Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2020 – 04:09 PM BST

PDB ID	:	5OYH
Title	:	crystal structure of the catalytic core of a rhodopsin-guanylyl cyclase with converted specificity in complex with ATPalphaS
Authors	:	Broser, M.; Scheib, U.; Hegemann, P.
Deposited on	:	2017-09-09
Resolution	:	2.25 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 following versions of software and data (see references (i)) were used in the production of this report:

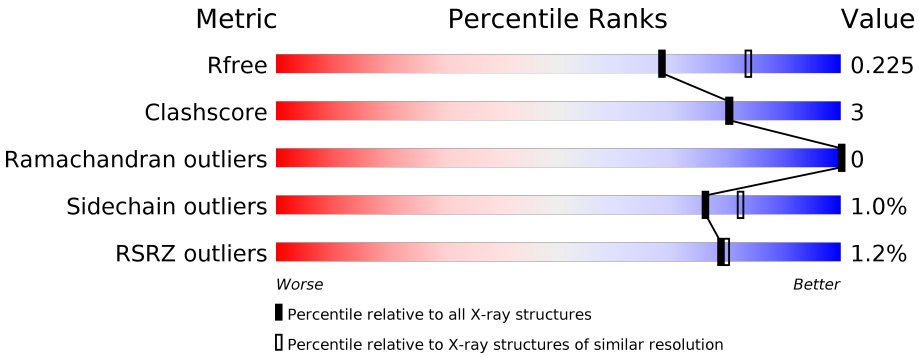
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 2.25 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 on 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	193	86% 8% • 5%
1	B	193	89% 6% 5%
1	C	193	91% • • 5%
1	D	193	91% 5% •
1	E	193	87% 7% 6%
1	F	193	89% 7% •

