



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:30 AM UTC

PDB ID : 7F9U / pdb_00007f9u
Title : Toxoplasma gondii Prolyl-tRNA Synthetase (TgPRS) in Complex with inhibitor T35 and Halofuginone
Authors : Manickam, Y.; Malhotra, N.; Sharma, A.
Deposited on : 2021-07-04
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

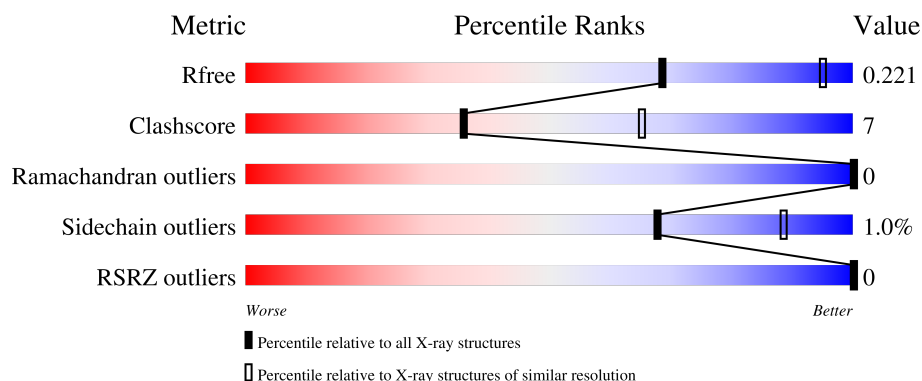
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

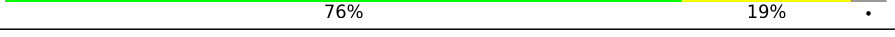
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 ≥ 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	500	
1	B	500	
1	C	500	
1	D	500	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15950 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.

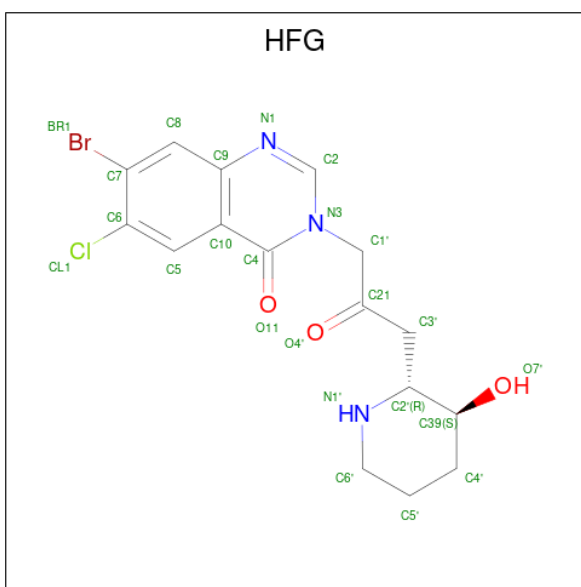
- Molecule 1 is a protein called Prolyl-tRNA synthetase (ProRS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3895	2504	670	700	21			
1	B	483	Total	C	N	O	S	0	0	0
			3922	2517	672	712	21			
1	C	489	Total	C	N	O	S	0	0	0
			3944	2530	673	718	23			
1	D	480	Total	C	N	O	S	0	0	0
			3885	2497	666	700	22			

There are 12 discrepancies between the modelled and reference sequences:

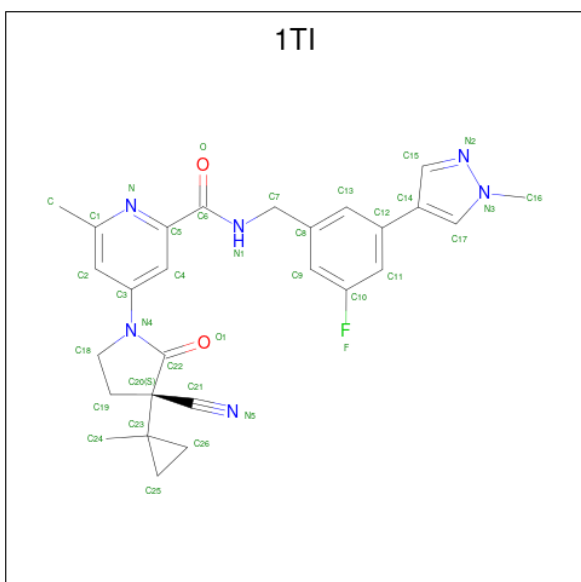
Chain	Residue	Modelled	Actual	Comment	Reference
A	331	GLY	-	expression tag	UNP A0A7J6JUK2
A	332	ALA	-	expression tag	UNP A0A7J6JUK2
A	333	MET	-	expression tag	UNP A0A7J6JUK2
B	331	GLY	-	expression tag	UNP A0A7J6JUK2
B	332	ALA	-	expression tag	UNP A0A7J6JUK2
B	333	MET	-	expression tag	UNP A0A7J6JUK2
C	331	GLY	-	expression tag	UNP A0A7J6JUK2
C	332	ALA	-	expression tag	UNP A0A7J6JUK2
C	333	MET	-	expression tag	UNP A0A7J6JUK2
D	331	GLY	-	expression tag	UNP A0A7J6JUK2
D	332	ALA	-	expression tag	UNP A0A7J6JUK2
D	333	MET	-	expression tag	UNP A0A7J6JUK2

- Molecule 2 is 7-bromo-6-chloro-3-{3-[(2R,3S)-3-hydroxypiperidin-2-yl]-2-oxopropyl}quinazolin-4(3H)-one (CCD ID: HFG) (formula: C₁₆H₁₇BrClN₃O₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	Cl	N	O	0	0
			24	1	16	1	3	3		
2	B	1	Total	Br	C	Cl	N	O	0	0
			24	1	16	1	3	3		
2	C	1	Total	Br	C	Cl	N	O	0	0
			24	1	16	1	3	3		
2	D	1	Total	Br	C	Cl	N	O	0	0
			24	1	16	1	3	3		

- Molecule 3 is 4-[(3S)-3-cyano-3-(1-methylcyclopropyl)-2-oxidanylidene-pyrrolidin-1-yl]-N-[[3-fluoranyl-5-(1-methylpyrazol-4-yl)phenyl]methyl]-6-methyl-pyridine-2-carboxamide (CCD ID: 1TI) (formula: C₂₇H₂₇FN₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			36	27	1	6	2		
3	B	1	Total	C	F	N	O	0	0
			36	27	1	6	2		
3	C	1	Total	C	F	N	O	0	0
			36	27	1	6	2		
3	D	1	Total	C	F	N	O	0	0
			36	27	1	6	2		

- Molecule 4 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Br	0	0
			1	1		
4	B	1	Total	Br	0	0
			1	1		
4	D	1	Total	Br	0	0
			1	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Cl	0	0
			3	3		
6	B	3	Total	Cl	0	0
			3	3		
6	C	2	Total	Cl	0	0
			2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	15	Total	O	0	0
			15	15		

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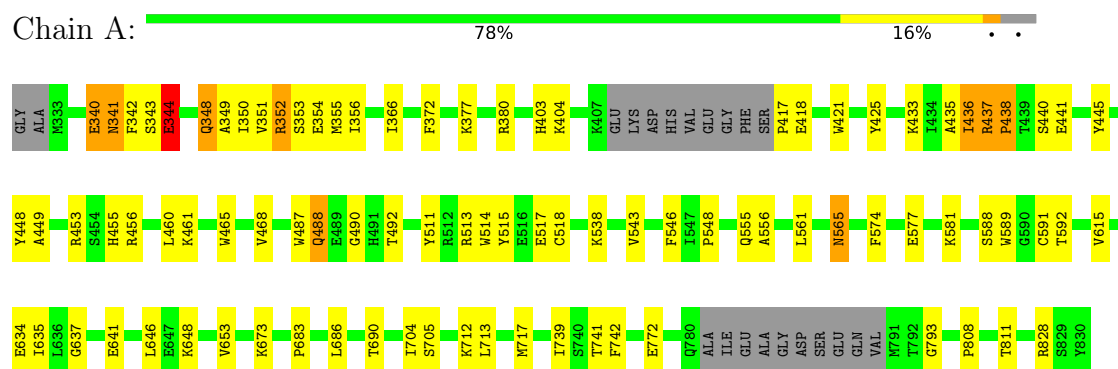
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	15	Total	O	0	0
			15	15		
7	C	14	Total	O	0	0
			14	14		
7	D	6	Total	O	0	0
			6	6		

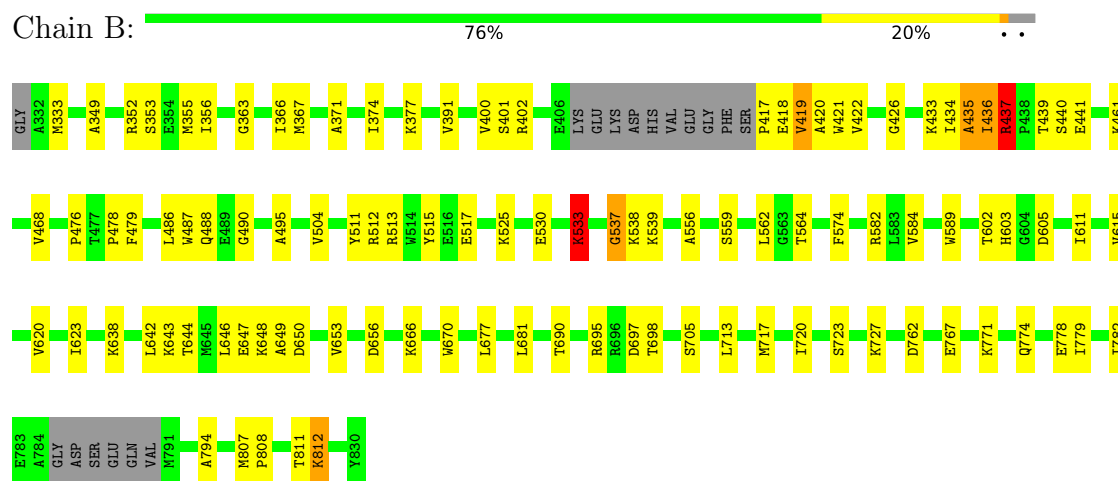
3 Residue-property plots [i](#)

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.

