Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2024 – 12:54 pm BST

PDB ID	:	5K09
Title	:	Crystal Structure of COMT in complex with a thiazole ligand
Authors	:	Ehler, A.; Rodriguez-Sarmiento, R.M.; Rudolph, M.G.
Deposited on	:	2016-05-17
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

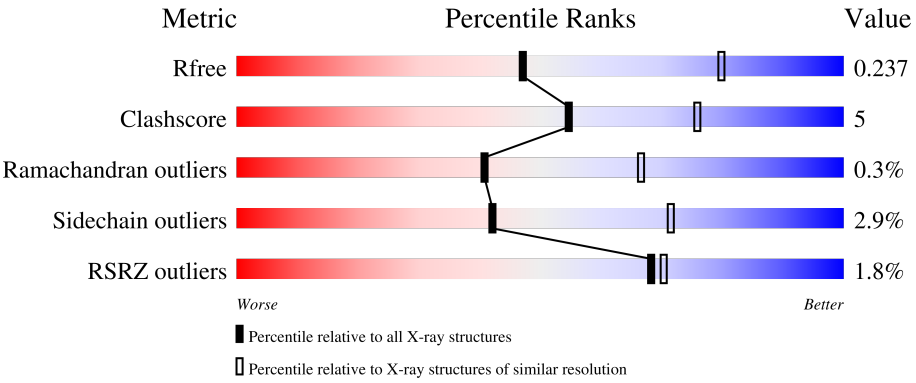
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	217	88% 12%
1	B	217	89% 10%
1	C	217	82% 16%
1	D	217	84% 14%
1	E	217	84% 14%

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Mol	Chain	Length	Quality of chain
1	F	217	86% 12%
1	G	217	82% 18%
1	H	217	84% 15%
1	I	217	82% 17%
1	J	217	83% 16%
1	K	217	81% 18%
1	L	217	80% 19%
1	M	217	85% 14%
1	N	217	86% 13%
1	O	217	83% 15%
1	P	217	82% 17%
1	Q	217	82% 18%
1	R	217	80% 19%
1	S	217	81% 17%
1	T	217	83% 16%
1	U	217	78% 21%
1	V	217	83% 15%
1	W	217	81% 18%
1	X	217	79% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	I	304	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 41639 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 Catechol O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1697	1075	281	329	12			
1	B	215	Total	C	N	O	S	0	0	0
			1683	1068	279	324	12			
1	C	216	Total	C	N	O	S	0	0	0
			1689	1071	280	326	12			
1	D	215	Total	C	N	O	S	0	0	0
			1683	1068	279	324	12			
1	E	215	Total	C	N	O	S	0	0	0
			1683	1068	279	324	12			
1	F	216	Total	C	N	O	S	0	0	0
			1689	1071	280	326	12			
1	G	217	Total	C	N	O	S	0	0	0
			1697	1075	281	329	12			
1	H	216	Total	C	N	O	S	0	0	0
			1689	1071	280	326	12			
1	I	215	Total	C	N	O	S	0	0	0
			1683	1068	279	324	12			
1	J	216	Total	C	N	O	S	0	0	0
			1689	1071	280	326	12			
1	K	215	Total	C	N	O	S	0	0	0
			1683	1068	279	324	12			
1	L	216	Total	C	N	O	S	0	0	0
			1689	1071	280	326	12			
1	M	215	Total	C	N	O	S	0	0	0
			1683	1068	279	324	12			
1	N	216	Total	C	N	O	S	0	0	0
			1689	1071	280	326	12			
1	O	216	Total	C	N	O	S	0	0	0
			1689	1071	280	326	12			
1	P	215	Total	C	N	O	S	0	0	0
			1683	1068	279	324	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	216	Total	C	N	O	S	0	0	0
			1689	1071	280	326	12			
1	R	217	Total	C	N	O	S	0	0	0
			1697	1075	281	329	12			
1	S	215	Total	C	N	O	S	0	0	0
			1683	1068	279	324	12			
1	T	215	Total	C	N	O	S	0	0	0
			1683	1068	279	324	12			
1	U	215	Total	C	N	O	S	0	0	0
			1683	1068	279	324	12			
1	V	215	Total	C	N	O	S	0	0	0
			1683	1068	279	324	12			
1	W	215	Total	C	N	O	S	0	0	0
			1683	1068	279	324	12			
1	X	215	Total	C	N	O	S	0	0	0
			1683	1068	279	324	12			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ILE	MET	engineered mutation	UNP P22734
A	95	CYS	TYR	engineered mutation	UNP P22734
A	156	GLU	LYS	engineered mutation	UNP P22734
A	218	ASP	-	expression tag	UNP P22734
B	91	ILE	MET	engineered mutation	UNP P22734
B	95	CYS	TYR	engineered mutation	UNP P22734
B	156	GLU	LYS	engineered mutation	UNP P22734
B	218	ASP	-	expression tag	UNP P22734
C	91	ILE	MET	engineered mutation	UNP P22734
C	95	CYS	TYR	engineered mutation	UNP P22734
C	156	GLU	LYS	engineered mutation	UNP P22734
C	218	ASP	-	expression tag	UNP P22734
D	91	ILE	MET	engineered mutation	UNP P22734
D	95	CYS	TYR	engineered mutation	UNP P22734
D	156	GLU	LYS	engineered mutation	UNP P22734
D	218	ASP	-	expression tag	UNP P22734
E	91	ILE	MET	engineered mutation	UNP P22734
E	95	CYS	TYR	engineered mutation	UNP P22734
E	156	GLU	LYS	engineered mutation	UNP P22734
E	218	ASP	-	expression tag	UNP P22734
F	91	ILE	MET	engineered mutation	UNP P22734
F	95	CYS	TYR	engineered mutation	UNP P22734
F	156	GLU	LYS	engineered mutation	UNP P22734

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Chain	Residue	Modelled	Actual	Comment	Reference
F	218	ASP	-	expression tag	UNP P22734
G	91	ILE	MET	engineered mutation	UNP P22734
G	95	CYS	TYR	engineered mutation	UNP P22734
G	156	GLU	LYS	engineered mutation	UNP P22734
G	218	ASP	-	expression tag	UNP P22734
H	91	ILE	MET	engineered mutation	UNP P22734
H	95	CYS	TYR	engineered mutation	UNP P22734
H	156	GLU	LYS	engineered mutation	UNP P22734
H	218	ASP	-	expression tag	UNP P22734
I	91	ILE	MET	engineered mutation	UNP P22734
I	95	CYS	TYR	engineered mutation	UNP P22734
I	156	GLU	LYS	engineered mutation	UNP P22734
I	218	ASP	-	expression tag	UNP P22734
J	91	ILE	MET	engineered mutation	UNP P22734
J	95	CYS	TYR	engineered mutation	UNP P22734
J	156	GLU	LYS	engineered mutation	UNP P22734
J	218	ASP	-	expression tag	UNP P22734
K	91	ILE	MET	engineered mutation	UNP P22734
K	95	CYS	TYR	engineered mutation	UNP P22734
K	156	GLU	LYS	engineered mutation	UNP P22734
K	218	ASP	-	expression tag	UNP P22734
L	91	ILE	MET	engineered mutation	UNP P22734
L	95	CYS	TYR	engineered mutation	UNP P22734
L	156	GLU	LYS	engineered mutation	UNP P22734
L	218	ASP	-	expression tag	UNP P22734
M	91	ILE	MET	engineered mutation	UNP P22734
M	95	CYS	TYR	engineered mutation	UNP P22734
M	156	GLU	LYS	engineered mutation	UNP P22734
M	218	ASP	-	expression tag	UNP P22734
N	91	ILE	MET	engineered mutation	UNP P22734
N	95	CYS	TYR	engineered mutation	UNP P22734
N	156	GLU	LYS	engineered mutation	UNP P22734
N	218	ASP	-	expression tag	UNP P22734
O	91	ILE	MET	engineered mutation	UNP P22734
O	95	CYS	TYR	engineered mutation	UNP P22734
O	156	GLU	LYS	engineered mutation	UNP P22734
O	218	ASP	-	expression tag	UNP P22734
P	91	ILE	MET	engineered mutation	UNP P22734
P	95	CYS	TYR	engineered mutation	UNP P22734
P	156	GLU	LYS	engineered mutation	UNP P22734
P	218	ASP	-	expression tag	UNP P22734
Q	91	ILE	MET	engineered mutation	UNP P22734

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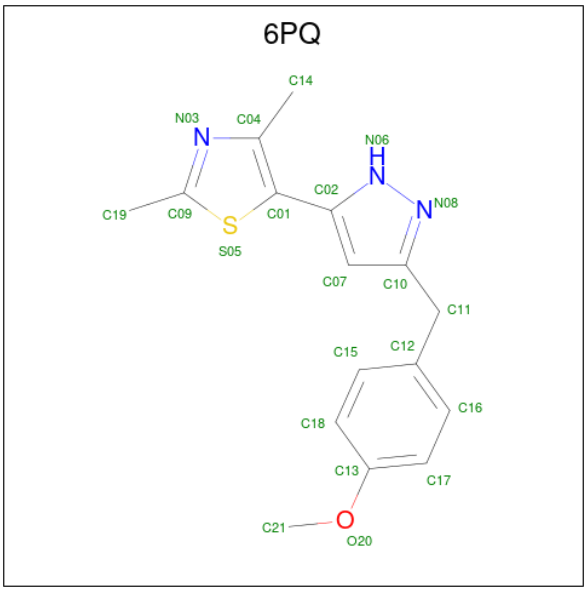
Chain	Residue	Modelled	Actual	Comment	Reference
Q	95	CYS	TYR	engineered mutation	UNP P22734
Q	156	GLU	LYS	engineered mutation	UNP P22734
Q	218	ASP	-	expression tag	UNP P22734
R	91	ILE	MET	engineered mutation	UNP P22734
R	95	CYS	TYR	engineered mutation	UNP P22734
R	156	GLU	LYS	engineered mutation	UNP P22734
R	218	ASP	-	expression tag	UNP P22734
S	91	ILE	MET	engineered mutation	UNP P22734
S	95	CYS	TYR	engineered mutation	UNP P22734
S	156	GLU	LYS	engineered mutation	UNP P22734
S	218	ASP	-	expression tag	UNP P22734
T	91	ILE	MET	engineered mutation	UNP P22734
T	95	CYS	TYR	engineered mutation	UNP P22734
T	156	GLU	LYS	engineered mutation	UNP P22734
T	218	ASP	-	expression tag	UNP P22734
U	91	ILE	MET	engineered mutation	UNP P22734
U	95	CYS	TYR	engineered mutation	UNP P22734
U	156	GLU	LYS	engineered mutation	UNP P22734
U	218	ASP	-	expression tag	UNP P22734
V	91	ILE	MET	engineered mutation	UNP P22734
V	95	CYS	TYR	engineered mutation	UNP P22734
V	156	GLU	LYS	engineered mutation	UNP P22734
V	218	ASP	-	expression tag	UNP P22734
W	91	ILE	MET	engineered mutation	UNP P22734
W	95	CYS	TYR	engineered mutation	UNP P22734
W	156	GLU	LYS	engineered mutation	UNP P22734
W	218	ASP	-	expression tag	UNP P22734
X	91	ILE	MET	engineered mutation	UNP P22734
X	95	CYS	TYR	engineered mutation	UNP P22734
X	156	GLU	LYS	engineered mutation	UNP P22734
X	218	ASP	-	expression tag	UNP P22734

- Molecule 2 is 5-{3-[(4-methoxyphenyl)methyl]-1H-pyrazol-5-yl}-2,4-dimethyl-1,3-thiazole (three-letter code: 6PQ) (formula: $C_{16}H_{17}N_3OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	B	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	C	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	D	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	E	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	F	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	G	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	H	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	I	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	J	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	K	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	L	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	M	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	N	1	Total	C	N	O	S	0	0
			21	16	3	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	P	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	Q	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	S	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	T	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	U	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	W	1	Total	C	N	O	S	0	0
			21	16	3	1	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	3	1	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	K	0	0
			3	3		
3	B	2	Total	K	0	0
			2	2		
3	C	2	Total	K	0	0
			2	2		
3	D	2	Total	K	0	0
			2	2		
3	E	2	Total	K	0	0
			2	2		
3	F	2	Total	K	0	0
			2	2		
3	G	3	Total	K	0	0
			3	3		
3	H	2	Total	K	0	0
			2	2		
3	I	2	Total	K	0	0
			2	2		

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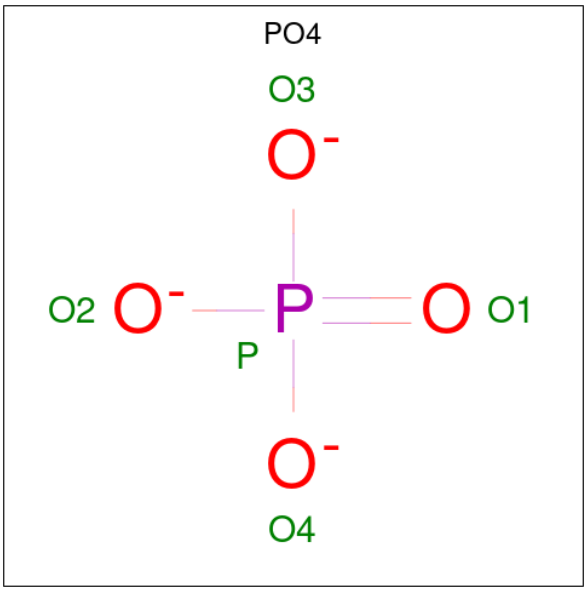
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	3	Total K 3 3	0	0
3	K	3	Total K 3 3	0	0
3	L	3	Total K 3 3	0	0
3	M	3	Total K 3 3	0	0
3	N	3	Total K 3 3	0	0
3	O	3	Total K 3 3	0	0
3	P	2	Total K 2 2	0	0
3	Q	2	Total K 2 2	0	0
3	R	3	Total K 3 3	0	0
3	S	3	Total K 3 3	0	0
3	T	2	Total K 2 2	0	0
3	U	2	Total K 2 2	0	0
3	V	2	Total K 2 2	0	0
3	W	2	Total K 2 2	0	0
3	X	2	Total K 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0
4	H	1	Total O P 5 4 1	0	0
4	I	1	Total O P 5 4 1	0	0
4	K	1	Total O P 5 4 1	0	0
4	M	1	Total O P 5 4 1	0	0
4	N	1	Total O P 5 4 1	0	0
4	Q	1	Total O P 5 4 1	0	0
4	S	1	Total O P 5 4 1	0	0
4	T	1	Total O P 5 4 1	0	0
4	V	1	Total O P 5 4 1	0	0
4	W	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	23	Total O 23 23	0	0
5	B	33	Total O 33 33	0	0
5	C	23	Total O 23 23	0	0
5	D	20	Total O 20 20	0	0
5	E	17	Total O 17 17	0	0
5	F	24	Total O 24 24	0	0
5	G	16	Total O 16 16	0	0
5	H	31	Total O 31 31	0	0
5	I	21	Total O 21 21	0	0
5	J	27	Total O 27 27	0	0
5	K	30	Total O 30 30	0	0
5	L	24	Total O 24 24	0	0
5	M	23	Total O 23 23	0	0
5	N	43	Total O 43 43	0	0
5	O	26	Total O 26 26	0	0
5	P	12	Total O 12 12	0	0
5	Q	24	Total O 24 24	0	0
5	R	27	Total O 27 27	0	0
5	S	22	Total O 22 22	0	0
5	T	23	Total O 23 23	0	0
5	U	10	Total O 10 10	0	0
5	V	15	Total O 15 15	0	0

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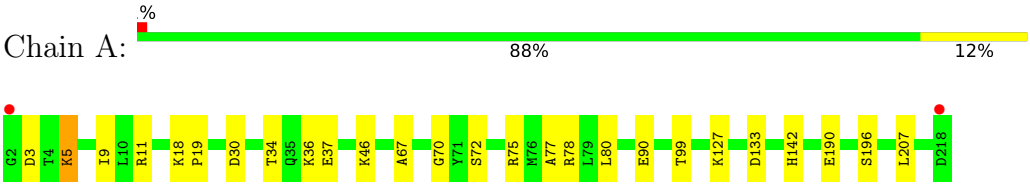
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	W	13	Total O 13 13	0	0
5	X	8	Total O 8 8	0	0

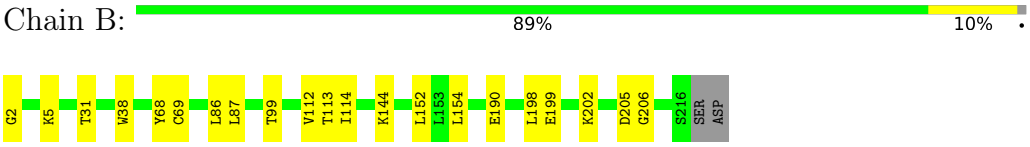
3 Residue-property plots (i)

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

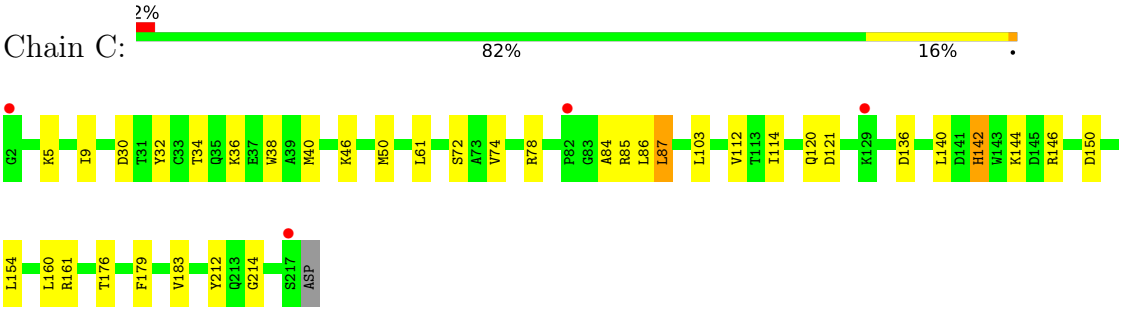
• Molecule 1: Catechol O-methyltransferase



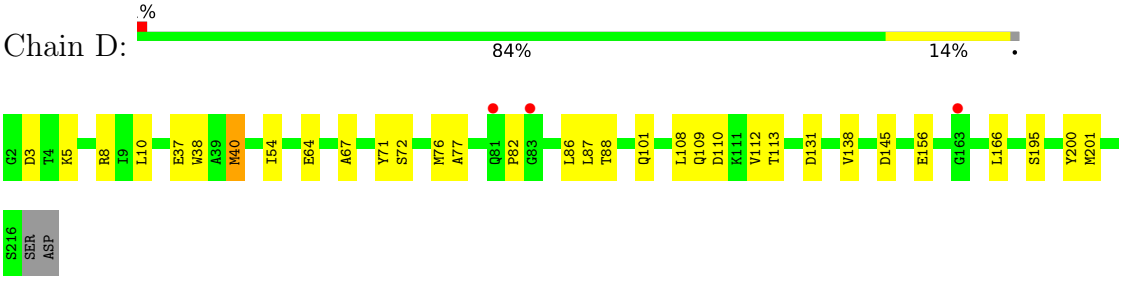
• Molecule 1: Catechol O-methyltransferase



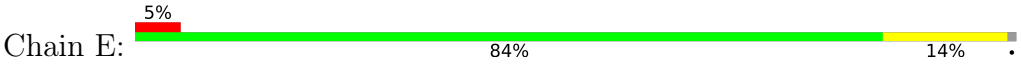
• Molecule 1: Catechol O-methyltransferase

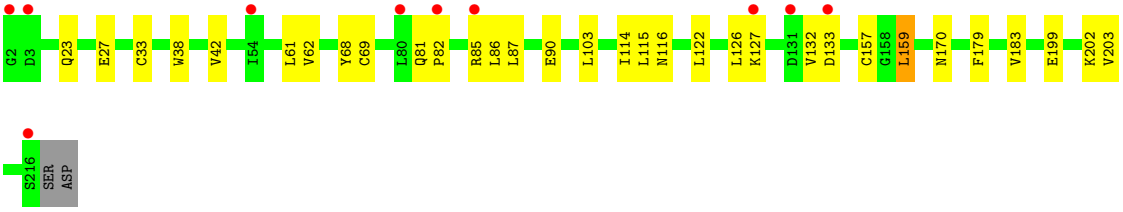


• Molecule 1: Catechol O-methyltransferase

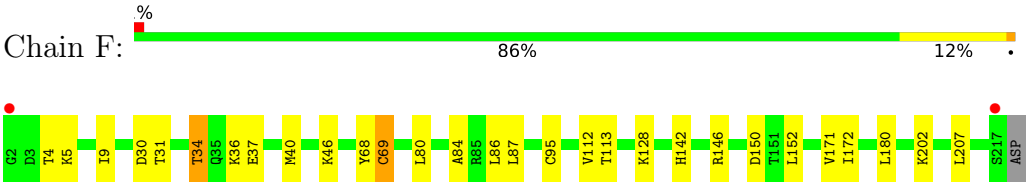


• Molecule 1: Catechol O-methyltransferase

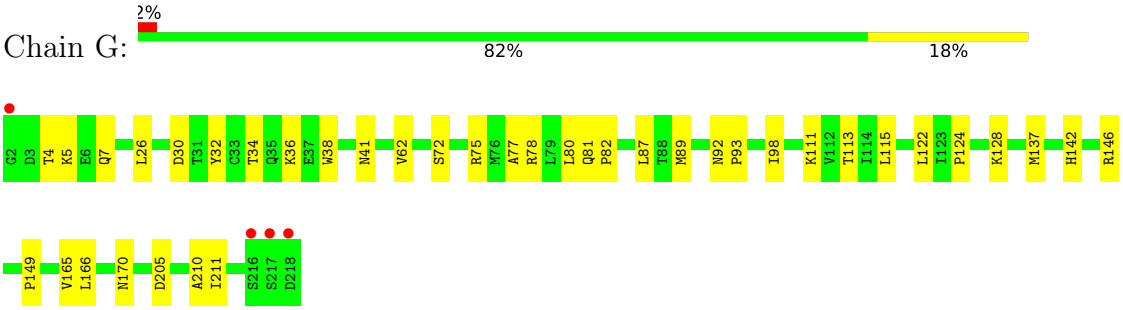




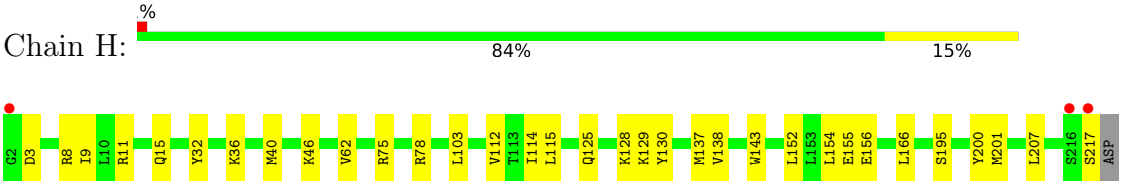
• Molecule 1: Catechol O-methyltransferase



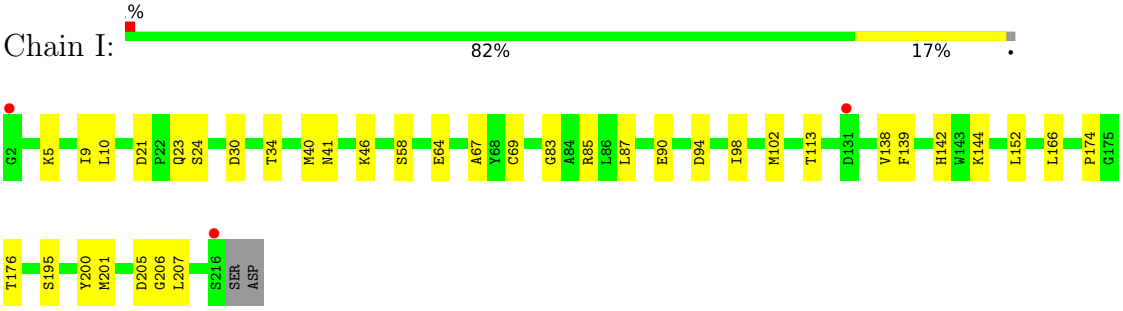
• Molecule 1: Catechol O-methyltransferase



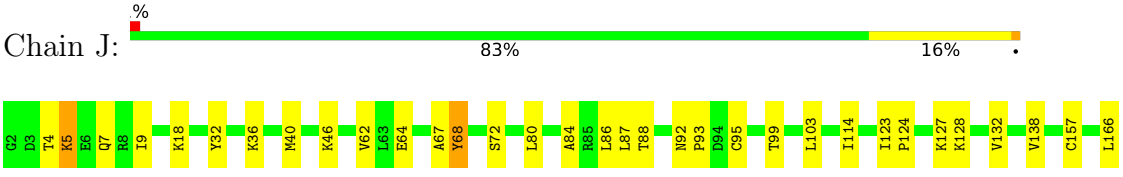
• Molecule 1: Catechol O-methyltransferase

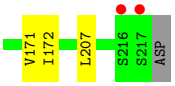


• Molecule 1: Catechol O-methyltransferase



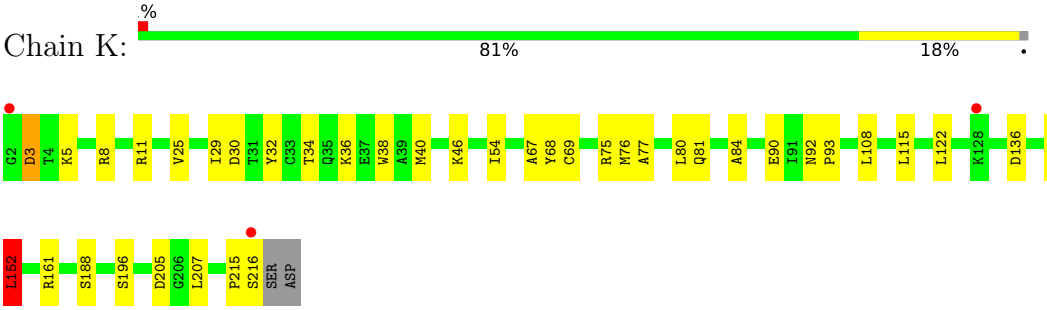
• Molecule 1: Catechol O-methyltransferase





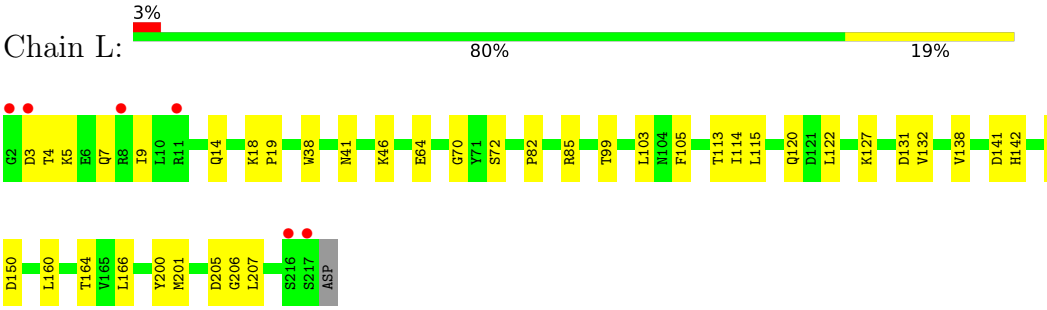
• Molecule 1: Catechol O-methyltransferase

Chain K:



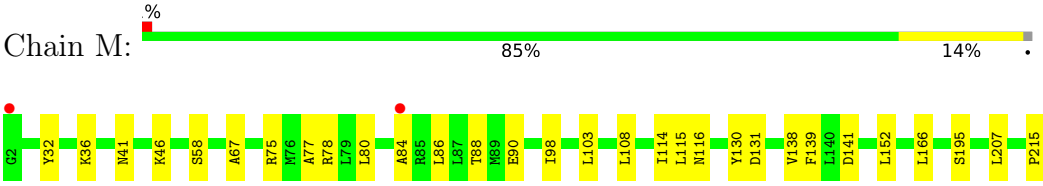
• Molecule 1: Catechol O-methyltransferase

Chain L:



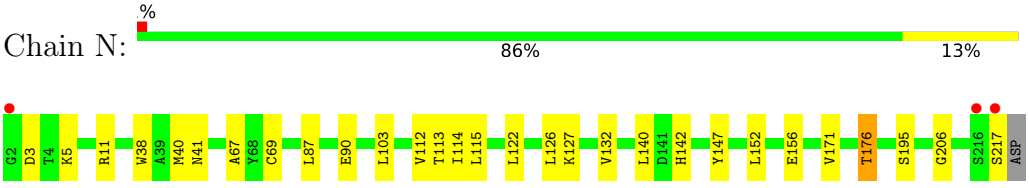
• Molecule 1: Catechol O-methyltransferase

Chain M:



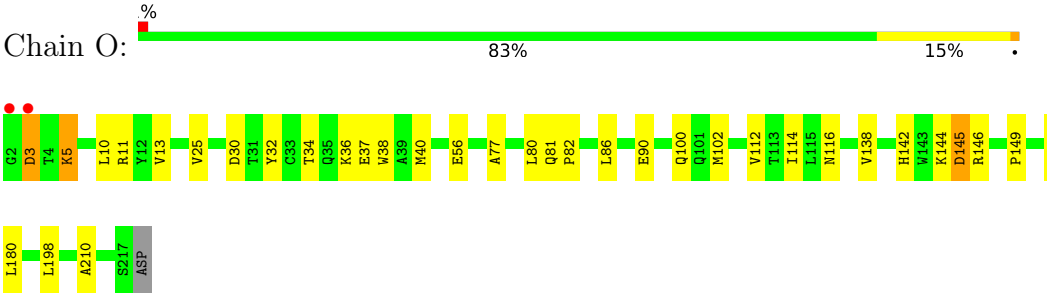
• Molecule 1: Catechol O-methyltransferase

Chain N:



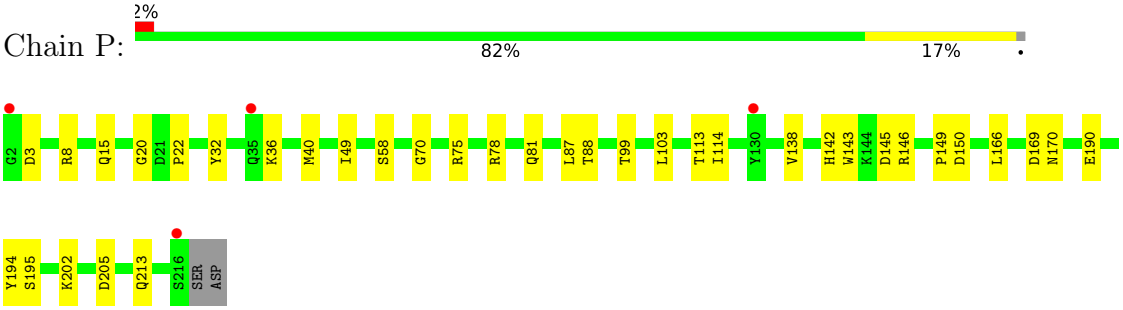
• Molecule 1: Catechol O-methyltransferase

Chain O:



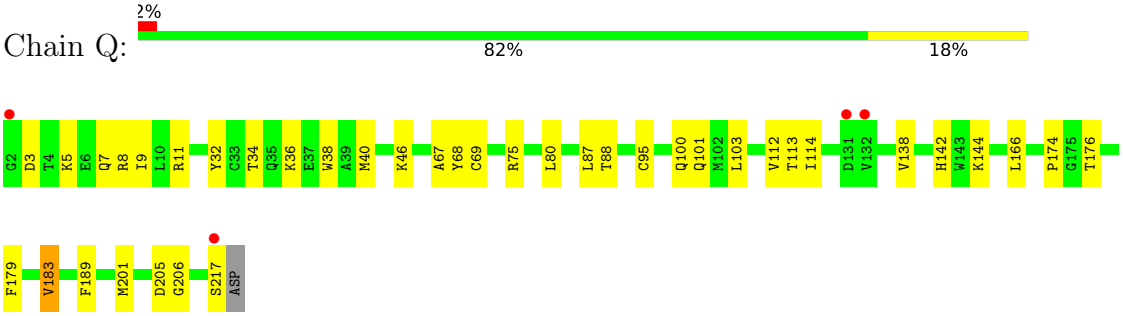
• Molecule 1: Catechol O-methyltransferase

