



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 06:02 am BST

PDB ID : 6E6I  
Title : Crystal structure of 4-methyl HOPDA bound to LigY from *Sphingobium* sp. strain SYK-6  
Authors : Kuatsjah, E.; Chan, A.C.; Hurst, T.E.; Snieckus, V.; Murphy, M.E.; Eltis, L.D.  
Deposited on : 2018-07-24  
Resolution : 2.40 Å(reported)

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

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

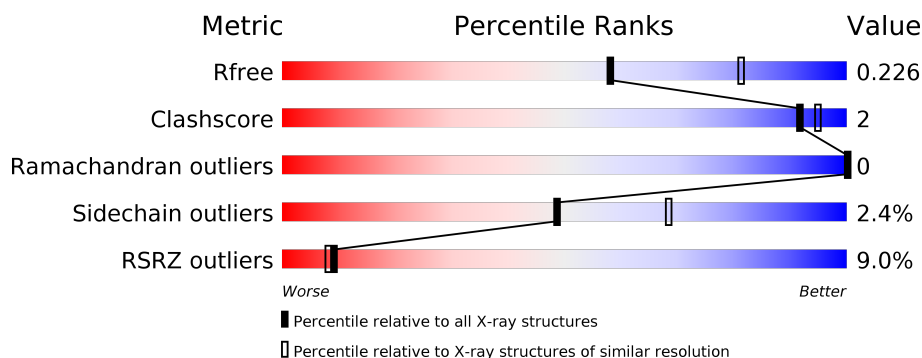
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	332	<div> <div>9%</div> <div>92%</div> <div>6%</div> </div>
1	B	332	<div> <div>8%</div> <div>94%</div> <div>6%</div> </div>
1	C	332	<div> <div>12%</div> <div>94%</div> <div>5%</div> </div>
1	D	332	<div> <div>7%</div> <div>94%</div> <div>6%</div> </div>
1	E	332	<div> <div>5%</div> <div>95%</div> <div>5%</div> </div>
1	F	332	<div> <div>6%</div> <div>97%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	332	<div><div></div><div>10%</div><div>95%</div><div></div><div></div></div>
1	H	332	<div><div></div><div>11%</div><div>94%</div><div>5%</div><div></div></div>
1	I	332	<div><div></div><div>12%</div><div>93%</div><div>7%</div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47089 atoms, of which 22616 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 2,2',3-trihydroxy-3'-methoxy-5,5'-dicarboxybiphenyl meta-cleavage compound hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	332	Total	C	H	N	O	S	0	2	0
			5083	1674	2459	450	483	17			
1	B	332	Total	C	H	N	O	S	0	4	0
			5159	1685	2515	455	487	17			
1	C	332	Total	C	H	N	O	S	0	4	0
			5165	1686	2520	457	485	17			
1	D	332	Total	C	H	N	O	S	0	2	0
			5120	1671	2500	449	483	17			
1	E	332	Total	C	H	N	O	S	0	5	0
			5165	1687	2517	455	489	17			
1	F	331	Total	C	H	N	O	S	0	3	0
			5128	1671	2506	450	484	17			
1	G	331	Total	C	H	N	O	S	0	3	0
			5128	1674	2502	451	484	17			
1	H	331	Total	C	H	N	O	S	0	3	0
			5124	1671	2502	450	484	17			
1	I	332	Total	C	H	N	O	S	0	3	0
			5135	1677	2505	451	485	17			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

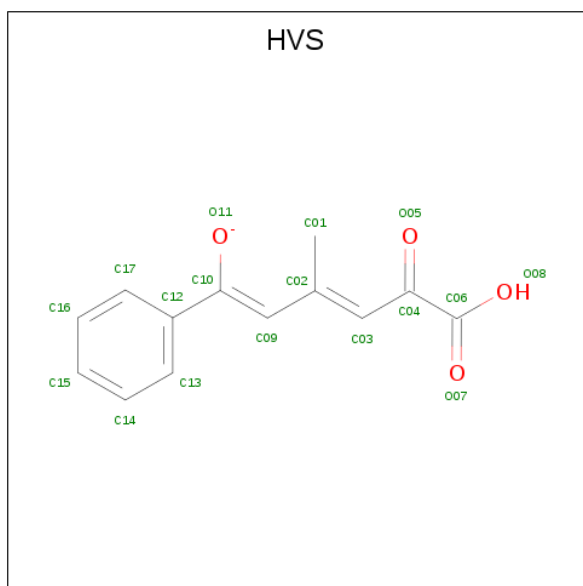
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (1Z,3E)-5-carboxy-3-methyl-5-oxo-1-phenylpenta-1,3-dien-1-olate (three-letter code: HVS) (formula: C<sub>13</sub>H<sub>11</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			27	13	10	4		
3	B	1	Total	C	H	O	0	0
			27	13	10	4		
3	C	1	Total	C	H	O	0	0
			27	13	10	4		
3	D	1	Total	C	H	O	0	0
			27	13	10	4		
3	E	1	Total	C	H	O	0	0
			27	13	10	4		
3	F	1	Total	C	H	O	0	0
			27	13	10	4		
3	G	1	Total	C	H	O	0	0
			27	13	10	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	H	O	0	0
			27	13	10	4		
3	I	1	Total	C	H	O	0	0
			27	13	10	4		

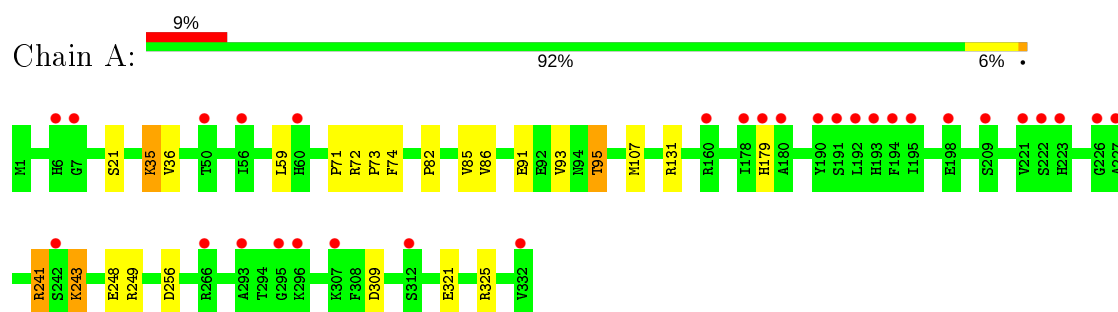
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		
4	B	110	Total	O	0	0
			110	110		
4	C	45	Total	O	0	0
			45	45		
4	D	72	Total	O	0	0
			72	72		
4	E	81	Total	O	0	0
			81	81		
4	F	81	Total	O	0	0
			81	81		
4	G	63	Total	O	0	0
			63	63		
4	H	48	Total	O	0	0
			48	48		
4	I	62	Total	O	0	0
			62	62		

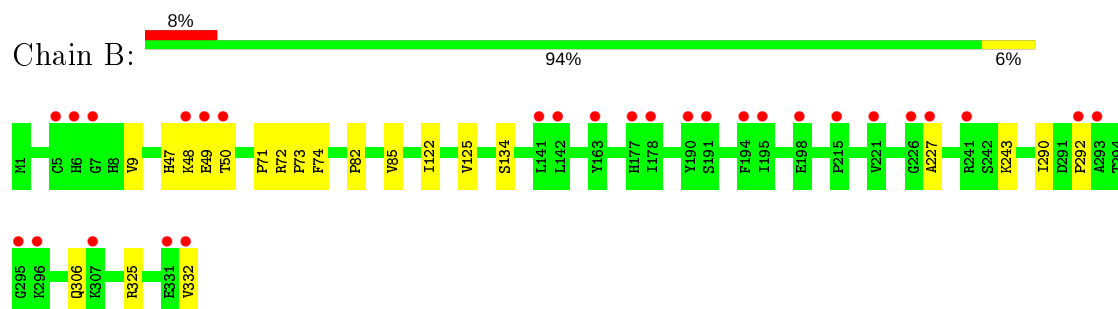
### 3 Residue-property plots

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.

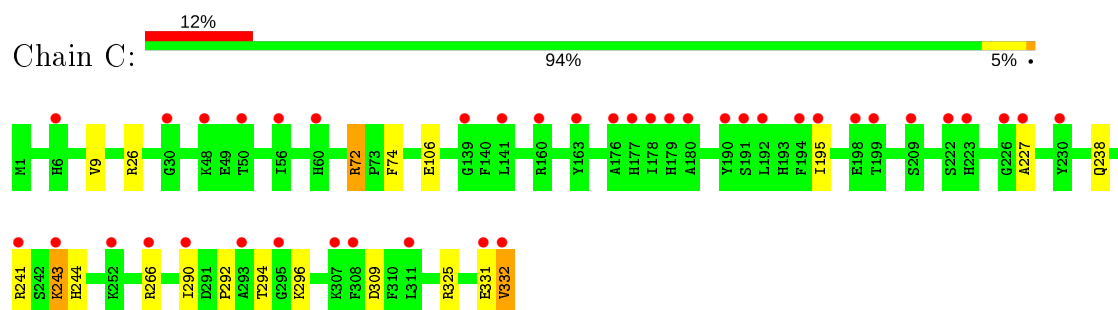
- Molecule 1: 2,2',3-trihydroxy-3'-methoxy-5,5'-dicarboxybiphenyl meta-cleavage compound hydrolase



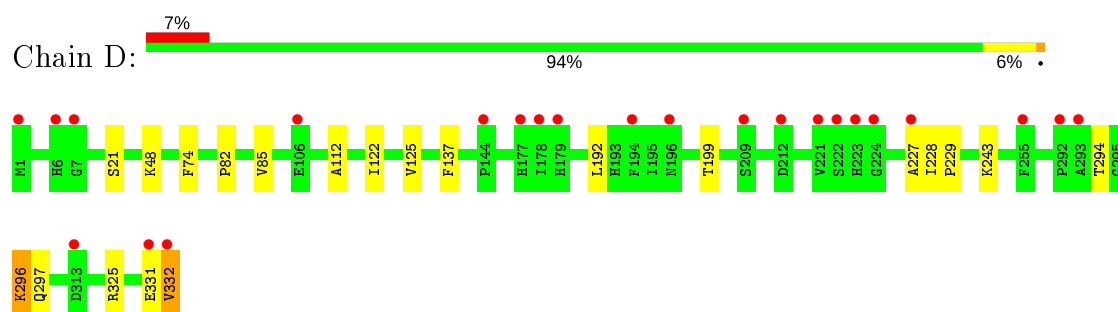
- Molecule 1: 2,2',3-trihydroxy-3'-methoxy-5,5'-dicarboxybiphenyl meta-cleavage compound hydrolase



