



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2026 – 12:39 am BST

PDB ID : 9S33 / pdb_00009s33
Title : Crystal structure of inhibitor-bound Helicobacter pylori urease
Authors : Chen, X.; Luecke, H.; Buitrago, A.
Deposited on : 2025-07-23
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.8.4, CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

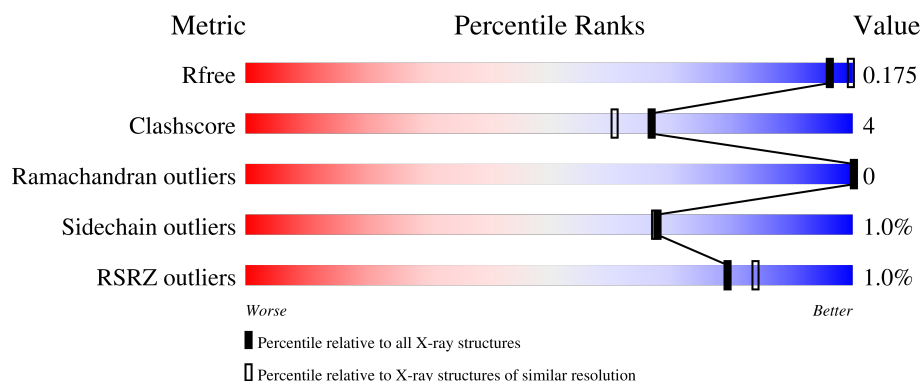
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	238	0% 92% 8%
1	C	238	0% 91% 9%
1	E	238	0% 92% 7%
1	G	238	3% 90% 10%
1	I	238	2% 93% 7%

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Mol	Chain	Length	Quality of chain
1	K	238	3% 94% 5%
2	B	569	93% 6%
2	D	569	92% 7%
2	F	569	% 91% 9%
2	H	569	% 92% 7%
2	J	569	2% 91% 8%
2	L	569	% 92% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 80455 atoms, of which 37196 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 Urease subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	238	Total	C	H	N	O	S	0	0	0
			3782	1177	1913	335	349	8			
1	C	238	Total	C	H	N	O	S	0	0	0
			3782	1177	1913	335	349	8			
1	E	238	Total	C	H	N	O	S	0	0	0
			3782	1177	1913	335	349	8			
1	G	238	Total	C	H	N	O	S	0	0	0
			3782	1177	1913	335	349	8			
1	I	238	Total	C	H	N	O	S	0	0	0
			3782	1177	1913	335	349	8			
1	K	238	Total	C	H	N	O	S	0	1	0
			3793	1180	1919	336	350	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ARG	LYS	conflict	UNP P14916
A	226	VAL	ALA	conflict	UNP P14916
C	21	ARG	LYS	conflict	UNP P14916
C	226	VAL	ALA	conflict	UNP P14916
E	21	ARG	LYS	conflict	UNP P14916
E	226	VAL	ALA	conflict	UNP P14916
G	21	ARG	LYS	conflict	UNP P14916
G	226	VAL	ALA	conflict	UNP P14916
I	21	ARG	LYS	conflict	UNP P14916
I	226	VAL	ALA	conflict	UNP P14916
K	21	ARG	LYS	conflict	UNP P14916
K	226	VAL	ALA	conflict	UNP P14916

- Molecule 2 is a protein called Urease subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	569	Total	C	H	N	O	S	0	0	0
			8610	2721	4270	746	852	21			
2	D	569	Total	C	H	N	O	S	0	1	0
			8618	2724	4273	746	854	21			
2	F	569	Total	C	H	N	O	S	0	1	0
			8626	2725	4281	746	852	22			
2	H	569	Total	C	H	N	O	S	0	0	0
			8610	2721	4270	746	852	21			
2	J	569	Total	C	H	N	O	S	0	0	0
			8610	2721	4270	746	852	21			
2	L	569	Total	C	H	N	O	S	0	0	0
			8610	2721	4270	746	852	21			

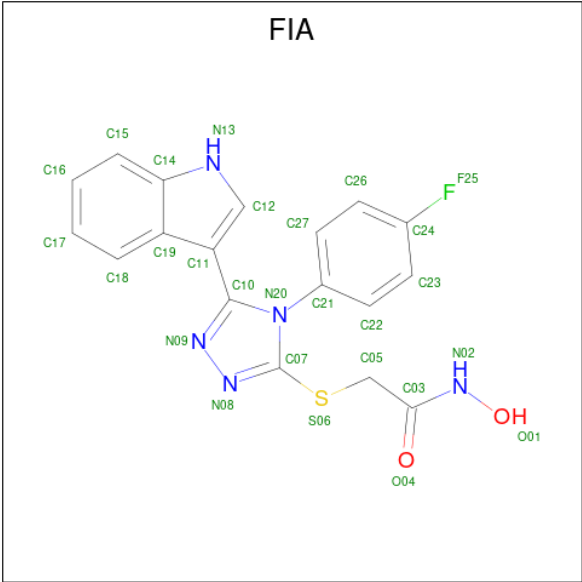
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	201	THR	ALA	conflict	UNP P69996
D	201	THR	ALA	conflict	UNP P69996
F	201	THR	ALA	conflict	UNP P69996
H	201	THR	ALA	conflict	UNP P69996
J	201	THR	ALA	conflict	UNP P69996
L	201	THR	ALA	conflict	UNP P69996

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

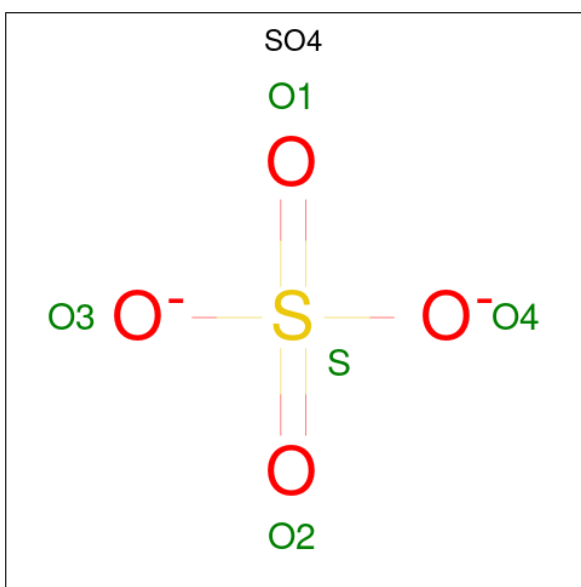
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ni	0	0
			2	2		
3	D	2	Total	Ni	0	0
			2	2		
3	F	2	Total	Ni	0	0
			2	2		
3	H	2	Total	Ni	0	0
			2	2		
3	J	2	Total	Ni	0	0
			2	2		
3	L	2	Total	Ni	0	0
			2	2		

- Molecule 4 is 2-{[4-(4-fluorophenyl)-5-(1H-indol-3-yl)-4H-1,2,4-triazol-3-yl]sulfanyl}-N-hydroxyacetamide (CCD ID: FIA) (formula: C₁₈H₁₄FN₅O₂S) (labeled as "Ligand of Interest" by depositor).