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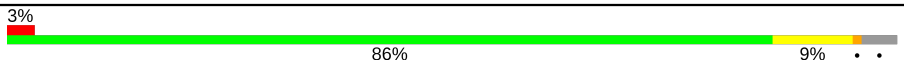
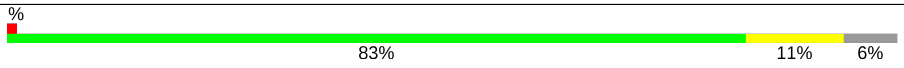
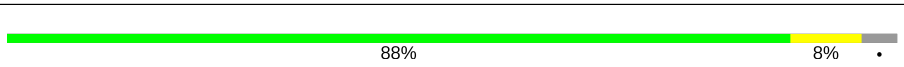
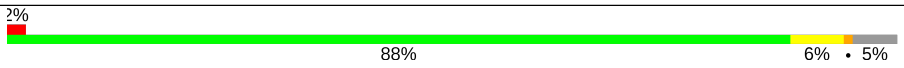
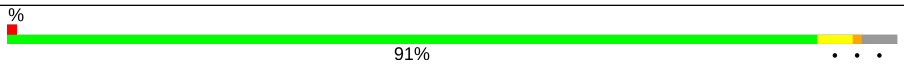
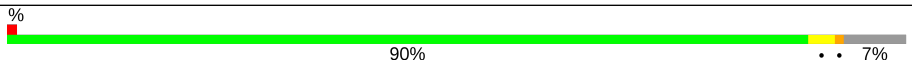
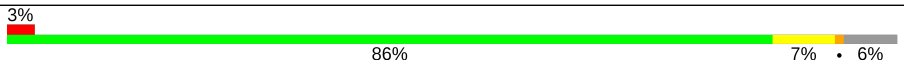
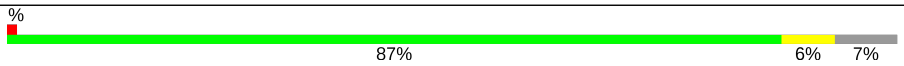
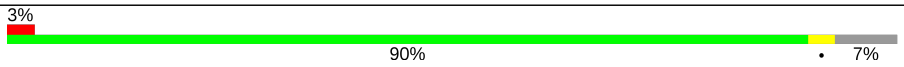
Mol	Chain	Length	Quality of chain
1	G	193	
1	H	193	
1	I	193	
1	J	193	
1	K	193	
1	L	193	
1	M	193	
1	N	193	
1	O	193	
1	P	193	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24979 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 Nucleotide cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1423	904	237	274	8			
1	B	184	Total	C	N	O	S	0	0	0
			1424	905	238	274	7			
1	C	184	Total	C	N	O	S	0	0	0
			1428	908	239	274	7			
1	D	185	Total	C	N	O	S	0	0	0
			1436	913	240	275	8			
1	E	182	Total	C	N	O	S	0	0	0
			1396	887	231	271	7			
1	F	185	Total	C	N	O	S	0	0	0
			1430	909	238	275	8			
1	G	185	Total	C	N	O	S	0	0	0
			1428	907	238	275	8			
1	H	185	Total	C	N	O	S	0	0	0
			1433	911	239	275	8			
1	I	182	Total	C	N	O	S	0	1	0
			1414	900	235	271	8			
1	J	185	Total	C	N	O	S	0	1	0
			1438	915	239	275	9			
1	K	183	Total	C	N	O	S	0	0	0
			1412	896	236	273	7			
1	L	185	Total	C	N	O	S	0	0	0
			1436	913	240	275	8			
1	M	180	Total	C	N	O	S	0	0	0
			1392	886	232	267	7			
1	N	181	Total	C	N	O	S	0	0	0
			1405	895	234	268	8			
1	O	179	Total	C	N	O	S	0	0	0
			1383	881	230	265	7			
1	P	179	Total	C	N	O	S	0	0	0
			1384	881	230	266	7			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
A	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
A	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
A	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
A	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
A	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
A	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
A	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
A	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
A	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
A	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
B	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
B	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
B	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
B	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
B	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
B	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
B	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
B	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
B	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
B	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
B	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
C	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
C	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
C	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
C	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
C	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
C	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
C	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
C	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
C	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
C	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
C	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
D	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
D	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
D	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
D	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
D	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
D	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
D	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
D	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
D	632	HIS	-	expression tag	UNP A0A1Y2HEJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
D	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
E	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
E	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
E	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
E	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
E	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
E	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
E	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
E	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
E	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
E	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
E	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
F	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
F	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
F	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
F	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
F	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
F	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
F	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
F	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
F	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
F	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
F	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
G	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
G	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
G	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
G	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
G	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
G	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
G	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
G	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
G	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
G	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
G	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
H	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
H	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
H	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
H	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
H	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
H	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
H	630	HIS	-	expression tag	UNP A0A1Y2HEJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
H	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
H	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
H	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
I	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
I	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
I	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
I	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
I	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
I	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
I	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
I	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
I	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
I	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
I	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
J	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
J	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
J	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
J	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
J	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
J	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
J	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
J	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
J	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
J	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
J	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
K	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
K	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
K	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
K	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
K	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
K	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
K	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
K	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
K	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
K	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
K	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
L	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
L	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
L	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
L	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
L	628	GLU	-	expression tag	UNP A0A1Y2HEJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
L	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
L	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
L	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
L	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
L	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
L	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
M	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
M	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
M	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
M	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
M	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
M	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
M	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
M	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
M	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
M	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
M	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
N	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
N	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
N	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
N	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
N	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
N	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
N	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
N	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
N	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
N	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
N	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
O	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
O	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
O	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3
O	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
O	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
O	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
O	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
O	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
O	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
O	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
O	634	HIS	-	expression tag	UNP A0A1Y2HEJ3
P	442	MET	-	initiating methionine	UNP A0A1Y2HEJ3
P	497	LYS	GLU	engineered mutation	UNP A0A1Y2HEJ3
P	566	ASP	CYS	engineered mutation	UNP A0A1Y2HEJ3

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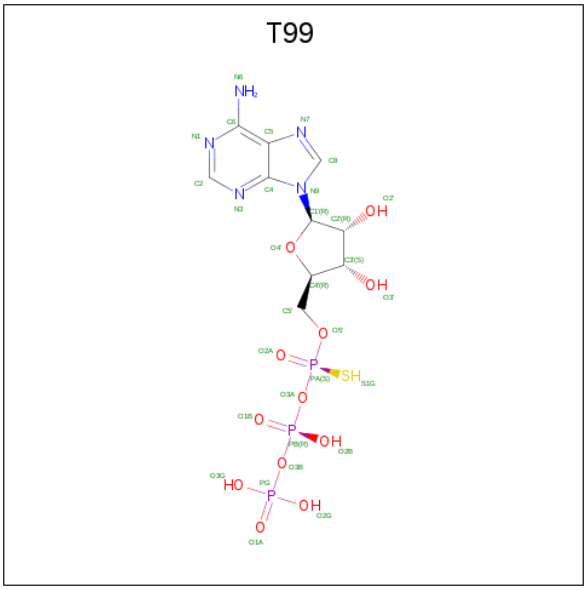
Chain	Residue	Modelled	Actual	Comment	Reference
P	627	LEU	-	expression tag	UNP A0A1Y2HEJ3
P	628	GLU	-	expression tag	UNP A0A1Y2HEJ3
P	629	HIS	-	expression tag	UNP A0A1Y2HEJ3
P	630	HIS	-	expression tag	UNP A0A1Y2HEJ3
P	631	HIS	-	expression tag	UNP A0A1Y2HEJ3
P	632	HIS	-	expression tag	UNP A0A1Y2HEJ3
P	633	HIS	-	expression tag	UNP A0A1Y2HEJ3
P	634	HIS	-	expression tag	UNP A0A1Y2HEJ3

