



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 11:42 PM JST

PDB ID : 7YHC  
Title : Crystal structure of VIM-2 MBL in complex with 3-(4-(3-aminophenyl)-1H-1,2,3-triazol-1-yl)phthalic acid  
Authors : Li, G.-B.; Yan, Y.-H.  
Deposited on : 2022-07-13  
Resolution : 2.15 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-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

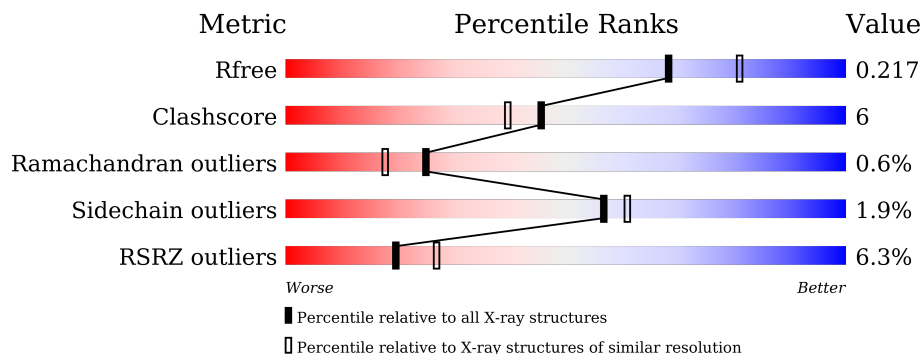
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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.



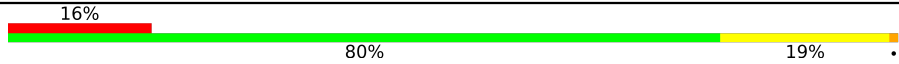

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	231	
1	B	231	
1	C	231	
1	D	231	
1	E	231	
1	F	231	

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Mol	Chain	Length	Quality of chain
1	G	231	 <p>16% 80% 19%</p>
1	H	231	 <p>10% 86% 14%</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14725 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 Beta-lactamase class B VIM-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	231	1733	1094	299	339	1	0	0	0
1	B	231	1733	1094	299	339	1	0	0	0
1	C	231	1733	1094	299	339	1	0	0	0
1	D	231	1733	1094	299	339	1	0	0	0
1	E	231	1733	1094	299	339	1	0	0	0
1	F	231	1733	1094	299	339	1	0	0	0
1	G	231	1733	1094	299	339	1	0	0	0
1	H	231	1733	1094	299	339	1	0	0	0

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

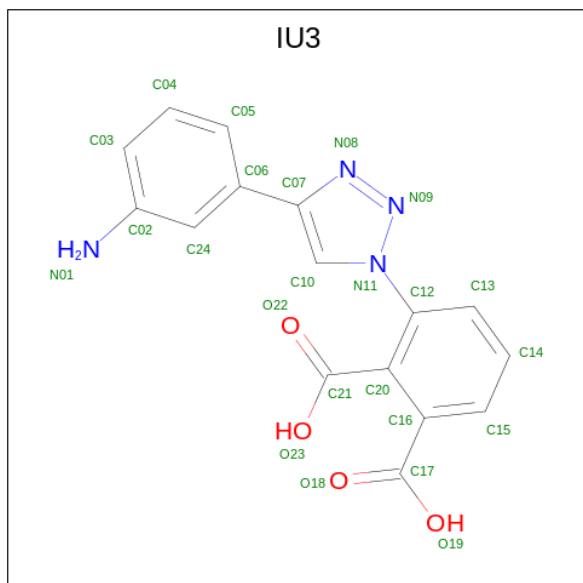
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0

- Molecule 3 is 3-[4-(3-aminophenyl)-1,2,3-triazol-1-yl]phthalic acid (three-letter code: IU3) (formula: C<sub>16</sub>H<sub>12</sub>N<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 24 16 4 4	0	0
3	B	1	Total C N O 24 16 4 4	0	0
3	C	1	Total C N O 24 16 4 4	0	0
3	D	1	Total C N O 24 16 4 4	0	0
3	E	1	Total C N O 24 16 4 4	0	0
3	F	1	Total C N O 24 16 4 4	0	0
3	G	1	Total C N O 24 16 4 4	0	0
3	H	1	Total C N O 24 16 4 4	0	0

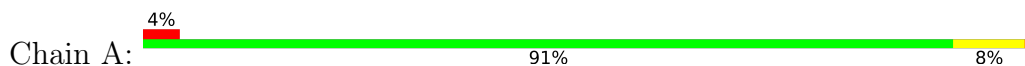
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	102	Total 102	O 102	0	0
4	B	68	Total 68	O 68	0	0
4	C	101	Total 101	O 101	0	0
4	D	98	Total 98	O 98	0	0
4	E	89	Total 89	O 89	0	0
4	F	87	Total 87	O 87	0	0
4	G	45	Total 45	O 45	0	0
4	H	63	Total 63	O 63	0	0

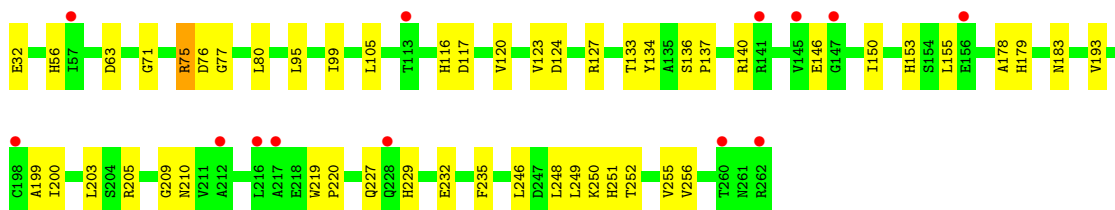
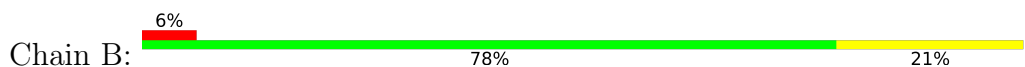
### 3 Residue-property plots [i](#)

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.

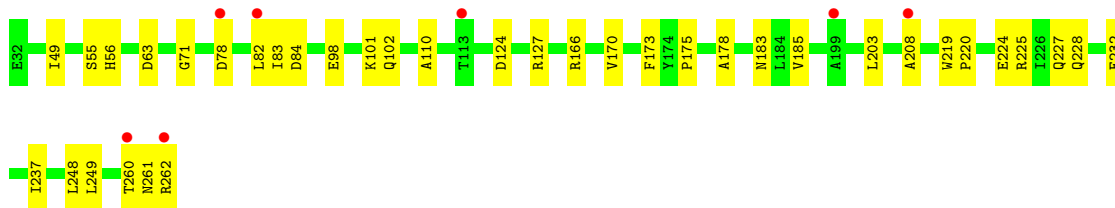
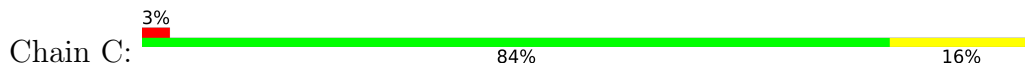
- Molecule 1: Beta-lactamase class B VIM-2



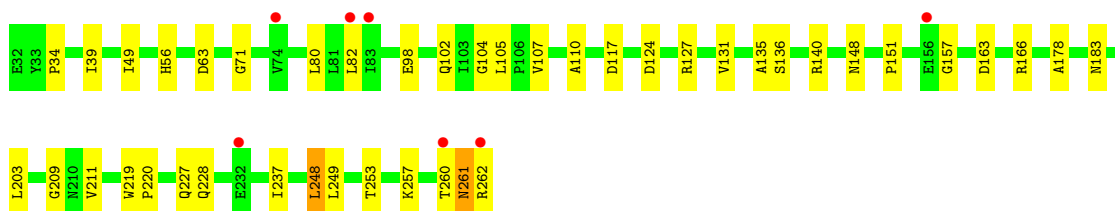
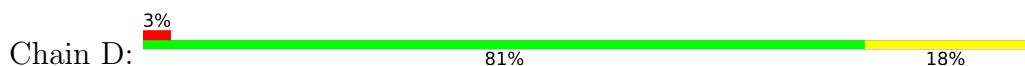
- Molecule 1: Beta-lactamase class B VIM-2



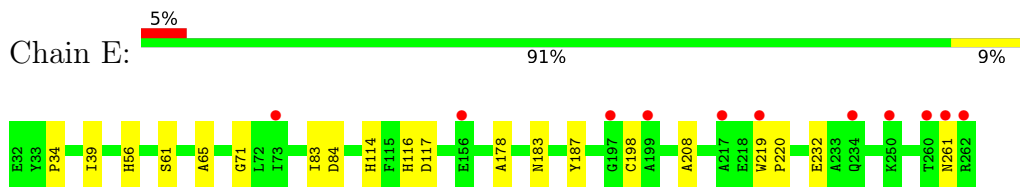
- Molecule 1: Beta-lactamase class B VIM-2



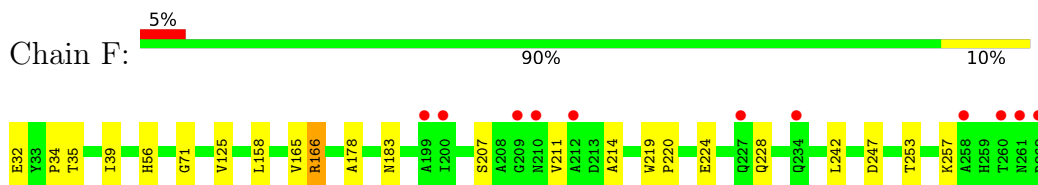
- Molecule 1: Beta-lactamase class B VIM-2



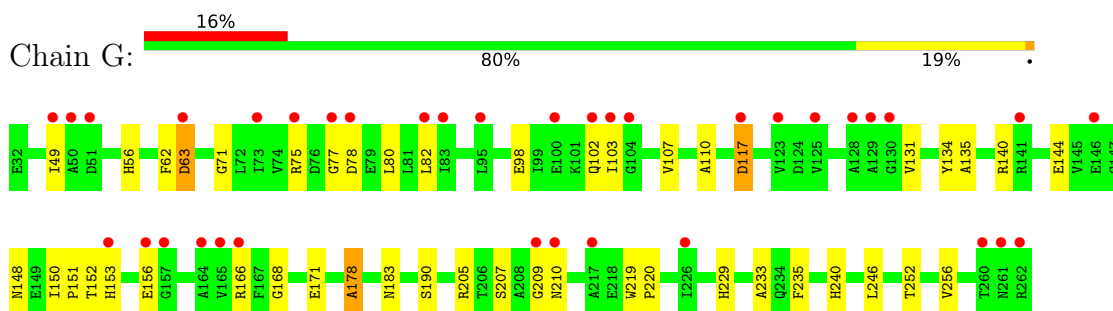
- Molecule 1: Beta-lactamase class B VIM-2