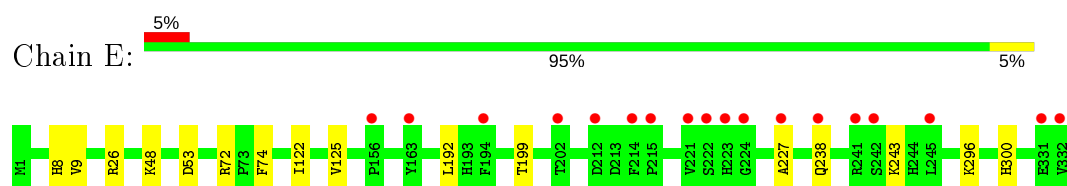
- Molecule 1: 2,2',3-trihydroxy-3'-methoxy-5,5'-dicarboxybiphenyl meta-cleavage compound hydrolase



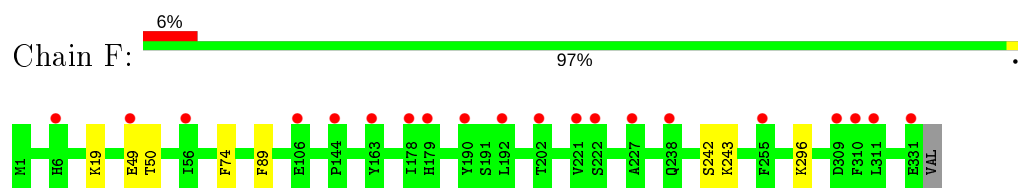
- Molecule 1: 2,2',3-trihydroxy-3'-methoxy-5,5'-dicarboxybiphenyl meta-cleavage compound hydrolase



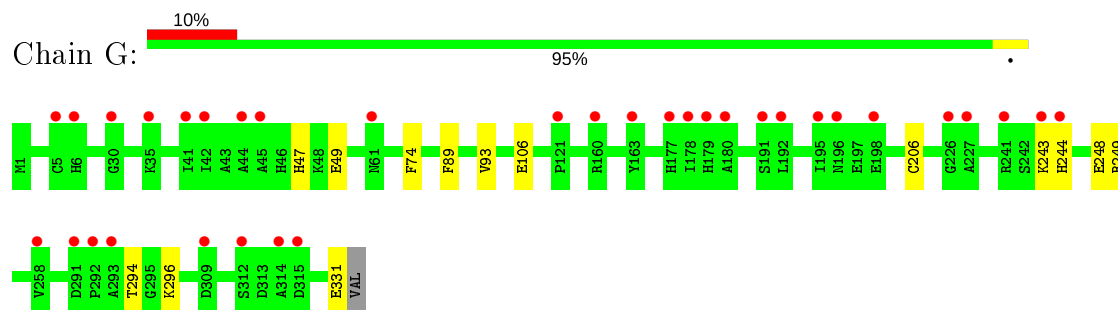
- Molecule 1: 2,2',3-trihydroxy-3'-methoxy-5,5'-dicarboxybiphenyl meta-cleavage compound hydrolase



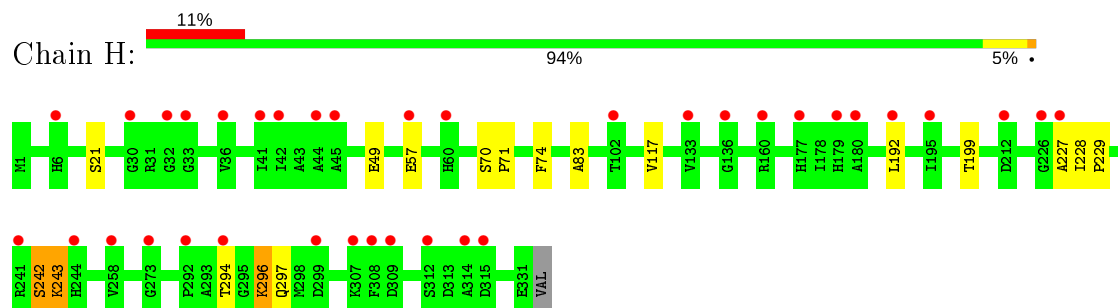
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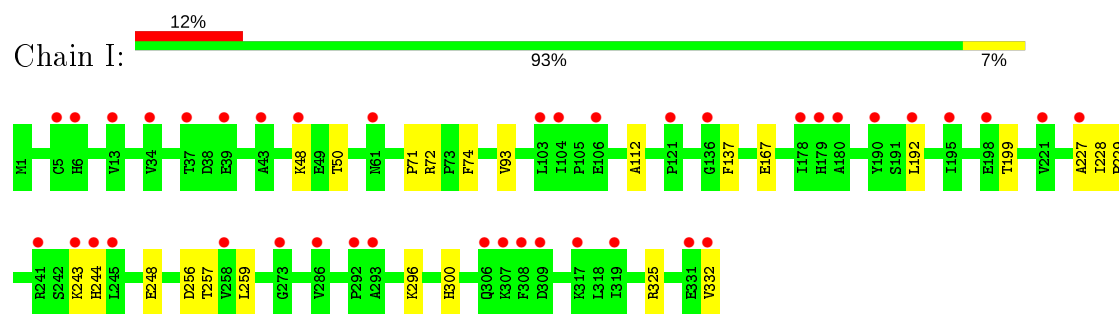


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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.65Å 195.10Å 179.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.14 – 2.40 38.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.14-2.40) 99.5 (38.73-2.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.39Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.183 , 0.219 0.194 , 0.226	Depositor DCC
$R_{free}$ test set	2005 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtrriage
Anisotropy	0.282	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 32.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	47089	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.87 % 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 4.7984e-06. 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, HVS

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	0.28	0/2711	0.46	0/3681
1	B	0.29	0/2731	0.46	0/3707
1	C	0.27	0/2733	0.45	0/3710
1	D	0.29	0/2707	0.45	0/3677
1	E	0.29	0/2736	0.46	0/3716
1	F	0.29	0/2709	0.46	0/3679
1	G	0.28	0/2713	0.46	0/3683
1	H	0.28	0/2709	0.45	0/3679
1	I	0.28	0/2717	0.46	0/3690
All	All	0.28	0/24466	0.46	0/33222

