



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:39 PM UTC

PDB ID : 7YHC / pdb_00007yhc
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

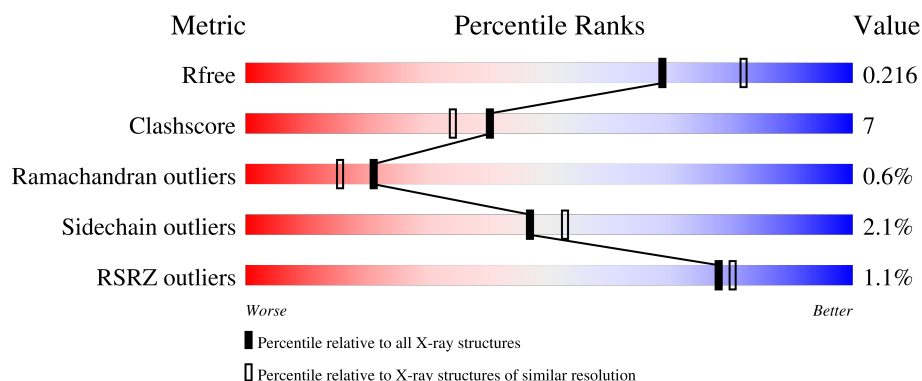
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 ≥ 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	

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Mol	Chain	Length	Quality of chain
1	F	231	2% 90% 10%
1	G	231	2% 80% 19%
1	H	231	% 86% 13%

2 Entry composition

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
1	A	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			
1	B	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			
1	C	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			
1	D	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			
1	E	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			
1	F	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			
1	G	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			
1	H	231	Total	C	N	O	S	0	0	0
			1733	1094	299	339	1			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

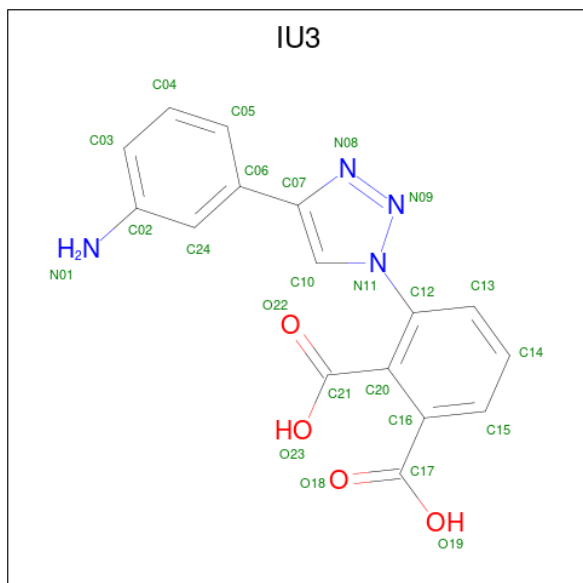
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

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

- Molecule 3 is 3-[4-(3-aminophenyl)-1,2,3-triazol-1-yl]phthalic acid (CCD ID: IU3) (formula: $C_{16}H_{12}N_4O_4$) (labeled as "Ligand of Interest" by depositor).



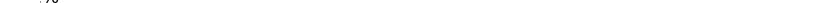
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	16	4	4		
3	B	1	Total	C	N	O	0	0
			24	16	4	4		
3	C	1	Total	C	N	O	0	0
			24	16	4	4		
3	D	1	Total	C	N	O	0	0
			24	16	4	4		
3	E	1	Total	C	N	O	0	0
			24	16	4	4		
3	F	1	Total	C	N	O	0	0
			24	16	4	4		
3	G	1	Total	C	N	O	0	0
			24	16	4	4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

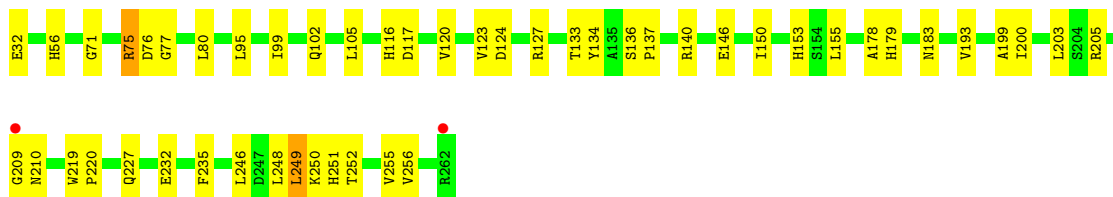
- Molecule 4 is water.

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

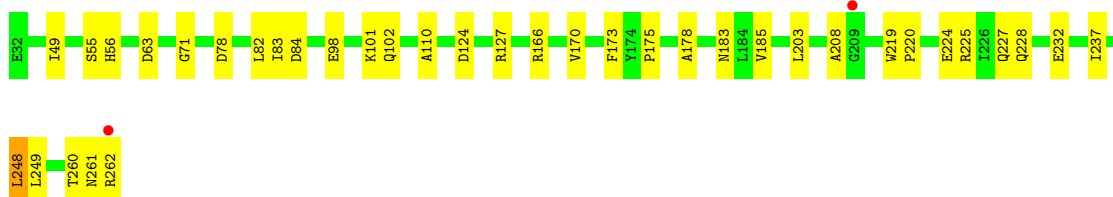
- Molecule 1: Beta-lactamase class B VIM-2



- Chain B:  79% 20% 1%



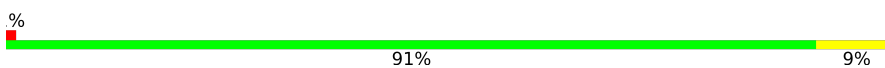
- Chain C: 84% 16%

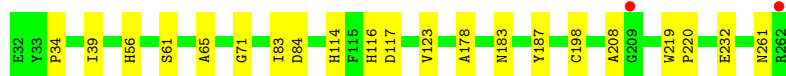


- Chain D: 81% 19%

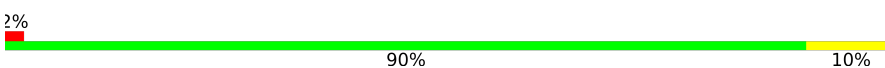


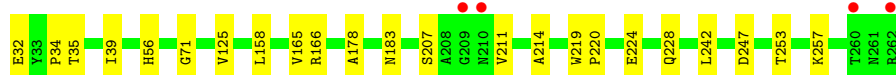
- Molecule 1: Beta-lactamase class B VIM-2

Chain E:  %



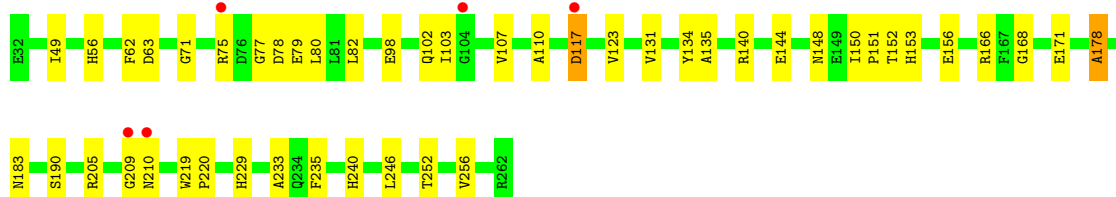
- Molecule 1: Beta-lactamase class B VIM-2

