wwPDB X-ray Structure Validation Summary Report (i)

Mar 3, 2024 – 10:32 PM EST

PDB ID	:	6EEE
Title	:	X-ray crystal structure of Pf-M17 in complex with inhibitor (6k) and regulatory zinc ion
Authors	:	Drinkwater, N.; McGowan, S.
Deposited on	:	2018-08-13
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

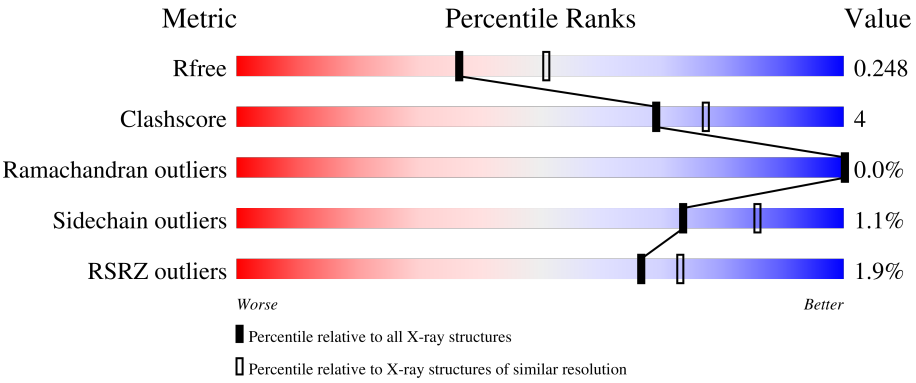
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	91% 8%
1	B	519	4% 89% 9%
1	C	519	92% 7%
1	D	519	2% 91% 9%
1	E	519	89% 9%

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Mol	Chain	Length	Quality of chain
1	F	519	2% 90% 8%
1	G	519	1% 91% 8%
1	H	519	7% 89% 10%
1	I	519	1% 91% 8%
1	J	519	1% 88% 11%
1	K	519	90% 9%
1	L	519	4% 87% 11%

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
7	1PE	D	1007	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 50000 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called M17 LEUCYL-AMINOPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	1	0
			3938	2525	634	760	19			
1	B	511	Total	C	N	O	S	0	0	0
			3859	2481	628	731	19			
1	C	518	Total	C	N	O	S	0	1	0
			3943	2537	639	748	19			
1	D	516	Total	C	N	O	S	0	1	0
			3933	2534	639	740	20			
1	E	510	Total	C	N	O	S	0	0	0
			3884	2504	626	735	19			
1	F	509	Total	C	N	O	S	0	0	0
			3847	2475	621	732	19			
1	G	517	Total	C	N	O	S	0	1	0
			3962	2544	637	761	20			
1	H	513	Total	C	N	O	S	0	1	0
			3865	2485	627	734	19			
1	I	518	Total	C	N	O	S	0	1	0
			3933	2526	638	750	19			
1	J	516	Total	C	N	O	S	0	1	0
			3951	2540	643	748	20			
1	K	510	Total	C	N	O	S	0	0	0
			3895	2508	628	740	19			
1	L	510	Total	C	N	O	S	0	0	0
			3831	2463	620	729	19			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
A	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
A	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
B	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
B	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6

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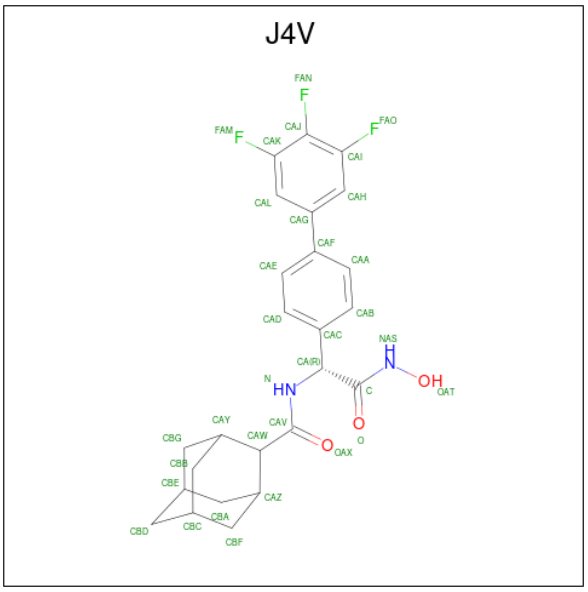
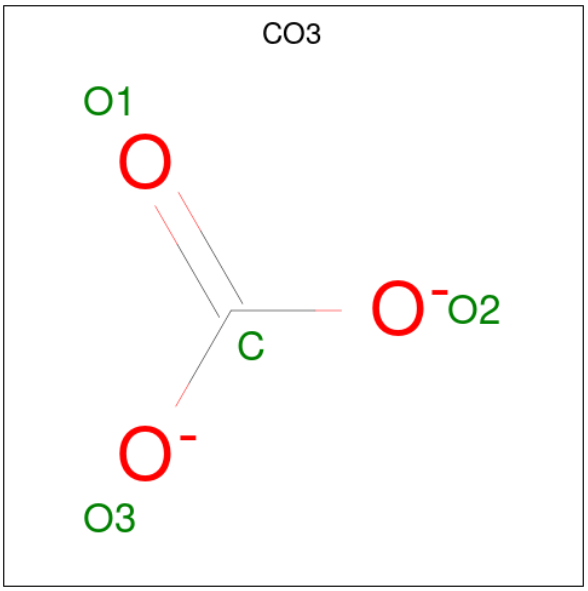
Chain	Residue	Modelled	Actual	Comment	Reference
B	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
C	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
C	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
C	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
D	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
D	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
D	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
E	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
E	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
E	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
F	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
F	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
F	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
G	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
G	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
G	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
H	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
H	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
H	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
I	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
I	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
I	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
J	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
J	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
J	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
K	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
K	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
K	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
L	152	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
L	515	GLN	ASN	engineered mutation	UNP A0A0L7KHE6
L	546	GLN	ASN	engineered mutation	UNP A0A0L7KHE6

- Molecule 2 is (1R,2r,3S,5R,7R)-N-[(1R)-2-(hydroxyamino)-2-oxo-1-(3',4',5'-trifluoro[1,1'-biphenyl]-4-yl)ethyl]tricyclo[3.3.1.1 3,7]decane-2-carboxamide (three-letter code: J4V) (formula: $C_{25}H_{25}F_3N_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			33	25	3	2	3		
2	B	1	Total	C	F	N	O	0	0
			33	25	3	2	3		
2	C	1	Total	C	F	N	O	0	0
			33	25	3	2	3		
2	D	1	Total	C	F	N	O	0	0
			33	25	3	2	3		
2	E	1	Total	C	F	N	O	0	0
			33	25	3	2	3		
2	F	1	Total	C	F	N	O	0	0
			33	25	3	2	3		
2	G	1	Total	C	F	N	O	0	0
			33	25	3	2	3		
2	H	1	Total	C	F	N	O	0	0
			33	25	3	2	3		
2	I	1	Total	C	F	N	O	0	0
			33	25	3	2	3		
2	J	1	Total	C	F	N	O	0	0
			33	25	3	2	3		
2	K	1	Total	C	F	N	O	0	0
			33	25	3	2	3		
2	L	1	Total	C	F	N	O	0	0
			33	25	3	2	3		

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).

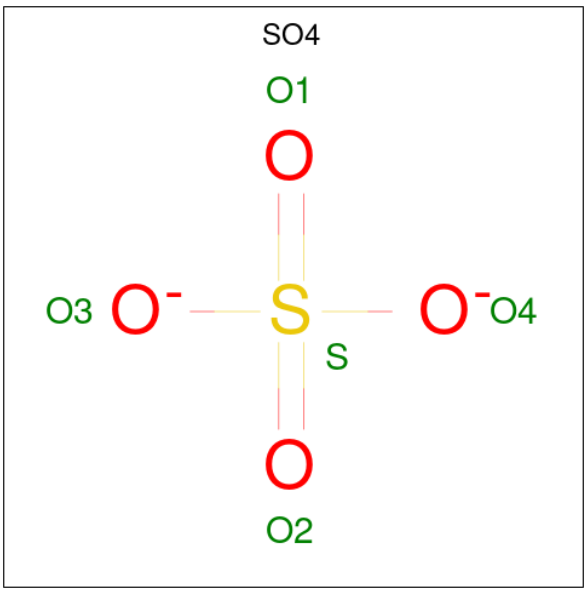


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 1 3	0	0
3	B	1	Total C O 4 1 3	0	0
3	C	1	Total C O 4 1 3	0	0
3	D	1	Total C O 4 1 3	0	0
3	E	1	Total C O 4 1 3	0	0
3	F	1	Total C O 4 1 3	0	0
3	G	1	Total C O 4 1 3	0	0
3	H	1	Total C O 4 1 3	0	0
3	I	1	Total C O 4 1 3	0	0
3	J	1	Total C O 4 1 3	0	0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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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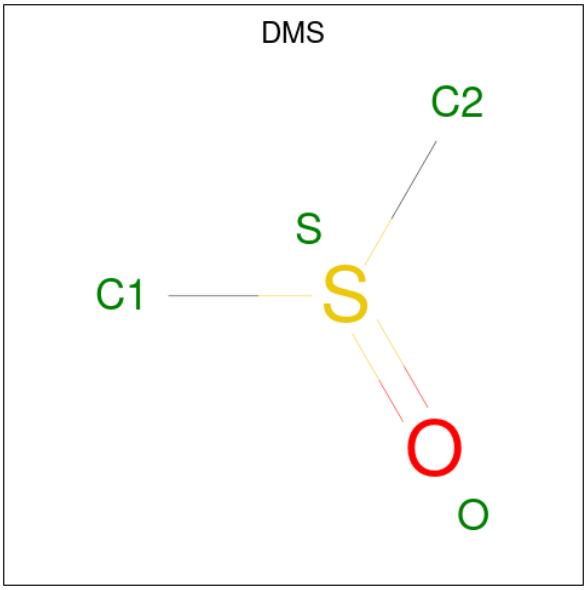
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total O S 5 4 1	0	0
5	J	1	Total O S 5 4 1	0	0
5	J	1	Total O S 5 4 1	0	0
5	K	1	Total O S 5 4 1	0	0
5	K	1	Total O S 5 4 1	0	0
5	K	1	Total O S 5 4 1	0	0
5	K	1	Total O S 5 4 1	0	0
5	L	1	Total O S 5 4 1	0	0
5	L	1	Total O S 5 4 1	0	0

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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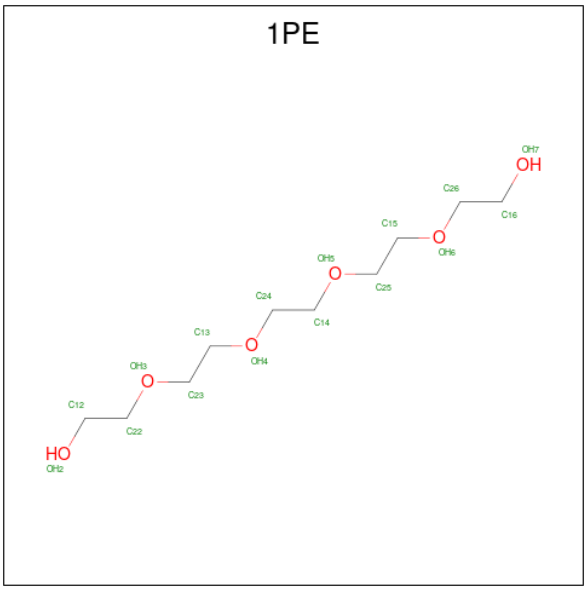
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O S 4 2 1 1	0	0
6	B	1	Total C O S 4 2 1 1	0	0
6	G	1	Total C O S 4 2 1 1	0	0
6	H	1	Total C O S 4 2 1 1	0	0

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 15 10 5	0	0
7	A	1	Total C O 12 8 4	0	0
7	B	1	Total C O 9 6 3	0	0
7	C	1	Total C O 15 10 5	0	0
7	C	1	Total C O 12 8 4	0	0
7	D	1	Total C O 12 8 4	0	0
7	D	1	Total C O 7 4 3	0	0

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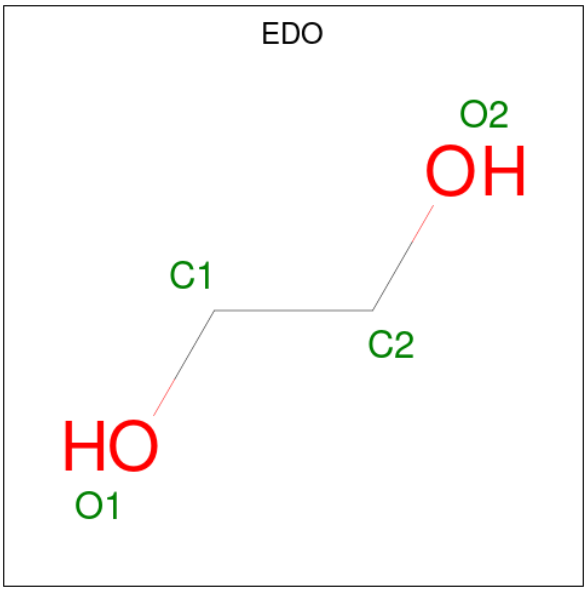
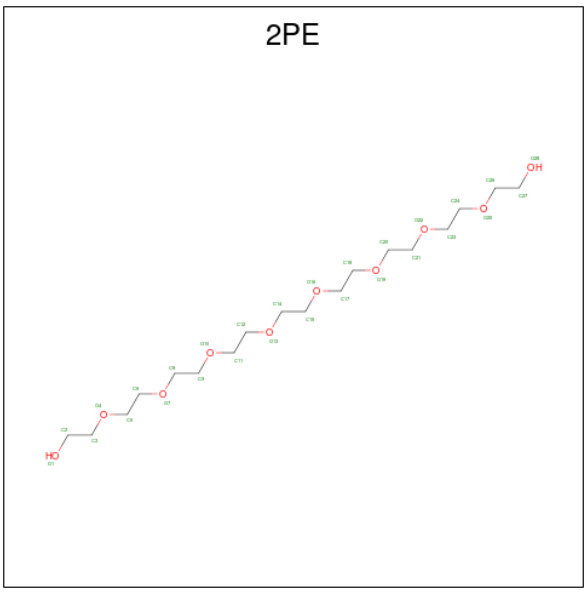
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C O 9 6 3	0	0
7	F	1	Total C O 9 6 3	0	0
7	G	1	Total C O 9 6 3	0	0
7	G	1	Total C O 9 6 3	0	0
7	H	1	Total C O 9 6 3	0	0
7	I	1	Total C O 12 8 4	0	0
7	I	1	Total C O 9 6 3	0	0
7	J	1	Total C O 9 6 3	0	0
7	J	1	Total C O 9 6 3	0	0
7	J	1	Total C O 13 9 4	0	0
7	K	1	Total C O 13 9 4	0	0
7	K	1	Total C O 15 10 5	0	0
7	L	1	Total C O 13 8 5	0	0
7	L	1	Total C O 12 8 4	0	0
7	L	1	Total C O 7 4 3	0	0
7	L	1	Total C O 5 3 2	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	1	Total C O 25 16 9	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	209	Total O 209 209	0	0
10	B	158	Total O 158 158	0	0
10	C	209	Total O 209 209	0	0
10	D	198	Total O 198 198	0	0
10	E	219	Total O 219 219	0	0
10	F	155	Total O 155 155	0	0
10	G	172	Total O 172 172	0	0
10	H	152	Total O 152 152	0	0
10	I	207	Total O 207 207	0	0
10	J	180	Total O 180 180	0	0

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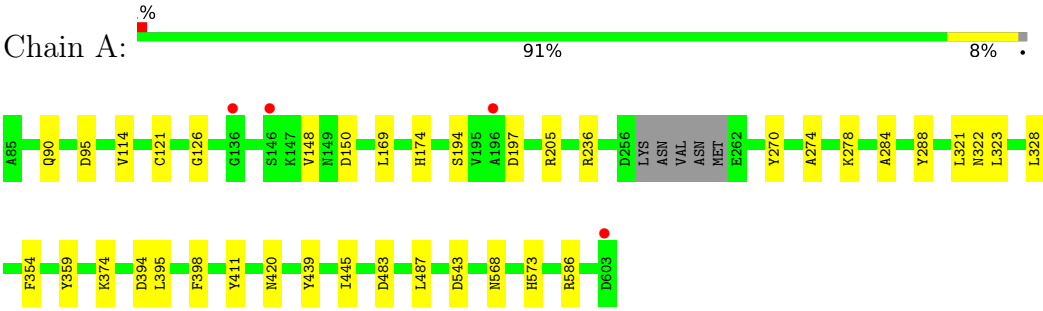
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	K	205	Total O 205 205	0	0
10	L	135	Total O 135 135	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

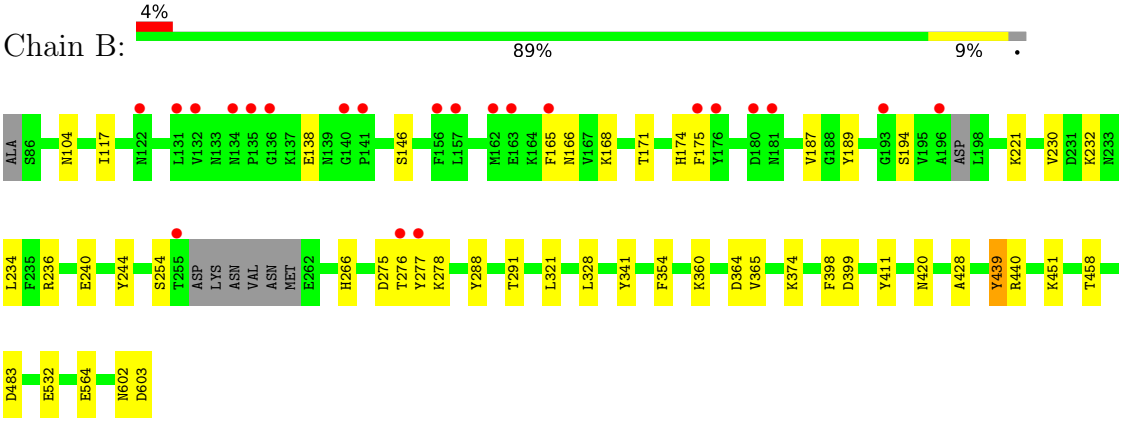
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE

Chain A:



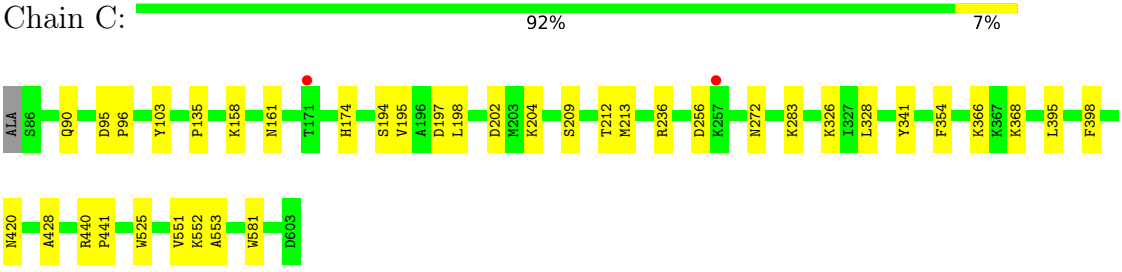
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE

Chain B:



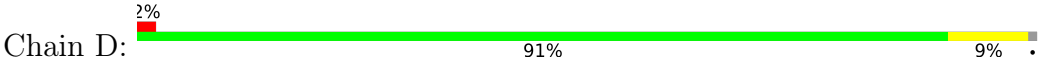
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE

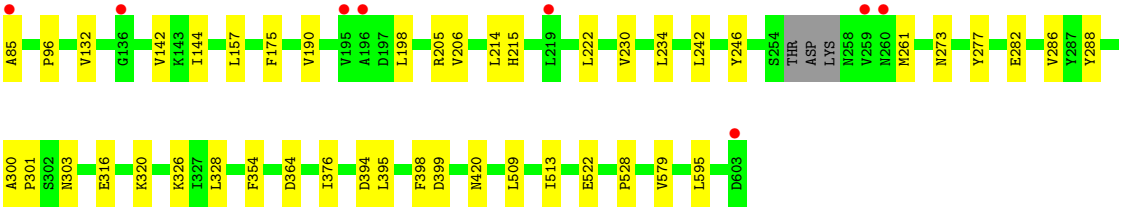
Chain C:



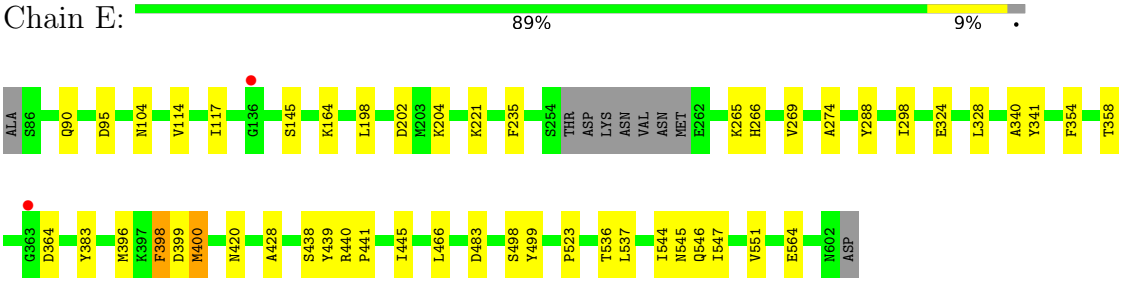
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE

Chain D:

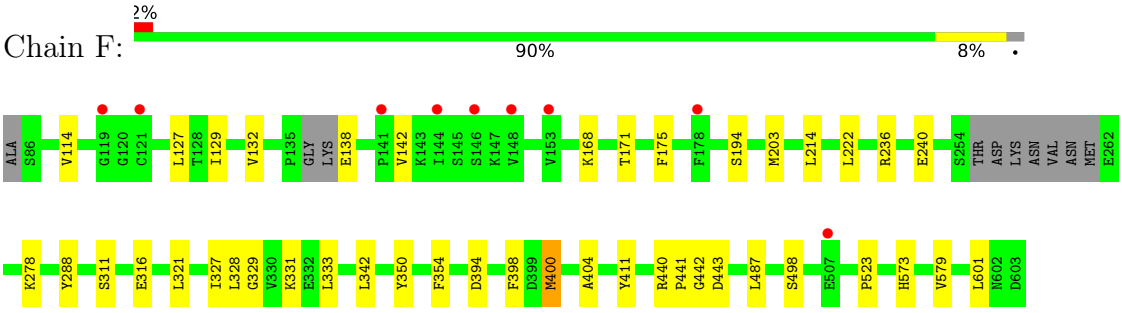




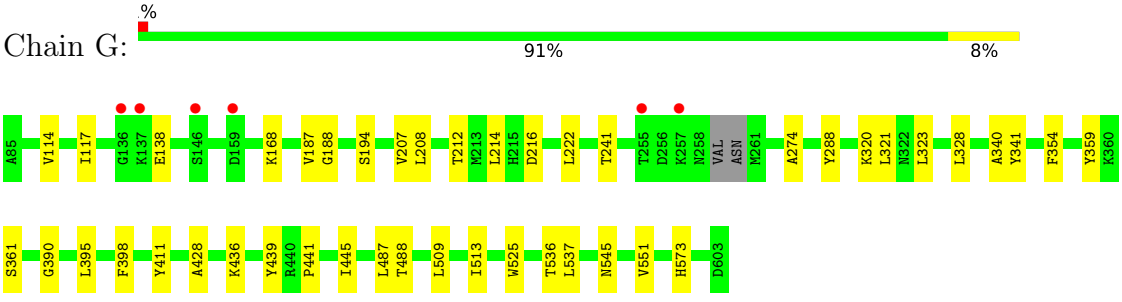
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE



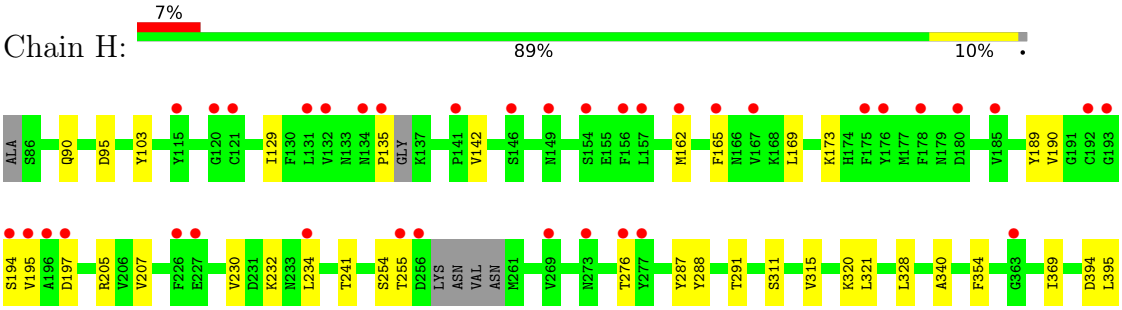
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE

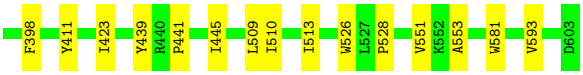


• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE



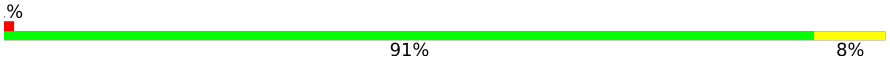
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE

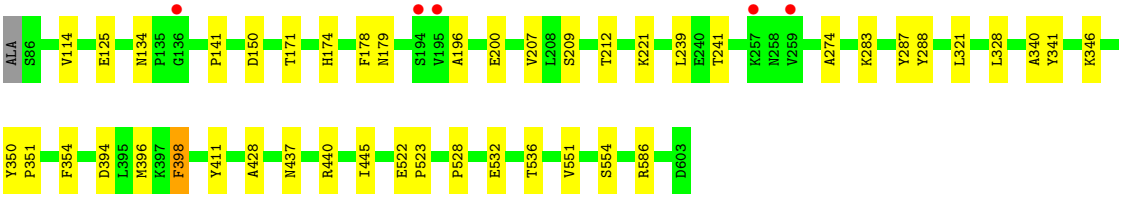




• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE

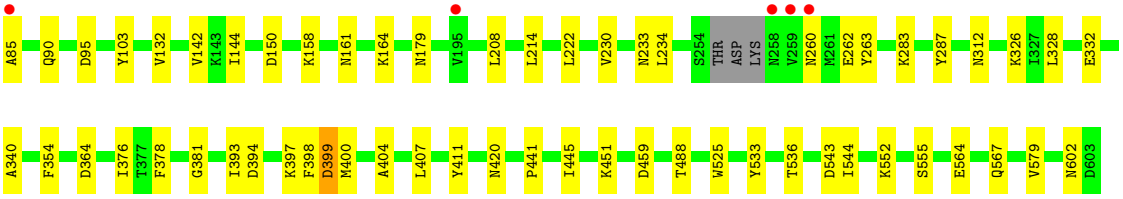
Chain I:





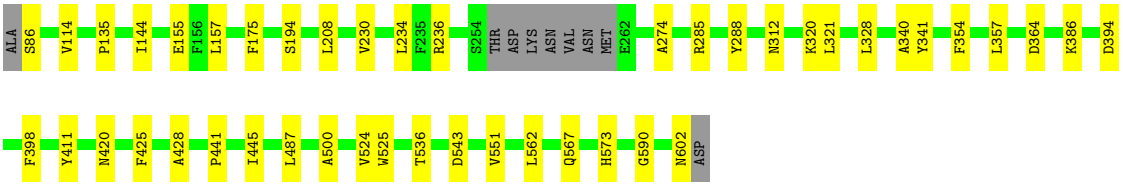
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE

Chain J:



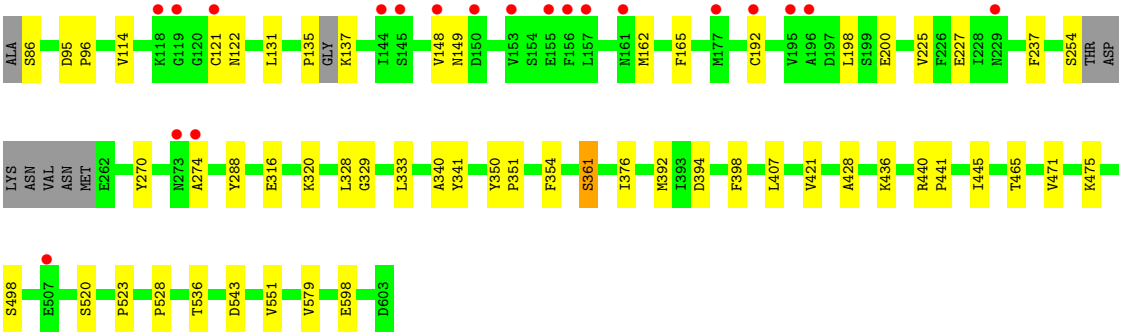
• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE

Chain K:



• Molecule 1: M17 LEUCYL-AMINOPEPTIDASE

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	173.68Å 177.40Å 229.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.30 48.19 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.17-2.30) 99.8 (48.19-2.30)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.193 , 0.246 0.198 , 0.248	Depositor DCC
R_{free} test set	15495 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.779	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	50000	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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 48.41 % 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 8.6342e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, 2PE, SO4, ZN, J4V, 1PE, CO3, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.41	0/4015	0.54	0/5450
1	B	0.39	0/3935	0.50	0/5346
1	C	0.41	0/4024	0.53	0/5463
1	D	0.41	0/4013	0.52	0/5443
1	E	0.43	0/3961	0.53	0/5376
1	F	0.39	0/3923	0.53	0/5332
1	G	0.40	0/4039	0.52	0/5478
1	H	0.40	0/3944	0.52	0/5363
1	I	0.41	0/4014	0.53	0/5452
1	J	0.43	0/4031	0.54	0/5466
1	K	0.42	0/3972	0.55	0/5390
1	L	0.37	0/3907	0.51	0/5313
All	All	0.41	0/47778	0.52	0/64872

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

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	3938	0	3854	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3859	0	3741	29	0
1	C	3943	0	3867	25	0
1	D	3933	0	3874	37	0
1	E	3884	0	3812	33	0
1	F	3847	0	3733	27	0
1	G	3962	0	3890	27	0
1	H	3865	0	3730	31	0
1	I	3933	0	3834	24	0
1	J	3951	0	3900	41	0
1	K	3895	0	3827	30	0
1	L	3831	0	3689	38	0
2	A	33	0	0	1	0
2	B	33	0	0	0	0
2	C	33	0	0	0	0
2	D	33	0	0	0	0
2	E	33	0	0	0	0
2	F	33	0	0	0	0
2	G	33	0	0	1	0
2	H	33	0	0	0	0
2	I	33	0	0	0	0
2	J	33	0	0	1	0
2	K	33	0	0	0	0
2	L	33	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
3	I	4	0	0	0	0
3	J	4	0	0	0	0
3	K	4	0	0	0	0
3	L	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	20	0	0	1	0
5	B	5	0	0	0	0
5	C	15	0	0	1	0
5	D	15	0	0	0	0
5	E	10	0	0	0	0
5	F	10	0	0	0	0
5	G	10	0	0	0	0
5	H	15	0	0	1	0
5	I	15	0	0	0	0
5	J	10	0	0	0	0
5	K	20	0	0	1	0
5	L	10	0	0	0	0
6	A	4	0	6	0	0
6	B	12	0	18	1	0
6	G	4	0	6	2	0
6	H	4	0	6	0	0
7	A	27	0	33	1	0
7	B	9	0	8	0	0
7	C	27	0	33	2	0
7	D	19	0	22	11	0
7	F	18	0	20	3	0
7	G	18	0	20	1	0
7	H	9	0	8	0	0
7	I	21	0	22	1	0
7	J	31	0	34	8	0
7	K	28	0	33	1	0
7	L	37	0	43	5	0
8	E	4	0	6	0	0
8	F	8	0	12	2	0
8	G	4	0	6	0	0
8	H	4	0	6	0	0
8	I	4	0	6	2	0
8	J	12	0	18	1	0
8	K	16	0	24	0	0
8	L	4	0	6	0	0
9	H	25	0	33	4	0
10	A	209	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	158	0	0	2	0
10	C	209	0	0	7	0
10	D	198	0	0	2	0
10	E	219	0	0	3	0
10	F	155	0	0	1	0
10	G	172	0	0	3	0
10	H	152	0	0	0	0
10	I	207	0	0	2	0
10	J	180	0	0	3	0
10	K	205	0	0	4	0
10	L	135	0	0	3	0
All	All	50000	0	46180	345	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 345 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)
2:J:1001:J4V:NAS	2:J:1001:J4V:OAT	1.58	1.33
1:E:298:ILE:HA	1:E:400:MET:HE2	1.38	1.04
1:E:298:ILE:HA	1:E:400:MET:CE	1.89	1.03
1:E:298:ILE:HG12	1:E:400:MET:HE1	1.43	0.97
1:J:451:LYS:HG2	7:J:1011:1PE:H131	1.48	0.95

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	510/519 (98%)	495 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	505/519 (97%)	491 (97%)	14 (3%)	0	100	100
1	C	517/519 (100%)	503 (97%)	14 (3%)	0	100	100
1	D	513/519 (99%)	499 (97%)	14 (3%)	0	100	100
1	E	506/519 (98%)	491 (97%)	15 (3%)	0	100	100
1	F	503/519 (97%)	487 (97%)	16 (3%)	0	100	100
1	G	513/519 (99%)	496 (97%)	17 (3%)	0	100	100
1	H	508/519 (98%)	496 (98%)	12 (2%)	0	100	100
1	I	517/519 (100%)	510 (99%)	6 (1%)	1 (0%)	47	58
1	J	513/519 (99%)	505 (98%)	8 (2%)	0	100	100
1	K	506/519 (98%)	496 (98%)	9 (2%)	1 (0%)	47	58
1	L	504/519 (97%)	493 (98%)	11 (2%)	0	100	100
All	All	6115/6228 (98%)	5962 (98%)	151 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	386	LYS
1	I	196	ALA

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	423/447 (95%)	417 (99%)	6 (1%)	67	81
1	B	402/447 (90%)	397 (99%)	5 (1%)	71	84
1	C	417/447 (93%)	416 (100%)	1 (0%)	93	97
1	D	415/447 (93%)	411 (99%)	4 (1%)	76	87
1	E	410/447 (92%)	402 (98%)	8 (2%)	55	72
1	F	404/447 (90%)	398 (98%)	6 (2%)	65	79
1	G	424/447 (95%)	420 (99%)	4 (1%)	78	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	402/447 (90%)	399 (99%)	3 (1%)	84 92
1	I	415/447 (93%)	409 (99%)	6 (1%)	67 81
1	J	422/447 (94%)	418 (99%)	4 (1%)	78 89
1	K	414/447 (93%)	411 (99%)	3 (1%)	84 92
1	L	398/447 (89%)	393 (99%)	5 (1%)	69 82
All	All	4946/5364 (92%)	4891 (99%)	55 (1%)	73 86

