Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:43 PM UTC

PDB ID	:	7W2H / pdb_00007w2h
Title	:	A double cysteine variant of the sigma-1 receptor from Xenopus laevis complexed with S1RA
Authors	:	Meng, F.; Sun, Z.; Zhou, X.
Deposited on	:	2021-11-23
Resolution	:	3.80 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*
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:

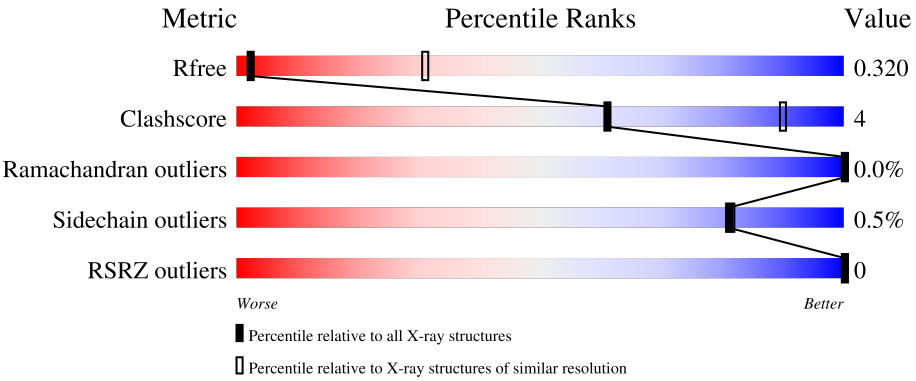
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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 <=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	225	85% 9% 5%
1	B	225	84% 10% 5%
1	C	225	83% 12% • 5%
1	D	225	84% 11% 5%
1	E	225	80% 11% 8%

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Mol	Chain	Length	Quality of chain
1	F	225	79% 12% 8%
1	G	225	84% 10% 5%
1	H	225	80% 14% 5%
1	I	225	81% 12% 7%
1	J	225	84% 10% • 5%
1	K	225	86% 9% 5%
1	L	225	82% 11% 7%
1	M	225	76% 11% 13%
1	N	225	82% 11% 7%
1	O	225	81% 13% 6%
1	P	225	80% 9% 10%
1	Q	225	84% 9% 6%
1	R	225	81% 13% 6%
1	S	225	84% 9% 7%
1	T	225	84% 10% • 5%
1	U	225	81% 13% 5%
1	V	225	80% 12% 7%
1	W	225	84% 10% 5%
1	X	225	81% 14% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 40341 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 Sigma non-opioid intracellular receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1671	1081	276	308	6			
1	C	214	Total	C	N	O	S	0	0	0
			1685	1092	278	309	6			
1	E	206	Total	C	N	O	S	0	0	0
			1620	1047	266	301	6			
1	B	213	Total	C	N	O	S	0	0	0
			1671	1081	276	308	6			
1	D	214	Total	C	N	O	S	0	0	0
			1685	1092	278	309	6			
1	F	206	Total	C	N	O	S	0	0	0
			1620	1047	266	301	6			
1	G	213	Total	C	N	O	S	0	0	0
			1671	1081	276	308	6			
1	H	213	Total	C	N	O	S	0	0	0
			1671	1081	276	308	6			
1	I	210	Total	C	N	O	S	0	0	0
			1651	1067	273	305	6			
1	J	213	Total	C	N	O	S	0	0	0
			1671	1081	276	308	6			
1	K	214	Total	C	N	O	S	0	0	0
			1685	1092	278	309	6			
1	L	210	Total	C	N	O	S	0	0	0
			1651	1067	273	305	6			
1	M	196	Total	C	N	O	S	0	0	0
			1552	1001	255	290	6			
1	N	210	Total	C	N	O	S	0	0	0
			1651	1067	273	305	6			
1	O	212	Total	C	N	O	S	0	0	0
			1663	1075	275	307	6			
1	P	202	Total	C	N	O	S	0	0	0
			1597	1032	262	297	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	212	Total	C	N	O	S	0	0	0
			1663	1075	275	307	6			
1	R	212	Total	C	N	O	S	0	0	0
			1663	1075	275	307	6			
1	S	209	Total	C	N	O	S	0	0	0
			1640	1061	269	304	6			
1	T	213	Total	C	N	O	S	0	0	0
			1671	1081	276	308	6			
1	U	213	Total	C	N	O	S	0	0	0
			1671	1081	276	308	6			
1	V	210	Total	C	N	O	S	0	0	0
			1651	1067	273	305	6			
1	W	213	Total	C	N	O	S	0	0	0
			1671	1081	276	308	6			
1	X	213	Total	C	N	O	S	0	0	0
			1671	1081	276	308	6			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP Q6DCU6
A	-2	VAL	-	expression tag	UNP Q6DCU6
A	-1	ASP	-	expression tag	UNP Q6DCU6
A	0	THR	-	expression tag	UNP Q6DCU6
A	179	CYS	LEU	engineered mutation	UNP Q6DCU6
A	203	CYS	TYR	engineered mutation	UNP Q6DCU6
C	-3	SER	-	expression tag	UNP Q6DCU6
C	-2	VAL	-	expression tag	UNP Q6DCU6
C	-1	ASP	-	expression tag	UNP Q6DCU6
C	0	THR	-	expression tag	UNP Q6DCU6
C	179	CYS	LEU	engineered mutation	UNP Q6DCU6
C	203	CYS	TYR	engineered mutation	UNP Q6DCU6
E	-3	SER	-	expression tag	UNP Q6DCU6
E	-2	VAL	-	expression tag	UNP Q6DCU6
E	-1	ASP	-	expression tag	UNP Q6DCU6
E	0	THR	-	expression tag	UNP Q6DCU6
E	179	CYS	LEU	engineered mutation	UNP Q6DCU6
E	203	CYS	TYR	engineered mutation	UNP Q6DCU6
B	-3	SER	-	expression tag	UNP Q6DCU6
B	-2	VAL	-	expression tag	UNP Q6DCU6
B	-1	ASP	-	expression tag	UNP Q6DCU6
B	0	THR	-	expression tag	UNP Q6DCU6
B	179	CYS	LEU	engineered mutation	UNP Q6DCU6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	203	CYS	TYR	engineered mutation	UNP Q6DCU6
D	-3	SER	-	expression tag	UNP Q6DCU6
D	-2	VAL	-	expression tag	UNP Q6DCU6
D	-1	ASP	-	expression tag	UNP Q6DCU6
D	0	THR	-	expression tag	UNP Q6DCU6
D	179	CYS	LEU	engineered mutation	UNP Q6DCU6
D	203	CYS	TYR	engineered mutation	UNP Q6DCU6
F	-3	SER	-	expression tag	UNP Q6DCU6
F	-2	VAL	-	expression tag	UNP Q6DCU6
F	-1	ASP	-	expression tag	UNP Q6DCU6
F	0	THR	-	expression tag	UNP Q6DCU6
F	179	CYS	LEU	engineered mutation	UNP Q6DCU6
F	203	CYS	TYR	engineered mutation	UNP Q6DCU6
G	-3	SER	-	expression tag	UNP Q6DCU6
G	-2	VAL	-	expression tag	UNP Q6DCU6
G	-1	ASP	-	expression tag	UNP Q6DCU6
G	0	THR	-	expression tag	UNP Q6DCU6
G	179	CYS	LEU	engineered mutation	UNP Q6DCU6
G	203	CYS	TYR	engineered mutation	UNP Q6DCU6
H	-3	SER	-	expression tag	UNP Q6DCU6
H	-2	VAL	-	expression tag	UNP Q6DCU6
H	-1	ASP	-	expression tag	UNP Q6DCU6
H	0	THR	-	expression tag	UNP Q6DCU6
H	179	CYS	LEU	engineered mutation	UNP Q6DCU6
H	203	CYS	TYR	engineered mutation	UNP Q6DCU6
I	-3	SER	-	expression tag	UNP Q6DCU6
I	-2	VAL	-	expression tag	UNP Q6DCU6
I	-1	ASP	-	expression tag	UNP Q6DCU6
I	0	THR	-	expression tag	UNP Q6DCU6
I	179	CYS	LEU	engineered mutation	UNP Q6DCU6
I	203	CYS	TYR	engineered mutation	UNP Q6DCU6
J	-3	SER	-	expression tag	UNP Q6DCU6
J	-2	VAL	-	expression tag	UNP Q6DCU6
J	-1	ASP	-	expression tag	UNP Q6DCU6
J	0	THR	-	expression tag	UNP Q6DCU6
J	179	CYS	LEU	engineered mutation	UNP Q6DCU6
J	203	CYS	TYR	engineered mutation	UNP Q6DCU6
K	-3	SER	-	expression tag	UNP Q6DCU6
K	-2	VAL	-	expression tag	UNP Q6DCU6
K	-1	ASP	-	expression tag	UNP Q6DCU6
K	0	THR	-	expression tag	UNP Q6DCU6
K	179	CYS	LEU	engineered mutation	UNP Q6DCU6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	203	CYS	TYR	engineered mutation	UNP Q6DCU6
L	-3	SER	-	expression tag	UNP Q6DCU6
L	-2	VAL	-	expression tag	UNP Q6DCU6
L	-1	ASP	-	expression tag	UNP Q6DCU6
L	0	THR	-	expression tag	UNP Q6DCU6
L	179	CYS	LEU	engineered mutation	UNP Q6DCU6
L	203	CYS	TYR	engineered mutation	UNP Q6DCU6
M	-3	SER	-	expression tag	UNP Q6DCU6
M	-2	VAL	-	expression tag	UNP Q6DCU6
M	-1	ASP	-	expression tag	UNP Q6DCU6
M	0	THR	-	expression tag	UNP Q6DCU6
M	179	CYS	LEU	engineered mutation	UNP Q6DCU6
M	203	CYS	TYR	engineered mutation	UNP Q6DCU6
N	-3	SER	-	expression tag	UNP Q6DCU6
N	-2	VAL	-	expression tag	UNP Q6DCU6
N	-1	ASP	-	expression tag	UNP Q6DCU6
N	0	THR	-	expression tag	UNP Q6DCU6
N	179	CYS	LEU	engineered mutation	UNP Q6DCU6
N	203	CYS	TYR	engineered mutation	UNP Q6DCU6
O	-3	SER	-	expression tag	UNP Q6DCU6
O	-2	VAL	-	expression tag	UNP Q6DCU6
O	-1	ASP	-	expression tag	UNP Q6DCU6
O	0	THR	-	expression tag	UNP Q6DCU6
O	179	CYS	LEU	engineered mutation	UNP Q6DCU6
O	203	CYS	TYR	engineered mutation	UNP Q6DCU6
P	-3	SER	-	expression tag	UNP Q6DCU6
P	-2	VAL	-	expression tag	UNP Q6DCU6
P	-1	ASP	-	expression tag	UNP Q6DCU6
P	0	THR	-	expression tag	UNP Q6DCU6
P	179	CYS	LEU	engineered mutation	UNP Q6DCU6
P	203	CYS	TYR	engineered mutation	UNP Q6DCU6
Q	-3	SER	-	expression tag	UNP Q6DCU6
Q	-2	VAL	-	expression tag	UNP Q6DCU6
Q	-1	ASP	-	expression tag	UNP Q6DCU6
Q	0	THR	-	expression tag	UNP Q6DCU6
Q	179	CYS	LEU	engineered mutation	UNP Q6DCU6
Q	203	CYS	TYR	engineered mutation	UNP Q6DCU6
R	-3	SER	-	expression tag	UNP Q6DCU6
R	-2	VAL	-	expression tag	UNP Q6DCU6
R	-1	ASP	-	expression tag	UNP Q6DCU6
R	0	THR	-	expression tag	UNP Q6DCU6
R	179	CYS	LEU	engineered mutation	UNP Q6DCU6

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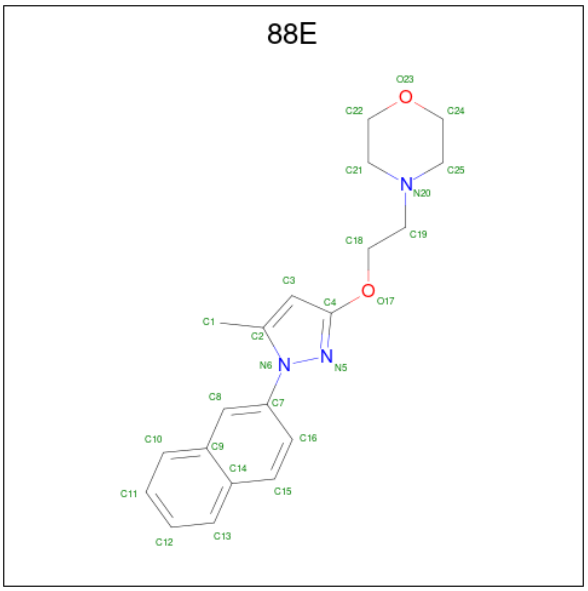
Chain	Residue	Modelled	Actual	Comment	Reference
R	203	CYS	TYR	engineered mutation	UNP Q6DCU6
S	-3	SER	-	expression tag	UNP Q6DCU6
S	-2	VAL	-	expression tag	UNP Q6DCU6
S	-1	ASP	-	expression tag	UNP Q6DCU6
S	0	THR	-	expression tag	UNP Q6DCU6
S	179	CYS	LEU	engineered mutation	UNP Q6DCU6
S	203	CYS	TYR	engineered mutation	UNP Q6DCU6
T	-3	SER	-	expression tag	UNP Q6DCU6
T	-2	VAL	-	expression tag	UNP Q6DCU6
T	-1	ASP	-	expression tag	UNP Q6DCU6
T	0	THR	-	expression tag	UNP Q6DCU6
T	179	CYS	LEU	engineered mutation	UNP Q6DCU6
T	203	CYS	TYR	engineered mutation	UNP Q6DCU6
U	-3	SER	-	expression tag	UNP Q6DCU6
U	-2	VAL	-	expression tag	UNP Q6DCU6
U	-1	ASP	-	expression tag	UNP Q6DCU6
U	0	THR	-	expression tag	UNP Q6DCU6
U	179	CYS	LEU	engineered mutation	UNP Q6DCU6
U	203	CYS	TYR	engineered mutation	UNP Q6DCU6
V	-3	SER	-	expression tag	UNP Q6DCU6
V	-2	VAL	-	expression tag	UNP Q6DCU6
V	-1	ASP	-	expression tag	UNP Q6DCU6
V	0	THR	-	expression tag	UNP Q6DCU6
V	179	CYS	LEU	engineered mutation	UNP Q6DCU6
V	203	CYS	TYR	engineered mutation	UNP Q6DCU6
W	-3	SER	-	expression tag	UNP Q6DCU6
W	-2	VAL	-	expression tag	UNP Q6DCU6
W	-1	ASP	-	expression tag	UNP Q6DCU6
W	0	THR	-	expression tag	UNP Q6DCU6
W	179	CYS	LEU	engineered mutation	UNP Q6DCU6
W	203	CYS	TYR	engineered mutation	UNP Q6DCU6
X	-3	SER	-	expression tag	UNP Q6DCU6
X	-2	VAL	-	expression tag	UNP Q6DCU6
X	-1	ASP	-	expression tag	UNP Q6DCU6
X	0	THR	-	expression tag	UNP Q6DCU6
X	179	CYS	LEU	engineered mutation	UNP Q6DCU6
X	203	CYS	TYR	engineered mutation	UNP Q6DCU6

- Molecule 2 is 4-[2-(5-methyl-1-naphthalen-2-yl-pyrazol-3-yl)oxyethyl]morpholine (CCD ID: 88E) (formula: $C_{20}H_{23}N_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	20	3	2		
2	C	1	Total	C	N	O	0	0
			25	20	3	2		
2	E	1	Total	C	N	O	0	0
			25	20	3	2		
2	B	1	Total	C	N	O	0	0
			25	20	3	2		
2	D	1	Total	C	N	O	0	0
			25	20	3	2		
2	F	1	Total	C	N	O	0	0
			25	20	3	2		
2	G	1	Total	C	N	O	0	0
			25	20	3	2		
2	H	1	Total	C	N	O	0	0
			25	20	3	2		
2	I	1	Total	C	N	O	0	0
			25	20	3	2		
2	J	1	Total	C	N	O	0	0
			25	20	3	2		
2	K	1	Total	C	N	O	0	0
			25	20	3	2		
2	L	1	Total	C	N	O	0	0
			25	20	3	2		
2	M	1	Total	C	N	O	0	0
			25	20	3	2		
2	N	1	Total	C	N	O	0	0
			25	20	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total	C	N	O	0	0
			25	20	3	2		
2	P	1	Total	C	N	O	0	0
			25	20	3	2		
2	P	1	Total	C	N	O	0	0
			25	20	3	2		
2	Q	1	Total	C	N	O	0	0
			25	20	3	2		
2	R	1	Total	C	N	O	0	0
			25	20	3	2		
2	S	1	Total	C	N	O	0	0
			25	20	3	2		
2	T	1	Total	C	N	O	0	0
			25	20	3	2		
2	U	1	Total	C	N	O	0	0
			25	20	3	2		
2	V	1	Total	C	N	O	0	0
			25	20	3	2		
2	W	1	Total	C	N	O	0	0
			25	20	3	2		
2	X	1	Total	C	N	O	0	0
			25	20	3	2		

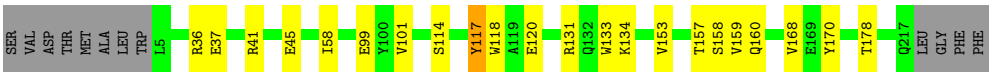
3 Residue-property plots (i)

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: Sigma non-opioid intracellular receptor 1

Chain A:

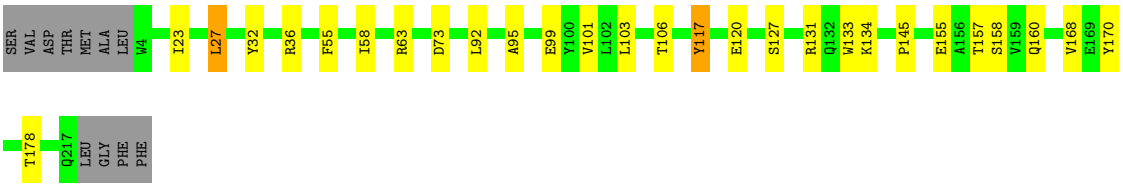




• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain C:

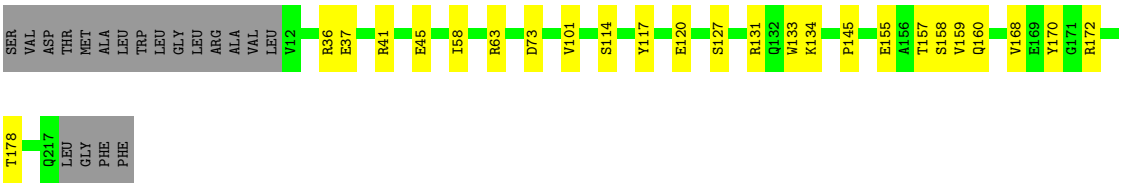




• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain E:

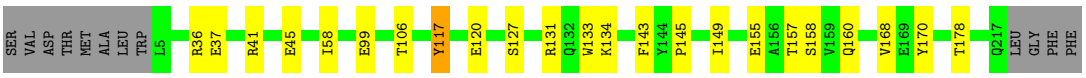




• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain B:

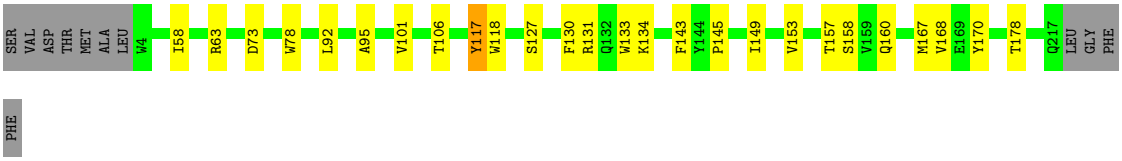




• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain D:

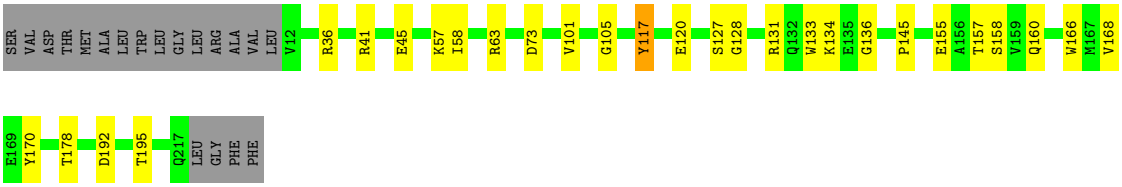




• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain F:





• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain G:

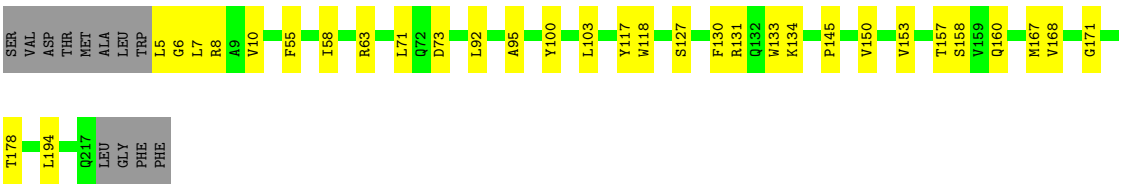




• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain H:

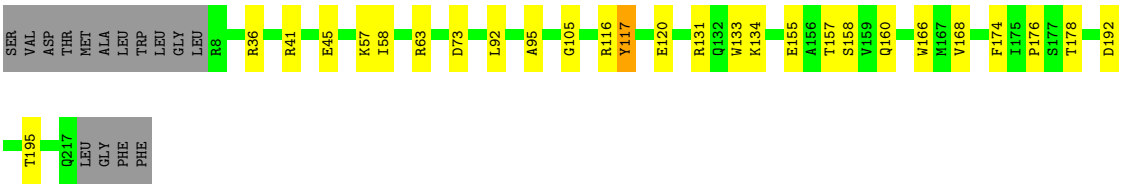




• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain I:

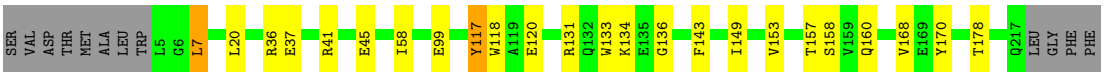




• Molecule 1: Sigma non-opioid intracellular receptor 1

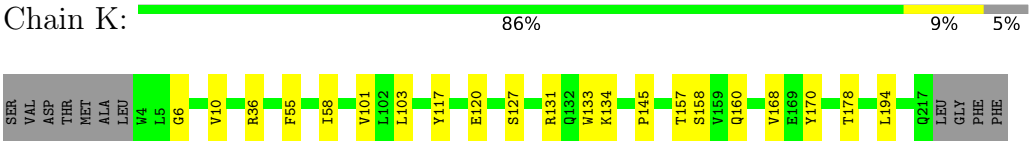
Chain J:





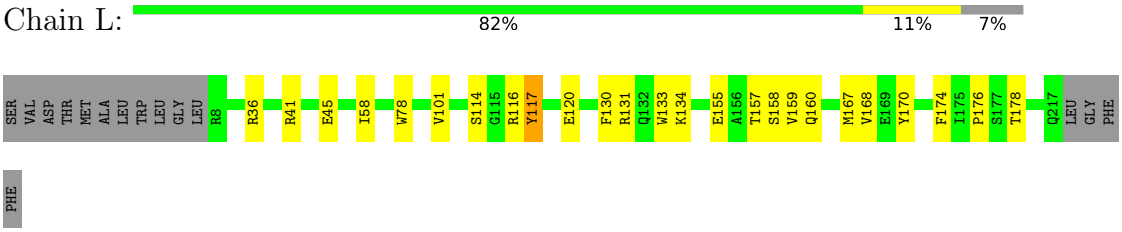
• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain K:



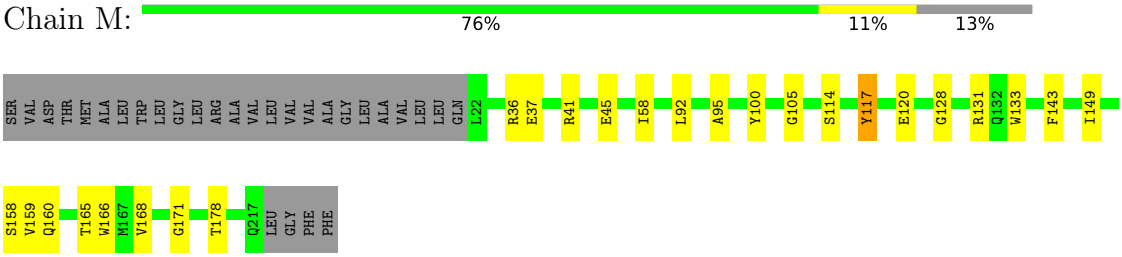
• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain L:



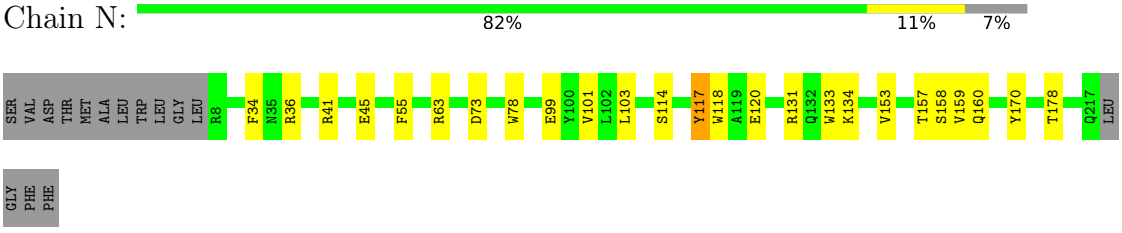
• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain M:



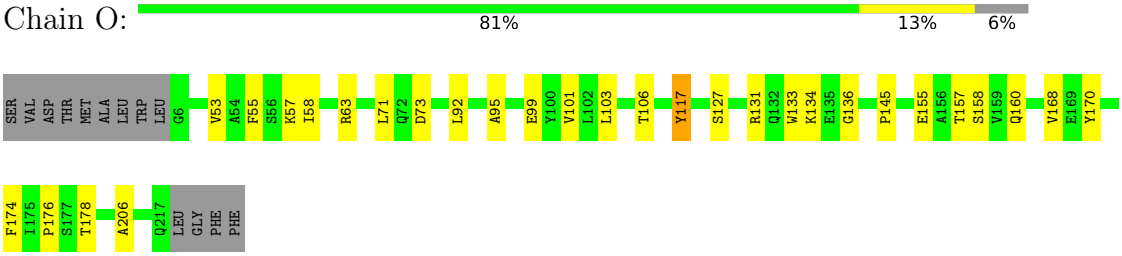
• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain N:



