



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 01:47 pm BST

PDB ID : 9I7K / pdb\_00009i7k  
Title : Pseudomonas aeruginosa FabF C164A in complex with N-(3-(2-(1H-pyrrol-1-yl)propanamido)-2-hydroxy-2-methylpropyl)-1H-pyrazole-3-carboxamide  
Authors : Yadrykhinsky, V.; Brenk, R.  
Deposited on : 2025-01-31  
Resolution : 1.83 Å(reported)

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

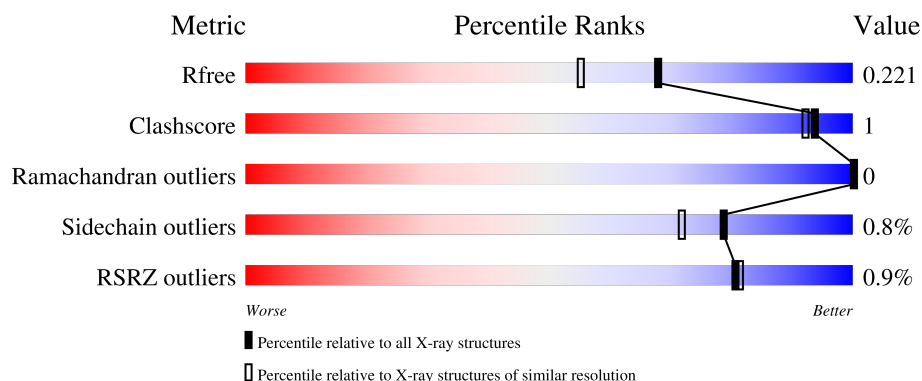
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.83 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))
$R_{free}$	164625	9242 (1.84-1.80)
Clashscore	180529	1080 (1.82-1.82)
Ramachandran outliers	177936	1073 (1.82-1.82)
Sidechain outliers	177891	1073 (1.82-1.82)
RSRZ outliers	164620	9241 (1.84-1.80)

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	419	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>..</div> </div> </div>
1	B	419	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12633 atoms, of which 6177 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 3-oxoacyl-[acyl-carrier-protein] synthase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	411	Total	C	H	N	O	S	182	8	0
			6105	1906	3039	557	584	19			
1	A	410	Total	C	H	N	O	S	141	6	0
			6076	1898	3024	555	581	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP G3XDA2
B	-3	HIS	-	expression tag	UNP G3XDA2
B	-2	MET	-	expression tag	UNP G3XDA2
B	-1	ALA	-	expression tag	UNP G3XDA2
B	0	SER	-	expression tag	UNP G3XDA2
B	164	ALA	CYS	engineered mutation	UNP G3XDA2
A	-4	GLY	-	expression tag	UNP G3XDA2
A	-3	HIS	-	expression tag	UNP G3XDA2
A	-2	MET	-	expression tag	UNP G3XDA2
A	-1	ALA	-	expression tag	UNP G3XDA2
A	0	SER	-	expression tag	UNP G3XDA2
A	164	ALA	CYS	engineered mutation	UNP G3XDA2

- Molecule 2 is FORMIC ACID (CCD ID: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



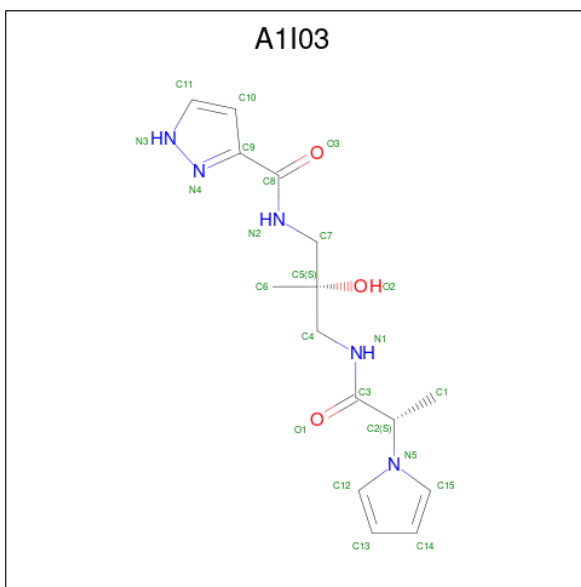
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	1	0
			5	1	2	2		
2	B	1	Total	C	H	O	1	0
			5	1	2	2		
2	B	1	Total	C	H	O	1	0
			5	1	2	2		
2	B	1	Total	C	H	O	1	0
			5	1	2	2		
2	A	1	Total	C	H	O	1	0
			5	1	2	2		
2	A	1	Total	C	H	O	1	0
			5	1	2	2		
2	A	1	Total	C	H	O	1	0
			5	1	2	2		
2	A	1	Total	C	H	O	1	0
			5	1	2	2		