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	579	VAL
1	H	398	PHE
1	L	579	VAL
1	K	602	ASN
1	F	601	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	420	ASN
1	K	273	ASN
1	K	420	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 111 ligands modelled in this entry, 12 are monoatomic - leaving 99 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	$\#\|Z\| > 2$
7	1PE	G	1008	-	8,8,15	0.57	0	7,7,14	0.40	0
2	J4V	C	1001	4	37,37,37	1.90	8 (21%)	51,55,55	2.52	9 (17%)
7	1PE	L	1007	-	12,12,15	0.56	0	11,11,14	0.54	0
2	J4V	D	1001	4	37,37,37	2.16	8 (21%)	51,55,55	2.34	6 (11%)
2	J4V	F	1001	4	37,37,37	2.30	11 (29%)	51,55,55	2.40	7 (13%)
5	SO4	C	1005	-	4,4,4	0.12	0	6,6,6	0.22	0
5	SO4	H	1006	-	4,4,4	0.11	0	6,6,6	0.16	0
5	SO4	L	1005	-	4,4,4	0.18	0	6,6,6	0.19	0
5	SO4	D	1005	-	4,4,4	0.15	0	6,6,6	0.16	0
5	SO4	E	1004	-	4,4,4	0.16	0	6,6,6	0.13	0
7	1PE	L	1010	-	4,4,15	0.45	0	3,3,14	0.35	0
2	J4V	J	1001	4	37,37,37	2.29	8 (21%)	51,55,55	2.27	7 (13%)
5	SO4	K	1006	-	4,4,4	0.10	0	6,6,6	0.20	0
5	SO4	I	1004	-	4,4,4	0.13	0	6,6,6	0.22	0
5	SO4	E	1005	-	4,4,4	0.13	0	6,6,6	0.20	0
3	CO3	K	1002	-	2,3,3	0.44	0	2,3,3	0.74	0
8	EDO	K	1010	-	3,3,3	0.51	0	2,2,2	0.44	0
5	SO4	H	1004	-	4,4,4	0.18	0	6,6,6	0.36	0
8	EDO	K	1008	-	3,3,3	0.49	0	2,2,2	0.33	0
5	SO4	J	1004	-	4,4,4	0.11	0	6,6,6	0.11	0
7	1PE	C	1007	-	14,14,15	0.52	0	13,13,14	0.47	0
2	J4V	A	1001	4	37,37,37	2.09	9 (24%)	51,55,55	2.35	7 (13%)
3	CO3	L	1002	-	2,3,3	0.33	0	2,3,3	0.35	0
3	CO3	D	1002	-	2,3,3	0.51	0	2,3,3	0.53	0
8	EDO	H	1009	-	3,3,3	0.49	0	2,2,2	0.56	0
8	EDO	J	1007	-	3,3,3	0.51	0	2,2,2	0.11	0
7	1PE	G	1009	-	8,8,15	0.56	0	7,7,14	0.40	0
8	EDO	G	1007	-	3,3,3	0.57	0	2,2,2	0.08	0
6	DMS	B	1007	-	3,3,3	0.72	0	3,3,3	0.72	0
3	CO3	B	1002	-	2,3,3	0.59	0	2,3,3	0.58	0
7	1PE	J	1010	-	8,8,15	0.53	0	7,7,14	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	DMS	B	1005	-	3,3,3	0.61	0	3,3,3	0.92	0
5	SO4	F	1004	-	4,4,4	0.23	0	6,6,6	0.15	0
3	CO3	H	1002	-	2,3,3	0.40	0	2,3,3	0.04	0
8	EDO	I	1007	-	3,3,3	0.42	0	2,2,2	0.72	0
5	SO4	B	1004	-	4,4,4	0.10	0	6,6,6	0.16	0
7	1PE	A	1010	-	11,11,15	0.51	0	10,10,14	0.44	0
8	EDO	K	1009	-	3,3,3	0.58	0	2,2,2	0.26	0
5	SO4	K	1007	-	4,4,4	0.15	0	6,6,6	0.10	0
5	SO4	J	1005	-	4,4,4	0.14	0	6,6,6	0.25	0
5	SO4	D	1004	-	4,4,4	0.17	0	6,6,6	0.14	0
5	SO4	C	1004	-	4,4,4	0.11	0	6,6,6	0.24	0
5	SO4	C	1006	-	4,4,4	0.23	0	6,6,6	0.15	0
7	1PE	J	1011	-	12,12,15	0.55	0	11,11,14	0.43	0
3	CO3	J	1002	-	2,3,3	0.48	0	2,3,3	0.56	0
3	CO3	I	1002	-	2,3,3	0.31	0	2,3,3	0.19	0
5	SO4	A	1004	-	4,4,4	0.11	0	6,6,6	0.07	0
3	CO3	C	1002	-	2,3,3	0.26	0	2,3,3	0.41	0
5	SO4	F	1005	-	4,4,4	0.17	0	6,6,6	0.20	0
3	CO3	F	1002	-	2,3,3	0.37	0	2,3,3	0.65	0
5	SO4	A	1005	-	4,4,4	0.16	0	6,6,6	0.33	0
7	1PE	A	1009	-	14,14,15	0.55	0	13,13,14	0.45	0
7	1PE	B	1008	-	8,8,15	0.51	0	7,7,14	0.47	0
7	1PE	D	1007	-	11,11,15	0.54	0	10,10,14	0.42	0
7	1PE	I	1009	-	8,8,15	0.45	0	7,7,14	0.44	0
9	2PE	H	1007	-	24,24,27	0.55	0	23,23,26	0.30	0
2	J4V	G	1001	4	37,37,37	1.89	7 (18%)	51,55,55	2.37	7 (13%)
7	1PE	L	1009	-	6,6,15	0.48	0	5,5,14	0.43	0
7	1PE	L	1008	-	11,11,15	0.56	0	10,10,14	0.43	0
5	SO4	A	1006	-	4,4,4	0.26	0	6,6,6	0.18	0
7	1PE	D	1008	-	6,6,15	0.44	0	5,5,14	0.37	0
2	J4V	H	1001	4	37,37,37	2.30	8 (21%)	51,55,55	2.25	7 (13%)
6	DMS	G	1006	-	3,3,3	0.71	0	3,3,3	0.46	0
8	EDO	J	1006	-	3,3,3	0.50	0	2,2,2	0.20	0
6	DMS	A	1008	-	3,3,3	0.65	0	3,3,3	0.35	0
5	SO4	H	1005	-	4,4,4	0.16	0	6,6,6	0.21	0
7	1PE	J	1009	-	8,8,15	0.57	0	7,7,14	0.44	0
8	EDO	L	1006	-	3,3,3	0.42	0	2,2,2	0.46	0
7	1PE	I	1008	-	11,11,15	0.54	0	10,10,14	0.42	0
2	J4V	K	1001	4	37,37,37	2.06	5 (13%)	51,55,55	2.22	7 (13%)
8	EDO	F	1006	-	3,3,3	0.48	0	2,2,2	0.48	0
2	J4V	B	1001	4	37,37,37	1.88	6 (16%)	51,55,55	2.45	6 (11%)
5	SO4	G	1004	-	4,4,4	0.20	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	1PE	K	1013	-	14,14,15	0.56	0	13,13,14	0.45	0
2	J4V	I	1001	4	37,37,37	1.87	5 (13%)	51,55,55	2.36	6 (11%)
7	1PE	C	1008	-	11,11,15	0.57	0	10,10,14	0.45	0
2	J4V	L	1001	4	37,37,37	2.01	8 (21%)	51,55,55	2.39	6 (11%)
5	SO4	A	1007	-	4,4,4	0.21	0	6,6,6	0.19	0
8	EDO	J	1008	-	3,3,3	0.49	0	2,2,2	0.30	0
6	DMS	B	1006	-	3,3,3	0.76	0	3,3,3	0.65	0
5	SO4	L	1004	-	4,4,4	0.16	0	6,6,6	0.10	0
2	J4V	E	1001	4	37,37,37	2.10	8 (21%)	51,55,55	2.38	6 (11%)
5	SO4	G	1005	-	4,4,4	0.18	0	6,6,6	0.20	0
7	1PE	F	1009	-	8,8,15	0.58	0	7,7,14	0.42	0
8	EDO	E	1006	-	3,3,3	0.56	0	2,2,2	0.16	0
5	SO4	K	1004	-	4,4,4	0.13	0	6,6,6	0.22	0
3	CO3	G	1002	-	2,3,3	0.54	0	2,3,3	1.13	0
5	SO4	I	1006	-	4,4,4	0.16	0	6,6,6	0.18	0
7	1PE	F	1008	-	8,8,15	0.55	0	7,7,14	0.49	0
8	EDO	K	1011	-	3,3,3	0.50	0	2,2,2	0.24	0
3	CO3	A	1002	-	2,3,3	0.42	0	2,3,3	0.12	0
5	SO4	K	1005	-	4,4,4	0.17	0	6,6,6	0.24	0
5	SO4	D	1006	-	4,4,4	0.11	0	6,6,6	0.13	0
8	EDO	F	1007	-	3,3,3	0.48	0	2,2,2	0.30	0
6	DMS	H	1010	-	3,3,3	0.75	0	3,3,3	0.40	0
7	1PE	K	1012	-	12,12,15	0.54	0	11,11,14	0.34	0
7	1PE	H	1008	-	8,8,15	0.48	0	7,7,14	0.54	0
3	CO3	E	1002	-	2,3,3	0.34	0	2,3,3	0.29	0
5	SO4	I	1005	-	4,4,4	0.17	0	6,6,6	0.22	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
7	1PE	G	1008	-	-	2/6/6/13	-
2	J4V	C	1001	4	-	2/22/50/50	0/6/5/5
7	1PE	B	1008	-	-	4/6/6/13	-
7	1PE	D	1007	-	-	5/9/9/13	-
7	1PE	I	1009	-	-	3/6/6/13	-
2	J4V	L	1001	4	-	2/22/50/50	0/6/5/5
9	2PE	H	1007	-	-	7/22/22/25	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1PE	L	1007	-	-	4/10/10/13	-
2	J4V	D	1001	4	-	2/22/50/50	0/6/5/5
2	J4V	G	1001	4	-	2/22/50/50	0/6/5/5
2	J4V	F	1001	4	-	2/22/50/50	0/6/5/5
8	EDO	J	1008	-	-	1/1/1/1	-
7	1PE	J	1010	-	-	3/6/6/13	-
7	1PE	L	1009	-	-	2/4/4/13	-
2	J4V	E	1001	4	-	2/22/50/50	0/6/5/5
7	1PE	L	1010	-	-	1/2/2/13	-
7	1PE	F	1009	-	-	3/6/6/13	-
7	1PE	L	1008	-	-	3/9/9/13	-
8	EDO	E	1006	-	-	1/1/1/1	-
2	J4V	J	1001	4	-	0/22/50/50	0/6/5/5
7	1PE	D	1008	-	-	3/4/4/13	-
8	EDO	I	1007	-	-	0/1/1/1	-
7	1PE	F	1008	-	-	5/6/6/13	-
7	1PE	A	1010	-	-	5/9/9/13	-
8	EDO	K	1011	-	-	0/1/1/1	-
2	J4V	H	1001	4	-	0/22/50/50	0/6/5/5
8	EDO	K	1009	-	-	0/1/1/1	-
8	EDO	J	1006	-	-	0/1/1/1	-
8	EDO	K	1010	-	-	1/1/1/1	-
8	EDO	K	1008	-	-	0/1/1/1	-
7	1PE	C	1007	-	-	3/12/12/13	-
7	1PE	J	1009	-	-	3/6/6/13	-
7	1PE	J	1011	-	-	4/10/10/13	-
2	J4V	A	1001	4	-	3/22/50/50	0/6/5/5
8	EDO	L	1006	-	-	0/1/1/1	-
7	1PE	I	1008	-	-	8/9/9/13	-
2	J4V	K	1001	4	-	0/22/50/50	0/6/5/5
8	EDO	F	1006	-	-	1/1/1/1	-
8	EDO	H	1009	-	-	1/1/1/1	-
2	J4V	B	1001	4	-	2/22/50/50	0/6/5/5
8	EDO	J	1007	-	-	0/1/1/1	-
7	1PE	K	1012	-	-	7/10/10/13	-
7	1PE	K	1013	-	-	5/12/12/13	-
7	1PE	H	1008	-	-	4/6/6/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	J4V	I	1001	4	-	2/22/50/50	0/6/5/5
7	1PE	G	1009	-	-	5/6/6/13	-
8	EDO	F	1007	-	-	0/1/1/1	-
8	EDO	G	1007	-	-	0/1/1/1	-
7	1PE	C	1008	-	-	6/9/9/13	-
7	1PE	A	1009	-	-	8/12/12/13	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1001	J4V	CAC-CA	-7.85	1.39	1.52
2	E	1001	J4V	CAC-CA	-7.84	1.39	1.52
2	L	1001	J4V	CAC-CA	-7.43	1.40	1.52
2	I	1001	J4V	CAC-CA	-7.35	1.40	1.52
2	B	1001	J4V	CAC-CA	-7.35	1.40	1.52

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1001	J4V	CAY-CBG-CBE	-8.61	94.88	110.17
2	B	1001	J4V	CAZ-CBA-CBE	-8.55	94.99	110.17
2	E	1001	J4V	CAY-CBG-CBE	-8.53	95.02	110.17
2	I	1001	J4V	CAY-CBG-CBE	-8.52	95.04	110.17
2	C	1001	J4V	CAZ-CBA-CBE	-8.51	95.05	110.17

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	J4V	OAX-CAV-CAW-CAZ
2	B	1001	J4V	N-CAV-CAW-CAZ
2	C	1001	J4V	N-CAV-CAW-CAZ
2	G	1001	J4V	N-CAV-CAW-CAZ
7	D	1007	1PE	C13-C23-OH3-C22

There are no ring outliers.

25 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	1007	1PE	2	0

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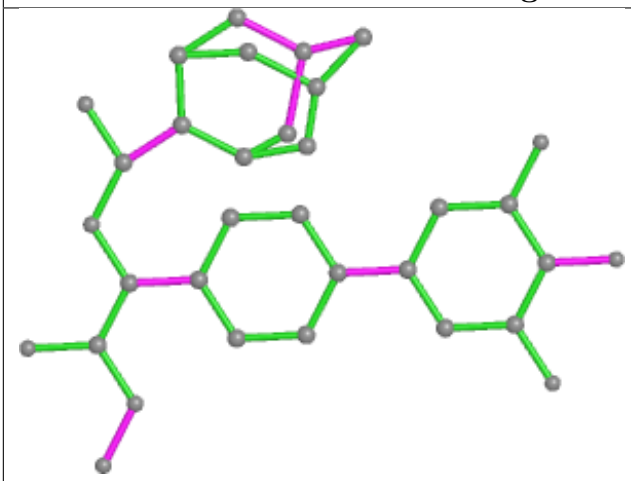
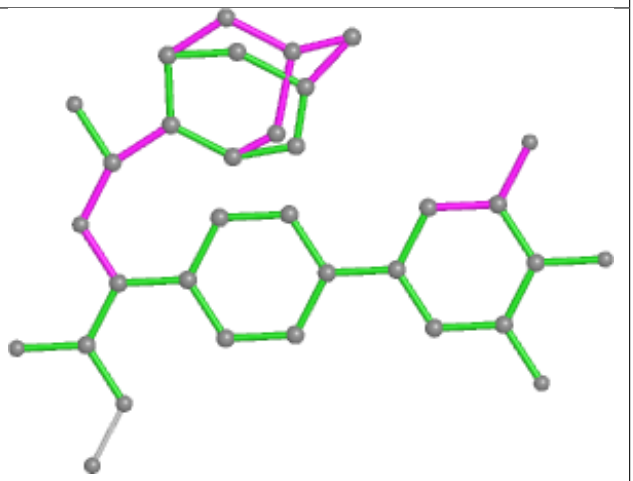
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1006	SO4	1	0
2	J	1001	J4V	1	0
7	C	1007	1PE	2	0
2	A	1001	J4V	1	0
8	J	1007	EDO	1	0
7	G	1009	1PE	1	0
6	B	1005	DMS	1	0
8	I	1007	EDO	2	0
7	A	1010	1PE	1	0
5	C	1004	SO4	1	0
7	J	1011	1PE	5	0
5	A	1005	SO4	1	0
7	D	1007	1PE	11	0
7	I	1009	1PE	1	0
9	H	1007	2PE	4	0
2	G	1001	J4V	1	0
7	L	1008	1PE	3	0
6	G	1006	DMS	2	0
7	J	1009	1PE	3	0
8	F	1006	EDO	2	0
7	F	1009	1PE	1	0
5	K	1004	SO4	1	0
7	F	1008	1PE	2	0
7	K	1012	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