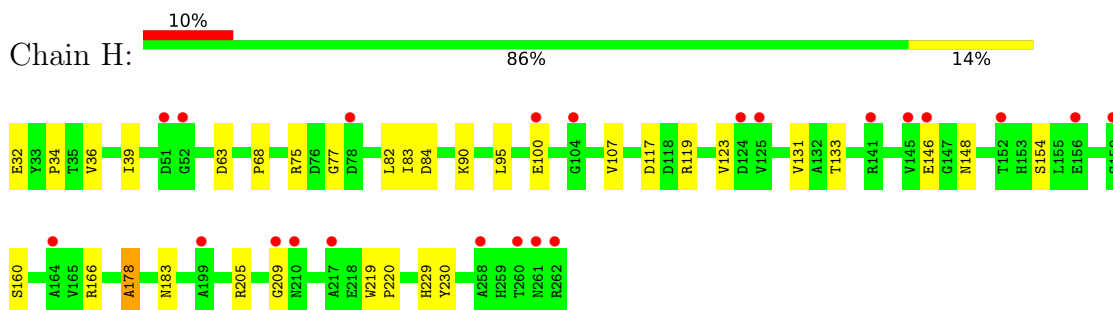
- Molecule 1: Beta-lactamase class B VIM-2



- Molecule 1: Beta-lactamase class B VIM-2



- Molecule 1: Beta-lactamase class B VIM-2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.24Å 246.24Å 88.28Å 90.00° 93.95° 90.00°	Depositor
Resolution (Å)	19.83 – 2.15 19.83 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.83-2.15) 98.4 (19.83-2.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.15Å)	Xtrriage
Refinement program	PHENIX 1.10.1	Depositor
R, $R_{free}$	0.172 , 0.217 0.173 , 0.217	Depositor DCC
$R_{free}$ test set	1996 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtrriage
Anisotropy	0.316	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 52.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14725	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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 51.05 % 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 5.9275e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, IU3

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	0/1774	0.60	0/2429
1	B	0.37	0/1774	0.55	0/2429
1	C	0.40	0/1774	0.59	0/2429
1	D	0.39	0/1774	0.58	1/2429 (0.0%)
1	E	0.39	0/1774	0.56	0/2429
1	F	0.38	0/1774	0.58	0/2429
1	G	0.36	0/1774	0.53	0/2429
1	H	0.38	0/1774	0.55	0/2429
All	All	0.39	0/14192	0.57	1/19432 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	248	LEU	CA-CB-CG	5.32	127.53	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1733	0	1676	14	1
1	B	1733	0	1676	37	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1733	0	1676	21	0
1	D	1733	0	1676	31	0
1	E	1733	0	1676	10	1
1	F	1733	0	1676	13	1
1	G	1733	0	1676	34	0
1	H	1733	0	1676	17	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	24	0	0	0	0
3	B	24	0	0	3	0
3	C	24	0	0	0	0
3	D	24	0	0	4	0
3	E	24	0	0	3	0
3	F	24	0	0	1	0
3	G	24	0	0	4	0
3	H	24	0	0	3	0
4	A	102	0	0	2	1
4	B	68	0	0	4	0
4	C	101	0	0	1	0
4	D	98	0	0	4	0
4	E	89	0	0	2	0
4	F	87	0	0	3	0
4	G	45	0	0	1	0
4	H	63	0	0	1	0
All	All	14725	0	13408	176	3

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 6.

All (176) 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:A:205:ARG:HH21	1:A:209:GLY:HA3	1.33	0.94
3:D:303:IU3:N01	4:D:401:HOH:O	2.08	0.86
1:D:124:ASP:OD1	1:D:127:ARG:NH2	2.09	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LEU:HG	1:B:248:LEU:HD21	1.61	0.82
1:D:203:LEU:HG	1:D:248:LEU:HD22	1.62	0.82
1:C:224:GLU:O	1:C:228:GLN:HG2	1.78	0.81
1:A:205:ARG:NH2	1:A:209:GLY:HA3	1.94	0.81
1:C:98:GLU:OE2	1:C:102:GLN:NE2	2.13	0.80
1:C:203:LEU:HG	1:C:248:LEU:HD22	1.65	0.78
1:A:203:LEU:HG	1:A:248:LEU:HD22	1.67	0.77
1:B:203:LEU:HG	1:B:248:LEU:CD2	2.17	0.74
1:F:35:THR:HG22	1:F:242:LEU:HD21	1.70	0.74
3:F:303:IU3:N01	4:F:401:HOH:O	2.21	0.73
1:G:98:GLU:OE2	1:G:102:GLN:NE2	2.21	0.70
1:D:228:GLN:HG3	1:G:190:SER:OG	1.91	0.70
1:B:250:LYS:NZ	4:B:401:HOH:O	2.23	0.70
3:E:303:IU3:N01	4:E:401:HOH:O	2.24	0.69
1:G:117:ASP:HB2	3:G:303:IU3:C24	2.22	0.69
1:G:75:ARG:HA	1:G:80:LEU:HD23	1.74	0.69
1:A:124:ASP:OD1	1:A:127:ARG:NH2	2.26	0.68
1:B:117:ASP:OD2	3:B:303:IU3:N01	2.27	0.68
1:E:261:ASN:ND2	4:E:402:HOH:O	2.26	0.67
1:B:116:HIS:O	1:B:120:VAL:HG22	1.96	0.66
1:H:123:VAL:HG13	1:H:133:THR:HG21	1.79	0.65
1:B:246:LEU:CD2	1:B:249:LEU:HD22	2.28	0.64
1:G:156:GLU:HA	1:G:156:GLU:OE1	1.96	0.64
1:A:203:LEU:HG	1:A:248:LEU:CD2	2.29	0.63
1:B:252:THR:O	1:B:256:VAL:HG23	1.99	0.62
1:F:34:PRO:HB2	1:F:39:ILE:HD11	1.82	0.62
1:A:205:ARG:NH2	1:A:208:ALA:O	2.32	0.61
1:C:261:ASN:ND2	4:C:402:HOH:O	2.32	0.61
1:B:227:GLN:HE22	1:B:246:LEU:HD13	1.65	0.61
1:G:140:ARG:NH2	1:G:152:THR:O	2.31	0.61
1:D:261:ASN:ND2	4:D:403:HOH:O	2.30	0.60
1:F:32:GLU:N	4:F:402:HOH:O	2.33	0.60
1:G:210:ASN:ND2	3:G:303:IU3:O23	2.34	0.60
1:G:75:ARG:HH12	1:G:77:GLY:HA2	1.67	0.60
1:H:148:ASN:OD1	3:H:303:IU3:N01	2.35	0.60
1:D:117:ASP:OD1	3:D:303:IU3:N01	2.34	0.60
1:B:32:GLU:N	4:B:403:HOH:O	2.34	0.60
1:G:62:PHE:CD1	1:G:63:ASP:HB2	2.38	0.58
1:D:104:GLY:O	4:D:402:HOH:O	2.17	0.58
1:G:166:ARG:NH1	1:G:168:GLY:O	2.37	0.57
1:C:56:HIS:CE1	1:C:71:GLY:HA3	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:117:ASP:OD2	3:H:303:IU3:N01	2.37	0.57
1:G:56:HIS:CE1	1:G:71:GLY:HA3	2.40	0.57
1:H:34:PRO:HB2	1:H:39:ILE:HD11	1.87	0.57
1:C:56:HIS:NE2	1:C:71:GLY:HA3	2.21	0.56
1:G:80:LEU:HD11	1:G:103:ILE:HG21	1.88	0.56
1:E:219:TRP:HB3	1:E:220:PRO:HD3	1.88	0.55
1:B:124:ASP:OD1	1:B:127:ARG:NH2	2.39	0.55
1:A:231:PRO:O	1:A:246:LEU:HD11	2.06	0.55
1:A:201:TYR:O	1:A:248:LEU:HD13	2.07	0.55
1:C:49:ILE:HD13	1:C:237:ILE:HD11	1.88	0.55
1:C:173:PHE:HB3	1:C:185:VAL:CG2	2.36	0.54
1:G:107:VAL:O	1:G:131:VAL:HG22	2.07	0.54
1:B:75:ARG:HD2	1:B:77:GLY:O	2.08	0.54
1:C:124:ASP:OD1	1:C:127:ARG:NH2	2.40	0.54
1:G:82:LEU:O	1:G:110:ALA:HA	2.07	0.54
1:C:203:LEU:HG	1:C:248:LEU:CD2	2.35	0.53
1:B:136:SER:O	1:B:140:ARG:HG3	2.08	0.53
1:B:56:HIS:CE1	1:B:71:GLY:HA3	2.44	0.53
1:D:228:GLN:HG3	1:G:190:SER:CB	2.39	0.52
1:E:56:HIS:CE1	1:E:71:GLY:HA3	2.44	0.52
1:A:56:HIS:NE2	1:A:71:GLY:HA3	2.24	0.52
1:B:219:TRP:HB3	1:B:220:PRO:HD3	1.92	0.52
1:D:148:ASN:OD1	3:D:303:IU3:N01	2.43	0.51
1:D:56:HIS:CE1	1:D:71:GLY:HA3	2.45	0.51
1:H:75:ARG:NH1	1:H:77:GLY:O	2.43	0.51
1:H:229:HIS:HD2	1:H:230:TYR:CZ	2.27	0.51
1:D:107:VAL:O	1:D:131:VAL:HG22	2.10	0.51
1:G:233:ALA:HB3	1:G:246:LEU:HD21	1.92	0.51
1:B:232:GLU:HG3	1:B:232:GLU:O	2.10	0.51
1:D:56:HIS:NE2	1:D:71:GLY:HA3	2.26	0.51
1:H:146:GLU:O	1:H:146:GLU:HG3	2.10	0.51
1:D:209:GLY:H	1:D:211:VAL:HG13	1.76	0.51
1:B:75:ARG:HG3	1:B:76:ASP:N	2.26	0.51
1:F:247:ASP:N	1:F:247:ASP:OD1	2.42	0.51
1:H:107:VAL:O	1:H:131:VAL:HG22	2.11	0.50
1:B:203:LEU:CD2	1:B:248:LEU:HD23	2.41	0.50
1:B:210:ASN:ND2	4:B:404:HOH:O	2.38	0.50
1:H:178:ALA:HB1	1:H:219:TRP:CD1	2.47	0.50
1:D:203:LEU:HG	1:D:248:LEU:CD2	2.38	0.50
1:H:205:ARG:HH21	1:H:209:GLY:HA3	1.75	0.50
1:B:123:VAL:HG13	1:B:133:THR:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ILE:HD13	1:D:237:ILE:HD11	1.92	0.50
1:B:193:VAL:HG22	1:B:235:PHE:HB3	1.94	0.49
1:G:171:GLU:OE1	1:G:229:HIS:HE1	1.95	0.49
1:D:117:ASP:H	3:D:303:IU3:C24	2.24	0.49
1:F:253:THR:HG22	1:F:257:LYS:HD2	1.94	0.49
1:G:56:HIS:NE2	1:G:71:GLY:HA3	2.28	0.48
1:G:49:ILE:HG12	1:G:235:PHE:CE2	2.48	0.48
1:G:75:ARG:NH1	1:G:77:GLY:HA2	2.26	0.48
1:A:228:GLN:NE2	4:A:404:HOH:O	2.43	0.48
1:B:227:GLN:NE2	1:B:246:LEU:HD13	2.29	0.48
1:A:261:ASN:ND2	4:A:407:HOH:O	2.47	0.48
1:B:56:HIS:NE2	1:B:71:GLY:HA3	2.29	0.47
1:D:98:GLU:OE2	1:D:102:GLN:NE2	2.47	0.47
1:G:117:ASP:H	3:G:303:IU3:C24	2.28	0.47
1:B:134:TYR:CD2	1:B:153:HIS:HB2	2.49	0.47
1:B:150:ILE:HD12	1:B:150:ILE:N	2.30	0.47
1:D:253:THR:HG23	1:D:257:LYS:HE3	1.97	0.47
1:G:134:TYR:CD2	1:G:153:HIS:HB2	2.49	0.47
1:F:56:HIS:CE1	1:F:71:GLY:HA3	2.50	0.46
1:G:205:ARG:HH21	1:G:209:GLY:HA3	1.80	0.46
1:D:260:THR:C	1:D:262:ARG:H	2.17	0.46
1:F:211:VAL:HB	1:F:214:ALA:CB	2.45	0.46
1:E:34:PRO:HB2	1:E:39:ILE:HD11	1.97	0.46
1:H:119:ARG:HA	1:H:119:ARG:HD3	1.85	0.46
1:F:219:TRP:HB3	1:F:220:PRO:HD3	1.96	0.46
1:D:219:TRP:HB3	1:D:220:PRO:HD3	1.97	0.46
1:F:158:LEU:HD21	1:F:165:VAL:HG22	1.98	0.46
1:D:135:ALA:HB2	1:D:151:PRO:HG2	1.99	0.45
1:B:150:ILE:HD11	4:B:437:HOH:O	2.15	0.45
1:D:148:ASN:OD1	4:D:401:HOH:O	2.21	0.45
1:D:82:LEU:O	1:D:110:ALA:HA	2.17	0.45
1:D:80:LEU:HG	1:D:105:LEU:HB2	1.98	0.45
1:B:95:LEU:O	1:B:99:ILE:HG13	2.16	0.45
1:C:173:PHE:HB3	1:C:185:VAL:HG23	1.97	0.45
1:B:137:PRO:HD3	1:B:155:LEU:O	2.17	0.45
1:F:125:VAL:HG23	4:F:470:HOH:O	2.16	0.44
1:C:166:ARG:HD3	1:C:170:VAL:O	2.16	0.44
1:B:75:ARG:HA	1:B:80:LEU:HD23	1.98	0.44
1:B:146:GLU:O	1:B:146:GLU:HG3	2.17	0.44
1:D:136:SER:O	1:D:140:ARG:HG3	2.17	0.44
1:C:78:ASP:OD1	1:C:78:ASP:N	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:PRO:O	1:C:225:ARG:HD2	2.18	0.44
1:G:75:ARG:NH1	1:G:77:GLY:CA	2.80	0.44
1:H:117:ASP:H	3:H:303:IU3:C24	2.31	0.43
1:B:199:ALA:O	1:B:200:ILE:HD13	2.18	0.43
1:A:257:LYS:O	1:A:260:THR:HB	2.18	0.43
1:C:49:ILE:HD11	1:C:55:SER:HB3	2.01	0.43
1:C:219:TRP:HB3	1:C:220:PRO:HD3	2.01	0.43
1:E:56:HIS:NE2	1:E:71:GLY:HA3	2.33	0.43
1:E:61:SER:HA	1:E:65:ALA:O	2.19	0.43
1:B:251:HIS:O	1:B:255:VAL:HG23	2.18	0.43
1:D:63:ASP:OD2	1:F:207:SER:OG	2.29	0.43
1:E:116:HIS:HB3	3:E:303:IU3:N08	2.34	0.43
1:G:252:THR:O	1:G:256:VAL:HG23	2.18	0.43
1:F:211:VAL:HB	1:F:214:ALA:HB3	1.99	0.43
1:C:261:ASN:O	1:C:262:ARG:CB	2.67	0.42
1:C:83:ILE:O	1:C:84:ASP:HB2	2.19	0.42
1:H:32:GLU:HA	4:H:426:HOH:O	2.19	0.42
1:B:205:ARG:HH21	1:B:209:GLY:HA3	1.84	0.42
1:A:246:LEU:HD23	1:A:249:LEU:HD22	2.02	0.42
1:F:224:GLU:O	1:F:228:GLN:HG2	2.19	0.42
1:H:83:ILE:O	1:H:84:ASP:HB2	2.18	0.42
1:A:56:HIS:CE1	1:A:71:GLY:HA3	2.54	0.42
1:B:117:ASP:H	3:B:303:IU3:C24	2.32	0.42
1:G:78:ASP:N	1:G:78:ASP:OD1	2.52	0.42
1:B:179:HIS:HA	1:B:219:TRP:CZ3	2.54	0.42
1:C:227:GLN:HB2	1:C:249:LEU:HD23	2.02	0.42
1:E:114:HIS:HE1	1:E:198:CYS:SG	2.43	0.42
1:G:240:HIS:O	4:G:401:HOH:O	2.21	0.42
1:C:82:LEU:O	1:C:110:ALA:HA	2.20	0.42
1:D:209:GLY:HA2	1:D:211:VAL:N	2.35	0.42
1:H:219:TRP:HB3	1:H:220:PRO:HD3	2.02	0.42
1:G:135:ALA:HB2	1:G:151:PRO:HG2	2.02	0.41
1:G:178:ALA:HB1	1:G:219:TRP:CD1	2.54	0.41
1:D:166:ARG:HD2	1:D:166:ARG:HA	1.90	0.41
1:G:75:ARG:NH1	1:G:77:GLY:H	2.18	0.41
1:D:157:GLY:O	1:D:163:ASP:HB3	2.20	0.41
1:D:228:GLN:OE1	1:G:75:ARG:NH2	2.53	0.41
1:C:260:THR:C	1:C:262:ARG:H	2.23	0.41
1:D:227:GLN:HB2	1:D:249:LEU:HD23	2.01	0.41
1:G:148:ASN:OD1	3:G:303:IU3:N01	2.54	0.41
1:G:144:GLU:HA	1:G:150:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:VAL:HB	1:H:68:PRO:HG3	2.02	0.41
1:B:246:LEU:HD23	1:B:246:LEU:HA	1.90	0.41
1:D:34:PRO:HB2	1:D:39:ILE:HD11	2.03	0.41
1:E:83:ILE:O	1:E:84:ASP:HB2	2.19	0.41
1:E:117:ASP:OD1	3:E:303:IU3:N01	2.54	0.40
1:H:82:LEU:HD11	1:H:95:LEU:HD21	2.03	0.40
1:B:75:ARG:HD3	1:B:105:LEU:CD1	2.52	0.40
1:B:116:HIS:CD2	3:B:303:IU3:C05	3.04	0.40
1:G:219:TRP:HB3	1:G:220:PRO:HD3	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLU:OE2	1:E:187:TYR:OH[2_848]	2.05	0.15
1:A:229:HIS:O	1:F:166:ARG:NH1[2_848]	2.14	0.06
4:A:494:HOH:O	4:A:496:HOH:O[1_455]	2.15	0.05