• Molecule 1: Sigma non-opioid intracellular receptor 1

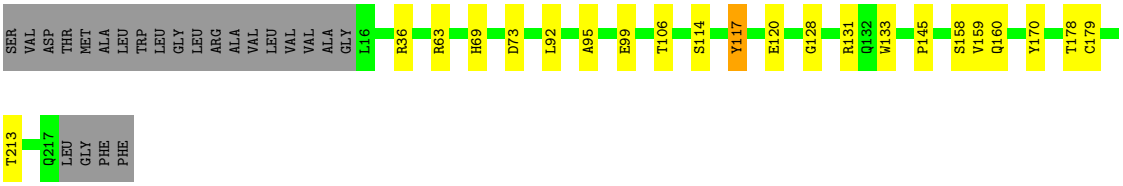
Chain O:



• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain P:





• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain Q:

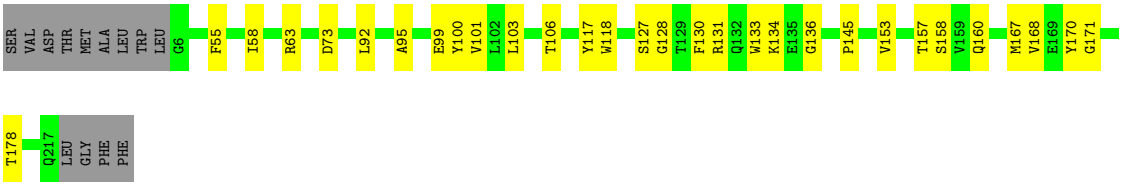




• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain R:





• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain S:

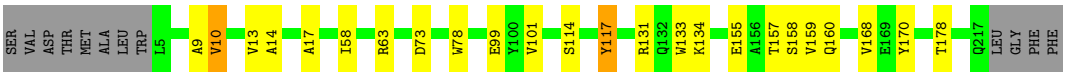




• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain T:

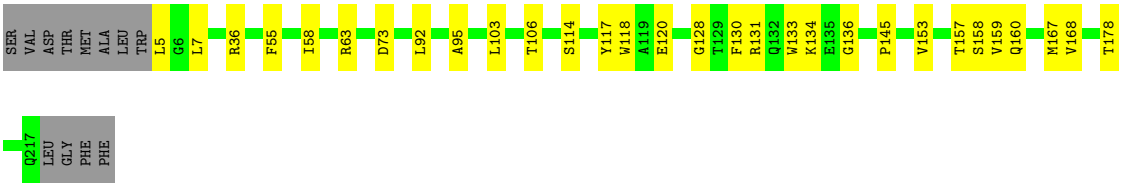




• Molecule 1: Sigma non-opioid intracellular receptor 1

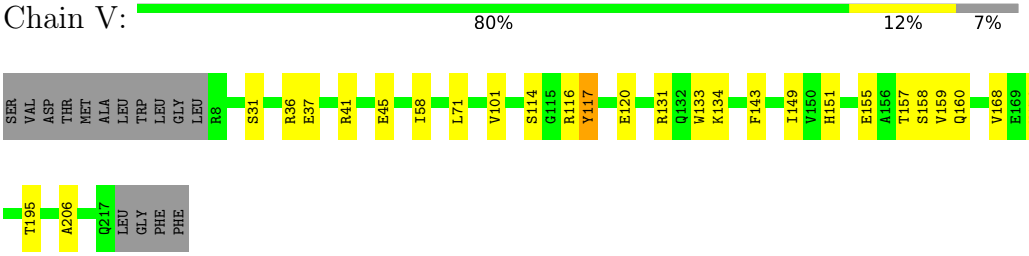
Chain U:





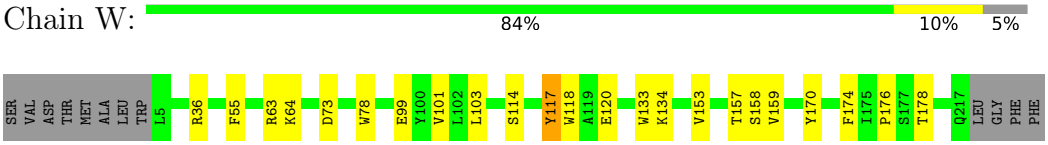
• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain V:



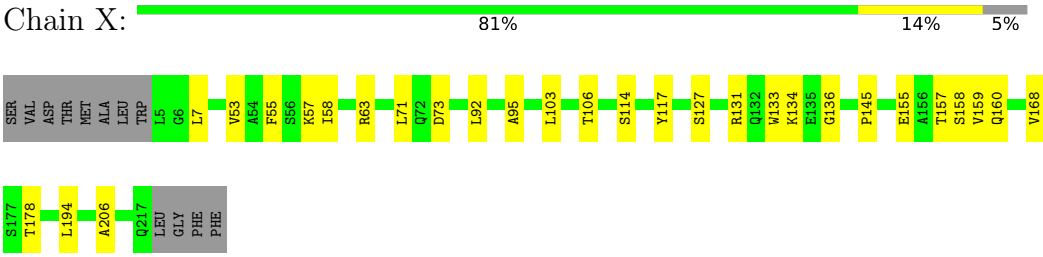
• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain W:



• Molecule 1: Sigma non-opioid intracellular receptor 1

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	134.45Å 200.75Å 160.59Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	19.85 – 3.80 19.85 – 3.80	Depositor EDS
% Data completeness (in resolution range)	80.8 (19.85-3.80) 81.0 (19.85-3.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 3.82Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.283 , 0.318 0.287 , 0.320	Depositor DCC
R_{free} test set	3342 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å^2)	73.0	Xtriage
Anisotropy	0.784	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 32.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.369 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	40341	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8494e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 88E

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	0.12	0/1712	0.28	0/2324
1	B	0.11	0/1712	0.28	0/2324
1	C	0.11	0/1728	0.28	0/2347
1	D	0.11	0/1728	0.26	0/2347
1	E	0.12	0/1661	0.28	0/2255
1	F	0.11	0/1661	0.26	0/2255
1	G	0.11	0/1712	0.28	0/2324
1	H	0.11	0/1712	0.27	0/2324
1	I	0.11	0/1692	0.27	0/2297
1	J	0.12	0/1712	0.27	0/2324
1	K	0.10	0/1728	0.27	0/2347
1	L	0.12	0/1692	0.28	0/2297
1	M	0.13	0/1593	0.29	0/2161
1	N	0.11	0/1692	0.27	0/2297
1	O	0.11	0/1704	0.27	0/2313
1	P	0.13	0/1638	0.30	0/2223
1	Q	0.11	0/1704	0.27	0/2313
1	R	0.12	0/1704	0.27	0/2313
1	S	0.12	0/1681	0.27	0/2283
1	T	0.11	0/1712	0.27	0/2324
1	U	0.11	0/1712	0.26	0/2324
1	V	0.11	0/1692	0.27	0/2297
1	W	0.12	0/1712	0.29	0/2324
1	X	0.12	0/1712	0.27	0/2324
All	All	0.11	0/40706	0.27	0/55261

There are no bond length outliers.

There are no bond angle outliers.

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	1671	0	1652	12	0
1	B	1671	0	1652	15	0
1	C	1685	0	1662	15	0
1	D	1685	0	1662	15	0
1	E	1620	0	1589	15	0
1	F	1620	0	1589	17	0
1	G	1671	0	1652	15	0
1	H	1671	0	1652	20	0
1	I	1651	0	1627	15	0
1	J	1671	0	1652	14	0
1	K	1685	0	1662	11	0
1	L	1651	0	1627	14	0
1	M	1552	0	1508	14	0
1	N	1651	0	1627	14	0
1	O	1663	0	1641	18	0
1	P	1597	0	1563	13	0
1	Q	1663	0	1641	13	0
1	R	1663	0	1641	17	0
1	S	1640	0	1614	11	0
1	T	1671	0	1652	15	0
1	U	1671	0	1652	16	0
1	V	1651	0	1627	16	0
1	W	1671	0	1652	15	0
1	X	1671	0	1652	18	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
2	C	25	0	0	0	0
2	D	25	0	0	0	0
2	E	25	0	0	0	0
2	F	25	0	0	0	0
2	G	25	0	0	0	0
2	H	25	0	0	0	0
2	I	25	0	0	0	0
2	J	25	0	0	0	0
2	K	25	0	0	0	0
2	L	25	0	0	0	0
2	M	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	25	0	0	0	0
2	O	25	0	0	0	0
2	P	50	0	0	1	0
2	Q	25	0	0	0	0
2	R	25	0	0	0	0
2	S	25	0	0	0	0
2	T	25	0	0	0	0
2	U	25	0	0	0	0
2	V	25	0	0	0	0
2	W	25	0	0	0	0
2	X	25	0	0	0	0
All	All	40341	0	39148	331	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.

All (331) 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:R:133:TRP:HB3	1:R:158:SER:HB3	1.71	0.72
1:R:131:ARG:HB3	1:R:160:GLN:HB3	1.75	0.69
1:K:133:TRP:HB3	1:K:158:SER:HB3	1.76	0.67
1:C:133:TRP:HB3	1:C:158:SER:HB3	1.77	0.67
1:H:133:TRP:HB3	1:H:158:SER:HB3	1.77	0.67
1:U:133:TRP:HB3	1:U:158:SER:HB3	1.75	0.66
1:T:10:VAL:O	1:T:14:ALA:N	2.29	0.65
1:P:133:TRP:HB3	1:P:158:SER:HB3	1.77	0.65
1:D:133:TRP:HB3	1:D:158:SER:HB3	1.79	0.65
1:B:36:ARG:NH1	1:B:120:GLU:OE2	2.29	0.65
1:J:117:TYR:HB2	1:J:178:THR:HG22	1.80	0.64
1:G:36:ARG:NH1	1:G:120:GLU:OE2	2.30	0.63
1:T:134:LYS:NZ	1:T:155:GLU:OE1	2.30	0.63
1:F:133:TRP:HB3	1:F:158:SER:HB3	1.78	0.63
1:S:133:TRP:HB3	1:S:158:SER:HB3	1.79	0.63
1:O:133:TRP:HB3	1:O:158:SER:HB3	1.78	0.63
1:L:133:TRP:HB3	1:L:158:SER:HB3	1.80	0.63
1:I:36:ARG:NH1	1:I:120:GLU:OE2	2.31	0.62
1:E:133:TRP:HB3	1:E:158:SER:HB3	1.82	0.61
1:X:134:LYS:HA	1:X:157:THR:HG22	1.82	0.61
1:A:36:ARG:NH1	1:A:120:GLU:OE2	2.34	0.61
1:F:36:ARG:NH1	1:F:120:GLU:OE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:LYS:HA	1:E:157:THR:HG22	1.82	0.61
1:V:133:TRP:HB3	1:V:158:SER:HB3	1.81	0.61
1:T:14:ALA:HA	1:T:17:ALA:HB3	1.83	0.61
1:Q:134:LYS:NZ	1:Q:155:GLU:OE1	2.33	0.60
1:C:134:LYS:HA	1:C:157:THR:HG22	1.84	0.60
1:G:117:TYR:HB2	1:G:178:THR:HG22	1.84	0.59
1:N:36:ARG:NH1	1:N:120:GLU:OE2	2.35	0.59
1:F:134:LYS:HA	1:F:157:THR:HG22	1.85	0.59
1:M:133:TRP:HB3	1:M:158:SER:HB3	1.84	0.59
1:B:117:TYR:HB2	1:B:178:THR:HG22	1.85	0.58
1:N:133:TRP:HB3	1:N:158:SER:HB3	1.85	0.58
1:Q:117:TYR:HB2	1:Q:178:THR:HG22	1.85	0.58
1:Q:133:TRP:HB3	1:Q:158:SER:HB3	1.85	0.58
1:T:117:TYR:HB2	1:T:178:THR:HG22	1.86	0.58
1:E:63:ARG:NH1	1:E:73:ASP:OD1	2.37	0.58
1:F:57:LYS:NZ	1:V:45:GLU:OE2	2.37	0.58
1:E:131:ARG:HB3	1:E:160:GLN:HB3	1.86	0.57
1:W:36:ARG:NH1	1:W:120:GLU:OE2	2.37	0.57
1:L:36:ARG:NH1	1:L:120:GLU:OE2	2.38	0.57
1:D:131:ARG:HB3	1:D:160:GLN:HB3	1.86	0.57
1:T:133:TRP:HB3	1:T:158:SER:HB3	1.87	0.57
1:X:133:TRP:HB3	1:X:158:SER:HB3	1.86	0.56
1:O:131:ARG:HB3	1:O:160:GLN:HB3	1.87	0.56
1:L:134:LYS:HA	1:L:157:THR:HG22	1.88	0.56
1:H:131:ARG:HB3	1:H:160:GLN:HB3	1.87	0.56
1:U:92:LEU:HD11	1:U:95:ALA:HB2	1.88	0.56
1:W:133:TRP:HB3	1:W:158:SER:HB3	1.88	0.56
1:B:45:GLU:HG2	1:X:53:VAL:HG11	1.88	0.56
1:I:133:TRP:HB3	1:I:158:SER:HB3	1.86	0.56
1:I:134:LYS:HA	1:I:157:THR:HG22	1.88	0.55
1:S:36:ARG:NH1	1:S:120:GLU:OE2	2.39	0.55
1:I:134:LYS:NZ	1:I:155:GLU:OE1	2.35	0.55
1:C:131:ARG:HB3	1:C:160:GLN:HB3	1.89	0.55
1:B:45:GLU:OE2	1:X:57:LYS:NZ	2.39	0.55
1:Q:134:LYS:HA	1:Q:157:THR:HG22	1.88	0.54
1:P:36:ARG:NH1	1:P:120:GLU:OE2	2.40	0.54
1:T:134:LYS:HA	1:T:157:THR:HG22	1.89	0.54
1:D:117:TYR:HB2	1:D:178:THR:HG22	1.89	0.54
1:B:134:LYS:HA	1:B:157:THR:HG22	1.89	0.54
1:G:45:GLU:HG2	1:O:53:VAL:HG11	1.89	0.54
1:G:134:LYS:HA	1:G:157:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:131:ARG:HB3	1:K:160:GLN:HB3	1.90	0.54
1:C:23:ILE:O	1:C:27:LEU:HD13	2.08	0.54
1:E:36:ARG:NH1	1:E:120:GLU:OE2	2.40	0.54
1:H:117:TYR:HB2	1:H:178:THR:HG22	1.89	0.54
1:U:131:ARG:HB3	1:U:160:GLN:HB3	1.88	0.54
1:J:58:ILE:HD13	1:J:168:VAL:HG21	1.89	0.54
1:J:134:LYS:HA	1:J:157:THR:HG22	1.90	0.53
1:A:131:ARG:HB3	1:A:160:GLN:HB3	1.90	0.53
1:A:134:LYS:HA	1:A:157:THR:HG22	1.91	0.53
1:M:117:TYR:HB2	1:M:178:THR:HG22	1.90	0.53
1:G:45:GLU:OE2	1:O:57:LYS:NZ	2.42	0.53
1:D:134:LYS:HA	1:D:157:THR:HG22	1.90	0.53
1:F:134:LYS:NZ	1:F:155:GLU:OE1	2.38	0.53
1:U:5:LEU:HD21	1:U:7:LEU:HD13	1.91	0.53
1:B:133:TRP:HB3	1:B:158:SER:HB3	1.90	0.53
1:J:131:ARG:HB3	1:J:160:GLN:HB3	1.90	0.53
1:C:36:ARG:NH1	1:C:120:GLU:OE2	2.41	0.53
1:A:117:TYR:HB2	1:A:178:THR:HG22	1.91	0.52
1:I:57:LYS:NZ	1:M:45:GLU:OE2	2.42	0.52
1:S:134:LYS:HA	1:S:157:THR:HG22	1.90	0.52
1:O:134:LYS:HA	1:O:157:THR:HG22	1.91	0.52
1:H:6:GLY:HA3	1:H:10:VAL:HG21	1.90	0.52
1:R:63:ARG:NH1	1:R:73:ASP:OD1	2.41	0.52
1:U:63:ARG:NH1	1:U:73:ASP:OD1	2.42	0.52
1:F:131:ARG:HB3	1:F:160:GLN:HB3	1.92	0.52
1:I:58:ILE:HD13	1:I:168:VAL:HG21	1.92	0.52
1:G:7:LEU:HD12	1:G:7:LEU:H	1.74	0.52
1:V:36:ARG:NH1	1:V:120:GLU:OE2	2.43	0.52
1:E:117:TYR:HB2	1:E:178:THR:HG22	1.93	0.51
1:N:78:TRP:HB2	1:O:136:GLY:HA2	1.93	0.51
1:U:117:TYR:HB2	1:U:178:THR:HG22	1.92	0.51
1:L:131:ARG:HB3	1:L:160:GLN:HB3	1.93	0.51
1:A:58:ILE:HD13	1:A:168:VAL:HG21	1.92	0.50
1:X:92:LEU:HD11	1:X:95:ALA:HB2	1.93	0.50
1:W:78:TRP:HB2	1:X:136:GLY:HA2	1.93	0.50
1:F:63:ARG:NH1	1:F:73:ASP:OD1	2.44	0.50
1:H:7:LEU:HG	1:H:8:ARG:HG2	1.94	0.50
1:J:133:TRP:HB3	1:J:158:SER:HB3	1.93	0.50
1:Q:101:VAL:HG22	1:Q:170:TYR:HD1	1.77	0.50
1:X:131:ARG:HB3	1:X:160:GLN:HB3	1.93	0.50
1:M:37:GLU:HB3	1:M:41:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:134:LYS:HA	1:R:157:THR:HG22	1.93	0.49
1:Q:78:TRP:HB2	1:R:136:GLY:HA2	1.94	0.49
1:H:92:LEU:HD11	1:H:95:ALA:HB2	1.94	0.49
1:R:58:ILE:HD13	1:R:168:VAL:HG21	1.94	0.49
1:G:133:TRP:HB3	1:G:158:SER:HB3	1.93	0.48
1:V:37:GLU:HB3	1:V:41:ARG:NH1	2.27	0.48
1:C:106:THR:HA	1:E:133:TRP:CH2	2.48	0.48
1:C:117:TYR:HB2	1:C:178:THR:HG22	1.94	0.48
1:K:117:TYR:HB2	1:K:178:THR:HG22	1.94	0.48
1:R:92:LEU:HD11	1:R:95:ALA:HB2	1.94	0.48
1:X:117:TYR:HB2	1:X:178:THR:HG22	1.95	0.48
1:K:134:LYS:HA	1:K:157:THR:HG22	1.96	0.48
1:U:134:LYS:HA	1:U:157:THR:HG22	1.96	0.48
1:R:130:PHE:HD1	1:R:167:MET:HE1	1.79	0.47
1:J:36:ARG:NH1	1:J:120:GLU:OE2	2.47	0.47
1:O:134:LYS:NZ	1:O:155:GLU:OE1	2.46	0.47
1:S:92:LEU:HD11	1:S:95:ALA:HB2	1.96	0.47
1:O:63:ARG:NH1	1:O:73:ASP:OD1	2.48	0.47
1:W:117:TYR:HB2	1:W:178:THR:HG22	1.95	0.47
1:B:58:ILE:HD13	1:B:168:VAL:HG21	1.97	0.47
1:H:150:VAL:H	1:W:64:LYS:HZ3	1.63	0.47
1:J:99:GLU:OE2	1:J:170:TYR:OH	2.30	0.47
1:W:134:LYS:HA	1:W:157:THR:HG22	1.96	0.47
1:X:127:SER:HA	1:X:145:PRO:HG3	1.96	0.47
1:A:133:TRP:HB3	1:A:158:SER:HB3	1.95	0.47
1:V:143:PHE:CG	1:V:149:ILE:HD11	2.50	0.46
1:C:101:VAL:HG22	1:C:170:TYR:HD1	1.80	0.46
1:R:117:TYR:HB2	1:R:178:THR:HG22	1.96	0.46
1:S:63:ARG:NH1	1:S:73:ASP:OD1	2.48	0.46
1:B:99:GLU:OE2	1:B:170:TYR:OH	2.32	0.46
1:D:127:SER:HA	1:D:145:PRO:HG3	1.98	0.46
1:N:99:GLU:OE2	1:N:170:TYR:OH	2.32	0.46
1:N:101:VAL:HG22	1:N:170:TYR:HD1	1.79	0.46
1:N:134:LYS:HA	1:N:157:THR:HG22	1.97	0.46
1:P:114:SER:HB3	1:P:159:VAL:HG13	1.98	0.46
1:B:131:ARG:HB3	1:B:160:GLN:HB3	1.97	0.46
1:N:117:TYR:HB2	1:N:178:THR:HG22	1.97	0.46
1:F:58:ILE:HD13	1:F:168:VAL:HG21	1.97	0.46
1:I:131:ARG:HB3	1:I:160:GLN:HB3	1.98	0.46
1:K:58:ILE:HD13	1:K:168:VAL:HG21	1.97	0.46
1:D:63:ARG:NH1	1:D:73:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:131:ARG:HB3	1:M:160:GLN:HB3	1.97	0.46
1:P:179:CYS:HB2	2:P:302:88E:C22	2.45	0.46
1:T:78:TRP:HB2	1:U:136:GLY:HA2	1.98	0.46
1:E:101:VAL:HG22	1:E:170:TYR:HD1	1.79	0.46
1:F:117:TYR:HB2	1:F:178:THR:HG22	1.96	0.46
1:L:114:SER:HB3	1:L:159:VAL:HG13	1.97	0.46
1:O:58:ILE:HD13	1:O:168:VAL:HG21	1.98	0.46
1:K:36:ARG:NH1	1:K:120:GLU:OE2	2.49	0.46
1:L:58:ILE:HD13	1:L:168:VAL:HG21	1.97	0.46
1:L:101:VAL:HG22	1:L:170:TYR:HD1	1.80	0.46
1:L:130:PHE:HD1	1:L:167:MET:HE1	1.81	0.46
1:O:92:LEU:HD11	1:O:95:ALA:HB2	1.97	0.46
1:S:99:GLU:OE2	1:S:170:TYR:OH	2.31	0.46
1:C:127:SER:HA	1:C:145:PRO:HG3	1.98	0.45
1:E:114:SER:HB3	1:E:159:VAL:HG13	1.97	0.45
1:K:55:PHE:CD1	1:K:103:LEU:HD13	2.50	0.45
1:O:117:TYR:HB2	1:O:178:THR:HG22	1.98	0.45
1:V:134:LYS:HA	1:V:157:THR:HG22	1.98	0.45
1:X:134:LYS:NZ	1:X:155:GLU:OE1	2.43	0.45
1:E:127:SER:HA	1:E:145:PRO:HG3	1.98	0.45
1:I:92:LEU:HD11	1:I:95:ALA:HB2	1.98	0.45
1:A:41:ARG:O	1:A:45:GLU:HG3	2.16	0.45
1:M:92:LEU:HD11	1:M:95:ALA:HB2	1.99	0.45
1:S:58:ILE:HD13	1:S:168:VAL:HG21	1.99	0.45
1:U:130:PHE:HD1	1:U:167:MET:HE1	1.81	0.45
1:W:63:ARG:NH1	1:W:73:ASP:OD1	2.50	0.45
1:W:101:VAL:HG22	1:W:170:TYR:HD1	1.81	0.45
1:M:133:TRP:CH2	1:O:106:THR:HA	2.51	0.45
1:C:134:LYS:NZ	1:C:155:GLU:OE1	2.50	0.45
1:H:150:VAL:HB	1:W:64:LYS:HD2	1.98	0.45
1:G:58:ILE:HD13	1:G:168:VAL:HG21	1.99	0.45
1:V:58:ILE:HD13	1:V:168:VAL:HG21	1.99	0.45
1:W:99:GLU:OE2	1:W:170:TYR:OH	2.32	0.45
1:E:134:LYS:NZ	1:E:155:GLU:OE1	2.42	0.45
1:K:127:SER:HA	1:K:145:PRO:HG3	1.98	0.45
1:M:114:SER:HB3	1:M:159:VAL:HG13	1.98	0.45
1:P:92:LEU:HD11	1:P:95:ALA:HB2	1.99	0.45
1:P:128:GLY:O	1:P:145:PRO:HD3	2.17	0.45
1:Q:63:ARG:NH1	1:Q:73:ASP:OD1	2.50	0.45
1:V:192:ASP:OD2	1:V:195:THR:OG1	2.28	0.45
1:I:41:ARG:O	1:I:45:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:117:TYR:HB2	1:S:178:THR:HG22	1.99	0.44
1:T:101:VAL:HG22	1:T:170:TYR:HD1	1.81	0.44
1:H:194:LEU:HD23	1:I:116:ARG:NH1	2.32	0.44
1:L:117:TYR:HB2	1:L:178:THR:HG22	1.99	0.44
1:D:58:ILE:HD13	1:D:168:VAL:HG21	1.99	0.44
1:J:41:ARG:O	1:J:45:GLU:HG3	2.17	0.44
1:N:55:PHE:CD1	1:N:103:LEU:HD13	2.53	0.44
1:H:127:SER:HA	1:H:145:PRO:HG3	2.00	0.44
1:O:55:PHE:CG	1:O:103:LEU:HD13	2.51	0.44
1:P:99:GLU:OE2	1:P:170:TYR:OH	2.34	0.44
1:D:78:TRP:HB2	1:F:136:GLY:HA2	2.00	0.44
1:H:134:LYS:HA	1:H:157:THR:HG22	1.99	0.44
1:S:131:ARG:HB3	1:S:160:GLN:HB3	1.99	0.44
1:T:131:ARG:HB3	1:T:160:GLN:HB3	1.99	0.44
1:P:131:ARG:HB3	1:P:160:GLN:HB3	1.98	0.44
1:T:9:ALA:O	1:T:13:VAL:N	2.51	0.44
1:V:131:ARG:HB3	1:V:160:GLN:HB3	1.99	0.44
1:A:114:SER:HB3	1:A:159:VAL:HG13	1.99	0.44
1:E:120:GLU:N	1:E:172:ARG:O	2.46	0.44
1:D:130:PHE:HD1	1:D:167:MET:HE1	1.82	0.44
1:F:192:ASP:OD2	1:F:195:THR:OG1	2.29	0.44
1:J:37:GLU:HB3	1:J:41:ARG:NH1	2.32	0.44
1:N:114:SER:HB3	1:N:159:VAL:HG13	2.00	0.44
1:O:71:LEU:HD21	1:O:206:ALA:HA	2.00	0.44
1:R:55:PHE:CG	1:R:103:LEU:HD13	2.53	0.44
1:X:71:LEU:HD21	1:X:206:ALA:HA	2.00	0.44
1:H:58:ILE:HD13	1:H:168:VAL:HG21	1.99	0.44
1:T:10:VAL:HA	1:T:13:VAL:HB	1.99	0.44
1:J:136:GLY:HA2	1:L:78:TRP:HB2	2.00	0.44
1:M:58:ILE:HD13	1:M:168:VAL:HG21	2.00	0.44
1:A:99:GLU:OE2	1:A:170:TYR:OH	2.32	0.43
1:C:58:ILE:HD13	1:C:168:VAL:HG21	1.99	0.43
1:D:118:TRP:HA	1:D:153:VAL:HG13	2.00	0.43
1:X:55:PHE:CG	1:X:103:LEU:HD13	2.53	0.43
1:J:118:TRP:HA	1:J:153:VAL:HG13	1.99	0.43
1:P:117:TYR:HB2	1:P:178:THR:HG22	2.00	0.43
1:D:106:THR:HA	1:F:133:TRP:CH2	2.53	0.43
1:H:130:PHE:HD1	1:H:167:MET:HE1	1.82	0.43
1:C:32:TYR:HB3	1:C:99:GLU:OE2	2.19	0.43
1:G:41:ARG:O	1:G:45:GLU:HG3	2.18	0.43
1:J:20:LEU:HD23	1:J:20:LEU:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:99:GLU:OE2	1:R:170:TYR:OH	2.32	0.43
1:I:192:ASP:OD2	1:I:195:THR:OG1	2.30	0.43
1:E:37:GLU:HB3	1:E:41:ARG:NH1	2.34	0.43
1:I:117:TYR:HB2	1:I:178:THR:HG22	1.99	0.43
1:O:127:SER:HA	1:O:145:PRO:HG3	1.99	0.43
1:R:127:SER:HA	1:R:145:PRO:HG3	2.00	0.43
1:V:114:SER:HB3	1:V:159:VAL:HG13	2.00	0.43
1:C:55:PHE:CD1	1:C:103:LEU:HD13	2.53	0.43
1:B:41:ARG:O	1:B:45:GLU:HG3	2.19	0.43
1:I:105:GLY:HA3	1:I:166:TRP:CE3	2.54	0.43
1:O:174:PHE:CD2	1:O:176:PRO:HD2	2.54	0.43
1:A:118:TRP:HA	1:A:153:VAL:HG13	2.00	0.43
1:F:41:ARG:O	1:F:45:GLU:HG3	2.19	0.43
1:F:105:GLY:HA3	1:F:166:TRP:CE3	2.54	0.43
1:J:143:PHE:CG	1:J:149:ILE:HD11	2.53	0.43
1:B:127:SER:HA	1:B:145:PRO:HG3	2.01	0.43
1:M:100:TYR:CE2	1:M:171:GLY:HA3	2.54	0.43
1:V:116:ARG:NH1	1:X:194:LEU:HD23	2.34	0.42
1:G:71:LEU:HD23	1:G:209:LEU:HD22	2.01	0.42
1:H:63:ARG:NH1	1:H:73:ASP:OD1	2.52	0.42
1:U:128:GLY:O	1:U:145:PRO:HD3	2.19	0.42
1:K:194:LEU:HD23	1:L:116:ARG:NH1	2.33	0.42
1:F:101:VAL:HG22	1:F:170:TYR:HD1	1.85	0.42
1:L:41:ARG:O	1:L:45:GLU:HG3	2.20	0.42
1:N:118:TRP:HA	1:N:153:VAL:HG13	2.02	0.42
1:E:41:ARG:O	1:E:45:GLU:HG3	2.20	0.42
1:D:143:PHE:CG	1:D:149:ILE:HD11	2.54	0.42
1:K:101:VAL:HG22	1:K:170:TYR:HD1	1.84	0.42
1:M:143:PHE:CG	1:M:149:ILE:HD11	2.54	0.42
1:V:101:VAL:HG22	1:V:170:TYR:HD1	1.83	0.42
1:V:117:TYR:HB2	1:V:178:THR:HG22	2.01	0.42
1:X:63:ARG:NH1	1:X:73:ASP:OD1	2.52	0.42
1:B:37:GLU:HB3	1:B:41:ARG:NH1	2.35	0.42
1:W:55:PHE:CD1	1:W:103:LEU:HD13	2.55	0.42
1:E:58:ILE:HD13	1:E:168:VAL:HG21	2.01	0.42
1:B:106:THR:HA	1:D:133:TRP:CH2	2.54	0.42
1:K:6:GLY:HA3	1:K:10:VAL:HB	2.01	0.42
1:S:37:GLU:HB3	1:S:41:ARG:NH1	2.34	0.42
1:C:63:ARG:NH1	1:C:73:ASP:OD1	2.53	0.42
1:V:133:TRP:CH2	1:X:106:THR:HA	2.55	0.42
1:G:106:THR:HA	1:H:133:TRP:CH2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:55:PHE:CG	1:U:103:LEU:HD13	2.54	0.42
1:Q:58:ILE:HD13	1:Q:168:VAL:HG21	2.02	0.42
1:Q:131:ARG:HB3	1:Q:160:GLN:HB3	2.02	0.42
1:T:114:SER:HB3	1:T:159:VAL:HG13	2.02	0.42
1:X:174:PHE:CD2	1:X:176:PRO:HD2	2.55	0.42
1:B:134:LYS:NZ	1:B:155:GLU:OE1	2.50	0.41
1:F:128:GLY:O	1:F:145:PRO:HD3	2.20	0.41
1:H:118:TRP:HA	1:H:153:VAL:HG13	2.02	0.41
1:M:36:ARG:NH1	1:M:120:GLU:OE2	2.52	0.41
1:N:41:ARG:O	1:N:45:GLU:HG3	2.20	0.41
1:N:131:ARG:HB3	1:N:160:GLN:HB3	2.02	0.41
1:T:99:GLU:OE2	1:T:170:TYR:OH	2.37	0.41
1:V:151:HIS:NE2	1:V:155:GLU:O	2.53	0.41
1:L:174:PHE:CD2	1:L:176:PRO:HD2	2.55	0.41
1:Q:114:SER:HB3	1:Q:159:VAL:HG13	2.02	0.41
1:U:58:ILE:HD13	1:U:168:VAL:HG21	2.02	0.41
1:G:37:GLU:HB3	1:G:41:ARG:NH1	2.36	0.41
1:H:55:PHE:CD1	1:H:103:LEU:HD13	2.56	0.41
1:Q:92:LEU:HD11	1:Q:95:ALA:HB2	2.01	0.41
1:V:71:LEU:HD21	1:V:206:ALA:HA	2.01	0.41
1:A:37:GLU:HB3	1:A:41:ARG:NH1	2.35	0.41
1:W:118:TRP:HA	1:W:153:VAL:HG13	2.03	0.41
1:A:101:VAL:HG22	1:A:170:TYR:HD1	1.84	0.41
1:P:63:ARG:NH1	1:P:73:ASP:OD1	2.54	0.41
1:S:133:TRP:CH2	1:U:106:THR:HA	2.56	0.41
1:C:92:LEU:HD11	1:C:95:ALA:HB2	2.01	0.41
1:J:7:LEU:HA	1:J:7:LEU:HD23	1.75	0.41
1:L:134:LYS:NZ	1:L:155:GLU:OE1	2.48	0.41
1:M:105:GLY:HA3	1:M:166:TRP:CE3	2.55	0.41
1:R:101:VAL:HG22	1:R:170:TYR:HD1	1.86	0.41
1:R:118:TRP:HA	1:R:153:VAL:HG13	2.03	0.41
1:U:118:TRP:HA	1:U:153:VAL:HG13	2.02	0.41
1:I:63:ARG:NH1	1:I:73:ASP:OD1	2.54	0.41
1:P:69:HIS:CE1	1:P:213:THR:HG21	2.55	0.41
1:R:128:GLY:O	1:R:145:PRO:HD3	2.20	0.41
1:D:101:VAL:HG22	1:D:170:TYR:HD1	1.85	0.41
1:H:63:ARG:NH2	1:H:71:LEU:O	2.54	0.41
1:O:101:VAL:HG22	1:O:170:TYR:HD1	1.86	0.41
1:I:174:PHE:CD2	1:I:176:PRO:HD2	2.56	0.41
1:R:100:TYR:CE2	1:R:171:GLY:HA3	2.56	0.41
1:X:58:ILE:HD13	1:X:168:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:106:THR:HA	1:Q:133:TRP:CH2	2.56	0.40
1:T:63:ARG:NH1	1:T:73:ASP:OD1	2.54	0.40
1:U:36:ARG:NH1	1:U:120:GLU:OE2	2.55	0.40
1:W:174:PHE:CD2	1:W:176:PRO:HD2	2.56	0.40
1:X:114:SER:HB3	1:X:159:VAL:HG13	2.03	0.40
1:B:143:PHE:CG	1:B:149:ILE:HD11	2.56	0.40
1:D:92:LEU:HD11	1:D:95:ALA:HB2	2.03	0.40
1:F:127:SER:HA	1:F:145:PRO:HG3	2.02	0.40
1:M:128:GLY:HA3	1:M:165:THR:HA	2.03	0.40
1:N:34:PHE:HB2	1:N:170:TYR:CE1	2.56	0.40
1:N:63:ARG:NH1	1:N:73:ASP:OD1	2.55	0.40
1:O:99:GLU:OE2	1:O:170:TYR:OH	2.38	0.40
1:P:133:TRP:CH2	1:R:106:THR:HA	2.56	0.40
1:T:58:ILE:HD13	1:T:168:VAL:HG21	2.02	0.40
1:U:114:SER:HB3	1:U:159:VAL:HG13	2.02	0.40
1:G:100:TYR:CE2	1:G:171:GLY:HA3	2.56	0.40
1:G:127:SER:HA	1:G:145:PRO:HG3	2.04	0.40
1:H:100:TYR:CE2	1:H:171:GLY:HA3	2.55	0.40
1:W:114:SER:HB3	1:W:159:VAL:HG13	2.02	0.40
1:G:143:PHE:CG	1:G:149:ILE:HD11	2.55	0.40
1:H:150:VAL:N	1:W:64:LYS:HZ3	2.19	0.40
1:Q:174:PHE:CD2	1:Q:176:PRO:HD2	2.56	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	211/225 (94%)	207 (98%)	4 (2%)	0	100	100
1	B	211/225 (94%)	206 (98%)	5 (2%)	0	100	100
1	C	212/225 (94%)	206 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	212/225 (94%)	206 (97%)	6 (3%)	0	100	100
1	E	204/225 (91%)	199 (98%)	5 (2%)	0	100	100
1	F	204/225 (91%)	199 (98%)	5 (2%)	0	100	100
1	G	211/225 (94%)	207 (98%)	4 (2%)	0	100	100
1	H	211/225 (94%)	207 (98%)	4 (2%)	0	100	100
1	I	208/225 (92%)	203 (98%)	5 (2%)	0	100	100
1	J	211/225 (94%)	207 (98%)	4 (2%)	0	100	100
1	K	212/225 (94%)	207 (98%)	5 (2%)	0	100	100
1	L	208/225 (92%)	203 (98%)	5 (2%)	0	100	100
1	M	194/225 (86%)	189 (97%)	5 (3%)	0	100	100
1	N	208/225 (92%)	203 (98%)	5 (2%)	0	100	100
1	O	210/225 (93%)	206 (98%)	4 (2%)	0	100	100
1	P	200/225 (89%)	196 (98%)	4 (2%)	0	100	100
1	Q	210/225 (93%)	205 (98%)	5 (2%)	0	100	100
1	R	210/225 (93%)	206 (98%)	4 (2%)	0	100	100
1	S	207/225 (92%)	203 (98%)	3 (1%)	1 (0%)	24	57
1	T	211/225 (94%)	205 (97%)	6 (3%)	0	100	100
1	U	211/225 (94%)	206 (98%)	5 (2%)	0	100	100
1	V	208/225 (92%)	204 (98%)	3 (1%)	1 (0%)	24	57
1	W	211/225 (94%)	205 (97%)	6 (3%)	0	100	100
1	X	211/225 (94%)	207 (98%)	4 (2%)	0	100	100
All	All	5006/5400 (93%)	4892 (98%)	112 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	31	SER
1	V	31	SER