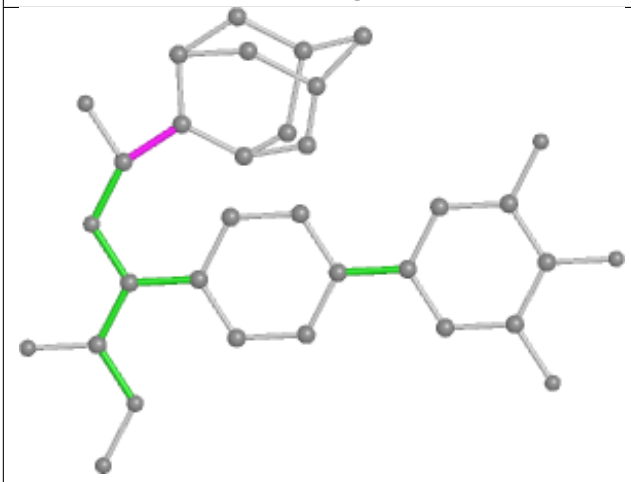
Ligand J4V C 1001



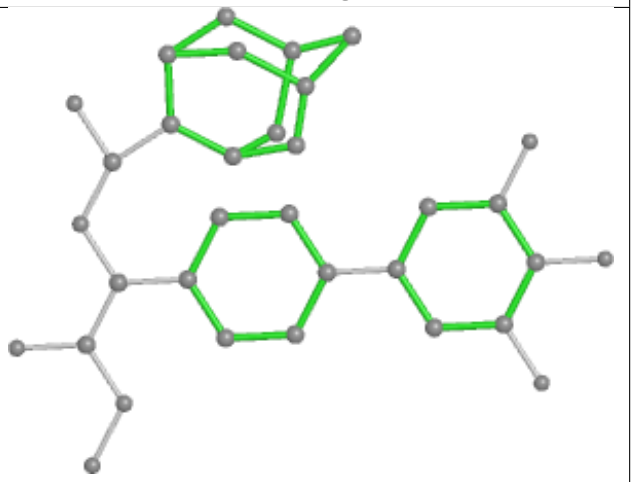
Bond lengths



Bond angles

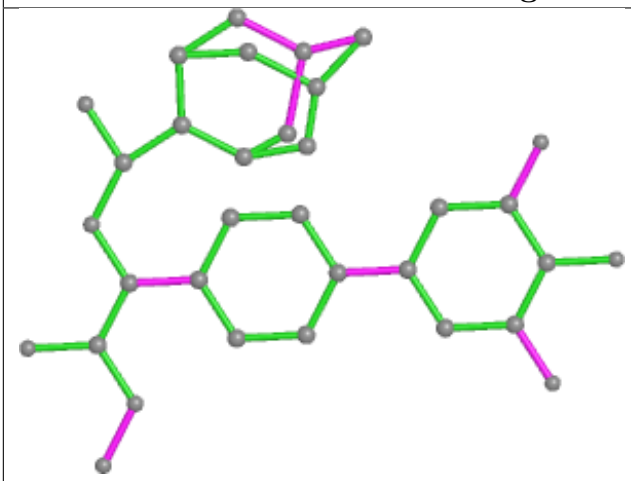


Torsions

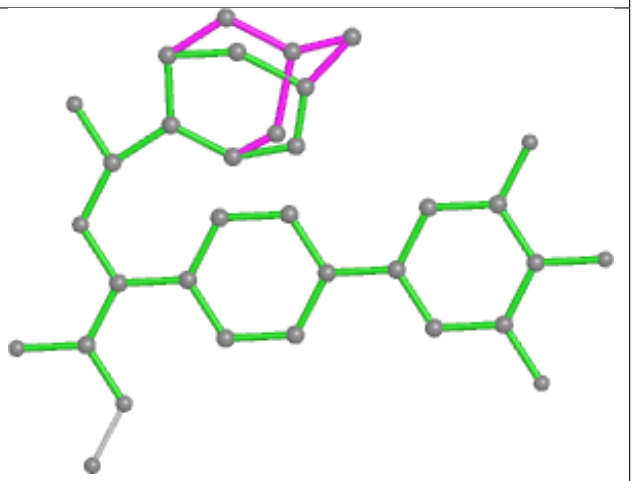


Rings

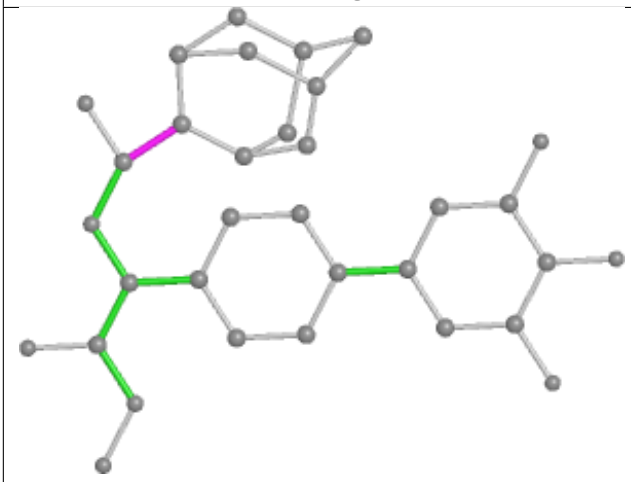
Ligand J4V D 1001



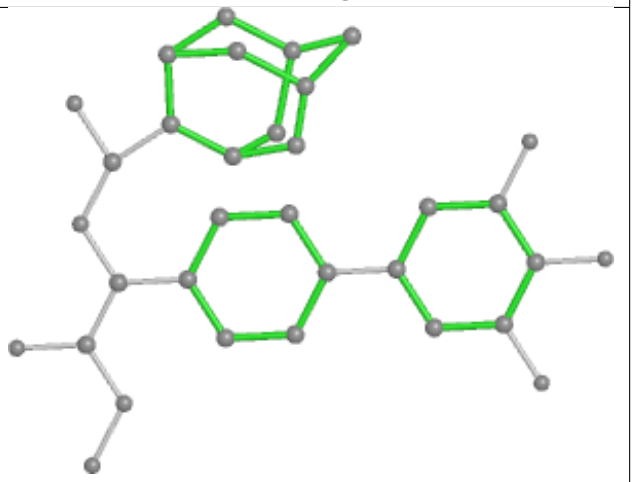
Bond lengths



Bond angles

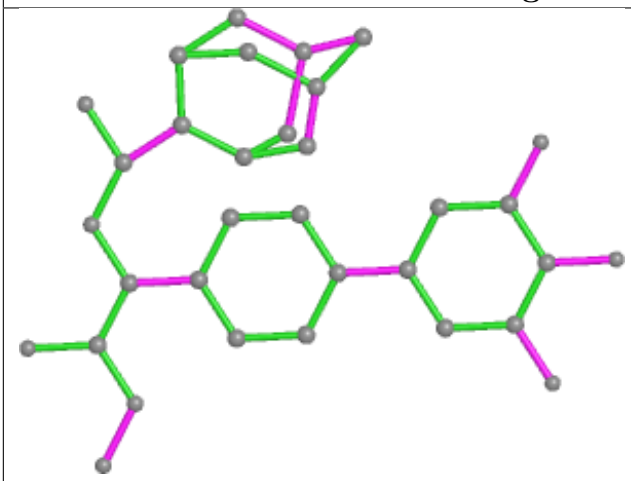


Torsions

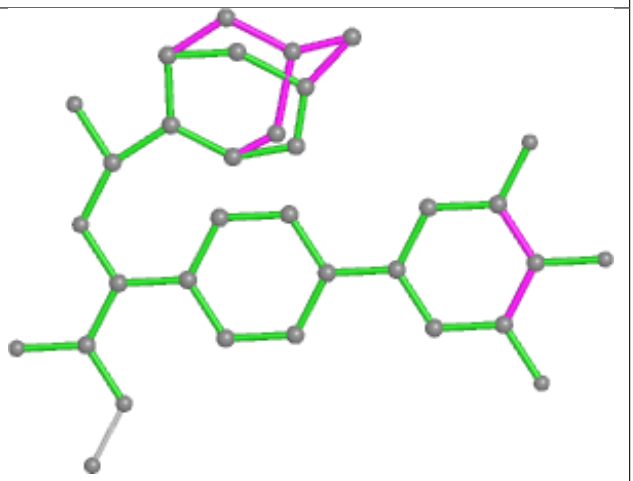


Rings

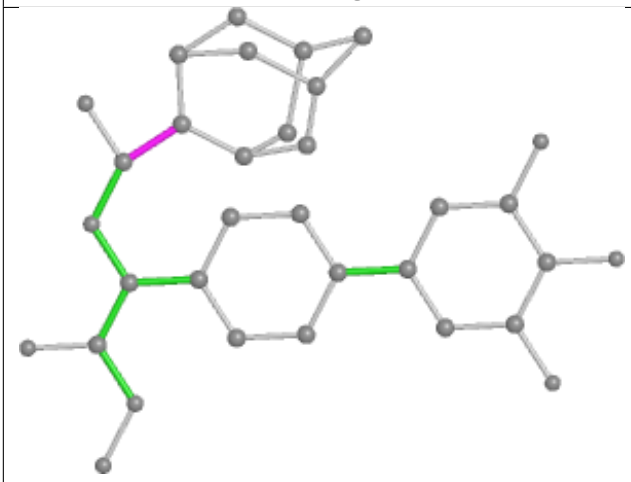
Ligand J4V F 1001



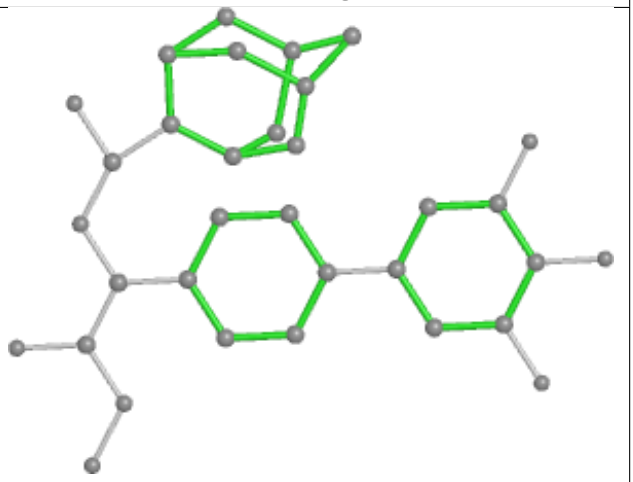
Bond lengths



Bond angles

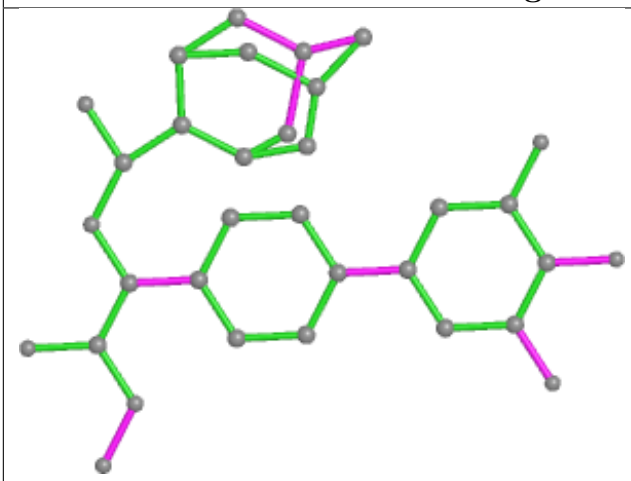


Torsions

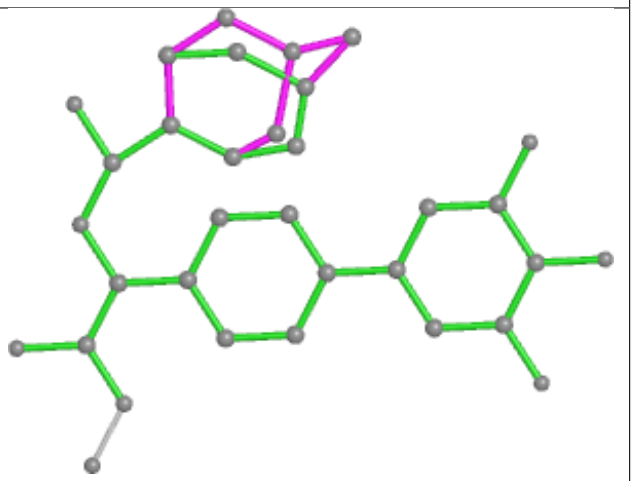


Rings

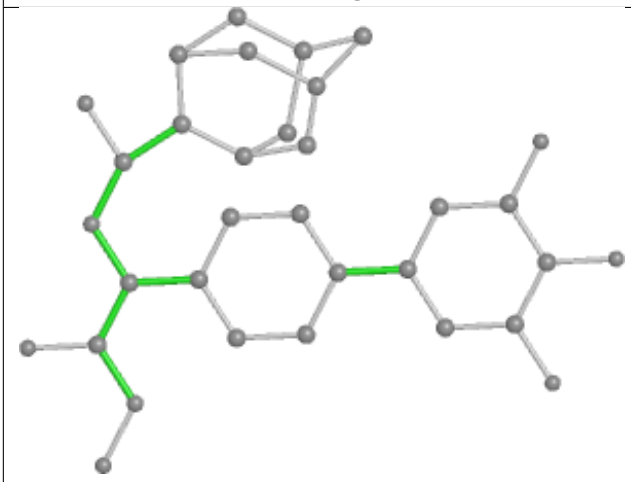
Ligand J4V J 1001



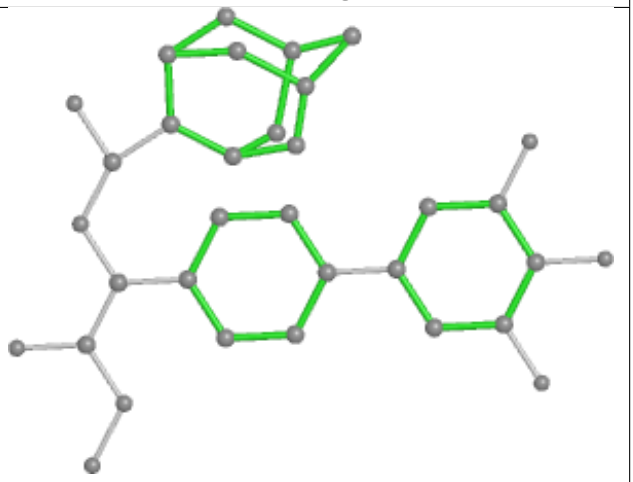
Bond lengths



Bond angles

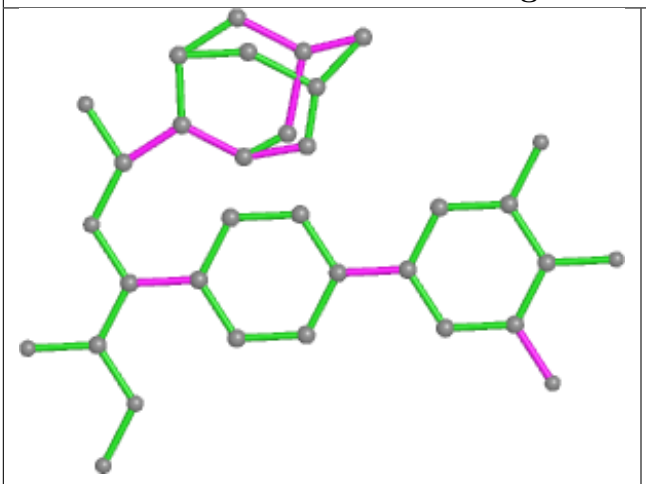


Torsions

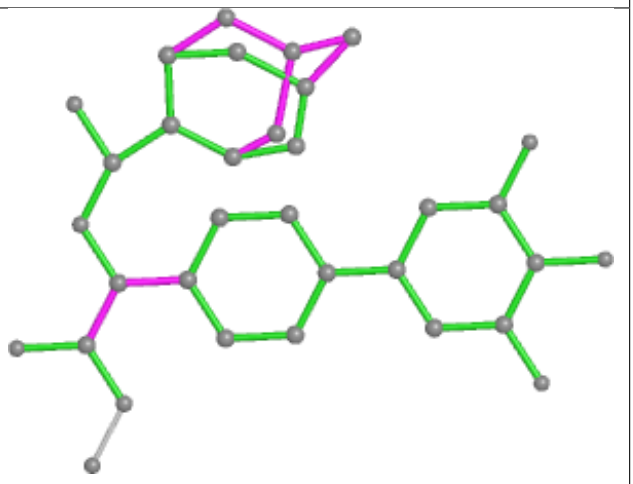


Rings

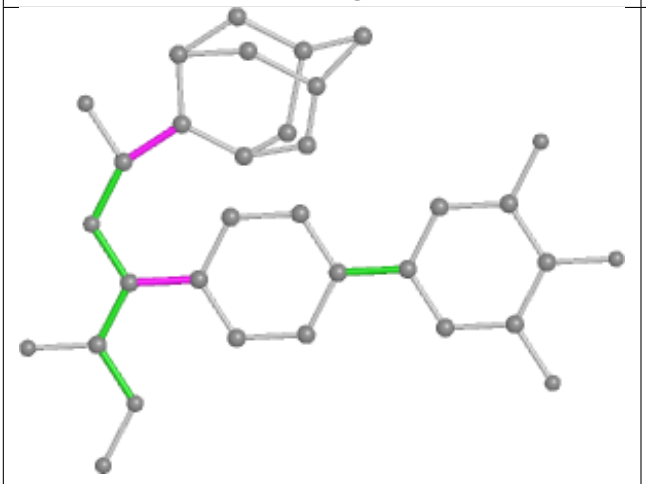
Ligand J4V A 1001



Bond lengths



Bond angles



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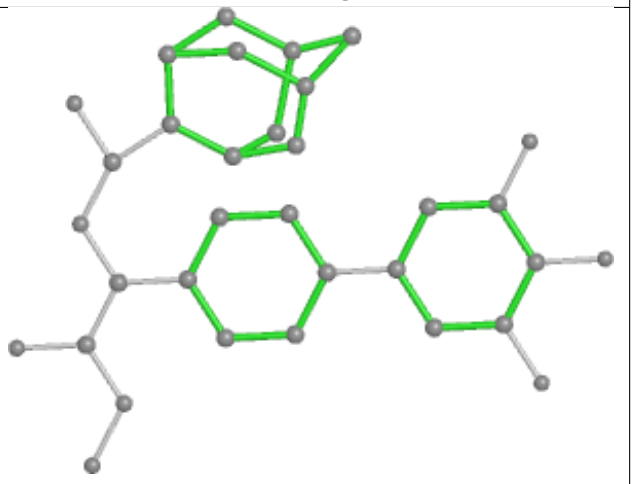
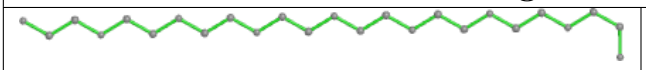
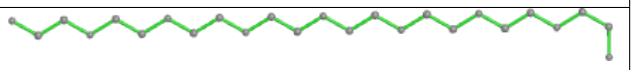


