



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2022 – 06:36 PM JST

PDB ID : 7F9U  
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.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

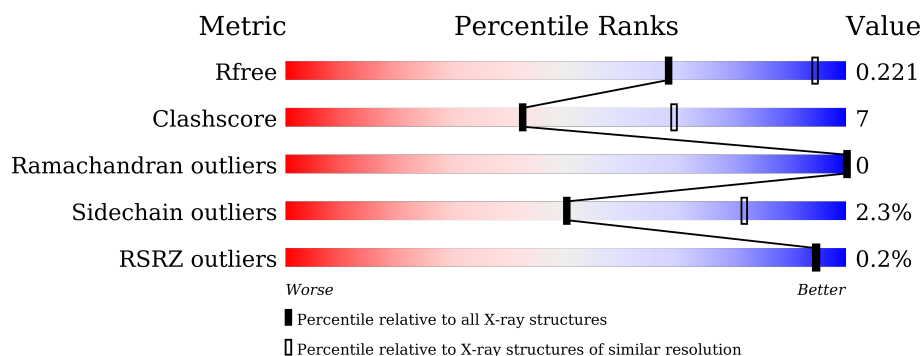
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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  $\geq 3$ , 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	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.

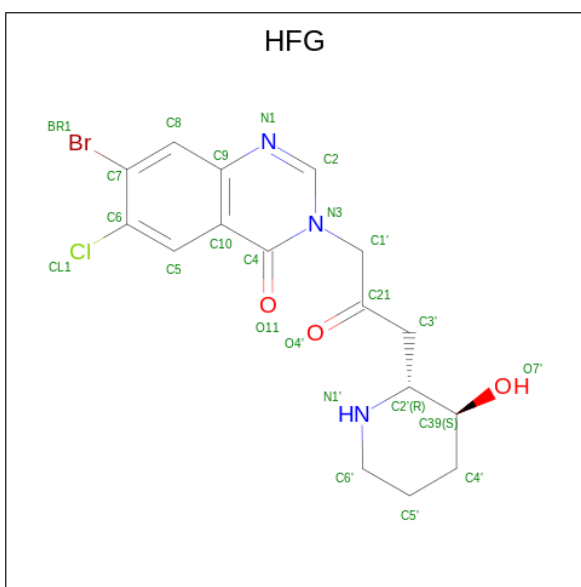
- Molecule 1 is a protein called Prolyl-tRNA synthetase (ProRS).

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:

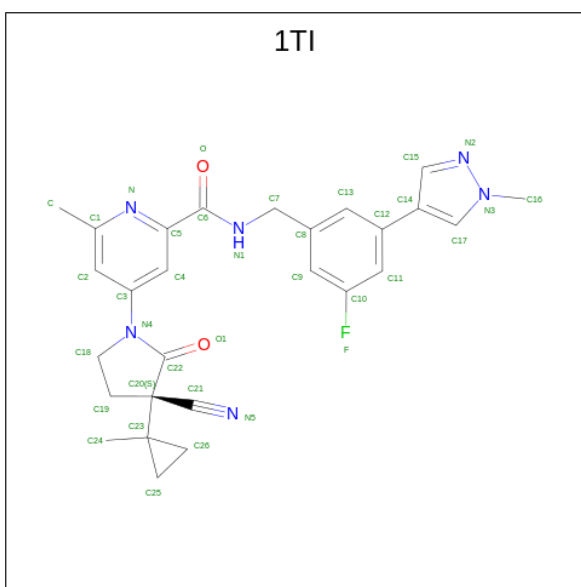
Chain	Residue	Modelled	Actual	Comment	Reference
A	331	GLY	-	expression tag	UNP A0A7J6JUK2
A	332	ALA	-	expression tag	UNP A0A7J6JUK2
A	333	MET	-	expression tag	UNP A0A7J6JUK2
B	331	GLY	-	expression tag	UNP A0A7J6JUK2
B	332	ALA	-	expression tag	UNP A0A7J6JUK2
B	333	MET	-	expression tag	UNP A0A7J6JUK2
C	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 (three-letter code: HFG) (formula: C<sub>16</sub>H<sub>17</sub>BrClN<sub>3</sub>O<sub>3</sub>).



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 (three-letter code: 1TI) (formula: C<sub>27</sub>H<sub>27</sub>FN<sub>6</sub>O<sub>2</sub>) (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 (three-letter code: 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 (three-letter code: 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 (three-letter code: CL) (formula: Cl).

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

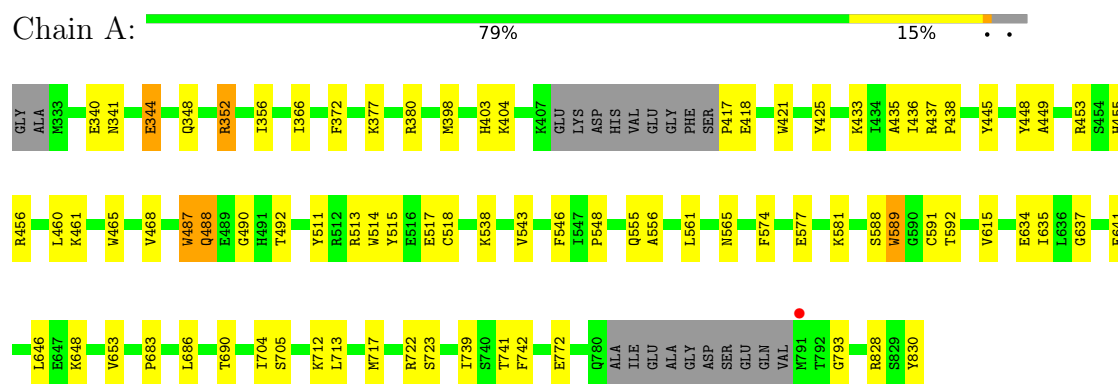
- Molecule 7 is water.

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

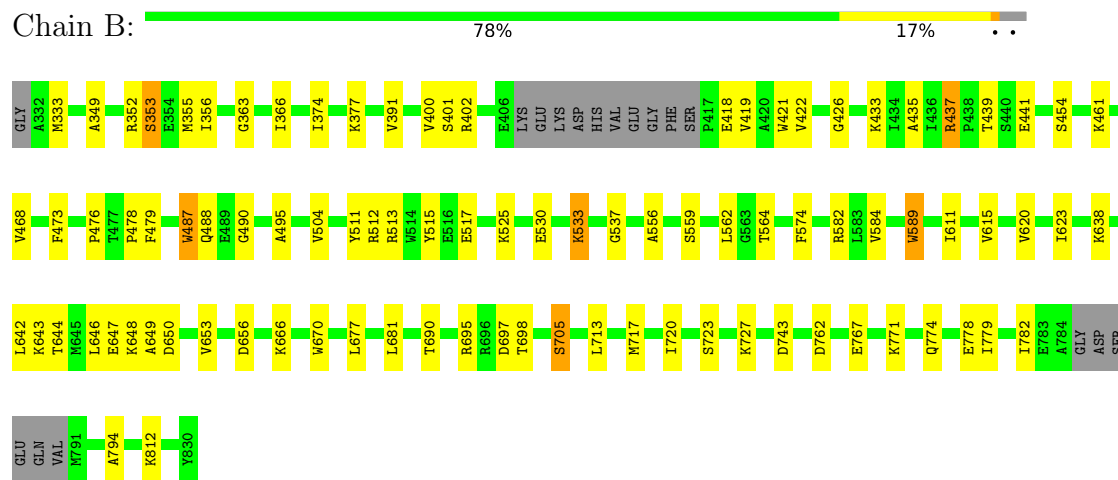
### 3 Residue-property plots [i](#)

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.