- Molecule 2 is ADENOSINE-5'-SP-ALPHA-THIO-TRIPHOSPHATE (three-letter code: T99) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	K	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	M	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	N	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	O	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	P	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		
3	J	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	K	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	I	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

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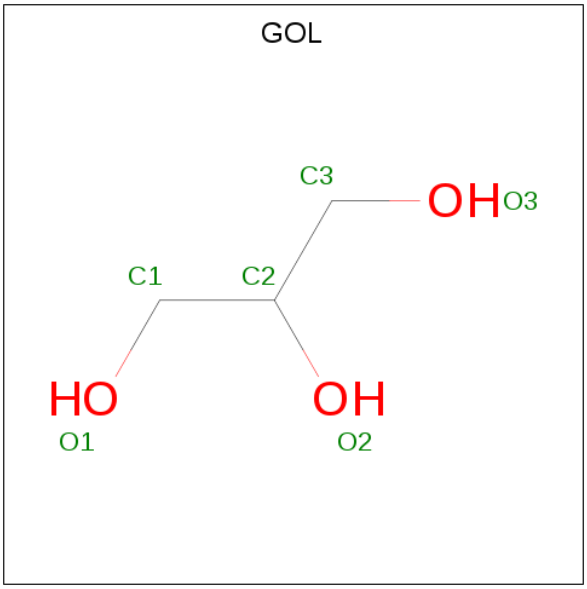
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	N	1	Total Ca 1 1	0	0
3	O	1	Total Ca 1 1	0	0
3	L	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	M	1	Total Ca 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0
4	K	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	O	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	100	Total O 100 100	0	0
5	B	139	Total O 139 139	0	0
5	C	123	Total O 123 123	0	0
5	D	176	Total O 176 176	0	0
5	E	89	Total O 89 89	0	0
5	F	115	Total O 115 115	0	0
5	G	125	Total O 125 125	0	0
5	H	169	Total O 169 169	0	0
5	I	72	Total O 72 72	0	0

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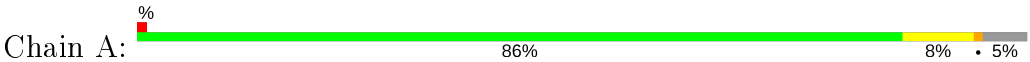
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	100	Total O 100 100	0	0
5	K	67	Total O 67 67	0	0
5	L	138	Total O 138 138	0	0
5	M	104	Total O 104 104	0	0
5	N	63	Total O 63 63	0	0
5	O	82	Total O 82 82	0	0
5	P	53	Total O 53 53	0	0

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: Nucleotide cyclase

Chain A:

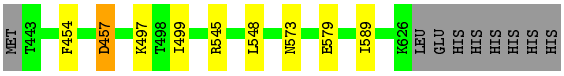


- Molecule 1: Nucleotide cyclase

Chain B:

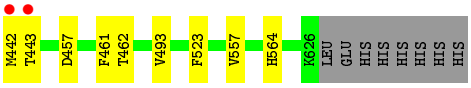
- Molecule 1: Nucleotide cyclase

Chain C:



- Molecule 1: Nucleotide cyclase

Chain D:

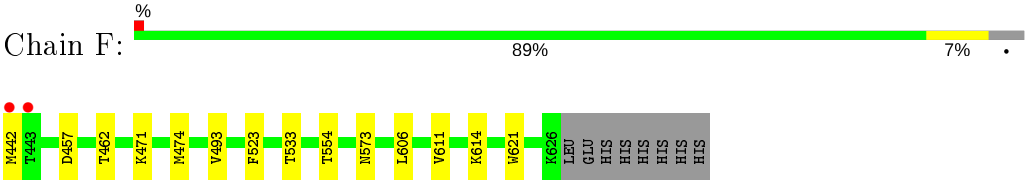


- Molecule 1: Nucleotide cyclase

Chain E:

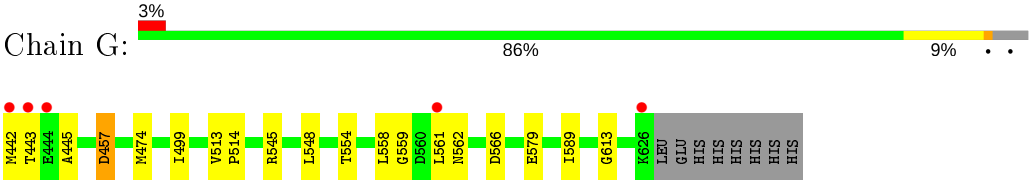
- Molecule 1: Nucleotide cyclase

Chain F:



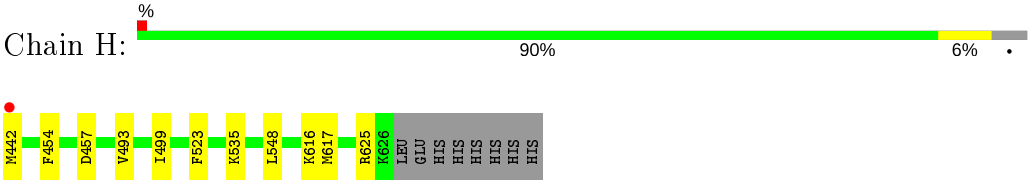
- Molecule 1: Nucleotide cyclase

Chain G:



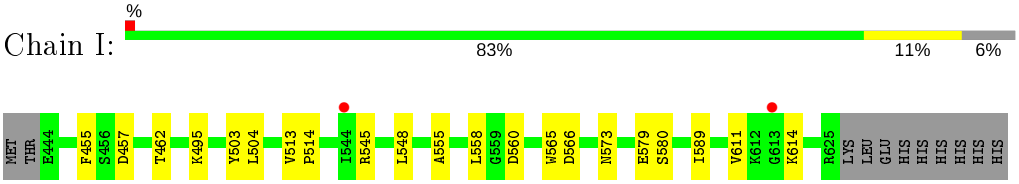
- Molecule 1: Nucleotide cyclase

Chain H:



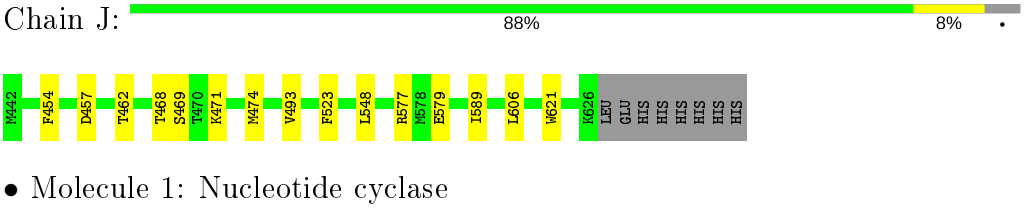
- Molecule 1: Nucleotide cyclase

Chain I:



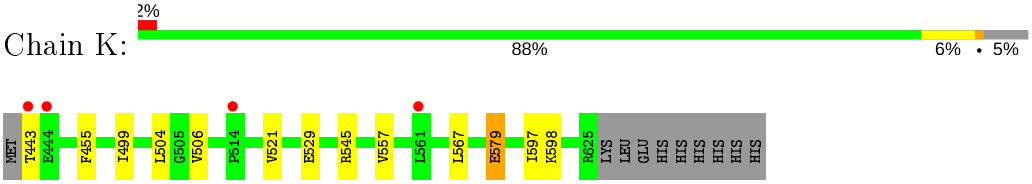
- Molecule 1: Nucleotide cyclase

Chain J:



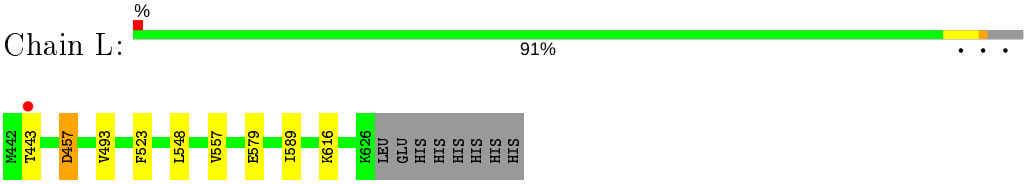
- Molecule 1: Nucleotide cyclase

Chain K:



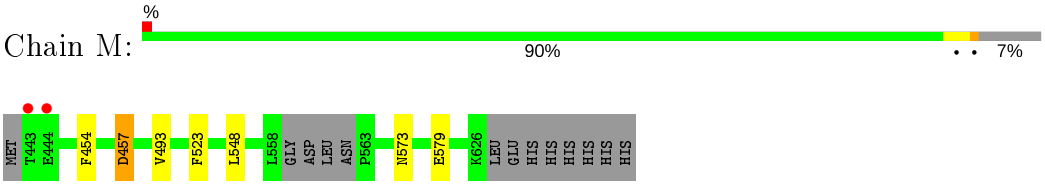
- Molecule 1: Nucleotide cyclase

Chain L:



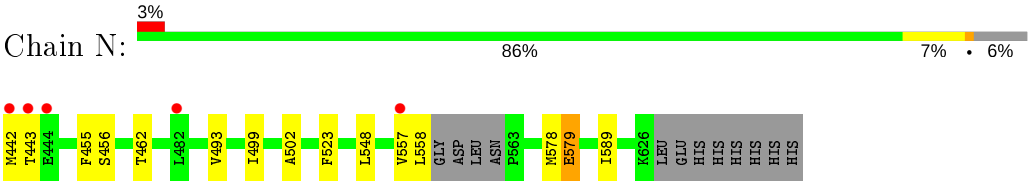
• Molecule 1: Nucleotide cyclase

Chain M:



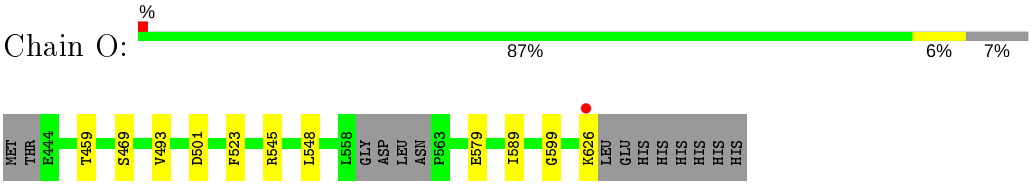
• Molecule 1: Nucleotide cyclase

Chain N:



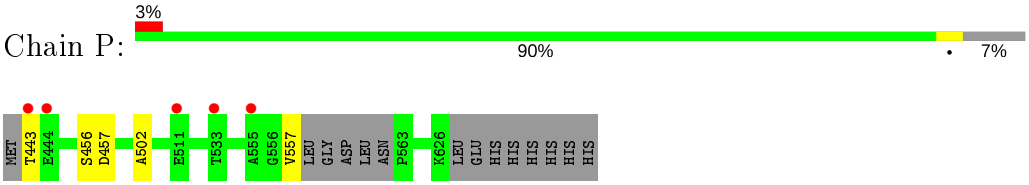
• Molecule 1: Nucleotide cyclase

Chain O:



• Molecule 1: Nucleotide cyclase

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	193.28Å 193.28Å 225.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.90 – 2.25 48.32 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.90-2.25) 99.8 (48.32-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.182 , 0.224 0.183 , 0.225	Depositor DCC
R_{free} test set	2100 reflections (1.08%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	24979	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8784e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, T99

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	0.42	0/1451	0.57	0/1968
1	B	0.50	0/1452	0.62	0/1969
1	C	0.44	0/1456	0.59	0/1973
1	D	0.51	0/1464	0.61	0/1983
1	E	0.38	0/1424	0.54	0/1934
1	F	0.42	0/1458	0.55	0/1977
1	G	0.46	0/1456	0.58	0/1975
1	H	0.53	0/1461	0.64	0/1980
1	I	0.38	0/1445	0.53	0/1959
1	J	0.44	0/1469	0.59	0/1990
1	K	0.40	0/1440	0.55	0/1954
1	L	0.50	0/1464	0.58	0/1983
1	M	0.42	0/1419	0.56	0/1923
1	N	0.37	0/1432	0.55	0/1938
1	O	0.38	0/1410	0.53	0/1911
1	P	0.36	0/1411	0.53	0/1912
All	All	0.44	0/23112	0.57	0/31329

