1PE	7	0
7	G	710	DMS	2	0
6	L	707	1PE	4	0
5	D	705	SO4	1	0
7	E	707	DMS	1	0
4	E	703	J1V	1	0
4	D	703	J1V	2	0
5	E	709	SO4	1	0
6	I	705	1PE	1	0

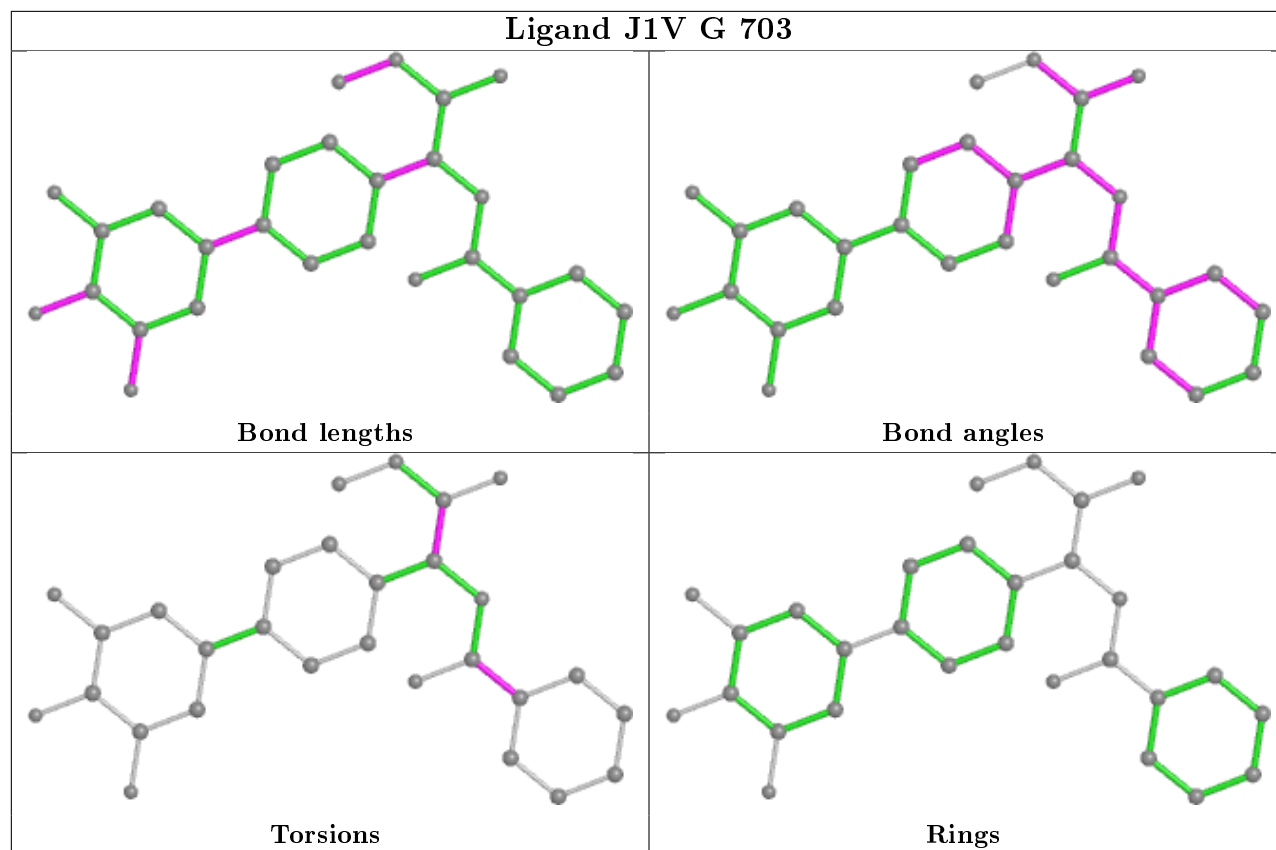
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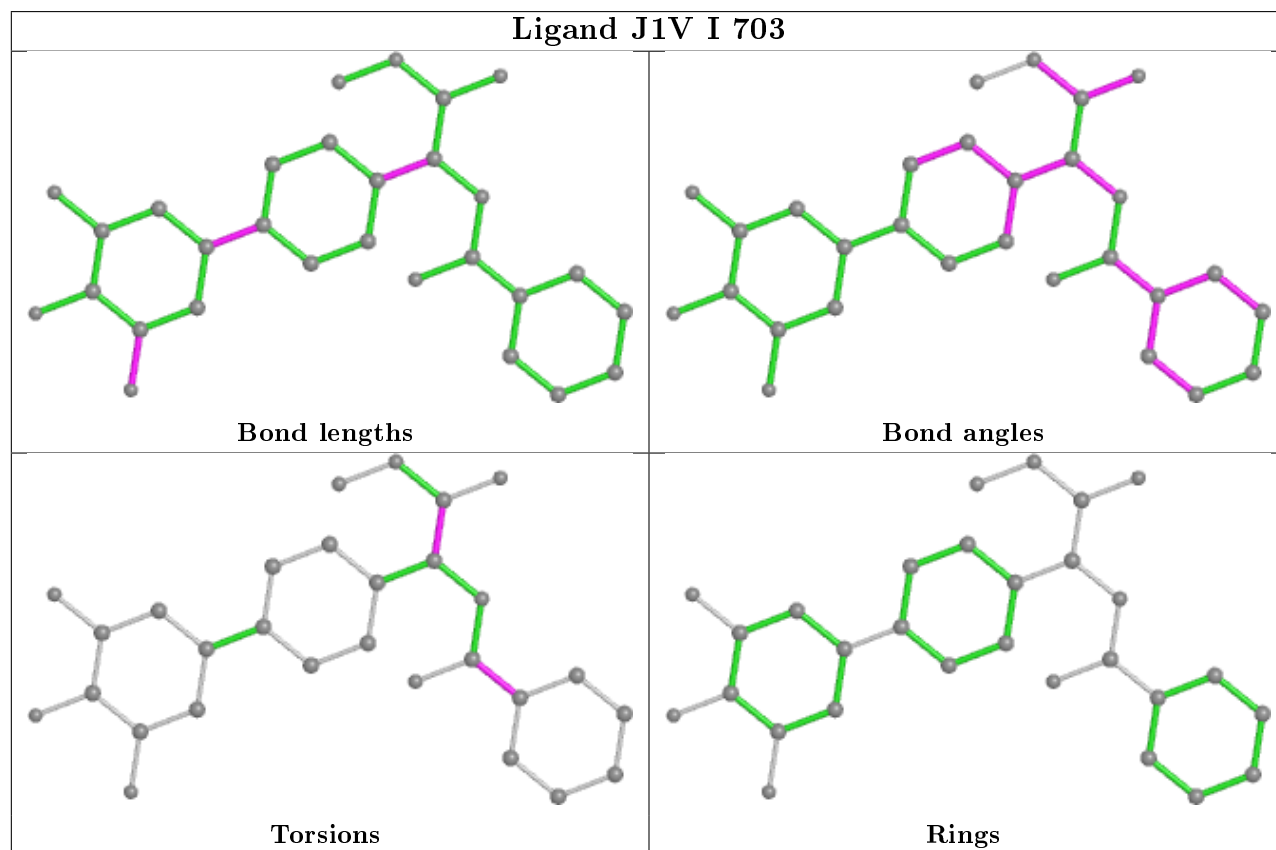
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	710	DMS	2	0
4	B	703	J1V	1	0
6	K	706	1PE	1	0
6	K	708	1PE	1	0
7	D	710	DMS	1	0
6	A	707	1PE	2	0
6	D	706	1PE	1	0
6	C	705	1PE	1	0
6	F	707	1PE	1	0
6	D	707	1PE	1	0
6	L	706	1PE	1	0
7	A	709	DMS	3	0
6	G	709	1PE	2	0
6	I	704	1PE	5	0
6	B	705	1PE	2	0
6	G	707	1PE	1	0
6	J	705	1PE	1	0
6	D	708	1PE	1	0
4	K	703	J1V	1	0
6	F	706	1PE	5	0
6	E	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.