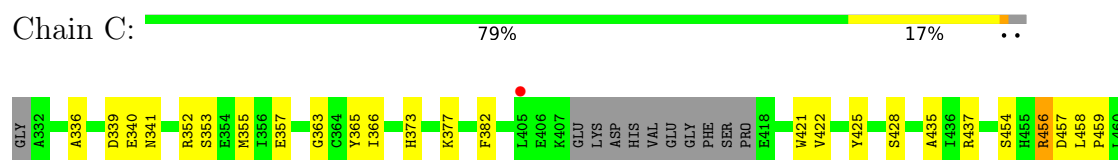
#### • Molecule 1: Prolyl-tRNA synthetase (ProRS)



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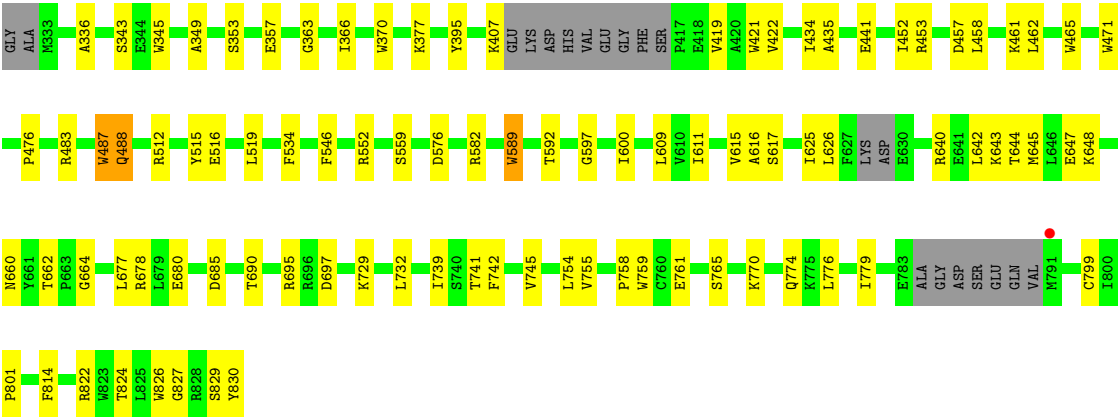
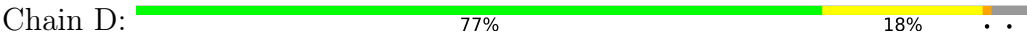


#### • Molecule 1: Prolyl-tRNA synthetase (ProRS)





• Molecule 1: Prolyl-tRNA synthetase (ProRS)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 9.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	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	0.94	EDS
Total number of atoms	15950	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.68	0/4000	0.66	0/5411
1	B	0.67	0/4026	0.68	0/5450
1	C	0.69	2/4047 (0.0%)	0.69	1/5479 (0.0%)
1	D	0.52	0/3988	0.62	0/5395
All	All	0.65	2/16061 (0.0%)	0.66	1/21735 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	761	GLU	CG-CD	-5.81	1.43	1.51
1	C	761	GLU	CD-OE1	-5.11	1.20	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	483	ARG	NE-CZ-NH2	-5.47	117.56	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3895	0	3851	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3922	0	3861	54	0
1	C	3944	0	3883	62	0
1	D	3885	0	3825	57	0
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	217	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 (217) 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:C:355:MET:HE1	1:C:600:ILE:HD11	1.75	0.68
1:B:402:ARG:HD2	1:B:433:LYS:HE2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:512:ARG:NH1	1:D:516:GLU:OE1	2.26	0.68
1:C:759:TRP:HE3	1:C:824:THR:HG1	1.43	0.67
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
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:764:GLU:HA	1:C:764:GLU:OE2	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:778:GLU:O	1:C:782:ILE:HG13	2.19	0.43
1:C:812:LYS:HB3	1:C:812:LYS:HE2	1.59	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: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:457:ASP:O	1:C:458:LEU:HD23	2.20	0.42
1:B:422:VAL:HG22	1:C:422:VAL:HG22	2.02	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:813:CYS:SG	1:C:816:THR:OG1	2.78	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: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:B:504:VAL:HG13	1:B:559:SER:OG	2.21	0.40
1:C:355:MET:HE3	1:C:355:MET:HB3	1.82	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	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 [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	413/436 (95%)	402 (97%)	11 (3%)	44	78
1	B	415/436 (95%)	403 (97%)	12 (3%)	42	76
1	C	416/436 (95%)	407 (98%)	9 (2%)	52	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	409/436 (94%)	403 (98%)	6 (2%)	65 89
All	All	1653/1744 (95%)	1615 (98%)	38 (2%)	50 82

All (38) 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	398	MET
1	A	436	ILE
1	A	487	TRP
1	A	488	GLN
1	A	589	TRP
1	A	722	ARG
1	A	723	SER
1	A	830	TYR
1	B	353	SER
1	B	401	SER
1	B	419	VAL
1	B	437	ARG
1	B	454	SER
1	B	473	PHE
1	B	487	TRP
1	B	533	LYS
1	B	589	TRP
1	B	705	SER
1	B	743	ASP
1	B	812	LYS
1	C	425	TYR
1	C	428	SER
1	C	456	ARG
1	C	487	TRP
1	C	488	GLN
1	C	589	TRP
1	C	627	PHE
1	C	764	GLU
1	C	767	GLU
1	D	343	SER
1	D	487	TRP
1	D	488	GLN
1	D	589	TRP

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Mol	Chain	Res	Type
1	D	774	GLN
1	D	830	TYR

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

Mol	Chain	Res	Type
1	A	565	ASN
1	C	750	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
3	1TI	D	902	-	35,40,40	0.99	2 (5%)	52,61,61	0.86	4 (7%)
2	HFG	A	901	-	25,26,26	0.28	0	27,37,37	0.71	1 (3%)
3	1TI	A	902	-	35,40,40	1.40	2 (5%)	52,61,61	0.73	0
3	1TI	C	902	-	35,40,40	0.94	2 (5%)	52,61,61	1.05	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HFG	B	901	-	25,26,26	0.46	0	27,37,37	0.93	1 (3%)
3	1TI	B	902	-	35,40,40	1.12	3 (8%)	52,61,61	1.09	3 (5%)
2	HFG	D	901	-	25,26,26	0.36	0	27,37,37	1.73	1 (3%)
2	HFG	C	901	-	25,26,26	0.27	0	27,37,37	1.06	1 (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
3	1TI	D	902	-	-	0/17/49/49	0/5/5/5
2	HFG	A	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	B	901	-	-	0/8/19/19	0/3/3/3
3	1TI	B	902	-	-	0/17/49/49	0/5/5/5
2	HFG	D	901	-	-	0/8/19/19	0/3/3/3
2	HFG	C	901	-	-	0/8/19/19	0/3/3/3