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1423	0	1419	15	0
1	B	1424	0	1423	7	0
1	C	1428	0	1434	6	0
1	D	1436	0	1443	9	0
1	E	1396	0	1374	8	0
1	F	1430	0	1425	10	0
1	G	1428	0	1421	15	0
1	H	1433	0	1434	9	0
1	I	1414	0	1414	13	0
1	J	1438	0	1443	8	0
1	K	1412	0	1401	7	0
1	L	1436	0	1443	5	0
1	M	1392	0	1388	4	0
1	N	1405	0	1410	10	0
1	O	1383	0	1374	6	0
1	P	1384	0	1374	2	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
2	C	31	0	0	1	0
2	D	31	0	0	1	0
2	E	31	0	0	0	0
2	F	31	0	0	1	0
2	G	31	0	0	0	0
2	H	31	0	0	0	0
2	I	31	0	0	0	0
2	J	31	0	0	1	0
2	K	31	0	0	0	0
2	L	31	0	0	0	0
2	M	31	0	0	0	0
2	N	31	0	0	0	0
2	O	31	0	0	1	0
2	P	31	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	A	12	0	16	0	0
4	C	12	0	16	0	0
4	D	6	0	8	0	0
4	E	6	0	8	0	0
4	F	12	0	16	0	0
4	G	6	0	8	0	0
4	I	6	0	8	0	0
4	J	12	0	16	0	0
4	K	6	0	8	0	0
4	L	6	0	8	0	0
4	O	6	0	8	0	0
5	A	100	0	0	0	0
5	B	139	0	0	1	0
5	C	123	0	0	0	0
5	D	176	0	0	1	0
5	E	89	0	0	1	0
5	F	115	0	0	1	0
5	G	125	0	0	2	0
5	H	169	0	0	3	0
5	I	72	0	0	0	0
5	J	100	0	0	1	0
5	K	67	0	0	1	0
5	L	138	0	0	0	0
5	M	104	0	0	0	0
5	N	63	0	0	0	0
5	O	82	0	0	0	0
5	P	53	0	0	0	0
All	All	24979	0	22740	123	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 3.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:THR:HG22	1:A:444:GLU:HG3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:443:THR:HB	1:L:557:VAL:HB	1.69	0.74
1:I:462:THR:OG1	1:J:577:ARG:NH2	2.23	0.71
1:D:443:THR:OG1	1:D:557:VAL:HB	1.91	0.69
1:I:513:VAL:CG2	1:I:514:PRO:HD2	2.30	0.62
1:N:578:MET:HE2	1:N:589:ILE:C	2.21	0.61
1:I:513:VAL:HG22	1:I:514:PRO:HD2	1.84	0.60
1:G:613:GLY:O	5:G:801:HOH:O	2.16	0.60
1:F:442:MET:HE1	1:F:554:THR:HG22	1.83	0.59
1:N:442:MET:HG2	1:N:443:THR:H	1.67	0.59
1:J:606:LEU:HD11	1:J:621:TRP:CE2	2.38	0.58
2:J:703:T99:N3	5:J:801:HOH:O	2.32	0.58
1:D:564:HIS:ND1	5:D:803:HOH:O	2.32	0.57
1:A:558:LEU:HD12	1:A:566:ASP:HB3	1.86	0.57
1:I:558:LEU:HD12	1:I:566:ASP:HB3	1.86	0.57
1:A:442:MET:CE	1:A:554:THR:HG22	2.36	0.56
1:M:573:ASN:HB3	1:N:462:THR:HG22	1.87	0.56
1:C:457:ASP:OD2	1:C:579:GLU:OE2	2.24	0.55
1:G:442:MET:HG3	1:G:558:LEU:HG	1.88	0.55
1:N:442:MET:CG	1:N:443:THR:H	2.20	0.55
1:K:506:VAL:HB	1:K:567:LEU:HD11	1.89	0.54
1:I:611:VAL:HG23	1:I:614:LYS:HB2	1.89	0.54
1:H:442:MET:N	5:H:803:HOH:O	2.42	0.52
1:I:457:ASP:OD1	1:I:579:GLU:OE2	2.28	0.52
1:K:598:LYS:HE3	1:O:469:SER:HA	1.92	0.52
1:F:533:THR:HG23	5:F:861:HOH:O	2.09	0.52
1:E:470:THR:O	1:E:474:MET:HG3	2.09	0.52
1:N:443:THR:OG1	1:N:557:VAL:HG23	2.10	0.52
1:O:493:VAL:HG21	1:O:523:PHE:CG	2.45	0.52
