



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2022 – 10:24 AM EST

PDB ID : 7THQ  
Title : Crystal structure of PltF trapped with PigG using a proline adenosine vinyl-sulfonamide inhibitor  
Authors : Corpuz, J.C.; Podust, L.M.  
Deposited on : 2022-01-11  
Resolution : 2.46 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>.

---

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 : 2.31.2  
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) : 2.31.2

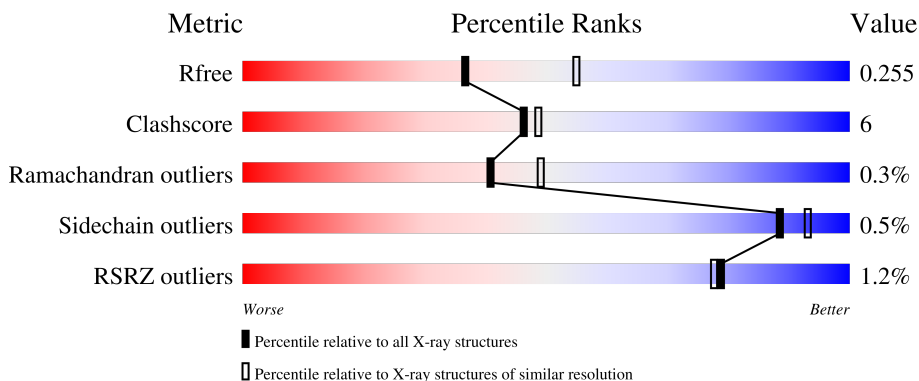
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	513	<div> <div>0%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	B	513	<div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	C	95	<div> <div>4%</div> <div>62%</div> <div>18%</div> <div>.</div> <div>19%</div> </div>
2	E	95	<div> <div>4%</div> <div>67%</div> <div>16%</div> <div>17%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8613 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 L-proline--[L-prolyl-carrier protein] ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	505	Total	C	N	O	S	0	1	0
			3744	2386	654	679	25			
1	A	500	Total	C	N	O	S	0	0	0
			3662	2333	633	672	24			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	499	LYS	-	expression tag	UNP Q4KCY5
B	500	LEU	-	expression tag	UNP Q4KCY5
B	501	ALA	-	expression tag	UNP Q4KCY5
B	502	ALA	-	expression tag	UNP Q4KCY5
B	503	ALA	-	expression tag	UNP Q4KCY5
B	504	LEU	-	expression tag	UNP Q4KCY5
B	505	GLU	-	expression tag	UNP Q4KCY5
B	506	HIS	-	expression tag	UNP Q4KCY5
B	507	HIS	-	expression tag	UNP Q4KCY5
B	508	HIS	-	expression tag	UNP Q4KCY5
B	509	HIS	-	expression tag	UNP Q4KCY5
B	510	HIS	-	expression tag	UNP Q4KCY5
B	511	HIS	-	expression tag	UNP Q4KCY5
B	512	HIS	-	expression tag	UNP Q4KCY5
B	513	HIS	-	expression tag	UNP Q4KCY5
A	499	LYS	-	expression tag	UNP Q4KCY5
A	500	LEU	-	expression tag	UNP Q4KCY5
A	501	ALA	-	expression tag	UNP Q4KCY5
A	502	ALA	-	expression tag	UNP Q4KCY5
A	503	ALA	-	expression tag	UNP Q4KCY5
A	504	LEU	-	expression tag	UNP Q4KCY5
A	505	GLU	-	expression tag	UNP Q4KCY5
A	506	HIS	-	expression tag	UNP Q4KCY5
A	507	HIS	-	expression tag	UNP Q4KCY5
A	508	HIS	-	expression tag	UNP Q4KCY5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	509	HIS	-	expression tag	UNP Q4KCY5
A	510	HIS	-	expression tag	UNP Q4KCY5
A	511	HIS	-	expression tag	UNP Q4KCY5
A	512	HIS	-	expression tag	UNP Q4KCY5
A	513	HIS	-	expression tag	UNP Q4KCY5

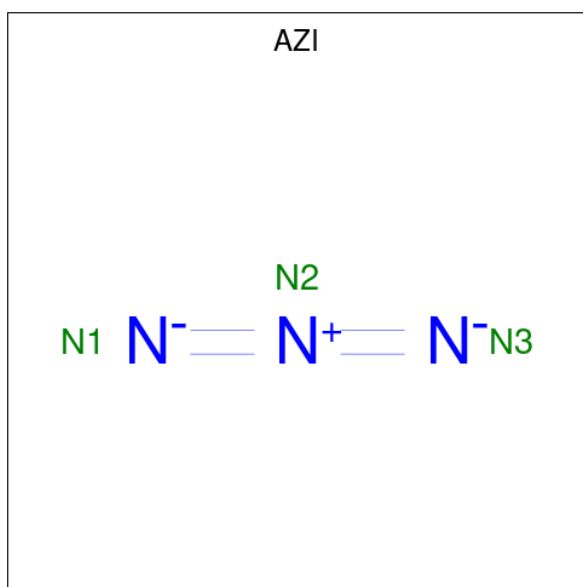
- Molecule 2 is a protein called Probable acyl carrier protein PigG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	79	Total	C	N	O	S	0	0	0
			528	344	85	97	2			
2	C	77	Total	C	N	O	S	0	0	0
			512	329	84	97	2			