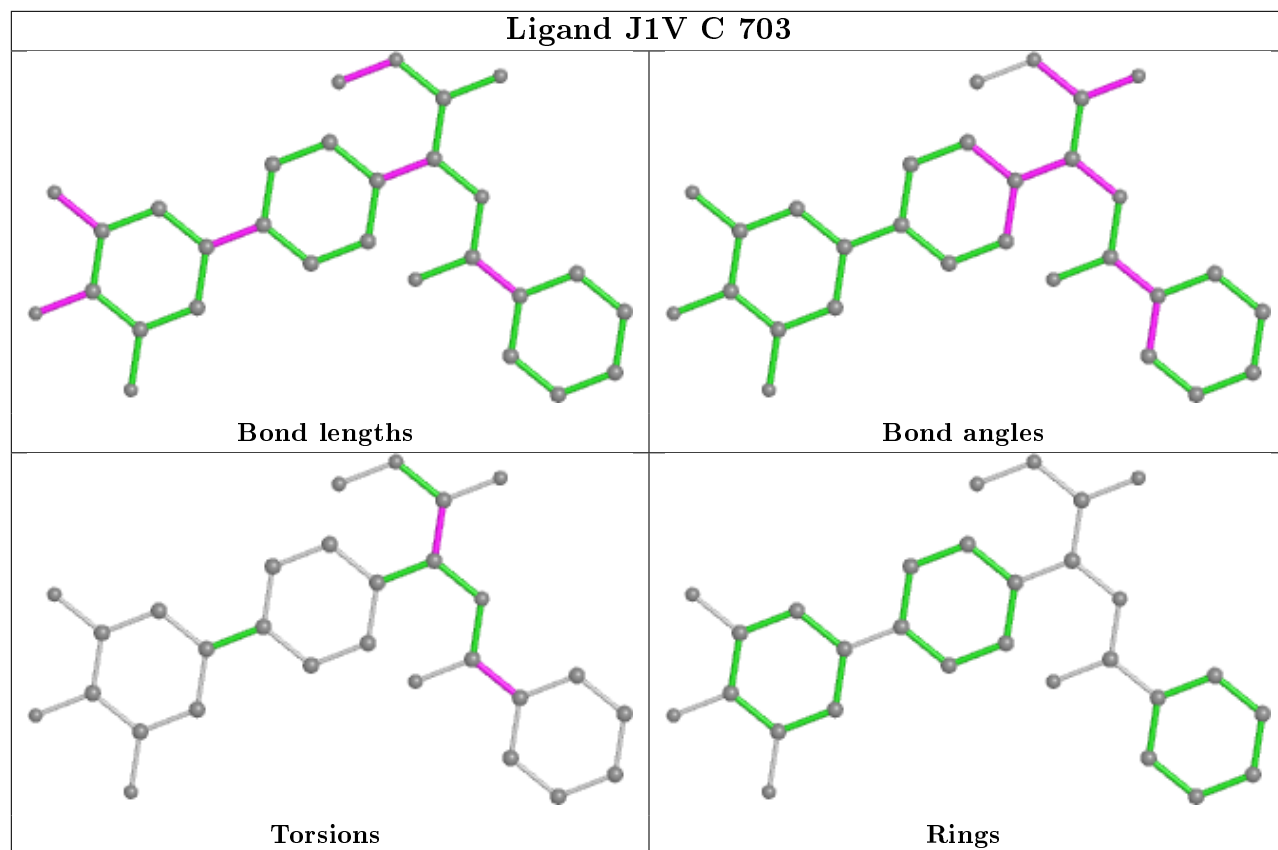
## Ligand J1V G 703



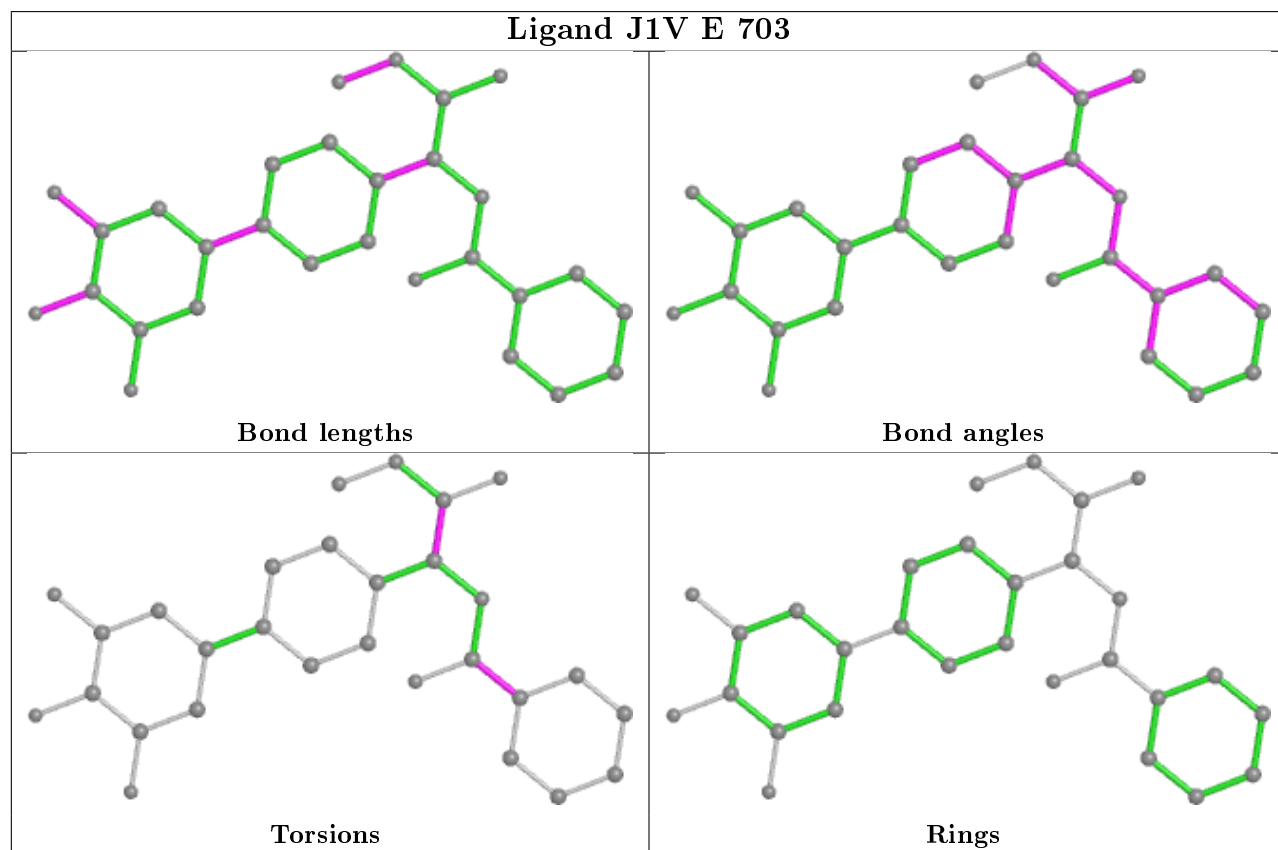
## Ligand J1V I 703



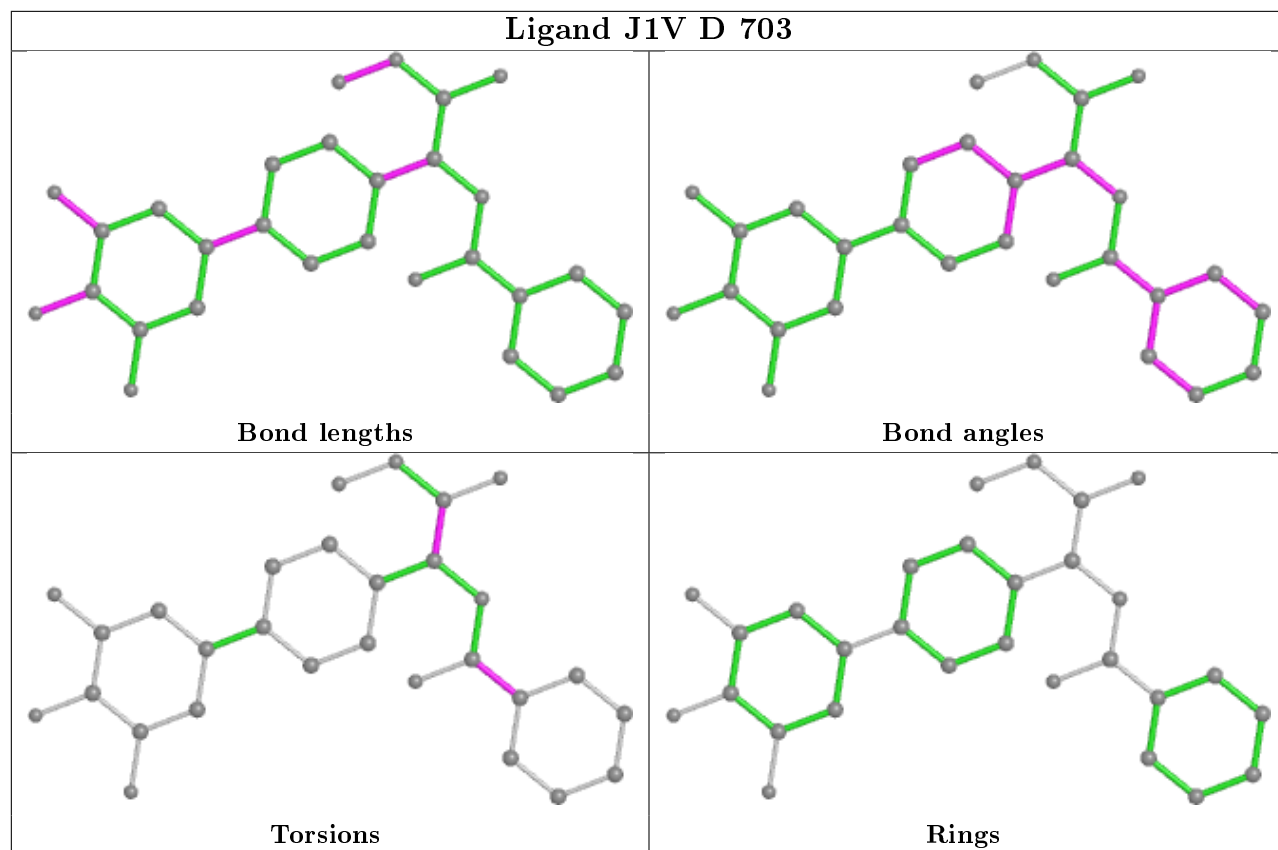
## Ligand J1V C 703