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
3	B	902	1TI	C17-N3	-2.32	1.33	1.35

All (14) 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
3	B	902	1TI	C23-C20-C22	4.58	113.97	108.10
3	C	902	1TI	C15-C14-C12	3.88	132.82	127.74
3	C	902	1TI	C17-C14-C12	-3.85	122.70	127.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	1TI	C23-C20-C22	3.66	112.78	108.10
3	B	902	1TI	C15-C14-C12	3.22	131.97	127.74
3	D	902	1TI	C15-C14-C12	3.14	131.85	127.74
3	B	902	1TI	C17-C14-C12	-3.09	123.70	127.74
3	D	902	1TI	C17-C14-C12	-3.01	123.79	127.74
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	D	902	1TI	C19-C20-C22	2.19	104.98	102.09
3	D	902	1TI	C26-C23-C20	-2.04	114.46	118.55

There are no chirality outliers.

There are no torsion outliers.

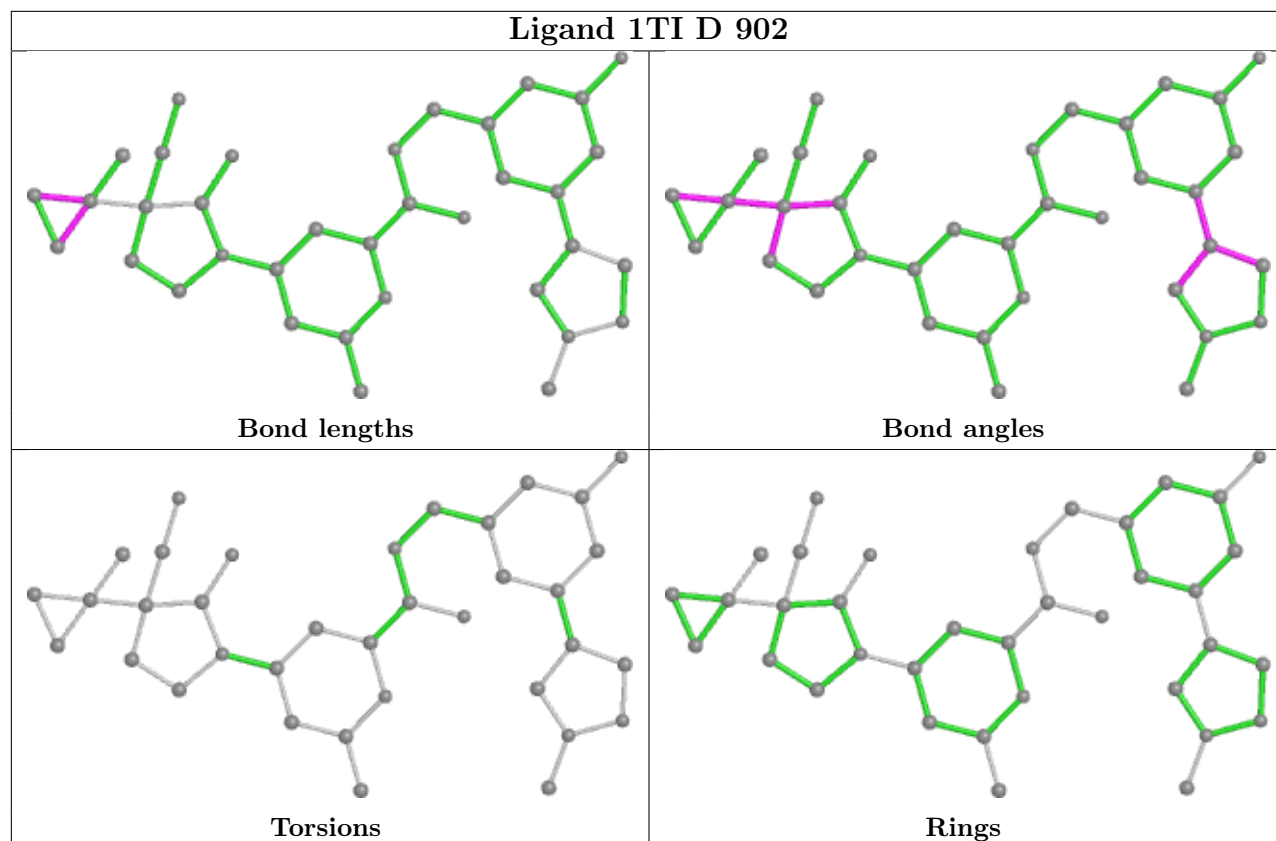
There are no ring outliers.

6 monomers are involved in 10 short contacts:

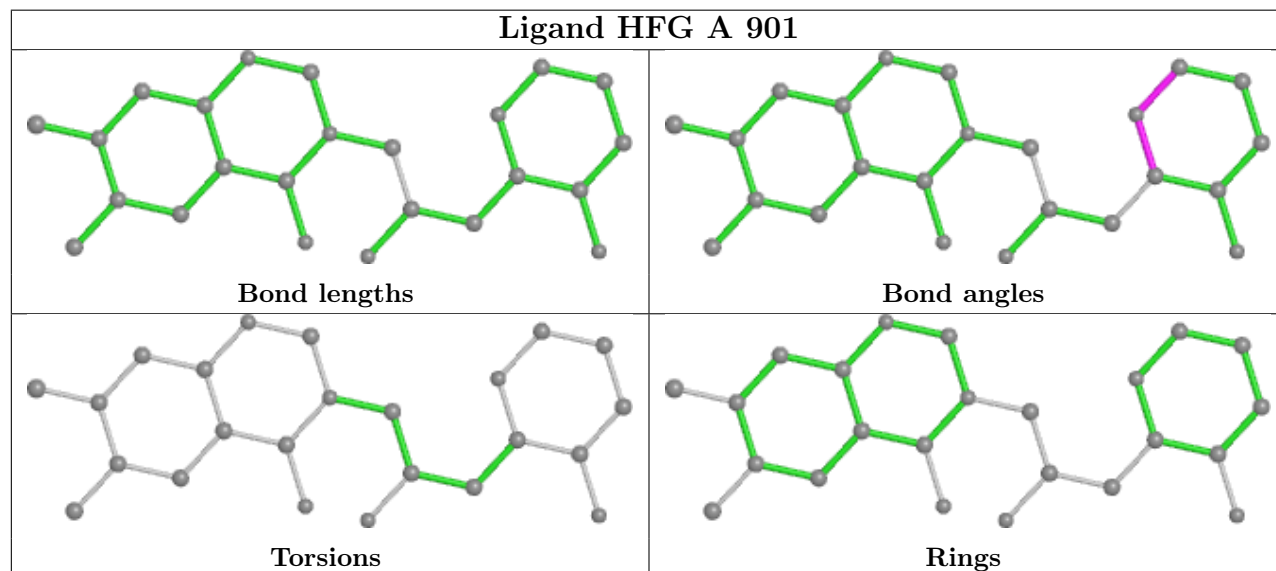
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	HFG	1	0
3	A	902	1TI	1	0
3	C	902	1TI	2	0
2	B	901	HFG	4	0
2	D	901	HFG	1	0
2	C	901	HFG	1	0

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.