1:D:442:MET:HG2	1:D:443:THR:N	2.25	0.52
1:N:548:LEU:HB2	1:N:589:ILE:HG22	1.92	0.52
1:A:442:MET:HE2	1:A:554:THR:HG22	1.92	0.51
1:D:442:MET:HG2	1:D:443:THR:H	1.75	0.51
1:A:442:MET:HB2	1:B:474:MET:CE	2.41	0.50
1:G:442:MET:CE	1:G:554:THR:HG22	2.42	0.50
1:O:501:ASP:OD1	2:O:701:T99:O2'	2.30	0.49
1:O:459:THR:HG22	1:O:545:ARG:HH11	1.77	0.49
1:P:443:THR:OG1	1:P:557:VAL:HG23	2.12	0.49
1:A:457:ASP:OD1	1:A:579:GLU:OE2	2.30	0.49
1:L:493:VAL:HG21	1:L:523:PHE:CG	2.48	0.49
1:G:442:MET:HE2	1:G:554:THR:HG22	1.95	0.49
1:N:493:VAL:HG21	1:N:523:PHE:CG	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:471:LYS:HA	1:F:474:MET:HE2	1.93	0.49
1:F:493:VAL:HG21	1:F:523:PHE:CG	2.48	0.48
1:I:548:LEU:HB2	1:I:589:ILE:HG22	1.96	0.48
1:B:493:VAL:HG21	1:B:523:PHE:CG	2.49	0.48
1:D:442:MET:CG	1:D:443:THR:H	2.25	0.48
1:O:548:LEU:HB2	1:O:589:ILE:HG22	1.95	0.48
1:G:474:MET:SD	1:H:442:MET:HE1	2.55	0.47
1:H:617:MET:HB3	5:H:872:HOH:O	2.15	0.47
1:C:454:PHE:HA	1:C:548:LEU:HD23	1.97	0.47
1:G:457:ASP:OD2	1:G:579:GLU:OE2	2.33	0.47
1:E:558:LEU:HD12	1:E:566:ASP:HB3	1.98	0.46
1:A:573:ASN:HB3	1:B:462:THR:HG22	1.96	0.46
1:H:493:VAL:HG21	1:H:523:PHE:CG	2.51	0.46
1:J:468:THR:HG22	1:J:469:SER:O	2.15	0.46
1:N:442:MET:HG3	1:N:558:LEU:HD23	1.97	0.46
1:C:545:ARG:HH22	2:C:702:T99:PG	2.39	0.46
1:E:545:ARG:HD3	1:E:579:GLU:O	2.16	0.46
1:G:513:VAL:HG22	1:G:514:PRO:HD2	1.97	0.46
1:G:442:MET:HE3	1:G:445:ALA:HA	1.97	0.46
1:F:442:MET:CE	1:F:554:THR:HG22	2.46	0.45
1:I:555:ALA:HB1	1:I:565:TRP:CZ2	2.51	0.45
1:K:455:PHE:CZ	1:K:504:LEU:HD13	2.52	0.45
1:K:443:THR:OG1	1:K:557:VAL:HG23	2.17	0.45
1:J:493:VAL:HG21	1:J:523:PHE:CG	2.52	0.45
1:E:497:LYS:HE3	2:F:702:T99:N1	2.32	0.45
1:J:471:LYS:HA	1:J:474:MET:HE2	1.98	0.45
1:O:599:GLY:O	1:O:626:LYS:HD3	2.17	0.45
1:B:564:HIS:ND1	5:B:801:HOH:O	2.35	0.44
1:C:497:LYS:HD2	1:C:499:ILE:HD11	1.99	0.44
1:M:457:ASP:OD1	1:M:579:GLU:OE2	2.35	0.44
1:A:462:THR:HG22	1:B:573:ASN:HB3	2.00	0.44
1:D:442:MET:CG	1:D:443:THR:N	2.81	0.43
1:E:493:VAL:HG21	1:E:523:PHE:CG	2.53	0.43
1:E:548:LEU:HB2	1:E:589:ILE:HG22	1.99	0.43
1:H:616:LYS:HB2	1:L:616:LYS:HB2	2.00	0.43
5:E:866:HOH:O	1:F:462:THR:HG23	2.19	0.43
1:L:457:ASP:OD1	1:L:579:GLU:OE2	2.37	0.43
1:G:558:LEU:HD12	1:G:566:ASP:HB3	2.00	0.43
1:F:471:LYS:HD3	1:F:474:MET:HE3	2.01	0.43
1:H:442:MET:HB3	1:H:442:MET:HE2	1.63	0.42
1:N:455:PHE:HB3	1:N:579:GLU:HG3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:535:LYS:HD3	1:H:535:LYS:HA	1.81	0.42
1:I:455:PHE:CZ	1:I:504:LEU:HD13	2.55	0.42