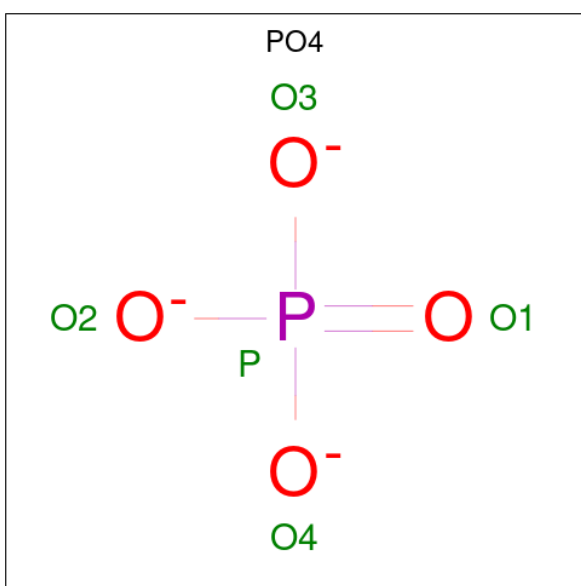
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	B	1	Total	C	F	H	N	O	S	0	0
			40	18	1	13	5	2	1		
4	D	1	Total	C	F	H	N	O	S	0	0
			40	18	1	13	5	2	1		
4	F	1	Total	C	F	H	N	O	S	0	0
			40	18	1	13	5	2	1		
4	H	1	Total	C	F	H	N	O	S	0	0
			40	18	1	13	5	2	1		
4	J	1	Total	C	F	H	N	O	S	0	0
			40	18	1	13	5	2	1		
4	L	1	Total	C	F	H	N	O	S	0	0
			40	18	1	13	5	2	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	O	P	0	0
			5	4	1		
6	H	1	Total	O	P	0	0
			5	4	1		

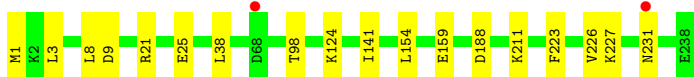
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	319	Total 319	O 319	0	0
7	B	671	Total 671	O 671	0	0
7	C	337	Total 337	O 337	0	0
7	D	619	Total 619	O 619	0	0
7	E	309	Total 309	O 309	0	0
7	F	640	Total 640	O 640	0	0
7	G	311	Total 311	O 311	0	0
7	H	631	Total 631	O 631	0	0
7	I	337	Total 337	O 337	0	0
7	J	664	Total 664	O 664	0	0
7	K	314	Total 314	O 314	0	0
7	L	644	Total 644	O 644	0	0

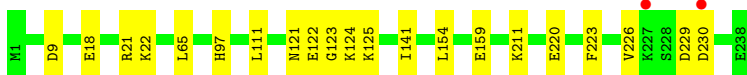
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Urease subunit alpha



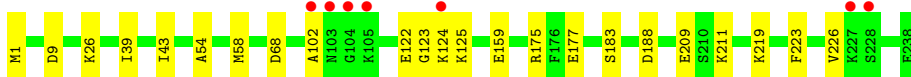
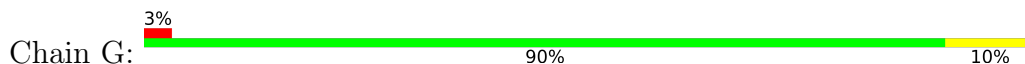
- Molecule 1: Urease subunit alpha



- Molecule 1: Urease subunit alpha



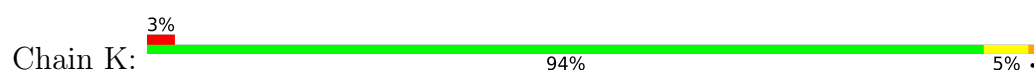
- Molecule 1: Urease subunit alpha



- Molecule 1: Urease subunit alpha



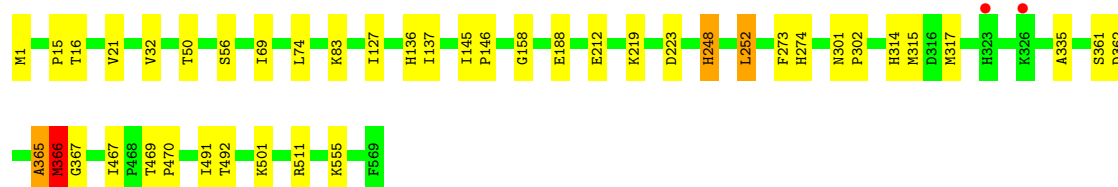
- Molecule 1: Urease subunit alpha



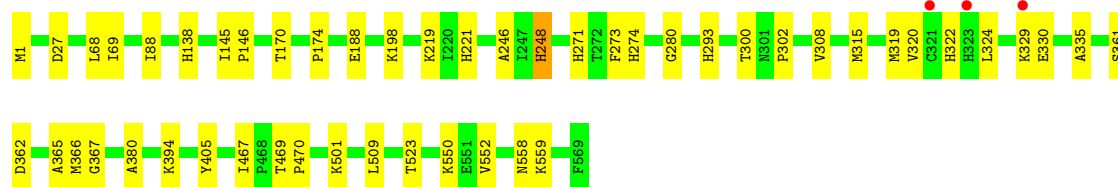
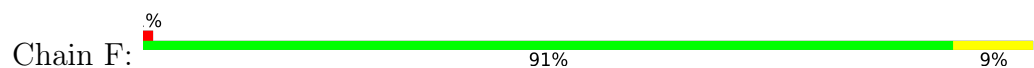
• Molecule 2: Urease subunit beta



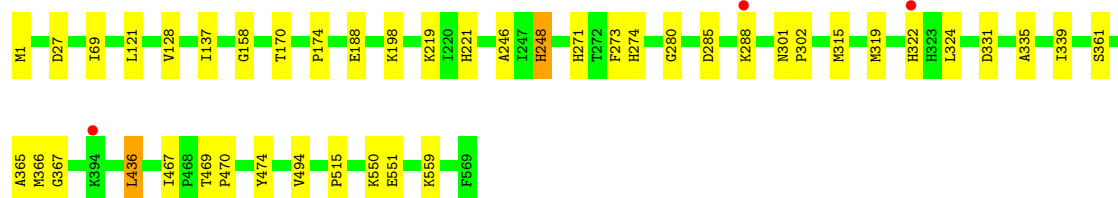
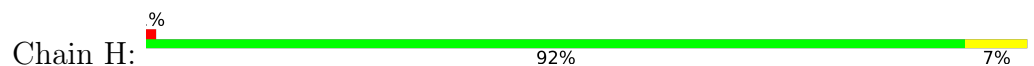
• Molecule 2: Urease subunit beta



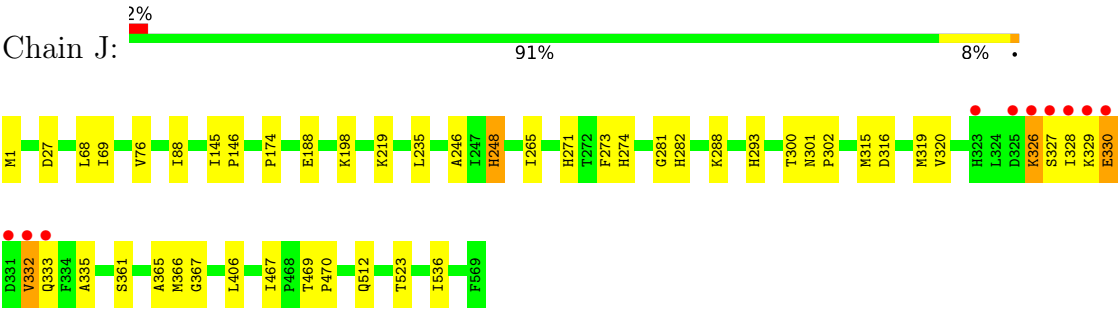
• Molecule 2: Urease subunit beta



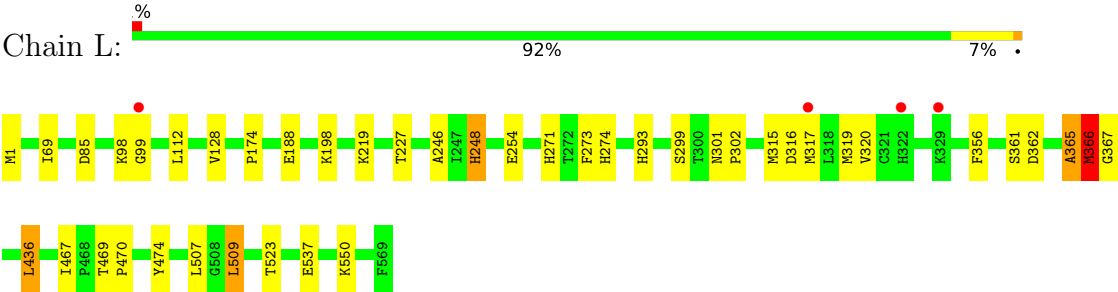
• Molecule 2: Urease subunit beta



• Molecule 2: Urease subunit beta



• Molecule 2: Urease subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	168.36Å 181.97Å 186.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.36 – 1.95 38.36 – 1.95	Depositor EDS
% Data completeness (in resolution range)	90.7 (38.36-1.95) 90.7 (38.36-1.95)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.137 , 0.175 0.137 , 0.175	Depositor DCC
R_{free} test set	18665 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	80455	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, KCX, PO4, NI, FIA