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	2624	2459	2532	13	0
1	B	2644	2515	2549	10	0
1	C	2645	2520	2550	10	0
1	D	2620	2500	2521	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2648	2517	2539	10	0
1	F	2622	2506	2519	2	0
1	G	2626	2502	2530	4	0
1	H	2622	2502	2519	12	0
1	I	2630	2505	2537	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
3	A	17	10	0	0	0
3	B	17	10	0	0	0
3	C	17	10	0	0	0
3	D	17	10	0	0	0
3	E	17	10	0	0	0
3	F	17	10	0	0	0
3	G	17	10	0	0	0
3	H	17	10	0	0	0
3	I	17	10	0	0	0
4	A	68	0	0	0	0
4	B	110	0	0	1	0
4	C	45	0	0	0	0
4	D	72	0	0	0	0
4	E	81	0	0	0	0
4	F	81	0	0	0	0
4	G	63	0	0	0	0
4	H	48	0	0	0	0
4	I	62	0	0	1	0
All	All	24473	22616	22796	74	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 2.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ARG:HD2	1:B:332:VAL:HG22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLU:O	1:A:95:THR:HG23	1.92	0.69
1:B:227:ALA:HB2	1:C:227:ALA:HB2	1.73	0.69
1:E:227:ALA:HB2	1:H:227:ALA:HB2	1.73	0.68
1:C:294:THR:HB	1:C:296:LYS:HE2	1.76	0.67
1:E:8:HIS:HB3	1:E:72:ARG:HD2	1.77	0.65
1:B:325:ARG:NH1	4:B:501:HOH:O	2.24	0.65
1:D:82:PRO:O	1:D:85:VAL:HG22	1.99	0.62
1:I:48:LYS:NZ	4:I:502:HOH:O	2.32	0.61
1:D:227:ALA:HB2	1:I:227:ALA:HB2	1.82	0.61
1:E:48:LYS:HE2	1:E:53:ASP:OD1	2.02	0.59
1:C:294:THR:CB	1:C:296:LYS:HE2	2.32	0.58
1:A:95:THR:HG22	1:A:131:ARG:HH12	1.67	0.58
1:E:296:LYS:HE3	1:E:300:HIS:O	2.04	0.58
1:D:192:LEU:HD11	1:I:199:THR:HG22	1.86	0.58
1:E:8:HIS:CB	1:E:72:ARG:HD2	2.35	0.57
1:B:325:ARG:CD	1:B:332:VAL:HG22	2.36	0.54
1:I:296:LYS:HE2	1:I:300:HIS:HB3	1.90	0.53
1:H:242:SER:OG	1:H:243:LYS:N	2.39	0.52
1:H:294:THR:CG2	1:H:296:LYS:HD3	2.40	0.51
1:A:59:LEU:HD12	1:A:107:MET:HE3	1.91	0.51
1:G:244:HIS:ND1	1:G:248:GLU:OE2	2.41	0.51
1:E:9:VAL:O	1:E:72:ARG:HD3	2.09	0.51
1:A:243:LYS:HD3	1:A:243:LYS:N	2.26	0.51
1:D:48:LYS:N	1:D:48:LYS:HD2	2.26	0.51
1:C:325:ARG:HD3	1:C:332:VAL:HG22	1.93	0.50
1:H:57:GLU:OE1	1:H:57:GLU:N	2.44	0.50
1:A:71:PRO:HB3	1:A:93:VAL:HG11	1.93	0.50
1:D:199:THR:HG22	1:I:192:LEU:HD11	1.93	0.49
1:C:309:ASP:N	1:C:309:ASP:OD1	2.46	0.48
1:E:192:LEU:HD11	1:H:199:THR:HG22	1.94	0.48
1:A:35:LYS:HD2	1:A:35:LYS:N	2.29	0.48
1:E:199:THR:HG22	1:H:192:LEU:HD11	1.96	0.47
1:A:309:ASP:N	1:A:309:ASP:OD1	2.47	0.47
1:B:9:VAL:O	1:B:72:ARG:HD3	2.16	0.46
1:H:294:THR:HG21	1:H:296:LYS:HD3	1.97	0.46
1:A:241:ARG:HG2	1:A:241:ARG:O	2.14	0.45
1:D:112:ALA:HB2	1:D:137:PHE:CD2	2.52	0.45
1:A:73:PRO:HG2	1:A:179:HIS:CE1	2.52	0.44
1:G:47:HIS:ND1	1:G:49:GLU:HG2	2.32	0.44
1:C:9:VAL:O	1:C:72:ARG:HD2	2.18	0.44
1:B:47:HIS:ND1	1:B:49:GLU:HG2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:LEU:CD1	1:H:199:THR:HG22	2.48	0.44
1:C:243:LYS:HG2	1:C:244:HIS:N	2.32	0.43
1:C:290:ILE:O	1:C:292:PRO:HD3	2.18	0.43
1:A:321:GLU:OE1	1:A:325:ARG:NH2	2.50	0.43
1:F:19:LYS:HB2	1:F:89:PHE:CE1	2.54	0.43
1:E:122:ILE:O	1:E:125:VAL:HG22	2.18	0.43
1:G:89:PHE:O	1:G:93:VAL:HG23	2.19	0.43
1:I:257:THR:O	1:I:259:LEU:N	2.50	0.42
1:B:290:ILE:O	1:B:292:PRO:HD3	2.18	0.42
1:D:228:ILE:HB	1:D:229:PRO:HD3	2.01	0.42
1:H:296:LYS:HG2	1:H:297:GLN:N	2.33	0.42
1:I:112:ALA:HB2	1:I:137:PHE:CD2	2.54	0.42
1:C:296:LYS:HB2	1:C:296:LYS:HE3	1.83	0.42
1:C:238:GLN:OE1	1:C:241:ARG:NH1	2.53	0.42
1:F:49:GLU:HB3	1:F:50:THR:H	1.70	0.41
1:G:206:CYS:HA	1:G:249:ARG:HB3	2.01	0.41
1:A:256:ASP:C	1:A:256:ASP:OD1	2.59	0.41
1:D:296:LYS:HG2	1:D:297:GLN:N	2.35	0.41
1:D:122:ILE:O	1:D:125:VAL:HG22	2.20	0.41
1:D:325:ARG:NH1	1:D:332:VAL:HB	2.35	0.41
1:I:325:ARG:HH11	1:I:332:VAL:HB	1.86	0.41
1:H:70:SER:HB2	1:H:71:PRO:HD2	2.03	0.41
1:H:83:ALA:HB1	1:H:117:VAL:HG21	2.03	0.41
1:A:82:PRO:O	1:A:85:VAL:HG22	2.21	0.40
1:B:122:ILE:O	1:B:125:VAL:HG22	2.21	0.40
1:I:256:ASP:C	1:I:256:ASP:OD1	2.60	0.40
1:A:59:LEU:CD1	1:A:107:MET:HE3	2.51	0.40
1:B:71:PRO:O	1:B:73:PRO:HD3	2.20	0.40
1:I:71:PRO:HB3	1:I:93:VAL:HG11	2.04	0.40
1:H:228:ILE:HB	1:H:229:PRO:HD3	2.04	0.40
1:I:228:ILE:HB	1:I:229:PRO:HD3	2.02	0.40
1:B:82:PRO:O	1:B:85:VAL:HG22	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/332 (100%)	326 (98%)	6 (2%)	0	100	100
1	B	334/332 (101%)	319 (96%)	15 (4%)	0	100	100
1	C	334/332 (101%)	325 (97%)	9 (3%)	0	100	100
1	D	332/332 (100%)	320 (96%)	12 (4%)	0	100	100
1	E	335/332 (101%)	326 (97%)	9 (3%)	0	100	100
1	F	332/332 (100%)	322 (97%)	10 (3%)	0	100	100
1	G	332/332 (100%)	323 (97%)	9 (3%)	0	100	100
1	H	332/332 (100%)	321 (97%)	11 (3%)	0	100	100
1	I	333/332 (100%)	323 (97%)	10 (3%)	0	100	100
All	All	2996/2988 (100%)	2905 (97%)	91 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	286/284 (101%)	275 (96%)	11 (4%)	33	51
1	B	288/284 (101%)	282 (98%)	6 (2%)	53	72
1	C	288/284 (101%)	279 (97%)	9 (3%)	40	60
1	D	285/284 (100%)	278 (98%)	7 (2%)	47	67
1	E	288/284 (101%)	284 (99%)	4 (1%)	67	82
1	F	285/284 (100%)	281 (99%)	4 (1%)	67	82
1	G	286/284 (101%)	280 (98%)	6 (2%)	53	72
1	H	285/284 (100%)	279 (98%)	6 (2%)	53	72
1	I	287/284 (101%)	280 (98%)	7 (2%)	49	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2578/2556 (101%)	2518 (98%)	60 (2%)	49 70

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	35	LYS
1	A	36	VAL
1	A	72	ARG
1	A	74	PHE
1	A	86	VAL
1	A	95	THR
1	A	241	ARG
1	A	243	LYS
1	A	248	GLU
1	A	249	ARG
1	B	48	LYS
1	B	50	THR
1	B	74	PHE
1	B	134	SER
1	B	243	LYS
1	B	306	GLN
1	C	26	ARG
1	C	72	ARG
1	C	74	PHE
1	C	106	GLU
1	C	195	ILE
1	C	243	LYS
1	C	266	ARG
1	C	331	GLU
1	C	332	VAL
1	D	21	SER
1	D	74	PHE
1	D	243	LYS
1	D	294	THR
1	D	296	LYS
1	D	331	GLU
1	D	332	VAL
1	E	26	ARG
1	E	74	PHE
1	E	238	GLN
1	E	243	LYS

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Mol	Chain	Res	Type
1	F	74	PHE
1	F	242	SER
1	F	243	LYS
1	F	296	LYS
1	G	74	PHE
1	G	106	GLU
1	G	243	LYS
1	G	294	THR
1	G	296	LYS
1	G	331	GLU
1	H	21	SER
1	H	49	GLU
1	H	74	PHE
1	H	242	SER
1	H	243	LYS
1	H	296	LYS
1	I	50	THR
1	I	72	ARG
1	I	74	PHE
1	I	167	GLU
1	I	243	LYS
1	I	244	HIS
1	I	248	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	60	HIS
1	D	60	HIS
1	F	238	GLN
1	G	204	ASN
1	I	300	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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
3	HVS	B	401	2	14,17,17	1.80	3 (21%)	15,22,22	2.03	2 (13%)
3	HVS	G	401	2	14,17,17	1.73	2 (14%)	15,22,22	2.16	3 (20%)
3	HVS	D	401	2	14,17,17	1.63	2 (14%)	15,22,22	2.15	2 (13%)
3	HVS	A	401	2	14,17,17	1.87	2 (14%)	15,22,22	2.01	3 (20%)
3	HVS	F	401	2	14,17,17	1.81	3 (21%)	15,22,22	2.00	3 (20%)
3	HVS	H	401	2	14,17,17	1.66	2 (14%)	15,22,22	1.95	3 (20%)
3	HVS	I	401	2	14,17,17	1.65	2 (14%)	15,22,22	1.83	2 (13%)
3	HVS	E	401	2	14,17,17	1.73	3 (21%)	15,22,22	2.07	3 (20%)
3	HVS	C	401	2	14,17,17	1.69	2 (14%)	15,22,22	1.97	2 (13%)

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
3	HVS	B	401	2	-	5/12/16/16	0/1/1/1
3	HVS	G	401	2	-	6/12/16/16	0/1/1/1
3	HVS	D	401	2	-	6/12/16/16	0/1/1/1
3	HVS	A	401	2	-	6/12/16/16	0/1/1/1
3	HVS	F	401	2	-	4/12/16/16	0/1/1/1
3	HVS	H	401	2	-	4/12/16/16	0/1/1/1
3	HVS	I	401	2	-	6/12/16/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HVS	E	401	2	-	4/12/16/16	0/1/1/1
3	HVS	C	401	2	-	5/12/16/16	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	HVS	C12-C10	4.88	1.56	1.47
3	F	401	HVS	C12-C10	4.54	1.55	1.47
3	B	401	HVS	C12-C10	4.41	1.55	1.47
3	G	401	HVS	C12-C10	4.25	1.55	1.47
3	C	401	HVS	C12-C10	4.08	1.54	1.47
3	E	401	HVS	O11-C10	-4.02	1.23	1.32
3	D	401	HVS	O11-C10	-3.99	1.23	1.32
3	G	401	HVS	O11-C10	-3.98	1.23	1.32
3	F	401	HVS	O11-C10	-3.98	1.23	1.32
3	H	401	HVS	O11-C10	-3.97	1.23	1.32
3	B	401	HVS	O11-C10	-3.97	1.23	1.32
3	I	401	HVS	O11-C10	-3.96	1.23	1.32
3	C	401	HVS	O11-C10	-3.94	1.23	1.32
3	A	401	HVS	O11-C10	-3.93	1.23	1.32
3	H	401	HVS	C12-C10	3.89	1.54	1.47
3	E	401	HVS	C12-C10	3.82	1.54	1.47
3	I	401	HVS	C12-C10	3.81	1.54	1.47
3	D	401	HVS	C12-C10	3.63	1.53	1.47
3	B	401	HVS	C03-C04	2.23	1.50	1.43
3	E	401	HVS	C03-C04	2.16	1.50	1.43
3	F	401	HVS	C03-C04	2.03	1.50	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	HVS	O11-C10-C09	5.23	128.41	121.09
3	D	401	HVS	O11-C10-C09	5.15	128.30	121.09
3	G	401	HVS	O11-C10-C09	5.10	128.22	121.09
3	B	401	HVS	O11-C10-C09	4.92	127.97	121.09
3	C	401	HVS	O11-C10-C09	4.80	127.80	121.09
3	A	401	HVS	O11-C10-C09	4.75	127.74	121.09
3	G	401	HVS	C12-C10-C09	-4.72	118.77	124.10
3	F	401	HVS	O11-C10-C09	4.62	127.55	121.09
3	D	401	HVS	C12-C10-C09	-4.61	118.89	124.10
3	H	401	HVS	O11-C10-C09	4.58	127.50	121.09
3	I	401	HVS	O11-C10-C09	4.41	127.26	121.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	HVS	C12-C10-C09	-4.18	119.38	124.10
3	B	401	HVS	C12-C10-C09	-4.10	119.47	124.10
3	A	401	HVS	C12-C10-C09	-3.93	119.66	124.10
3	E	401	HVS	C12-C10-C09	-3.86	119.74	124.10
3	C	401	HVS	C12-C10-C09	-3.75	119.87	124.10
3	H	401	HVS	C12-C10-C09	-3.67	119.96	124.10
3	I	401	HVS	C12-C10-C09	-3.50	120.14	124.10
3	E	401	HVS	O11-C10-C12	-2.16	111.84	114.89
3	F	401	HVS	C13-C12-C10	2.09	124.02	120.88
3	H	401	HVS	C13-C12-C10	2.04	123.93	120.88
3	G	401	HVS	C13-C12-C10	2.03	123.91	120.88
3	A	401	HVS	C17-C12-C13	-2.03	115.70	118.59