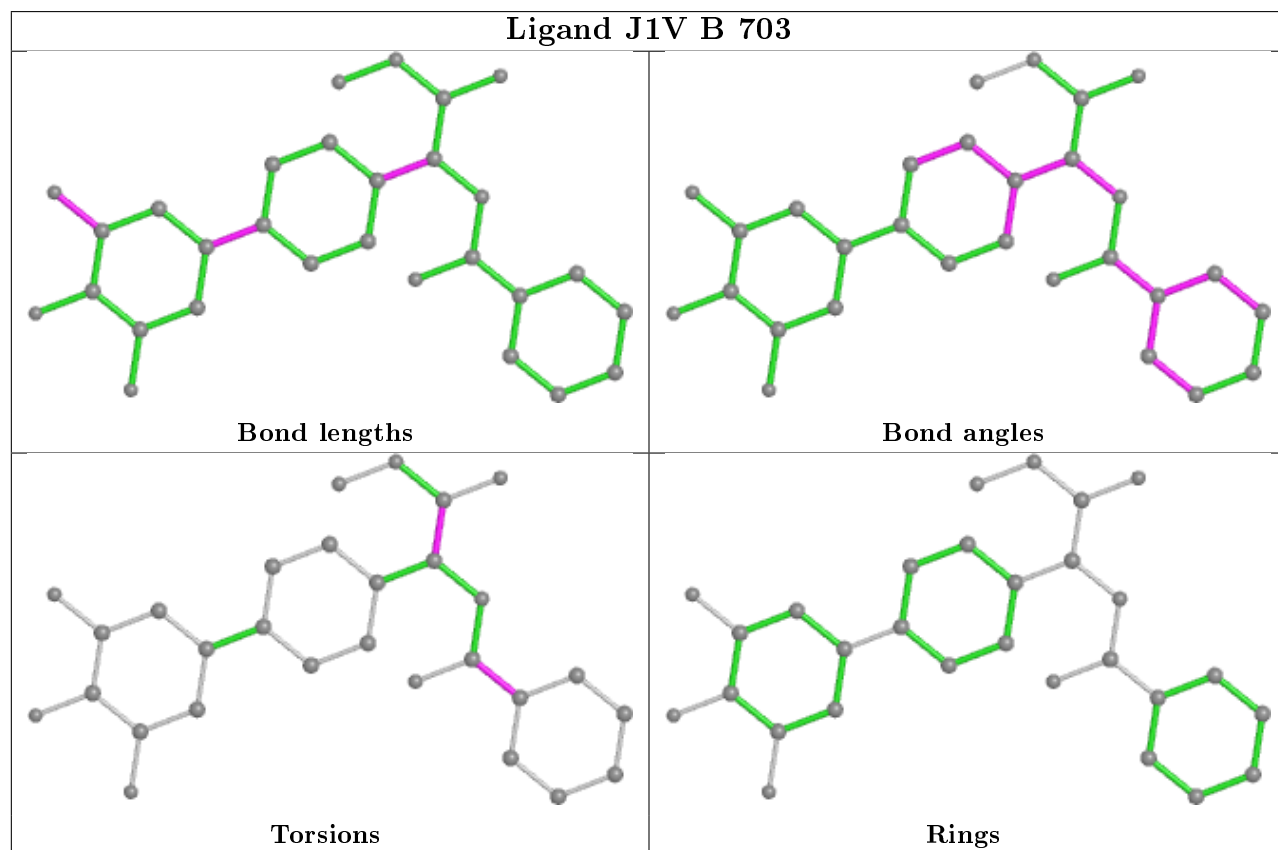
## Ligand J1V E 703



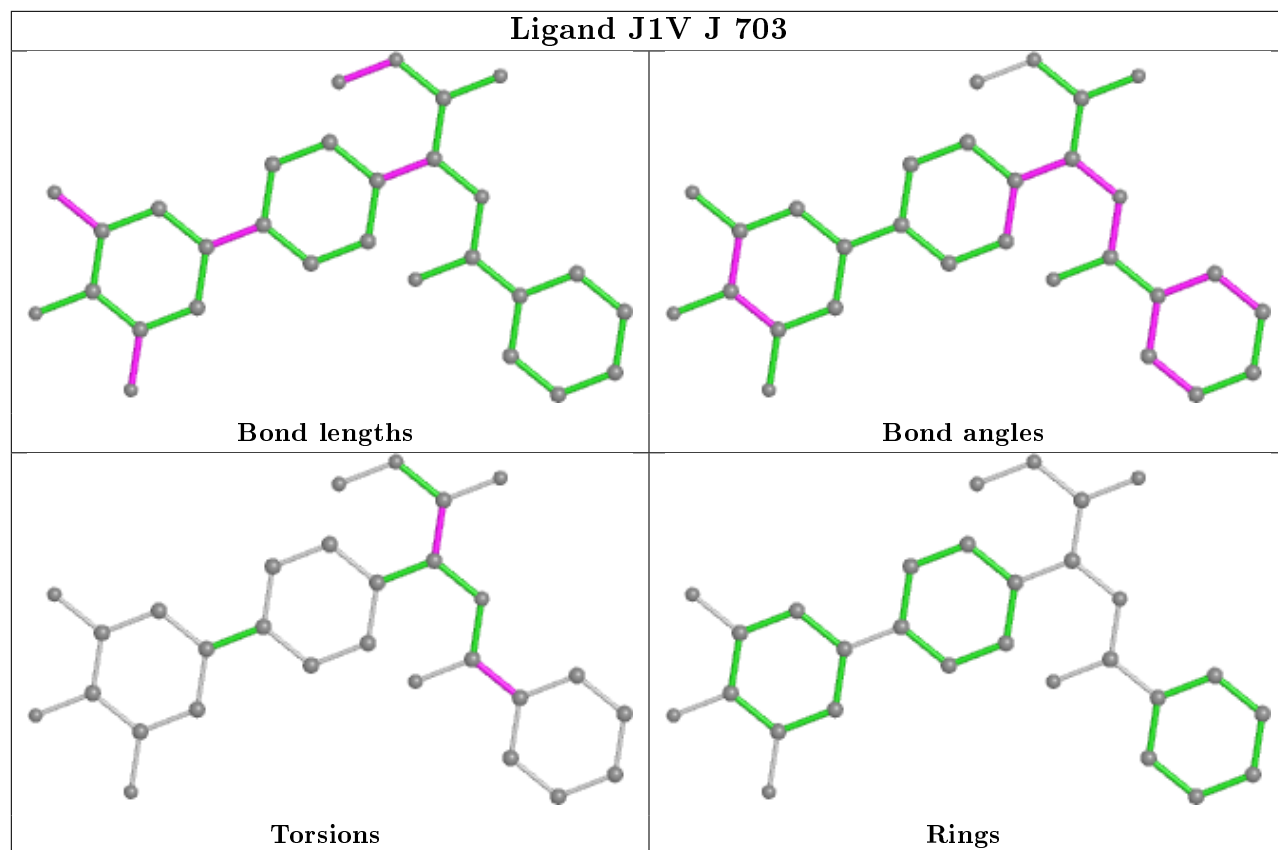
## Ligand J1V D 703



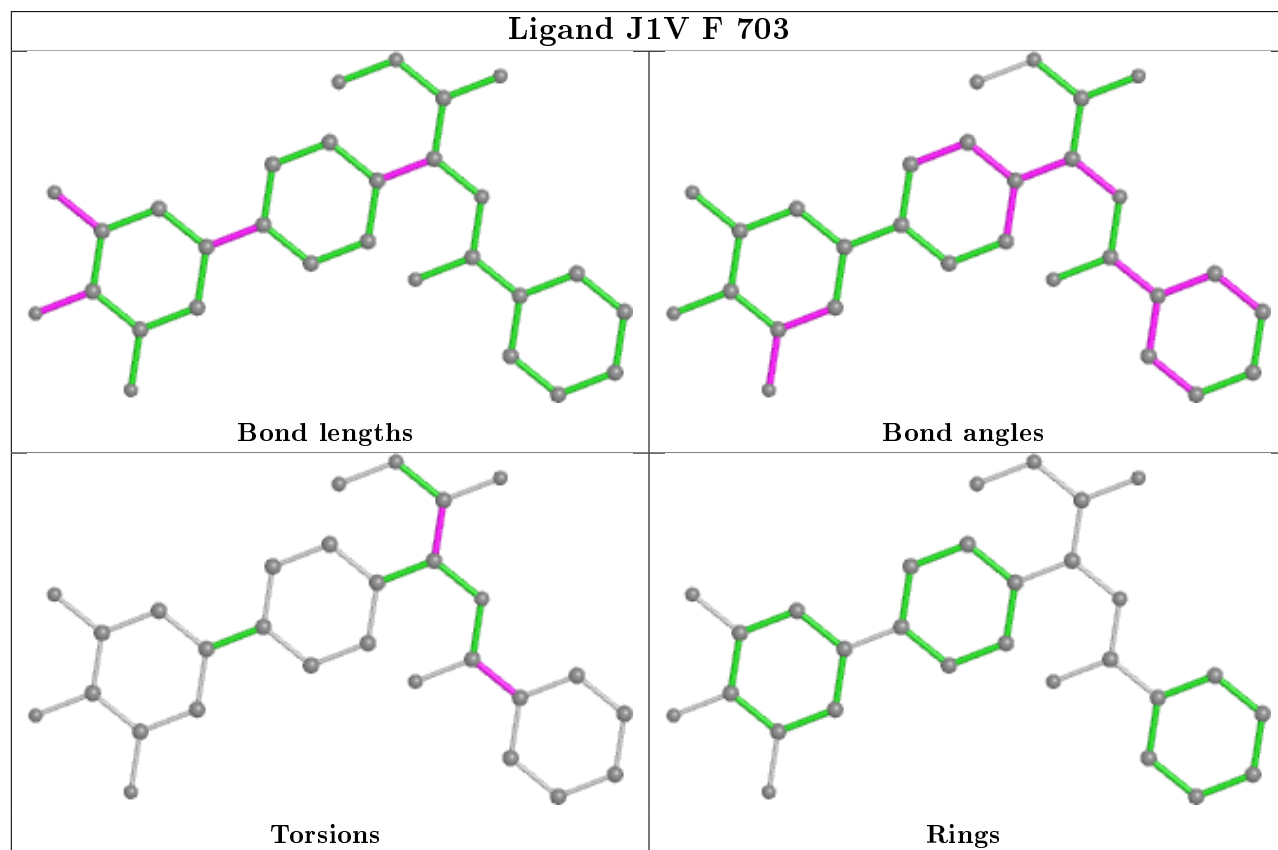
## Ligand J1V B 703



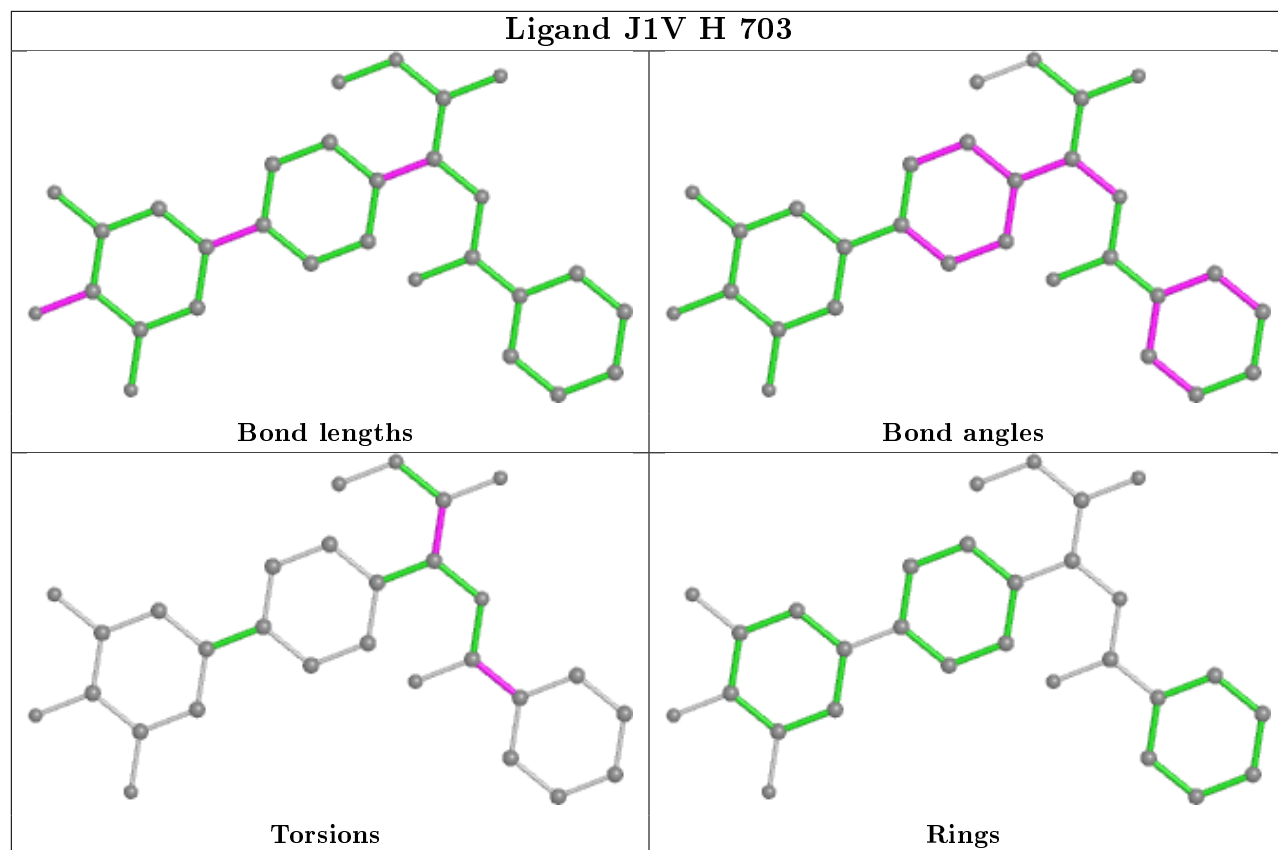