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
3	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
3	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
3	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
3	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 4 is {N}-[(2 {S})-2-methyl-2-oxidanyl-3-[(2 {S})-2-pyrrol-1-ylpropanoyl]amino]propyl]-1 {H}-pyrazole-3-carboxamide (CCD ID: A1I03) (formula: C<sub>15</sub>H<sub>21</sub>N<sub>5</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	1	0
			44	15	21	5	3		
4	B	1	Total	C	H	N	O	1	0
			19	7	9	2	1		
4	A	1	Total	C	H	N	O	1	0
			44	15	21	5	3		
4	A	1	Total	C	H	N	O	1	0
			19	7	9	2	1		

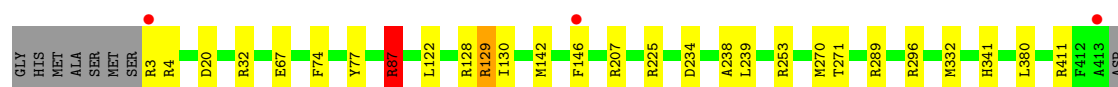
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	102	Total	O	0	0
			102	102		
5	A	119	Total	O	0	0
			119	119		

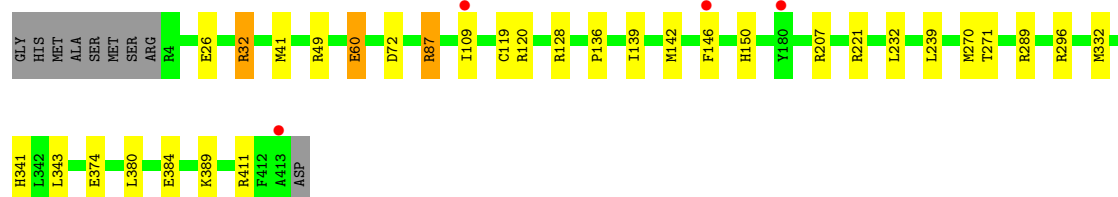
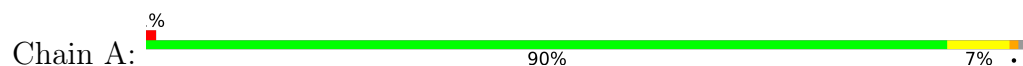
### 3 Residue-property plots [i](#)

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: 3-oxoacyl-[acyl-carrier-protein] synthase 2



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.74Å 104.19Å 142.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.43 – 1.83 72.43 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.4 (72.43-1.83) 99.4 (72.43-1.83)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.173 , 0.217 0.176 , 0.221	Depositor DCC
$R_{free}$ test set	3281 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 28.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.038 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, A1I03, DMS

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	0.85	4/3126 (0.1%)	1.19	21/4223 (0.5%)
1	B	2.43	7/3146 (0.2%)	1.50	21/4249 (0.5%)
All	All	1.82	11/6272 (0.2%)	1.36	42/8472 (0.5%)

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	6
1	B	0	5
All	All	0	11

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	ARG	CZ-NH1	127.11	2.98	1.33
1	B	207	ARG	CD-NE	-23.02	1.07	1.46
1	A	87	ARG	CD-NE	15.13	1.72	1.46
1	A	384	GLU	CG-CD	-14.57	1.30	1.51
1	A	374	GLU	CG-CD	-13.57	1.31	1.51
1	B	128	ARG	CA-CB	-12.13	1.27	1.53
1	B	129	ARG	CZ-NH2	-11.99	1.17	1.33
1	A	60	GLU	CB-CG	11.65	1.74	1.52
1	B	3	ARG	CB-CG	-7.50	1.32	1.52
1	B	129	ARG	CA-CB	-7.22	1.38	1.53
1	B	67	GLU	CD-OE1	6.16	1.32	1.25