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	0.25	0/1897	0.47	0/2539
1	C	0.26	0/1897	0.45	0/2539
1	E	0.29	1/1897 (0.1%)	0.48	0/2539
1	G	0.24	0/1897	0.48	0/2539
1	I	0.28	0/1897	0.48	0/2539
1	K	0.43	2/1905 (0.1%)	0.49	0/2550
2	B	0.26	0/4411	0.55	0/5966
2	D	0.25	0/4419	0.53	3/5977 (0.1%)
2	F	0.26	0/4419	0.54	0/5976
2	H	0.27	0/4411	0.54	0/5966
2	J	0.26	0/4411	0.55	0/5966
2	L	0.27	0/4411	0.55	2/5966 (0.0%)
All	All	0.27	3/37872 (0.0%)	0.52	5/51062 (0.0%)

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	K	0	1
2	B	0	1
2	D	0	3
2	F	0	1
2	H	0	1
2	J	0	1
2	L	0	3
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	22	LYS	CE-NZ	11.19	1.82	1.49
1	K	22	LYS	CD-CE	-8.66	1.26	1.52
1	E	101	GLU	CB-CG	-5.21	1.36	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	366	MET	N-CA-C	5.97	122.58	113.51
2	L	366	MET	N-CA-C	5.90	122.47	113.51
2	L	366	MET	N-CA-CB	-5.77	108.33	114.10
2	D	366	MET	CB-CA-C	-5.38	104.51	109.83
2	D	366	MET	N-CA-CB	-5.01	109.09	114.10

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	188	GLU	Peptide
2	D	188	GLU	Peptide
2	D	365	ALA	Mainchain
2	D	366	MET	Mainchain
2	F	188	GLU	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	1869	1913	1913	11	0
1	C	1869	1913	1913	15	0
1	E	1869	1913	1913	19	0
1	G	1869	1913	1913	18	0
1	I	1869	1913	1913	20	0
1	K	1874	1919	1919	18	0
2	B	4340	4270	4269	26	0
2	D	4345	4273	4273	35	0
2	F	4345	4281	4280	33	0
2	H	4340	4270	4269	32	0
2	J	4340	4270	4269	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	4340	4270	4269	33	0
3	B	2	0	0	0	0
3	D	2	0	0	0	0
3	F	2	0	0	0	0
3	H	2	0	0	0	0
3	J	2	0	0	0	0
3	L	2	0	0	0	0
4	B	27	13	0	1	0
4	D	27	13	0	1	0
4	F	27	13	0	1	0
4	H	27	13	0	0	0
4	J	27	13	0	0	0
4	L	27	13	0	1	0
5	C	5	0	0	1	0
5	K	5	0	0	0	0
6	G	5	0	0	0	0
6	H	5	0	0	0	0
7	A	319	0	0	4	0
7	B	671	0	0	6	0
7	C	337	0	0	6	0
7	D	619	0	0	14	0
7	E	309	0	0	8	0
7	F	640	0	0	6	0
7	G	311	0	0	8	0
7	H	631	0	0	4	0
7	I	337	0	0	11	0
7	J	664	0	0	7	0
7	K	314	0	0	6	0
7	L	644	0	0	8	0
All	All	43259	37196	37113	275	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 4.

The worst 5 of 275 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:K:22:LYS:NZ	1:K:22:LYS:CE	1.82	1.40
2:B:320:VAL:HG21	7:I:546:HOH:O	1.69	0.91
1:E:67:PRO:HG3	1:E:101:GLU:CG	2.07	0.84
2:D:511:ARG:HD3	7:D:3101:HOH:O	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:PRO:HG3	1:E:101:GLU:HG3	1.62	0.82

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	236/238 (99%)	229 (97%)	7 (3%)	0	100	100
1	C	236/238 (99%)	225 (95%)	11 (5%)	0	100	100
1	E	236/238 (99%)	226 (96%)	10 (4%)	0	100	100
1	G	236/238 (99%)	229 (97%)	7 (3%)	0	100	100
1	I	236/238 (99%)	225 (95%)	11 (5%)	0	100	100
1	K	237/238 (100%)	227 (96%)	10 (4%)	0	100	100
2	B	566/569 (100%)	544 (96%)	22 (4%)	0	100	100
2	D	567/569 (100%)	543 (96%)	24 (4%)	0	100	100
2	F	566/569 (100%)	545 (96%)	21 (4%)	0	100	100
2	H	566/569 (100%)	544 (96%)	22 (4%)	0	100	100
2	J	566/569 (100%)	541 (96%)	25 (4%)	0	100	100
2	L	566/569 (100%)	545 (96%)	21 (4%)	0	100	100
All	All	4814/4842 (99%)	4623 (96%)	191 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	199/199 (100%)	196 (98%)	3 (2%)	57	54
1	C	199/199 (100%)	198 (100%)	1 (0%)	81	82
1	E	199/199 (100%)	198 (100%)	1 (0%)	81	82
1	G	199/199 (100%)	197 (99%)	2 (1%)	68	67
1	I	199/199 (100%)	198 (100%)	1 (0%)	81	82
1	K	200/199 (100%)	197 (98%)	3 (2%)	57	54
2	B	460/460 (100%)	457 (99%)	3 (1%)	76	76
2	D	461/460 (100%)	457 (99%)	4 (1%)	70	70
2	F	461/460 (100%)	456 (99%)	5 (1%)	65	64
2	H	460/460 (100%)	456 (99%)	4 (1%)	70	70
2	J	460/460 (100%)	453 (98%)	7 (2%)	57	54
2	L	460/460 (100%)	454 (99%)	6 (1%)	61	58
All	All	3957/3954 (100%)	3917 (99%)	40 (1%)	68	67

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	330	GLU
2	L	69	ILE
2	J	332	VAL
1	K	21	ARG
2	L	436	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	314	HIS
2	L	535	HIS
2	F	528	GLN
2	L	253	ASN
2	F	496	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	KCX	H	219	3,2	9,11,12	1.48	1 (11%)	5,12,14	2.41	1 (20%)
2	KCX	F	219	3,2	9,11,12	1.49	2 (22%)	5,12,14	2.33	1 (20%)
2	KCX	J	219	3,2	9,11,12	1.59	2 (22%)	5,12,14	2.30	1 (20%)
2	KCX	L	219	3,2	9,11,12	1.41	1 (11%)	5,12,14	2.16	1 (20%)
2	KCX	D	219	3,2	9,11,12	1.51	1 (11%)	5,12,14	2.06	1 (20%)
2	KCX	B	219	3,2	9,11,12	1.55	2 (22%)	5,12,14	2.43	1 (20%)

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
2	KCX	H	219	3,2	-	0/9/10/12	-
2	KCX	F	219	3,2	-	0/9/10/12	-
2	KCX	J	219	3,2	-	0/9/10/12	-
2	KCX	L	219	3,2	-	0/9/10/12	-
2	KCX	D	219	3,2	-	0/9/10/12	-
2	KCX	B	219	3,2	-	0/9/10/12	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	219	KCX	CX-NZ	3.75	1.41	1.35
2	B	219	KCX	CX-NZ	3.63	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	219	KCX	CX-NZ	3.57	1.41	1.35
2	H	219	KCX	CX-NZ	3.53	1.41	1.35
2	F	219	KCX	CX-NZ	3.45	1.41	1.35