## Ligand J1V J 703



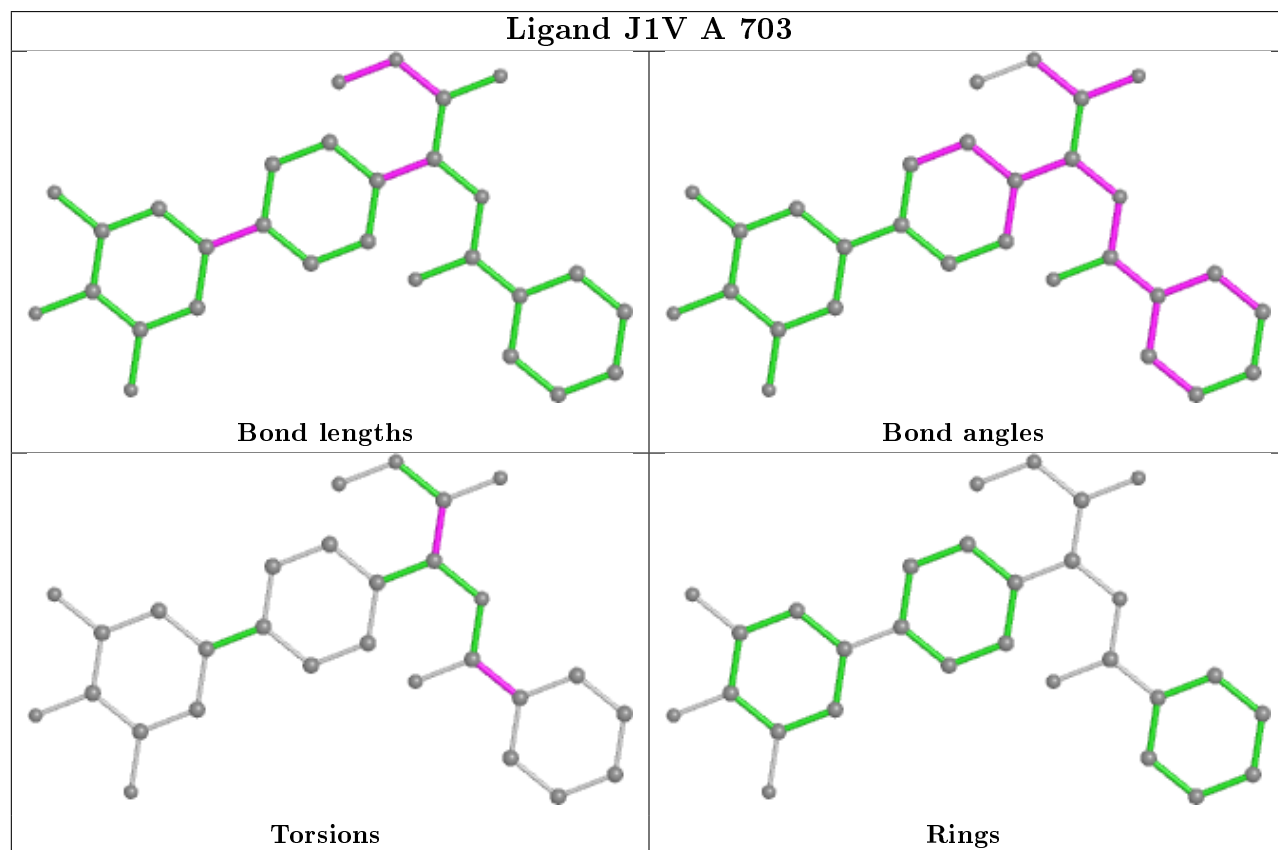
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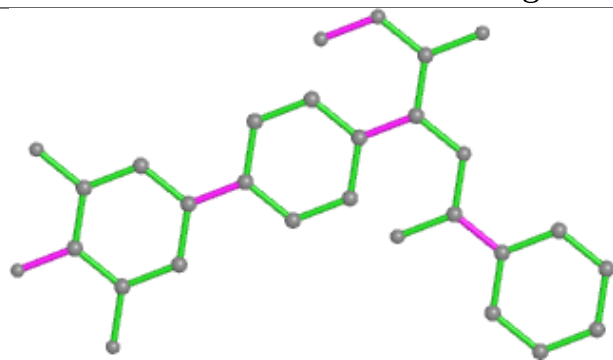
## Ligand J1V H 703



