



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 05:04 PM JST

PDB ID : 8HXE  
Title : Crystal structure of B3 L1 MBL in complex with 2-amino-5-(4-propylbenzyl)thiazole-4-carboxylic acid  
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Deposited on : 2023-01-04  
Resolution : 2.38 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

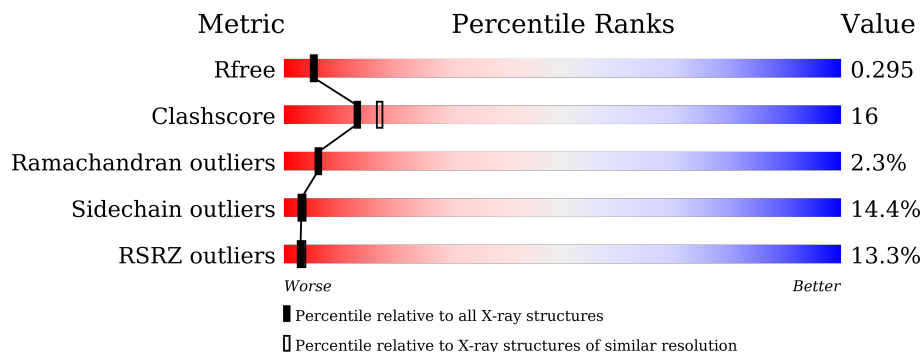
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	266	 12% 61% 32% 5% •
1	B	266	 14% 67% 25% 7% •

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4069 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.

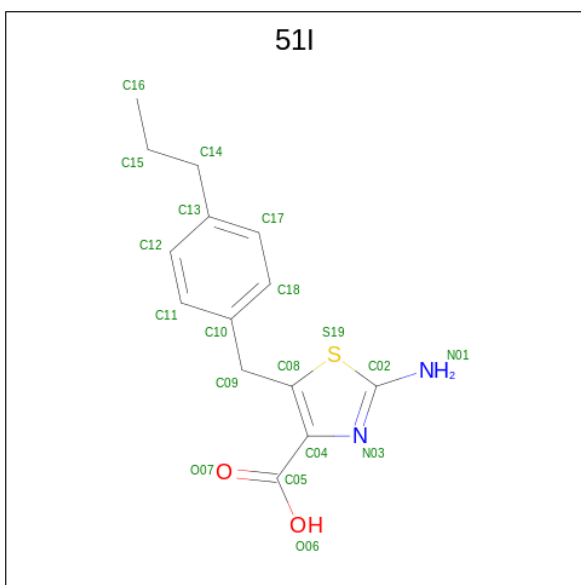
- Molecule 1 is a protein called Metallo-beta-lactamase L1 type 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	2001	1258	360	375	8	0	0	0
1	B	266	2001	1258	360	375	8	0	0	0

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

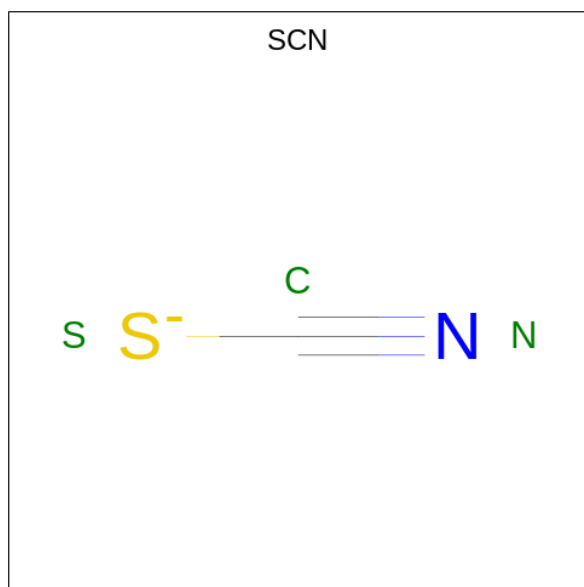
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 2-azanyl-5-[(4-propylphenyl)methyl]-1,3-thiazole-4-carboxylic acid (three-letter code: 51I) (formula: C<sub>14</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			19	14	2	2	1		
3	B	1	Total	C	N	O	S	0	0
			19	14	2	2	1		

- Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			3	1	1	1		
4	B	1	Total	C	N	S	0	0
			3	1	1	1		