There are 16 discrepancies between the modelled and reference sequences:

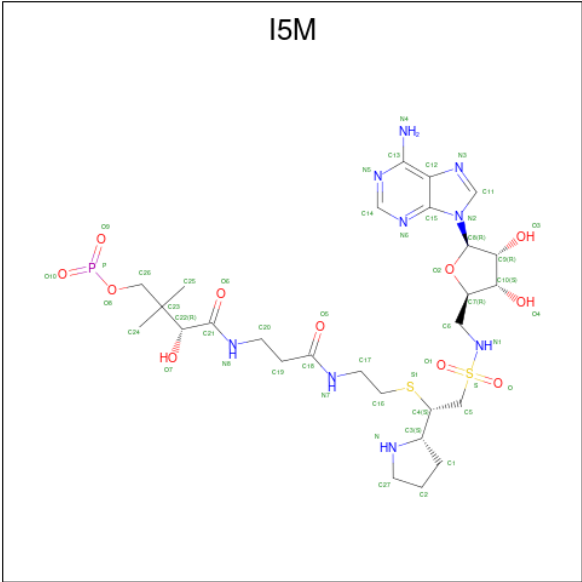
Chain	Residue	Modelled	Actual	Comment	Reference
E	88	TRP	-	expression tag	UNP Q5W265
E	89	GLU	-	expression tag	UNP Q5W265
E	90	HIS	-	expression tag	UNP Q5W265
E	91	HIS	-	expression tag	UNP Q5W265
E	92	HIS	-	expression tag	UNP Q5W265
E	93	HIS	-	expression tag	UNP Q5W265
E	94	HIS	-	expression tag	UNP Q5W265
E	95	HIS	-	expression tag	UNP Q5W265
C	88	TRP	-	expression tag	UNP Q5W265
C	89	GLU	-	expression tag	UNP Q5W265
C	90	HIS	-	expression tag	UNP Q5W265
C	91	HIS	-	expression tag	UNP Q5W265
C	92	HIS	-	expression tag	UNP Q5W265
C	93	HIS	-	expression tag	UNP Q5W265
C	94	HIS	-	expression tag	UNP Q5W265
C	95	HIS	-	expression tag	UNP Q5W265

- Molecule 3 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



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

- Molecule 4 is 5'-deoxy-5'-({(2S)-2-({2-[(N-{(2R)-4-[(dioxo-lambda 5 -phosphanyl)oxy]-2-hydroxy-3,3-dimethylbutanoyl}-beta-alanyl)amino]ethyl}sulfanyl)-2-[(2S)-pyrrolidin-2-yl]ethanesulfonyl}amino)adenosine (three-letter code: I5M) (formula: C<sub>27</sub>H<sub>44</sub>N<sub>9</sub>O<sub>11</sub>PS<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	S	0	0
			50	27	9	11	1	2		
4	C	1	Total	C	N	O	P	S	0	0
			50	27	9	11	1	2		

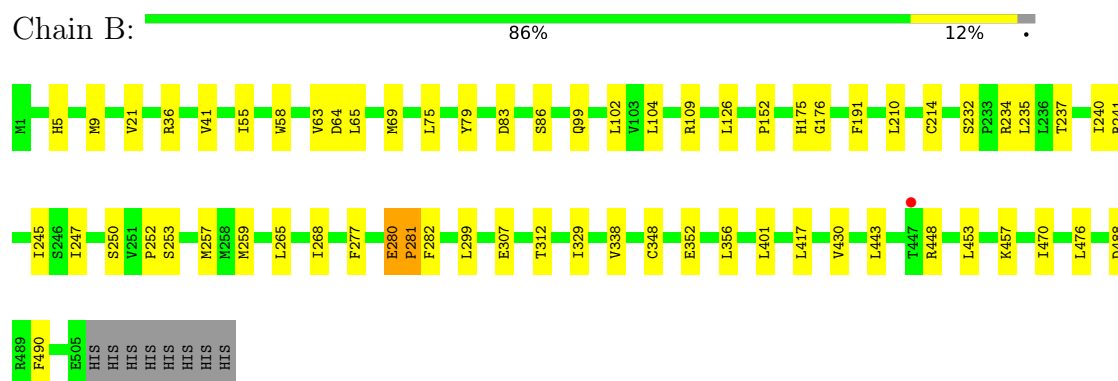
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	26	Total	O	0	0
			26	26		
5	E	1	Total	O	0	0
			1	1		
5	A	20	Total	O	0	0
			20	20		
5	C	2	Total	O	0	0
			2	2		