Chain F:  %

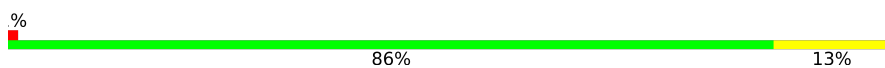


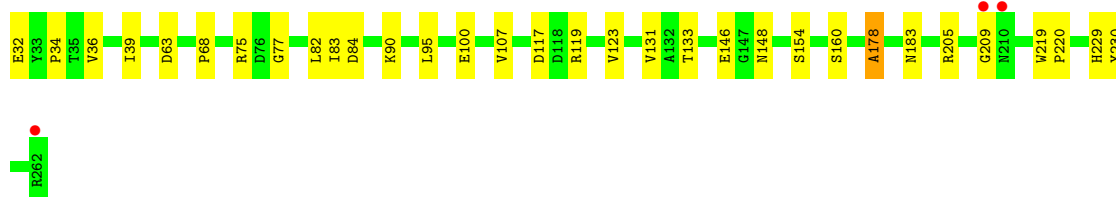
- Molecule 1: Beta-lactamase class B VIM-2

Chain G:  %



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

Chain H:  %



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 98.2 (19.83-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.15Å)	Xtriage
Refinement program	PHENIX 1.10.1	Depositor
R, R_{free}	0.172 , 0.217 0.173 , 0.216	Depositor DCC
R_{free} test set	1997 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14725	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.35	0/1774	0.53	0/2429
1	B	0.31	0/1774	0.48	0/2429
1	C	0.35	0/1774	0.55	0/2429
1	D	0.34	0/1774	0.53	0/2429
1	E	0.33	0/1774	0.50	0/2429
1	F	0.33	0/1774	0.53	0/2429
1	G	0.28	0/1774	0.46	0/2429
1	H	0.31	0/1774	0.49	0/2429
All	All	0.33	0/14192	0.51	0/19432

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1733	0	1676	16	1
1	B	1733	0	1676	37	1
1	C	1733	0	1676	22	0
1	D	1733	0	1676	32	0
1	E	1733	0	1676	10	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1733	0	1676	13	1
1	G	1733	0	1676	35	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	180	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 7.

All (180) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:201:TYR:OH	1:A:208:ALA:O	2.25	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:228:GLN:HG3	1:G:190:SER:HG	1.74	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:D:260:THR:C	1:D:262:ARG:H	2.17	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: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:C:260:THR:C	1:C:262:ARG:H	2.23	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: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
1:H:36:VAL:HB	1:H:68:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:260:THR:C	1:C:262:ARG:N	2.79	0.40
1:A:260:THR:C	1:A:262:ARG:H	2.28	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 ⓘ

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	229/231 (99%)	223 (97%)	5 (2%)	1 (0%)	30	26
1	B	229/231 (99%)	223 (97%)	5 (2%)	1 (0%)	30	26
1	C	229/231 (99%)	223 (97%)	4 (2%)	2 (1%)	14	9
1	D	229/231 (99%)	222 (97%)	5 (2%)	2 (1%)	14	9
1	E	229/231 (99%)	224 (98%)	3 (1%)	2 (1%)	14	9
1	F	229/231 (99%)	224 (98%)	4 (2%)	1 (0%)	30	26
1	G	229/231 (99%)	220 (96%)	8 (4%)	1 (0%)	30	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	229/231 (99%)	220 (96%)	8 (4%)	1 (0%)	30 26
All	All	1832/1848 (99%)	1779 (97%)	42 (2%)	11 (1%)	21 15

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 ⓘ

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%)	45 51
1	B	182/184 (99%)	178 (98%)	4 (2%)	45 51
1	C	182/184 (99%)	177 (97%)	5 (3%)	39 41
1	D	182/184 (99%)	178 (98%)	4 (2%)	45 51
1	E	182/184 (99%)	179 (98%)	3 (2%)	55 61
1	F	182/184 (99%)	181 (100%)	1 (0%)	81 87
1	G	182/184 (99%)	178 (98%)	4 (2%)	45 51
1	H	182/184 (99%)	176 (97%)	6 (3%)	33 34
All	All	1456/1472 (99%)	1425 (98%)	31 (2%)	47 52

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	VAL
1	A	183	ASN
1	A	229	HIS
1	A	248	LEU
1	B	75	ARG
1	B	102	GLN
1	B	183	ASN
1	B	249	LEU
1	C	63	ASP
1	C	101	LYS
1	C	183	ASN
1	C	232	GLU
1	C	248	LEU
1	D	123	VAL
1	D	183	ASN
1	D	224	GLU
1	D	248	LEU
1	E	123	VAL
1	E	183	ASN
1	E	232	GLU
1	F	183	ASN
1	G	79	GLU
1	G	117	ASP
1	G	123	VAL
1	G	183	ASN
1	H	63	ASP
1	H	90	LYS
1	H	100	GLU
1	H	154	SER
1	H	160	SER
1	H	183	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	HIS
1	B	102	GLN
1	B	227	GLN
1	D	102	GLN
1	D	210	ASN
1	H	234	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 oligosaccharides 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	C	303	2	26,26,26	1.46	4 (15%)	37,37,37	1.88	11 (29%)
3	IU3	E	303	2	26,26,26	1.60	3 (11%)	37,37,37	1.49	7 (18%)
3	IU3	G	303	2	26,26,26	1.76	4 (15%)	37,37,37	1.37	5 (13%)
3	IU3	B	303	2	26,26,26	1.65	3 (11%)	37,37,37	1.59	8 (21%)
3	IU3	A	303	2	26,26,26	1.61	4 (15%)	37,37,37	1.72	9 (24%)
3	IU3	F	303	2	26,26,26	1.49	4 (15%)	37,37,37	1.52	7 (18%)
3	IU3	H	303	2	26,26,26	1.76	5 (19%)	37,37,37	1.68	10 (27%)
3	IU3	D	303	2	26,26,26	1.60	3 (11%)	37,37,37	1.47	9 (24%)

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	C	303	2	-	1/16/16/16	0/3/3/3
3	IU3	E	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	-	3/16/16/16	0/3/3/3
3	IU3	A	303	2	-	3/16/16/16	0/3/3/3
3	IU3	F	303	2	-	1/16/16/16	0/3/3/3
3	IU3	H	303	2	-	5/16/16/16	0/3/3/3
3	IU3	D	303	2	-	2/16/16/16	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	303	IU3	C10-C07	4.75	1.45	1.37
3	G	303	IU3	C10-C07	4.71	1.45	1.37
3	H	303	IU3	C06-C07	4.61	1.54	1.47
3	B	303	IU3	C10-C07	4.47	1.44	1.37
3	B	303	IU3	C06-C07	4.42	1.54	1.47
3	D	303	IU3	C10-C07	4.39	1.44	1.37
3	A	303	IU3	C10-C07	4.24	1.44	1.37
3	E	303	IU3	C10-C07	4.09	1.44	1.37
3	D	303	IU3	C06-C07	4.07	1.53	1.47
3	A	303	IU3	C06-C07	3.97	1.53	1.47
3	G	303	IU3	C06-C07	3.95	1.53	1.47
3	F	303	IU3	C10-C07	3.75	1.43	1.37
3	E	303	IU3	C06-C07	3.57	1.53	1.47
3	C	303	IU3	C10-C07	3.53	1.43	1.37
3	F	303	IU3	C06-C07	3.41	1.52	1.47
3	C	303	IU3	C06-C07	3.13	1.52	1.47
3	E	303	IU3	C02-N01	2.69	1.47	1.38
3	H	303	IU3	C02-N01	2.62	1.47	1.38
3	G	303	IU3	C02-N01	2.60	1.47	1.38
3	H	303	IU3	C16-C17	2.55	1.55	1.49
3	A	303	IU3	C02-N01	2.54	1.47	1.38
3	G	303	IU3	N11-N09	-2.46	1.31	1.35
3	B	303	IU3	C02-N01	2.33	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	F	303	IU3	C16-C17	2.11	1.54	1.49
3	F	303	IU3	C02-N01	2.11	1.45	1.38
3	C	303	IU3	N11-N09	-2.07	1.32	1.35
3	H	303	IU3	C12-N11	2.01	1.46	1.43
3	D	303	IU3	C02-N01	2.01	1.45	1.38