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ARG	NE-CZ-NH2	38.76	139.68	120.30
1	B	129	ARG	NE-CZ-NH1	34.31	137.46	120.30
1	B	129	ARG	NH1-CZ-NH2	-33.36	82.70	119.40
1	B	128	ARG	N-CA-CB	-18.10	78.01	110.60
1	A	60	GLU	CG-CD-OE1	-13.84	90.62	118.30
1	A	87	ARG	CG-CD-NE	-12.43	85.69	111.80
1	B	128	ARG	CA-CB-CG	-10.37	90.59	113.40
1	B	207	ARG	CD-NE-CZ	10.01	137.61	123.60
1	A	384	GLU	CG-CD-OE2	-8.90	100.49	118.30
1	B	128	ARG	CB-CA-C	8.46	127.33	110.40
1	A	60	GLU	CB-CG-CD	7.92	135.58	114.20
1	A	384	GLU	CG-CD-OE1	7.92	134.13	118.30
1	A	32[A]	ARG	NE-CZ-NH1	-7.69	116.46	120.30
1	A	32[B]	ARG	NE-CZ-NH1	-7.69	116.46	120.30
1	B	207	ARG	NE-CZ-NH2	7.47	124.03	120.30
1	B	3	ARG	CA-CB-CG	7.26	129.37	113.40
1	A	384	GLU	CB-CG-CD	7.21	133.66	114.20
1	A	41	MET	CG-SD-CE	-7.16	88.75	100.20
1	B	32[A]	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	B	32[B]	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	A	60	GLU	CG-CD-OE2	6.51	131.32	118.30
1	A	49	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	B	225	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	221	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	296	ARG	NE-CZ-NH2	6.17	123.38	120.30
1	A	120	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	128	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	A	60	GLU	CA-CB-CG	-5.74	100.76	113.40
1	B	253	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	4	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	20	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	B	87	ARG	CG-CD-NE	5.44	123.23	111.80
1	B	87	ARG	CD-NE-CZ	5.37	131.12	123.60
1	A	49	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	A	119	CYS	CB-CA-C	-5.30	99.81	110.40
1	A	221	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	109	ILE	CB-CA-C	5.16	121.92	111.60
1	B	77	TYR	CB-CG-CD1	5.12	124.07	121.00
1	A	72	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	32[A]	ARG	NH1-CZ-NH2	5.05	124.96	119.40
1	B	32[B]	ARG	NH1-CZ-NH2	5.05	124.96	119.40
1	B	74	PHE	N-CA-CB	5.03	119.66	110.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	ARG	Sidechain
1	A	289[A]	ARG	Sidechain
1	A	289[B]	ARG	Sidechain
1	A	411	ARG	Sidechain
1	A	60	GLU	Sidechain
1	A	87	ARG	Sidechain
1	B	129	ARG	Sidechain
1	B	289	ARG	Sidechain
1	B	296	ARG	Sidechain
1	B	411	ARG	Sidechain
1	B	87	ARG	Sidechain

## 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	3052	3024	3007	9	0
1	B	3066	3039	3016	7	0
2	A	15	10	5	0	0
2	B	12	8	4	0	0
3	A	16	24	24	0	0
3	B	8	12	12	0	0
4	A	33	30	0	0	0
4	B	33	30	0	0	0
5	A	119	0	0	0	0
5	B	102	0	0	0	0
All	All	6456	6177	6068	16	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 1.

All (16) 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:142:MET:HE2	1:B:146:PHE:CE2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:MET:HE2	1:A:146:PHE:CE2	2.40	0.56
1:B:270:MET:HG3	1:B:271:THR:HG23	1.89	0.55
1:A:26:GLU:OE1	1:A:32[A]:ARG:NH1	2.41	0.53
1:B:239:LEU:HD12	1:B:239:LEU:N	2.23	0.53
1:B:332:MET:O	1:B:380:LEU:HA	2.12	0.49
1:B:87:ARG:HH11	1:B:87:ARG:HG3	1.80	0.47
1:A:239:LEU:HD12	1:A:239:LEU:N	2.30	0.46
1:A:332:MET:O	1:A:380:LEU:HA	2.16	0.46
1:B:122:LEU:HD13	1:B:130:ILE:HD11	1.98	0.45
1:A:136:PRO:O	1:A:142:MET:HG3	2.16	0.45
1:A:270:MET:HG3	1:A:271:THR:HG23	1.99	0.45
1:A:232:LEU:HD11	1:A:343:LEU:HD11	1.99	0.44
1:A:139:ILE:HG13	1:A:142:MET:HG2	2.02	0.41
1:A:232:LEU:CD1	1:A:343:LEU:HD11	2.51	0.41
1:B:238:ALA:C	1:B:239:LEU:HD12	2.41	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	414/419 (99%)	402 (97%)	12 (3%)	0	100	100
1	B	417/419 (100%)	407 (98%)	10 (2%)	0	100	100
All	All	831/838 (99%)	809 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/313 (100%)	309 (99%)	3 (1%)	73	62
1	B	315/313 (101%)	313 (99%)	2 (1%)	84	78
All	All	627/626 (100%)	622 (99%)	5 (1%)	79	72

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	234	ASP
1	B	341	HIS
1	A	150	HIS
1	A	341	HIS
1	A	389	LYS