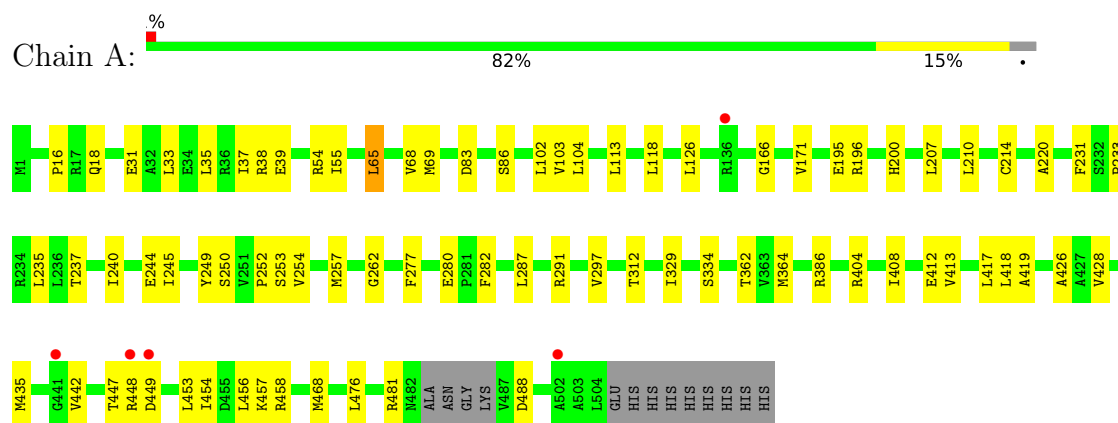
### 3 Residue-property plots

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.

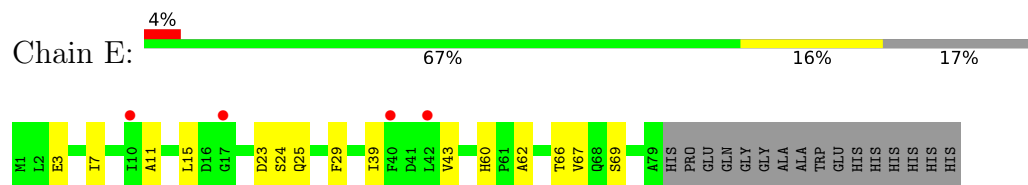
- Molecule 1: L-proline--[L-prolyl-carrier protein] ligase



- Molecule 1: L-proline--[L-prolyl-carrier protein] ligase

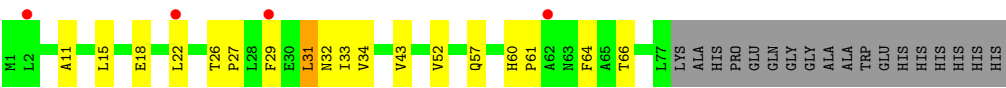


- Molecule 2: Probable acyl carrier protein PigG



- Molecule 2: Probable acyl carrier protein PigG







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.73Å 132.68Å 140.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.61 – 2.46 96.61 – 2.46	Depositor EDS
% Data completeness (in resolution range)	98.2 (96.61-2.46) 98.2 (96.61-2.46)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.206 , 0.255 0.207 , 0.255	Depositor DCC
$R_{free}$ test set	2303 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.8	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8613	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: AZI, I5M

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	0.31	0/3736	0.56	2/5100 (0.0%)
1	B	0.36	2/3823 (0.1%)	0.54	3/5216 (0.1%)
2	C	0.27	0/519	0.57	1/714 (0.1%)
2	E	0.29	0/536	0.58	0/734
All	All	0.33	2/8614 (0.0%)	0.55	6/11764 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	PRO	N-CA	12.56	1.68	1.47
1	B	280	GLU	C-N	5.25	1.44	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	PRO	CA-N-CD	-6.94	101.79	111.50
1	A	18	GLN	CA-CB-CG	5.39	125.25	113.40
1	B	281	PRO	N-CA-C	-5.22	98.54	112.10
2	C	31	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	A	65	LEU	CB-CG-CD2	-5.15	102.25	111.00
1	B	476	LEU	CB-CG-CD2	-5.01	102.48	111.00