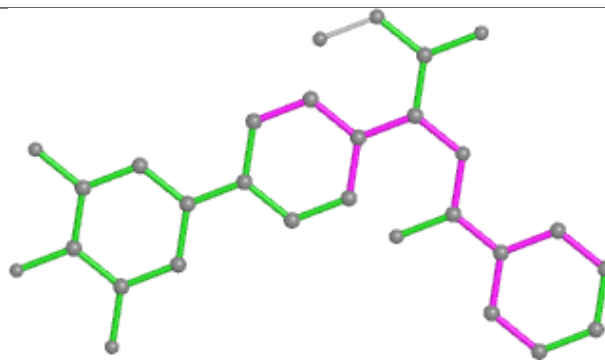
## Ligand J1V A 703



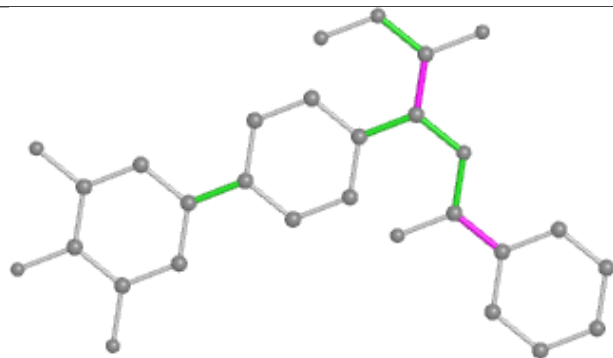
## Ligand J1V L 704



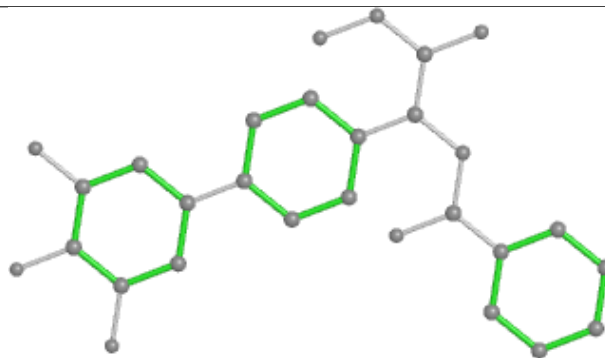
Bond lengths



Bond angles

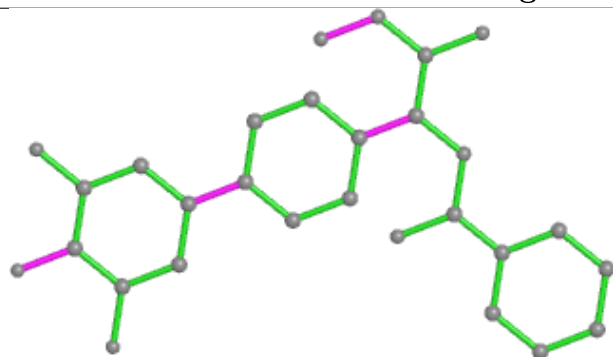


Torsions

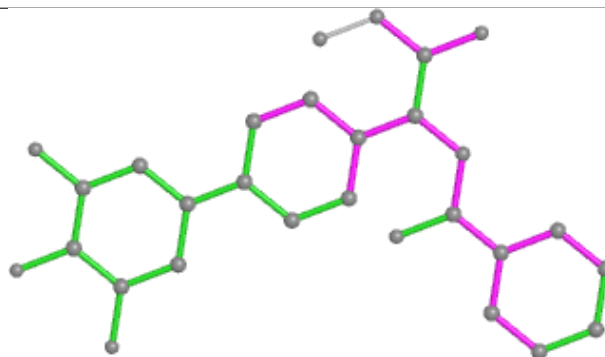


Rings

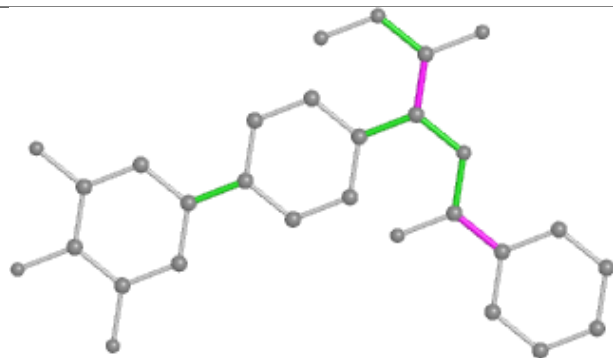
## Ligand J1V K 703



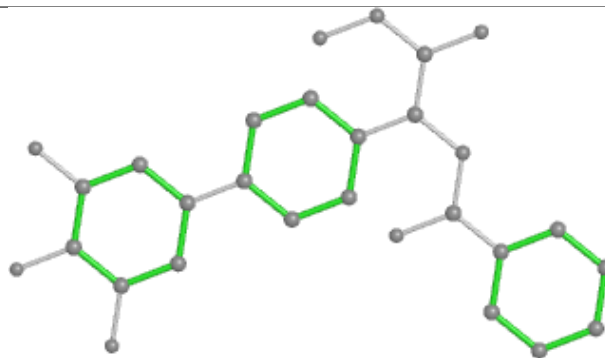
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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	519/526 (98%)	-0.51	5 (0%) 82 85	9, 17, 34, 57	3 (0%)
1	B	518/526 (98%)	-0.42	7 (1%) 75 78	9, 19, 44, 62	4 (0%)
1	C	520/526 (98%)	-0.53	3 (0%) 89 91	9, 17, 35, 51	7 (1%)
1	D	516/526 (98%)	-0.44	7 (1%) 75 78	10, 17, 34, 84	12 (2%)
1	E	510/526 (96%)	-0.65	0 100 100	9, 16, 29, 44	9 (1%)
1	F	510/526 (96%)	-0.42	0 100 100	11, 20, 38, 49	8 (1%)
1	G	519/526 (98%)	-0.54	2 (0%) 92 93	9, 17, 33, 52	6 (1%)
1	H	520/526 (98%)	-0.44	8 (1%) 73 77	9, 18, 45, 74	10 (1%)
1	I	523/526 (99%)	-0.52	4 (0%) 86 88	9, 17, 35, 61	6 (1%)
1	J	512/526 (97%)	-0.48	2 (0%) 92 93	9, 17, 34, 53	8 (1%)
1	K	509/526 (96%)	-0.64	1 (0%) 95 95	10, 16, 29, 50	5 (0%)
1	L	513/526 (97%)	-0.47	1 (0%) 95 95	9, 19, 37, 48	13 (2%)
All	All	6189/6312 (98%)	-0.51	40 (0%) 89 91	9, 17, 37, 84	91 (1%)

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	259	VAL	5.1
1	J	85	ALA	4.1
1	D	260	ASN	3.8
1	B	136	GLY	3.7
1	D	603	ASP	3.4