Rings

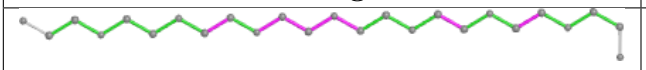
Ligand 2PE H 1007



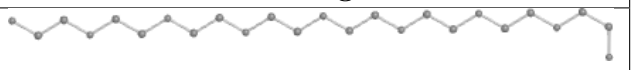
Bond lengths



Bond angles

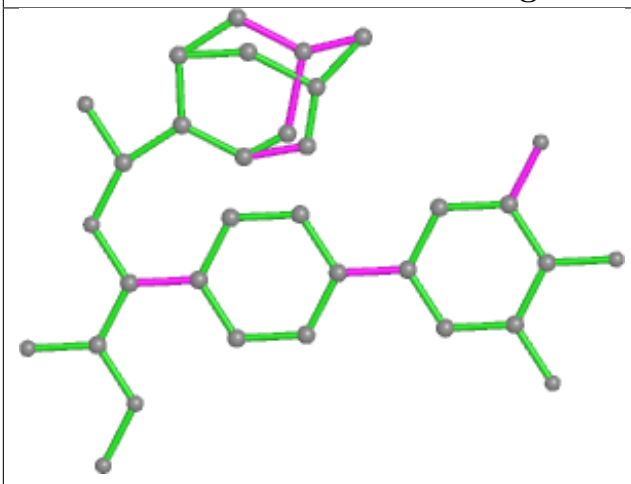


Torsions

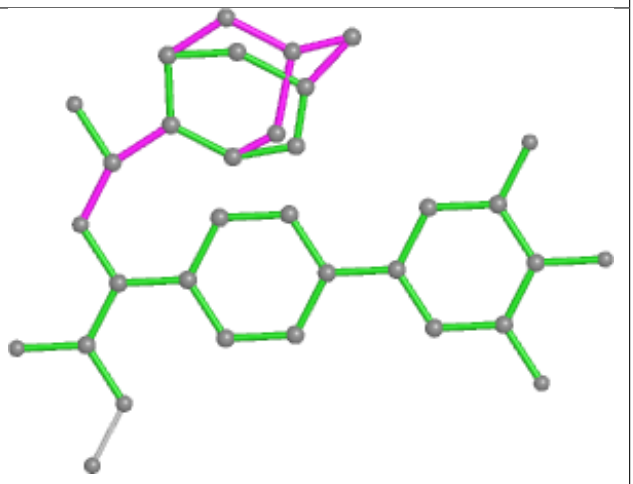


Rings

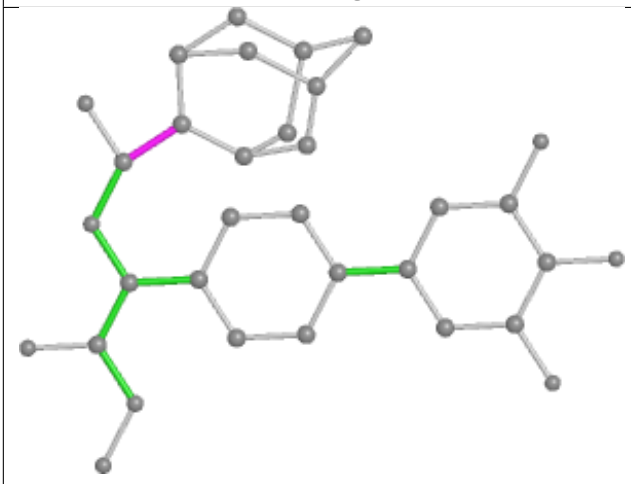
Ligand J4V G 1001



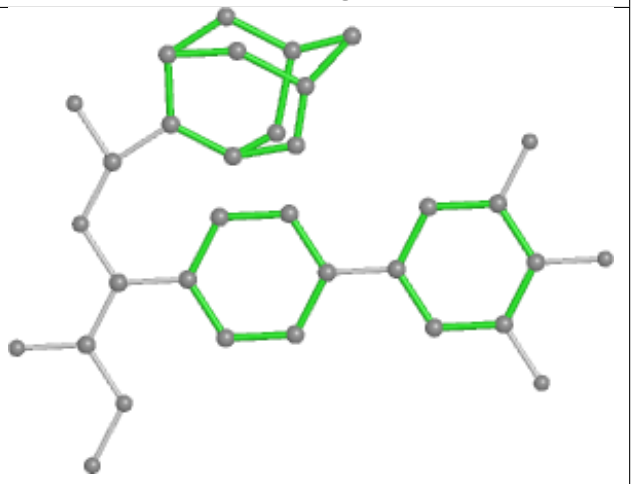
Bond lengths



Bond angles

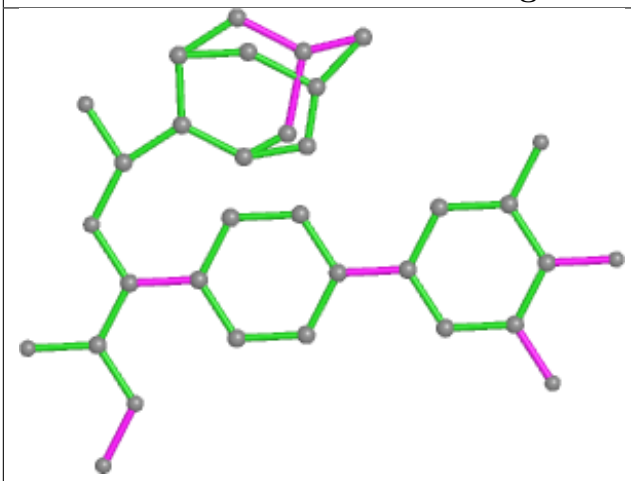


Torsions

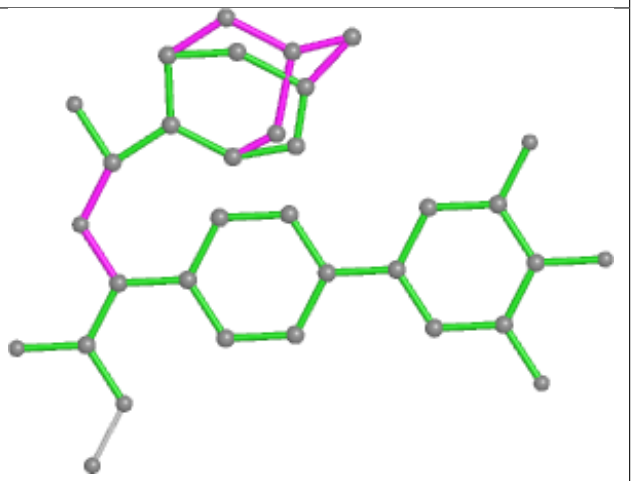


Rings

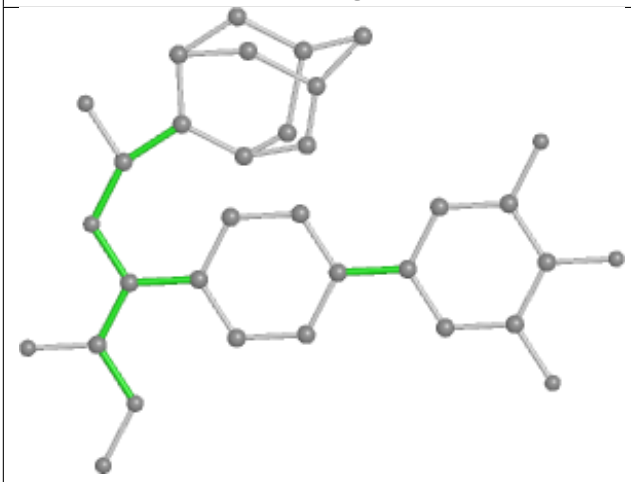
Ligand J4V H 1001



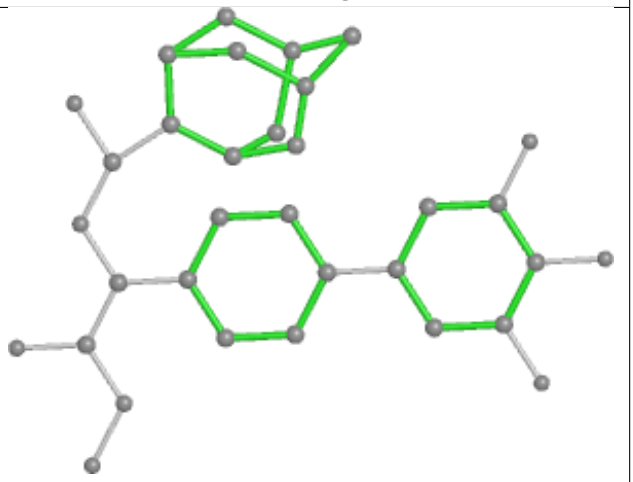
Bond lengths



Bond angles

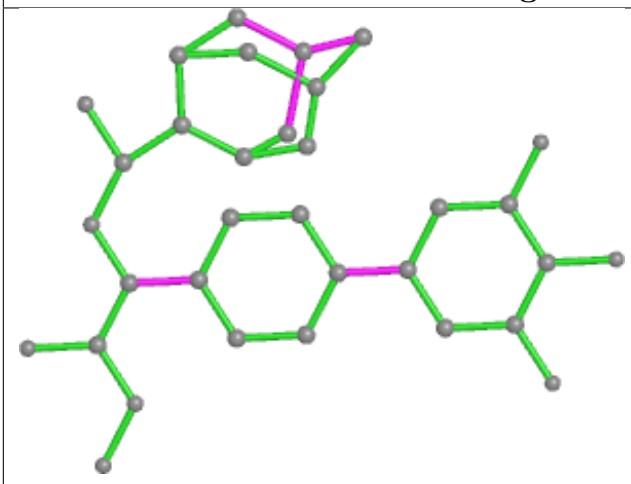


Torsions

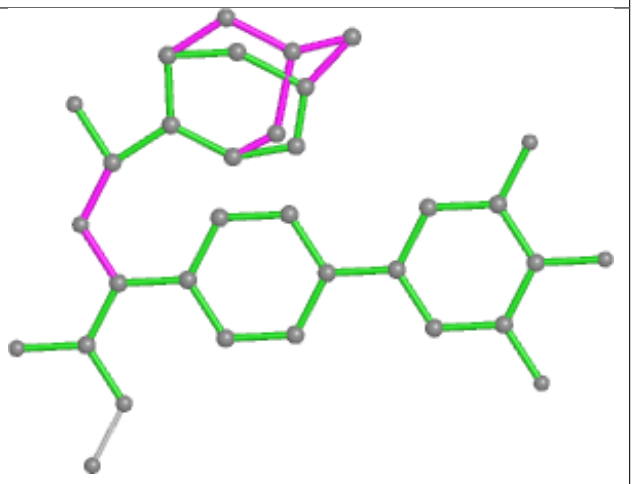


Rings

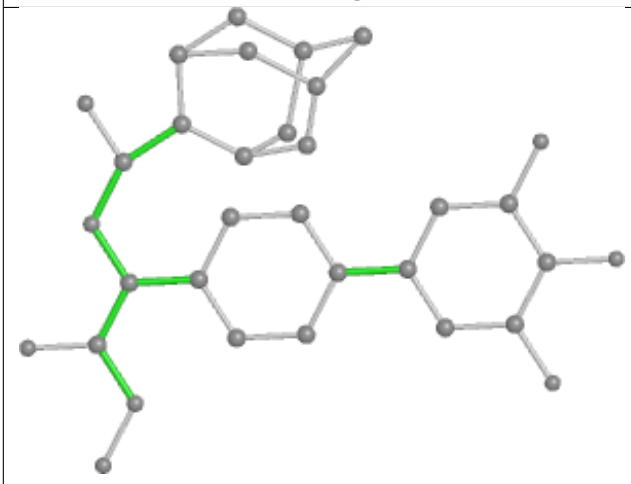
Ligand J4V K 1001



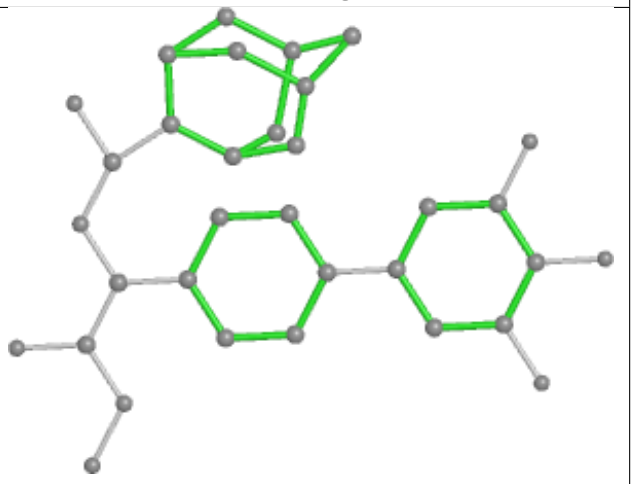
Bond lengths



Bond angles

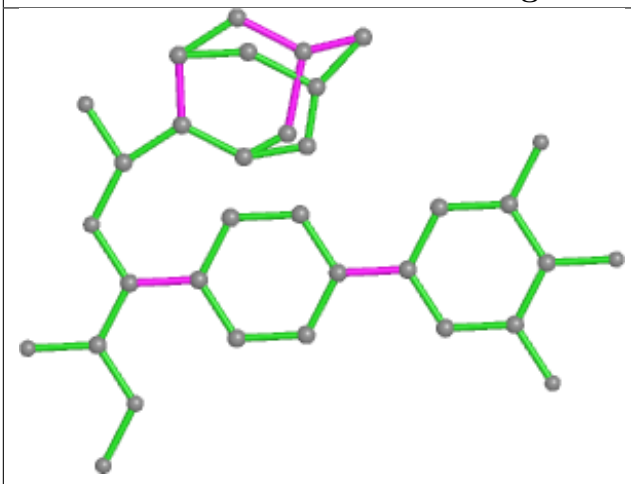


Torsions

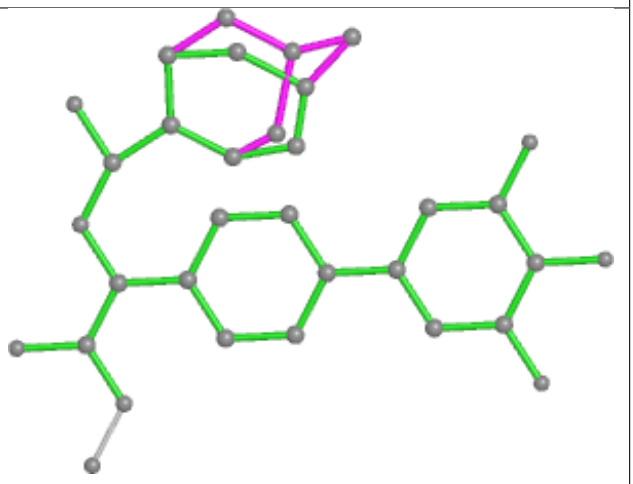


Rings

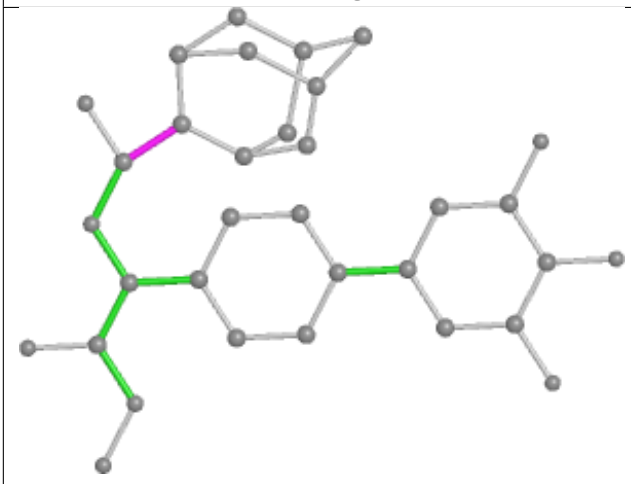
Ligand J4V B 1001



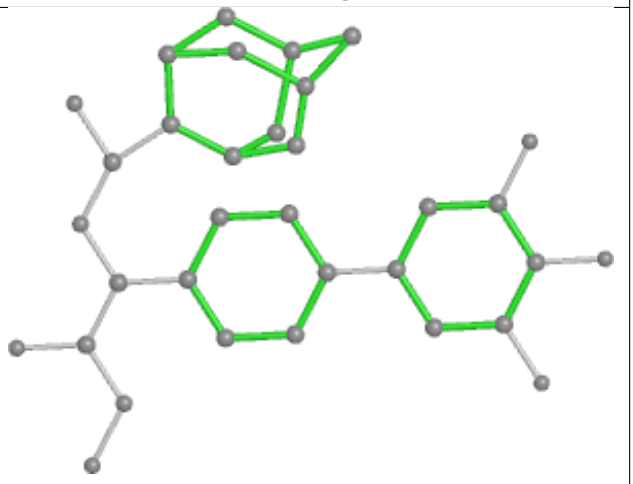
Bond lengths



Bond angles

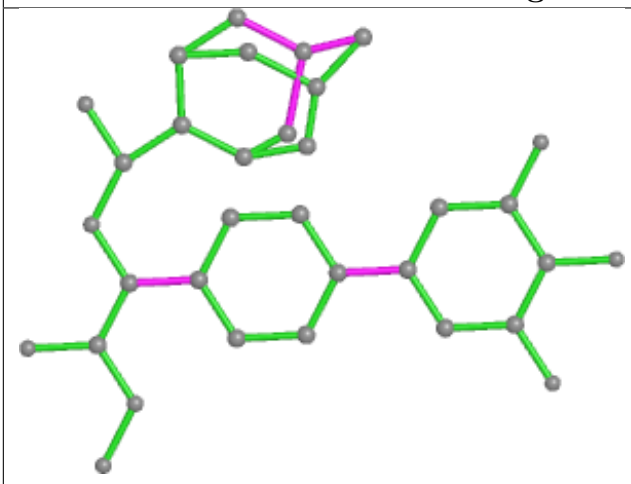


Torsions

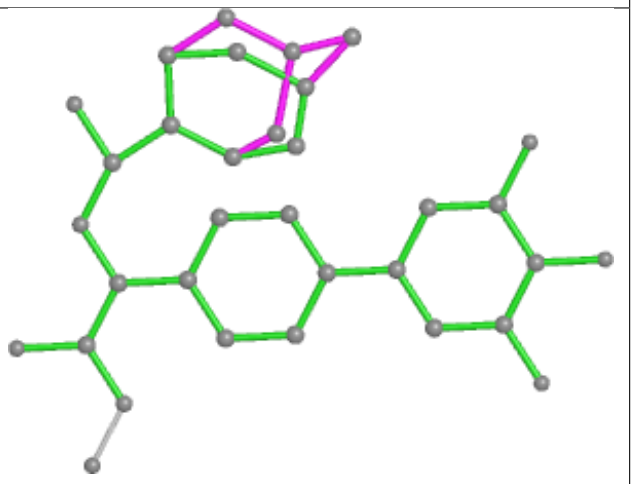


Rings

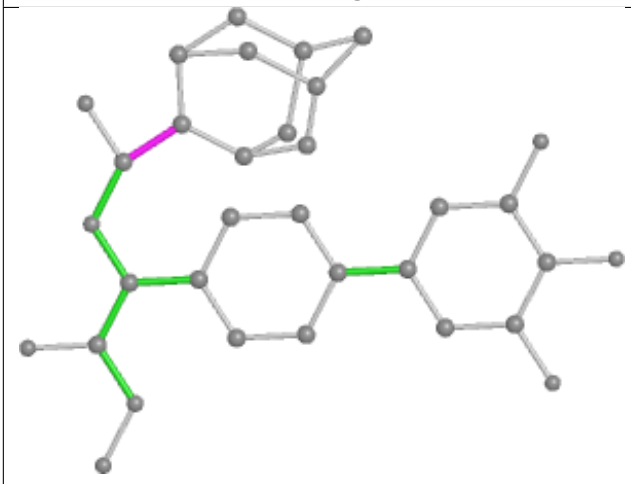
Ligand J4V I 1001



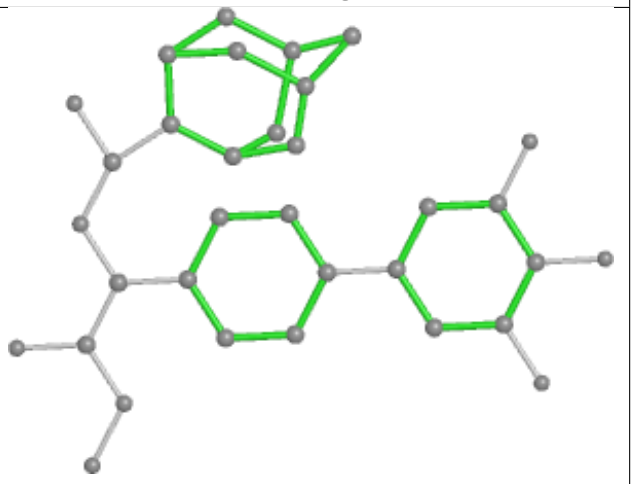
Bond lengths



Bond angles

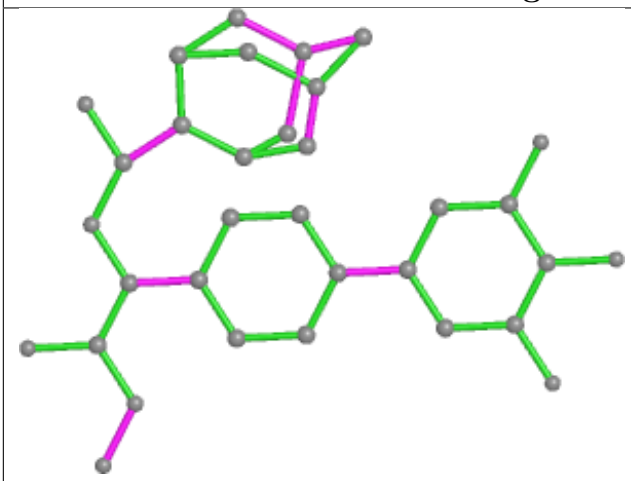


Torsions

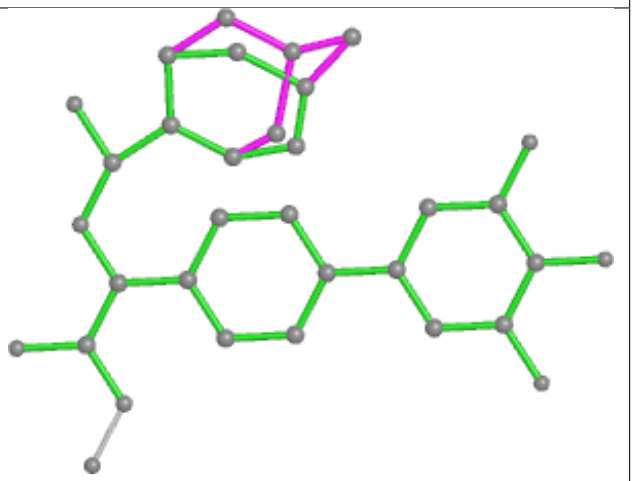


Rings

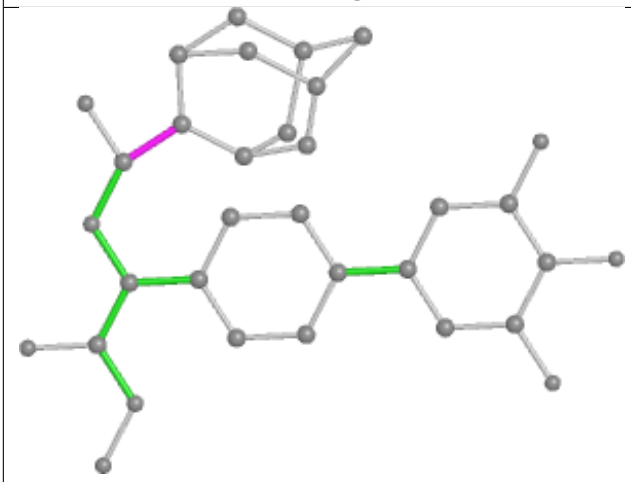
Ligand J4V L 1001



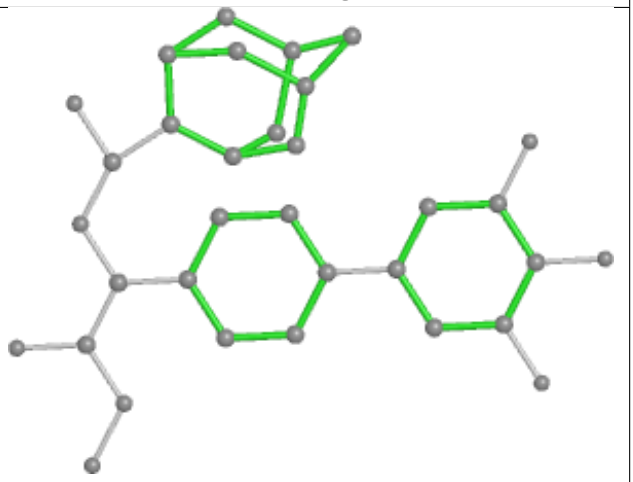
Bond lengths



Bond angles

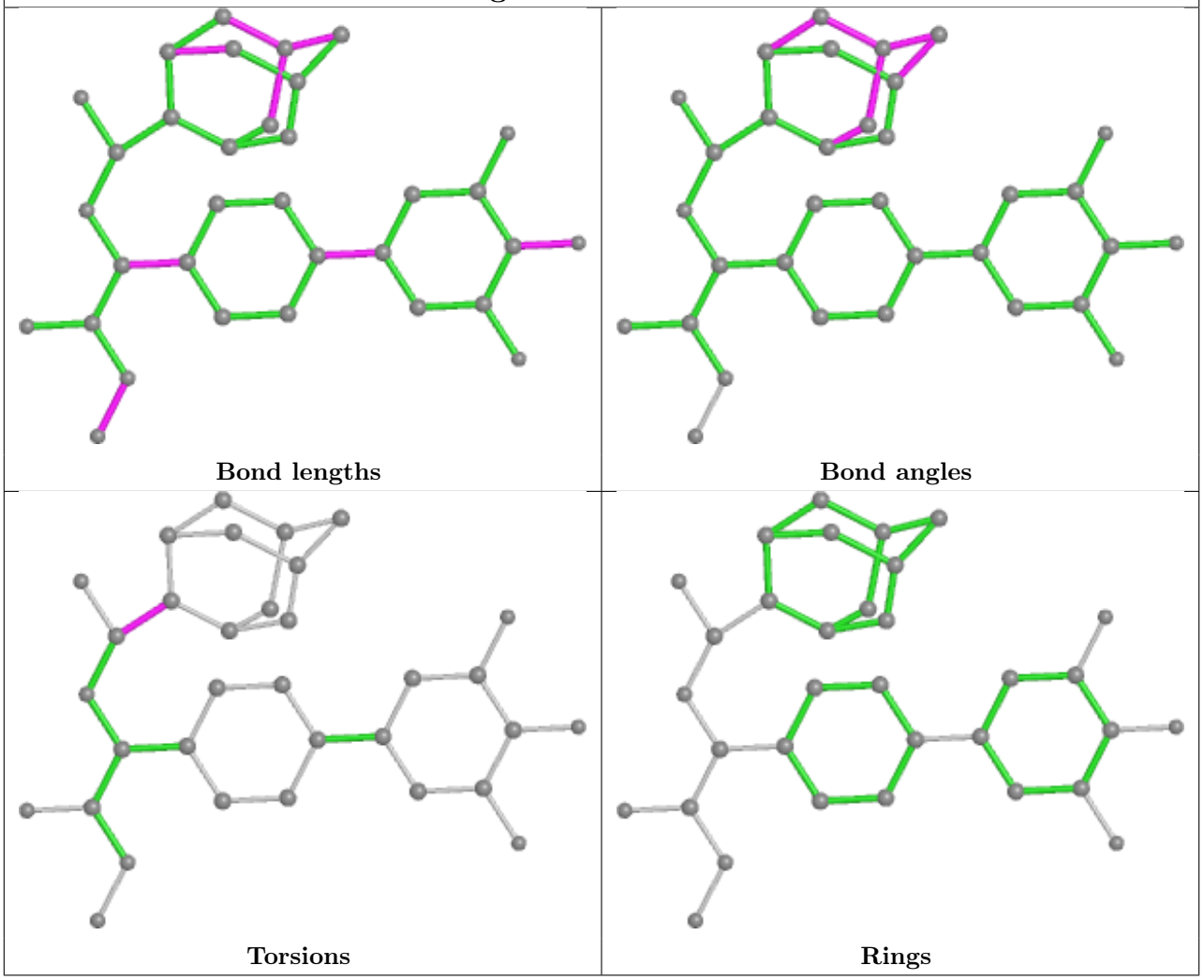


Torsions



Rings

Ligand J4V E 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	514/519 (99%)	-0.16	4 (0%) 86 89	19, 28, 45, 63	9 (1%)
1	B	511/519 (98%)	0.03	22 (4%) 35 42	19, 29, 60, 75	4 (0%)
1	C	518/519 (99%)	-0.17	2 (0%) 92 95	19, 29, 47, 70	4 (0%)
1	D	516/519 (99%)	-0.31	8 (1%) 72 77	19, 28, 43, 67	2 (0%)
1	E	510/519 (98%)	-0.32	2 (0%) 92 95	20, 27, 38, 53	6 (1%)
1	F	509/519 (98%)	-0.08	9 (1%) 68 74	22, 31, 58, 67	8 (1%)
1	G	517/519 (99%)	-0.19	6 (1%) 79 83	19, 29, 47, 65	9 (1%)
1	H	513/519 (98%)	0.06	37 (7%) 15 20	18, 29, 62, 74	17 (3%)
1	I	518/519 (99%)	-0.18	5 (0%) 82 86	19, 28, 47, 66	5 (0%)
1	J	516/519 (99%)	-0.29	5 (0%) 82 86	19, 28, 44, 69	10 (1%)
1	K	510/519 (98%)	-0.32	0 100 100	19, 26, 37, 49	7 (1%)
1	L	510/519 (98%)	-0.05	20 (3%) 39 46	21, 33, 61, 70	11 (2%)
All	All	6162/6228 (98%)	-0.16	120 (1%) 66 73	18, 28, 53, 75	92 (1%)

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	121	CYS	4.9
1	A	136	GLY	4.8
1	J	259	VAL	4.6
1	B	140	GLY	4.6
1	B	136	GLY	4.5

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	1PE	F	1009	9/16	0.77	0.20	39,46,52,55	0
7	1PE	L	1008	12/16	0.77	0.20	33,44,53,55	0
8	EDO	F	1007	4/4	0.77	0.30	44,45,46,46	0
7	1PE	J	1010	9/16	0.79	0.19	37,37,50,55	0
6	DMS	H	1010	4/4	0.81	0.20	44,48,49,55	0
7	1PE	L	1007	13/16	0.83	0.18	29,42,49,50	0