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	3662	0	3515	47	0
1	B	3744	0	3664	41	0
2	C	512	0	436	13	0
2	E	528	0	457	10	0
3	A	6	0	0	0	0
3	B	9	0	0	0	0
3	C	3	0	0	0	0
4	C	50	0	0	1	0
4	E	50	0	0	0	0
5	A	20	0	0	1	0
5	B	26	0	0	0	0
5	C	2	0	0	0	0
5	E	1	0	0	0	0
All	All	8613	0	8072	104	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:PRO:CA	1:B:281:PRO:N	1.68	1.38
1:A:458:ARG:HE	2:C:31:LEU:HD21	1.40	0.86
1:A:404:ARG:HG2	1:A:435:MET:HE1	1.60	0.83
2:E:60:HIS:HD2	2:E:62:ALA:H	1.25	0.80
1:A:237:THR:HG21	1:A:262:GLY:O	1.86	0.75
1:B:281:PRO:N	1:B:281:PRO:C	2.43	0.72
1:B:453:LEU:O	1:B:457:LYS:HG3	1.92	0.69
1:A:33:LEU:O	1:A:37:ILE:HG13	1.96	0.66
1:A:166:GLY:HA2	1:A:412:GLU:HG3	1.78	0.66
1:B:240:ILE:HG23	1:B:245:ILE:HB	1.79	0.65
2:C:27:PRO:HG2	2:C:31:LEU:HD13	1.78	0.65
2:C:11:ALA:HA	2:C:15:LEU:HB2	1.84	0.60
2:E:24:SER:HA	2:E:67:VAL:HB	1.82	0.59
2:E:66:THR:HG23	2:E:69:SER:H	1.68	0.58
1:A:334:SER:HB3	1:A:362:THR:HG21	1.86	0.57
2:E:29:PHE:HZ	2:E:39:ILE:HD13	1.69	0.57
1:B:55:ILE:HG22	1:B:102:LEU:HB3	1.87	0.56
1:B:104:LEU:HB3	1:B:126:LEU:HD11	1.88	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:HG22	1:A:102:LEU:HB3	1.88	0.56
1:B:83:ASP:HB3	1:B:86:SER:HB2	1.88	0.56
1:A:447:THR:O	1:A:449:ASP:N	2.39	0.56
1:A:458:ARG:NE	2:C:31:LEU:HD21	2.17	0.55
2:E:60:HIS:CD2	2:E:62:ALA:H	2.16	0.55
2:E:11:ALA:HA	2:E:15:LEU:HB2	1.88	0.55
1:A:253:SER:O	1:A:257:MET:HG3	2.07	0.54
1:A:65:LEU:O	1:A:69:MET:HG3	2.08	0.54
1:B:453:LEU:HG	1:B:457:LYS:HE3	1.89	0.53
1:A:207:LEU:HD22	1:A:249:TYR:CZ	2.43	0.53
1:B:348:CYS:HB3	1:B:352:GLU:HB2	1.91	0.53
1:A:457:LYS:NZ	2:C:32:ASN:O	2.39	0.53
1:B:152:PRO:O	1:B:175:HIS:HB2	2.09	0.52
1:B:241:ARG:NH2	1:B:268:ILE:O	2.43	0.52
2:E:3:GLU:O	2:E:7:ILE:HG13	2.10	0.52
1:A:233:PRO:O	1:A:237:THR:HG22	2.09	0.52
1:B:232:SER:HB3	1:B:235:LEU:HB2	1.92	0.51
1:B:36:ARG:NH1	1:B:64:ASP:OD1	2.44	0.50
1:B:312:THR:HG22	1:B:329:ILE:O	2.11	0.50
1:A:240:ILE:HG23	1:A:245:ILE:HB	1.94	0.50
1:A:418:LEU:HD22	1:A:426:ALA:HB3	1.93	0.50
1:B:234:ARG:NH2	1:B:237:THR:OG1	2.45	0.50
1:A:291:ARG:NH2	1:A:297:VAL:O	2.39	0.50
1:B:252:PRO:HD2	1:B:280:GLU:HG2	1.93	0.49
1:A:35:LEU:O	1:A:39:GLU:HG3	2.12	0.49
1:A:235:LEU:HD21	2:C:57:GLN:O	2.11	0.49
1:B:5:HIS:O	1:B:9:MET:HG3	2.12	0.49
1:A:312:THR:HG22	1:A:329:ILE:O	2.13	0.49
1:B:417:LEU:HD13	1:B:443:LEU:HD21	1.95	0.48
2:E:39:ILE:O	2:E:43:VAL:HG23	2.13	0.48
1:B:253:SER:O	1:B:257:MET:HG3	2.13	0.48
1:A:210:LEU:O	1:A:214:CYS:HB2	2.14	0.47
2:C:43:VAL:HG22	2:C:64:PHE:CZ	2.49	0.47
1:B:277:PHE:HE2	1:B:299:LEU:CD2	2.27	0.47
1:B:152:PRO:O	1:B:176:GLY:N	2.47	0.47
1:B:338:VAL:CG1	1:B:356:LEU:HD11	2.45	0.47