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

19 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	$\# Z  > 2$
2	FMT	A	505	-	2,2,2	0.85	0	1,1,1	0.36	0
2	FMT	B	504	-	2,2,2	0.51	0	1,1,1	0.58	0
3	DMS	A	507	-	3,3,3	0.60	0	3,3,3	0.24	0
2	FMT	B	501	-	2,2,2	0.88	0	1,1,1	0.33	0
4	A1I03	A	504	-	10,10,24	1.93	2 (20%)	9,13,33	1.73	2 (22%)
2	FMT	A	501	-	2,2,2	0.62	0	1,1,1	0.67	0
2	FMT	A	508	-	2,2,2	0.86	0	1,1,1	0.27	0
2	FMT	B	502	-	2,2,2	0.66	0	1,1,1	0.41	0
2	FMT	A	510	-	2,2,2	0.98	0	1,1,1	0.34	0
3	DMS	A	511	-	3,3,3	0.30	0	3,3,3	0.37	0
4	A1I03	A	503	-	21,24,24	1.46	2 (9%)	19,33,33	3.07	5 (26%)
4	A1I03	B	508	-	10,10,24	1.16	1 (10%)	9,13,33	1.56	1 (11%)
3	DMS	A	509	-	3,3,3	0.47	0	3,3,3	0.27	0
3	DMS	B	505	-	3,3,3	0.51	0	3,3,3	0.62	0
4	A1I03	B	506	-	21,24,24	1.39	2 (9%)	19,33,33	1.59	5 (26%)
2	FMT	A	502	-	2,2,2	0.86	0	1,1,1	0.37	0
2	FMT	B	503	-	2,2,2	0.96	0	1,1,1	0.49	0
3	DMS	A	506	-	3,3,3	0.40	0	3,3,3	0.37	0
3	DMS	B	507	-	3,3,3	0.47	0	3,3,3	0.65	0

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	A1I03	A	504	-	-	2/8/8/24	0/1/1/2
4	A1I03	A	503	-	-	9/21/24/24	0/2/2/2
4	A1I03	B	506	-	-	8/21/24/24	0/2/2/2
4	A1I03	B	508	-	-	2/8/8/24	0/1/1/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	A1I03	C15-N5	5.58	1.42	1.37
4	A	503	A1I03	C12-N5	5.12	1.41	1.37
4	B	506	A1I03	C12-N5	4.81	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	508	A1I03	C15-N5	3.12	1.40	1.37
4	A	503	A1I03	C15-N5	3.06	1.40	1.37
4	B	506	A1I03	C15-N5	2.71	1.39	1.37
4	A	504	A1I03	C12-N5	-2.17	1.36	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	A1I03	C7-N2-C8	9.81	139.07	122.89
4	A	503	A1I03	C9-C8-N2	4.73	122.21	115.59
4	A	503	A1I03	O2-C5-C4	4.43	118.70	106.44
4	A	503	A1I03	O1-C3-C2	-4.35	110.24	120.92
4	A	504	A1I03	C14-C15-N5	3.24	109.68	107.53
4	B	508	A1I03	C14-C15-N5	3.21	109.66	107.53
4	B	506	A1I03	O2-C5-C4	2.79	114.15	106.44
4	B	506	A1I03	O2-C5-C6	2.59	114.64	108.19
4	A	504	A1I03	C13-C12-N5	2.48	109.18	107.53
4	B	506	A1I03	C4-N1-C3	2.27	126.37	122.79
4	A	503	A1I03	O2-C5-C7	-2.23	100.27	106.44
4	B	506	A1I03	O1-C3-N1	-2.06	118.57	122.99
4	B	506	A1I03	C13-C12-N5	2.01	108.87	107.53

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	506	A1I03	C1-C2-N5-C15
4	B	506	A1I03	C3-C2-N5-C12
4	B	506	A1I03	C3-C2-N5-C15
4	B	508	A1I03	C1-C2-C3-N1
4	A	503	A1I03	C3-C2-N5-C12
4	A	503	A1I03	C3-C2-N5-C15
4	A	503	A1I03	C4-C5-C7-N2
4	A	503	A1I03	O2-C5-C7-N2
4	A	503	A1I03	C9-C8-N2-C7
4	A	504	A1I03	C1-C2-C3-N1
4	A	503	A1I03	O3-C8-N2-C7
4	A	503	A1I03	C6-C5-C7-N2
4	B	506	A1I03	C1-C2-N5-C12
4	B	506	A1I03	C1-C2-C3-O1
4	B	506	A1I03	C1-C2-C3-N1
4	B	508	A1I03	C1-C2-C3-O1