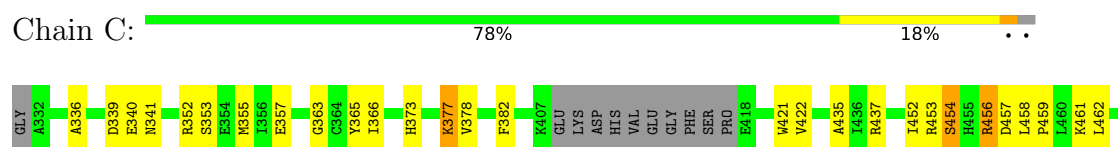
• Molecule 1: Prolyl-tRNA synthetase (ProRS)

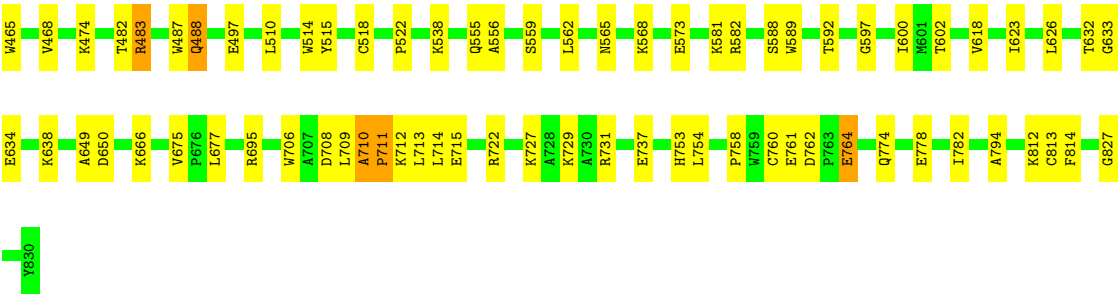


• Molecule 1: Prolyl-tRNA synthetase (ProRS)

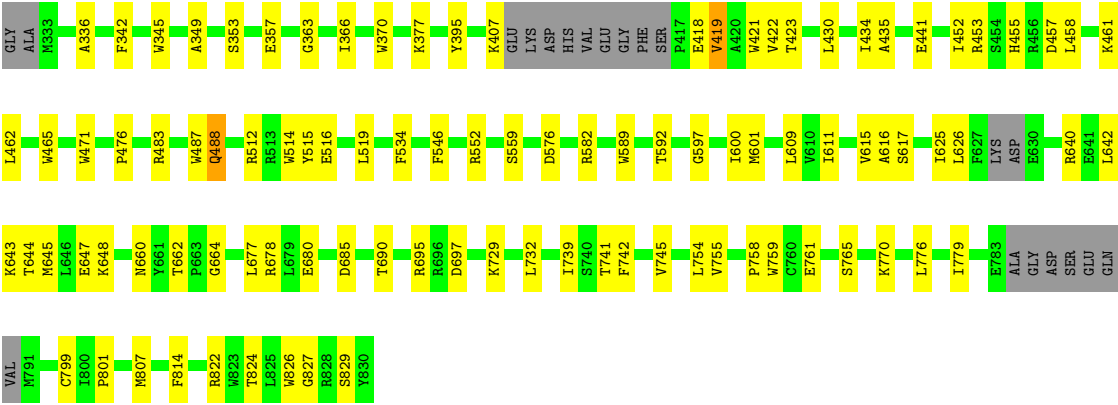


• Molecule 1: Prolyl-tRNA synthetase (ProRS)





- Molecule 1: Prolyl-tRNA synthetase (ProRS)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	76.57Å 76.57Å 403.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.57 – 2.80 76.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (76.57-2.80) 99.9 (76.57-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.15rc1_3423	Depositor
R, R_{free}	0.164 , 0.224 0.164 , 0.221	Depositor DCC
R_{free} test set	982 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 7.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.159 for h,-k,-l	Xtriage
Reported twinning fraction	0.150 for h,-k,-l	Depositor
Outliers	0 of 56768 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15950	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 1TI, BR, CA, HFG

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	0.79	21/4000 (0.5%)	0.74	8/5411 (0.1%)
1	B	0.79	19/4026 (0.5%)	0.79	12/5450 (0.2%)
1	C	0.82	22/4047 (0.5%)	0.74	4/5479 (0.1%)
1	D	0.49	2/3988 (0.1%)	0.64	0/5395
All	All	0.74	64/16061 (0.4%)	0.73	24/21735 (0.1%)

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	539	LYS	C-O	-8.63	1.14	1.23
1	B	436	ILE	C-O	-8.48	1.14	1.24
1	A	348	GLN	C-O	-8.28	1.14	1.24
1	A	349	ALA	C-O	-7.54	1.15	1.24
1	C	711	PRO	C-O	-7.47	1.14	1.24
1	C	715	GLU	C-O	-7.37	1.15	1.24
1	B	602	THR	C-O	-7.25	1.14	1.24
1	C	709	LEU	C-O	-7.25	1.15	1.24
1	C	714	LEU	C-O	-7.18	1.14	1.24
1	C	712	LYS	C-O	-7.18	1.15	1.24
1	A	441	GLU	C-O	-7.16	1.15	1.24
1	A	353	SER	C-O	-7.14	1.14	1.24
1	A	348	GLN	CA-C	-7.12	1.43	1.52
1	A	350	ILE	C-O	-7.06	1.15	1.24
1	A	342	PHE	C-O	-7.01	1.16	1.24
1	C	378	VAL	C-O	-6.99	1.15	1.24
1	A	341	ASN	CA-C	-6.79	1.46	1.53
1	D	455	HIS	C-O	-6.76	1.16	1.24
1	C	483	ARG	C-O	-6.69	1.15	1.24
1	A	436	ILE	CA-C	-6.62	1.44	1.52
1	B	434	ILE	C-O	-6.51	1.17	1.24
1	C	722	ARG	C-O	-6.47	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	GLU	C-O	-6.46	1.15	1.24
1	A	436	ILE	C-O	-6.32	1.16	1.24
1	C	454	SER	C-O	-6.30	1.15	1.23
1	B	811	THR	CA-C	-6.28	1.44	1.52
1	B	811	THR	C-O	-6.24	1.16	1.23
1	A	440	SER	C-O	-6.17	1.15	1.23
1	A	351	VAL	C-O	-6.11	1.16	1.24
1	C	377	LYS	C-O	-6.08	1.16	1.24
1	D	419	VAL	C-O	-6.04	1.17	1.24
1	C	483	ARG	CA-C	-6.02	1.44	1.52
1	A	344	GLU	CA-C	-6.00	1.44	1.52
1	C	710	ALA	C-O	-5.92	1.16	1.24
1	C	711	PRO	CA-C	-5.89	1.43	1.52
1	A	673	LYS	C-O	-5.76	1.16	1.24
1	C	634	GLU	C-O	-5.72	1.17	1.24
1	C	715	GLU	N-CA	-5.72	1.39	1.46
1	B	538	LYS	N-CA	-5.69	1.39	1.46
1	B	440	SER	C-O	-5.65	1.16	1.24
1	A	355	MET	CA-C	-5.64	1.44	1.52
1	B	435	ALA	C-O	-5.57	1.16	1.23
1	C	762	ASP	C-O	-5.56	1.16	1.24
1	C	452	ILE	C-O	-5.50	1.17	1.24
1	B	436	ILE	CA-C	-5.46	1.46	1.52
1	C	762	ASP	CA-C	-5.46	1.47	1.53
1	B	539	LYS	CA-C	-5.40	1.46	1.52
1	B	533	LYS	C-O	-5.38	1.16	1.23
1	C	454	SER	CA-C	-5.38	1.45	1.52
1	B	812	LYS	N-CA	-5.36	1.39	1.45
1	B	603	HIS	C-O	-5.36	1.16	1.24
1	A	340	GLU	C-O	-5.30	1.15	1.23
1	A	341	ASN	C-O	-5.29	1.17	1.23
1	A	355	MET	C-O	-5.27	1.17	1.24
1	B	420	ALA	C-O	-5.26	1.17	1.24
1	B	602	THR	CA-C	-5.25	1.45	1.52
1	A	349	ALA	CA-C	-5.25	1.46	1.52
1	B	605	ASP	C-O	-5.14	1.17	1.24
1	B	602	THR	N-CA	-5.13	1.39	1.46
1	C	708	ASP	C-O	-5.11	1.16	1.23
1	A	354	GLU	CA-C	-5.08	1.46	1.53
1	C	453	ARG	C-O	-5.07	1.17	1.24
1	C	633	GLY	C-O	-5.05	1.17	1.24
1	B	419	VAL	C-O	-5.02	1.17	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	709	LEU	N-CA-C	9.89	121.82	111.14
1	C	632	THR	N-CA-C	8.17	123.47	113.17
1	A	440	SER	N-CA-C	7.85	122.62	112.26
1	B	437	ARG	N-CA-C	7.38	120.11	109.48
1	B	437	ARG	CA-C-N	7.09	128.70	119.84
1	B	437	ARG	C-N-CA	7.09	128.70	119.84
1	B	537	GLY	N-CA-C	6.89	123.06	112.51
1	A	437	ARG	CA-C-N	6.70	128.21	119.84
1	A	437	ARG	C-N-CA	6.70	128.21	119.84
1	A	351	VAL	N-CA-C	6.36	117.15	110.72
1	C	377	LYS	N-CA-C	6.26	118.19	111.36
1	B	440	SER	N-CA-C	6.18	120.44	112.41
1	A	343	SER	N-CA-C	6.13	117.97	111.28
1	B	807	MET	CA-C-N	6.02	126.37	119.93
1	B	807	MET	C-N-CA	6.02	126.37	119.93
1	B	808	PRO	CB-CA-C	-5.63	104.49	111.64
1	A	437	ARG	N-CA-C	5.62	117.57	109.48
1	A	438	PRO	CA-C-N	5.49	132.03	121.54
1	A	438	PRO	C-N-CA	5.49	132.03	121.54
1	B	419	VAL	N-CA-C	5.44	117.06	109.55
1	C	761	GLU	N-CA-C	5.44	119.50	112.86
1	B	808	PRO	CA-C-O	-5.23	115.62	121.32
1	B	417	PRO	CA-C-N	5.09	131.26	121.54
1	B	417	PRO	C-N-CA	5.09	131.26	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3895	0	3851	53	0
1	B	3922	0	3861	57	0
1	C	3944	0	3883	62	0
1	D	3885	0	3825	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	24	0	17	1	0
2	B	24	0	17	4	0
2	C	24	0	17	1	0
2	D	24	0	17	1	0
3	A	36	0	0	1	0
3	B	36	0	0	0	0
3	C	36	0	0	2	0
3	D	36	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
6	C	2	0	0	0	0
7	A	15	0	0	0	0
7	B	15	0	0	1	0
7	C	14	0	0	2	0
7	D	6	0	0	0	0
All	All	15950	0	15488	228	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 7.