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	IU3	C12-N11-N09	4.73	127.67	119.81
3	B	303	IU3	C12-C20-C21	-4.34	116.10	122.27
3	C	303	IU3	C06-C07-N08	4.34	129.03	122.05
3	A	303	IU3	C06-C07-N08	3.97	128.44	122.05
3	A	303	IU3	N11-N09-N08	3.95	111.38	107.02
3	A	303	IU3	C12-C20-C21	-3.87	116.77	122.27
3	G	303	IU3	N11-N09-N08	3.85	111.27	107.02
3	H	303	IU3	N11-N09-N08	3.84	111.26	107.02
3	E	303	IU3	C06-C07-N08	3.83	128.20	122.05
3	F	303	IU3	C06-C07-N08	3.69	127.97	122.05
3	H	303	IU3	C06-C07-N08	3.54	127.73	122.05
3	D	303	IU3	N11-N09-N08	3.45	110.83	107.02
3	F	303	IU3	N11-N09-N08	3.40	110.77	107.02
3	H	303	IU3	C12-C20-C21	-3.37	117.48	122.27
3	H	303	IU3	C10-C07-N08	-3.36	104.61	107.85
3	B	303	IU3	N11-N09-N08	3.35	110.72	107.02
3	C	303	IU3	C12-N11-C10	-3.31	123.34	129.51
3	B	303	IU3	C06-C07-N08	3.21	127.20	122.05
3	A	303	IU3	C12-N11-N09	3.18	125.08	119.81
3	D	303	IU3	C10-C07-N08	-3.15	104.82	107.85
3	D	303	IU3	C12-N11-N09	3.07	124.91	119.81
3	B	303	IU3	C10-C07-N08	-2.98	104.98	107.85
3	G	303	IU3	C10-C07-N08	-2.88	105.08	107.85
3	H	303	IU3	C12-N11-N09	2.87	124.57	119.81
3	E	303	IU3	N11-N09-N08	2.84	110.15	107.02
3	C	303	IU3	N11-N09-N08	2.84	110.15	107.02
3	C	303	IU3	C06-C07-C10	-2.83	125.33	129.65
3	F	303	IU3	C13-C12-N11	2.76	122.20	118.36
3	F	303	IU3	C12-C20-C21	-2.76	118.35	122.27
3	E	303	IU3	C10-C07-N08	-2.65	105.30	107.85
3	B	303	IU3	C13-C12-N11	2.63	122.02	118.36
3	A	303	IU3	O19-C17-O18	-2.62	117.72	123.35
3	A	303	IU3	C16-C20-C12	2.61	121.38	118.73
3	E	303	IU3	C12-N11-N09	2.60	124.14	119.81
3	D	303	IU3	C06-C07-N08	2.59	126.21	122.05
3	H	303	IU3	C16-C20-C12	2.58	121.35	118.73
3	C	303	IU3	C06-C24-C02	-2.55	118.56	120.66
3	F	303	IU3	C12-N11-N09	2.52	123.99	119.81
3	A	303	IU3	C06-C07-C10	-2.51	125.81	129.65
3	D	303	IU3	O19-C17-O18	-2.48	118.02	123.35
3	C	303	IU3	C10-C07-N08	-2.42	105.52	107.85
3	C	303	IU3	O19-C17-O18	-2.42	118.15	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	IU3	C13-C12-N11	2.34	121.62	118.36
3	F	303	IU3	C06-C07-C10	-2.31	126.12	129.65
3	G	303	IU3	C13-C12-N11	2.30	121.56	118.36
3	C	303	IU3	C12-C20-C21	-2.30	119.00	122.27
3	D	303	IU3	C16-C20-C12	2.30	121.06	118.73
3	H	303	IU3	O19-C17-C16	2.29	121.80	115.28
3	G	303	IU3	C06-C07-N08	2.27	125.69	122.05
3	B	303	IU3	C16-C20-C12	2.25	121.01	118.73
3	H	303	IU3	O19-C17-O18	-2.24	118.53	123.35
3	H	303	IU3	C13-C12-N11	2.23	121.46	118.36
3	D	303	IU3	C12-C20-C21	-2.19	119.16	122.27
3	H	303	IU3	C10-N11-N09	-2.19	107.70	110.31
3	A	303	IU3	C10-C07-N08	-2.18	105.75	107.85
3	E	303	IU3	C06-C07-C10	-2.17	126.34	129.65
3	G	303	IU3	C12-C20-C21	-2.16	119.21	122.27
3	E	303	IU3	C12-C20-C21	-2.11	119.27	122.27
3	B	303	IU3	C12-N11-N09	2.08	123.27	119.81
3	B	303	IU3	O19-C17-O18	-2.08	118.88	123.35
3	D	303	IU3	C10-N11-N09	-2.07	107.84	110.31
3	E	303	IU3	C13-C12-N11	2.06	121.23	118.36
3	C	303	IU3	C16-C20-C12	2.05	120.81	118.73
3	A	303	IU3	O19-C17-C16	2.05	121.10	115.28
3	F	303	IU3	C10-C07-N08	-2.02	105.90	107.85
3	D	303	IU3	O19-C17-C16	2.02	121.02	115.28

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	303	IU3	C13-C12-N11-N09
3	H	303	IU3	C15-C16-C17-O19
3	E	303	IU3	C13-C12-N11-C10
3	A	303	IU3	C15-C16-C17-O18
3	A	303	IU3	C15-C16-C17-O19
3	B	303	IU3	C15-C16-C17-O19
3	A	303	IU3	C13-C12-N11-C10
3	C	303	IU3	C13-C12-N11-C10
3	F	303	IU3	C13-C12-N11-C10
3	G	303	IU3	C13-C12-N11-C10
3	H	303	IU3	C13-C12-N11-C10
3	H	303	IU3	C15-C16-C17-O18
3	B	303	IU3	C15-C16-C17-O18

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Mol	Chain	Res	Type	Atoms
3	B	303	IU3	C13-C12-N11-C10
3	H	303	IU3	C13-C12-N11-N09
3	H	303	IU3	C20-C16-C17-O19
3	D	303	IU3	C13-C12-N11-C10