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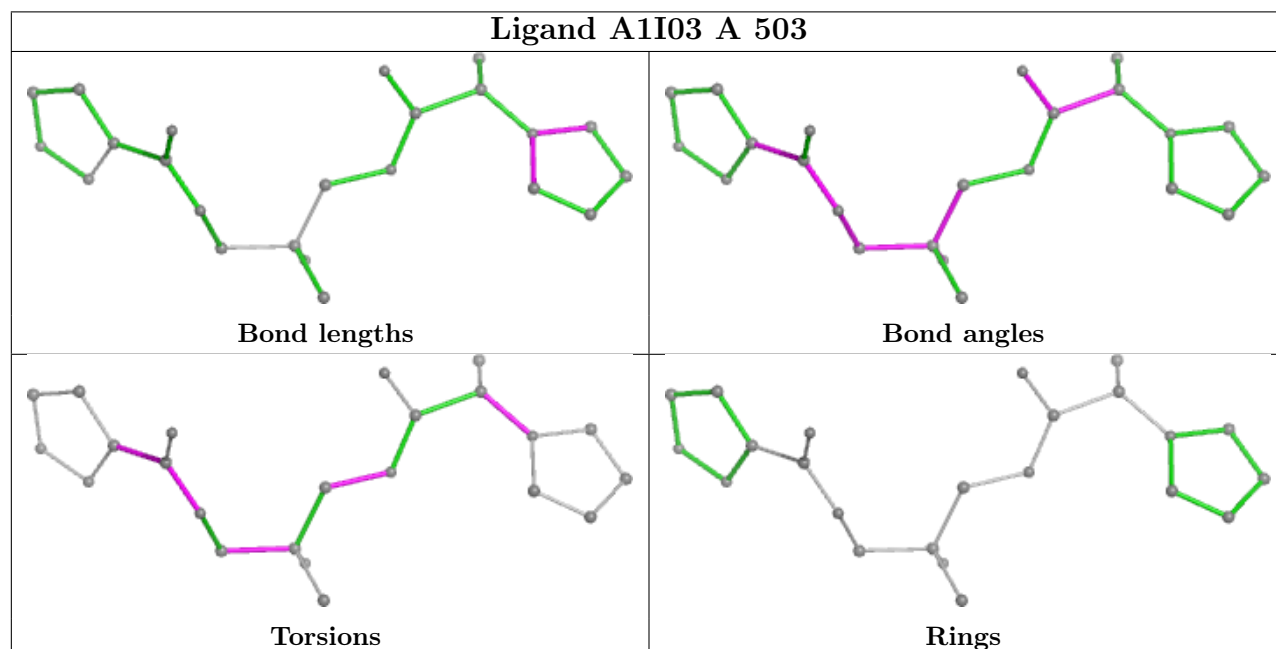
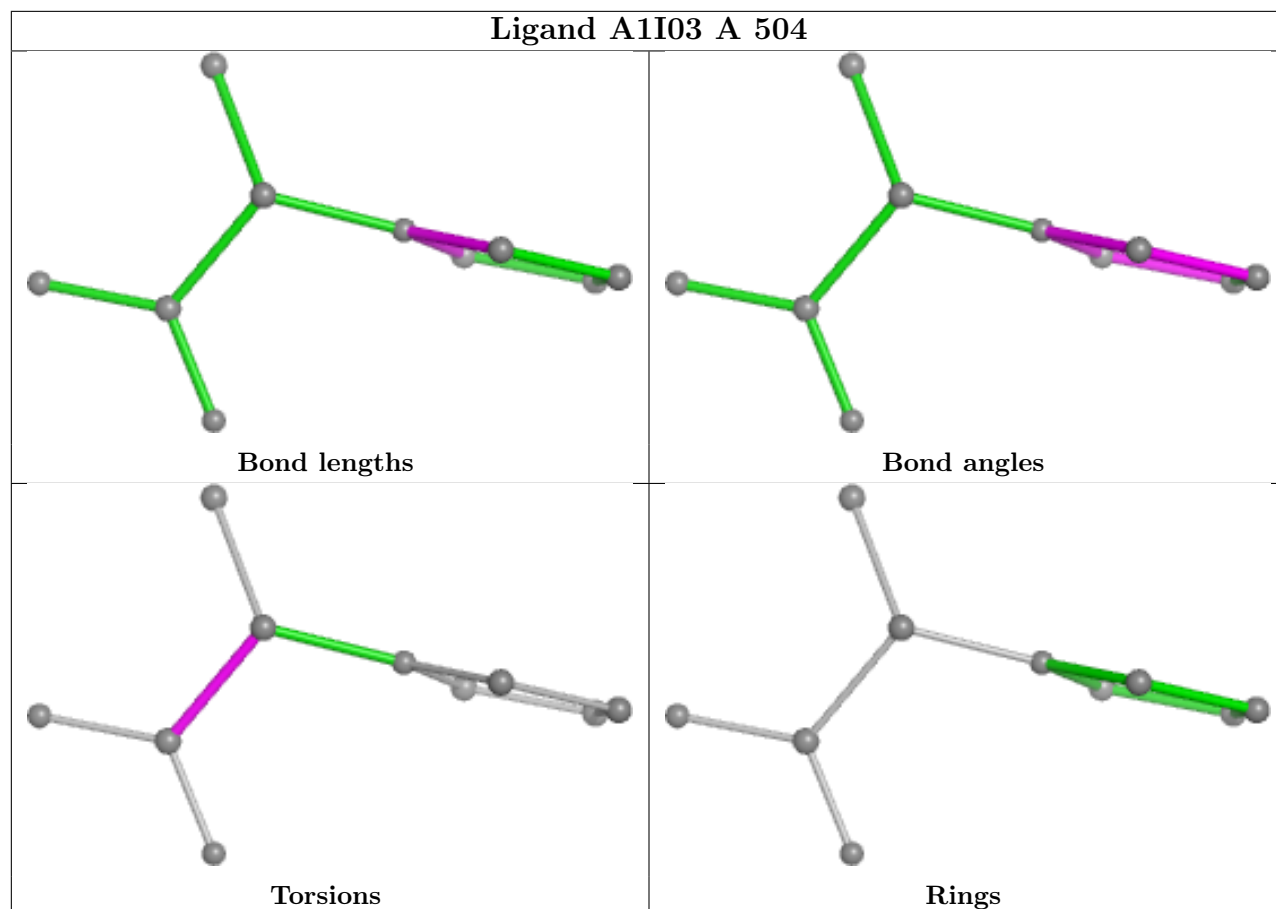
Mol	Chain	Res	Type	Atoms
4	A	504	A1I03	C1-C2-C3-O1
4	B	506	A1I03	C5-C4-N1-C3
4	A	503	A1I03	C5-C4-N1-C3
4	B	506	A1I03	O3-C8-C9-C10
4	A	503	A1I03	O3-C8-C9-C10