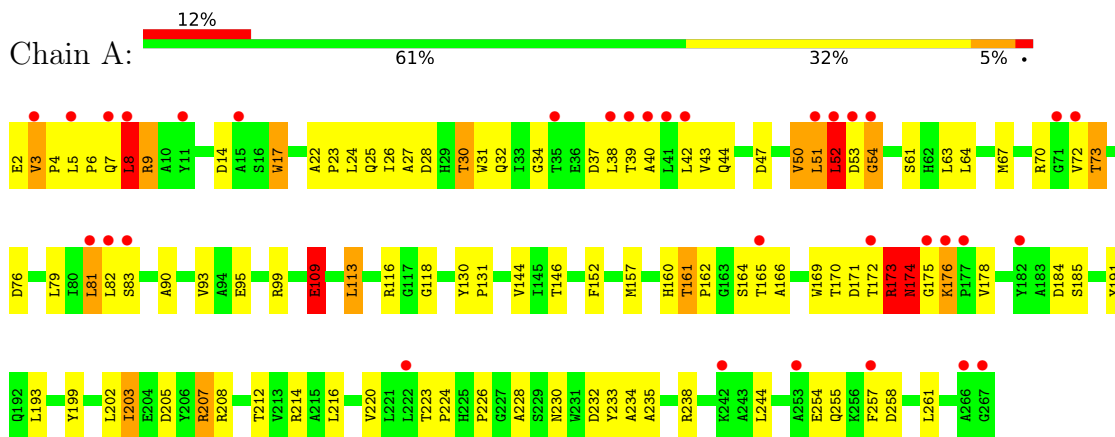
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	10	Total	O	0	0
			10	10		

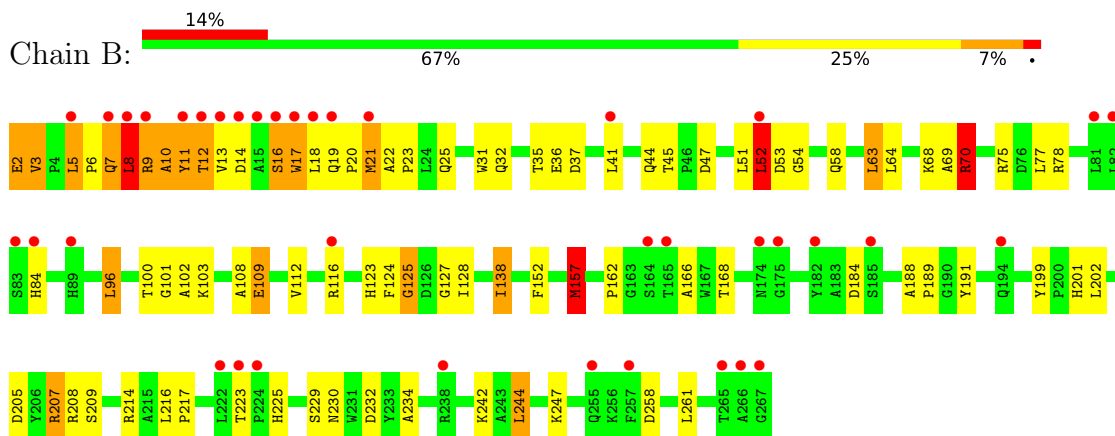
### 3 Residue-property plots [i](#)

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: Metallo-beta-lactamase L1 type 3



- Molecule 1: Metallo-beta-lactamase L1 type 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.53Å 75.53Å 181.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.65 – 2.38 32.65 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.65-2.38) 99.8 (32.65-2.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.214 , 0.299 0.219 , 0.295	Depositor DCC
$R_{free}$ test set	1999 reflections (9.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.1	Xtrriage
Anisotropy	0.223	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4069	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, SCN, 51I

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	0.67	2/2051 (0.1%)	0.84	3/2801 (0.1%)
1	B	0.66	0/2051	0.85	4/2801 (0.1%)
All	All	0.67	2/4102 (0.0%)	0.85	7/5602 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	GLU	CG-CD	-6.42	1.42	1.51
1	A	17	TRP	CB-CG	-5.29	1.40	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	70	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	B	8	LEU	CB-CG-CD1	5.42	120.22	111.00
1	B	157	MET	CG-SD-CE	-5.41	91.55	100.20
1	A	52	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	116	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	9	ARG	N-CA-C	5.06	124.66	111.00
1	B	52	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	LEU	Peptide
1	B	217	PRO	Peptide

## 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	2001	0	1958	71	1
1	B	2001	0	1958	59	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	19	0	0	0	0
3	B	19	0	0	0	0
4	A	3	0	0	1	0
4	B	3	0	0	0	0
5	A	9	0	0	4	0
5	B	10	0	0	1	0
All	All	4069	0	3916	130	1

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 16.