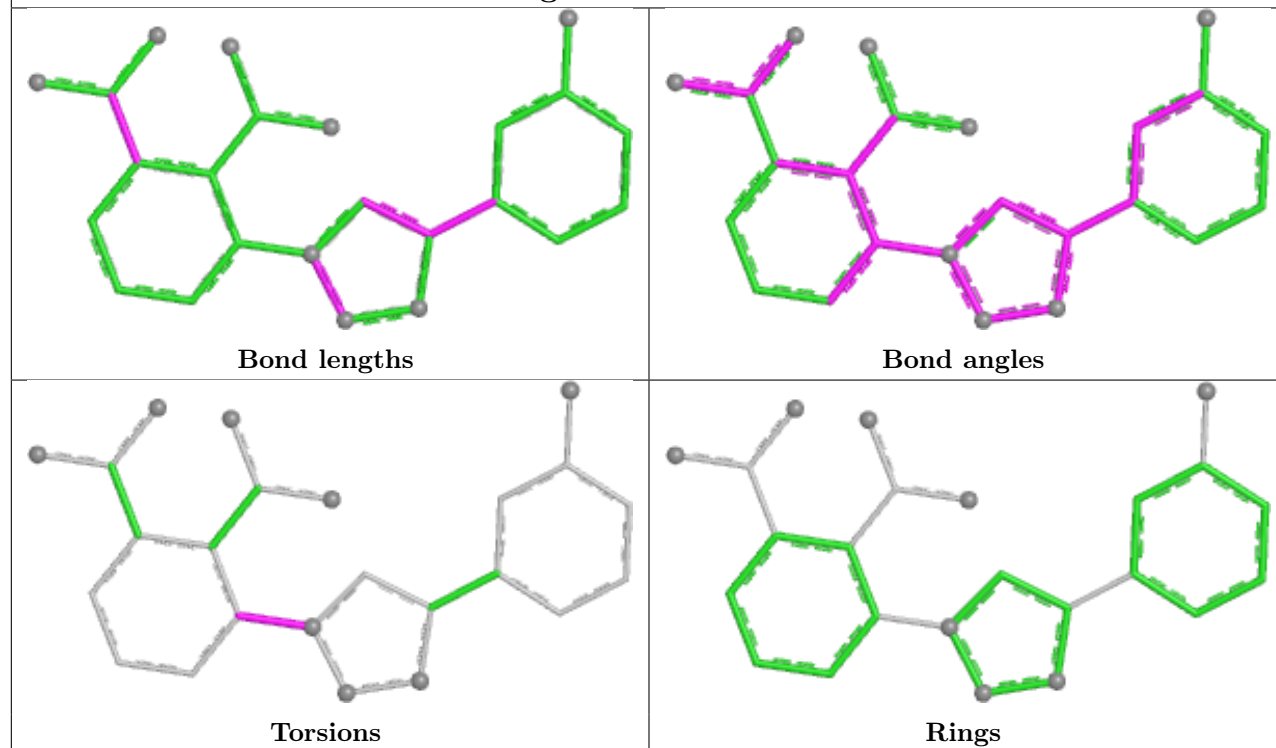
There are no ring outliers.

6 monomers are involved in 18 short contacts:

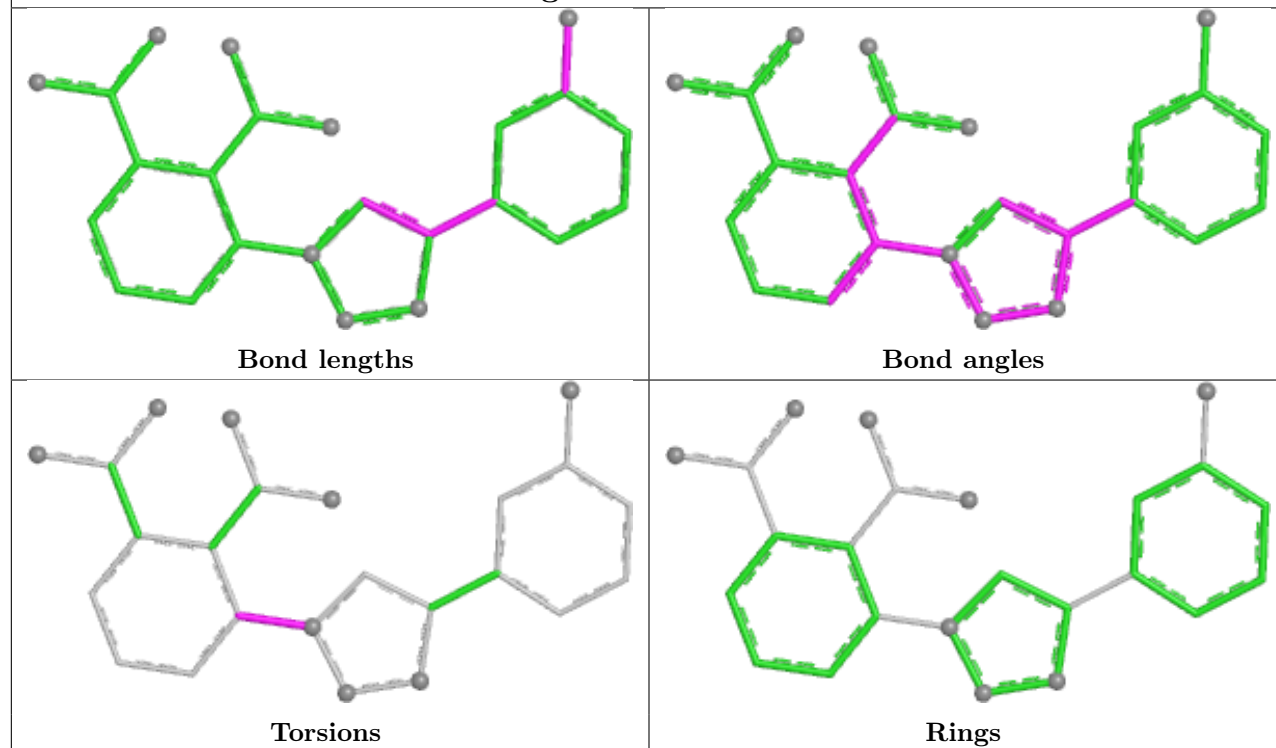
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	303	IU3	3	0
3	G	303	IU3	4	0
3	B	303	IU3	3	0
3	F	303	IU3	1	0
3	H	303	IU3	3	0
3	D	303	IU3	4	0