1:A:171:VAL:HG13	1:A:364:MET:HE3	1.97	0.47
1:A:417:LEU:HD21	1:A:456:LEU:HD21	1.97	0.47
2:C:60:HIS:CG	2:C:61:PRO:HD2	2.49	0.46
1:A:200:HIS:CE1	1:A:254:VAL:HG21	2.50	0.46
1:A:103:VAL:HG21	1:A:118:LEU:HD12	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:GLN:NE2	1:A:419:ALA:HA	2.31	0.46
1:B:401:LEU:HD23	1:B:430:VAL:HG23	1.97	0.46
2:C:29:PHE:CE1	2:C:34:VAL:HG12	2.51	0.46
1:A:386:ARG:HG2	5:A:810:HOH:O	2.15	0.45
1:A:196:ARG:HG3	1:A:244:GLU:O	2.16	0.45
1:B:41:VAL:HG13	1:B:75:LEU:HD21	1.97	0.45
2:E:23:ASP:OD2	2:E:25:GLN:N	2.38	0.45
1:A:195:GLU:O	1:A:220:ALA:HB1	2.16	0.45
1:A:282:PHE:CE2	1:A:287:LEU:HD13	2.52	0.45
1:B:21:VAL:HG22	1:B:63:VAL:HG12	1.98	0.44
1:B:488:ASP:C	1:B:490:PHE:H	2.20	0.44
1:B:259:MET:HE2	1:B:265:LEU:HD11	1.98	0.44
1:B:457:LYS:HE2	1:B:470:ILE:O	2.18	0.44
2:C:15:LEU:HA	2:C:15:LEU:HD23	1.69	0.44
1:A:442:VAL:HG13	1:A:476:LEU:HD23	2.01	0.43
1:A:83:ASP:O	1:A:86:SER:HB3	2.19	0.43
1:B:210:LEU:O	1:B:214:CYS:HB2	2.19	0.43
1:A:408:ILE:HG12	1:A:468:MET:HG2	1.99	0.43
1:B:252:PRO:HD2	1:B:280:GLU:CG	2.49	0.43
1:A:250:SER:O	1:A:277:PHE:HA	2.18	0.43
1:B:191:PHE:CE1	1:B:247:ILE:HG12	2.55	0.42
1:B:65:LEU:HD23	1:B:65:LEU:HA	1.76	0.42
1:A:453:LEU:O	1:A:457:LYS:HG3	2.19	0.42
1:A:104:LEU:HD23	1:A:126:LEU:HD21	2.01	0.42
1:A:435:MET:HA	1:A:435:MET:CE	2.49	0.42
1:A:404:ARG:NH1	4:C:901:I5M:O10	2.52	0.42
2:C:26:THR:O	2:C:66:THR:HG22	2.20	0.42
1:B:58:TRP:HZ2	1:B:109:ARG:NH2	2.17	0.42
1:A:68:VAL:HG11	1:A:104:LEU:HD22	2.02	0.41
1:A:252:PRO:HD2	1:A:280:GLU:CG	2.51	0.41
2:C:15:LEU:HD12	2:C:22:LEU:HD22	2.03	0.41
1:B:250:SER:O	1:B:277:PHE:HA	2.20	0.41
1:A:171:VAL:HG22	1:A:364:MET:HE3	2.01	0.41
1:A:252:PRO:HB3	1:A:282:PHE:CD1	2.56	0.41
1:B:58:TRP:CZ2	1:B:109:ARG:NH2	2.89	0.41
1:B:234:ARG:HA	1:B:234:ARG:HD2	1.61	0.41
1:A:16:PRO:HB2	1:A:31:GLU:HG3	2.03	0.41
1:B:69:MET:HG2	1:B:79:TYR:CE1	2.55	0.41
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.82	0.41
1:A:413:VAL:HG12	1:A:428:VAL:HG21	2.03	0.41
1:B:307:GLU:OE1	1:B:307:GLU:N	2.46	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ARG:CB	1:A:488:ASP:HA	2.51	0.40
1:A:454:ILE:HG23	2:C:33:ILE:HD11	2.03	0.40
1:B:338:VAL:HG13	1:B:356:LEU:HD11	2.03	0.40
1:B:453:LEU:HD23	2:E:15:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	496/513 (97%)	485 (98%)	10 (2%)	1 (0%)	47	57
1	B	504/513 (98%)	493 (98%)	10 (2%)	1 (0%)	47	57
2	C	75/95 (79%)	70 (93%)	3 (4%)	2 (3%)	5	2
2	E	77/95 (81%)	76 (99%)	1 (1%)	0	100	100
All	All	1152/1216 (95%)	1124 (98%)	24 (2%)	4 (0%)	41	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	448	ARG
2	C	18	GLU
1	B	448	ARG
2	C	52	VAL