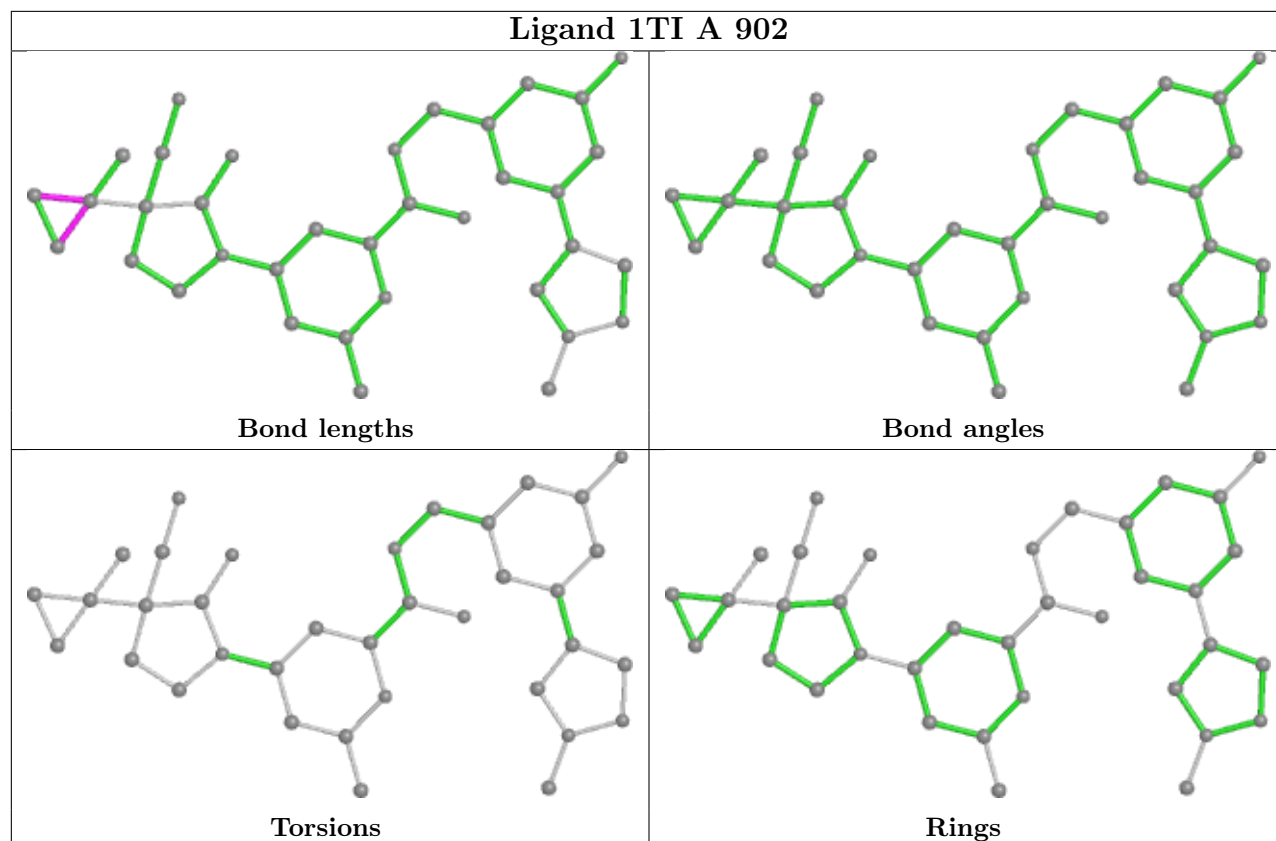
## Ligand 1TI D 902



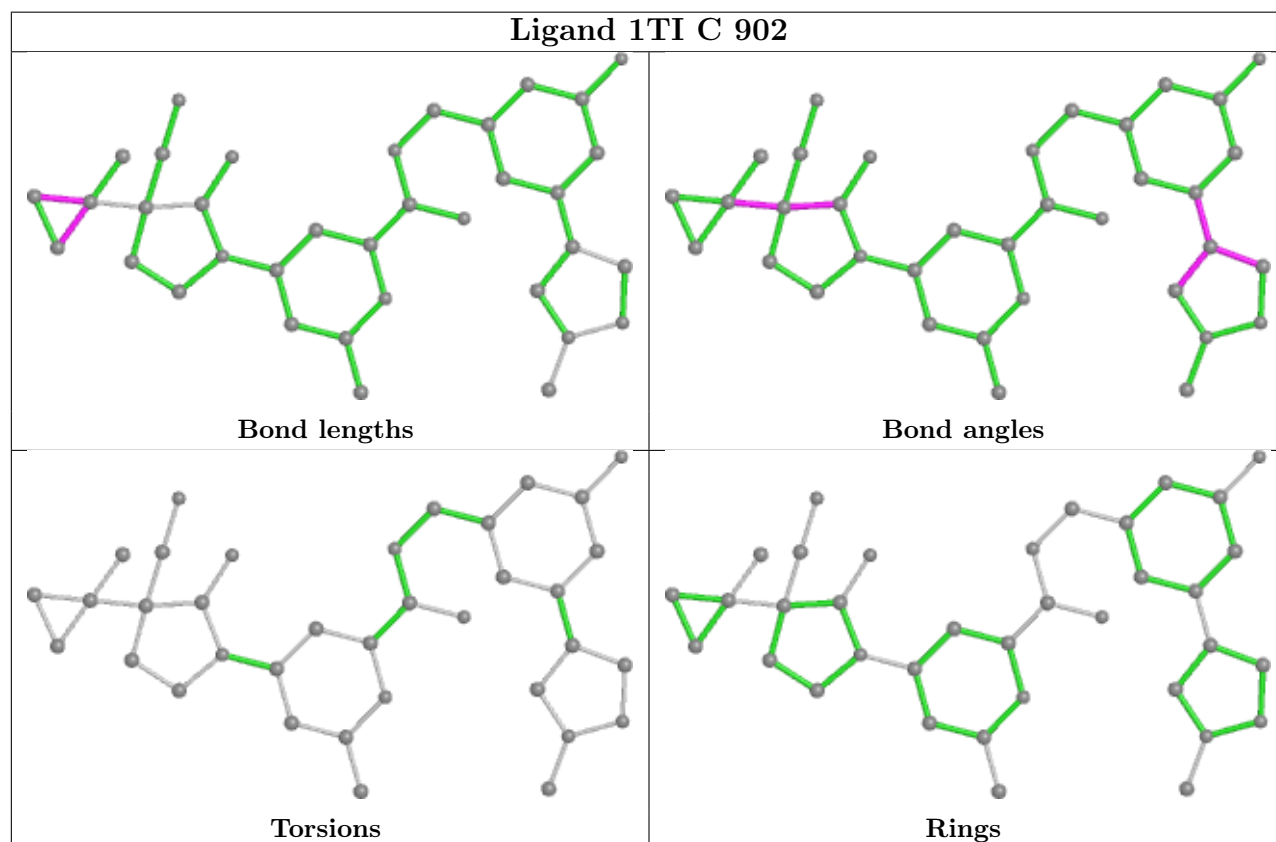