8	EDO	K	1009	4/4	0.83	0.15	29,30,31,33	0
8	EDO	J	1007	4/4	0.84	0.18	39,39,43,44	0
7	1PE	B	1008	9/16	0.84	0.20	37,44,48,49	0
7	1PE	J	1011	13/16	0.85	0.25	35,40,50,59	0
7	1PE	H	1008	9/16	0.85	0.21	31,40,45,48	0
7	1PE	L	1010	5/16	0.86	0.25	38,42,44,45	0
7	1PE	C	1007	15/16	0.86	0.22	35,41,58,64	0
9	2PE	H	1007	25/28	0.86	0.17	34,45,53,54	0
6	DMS	A	1008	4/4	0.87	0.19	37,48,57,67	0
7	1PE	G	1009	9/16	0.88	0.16	37,45,47,50	0
8	EDO	F	1006	4/4	0.88	0.17	34,36,38,48	0
7	1PE	D	1007	12/16	0.88	0.15	40,44,48,51	0
7	1PE	C	1008	12/16	0.89	0.14	33,42,47,49	0
7	1PE	K	1012	13/16	0.89	0.13	32,37,42,46	0
8	EDO	G	1007	4/4	0.89	0.12	31,33,36,40	0
8	EDO	H	1009	4/4	0.89	0.16	33,34,37,38	0
6	DMS	B	1007	4/4	0.89	0.20	35,38,53,59	0
7	1PE	J	1009	9/16	0.89	0.15	31,33,39,39	0
7	1PE	A	1009	15/16	0.89	0.17	41,47,52,52	0
7	1PE	A	1010	12/16	0.90	0.15	33,37,49,55	0
8	EDO	K	1008	4/4	0.90	0.11	37,43,44,44	0
7	1PE	G	1008	9/16	0.90	0.16	34,40,42,43	0
7	1PE	D	1008	7/16	0.90	0.12	28,32,37,37	0
7	1PE	I	1008	12/16	0.91	0.14	31,39,44,50	0
2	J4V	E	1001	33/33	0.91	0.14	22,30,37,40	0
7	1PE	L	1009	7/16	0.91	0.10	34,38,40,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	J4V	J	1001	33/33	0.91	0.13	22,29,34,36	0
2	J4V	D	1001	33/33	0.91	0.14	23,30,35,37	0
8	EDO	K	1011	4/4	0.91	0.19	34,40,42,44	0
7	1PE	F	1008	9/16	0.91	0.13	31,36,41,48	0
2	J4V	L	1001	33/33	0.92	0.13	22,30,39,41	0
2	J4V	H	1001	33/33	0.92	0.13	21,30,36,43	0
6	DMS	B	1005	4/4	0.92	0.20	42,48,49,54	0
6	DMS	B	1006	4/4	0.92	0.14	39,42,48,61	0
2	J4V	I	1001	33/33	0.92	0.14	23,29,35,43	0
2	J4V	F	1001	33/33	0.92	0.14	24,31,36,43	0
2	J4V	C	1001	33/33	0.93	0.13	20,26,34,37	0
2	J4V	K	1001	33/33	0.93	0.13	21,28,35,39	0
7	1PE	K	1013	15/16	0.93	0.15	26,34,42,45	0
8	EDO	I	1007	4/4	0.93	0.19	17,25,29,41	0
8	EDO	J	1006	4/4	0.93	0.22	38,38,44,49	0
2	J4V	G	1001	33/33	0.93	0.14	23,31,41,45	0
4	ZN	K	1003	1/1	0.93	0.10	37,37,37,37	1
7	1PE	I	1009	9/16	0.93	0.16	29,33,38,39	0
2	J4V	A	1001	33/33	0.93	0.14	22,28,40,45	0
2	J4V	B	1001	33/33	0.93	0.12	21,28,33,38	0
8	EDO	J	1008	4/4	0.94	0.12	32,33,42,44	0
5	SO4	E	1004	5/5	0.94	0.12	35,37,40,46	5
3	CO3	J	1002	4/4	0.94	0.20	23,24,29,30	0
4	ZN	E	1003	1/1	0.94	0.05	36,36,36,36	1
3	CO3	C	1002	4/4	0.94	0.17	19,23,31,32	0
5	SO4	H	1005	5/5	0.95	0.15	38,39,49,49	5
5	SO4	L	1004	5/5	0.95	0.15	46,54,56,56	0
4	ZN	D	1003	1/1	0.95	0.04	34,34,34,34	1
8	EDO	E	1006	4/4	0.95	0.14	24,24,25,27	0
5	SO4	D	1005	5/5	0.95	0.11	31,38,43,44	5
4	ZN	H	1003	1/1	0.95	0.07	40,40,40,40	1
8	EDO	K	1010	4/4	0.95	0.15	25,31,37,40	0
5	SO4	F	1004	5/5	0.95	0.10	48,49,56,58	0
6	DMS	G	1006	4/4	0.95	0.16	37,42,48,50	0
5	SO4	K	1007	5/5	0.96	0.15	35,37,37,38	5
4	ZN	B	1003	1/1	0.96	0.06	37,37,37,37	1
3	CO3	G	1002	4/4	0.96	0.15	18,23,30,31	0
3	CO3	H	1002	4/4	0.96	0.09	19,24,28,29	0
3	CO3	E	1002	4/4	0.96	0.12	25,27,32,38	0
4	ZN	I	1003	1/1	0.96	0.04	34,34,34,34	1
5	SO4	H	1006	5/5	0.96	0.09	42,44,51,55	0
5	SO4	I	1004	5/5	0.96	0.13	42,45,51,54	0