All (130) 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:214:ARG:NH2	1:A:254:GLU:OE1	2.15	0.79
1:A:207:ARG:NH2	1:A:258:ASP:OD1	2.18	0.76
1:B:157:MET:HE2	1:B:166:ALA:HB2	1.69	0.75
1:A:44:GLN:NE2	1:A:70:ARG:O	2.26	0.69
1:B:157:MET:CE	1:B:166:ALA:HB2	2.23	0.68
1:B:9:ARG:HG3	1:B:10:ALA:N	2.09	0.67
1:A:203:ILE:HG22	5:A:407:HOH:O	1.95	0.65
1:B:205:ASP:OD1	1:B:208:ARG:NH2	2.31	0.64
1:B:100:THR:HG22	1:B:102:ALA:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLU:HG2	1:A:162:PRO:HB2	1.81	0.62
1:B:10:ALA:O	1:B:11:TYR:HB2	2.01	0.61
1:A:161:THR:HG21	5:A:401:HOH:O	1.99	0.61
1:B:35:THR:HG22	1:B:37:ASP:H	1.65	0.60
1:A:51:LEU:HD23	1:A:53:ASP:O	2.01	0.60
1:B:77:LEU:HD23	1:B:100:THR:HG21	1.83	0.60
1:A:161:THR:HG22	1:A:164:SER:N	2.17	0.60
1:B:6:PRO:O	1:B:9:ARG:HG2	2.02	0.59
1:A:113:LEU:HD22	1:A:118:GLY:HA2	1.83	0.59
1:B:2:GLU:O	1:B:3:VAL:CG1	2.51	0.59
1:A:27:ALA:O	1:A:28:ASP:C	2.41	0.58
1:B:44:GLN:OE1	1:B:70:ARG:HG3	2.03	0.58
1:A:30:THR:HB	1:A:43:VAL:HG12	1.86	0.57
1:A:63:LEU:O	1:A:67:MET:HG3	2.05	0.56
1:A:31:TRP:NE1	1:A:70:ARG:NH1	2.54	0.56
1:A:212:THR:O	1:A:216:LEU:HD13	2.05	0.56
1:A:161:THR:HG22	1:A:164:SER:H	1.70	0.56
1:A:205:ASP:OD1	1:A:208:ARG:NH2	2.36	0.56
1:B:2:GLU:O	1:B:3:VAL:HG12	2.05	0.56
1:A:95:GLU:OE2	1:A:99:ARG:NH1	2.39	0.56
1:A:43:VAL:CG2	1:A:50:VAL:HG13	2.35	0.55
1:A:39:THR:HB	1:A:224:PRO:HA	1.88	0.55
1:B:96:LEU:O	1:B:100:THR:HB	2.06	0.55
1:B:223:THR:HG23	1:B:225:HIS:O	2.08	0.53
1:B:13:VAL:O	1:B:13:VAL:HG23	2.06	0.53
1:A:24:LEU:O	1:A:24:LEU:HD23	2.08	0.53
1:B:223:THR:HG22	1:B:229:SER:OG	2.08	0.53
1:A:52:LEU:HD12	1:A:81:LEU:HB2	1.90	0.53
1:B:18:LEU:O	1:B:20:PRO:HD3	2.09	0.53
1:B:2:GLU:O	5:B:401:HOH:O	2.18	0.53
1:B:21:MET:CE	1:B:35:THR:C	2.78	0.52
1:A:37:ASP:O	1:A:38:LEU:HD12	2.09	0.51
1:A:44:GLN:OE1	1:A:70:ARG:NH1	2.42	0.51
1:A:160:HIS:CE1	4:A:304:SCN:S	3.04	0.51
1:B:100:THR:HG22	1:B:102:ALA:N	2.26	0.50
1:A:79:LEU:HG	1:A:81:LEU:HD13	1.93	0.50
1:B:109:GLU:HG2	1:B:162:PRO:HB2	1.93	0.50
1:B:127:GLY:O	1:B:128:ILE:HD13	2.12	0.49
1:B:124:PHE:O	1:B:125:GLY:C	2.51	0.49
1:B:41:LEU:O	1:B:51:LEU:HD12	2.14	0.48
1:B:157:MET:HB2	1:B:209:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:THR:O	1:A:76:ASP:N	2.45	0.48
1:A:171:ASP:O	1:A:178:VAL:HG22	2.13	0.48
1:A:67:MET:O	1:A:72:VAL:HB	2.13	0.48
1:A:67:MET:O	1:A:72:VAL:N	2.46	0.48
1:B:9:ARG:CG	1:B:10:ALA:N	2.77	0.48
1:B:54:GLY:O	1:B:63:LEU:HD21	2.14	0.48
1:A:230:ASN:HB2	1:A:244:LEU:CD1	2.43	0.48
1:B:14:ASP:HB3	1:B:17:TRP:CE3	2.49	0.47
1:A:61:SER:OG	1:A:99:ARG:NH2	2.44	0.47
1:A:223:THR:OG1	1:A:228:ALA:HB3	2.14	0.47
1:A:23:PRO:HG2	1:A:70:ARG:HG2	1.96	0.47
1:A:54:GLY:O	1:A:63:LEU:HD11	2.14	0.47
1:A:22:ALA:HB1	1:A:23:PRO:HD2	1.97	0.47
1:A:51:LEU:CD2	1:A:53:ASP:O	2.62	0.47