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	HVS	C03-C02-C09-C10
3	H	401	HVS	C09-C10-C12-C13
3	H	401	HVS	C09-C10-C12-C17
3	H	401	HVS	O11-C10-C12-C13
3	H	401	HVS	O11-C10-C12-C17
3	I	401	HVS	C09-C10-C12-C13
3	I	401	HVS	C09-C10-C12-C17
3	I	401	HVS	O11-C10-C12-C13
3	I	401	HVS	O11-C10-C12-C17
3	G	401	HVS	C01-C02-C09-C10
3	G	401	HVS	C03-C02-C09-C10
3	F	401	HVS	C09-C10-C12-C13
3	F	401	HVS	O11-C10-C12-C13
3	F	401	HVS	O11-C10-C12-C17
3	B	401	HVS	O11-C10-C12-C13
3	G	401	HVS	O11-C10-C12-C13
3	F	401	HVS	C09-C10-C12-C17
3	G	401	HVS	O11-C10-C12-C17
3	B	401	HVS	C09-C10-C12-C13
3	B	401	HVS	C09-C10-C12-C17
3	G	401	HVS	C09-C10-C12-C13
3	G	401	HVS	C09-C10-C12-C17
3	B	401	HVS	O11-C10-C12-C17
3	D	401	HVS	O11-C10-C12-C13
3	D	401	HVS	C09-C10-C12-C13

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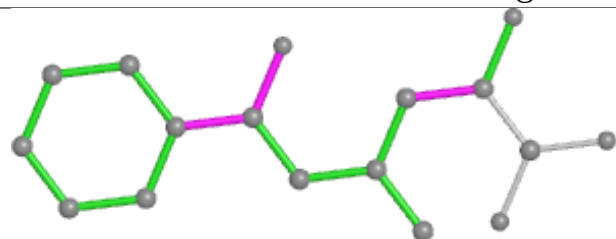
Mol	Chain	Res	Type	Atoms
3	D	401	HVS	O11-C10-C12-C17
3	D	401	HVS	C09-C10-C12-C17
3	A	401	HVS	O11-C10-C12-C13
3	A	401	HVS	O11-C10-C12-C17
3	A	401	HVS	C09-C10-C12-C17
3	A	401	HVS	C09-C10-C12-C13
3	A	401	HVS	C01-C02-C09-C10
3	E	401	HVS	C01-C02-C09-C10
3	B	401	HVS	C03-C02-C09-C10
3	D	401	HVS	C03-C02-C09-C10
3	C	401	HVS	C03-C02-C09-C10
3	E	401	HVS	C03-C02-C09-C10
3	C	401	HVS	O11-C10-C12-C13
3	C	401	HVS	O11-C10-C12-C17
3	I	401	HVS	C01-C02-C09-C10
3	D	401	HVS	C01-C02-C09-C10
3	C	401	HVS	C09-C10-C12-C17
3	I	401	HVS	C03-C02-C09-C10
3	C	401	HVS	C09-C10-C12-C13
3	E	401	HVS	O11-C10-C12-C13
3	E	401	HVS	C09-C10-C12-C17

There are no ring outliers.

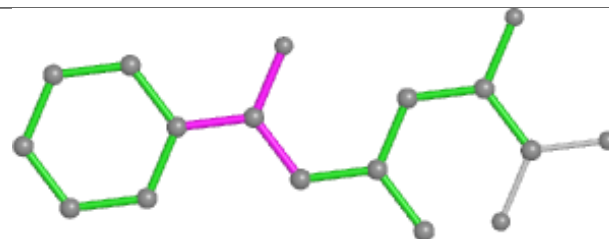
No monomer is involved in short contacts.

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.

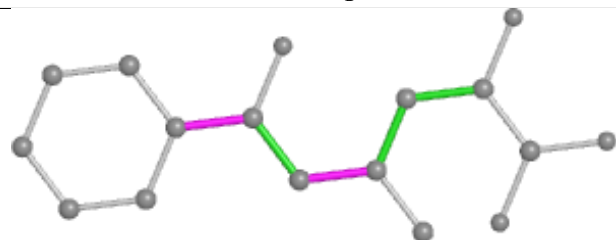
## Ligand HVS B 401



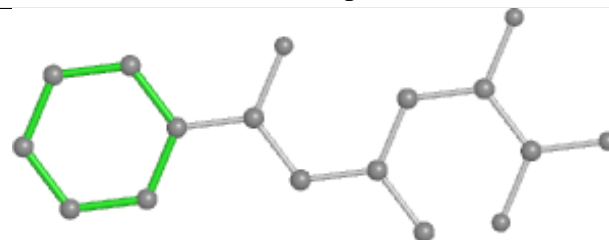
Bond lengths



Bond angles

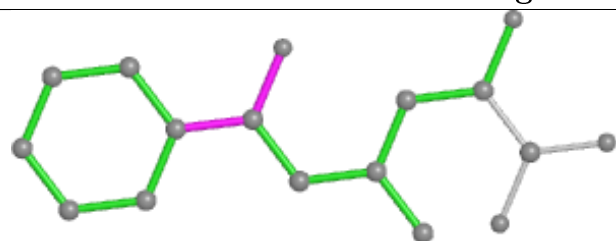


Torsions

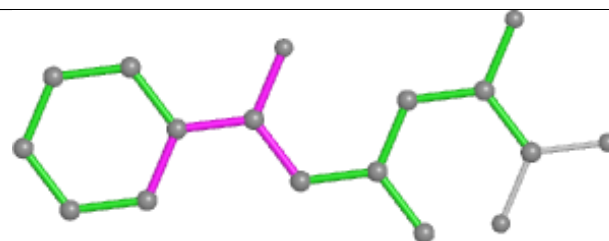


Rings

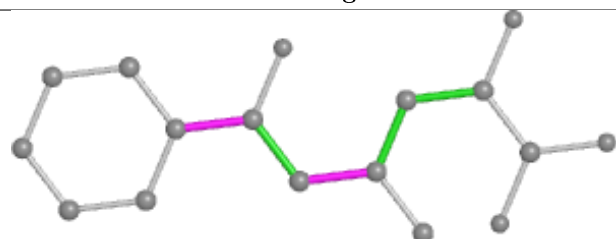
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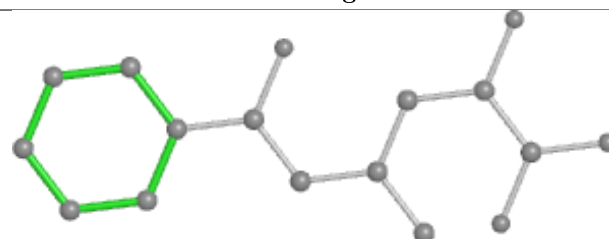
Bond lengths