### 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	350/418 (84%)	347 (99%)	3 (1%)	78	86
1	B	368/418 (88%)	367 (100%)	1 (0%)	92	95
2	C	41/81 (51%)	41 (100%)	0	100	100
2	E	41/81 (51%)	41 (100%)	0	100	100
All	All	800/998 (80%)	796 (100%)	4 (0%)	88	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	282	PHE
1	A	38	ARG
1	A	54	ARG
1	A	231	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	60	HIS
1	A	420	HIS

### 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](#)

8 ligands are modelled in this entry.

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	AZI	B	701	-	0,2,2	-	-	0,1,1	-	-
3	AZI	C	902	-	0,2,2	-	-	0,1,1	-	-
3	AZI	A	702	-	0,2,2	-	-	0,1,1	-	-
3	AZI	B	702	-	0,2,2	-	-	0,1,1	-	-
3	AZI	A	701	-	0,2,2	-	-	0,1,1	-	-
4	I5M	C	901	2	42,53,53	1.34	4 (9%)	47,76,76	2.37	13 (27%)
3	AZI	B	703	-	0,2,2	-	-	0,1,1	-	-
4	I5M	E	1001	2	42,53,53	2.26	14 (33%)	47,76,76	2.02	8 (17%)

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
4	I5M	C	901	2	-	13/40/71/71	0/4/4/4
4	I5M	E	1001	2	-	16/40/71/71	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1001	I5M	C16-S1	-5.64	1.74	1.81
4	E	1001	I5M	C4-S1	-5.17	1.73	1.82
4	E	1001	I5M	O1-S	-4.83	1.36	1.43
4	E	1001	I5M	C5-S	-4.72	1.63	1.77
4	E	1001	I5M	O-S	-4.45	1.37	1.43
4	C	901	I5M	C16-S1	-4.18	1.76	1.81
4	C	901	I5M	C13-N4	4.13	1.49	1.34
4	C	901	I5M	C4-S1	-3.57	1.76	1.82
4	C	901	I5M	C5-S	-3.52	1.66	1.77
4	E	1001	I5M	C13-N4	3.13	1.45	1.34
4	E	1001	I5M	C9-C8	-2.93	1.49	1.53
4	E	1001	I5M	C1-C3	-2.60	1.49	1.53
4	E	1001	I5M	C12-N3	-2.24	1.31	1.39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1001	I5M	O2-C7	-2.21	1.40	1.45
4	E	1001	I5M	C15-N6	-2.16	1.32	1.35
4	E	1001	I5M	C12-C15	-2.13	1.35	1.40
4	E	1001	I5M	O8-C26	-2.13	1.39	1.44
4	E	1001	I5M	S-N1	-2.11	1.55	1.61

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1001	I5M	O-S-O1	-8.89	106.47	119.35
4	C	901	I5M	O-S-O1	-8.07	107.67	119.35
4	C	901	I5M	C6-N1-S	-6.34	107.99	120.63
4	E	1001	I5M	C6-N1-S	-5.78	109.09	120.63
4	C	901	I5M	N6-C14-N5	-5.06	120.78	128.68
4	E	1001	I5M	N6-C14-N5	-4.50	121.65	128.68
4	C	901	I5M	C25-C23-C26	-4.05	101.63	108.23
4	C	901	I5M	C17-N7-C18	-4.02	115.37	122.84
4	C	901	I5M	C19-C20-N8	-3.63	104.57	111.90
4	C	901	I5M	O2-C7-C10	3.50	112.04	105.11
4	C	901	I5M	C10-C9-C8	3.05	105.57	100.98
4	C	901	I5M	C25-C23-C22	3.01	114.03	108.82
4	C	901	I5M	C5-S-N1	2.61	112.75	107.34
4	E	1001	I5M	C5-S-N1	2.53	112.58	107.34
4	C	901	I5M	C7-C6-N1	-2.52	107.46	112.51
4	C	901	I5M	C9-C10-C7	-2.37	98.05	102.64
4	E	1001	I5M	C20-N8-C21	-2.19	118.69	122.59
4	E	1001	I5M	C15-C12-N3	-2.12	107.19	109.40
4	E	1001	I5M	C20-C19-C18	-2.07	108.91	112.36
4	E	1001	I5M	C22-C21-N8	2.04	120.64	116.58
4	C	901	I5M	C19-C18-N7	2.00	119.80	116.42

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1001	I5M	C4-C5-S-N1
4	E	1001	I5M	C19-C18-N7-C17
4	E	1001	I5M	O5-C18-N7-C17
4	E	1001	I5M	C21-C22-C23-C26
4	E	1001	I5M	C21-C22-C23-C25
4	E	1001	I5M	C22-C21-N8-C20
4	E	1001	I5M	C18-C19-C20-N8