Chain P:



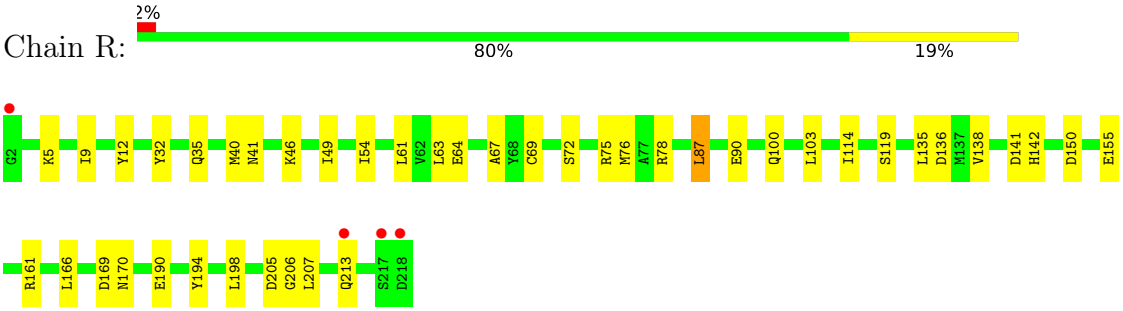
• Molecule 1: Catechol O-methyltransferase

Chain Q:



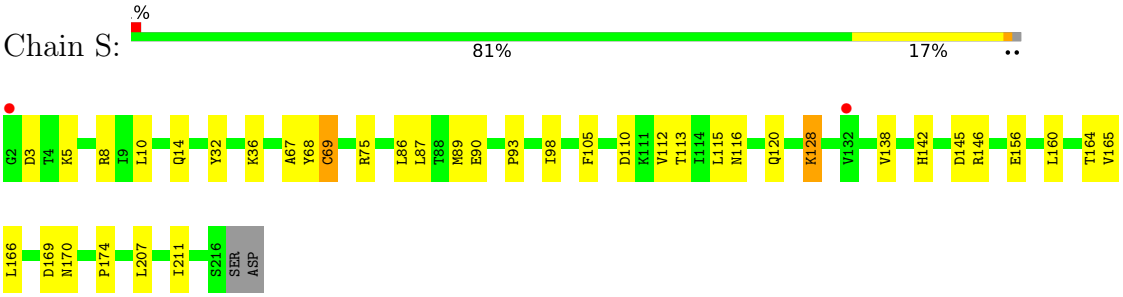
• Molecule 1: Catechol O-methyltransferase

Chain R:



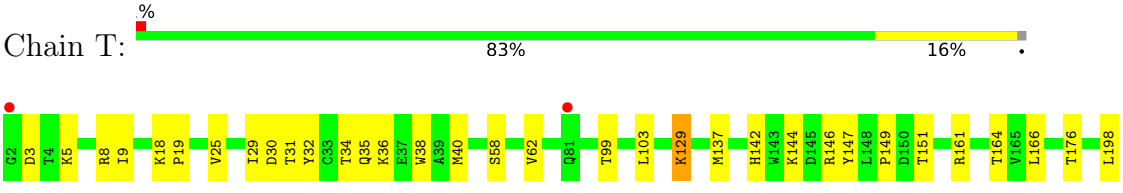
• Molecule 1: Catechol O-methyltransferase

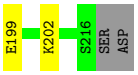
Chain S:



• Molecule 1: Catechol O-methyltransferase

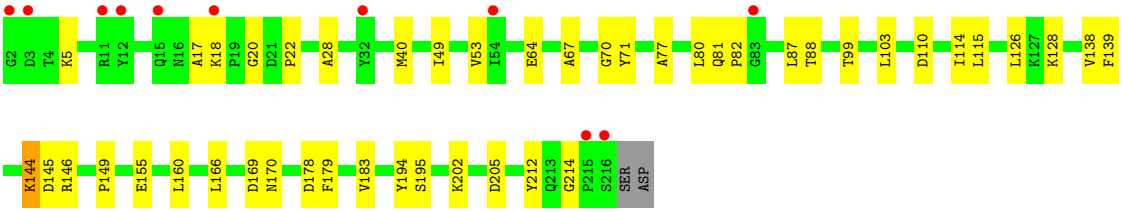
Chain T:





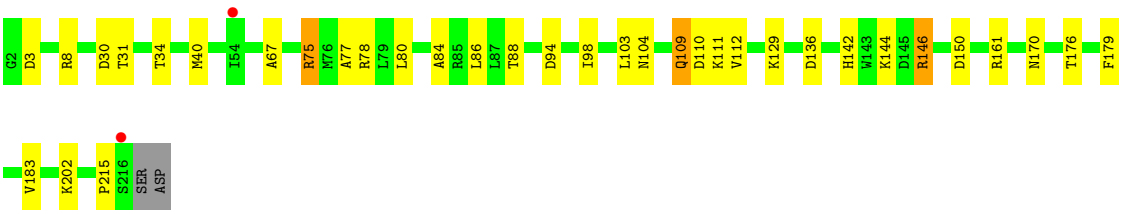
• Molecule 1: Catechol O-methyltransferase

Chain U:



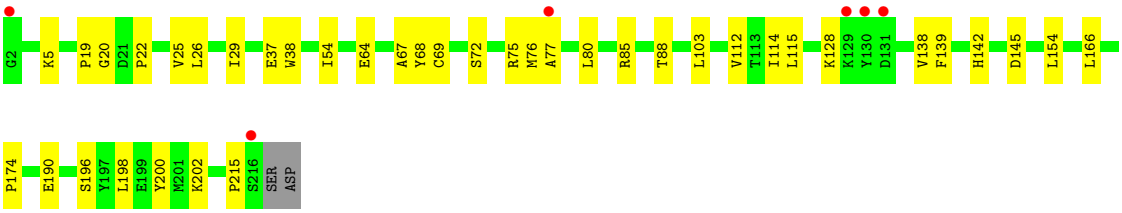
• Molecule 1: Catechol O-methyltransferase

Chain V:



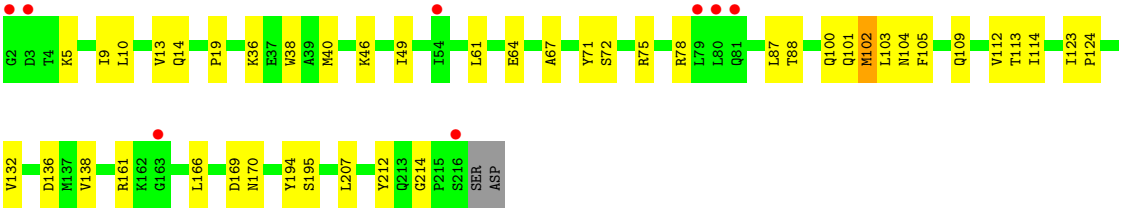
• Molecule 1: Catechol O-methyltransferase

Chain W:



• Molecule 1: Catechol O-methyltransferase

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	84.03Å 138.42Å 158.50Å 91.48° 97.19° 90.16°	Depositor
Resolution (Å)	48.84 – 2.70 48.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.84-2.70) 87.3 (48.83-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.165 , 0.236 0.168 , 0.237	Depositor DCC
R_{free} test set	9582 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.042 for -h,k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	41639	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 6PQ, K, PO4

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	0.40	0/1728	0.54	0/2343
1	B	0.43	0/1714	0.58	0/2324
1	C	0.40	0/1720	0.55	0/2332
1	D	0.40	0/1714	0.54	0/2324
1	E	0.36	0/1714	0.51	0/2324
1	F	0.44	1/1720 (0.1%)	0.57	0/2332
1	G	0.40	0/1728	0.55	0/2343
1	H	0.44	0/1720	0.58	0/2332
1	I	0.39	0/1714	0.55	0/2324
1	J	0.42	0/1720	0.57	0/2332
1	K	0.45	0/1714	0.59	1/2324 (0.0%)
1	L	0.42	0/1720	0.57	0/2332
1	M	0.41	0/1714	0.58	0/2324
1	N	0.44	1/1720 (0.1%)	0.57	0/2332
1	O	0.42	0/1720	0.59	0/2332
1	P	0.38	0/1714	0.54	0/2324
1	Q	0.42	0/1720	0.57	0/2332
1	R	0.40	0/1728	0.53	0/2343
1	S	0.39	0/1714	0.54	0/2324
1	T	0.41	0/1714	0.58	0/2324
1	U	0.36	0/1714	0.52	0/2324
1	V	0.39	0/1714	0.53	0/2324
1	W	0.36	0/1714	0.51	0/2324
1	X	0.36	0/1714	0.51	0/2324
All	All	0.40	2/41226 (0.0%)	0.55	1/55897 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	69	CYS	CB-SG	-6.30	1.71	1.82
1	F	69	CYS	CB-SG	-5.21	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	152	LEU	CA-CB-CG	-6.05	101.38	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	40	MET	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1697	0	1689	13	0
1	B	1683	0	1681	10	0
1	C	1689	0	1686	21	0
1	D	1683	0	1681	14	0
1	E	1683	0	1681	20	0
1	F	1689	0	1686	14	0
1	G	1697	0	1690	19	0
1	H	1689	0	1686	19	0
1	I	1683	0	1681	18	0
1	J	1689	0	1685	19	0
1	K	1683	0	1680	20	0
1	L	1689	0	1685	20	0
1	M	1683	0	1681	12	0
1	N	1689	0	1685	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1689	0	1685	18	0
1	P	1683	0	1681	20	0
1	Q	1689	0	1686	21	0
1	R	1697	0	1690	22	0
1	S	1683	0	1680	18	0
1	T	1683	0	1681	19	0
1	U	1683	0	1681	25	0
1	V	1683	0	1681	18	0
1	W	1683	0	1681	19	0
1	X	1683	0	1681	25	0
2	A	21	0	0	0	0
2	B	21	0	0	0	0
2	C	21	0	0	0	0
2	D	21	0	0	0	0
2	E	21	0	0	0	0
2	F	21	0	0	1	0
2	G	21	0	0	0	0
2	H	21	0	0	0	0
2	I	21	0	0	0	0
2	J	21	0	0	0	0
2	K	21	0	0	0	0
2	L	21	0	0	0	0
2	M	21	0	0	0	0
2	N	21	0	0	0	0
2	O	21	0	0	0	0
2	P	21	0	0	0	0
2	Q	21	0	0	0	0
2	R	21	0	0	0	0
2	S	21	0	0	0	0
2	T	21	0	0	0	0
2	U	21	0	0	0	0
2	V	21	0	0	0	0
2	W	21	0	0	0	0
2	X	21	0	0	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	2	0	0	0	0
3	J	3	0	0	1	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
3	M	3	0	0	0	0
3	N	3	0	0	0	0
3	O	3	0	0	0	0
3	P	2	0	0	0	0
3	Q	2	0	0	0	0
3	R	3	0	0	0	0
3	S	3	0	0	0	0
3	T	2	0	0	0	0
3	U	2	0	0	0	0
3	V	2	0	0	0	0
3	W	2	0	0	0	0
3	X	2	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	H	5	0	0	0	0
4	I	5	0	0	2	0
4	K	5	0	0	0	0
4	M	5	0	0	0	0
4	N	5	0	0	0	0
4	Q	5	0	0	0	0
4	S	5	0	0	0	0
4	T	5	0	0	0	0
4	V	5	0	0	0	0
4	W	5	0	0	1	0
5	A	23	0	0	0	0
5	B	33	0	0	0	0
5	C	23	0	0	0	0
5	D	20	0	0	0	0
5	E	17	0	0	0	0
5	F	24	0	0	0	0
5	G	16	0	0	0	0
5	H	31	0	0	1	0
5	I	21	0	0	0	0
5	J	27	0	0	2	0
5	K	30	0	0	0	0
5	L	24	0	0	0	0
5	M	23	0	0	0	0
5	N	43	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	O	26	0	0	0	0
5	P	12	0	0	0	0
5	Q	24	0	0	0	0
5	R	27	0	0	1	0
5	S	22	0	0	0	0
5	T	23	0	0	0	0
5	U	10	0	0	0	0
5	V	15	0	0	1	0
5	W	13	0	0	0	0
5	X	8	0	0	0	0
All	All	41639	0	40404	421	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 5.

All (421) 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:E:127:LYS:HE3	1:E:159:LEU:HD22	1.48	0.94
3:J:302:K:K	5:J:419:HOH:O	1.85	0.88
1:O:3:ASP:OD2	1:O:11:ARG:NH2	2.11	0.81
1:R:103:LEU:HD12	1:R:114:ILE:HD11	1.65	0.77
1:L:41:ASN:ND2	1:L:141:ASP:OD2	2.23	0.71
1:Q:3:ASP:O	1:Q:8:ARG:NH2	2.23	0.71
1:L:146:ARG:NH1	1:L:150:ASP:OD1	2.26	0.69
1:O:86:LEU:HB3	1:O:112:VAL:HG22	1.74	0.69
1:L:85:ARG:NH1	1:L:113:THR:OG1	2.26	0.69
1:J:46:LYS:HG2	1:J:207:LEU:HD11	1.75	0.67
1:I:87:LEU:HD23	1:I:113:THR:HB	1.77	0.67
1:R:46:LYS:HG2	1:R:207:LEU:HD11	1.77	0.67
1:R:136:ASP:OD1	1:R:161:ARG:NH2	2.26	0.67
1:X:75:ARG:HG3	1:X:78:ARG:HH12	1.59	0.66
1:L:138:VAL:HB	1:L:166:LEU:HD23	1.78	0.66
1:I:67:ALA:HB3	1:I:90:GLU:HB2	1.78	0.66
1:J:103:LEU:HD12	1:J:114:ILE:HD11	1.78	0.65
1:W:54:ILE:HD11	1:W:76:MET:HG2	1.78	0.65
1:X:40:MET:HE2	1:X:71:TYR:HB2	1.78	0.65
1:P:3:ASP:O	1:P:8:ARG:NH2	2.30	0.64
1:K:46:LYS:HG2	1:K:207:LEU:HD11	1.79	0.64
1:P:146:ARG:HD3	1:P:149:PRO:HG2	1.78	0.64
1:G:5:LYS:HD2	1:G:38:TRP:CE2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:103:LEU:HD12	1:U:114:ILE:HD11	1.81	0.63
1:D:3:ASP:O	1:D:8:ARG:NH2	2.33	0.62
1:N:67:ALA:HB3	1:N:90:GLU:HB2	1.81	0.62
1:Q:3:ASP:OD2	1:Q:11:ARG:NH2	2.32	0.62
1:X:103:LEU:HD22	1:X:112:VAL:HG21	1.81	0.62
1:P:70:GLY:HA3	1:P:99:THR:HG23	1.81	0.62
1:V:94:ASP:O	1:V:98:ILE:HG12	2.00	0.62
1:F:80:LEU:HB3	1:F:84:ALA:HB3	1.81	0.61
1:M:32:TYR:CZ	1:M:36:LYS:HG3	2.35	0.61
1:D:77:ALA:HB3	1:D:108:LEU:HD13	1.82	0.61
1:T:62:VAL:HG13	1:T:137:MET:HG2	1.83	0.61
1:L:46:LYS:HG2	1:L:207:LEU:HD11	1.83	0.61
1:C:146:ARG:NH1	1:C:150:ASP:OD1	2.31	0.61
1:X:138:VAL:HB	1:X:166:LEU:HD22	1.84	0.60
1:C:84:ALA:O	1:C:85:ARG:NH1	2.33	0.60
1:H:103:LEU:HD12	1:H:114:ILE:HD11	1.83	0.59
1:R:138:VAL:HB	1:R:166:LEU:HD22	1.84	0.59
1:U:64:GLU:HG3	1:U:139:PHE:HD2	1.68	0.59
1:F:30:ASP:O	1:F:34:THR:HG23	2.01	0.59
1:V:144:LYS:HB2	1:V:176:THR:HG22	1.84	0.59
1:V:103:LEU:HD13	1:V:112:VAL:HG11	1.85	0.59
1:H:46:LYS:HG2	1:H:207:LEU:HD11	1.84	0.58
1:J:64:GLU:OE2	1:J:72:SER:OG	2.18	0.58
1:H:62:VAL:HG13	1:H:137:MET:HG2	1.85	0.58
1:S:93:PRO:HA	1:S:116:ASN:HD21	1.68	0.58
1:W:64:GLU:OE2	1:W:72:SER:OG	2.18	0.58
1:I:138:VAL:HB	1:I:166:LEU:HD22	1.84	0.58
1:O:144:LYS:HB2	1:O:176:THR:HG22	1.85	0.58
1:P:190:GLU:HB2	1:P:213:GLN:HE21	1.68	0.58
1:G:166:LEU:HB2	1:G:210:ALA:HB3	1.85	0.58
1:B:205:ASP:OD1	1:B:206:GLY:N	2.33	0.58
1:K:3:ASP:OD2	1:K:11:ARG:NH2	2.36	0.58
1:L:120:GLN:HB3	1:L:146:ARG:NH1	2.17	0.58
1:F:46:LYS:HG2	1:F:207:LEU:HD11	1.84	0.58
1:P:49:ILE:HD13	1:P:194:TYR:HB3	1.86	0.58
1:R:40:MET:HE1	1:R:69:CYS:HB2	1.86	0.57
1:V:3:ASP:O	1:V:8:ARG:NH2	2.36	0.57
1:O:32:TYR:CZ	1:O:36:LYS:HG3	2.39	0.57
1:C:5:LYS:O	1:C:9:ILE:HG13	2.04	0.57
1:K:136:ASP:OD2	1:K:161:ARG:NH2	2.32	0.57
1:F:87:LEU:HD23	1:F:113:THR:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:ASP:O	1:K:34:THR:HG23	2.05	0.57
1:M:80:LEU:HB3	1:M:84:ALA:HB3	1.85	0.57
1:N:87:LEU:HD23	1:N:113:THR:HB	1.85	0.57
1:V:80:LEU:HB3	1:V:84:ALA:HB3	1.86	0.57
1:U:49:ILE:HD13	1:U:194:TYR:HB3	1.87	0.56
1:O:166:LEU:HB2	1:O:210:ALA:HB3	1.88	0.56
1:G:75:ARG:O	1:G:78:ARG:NH1	2.38	0.56
1:H:138:VAL:HB	1:H:166:LEU:HD22	1.86	0.56
1:L:14:GLN:HA	1:L:105:PHE:CE2	2.40	0.56
1:S:174:PRO:HD3	1:T:202:LYS:HB3	1.87	0.56
1:O:81:GLN:HG3	1:O:82:PRO:HD2	1.87	0.56
1:Q:87:LEU:HD23	1:Q:113:THR:HB	1.88	0.56
1:P:88:THR:HG23	1:P:114:ILE:HG23	1.86	0.56
1:X:5:LYS:HD2	1:X:38:TRP:CE2	2.40	0.56
1:X:61:LEU:HD21	1:X:132:VAL:HG13	1.86	0.56
1:H:32:TYR:CZ	1:H:36:LYS:HG3	2.41	0.55
1:X:104:ASN:HA	1:X:109:GLN:HB3	1.89	0.55
1:E:62:VAL:HB	1:E:86:LEU:HD13	1.87	0.55
1:P:103:LEU:HD12	1:P:114:ILE:HD11	1.89	0.55
1:Q:138:VAL:HB	1:Q:166:LEU:HD22	1.89	0.55
1:R:61:LEU:HD11	1:R:87:LEU:HD12	1.89	0.55
1:X:46:LYS:HG2	1:X:207:LEU:HD11	1.88	0.55
1:R:64:GLU:OE2	1:R:72:SER:OG	2.21	0.55
1:H:128:LYS:HE2	1:H:129:LYS:HG3	1.89	0.54
1:O:5:LYS:HD2	1:O:38:TRP:CE2	2.43	0.54
1:S:86:LEU:HB3	1:S:112:VAL:HG22	1.90	0.54
1:I:5:LYS:O	1:I:9:ILE:HG13	2.07	0.54
1:F:202:LYS:HB3	1:I:174:PRO:HD3	1.89	0.54
1:Q:103:LEU:HD12	1:Q:114:ILE:HD11	1.89	0.54
1:R:54:ILE:HD11	1:R:76:MET:HG2	1.89	0.54
1:L:146:ARG:HA	1:L:149:PRO:HG2	1.90	0.53
1:H:143:TRP:CZ2	1:K:152:LEU:HD13	2.43	0.53
1:S:32:TYR:CZ	1:S:36:LYS:HG3	2.44	0.53
1:G:87:LEU:HD23	1:G:113:THR:HB	1.91	0.53
1:E:61:LEU:HD13	1:E:85:ARG:HB2	1.91	0.52
1:M:138:VAL:HB	1:M:166:LEU:HD22	1.91	0.52
1:V:136:ASP:OD1	1:V:161:ARG:NH2	2.38	0.52
1:F:86:LEU:HB3	1:F:112:VAL:HG22	1.90	0.52
1:V:75:ARG:O	1:V:78:ARG:NH1	2.42	0.52
1:O:145:ASP:OD1	1:O:145:ASP:N	2.28	0.52
1:B:87:LEU:HD23	1:B:113:THR:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:138:VAL:HB	1:J:166:LEU:HD22	1.92	0.52
1:P:87:LEU:HD23	1:P:113:THR:HB	1.91	0.52
1:B:5:LYS:HD2	1:B:38:TRP:CE2	2.44	0.52
1:D:86:LEU:HB3	1:D:112:VAL:HG22	1.92	0.52
1:J:68:TYR:O	1:J:95:CYS:HB3	2.10	0.52
1:O:30:ASP:O	1:O:34:THR:HG23	2.10	0.52
1:U:67:ALA:HB2	1:U:88:THR:OG1	2.10	0.52
1:C:136:ASP:OD1	1:C:161:ARG:NH2	2.37	0.52
1:C:212:TYR:CE2	1:C:214:GLY:HA2	2.45	0.51
1:J:80:LEU:HB3	1:J:84:ALA:HB3	1.92	0.51
1:N:115:LEU:HB3	1:N:122:LEU:HD13	1.91	0.51
1:U:77:ALA:HA	1:U:80:LEU:HG	1.91	0.51
1:V:77:ALA:HA	1:V:80:LEU:HG	1.92	0.51
1:S:10:LEU:HD22	1:S:98:ILE:HG23	1.91	0.51
1:N:5:LYS:HD3	1:N:38:TRP:CD2	2.45	0.51
1:R:155:GLU:OE2	5:R:401:HOH:O	2.19	0.51
1:B:202:LYS:HB3	1:Q:174:PRO:HD3	1.93	0.51
1:E:87:LEU:HD22	1:E:115:LEU:HD11	1.92	0.51
1:X:87:LEU:HD23	1:X:113:THR:HB	1.92	0.51
1:C:9:ILE:HG12	1:C:32:TYR:CE2	2.46	0.51
1:B:2:GLY:N	1:H:217:SER:O	2.44	0.51
1:U:70:GLY:HA3	1:U:99:THR:HG23	1.91	0.51
1:V:86:LEU:HB3	1:V:112:VAL:HG22	1.92	0.51
1:V:202:LYS:HD2	5:V:411:HOH:O	2.10	0.51
1:O:144:LYS:NZ	1:U:178:ASP:OD2	2.45	0.50
1:W:5:LYS:HD2	1:W:38:TRP:CE2	2.46	0.50
1:J:171:VAL:HG23	1:J:172:ILE:HG12	1.93	0.50
1:T:146:ARG:HA	1:T:149:PRO:HG2	1.92	0.50
1:X:136:ASP:OD1	1:X:161:ARG:NH2	2.26	0.50
1:D:64:GLU:OE2	1:D:72:SER:OG	2.20	0.50
1:G:146:ARG:HA	1:G:149:PRO:HG2	1.93	0.50
1:I:21:ASP:HB3	1:I:24:SER:HB3	1.94	0.50
1:X:75:ARG:HG3	1:X:78:ARG:NH1	2.27	0.50
1:O:77:ALA:HA	1:O:80:LEU:HG	1.93	0.50
1:N:103:LEU:HD12	1:N:114:ILE:HD11	1.94	0.50
1:N:171:VAL:HA	1:N:176:THR:OG1	2.12	0.50
1:A:70:GLY:CA	1:A:99:THR:HG23	2.41	0.50
1:C:5:LYS:HE3	1:C:38:TRP:CD2	2.47	0.50
1:J:62:VAL:HB	1:J:86:LEU:HD12	1.94	0.50
1:M:46:LYS:HG2	1:M:207:LEU:HD11	1.92	0.50
1:M:75:ARG:HG3	1:M:78:ARG:HH12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:144:LYS:HB2	1:Q:176:THR:HG22	1.93	0.50
1:T:32:TYR:CZ	1:T:36:LYS:HD2	2.47	0.50
1:I:10:LEU:HD13	1:I:102:MET:HE2	1.92	0.49
1:I:40:MET:HE1	1:I:69:CYS:HB2	1.93	0.49
1:V:146:ARG:NH1	1:V:150:ASP:OD1	2.42	0.49
1:X:9:ILE:O	1:X:13:VAL:HG23	2.11	0.49
1:O:146:ARG:HA	1:O:149:PRO:HG2	1.94	0.49
1:S:138:VAL:HB	1:S:166:LEU:HD22	1.93	0.49
1:S:89:MET:HG2	1:S:115:LEU:HB2	1.94	0.49
1:W:26:LEU:HD11	1:W:75:ARG:HA	1.93	0.49
1:D:200:TYR:CE2	1:D:201:MET:HG2	2.47	0.49
1:P:202:LYS:HD2	1:X:170:ASN:OD1	2.12	0.49
1:R:67:ALA:HB3	1:R:90:GLU:HB2	1.95	0.49
1:T:30:ASP:O	1:T:34:THR:HG23	2.12	0.49
1:B:99:THR:HG22	1:B:114:ILE:HD11	1.94	0.49
1:E:23:GLN:O	1:E:27:GLU:HG3	2.12	0.49
1:X:103:LEU:HD12	1:X:114:ILE:HD11	1.94	0.49
1:P:32:TYR:CZ	1:P:36:LYS:HG3	2.47	0.49
1:X:14:GLN:HA	1:X:105:PHE:CZ	2.48	0.49
1:X:19:PRO:HG3	1:X:105:PHE:CZ	2.47	0.49
1:X:169:ASP:OD1	1:X:170:ASN:N	2.46	0.49
1:O:10:LEU:HD13	1:O:102:MET:HE2	1.94	0.49
1:R:63:LEU:HB2	1:R:135:LEU:HD22	1.95	0.48
1:S:87:LEU:HD23	1:S:113:THR:HB	1.95	0.48
1:G:7:GLN:HG3	1:G:98:ILE:HD11	1.94	0.48
1:H:143:TRP:HZ2	1:K:152:LEU:HD13	1.79	0.48
1:L:200:TYR:CE2	1:L:201:MET:HG2	2.49	0.48
1:E:179:PHE:O	1:E:183:VAL:HG22	2.12	0.48
1:K:5:LYS:HD2	1:K:38:TRP:CE2	2.48	0.48
1:F:171:VAL:HG23	1:F:172:ILE:HG12	1.96	0.48
1:P:138:VAL:HB	1:P:166:LEU:HD22	1.96	0.48
1:D:138:VAL:HB	1:D:166:LEU:HD22	1.95	0.48
1:N:3:ASP:OD2	1:N:11:ARG:NH2	2.46	0.48
1:V:30:ASP:O	1:V:34:THR:HG23	2.14	0.48
1:A:5:LYS:O	1:A:9:ILE:HG13	2.13	0.48
1:K:67:ALA:HB3	1:K:90:GLU:HB2	1.96	0.48
1:T:161:ARG:HG3	1:T:164:THR:OG1	2.14	0.48
1:W:114:ILE:O	1:W:115:LEU:HD23	2.14	0.48
1:A:127:LYS:NZ	1:A:133:ASP:O	2.47	0.47
1:F:152:LEU:HD22	1:P:143:TRP:CZ2	2.49	0.47
1:W:103:LEU:HD12	1:W:114:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5:LYS:HD2	1:L:38:TRP:CE2	2.49	0.47
1:V:104:ASN:OD1	1:V:109:GLN:HG3	2.14	0.47
1:I:30:ASP:O	1:I:34:THR:HG23	2.15	0.47
1:X:101:GLN:HA	1:X:104:ASN:HB2	1.96	0.47
1:C:32:TYR:CE1	1:C:36:LYS:HG3	2.50	0.47
1:P:75:ARG:O	1:P:78:ARG:NH1	2.47	0.47
1:Q:179:PHE:O	1:Q:183:VAL:HG22	2.15	0.47
1:M:115:LEU:HD22	1:M:130:TYR:CE1	2.49	0.47
1:U:17:ALA:HB2	1:U:28:ALA:HB2	1.96	0.47
1:H:9:ILE:HG12	1:H:32:TYR:CD2	2.49	0.47
1:H:154:LEU:HD23	1:H:154:LEU:HA	1.73	0.47
1:M:67:ALA:HB2	1:M:88:THR:OG1	2.14	0.47
1:M:139:PHE:CE2	1:M:141:ASP:HB2	2.50	0.47
1:S:160:LEU:HD22	1:S:164:THR:HG21	1.97	0.47
1:T:31:THR:O	1:T:35:GLN:HG3	2.14	0.47
1:T:147:TYR:CD2	1:T:176:THR:HG21	2.49	0.47
1:Q:103:LEU:HD22	1:Q:112:VAL:HG21	1.96	0.47
1:C:32:TYR:CZ	1:C:36:LYS:HG3	2.50	0.47
1:E:81:GLN:HB3	1:E:82:PRO:HD2	1.97	0.47
1:Q:5:LYS:HD2	1:Q:38:TRP:CE2	2.49	0.47
1:X:101:GLN:O	1:X:105:PHE:HB2	2.14	0.47
1:J:5:LYS:O	1:J:9:ILE:HG13	2.15	0.47
1:A:70:GLY:HA3	1:A:99:THR:HG23	1.97	0.46
1:U:138:VAL:HB	1:U:166:LEU:HD22	1.96	0.46
1:I:83:GLY:N	4:I:304:PO4:O2	2.41	0.46
1:K:80:LEU:HB3	1:K:84:ALA:HB3	1.96	0.46
1:S:14:GLN:HA	1:S:105:PHE:CE2	2.50	0.46
1:A:75:ARG:O	1:A:78:ARG:NH1	2.49	0.46
1:E:127:LYS:HZ2	1:E:133:ASP:C	2.19	0.46
1:K:46:LYS:NZ	1:K:205:ASP:OD2	2.40	0.46
1:Q:68:TYR:O	1:Q:95:CYS:HB3	2.15	0.46
1:W:138:VAL:HB	1:W:166:LEU:HD23	1.97	0.46
1:G:115:LEU:HB3	1:G:122:LEU:HD13	1.96	0.46
1:H:11:ARG:O	1:H:15:GLN:HG3	2.16	0.46
1:I:205:ASP:OD1	1:I:206:GLY:N	2.42	0.46
1:M:90:GLU:O	1:M:116:ASN:ND2	2.45	0.46
1:T:151:THR:HG23	1:T:166:LEU:HD11	1.97	0.46
1:F:68:TYR:O	1:F:95:CYS:HB3	2.15	0.46
1:K:25:VAL:O	1:K:29:ILE:HG13	2.15	0.46
1:I:46:LYS:HG2	1:I:207:LEU:HD11	1.97	0.46
1:M:75:ARG:O	1:M:78:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:25:VAL:O	1:T:29:ILE:HG13	2.16	0.46
1:J:99:THR:HG22	1:J:114:ILE:HD11	1.97	0.45
1:S:165:VAL:HG22	1:S:211:ILE:HG12	1.97	0.45
1:R:9:ILE:HG12	1:R:32:TYR:CE1	2.50	0.45
1:T:9:ILE:HG12	1:T:32:TYR:CD2	2.52	0.45
1:E:126:LEU:HD23	1:E:126:LEU:HA	1.73	0.45
1:G:124:PRO:O	1:G:128:LYS:NZ	2.49	0.45
1:H:155:GLU:OE2	5:H:401:HOH:O	2.21	0.45
1:Q:100:GLN:HE21	1:Q:101:GLN:HG3	1.82	0.45
1:E:115:LEU:HB3	1:E:122:LEU:HD13	1.99	0.45
1:J:92:ASN:HA	1:J:93:PRO:HD3	1.86	0.45
1:L:64:GLU:OE2	1:L:72:SER:OG	2.16	0.45
1:W:67:ALA:HB2	1:W:88:THR:OG1	2.16	0.45
1:J:32:TYR:CZ	1:J:36:LYS:HG3	2.51	0.45
1:K:77:ALA:HA	1:K:80:LEU:HG	1.98	0.45
1:P:170:ASN:HA	1:P:205:ASP:OD2	2.17	0.45
1:G:41:ASN:HD22	1:G:72:SER:HB3	1.81	0.45
1:K:68:TYR:CG	1:K:69:CYS:N	2.83	0.45
1:R:190:GLU:HB2	1:R:213:GLN:NE2	2.32	0.45
1:S:128:LYS:HD2	1:S:128:LYS:HA	1.54	0.45
1:E:68:TYR:CG	1:E:69:CYS:N	2.83	0.45
1:E:103:LEU:HD12	1:E:114:ILE:HD11	1.99	0.45
1:E:127:LYS:HD3	1:E:132:VAL:O	2.17	0.45
2:F:301:6PQ:C17	1:I:201:MET:HG3	2.48	0.45
1:G:62:VAL:HG22	1:G:137:MET:HB3	1.98	0.45
1:U:146:ARG:HA	1:U:149:PRO:HG2	1.99	0.45
1:U:155:GLU:HG2	1:U:160:LEU:HD12	1.99	0.44
1:U:169:ASP:OD1	1:U:170:ASN:N	2.51	0.44
1:E:199:GLU:HB3	1:E:203:VAL:HB	1.99	0.44
1:L:70:GLY:HA3	1:L:99:THR:HG23	1.99	0.44
1:T:3:ASP:O	1:T:8:ARG:NH2	2.50	0.44
1:C:5:LYS:HE3	1:C:38:TRP:CG	2.52	0.44
1:P:20:GLY:O	1:P:22:PRO:HD3	2.17	0.44
1:S:3:ASP:O	1:S:8:ARG:NH2	2.51	0.44
1:C:120:GLN:HG2	1:C:121:ASP:N	2.33	0.44
1:D:54:ILE:HD11	1:D:76:MET:HG2	1.99	0.44
1:F:36:LYS:O	1:F:37:GLU:HG2	2.17	0.44
1:R:5:LYS:O	1:R:9:ILE:HG13	2.17	0.44
1:G:82:PRO:HA	1:G:111:LYS:HZ1	1.83	0.44
1:G:170:ASN:HA	1:G:205:ASP:OD2	2.18	0.44
1:K:3:ASP:O	1:K:8:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:90:GLU:O	1:O:116:ASN:ND2	2.51	0.44
1:S:67:ALA:HB3	1:S:90:GLU:HB2	2.00	0.44
1:U:128:LYS:HE2	1:U:128:LYS:HB3	1.85	0.44
1:V:80:LEU:HB2	1:V:111:LYS:HE3	1.99	0.44
1:X:10:LEU:HD13	1:X:102:MET:HE2	1.98	0.44
1:B:68:TYR:CG	1:B:69:CYS:N	2.85	0.44
1:Q:40:MET:HE1	1:Q:69:CYS:HB2	2.00	0.44
1:Q:183:VAL:HG12	1:Q:189:PHE:CD2	2.53	0.44
1:T:5:LYS:HD2	1:T:38:TRP:CE2	2.52	0.44
1:F:180:LEU:HD23	1:F:180:LEU:HA	1.80	0.44
1:H:103:LEU:HD22	1:H:112:VAL:HG21	2.00	0.44
1:W:154:LEU:HD23	1:W:154:LEU:HA	1.84	0.44
1:X:64:GLU:OE2	1:X:72:SER:OG	2.15	0.44
1:T:9:ILE:HG12	1:T:32:TYR:CE2	2.53	0.43
1:U:144:LYS:HE2	1:U:144:LYS:HB3	1.77	0.43
1:J:87:LEU:HD11	1:J:132:VAL:HG21	2.00	0.43
1:R:49:ILE:HD13	1:R:194:TYR:HB3	1.99	0.43
1:L:4:THR:OG1	1:L:7:GLN:HG3	2.18	0.43
1:P:190:GLU:HB2	1:P:213:GLN:NE2	2.32	0.43
1:T:5:LYS:O	1:T:9:ILE:HG13	2.18	0.43
1:Q:32:TYR:CZ	1:Q:36:LYS:HG3	2.53	0.43
1:Q:205:ASP:CG	1:Q:206:GLY:H	2.21	0.43
1:X:67:ALA:HB2	1:X:88:THR:OG1	2.19	0.43
1:N:147:TYR:CD2	1:N:176:THR:HG21	2.53	0.43
1:A:36:LYS:HD3	1:A:36:LYS:HA	1.87	0.43
1:D:40:MET:HG3	1:D:71:TYR:CG	2.53	0.43
1:D:86:LEU:HD23	1:D:112:VAL:HG13	2.00	0.43
1:L:160:LEU:HD22	1:L:164:THR:HG21	2.00	0.43
1:T:18:LYS:HA	1:T:19:PRO:HD3	1.72	0.43
1:K:77:ALA:HB3	1:K:108:LEU:HD13	2.00	0.43
1:R:169:ASP:OD1	1:R:170:ASN:N	2.52	0.43
1:U:81:GLN:HG3	1:U:82:PRO:HD2	2.01	0.43
1:W:20:GLY:O	1:W:22:PRO:HD3	2.18	0.43
1:W:85:ARG:NH2	4:W:304:PO4:O1	2.48	0.43
1:C:74:VAL:O	1:C:78:ARG:HB3	2.19	0.43
1:C:144:LYS:HB2	1:C:176:THR:HG22	2.01	0.43
1:D:145:ASP:OD1	1:D:145:ASP:N	2.43	0.43
1:F:5:LYS:O	1:F:9:ILE:HG13	2.18	0.43
1:H:200:TYR:CE2	1:H:201:MET:HG2	2.54	0.43
1:I:200:TYR:CE2	1:I:201:MET:HG2	2.54	0.43
1:K:92:ASN:HA	1:K:93:PRO:HD3	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:9:ILE:HG12	1:Q:32:TYR:CD1	2.54	0.43
1:S:169:ASP:HA	1:S:207:LEU:HG	2.01	0.43
1:U:87:LEU:HD22	1:U:115:LEU:HD11	2.01	0.43
1:G:32:TYR:CZ	1:G:36:LYS:HG3	2.54	0.43
1:P:146:ARG:HD2	1:P:150:ASP:OD1	2.19	0.43
1:D:87:LEU:HD23	1:D:113:THR:HB	2.00	0.42
1:E:90:GLU:O	1:E:116:ASN:ND2	2.43	0.42
1:G:92:ASN:HA	1:G:93:PRO:HD3	1.89	0.42
1:J:67:ALA:HB2	1:J:88:THR:OG1	2.19	0.42
1:J:128:LYS:HB2	1:J:128:LYS:HE3	1.68	0.42
1:U:126:LEU:HD23	1:U:126:LEU:HA	1.84	0.42
1:V:129:LYS:HB3	1:V:129:LYS:HE2	1.71	0.42
1:I:64:GLU:HG3	1:I:139:PHE:HD2	1.83	0.42
1:U:212:TYR:CE2	1:U:214:GLY:HA2	2.55	0.42
1:V:179:PHE:O	1:V:183:VAL:HG22	2.19	0.42
1:B:154:LEU:HD23	1:B:154:LEU:HA	1.88	0.42
1:G:30:ASP:O	1:G:34:THR:HG23	2.19	0.42
1:D:5:LYS:HD2	1:D:38:TRP:CE2	2.54	0.42
1:N:140:LEU:N	1:N:140:LEU:HD12	2.34	0.42
1:S:170:ASN:ND2	1:T:199:GLU:OE2	2.41	0.42
1:U:145:ASP:OD1	1:U:145:ASP:N	2.34	0.42
1:A:46:LYS:HG2	1:A:207:LEU:HD11	2.00	0.42
1:J:127:LYS:HE3	1:J:157:CYS:O	2.19	0.42
1:L:18:LYS:HA	1:L:19:PRO:HD3	1.91	0.42
1:Q:67:ALA:HB2	1:Q:88:THR:OG1	2.19	0.42
1:U:20:GLY:O	1:U:22:PRO:HD3	2.20	0.42
1:H:3:ASP:O	1:H:8:ARG:NH2	2.52	0.42
1:L:103:LEU:HD12	1:L:114:ILE:HD11	2.00	0.42
1:M:77:ALA:HB3	1:M:108:LEU:HD13	2.00	0.42
1:N:127:LYS:HG2	1:N:132:VAL:O	2.19	0.42
1:U:170:ASN:HA	1:U:205:ASP:OD2	2.20	0.42
1:X:49:ILE:HD13	1:X:194:TYR:HB3	2.02	0.42
1:F:40:MET:HE1	1:F:69:CYS:HB2	2.02	0.42
1:G:89:MET:HG2	1:G:115:LEU:HB2	2.01	0.42
1:T:99:THR:HG22	1:T:103:LEU:HD12	2.01	0.42
1:L:205:ASP:CG	1:L:206:GLY:H	2.23	0.42
1:I:94:ASP:O	1:I:98:ILE:HG12	2.20	0.42
1:I:144:LYS:HB2	1:I:176:THR:HG22	2.02	0.42
1:N:103:LEU:HD13	1:N:112:VAL:HB	2.01	0.42
1:R:75:ARG:O	1:R:78:ARG:NH1	2.53	0.42
1:A:77:ALA:HA	1:A:80:LEU:HG	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LEU:HD11	1:C:87:LEU:HD12	2.01	0.42
1:L:5:LYS:O	1:L:9:ILE:HG13	2.20	0.42
1:O:13:VAL:HG11	1:O:25:VAL:HG13	2.01	0.42
1:U:40:MET:HG2	1:U:71:TYR:CG	2.55	0.42
1:X:123:ILE:HB	1:X:124:PRO:HD3	2.02	0.42
1:A:18:LYS:HA	1:A:19:PRO:HD3	1.95	0.41
1:C:179:PHE:O	1:C:183:VAL:HG22	2.19	0.41
1:S:120:GLN:HB3	1:S:146:ARG:NH2	2.35	0.41
1:C:30:ASP:O	1:C:34:THR:HG23	2.20	0.41
1:C:86:LEU:HB3	1:C:112:VAL:HG22	2.02	0.41
1:W:103:LEU:HD22	1:W:112:VAL:HG21	2.02	0.41
1:C:46:LYS:O	1:C:50:MET:HG3	2.20	0.41
1:G:165:VAL:HG22	1:G:211:ILE:HG12	2.02	0.41
1:H:75:ARG:O	1:H:78:ARG:NH1	2.52	0.41
1:L:115:LEU:HB2	1:L:122:LEU:HD13	2.02	0.41
1:R:100:GLN:OE1	1:R:114:ILE:HD12	2.20	0.41
1:B:199:GLU:CD	1:Q:46:LYS:HZ2	2.24	0.41
1:N:126:LEU:HD23	1:N:126:LEU:HA	1.88	0.41
1:N:217:SER:HB2	1:Q:7:GLN:HE22	1.84	0.41
1:J:18:LYS:NZ	5:J:404:HOH:O	2.52	0.41
1:V:67:ALA:HB2	1:V:88:THR:OG1	2.20	0.41
1:B:86:LEU:HB3	1:B:112:VAL:HG22	2.03	0.41
1:C:103:LEU:HD12	1:C:114:ILE:HD11	2.02	0.41
1:E:202:LYS:HB3	1:W:174:PRO:HD3	2.03	0.41
1:G:26:LEU:HD23	1:G:26:LEU:HA	1.82	0.41
1:N:171:VAL:HG22	1:N:206:GLY:O	2.20	0.41
1:R:41:ASN:HB2	1:R:141:ASP:OD2	2.20	0.41
1:X:212:TYR:CE2	1:X:214:GLY:HA2	2.56	0.41
1:D:10:LEU:HD21	1:D:101:GLN:OE1	2.21	0.41
1:L:127:LYS:HG2	1:L:132:VAL:O	2.20	0.41
1:O:138:VAL:HB	1:O:166:LEU:HD22	2.02	0.41
1:U:202:LYS:HD2	1:V:170:ASN:CG	2.40	0.41
1:D:67:ALA:HB2	1:D:88:THR:OG1	2.21	0.41
1:M:103:LEU:HD12	1:M:114:ILE:HD11	2.03	0.41
1:T:129:LYS:HA	1:T:129:LYS:HD2	1.81	0.41
1:U:179:PHE:O	1:U:183:VAL:HG22	2.20	0.41
1:W:77:ALA:HA	1:W:80:LEU:HG	2.03	0.41
1:A:30:ASP:O	1:A:34:THR:HG23	2.20	0.41
1:E:68:TYR:CE1	1:W:200:TYR:CZ	3.09	0.41
1:H:115:LEU:HD22	1:H:130:TYR:CE1	2.55	0.41
1:H:125:GLN:O	1:H:129:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4:THR:HG23	1:J:7:GLN:OE1	2.20	0.41
1:K:32:TYR:CZ	1:K:36:LYS:HG3	2.56	0.41
1:O:100:GLN:HB3	1:O:114:ILE:HD12	2.03	0.41
1:S:68:TYR:CG	1:S:69:CYS:N	2.88	0.41
1:U:49:ILE:O	1:U:53:VAL:HG23	2.21	0.41
1:W:64:GLU:HG3	1:W:139:PHE:HD2	1.85	0.41
1:A:67:ALA:HB3	1:A:90:GLU:HB2	2.03	0.41
1:P:169:ASP:OD1	1:P:170:ASN:N	2.54	0.41
1:R:119:SER:OG	1:R:150:ASP:OD2	2.28	0.41
1:W:68:TYR:CG	1:W:69:CYS:N	2.89	0.41
1:A:11:ARG:HH21	1:P:15:GLN:HG2	1.85	0.40
1:A:11:ARG:NH2	1:P:15:GLN:HG2	2.36	0.40
1:C:154:LEU:HD13	1:C:160:LEU:HD21	2.03	0.40
1:E:157:CYS:HB3	1:E:159:LEU:HD21	2.03	0.40
1:K:115:LEU:HB3	1:K:122:LEU:HD13	2.03	0.40
1:Q:80:LEU:HD23	1:Q:80:LEU:HA	1.83	0.40
1:C:140:LEU:HD23	1:C:142:HIS:HE1	1.85	0.40
1:E:170:ASN:OD1	1:W:202:LYS:HD2	2.22	0.40
1:I:85:ARG:NH2	4:I:304:PO4:O1	2.54	0.40
1:J:123:ILE:HB	1:J:124:PRO:HD3	2.03	0.40
1:K:54:ILE:HD11	1:K:76:MET:HG2	2.04	0.40
1:E:33:CYS:HB3	1:E:38:TRP:O	2.21	0.40
1:R:12:TYR:CD2	1:R:32:TYR:HB2	2.57	0.40
1:F:146:ARG:NH2	1:F:150:ASP:OD1	2.50	0.40
1:K:122:LEU:HA	1:K:122:LEU:HD23	1.91	0.40
1:O:180:LEU:HA	1:O:180:LEU:HD23	1.80	0.40
1:R:205:ASP:CG	1:R:206:GLY:H	2.25	0.40
1:W:25:VAL:O	1:W:29:ILE:HG13	2.21	0.40
1:G:77:ALA:HA	1:G:80:LEU:HG	2.04	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	215/217 (99%)	207 (96%)	7 (3%)	1 (0%)	29	54
1	B	213/217 (98%)	204 (96%)	9 (4%)	0	100	100
1	C	214/217 (99%)	203 (95%)	11 (5%)	0	100	100
1	D	213/217 (98%)	199 (93%)	12 (6%)	2 (1%)	17	40
1	E	213/217 (98%)	198 (93%)	15 (7%)	0	100	100
1	F	214/217 (99%)	201 (94%)	13 (6%)	0	100	100
1	G	215/217 (99%)	201 (94%)	14 (6%)	0	100	100
1	H	214/217 (99%)	200 (94%)	14 (6%)	0	100	100
1	I	213/217 (98%)	199 (93%)	14 (7%)	0	100	100
1	J	214/217 (99%)	206 (96%)	7 (3%)	1 (0%)	29	54
1	K	213/217 (98%)	199 (93%)	13 (6%)	1 (0%)	29	54
1	L	214/217 (99%)	194 (91%)	19 (9%)	1 (0%)	29	54
1	M	213/217 (98%)	200 (94%)	11 (5%)	2 (1%)	17	40
1	N	214/217 (99%)	202 (94%)	11 (5%)	1 (0%)	29	54
1	O	214/217 (99%)	200 (94%)	13 (6%)	1 (0%)	29	54
1	P	213/217 (98%)	201 (94%)	12 (6%)	0	100	100
1	Q	214/217 (99%)	203 (95%)	10 (5%)	1 (0%)	29	54
1	R	215/217 (99%)	201 (94%)	14 (6%)	0	100	100
1	S	213/217 (98%)	200 (94%)	13 (6%)	0	100	100
1	T	213/217 (98%)	201 (94%)	12 (6%)	0	100	100
1	U	213/217 (98%)	196 (92%)	17 (8%)	0	100	100
1	V	213/217 (98%)	203 (95%)	9 (4%)	1 (0%)	29	54
1	W	213/217 (98%)	197 (92%)	13 (6%)	3 (1%)	11	28
1	X	213/217 (98%)	200 (94%)	13 (6%)	0	100	100
All	All	5126/5208 (98%)	4815 (94%)	296 (6%)	15 (0%)	41	66