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	178/188 (95%)	177 (99%)	1 (1%)	78	79
1	B	178/188 (95%)	177 (99%)	1 (1%)	78	79
1	C	179/188 (95%)	177 (99%)	2 (1%)	65	73
1	D	179/188 (95%)	178 (99%)	1 (1%)	78	79
1	E	173/188 (92%)	173 (100%)	0	100	100
1	F	173/188 (92%)	172 (99%)	1 (1%)	78	79
1	G	178/188 (95%)	177 (99%)	1 (1%)	78	79
1	H	178/188 (95%)	177 (99%)	1 (1%)	78	79
1	I	176/188 (94%)	175 (99%)	1 (1%)	78	79
1	J	178/188 (95%)	176 (99%)	2 (1%)	65	73
1	K	179/188 (95%)	179 (100%)	0	100	100
1	L	176/188 (94%)	175 (99%)	1 (1%)	78	79
1	M	166/188 (88%)	165 (99%)	1 (1%)	78	79
1	N	176/188 (94%)	175 (99%)	1 (1%)	78	79
1	O	177/188 (94%)	176 (99%)	1 (1%)	78	79
1	P	171/188 (91%)	170 (99%)	1 (1%)	78	79
1	Q	177/188 (94%)	176 (99%)	1 (1%)	78	79
1	R	177/188 (94%)	177 (100%)	0	100	100
1	S	175/188 (93%)	174 (99%)	1 (1%)	78	79
1	T	178/188 (95%)	176 (99%)	2 (1%)	65	73
1	U	178/188 (95%)	178 (100%)	0	100	100
1	V	176/188 (94%)	175 (99%)	1 (1%)	78	79
1	W	178/188 (95%)	177 (99%)	1 (1%)	78	79
1	X	178/188 (95%)	177 (99%)	1 (1%)	78	79
All	All	4232/4512 (94%)	4209 (100%)	23 (0%)	81	81

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	TYR
1	C	27	LEU
1	C	117	TYR

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Mol	Chain	Res	Type
1	B	117	TYR
1	D	117	TYR
1	F	117	TYR
1	G	117	TYR
1	H	5	LEU
1	I	117	TYR
1	J	7	LEU
1	J	117	TYR
1	L	117	TYR
1	M	117	TYR
1	N	117	TYR
1	O	117	TYR
1	P	117	TYR
1	Q	117	TYR
1	S	117	TYR
1	T	10	VAL
1	T	117	TYR
1	V	117	TYR
1	W	117	TYR
1	X	7	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	HIS
1	C	191	GLN
1	E	69	HIS
1	E	191	GLN
1	E	214	HIS
1	B	69	HIS
1	F	82	ASN
1	F	214	HIS
1	H	82	ASN
1	I	82	ASN
1	I	191	GLN
1	J	191	GLN
1	K	191	GLN
1	L	82	ASN
1	L	94	HIS
1	L	191	GLN
1	L	214	HIS
1	M	69	HIS

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Mol	Chain	Res	Type
1	M	94	HIS
1	N	66	HIS
1	N	82	ASN
1	N	191	GLN
1	P	69	HIS
1	P	151	HIS
1	R	82	ASN
1	S	69	HIS
1	U	82	ASN
1	V	94	HIS
1	V	191	GLN
1	W	66	HIS
1	W	82	ASN
1	W	191	GLN
1	W	214	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)

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	88E	F	301	-	28,28,28	2.46	8 (28%)	36,38,38	2.46	7 (19%)
2	88E	K	301	-	28,28,28	2.48	8 (28%)	36,38,38	2.42	6 (16%)
2	88E	Q	301	-	28,28,28	2.48	8 (28%)	36,38,38	2.45	7 (19%)
2	88E	S	301	-	28,28,28	2.45	8 (28%)	36,38,38	2.48	8 (22%)
2	88E	W	301	-	28,28,28	2.50	8 (28%)	36,38,38	2.58	7 (19%)
2	88E	J	301	-	28,28,28	2.51	8 (28%)	36,38,38	2.48	7 (19%)
2	88E	O	301	-	28,28,28	2.51	8 (28%)	36,38,38	2.39	6 (16%)
2	88E	R	301	-	28,28,28	2.50	8 (28%)	36,38,38	2.44	7 (19%)
2	88E	T	301	-	28,28,28	2.49	8 (28%)	36,38,38	2.45	7 (19%)
2	88E	X	301	-	28,28,28	2.51	8 (28%)	36,38,38	2.40	6 (16%)
2	88E	C	301	-	28,28,28	2.49	8 (28%)	36,38,38	2.38	6 (16%)
2	88E	I	301	-	28,28,28	2.46	8 (28%)	36,38,38	2.46	7 (19%)
2	88E	M	301	-	28,28,28	2.46	7 (25%)	36,38,38	2.42	6 (16%)
2	88E	P	302	-	28,28,28	2.48	8 (28%)	36,38,38	2.33	8 (22%)
2	88E	L	301	-	28,28,28	2.46	8 (28%)	36,38,38	2.43	7 (19%)
2	88E	D	301	-	28,28,28	2.47	8 (28%)	36,38,38	2.33	6 (16%)
2	88E	A	301	-	28,28,28	2.51	8 (28%)	36,38,38	2.51	8 (22%)
2	88E	V	301	-	28,28,28	2.47	8 (28%)	36,38,38	2.49	7 (19%)
2	88E	P	301	-	28,28,28	2.46	9 (32%)	36,38,38	2.43	7 (19%)
2	88E	G	301	-	28,28,28	2.51	8 (28%)	36,38,38	2.44	7 (19%)
2	88E	U	301	-	28,28,28	2.49	8 (28%)	36,38,38	2.40	6 (16%)
2	88E	E	301	-	28,28,28	2.47	8 (28%)	36,38,38	2.43	6 (16%)
2	88E	B	301	-	28,28,28	2.50	8 (28%)	36,38,38	2.45	8 (22%)
2	88E	N	301	-	28,28,28	2.49	8 (28%)	36,38,38	2.56	7 (19%)
2	88E	H	301	-	28,28,28	2.48	8 (28%)	36,38,38	2.33	6 (16%)

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	88E	F	301	-	-	3/10/18/18	0/4/4/4
2	88E	K	301	-	-	3/10/18/18	0/4/4/4
2	88E	Q	301	-	-	3/10/18/18	0/4/4/4
2	88E	S	301	-	-	3/10/18/18	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	88E	W	301	-	-	3/10/18/18	0/4/4/4
2	88E	J	301	-	-	3/10/18/18	0/4/4/4
2	88E	O	301	-	-	3/10/18/18	0/4/4/4
2	88E	R	301	-	-	3/10/18/18	0/4/4/4
2	88E	T	301	-	-	3/10/18/18	0/4/4/4
2	88E	X	301	-	-	3/10/18/18	0/4/4/4
2	88E	C	301	-	-	3/10/18/18	0/4/4/4
2	88E	I	301	-	-	3/10/18/18	0/4/4/4
2	88E	M	301	-	-	3/10/18/18	0/4/4/4
2	88E	P	302	-	-	3/10/18/18	0/4/4/4
2	88E	L	301	-	-	3/10/18/18	0/4/4/4
2	88E	D	301	-	-	3/10/18/18	0/4/4/4
2	88E	A	301	-	-	3/10/18/18	0/4/4/4
2	88E	V	301	-	-	3/10/18/18	0/4/4/4
2	88E	P	301	-	-	3/10/18/18	0/4/4/4
2	88E	G	301	-	-	3/10/18/18	0/4/4/4
2	88E	U	301	-	-	3/10/18/18	0/4/4/4
2	88E	E	301	-	-	3/10/18/18	0/4/4/4
2	88E	B	301	-	-	3/10/18/18	0/4/4/4
2	88E	N	301	-	-	3/10/18/18	0/4/4/4
2	88E	H	301	-	-	3/10/18/18	0/4/4/4

All (200) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	302	88E	C19-N20	-8.94	1.27	1.47
2	J	301	88E	C19-N20	-8.90	1.27	1.47
2	E	301	88E	C19-N20	-8.87	1.27	1.47
2	A	301	88E	C19-N20	-8.87	1.27	1.47
2	O	301	88E	C19-N20	-8.86	1.27	1.47
2	B	301	88E	C19-N20	-8.85	1.27	1.47
2	G	301	88E	C19-N20	-8.85	1.27	1.47
2	M	301	88E	C19-N20	-8.84	1.27	1.47
2	T	301	88E	C19-N20	-8.84	1.27	1.47
2	P	301	88E	C19-N20	-8.81	1.27	1.47
2	X	301	88E	C19-N20	-8.81	1.27	1.47
2	V	301	88E	C19-N20	-8.79	1.27	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	88E	C19-N20	-8.79	1.27	1.47
2	H	301	88E	C19-N20	-8.78	1.27	1.47
2	R	301	88E	C19-N20	-8.78	1.27	1.47
2	K	301	88E	C19-N20	-8.78	1.27	1.47
2	C	301	88E	C19-N20	-8.77	1.27	1.47
2	Q	301	88E	C19-N20	-8.77	1.27	1.47
2	S	301	88E	C19-N20	-8.75	1.27	1.47
2	D	301	88E	C19-N20	-8.75	1.27	1.47
2	F	301	88E	C19-N20	-8.75	1.27	1.47
2	U	301	88E	C19-N20	-8.75	1.27	1.47
2	W	301	88E	C19-N20	-8.75	1.27	1.47
2	I	301	88E	C19-N20	-8.73	1.27	1.47
2	N	301	88E	C19-N20	-8.72	1.27	1.47
2	W	301	88E	O17-C4	4.81	1.40	1.35
2	N	301	88E	O17-C4	4.73	1.40	1.35
2	X	301	88E	O17-C4	4.65	1.40	1.35
2	U	301	88E	O17-C4	4.65	1.40	1.35
2	A	301	88E	O17-C4	4.61	1.40	1.35
2	X	301	88E	C2-N6	-4.61	1.31	1.37
2	O	301	88E	O17-C4	4.60	1.40	1.35
2	R	301	88E	O17-C4	4.59	1.40	1.35
2	J	301	88E	O17-C4	4.55	1.40	1.35
2	O	301	88E	C2-N6	-4.55	1.31	1.37
2	C	301	88E	O17-C4	4.54	1.40	1.35
2	T	301	88E	O17-C4	4.54	1.40	1.35
2	Q	301	88E	O17-C4	4.51	1.40	1.35
2	G	301	88E	O17-C4	4.47	1.40	1.35
2	P	301	88E	C2-N6	-4.46	1.31	1.37
2	K	301	88E	O17-C4	4.45	1.40	1.35
2	D	301	88E	O17-C4	4.44	1.40	1.35
2	B	301	88E	O17-C4	4.43	1.40	1.35
2	I	301	88E	C2-N6	-4.42	1.31	1.37
2	S	301	88E	C2-N6	-4.42	1.31	1.37
2	H	301	88E	O17-C4	4.39	1.40	1.35
2	V	301	88E	O17-C4	4.39	1.40	1.35
2	R	301	88E	C2-N6	-4.39	1.31	1.37
2	H	301	88E	C2-N6	-4.37	1.31	1.37
2	I	301	88E	O17-C4	4.36	1.40	1.35
2	F	301	88E	C2-N6	-4.36	1.31	1.37
2	K	301	88E	C2-N6	-4.36	1.31	1.37
2	W	301	88E	C2-N6	-4.35	1.31	1.37
2	U	301	88E	C2-N6	-4.35	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	88E	C2-N6	-4.35	1.31	1.37
2	C	301	88E	C2-N6	-4.34	1.31	1.37
2	D	301	88E	C2-N6	-4.34	1.31	1.37
2	F	301	88E	O17-C4	4.32	1.40	1.35
2	V	301	88E	C2-N6	-4.32	1.31	1.37
2	L	301	88E	O17-C4	4.31	1.40	1.35
2	G	301	88E	C2-N6	-4.31	1.31	1.37
2	L	301	88E	C2-N6	-4.30	1.31	1.37
2	M	301	88E	C2-N6	-4.30	1.31	1.37
2	N	301	88E	C2-N6	-4.30	1.31	1.37
2	A	301	88E	C2-N6	-4.30	1.31	1.37
2	Q	301	88E	C2-N6	-4.29	1.31	1.37
2	E	301	88E	O17-C4	4.28	1.40	1.35
2	M	301	88E	O17-C4	4.27	1.40	1.35
2	J	301	88E	C2-N6	-4.24	1.31	1.37
2	T	301	88E	C2-N6	-4.22	1.31	1.37
2	B	301	88E	C2-N6	-4.20	1.31	1.37
2	P	301	88E	O17-C4	4.04	1.40	1.35
2	S	301	88E	O17-C4	4.04	1.40	1.35
2	P	302	88E	O17-C4	4.02	1.40	1.35
2	P	302	88E	C2-N6	-4.02	1.31	1.37
2	P	302	88E	C21-N20	-3.27	1.38	1.46
2	G	301	88E	C25-N20	-3.23	1.38	1.46
2	O	301	88E	C25-N20	-3.22	1.38	1.46
2	J	301	88E	C25-N20	-3.22	1.38	1.46
2	A	301	88E	C25-N20	-3.21	1.38	1.46
2	M	301	88E	C25-N20	-3.21	1.38	1.46
2	B	301	88E	C25-N20	-3.20	1.38	1.46
2	X	301	88E	C25-N20	-3.20	1.38	1.46
2	N	301	88E	C25-N20	-3.20	1.38	1.46
2	K	301	88E	C25-N20	-3.20	1.38	1.46
2	P	301	88E	C21-N20	-3.20	1.38	1.46
2	U	301	88E	C21-N20	-3.19	1.38	1.46
2	T	301	88E	C25-N20	-3.19	1.38	1.46
2	P	302	88E	C25-N20	-3.19	1.38	1.46
2	R	301	88E	C21-N20	-3.19	1.38	1.46
2	C	301	88E	C25-N20	-3.19	1.38	1.46
2	W	301	88E	C25-N20	-3.19	1.38	1.46
2	P	301	88E	C25-N20	-3.19	1.38	1.46
2	O	301	88E	C21-N20	-3.18	1.38	1.46
2	D	301	88E	C21-N20	-3.18	1.38	1.46
2	S	301	88E	C25-N20	-3.18	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	301	88E	C21-N20	-3.18	1.38	1.46
2	K	301	88E	C21-N20	-3.18	1.38	1.46
2	R	301	88E	C25-N20	-3.18	1.38	1.46
2	H	301	88E	C25-N20	-3.17	1.38	1.46
2	V	301	88E	C25-N20	-3.17	1.38	1.46
2	Q	301	88E	C25-N20	-3.17	1.38	1.46
2	B	301	88E	C21-N20	-3.17	1.38	1.46
2	S	301	88E	C21-N20	-3.17	1.38	1.46
2	H	301	88E	C21-N20	-3.17	1.38	1.46
2	A	301	88E	C21-N20	-3.17	1.38	1.46
2	E	301	88E	C21-N20	-3.17	1.38	1.46
2	G	301	88E	C21-N20	-3.16	1.38	1.46
2	U	301	88E	C25-N20	-3.16	1.38	1.46
2	T	301	88E	C21-N20	-3.16	1.38	1.46
2	L	301	88E	C25-N20	-3.16	1.38	1.46
2	E	301	88E	C25-N20	-3.16	1.38	1.46
2	L	301	88E	C21-N20	-3.15	1.38	1.46
2	V	301	88E	C21-N20	-3.15	1.38	1.46
2	C	301	88E	C21-N20	-3.14	1.38	1.46
2	I	301	88E	C25-N20	-3.14	1.38	1.46
2	M	301	88E	C21-N20	-3.14	1.38	1.46
2	Q	301	88E	C21-N20	-3.14	1.38	1.46
2	J	301	88E	C21-N20	-3.14	1.38	1.46
2	D	301	88E	C25-N20	-3.13	1.38	1.46
2	N	301	88E	C21-N20	-3.13	1.38	1.46
2	F	301	88E	C21-N20	-3.13	1.38	1.46
2	F	301	88E	C25-N20	-3.12	1.38	1.46
2	W	301	88E	C21-N20	-3.12	1.38	1.46
2	I	301	88E	C21-N20	-3.09	1.38	1.46
2	P	302	88E	N6-N5	-2.69	1.33	1.39
2	M	301	88E	N6-N5	-2.57	1.33	1.39
2	P	301	88E	N6-N5	-2.56	1.33	1.39
2	G	301	88E	N6-N5	-2.55	1.33	1.39
2	D	301	88E	N6-N5	-2.53	1.33	1.39
2	B	301	88E	N6-N5	-2.52	1.33	1.39
2	S	301	88E	N6-N5	-2.51	1.33	1.39
2	O	301	88E	N6-N5	-2.51	1.33	1.39
2	H	301	88E	N6-N5	-2.50	1.33	1.39
2	T	301	88E	N6-N5	-2.50	1.33	1.39
2	E	301	88E	N6-N5	-2.49	1.33	1.39
2	T	301	88E	C9-C14	-2.49	1.36	1.42
2	X	301	88E	N6-N5	-2.48	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	301	88E	N6-N5	-2.48	1.33	1.39
2	U	301	88E	N6-N5	-2.48	1.33	1.39
2	V	301	88E	N6-N5	-2.48	1.33	1.39
2	C	301	88E	N6-N5	-2.47	1.33	1.39
2	C	301	88E	C9-C14	-2.46	1.36	1.42
2	A	301	88E	N6-N5	-2.46	1.33	1.39
2	E	301	88E	C9-C14	-2.46	1.36	1.42
2	F	301	88E	C9-C14	-2.46	1.36	1.42
2	V	301	88E	C9-C14	-2.45	1.36	1.42
2	L	301	88E	N6-N5	-2.45	1.33	1.39
2	I	301	88E	C9-C14	-2.45	1.36	1.42
2	D	301	88E	C9-C14	-2.45	1.36	1.42
2	J	301	88E	N6-N5	-2.45	1.33	1.39
2	A	301	88E	C9-C14	-2.44	1.36	1.42
2	K	301	88E	N6-N5	-2.44	1.33	1.39
2	Q	301	88E	N6-N5	-2.44	1.33	1.39
2	I	301	88E	N6-N5	-2.44	1.33	1.39
2	J	301	88E	C9-C14	-2.43	1.36	1.42
2	X	301	88E	C9-C14	-2.43	1.36	1.42
2	P	302	88E	C3-C2	2.43	1.41	1.37
2	Q	301	88E	C9-C14	-2.42	1.36	1.42
2	K	301	88E	C9-C14	-2.42	1.36	1.42
2	W	301	88E	C9-C14	-2.42	1.36	1.42
2	G	301	88E	C9-C14	-2.42	1.36	1.42
2	B	301	88E	C3-C2	2.42	1.41	1.37
2	P	301	88E	C9-C14	-2.42	1.36	1.42
2	P	302	88E	C9-C14	-2.42	1.36	1.42
2	H	301	88E	C9-C14	-2.42	1.36	1.42
2	B	301	88E	C9-C14	-2.41	1.36	1.42
2	F	301	88E	N6-N5	-2.41	1.33	1.39
2	S	301	88E	C9-C14	-2.40	1.36	1.42
2	L	301	88E	C9-C14	-2.40	1.36	1.42
2	N	301	88E	C9-C14	-2.39	1.36	1.42
2	O	301	88E	C9-C14	-2.39	1.36	1.42
2	J	301	88E	C3-C2	2.39	1.41	1.37
2	U	301	88E	C9-C14	-2.39	1.36	1.42
2	R	301	88E	C9-C14	-2.39	1.36	1.42
2	M	301	88E	C9-C14	-2.38	1.36	1.42
2	G	301	88E	C3-C2	2.36	1.41	1.37
2	A	301	88E	C3-C2	2.32	1.41	1.37
2	R	301	88E	C3-C2	2.32	1.41	1.37
2	N	301	88E	N6-N5	-2.31	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	301	88E	C3-C2	2.29	1.41	1.37
2	T	301	88E	C3-C2	2.28	1.41	1.37
2	Q	301	88E	C3-C2	2.27	1.41	1.37
2	H	301	88E	C3-C2	2.27	1.41	1.37
2	N	301	88E	C3-C2	2.25	1.41	1.37
2	W	301	88E	N6-N5	-2.24	1.34	1.39
2	W	301	88E	C3-C2	2.24	1.41	1.37
2	C	301	88E	C3-C2	2.23	1.41	1.37
2	X	301	88E	C3-C2	2.21	1.41	1.37
2	D	301	88E	C3-C2	2.21	1.41	1.37
2	K	301	88E	C3-C2	2.20	1.41	1.37
2	O	301	88E	C3-C2	2.19	1.41	1.37
2	L	301	88E	C3-C2	2.16	1.41	1.37
2	I	301	88E	C3-C2	2.14	1.41	1.37
2	F	301	88E	C3-C2	2.12	1.41	1.37
2	E	301	88E	C3-C2	2.09	1.41	1.37
2	P	301	88E	C3-C2	2.07	1.41	1.37
2	S	301	88E	O17-C18	-2.05	1.39	1.45
2	P	301	88E	O17-C18	-2.04	1.39	1.45
2	V	301	88E	C3-C2	2.04	1.41	1.37