1:B:21:MET:HG3	1:B:22:ALA:N	2.30	0.47
1:B:14:ASP:O	1:B:17:TRP:O	2.33	0.47
1:A:191:TYR:O	1:A:193:LEU:CD1	2.63	0.47
1:B:47:ASP:OD2	1:B:78:ARG:NH1	2.48	0.47
1:B:23:PRO:HA	1:B:32:GLN:O	2.15	0.46
1:B:230:ASN:HB2	1:B:244:LEU:HD13	1.97	0.46
1:A:235:ALA:O	1:A:238:ARG:N	2.44	0.46
1:B:13:VAL:O	1:B:13:VAL:CG2	2.64	0.46
1:A:31:TRP:CD1	1:A:70:ARG:NH1	2.84	0.46
1:B:8:LEU:CA	1:B:9:ARG:HB3	2.45	0.46
1:A:230:ASN:HB2	1:A:244:LEU:HD13	1.97	0.46
5:A:408:HOH:O	1:B:138:ILE:HG23	2.16	0.46
1:B:17:TRP:HD1	1:B:37:ASP:OD2	1.99	0.46
1:B:21:MET:HG3	1:B:22:ALA:O	2.15	0.46
1:B:25:GLN:HB2	1:B:31:TRP:CZ3	2.51	0.46
1:B:18:LEU:O	1:B:18:LEU:HD23	2.15	0.46
1:A:25:GLN:HB2	1:A:31:TRP:CZ3	2.51	0.45
1:A:43:VAL:O	1:A:43:VAL:HG23	2.15	0.45
1:A:203:ILE:HD13	1:A:257:PHE:HE2	1.81	0.45
1:A:2:GLU:O	1:A:3:VAL:O	2.34	0.45
1:A:34:GLY:CA	1:A:40:ALA:HB3	2.47	0.45
1:A:173:ARG:C	1:A:175:GLY:H	2.20	0.45
1:A:202:LEU:C	1:A:202:LEU:HD23	2.36	0.45
1:A:83:SER:OG	1:A:184:ASP:OD1	2.35	0.45
1:A:172:THR:O	1:A:173:ARG:HB2	2.16	0.45
1:A:79:LEU:HD21	1:A:81:LEU:HD11	2.00	0.44
1:A:39:THR:OG1	1:A:223:THR:O	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PRO:HG3	1:A:233:TYR:CE2	2.53	0.44
1:B:232:ASP:OD1	1:B:234:ALA:HB3	2.17	0.44
1:B:7:GLN:O	1:B:8:LEU:HD12	2.17	0.44
1:A:90:ALA:O	1:A:93:VAL:HG23	2.18	0.44
1:B:108:ALA:O	1:B:112:VAL:HG23	2.18	0.44
1:A:130:TYR:HB2	1:A:131:PRO:HD2	2.00	0.43
1:A:7:GLN:C	1:A:8:LEU:HG	2.38	0.43
1:B:6:PRO:HA	1:B:9:ARG:NH1	2.34	0.43
1:A:174:ASN:HB3	1:A:176:LYS:HE3	1.99	0.43
1:A:5:LEU:H	1:A:6:PRO:HD2	1.83	0.43
1:B:214:ARG:HG3	1:B:247:LYS:HA	2.00	0.43
1:B:84:HIS:HB3	1:B:184:ASP:OD2	2.18	0.43
1:B:188:ALA:N	1:B:189:PRO:HD3	2.33	0.43
1:A:52:LEU:O	1:A:53:ASP:HB2	2.19	0.43
1:B:100:THR:HG22	1:B:101:GLY:N	2.34	0.43
1:A:130:TYR:HB2	1:A:131:PRO:CD	2.49	0.43
1:A:193:LEU:HD23	1:A:261:LEU:HG	2.02	0.42
1:B:52:LEU:O	1:B:53:ASP:HB2	2.19	0.42
1:A:232:ASP:C	1:A:234:ALA:H	2.23	0.42
5:A:408:HOH:O	1:B:138:ILE:CG2	2.67	0.42
1:A:14:ASP:HB3	1:A:17:TRP:CD2	2.55	0.42
1:B:5:LEU:N	1:B:6:PRO:HD2	2.35	0.42
1:B:207:ARG:NH1	1:B:258:ASP:OD1	2.51	0.42
1:A:7:GLN:O	1:A:8:LEU:CB	2.68	0.41
1:B:35:THR:HG22	1:B:36:GLU:N	2.35	0.41
1:A:157:MET:HE1	1:A:184:ASP:O	2.21	0.41
1:B:52:LEU:CD2	1:B:52:LEU:N	2.84	0.41
1:A:22:ALA:HB1	1:A:23:PRO:CD	2.51	0.41
1:A:165:THR:HG22	1:A:166:ALA:N	2.35	0.41
1:B:12:THR:O	1:B:12:THR:HG22	2.20	0.41
1:A:23:PRO:HB2	1:A:31:TRP:CE3	2.56	0.41
1:A:32:GLN:O	1:A:32:GLN:HG3	2.21	0.41
1:A:173:ARG:HD2	1:A:178:VAL:HG11	2.02	0.41
1:B:8:LEU:HA	1:B:9:ARG:HB3	2.02	0.41
1:B:70:ARG:HH11	1:B:70:ARG:CA	2.34	0.41
1:B:152:PHE:HA	1:B:168:THR:O	2.21	0.41
1:A:30:THR:HG21	1:A:169:TRP:HE1	1.86	0.40
1:A:144:VAL:HA	1:A:152:PHE:O	2.21	0.40
1:B:123:HIS:CE1	1:B:191:TYR:CD2	3.10	0.40