*Continued on next page...*

*Continued from previous page...*

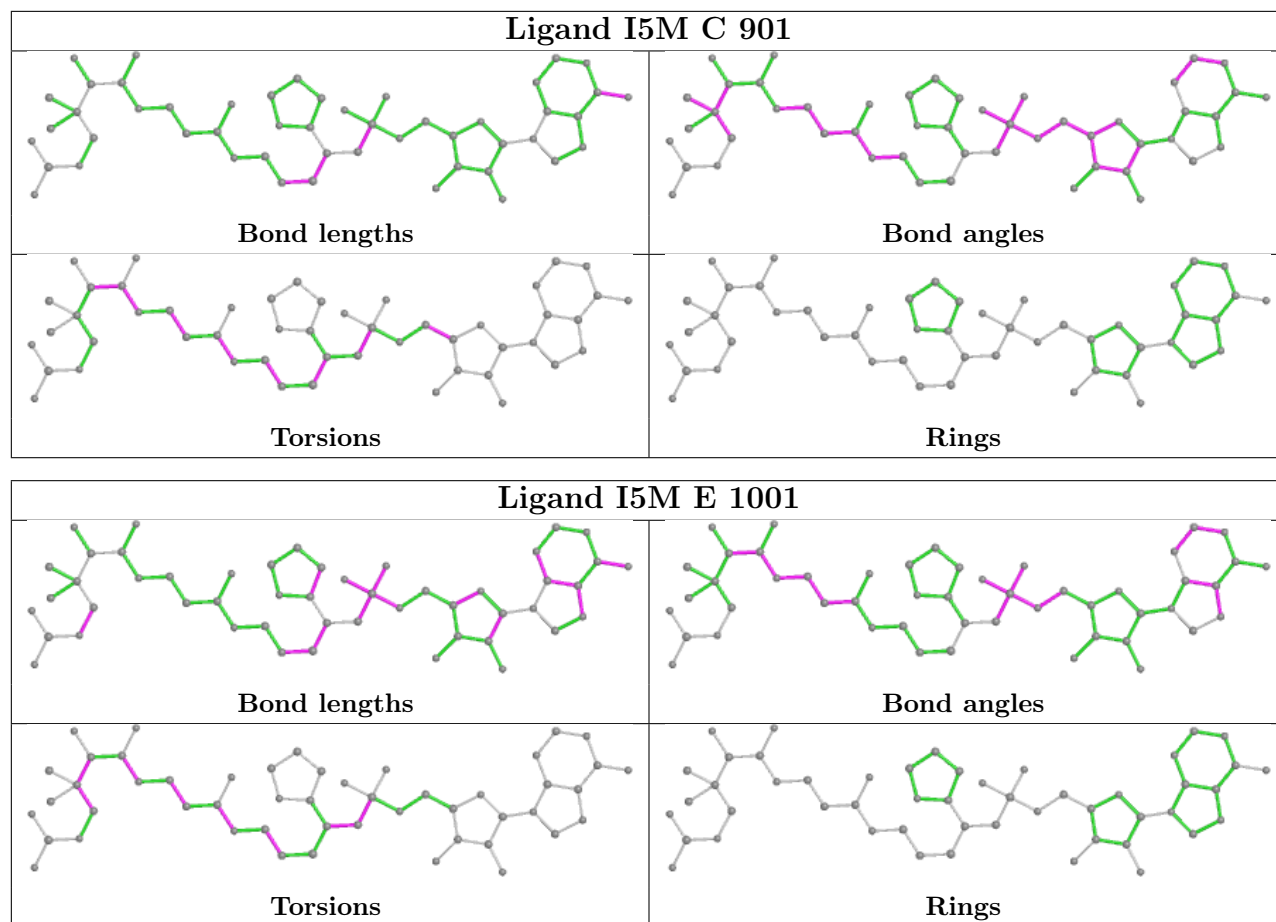
Mol	Chain	Res	Type	Atoms
4	C	901	I5M	C4-C5-S-N1
4	C	901	I5M	C5-C4-S1-C16
4	C	901	I5M	N1-C6-C7-O2
4	C	901	I5M	N1-C6-C7-C10
4	C	901	I5M	C22-C21-N8-C20
4	E	1001	I5M	O6-C21-N8-C20
4	E	1001	I5M	S1-C16-C17-N7
4	C	901	I5M	O6-C21-N8-C20
4	C	901	I5M	O5-C18-N7-C17
4	C	901	I5M	C18-C19-C20-N8
4	E	1001	I5M	C21-C22-C23-C24
4	E	1001	I5M	C3-C4-C5-S
4	E	1001	I5M	C4-C5-S-O1
4	E	1001	I5M	C4-C5-S-O
4	E	1001	I5M	O7-C22-C23-C26
4	C	901	I5M	C4-C5-S-O1
4	C	901	I5M	C4-C5-S-O
4	E	1001	I5M	O7-C22-C23-C24
4	C	901	I5M	C19-C18-N7-C17
4	E	1001	I5M	C24-C23-C26-O8
4	C	901	I5M	O6-C21-C22-C23
4	C	901	I5M	S1-C16-C17-N7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	901	I5M	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	500/513 (97%)	-0.03	5 (1%) 82 83	45, 66, 101, 127	0
1	B	505/513 (98%)	-0.07	1 (0%) 95 95	44, 59, 83, 106	0
2	C	77/95 (81%)	0.63	4 (5%) 27 24	85, 100, 113, 115	0
2	E	79/95 (83%)	0.27	4 (5%) 28 25	72, 93, 108, 112	0
All	All	1161/1216 (95%)	0.02	14 (1%) 79 77	44, 65, 103, 127	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	42	LEU	3.4
1	B	447	THR	3.1
2	C	62	ALA	2.9
1	A	502	ALA	2.8
2	E	10	ILE	2.8
1	A	448	ARG	2.8
1	A	136	ARG	2.8
1	A	441	GLY	2.6
2	C	29	PHE	2.6
2	E	17	GLY	2.5
2	E	40	PHE	2.4
1	A	449	ASP	2.3
2	C	22	LEU	2.1
2	C	2	LEU	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](#)