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	301	88E	C3-C4-N5	-8.39	107.46	113.77
2	A	301	88E	C3-C4-N5	-8.38	107.47	113.77
2	N	301	88E	C3-C4-N5	-8.34	107.50	113.77
2	J	301	88E	C3-C4-N5	-8.30	107.53	113.77
2	R	301	88E	C3-C4-N5	-8.29	107.53	113.77
2	O	301	88E	C3-C4-N5	-8.28	107.54	113.77
2	Q	301	88E	C3-C4-N5	-8.25	107.57	113.77
2	T	301	88E	C3-C4-N5	-8.24	107.57	113.77
2	G	301	88E	C3-C4-N5	-8.23	107.58	113.77
2	X	301	88E	C3-C4-N5	-8.22	107.58	113.77
2	U	301	88E	C3-C4-N5	-8.20	107.61	113.77
2	B	301	88E	C3-C4-N5	-8.12	107.67	113.77
2	K	301	88E	C3-C4-N5	-8.04	107.72	113.77
2	P	302	88E	C4-N5-N6	8.00	110.10	103.11
2	J	301	88E	C4-N5-N6	7.96	110.06	103.11
2	A	301	88E	C4-N5-N6	7.96	110.06	103.11
2	D	301	88E	C3-C4-N5	-7.94	107.80	113.77
2	B	301	88E	C4-N5-N6	7.93	110.04	103.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	301	88E	C3-C4-N5	-7.91	107.82	113.77
2	C	301	88E	C3-C4-N5	-7.91	107.82	113.77
2	G	301	88E	C4-N5-N6	7.85	109.96	103.11
2	T	301	88E	C4-N5-N6	7.84	109.95	103.11
2	I	301	88E	C3-C4-N5	-7.83	107.88	113.77
2	P	302	88E	C3-C4-N5	-7.83	107.88	113.77
2	L	301	88E	C3-C4-N5	-7.78	107.92	113.77
2	N	301	88E	C4-N5-N6	7.76	109.89	103.11
2	R	301	88E	C4-N5-N6	7.73	109.86	103.11
2	Q	301	88E	C4-N5-N6	7.71	109.84	103.11
2	W	301	88E	C4-N5-N6	7.71	109.84	103.11
2	F	301	88E	C3-C4-N5	-7.59	108.06	113.77
2	U	301	88E	C4-N5-N6	7.56	109.71	103.11
2	E	301	88E	C3-C4-N5	-7.55	108.09	113.77
2	V	301	88E	C3-C4-N5	-7.54	108.10	113.77
2	O	301	88E	C4-N5-N6	7.49	109.66	103.11
2	P	301	88E	C3-C4-N5	-7.47	108.15	113.77
2	X	301	88E	C4-N5-N6	7.45	109.61	103.11
2	M	301	88E	C3-C4-N5	-7.42	108.19	113.77
2	K	301	88E	C4-N5-N6	7.41	109.58	103.11
2	S	301	88E	C3-C4-N5	-7.40	108.20	113.77
2	I	301	88E	C4-N5-N6	7.33	109.52	103.11
2	H	301	88E	C4-N5-N6	7.31	109.50	103.11
2	L	301	88E	C4-N5-N6	7.26	109.45	103.11
2	C	301	88E	C4-N5-N6	7.23	109.43	103.11
2	F	301	88E	C4-N5-N6	7.21	109.40	103.11
2	D	301	88E	C4-N5-N6	7.19	109.39	103.11
2	V	301	88E	C4-N5-N6	7.05	109.27	103.11
2	E	301	88E	C4-N5-N6	7.04	109.26	103.11
2	P	301	88E	C4-N5-N6	7.03	109.25	103.11
2	S	301	88E	C4-N5-N6	6.96	109.19	103.11
2	M	301	88E	C4-N5-N6	6.92	109.15	103.11
2	S	301	88E	C7-N6-C2	-6.20	122.74	129.43
2	V	301	88E	C7-N6-C2	-6.16	122.79	129.43
2	W	301	88E	C7-N6-C2	-5.96	123.00	129.43
2	M	301	88E	C7-N6-C2	-5.88	123.09	129.43
2	F	301	88E	C7-N6-C2	-5.85	123.12	129.43
2	E	301	88E	C7-N6-C2	-5.79	123.19	129.43
2	P	301	88E	C7-N6-C2	-5.71	123.27	129.43
2	N	301	88E	C7-N6-C2	-5.65	123.33	129.43
2	I	301	88E	C7-N6-C2	-5.63	123.36	129.43
2	L	301	88E	C7-N6-C2	-5.54	123.45	129.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	301	88E	C7-N6-N5	5.51	126.66	118.67
2	V	301	88E	C7-N6-N5	5.48	126.61	118.67
2	S	301	88E	C7-N6-N5	5.48	126.61	118.67
2	N	301	88E	C7-N6-N5	5.34	126.41	118.67
2	K	301	88E	C7-N6-C2	-5.33	123.69	129.43
2	C	301	88E	C7-N6-C2	-5.32	123.70	129.43
2	F	301	88E	C7-N6-N5	5.31	126.37	118.67
2	M	301	88E	C7-N6-N5	5.17	126.16	118.67
2	X	301	88E	C7-N6-C2	-5.16	123.87	129.43
2	I	301	88E	C7-N6-N5	5.14	126.13	118.67
2	E	301	88E	C7-N6-N5	5.14	126.11	118.67
2	D	301	88E	C7-N6-C2	-5.13	123.90	129.43
2	P	301	88E	C7-N6-N5	5.00	125.92	118.67
2	A	301	88E	C7-N6-C2	-4.97	124.07	129.43
2	L	301	88E	C7-N6-N5	4.97	125.87	118.67
2	H	301	88E	C7-N6-C2	-4.89	124.16	129.43
2	R	301	88E	C7-N6-C2	-4.88	124.16	129.43
2	O	301	88E	C7-N6-C2	-4.87	124.18	129.43
2	Q	301	88E	C7-N6-C2	-4.87	124.18	129.43
2	U	301	88E	C7-N6-C2	-4.86	124.18	129.43
2	A	301	88E	C7-N6-N5	4.83	125.67	118.67
2	K	301	88E	C7-N6-N5	4.80	125.63	118.67
2	J	301	88E	C7-N6-C2	-4.76	124.30	129.43
2	T	301	88E	C7-N6-C2	-4.69	124.38	129.43
2	C	301	88E	C7-N6-N5	4.66	125.42	118.67
2	J	301	88E	C7-N6-N5	4.64	125.39	118.67
2	Q	301	88E	C7-N6-N5	4.60	125.34	118.67
2	B	301	88E	C7-N6-C2	-4.58	124.49	129.43
2	X	301	88E	C7-N6-N5	4.57	125.30	118.67
2	G	301	88E	C7-N6-C2	-4.56	124.51	129.43
2	R	301	88E	C7-N6-N5	4.56	125.27	118.67
2	T	301	88E	C7-N6-N5	4.53	125.24	118.67
2	B	301	88E	C7-N6-N5	4.49	125.17	118.67
2	U	301	88E	C7-N6-N5	4.43	125.09	118.67
2	O	301	88E	C7-N6-N5	4.38	125.02	118.67
2	G	301	88E	C7-N6-N5	4.37	125.01	118.67
2	D	301	88E	C7-N6-N5	4.37	125.00	118.67
2	H	301	88E	C7-N6-N5	4.29	124.90	118.67
2	F	301	88E	C3-C2-N6	3.37	107.58	105.39
2	I	301	88E	C3-C2-N6	3.34	107.56	105.39
2	V	301	88E	C3-C2-N6	3.34	107.56	105.39
2	S	301	88E	C3-C2-N6	3.29	107.53	105.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	301	88E	C3-C2-N6	3.27	107.52	105.39
2	P	302	88E	C18-O17-C4	-3.23	110.72	117.09
2	E	301	88E	C3-C2-N6	3.22	107.48	105.39
2	M	301	88E	C3-C2-N6	3.14	107.43	105.39
2	A	301	88E	C3-C2-N6	3.13	107.42	105.39
2	W	301	88E	C3-C2-N6	3.12	107.42	105.39
2	L	301	88E	C3-C2-N6	3.05	107.38	105.39
2	P	301	88E	C3-C2-N6	3.05	107.38	105.39
2	P	302	88E	C7-N6-N5	3.02	123.06	118.67
2	J	301	88E	C3-C2-N6	3.02	107.36	105.39
2	T	301	88E	C3-C2-N6	3.02	107.35	105.39
2	B	301	88E	C3-C2-N6	3.01	107.35	105.39
2	Q	301	88E	C3-C2-N6	2.94	107.30	105.39
2	G	301	88E	C3-C2-N6	2.92	107.29	105.39
2	R	301	88E	C3-C2-N6	2.91	107.29	105.39
2	P	302	88E	C3-C2-N6	2.84	107.24	105.39
2	K	301	88E	C3-C2-N6	2.81	107.22	105.39
2	X	301	88E	C3-C2-N6	2.76	107.19	105.39
2	P	302	88E	C1-C2-C3	-2.75	125.29	129.90
2	U	301	88E	C3-C2-N6	2.73	107.17	105.39
2	O	301	88E	C3-C2-N6	2.70	107.15	105.39
2	N	301	88E	C2-N6-N5	-2.66	110.24	111.97
2	A	301	88E	C2-N6-N5	-2.63	110.27	111.97
2	V	301	88E	C1-C2-C3	-2.62	125.52	129.90
2	P	302	88E	C7-N6-C2	-2.61	126.61	129.43
2	M	301	88E	C1-C2-C3	-2.61	125.54	129.90
2	C	301	88E	C3-C2-N6	2.57	107.06	105.39
2	J	301	88E	C2-N6-N5	-2.57	110.30	111.97
2	B	301	88E	C2-N6-N5	-2.54	110.33	111.97
2	W	301	88E	C2-N6-N5	-2.53	110.33	111.97
2	P	302	88E	C2-N6-N5	-2.53	110.33	111.97
2	E	301	88E	C1-C2-C3	-2.52	125.69	129.90
2	N	301	88E	C1-C2-C3	-2.49	125.74	129.90
2	S	301	88E	C1-C2-C3	-2.48	125.75	129.90
2	P	301	88E	C18-O17-C4	-2.46	112.23	117.09
2	T	301	88E	C2-N6-N5	-2.45	110.38	111.97
2	F	301	88E	C1-C2-C3	-2.45	125.80	129.90
2	H	301	88E	C3-C2-N6	2.44	106.98	105.39
2	L	301	88E	C1-C2-C3	-2.44	125.81	129.90
2	T	301	88E	C1-C2-C3	-2.44	125.82	129.90
2	Q	301	88E	C1-C2-C3	-2.40	125.88	129.90
2	J	301	88E	C1-C2-C3	-2.39	125.90	129.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	88E	C1-C2-C3	-2.38	125.92	129.90
2	W	301	88E	C1-C2-C3	-2.37	125.93	129.90
2	I	301	88E	C1-C2-C3	-2.37	125.94	129.90
2	S	301	88E	C18-O17-C4	-2.36	112.43	117.09
2	K	301	88E	C1-C2-C3	-2.35	125.97	129.90
2	A	301	88E	C1-C2-C3	-2.33	126.01	129.90
2	P	301	88E	C1-C2-C3	-2.32	126.02	129.90
2	B	301	88E	C1-C2-C3	-2.31	126.03	129.90
2	D	301	88E	C3-C2-N6	2.30	106.89	105.39
2	G	301	88E	C2-N6-N5	-2.30	110.48	111.97
2	Q	301	88E	C2-N6-N5	-2.30	110.48	111.97
2	F	301	88E	C2-N6-N5	-2.27	110.50	111.97
2	U	301	88E	C1-C2-C3	-2.27	126.11	129.90
2	D	301	88E	C1-C2-C3	-2.26	126.13	129.90
2	H	301	88E	C1-C2-C3	-2.25	126.14	129.90
2	I	301	88E	C2-N6-N5	-2.25	110.51	111.97
2	G	301	88E	C1-C2-C3	-2.23	126.17	129.90
2	O	301	88E	C1-C2-C3	-2.21	126.21	129.90
2	R	301	88E	C1-C2-C3	-2.19	126.25	129.90
2	R	301	88E	C2-N6-N5	-2.18	110.56	111.97
2	V	301	88E	C2-N6-N5	-2.12	110.59	111.97
2	X	301	88E	C1-C2-C3	-2.11	126.38	129.90
2	B	301	88E	C18-O17-C4	-2.11	112.93	117.09
2	A	301	88E	C18-O17-C4	-2.10	112.93	117.09
2	S	301	88E	C2-N6-N5	-2.05	110.64	111.97
2	L	301	88E	C2-N6-N5	-2.01	110.67	111.97

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	88E	C3-C4-O17-C18
2	C	301	88E	C3-C4-O17-C18
2	E	301	88E	C3-C4-O17-C18
2	B	301	88E	C3-C4-O17-C18
2	D	301	88E	C3-C4-O17-C18
2	F	301	88E	C3-C4-O17-C18
2	G	301	88E	C3-C4-O17-C18
2	H	301	88E	C3-C4-O17-C18
2	I	301	88E	C3-C4-O17-C18
2	J	301	88E	C3-C4-O17-C18
2	K	301	88E	C3-C4-O17-C18

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Mol	Chain	Res	Type	Atoms
2	L	301	88E	C3-C4-O17-C18
2	M	301	88E	C3-C4-O17-C18
2	N	301	88E	C3-C4-O17-C18
2	O	301	88E	C3-C4-O17-C18
2	P	301	88E	C3-C4-O17-C18
2	P	302	88E	C3-C4-O17-C18
2	P	302	88E	N5-C4-O17-C18
2	Q	301	88E	C3-C4-O17-C18
2	R	301	88E	C3-C4-O17-C18
2	S	301	88E	C3-C4-O17-C18
2	T	301	88E	C3-C4-O17-C18
2	U	301	88E	C3-C4-O17-C18
2	V	301	88E	C3-C4-O17-C18
2	W	301	88E	C3-C4-O17-C18
2	X	301	88E	C3-C4-O17-C18
2	E	301	88E	C18-C19-N20-C25
2	F	301	88E	C18-C19-N20-C25
2	I	301	88E	C18-C19-N20-C25
2	L	301	88E	C18-C19-N20-C25
2	M	301	88E	C18-C19-N20-C25
2	D	301	88E	C18-C19-N20-C25
2	N	301	88E	C18-C19-N20-C25
2	Q	301	88E	C18-C19-N20-C25
2	S	301	88E	C18-C19-N20-C25
2	U	301	88E	C18-C19-N20-C25
2	V	301	88E	C18-C19-N20-C25
2	X	301	88E	C18-C19-N20-C25
2	A	301	88E	C18-C19-N20-C25
2	C	301	88E	C18-C19-N20-C25
2	B	301	88E	C18-C19-N20-C25
2	G	301	88E	C18-C19-N20-C25
2	H	301	88E	C18-C19-N20-C25
2	K	301	88E	C18-C19-N20-C25
2	O	301	88E	C18-C19-N20-C25
2	P	301	88E	C18-C19-N20-C25
2	R	301	88E	C18-C19-N20-C25
2	T	301	88E	C18-C19-N20-C25
2	W	301	88E	C18-C19-N20-C25
2	J	301	88E	C18-C19-N20-C25
2	P	302	88E	O17-C18-C19-N20
2	A	301	88E	N5-C4-O17-C18
2	C	301	88E	N5-C4-O17-C18

Continued on next page...

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Mol	Chain	Res	Type	Atoms
2	E	301	88E	N5-C4-O17-C18
2	B	301	88E	N5-C4-O17-C18
2	D	301	88E	N5-C4-O17-C18
2	F	301	88E	N5-C4-O17-C18
2	G	301	88E	N5-C4-O17-C18
2	H	301	88E	N5-C4-O17-C18
2	I	301	88E	N5-C4-O17-C18
2	J	301	88E	N5-C4-O17-C18
2	K	301	88E	N5-C4-O17-C18
2	L	301	88E	N5-C4-O17-C18
2	M	301	88E	N5-C4-O17-C18
2	N	301	88E	N5-C4-O17-C18
2	O	301	88E	N5-C4-O17-C18
2	P	301	88E	N5-C4-O17-C18
2	Q	301	88E	N5-C4-O17-C18
2	R	301	88E	N5-C4-O17-C18
2	S	301	88E	N5-C4-O17-C18
2	T	301	88E	N5-C4-O17-C18
2	U	301	88E	N5-C4-O17-C18
2	V	301	88E	N5-C4-O17-C18
2	W	301	88E	N5-C4-O17-C18
2	X	301	88E	N5-C4-O17-C18

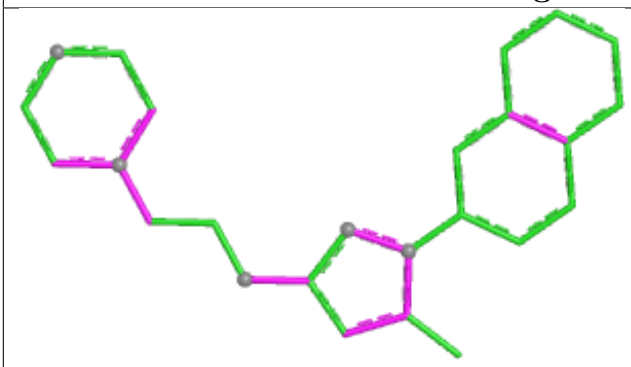
There are no ring outliers.

1 monomer is involved in 1 short contact:

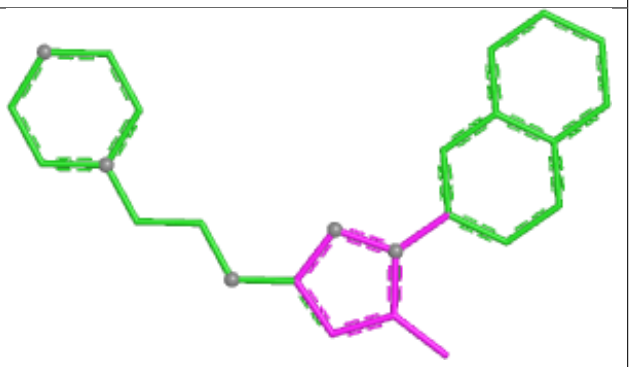
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	302	88E	1	0

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 then 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.