### 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 ⓘ

There are no carbohydrates 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, 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
6	1PE	K	707	11/16	0.71	0.27	33,37,45,50	0
7	DMS	A	710	4/4	0.76	0.17	18,28,52,59	0
5	SO4	A	705	5/5	0.78	0.18	60,63,78,83	0
6	1PE	L	709	12/16	0.79	0.32	25,32,38,51	0
6	1PE	F	706	10/16	0.79	0.18	41,46,49,52	0
6	1PE	G	709	12/16	0.80	0.17	30,47,52,57	0
6	1PE	H	705	10/16	0.80	0.18	30,43,46,47	0
6	1PE	K	708	6/16	0.80	0.14	25,32,40,43	0
6	1PE	E	706	8/16	0.80	0.25	31,38,39,43	0
6	1PE	L	701	7/16	0.80	0.18	24,35,43,45	0
6	1PE	D	707	11/16	0.81	0.42	31,39,45,46	0
5	SO4	E	709	5/5	0.81	0.33	53,53,55,58	5
6	1PE	A	707	12/16	0.81	0.19	33,43,49,53	0
6	1PE	I	704	15/16	0.82	0.22	27,40,49,55	0
6	1PE	C	704	13/16	0.82	0.24	27,41,49,54	0
6	1PE	D	708	10/16	0.82	0.17	27,36,45,49	0
7	DMS	K	709	4/4	0.82	0.21	27,36,38,52	0
6	1PE	D	709	7/16	0.82	0.17	18,25,33,34	0
7	DMS	E	707	4/4	0.82	0.19	23,28,43,46	0
6	1PE	L	708	11/16	0.83	0.19	38,45,50,52	0
6	1PE	B	705	10/16	0.84	0.14	30,34,42,43	0
6	1PE	K	705	12/16	0.84	0.14	35,38,46,47	0
5	SO4	I	710	5/5	0.84	0.40	52,59,67,68	5
6	1PE	J	704	6/16	0.85	0.19	21,27,34,36	0
6	1PE	J	706	9/16	0.85	0.16	29,37,41,43	0
6	1PE	F	707	10/16	0.86	0.22	28,39,44,44	0
6	1PE	E	704	12/16	0.86	0.17	30,34,41,42	0
7	DMS	G	710	4/4	0.86	0.18	19,19,27,40	0
8	EDO	I	707	4/4	0.87	0.12	24,26,30,35	0
6	1PE	L	707	12/16	0.87	0.28	30,41,51,53	0
5	SO4	E	708	5/5	0.87	0.27	28,41,46,48	5
6	1PE	G	708	6/16	0.88	0.14	23,31,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	DMS	C	706	4/4	0.88	0.21	28,29,35,44	0
6	1PE	I	705	11/16	0.88	0.12	25,27,41,44	0
6	1PE	G	706	9/16	0.89	0.14	26,29,41,41	0
6	1PE	F	705	10/16	0.90	0.11	25,30,35,35	0
6	1PE	H	704	10/16	0.90	0.12	25,29,38,40	0
6	1PE	I	706	7/16	0.90	0.14	24,33,36,37	0
5	SO4	A	712	5/5	0.90	0.32	81,84,87,87	0
5	SO4	L	710	5/5	0.90	0.23	45,46,49,51	5
6	1PE	C	705	9/16	0.90	0.13	17,22,34,37	0
5	SO4	D	704	5/5	0.91	0.29	62,62,65,80	0
5	SO4	A	711	5/5	0.91	0.28	63,64,72,76	0
4	J1V	K	703	29/29	0.91	0.11	16,24,31,33	0
7	DMS	D	710	4/4	0.91	0.16	21,31,36,39	0
6	1PE	J	705	9/16	0.92	0.10	19,26,30,30	0
4	J1V	E	703	29/29	0.92	0.10	18,23,32,33	0
4	J1V	D	703	29/29	0.92	0.11	17,24,36,39	0
3	ZN	J	702	1/1	0.92	0.07	45,45,45,45	1
4	J1V	F	703	29/29	0.92	0.12	17,22,32,36	0
4	J1V	C	703	29/29	0.92	0.11	14,24,34,38	0
4	J1V	J	703	29/29	0.92	0.12	17,22,31,31	0
6	1PE	G	707	6/16	0.92	0.14	31,32,34,38	0
6	1PE	D	706	10/16	0.92	0.11	23,29,35,36	0
4	J1V	A	703	29/29	0.93	0.12	17,22,32,33	0
6	1PE	L	706	10/16	0.93	0.13	21,32,38,46	0
5	SO4	I	709	5/5	0.93	0.15	42,49,50,53	5
7	DMS	B	706	4/4	0.93	0.20	26,26,34,45	0
6	1PE	A	706	9/16	0.93	0.12	19,28,32,33	0
7	DMS	A	709	4/4	0.93	0.18	26,28,41,49	0
4	J1V	B	703	29/29	0.93	0.12	17,22,31,34	0
6	1PE	B	704	10/16	0.93	0.12	21,28,42,51	0
4	J1V	H	703	29/29	0.93	0.12	14,20,34,40	0
5	SO4	L	711	5/5	0.94	0.25	44,54,57,62	0
4	J1V	L	704	29/29	0.94	0.11	15,24,31,32	0
8	EDO	I	708	4/4	0.94	0.11	31,33,34,35	0
4	J1V	I	703	29/29	0.94	0.10	16,23,30,31	0
5	SO4	F	704	5/5	0.94	0.22	52,53,58,70	0
5	SO4	L	705	5/5	0.94	0.31	50,58,63,81	0
6	1PE	K	706	12/16	0.94	0.14	23,27,45,48	0
6	1PE	E	705	12/16	0.94	0.15	23,28,42,45	0
4	J1V	G	703	29/29	0.94	0.11	16,23,32,41	0
5	SO4	K	710	5/5	0.95	0.16	25,29,37,38	5
5	SO4	K	704	5/5	0.95	0.28	63,68,71,77	0

*Continued on next page...*

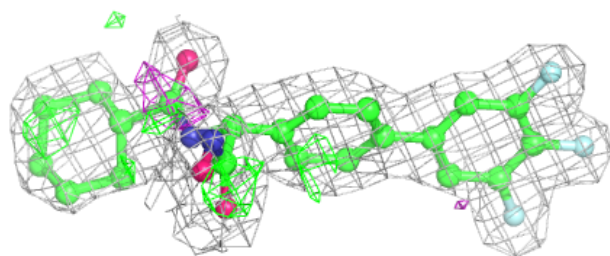
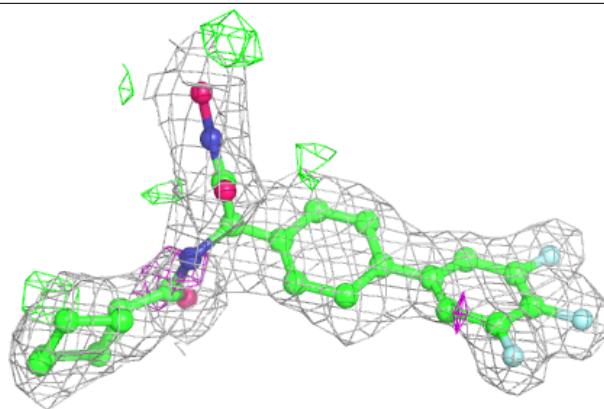
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CO3	D	701	4/4	0.95	0.09	13,15,19,22	0
5	SO4	A	704	5/5	0.95	0.23	46,54,66,66	0
2	CO3	B	701	4/4	0.95	0.11	13,13,15,20	0
5	SO4	C	707	5/5	0.95	0.20	22,26,27,32	5
5	SO4	B	707	5/5	0.95	0.35	40,50,53,53	5
5	SO4	G	711	5/5	0.96	0.28	57,59,63,66	0
2	CO3	L	702	4/4	0.96	0.11	13,14,16,21	0
2	CO3	G	701	4/4	0.96	0.09	12,15,18,29	0
7	DMS	J	707	4/4	0.96	0.14	25,25,33,36	0
3	ZN	F	702	1/1	0.96	0.04	40,40,40,40	1
2	CO3	C	701	4/4	0.96	0.10	13,15,20,23	0
2	CO3	I	702	4/4	0.96	0.10	13,14,16,22	0
3	ZN	L	703	1/1	0.97	0.03	41,41,41,41	1
3	ZN	K	702	1/1	0.97	0.05	44,44,44,44	1
2	CO3	A	701	4/4	0.97	0.12	8,13,14,25	0
3	ZN	H	702	1/1	0.97	0.05	41,41,41,41	1
3	ZN	I	701	1/1	0.97	0.06	44,44,44,44	1
2	CO3	J	701	4/4	0.97	0.09	11,11,16,23	0
5	SO4	G	705	5/5	0.97	0.15	49,49,56,57	0
3	ZN	B	702	1/1	0.97	0.06	42,42,42,42	1
3	ZN	E	702	1/1	0.97	0.07	45,45,45,45	1
2	CO3	E	701	4/4	0.98	0.09	13,13,18,19	0
3	ZN	D	702	1/1	0.98	0.04	41,41,41,41	1
2	CO3	F	701	4/4	0.98	0.05	14,15,21,22	0
2	CO3	H	701	4/4	0.98	0.08	10,15,20,22	0
2	CO3	K	701	4/4	0.98	0.08	12,15,17,20	0
3	ZN	G	702	1/1	0.98	0.04	39,39,39,39	1
3	ZN	A	702	1/1	0.99	0.05	40,40,40,40	1
5	SO4	D	705	5/5	0.99	0.09	12,14,15,17	0
5	SO4	K	711	5/5	0.99	0.08	15,16,20,21	0
3	ZN	C	702	1/1	0.99	0.04	37,37,37,37	1
5	SO4	A	708	5/5	1.00	0.06	13,13,17,18	0
5	SO4	G	704	5/5	1.00	0.05	10,10,13,15	0