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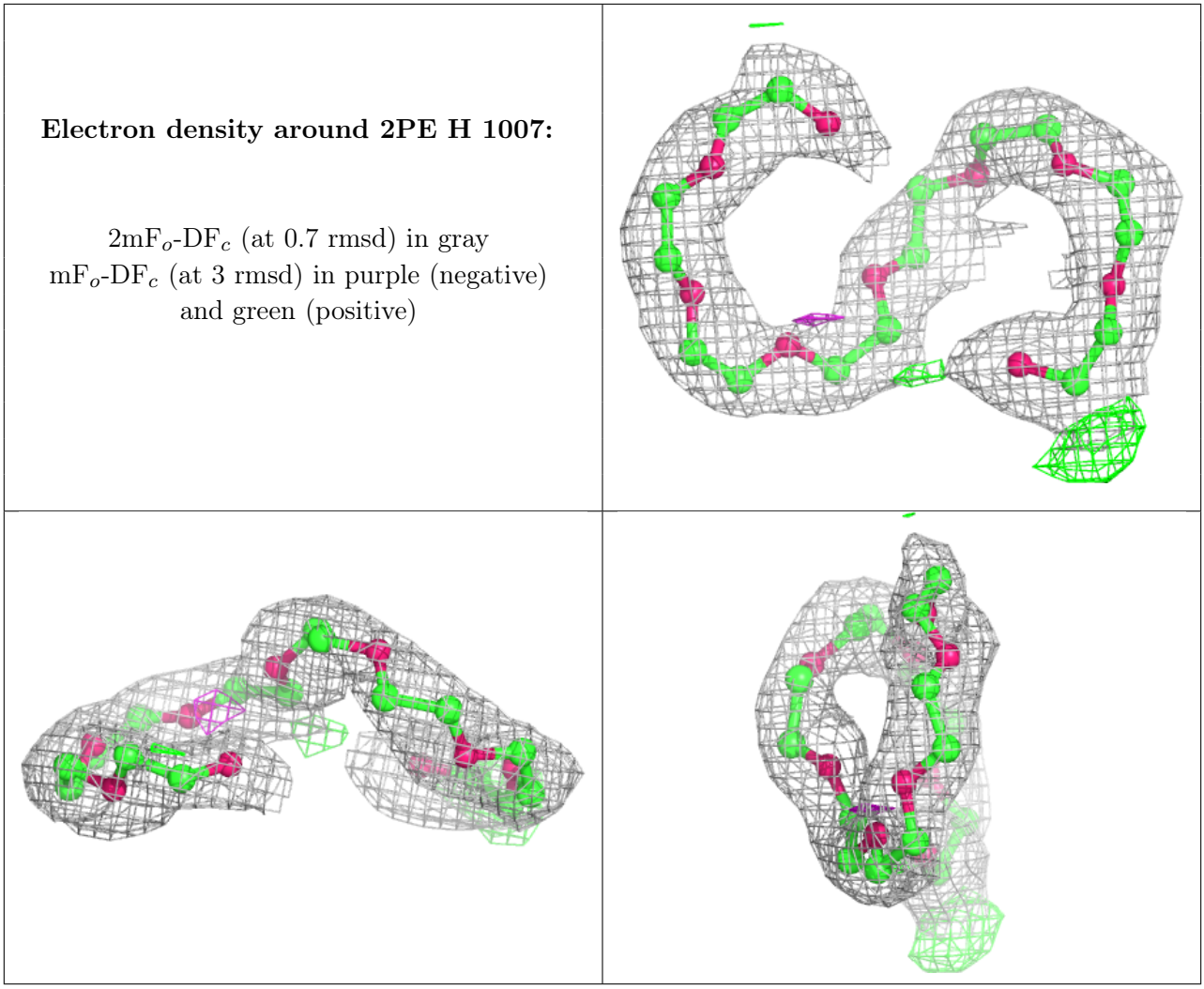
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	EDO	L	1006	4/4	0.96	0.09	23,28,37,39	0
5	SO4	I	1006	5/5	0.96	0.12	37,39,41,43	5
5	SO4	L	1005	5/5	0.97	0.13	46,49,58,58	0
3	CO3	A	1002	4/4	0.97	0.11	22,27,32,33	0
3	CO3	L	1002	4/4	0.97	0.11	24,27,31,33	0
3	CO3	F	1002	4/4	0.97	0.17	22,25,30,31	0
5	SO4	F	1005	5/5	0.97	0.15	43,47,52,65	0
4	ZN	J	1003	1/1	0.97	0.03	35,35,35,35	1
3	CO3	I	1002	4/4	0.97	0.12	21,27,30,33	0
5	SO4	A	1005	5/5	0.97	0.08	43,43,49,57	0
5	SO4	I	1005	5/5	0.97	0.09	40,45,46,49	0
5	SO4	A	1007	5/5	0.97	0.11	39,40,49,51	0
5	SO4	J	1005	5/5	0.97	0.17	41,49,52,52	0
5	SO4	K	1005	5/5	0.97	0.13	39,43,47,53	0
5	SO4	K	1006	5/5	0.97	0.11	29,32,36,46	5
5	SO4	B	1004	5/5	0.97	0.11	40,43,50,51	0
5	SO4	C	1006	5/5	0.97	0.10	31,33,36,41	0
3	CO3	D	1002	4/4	0.98	0.13	20,24,28,30	0
4	ZN	C	1003	1/1	0.98	0.05	34,34,34,34	1
5	SO4	G	1005	5/5	0.98	0.11	39,44,51,53	0
5	SO4	H	1004	5/5	0.98	0.10	22,24,29,29	0
5	SO4	C	1004	5/5	0.98	0.07	50,50,53,54	0
5	SO4	C	1005	5/5	0.98	0.16	44,47,48,48	0
3	CO3	K	1002	4/4	0.98	0.11	21,22,27,27	0
5	SO4	D	1004	5/5	0.98	0.08	47,47,52,52	0
3	CO3	B	1002	4/4	0.98	0.14	19,21,27,28	0
5	SO4	J	1004	5/5	0.98	0.06	44,46,50,54	0
4	ZN	G	1003	1/1	0.98	0.08	34,34,34,34	1
5	SO4	E	1005	5/5	0.98	0.10	39,47,49,52	0
4	ZN	F	1003	1/1	0.99	0.06	33,33,33,33	1
5	SO4	A	1006	5/5	0.99	0.08	21,24,27,30	0
4	ZN	A	1003	1/1	0.99	0.08	35,35,35,35	1
5	SO4	G	1004	5/5	0.99	0.12	33,36,39,44	5
4	ZN	L	1003	1/1	0.99	0.07	35,35,35,35	1
5	SO4	D	1006	5/5	0.99	0.09	26,27,27,29	0
5	SO4	K	1004	5/5	0.99	0.08	25,27,29,29	0
5	SO4	A	1004	5/5	0.99	0.06	44,47,48,51	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.

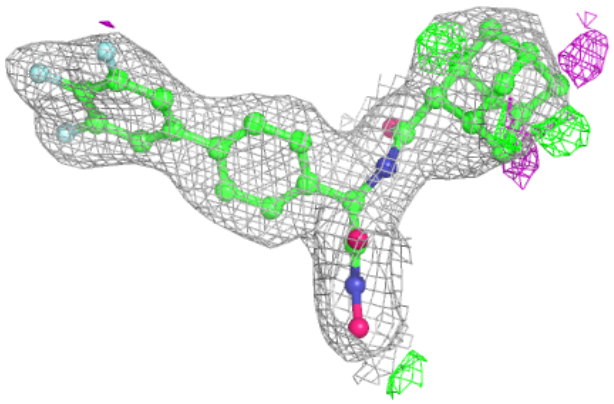
Electron density around 2PE H 1007:

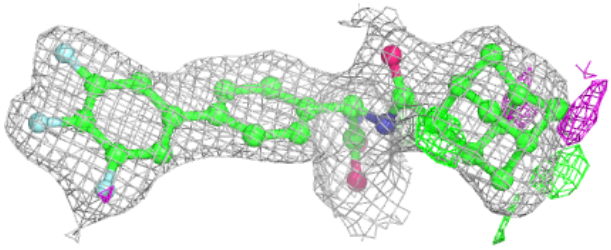
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

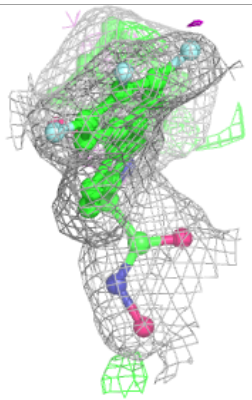


Electron density around J4V E 1001:

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

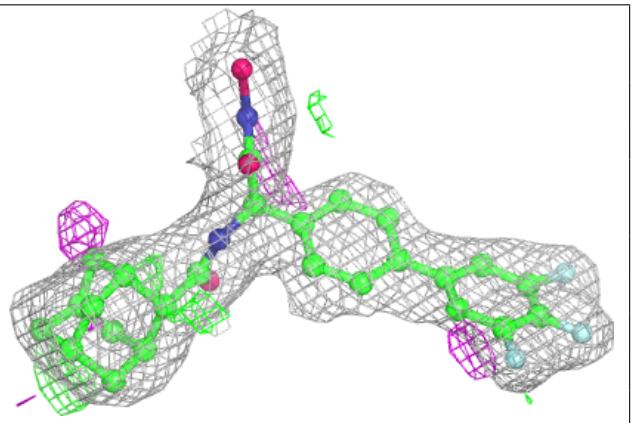


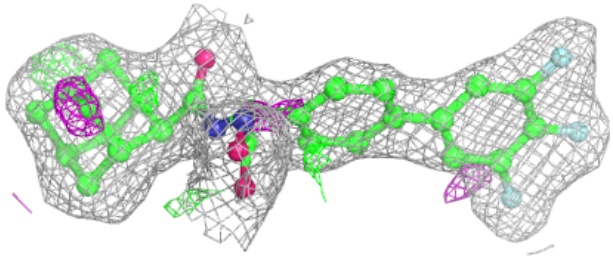


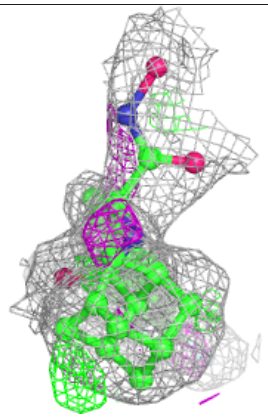


Electron density around J4V J 1001:

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

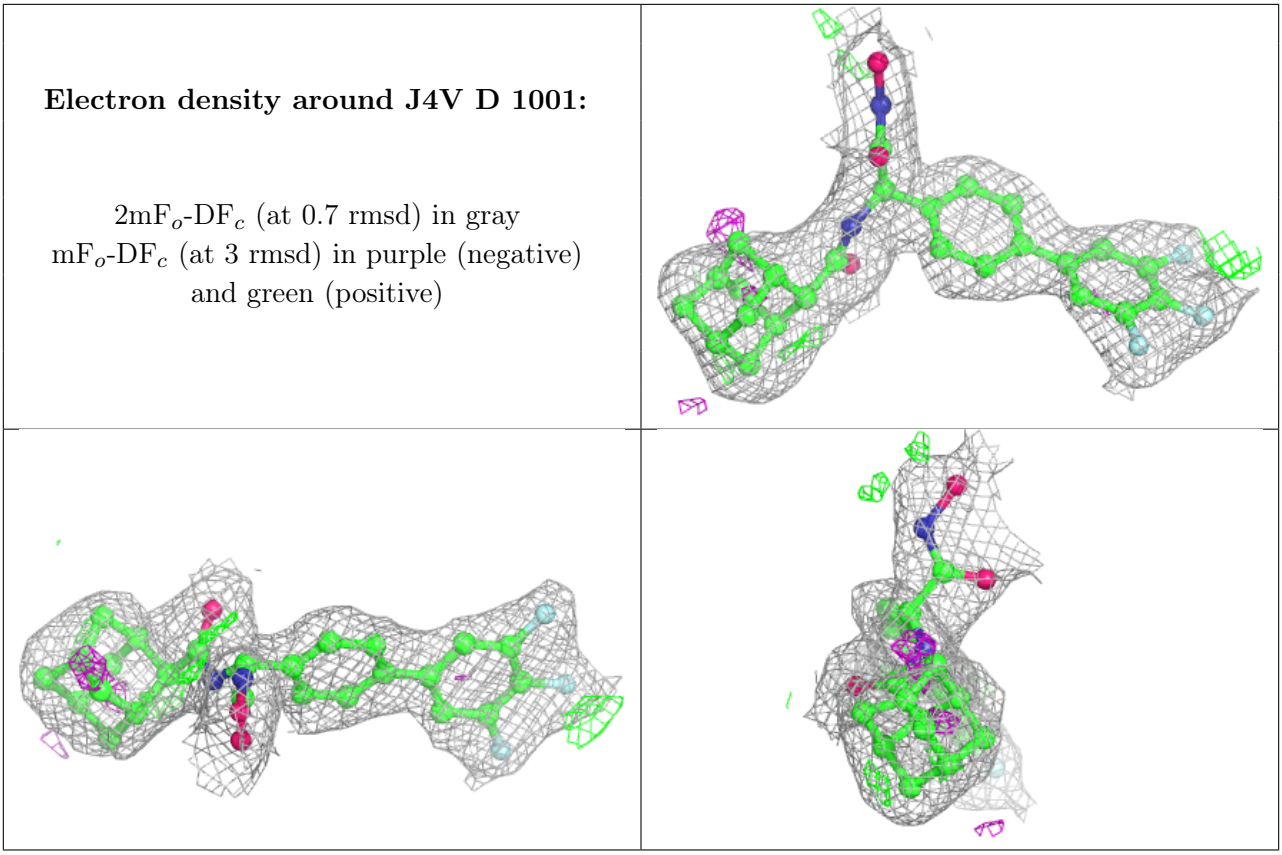






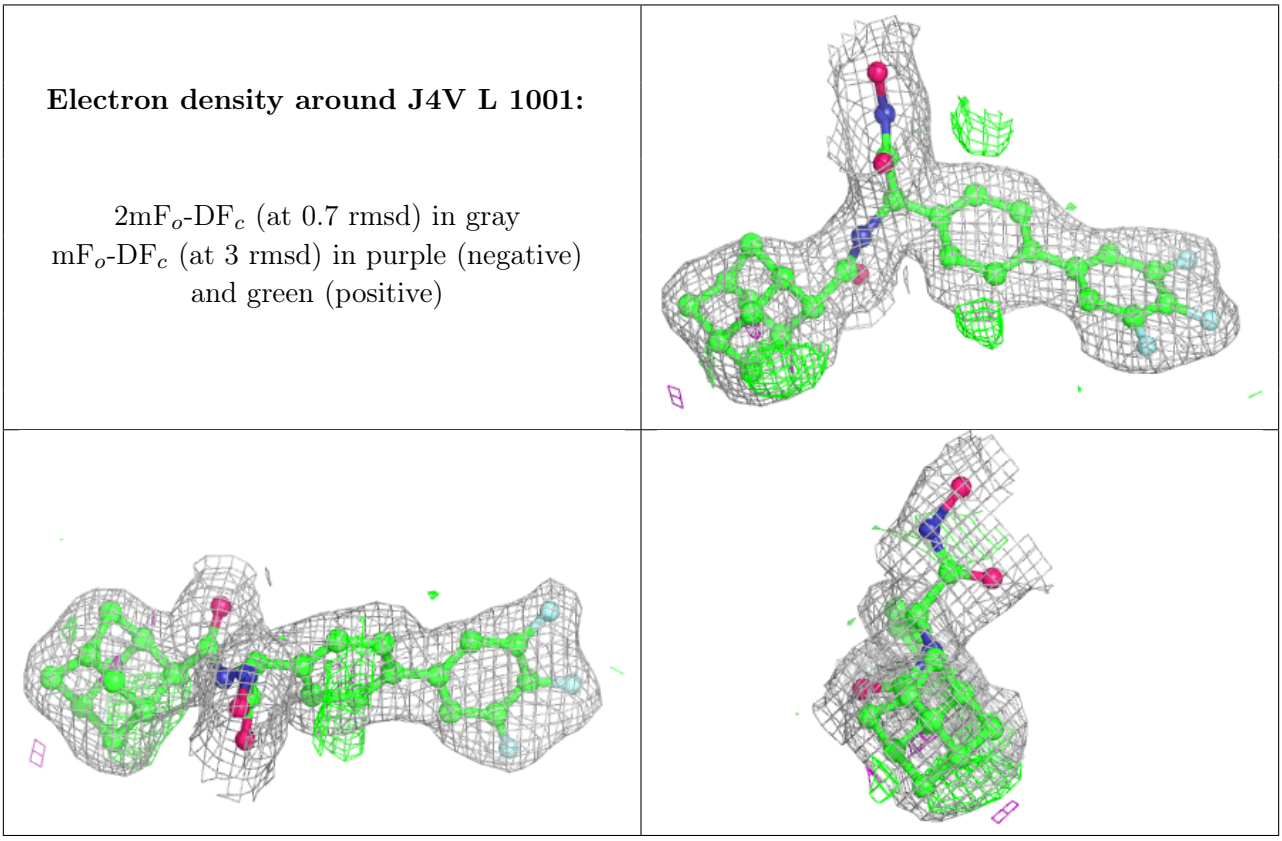
Electron density around J4V D 1001:

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



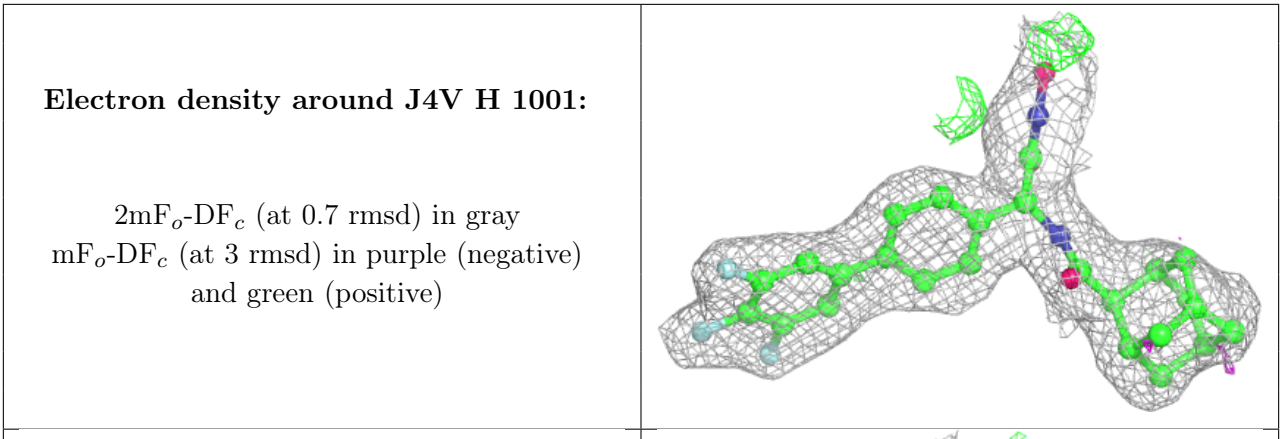
Electron density around J4V L 1001:

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



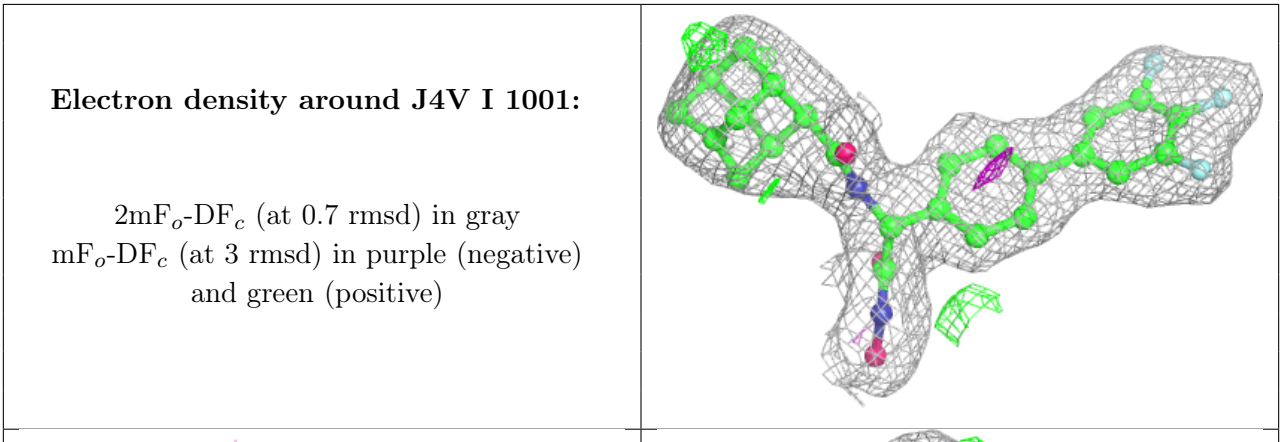
Electron density around J4V H 1001:

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



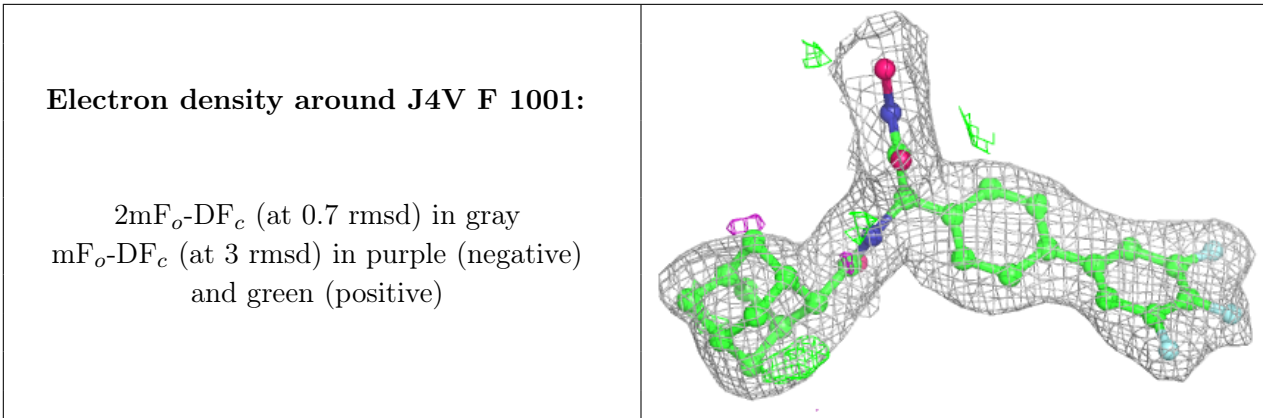
Electron density around J4V I 1001:

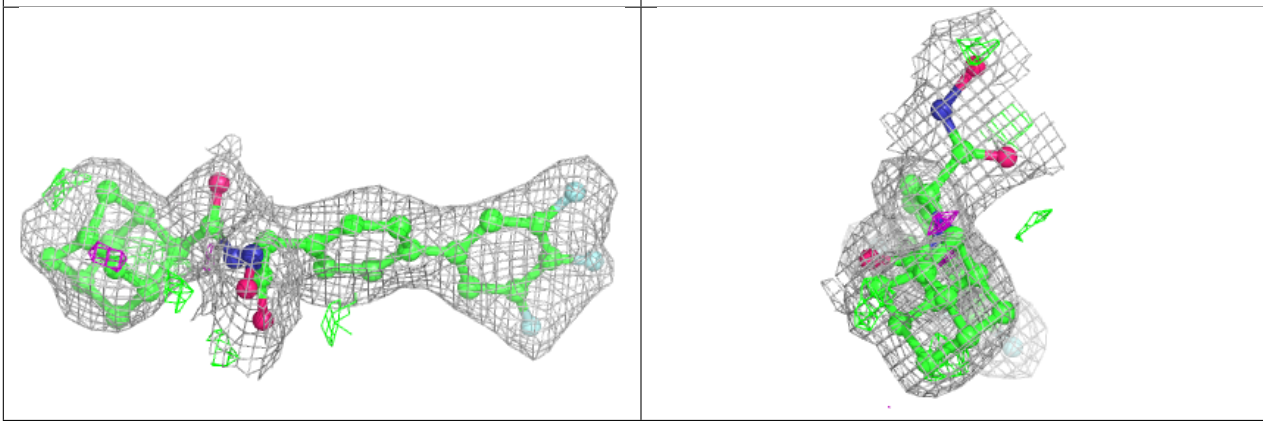
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around J4V F 1001:

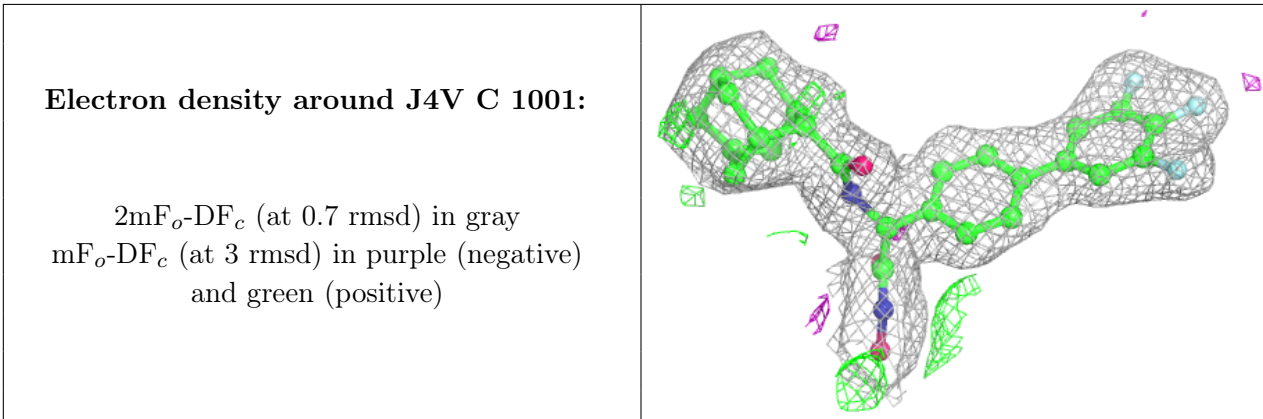
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

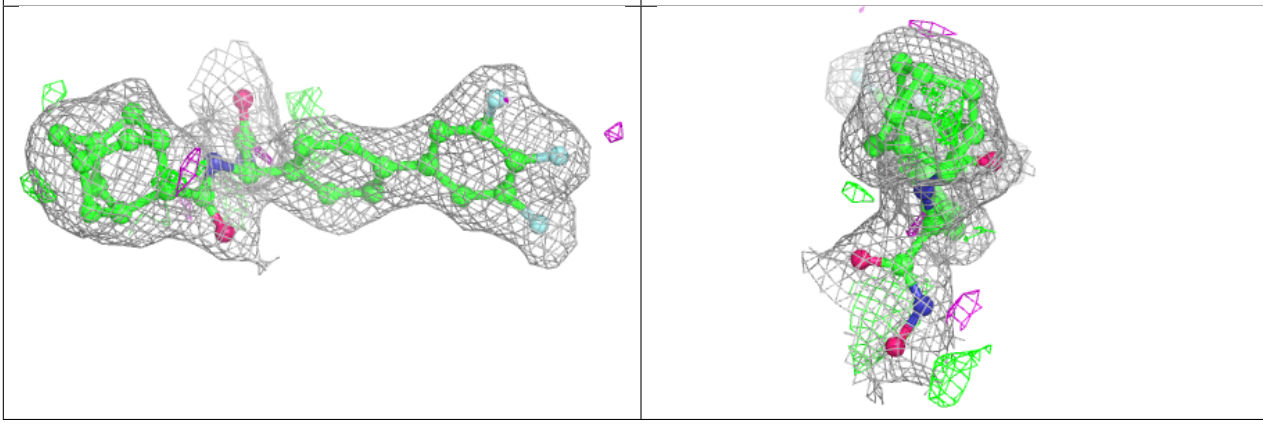




Electron density around J4V C 1001:

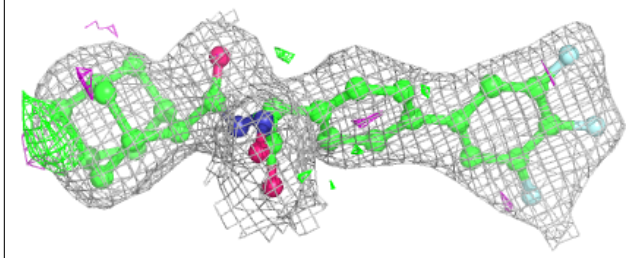
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

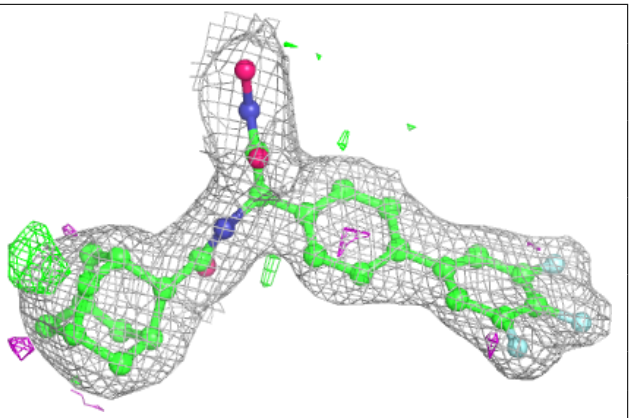


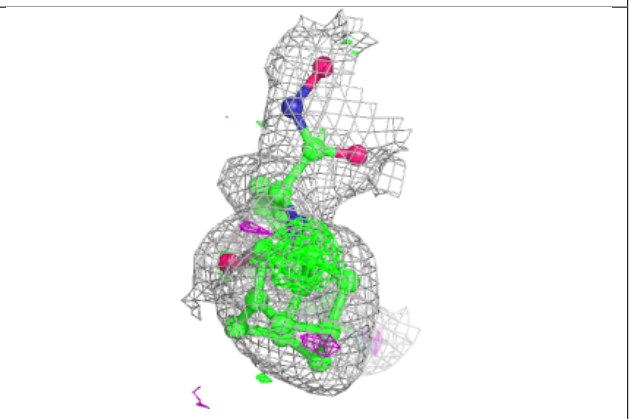


Electron density around J4V K 1001:

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

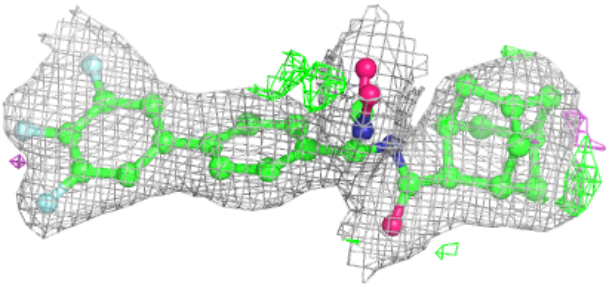


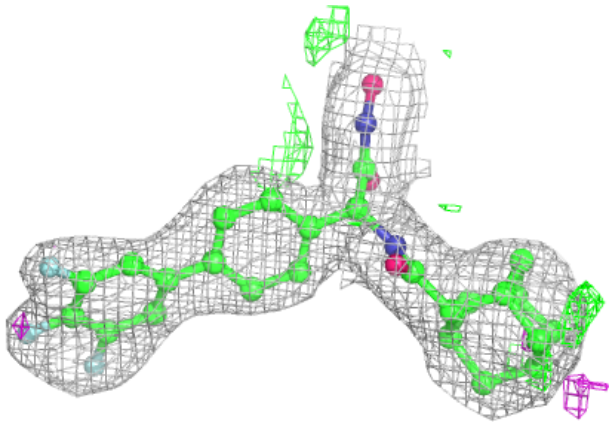


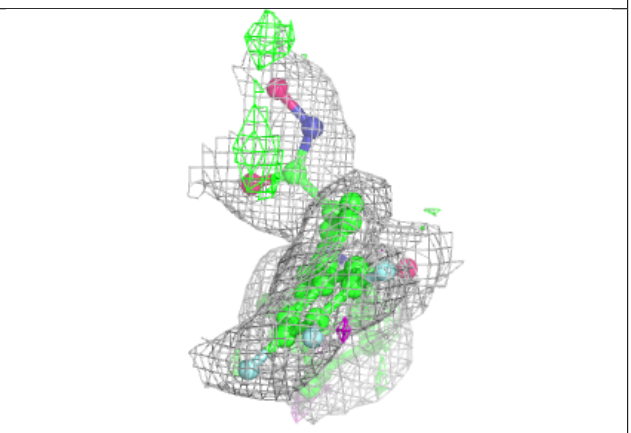


Electron density around J4V G 1001:

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

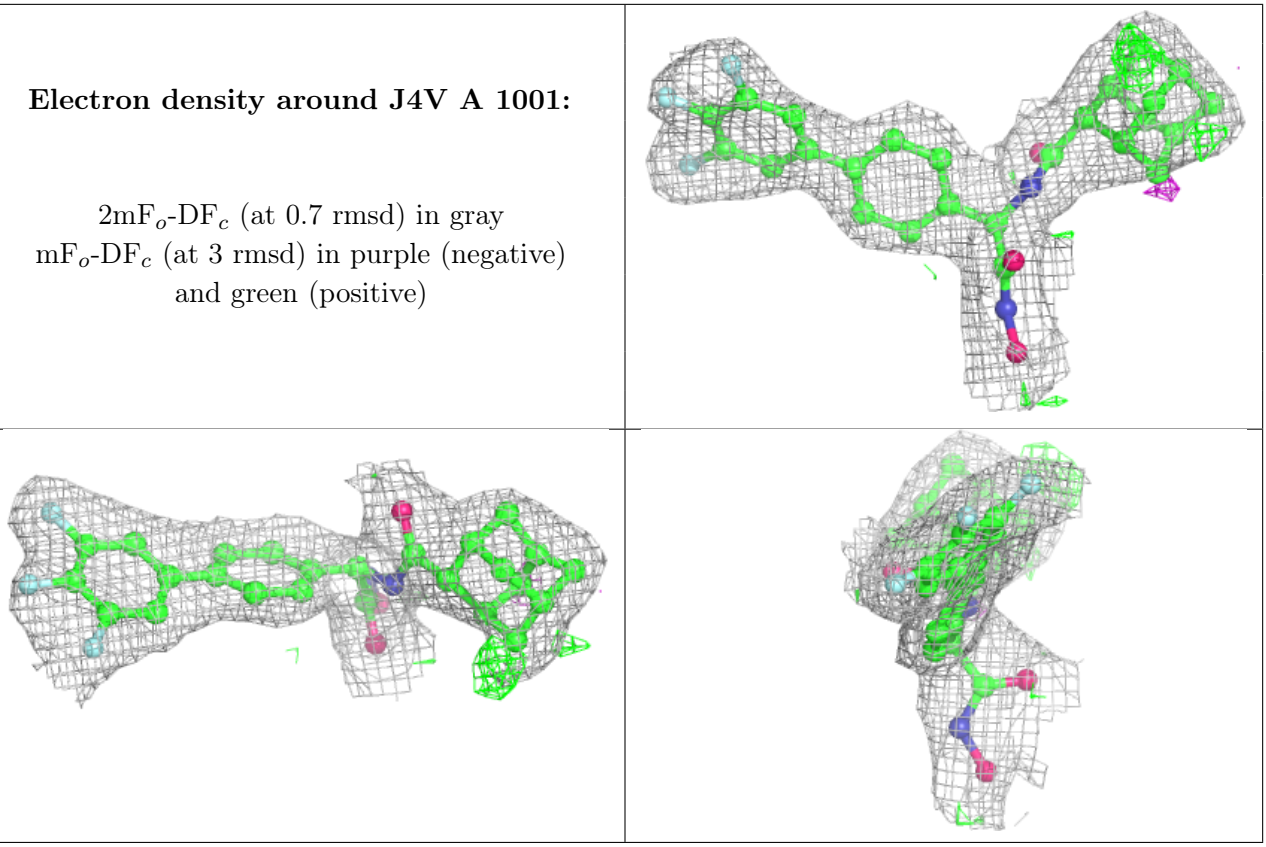






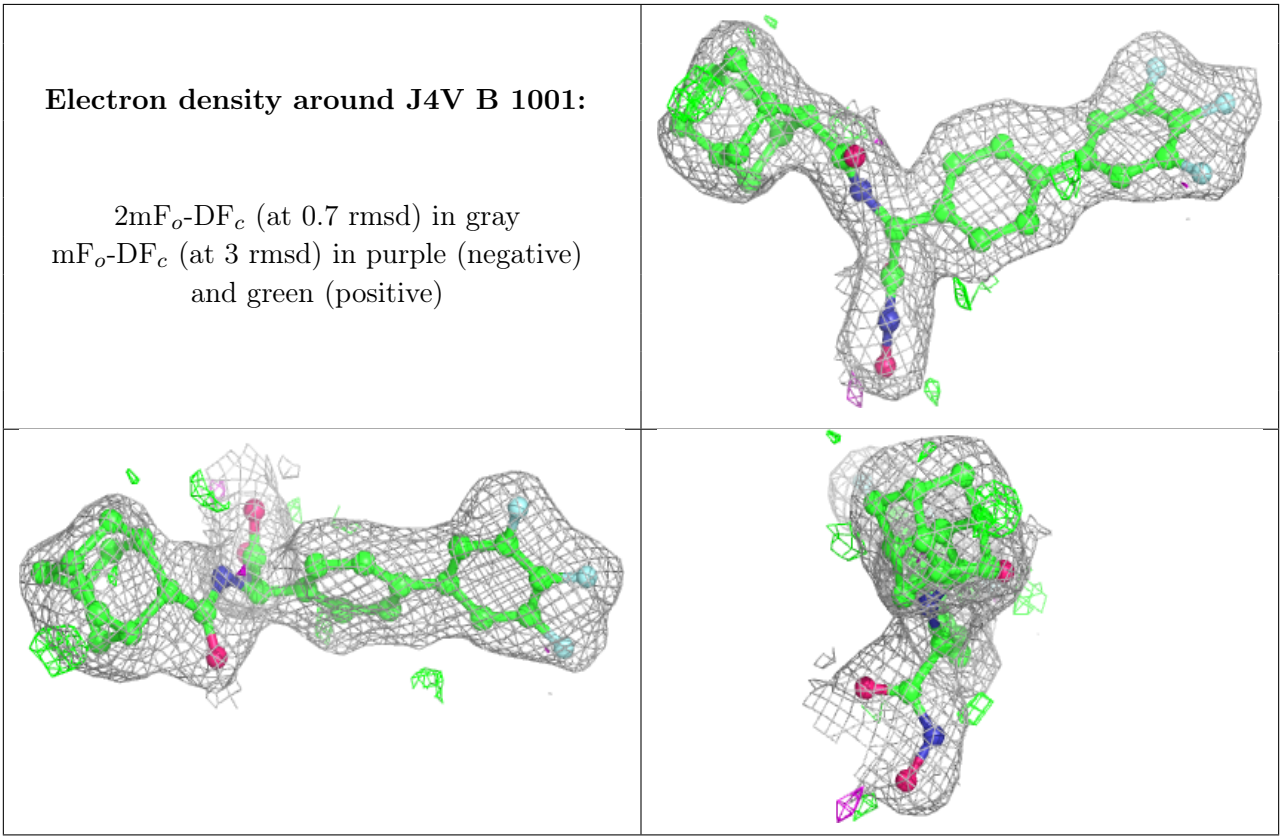
Electron density around J4V A 1001:

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



Electron density around J4V B 1001:

$2mF_o$-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.