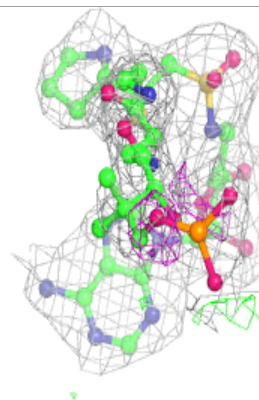
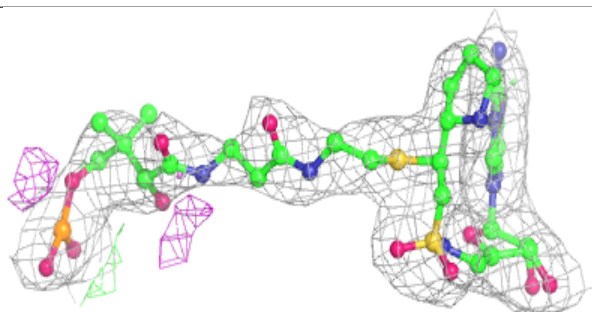
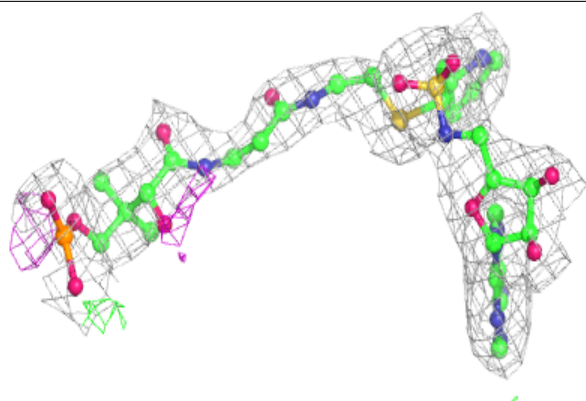
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AZI	B	702	3/3	0.58	0.20	73,73,77,87	0
3	AZI	C	902	3/3	0.63	0.25	99,99,103,106	0
3	AZI	B	703	3/3	0.71	0.25	74,74,114,117	0
3	AZI	B	701	3/3	0.82	0.13	76,76,86,89	0
3	AZI	A	702	3/3	0.88	0.18	71,71,79,80	0
3	AZI	A	701	3/3	0.95	0.14	65,65,74,76	0
4	I5M	C	901	50/50	0.95	0.19	44,56,83,133	0
4	I5M	E	1001	50/50	0.97	0.14	43,56,80,117	0

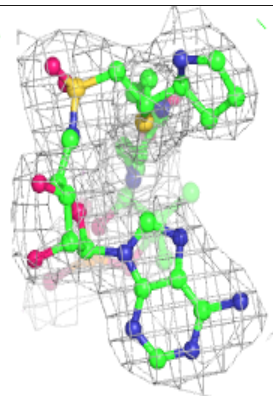
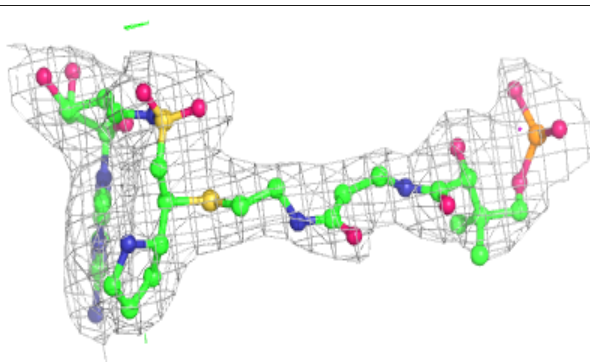
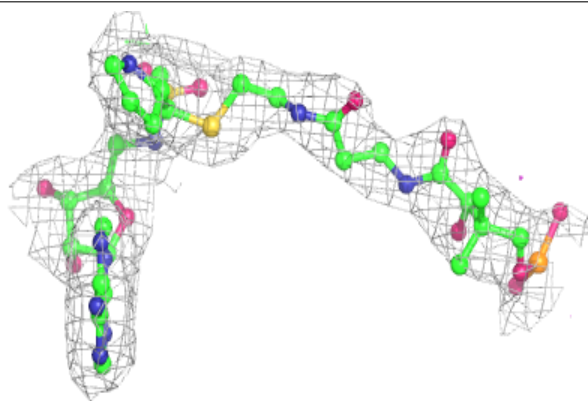
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around I5M C 901:**

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

**Electron density around I5M E 1001:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.