All (1) 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:A:238:ARG:NH2	1:B:69:ALA:O[3_545]	2.19	0.01

### 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	264/266 (99%)	224 (85%)	33 (12%)	7 (3%)	5	4
1	B	264/266 (99%)	240 (91%)	19 (7%)	5 (2%)	8	9
All	All	528/532 (99%)	464 (88%)	52 (10%)	12 (2%)	6	6

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	4	PRO
1	A	173	ARG
1	B	11	TYR
1	A	9	ARG
1	B	16	SER
1	A	8	LEU
1	B	3	VAL
1	B	10	ALA
1	B	125	GLY
1	A	174	ASN
1	A	54	GLY

#### 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	201/201 (100%)	175 (87%)	26 (13%)	4	4
1	B	201/201 (100%)	169 (84%)	32 (16%)	2	2
All	All	402/402 (100%)	344 (86%)	58 (14%)	3	3

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	26	ILE
1	A	30	THR
1	A	42	LEU
1	A	47	ASP
1	A	50	VAL
1	A	51	LEU
1	A	52	LEU
1	A	64	LEU
1	A	73	THR
1	A	81	LEU
1	A	82	LEU
1	A	109	GLU
1	A	113	LEU
1	A	146	THR
1	A	161	THR
1	A	170	THR
1	A	173	ARG
1	A	174	ASN
1	A	176	LYS
1	A	185	SER
1	A	199	TYR
1	A	203	ILE
1	A	207	ARG
1	A	220	VAL
1	A	255	GLN
1	B	2	GLU
1	B	5	LEU
1	B	7	GLN
1	B	8	LEU
1	B	9	ARG
1	B	12	THR
1	B	16	SER
1	B	17	TRP

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Mol	Chain	Res	Type
1	B	19	GLN
1	B	21	MET
1	B	45	THR
1	B	52	LEU
1	B	58	GLN
1	B	63	LEU
1	B	64	LEU
1	B	68	LYS
1	B	70	ARG
1	B	75	ARG
1	B	96	LEU
1	B	103	LYS
1	B	109	GLU
1	B	116	ARG
1	B	138	ILE
1	B	157	MET
1	B	199	TYR
1	B	201	HIS
1	B	202	LEU
1	B	207	ARG
1	B	216	LEU
1	B	242	LYS
1	B	244	LEU
1	B	261	LEU

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	51I	B	303	2	16,20,20	1.63	2 (12%)	19,27,27	1.08	3 (15%)
4	SCN	B	304	-	1,2,2	0.75	0	0,1,1	-	-
3	51I	A	303	2	16,20,20	1.55	2 (12%)	19,27,27	1.22	2 (10%)
4	SCN	A	304	2	1,2,2	0.64	0	0,1,1	-	-

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	51I	B	303	2	-	3/10/11/11	0/2/2/2
3	51I	A	303	2	-	2/10/11/11	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	51I	C09-C08	4.59	1.55	1.51
3	A	303	51I	C08-S19	-4.13	1.66	1.74
3	B	303	51I	C02-N01	3.52	1.45	1.35
3	A	303	51I	C02-N01	3.10	1.44	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	51I	C08-C04-C05	-3.23	121.33	130.50
3	A	303	51I	N01-C02-N03	2.46	126.37	123.19
3	B	303	51I	C08-C04-C05	-2.23	124.17	130.50
3	B	303	51I	O06-C05-C04	2.13	121.35	114.46
3	B	303	51I	C10-C09-C08	-2.00	107.25	112.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	51I	N03-C04-C05-O06
3	A	303	51I	C04-C08-C09-C10
3	B	303	51I	C13-C14-C15-C16
3	B	303	51I	C17-C13-C14-C15
3	B	303	51I	C12-C13-C14-C15