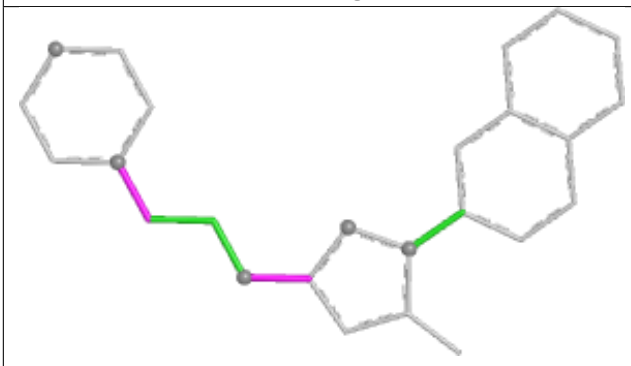
Ligand 88E F 301



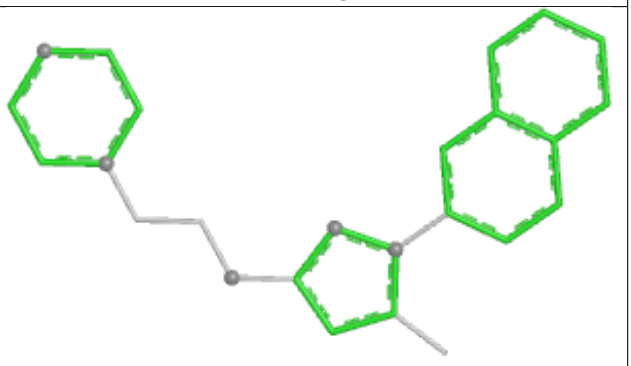
Bond lengths



Bond angles

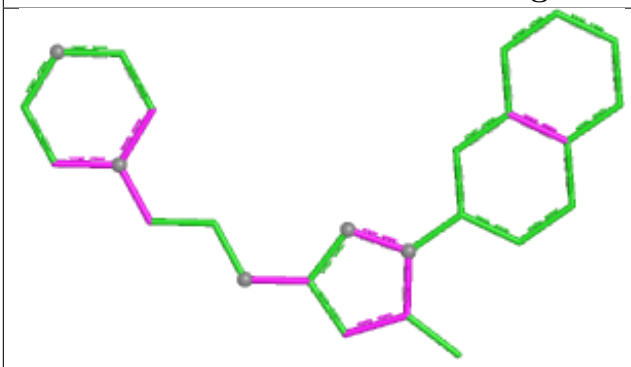


Torsions



Rings

Ligand 88E K 301



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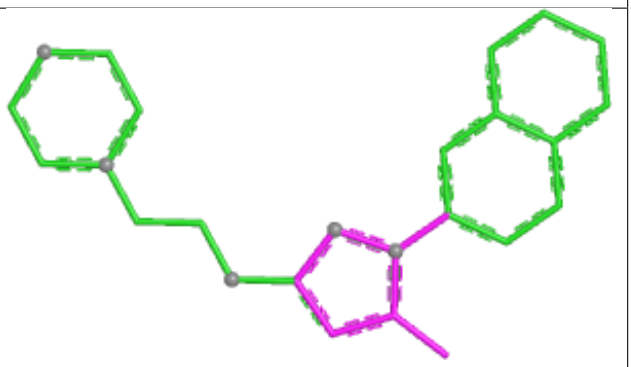
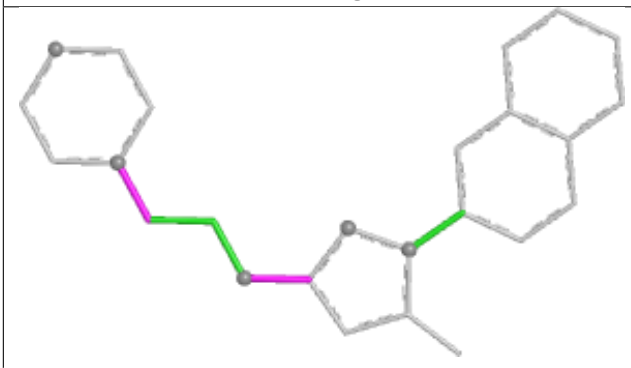


Bond angles



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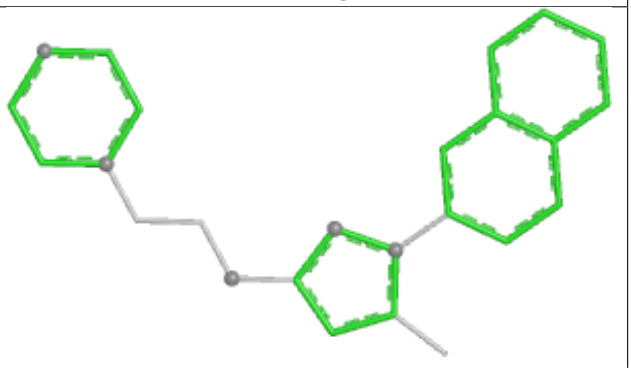

Rings

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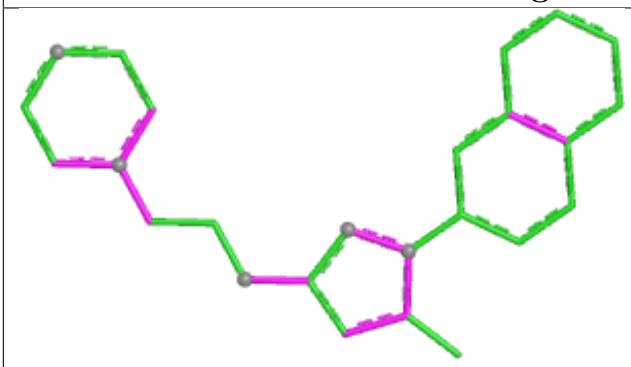

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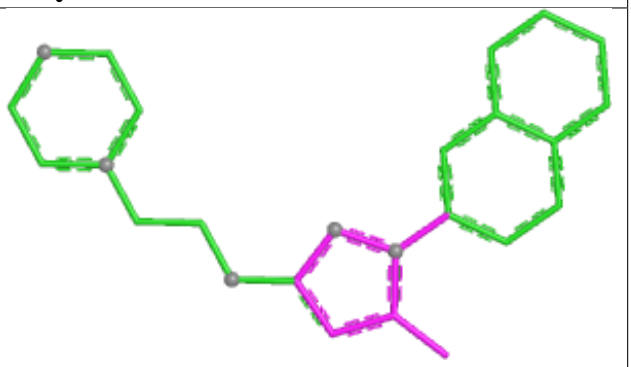

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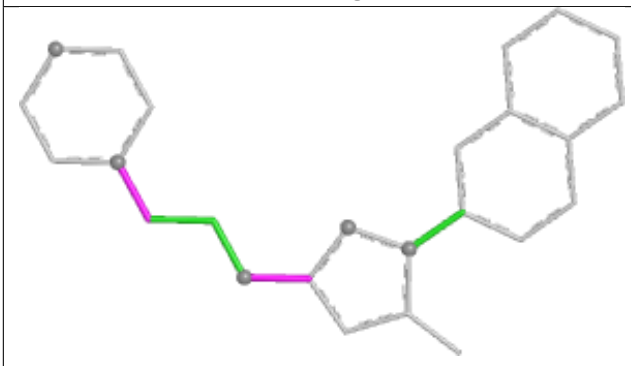

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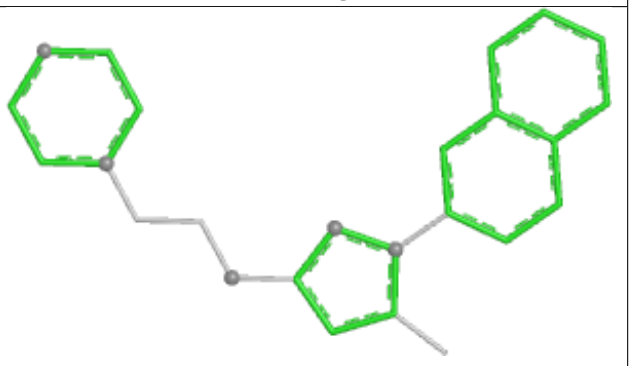
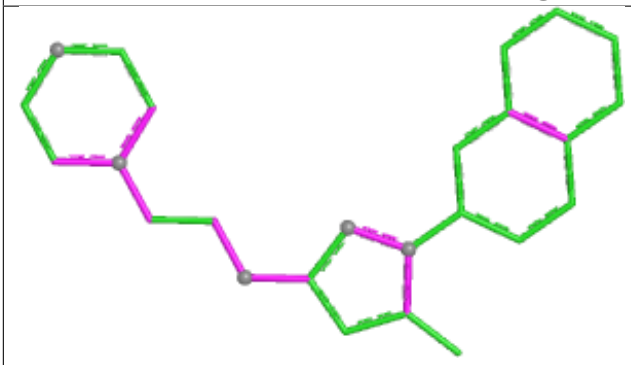


Rings

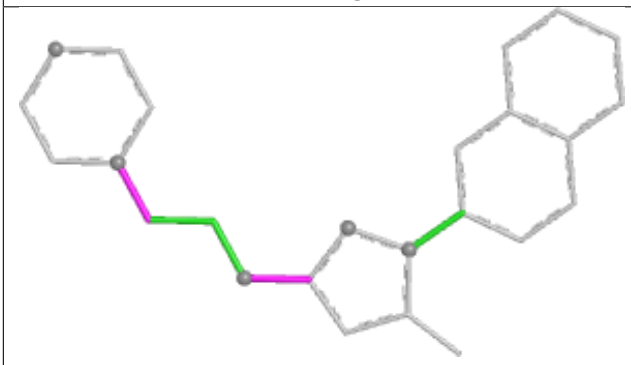
Ligand 88E S 301



Bond lengths



Bond angles



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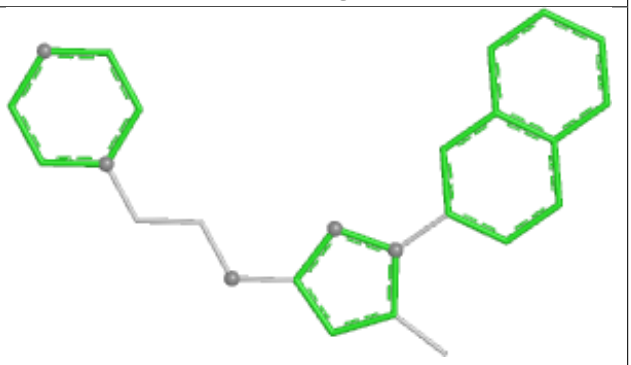

Rings

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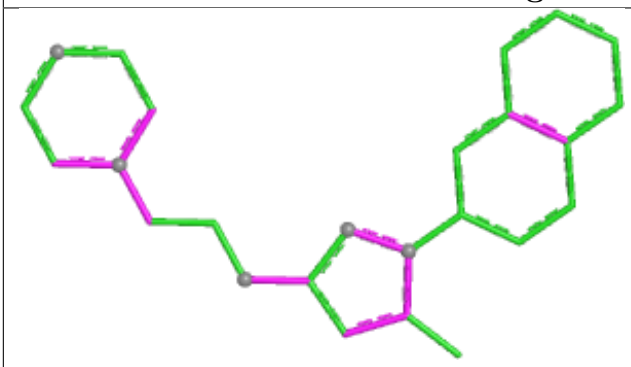

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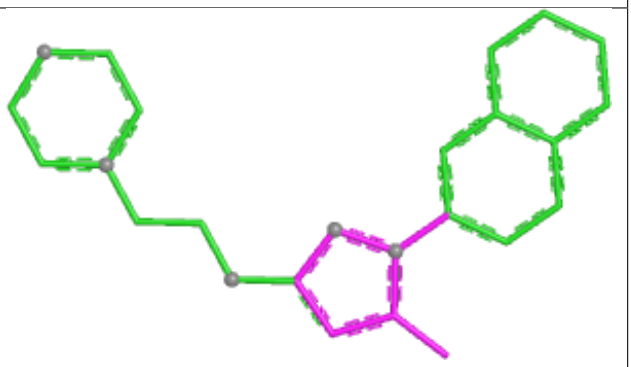

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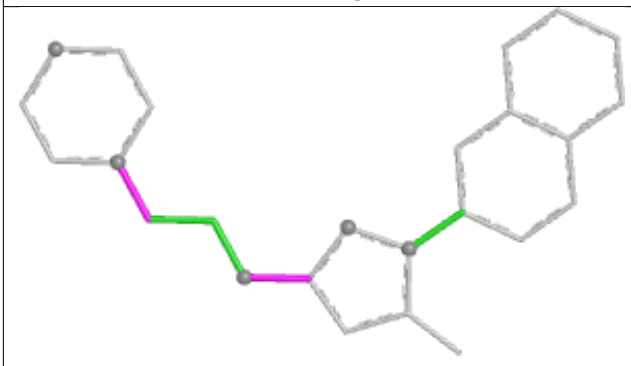

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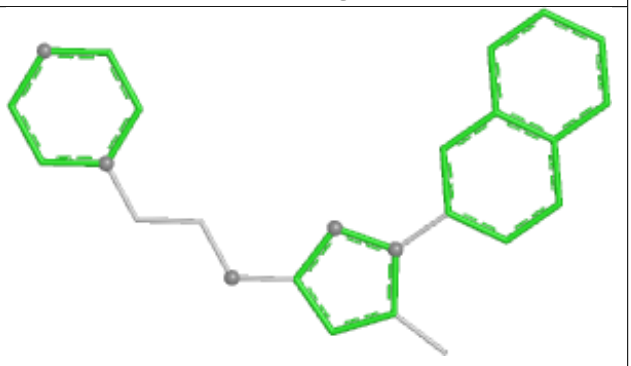

Rings

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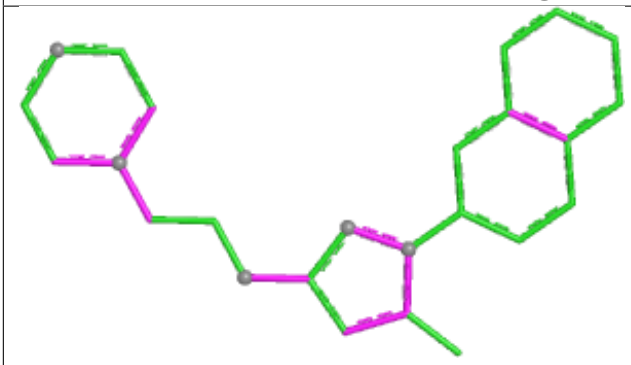

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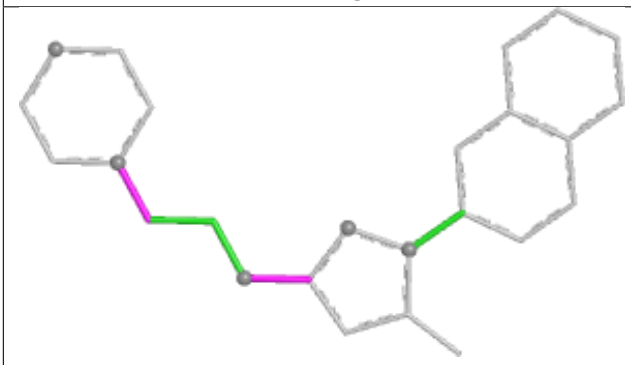

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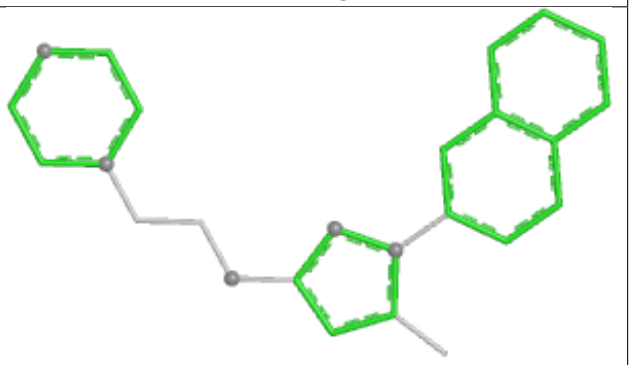

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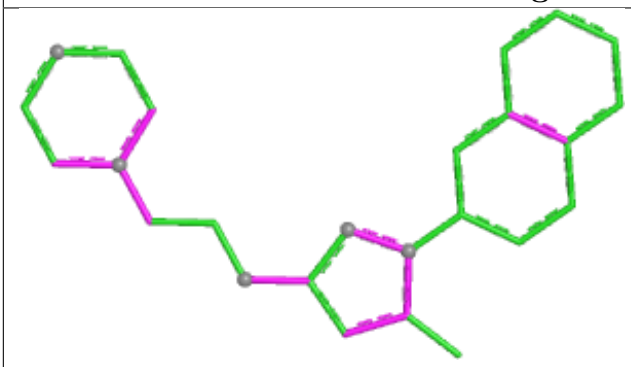

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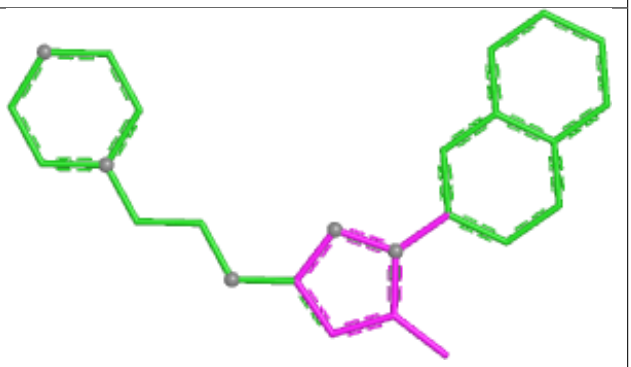

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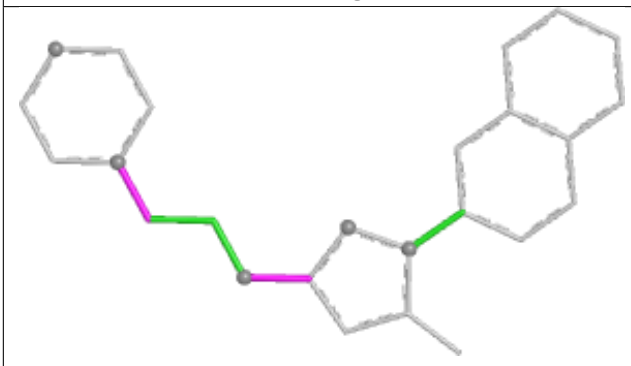

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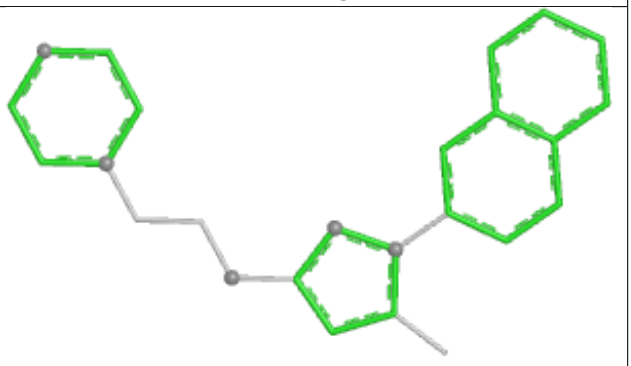

Rings

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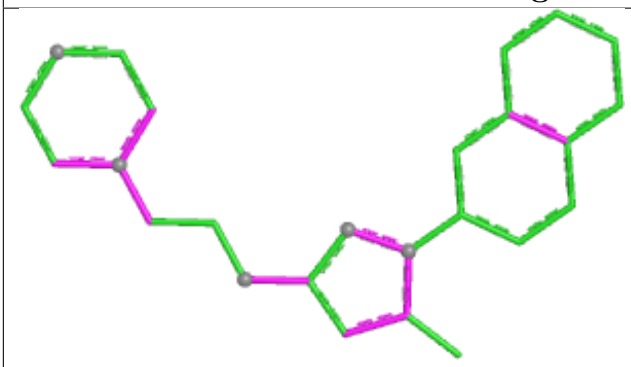

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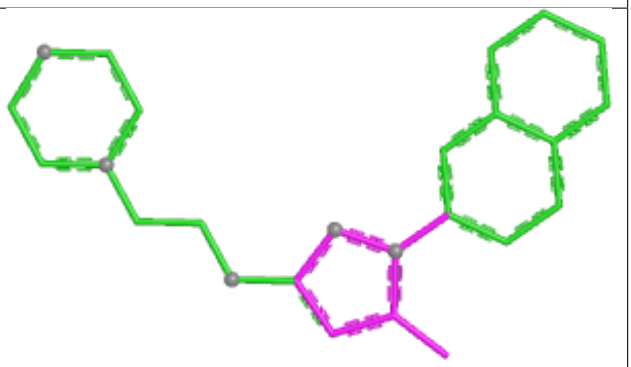

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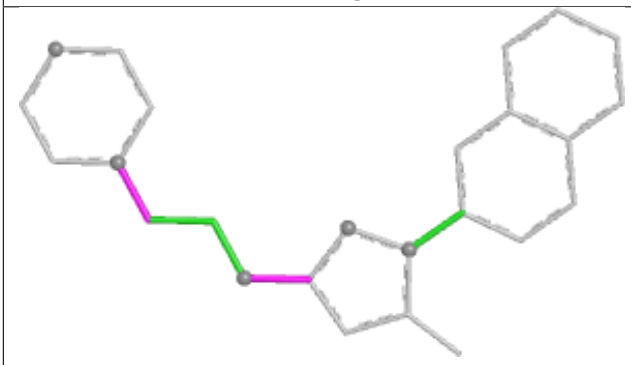

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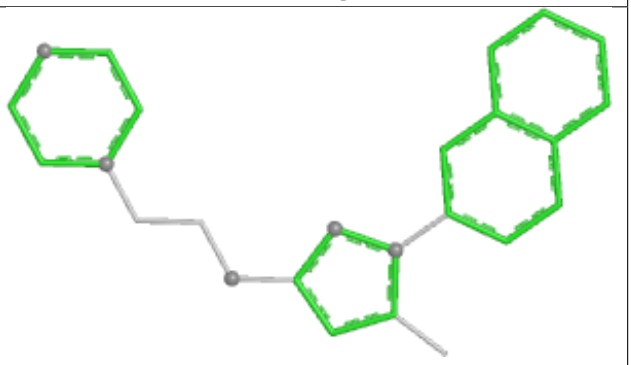
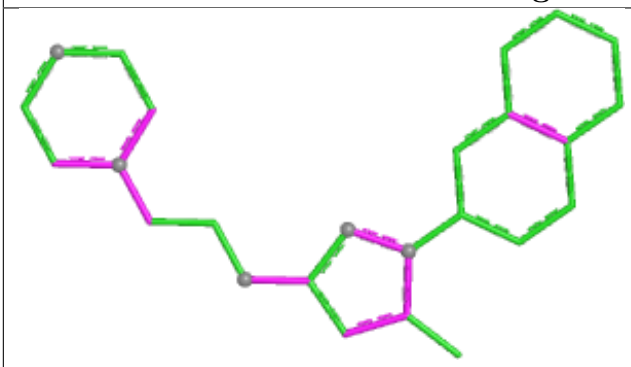


Rings

Ligand 88E T 301



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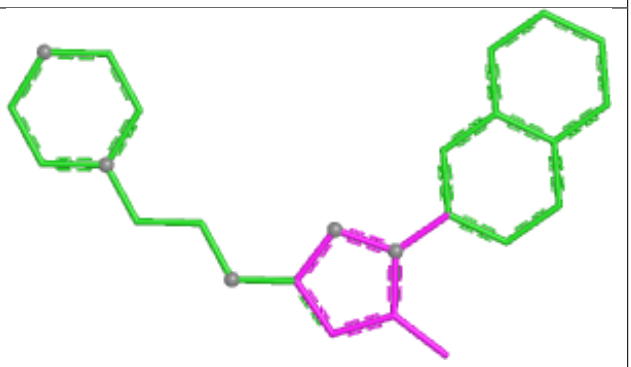

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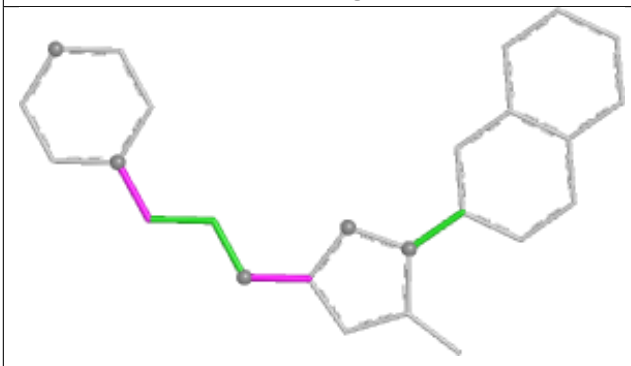

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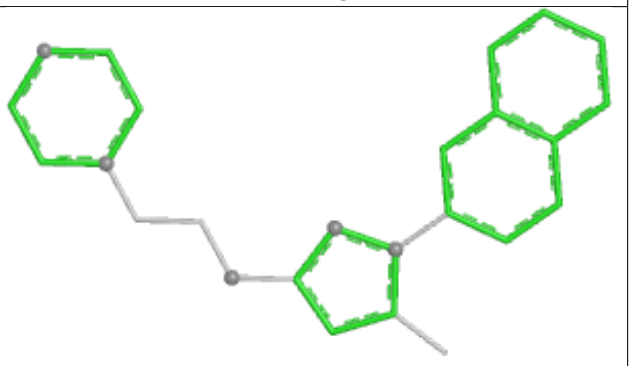

Rings

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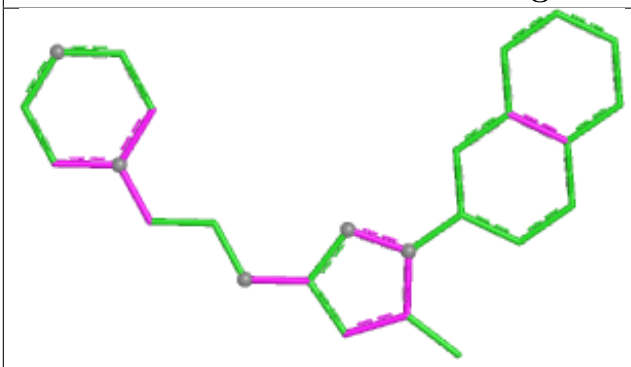

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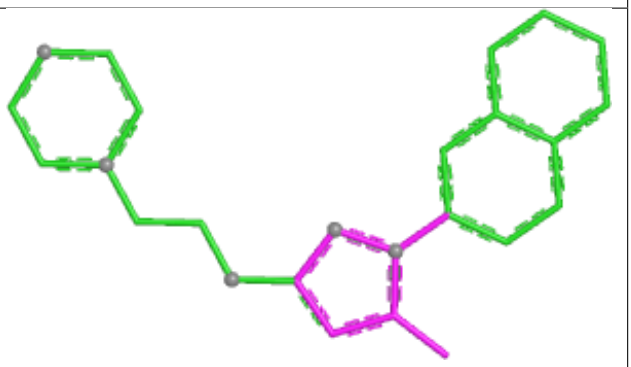

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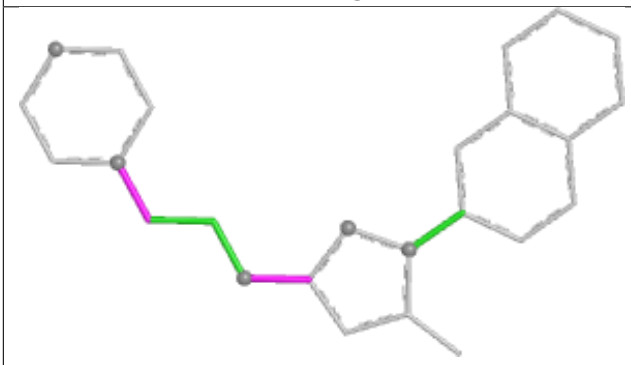

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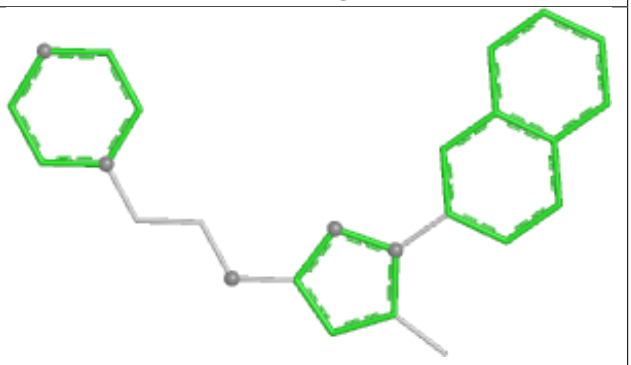

Rings

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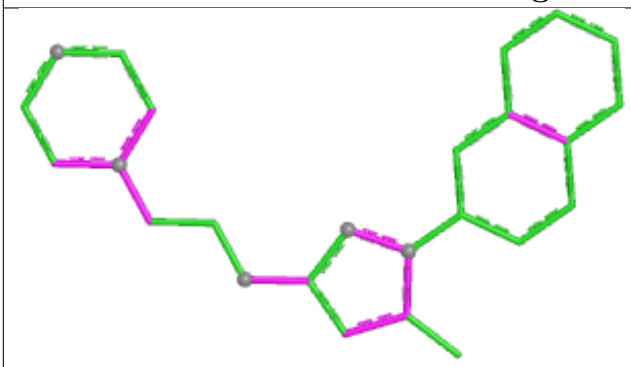