## Ligand HFG A 901

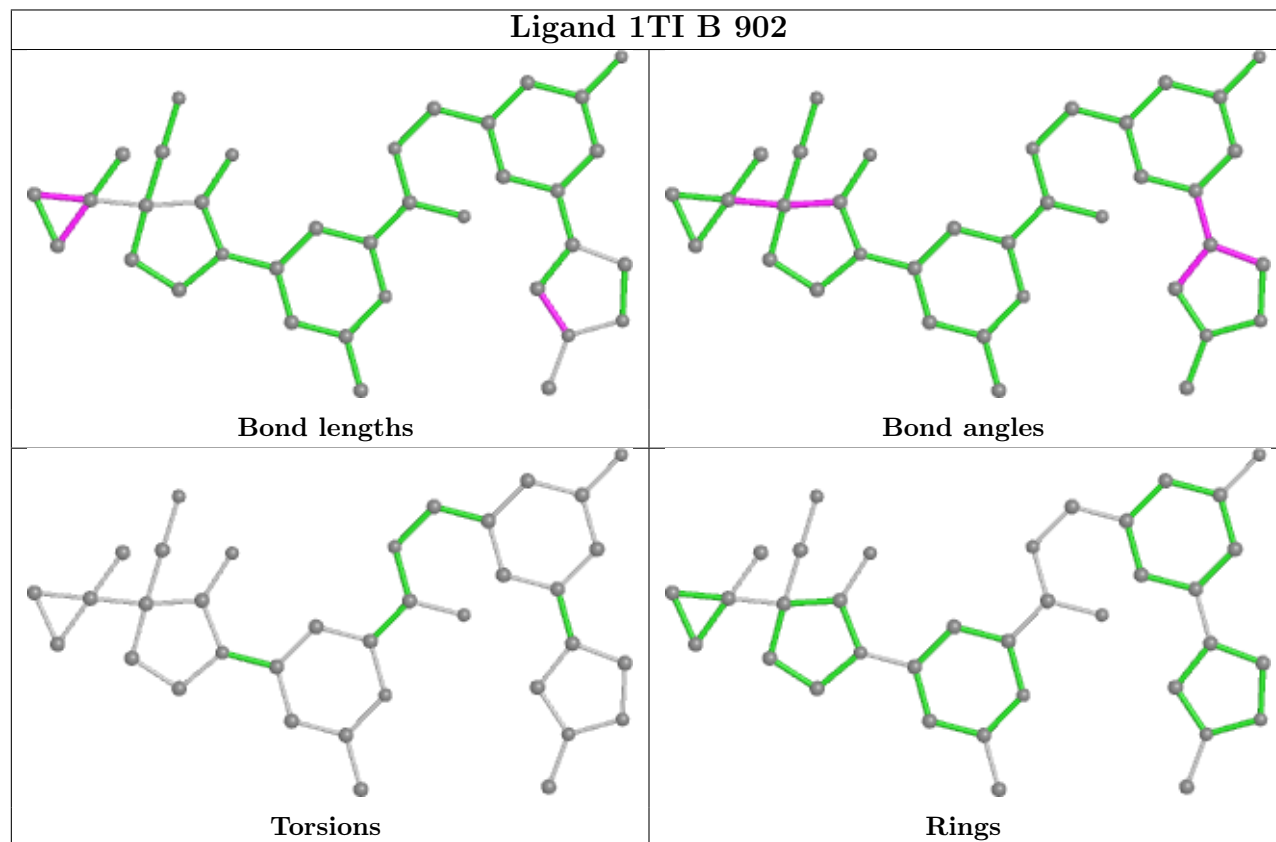
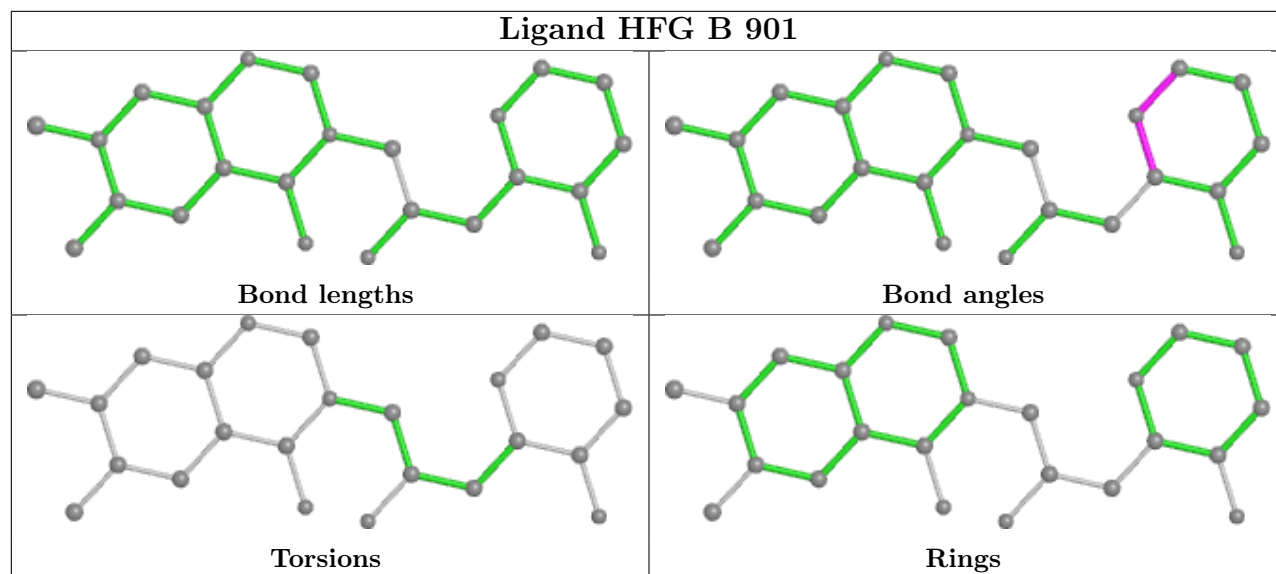