## 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	229/231 (99%)	223 (97%)	5 (2%)	1 (0%)	34 29
1	B	229/231 (99%)	223 (97%)	5 (2%)	1 (0%)	34 29
1	C	229/231 (99%)	223 (97%)	4 (2%)	2 (1%)	17 11
1	D	229/231 (99%)	222 (97%)	5 (2%)	2 (1%)	17 11
1	E	229/231 (99%)	224 (98%)	3 (1%)	2 (1%)	17 11
1	F	229/231 (99%)	224 (98%)	4 (2%)	1 (0%)	34 29
1	G	229/231 (99%)	220 (96%)	8 (4%)	1 (0%)	34 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	229/231 (99%)	220 (96%)	8 (4%)	1 (0%)	34 29
All	All	1832/1848 (99%)	1779 (97%)	42 (2%)	11 (1%)	25 18

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	ALA
1	C	208	ALA
1	D	178	ALA
1	E	208	ALA
1	A	178	ALA
1	D	261	ASN
1	E	178	ALA
1	F	178	ALA
1	H	178	ALA
1	C	178	ALA
1	G	178	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	182/184 (99%)	178 (98%)	4 (2%)	52 55
1	B	182/184 (99%)	178 (98%)	4 (2%)	52 55
1	C	182/184 (99%)	178 (98%)	4 (2%)	52 55
1	D	182/184 (99%)	181 (100%)	1 (0%)	88 92
1	E	182/184 (99%)	180 (99%)	2 (1%)	73 78
1	F	182/184 (99%)	180 (99%)	2 (1%)	73 78
1	G	182/184 (99%)	178 (98%)	4 (2%)	52 55
1	H	182/184 (99%)	175 (96%)	7 (4%)	33 31
All	All	1456/1472 (99%)	1428 (98%)	28 (2%)	57 61

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	183	ASN
1	A	229	HIS
1	A	248	LEU
1	B	63	ASP
1	B	75	ARG
1	B	183	ASN
1	B	229	HIS
1	C	63	ASP
1	C	101	LYS
1	C	183	ASN
1	C	232	GLU
1	D	183	ASN
1	E	183	ASN
1	E	232	GLU
1	F	166	ARG
1	F	183	ASN
1	G	63	ASP
1	G	117	ASP
1	G	183	ASN
1	G	207	SER
1	H	63	ASP
1	H	90	LYS
1	H	100	GLU
1	H	154	SER
1	H	160	SER
1	H	166	ARG
1	H	183	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	227	GLN