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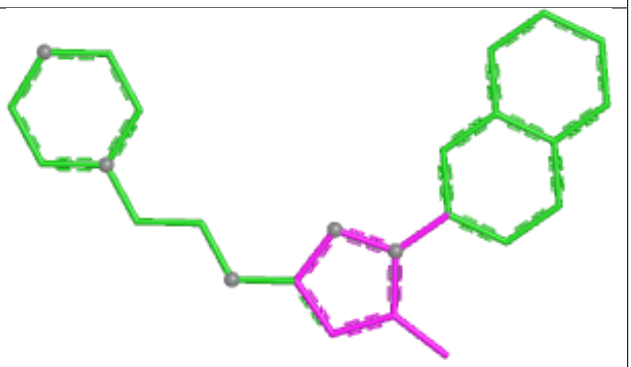

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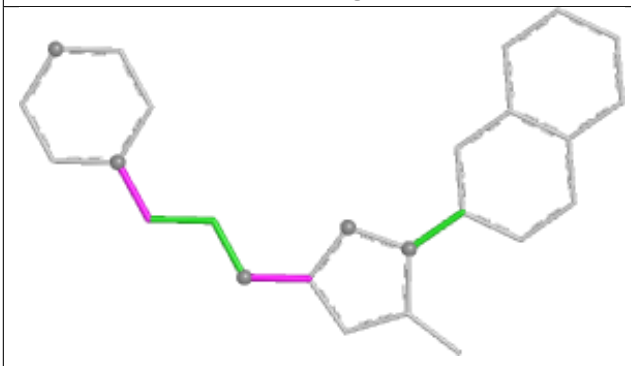

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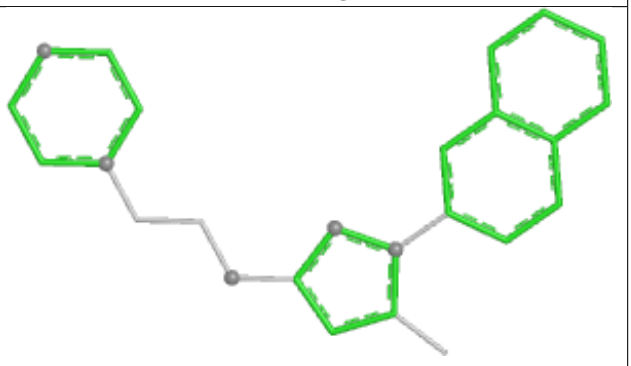
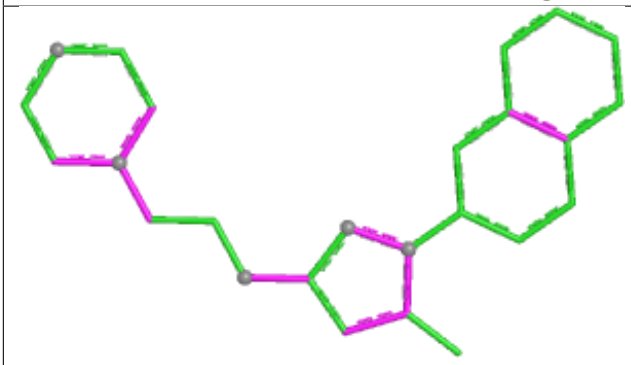


Rings

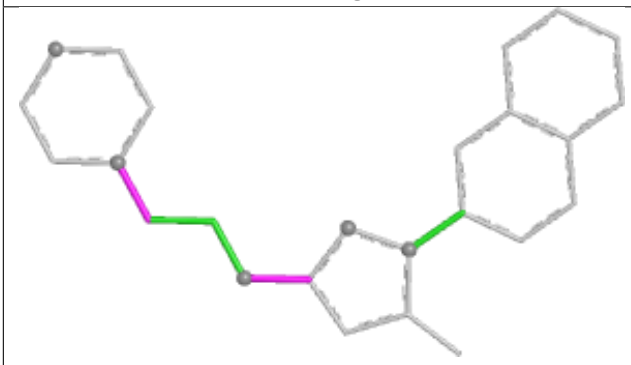
Ligand 88E I 301



Bond lengths



Bond angles



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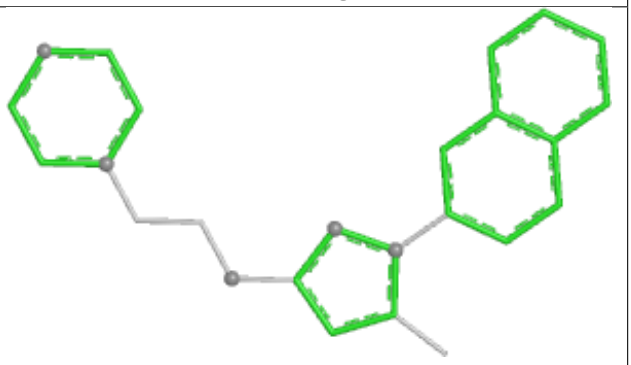
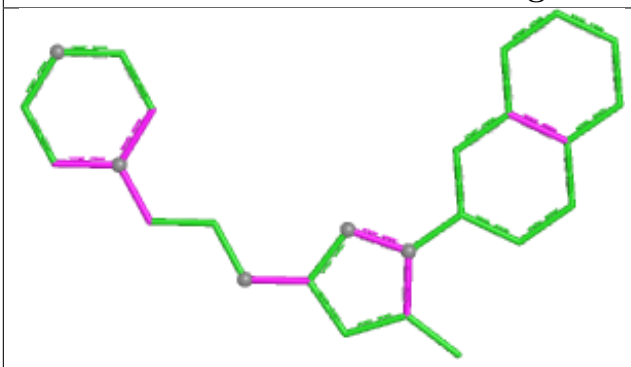


Rings

Ligand 88E M 301



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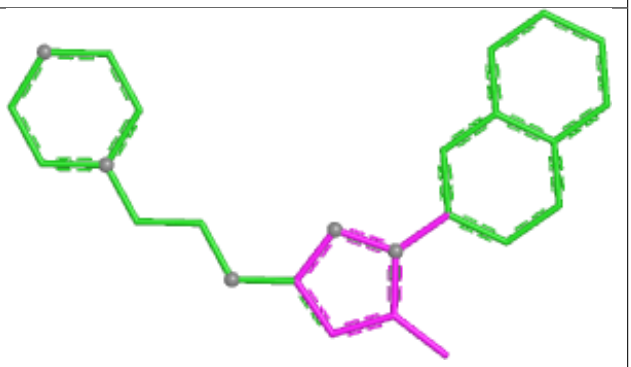
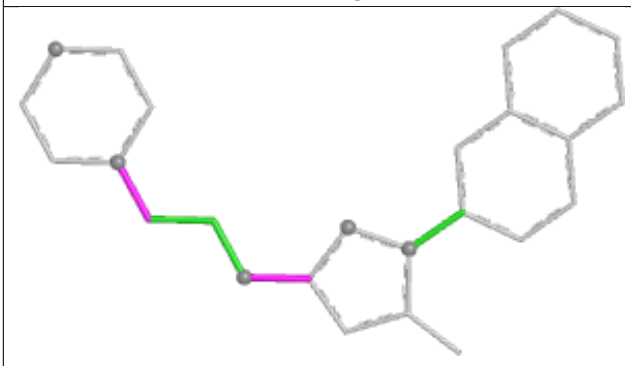


Bond angles



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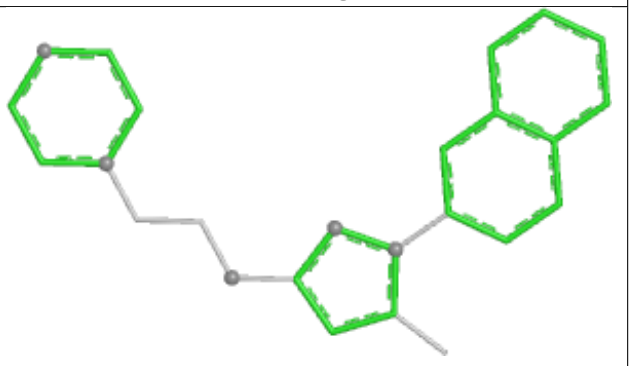

Rings

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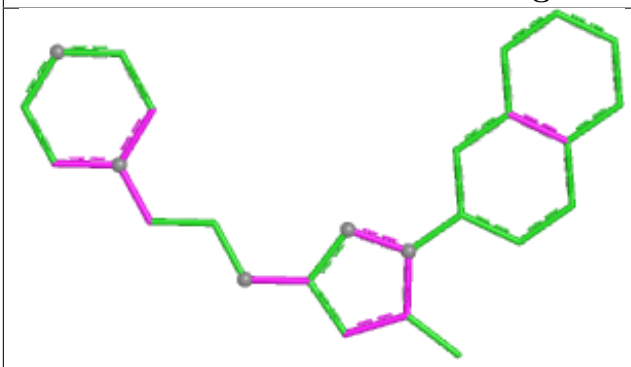

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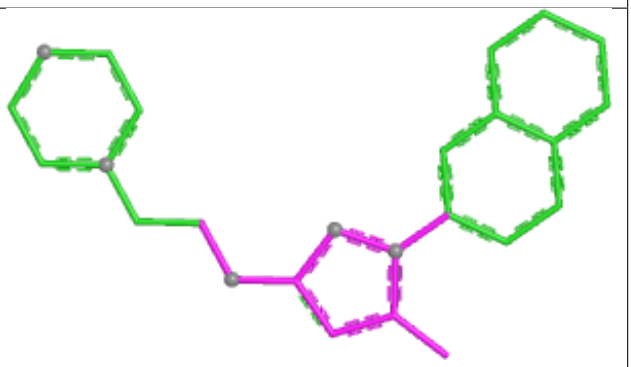
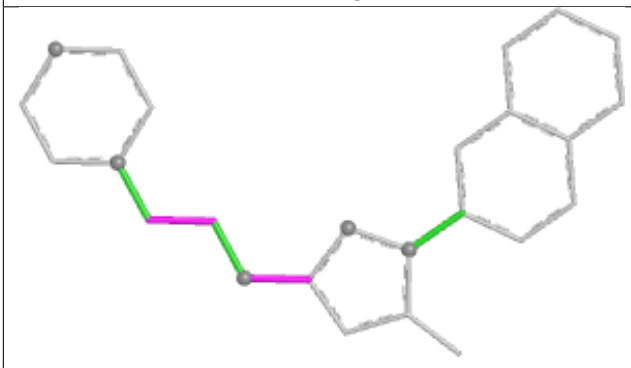
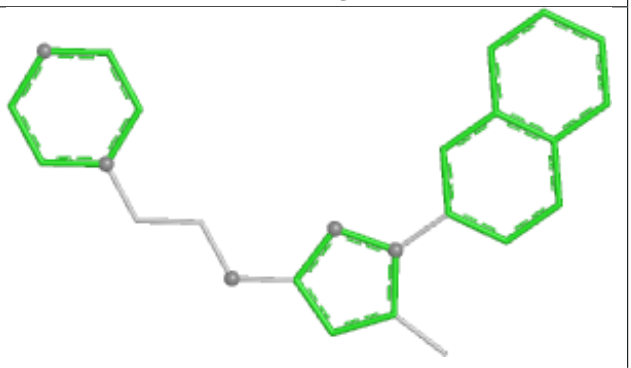


Bond angles

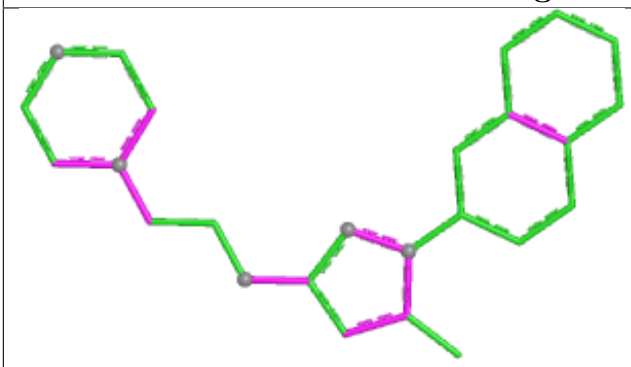


Torsions

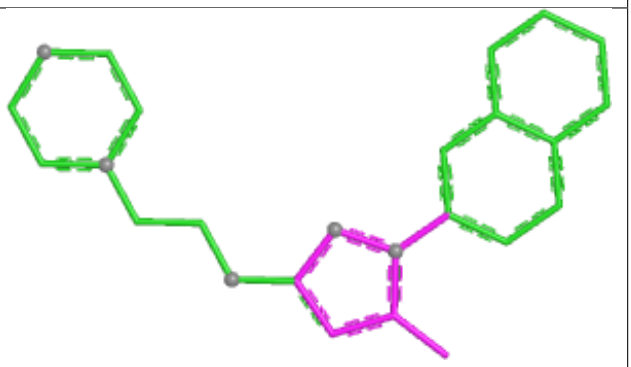


Rings

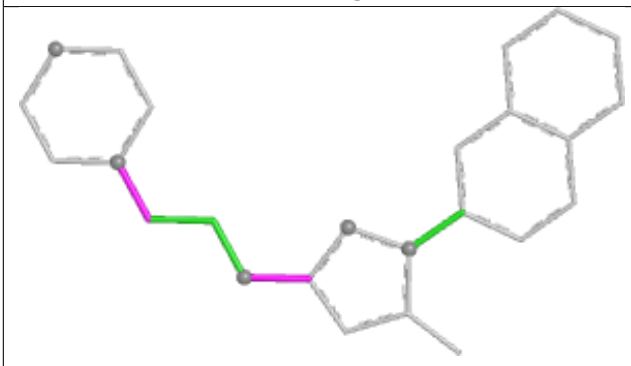
Ligand 88E L 301



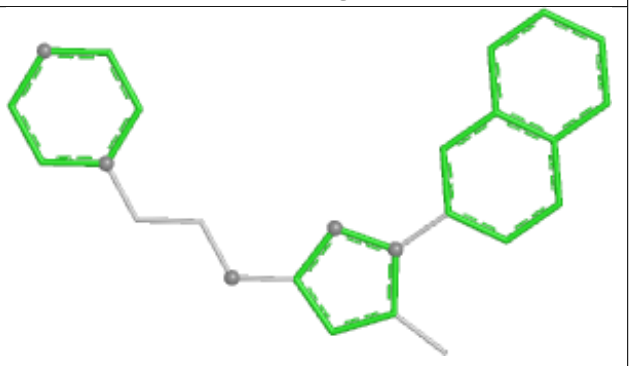
Bond lengths



Bond angles

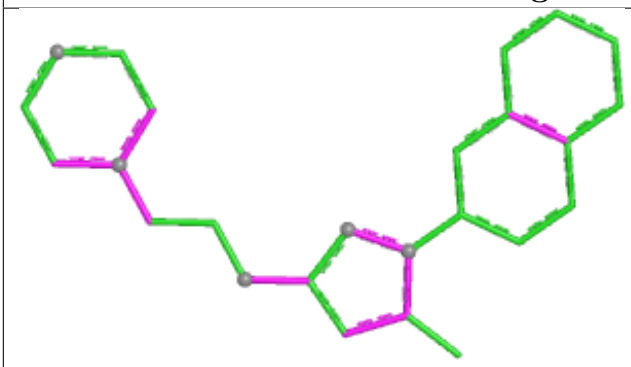


Torsions

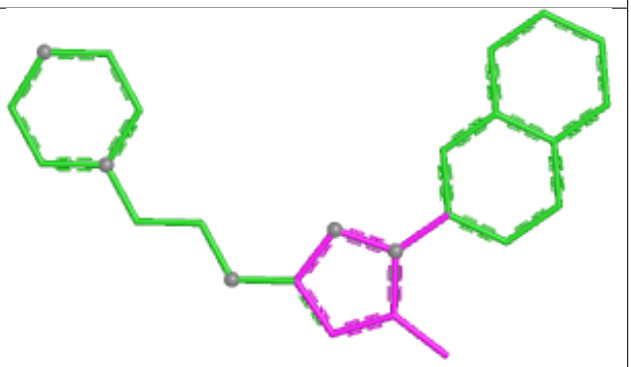


Rings

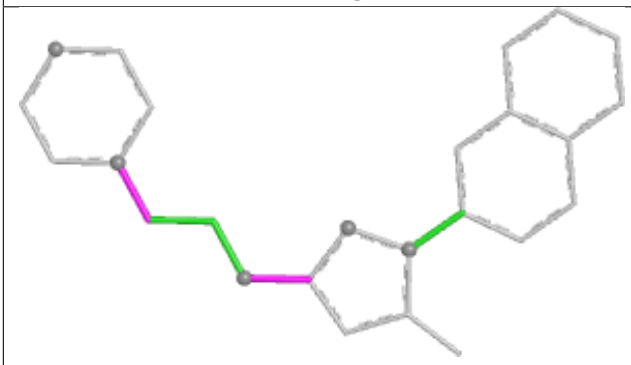
Ligand 88E D 301



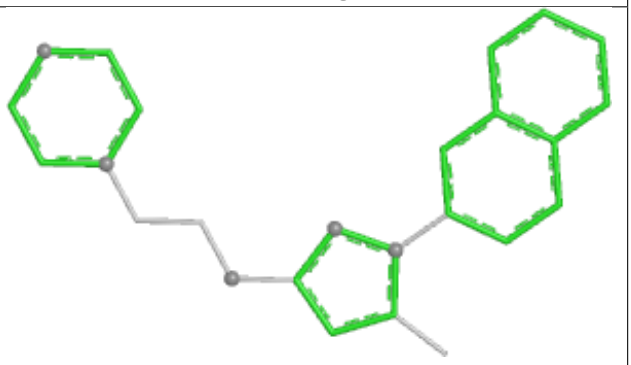
Bond lengths



Bond angles

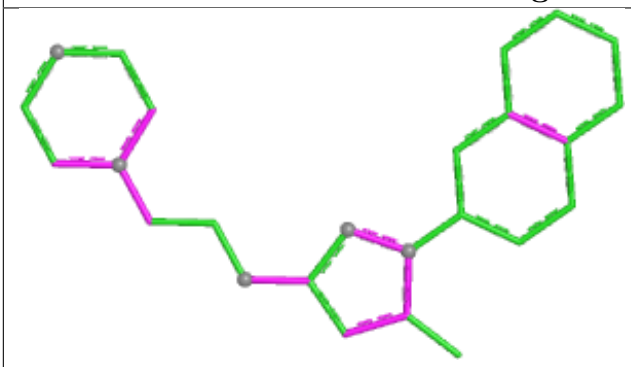


Torsions

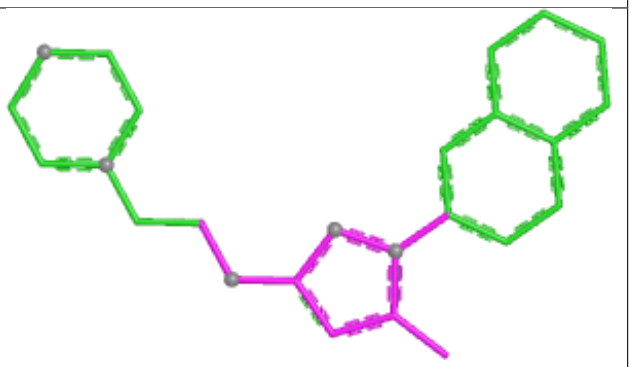


Rings

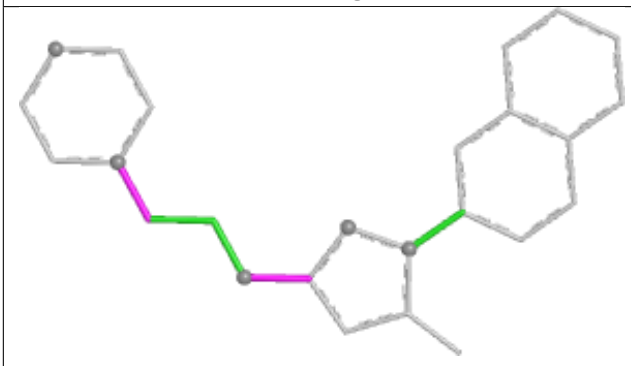
Ligand 88E A 301



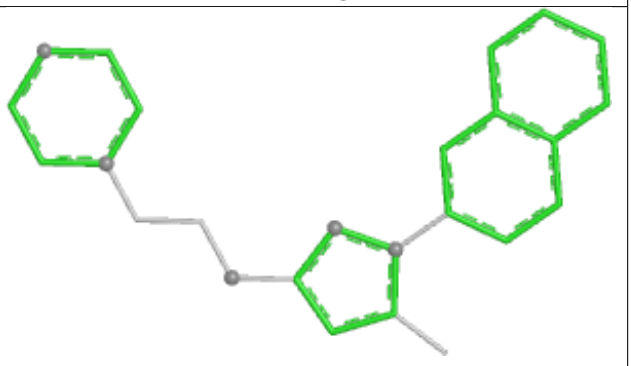
Bond lengths



Bond angles

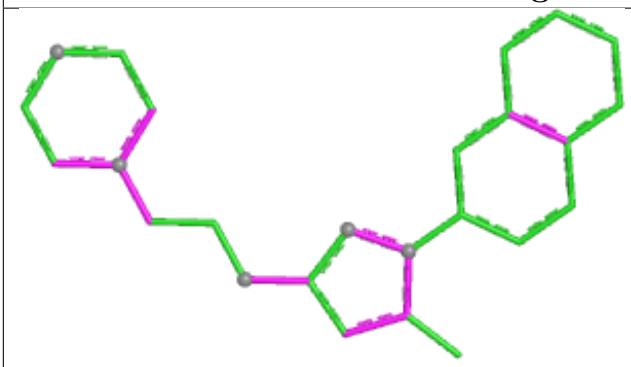


Torsions

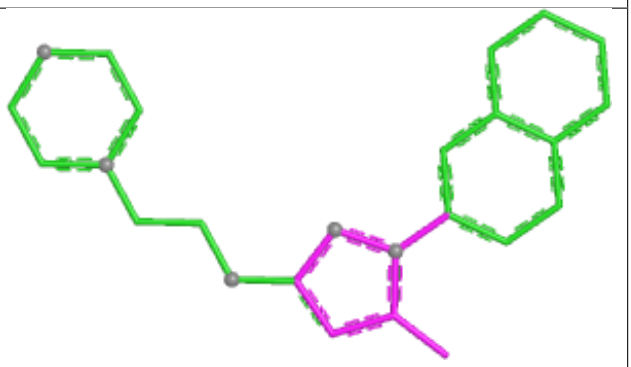


Rings

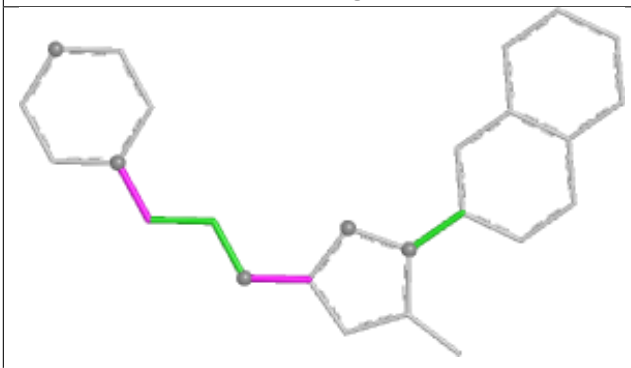
Ligand 88E V 301



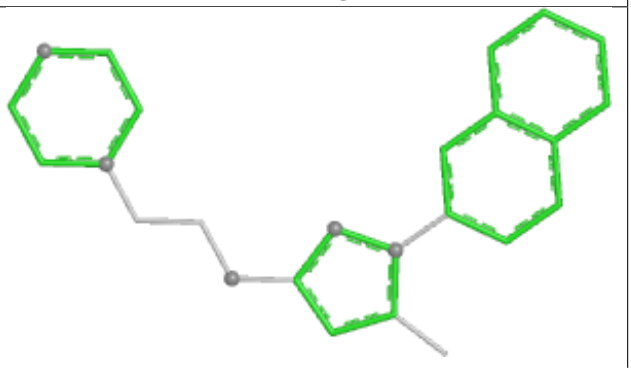
Bond lengths



Bond angles

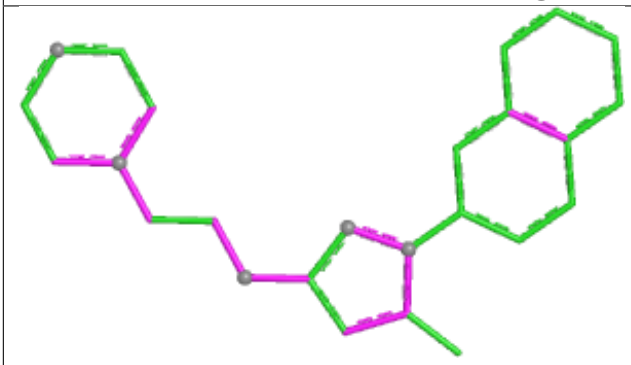


Torsions



Rings

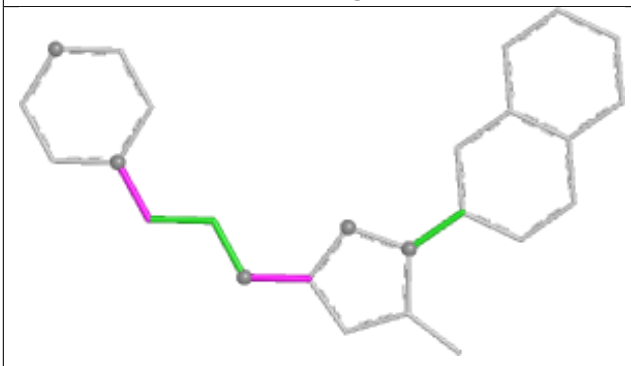
Ligand 88E P 301



Bond lengths



Bond angles



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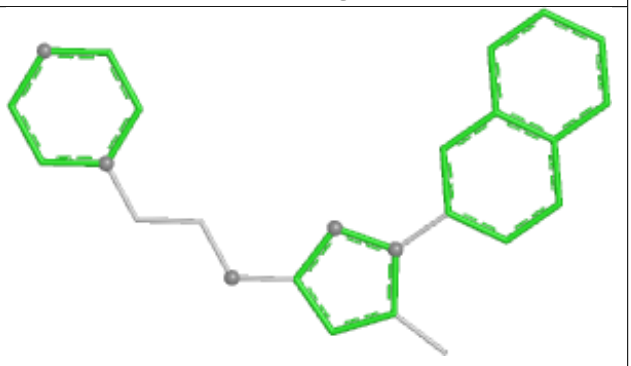
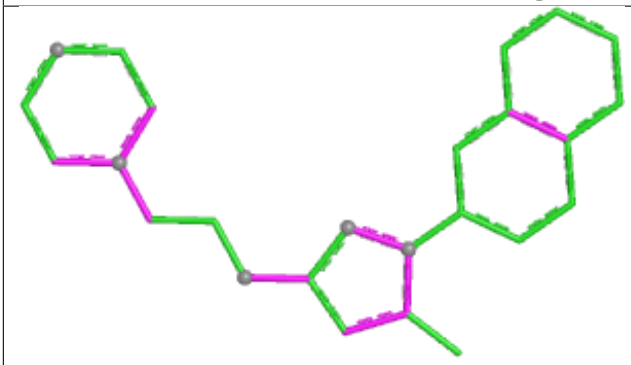