Bond angles

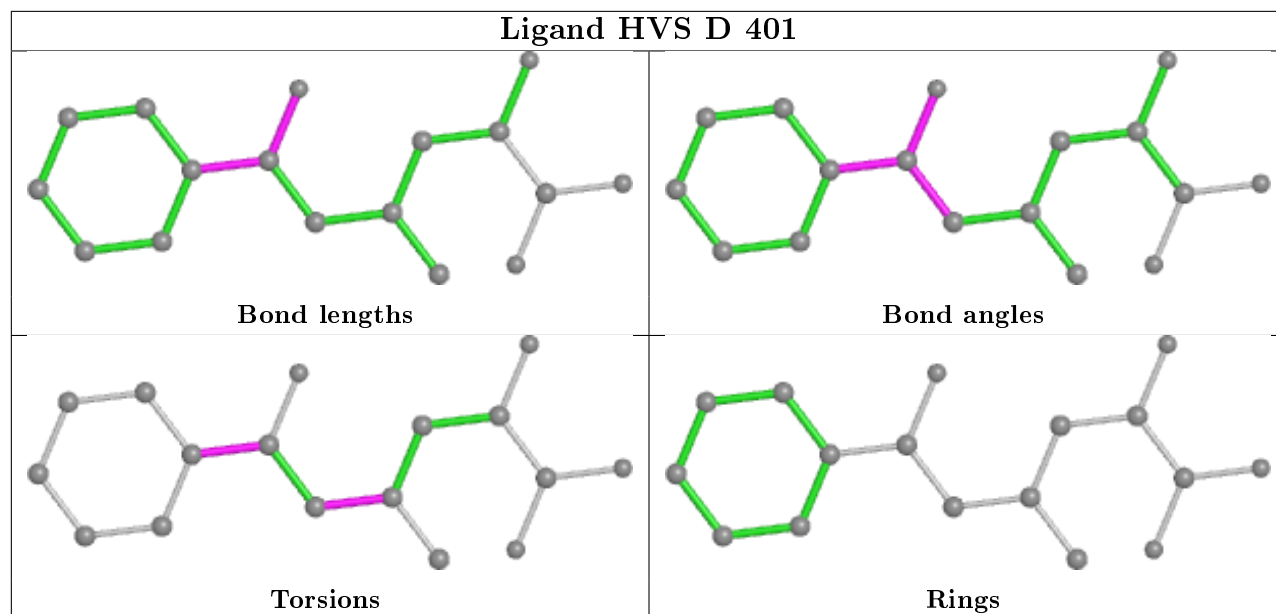


Torsions

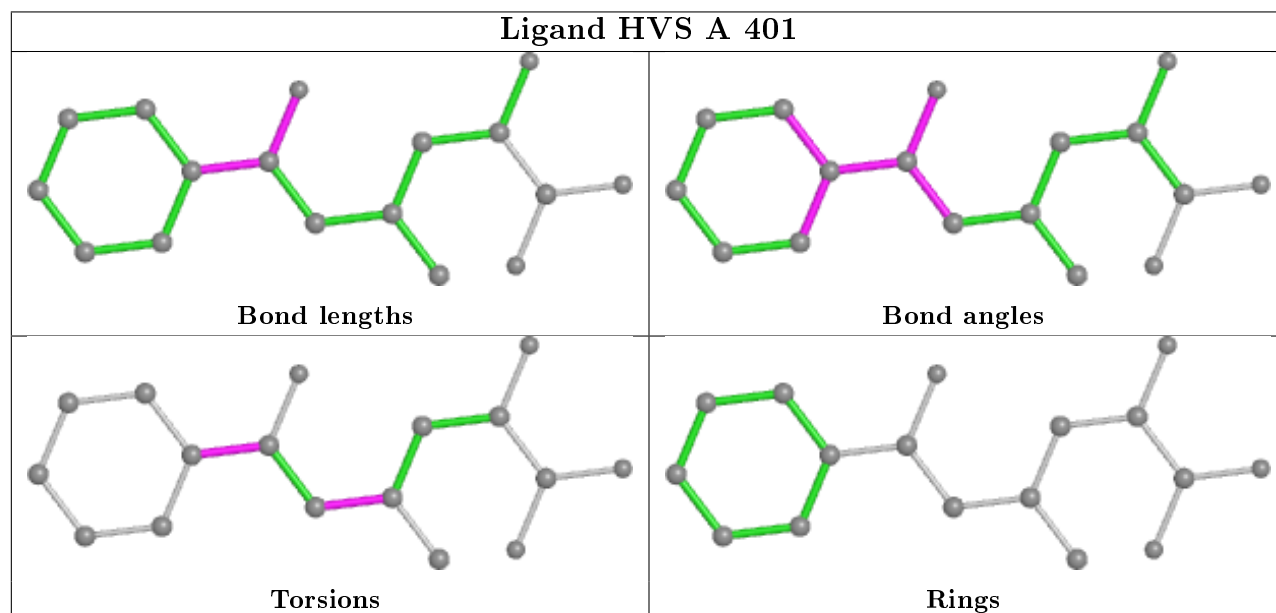


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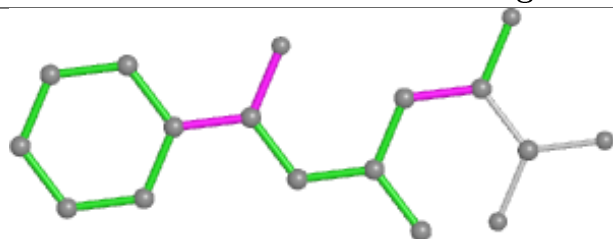
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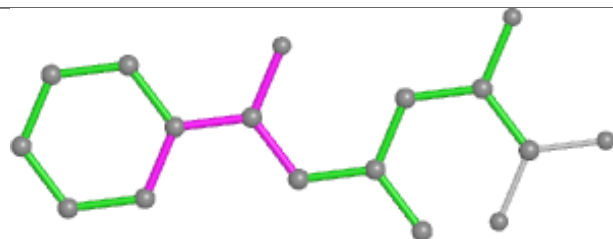
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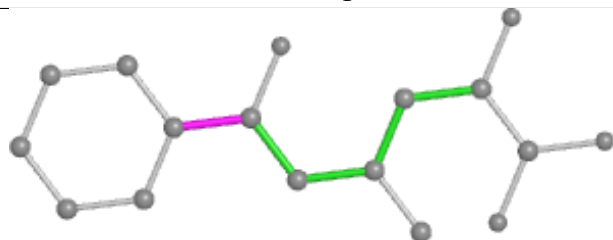
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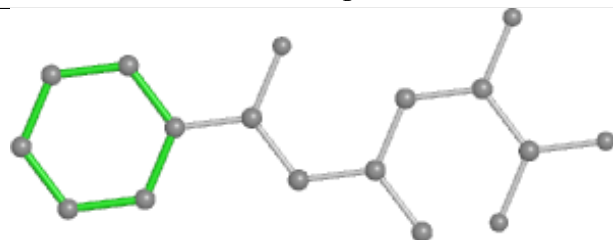
Bond lengths



Bond angles

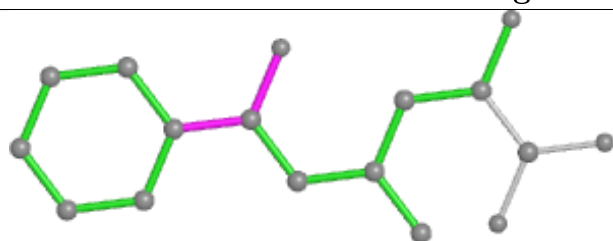


Torsions

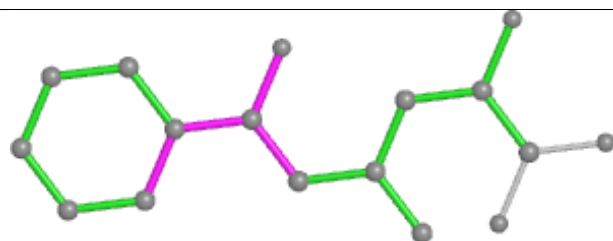


Rings

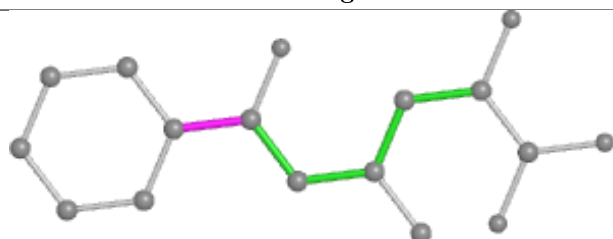
## Ligand HVS H 401



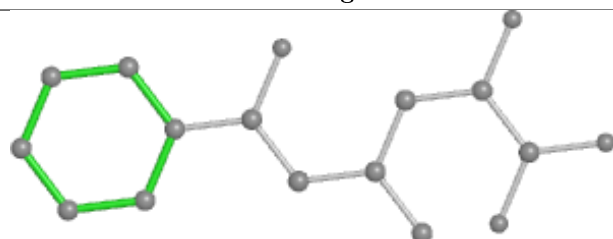
Bond lengths



Bond angles



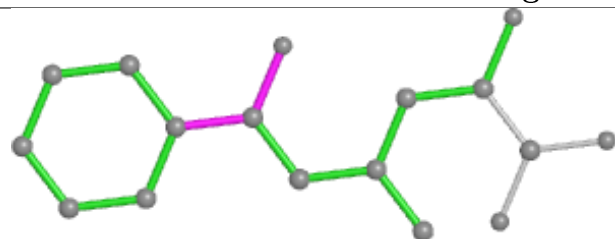
Torsions



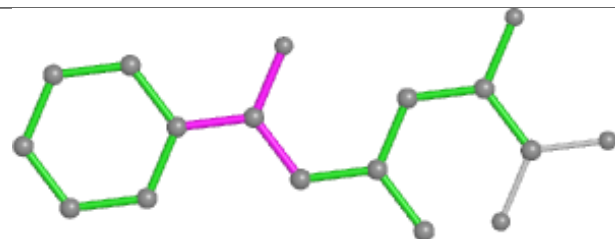
Rings



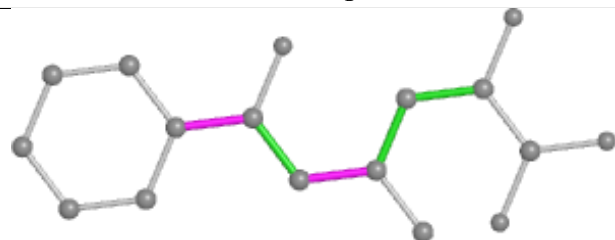
## Ligand HVS I 401



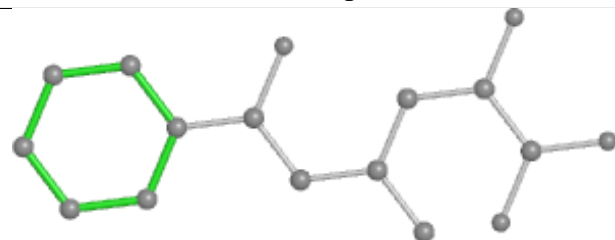
Bond lengths



Bond angles

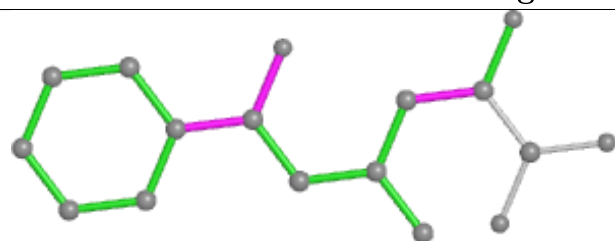


Torsions

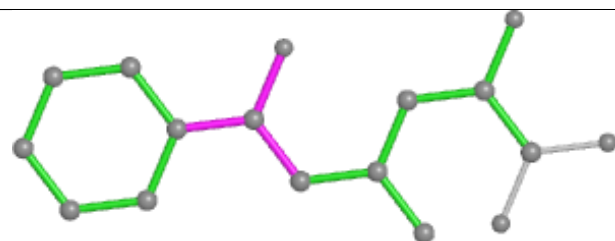


Rings

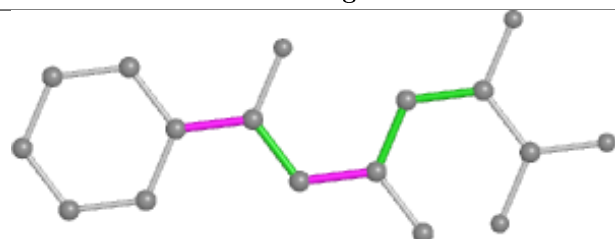
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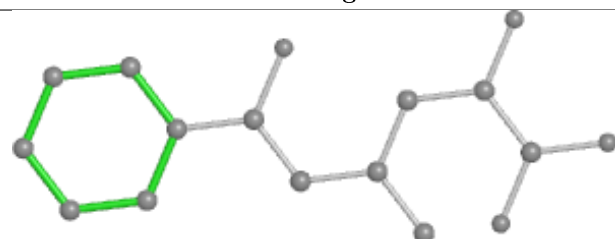
Bond lengths