## Ligand 1TI A 902

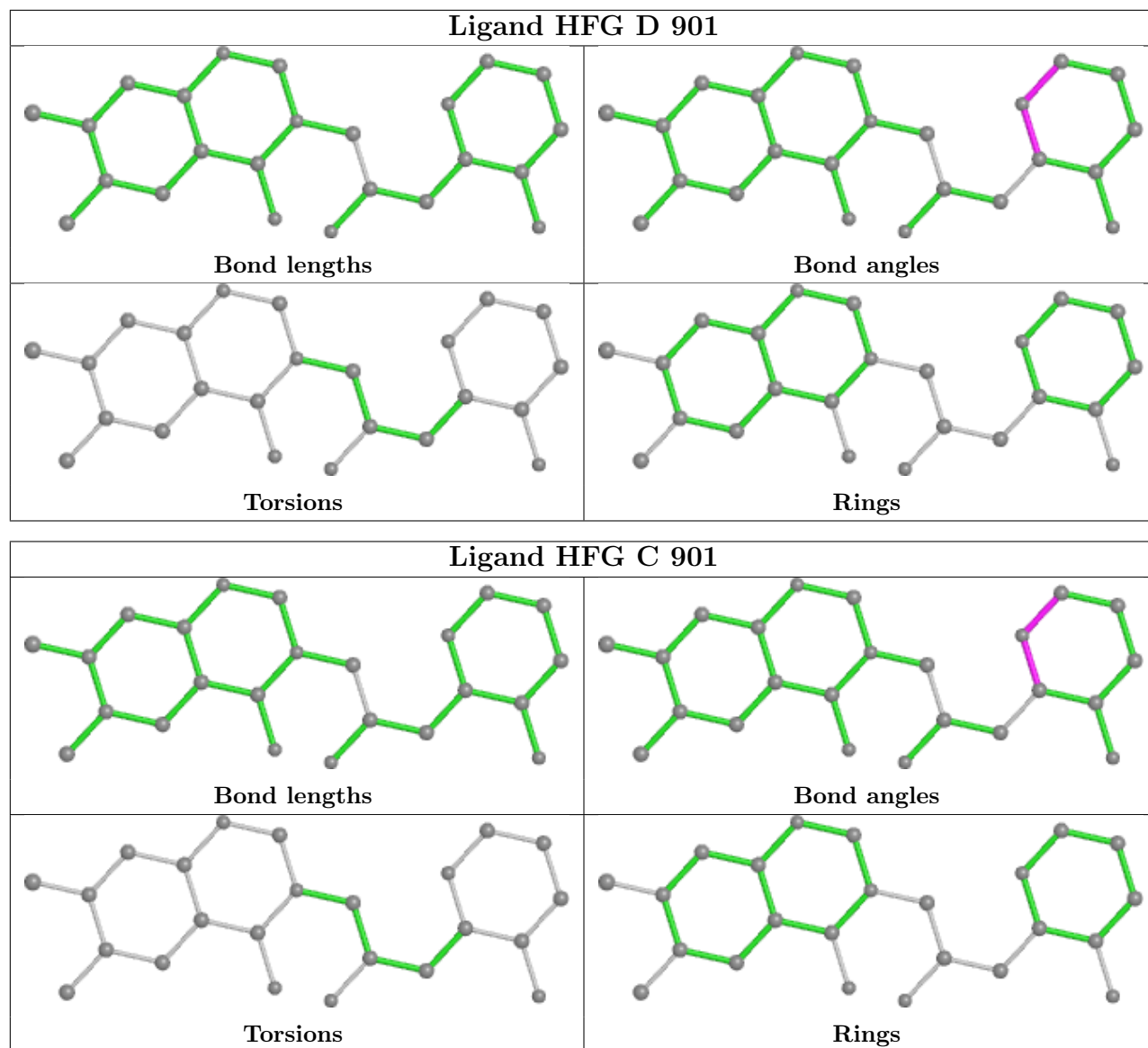


## Ligand 1TI C 902









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	479/500 (95%)	-0.63	1 (0%) 95 94	14, 28, 54, 79	0
1	B	483/500 (96%)	-0.59	0 100 100	15, 28, 57, 89	0
1	C	489/500 (97%)	-0.57	1 (0%) 95 94	18, 32, 61, 84	0
1	D	480/500 (96%)	-0.57	1 (0%) 95 94	20, 33, 64, 79	0
All	All	1931/2000 (96%)	-0.59	3 (0%) 95 94	14, 30, 59, 89	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	791	MET	2.4
1	D	791	MET	2.3
1	C	405	LEU	2.1

### 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](#)

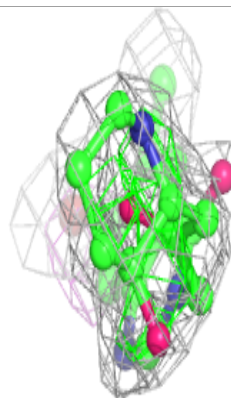
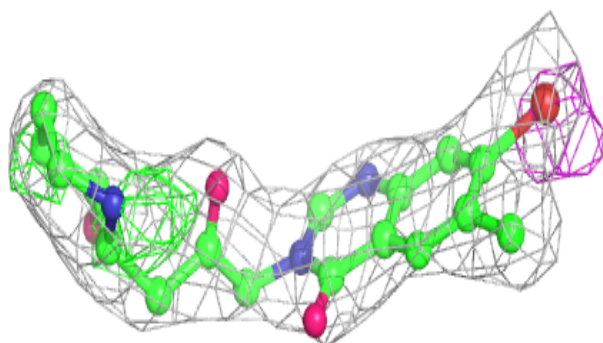
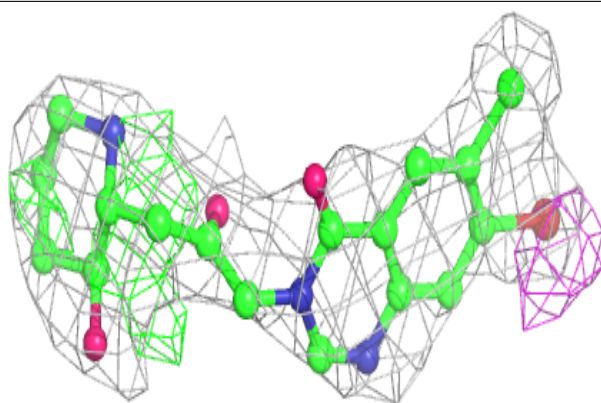
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	HFG	C	901	24/24	0.87	0.25	20,24,40,64	24
5	CA	A	905	1/1	0.91	0.12	69,69,69,69	0
4	BR	A	903	1/1	0.92	0.16	20,20,20,20	1
2	HFG	A	901	24/24	0.92	0.21	19,21,39,69	24
6	CL	A	908	1/1	0.93	0.08	55,55,55,55	0
6	CL	A	907	1/1	0.94	0.07	45,45,45,45	0
2	HFG	B	901	24/24	0.94	0.19	18,26,99,215	0
6	CL	B	907	1/1	0.94	0.09	58,58,58,58	0
6	CL	A	906	1/1	0.96	0.08	50,50,50,50	0
6	CL	B	905	1/1	0.96	0.07	55,55,55,55	0
2	HFG	D	901	24/24	0.96	0.18	21,27,112,191	0
3	1TI	D	902	36/36	0.97	0.17	22,31,47,49	0
3	1TI	C	902	36/36	0.97	0.19	20,24,34,35	36
6	CL	B	906	1/1	0.97	0.20	22,22,22,22	1
4	BR	D	903	1/1	0.97	0.09	84,84,84,84	0
3	1TI	B	902	36/36	0.98	0.17	16,23,35,36	0
5	CA	A	904	1/1	0.98	0.12	44,44,44,44	0
3	1TI	A	902	36/36	0.98	0.18	17,19,28,40	0
6	CL	C	904	1/1	0.98	0.08	44,44,44,44	0
5	CA	B	904	1/1	0.99	0.12	36,36,36,36	0
6	CL	C	903	1/1	0.99	0.09	36,36,36,36	0
4	BR	B	903	1/1	0.99	0.09	81,81,81,81	1