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	219	KCX	OQ1-CX-NZ	-5.31	116.73	124.96
2	B	219	KCX	OQ1-CX-NZ	-5.27	116.79	124.96
2	F	219	KCX	OQ1-CX-NZ	-5.18	116.93	124.96
2	J	219	KCX	OQ1-CX-NZ	-5.01	117.19	124.96
2	L	219	KCX	OQ1-CX-NZ	-4.76	117.58	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 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
4	FIA	D	3003	3	30,30,30	2.54	7 (23%)	36,42,42	1.89	8 (22%)
5	SO4	K	301	-	4,4,4	0.60	0	6,6,6	0.13	0
4	FIA	H	3003	3	30,30,30	2.55	7 (23%)	36,42,42	1.71	8 (22%)
4	FIA	B	3003	3	30,30,30	2.51	9 (30%)	36,42,42	2.01	11 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FIA	L	3003	3	30,30,30	2.55	7 (23%)	36,42,42	1.73	7 (19%)
4	FIA	F	3003	3	30,30,30	2.47	8 (26%)	36,42,42	1.72	10 (27%)
5	SO4	C	301	-	4,4,4	0.62	0	6,6,6	0.14	0
6	PO4	G	301	-	4,4,4	1.58	1 (25%)	6,6,6	0.41	0
4	FIA	J	3003	3	30,30,30	2.54	8 (26%)	36,42,42	1.79	8 (22%)
6	PO4	H	3004	-	4,4,4	1.60	1 (25%)	6,6,6	0.36	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	FIA	D	3003	3	-	3/15/15/15	0/4/4/4
4	FIA	H	3003	3	-	3/15/15/15	0/4/4/4
4	FIA	B	3003	3	-	2/15/15/15	0/4/4/4
4	FIA	L	3003	3	-	3/15/15/15	0/4/4/4
4	FIA	F	3003	3	-	3/15/15/15	0/4/4/4
4	FIA	J	3003	3	-	3/15/15/15	0/4/4/4

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	3003	FIA	C03-N02	11.25	1.44	1.32
4	H	3003	FIA	C03-N02	11.08	1.44	1.32
4	D	3003	FIA	C03-N02	11.04	1.44	1.32
4	J	3003	FIA	C03-N02	11.01	1.44	1.32
4	B	3003	FIA	C03-N02	10.51	1.43	1.32

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3003	FIA	N20-C10-N09	-6.05	106.49	110.71
4	L	3003	FIA	N20-C10-N09	-5.92	106.58	110.71
4	H	3003	FIA	N20-C10-N09	-5.64	106.78	110.71
4	J	3003	FIA	N20-C10-N09	-5.39	106.95	110.71
4	B	3003	FIA	N20-C10-N09	-5.20	107.08	110.71

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

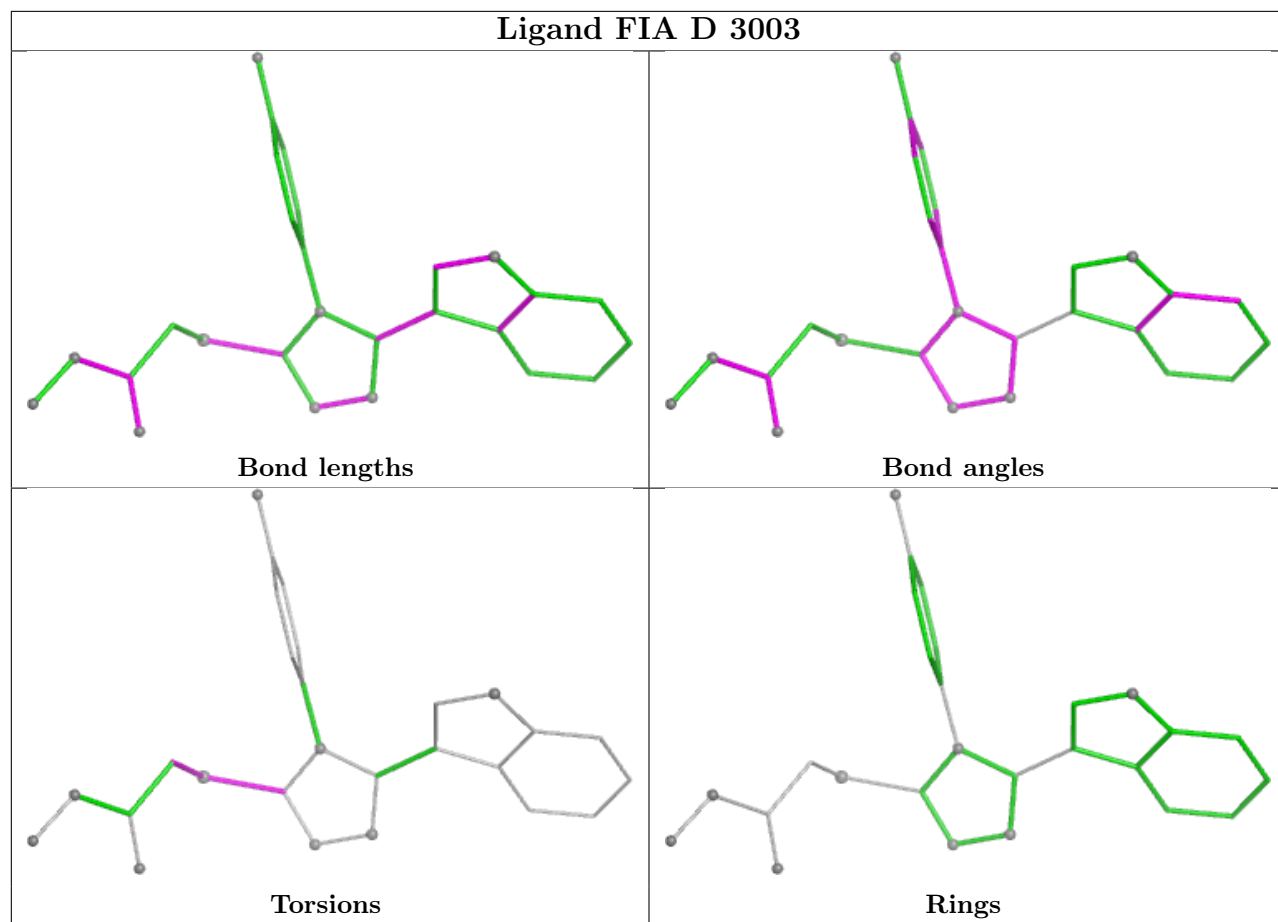
Mol	Chain	Res	Type	Atoms
4	B	3003	FIA	N08-C07-S06-C05
4	B	3003	FIA	N20-C07-S06-C05
4	D	3003	FIA	C03-C05-S06-C07
4	F	3003	FIA	C03-C05-S06-C07
4	H	3003	FIA	C03-C05-S06-C07

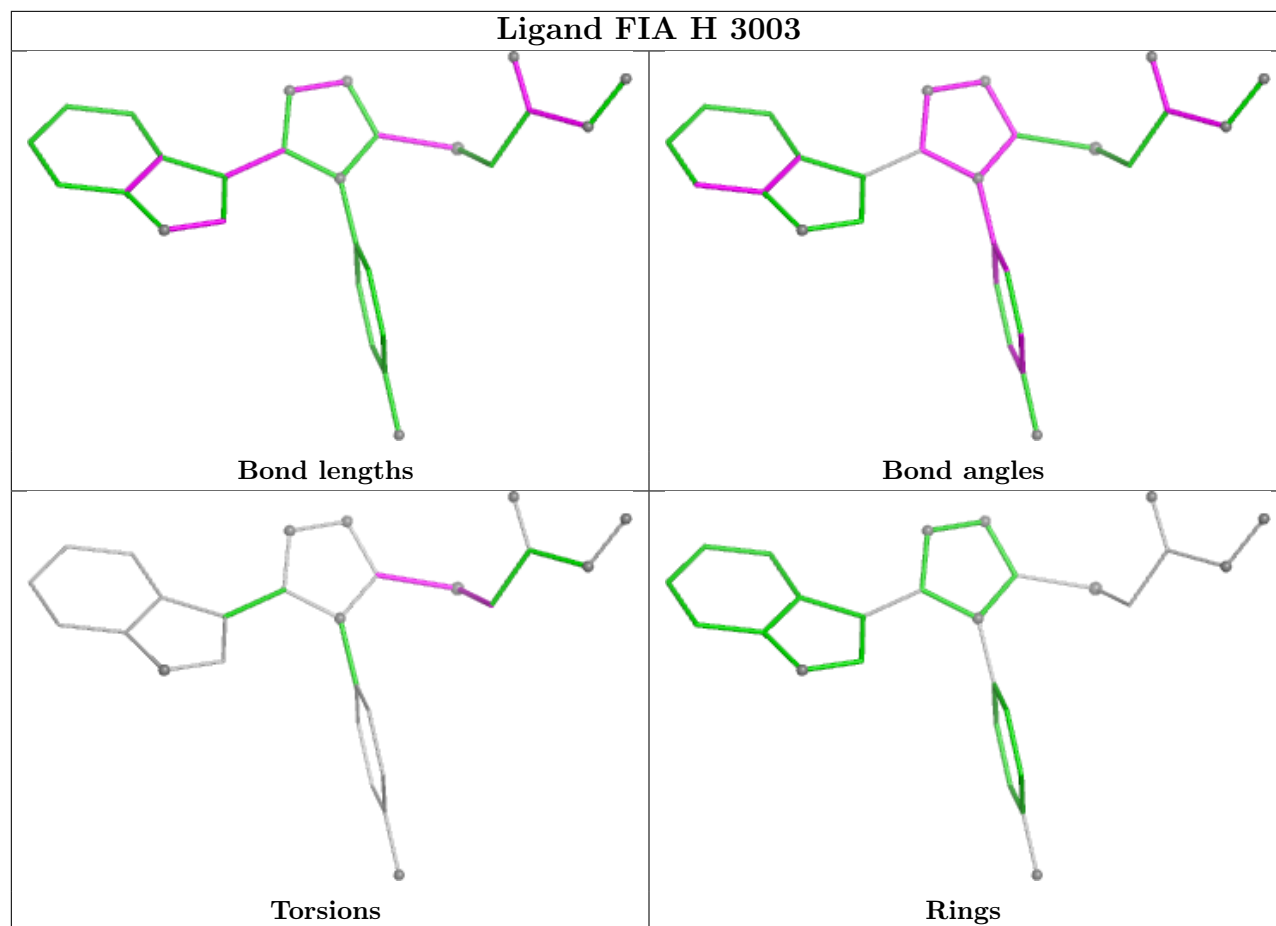
There are no ring outliers.