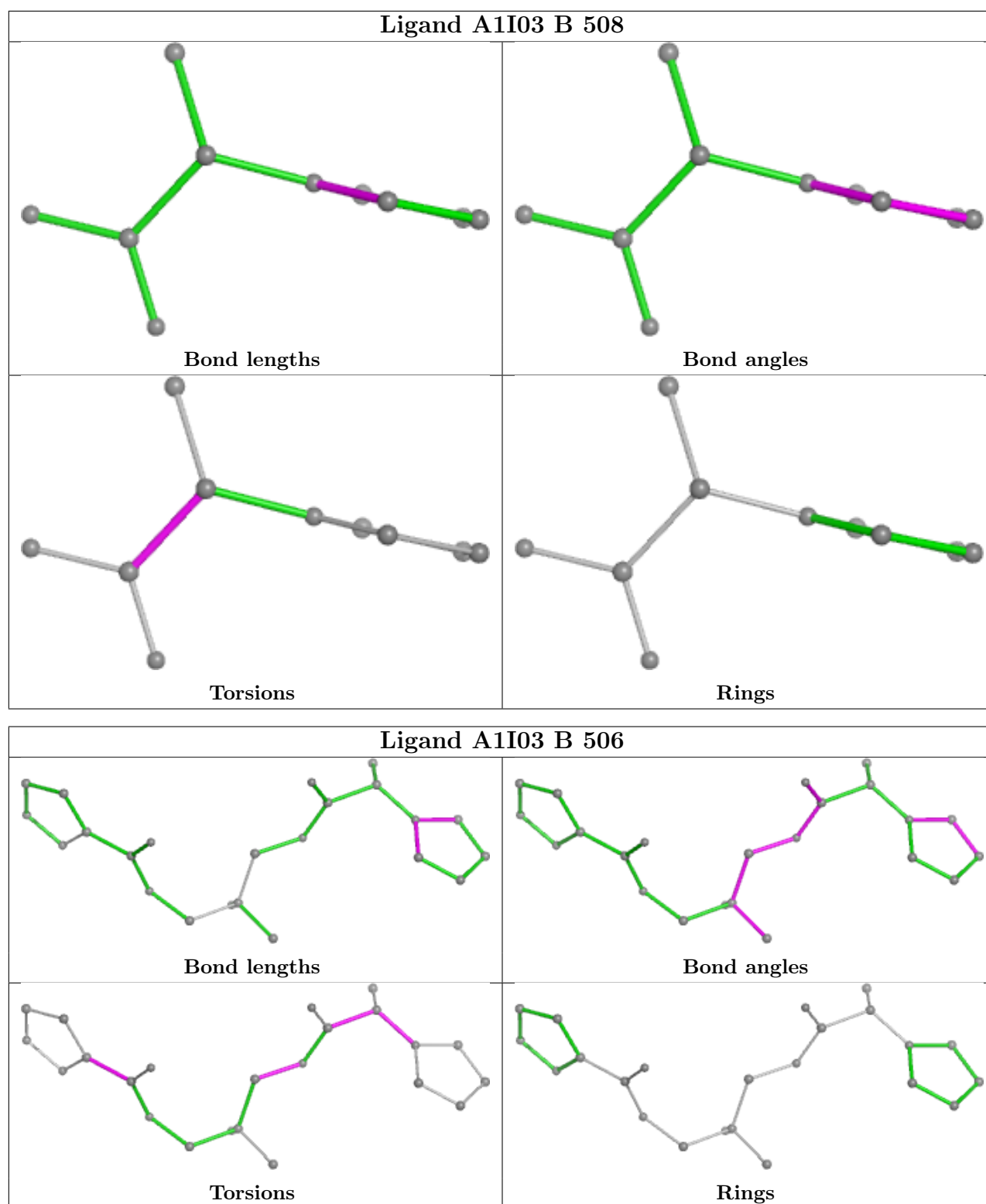
There are no ring outliers.