### 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 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	IU3	E	303	2	23,26,26	1.36	3 (13%)	29,37,37	1.77	4 (13%)
3	IU3	A	303	2	23,26,26	1.34	4 (17%)	29,37,37	2.01	6 (20%)
3	IU3	D	303	2	23,26,26	1.32	3 (13%)	29,37,37	1.78	5 (17%)
3	IU3	C	303	2	23,26,26	1.31	3 (13%)	29,37,37	1.90	6 (20%)
3	IU3	G	303	2	23,26,26	1.52	3 (13%)	29,37,37	1.57	4 (13%)
3	IU3	B	303	2	23,26,26	1.36	3 (13%)	29,37,37	1.95	5 (17%)
3	IU3	H	303	2	23,26,26	1.44	4 (17%)	29,37,37	1.99	6 (20%)
3	IU3	F	303	2	23,26,26	1.32	4 (17%)	29,37,37	1.77	4 (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	IU3	E	303	2	-	1/16/16/16	0/3/3/3
3	IU3	A	303	2	-	2/16/16/16	0/3/3/3
3	IU3	D	303	2	-	0/16/16/16	0/3/3/3
3	IU3	C	303	2	-	1/16/16/16	0/3/3/3
3	IU3	G	303	2	-	1/16/16/16	0/3/3/3
3	IU3	B	303	2	-	2/16/16/16	0/3/3/3
3	IU3	H	303	2	-	3/16/16/16	0/3/3/3
3	IU3	F	303	2	-	0/16/16/16	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	303	IU3	N09-N11	-3.80	1.31	1.37
3	H	303	IU3	C06-C07	3.54	1.54	1.48
3	B	303	IU3	C06-C07	3.37	1.54	1.48
3	C	303	IU3	N09-N11	-3.32	1.32	1.37
3	D	303	IU3	N09-N11	-3.20	1.32	1.37
3	F	303	IU3	N09-N11	-3.15	1.32	1.37
3	B	303	IU3	N09-N11	-3.15	1.32	1.37
3	H	303	IU3	N09-N11	-3.15	1.32	1.37
3	D	303	IU3	C06-C07	3.04	1.53	1.48
3	A	303	IU3	C06-C07	2.94	1.53	1.48
3	G	303	IU3	C06-C07	2.92	1.53	1.48
3	E	303	IU3	N09-N11	-2.84	1.33	1.37
3	E	303	IU3	C02-N01	2.69	1.47	1.38
3	A	303	IU3	N09-N11	-2.65	1.33	1.37
3	H	303	IU3	C02-N01	2.63	1.47	1.38
3	G	303	IU3	C02-N01	2.61	1.47	1.38
3	E	303	IU3	C06-C07	2.57	1.53	1.48
3	H	303	IU3	C16-C17	2.55	1.55	1.49
3	A	303	IU3	C02-N01	2.55	1.47	1.38
3	F	303	IU3	C06-C07	2.41	1.52	1.48
3	B	303	IU3	C02-N01	2.34	1.46	1.38
3	A	303	IU3	C16-C17	2.33	1.54	1.49
3	C	303	IU3	C16-C17	2.25	1.54	1.49
3	C	303	IU3	C06-C07	2.15	1.52	1.48
3	F	303	IU3	C16-C17	2.11	1.54	1.49
3	F	303	IU3	C02-N01	2.11	1.45	1.38
3	D	303	IU3	C02-N01	2.01	1.45	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	IU3	C16-C20-C12	6.10	121.38	116.69
3	H	303	IU3	C16-C20-C12	6.06	121.35	116.69
3	D	303	IU3	C16-C20-C12	5.68	121.06	116.69
3	B	303	IU3	C16-C20-C12	5.62	121.01	116.69
3	C	303	IU3	C16-C20-C12	5.36	120.81	116.69
3	E	303	IU3	C16-C20-C12	5.28	120.75	116.69
3	C	303	IU3	C06-C07-N08	5.05	129.03	120.96
3	F	303	IU3	C16-C20-C12	4.97	120.51	116.69
3	B	303	IU3	C12-C20-C21	-4.94	116.10	122.41
3	A	303	IU3	C06-C07-N08	4.68	128.44	120.96
3	D	303	IU3	C13-C12-C20	-4.64	119.53	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	303	IU3	C13-C12-C20	-4.58	119.57	122.21
3	E	303	IU3	C06-C07-N08	4.53	128.20	120.96
3	A	303	IU3	C12-C20-C21	-4.41	116.77	122.41
3	F	303	IU3	C06-C07-N08	4.39	127.97	120.96
3	G	303	IU3	C16-C20-C12	4.27	119.97	116.69
3	H	303	IU3	C06-C07-N08	4.24	127.73	120.96
3	B	303	IU3	C13-C12-C20	-4.21	119.78	122.21
3	G	303	IU3	C13-C12-C20	-3.95	119.93	122.21
3	B	303	IU3	C06-C07-N08	3.91	127.20	120.96
3	H	303	IU3	C12-C20-C21	-3.85	117.48	122.41
3	F	303	IU3	C13-C12-C20	-3.42	120.23	122.21
3	E	303	IU3	C13-C12-C20	-3.36	120.27	122.21
3	A	303	IU3	C13-C12-C20	-3.30	120.30	122.21
3	D	303	IU3	C06-C07-N08	3.29	126.21	120.96
3	F	303	IU3	C12-C20-C21	-3.17	118.35	122.41
3	G	303	IU3	C06-C07-N08	2.96	125.69	120.96
3	C	303	IU3	C12-C20-C21	-2.66	119.00	122.41
3	D	303	IU3	C12-C20-C21	-2.55	119.16	122.41
3	A	303	IU3	O19-C17-O18	-2.53	117.72	123.35
3	G	303	IU3	C12-C20-C21	-2.50	119.21	122.41
3	E	303	IU3	C12-C20-C21	-2.45	119.27	122.41
3	C	303	IU3	C06-C24-C02	-2.43	118.56	120.66
3	D	303	IU3	O19-C17-O18	-2.40	118.02	123.35
3	C	303	IU3	O19-C17-O18	-2.34	118.15	123.35
3	H	303	IU3	O19-C17-C16	2.25	121.80	115.31
3	H	303	IU3	O19-C17-O18	-2.17	118.53	123.35
3	C	303	IU3	C20-C12-N11	-2.16	116.84	120.36
3	A	303	IU3	O19-C17-C16	2.01	121.10	115.31
3	B	303	IU3	O19-C17-O18	-2.01	118.88	123.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	303	IU3	C13-C12-N11-N09
3	G	303	IU3	C13-C12-N11-N09
3	A	303	IU3	C15-C16-C17-O18
3	A	303	IU3	C15-C16-C17-O19
3	H	303	IU3	C15-C16-C17-O19
3	B	303	IU3	C15-C16-C17-O19
3	C	303	IU3	C13-C12-N11-N09
3	H	303	IU3	C15-C16-C17-O18

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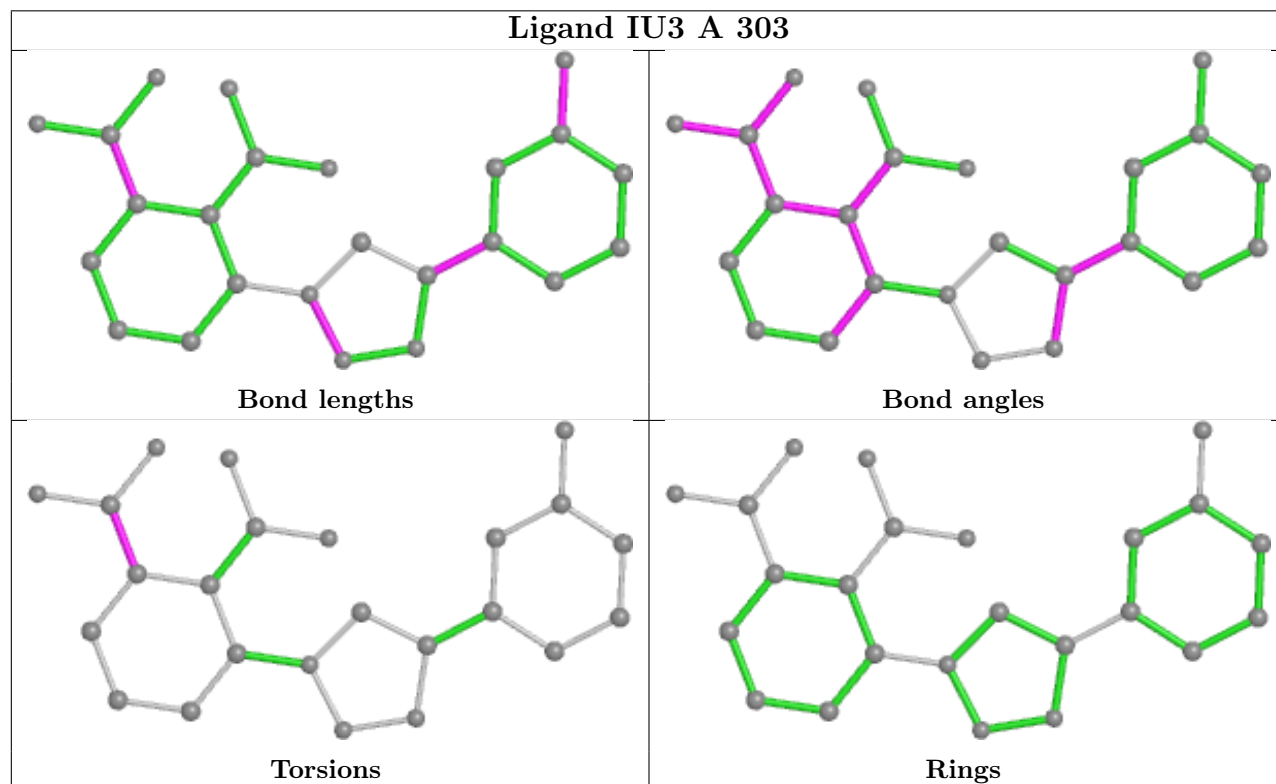
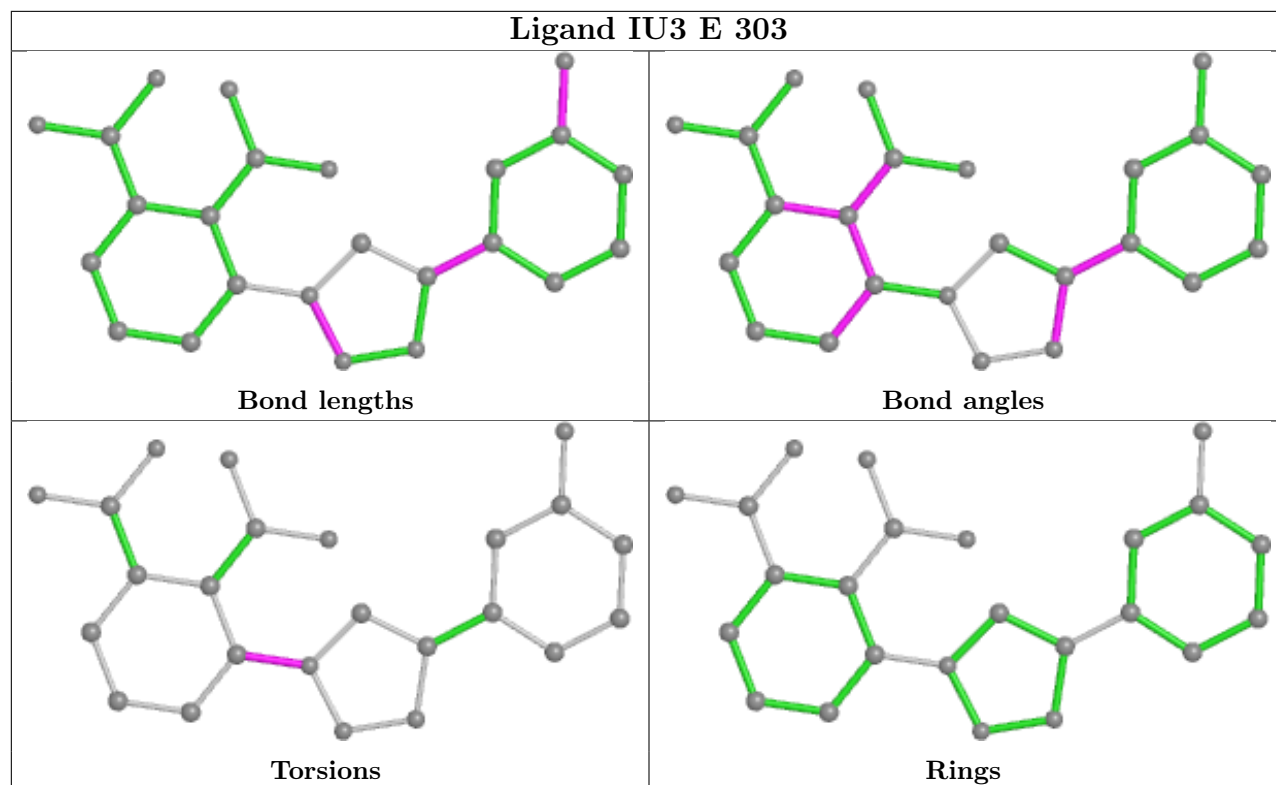
Mol	Chain	Res	Type	Atoms
3	B	303	IU3	C15-C16-C17-O18
3	H	303	IU3	C20-C16-C17-O19