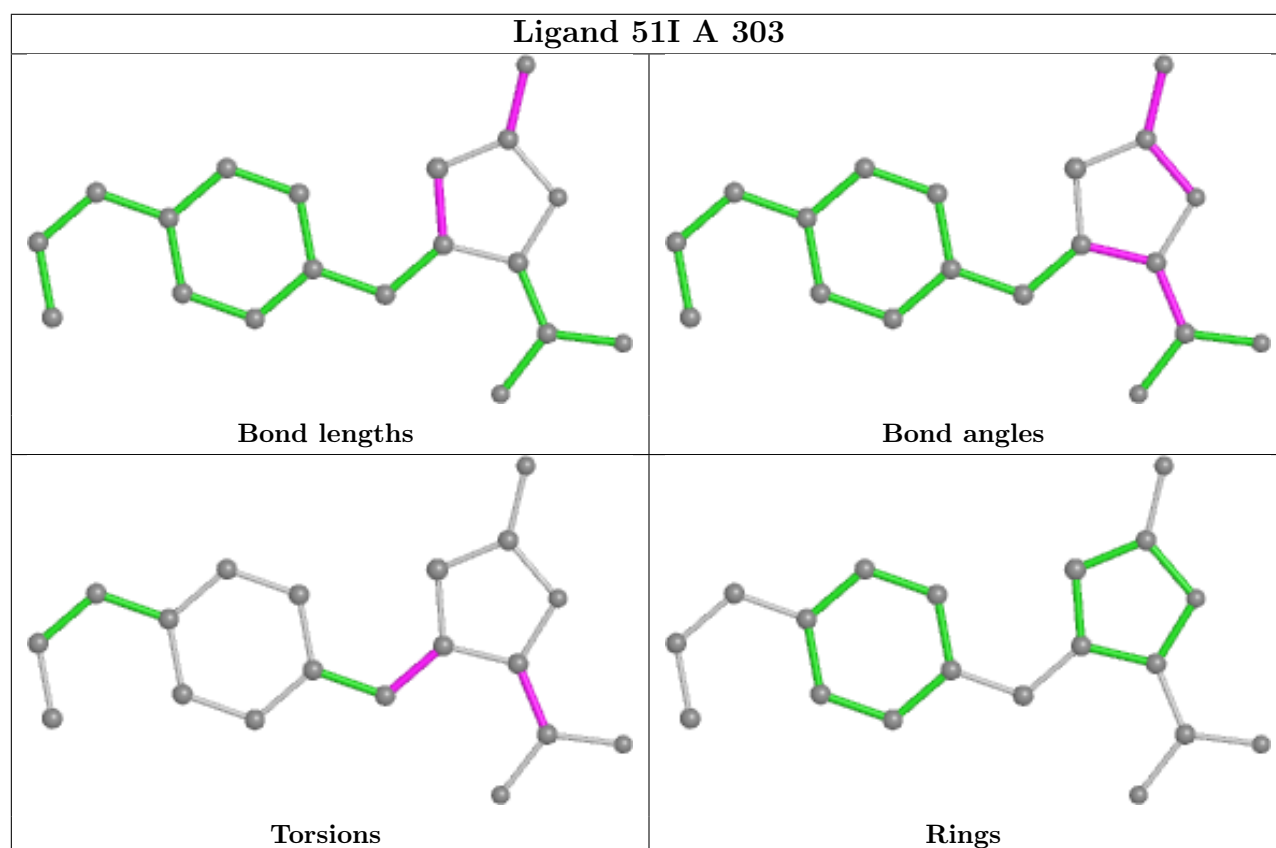
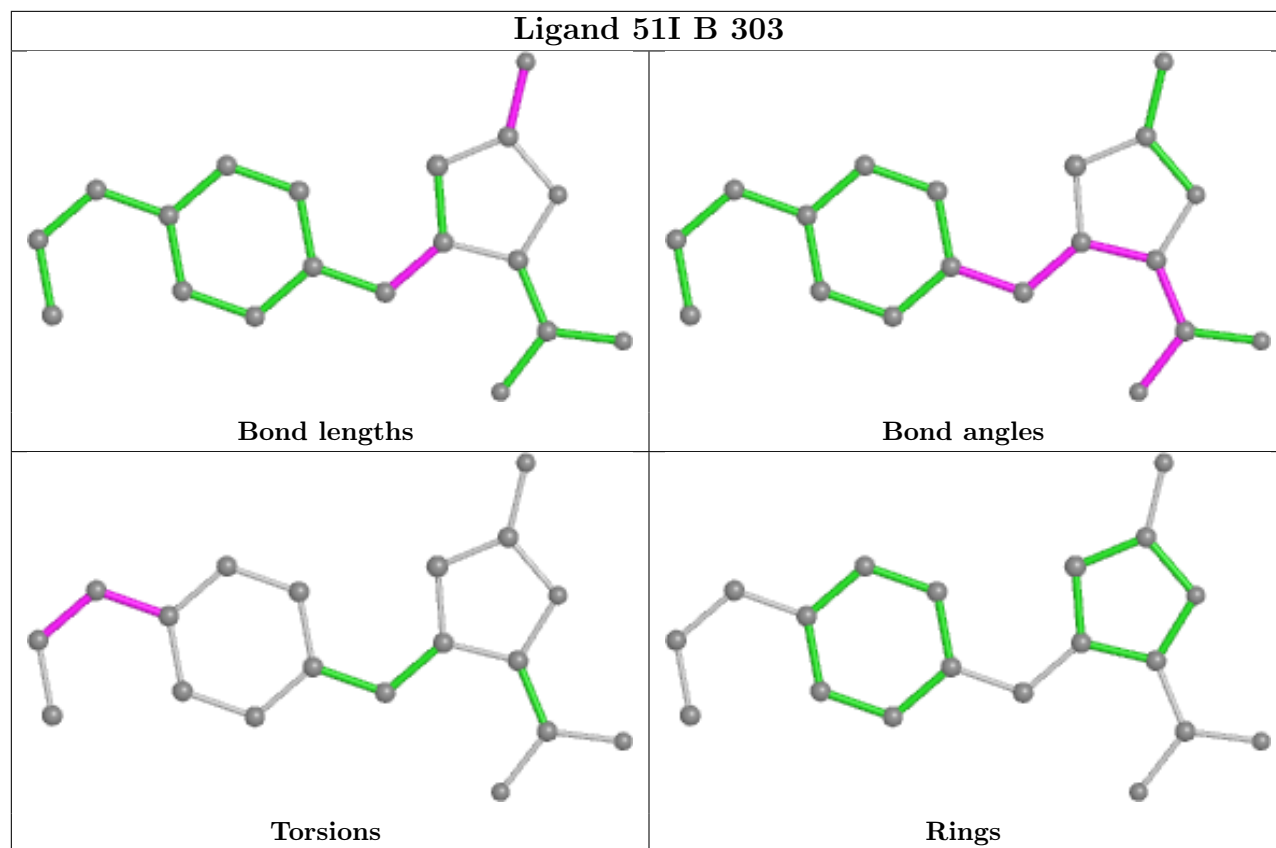
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	SCN	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 [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	266/266 (100%)	0.68	33 (12%) <b>4</b>   <b>4</b>	48, 79, 112, 149	0
1	B	266/266 (100%)	0.80	38 (14%) <b>2</b>   <b>2</b>	49, 69, 112, 152	1 (0%)
All	All	532/532 (100%)	0.74	71 (13%) <b>3</b>   <b>3</b>	48, 73, 112, 152	1 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	17	TRP	9.8
1	B	15	ALA	8.1
1	B	16	SER	8.1
1	B	12	THR	7.7
1	B	9	ARG	7.1
1	A	41	LEU	6.1
1	B	267	GLY	6.0
1	B	266	ALA	5.4
1	A	182	TYR	5.1
1	B	8	LEU	5.0
1	B	182	TYR	4.8
1	B	19	GLN	4.7
1	A	51	LEU	4.7
1	B	13	VAL	4.6
1	B	255	GLN	4.6
1	B	223	THR	4.3
1	A	222	LEU	4.1
1	B	82	LEU	4.1
1	B	224	PRO	4.0
1	A	267	GLY	4.0
1	B	83	SER	3.8
1	A	8	LEU	3.8
1	A	52	LEU	3.6
1	B	175	GLY	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	83	SER	3.4
1	B	11	TYR	3.4
1	A	266	ALA	3.3
1	A	176	LYS	3.2
1	B	174	ASN	3.1
1	A	82	LEU	3.1
1	A	39	THR	3.0
1	A	40	ALA	3.0
1	B	7	GLN	2.9
1	B	257	PHE	2.9
1	B	81	LEU	2.9
1	A	3	VAL	2.9
1	A	253	ALA	2.7
1	A	177	PRO	2.7
1	B	165	THR	2.7
1	B	194	GLN	2.7
1	B	52	LEU	2.7
1	B	89	HIS	2.7
1	A	257	PHE	2.6
1	B	238	ARG	2.6
1	A	71	GLY	2.6
1	A	172	THR	2.5
1	B	222	LEU	2.5
1	B	84	HIS	2.5
1	B	116	ARG	2.5
1	A	81	LEU	2.5
1	B	41	LEU	2.5
1	A	72	VAL	2.4
1	A	35	THR	2.4
1	A	175	GLY	2.4
1	B	164	SER	2.4
1	B	21	MET	2.4
1	A	7	GLN	2.4
1	A	242	LYS	2.3
1	A	38	LEU	2.3
1	A	53	ASP	2.2
1	A	15	ALA	2.2
1	B	14	ASP	2.2
1	B	18	LEU	2.2
1	B	5	LEU	2.1
1	B	185	SER	2.1
1	A	54	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	11	TYR	2.1
1	B	265	THR	2.1
1	A	5	LEU	2.1
1	A	42	LEU	2.0
1	A	165	THR	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](#)