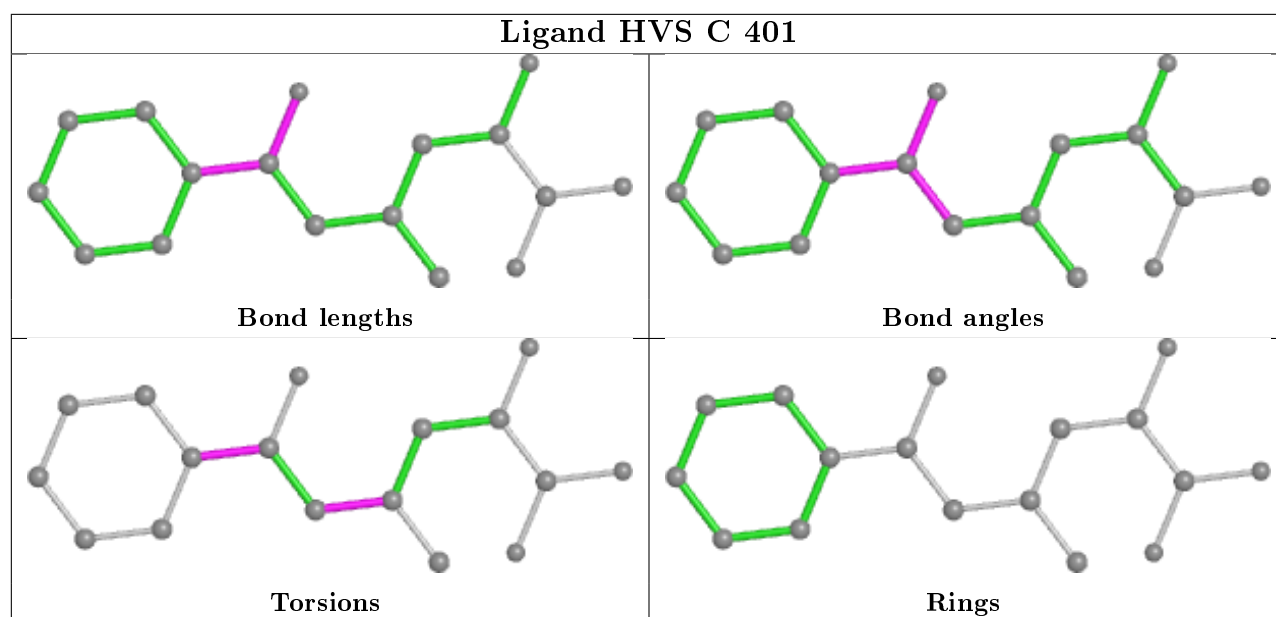
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	332/332 (100%)	0.48	30 (9%) 9 8	29, 44, 63, 98	0
1	B	332/332 (100%)	0.42	28 (8%) 11 10	27, 37, 63, 106	0
1	C	332/332 (100%)	0.72	40 (12%) 4 3	32, 53, 79, 112	0
1	D	332/332 (100%)	0.37	23 (6%) 16 15	30, 44, 66, 109	0
1	E	332/332 (100%)	0.37	18 (5%) 25 24	28, 39, 59, 102	0
1	F	331/332 (99%)	0.35	20 (6%) 21 20	29, 43, 64, 102	0
1	G	331/332 (99%)	0.60	34 (10%) 6 6	30, 47, 73, 111	0
1	H	331/332 (99%)	0.71	36 (10%) 5 5	31, 49, 74, 112	0
1	I	332/332 (100%)	0.68	40 (12%) 4 3	30, 46, 68, 100	0
All	All	2985/2988 (99%)	0.52	269 (9%) 9 8	27, 44, 70, 112	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	332	VAL	16.6
1	C	332	VAL	8.6
1	D	332	VAL	8.5
1	E	332	VAL	8.5
1	G	292	PRO	7.7
1	A	332	VAL	7.3
1	I	292	PRO	7.0
1	H	42	ILE	6.1
1	H	41	ILE	6.0
1	B	295	GLY	5.8
1	C	160	ARG	5.8
1	B	50	THR	5.3
1	C	243	LYS	5.2
1	B	178	ILE	5.2
1	I	104	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	H	309	ASP	5.0
1	I	309	ASP	5.0
1	I	332	VAL	4.8
1	A	227	ALA	4.7
1	D	331	GLU	4.6
1	A	209	SER	4.5
1	C	178	ILE	4.5
1	D	227	ALA	4.4
1	H	44	ALA	4.4
1	G	44	ALA	4.3
1	I	293	ALA	4.3
1	E	227	ALA	4.1
1	A	178	ILE	4.1
1	H	292	PRO	4.1
1	G	42	ILE	4.1
1	I	39	GLU	4.1
1	H	45	ALA	4.1
1	G	195	ILE	4.0
1	B	331[A]	GLU	4.0
1	B	241	ARG	3.9
1	I	34	VAL	3.9
1	C	50	THR	3.9
1	C	227	ALA	3.9
1	F	331	GLU	3.8
1	H	195	ILE	3.8
1	I	244	HIS	3.8
1	A	195	ILE	3.7
1	G	244	HIS	3.7
1	F	49	GLU	3.7
1	H	312	SER	3.7
1	C	226	GLY	3.7
1	G	41	ILE	3.7
1	C	290	ILE	3.6
1	A	312	SER	3.6
1	A	194	PHE	3.6
1	E	222	SER	3.6
1	E	245	LEU	3.6
1	H	294	THR	3.5
1	C	241	ARG	3.5
1	F	221	VAL	3.5
1	C	195	ILE	3.4
1	I	179	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	194	PHE	3.4
1	G	241	ARG	3.4
1	C	223	HIS	3.4
1	C	222	SER	3.3
1	E	163	TYR	3.3
1	B	307	LYS	3.3
1	H	32	GLY	3.3
1	C	293	ALA	3.3
1	F	179	HIS	3.3
1	B	227	ALA	3.2
1	E	241	ARG	3.2
1	H	102	THR	3.2
1	C	191	SER	3.2
1	C	180	ALA	3.2
1	C	194	PHE	3.2
1	G	309	ASP	3.2
1	G	312	SER	3.2
1	E	242	SER	3.1
1	D	106	GLU	3.1
1	H	30	GLY	3.1
1	I	243	LYS	3.1
1	B	49	GLU	3.1
1	C	179	HIS	3.1
1	C	307	LYS	3.1
1	G	121	PRO	3.1
1	B	226	GLY	3.1
1	C	252	LYS	3.0
1	B	198	GLU	3.0
1	I	227	ALA	3.0
1	A	226	GLY	3.0
1	A	191	SER	3.0
1	I	43	ALA	3.0
1	I	136	GLY	3.0
1	D	221	VAL	2.9
1	E	221	VAL	2.9
1	I	106	GLU	2.9
1	C	199	THR	2.9
1	I	103	LEU	2.9
1	F	311	LEU	2.9
1	H	180	ALA	2.9
1	G	258	VAL	2.9
1	C	295	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	315	ASP	2.9
1	H	160	ARG	2.9
1	I	5	CYS	2.9
1	D	179	HIS	2.9
1	A	307	LYS	2.8
1	H	241	ARG	2.8
1	H	36	VAL	2.8
1	C	60	HIS	2.8
1	F	255	PHE	2.8
1	H	133	VAL	2.8
1	A	179	HIS	2.8
1	A	223	HIS	2.8
1	E	223	HIS	2.8
1	C	30	GLY	2.7
1	C	311	LEU	2.7
1	A	198	GLU	2.7
1	C	331	GLU	2.7
1	G	6	HIS	2.7
1	H	60	HIS	2.7
1	A	242	SER	2.7
1	C	198	GLU	2.7
1	I	258	VAL	2.7
1	I	37	THR	2.7
1	H	258	VAL	2.7
1	I	286	VAL	2.7
1	G	315	ASP	2.7
1	I	180	ALA	2.7
1	A	190	TYR	2.7
1	B	221	VAL	2.7
1	F	106	GLU	2.7
1	C	192	LEU	2.7
1	G	291	ASP	2.7
1	G	192	LEU	2.6
1	F	238	GLN	2.6
1	A	180	ALA	2.6
1	H	244	HIS	2.6
1	F	227	ALA	2.6
1	G	179	HIS	2.6
1	A	295	GLY	2.6
1	A	56	ILE	2.6
1	D	209	SER	2.6
1	G	227	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	273	GLY	2.6
1	H	307	LYS	2.6
1	B	293	ALA	2.6
1	I	245	LEU	2.6
1	C	56	ILE	2.6
1	I	195	ILE	2.6
1	I	306	GLN	2.6
1	H	179	HIS	2.6
1	B	215	PRO	2.5
1	E	215	PRO	2.5
1	A	266	ARG	2.5
1	A	6	HIS	2.5
1	F	202	THR	2.5
1	H	227	ALA	2.5
1	G	226	GLY	2.5
1	A	222	SER	2.5
1	G	191	SER	2.5
1	G	314	ALA	2.5
1	H	192	LEU	2.5
1	B	48	LYS	2.5
1	D	293	ALA	2.5
1	H	226	GLY	2.5
1	G	178	ILE	2.4
1	C	139	GLY	2.4
1	G	45	ALA	2.4
1	D	222	SER	2.4
1	C	163	TYR	2.4
1	C	177	HIS	2.4
1	E	238	GLN	2.4
1	H	308	PHE	2.4
1	E	331	GLU	2.4
1	E	212	ASP	2.4
1	I	319	ILE	2.4
1	H	57	GLU	2.4
1	G	180	ALA	2.4
1	I	178	ILE	2.4
1	A	60	HIS	2.4
1	A	221	VAL	2.4
1	G	160	ARG	2.3
1	D	6	HIS	2.3
1	D	1	MET	2.3
1	E	214	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	50	THR	2.3
1	I	192	LEU	2.3
1	D	255	PHE	2.3
1	B	190	TYR	2.3
1	G	293	ALA	2.3
1	C	266	ARG	2.3
1	D	223	HIS	2.3
1	G	243	LYS	2.3
1	A	7	GLY	2.3
1	A	193	HIS	2.3
1	G	30	GLY	2.3
1	C	141	LEU	2.3
1	I	221	VAL	2.3
1	I	198	GLU	2.3
1	H	136	GLY	2.2
1	B	163	TYR	2.2
1	B	191	SER	2.2
1	B	142	LEU	2.2
1	G	196	ASN	2.2
1	D	212	ASP	2.2
1	H	299	ASP	2.2
1	C	209	SER	2.2
1	D	178	ILE	2.2
1	F	178	ILE	2.2
1	C	308	PHE	2.2
1	A	192	LEU	2.2
1	I	61	ASN	2.2
1	G	198	GLU	2.2
1	F	163	TYR	2.2
1	F	190	TYR	2.2
1	B	6	HIS	2.2
1	F	6	HIS	2.2
1	H	314	ALA	2.2
1	I	317	LYS	2.2
1	B	177	HIS	2.2
1	D	196	ASN	2.2
1	E	202	THR	2.2
1	D	7	GLY	2.2
1	D	224	GLY	2.2
1	E	156	PRO	2.2
1	B	141	LEU	2.2
1	H	177	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	6	HIS	2.1
1	G	163	TYR	2.1
1	H	212	ASP	2.1
1	D	292	PRO	2.1
1	F	144	PRO	2.1
1	I	121	PRO	2.1
1	I	308	PHE	2.1
1	I	307	LYS	2.1
1	E	224	GLY	2.1
1	I	273	GLY	2.1
1	F	192	LEU	2.1
1	C	6	HIS	2.1
1	B	5	CYS	2.1
1	B	7	GLY	2.1
1	B	296	LYS	2.1
1	C	48	LYS	2.1
1	C	176	ALA	2.1
1	D	144	PRO	2.1
1	F	222	SER	2.1
1	D	313	ASP	2.1
1	G	61	ASN	2.1
1	C	230	TYR	2.1
1	I	190	TYR	2.1
1	G	5	CYS	2.1
1	I	48	LYS	2.1
1	E	194	PHE	2.1
1	B	292	PRO	2.1
1	I	13	VAL	2.1
1	D	177	HIS	2.1
1	G	177	HIS	2.1
1	D	194	PHE	2.1
1	G	35	LYS	2.1
1	F	309	ASP	2.0
1	H	6	HIS	2.0
1	B	195	ILE	2.0
1	I	331	GLU	2.0
1	F	56	ILE	2.0
1	A	160	ARG	2.0
1	C	190	TYR	2.0
1	F	310	PHE	2.0
1	I	241	ARG	2.0
1	A	293	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	33	GLY	2.0
1	A	296	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