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

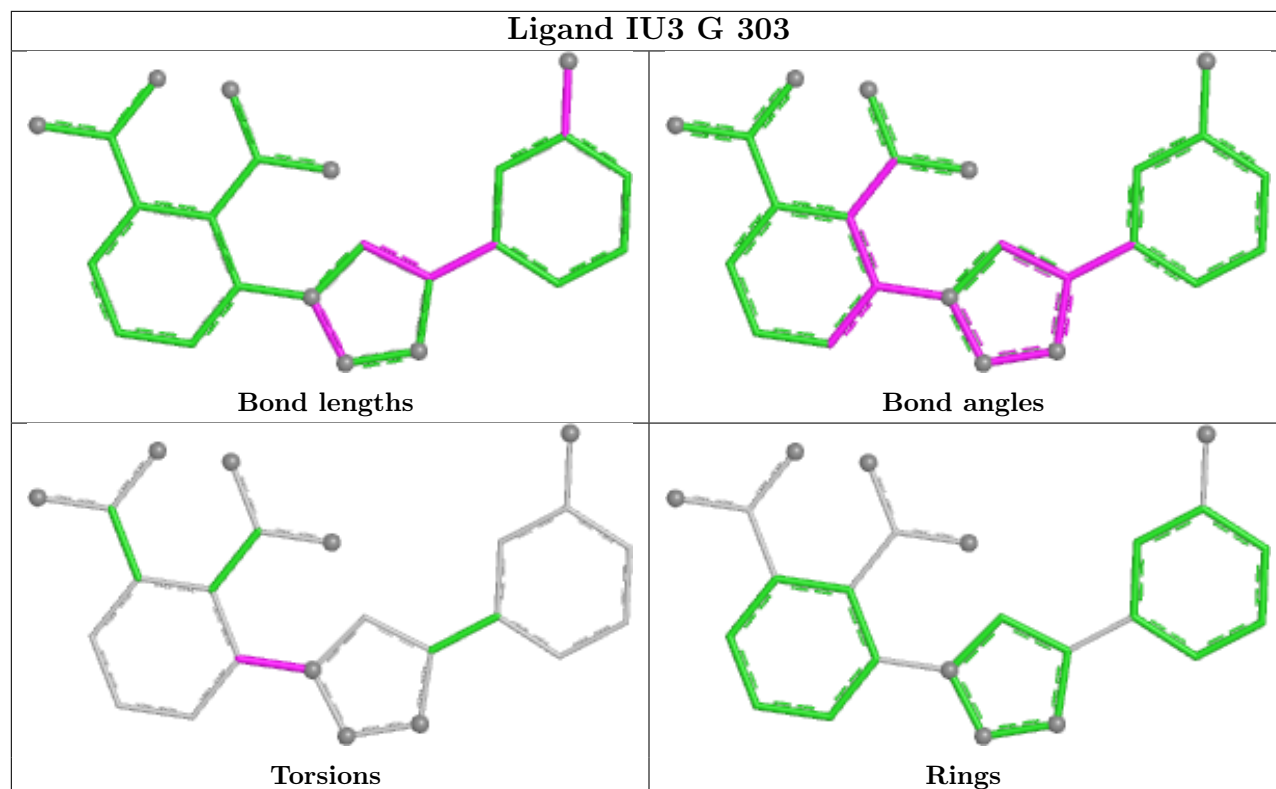
Ligand IU3 C 303



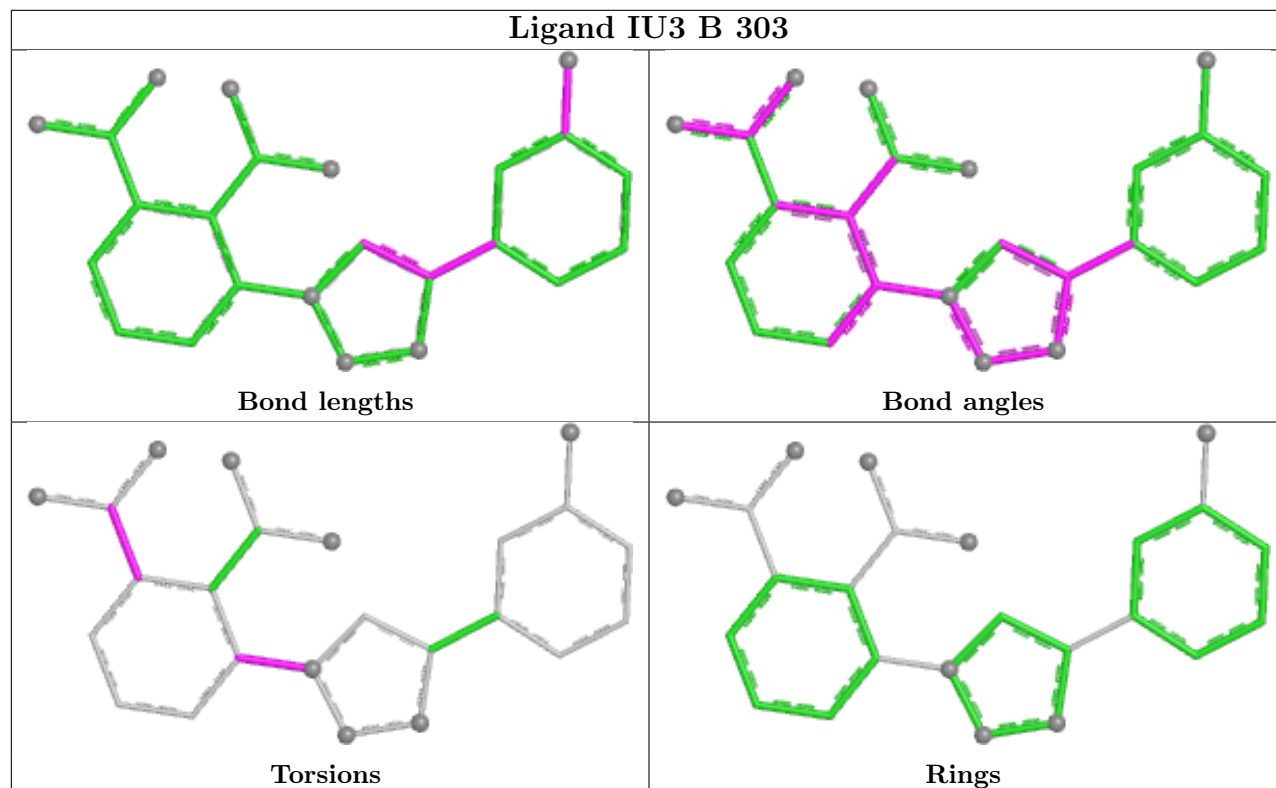
Ligand IU3 E 303



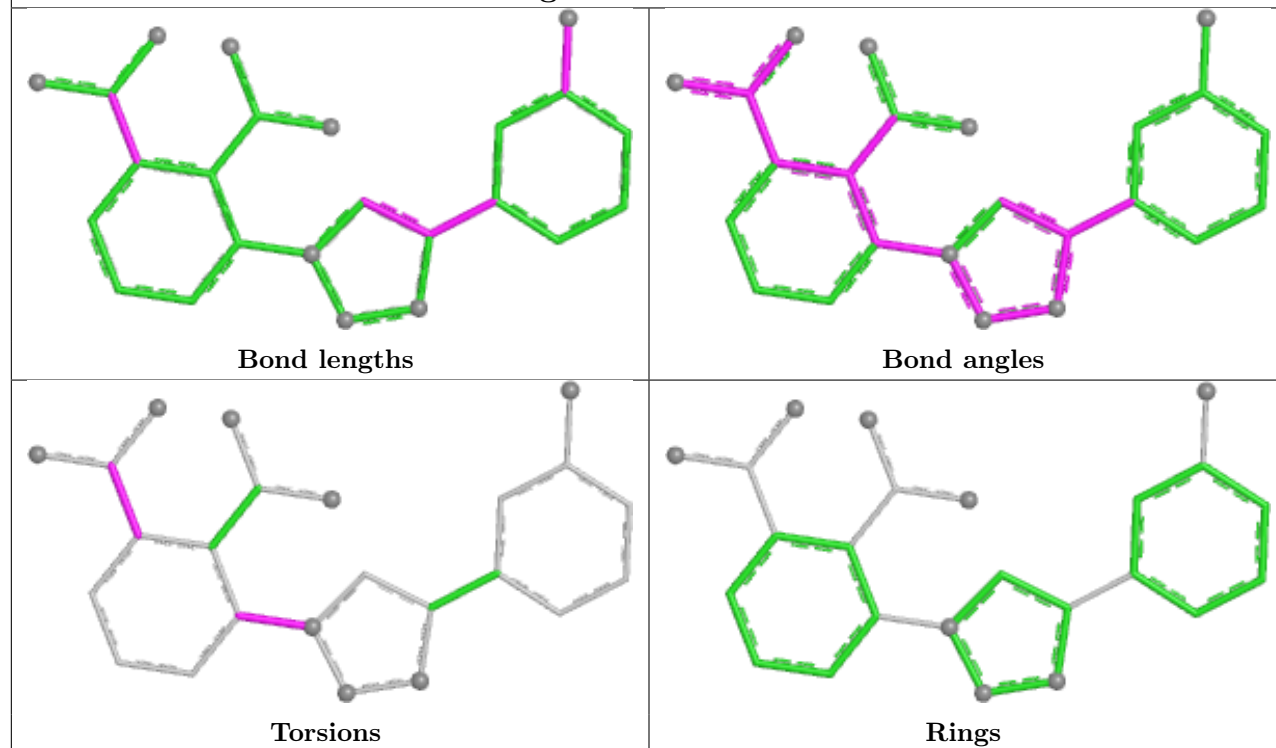
Ligand IU3 G 303



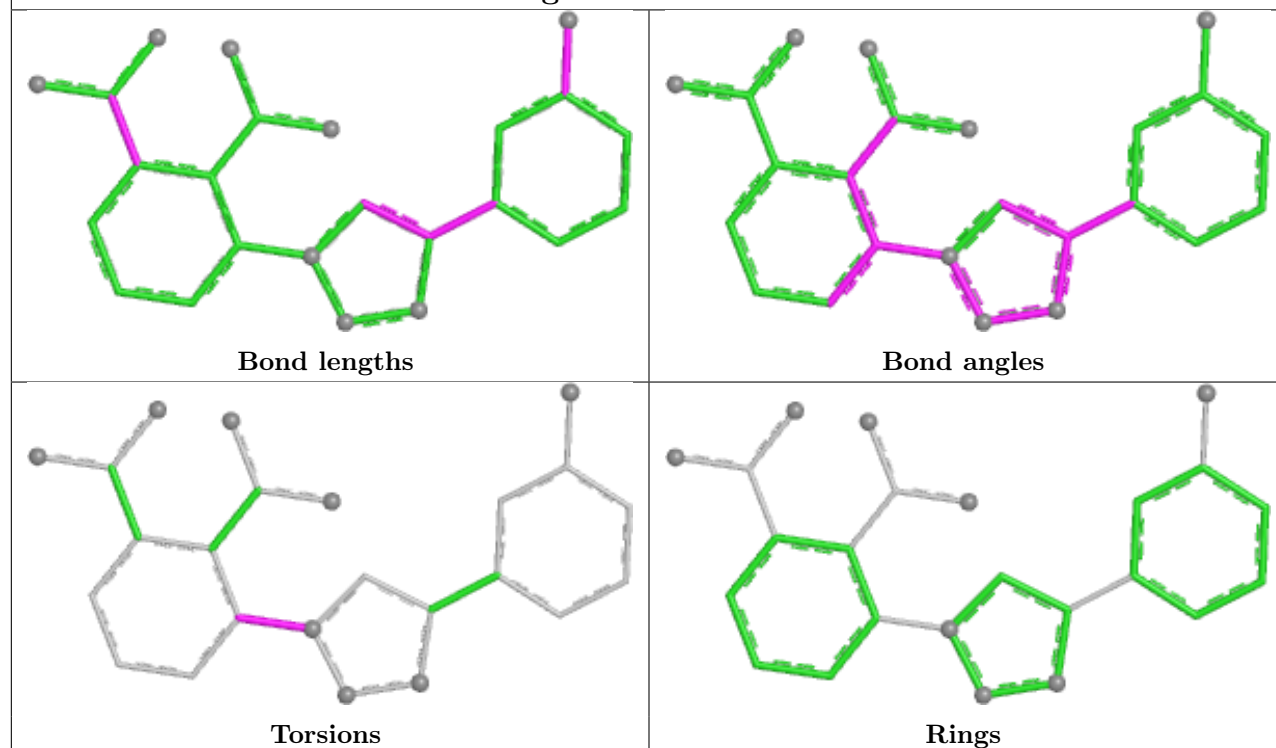
Ligand IU3 B 303

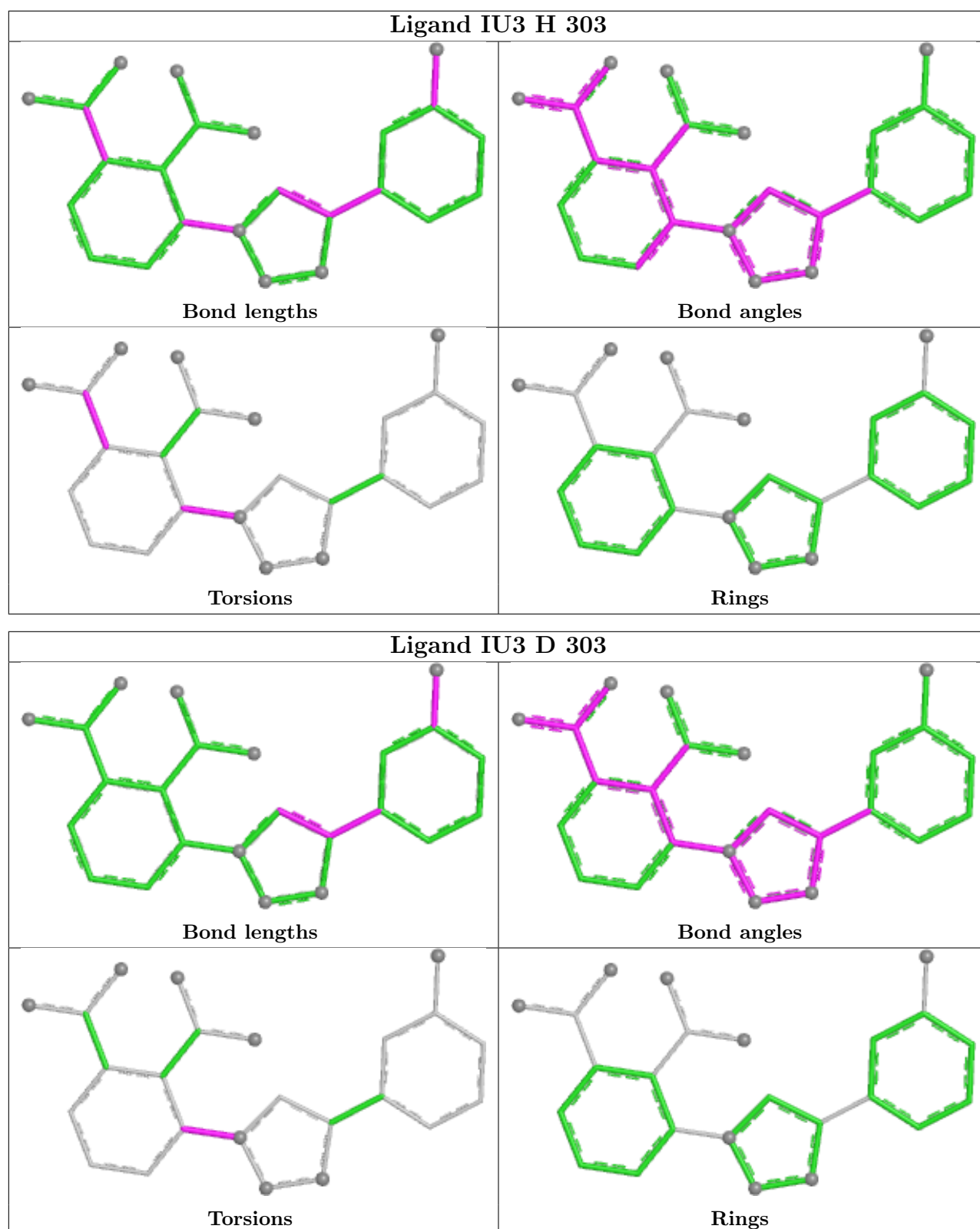


Ligand IU3 A 303



Ligand IU3 F 303





5.7 Other polymers ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/231 (100%)	-0.50	1 (0%) 88 90	21, 29, 42, 67	0
1	B	231/231 (100%)	-0.17	2 (0%) 81 83	26, 37, 52, 72	0
1	C	231/231 (100%)	-0.51	2 (0%) 81 83	21, 30, 41, 64	0
1	D	231/231 (100%)	-0.45	1 (0%) 88 90	22, 31, 44, 74	0
1	E	231/231 (100%)	-0.43	2 (0%) 81 83	23, 32, 48, 69	0
1	F	231/231 (100%)	-0.40	4 (1%) 69 73	22, 32, 46, 70	0
1	G	231/231 (100%)	0.07	5 (2%) 62 66	29, 42, 58, 67	0
1	H	231/231 (100%)	-0.10	3 (1%) 75 78	26, 37, 51, 68	0
All	All	1848/1848 (100%)	-0.31	20 (1%) 78 80	21, 34, 52, 74	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	210	ASN	3.3
1	F	210	ASN	3.2