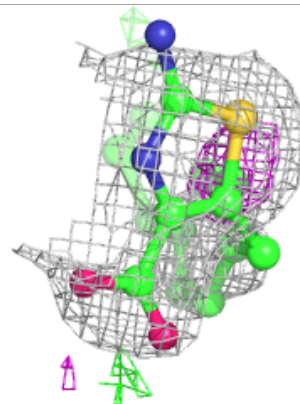
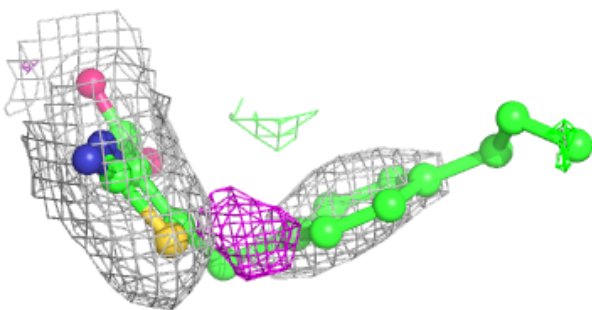
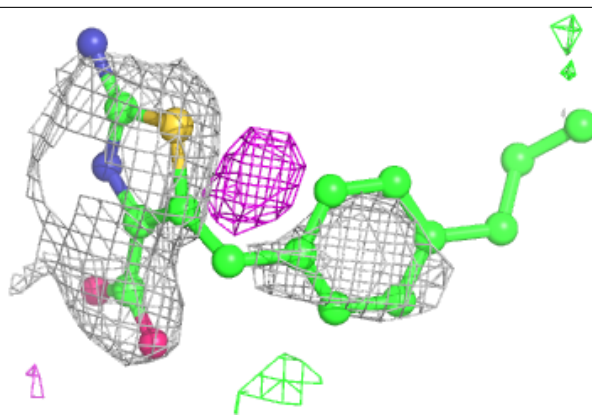
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	SCN	B	304	3/3	0.77	0.39	97,97,163,254	0
4	SCN	A	304	3/3	0.81	0.20	62,62,72,88	0
3	51I	B	303	19/19	0.88	0.25	78,98,114,121	0
3	51I	A	303	19/19	0.93	0.16	67,81,112,115	0
2	ZN	B	302	1/1	0.98	0.10	75,75,75,75	0
2	ZN	B	301	1/1	0.99	0.15	69,69,69,69	0
2	ZN	A	301	1/1	0.99	0.10	71,71,71,71	0
2	ZN	A	302	1/1	0.99	0.10	71,71,71,71	0