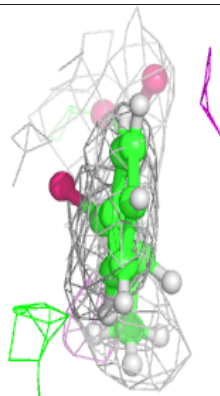
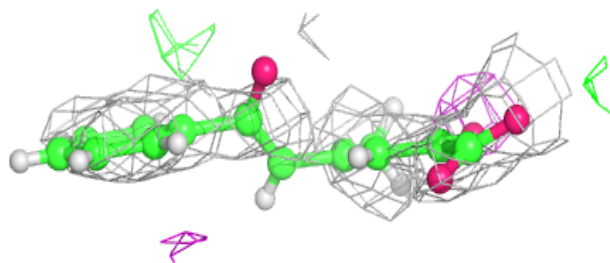
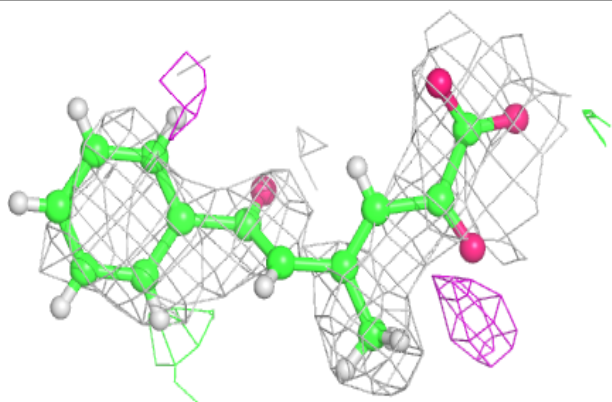
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HVS	I	401	17/17	0.81	0.30	43,70,84,84	0
3	HVS	D	401	17/17	0.85	0.53	36,45,54,54	27
3	HVS	H	401	17/17	0.89	0.27	39,62,75,75	0
3	HVS	F	401	17/17	0.90	0.24	39,60,72,73	0
3	HVS	B	401	17/17	0.90	0.23	33,54,65,66	0
3	HVS	E	401	17/17	0.90	0.28	34,56,68,69	0
3	HVS	C	401	17/17	0.93	0.24	42,62,75,75	0
3	HVS	G	401	17/17	0.93	0.23	38,59,72,72	0
3	HVS	A	401	17/17	0.94	0.23	38,56,67,67	0
2	ZN	C	400	1/1	0.97	0.07	33,33,33,33	0
2	ZN	A	400	1/1	0.97	0.11	29,29,29,29	0
2	ZN	H	400	1/1	0.98	0.10	32,32,32,32	0
2	ZN	G	400	1/1	0.99	0.10	30,30,30,30	0
2	ZN	I	400	1/1	0.99	0.11	29,29,29,29	0
2	ZN	E	400	1/1	0.99	0.12	29,29,29,29	0
2	ZN	D	400	1/1	0.99	0.11	30,30,30,30	0
2	ZN	B	400	1/1	0.99	0.11	26,26,26,26	0
2	ZN	F	400	1/1	0.99	0.11	31,31,31,31	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.

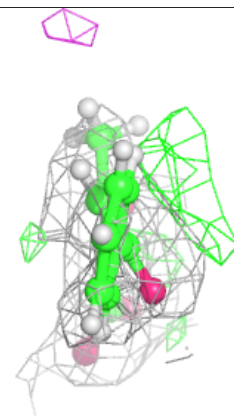
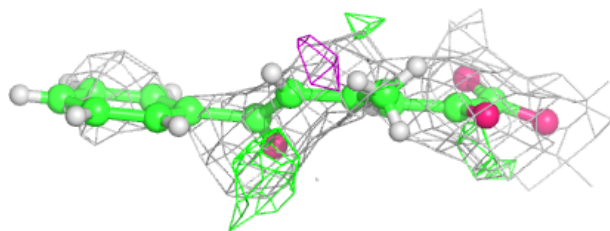
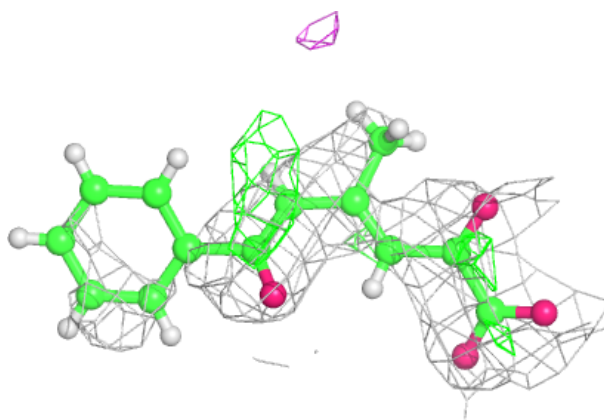
**Electron density around HVS I 401:**

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

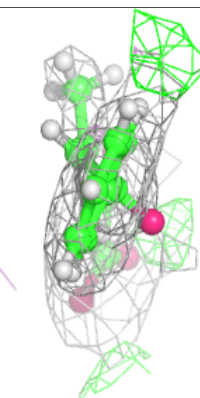
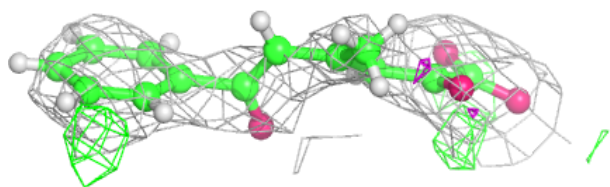
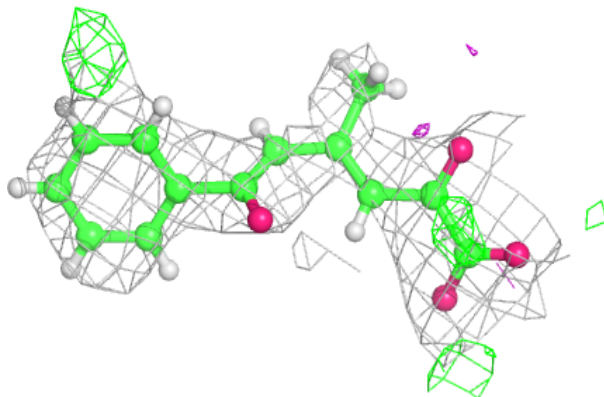