1	G	117	ASP	3.1
1	F	262	ARG	3.1
1	G	209	GLY	3.0
1	E	262	ARG	2.9
1	C	262	ARG	2.8
1	D	209	GLY	2.6
1	H	209	GLY	2.5
1	G	75	ARG	2.4
1	B	262	ARG	2.3
1	F	260	THR	2.3
1	A	262	ARG	2.3
1	G	210	ASN	2.2
1	F	209	GLY	2.2
1	B	209	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	209	GLY	2.0
1	G	104	GLY	2.0
1	H	262	ARG	2.0
1	C	209	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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	IU3	G	303	24/24	0.84	0.12	36,41,64,71	0
3	IU3	B	303	24/24	0.87	0.11	37,42,55,59	0
3	IU3	H	303	24/24	0.87	0.10	36,39,54,61	0
3	IU3	E	303	24/24	0.88	0.11	32,34,55,61	0
3	IU3	F	303	24/24	0.89	0.10	28,34,45,59	0
3	IU3	A	303	24/24	0.90	0.10	29,34,48,57	0
3	IU3	D	303	24/24	0.90	0.10	33,36,45,52	0
3	IU3	C	303	24/24	0.92	0.09	26,31,51,57	0
2	ZN	H	302	1/1	0.99	0.03	36,36,36,36	0
2	ZN	A	301	1/1	0.99	0.02	32,32,32,32	0
2	ZN	B	301	1/1	0.99	0.03	40,40,40,40	0
2	ZN	B	302	1/1	0.99	0.02	35,35,35,35	0
2	ZN	D	302	1/1	0.99	0.02	34,34,34,34	0
2	ZN	E	301	1/1	0.99	0.02	35,35,35,35	0
2	ZN	F	301	1/1	0.99	0.02	35,35,35,35	0