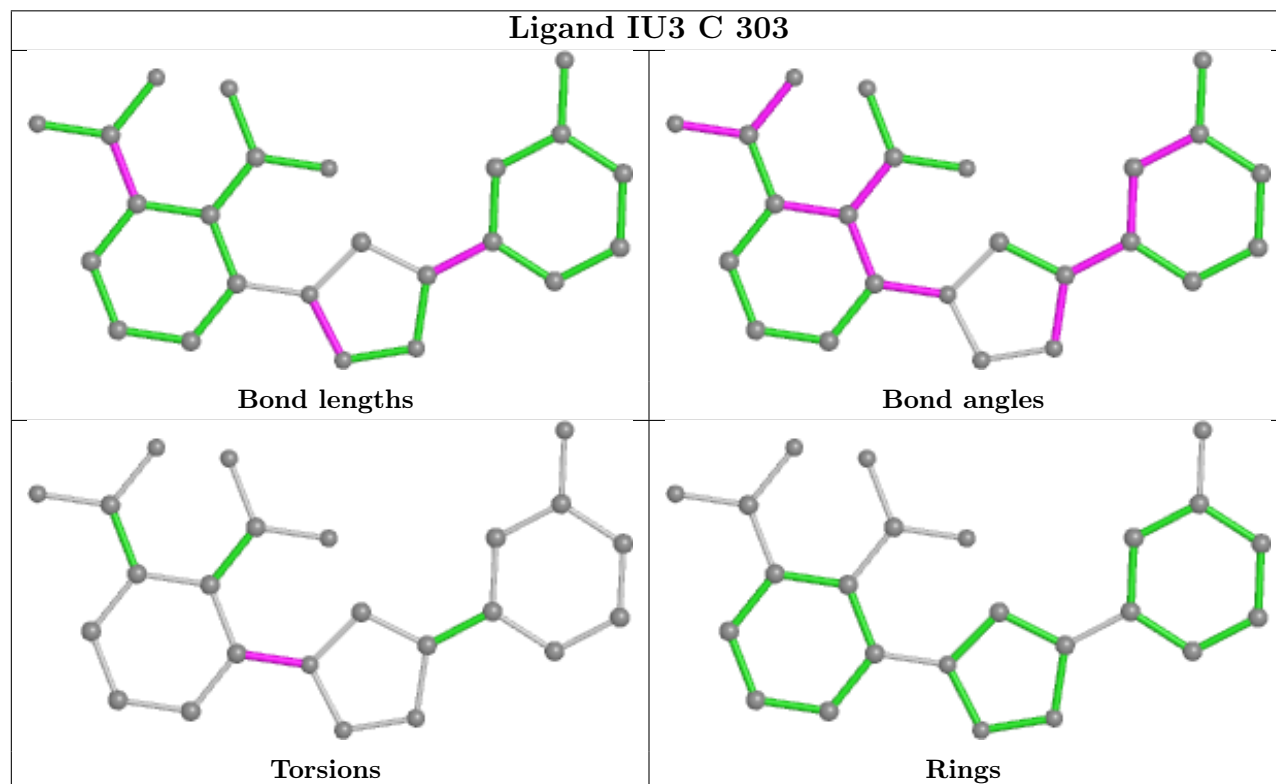
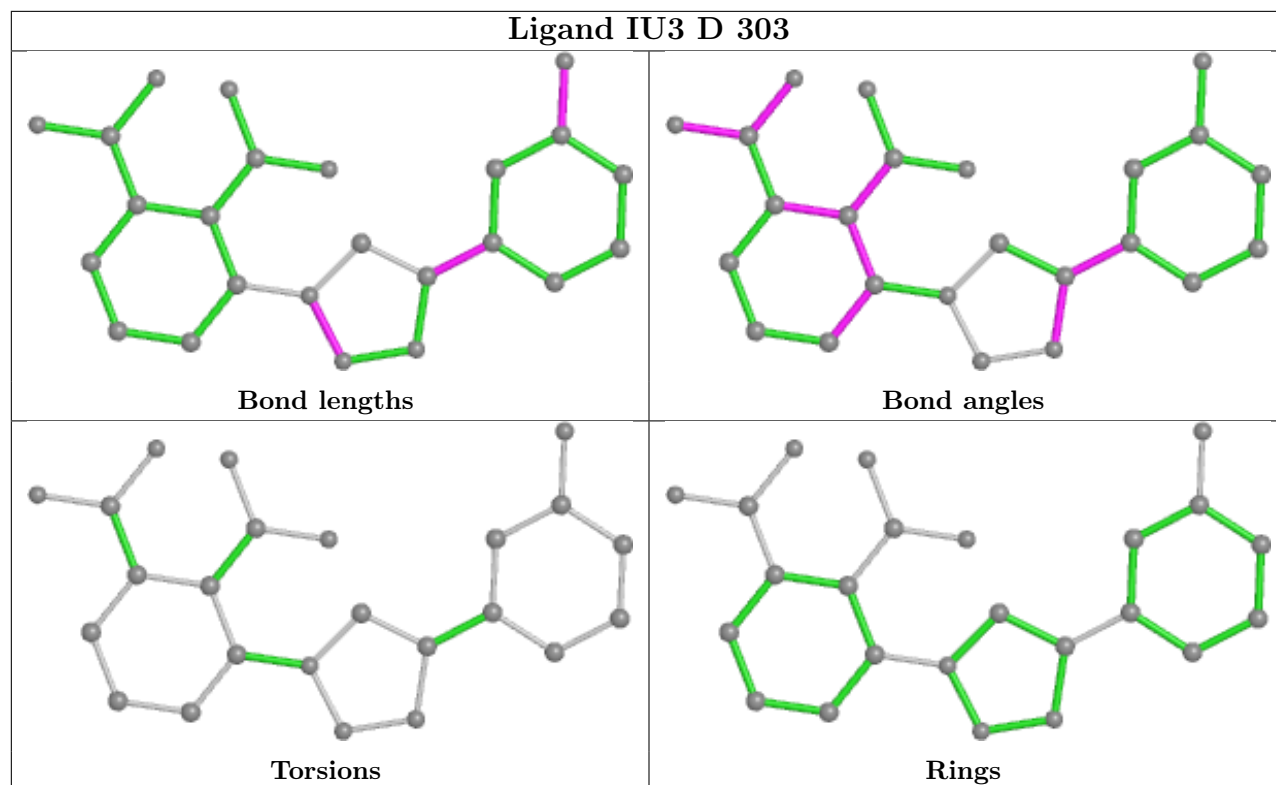
There are no ring outliers.

6 monomers are involved in 18 short contacts:

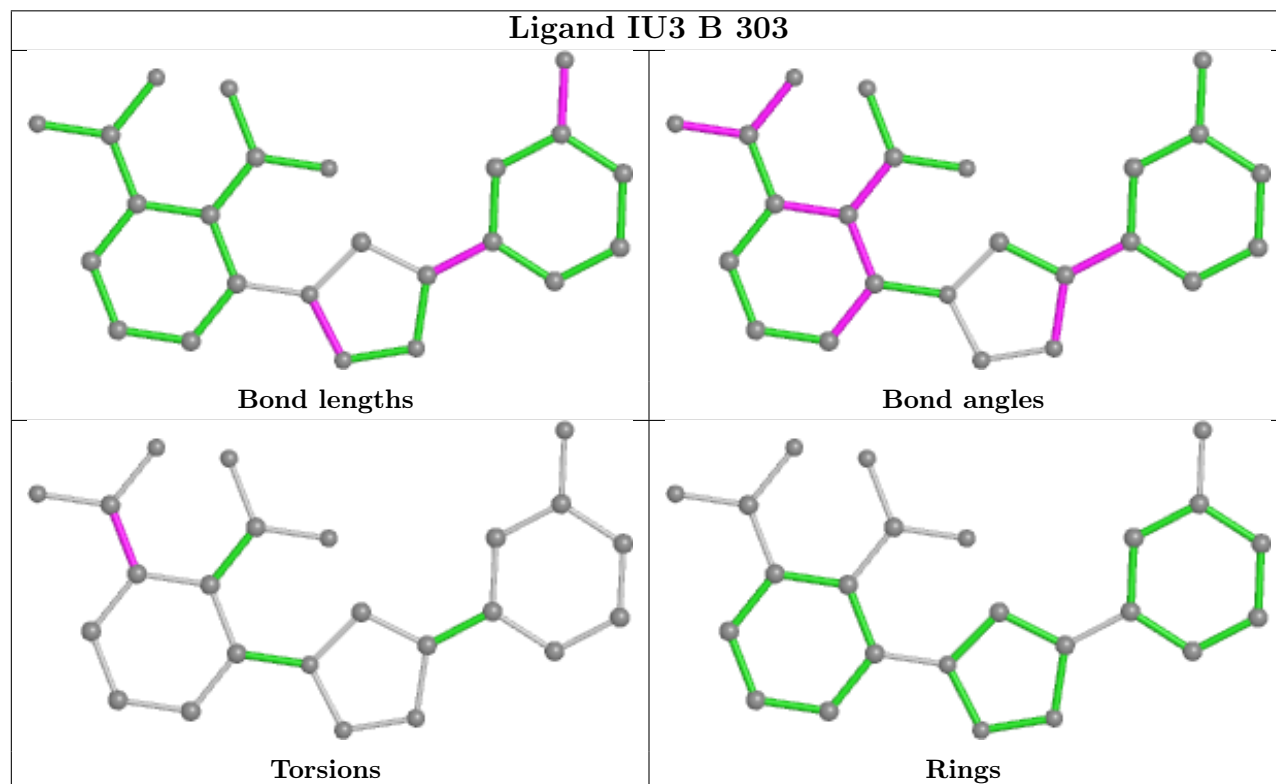
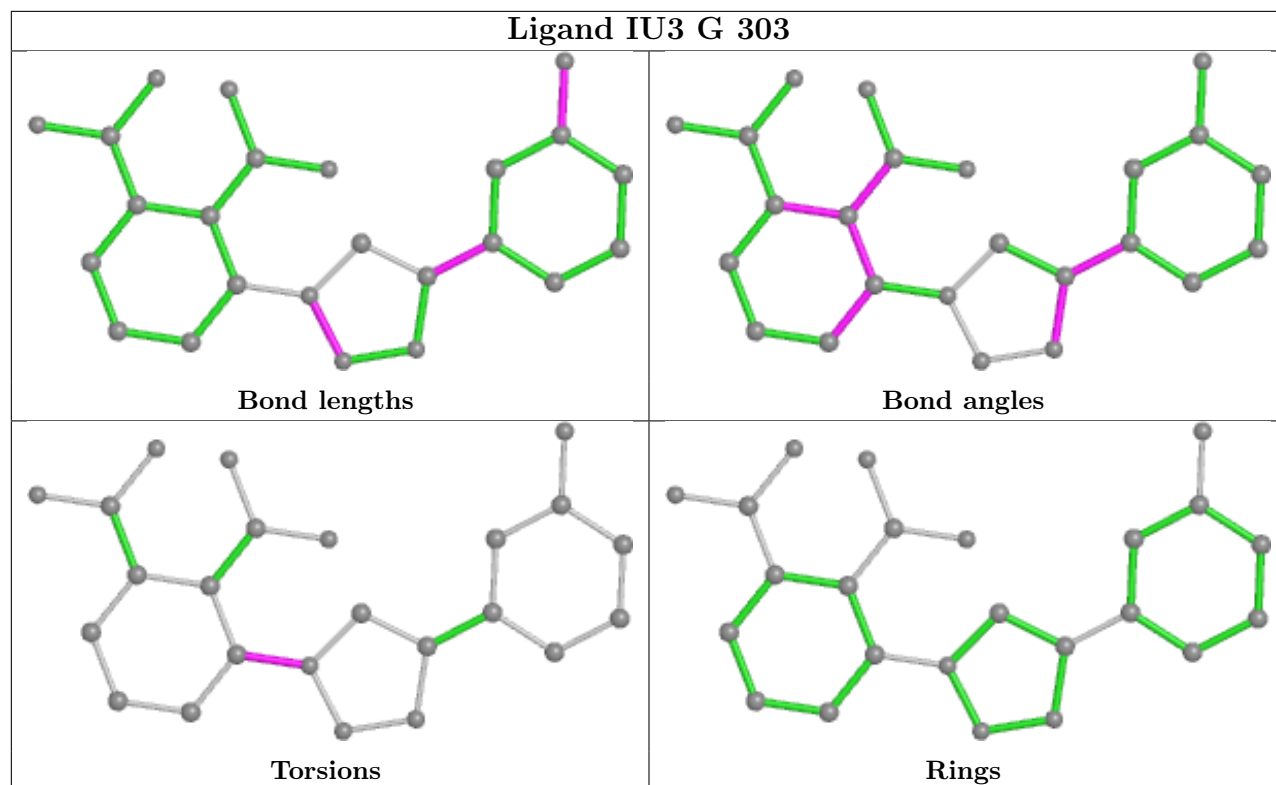
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	303	IU3	3	0
3	D	303	IU3	4	0
3	G	303	IU3	4	0
3	B	303	IU3	3	0
3	H	303	IU3	3	0
3	F	303	IU3	1	0

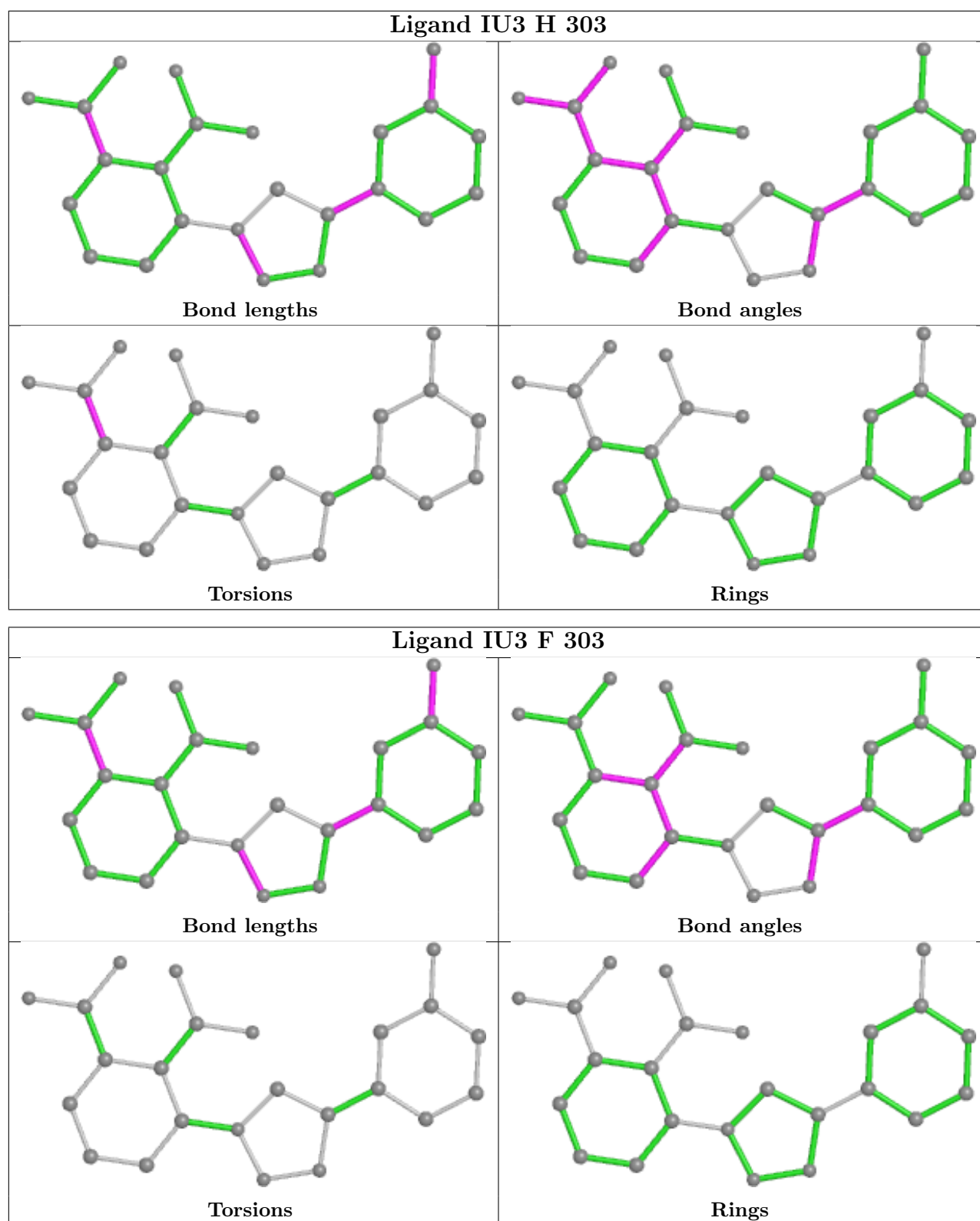
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	231/231 (100%)	0.14	9 (3%) 39 48	21, 29, 42, 67	0
1	B	231/231 (100%)	0.39	13 (5%) 24 33	26, 37, 52, 72	0
1	C	231/231 (100%)	0.11	7 (3%) 50 59	21, 30, 41, 64	0
1	D	231/231 (100%)	0.14	7 (3%) 50 59	22, 31, 44, 74	0
1	E	231/231 (100%)	0.21	11 (4%) 30 39	23, 32, 48, 69	0
1	F	231/231 (100%)	0.25	11 (4%) 30 39	22, 32, 46, 70	0
1	G	231/231 (100%)	0.77	36 (15%) 2 2	29, 42, 58, 67	0
1	H	231/231 (100%)	0.53	22 (9%) 8 12	26, 37, 51, 68	0
All	All	1848/1848 (100%)	0.32	116 (6%) 20 27	21, 34, 52, 74	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	ARG	8.7
1	F	262	ARG	6.6
1	E	261	ASN	6.4
1	C	262	ARG	5.5
1	H	78	ASP	5.3
1	G	78	ASP	5.2
1	H	145	VAL	5.1
1	B	260	THR	5.0
1	A	261	ASN	4.7
1	H	261	ASN	4.7
1	A	262	ARG	4.5
1	A	260	THR	4.5
1	F	210	ASN	4.4
1	G	130	GLY	4.3
1	E	260	THR	4.2
1	G	128	ALA	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	262	ARG	4.1
1	F	209	GLY	4.1
1	D	262	ARG	4.1
1	F	260	THR	4.0
1	G	157	GLY	3.9
1	G	261	ASN	3.9
1	E	262	ARG	3.9
1	G	51	ASP	3.9
1	H	100	GLU	3.8
1	H	260	THR	3.8
1	F	199	ALA	3.7
1	C	78	ASP	3.7
1	F	261	ASN	3.5
1	G	50	ALA	3.5
1	F	258	ALA	3.4
1	B	147	GLY	3.4
1	F	212	ALA	3.4
1	G	63	ASP	3.4
1	G	77	GLY	3.3
1	D	82	LEU	3.2
1	H	210	ASN	3.2
1	D	156	GLU	3.1
1	G	146	GLU	3.1
1	H	51	ASP	3.1
1	G	104	GLY	3.1
1	G	260	THR	3.1
1	E	199	ALA	3.1
1	H	258	ALA	3.0
1	G	164	ALA	3.0
1	E	250	LYS	3.0
1	B	228	GLN	3.0
1	C	260	THR	3.0
1	G	100	GLU	3.0
1	B	145	VAL	3.0
1	E	234	GLN	3.0
1	B	57	ILE	2.9
1	G	123	VAL	2.9
1	A	57	ILE	2.8
1	F	234	GLN	2.8
1	G	262	ARG	2.8
1	H	141	ARG	2.8
1	G	210	ASN	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	117	ASP	2.8
1	B	217	ALA	2.8
1	A	69	SER	2.8
1	H	104	GLY	2.7
1	G	75	ARG	2.6
1	D	260	THR	2.6
1	H	209	GLY	2.6
1	G	73	ILE	2.6
1	E	219	TRP	2.6
1	G	102	GLN	2.6
1	H	159	SER	2.6
1	E	73	ILE	2.6
1	B	156	GLU	2.5
1	F	200	ILE	2.5
1	H	125	VAL	2.5
1	H	217	ALA	2.5
1	G	49	ILE	2.5
1	G	125	VAL	2.4
1	G	156	GLU	2.4
1	A	228	GLN	2.4
1	C	113	THR	2.4
1	B	198	CYS	2.4
1	H	156	GLU	2.4
1	G	82	LEU	2.4
1	G	95	LEU	2.4
1	H	152	THR	2.4
1	G	141	ARG	2.3
1	E	197	GLY	2.3
1	C	82	LEU	2.3
1	G	129	ALA	2.3
1	H	52	GLY	2.3
1	B	212	ALA	2.3
1	G	165	VAL	2.3
1	G	217	ALA	2.3
1	G	153	HIS	2.3
1	E	217	ALA	2.2
1	B	113	THR	2.2
1	H	124	ASP	2.2
1	G	166	ARG	2.2
1	C	199	ALA	2.2
1	D	74	VAL	2.2
1	B	141	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	208	ALA	2.1
1	H	164	ALA	2.1
1	H	199	ALA	2.1
1	D	232	GLU	2.1
1	G	226	ILE	2.1
1	F	227	GLN	2.1
1	G	209	GLY	2.1
1	G	83	ILE	2.0
1	E	156	GLU	2.0
1	H	146	GLU	2.0
1	D	83	ILE	2.0
1	A	156	GLU	2.0
1	A	252	THR	2.0
1	B	216	LEU	2.0
1	C	208	ALA	2.0
1	G	103	ILE	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 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