All (228) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ARG:HG3	1:A:352:ARG:HH11	1.38	0.85
1:B:418:GLU:CB	2:B:901:HFG:BR1	2.81	0.84
1:B:418:GLU:HB2	2:B:901:HFG:BR1	2.37	0.79
1:B:418:GLU:HB3	2:B:901:HFG:BR1	2.39	0.78
1:A:344:GLU:O	1:A:348:GLN:HG3	1.88	0.73
1:D:755:VAL:HG22	1:D:826:TRP:HB2	1.74	0.69
1:A:352:ARG:HH11	1:A:352:ARG:CG	2.06	0.69
1:D:761:GLU:OE1	1:D:822:ARG:NE	2.21	0.68
1:B:402:ARG:HD2	1:B:433:LYS:HE2	1.76	0.68
1:D:512:ARG:NH1	1:D:516:GLU:OE1	2.26	0.68
1:C:497:GLU:OE2	1:C:538:LYS:NZ	2.25	0.67
1:D:552:ARG:NH1	1:D:829:SER:O	2.28	0.66
1:D:471:TRP:HA	1:D:483:ARG:HG2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:GLN:NE2	1:B:511:TYR:OH	2.29	0.63
1:B:349:ALA:O	1:B:353:SER:HB3	1.97	0.63
1:B:437:ARG:HG3	1:B:468:VAL:HG12	1.81	0.62
1:D:678:ARG:NH1	1:D:680:GLU:OE2	2.32	0.62
1:A:341:ASN:OD1	1:A:344:GLU:HB2	1.99	0.62
1:C:568:LYS:HD2	7:C:1001:HOH:O	2.00	0.62
1:B:564:THR:HG22	1:B:584:VAL:O	2.00	0.61
1:C:437:ARG:HG3	1:C:468:VAL:HG12	1.82	0.61
1:A:377:LYS:HG2	1:A:615:VAL:HA	1.81	0.61
1:D:759:TRP:NE1	1:D:765:SER:OG	2.33	0.61
1:C:764:GLU:HA	1:C:764:GLU:OE2	2.00	0.60
1:C:355:MET:HE1	1:C:600:ILE:HD11	1.82	0.60
1:C:461:LYS:O	1:C:462:LEU:HD23	2.01	0.60
1:C:363:GLY:HA3	1:C:483:ARG:HG3	1.85	0.59
1:D:421:TRP:CZ3	1:D:435:ALA:HB2	2.38	0.58
1:A:437:ARG:HG3	1:A:468:VAL:HG12	1.84	0.58
1:B:559:SER:HA	1:B:589:TRP:HB3	1.85	0.57
1:A:456:ARG:NH1	1:D:660:ASN:HB2	2.19	0.57
1:A:490:GLY:O	1:A:588:SER:HA	2.03	0.57
1:D:799:CYS:O	1:D:801:PRO:HD3	2.05	0.57
1:B:490:GLY:HA3	1:B:589:TRP:CH2	2.40	0.57
1:C:710:ALA:HB3	1:C:711:PRO:CD	2.35	0.57
1:C:454:SER:HB2	1:C:456:ARG:HG2	1.87	0.56
1:C:336:ALA:HB1	1:C:341:ASN:HB2	1.86	0.56
1:A:461:LYS:HA	1:A:492:THR:HG22	1.88	0.56
1:D:471:TRP:CD2	1:D:483:ARG:HD3	2.41	0.56
1:B:421:TRP:CE3	1:B:433:LYS:HE3	2.41	0.55
1:C:515:TYR:CZ	1:C:556:ALA:HB1	2.41	0.55
1:A:513:ARG:O	1:A:517:GLU:HB2	2.06	0.55
1:C:353:SER:OG	1:C:355:MET:HG3	2.07	0.55
1:D:754:LEU:HD22	1:D:827:GLY:HA3	1.89	0.55
1:B:723:SER:O	1:B:727:LYS:HG3	2.08	0.54
1:C:565:ASN:ND2	7:C:1001:HOH:O	2.39	0.54
1:B:333:MET:O	1:B:352:ARG:NH1	2.40	0.54
1:D:776:LEU:HA	1:D:779:ILE:HG12	1.89	0.54
1:A:465:TRP:CE3	1:A:488:GLN:HB3	2.44	0.53
1:C:456:ARG:CG	1:C:456:ARG:HH11	2.22	0.53
1:A:460:LEU:O	1:A:492:THR:HA	2.07	0.53
1:B:646:LEU:HB2	1:B:653:VAL:HG21	1.91	0.53
1:C:454:SER:CB	1:C:456:ARG:HG2	2.39	0.53
1:A:634:GLU:HB3	1:A:686:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:662:THR:HG22	1:D:664:GLY:H	1.72	0.53
1:A:704:ILE:HD13	1:A:712:LYS:HG2	1.91	0.52
1:C:573:GLU:HB2	1:C:582:ARG:O	2.09	0.52
1:D:625:ILE:O	1:D:626:LEU:HD23	2.09	0.52
1:A:490:GLY:HA3	1:A:589:TRP:CE2	2.45	0.52
1:B:513:ARG:O	1:B:517:GLU:HB2	2.10	0.52
1:A:490:GLY:HA3	1:A:589:TRP:CZ2	2.44	0.52
1:A:421:TRP:CZ3	1:A:435:ALA:HB2	2.45	0.52
1:C:487:TRP:HB3	1:C:592:THR:HG22	1.93	0.51
1:D:758:PRO:HD2	1:D:814:PHE:HB3	1.92	0.51
1:D:471:TRP:CE2	1:D:483:ARG:HD3	2.45	0.51
1:C:774:GLN:HB2	1:C:794:ALA:HB2	1.92	0.51
1:B:779:ILE:O	1:B:782:ILE:HG22	2.11	0.50
1:B:638:LYS:HB3	1:B:681:LEU:HD21	1.94	0.50
1:A:515:TYR:CZ	1:A:556:ALA:HB1	2.46	0.50
1:B:515:TYR:CZ	1:B:556:ALA:HB1	2.46	0.50
1:A:543:VAL:HG23	1:A:556:ALA:HB3	1.93	0.50
1:D:370:TRP:CZ3	1:D:617:SER:HB3	2.47	0.50
1:B:356:ILE:HA	1:B:366:ILE:O	2.12	0.49
1:D:357:GLU:HB3	1:D:366:ILE:HB	1.95	0.49
1:B:656:ASP:OD2	1:B:670:TRP:NE1	2.38	0.49
1:C:649:ALA:O	1:C:650:ASP:HB2	2.12	0.49
1:D:377:LYS:HG2	1:D:615:VAL:HA	1.94	0.49
1:D:695:ARG:NH2	1:D:697:ASP:OD2	2.34	0.49
1:C:710:ALA:N	1:C:711:PRO:HD2	2.28	0.49
1:C:737:GLU:OE2	1:C:753:HIS:ND1	2.38	0.49
1:D:349:ALA:O	1:D:353:SER:HB3	2.13	0.49
1:B:537:GLY:HA2	1:B:562:LEU:HA	1.95	0.48
1:D:407:LYS:HB2	1:D:407:LYS:HE3	1.63	0.48
1:D:770:LYS:NZ	1:D:770:LYS:HB3	2.28	0.48
1:A:487:TRP:CH2	2:A:901:HFG:H8	2.48	0.48
1:C:774:GLN:O	1:C:778:GLU:HG3	2.13	0.48
1:C:514:TRP:O	1:C:518:CYS:HB2	2.13	0.48
1:C:555:GLN:HG2	3:C:902:1TI:N5	2.29	0.48
1:D:640:ARG:O	1:D:644:THR:HG23	2.13	0.48
1:C:677:LEU:HD23	1:C:695:ARG:HA	1.95	0.48
1:B:487:TRP:CH2	2:B:901:HFG:H8	2.48	0.48
1:C:465:TRP:CE3	1:C:488:GLN:HB3	2.49	0.48
1:D:559:SER:HA	1:D:589:TRP:HB3	1.96	0.48
1:A:713:LEU:O	1:A:717:MET:HG3	2.14	0.48
1:C:522:PRO:HG3	1:C:729:LYS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:487:TRP:HB3	1:D:592:THR:HG22	1.96	0.48
1:A:646:LEU:HB2	1:A:653:VAL:HG21	1.95	0.47
1:B:690:THR:HA	1:B:705:SER:HA	1.96	0.47
1:D:576:ASP:OD2	1:D:582:ARG:NE	2.46	0.47
1:A:425:TYR:HA	1:D:419:VAL:O	2.14	0.47
1:A:793:GLY:O	1:A:828:ARG:NE	2.45	0.47
1:B:439:THR:OG1	1:B:441:GLU:OE1	2.30	0.47
1:C:352:ARG:HH11	1:C:352:ARG:HG3	1.79	0.47
1:C:421:TRP:CZ3	1:C:435:ALA:HB2	2.49	0.47
1:C:602:THR:O	1:C:731:ARG:NH2	2.48	0.47
1:D:441:GLU:N	1:D:441:GLU:OE1	2.46	0.47
1:A:417:PRO:HB2	1:A:418:GLU:H	1.57	0.47
1:A:514:TRP:O	1:A:518:CYS:HB2	2.14	0.47
1:C:754:LEU:HD22	1:C:827:GLY:HA3	1.95	0.47
1:D:597:GLY:HA2	1:D:600:ILE:HD12	1.97	0.47
1:A:380:ARG:HA	1:A:380:ARG:HD3	1.78	0.47
1:D:461:LYS:O	1:D:462:LEU:HD23	2.16	0.46
1:C:760:CYS:HB3	1:C:813:CYS:HB2	1.98	0.46