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	41	ASN
1	N	41	ASN
1	W	215	PRO
1	A	37	GLU
1	L	82	PRO
1	Q	201	MET

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Mol	Chain	Res	Type
1	W	37	GLU
1	D	37	GLU
1	M	215	PRO
1	O	37	GLU
1	J	68	TYR
1	K	215	PRO
1	W	19	PRO
1	D	82	PRO
1	V	215	PRO

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	186/186 (100%)	180 (97%)	6 (3%)	39	68
1	B	184/186 (99%)	179 (97%)	5 (3%)	44	74
1	C	185/186 (100%)	181 (98%)	4 (2%)	52	79
1	D	184/186 (99%)	178 (97%)	6 (3%)	38	67
1	E	184/186 (99%)	182 (99%)	2 (1%)	73	90
1	F	185/186 (100%)	180 (97%)	5 (3%)	44	74
1	G	186/186 (100%)	183 (98%)	3 (2%)	62	85
1	H	185/186 (100%)	181 (98%)	4 (2%)	52	79
1	I	184/186 (99%)	178 (97%)	6 (3%)	38	67
1	J	185/186 (100%)	183 (99%)	2 (1%)	73	90
1	K	184/186 (99%)	174 (95%)	10 (5%)	22	47
1	L	185/186 (100%)	180 (97%)	5 (3%)	44	74
1	M	184/186 (99%)	178 (97%)	6 (3%)	38	67
1	N	185/186 (100%)	180 (97%)	5 (3%)	44	74
1	O	185/186 (100%)	178 (96%)	7 (4%)	33	62
1	P	184/186 (99%)	178 (97%)	6 (3%)	38	67
1	Q	185/186 (100%)	180 (97%)	5 (3%)	44	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	R	186/186 (100%)	182 (98%)	4 (2%)	52 79
1	S	184/186 (99%)	176 (96%)	8 (4%)	29 57
1	T	184/186 (99%)	178 (97%)	6 (3%)	38 67
1	U	184/186 (99%)	179 (97%)	5 (3%)	44 74
1	V	184/186 (99%)	177 (96%)	7 (4%)	33 62
1	W	184/186 (99%)	178 (97%)	6 (3%)	38 67
1	X	184/186 (99%)	180 (98%)	4 (2%)	52 79
All	All	4430/4464 (99%)	4303 (97%)	127 (3%)	42 71

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	5	LYS
1	A	72	SER
1	A	142	HIS
1	A	190	GLU
1	A	196	SER
1	B	31	THR
1	B	144	LYS
1	B	152	LEU
1	B	190	GLU
1	B	198	LEU
1	C	40	MET
1	C	72	SER
1	C	87	LEU
1	C	142	HIS
1	D	40	MET
1	D	109	GLN
1	D	110	ASP
1	D	131	ASP
1	D	156	GLU
1	D	195	SER
1	E	42	VAL
1	E	159	LEU
1	F	4	THR
1	F	31	THR
1	F	34	THR
1	F	128	LYS
1	F	142	HIS

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Mol	Chain	Res	Type
1	G	4	THR
1	G	81	GLN
1	G	142	HIS
1	H	40	MET
1	H	152	LEU
1	H	156	GLU
1	H	195	SER
1	I	23	GLN
1	I	41	ASN
1	I	58	SER
1	I	142	HIS
1	I	152	LEU
1	I	195	SER
1	J	5	LYS
1	J	40	MET
1	K	3	ASP
1	K	40	MET
1	K	75	ARG
1	K	81	GLN
1	K	142	HIS
1	K	145	ASP
1	K	152	LEU
1	K	188	SER
1	K	196	SER
1	K	216	SER
1	L	3	ASP
1	L	131	ASP
1	L	142	HIS
1	L	145	ASP
1	L	146	ARG
1	M	58	SER
1	M	86	LEU
1	M	98	ILE
1	M	131	ASP
1	M	152	LEU
1	M	195	SER
1	N	142	HIS
1	N	152	LEU
1	N	156	GLU
1	N	176	THR
1	N	195	SER
1	O	3	ASP

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Mol	Chain	Res	Type
1	O	5	LYS
1	O	40	MET
1	O	56	GLU
1	O	142	HIS
1	O	145	ASP
1	O	198	LEU
1	P	40	MET
1	P	58	SER
1	P	81	GLN
1	P	142	HIS
1	P	145	ASP
1	P	195	SER
1	Q	34	THR
1	Q	75	ARG
1	Q	142	HIS
1	Q	183	VAL
1	Q	217	SER
1	R	35	GLN
1	R	87	LEU
1	R	142	HIS
1	R	198	LEU
1	S	5	LYS
1	S	69	CYS
1	S	75	ARG
1	S	110	ASP
1	S	128	LYS
1	S	142	HIS
1	S	145	ASP
1	S	156	GLU
1	T	40	MET
1	T	58	SER
1	T	129	LYS
1	T	142	HIS
1	T	144	LYS
1	T	198	LEU
1	U	5	LYS
1	U	18	LYS
1	U	110	ASP
1	U	144	LYS
1	U	195	SER
1	V	31	THR
1	V	40	MET

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Mol	Chain	Res	Type
1	V	75	ARG
1	V	109	GLN
1	V	110	ASP
1	V	142	HIS
1	V	146	ARG
1	W	128	LYS
1	W	142	HIS
1	W	145	ASP
1	W	190	GLU
1	W	196	SER
1	W	198	LEU
1	X	36	LYS
1	X	100	GLN
1	X	102	MET
1	X	195	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	41	ASN
1	Q	100	GLN
1	S	116	ASN
1	W	81	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 94 ligands modelled in this entry, 58 are monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	6PQ	S	301	-	19,23,23	1.19	1 (5%)	17,32,32	1.68	3 (17%)
4	PO4	N	305	-	4,4,4	0.84	0	6,6,6	0.83	0
2	6PQ	K	301	-	19,23,23	1.18	1 (5%)	17,32,32	1.84	3 (17%)
2	6PQ	N	301	-	19,23,23	1.13	1 (5%)	17,32,32	1.75	3 (17%)
4	PO4	Q	304	-	4,4,4	0.90	0	6,6,6	0.48	0
2	6PQ	D	301	-	19,23,23	1.23	1 (5%)	17,32,32	1.67	3 (17%)
2	6PQ	G	301	-	19,23,23	1.23	1 (5%)	17,32,32	1.66	3 (17%)
4	PO4	T	304	-	4,4,4	0.88	0	6,6,6	0.41	0
4	PO4	V	304	-	4,4,4	0.90	0	6,6,6	0.35	0
4	PO4	W	304	-	4,4,4	0.91	0	6,6,6	0.38	0
4	PO4	H	304	-	4,4,4	0.87	0	6,6,6	0.41	0
2	6PQ	T	301	-	19,23,23	1.24	1 (5%)	17,32,32	1.60	3 (17%)
2	6PQ	X	301	-	19,23,23	1.24	2 (10%)	17,32,32	1.50	3 (17%)
2	6PQ	V	301	-	19,23,23	1.16	1 (5%)	17,32,32	1.67	3 (17%)
2	6PQ	A	301	-	19,23,23	1.12	1 (5%)	17,32,32	1.80	3 (17%)
2	6PQ	I	301	-	19,23,23	1.20	1 (5%)	17,32,32	1.66	3 (17%)
4	PO4	I	304	-	4,4,4	0.86	0	6,6,6	0.58	0
2	6PQ	Q	301	-	19,23,23	1.19	1 (5%)	17,32,32	1.70	3 (17%)
4	PO4	C	304	-	4,4,4	0.92	0	6,6,6	0.42	0
2	6PQ	M	301	-	19,23,23	1.20	2 (10%)	17,32,32	1.76	3 (17%)
4	PO4	D	304	-	4,4,4	0.92	0	6,6,6	0.44	0
2	6PQ	B	301	-	19,23,23	1.20	1 (5%)	17,32,32	1.83	3 (17%)
4	PO4	S	305	-	4,4,4	0.91	0	6,6,6	0.53	0
2	6PQ	C	301	-	19,23,23	1.21	1 (5%)	17,32,32	1.62	3 (17%)
2	6PQ	O	301	-	19,23,23	1.27	1 (5%)	17,32,32	1.53	3 (17%)
2	6PQ	U	301	-	19,23,23	1.22	1 (5%)	17,32,32	1.65	3 (17%)
2	6PQ	P	301	-	19,23,23	1.25	1 (5%)	17,32,32	1.77	4 (23%)
2	6PQ	W	301	-	19,23,23	1.23	1 (5%)	17,32,32	1.69	2 (11%)
4	PO4	K	305	-	4,4,4	0.83	0	6,6,6	0.53	0
2	6PQ	H	301	-	19,23,23	1.24	2 (10%)	17,32,32	1.67	3 (17%)
2	6PQ	J	301	-	19,23,23	1.25	2 (10%)	17,32,32	1.68	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	6PQ	L	301	-	19,23,23	1.22	1 (5%)	17,32,32	1.75	3 (17%)
2	6PQ	F	301	-	19,23,23	1.28	2 (10%)	17,32,32	1.71	4 (23%)
2	6PQ	R	301	-	19,23,23	1.15	1 (5%)	17,32,32	1.71	3 (17%)
2	6PQ	E	301	-	19,23,23	1.21	2 (10%)	17,32,32	1.71	3 (17%)
4	PO4	M	305	-	4,4,4	0.83	0	6,6,6	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6PQ	S	301	-	-	2/6/10/10	0/3/3/3
2	6PQ	K	301	-	-	2/6/10/10	0/3/3/3
2	6PQ	N	301	-	-	2/6/10/10	0/3/3/3
2	6PQ	D	301	-	-	0/6/10/10	0/3/3/3
2	6PQ	G	301	-	-	2/6/10/10	0/3/3/3
2	6PQ	T	301	-	-	0/6/10/10	0/3/3/3
2	6PQ	X	301	-	-	2/6/10/10	0/3/3/3
2	6PQ	V	301	-	-	0/6/10/10	0/3/3/3
2	6PQ	A	301	-	-	2/6/10/10	0/3/3/3
2	6PQ	I	301	-	-	2/6/10/10	0/3/3/3
2	6PQ	Q	301	-	-	0/6/10/10	0/3/3/3
2	6PQ	M	301	-	-	0/6/10/10	0/3/3/3
2	6PQ	B	301	-	-	2/6/10/10	0/3/3/3
2	6PQ	C	301	-	-	0/6/10/10	0/3/3/3
2	6PQ	O	301	-	-	0/6/10/10	0/3/3/3
2	6PQ	U	301	-	-	2/6/10/10	0/3/3/3
2	6PQ	P	301	-	-	2/6/10/10	0/3/3/3
2	6PQ	W	301	-	-	2/6/10/10	0/3/3/3
2	6PQ	H	301	-	-	0/6/10/10	0/3/3/3
2	6PQ	J	301	-	-	0/6/10/10	0/3/3/3
2	6PQ	L	301	-	-	0/6/10/10	0/3/3/3
2	6PQ	F	301	-	-	2/6/10/10	0/3/3/3
2	6PQ	R	301	-	-	0/6/10/10	0/3/3/3
2	6PQ	E	301	-	-	2/6/10/10	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	6PQ	N08-N06	-3.84	1.30	1.37
2	U	301	6PQ	N08-N06	-3.70	1.30	1.37
2	H	301	6PQ	N08-N06	-3.64	1.30	1.37
2	T	301	6PQ	N08-N06	-3.64	1.30	1.37
2	S	301	6PQ	N08-N06	-3.62	1.30	1.37
2	C	301	6PQ	N08-N06	-3.60	1.30	1.37
2	P	301	6PQ	N08-N06	-3.54	1.30	1.37
2	W	301	6PQ	N08-N06	-3.51	1.30	1.37
2	V	301	6PQ	N08-N06	-3.50	1.30	1.37
2	D	301	6PQ	N08-N06	-3.50	1.30	1.37
2	A	301	6PQ	N08-N06	-3.49	1.30	1.37
2	K	301	6PQ	N08-N06	-3.47	1.30	1.37
2	I	301	6PQ	N08-N06	-3.46	1.30	1.37
2	X	301	6PQ	N08-N06	-3.44	1.30	1.37
2	R	301	6PQ	N08-N06	-3.42	1.30	1.37
2	E	301	6PQ	N08-N06	-3.41	1.30	1.37
2	Q	301	6PQ	N08-N06	-3.37	1.31	1.37
2	O	301	6PQ	N08-N06	-3.35	1.31	1.37
2	M	301	6PQ	N08-N06	-3.27	1.31	1.37
2	J	301	6PQ	N08-N06	-3.27	1.31	1.37
2	G	301	6PQ	N08-N06	-3.23	1.31	1.37
2	N	301	6PQ	N08-N06	-3.23	1.31	1.37
2	L	301	6PQ	N08-N06	-3.14	1.31	1.37
2	B	301	6PQ	N08-N06	-3.02	1.31	1.37
2	H	301	6PQ	C07-C10	2.13	1.43	1.39
2	F	301	6PQ	C07-C10	2.13	1.43	1.39
2	E	301	6PQ	O20-C13	2.12	1.42	1.37
2	J	301	6PQ	O20-C13	2.10	1.41	1.37
2	X	301	6PQ	C07-C10	2.08	1.42	1.39
2	M	301	6PQ	O20-C13	2.07	1.41	1.37