**Electron density around HVS D 401:**

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

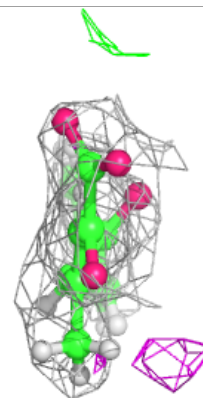
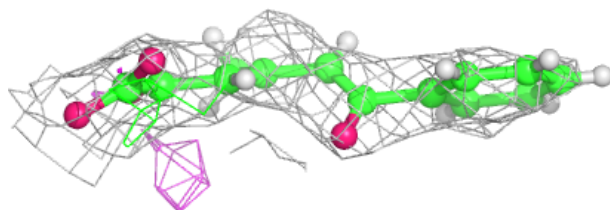
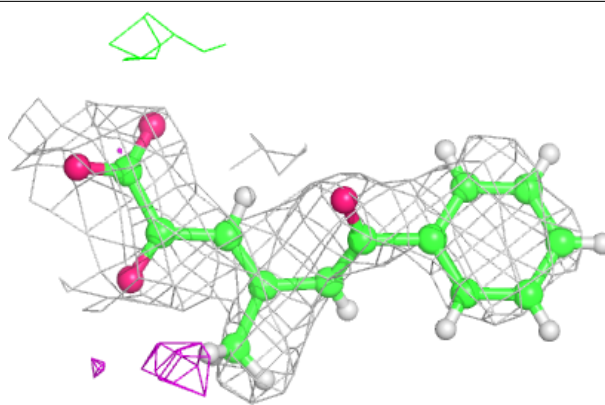
**Electron density around HVS H 401:**

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

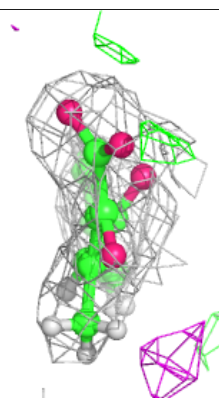
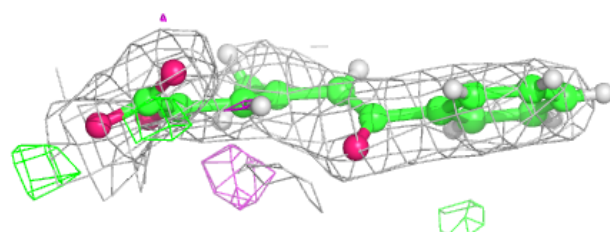
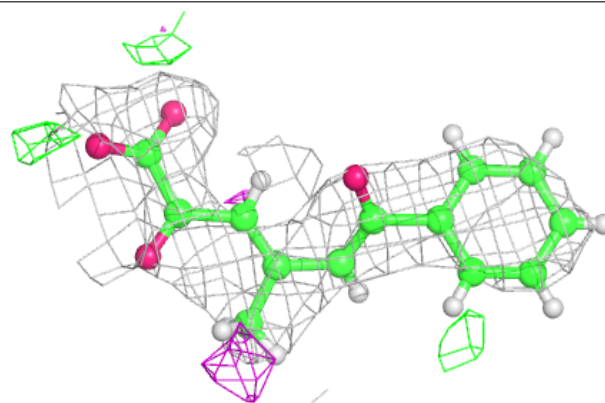


**Electron density around HVS F 401:**

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

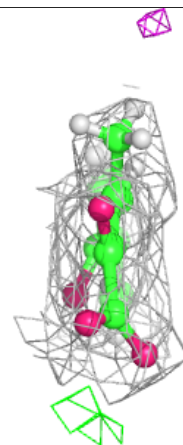
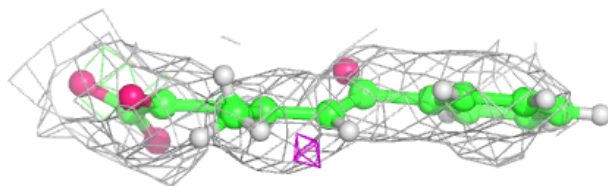
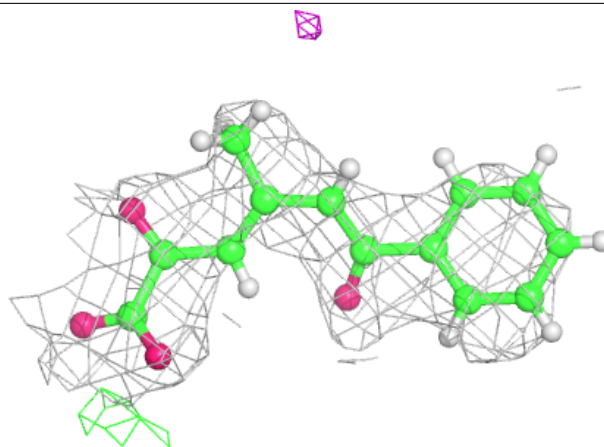
**Electron density around HVS B 401:**

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

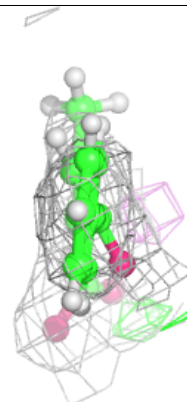
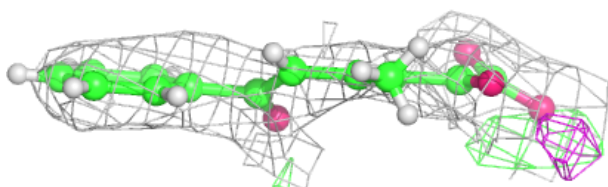
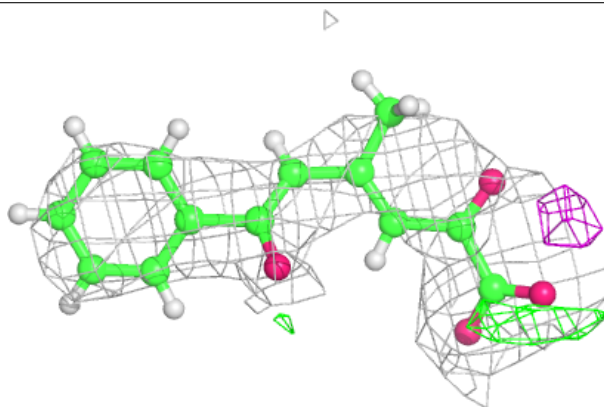


**Electron density around HVS E 401:**

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

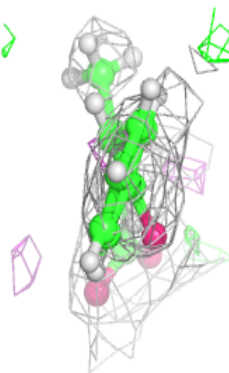
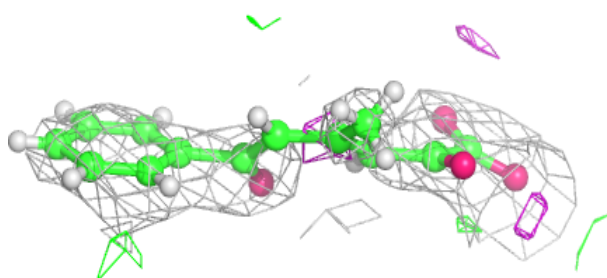
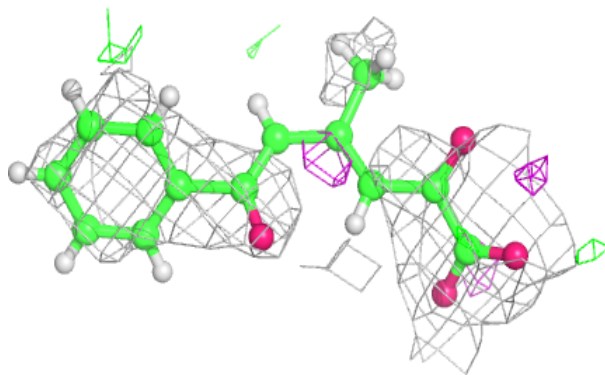
**Electron density around HVS C 401:**

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

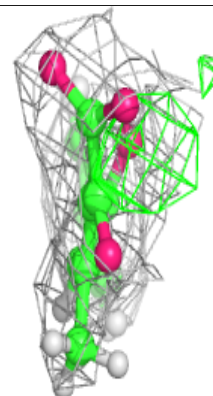
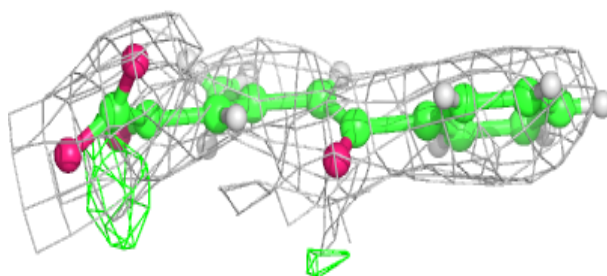
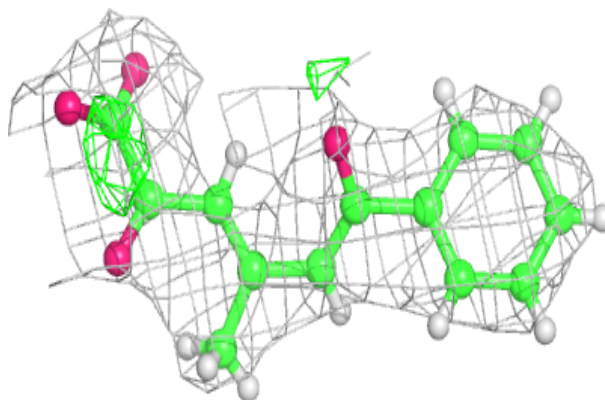


**Electron density around HVS G 401:**

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

**Electron density around HVS A 401:**

$2mF_o-DF_c$  (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.