2	ZN	F	302	1/1	0.99	0.01	30,30,30,30	0
2	ZN	H	301	1/1	0.99	0.03	42,42,42,42	0
2	ZN	C	302	1/1	1.00	0.01	26,26,26,26	0
2	ZN	D	301	1/1	1.00	0.01	30,30,30,30	0

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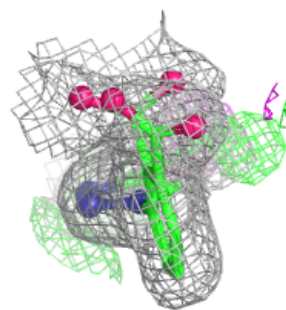
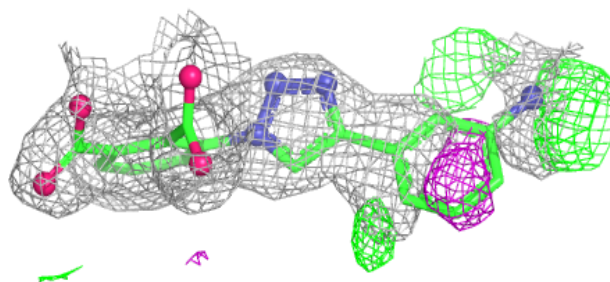
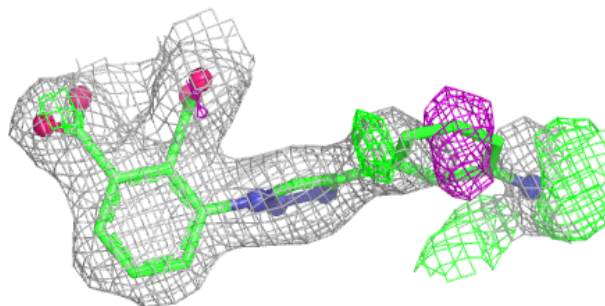
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	G	301	1/1	1.00	0.01	36,36,36,36	0
2	ZN	G	302	1/1	1.00	0.02	39,39,39,39	0
2	ZN	A	302	1/1	1.00	0.01	26,26,26,26	0
2	ZN	C	301	1/1	1.00	0.02	30,30,30,30	0
2	ZN	E	302	1/1	1.00	0.01	30,30,30,30	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.

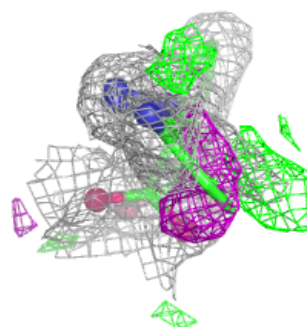
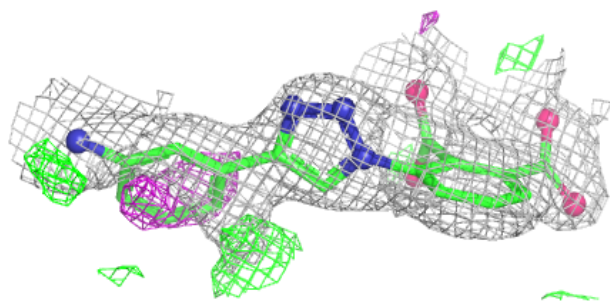
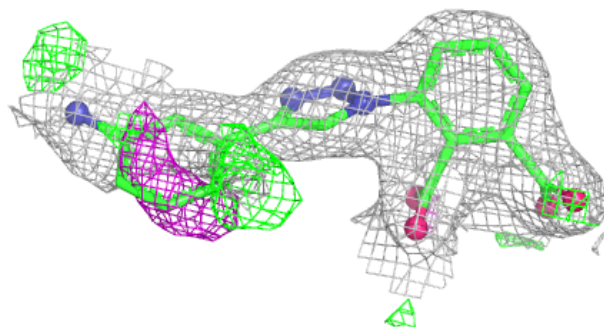
Electron density around IU3 G 303:

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

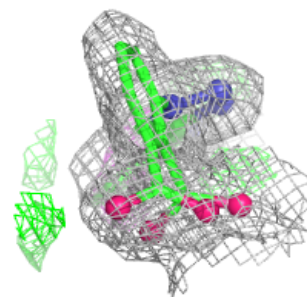
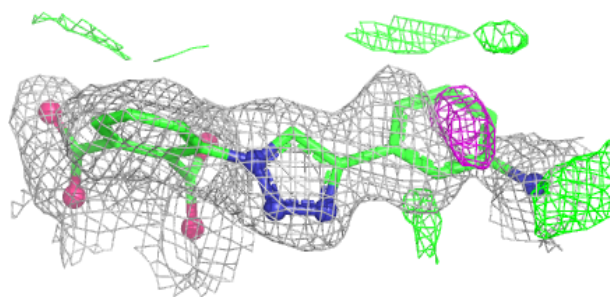
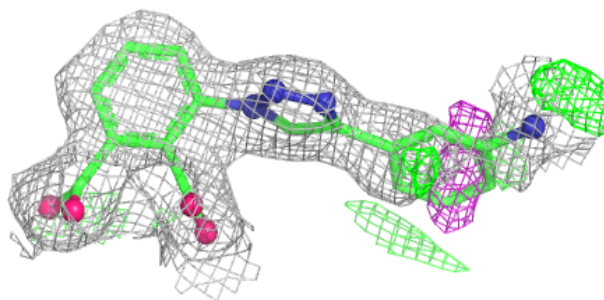


Electron density around IU3 B 303:

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

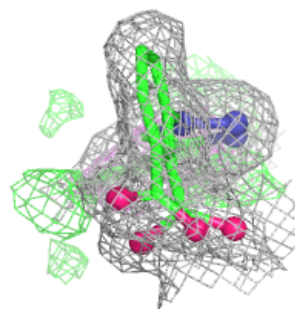
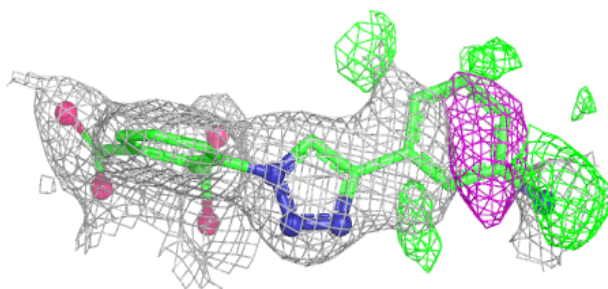
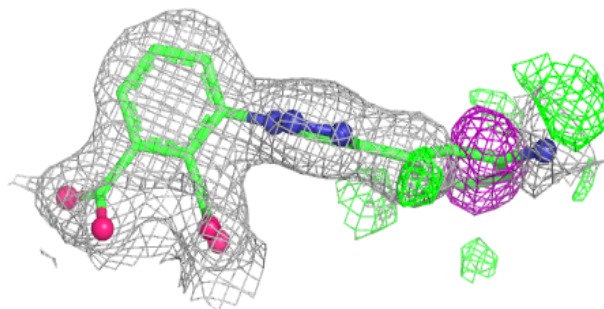
**Electron density around IU3 H 303:**

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and green (positive)

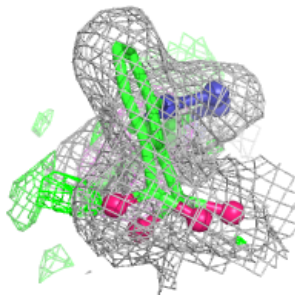
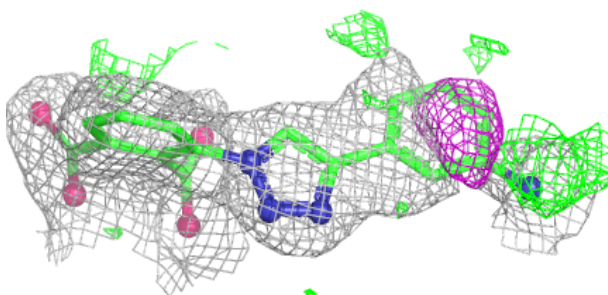
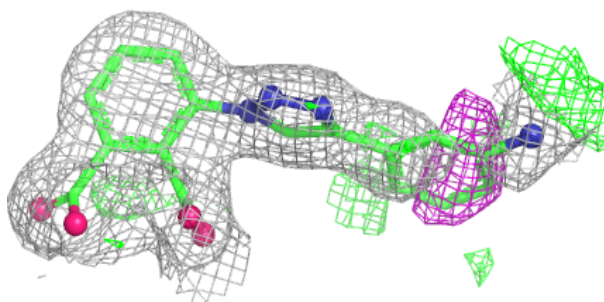


Electron density around IU3 E 303:

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

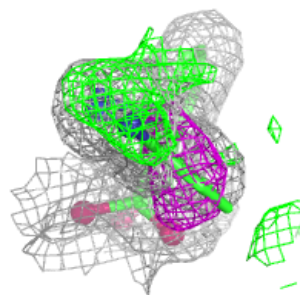
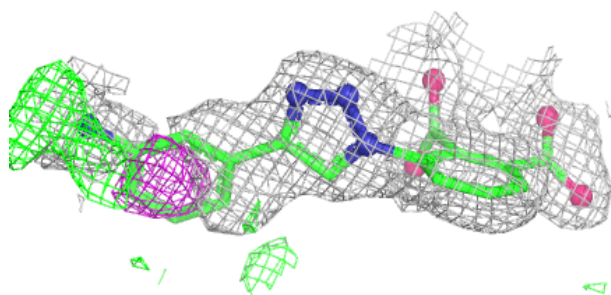
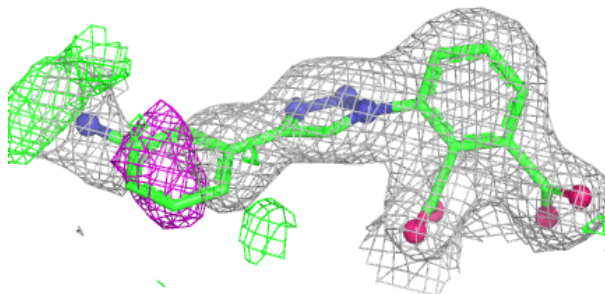
**Electron density around IU3 F 303:**

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

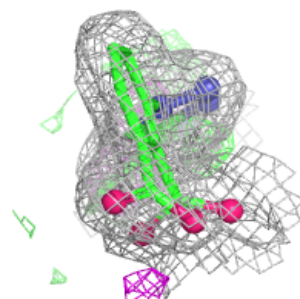
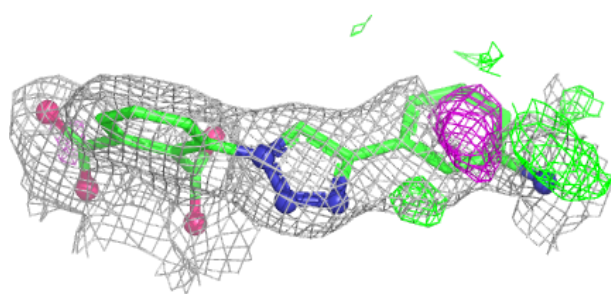
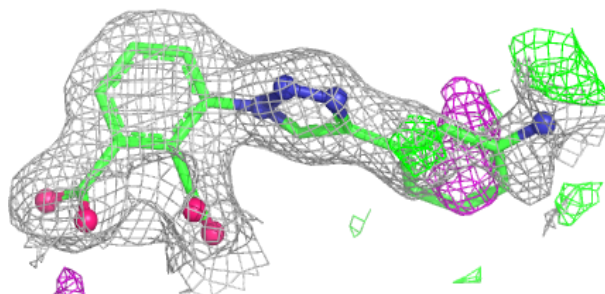


Electron density around IU3 A 303:

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

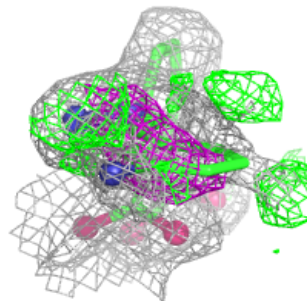
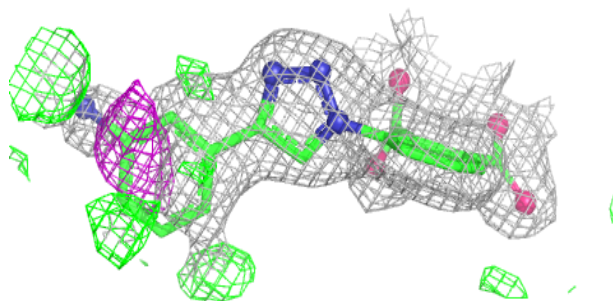
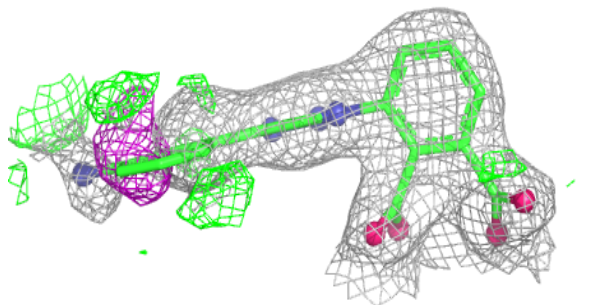
**Electron density around IU3 D 303:**

$2mF_o-DF_c$ (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.