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	6PQ	C19-C09-S05	5.60	127.65	120.12
2	W	301	6PQ	C19-C09-S05	5.26	127.19	120.12
2	B	301	6PQ	C19-C09-S05	5.24	127.16	120.12
2	A	301	6PQ	C19-C09-S05	5.14	127.03	120.12
2	K	301	6PQ	C19-C09-S05	5.08	126.95	120.12
2	V	301	6PQ	C19-C09-S05	4.97	126.80	120.12
2	L	301	6PQ	C19-C09-S05	4.87	126.67	120.12
2	M	301	6PQ	C19-C09-S05	4.82	126.59	120.12
2	H	301	6PQ	C19-C09-S05	4.79	126.56	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	301	6PQ	C19-C09-S05	4.77	126.53	120.12
2	Q	301	6PQ	C19-C09-S05	4.76	126.51	120.12
2	J	301	6PQ	C19-C09-S05	4.73	126.48	120.12
2	E	301	6PQ	C19-C09-S05	4.62	126.33	120.12
2	N	301	6PQ	C07-C02-C01	-4.38	122.93	129.32
2	U	301	6PQ	C19-C09-S05	4.38	126.01	120.12
2	T	301	6PQ	C19-C09-S05	4.33	125.94	120.12
2	R	301	6PQ	C07-C02-C01	-4.28	123.08	129.32
2	C	301	6PQ	C19-C09-S05	4.14	125.68	120.12
2	S	301	6PQ	C19-C09-S05	4.10	125.63	120.12
2	X	301	6PQ	C19-C09-S05	4.02	125.53	120.12
2	D	301	6PQ	C19-C09-S05	3.99	125.49	120.12
2	O	301	6PQ	C19-C09-S05	3.97	125.45	120.12
2	G	301	6PQ	C19-C09-S05	3.84	125.28	120.12
2	R	301	6PQ	C19-C09-S05	3.75	125.16	120.12
2	K	301	6PQ	C07-C02-C01	-3.73	123.88	129.32
2	D	301	6PQ	C07-C10-N08	-3.70	106.23	111.44
2	B	301	6PQ	C07-C10-N08	-3.65	106.30	111.44
2	N	301	6PQ	C19-C09-S05	3.60	124.96	120.12
2	I	301	6PQ	C07-C10-N08	-3.57	106.42	111.44
2	I	301	6PQ	C19-C09-S05	3.56	124.91	120.12
2	G	301	6PQ	C07-C02-C01	-3.54	124.15	129.32
2	S	301	6PQ	C07-C02-C01	-3.51	124.20	129.32
2	E	301	6PQ	C07-C10-N08	-3.49	106.53	111.44
2	Q	301	6PQ	C07-C02-C01	-3.47	124.25	129.32
2	M	301	6PQ	C07-C02-C01	-3.43	124.32	129.32
2	I	301	6PQ	C07-C02-C01	-3.40	124.36	129.32
2	O	301	6PQ	C07-C10-N08	-3.37	106.70	111.44
2	L	301	6PQ	C07-C02-C01	-3.28	124.53	129.32
2	N	301	6PQ	C07-C10-N08	-3.27	106.84	111.44
2	D	301	6PQ	C07-C02-C01	-3.23	124.61	129.32
2	A	301	6PQ	C07-C02-C01	-3.21	124.64	129.32
2	H	301	6PQ	C07-C10-N08	-3.20	106.94	111.44
2	T	301	6PQ	C07-C02-C01	-3.18	124.67	129.32
2	G	301	6PQ	C07-C10-N08	-3.16	107.00	111.44
2	K	301	6PQ	C07-C10-N08	-3.13	107.03	111.44
2	J	301	6PQ	C07-C02-C01	-3.11	124.78	129.32
2	M	301	6PQ	C07-C10-N08	-3.09	107.09	111.44
2	B	301	6PQ	C07-C02-C01	-3.08	124.83	129.32
2	E	301	6PQ	C07-C02-C01	-3.07	124.84	129.32
2	L	301	6PQ	C07-C10-N08	-3.07	107.12	111.44
2	U	301	6PQ	C07-C02-C01	-3.05	124.87	129.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	301	6PQ	C07-C10-N08	-2.98	107.24	111.44
2	S	301	6PQ	C07-C10-N08	-2.93	107.31	111.44
2	C	301	6PQ	C07-C02-C01	-2.91	125.08	129.32
2	X	301	6PQ	C07-C10-N08	-2.89	107.36	111.44
2	P	301	6PQ	C07-C10-N08	-2.88	107.39	111.44
2	Q	301	6PQ	C07-C10-N08	-2.87	107.40	111.44
2	R	301	6PQ	C07-C10-N08	-2.87	107.40	111.44
2	W	301	6PQ	C07-C10-N08	-2.86	107.41	111.44
2	U	301	6PQ	C07-C10-N08	-2.80	107.50	111.44
2	V	301	6PQ	C07-C02-C01	-2.79	125.25	129.32
2	A	301	6PQ	C07-C10-N08	-2.77	107.54	111.44
2	V	301	6PQ	C07-C10-N08	-2.48	107.95	111.44
2	P	301	6PQ	C07-C02-C01	-2.40	125.83	129.32
2	T	301	6PQ	C07-C10-N08	-2.39	108.07	111.44
2	X	301	6PQ	C07-C02-C01	-2.38	125.86	129.32
2	C	301	6PQ	C07-C10-N08	-2.30	108.21	111.44
2	F	301	6PQ	C07-C10-N08	-2.24	108.28	111.44
2	P	301	6PQ	C21-O20-C13	-2.20	112.75	117.51
2	O	301	6PQ	C07-C02-C01	-2.19	126.12	129.32
2	H	301	6PQ	C07-C02-C01	-2.17	126.16	129.32
2	F	301	6PQ	C07-C02-C01	-2.16	126.17	129.32
2	F	301	6PQ	C10-C07-C02	-2.15	102.44	105.29

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	301	6PQ	C17-C13-O20-C21
2	I	301	6PQ	C18-C13-O20-C21
2	P	301	6PQ	C18-C13-O20-C21
2	P	301	6PQ	C17-C13-O20-C21
2	N	301	6PQ	C17-C13-O20-C21
2	N	301	6PQ	C18-C13-O20-C21
2	U	301	6PQ	C18-C13-O20-C21
2	U	301	6PQ	C17-C13-O20-C21
2	A	301	6PQ	C17-C13-O20-C21
2	A	301	6PQ	C18-C13-O20-C21
2	E	301	6PQ	C18-C13-O20-C21
2	E	301	6PQ	C17-C13-O20-C21
2	S	301	6PQ	C18-C13-O20-C21
2	S	301	6PQ	C17-C13-O20-C21
2	X	301	6PQ	C18-C13-O20-C21

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Mol	Chain	Res	Type	Atoms
2	X	301	6PQ	C17-C13-O20-C21
2	F	301	6PQ	C18-C13-O20-C21
2	F	301	6PQ	C17-C13-O20-C21
2	W	301	6PQ	C18-C13-O20-C21
2	W	301	6PQ	C17-C13-O20-C21
2	B	301	6PQ	C18-C13-O20-C21
2	B	301	6PQ	C17-C13-O20-C21
2	G	301	6PQ	C17-C13-O20-C21
2	G	301	6PQ	C18-C13-O20-C21
2	K	301	6PQ	C17-C13-O20-C21
2	K	301	6PQ	C18-C13-O20-C21

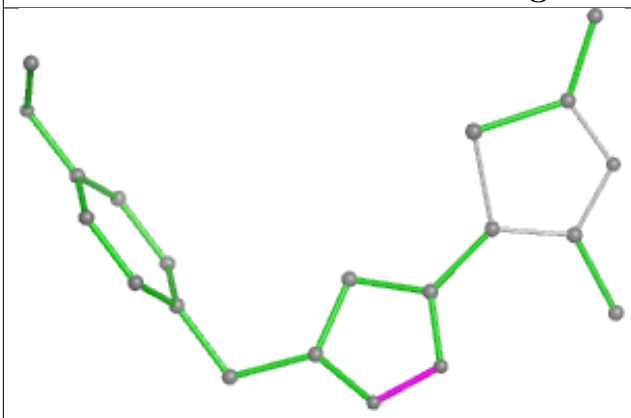
There are no ring outliers.

3 monomers are involved in 4 short contacts:

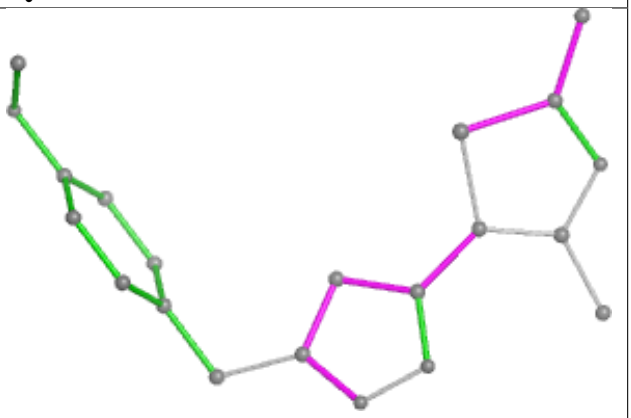
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	W	304	PO4	1	0
4	I	304	PO4	2	0
2	F	301	6PQ	1	0

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.

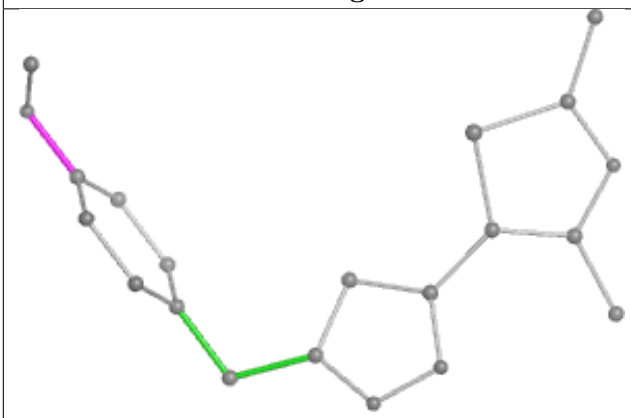
Ligand 6PQ S 301



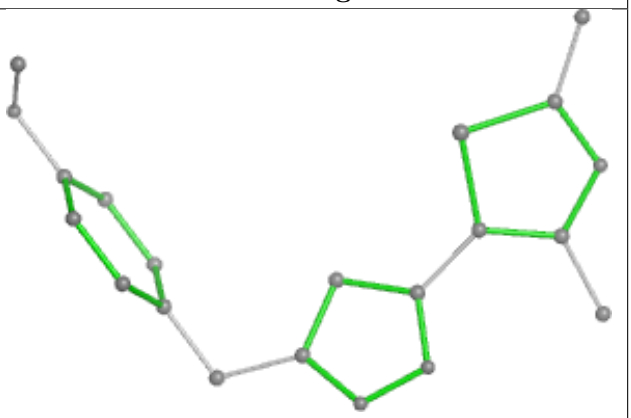
Bond lengths



Bond angles

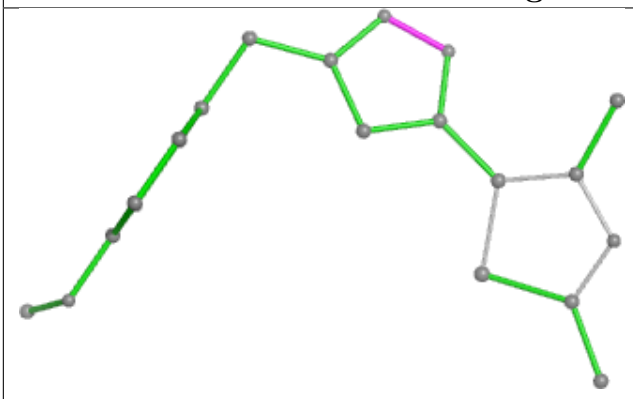


Torsions

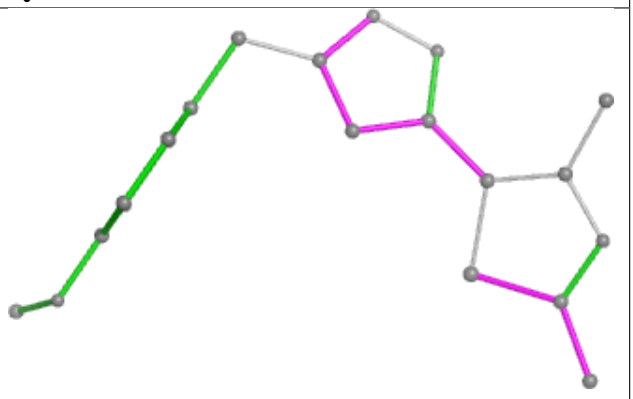


Rings

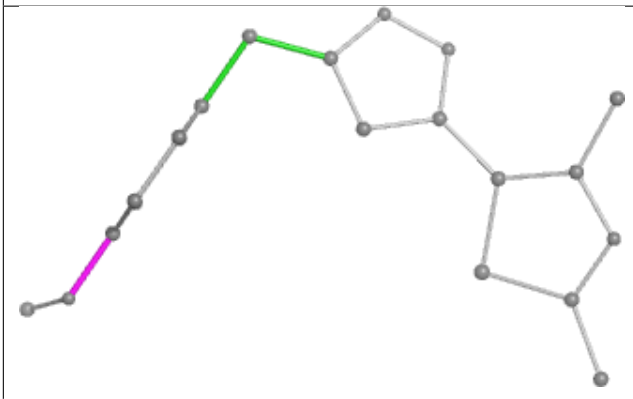
Ligand 6PQ K 301



Bond lengths



Bond angles



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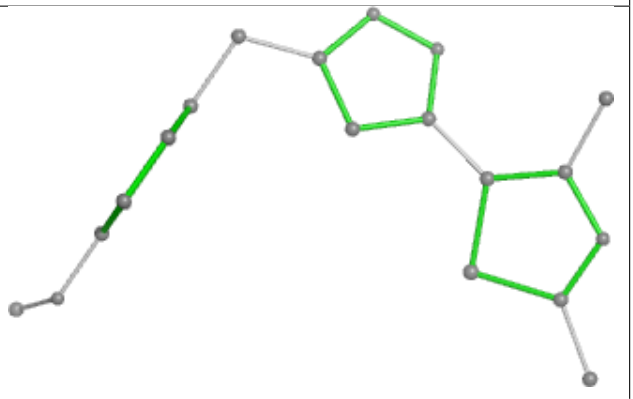
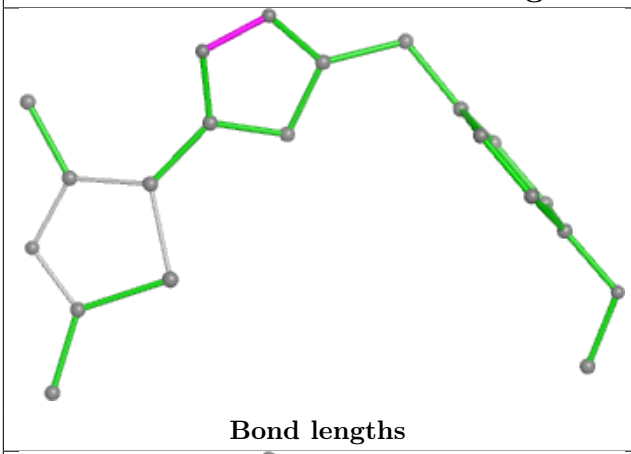


Rings

Ligand 6PQ N 301



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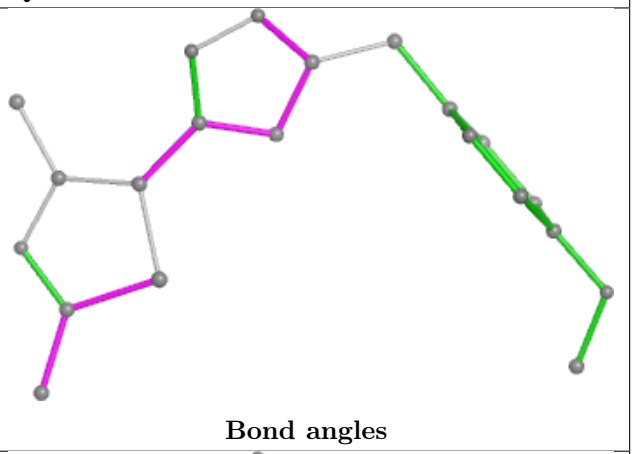
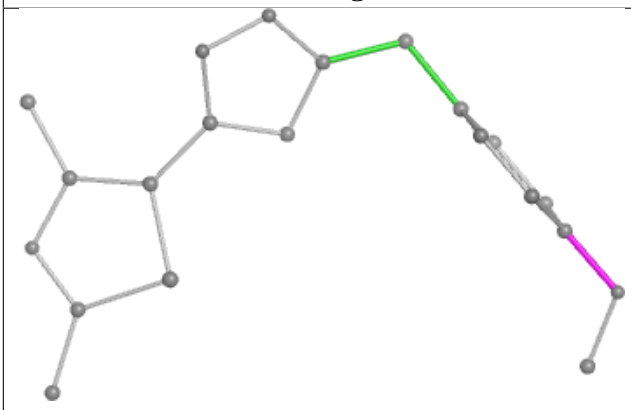
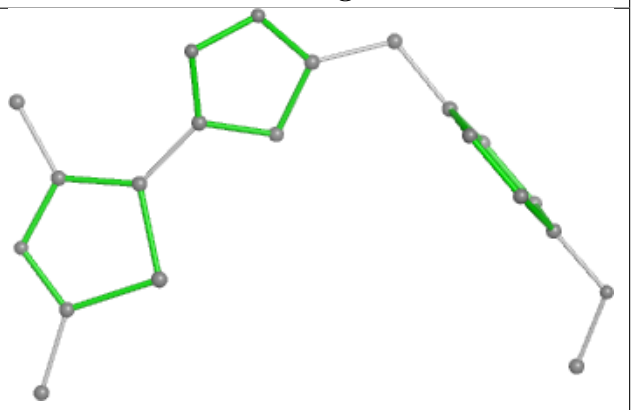


Bond angles

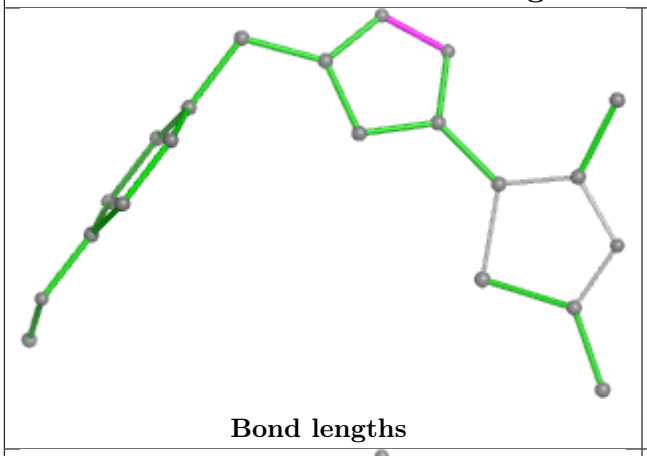


Torsions



Rings

Ligand 6PQ D 301



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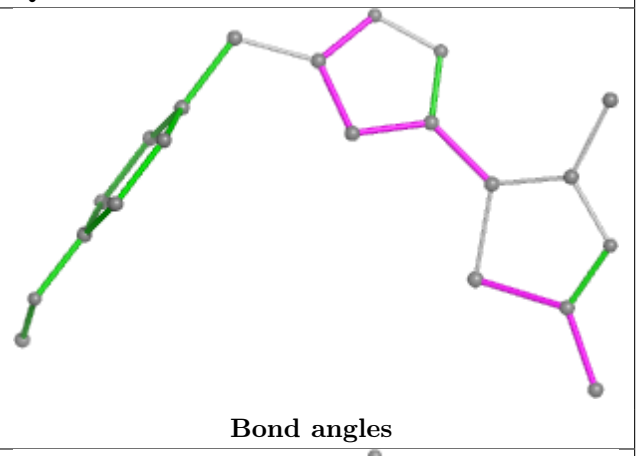

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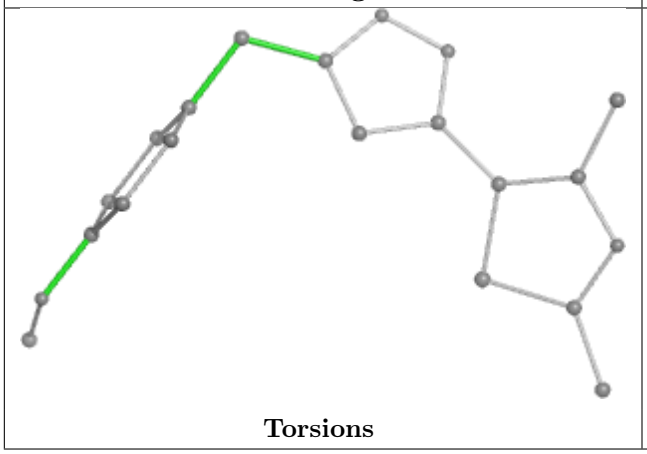

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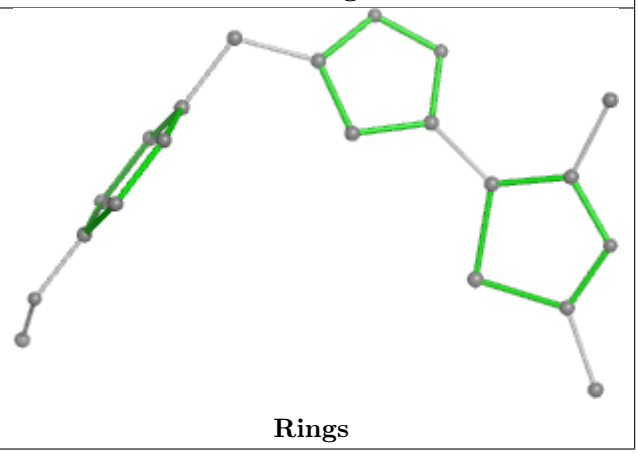
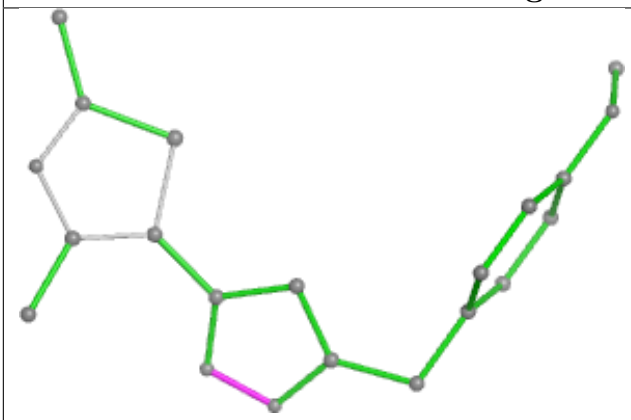


Rings

Ligand 6PQ G 301



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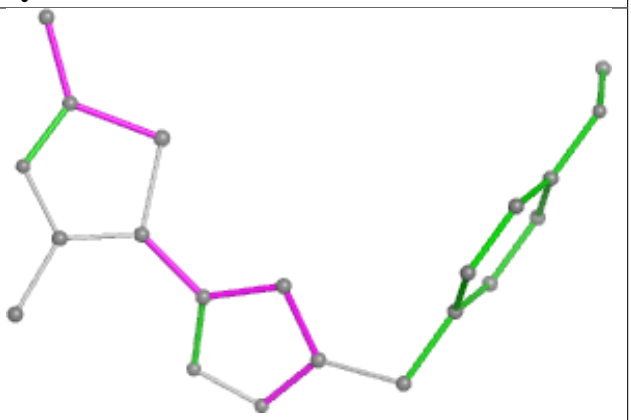

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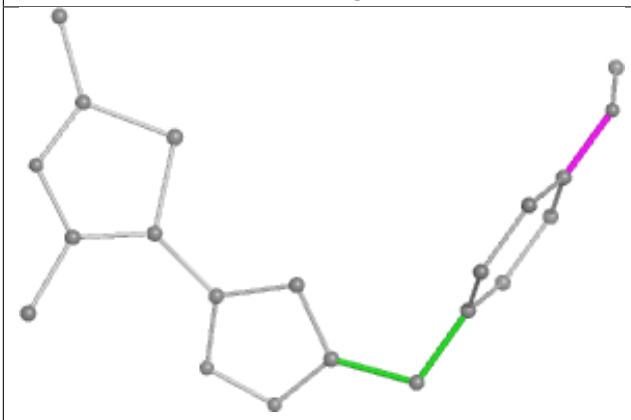

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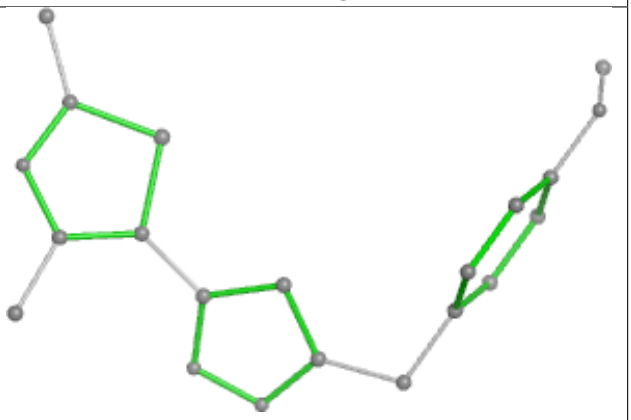
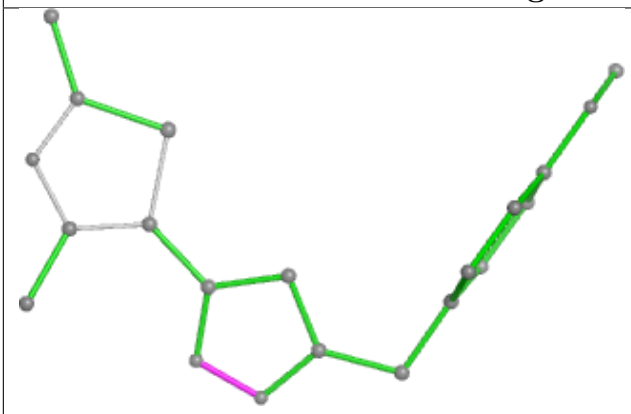


Rings

Ligand 6PQ T 301



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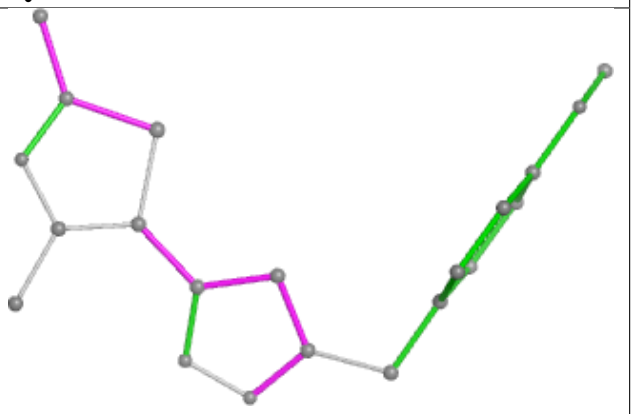

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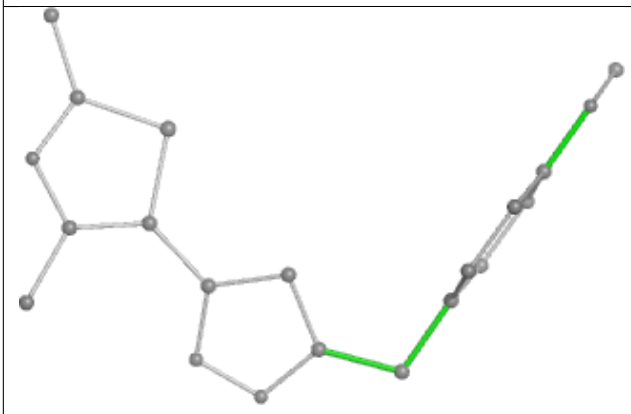

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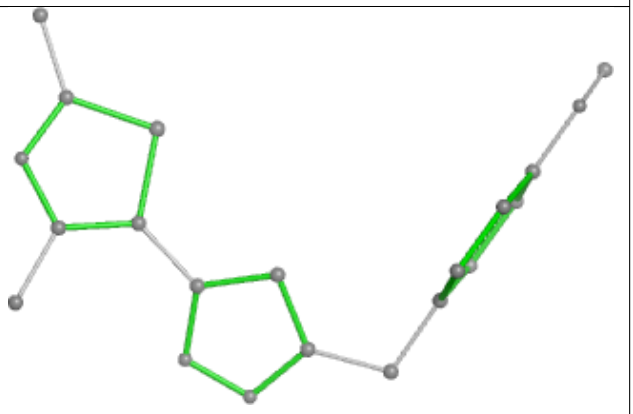

Rings

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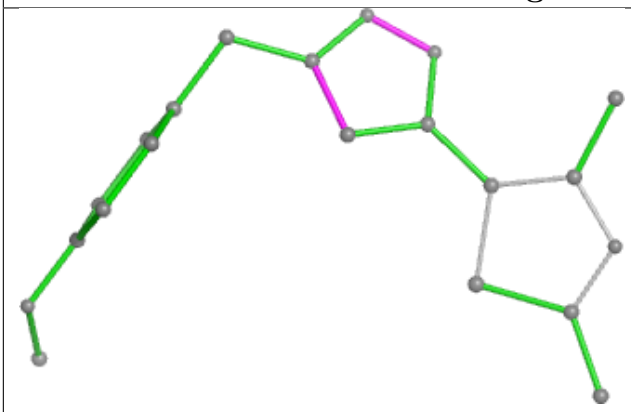

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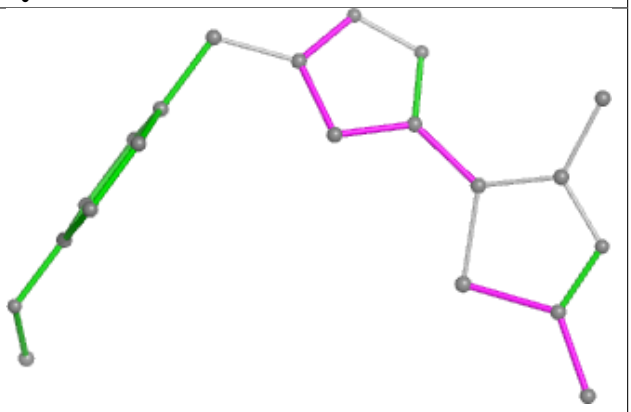

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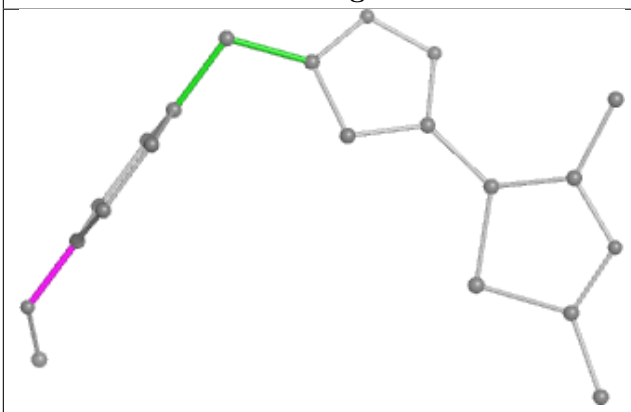

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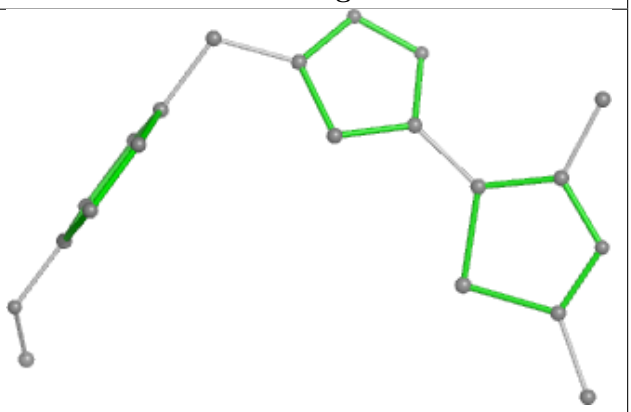

Rings

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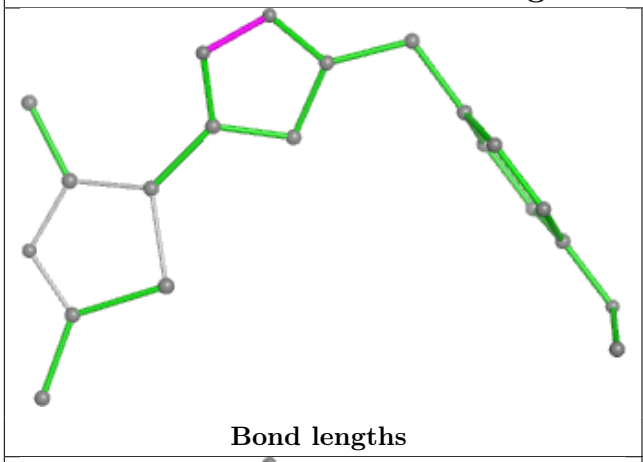