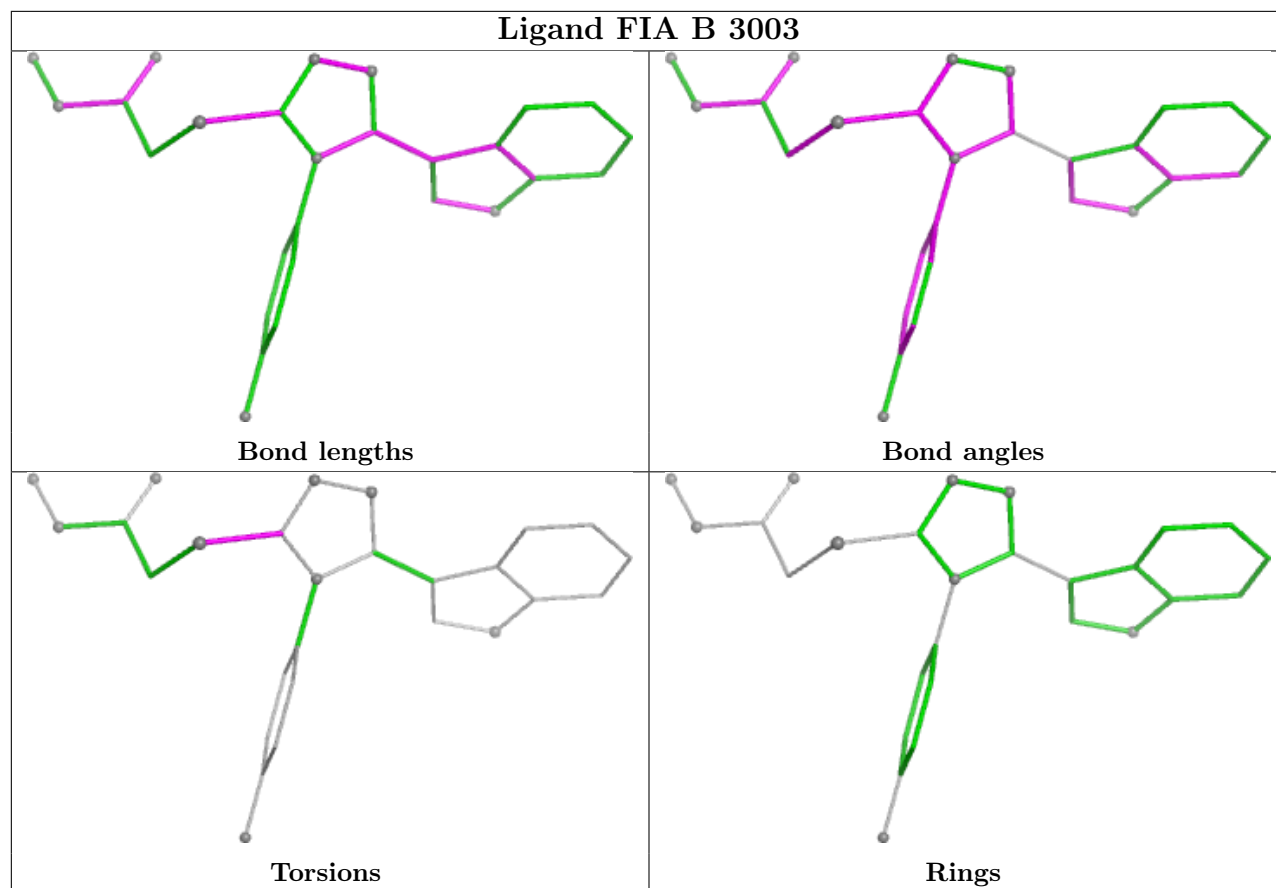
5 monomers are involved in 5 short contacts:

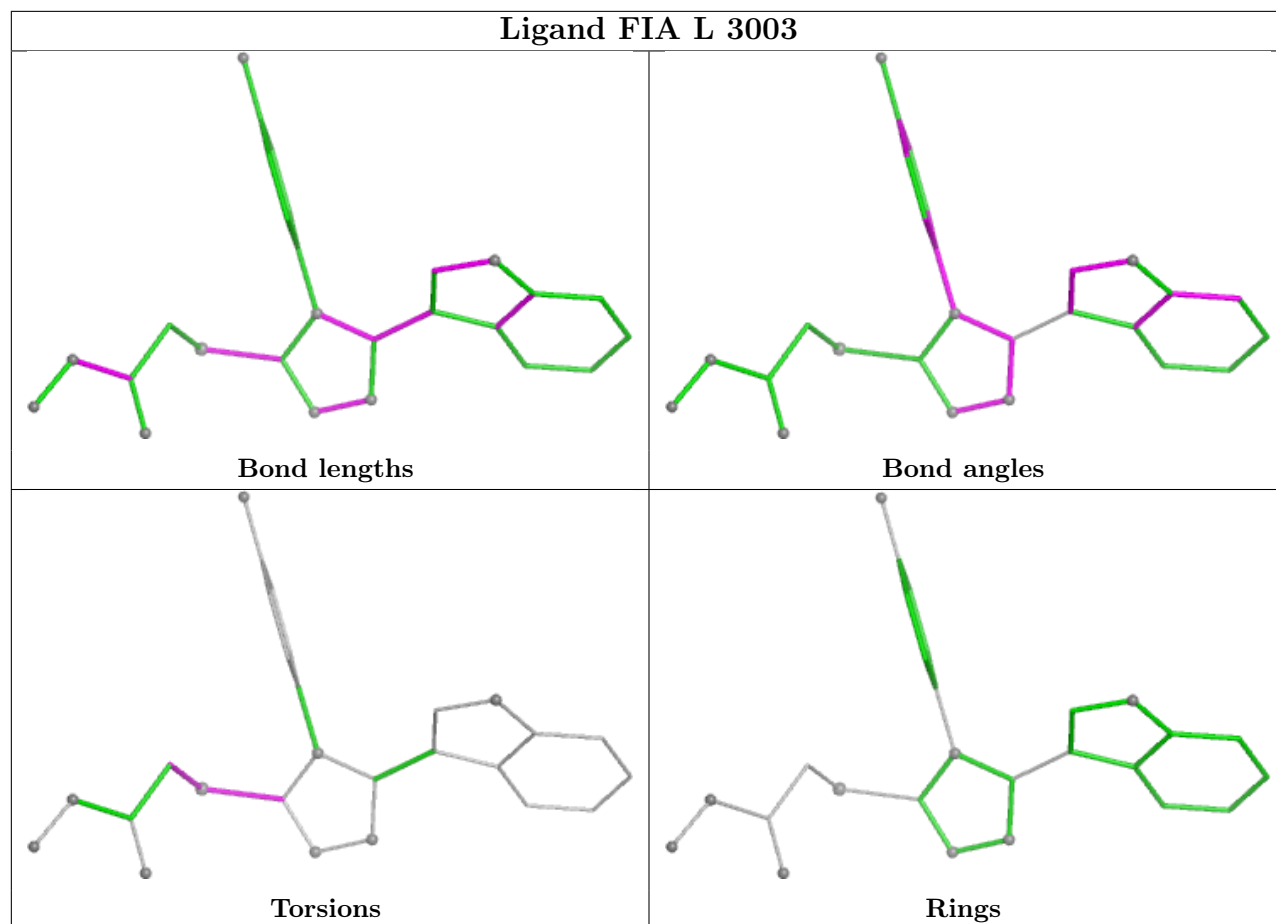
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3003	FIA	1	0
4	B	3003	FIA	1	0
4	L	3003	FIA	1	0
4	F	3003	FIA	1	0
5	C	301	SO4	1	0