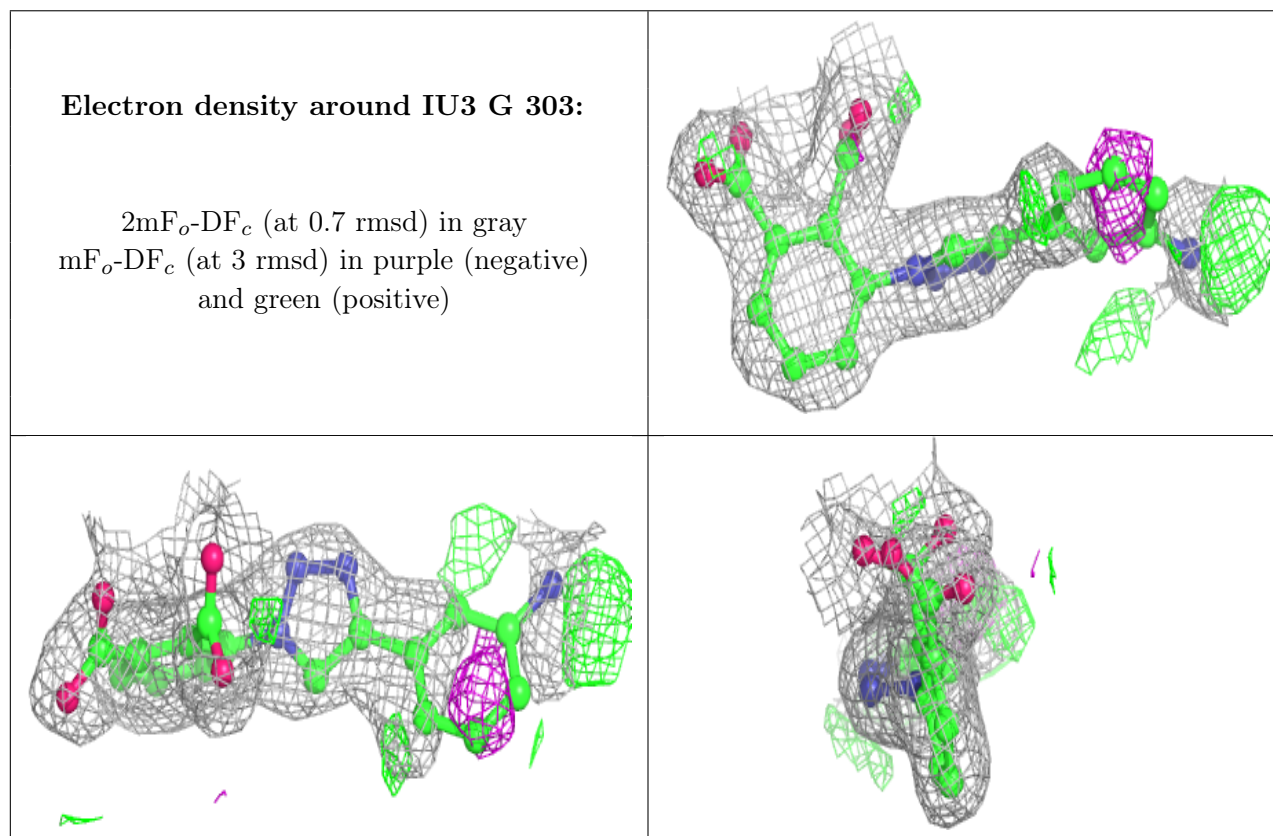
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	IU3	G	303	24/24	0.82	0.19	36,41,64,71	0
3	IU3	E	303	24/24	0.84	0.19	32,34,55,61	0
3	IU3	F	303	24/24	0.84	0.18	28,34,45,59	0
3	IU3	B	303	24/24	0.84	0.17	37,42,55,59	0
3	IU3	A	303	24/24	0.87	0.17	29,34,48,57	0
3	IU3	H	303	24/24	0.89	0.16	36,39,54,61	0
3	IU3	C	303	24/24	0.90	0.17	26,31,51,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	IU3	D	303	24/24	0.91	0.16	33,36,45,52	0
2	ZN	B	301	1/1	0.98	0.06	40,40,40,40	0
2	ZN	H	301	1/1	0.99	0.04	42,42,42,42	0
2	ZN	H	302	1/1	0.99	0.05	36,36,36,36	0
2	ZN	A	301	1/1	0.99	0.06	32,32,32,32	0
2	ZN	B	302	1/1	0.99	0.06	35,35,35,35	0
2	ZN	C	301	1/1	0.99	0.05	30,30,30,30	0
2	ZN	D	301	1/1	0.99	0.07	30,30,30,30	0
2	ZN	D	302	1/1	0.99	0.06	34,34,34,34	0
2	ZN	E	302	1/1	0.99	0.06	30,30,30,30	0
2	ZN	F	301	1/1	0.99	0.05	35,35,35,35	0
2	ZN	F	302	1/1	0.99	0.06	30,30,30,30	0
2	ZN	A	302	1/1	1.00	0.07	26,26,26,26	0
2	ZN	C	302	1/1	1.00	0.05	26,26,26,26	0
2	ZN	E	301	1/1	1.00	0.06	35,35,35,35	0
2	ZN	G	301	1/1	1.00	0.07	36,36,36,36	0
2	ZN	G	302	1/1	1.00	0.04	39,39,39,39	0

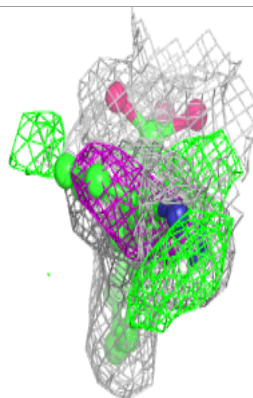
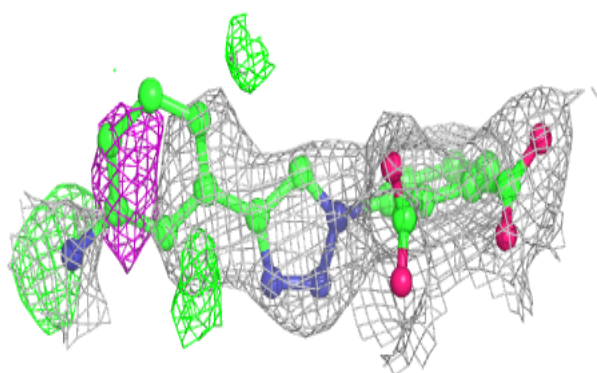
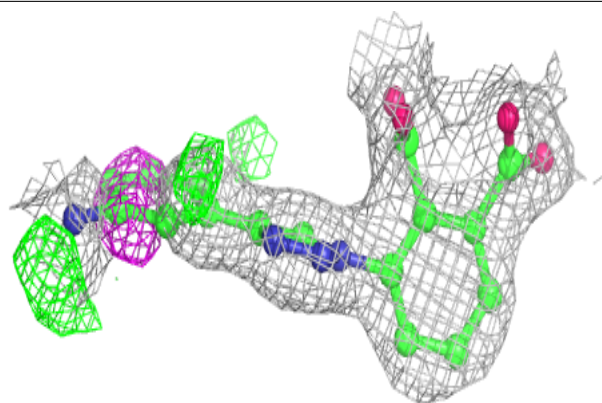
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



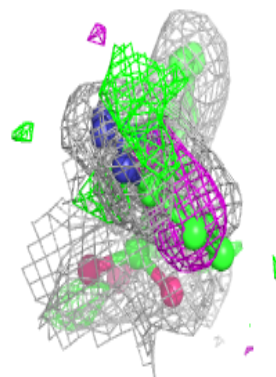
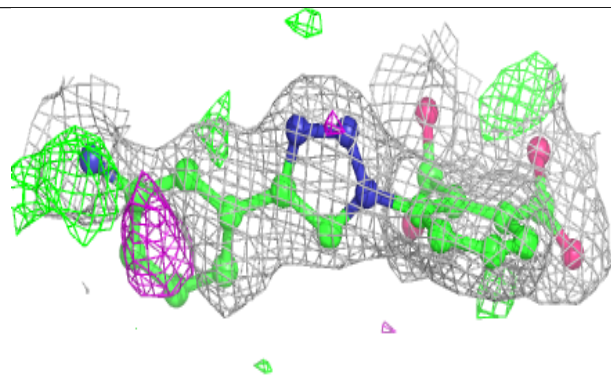
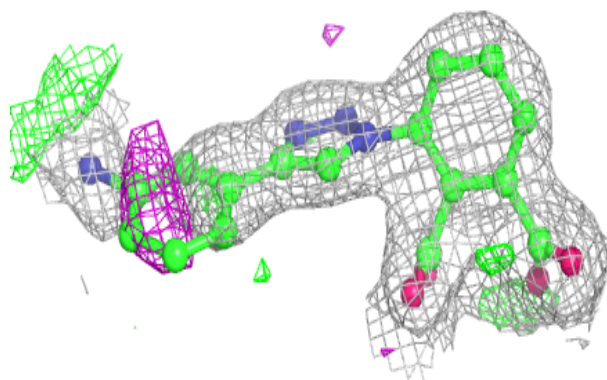