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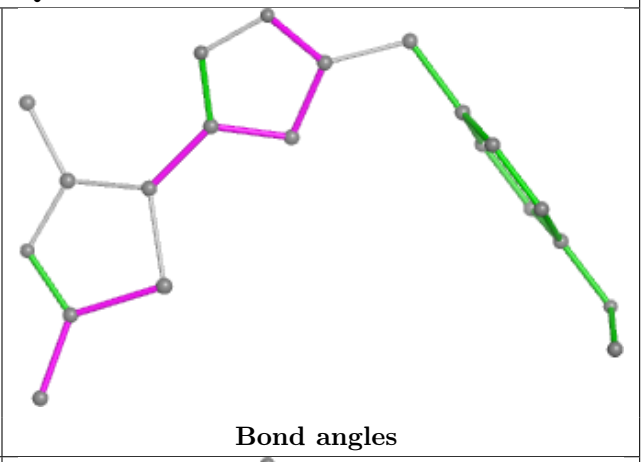

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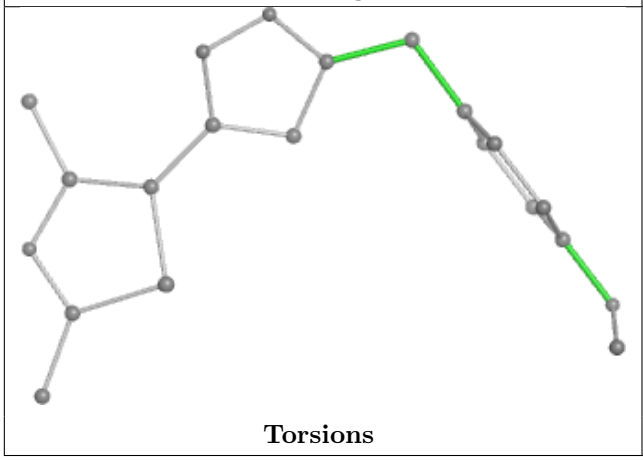

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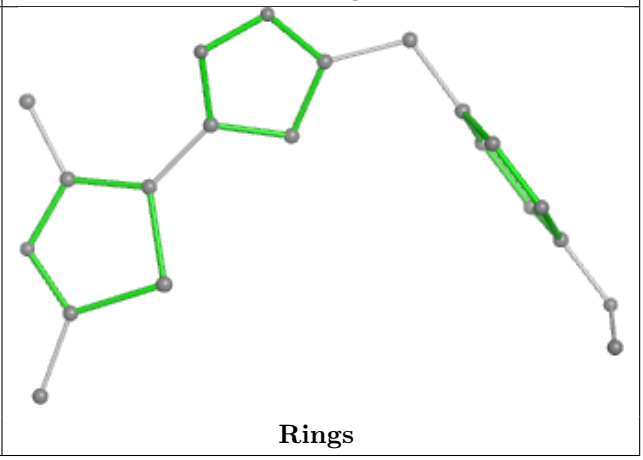
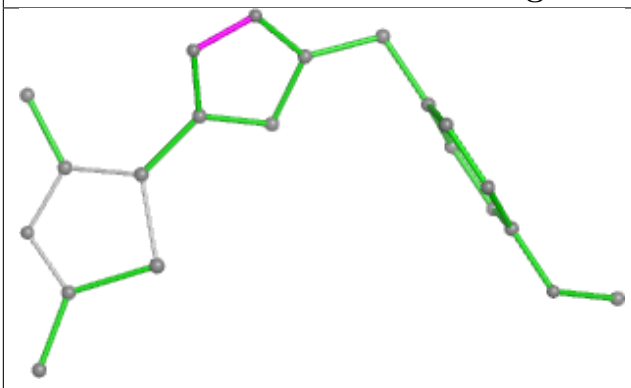


Rings

Ligand 6PQ A 301



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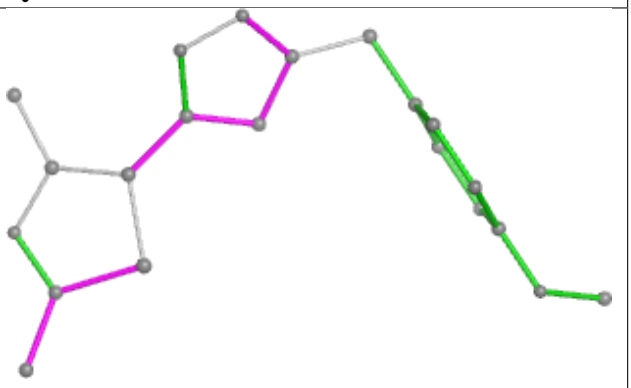

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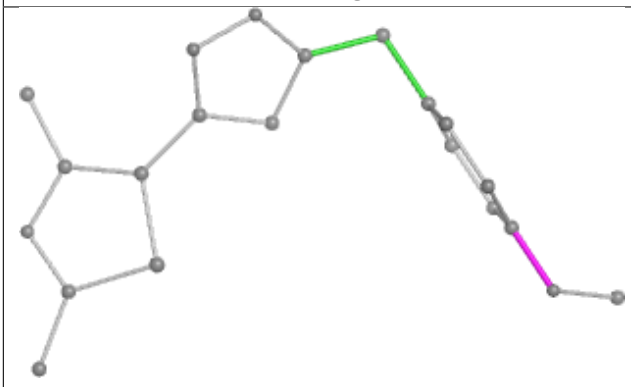

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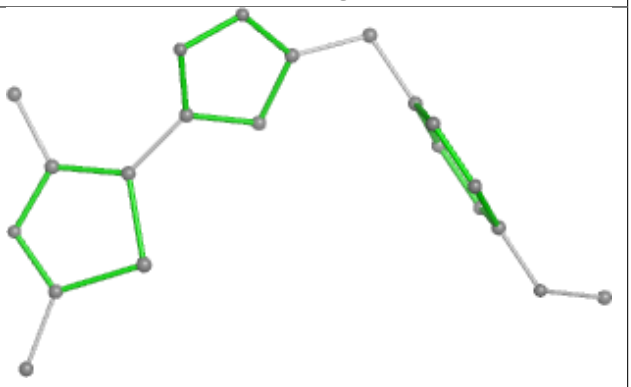
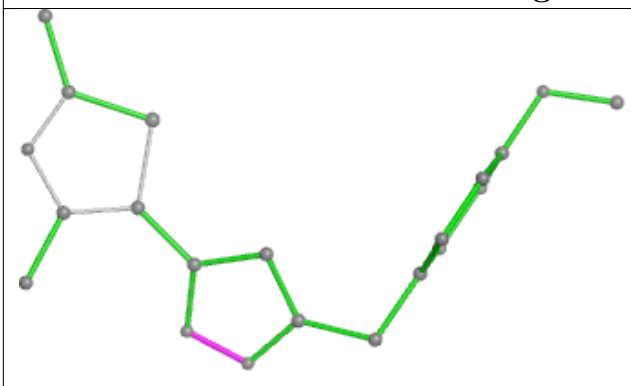


Rings

Ligand 6PQ I 301



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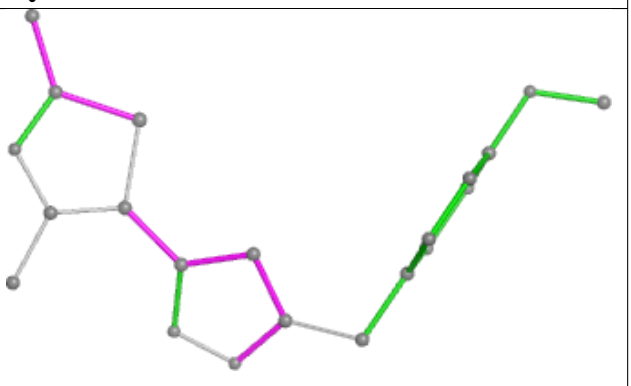

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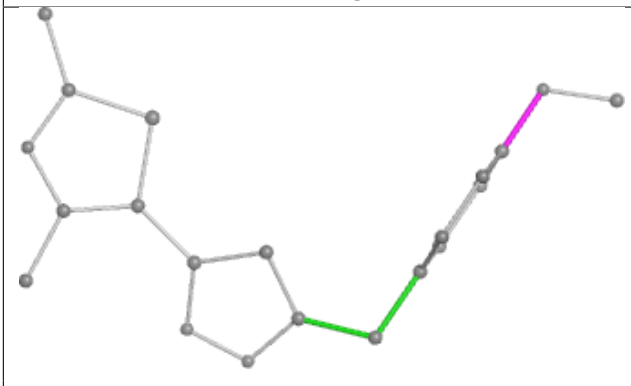

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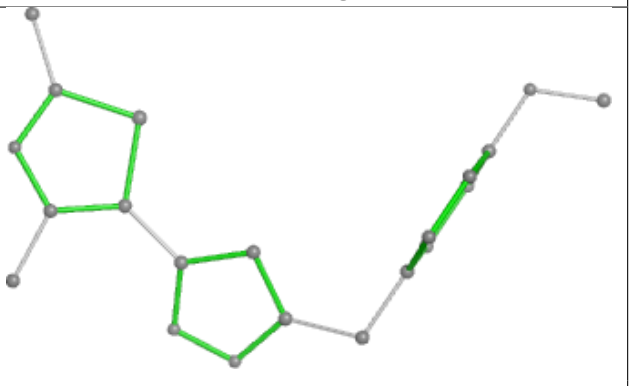
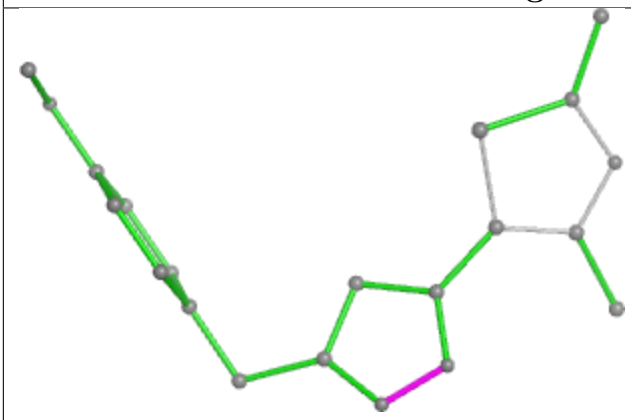


Rings

Ligand 6PQ Q 301



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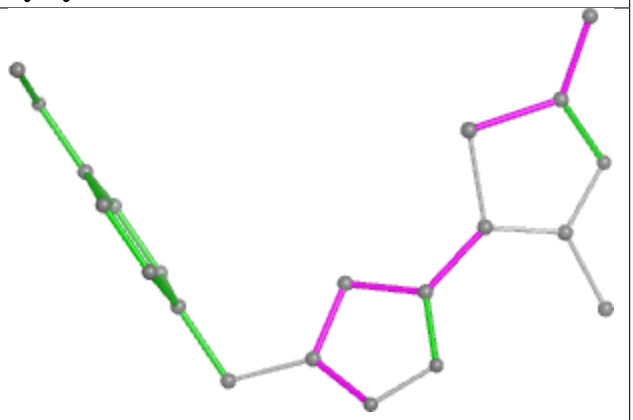

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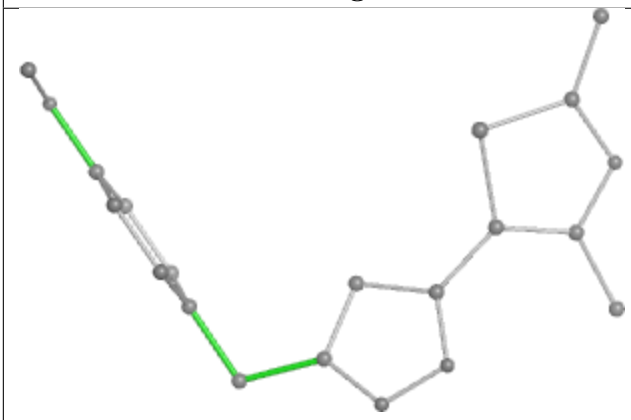

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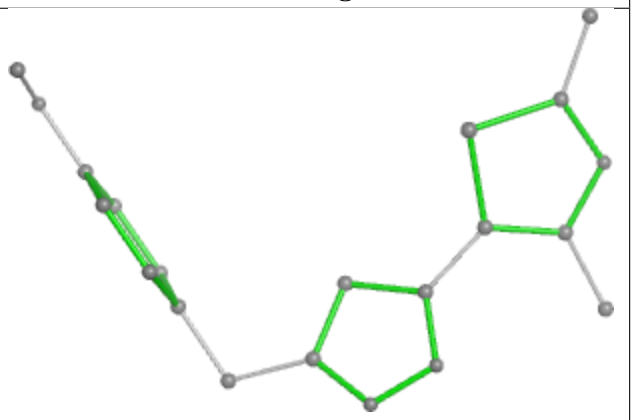
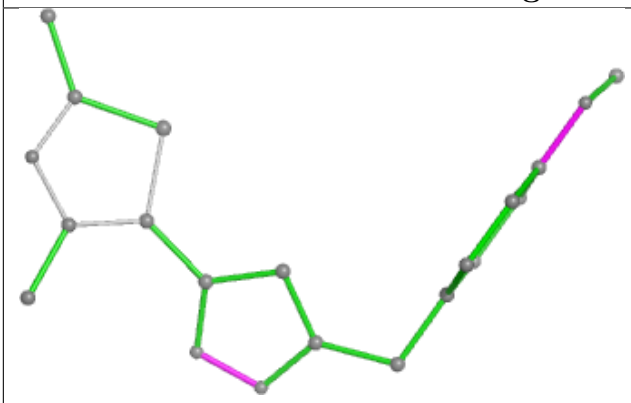


Rings

Ligand 6PQ M 301



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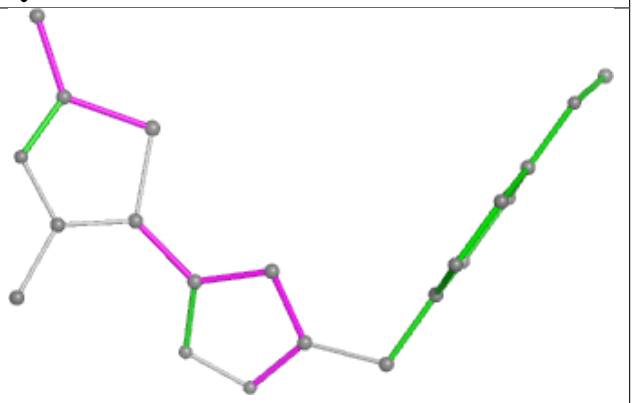

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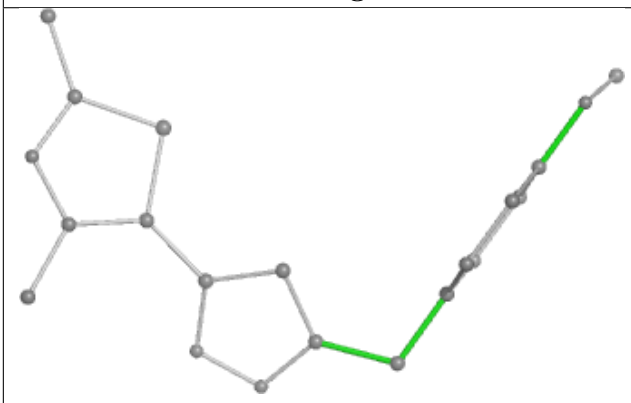

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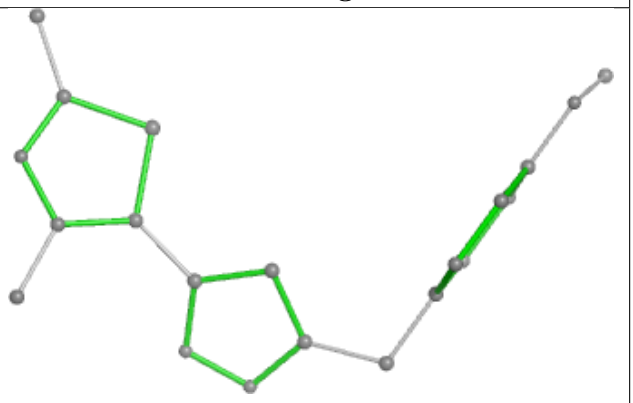

Rings

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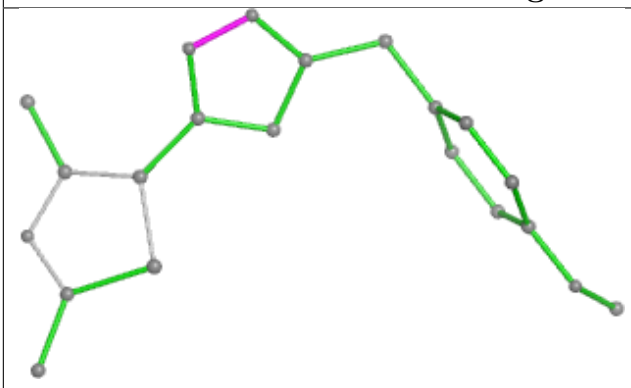

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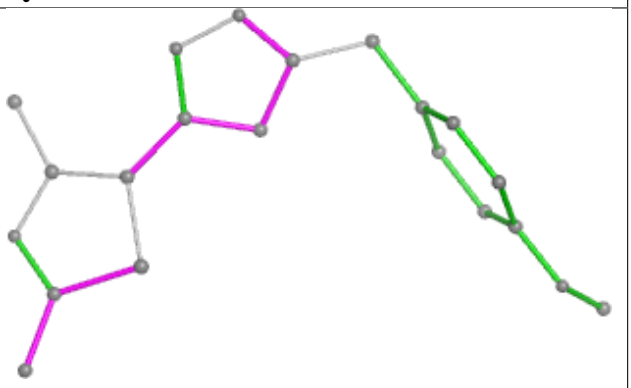

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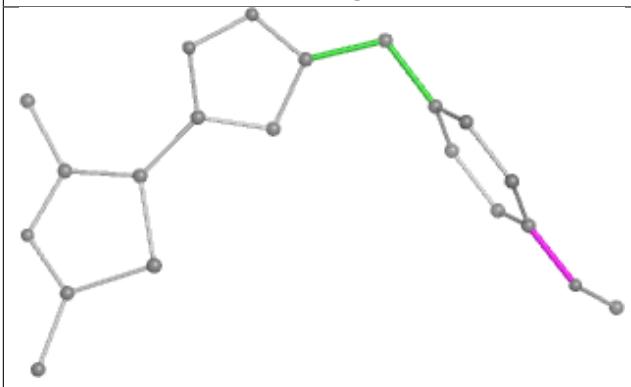

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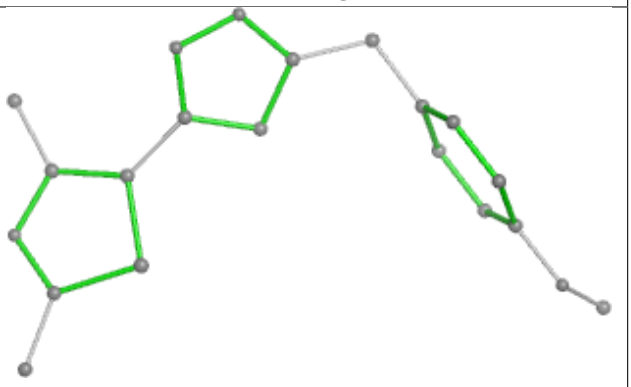
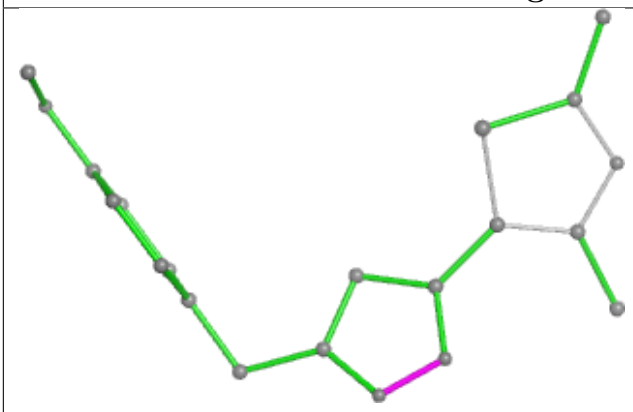


Rings

Ligand 6PQ C 301



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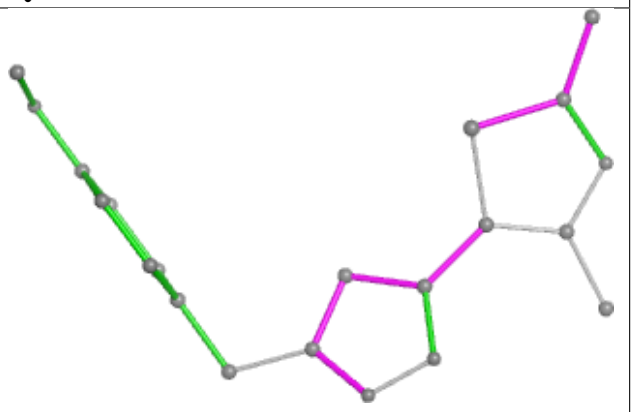

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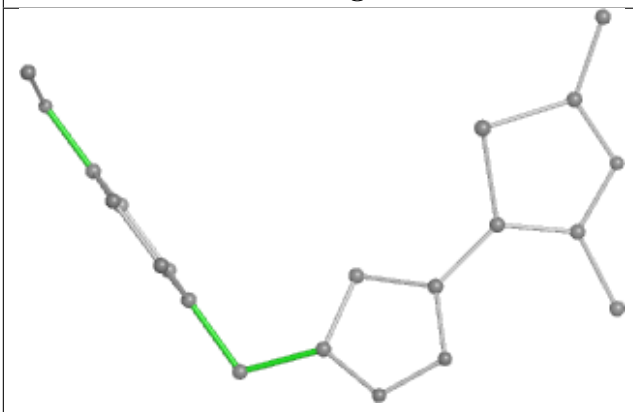

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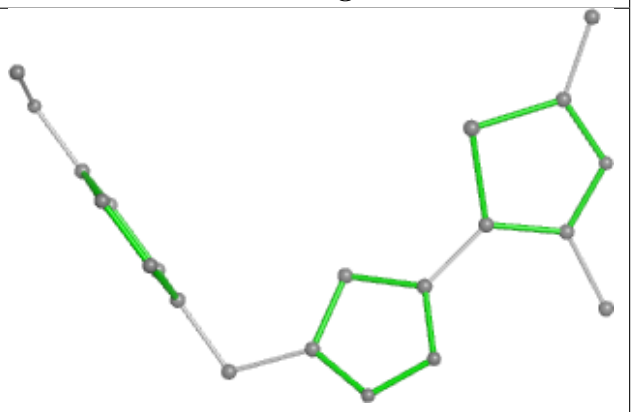
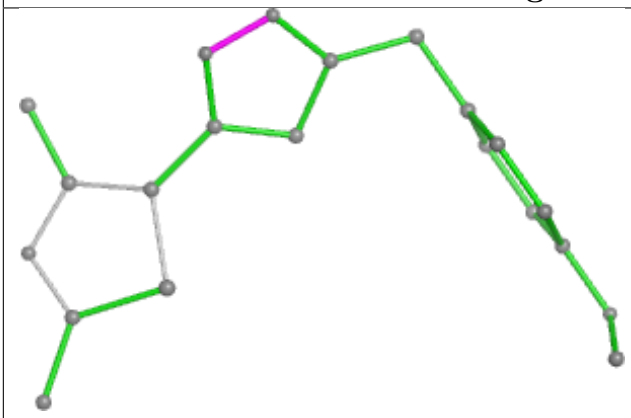


Rings

Ligand 6PQ O 301



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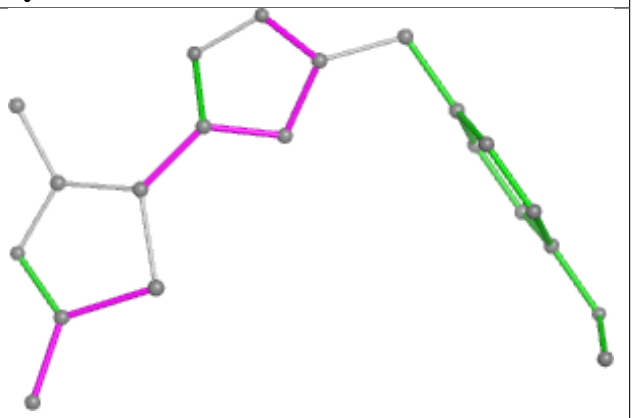

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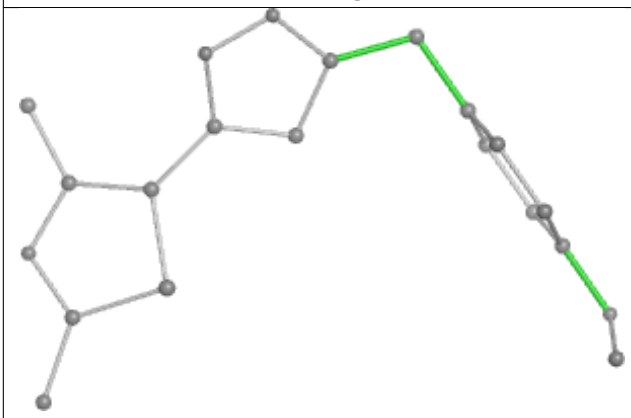

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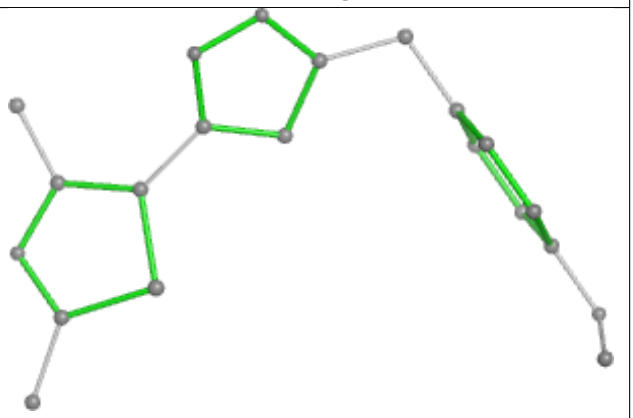
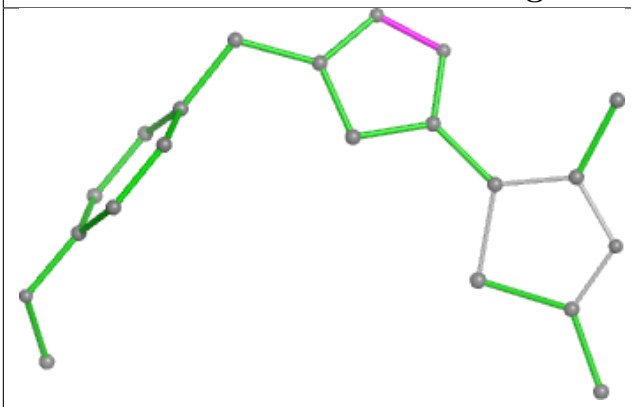


Rings

Ligand 6PQ U 301



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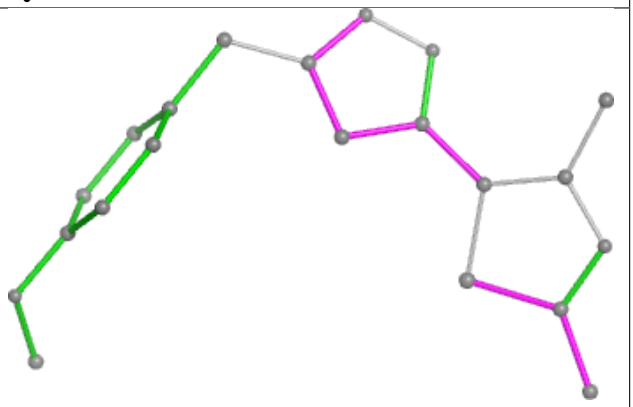

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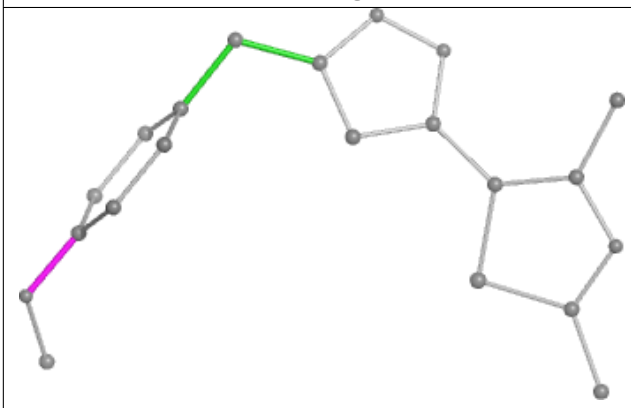

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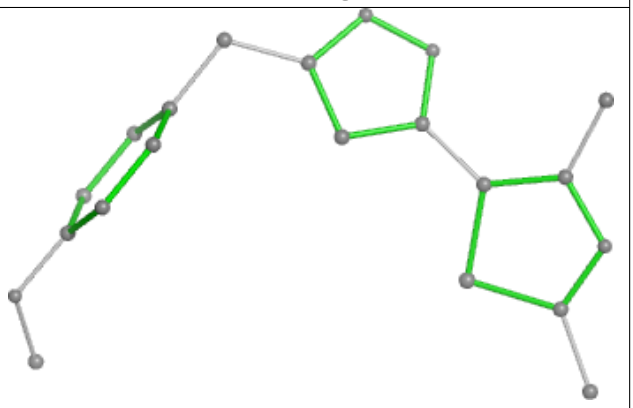
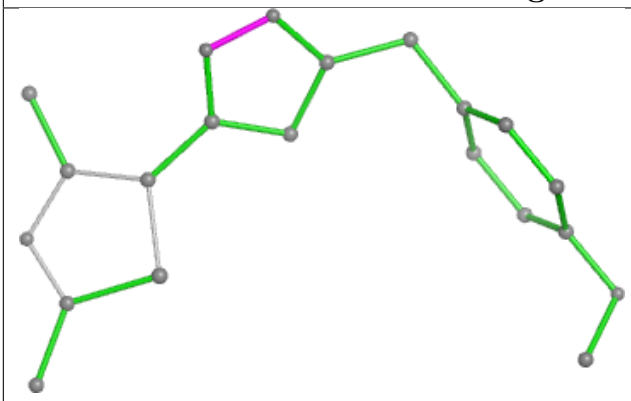


Rings

Ligand 6PQ P 301



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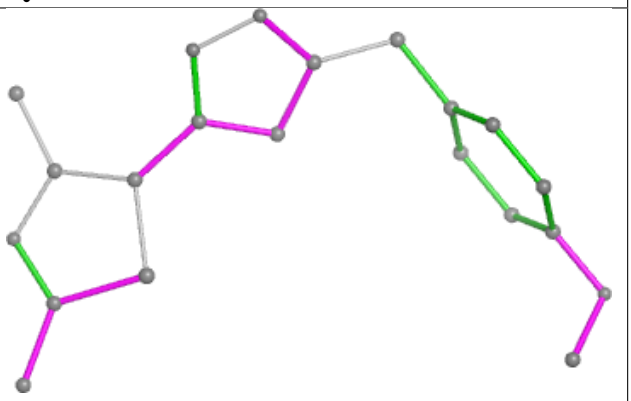
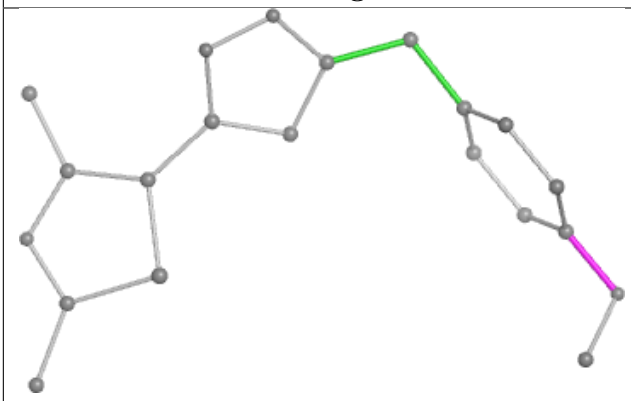