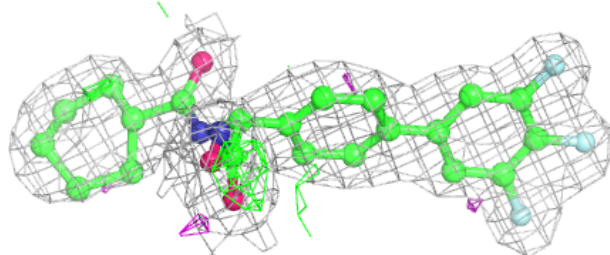
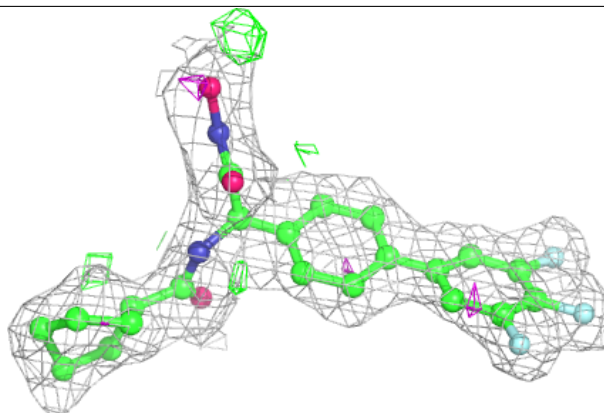
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around J1V K 703:**

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

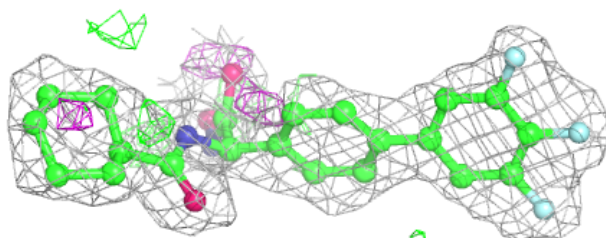
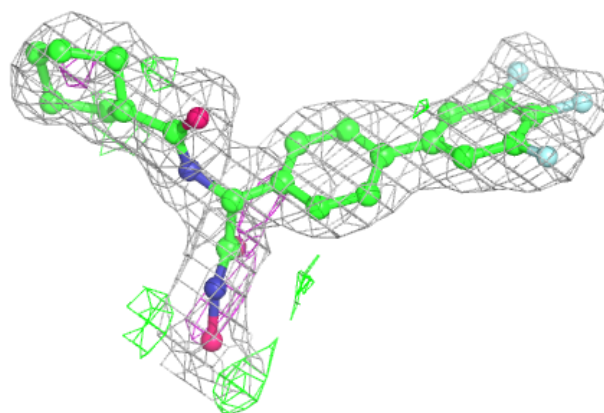
**Electron density around J1V E 703:**

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

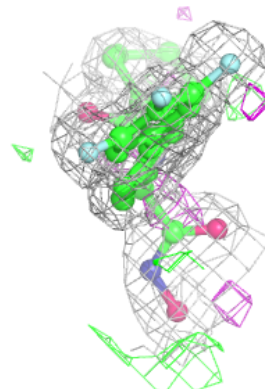
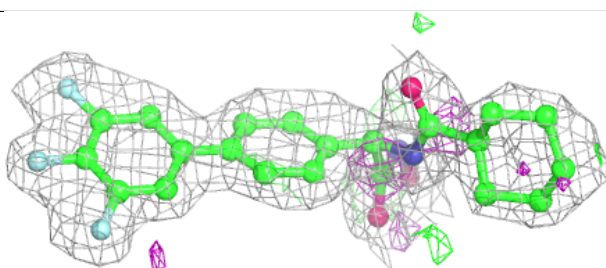
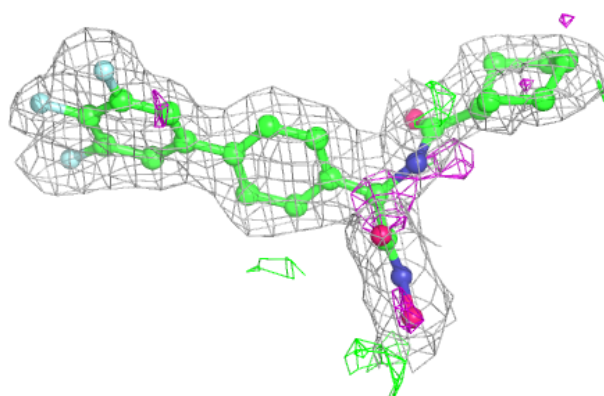


**Electron density around J1V D 703:**

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

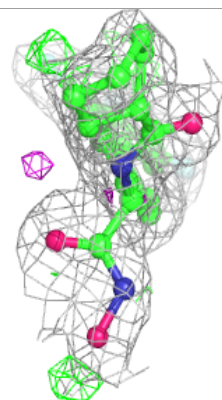
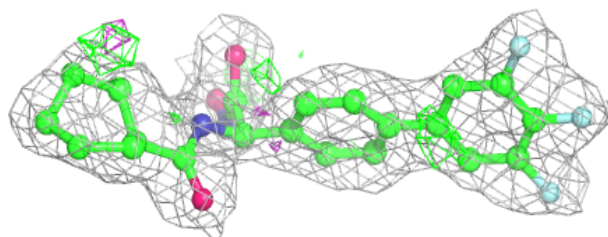
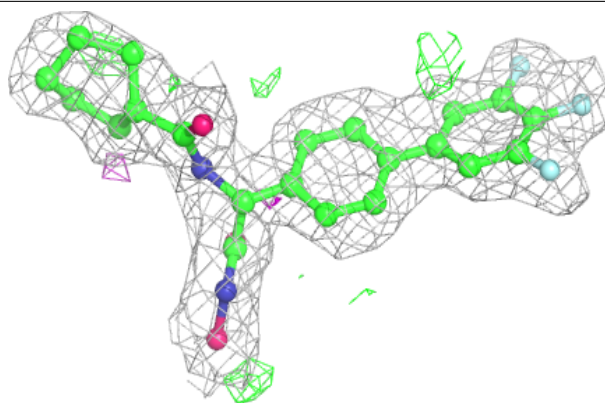
**Electron density around J1V F 703:**

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

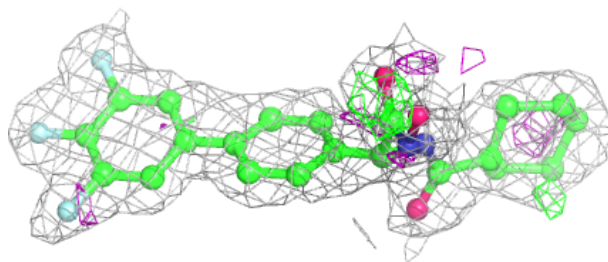
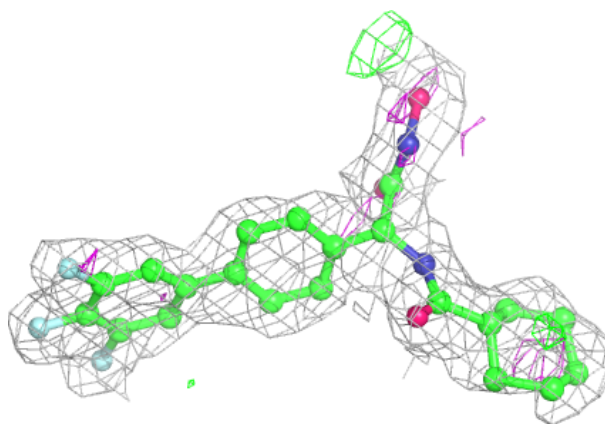


**Electron density around J1V C 703:**

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

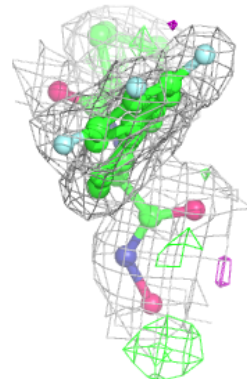
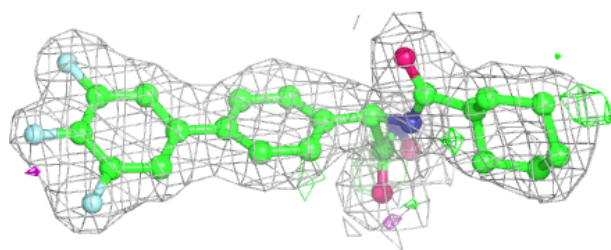
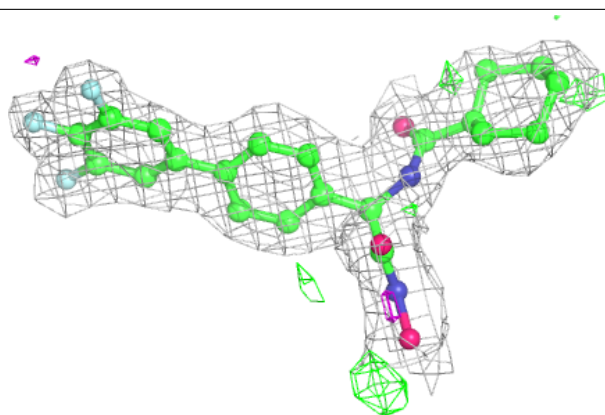
**Electron density around J1V J 703:**