1:B:642:LEU:O	1:B:646:LEU:HG	2.16	0.46
1:A:449:ALA:O	1:A:453:ARG:NH1	2.49	0.46
1:B:643:LYS:O	1:B:647:GLU:HG3	2.16	0.46
1:C:559:SER:HA	1:C:589:TRP:HB3	1.98	0.46
1:A:455:HIS:CD2	1:A:456:ARG:HG3	2.52	0.46
1:A:555:GLN:HG2	3:A:902:1TI:N5	2.31	0.46
1:A:635:ILE:HD11	1:A:683:PRO:HD3	1.97	0.46
1:C:474:LYS:HB2	3:C:902:1TI:C15	2.46	0.45
1:D:600:ILE:HG23	1:D:609:LEU:HD22	1.98	0.45
1:B:374:ILE:HD11	1:B:611:ILE:HD13	1.97	0.45
1:A:372:PHE:HE2	1:D:395:TYR:HB2	1.81	0.45
1:A:742:PHE:CZ	1:A:772:GLU:HG2	2.52	0.45
1:A:648:LYS:HE2	1:A:648:LYS:HB3	1.64	0.45
1:D:729:LYS:O	1:D:732:LEU:HB3	2.16	0.45
1:B:353:SER:OG	1:B:355:MET:HG3	2.17	0.45
1:D:336:ALA:HB3	1:D:345:TRP:HA	1.97	0.45
1:D:342:PHE:CE2	1:D:601:MET:HE2	2.52	0.45
1:B:495:ALA:HB3	7:B:1006:HOH:O	2.17	0.45
1:C:727:LYS:O	1:C:731:ARG:HG3	2.17	0.45
1:B:713:LEU:O	1:B:717:MET:HG3	2.16	0.45
1:B:574:PHE:CE1	1:B:582:ARG:HB2	2.52	0.44
1:C:562:LEU:HD11	1:C:588:SER:HB3	1.99	0.44
1:D:645:MET:HA	1:D:648:LYS:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:ASP:OD1	1:B:762:ASP:N	2.50	0.44
1:A:403:HIS:ND1	1:A:404:LYS:HG3	2.33	0.44
1:A:565:ASN:N	1:A:565:ASN:ND2	2.66	0.44
1:C:623:ILE:HD12	1:C:666:LYS:HB3	2.00	0.44
1:B:377:LYS:HG2	1:B:615:VAL:HA	1.99	0.44
1:B:487:TRP:CD1	1:B:487:TRP:C	2.94	0.44
1:A:577:GLU:OE2	1:A:577:GLU:N	2.42	0.44
1:C:487:TRP:CH2	2:C:901:HFG:H8	2.52	0.44
1:D:755:VAL:CG2	1:D:826:TRP:HB2	2.44	0.44
1:A:546:PHE:O	1:A:548:PRO:HD3	2.18	0.44
1:B:530:GLU:HA	1:B:533:LYS:HD3	2.00	0.44
1:D:824:THR:HB	1:D:826:TRP:HE1	1.83	0.44
1:A:538:LYS:N	1:A:561:LEU:O	2.49	0.43
1:B:490:GLY:HA3	1:B:589:TRP:CZ3	2.53	0.43
1:A:793:GLY:C	1:A:828:ARG:HE	2.27	0.43
1:C:778:GLU:O	1:C:782:ILE:HG13	2.19	0.43
1:A:487:TRP:C	1:A:487:TRP:CD1	2.96	0.43
1:B:367:MET:HE1	1:B:486:LEU:HD12	2.00	0.43
1:C:812:LYS:HB3	1:C:812:LYS:HE2	1.59	0.43
1:D:758:PRO:HB3	1:D:807:MET:HE1	2.01	0.43
1:B:478:PRO:O	1:B:479:PHE:HB2	2.19	0.43
1:B:512:ARG:HD3	1:B:525:LYS:HE3	1.99	0.43
1:C:459:PRO:HG2	1:C:461:LYS:HE3	1.99	0.43
1:C:618:VAL:O	1:C:675:VAL:HG13	2.19	0.43
1:A:421:TRP:CE3	1:A:433:LYS:HG3	2.53	0.43
1:C:510:LEU:HD23	1:C:510:LEU:HA	1.85	0.43
1:D:363:GLY:HA2	1:D:476:PRO:HG3	2.01	0.43
1:D:534:PHE:CE1	2:D:901:HFG:H15	2.54	0.43
1:D:662:THR:HG22	1:D:664:GLY:N	2.33	0.43
1:C:487:TRP:CB	1:C:592:THR:HG22	2.48	0.43
1:D:643:LYS:HE3	1:D:647:GLU:OE2	2.19	0.43
1:A:637:GLY:O	1:A:641:GLU:HG3	2.19	0.43
1:B:355:MET:HE2	1:B:371:ALA:HB2	2.00	0.42
1:A:808:PRO:O	1:A:811:THR:OG1	2.28	0.42
1:B:774:GLN:HB2	1:B:794:ALA:HB2	2.02	0.42
1:D:457:ASP:O	1:D:458:LEU:HD23	2.18	0.42
1:A:690:THR:HG22	1:A:705:SER:HA	2.02	0.42
1:C:355:MET:HB3	1:C:355:MET:HE3	1.62	0.42
1:C:457:ASP:O	1:C:458:LEU:HD23	2.20	0.42
1:C:514:TRP:CD1	1:C:514:TRP:C	2.97	0.42
1:B:422:VAL:HG22	1:C:422:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:ASP:OD1	1:B:698:THR:HG23	2.20	0.42
1:B:767:GLU:O	1:B:771:LYS:HG2	2.20	0.42
1:C:357:GLU:HB3	1:C:366:ILE:HB	2.02	0.42
1:C:626:LEU:HD23	1:C:626:LEU:HA	1.67	0.42
1:B:490:GLY:HA3	1:B:589:TRP:CZ2	2.55	0.42
1:B:695:ARG:HB2	1:B:720:ILE:HD11	2.02	0.42
1:C:365:TYR:HE2	1:C:482:THR:HG22	1.84	0.42
1:C:597:GLY:HA2	1:C:600:ILE:HD12	2.01	0.42
1:C:758:PRO:HD2	1:C:814:PHE:HB3	2.01	0.42
1:A:487:TRP:HB3	1:A:592:THR:HG22	2.02	0.42
1:B:363:GLY:HA2	1:B:476:PRO:HG3	2.02	0.42
1:C:382:PHE:CE2	1:C:488:GLN:NE2	2.88	0.41
1:D:377:LYS:HA	1:D:377:LYS:HD3	1.89	0.41
1:D:739:ILE:HD12	1:D:741:THR:O	2.20	0.41
1:C:373:HIS:NE2	1:C:377:LYS:HE3	2.35	0.41
1:D:465:TRP:CE3	1:D:488:GLN:HB3	2.54	0.41
1:D:685:ASP:HB3	1:D:690:THR:O	2.19	0.41
1:B:620:VAL:HG22	1:B:677:LEU:HB2	2.03	0.41
1:C:710:ALA:HB3	1:C:711:PRO:HD2	2.01	0.41
1:C:713:LEU:HD23	1:C:713:LEU:HA	1.61	0.41
1:D:546:PHE:CE1	1:D:754:LEU:HG	2.55	0.41
1:A:445:TYR:O	1:A:448:TYR:HB2	2.21	0.41
1:D:423:THR:C	1:D:430:LEU:HD12	2.45	0.41
1:D:642:LEU:HA	1:D:642:LEU:HD23	1.83	0.41
1:B:697:ASP:OD1	1:B:698:THR:N	2.53	0.41
1:D:515:TYR:O	1:D:519:LEU:HB2	2.20	0.41
1:A:514:TRP:CD1	1:A:514:TRP:C	2.99	0.41
1:B:623:ILE:HD12	1:B:666:LYS:HB3	2.03	0.41
1:B:391:VAL:HA	1:B:461:LYS:HB2	2.03	0.41
1:B:649:ALA:O	1:B:650:ASP:HB2	2.20	0.41
1:C:339:ASP:OD1	1:C:340:GLU:HG3	2.21	0.41
1:D:611:ILE:HG21	1:D:616:ALA:HA	2.02	0.41
1:D:742:PHE:O	1:D:745:VAL:HB	2.20	0.41
1:A:356:ILE:HA	1:A:366:ILE:O	2.21	0.41
1:A:437:ARG:HA	1:A:438:PRO:HD3	1.81	0.41
1:D:514:TRP:CD1	1:D:514:TRP:C	3.00	0.41
1:B:504:VAL:HG13	1:B:559:SER:OG	2.21	0.40
1:D:452:ILE:O	1:D:453:ARG:HD3	2.21	0.40
1:B:400:VAL:HG13	1:B:435:ALA:HB3	2.04	0.40
1:B:426:GLY:O	1:C:421:TRP:CD1	2.75	0.40
1:B:774:GLN:O	1:B:778:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:677:LEU:HD23	1:D:695:ARG:HA	2.02	0.40
1:A:511:TYR:CE1	1:A:591:CYS:HB2	2.57	0.40
1:A:739:ILE:HD12	1:A:741:THR:O	2.21	0.40
1:A:574:PHE:O	1:A:581:LYS:HA	2.21	0.40
1:C:487:TRP:CD1	1:C:487:TRP:C	2.99	0.40
1:C:573:GLU:HG3	1:C:581:LYS:HG2	2.03	0.40
1:C:638:LYS:HE2	1:C:706:TRP:CE3	2.57	0.40
1:B:644:THR:O	1:B:648:LYS:HG2	2.22	0.40
1:D:422:VAL:HB	1:D:434:ILE:HG12	2.03	0.40
1:D:515:TYR:HA	1:D:519:LEU:HD12	2.03	0.40