Bond angles



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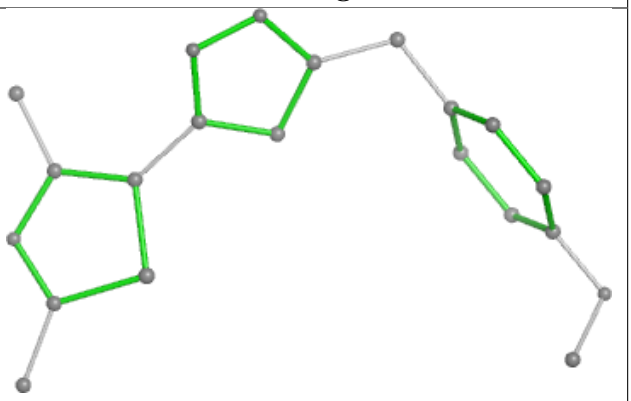
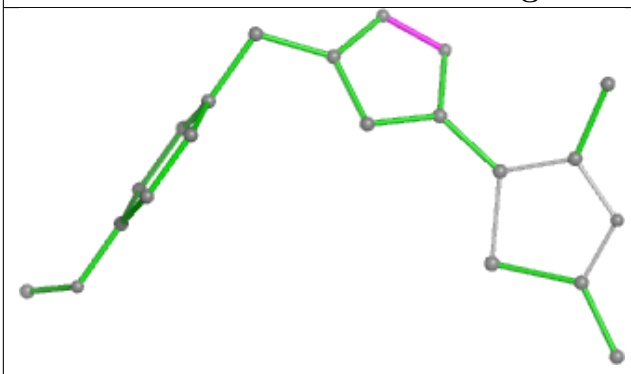


Rings

Ligand 6PQ W 301



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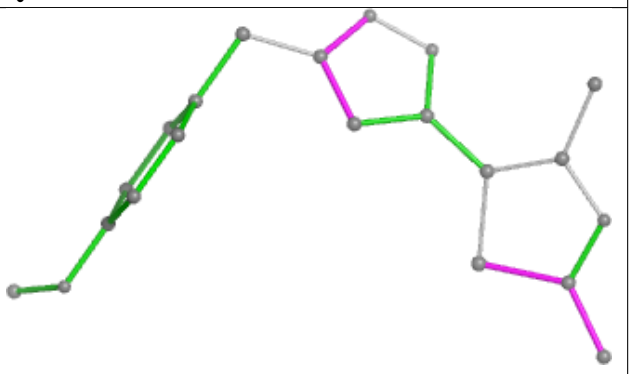
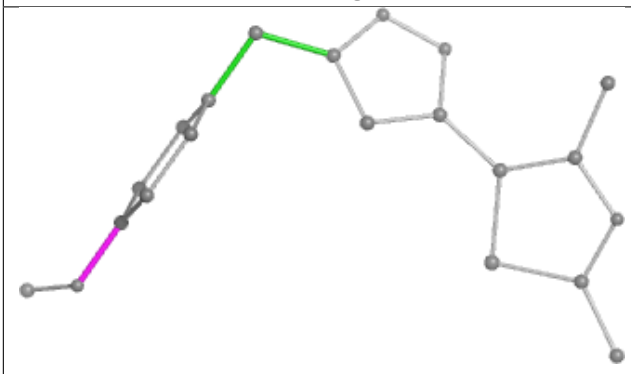
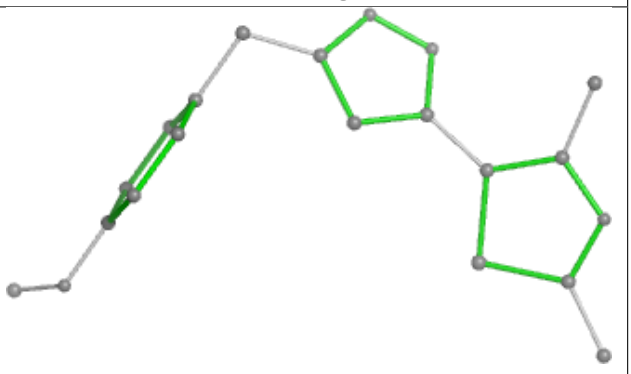


Bond angles

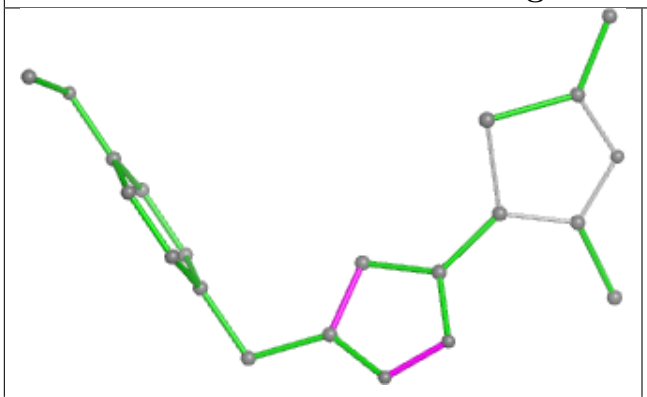


Torsions

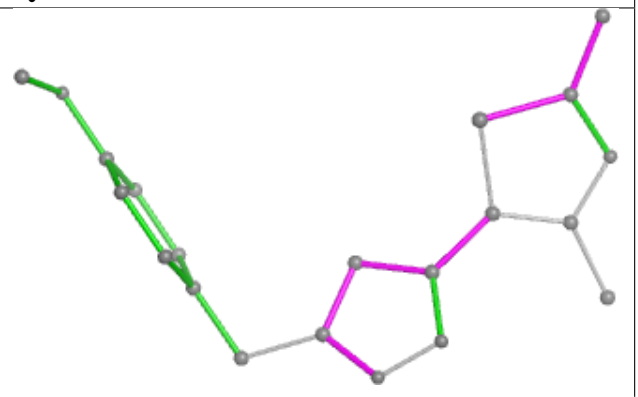


Rings

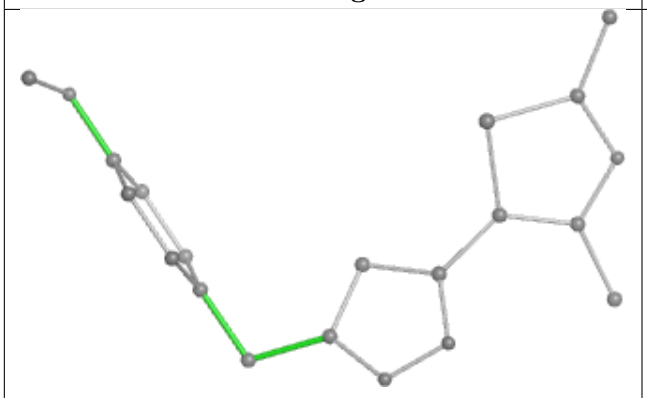
Ligand 6PQ H 301



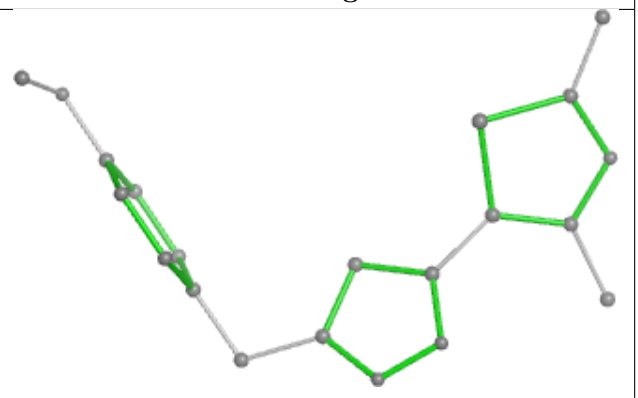
Bond lengths



Bond angles

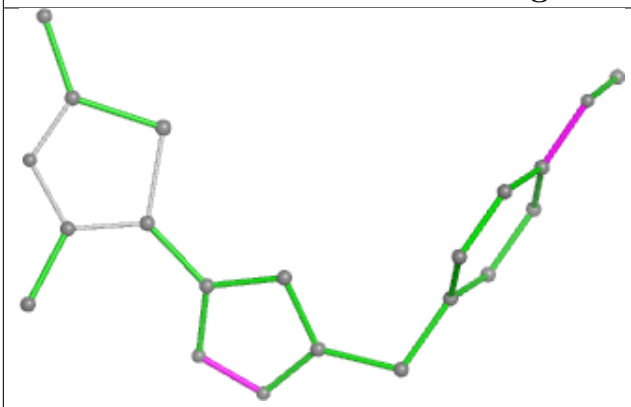


Torsions

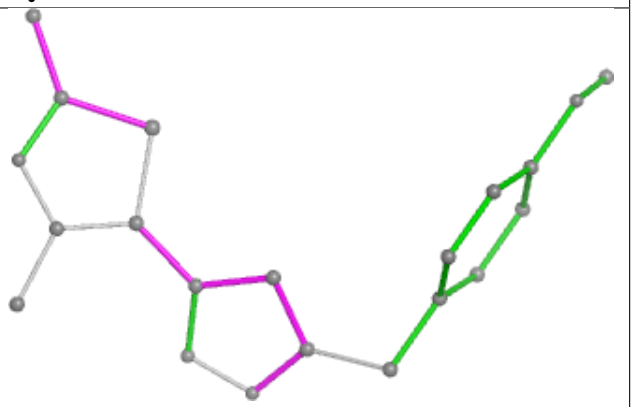


Rings

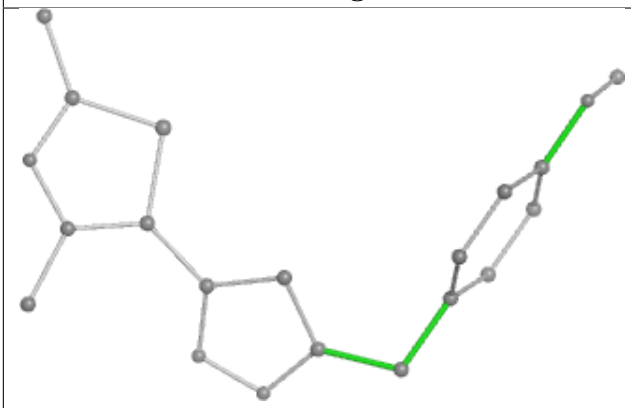
Ligand 6PQ J 301



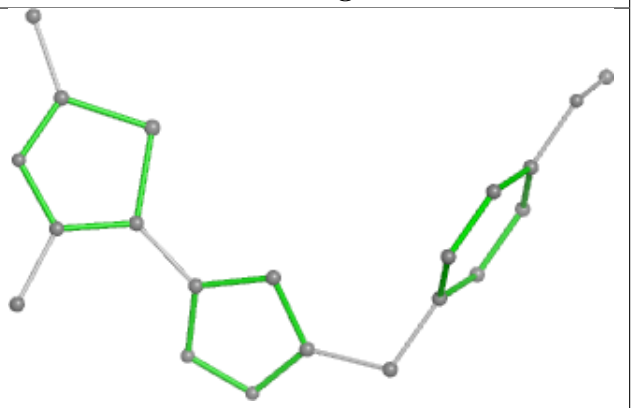
Bond lengths



Bond angles

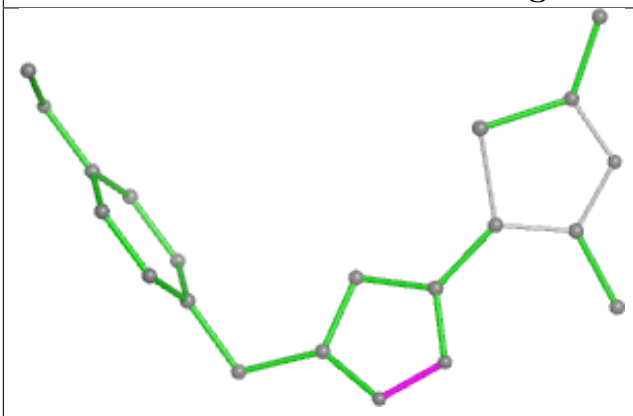


Torsions

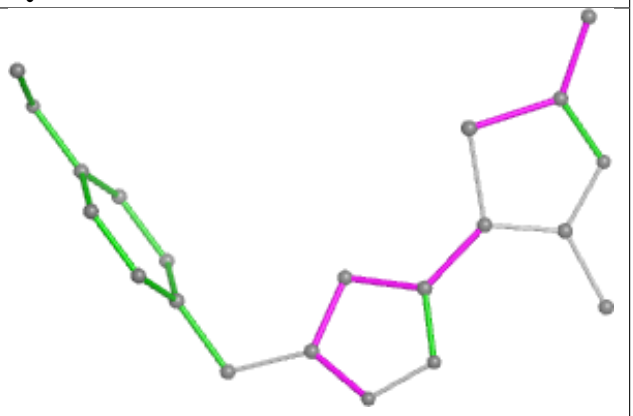


Rings

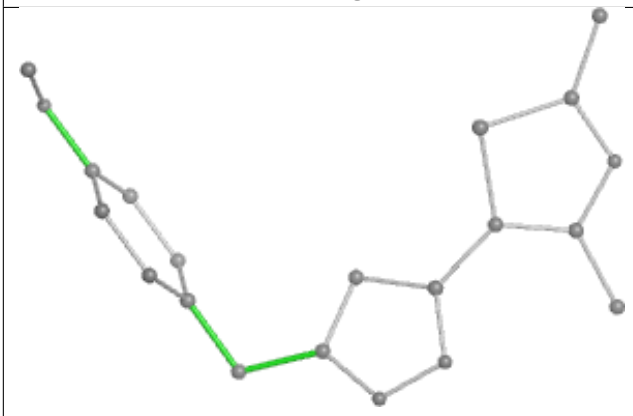
Ligand 6PQ L 301



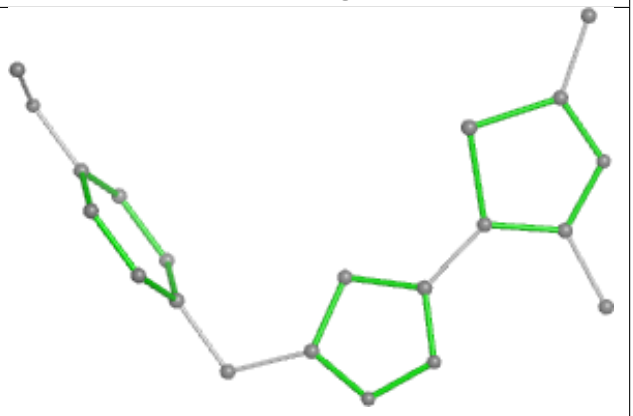
Bond lengths



Bond angles

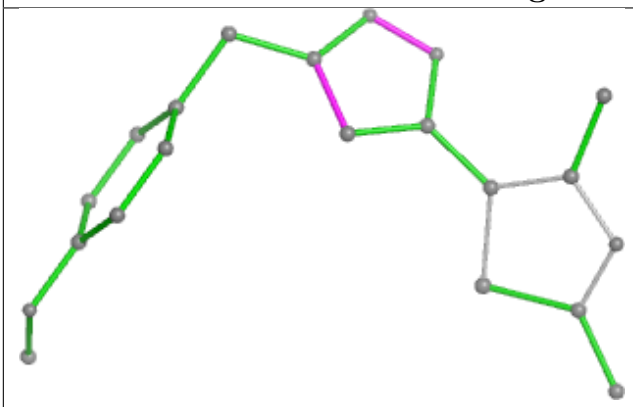


Torsions

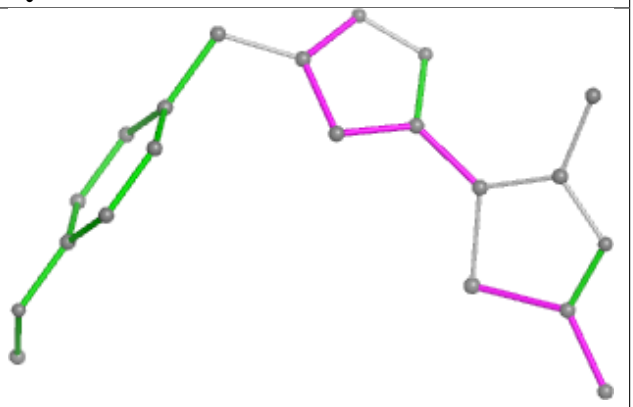


Rings

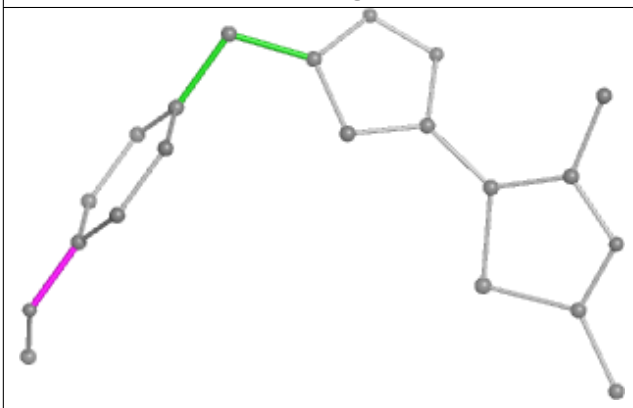
Ligand 6PQ F 301



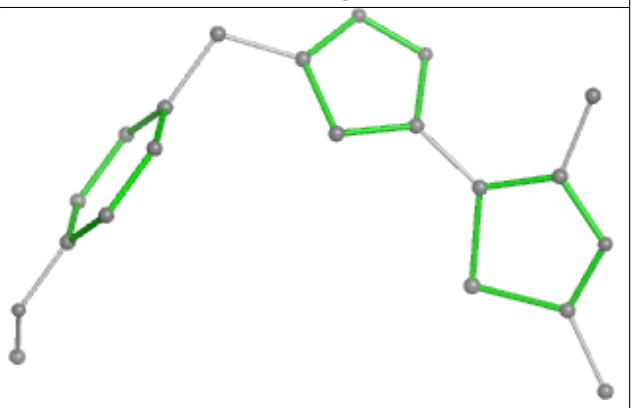
Bond lengths



Bond angles

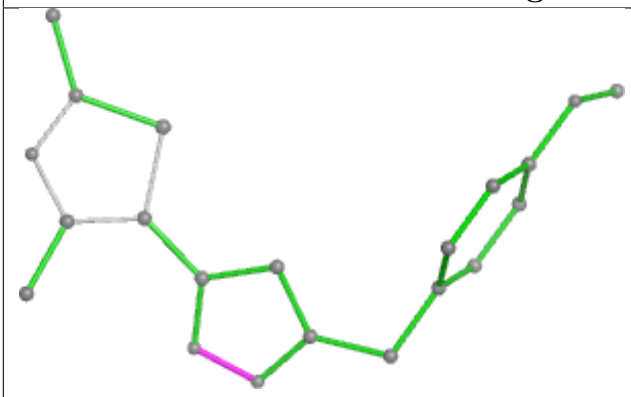


Torsions

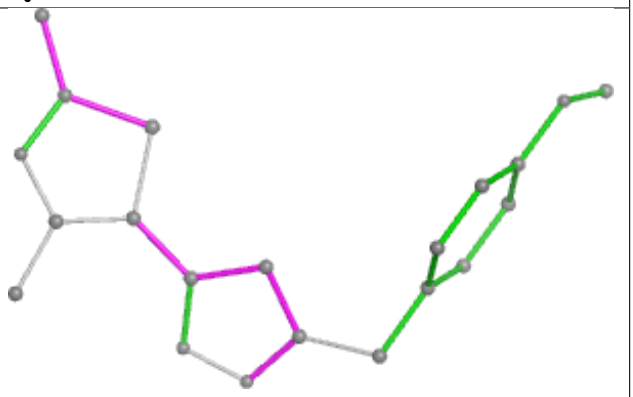


Rings

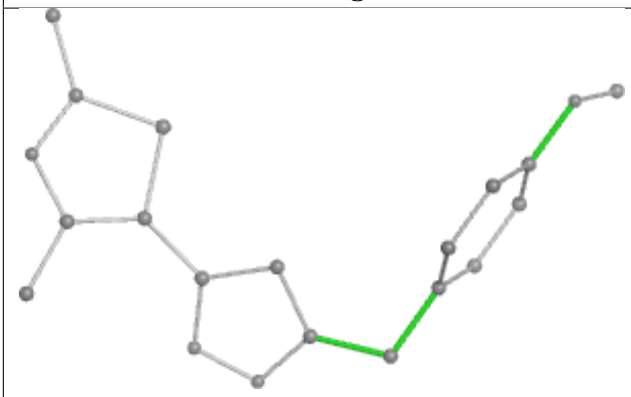
Ligand 6PQ R 301



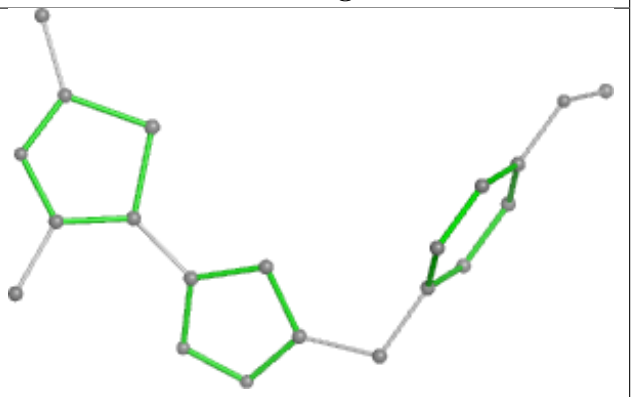
Bond lengths



Bond angles

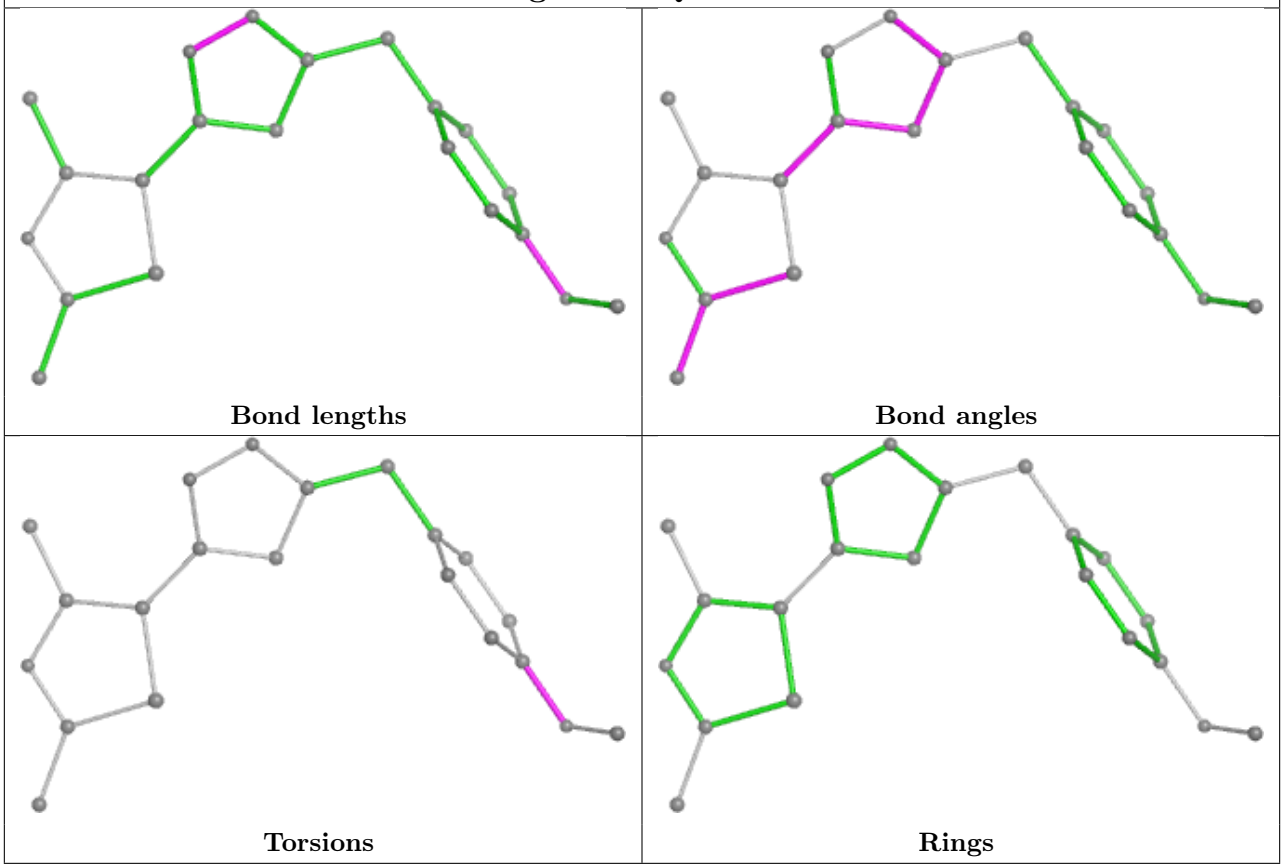


Torsions



Rings

Ligand 6PQ E 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	217/217 (100%)	-0.23	2 (0%) 84 85	32, 46, 72, 141	0
1	B	215/217 (99%)	-0.32	0 100 100	28, 40, 74, 114	0
1	C	216/217 (99%)	0.01	4 (1%) 66 69	31, 50, 73, 126	0
1	D	215/217 (99%)	0.07	3 (1%) 75 77	31, 49, 75, 114	0
1	E	215/217 (99%)	0.22	10 (4%) 31 30	42, 69, 104, 148	0
1	F	216/217 (99%)	-0.24	2 (0%) 84 85	29, 43, 72, 114	0
1	G	217/217 (100%)	-0.09	4 (1%) 68 70	31, 48, 79, 151	0
1	H	216/217 (99%)	-0.07	3 (1%) 75 77	31, 44, 69, 143	0
1	I	215/217 (99%)	0.06	3 (1%) 75 77	32, 51, 78, 121	0
1	J	216/217 (99%)	-0.22	2 (0%) 84 85	33, 46, 73, 116	0
1	K	215/217 (99%)	-0.25	3 (1%) 75 77	29, 39, 66, 120	0
1	L	216/217 (99%)	-0.10	6 (2%) 53 54	35, 47, 79, 107	0
1	M	215/217 (99%)	-0.02	3 (1%) 75 77	33, 49, 77, 131	0
1	N	216/217 (99%)	-0.17	3 (1%) 75 77	32, 46, 77, 126	0
1	O	216/217 (99%)	-0.18	2 (0%) 84 85	34, 48, 74, 124	0
1	P	215/217 (99%)	0.21	4 (1%) 66 69	36, 62, 96, 125	0
1	Q	216/217 (99%)	-0.12	4 (1%) 66 69	32, 47, 76, 110	0
1	R	217/217 (100%)	0.07	4 (1%) 68 70	33, 60, 90, 136	0
1	S	215/217 (99%)	0.09	2 (0%) 84 85	34, 57, 92, 124	0
1	T	215/217 (99%)	0.03	2 (0%) 84 85	31, 49, 78, 111	0
1	U	215/217 (99%)	0.43	11 (5%) 28 26	34, 69, 107, 124	0
1	V	215/217 (99%)	0.05	2 (0%) 84 85	37, 56, 83, 134	0
1	W	215/217 (99%)	0.20	6 (2%) 53 54	37, 62, 97, 118	0
1	X	215/217 (99%)	0.31	8 (3%) 41 41	37, 76, 111, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	5174/5208 (99%)	-0.01	93 (1%) 68 70	28, 51, 91, 151	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	ASP	5.6
1	H	216	SER	5.2
1	V	216	SER	5.0
1	N	216	SER	4.9
1	O	2	GLY	4.9
1	F	2	GLY	4.7
1	E	216	SER	4.7
1	T	2	GLY	4.6
1	R	218	ASP	4.4
1	I	2	GLY	4.4
1	X	2	GLY	4.3
1	L	2	GLY	4.3
1	M	2	GLY	4.3
1	P	2	GLY	4.2
1	K	2	GLY	4.0
1	H	217	SER	4.0
1	W	216	SER	4.0
1	Q	2	GLY	3.9
1	U	2	GLY	3.8
1	G	2	GLY	3.7
1	R	2	GLY	3.6
1	U	11	ARG	3.6
1	J	217	SER	3.6
1	W	2	GLY	3.5
1	U	215	PRO	3.5
1	X	216	SER	3.4
1	N	2	GLY	3.4
1	P	216	SER	3.3
1	C	2	GLY	3.3
1	N	217	SER	3.3
1	W	77	ALA	3.3
1	E	2	GLY	3.2
1	H	2	GLY	3.2
1	U	3	ASP	3.2
1	O	3	ASP	3.1
1	E	127	LYS	3.1
1	A	2	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	54	ILE	3.0
1	E	82	PRO	3.0
1	I	216	SER	2.8
1	C	217	SER	2.8
1	P	35	GLN	2.8
1	L	3	ASP	2.8
1	F	217	SER	2.8
1	R	217	SER	2.7
1	Q	131	ASP	2.7
1	G	218	ASP	2.7
1	Q	132	VAL	2.6
1	G	217	SER	2.6
1	X	3	ASP	2.6
1	U	216	SER	2.6
1	X	163	GLY	2.6
1	X	80	LEU	2.6
1	U	15	GLN	2.5
1	M	84	ALA	2.5
1	K	216	SER	2.5
1	M	216	SER	2.4
1	X	79	LEU	2.4
1	D	83	GLY	2.4
1	S	2	GLY	2.3
1	E	131	ASP	2.3
1	E	133	ASP	2.3
1	L	217	SER	2.3
1	U	18	LYS	2.3
1	R	213	GLN	2.3
1	V	54	ILE	2.3
1	E	3	ASP	2.3
1	X	81	GLN	2.2
1	C	129	LYS	2.2
1	S	132	VAL	2.2
1	C	82	PRO	2.2
1	U	32	TYR	2.2
1	T	81	GLN	2.2
1	P	130	TYR	2.2
1	U	83	GLY	2.2
1	E	80	LEU	2.2
1	W	130	TYR	2.2
1	J	216	SER	2.1
1	L	11	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	216	SER	2.1
1	X	54	ILE	2.1
1	W	129	LYS	2.1
1	L	8	ARG	2.1
1	L	216	SER	2.1
1	W	131	ASP	2.1
1	D	81	GLN	2.1
1	U	12	TYR	2.1
1	D	163	GLY	2.0
1	K	128	LYS	2.0
1	U	54	ILE	2.0
1	Q	217	SER	2.0
1	I	131	ASP	2.0
1	E	85	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
3	K	K	304	1/1	0.55	0.22	110,110,110,110	0
3	K	A	304	1/1	0.71	0.11	96,96,96,96	0
3	K	S	303	1/1	0.73	0.10	115,115,115,115	0
3	K	M	304	1/1	0.74	0.16	101,101,101,101	0
4	PO4	W	304	5/5	0.76	0.30	135,136,139,143	0
3	K	Q	303	1/1	0.80	0.12	82,82,82,82	0
3	K	R	303	1/1	0.80	0.17	105,105,105,105	0
4	PO4	V	304	5/5	0.88	0.15	109,109,112,113	0
3	K	L	304	1/1	0.88	0.08	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K	G	302	1/1	0.89	0.16	100,100,100,100	0
4	PO4	K	305	5/5	0.91	0.31	119,120,122,125	0
3	K	S	304	1/1	0.91	0.08	70,70,70,70	0
4	PO4	H	304	5/5	0.91	0.22	99,100,101,104	0
3	K	N	304	1/1	0.92	0.06	85,85,85,85	0
4	PO4	I	304	5/5	0.92	0.31	102,102,105,111	0
3	K	P	303	1/1	0.92	0.14	62,62,62,62	0
4	PO4	S	305	5/5	0.92	0.12	96,98,102,105	0
3	K	E	303	1/1	0.92	0.09	68,68,68,68	0
4	PO4	D	304	5/5	0.92	0.20	88,88,95,107	0
4	PO4	M	305	5/5	0.93	0.22	90,91,99,100	0
3	K	J	302	1/1	0.93	0.29	64,64,64,64	0
3	K	F	303	1/1	0.94	0.08	69,69,69,69	0
3	K	F	302	1/1	0.94	0.26	41,41,41,41	0
3	K	J	304	1/1	0.95	0.07	81,81,81,81	0
3	K	M	303	1/1	0.95	0.09	56,56,56,56	0
3	K	Q	302	1/1	0.95	0.13	37,37,37,37	0
3	K	U	303	1/1	0.95	0.06	65,65,65,65	0
4	PO4	Q	304	5/5	0.95	0.11	86,88,91,92	0
3	K	V	303	1/1	0.95	0.11	54,54,54,54	0
4	PO4	T	304	5/5	0.95	0.19	90,90,92,99	0
4	PO4	C	304	5/5	0.95	0.15	94,96,99,103	0
3	K	I	303	1/1	0.95	0.07	49,49,49,49	0
3	K	W	303	1/1	0.96	0.08	58,58,58,58	0
2	6PQ	N	301	21/21	0.96	0.17	26,36,56,63	0
2	6PQ	R	301	21/21	0.96	0.15	33,50,59,62	0
2	6PQ	L	301	21/21	0.96	0.14	29,41,48,51	0
3	K	R	302	1/1	0.96	0.17	42,42,42,42	0
3	K	C	302	1/1	0.96	0.20	38,38,38,38	0
3	K	D	302	1/1	0.96	0.14	43,43,43,43	0
3	K	N	303	1/1	0.96	0.07	52,52,52,52	0
3	K	D	303	1/1	0.96	0.08	45,45,45,45	0
3	K	V	302	1/1	0.96	0.21	45,45,45,45	0
3	K	O	304	1/1	0.96	0.15	72,72,72,72	0
3	K	W	302	1/1	0.96	0.16	45,45,45,45	0
2	6PQ	W	301	21/21	0.97	0.15	35,40,49,51	0
3	K	U	302	1/1	0.97	0.13	39,39,39,39	0
3	K	A	303	1/1	0.97	0.09	64,64,64,64	0
2	6PQ	F	301	21/21	0.97	0.17	29,39,50,53	0
3	K	B	303	1/1	0.97	0.12	48,48,48,48	0
2	6PQ	I	301	21/21	0.97	0.13	29,44,56,57	0
2	6PQ	J	301	21/21	0.97	0.16	36,43,51,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K	X	303	1/1	0.97	0.10	64,64,64,64	0
2	6PQ	B	301	21/21	0.97	0.17	28,37,45,49	0
3	K	O	302	1/1	0.97	0.16	39,39,39,39	0
3	K	O	303	1/1	0.97	0.06	46,46,46,46	0
3	K	E	302	1/1	0.97	0.17	53,53,53,53	0
2	6PQ	M	301	21/21	0.97	0.14	29,38,46,50	0
2	6PQ	D	301	21/21	0.97	0.16	35,42,49,52	0
4	PO4	N	305	5/5	0.97	0.12	46,55,59,66	0
2	6PQ	O	301	21/21	0.97	0.13	32,45,53,54	0
2	6PQ	P	301	21/21	0.97	0.18	32,52,57,61	0
2	6PQ	E	301	21/21	0.97	0.18	43,52,58,60	0
3	K	R	304	1/1	0.97	0.07	60,60,60,60	0
2	6PQ	S	301	21/21	0.97	0.15	44,55,62,63	0
3	K	K	302	1/1	0.98	0.25	43,43,43,43	0
3	K	K	303	1/1	0.98	0.08	45,45,45,45	0
3	K	T	303	1/1	0.98	0.09	43,43,43,43	0
2	6PQ	G	301	21/21	0.98	0.13	25,41,49,50	0
3	K	L	303	1/1	0.98	0.09	64,64,64,64	0
3	K	C	303	1/1	0.98	0.12	46,46,46,46	0
3	K	M	302	1/1	0.98	0.22	38,38,38,38	0
2	6PQ	H	301	21/21	0.98	0.15	28,40,49,52	0
2	6PQ	T	301	21/21	0.98	0.15	20,36,47,55	0
3	K	N	302	1/1	0.98	0.19	42,42,42,42	0
2	6PQ	U	301	21/21	0.98	0.14	35,43,55,64	0
2	6PQ	V	301	21/21	0.98	0.13	32,41,53,56	0
2	6PQ	C	301	21/21	0.98	0.14	22,43,51,55	0
2	6PQ	X	301	21/21	0.98	0.15	45,53,66,69	0
3	K	A	302	1/1	0.98	0.24	37,37,37,37	0
3	K	G	303	1/1	0.98	0.04	56,56,56,56	0
3	K	G	304	1/1	0.98	0.22	36,36,36,36	0
2	6PQ	A	301	21/21	0.98	0.15	35,41,48,56	0
2	6PQ	K	301	21/21	0.98	0.16	11,28,36,44	0
3	K	J	303	1/1	0.98	0.09	48,48,48,48	0
2	6PQ	Q	301	21/21	0.98	0.14	28,35,46,51	0
3	K	S	302	1/1	0.98	0.16	39,39,39,39	0
3	K	H	303	1/1	0.99	0.08	46,46,46,46	0
3	K	T	302	1/1	0.99	0.21	38,38,38,38	0
3	K	X	302	1/1	0.99	0.19	51,51,51,51	0
3	K	L	302	1/1	0.99	0.16	29,29,29,29	0
3	K	I	302	1/1	0.99	0.12	32,32,32,32	0
3	K	P	302	1/1	0.99	0.16	47,47,47,47	0
3	K	B	302	1/1	0.99	0.17	25,25,25,25	0