Rings

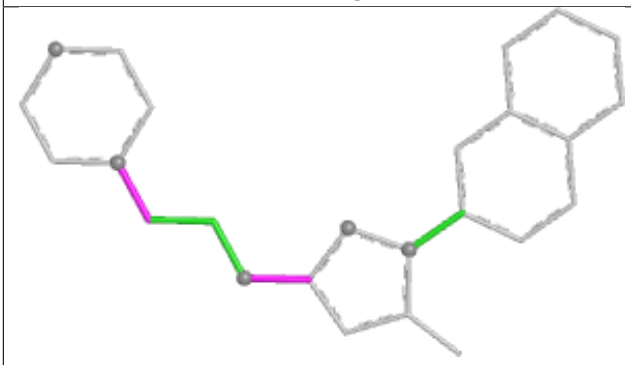
Ligand 88E G 301



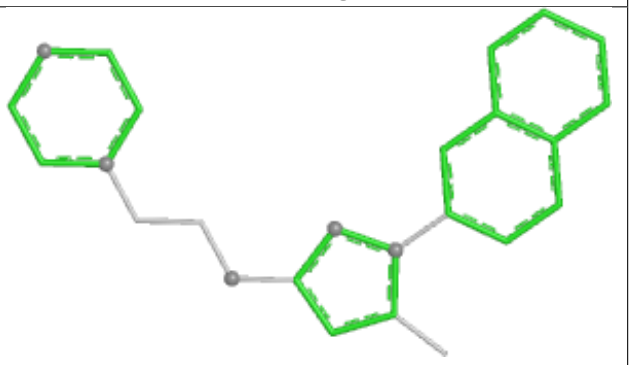
Bond lengths



Bond angles

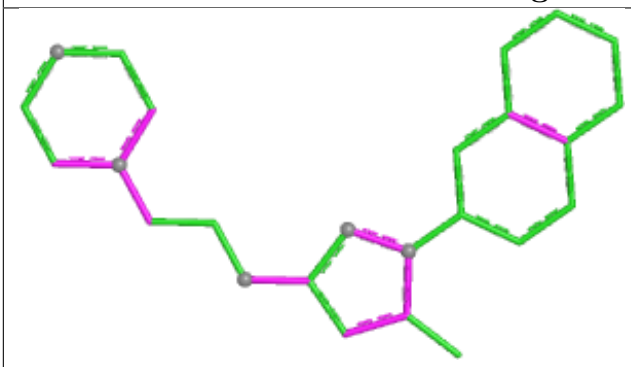


Torsions

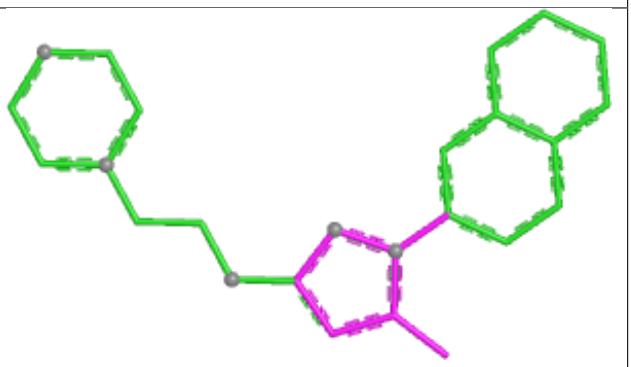


Rings

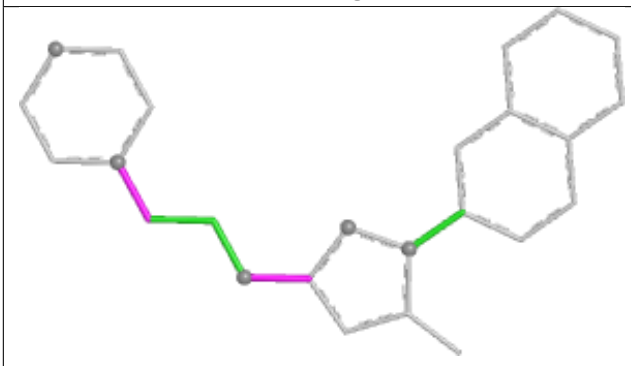
Ligand 88E U 301



Bond lengths



Bond angles



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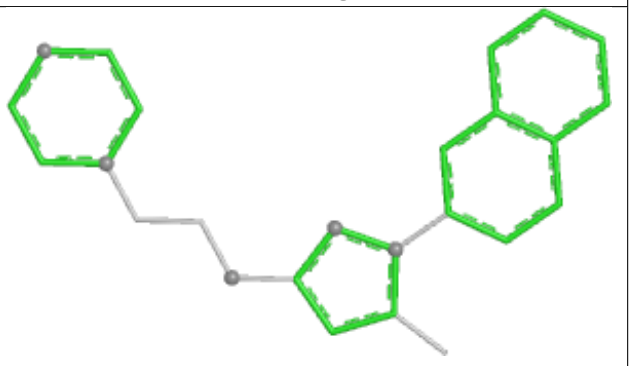
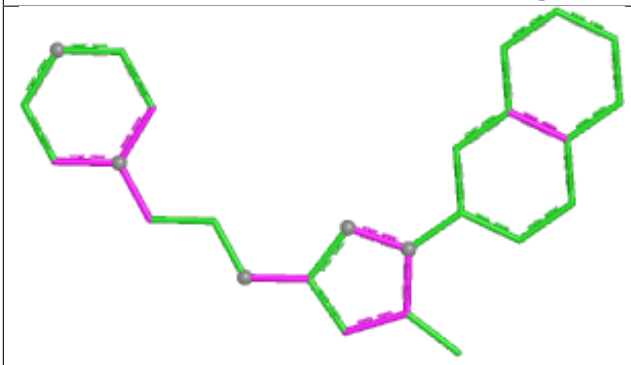


Rings

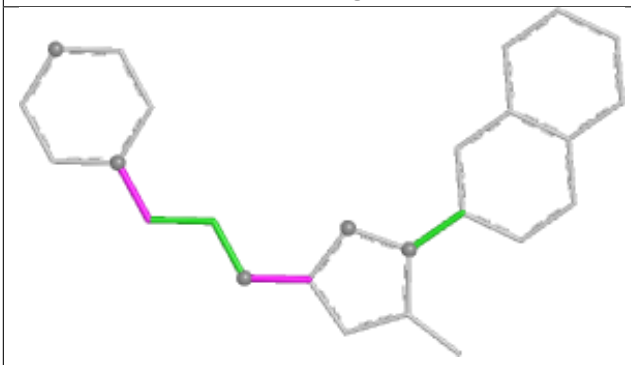
Ligand 88E E 301



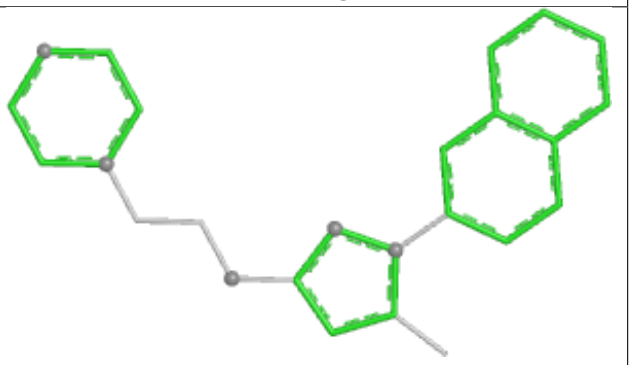
Bond lengths



Bond angles

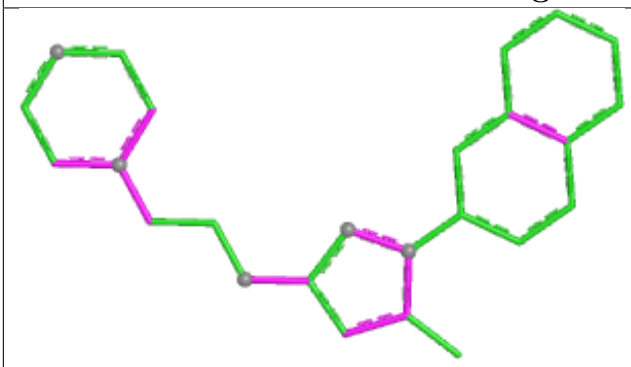


Torsions

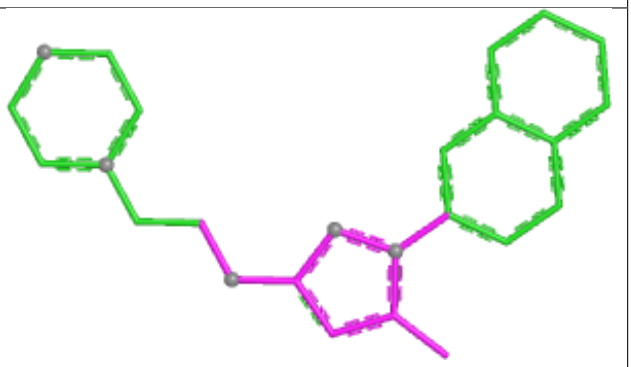


Rings

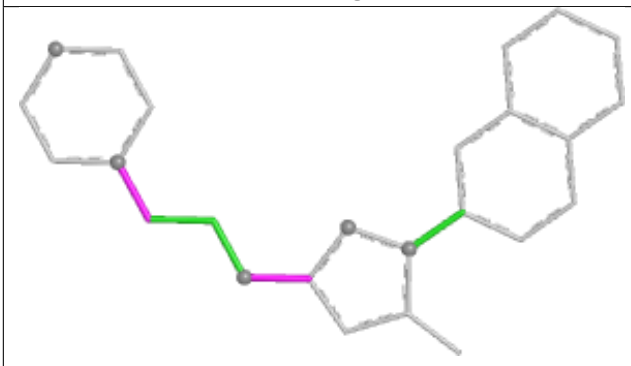
Ligand 88E B 301



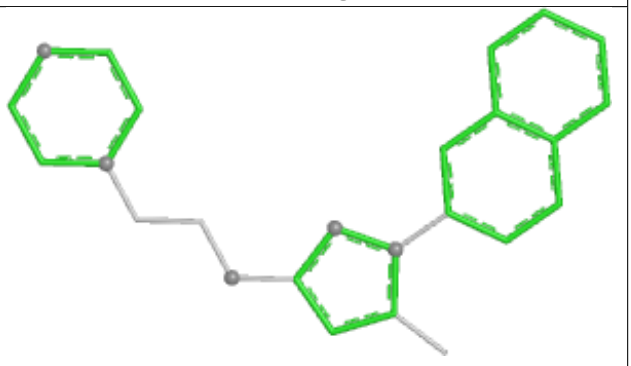
Bond lengths



Bond angles

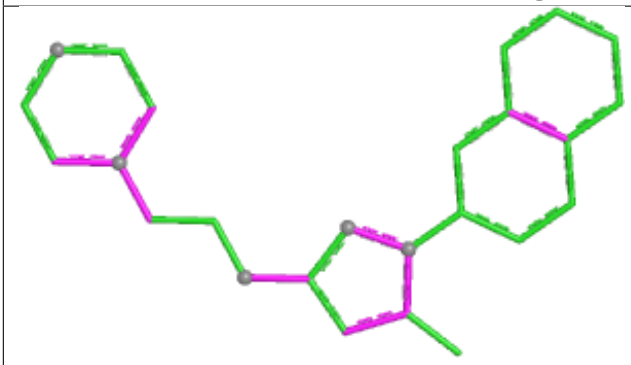


Torsions



Rings

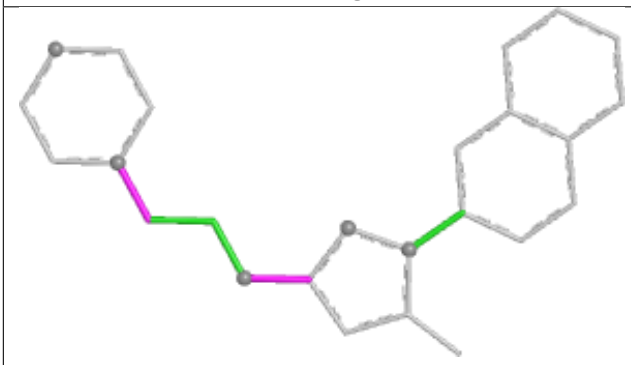
Ligand 88E N 301



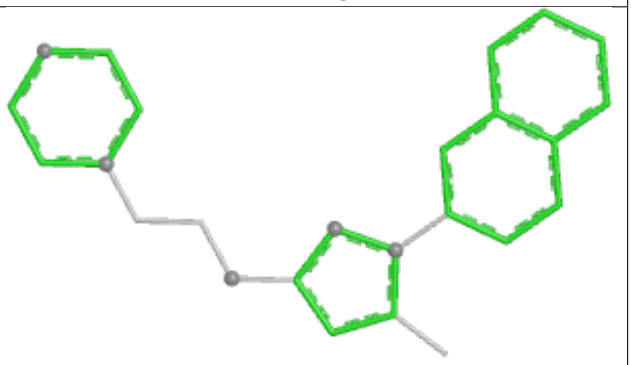
Bond lengths



Bond angles

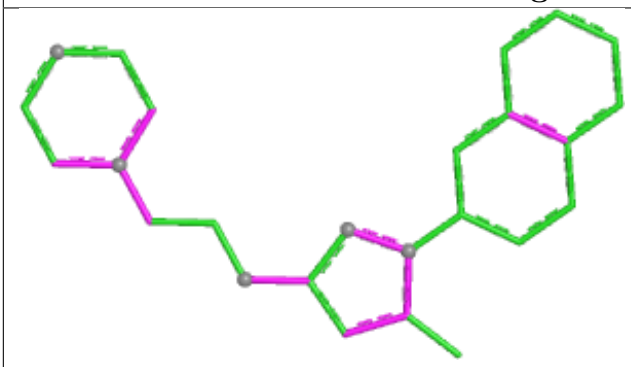


Torsions

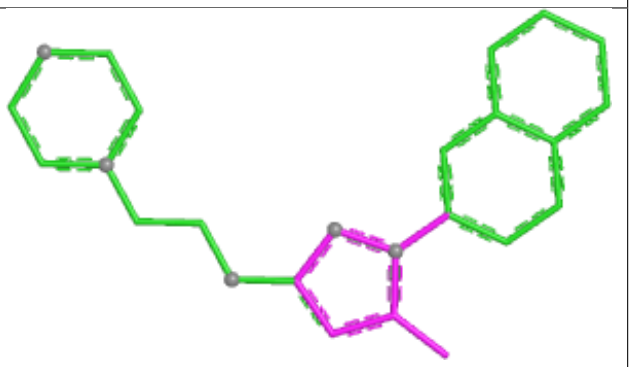


Rings

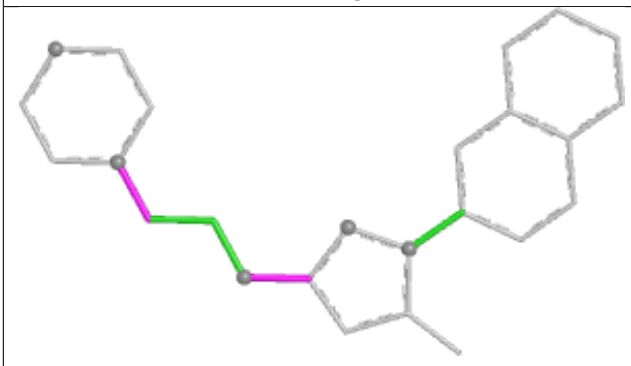
Ligand 88E H 301



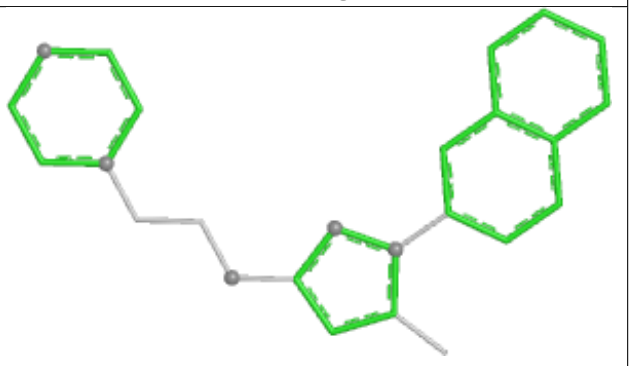
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	213/225 (94%)	-1.14	0	100	100	47, 78, 105, 125	0
1	B	213/225 (94%)	-1.09	0	100	100	59, 84, 111, 135	0
1	C	214/225 (95%)	-1.07	0	100	100	59, 82, 109, 126	0
1	D	214/225 (95%)	-1.07	0	100	100	52, 79, 106, 122	0
1	E	206/225 (91%)	-1.10	0	100	100	53, 73, 97, 107	0
1	F	206/225 (91%)	-1.15	0	100	100	43, 64, 108, 120	0
1	G	213/225 (94%)	-1.12	0	100	100	56, 83, 109, 118	0
1	H	213/225 (94%)	-1.06	0	100	100	65, 91, 109, 134	0
1	I	210/225 (93%)	-1.15	0	100	100	44, 73, 102, 122	0
1	J	213/225 (94%)	-1.14	0	100	100	57, 74, 99, 123	0
1	K	214/225 (95%)	-1.12	0	100	100	44, 76, 102, 124	0
1	L	210/225 (93%)	-1.13	0	100	100	46, 70, 101, 129	0
1	M	196/225 (87%)	-1.17	0	100	100	51, 70, 97, 111	0
1	N	210/225 (93%)	-1.12	0	100	100	53, 79, 108, 121	0
1	O	212/225 (94%)	-1.14	0	100	100	54, 77, 98, 116	0
1	P	202/225 (89%)	-1.14	0	100	100	49, 73, 108, 124	0
1	Q	212/225 (94%)	-1.02	0	100	100	74, 103, 129, 142	0
1	R	212/225 (94%)	-0.99	0	100	100	73, 103, 121, 131	0
1	S	209/225 (92%)	-1.16	0	100	100	49, 75, 109, 122	0
1	T	213/225 (94%)	-1.01	0	100	100	75, 93, 120, 141	0
1	U	213/225 (94%)	-1.03	0	100	100	67, 95, 115, 122	0
1	V	210/225 (93%)	-1.17	0	100	100	50, 73, 105, 124	0
1	W	213/225 (94%)	-1.10	0	100	100	55, 79, 121, 141	0
1	X	213/225 (94%)	-1.10	0	100	100	52, 77, 97, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
All	All	5054/5400 (93%)	-1.10	0	100 100	43, 80, 113, 142	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	88E	P	302	25/25	0.97	0.07	85,85,85,85	0
2	88E	C	301	25/25	0.99	0.05	80,80,80,80	0
2	88E	E	301	25/25	0.99	0.04	74,74,74,74	0
2	88E	B	301	25/25	0.99	0.05	74,74,74,74	0
2	88E	D	301	25/25	0.99	0.06	79,79,79,79	0
2	88E	F	301	25/25	0.99	0.04	69,69,69,69	0
2	88E	G	301	25/25	0.99	0.06	76,76,76,76	0
2	88E	H	301	25/25	0.99	0.06	84,84,84,84	0
2	88E	I	301	25/25	0.99	0.05	70,70,70,70	0
2	88E	J	301	25/25	0.99	0.05	69,69,69,69	0
2	88E	K	301	25/25	0.99	0.05	74,74,74,74	0
2	88E	L	301	25/25	0.99	0.05	70,70,70,70	0
2	88E	M	301	25/25	0.99	0.05	69,69,69,69	0
2	88E	N	301	25/25	0.99	0.06	77,77,77,77	0
2	88E	O	301	25/25	0.99	0.06	76,76,76,76	0
2	88E	P	301	25/25	0.99	0.05	68,68,68,68	0
2	88E	A	301	25/25	0.99	0.05	73,73,73,73	0
2	88E	Q	301	25/25	0.99	0.06	95,95,95,95	0
2	88E	R	301	25/25	0.99	0.06	97,97,97,97	0

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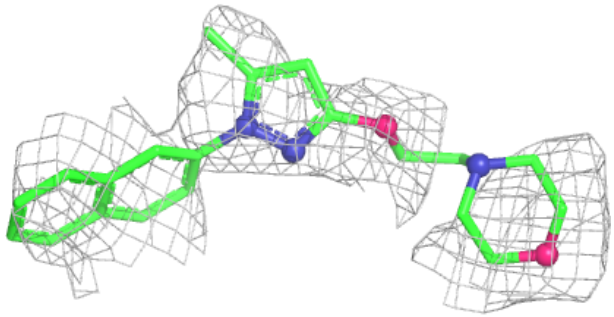
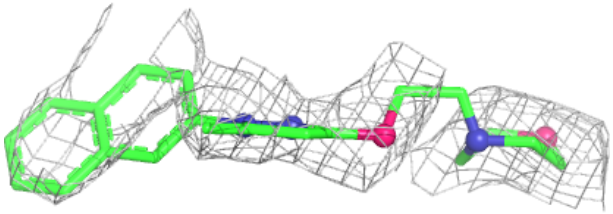
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	88E	S	301	25/25	0.99	0.05	75,75,75,75	0
2	88E	T	301	25/25	0.99	0.05	91,91,91,91	0
2	88E	U	301	25/25	0.99	0.06	94,94,94,94	0
2	88E	V	301	25/25	0.99	0.05	69,69,69,69	0
2	88E	W	301	25/25	0.99	0.07	78,78,78,78	0
2	88E	X	301	25/25	0.99	0.05	76,76,76,76	0

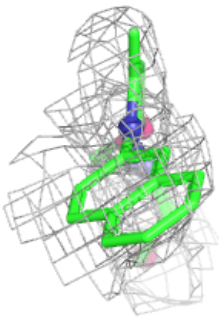
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 88E P 302:

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

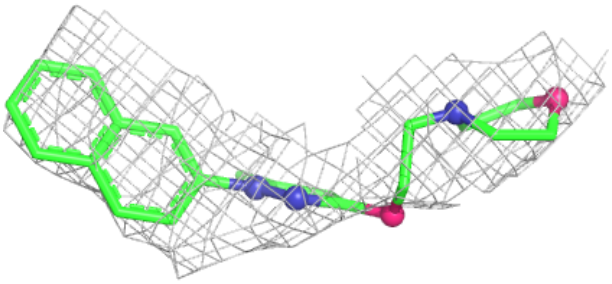


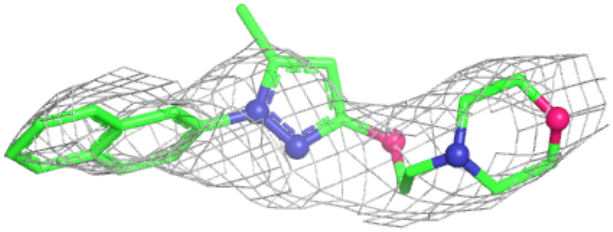


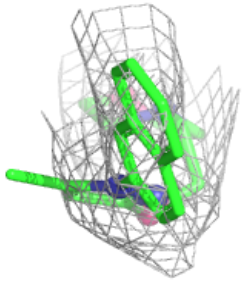


Electron density around 88E C 301:

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

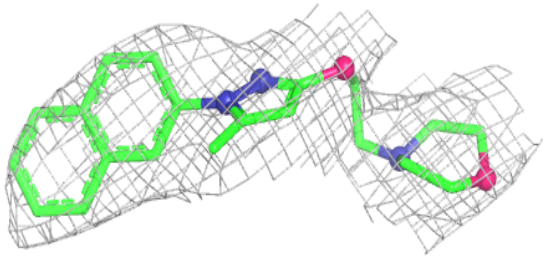


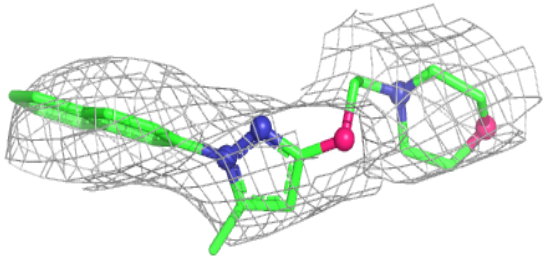


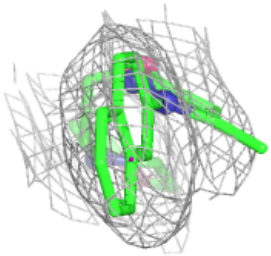


Electron density around 88E E 301:

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

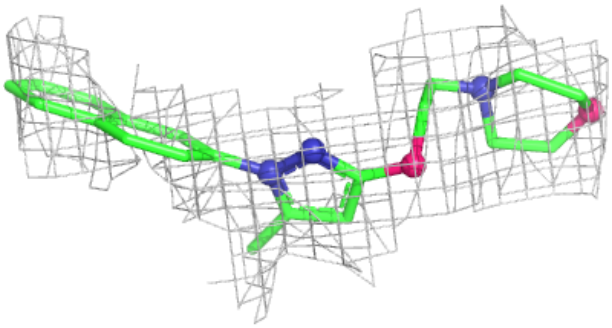


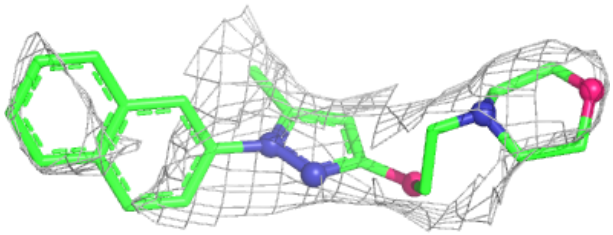


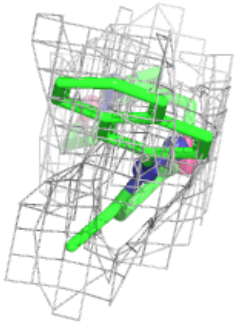


Electron density around 88E B 301:

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

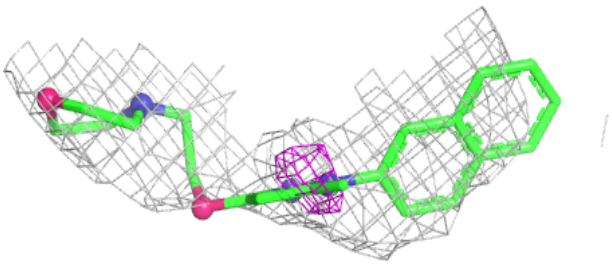


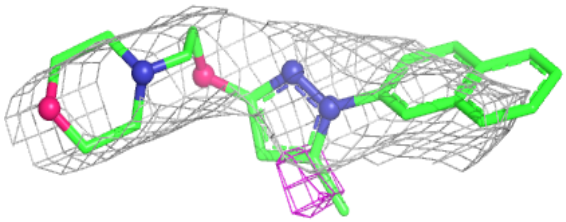


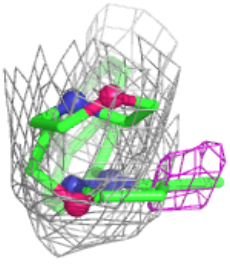


Electron density around 88E D 301:

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

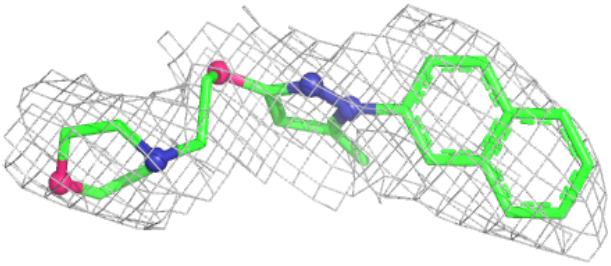


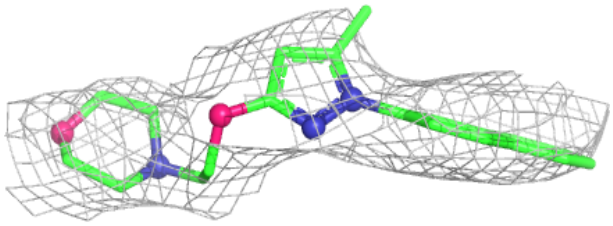


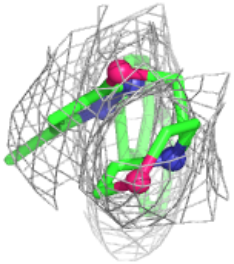


Electron density around 88E F 301:

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

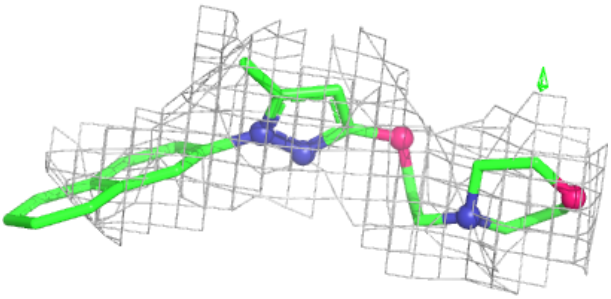


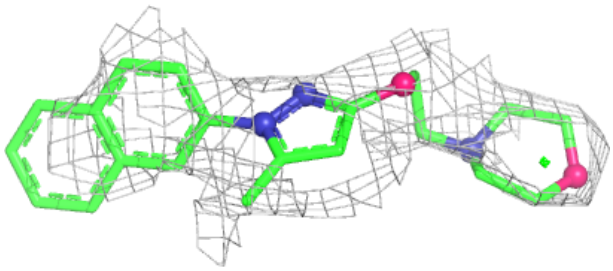


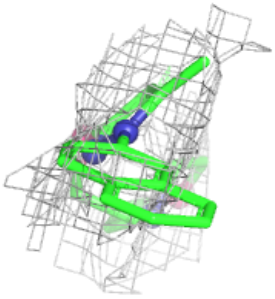


Electron density around 88E G 301:

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



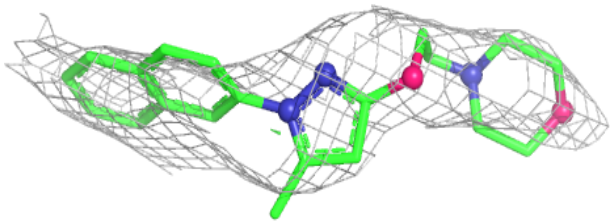


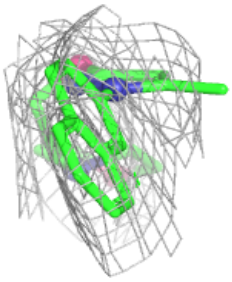


Electron density around 88E H 301:

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

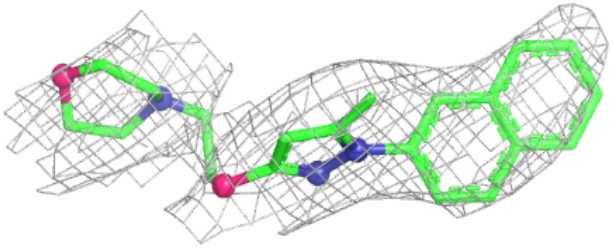


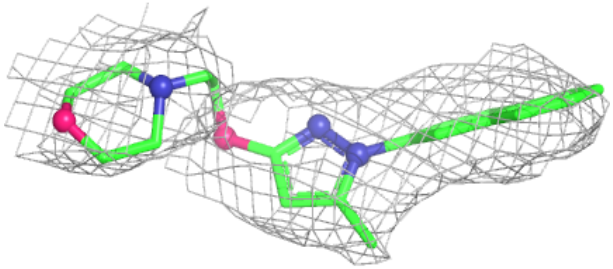


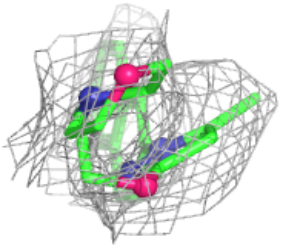


Electron density around 88E I 301:

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

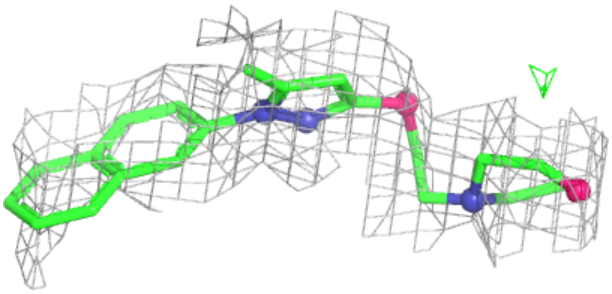


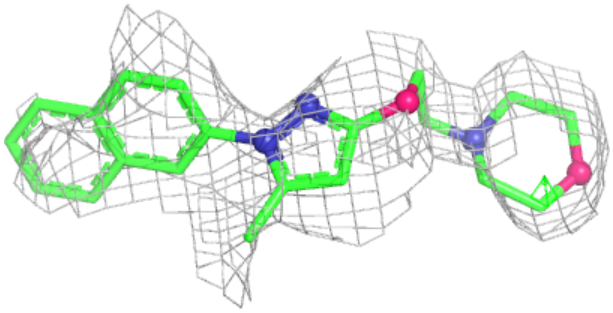


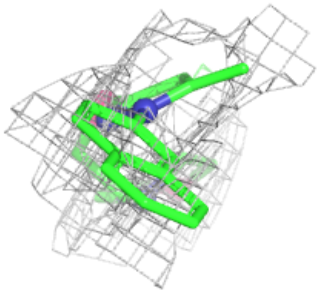


Electron density around 88E J 301:

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

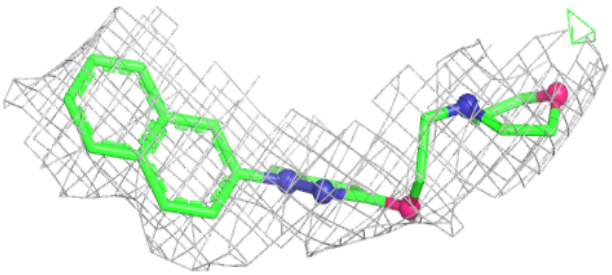


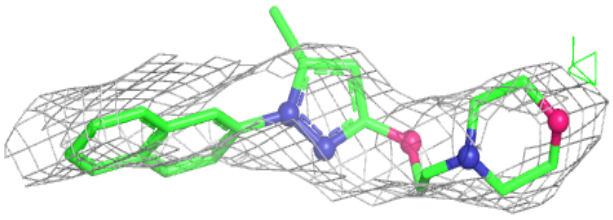


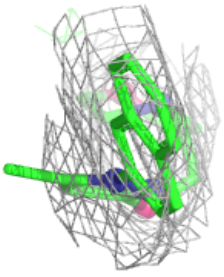


Electron density around 88E K 301:

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

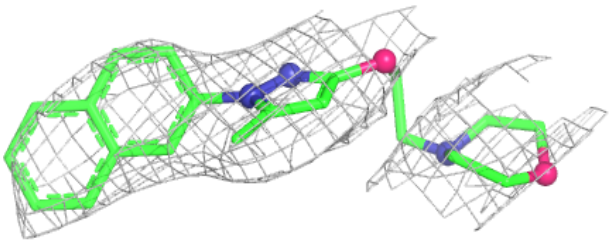


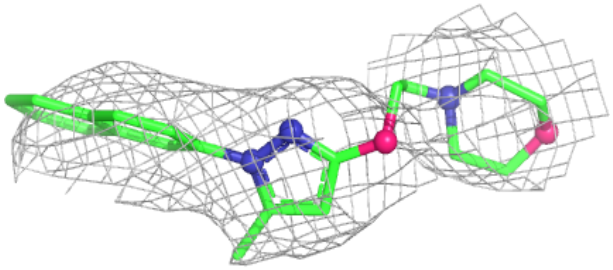


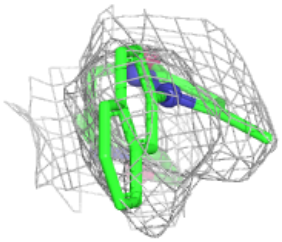


Electron density around 88E L 301:

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

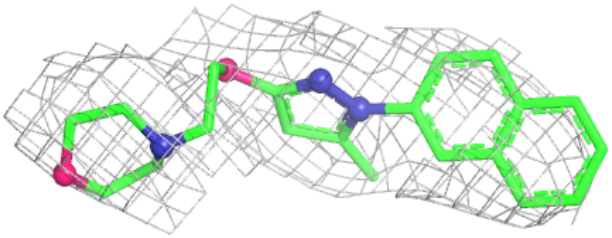


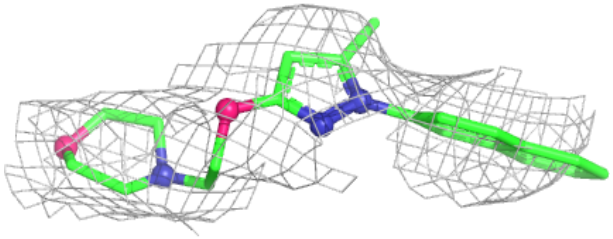


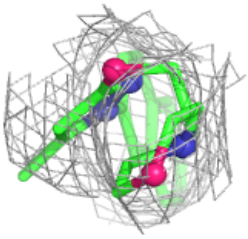


Electron density around 88E M 301:

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

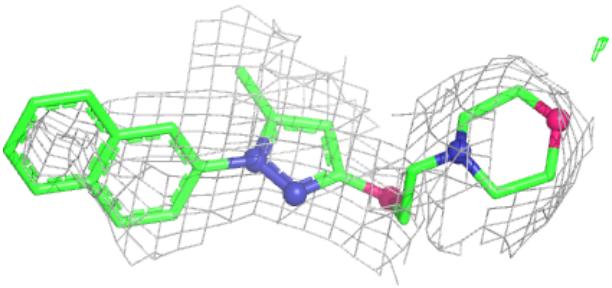


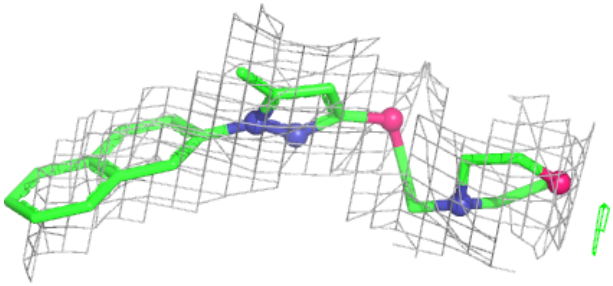


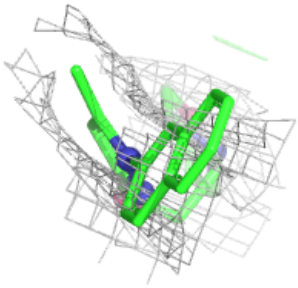


Electron density around 88E N 301:

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



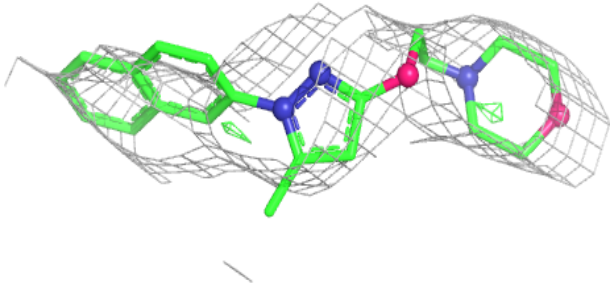


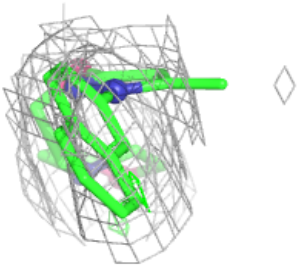


Electron density around 88E O 301:

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

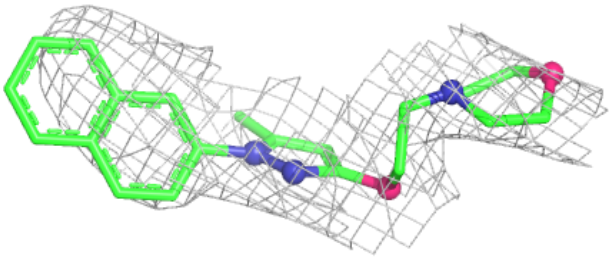


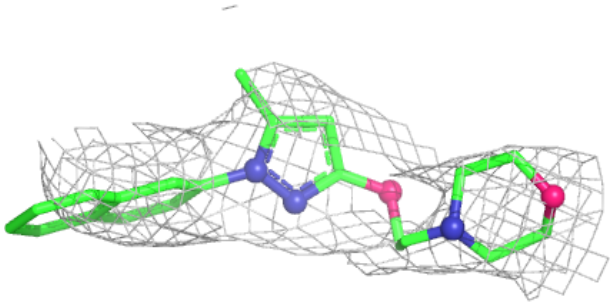


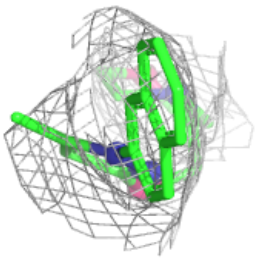


Electron density around 88E P 301:

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

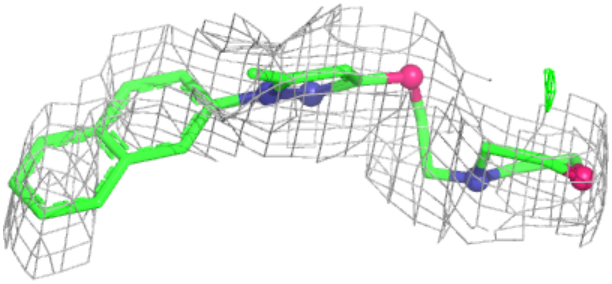


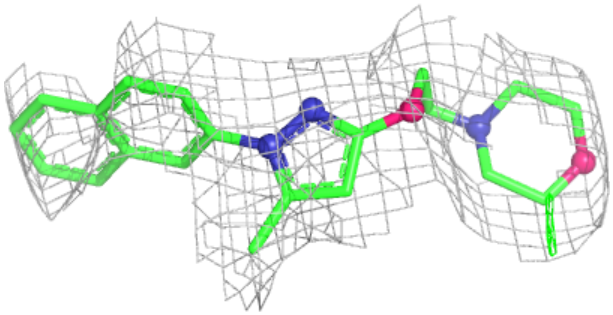


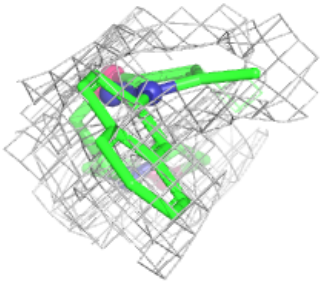


Electron density around 88E A 301:

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

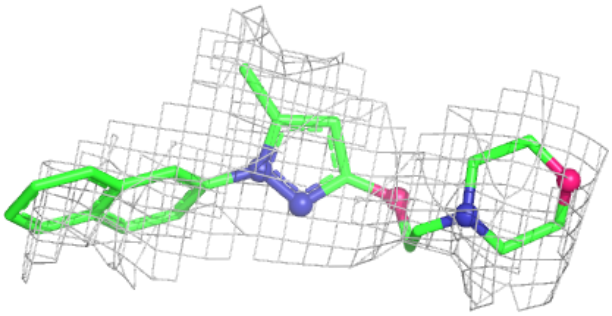


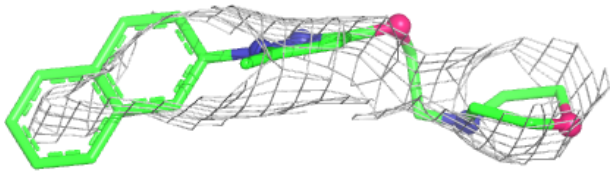


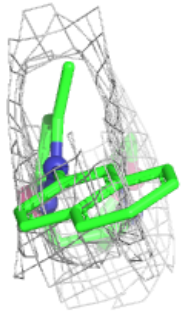


Electron density around 88E Q 301:

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

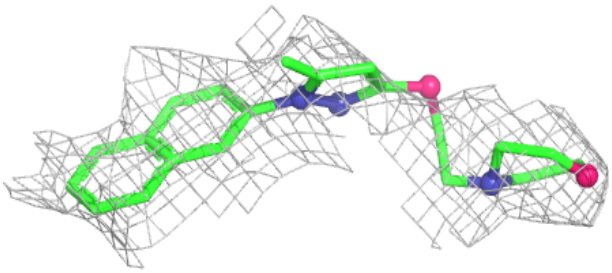


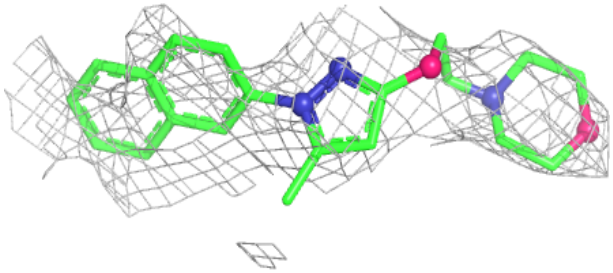


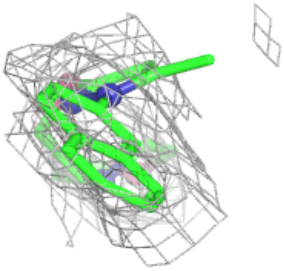


Electron density around 88E R 301:

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

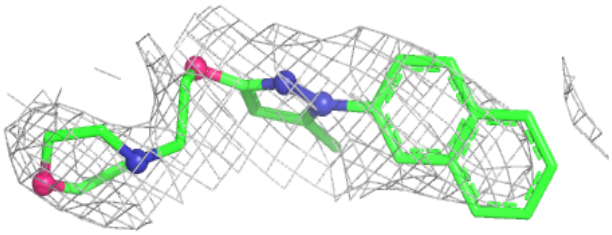


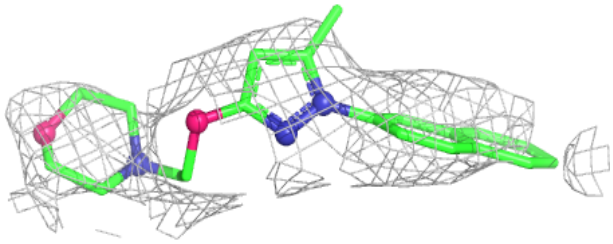


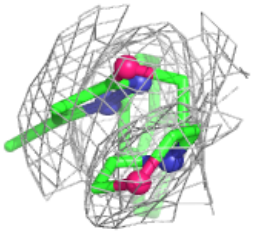


Electron density around 88E S 301:

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

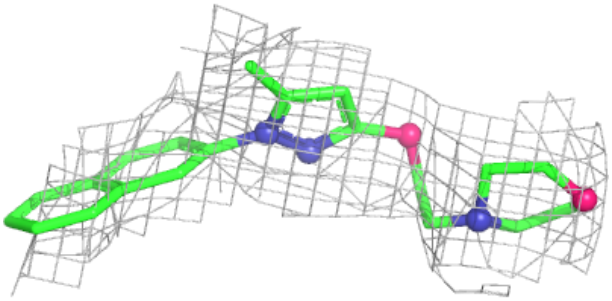


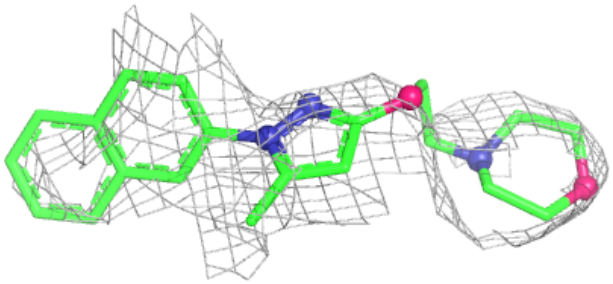


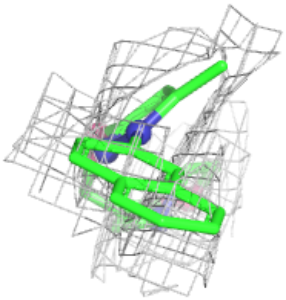


Electron density around 88E T 301:

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

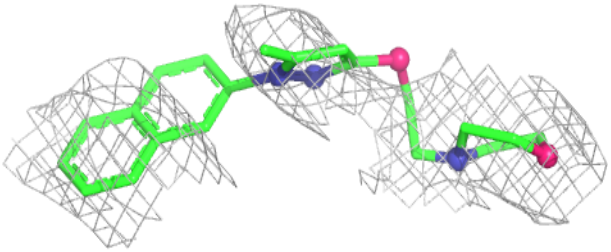


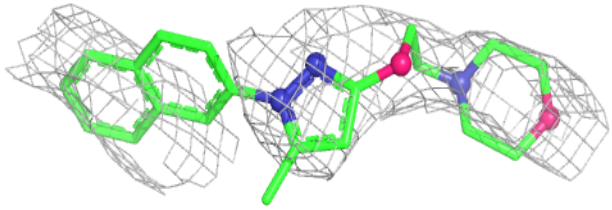


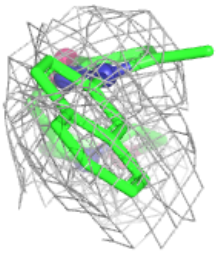


Electron density around 88E U 301:

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

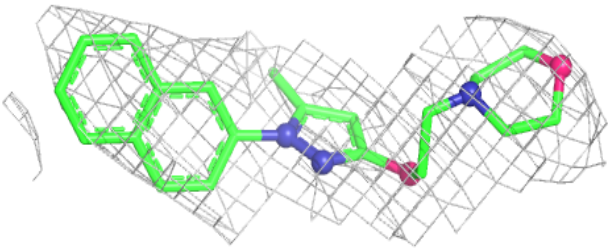


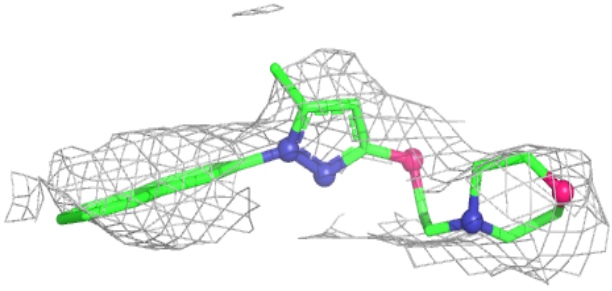


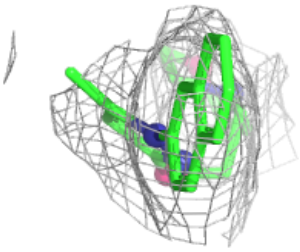


Electron density around 88E V 301:

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

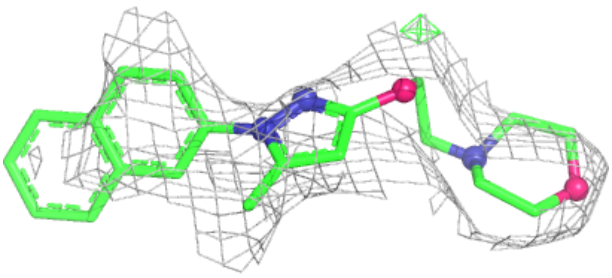


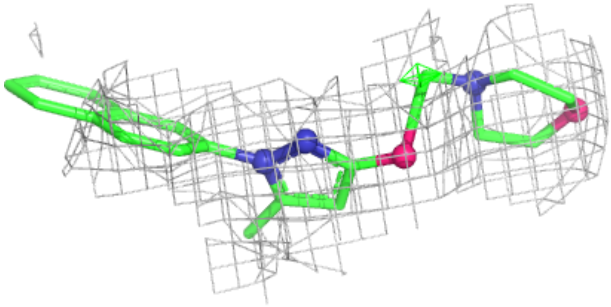


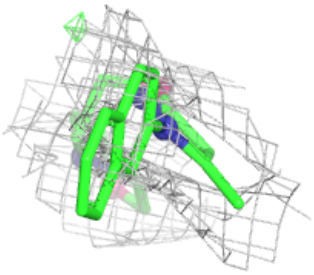


Electron density around 88E W 301:

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

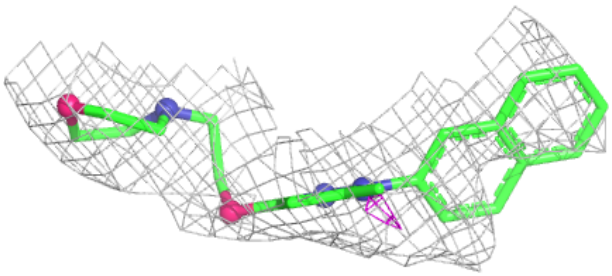


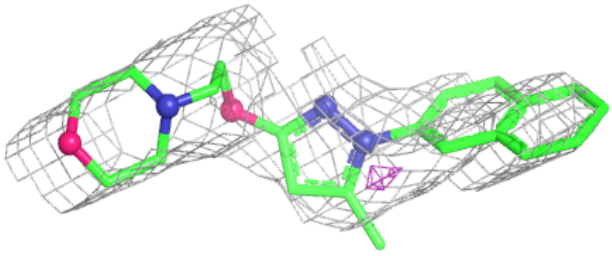


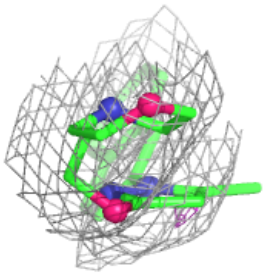


Electron density around 88E X 301:

$2mF_o$-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.