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	473/500 (95%)	458 (97%)	15 (3%)	0	100	100
1	B	477/500 (95%)	458 (96%)	19 (4%)	0	100	100
1	C	485/500 (97%)	466 (96%)	19 (4%)	0	100	100
1	D	472/500 (94%)	451 (96%)	21 (4%)	0	100	100
All	All	1907/2000 (95%)	1833 (96%)	74 (4%)	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	413/436 (95%)	407 (98%)	6 (2%)	57	84
1	B	415/436 (95%)	409 (99%)	6 (1%)	59	85
1	C	416/436 (95%)	413 (99%)	3 (1%)	76	91
1	D	409/436 (94%)	407 (100%)	2 (0%)	81	93
All	All	1653/1744 (95%)	1636 (99%)	17 (1%)	68	88

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	GLU
1	A	344	GLU
1	A	352	ARG
1	A	436	ILE
1	A	488	GLN
1	A	565	ASN
1	B	401	SER
1	B	419	VAL
1	B	436	ILE
1	B	437	ARG
1	B	533	LYS
1	B	812	LYS
1	C	456	ARG
1	C	488	GLN
1	C	764	GLU
1	D	418	GLU
1	D	488	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	488	GLN
1	A	565	ASN
1	B	669	HIS
1	C	341	ASN
1	C	668	ASN
1	C	669	HIS
1	C	750	ASN
1	D	463	ASN

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Mol	Chain	Res	Type
1	D	488	GLN
1	D	585	HIS
1	D	733	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HFG	A	901	-	26,26,26	0.43	0	29,37,37	0.67	1 (3%)
2	HFG	C	901	-	26,26,26	0.37	0	29,37,37	1.02	1 (3%)
2	HFG	B	901	-	26,26,26	0.50	0	29,37,37	0.89	1 (3%)
3	1TI	A	902	-	38,40,40	1.35	2 (5%)	54,61,61	0.70	0
3	1TI	C	902	-	38,40,40	0.90	2 (5%)	54,61,61	0.73	1 (1%)
2	HFG	D	901	-	26,26,26	0.57	1 (3%)	29,37,37	1.67	1 (3%)
3	1TI	B	902	-	38,40,40	1.03	2 (5%)	54,61,61	0.78	2 (3%)
3	1TI	D	902	-	38,40,40	0.93	2 (5%)	54,61,61	0.69	2 (3%)

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	HFG	A	901	-	-	0/8/19/19	0/3/3/3
2	HFG	C	901	-	-	0/8/19/19	0/3/3/3
2	HFG	B	901	-	-	0/8/19/19	0/3/3/3
3	1TI	A	902	-	-	0/17/49/49	0/5/5/5
3	1TI	C	902	-	-	0/17/49/49	0/5/5/5
2	HFG	D	901	-	-	0/8/19/19	0/3/3/3
3	1TI	B	902	-	-	0/17/49/49	0/5/5/5
3	1TI	D	902	-	-	0/17/49/49	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	1TI	C25-C23	-6.42	1.45	1.50
3	A	902	1TI	C26-C23	-4.94	1.46	1.50
3	D	902	1TI	C25-C23	-4.50	1.47	1.50
3	B	902	1TI	C25-C23	-4.49	1.47	1.50
3	B	902	1TI	C26-C23	-4.08	1.47	1.50
3	C	902	1TI	C25-C23	-3.98	1.47	1.50
3	C	902	1TI	C26-C23	-3.55	1.47	1.50
3	D	902	1TI	C26-C23	-3.30	1.48	1.50
2	D	901	HFG	C1'-C21	2.24	1.54	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	HFG	C6'-N1'-C2'	-8.17	106.52	111.62
2	C	901	HFG	C6'-N1'-C2'	-5.03	108.48	111.62
2	B	901	HFG	C6'-N1'-C2'	2.81	113.37	111.62
2	A	901	HFG	C6'-N1'-C2'	-2.36	110.15	111.62
3	B	902	1TI	C15-N2-N3	-2.23	103.18	104.41
3	D	902	1TI	C19-C20-C22	2.19	104.98	102.09
3	B	902	1TI	C17-N3-N2	2.06	113.26	112.08
3	D	902	1TI	C26-C23-C20	-2.04	114.46	118.55
3	C	902	1TI	C12-C14-C17	-2.01	122.70	127.14

There are no chirality outliers.

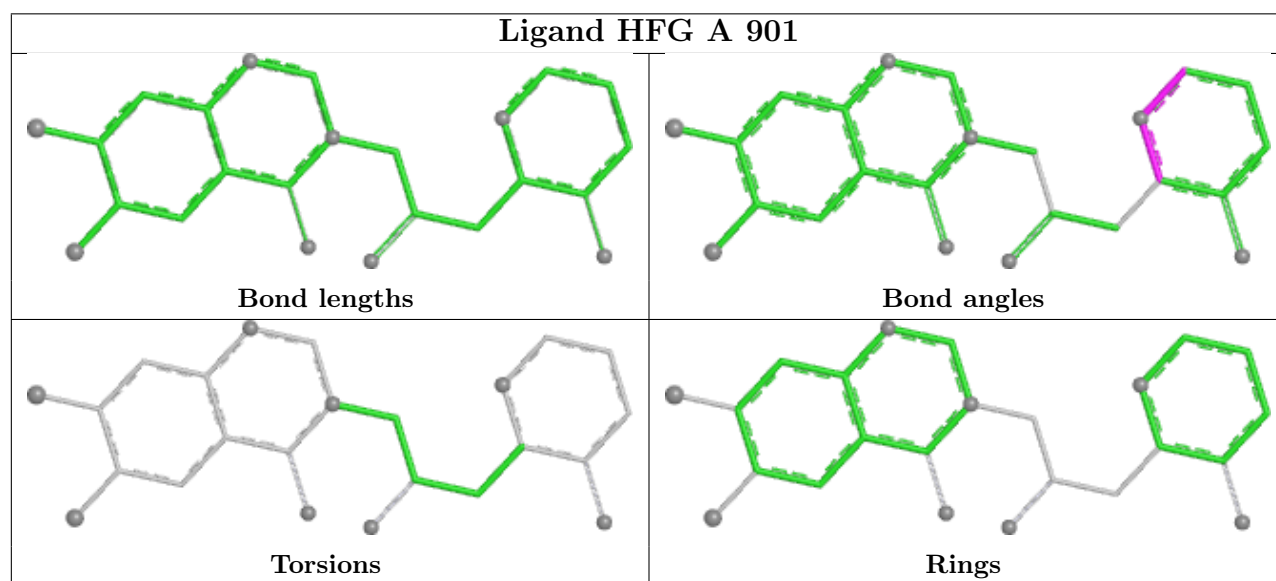
There are no torsion outliers.

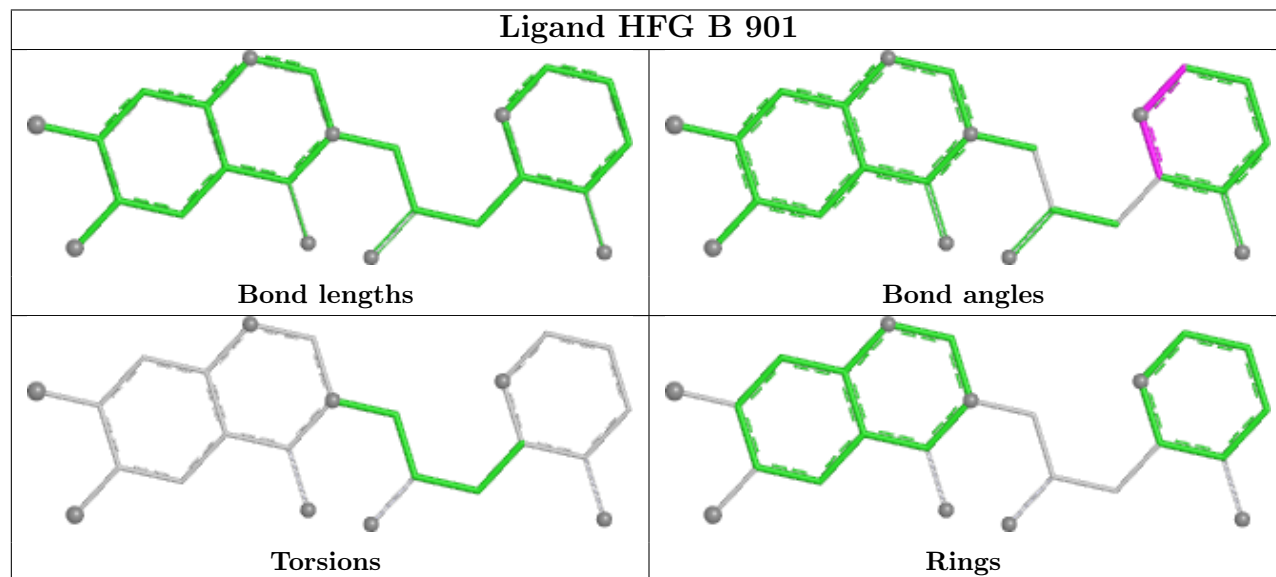
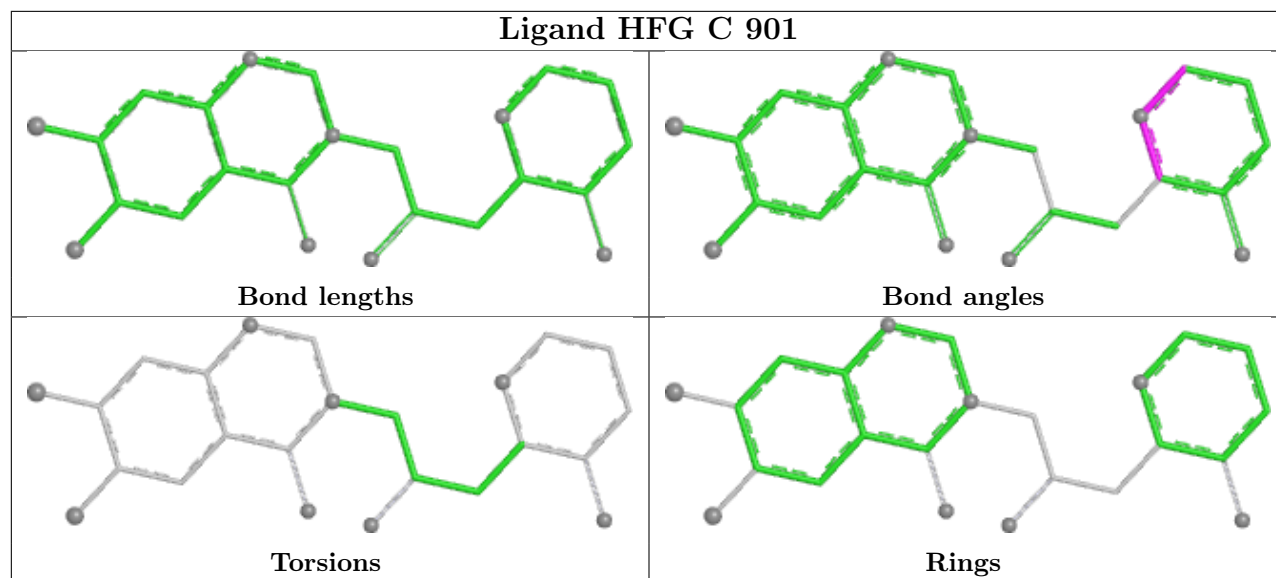
There are no ring outliers.