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

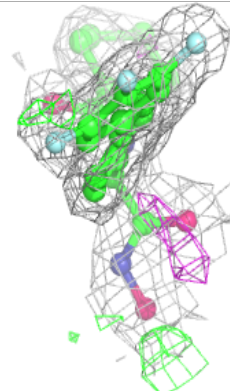
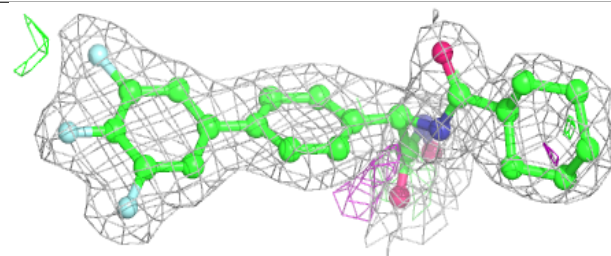
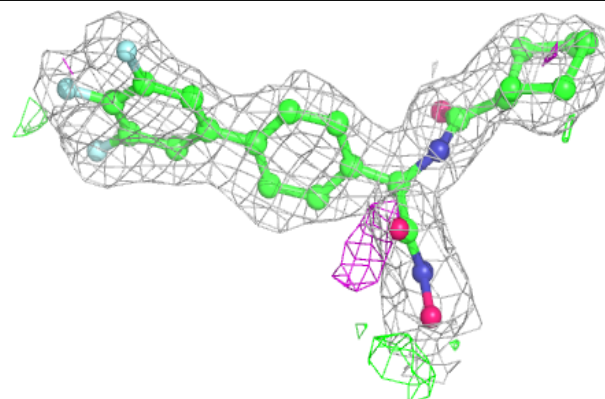


**Electron density around J1V A 703:**

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

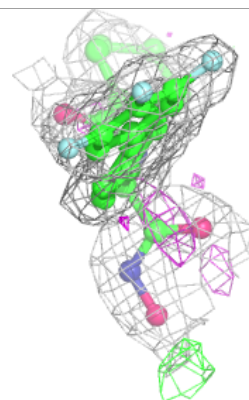
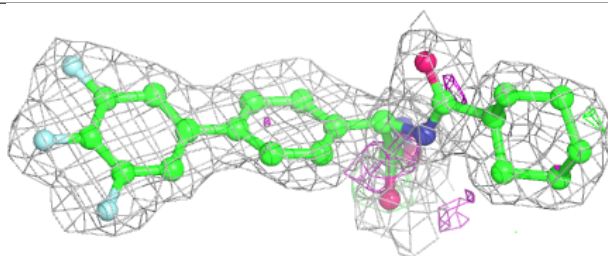
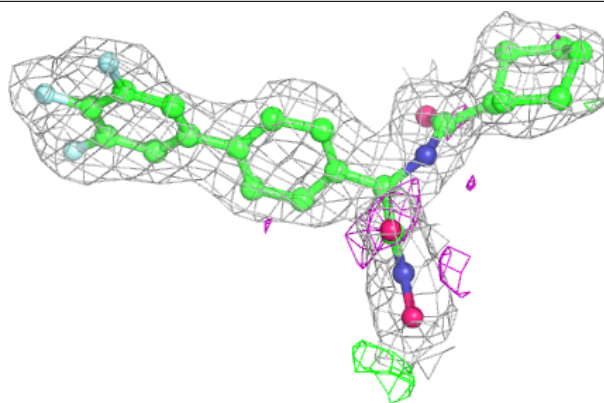
**Electron density around J1V B 703:**

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

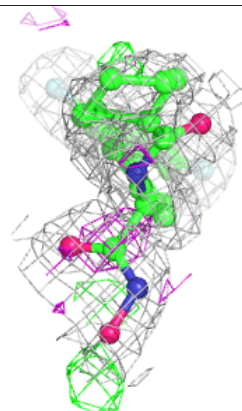
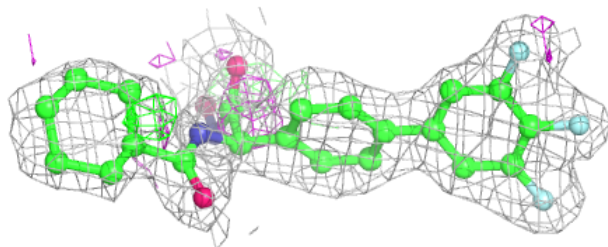
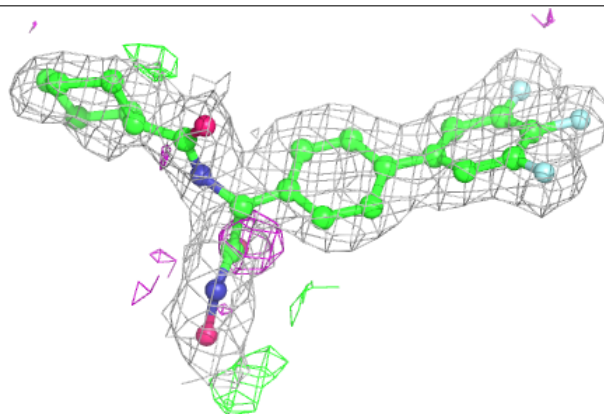


**Electron density around J1V H 703:**

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

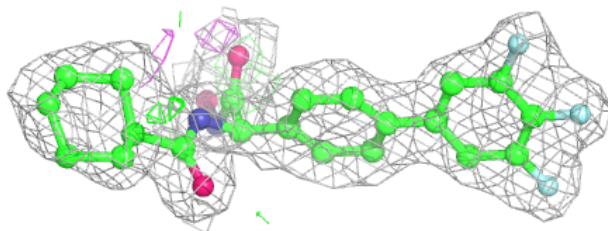
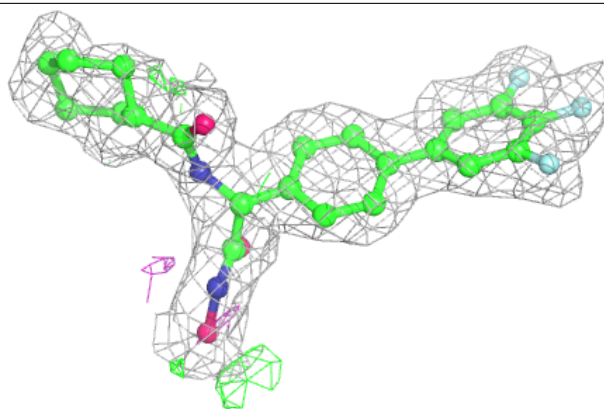
**Electron density around J1V L 704:**

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

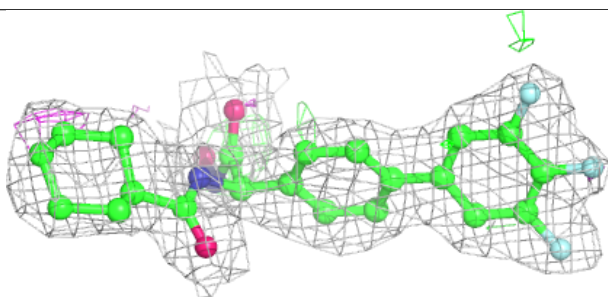
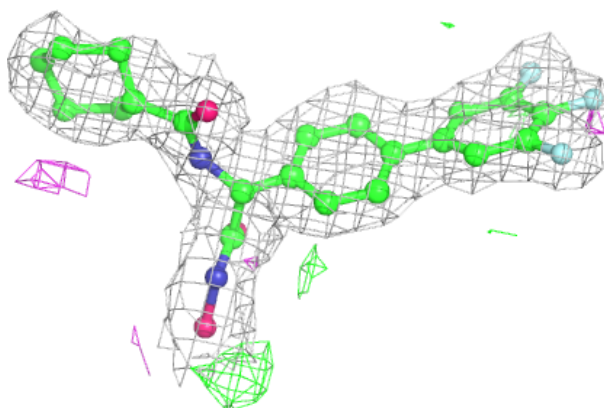


**Electron density around J1V I 703:**

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

**Electron density around J1V G 703:**

$2mF_o-DF_c$  (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.