**Electron density around IU3 E 303:**

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

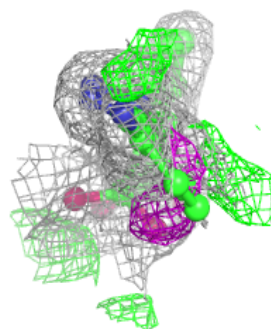
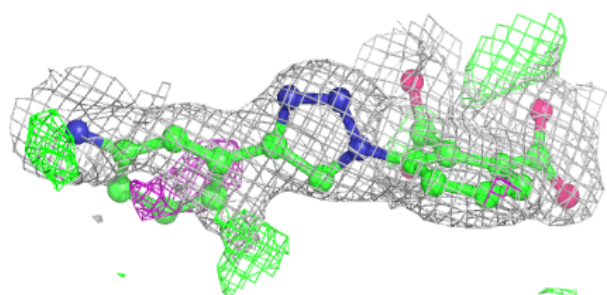
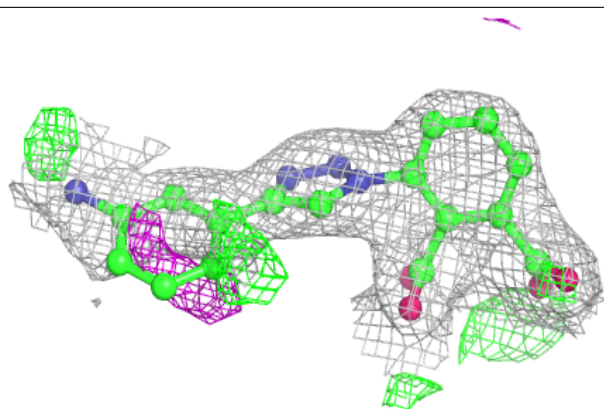
**Electron density around IU3 F 303:**

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

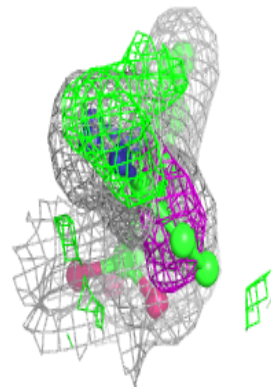
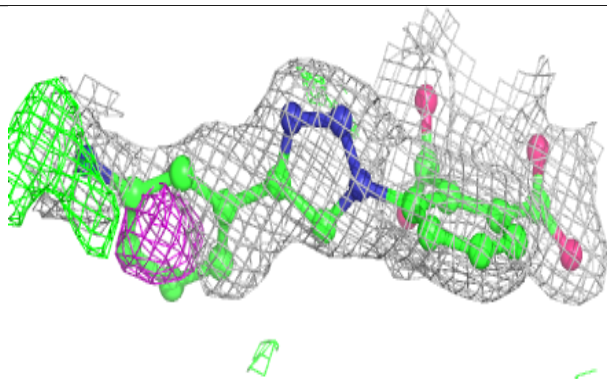
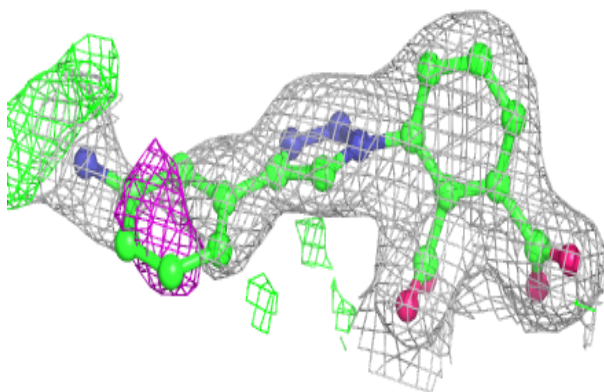


**Electron density around IU3 B 303:**

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

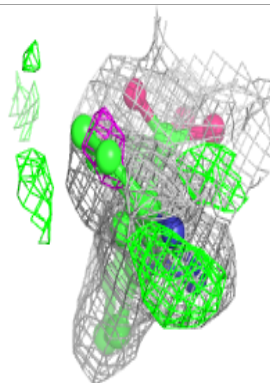
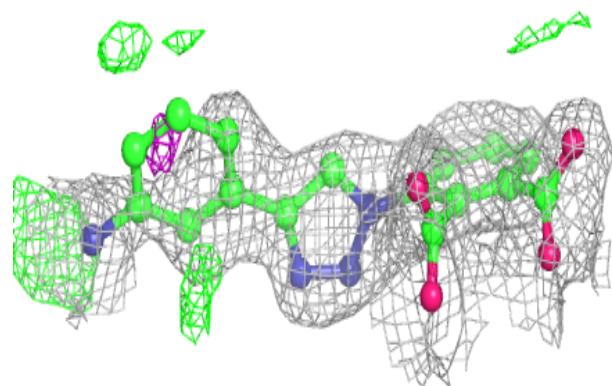
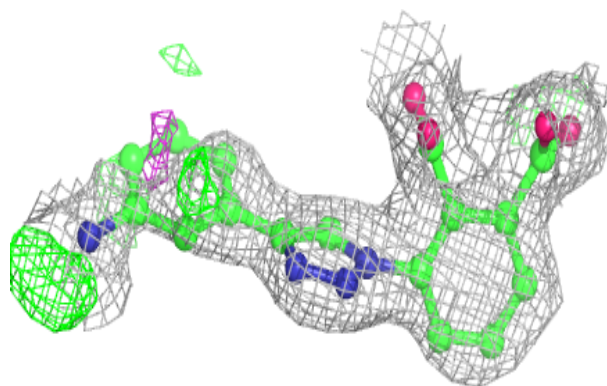
**Electron density around IU3 A 303:**

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

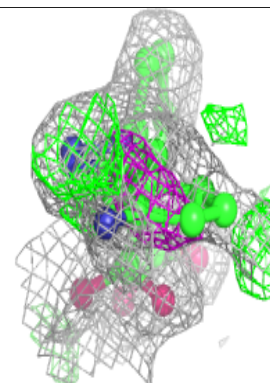
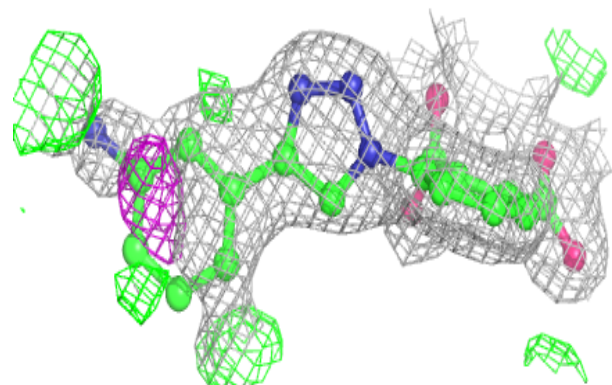
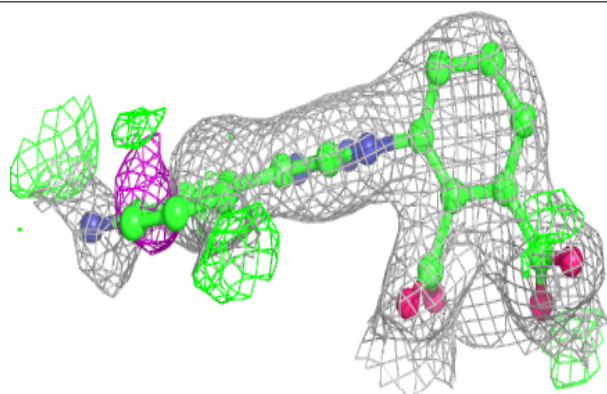


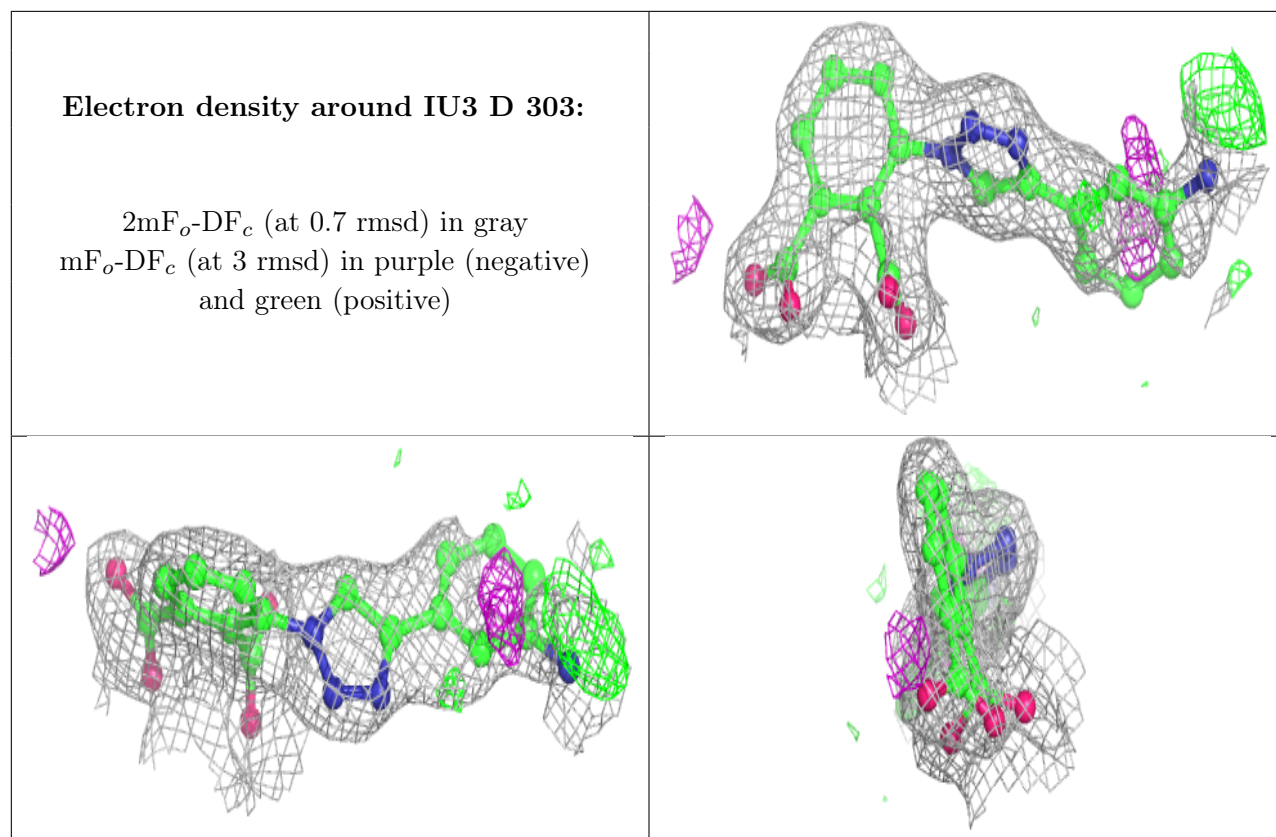
**Electron density around IU3 H 303:**

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

**Electron density around IU3 C 303:**

$2mF_o-DF_c$  (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.