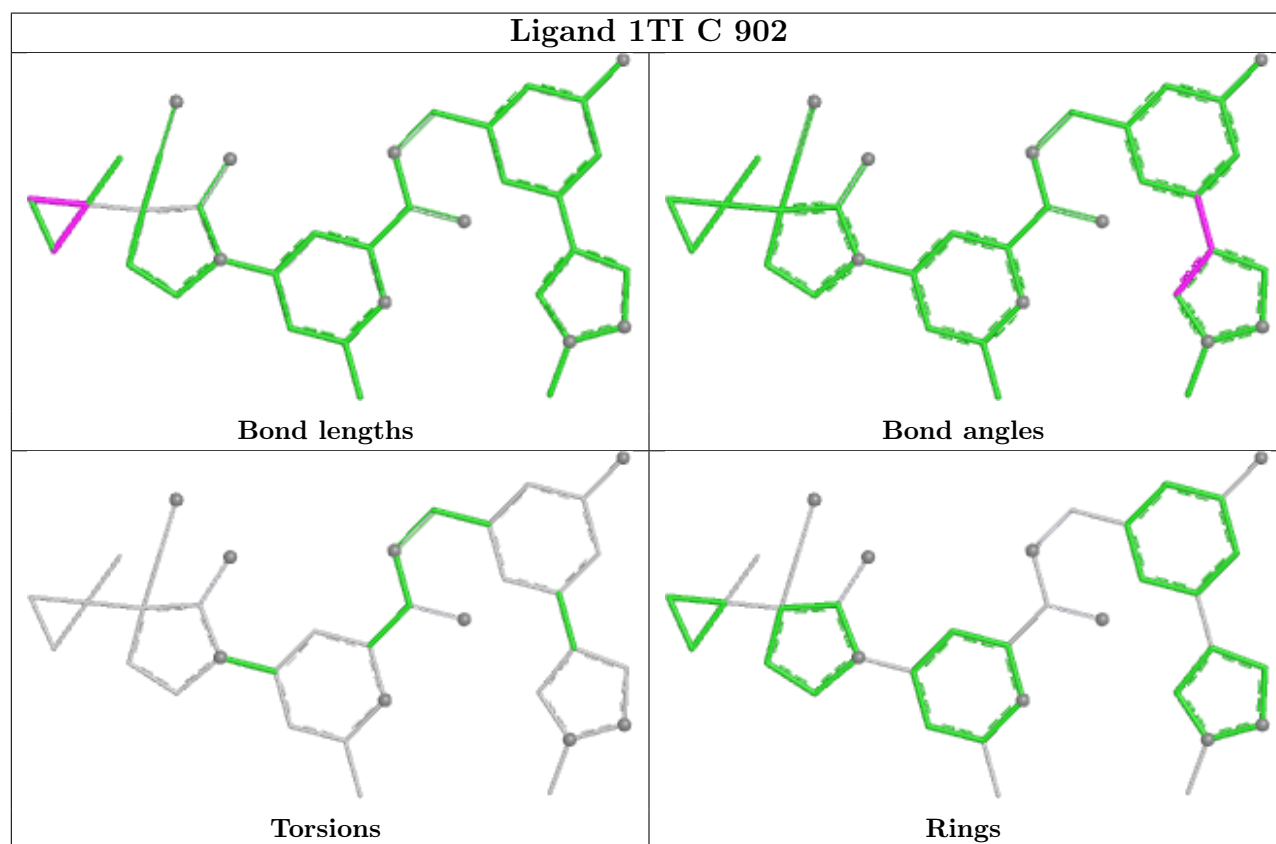
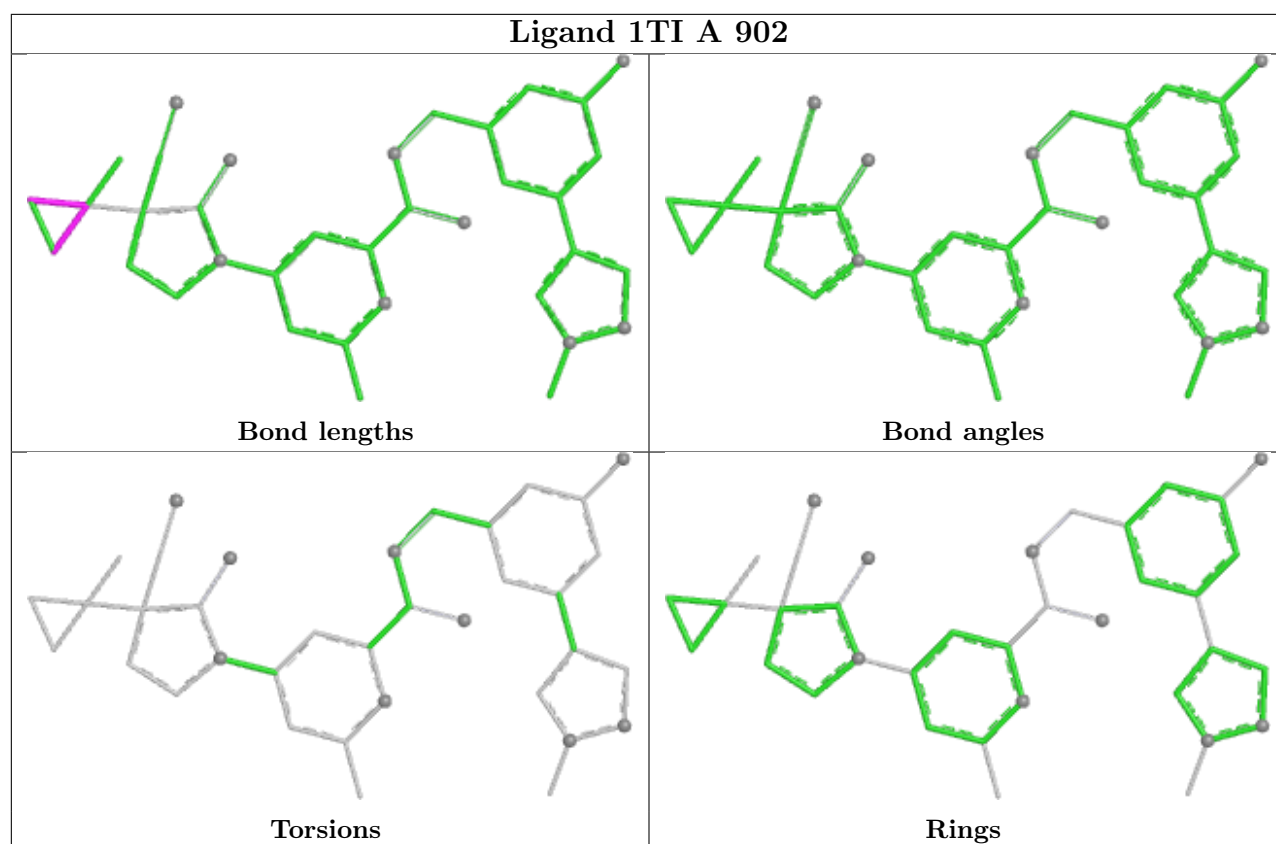
6 monomers are involved in 10 short contacts:

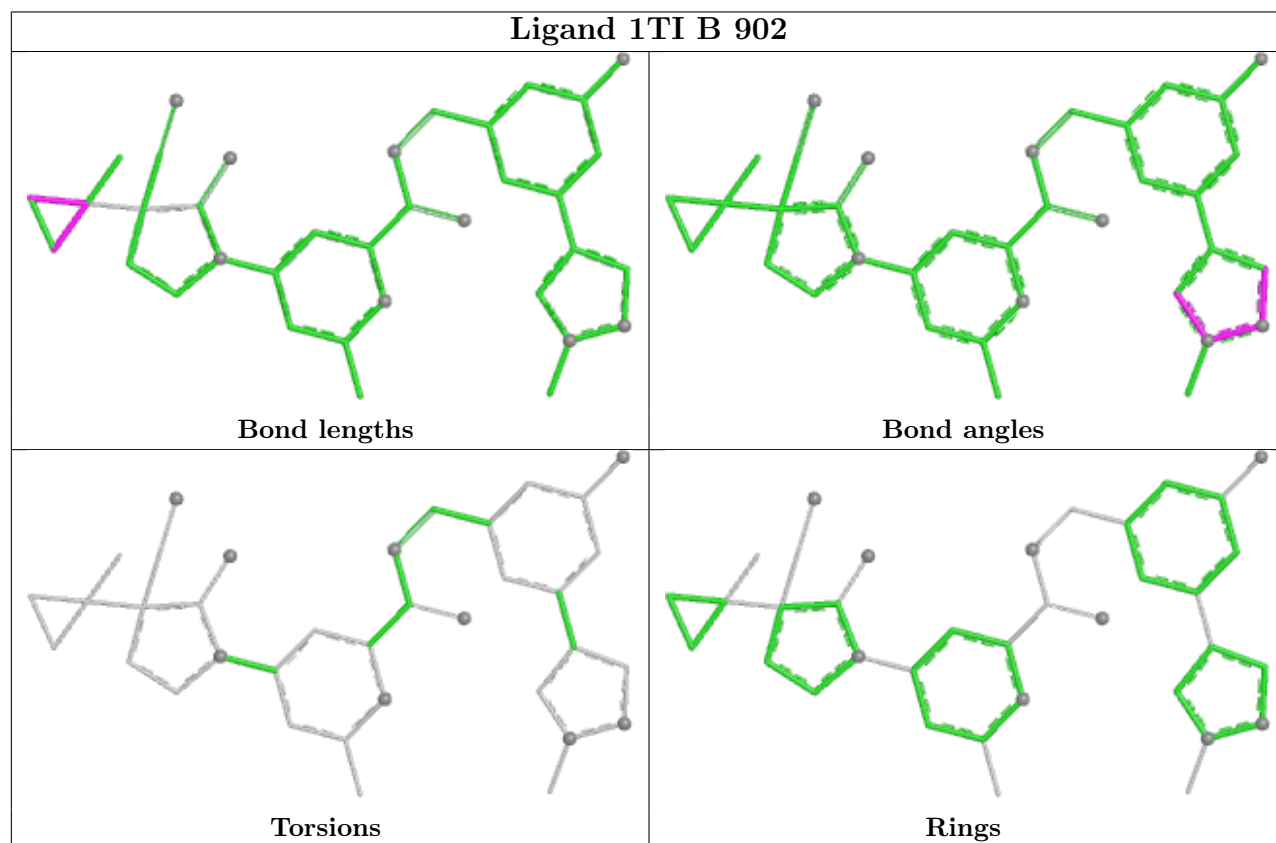
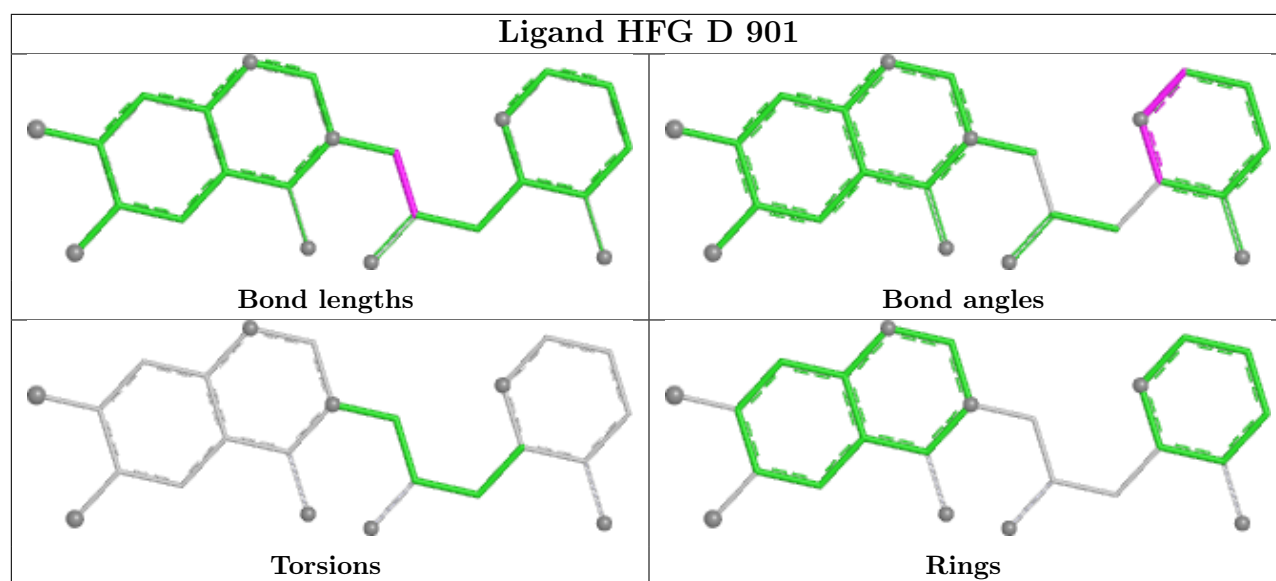
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	HFG	1	0
2	C	901	HFG	1	0
2	B	901	HFG	4	0
3	A	902	1TI	1	0
3	C	902	1TI	2	0
2	D	901	HFG	1	0