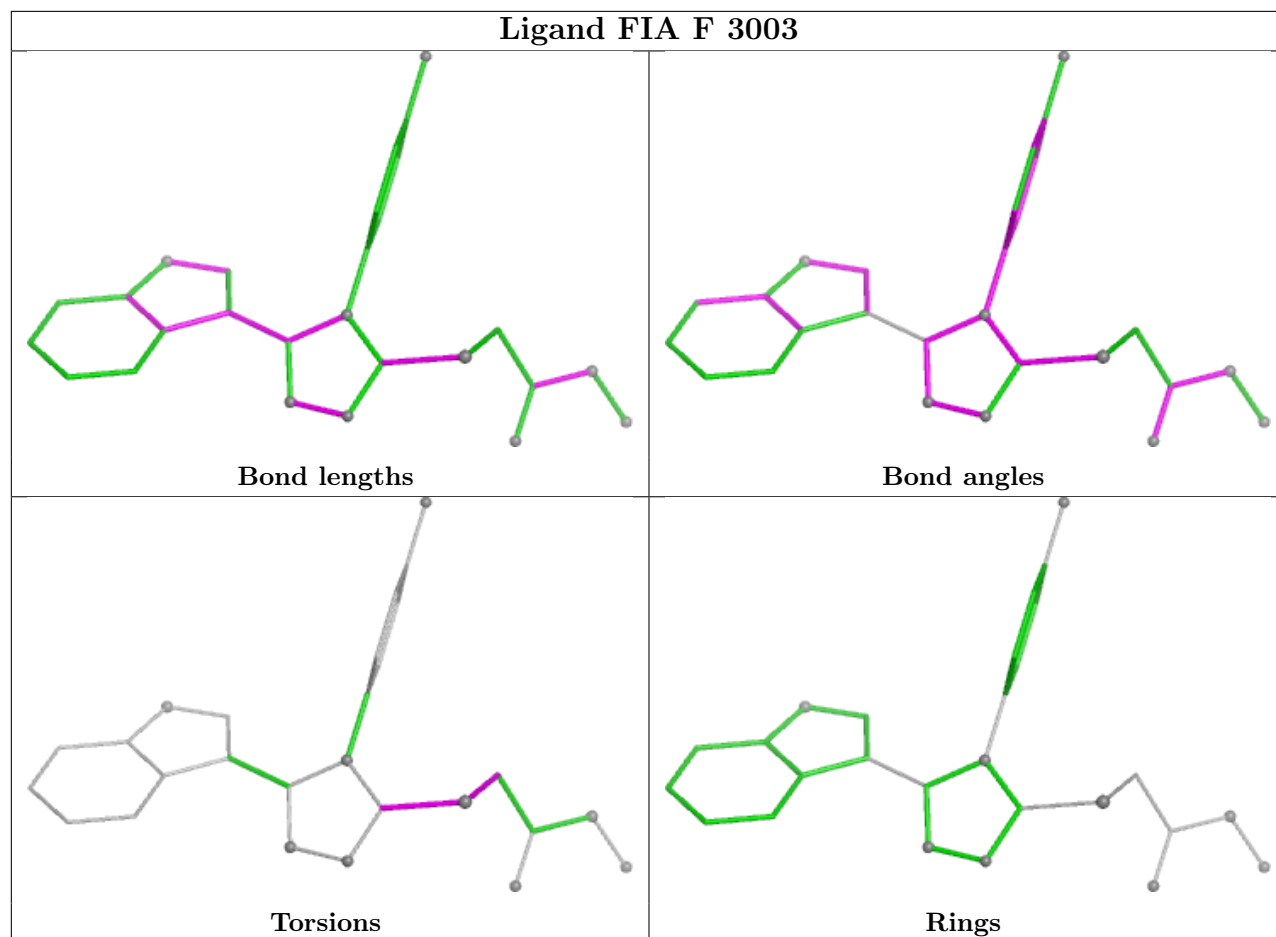
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