No monomer is involved in short contacts.

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [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	410/419 (97%)	-0.69	4 (0%) 79 80	8, 21, 37, 62	12 (2%)
1	B	411/419 (98%)	-0.58	3 (0%) 84 85	10, 22, 42, 72	14 (3%)
All	All	821/838 (97%)	-0.63	7 (0%) 81 81	8, 21, 41, 72	26 (3%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	ALA	5.0
1	B	413	ALA	4.8
1	A	109	ILE	3.5
1	A	180	TYR	2.8
1	B	146	PHE	2.4
1	A	146	PHE	2.3
1	B	3	ARG	2.2

### 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](#)

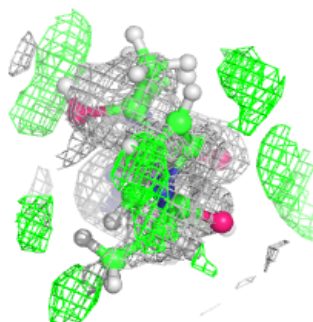
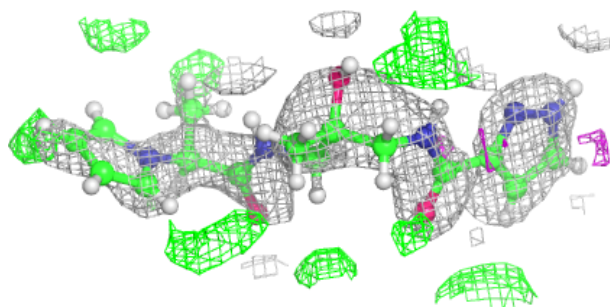
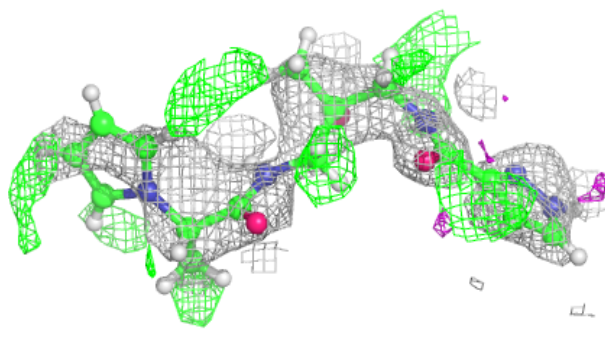
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 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
2	FMT	A	502	3/3	0.69	0.21	51,51,56,60	1
4	A1I03	B	506	23/23	0.79	0.22	36,63,94,100	1
4	A1I03	A	503	23/23	0.80	0.21	34,60,85,91	1
3	DMS	B	507	4/4	0.81	0.19	60,62,64,70	0
2	FMT	B	503	3/3	0.82	0.18	38,41,45,51	1
3	DMS	A	507	4/4	0.82	0.21	63,66,74,76	0
2	FMT	B	504	3/3	0.84	0.19	46,50,55,58	1
3	DMS	A	509	4/4	0.84	0.18	48,64,67,73	0
2	FMT	A	505	3/3	0.86	0.16	39,41,50,53	1
2	FMT	B	501	3/3	0.87	0.15	47,48,49,49	1
3	DMS	A	506	4/4	0.88	0.17	42,58,61,62	0
2	FMT	A	501	3/3	0.89	0.16	31,36,45,46	1
2	FMT	A	508	3/3	0.90	0.16	44,44,46,47	1
4	A1I03	B	508	10/23	0.91	0.10	27,35,45,50	1
2	FMT	A	510	3/3	0.93	0.10	42,45,46,46	1
3	DMS	B	505	4/4	0.93	0.17	40,44,61,62	0
2	FMT	B	502	3/3	0.93	0.12	37,38,46,58	1
4	A1I03	A	504	10/23	0.95	0.08	23,26,34,39	1
3	DMS	A	511	4/4	0.96	0.09	32,39,46,47	0

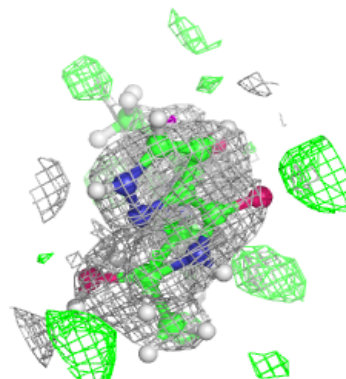
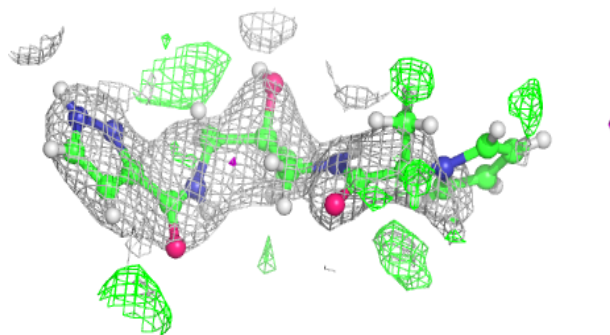
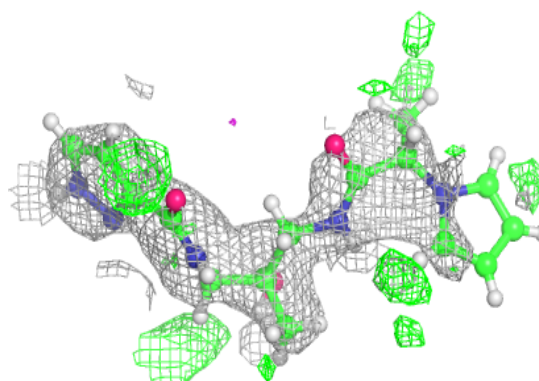
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1I03 B 506:**