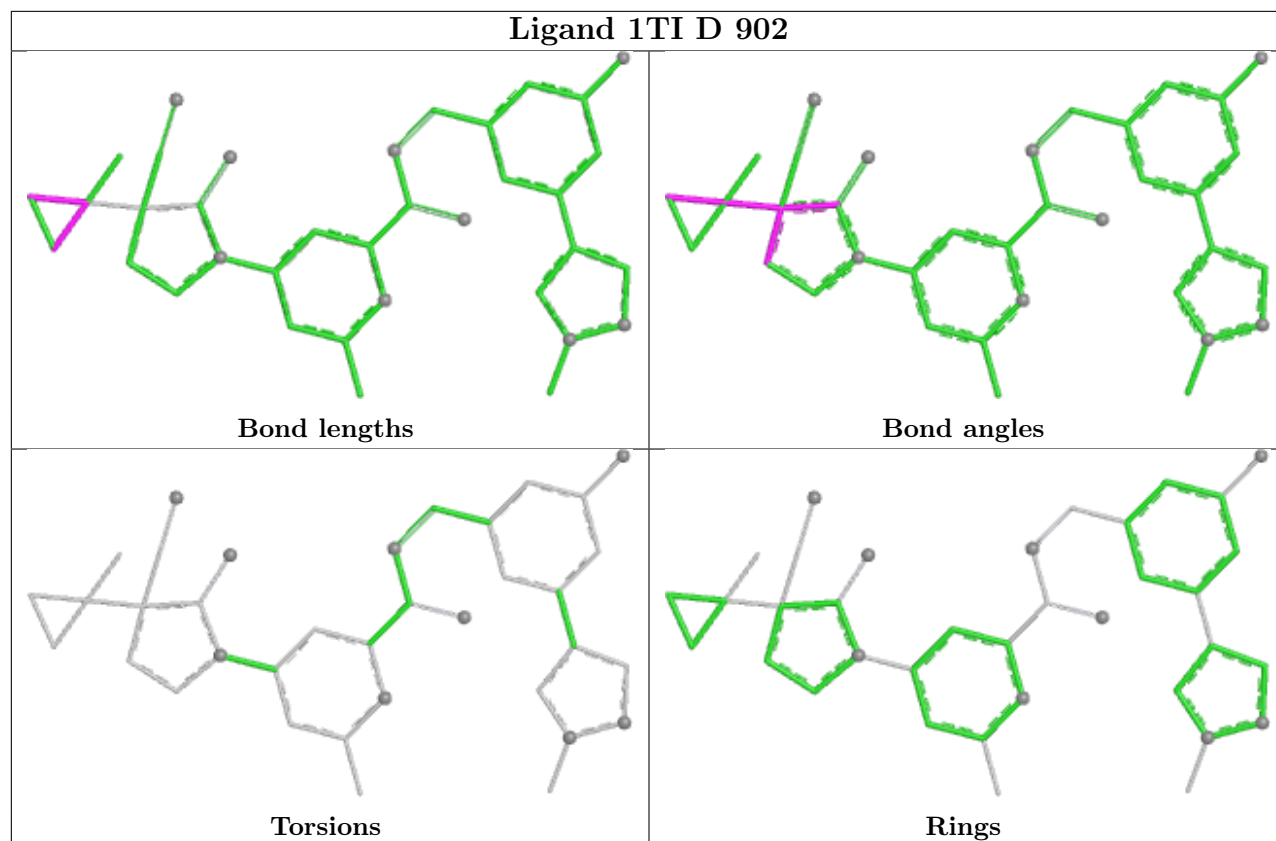
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	479/500 (95%)	-1.77	0 100 100	14, 28, 54, 79	0
1	B	483/500 (96%)	-1.75	0 100 100	15, 28, 57, 89	0
1	C	489/500 (97%)	-1.75	0 100 100	18, 32, 61, 84	0
1	D	480/500 (96%)	-1.71	0 100 100	20, 33, 64, 79	0
All	All	1931/2000 (96%)	-1.74	0 100 100	14, 30, 59, 89	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HFG	A	901	24/24	0.99	0.03	19,21,39,69	24
2	HFG	C	901	24/24	0.99	0.05	20,24,40,64	24
5	CA	A	905	1/1	0.99	0.05	69,69,69,69	0
6	CL	A	906	1/1	0.99	0.03	50,50,50,50	0

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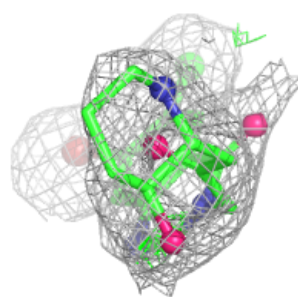
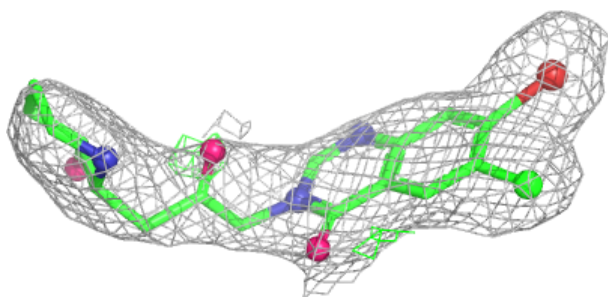
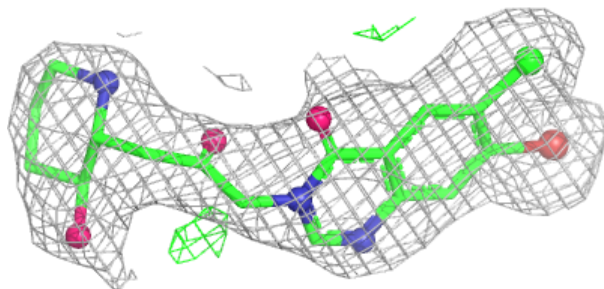
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CL	A	907	1/1	0.99	0.03	45,45,45,45	0
6	CL	B	905	1/1	0.99	0.04	55,55,55,55	0
6	CL	B	907	1/1	0.99	0.04	58,58,58,58	0
6	CL	C	904	1/1	0.99	0.03	44,44,44,44	0
4	BR	A	903	1/1	1.00	0.07	20,20,20,20	1
4	BR	B	903	1/1	1.00	0.04	81,81,81,81	1
4	BR	D	903	1/1	1.00	0.06	84,84,84,84	0
5	CA	A	904	1/1	1.00	0.03	44,44,44,44	0
2	HFG	B	901	24/24	1.00	0.03	18,26,99,215	0
5	CA	B	904	1/1	1.00	0.02	36,36,36,36	0
2	HFG	D	901	24/24	1.00	0.03	21,27,112,191	0
3	1TI	A	902	36/36	1.00	0.02	17,19,28,40	0
6	CL	A	908	1/1	1.00	0.02	55,55,55,55	0
3	1TI	B	902	36/36	1.00	0.02	16,23,35,36	0
6	CL	B	906	1/1	1.00	0.02	22,22,22,22	1
3	1TI	C	902	36/36	1.00	0.03	20,24,34,35	36
6	CL	C	903	1/1	1.00	0.01	36,36,36,36	0
3	1TI	D	902	36/36	1.00	0.02	22,31,47,49	0