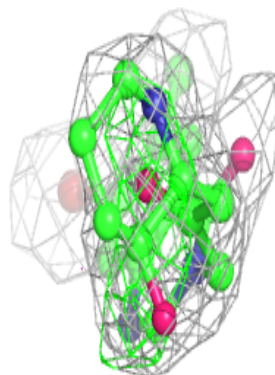
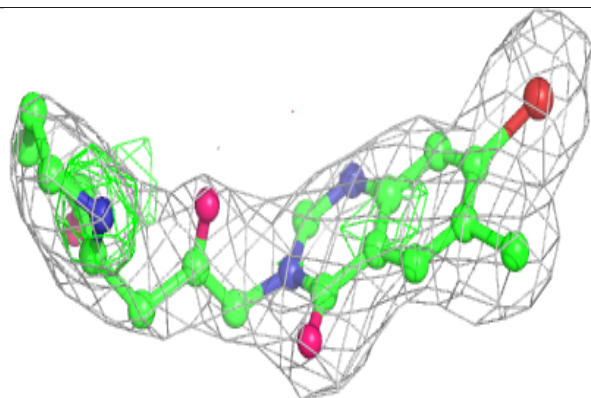
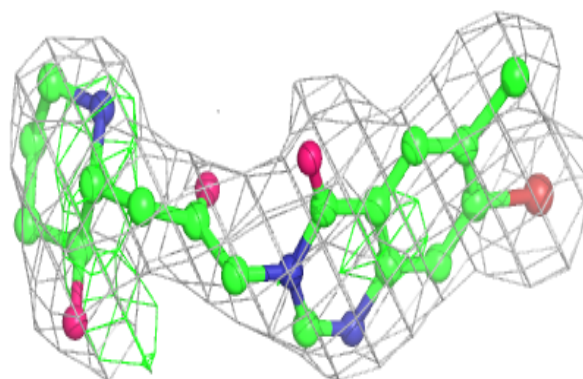
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HFG 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)

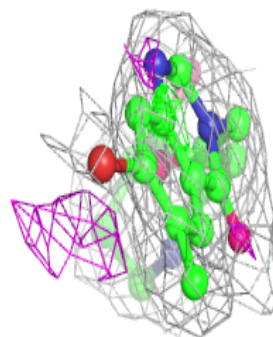
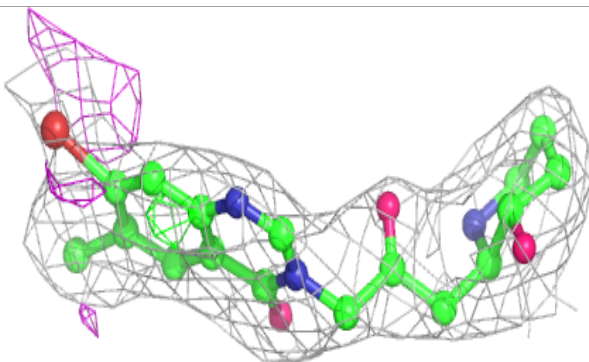
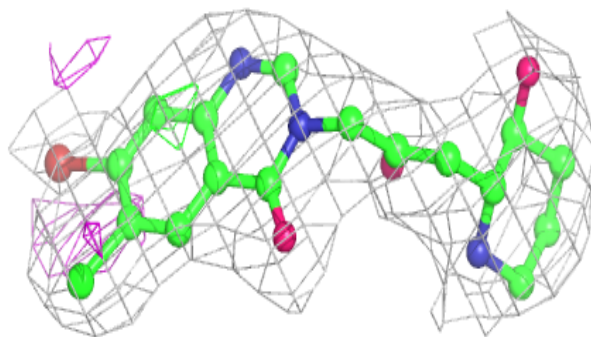
**Electron density around HFG A 901:**

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

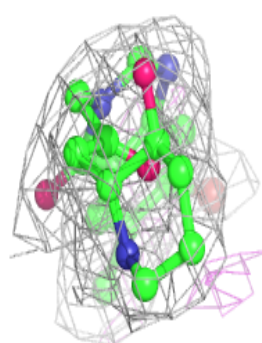
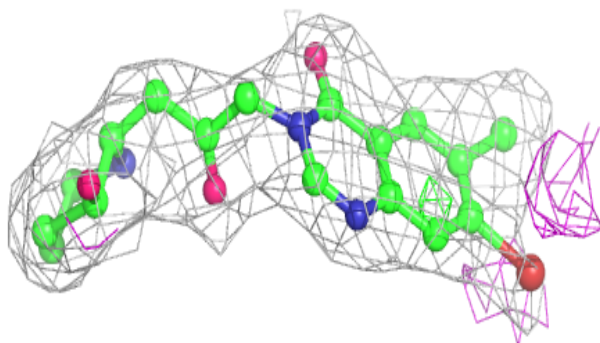
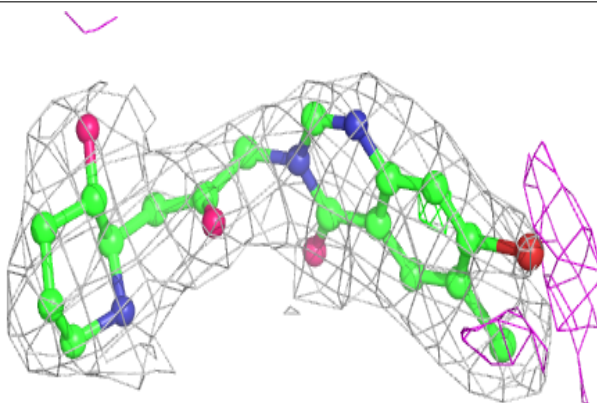