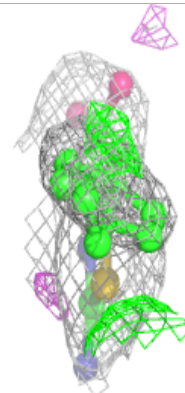
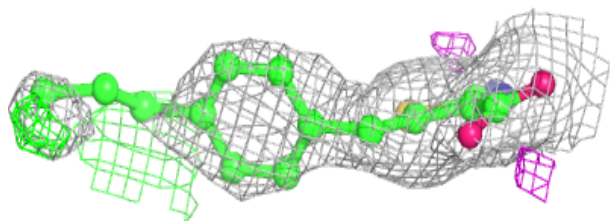
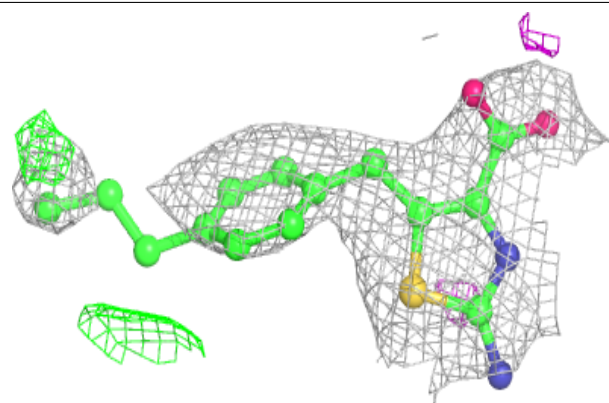
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 51I 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 51I 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.