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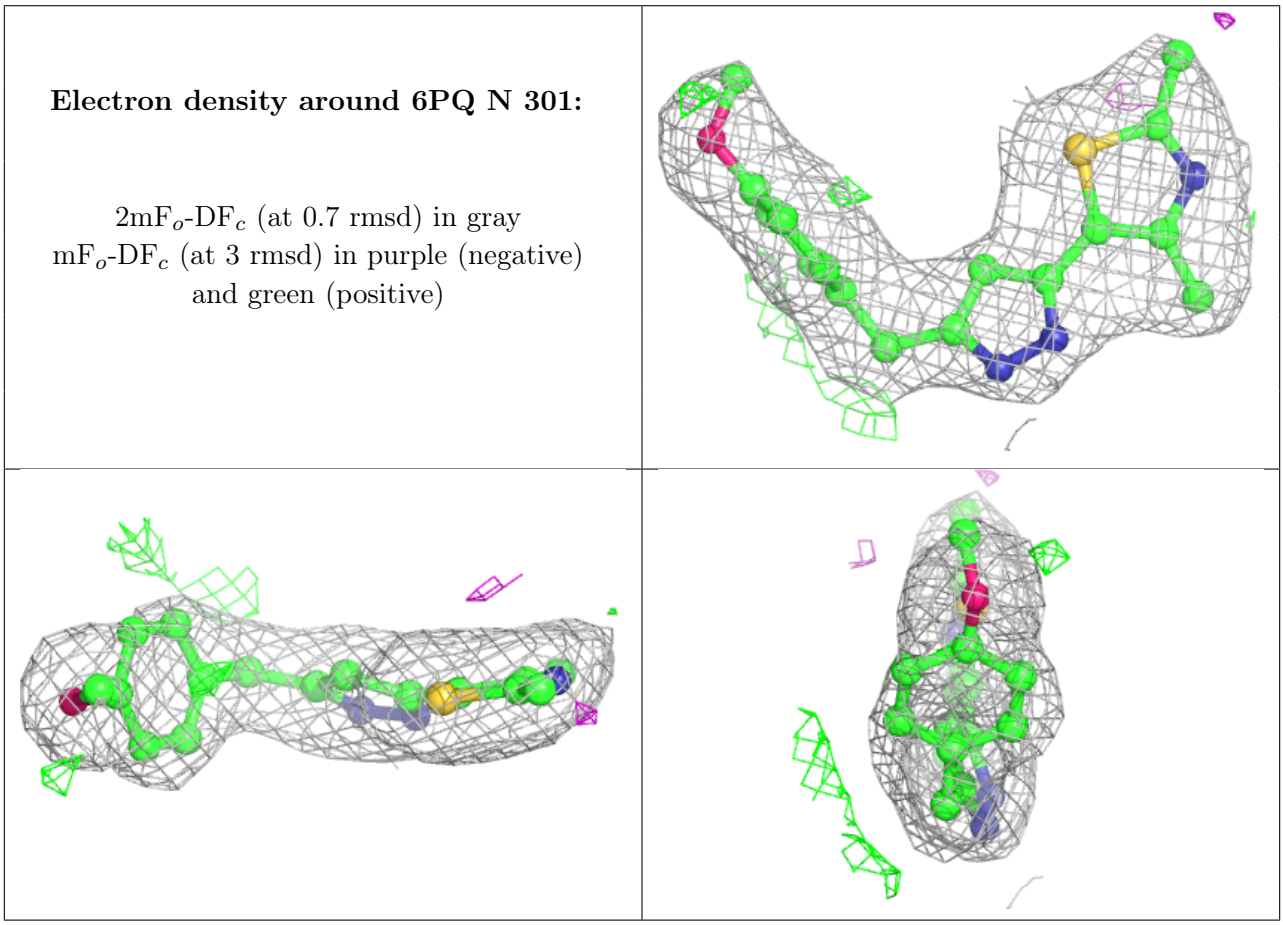
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K	H	302	1/1	0.99	0.22	38,38,38,38	0

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.

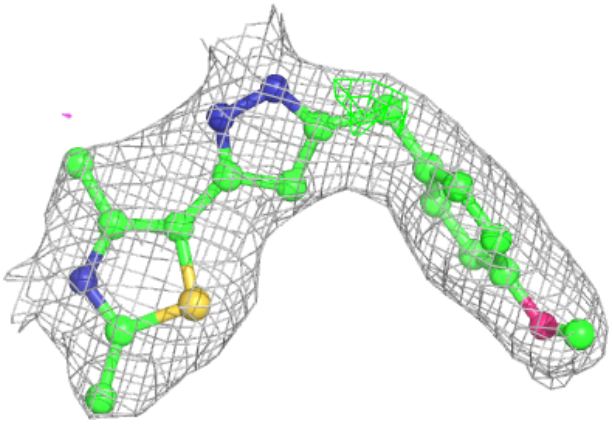
Electron density around 6PQ N 301:

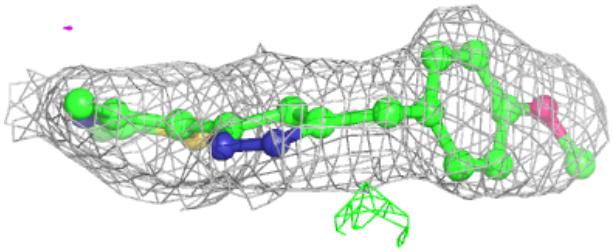
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

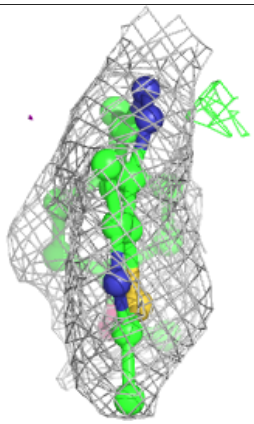


Electron density around 6PQ R 301:

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

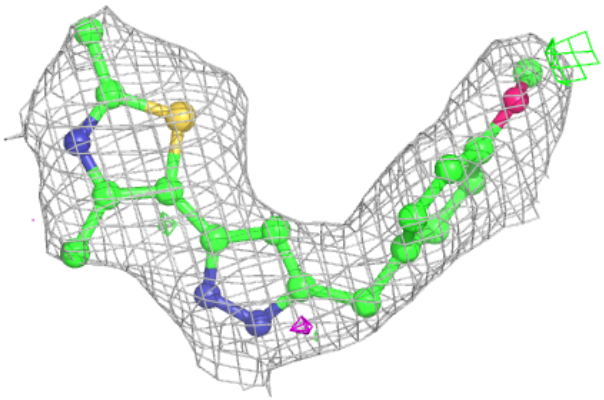


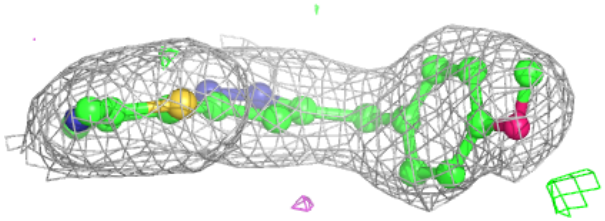


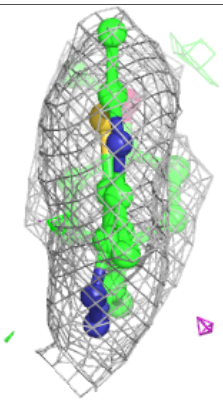


Electron density around 6PQ L 301:

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

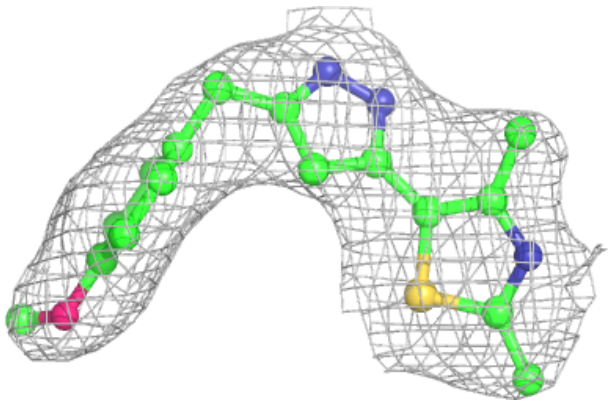


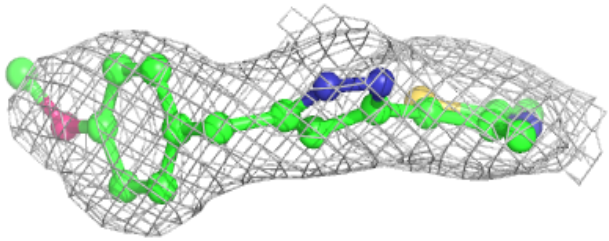


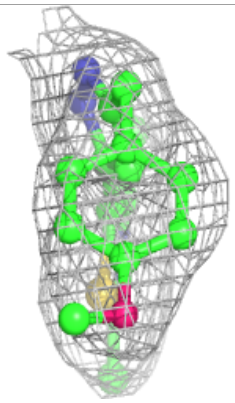


Electron density around 6PQ W 301:

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

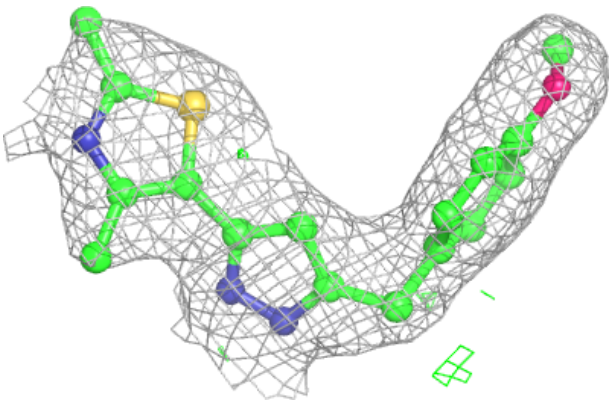


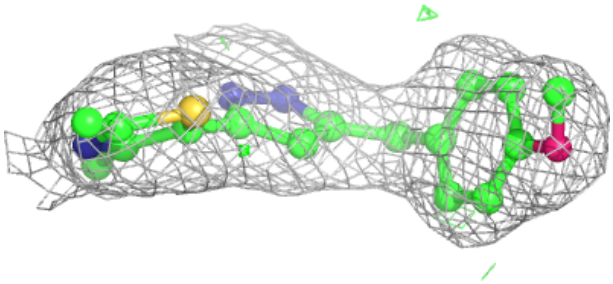


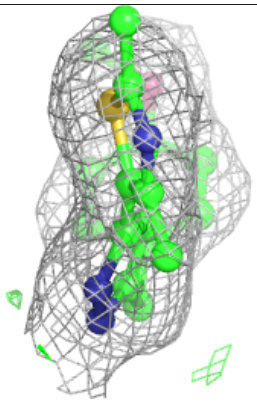


Electron density around 6PQ F 301:

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

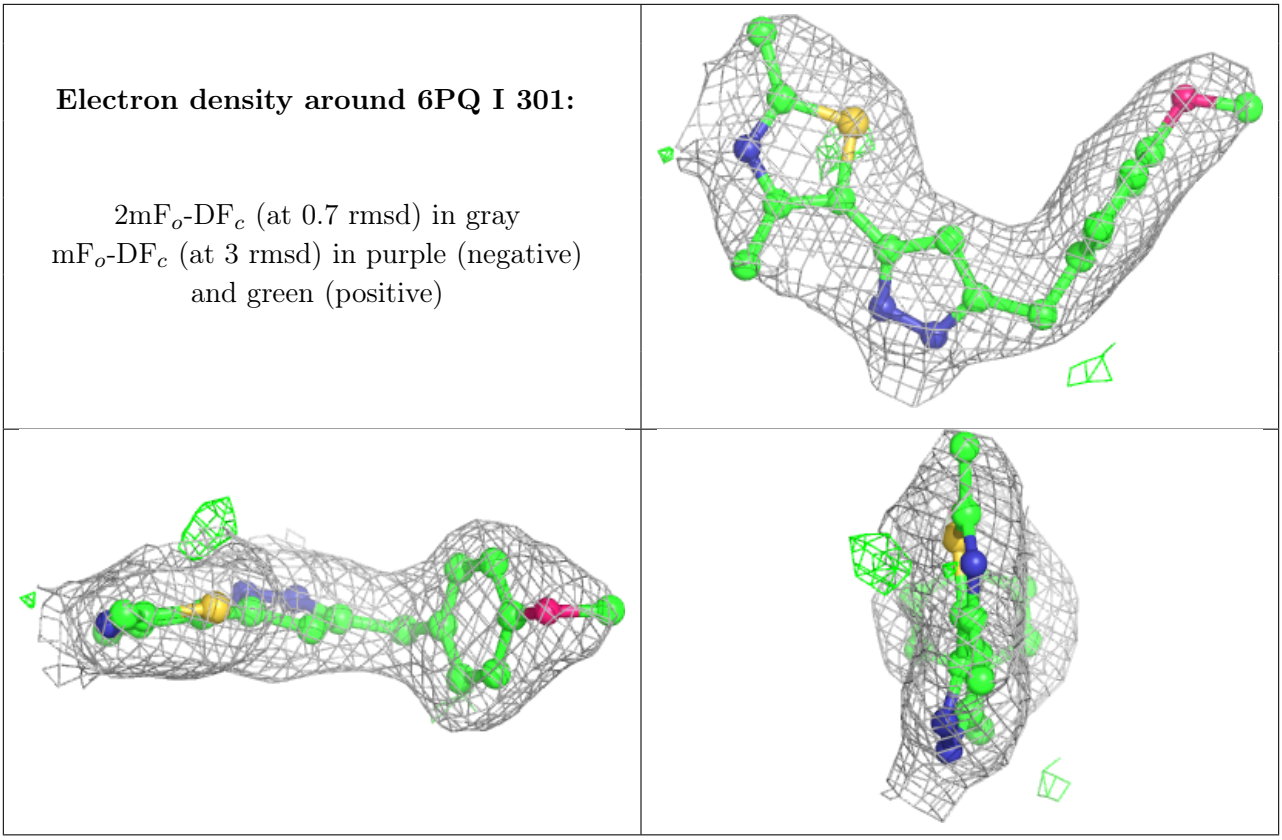






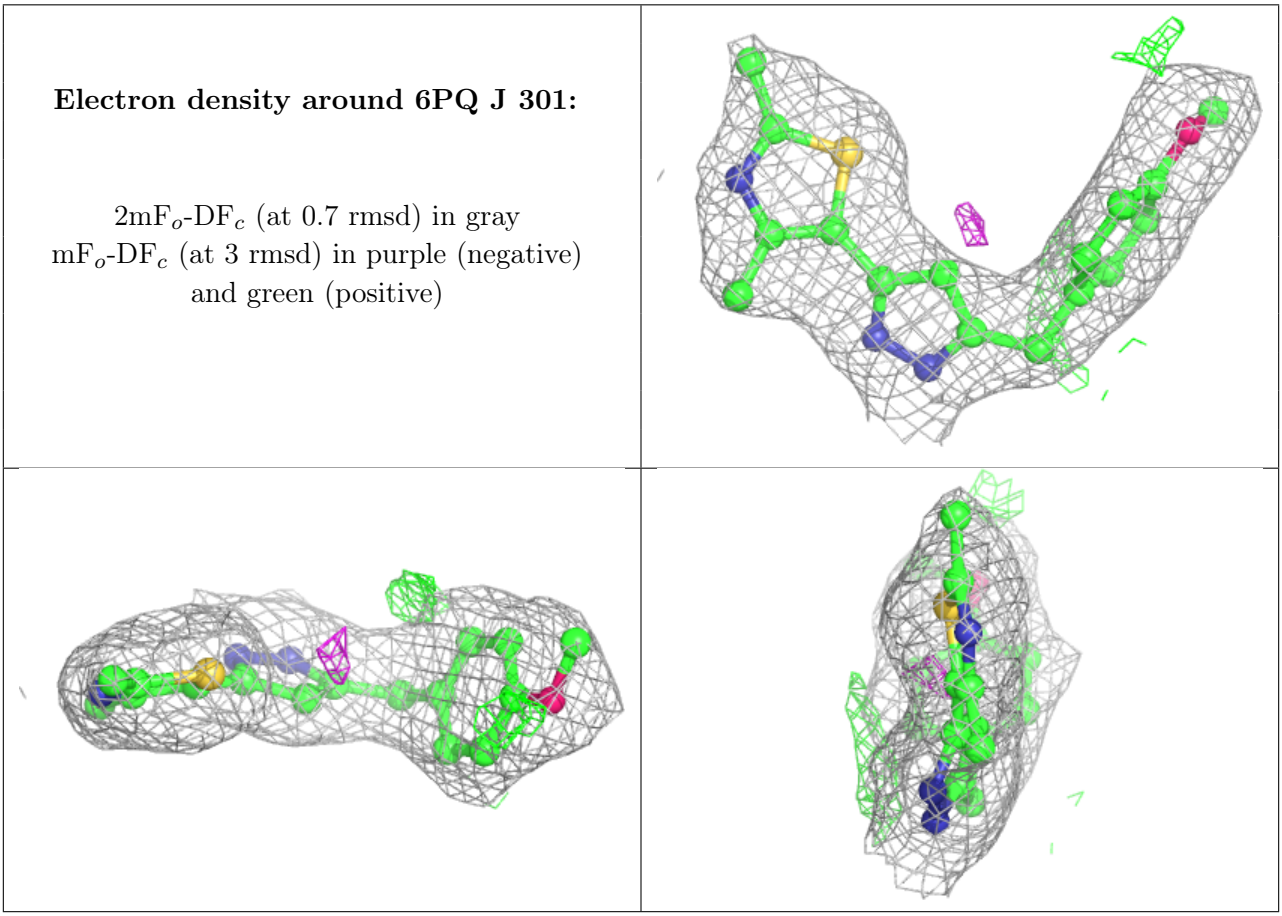
Electron density around 6PQ I 301:

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



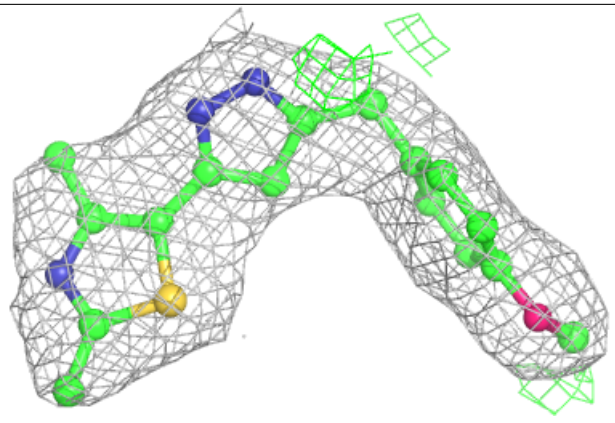
Electron density around 6PQ J 301:

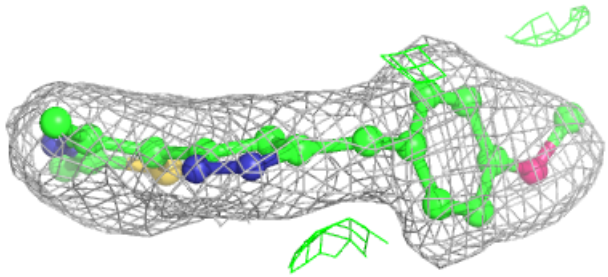
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

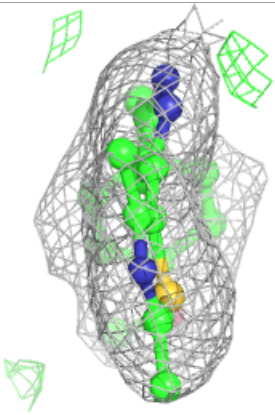


Electron density around 6PQ B 301:

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

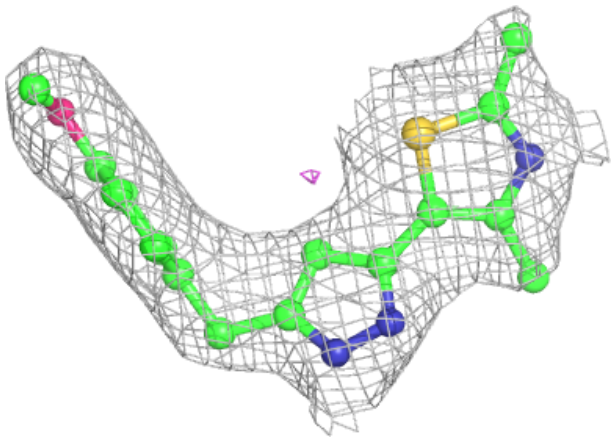


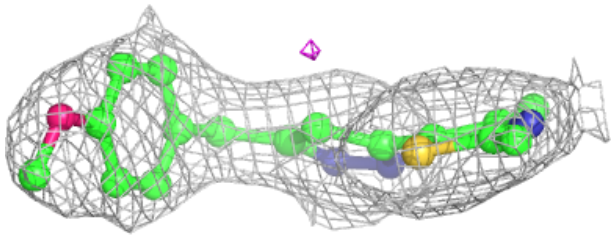


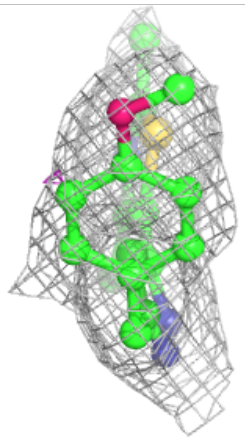


Electron density around 6PQ M 301:

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

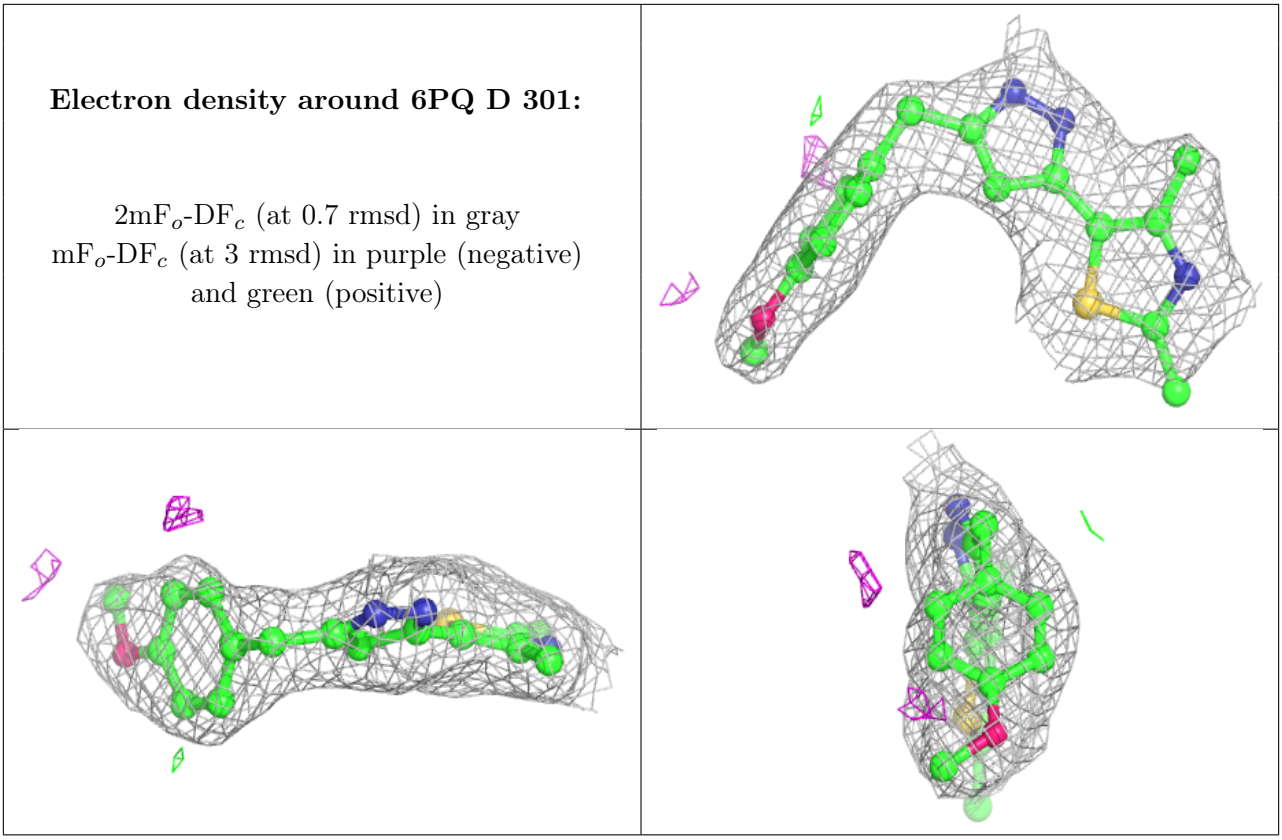






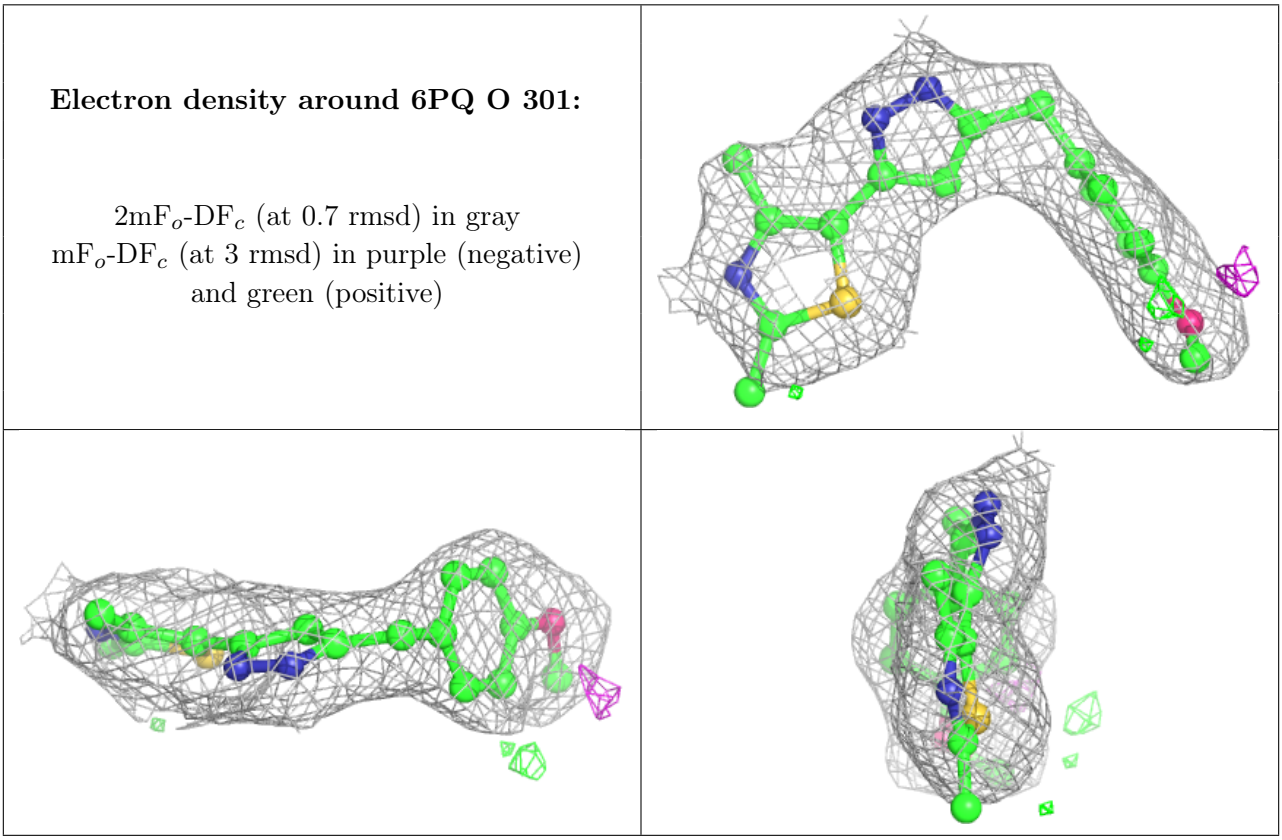
Electron density around 6PQ D 301:

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



Electron density around 6PQ 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 6PQ P 301:

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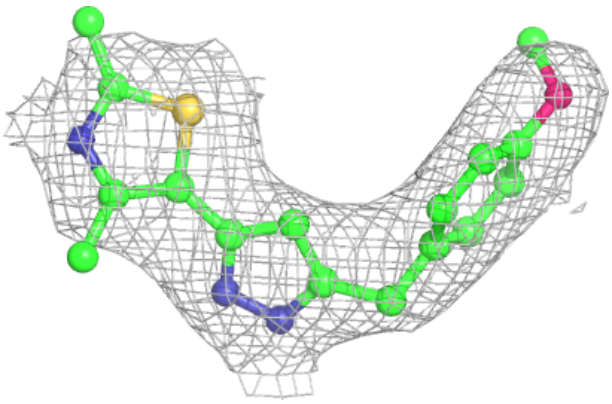
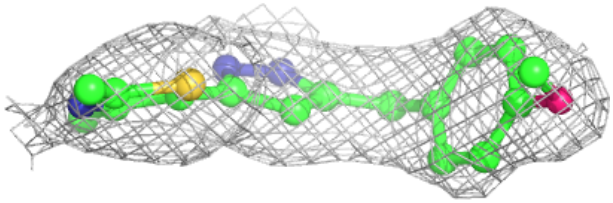
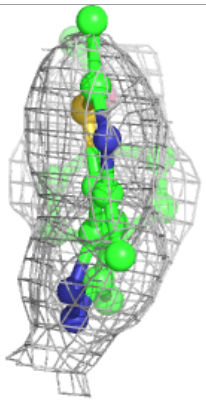
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

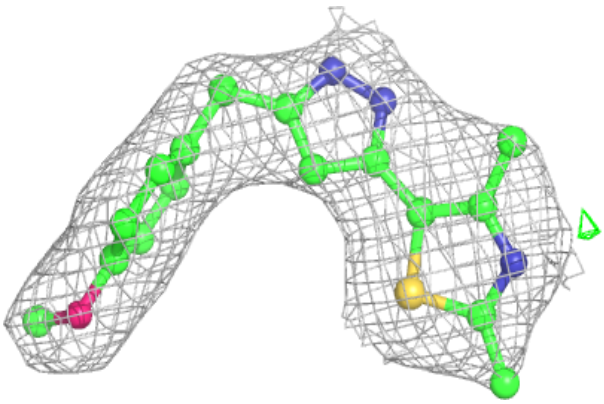


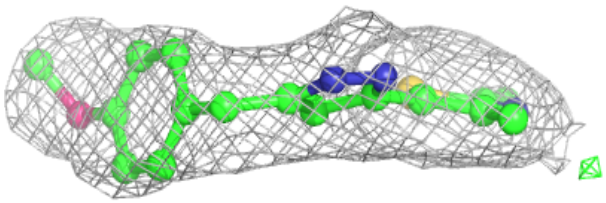


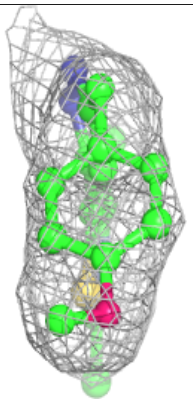


Electron density around 6PQ E 301:

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

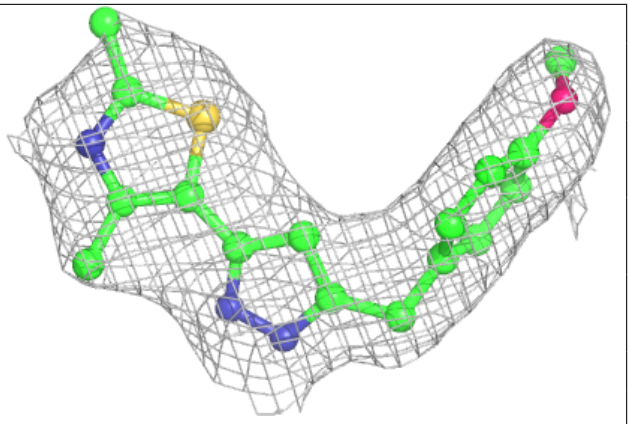


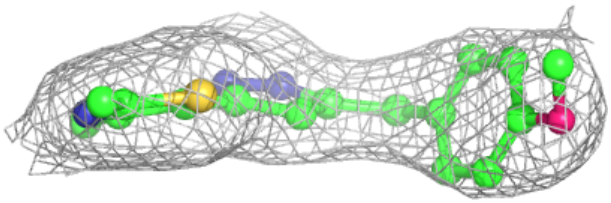


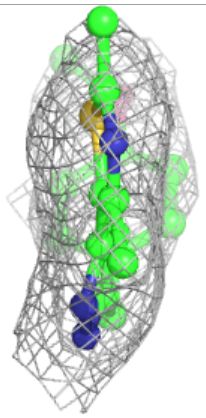


Electron density around 6PQ S 301:

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

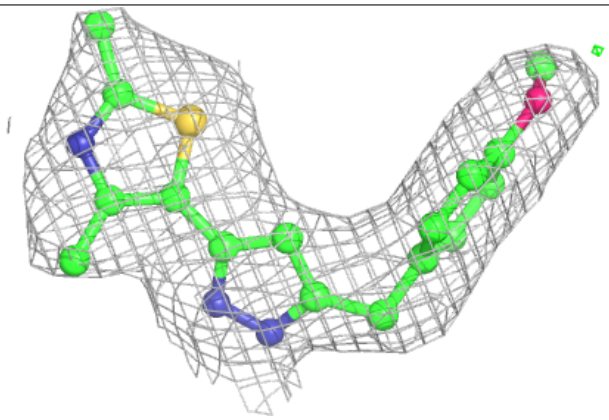


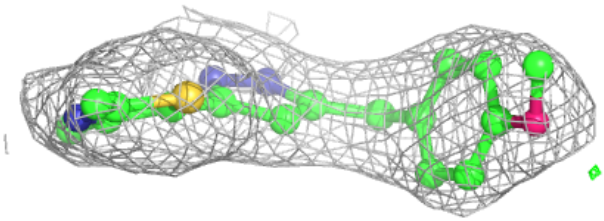


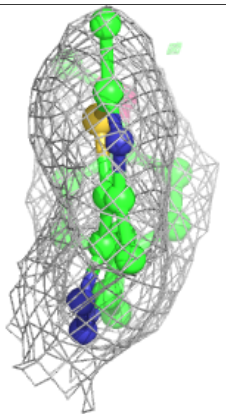


Electron density around 6PQ G 301:

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

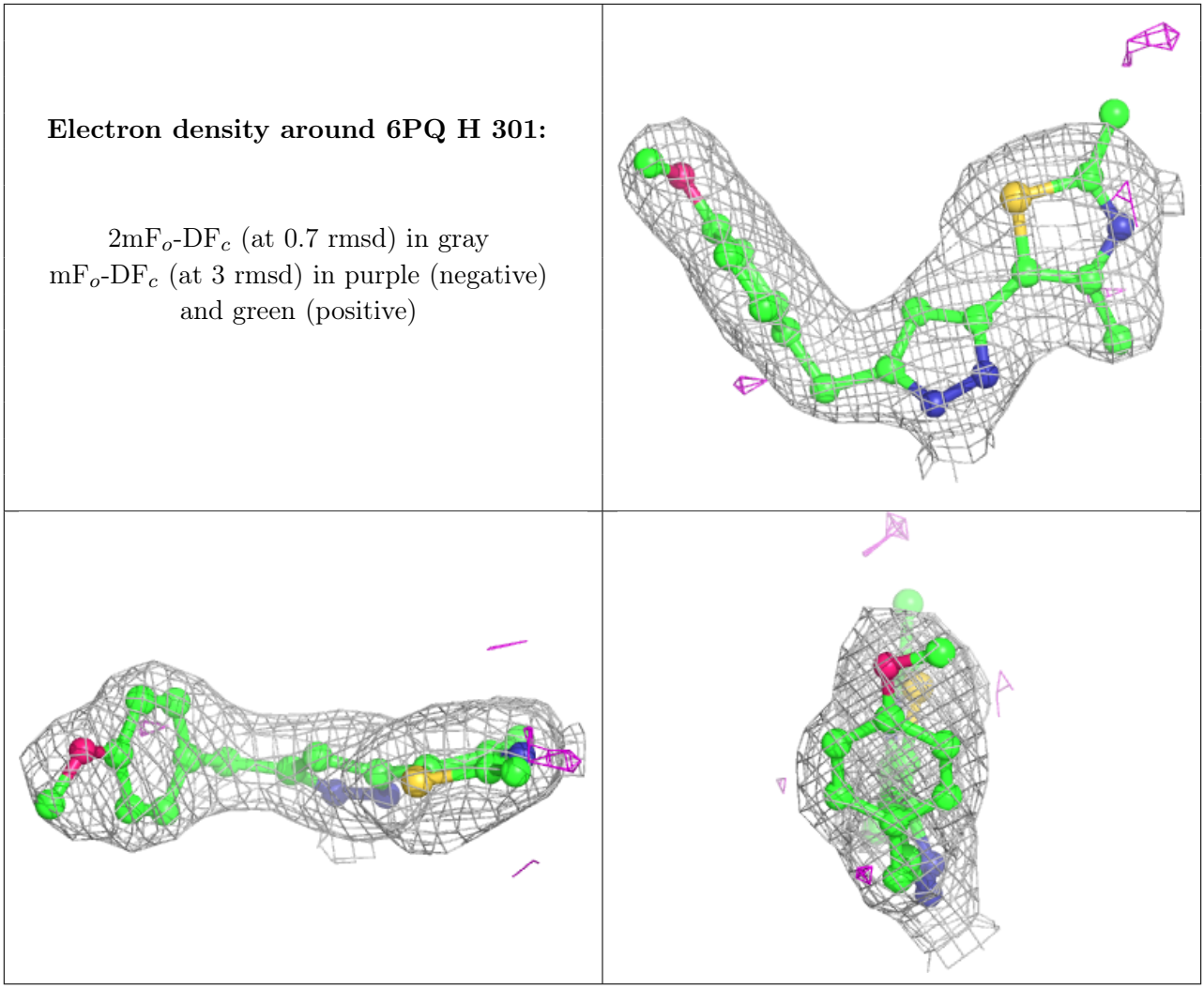






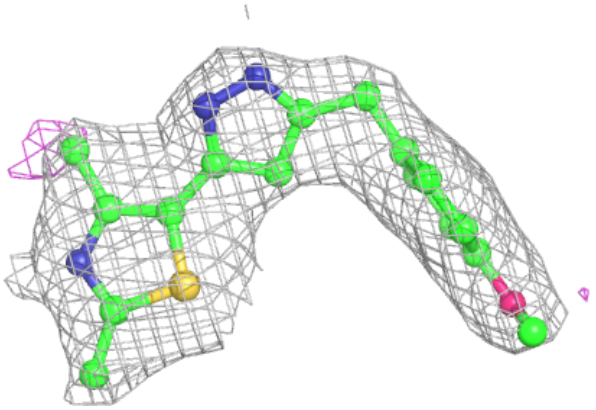
Electron density around 6PQ H 301:

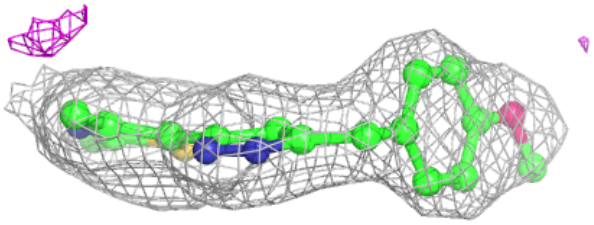
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

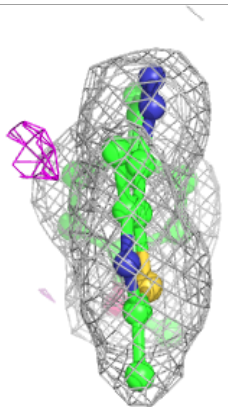


Electron density around 6PQ T 301:

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







Electron density around 6PQ U 301:

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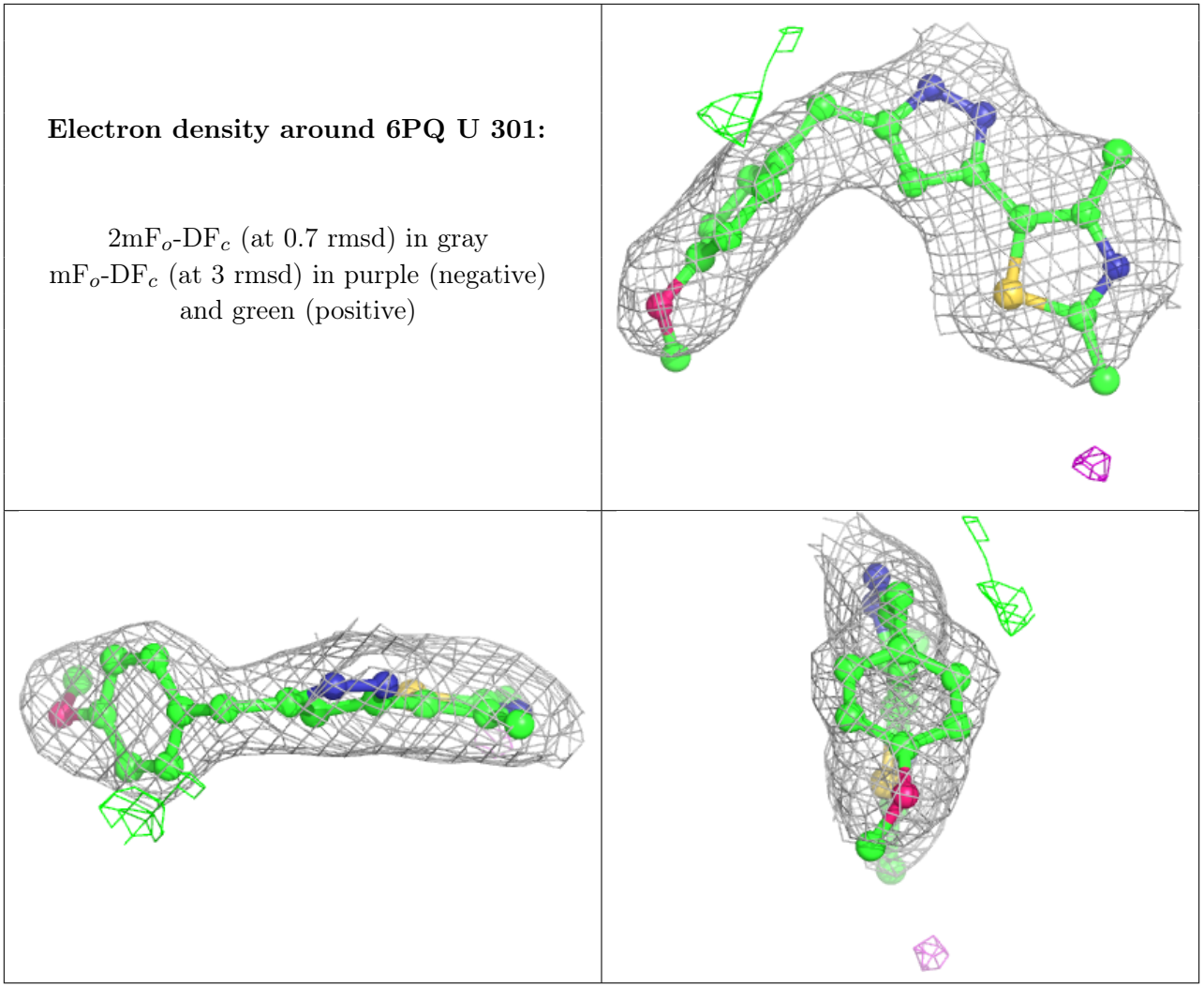
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 6PQ V 301:

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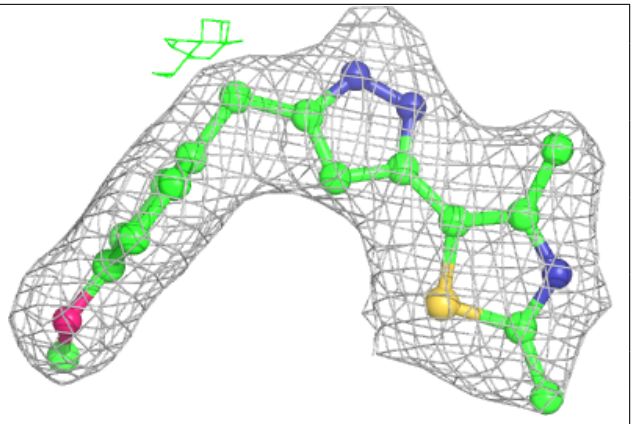
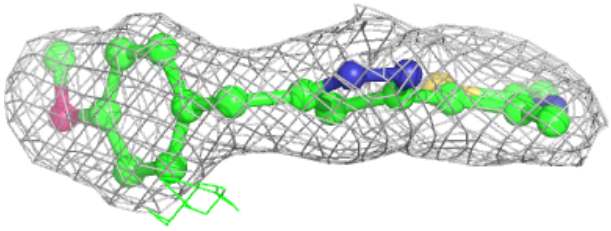
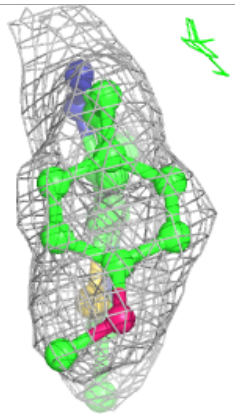
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

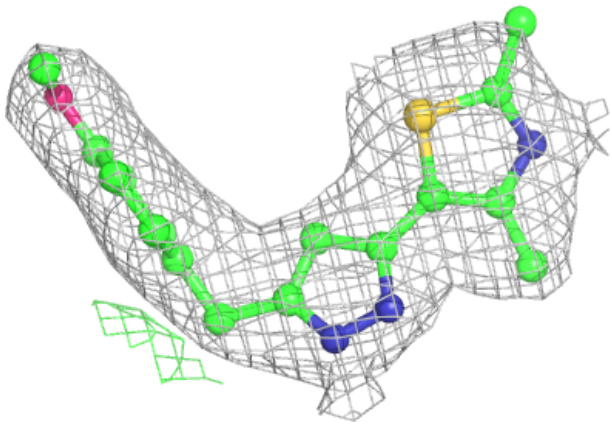


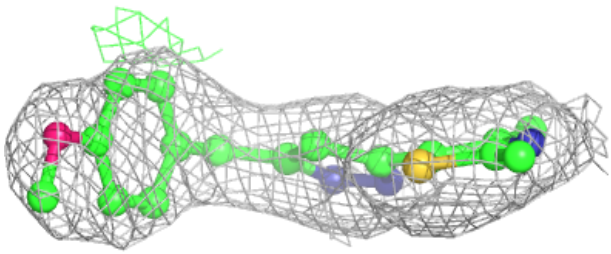


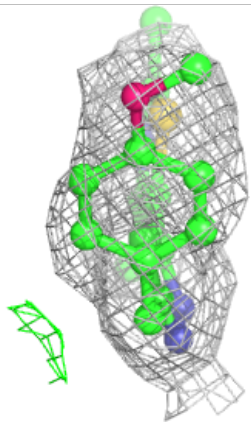


Electron density around 6PQ C 301:

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

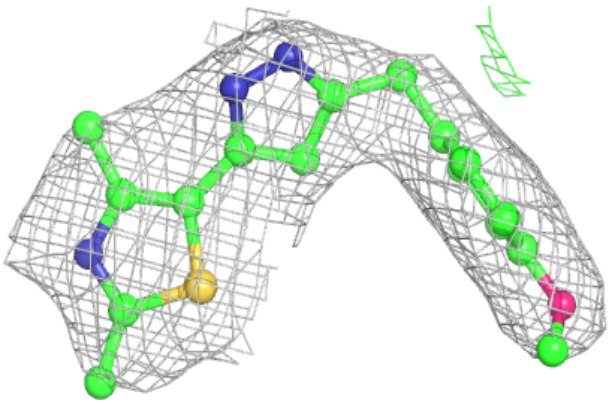


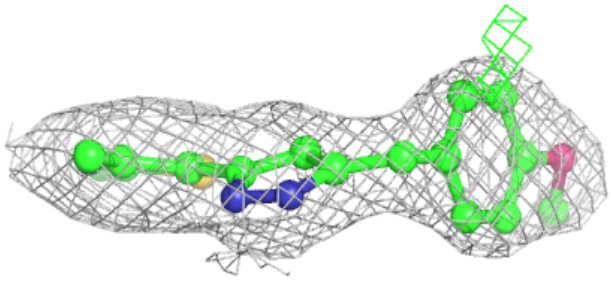


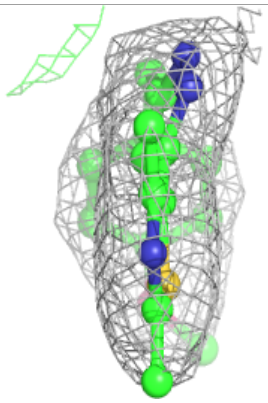


Electron density around 6PQ X 301:

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

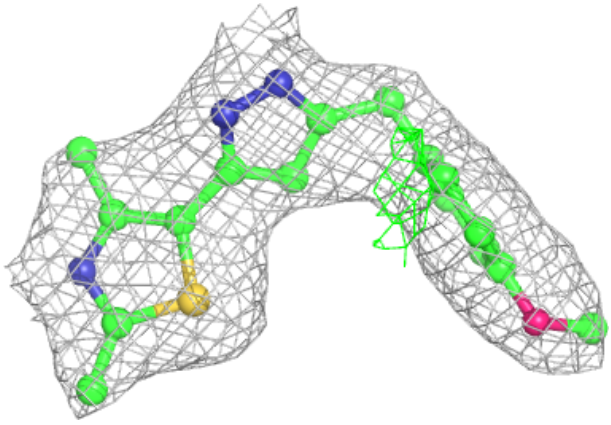


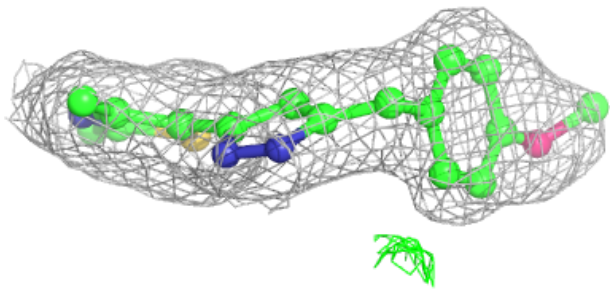


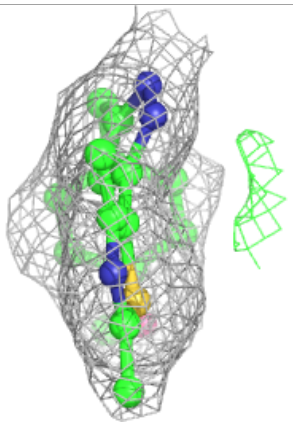


Electron density around 6PQ A 301:

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

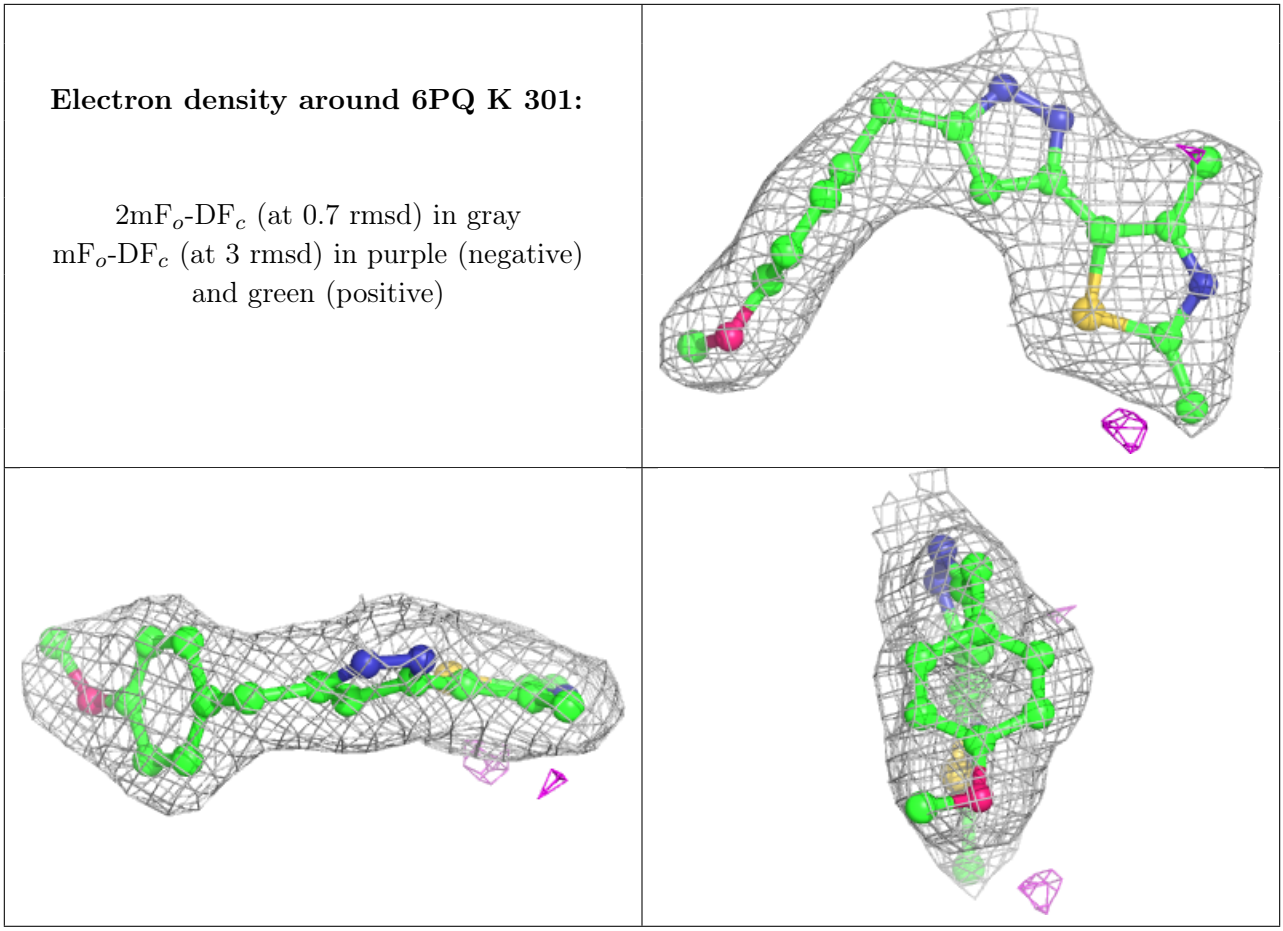






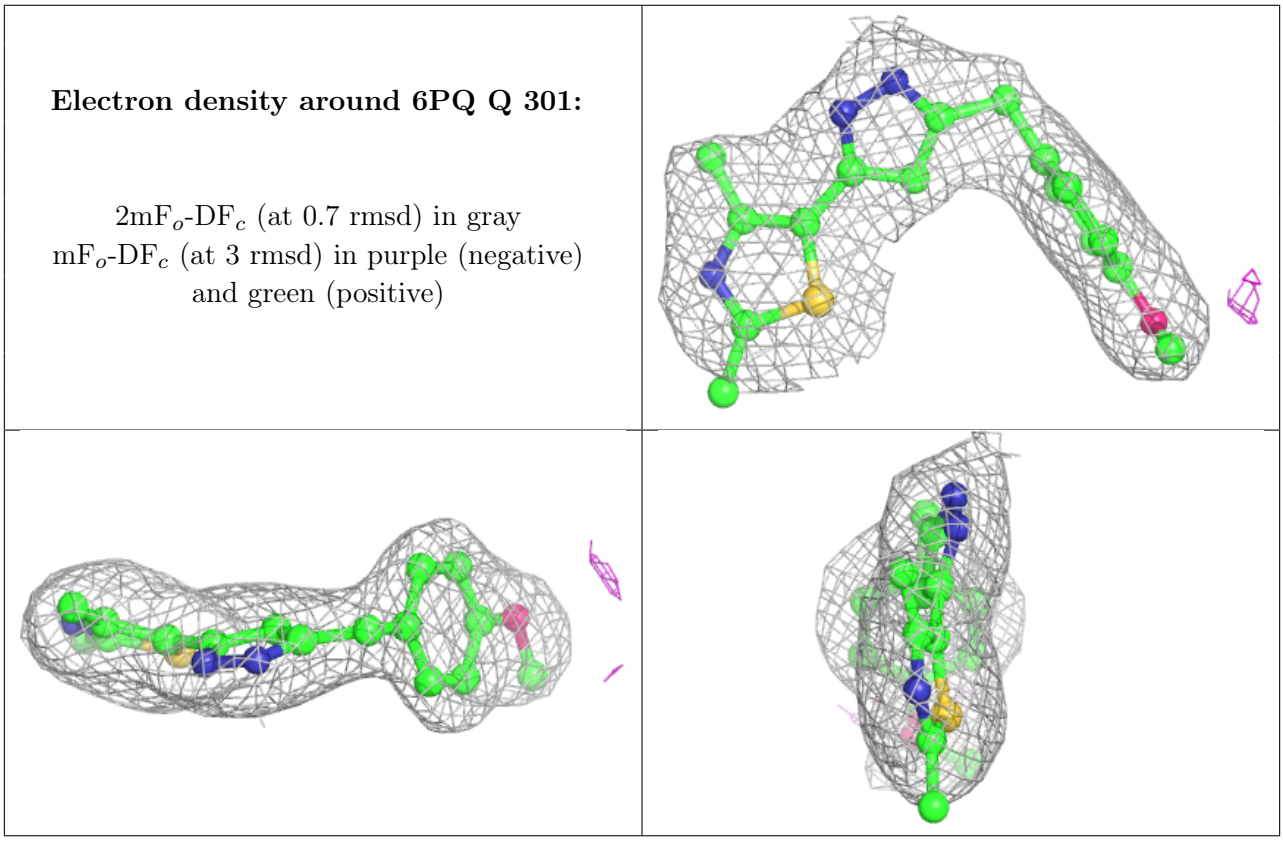
Electron density around 6PQ K 301:

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



Electron density around 6PQ 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)



6.5 Other polymers (i)

There are no such residues in this entry.