**Electron density around HFG B 901:**

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

**Electron density around HFG D 901:**

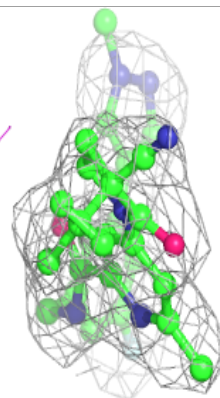
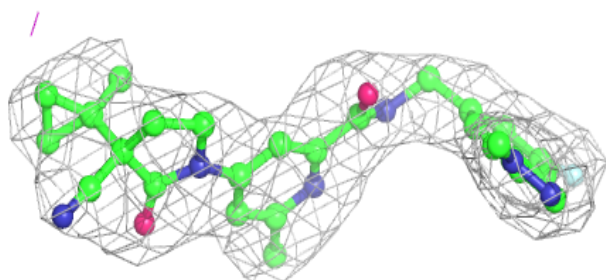
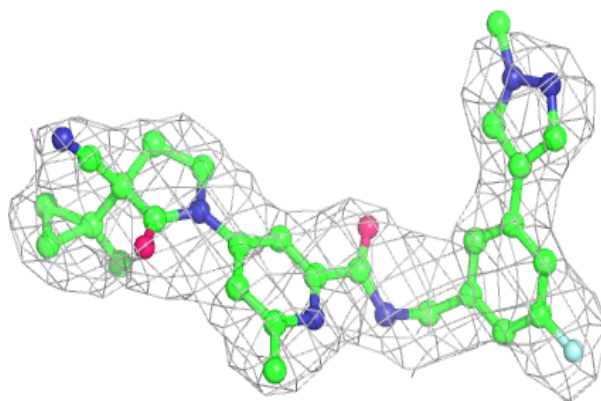
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



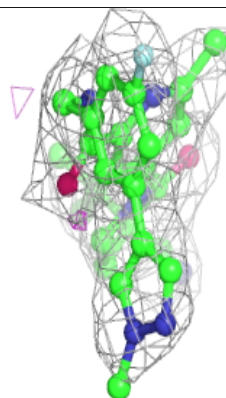
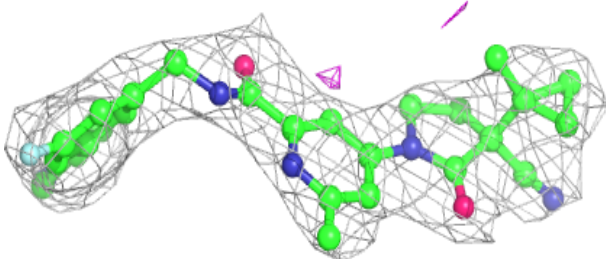
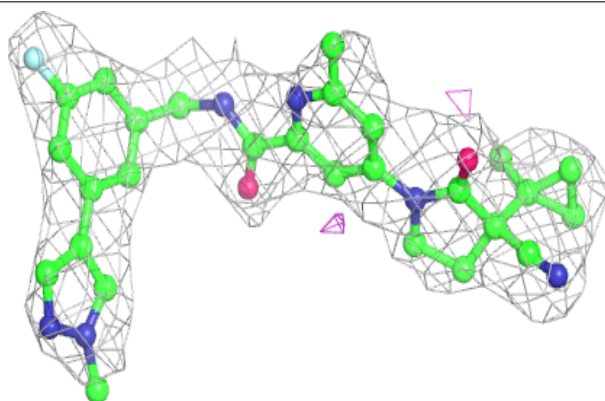


**Electron density around 1TI D 902:**

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

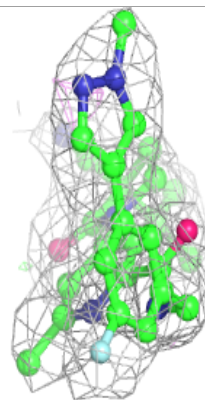
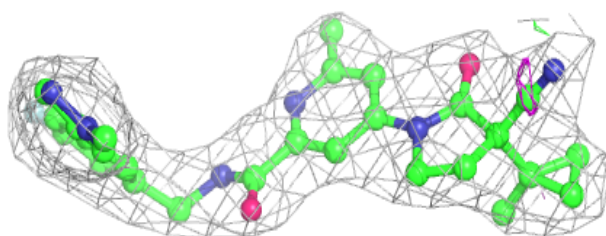
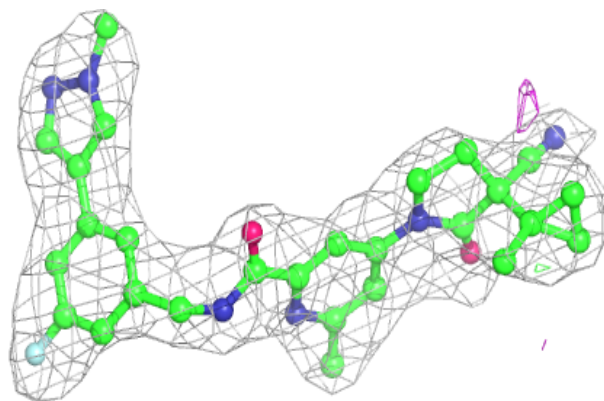
**Electron density around 1TI C 902:**

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

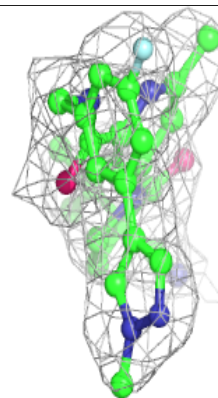
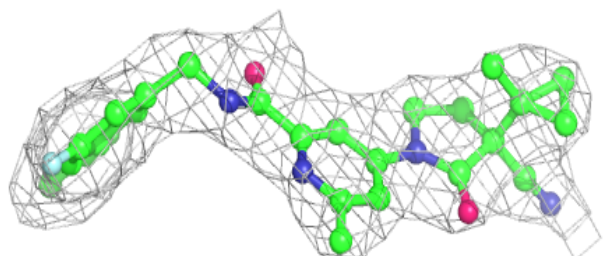
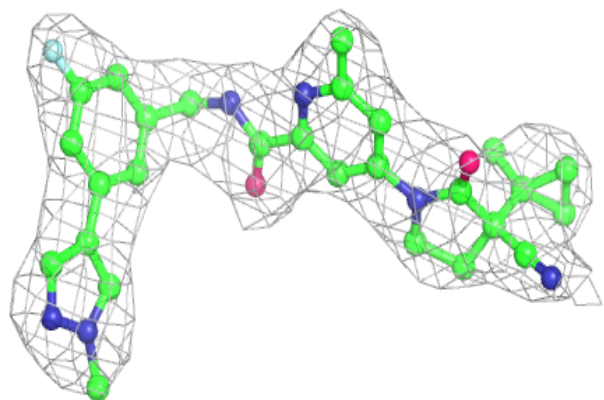


**Electron density around 1TI B 902:**

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

**Electron density around 1TI A 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 [i](#)

There are no such residues in this entry.