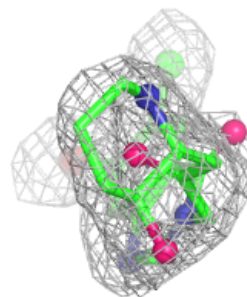
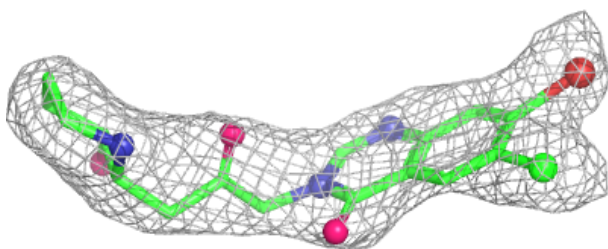
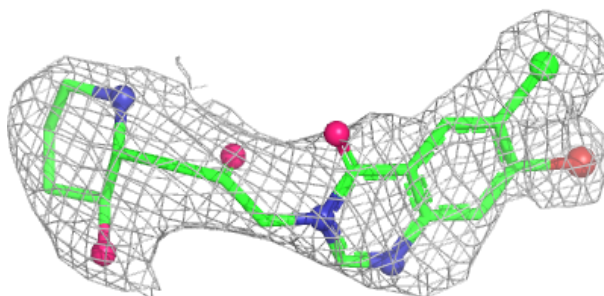
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HFG A 901:

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

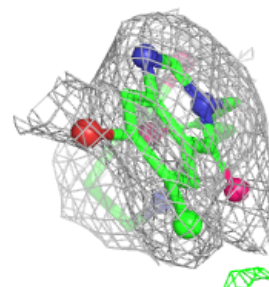
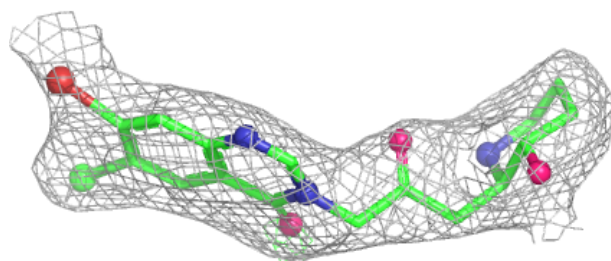
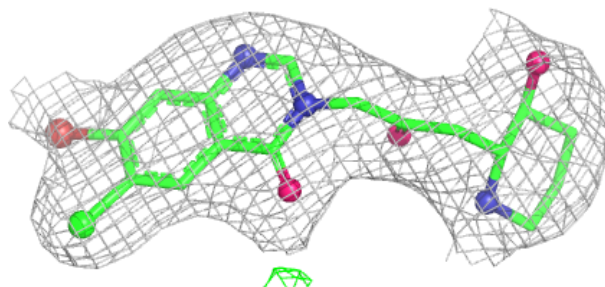
**Electron density around HFG C 901:**

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

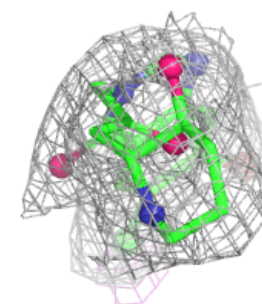
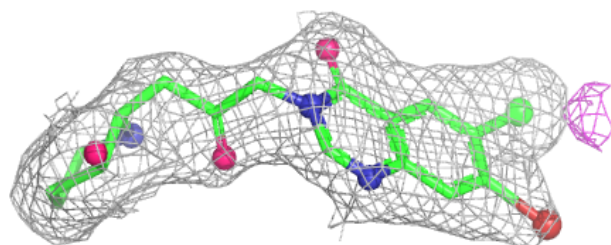
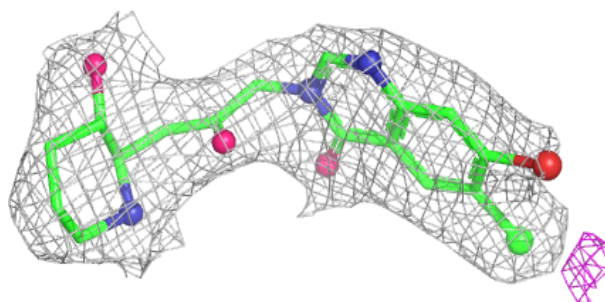


Electron density around HFG B 901:

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

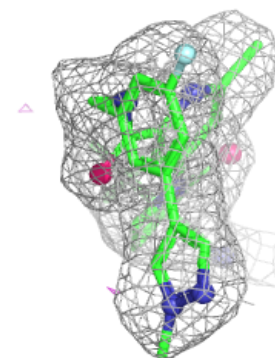
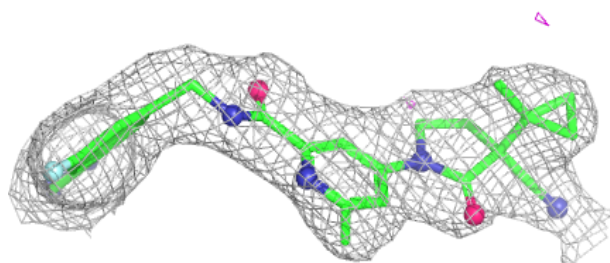
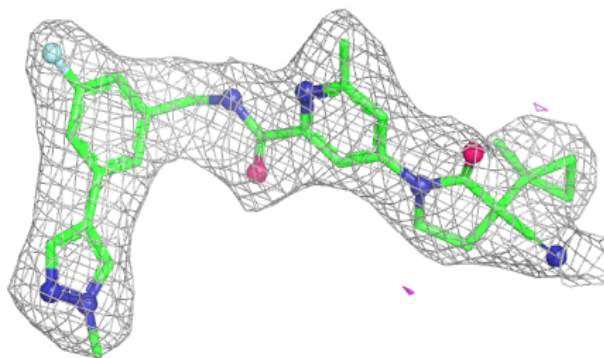
**Electron density around HFG D 901:**

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and green (positive)

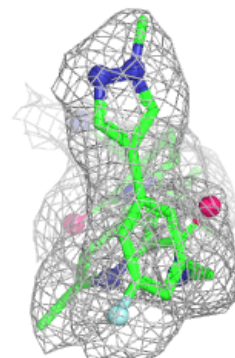
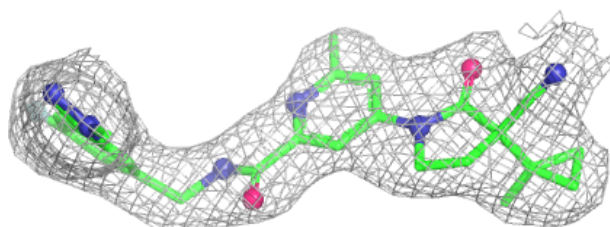
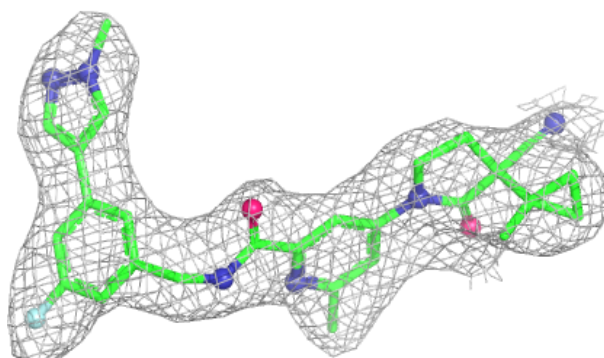


Electron density around 1TI A 902:

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

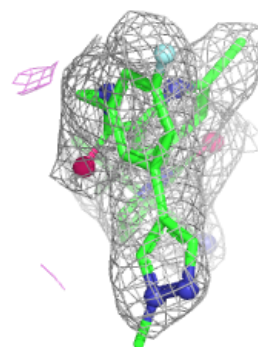
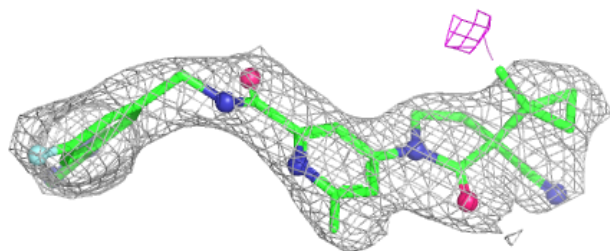
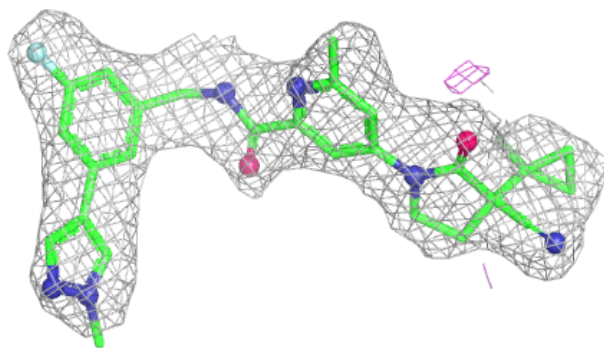
**Electron density around 1TI B 902:**

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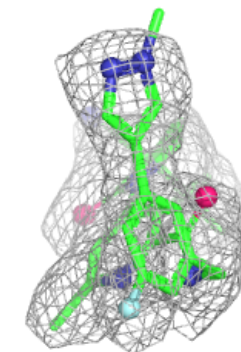
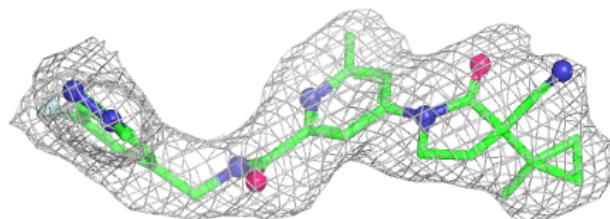
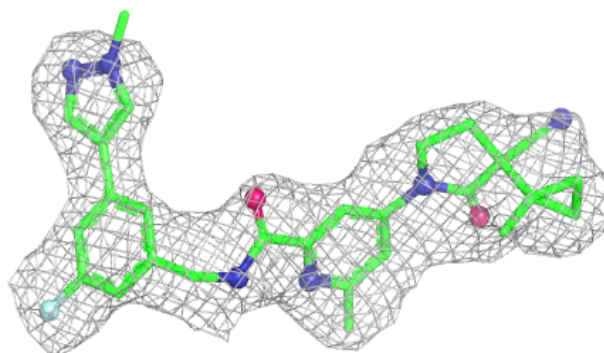


Electron density around 1TI C 902:

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

**Electron density around 1TI D 902:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.