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

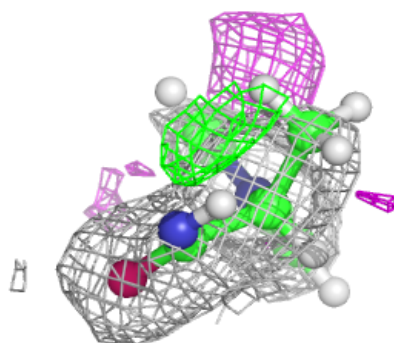
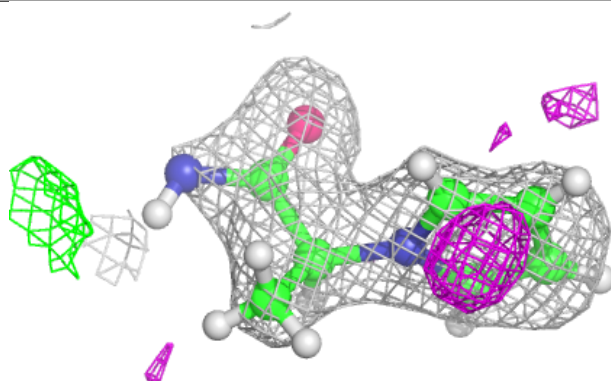
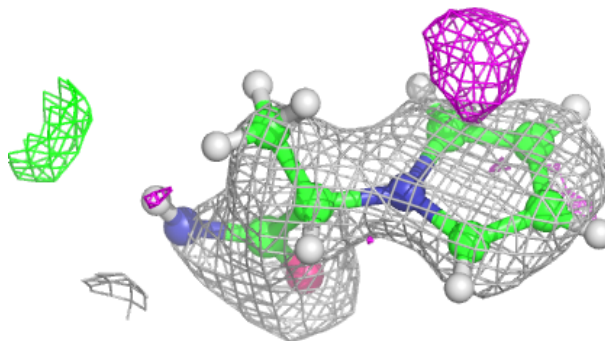
**Electron density around A1I03 A 503:**

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

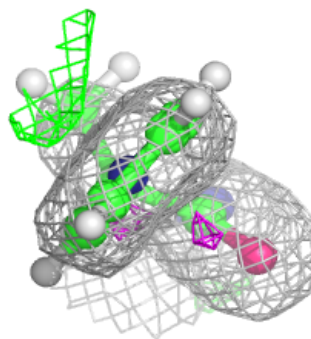
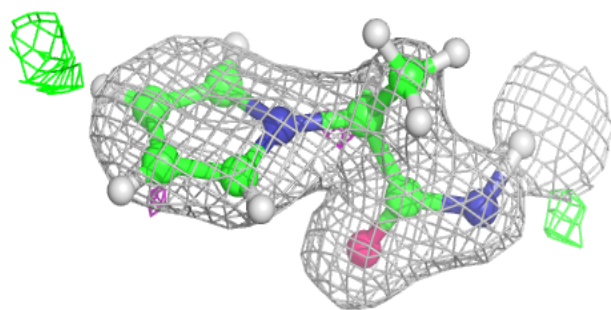
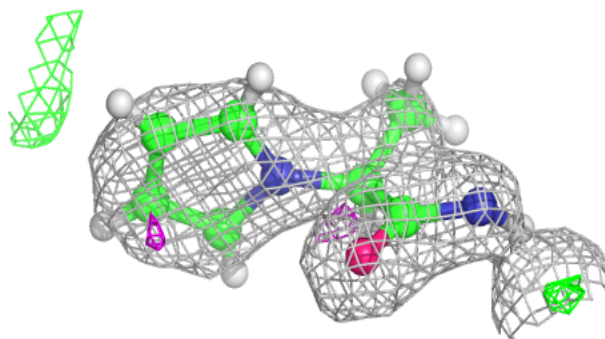


**Electron density around A1I03 B 508:**

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

**Electron density around A1I03 A 504:**

$2mF_o-DF_c$  (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.