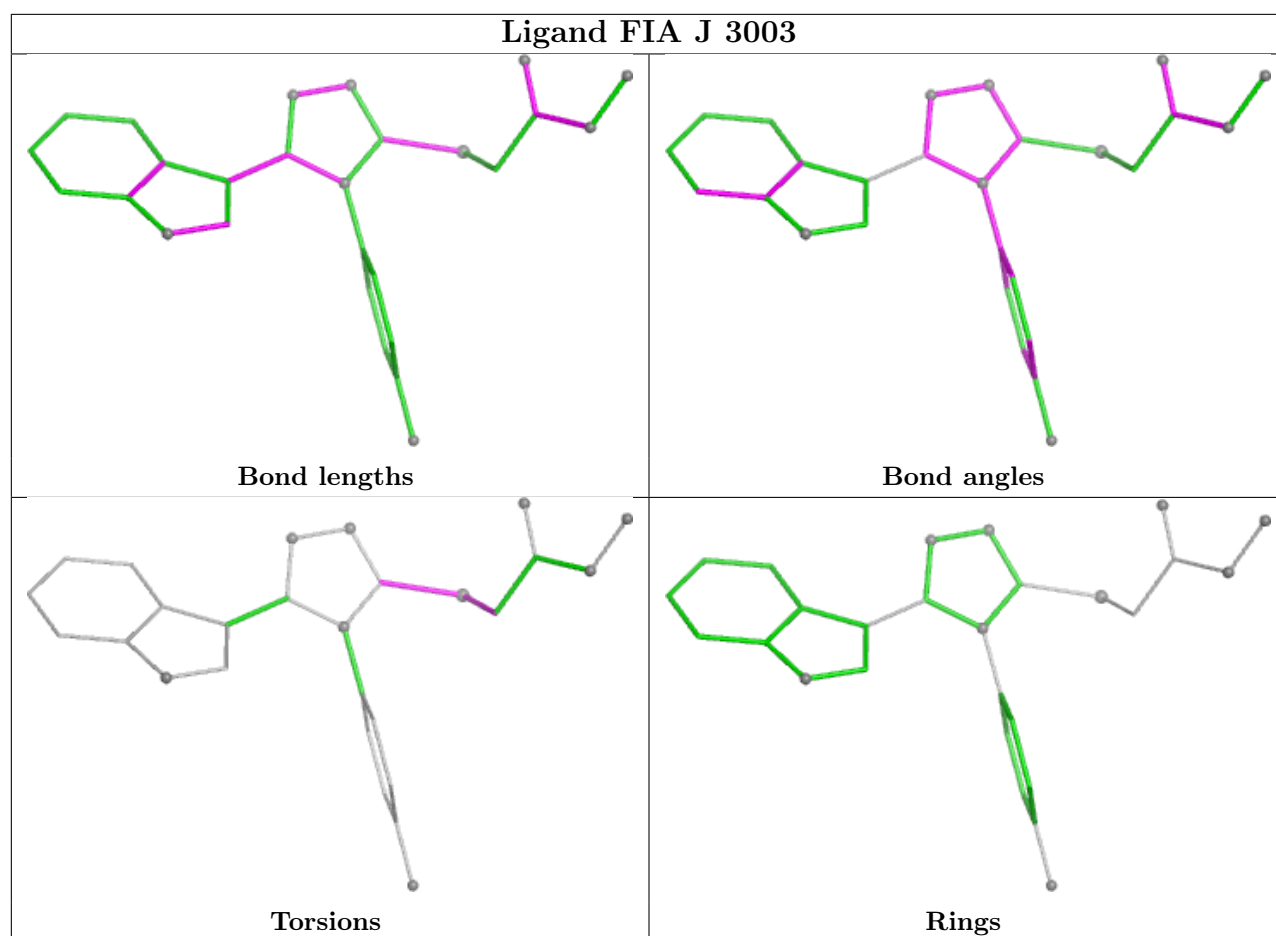












5.7 Other polymers [i](#)

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, 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	238/238 (100%)	-0.72	2 (0%) 82 86	9, 15, 34, 63	0
1	C	238/238 (100%)	-0.73	2 (0%) 82 86	9, 15, 34, 68	0
1	E	238/238 (100%)	-0.80	1 (0%) 88 91	8, 14, 31, 50	0
1	G	238/238 (100%)	-0.69	7 (2%) 53 60	9, 15, 37, 87	0
1	I	238/238 (100%)	-0.78	5 (2%) 63 70	8, 13, 34, 102	0
1	K	238/238 (100%)	-0.62	8 (3%) 48 54	9, 16, 39, 109	1 (0%)
2	B	568/569 (99%)	-0.93	2 (0%) 88 91	5, 11, 28, 65	0
2	D	568/569 (99%)	-0.91	2 (0%) 88 91	6, 11, 29, 85	1 (0%)
2	F	568/569 (99%)	-0.92	3 (0%) 87 90	5, 10, 28, 73	1 (0%)
2	H	568/569 (99%)	-0.92	3 (0%) 87 90	6, 11, 29, 65	0
2	J	568/569 (99%)	-0.87	10 (1%) 67 75	5, 10, 28, 114	0
2	L	568/569 (99%)	-0.91	4 (0%) 84 88	6, 11, 27, 70	0
All	All	4836/4842 (99%)	-0.85	49 (1%) 79 84	5, 12, 31, 114	3 (0%)

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	332	VAL	9.1
2	J	330	GLU	8.9
2	J	328	ILE	7.0
1	I	230	ASP	5.9
1	G	227	LYS	5.4

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	KCX	D	219	12/13	0.97	0.05	6,9,13,14	0
2	KCX	F	219	12/13	0.98	0.04	5,9,13,14	0
2	KCX	H	219	12/13	0.98	0.04	5,9,11,11	0
2	KCX	J	219	12/13	0.98	0.04	5,9,12,13	0
2	KCX	L	219	12/13	0.98	0.04	5,8,13,13	0
2	KCX	B	219	12/13	0.99	0.04	5,8,13,13	0

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(Å ²)	Q<0.9
5	SO4	C	301	5/5	0.74	0.20	49,49,61,79	0
6	PO4	H	3004	5/5	0.77	0.17	40,49,62,66	0
5	SO4	K	301	5/5	0.90	0.11	45,47,49,77	0
6	PO4	G	301	5/5	0.90	0.13	45,46,53,64	0
4	FIA	B	3003	27/27	0.90	0.12	15,21,29,30	40
4	FIA	F	3003	27/27	0.91	0.12	14,22,30,35	40
4	FIA	L	3003	27/27	0.92	0.10	16,27,39,46	0
4	FIA	H	3003	27/27	0.94	0.09	13,21,29,30	40
4	FIA	J	3003	27/27	0.95	0.09	8,21,31,37	40
4	FIA	D	3003	27/27	0.96	0.08	9,22,31,33	40
3	NI	L	3001	1/1	1.00	0.03	10,10,10,10	0
3	NI	L	3002	1/1	1.00	0.02	13,13,13,13	0
3	NI	B	3001	1/1	1.00	0.02	11,11,11,11	0
3	NI	B	3002	1/1	1.00	0.02	13,13,13,13	0
3	NI	D	3001	1/1	1.00	0.03	12,12,12,12	0
3	NI	D	3002	1/1	1.00	0.02	12,12,12,12	0
3	NI	F	3001	1/1	1.00	0.04	10,10,10,10	0
3	NI	F	3002	1/1	1.00	0.02	13,13,13,13	0
3	NI	H	3001	1/1	1.00	0.03	11,11,11,11	0
3	NI	H	3002	1/1	1.00	0.03	12,12,12,12	0

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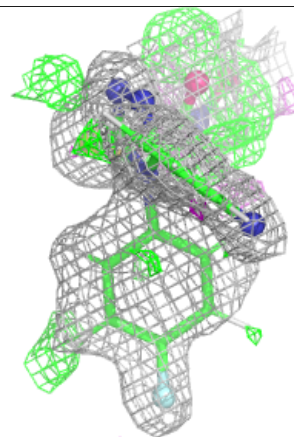
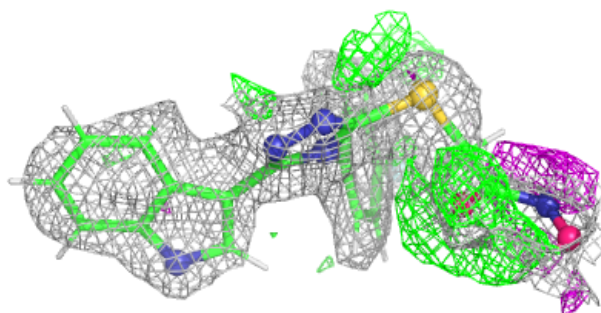
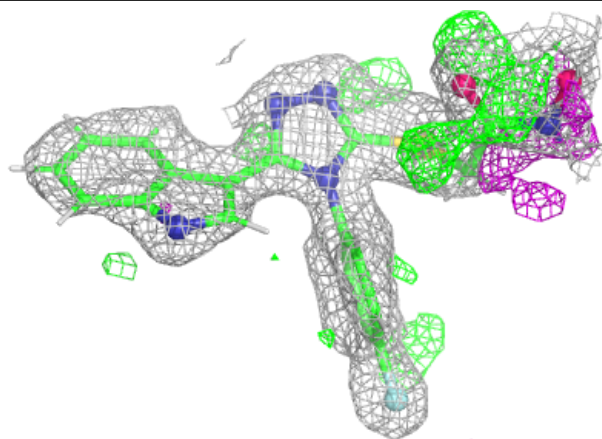
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NI	J	3001	1/1	1.00	0.02	11,11,11,11	0
3	NI	J	3002	1/1	1.00	0.01	12,12,12,12	0

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.

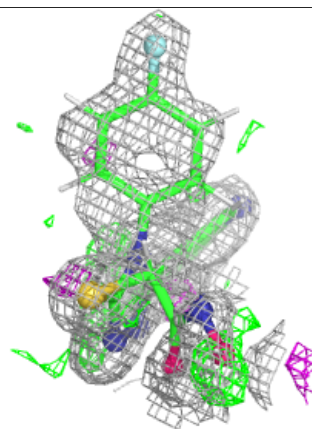
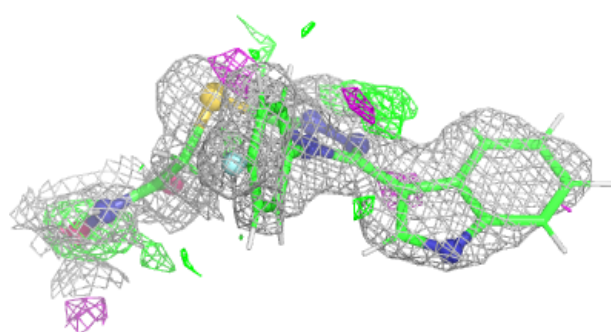
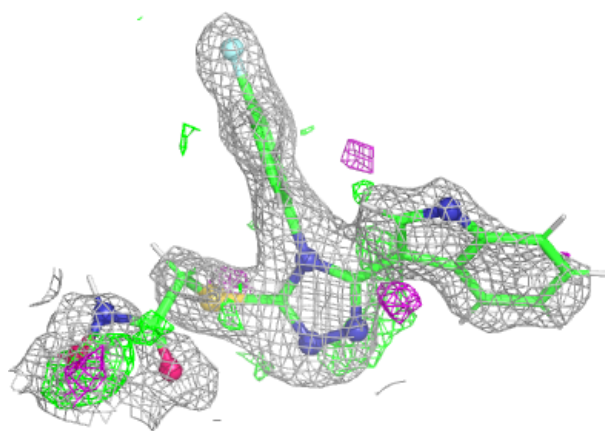
Electron density around FIA B 3003:

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

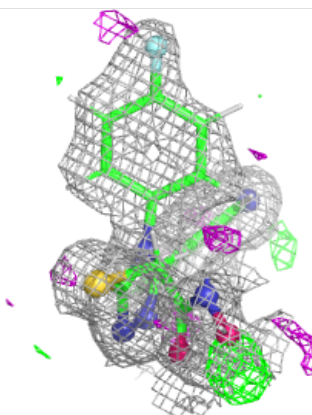
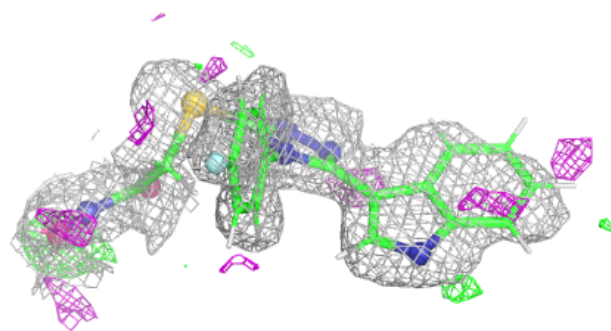
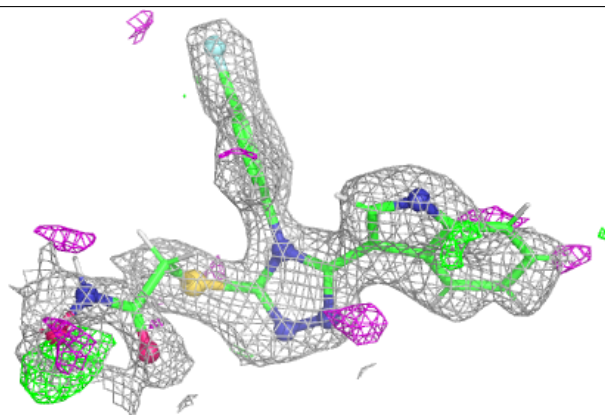


Electron density around FIA F 3003:

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

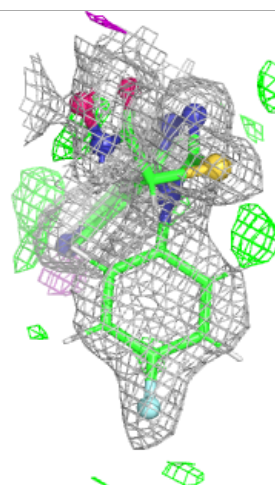
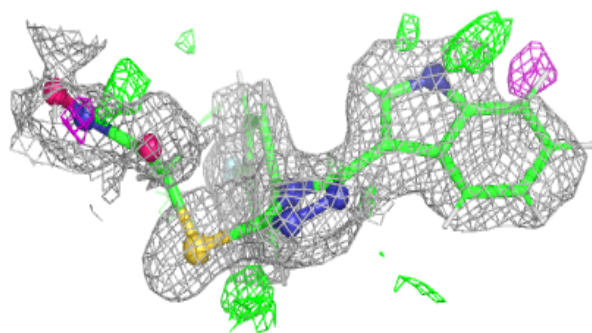
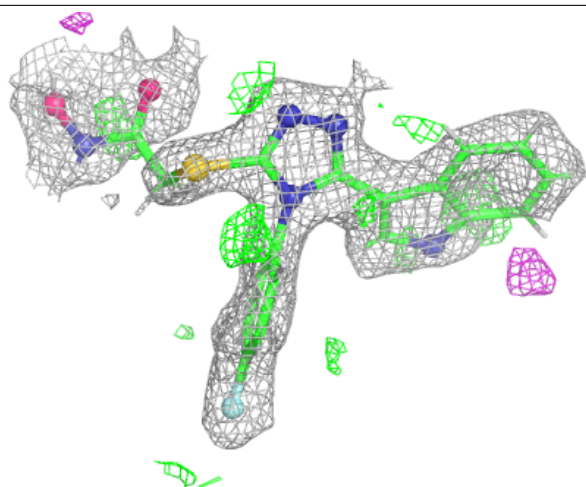
**Electron density around FIA L 3003:**

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



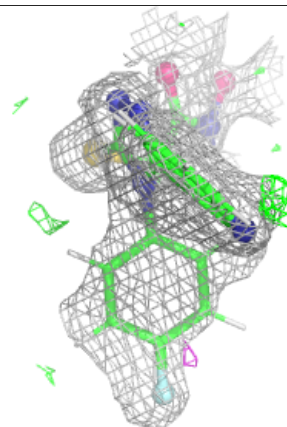
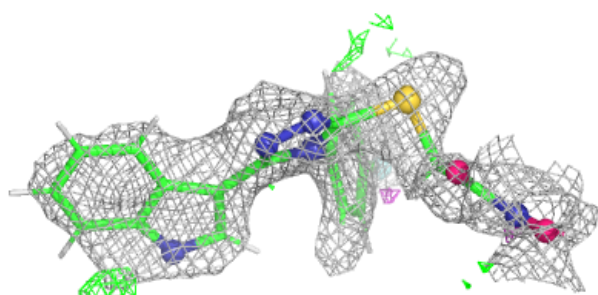
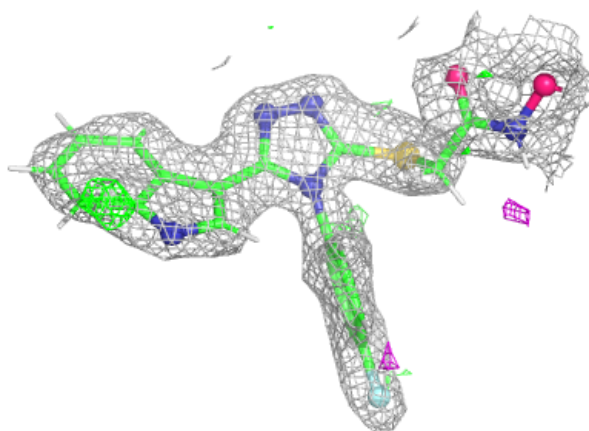
Electron density around FIA H 3003:

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



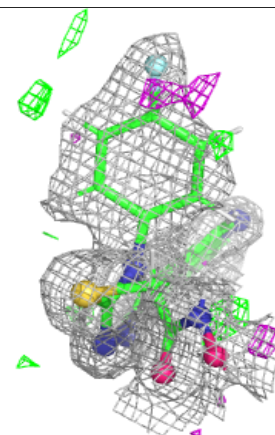
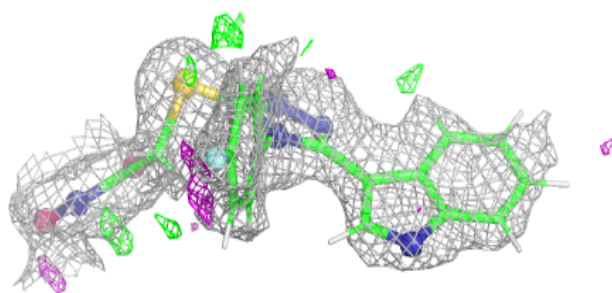
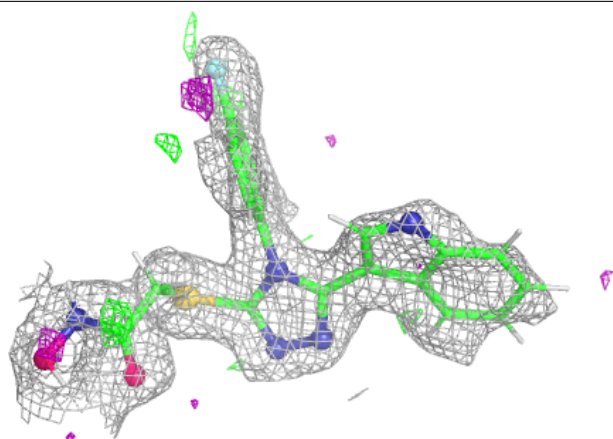
Electron density around FIA J 3003:

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



Electron density around FIA D 3003:

$2mF_o-DF_c$ (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.