1:A:545:ARG:HD3	1:A:579:GLU:O	2.18	0.42
1:G:442:MET:CG	1:G:443:THR:H	2.32	0.42
1:I:573:ASN:HB3	1:J:462:THR:HG22	2.02	0.42
1:M:454:PHE:HA	1:M:548:LEU:HD23	2.01	0.42
1:G:442:MET:HG2	1:G:443:THR:H	1.84	0.42
1:A:493:VAL:HG21	1:A:523:PHE:CG	2.55	0.42
1:J:548:LEU:HD12	1:J:589:ILE:HG22	2.02	0.42
1:K:545:ARG:HD3	1:K:579:GLU:O	2.18	0.42
1:D:461:PHE:HB3	2:D:701:T99:O2B	2.20	0.41
1:G:545:ARG:HD3	1:G:579:GLU:O	2.19	0.41
1:A:442:MET:HE3	1:A:445:ALA:HA	2.02	0.41
1:B:456:SER:O	1:B:502:ALA:HA	2.19	0.41
1:C:573:ASN:HB3	1:D:462:THR:HG22	2.03	0.41
1:P:456:SER:O	1:P:502:ALA:HA	2.21	0.41
1:C:548:LEU:HB2	1:C:589:ILE:HG22	2.02	0.41
1:H:625:ARG:NH2	5:H:806:HOH:O	2.53	0.41
1:I:545:ARG:NH1	1:I:580:SER:HA	2.35	0.41
1:M:493:VAL:HG21	1:M:523:PHE:CG	2.56	0.41
1:A:467:ARG:HH22	1:A:540:GLU:CD	2.24	0.41
1:A:474:MET:SD	1:B:568:VAL:HG21	2.61	0.41
1:I:495:LYS:HG3	1:I:503:TYR:CE2	2.55	0.41
1:I:513:VAL:HG23	1:I:514:PRO:HD2	2.03	0.41
1:K:521:VAL:HG21	1:K:597:ILE:HG21	2.02	0.41
1:E:454:PHE:HA	1:E:548:LEU:HD23	2.02	0.41
1:F:606:LEU:HD11	1:F:621:TRP:CE2	2.55	0.41
1:F:611:VAL:HB	1:F:614:LYS:HB2	2.03	0.41
1:G:562:ASN:HB2	5:G:908:HOH:O	2.21	0.41
1:N:456:SER:O	1:N:502:ALA:HA	2.21	0.41
1:E:462:THR:HG22	1:F:573:ASN:HB3	2.02	0.41
1:A:442:MET:HG3	1:A:557:VAL:O	2.21	0.41
1:G:559:GLY:O	1:G:561:LEU:N	2.49	0.41
1:G:548:LEU:HB2	1:G:589:ILE:HG22	2.02	0.40
1:H:454:PHE:HA	1:H:548:LEU:HD23	2.03	0.40
1:K:529:GLU:HG2	5:K:830:HOH:O	2.21	0.40
1:A:442:MET:HE1	1:A:554:THR:HG22	2.01	0.40
1:J:454:PHE:HA	1:J:548:LEU:HD23	2.03	0.40
1:D:493:VAL:HG21	1:D:523:PHE:CG	2.56	0.40
1:L:548:LEU:HB2	1:L:589:ILE:HG22	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	182/193 (94%)	180 (99%)	2 (1%)	0	100	100
1	B	182/193 (94%)	178 (98%)	4 (2%)	0	100	100
1	C	182/193 (94%)	180 (99%)	2 (1%)	0	100	100
1	D	183/193 (95%)	178 (97%)	5 (3%)	0	100	100
1	E	180/193 (93%)	179 (99%)	1 (1%)	0	100	100
1	F	183/193 (95%)	180 (98%)	3 (2%)	0	100	100
1	G	183/193 (95%)	180 (98%)	3 (2%)	0	100	100
1	H	183/193 (95%)	178 (97%)	5 (3%)	0	100	100
1	I	181/193 (94%)	179 (99%)	2 (1%)	0	100	100
1	J	184/193 (95%)	182 (99%)	2 (1%)	0	100	100
1	K	181/193 (94%)	176 (97%)	5 (3%)	0	100	100
1	L	183/193 (95%)	178 (97%)	5 (3%)	0	100	100
1	M	176/193 (91%)	172 (98%)	4 (2%)	0	100	100
1	N	177/193 (92%)	175 (99%)	2 (1%)	0	100	100
1	O	175/193 (91%)	172 (98%)	3 (2%)	0	100	100
1	P	175/193 (91%)	173 (99%)	2 (1%)	0	100	100
All	All	2890/3088 (94%)	2840 (98%)	50 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	155/165 (94%)	153 (99%)	2 (1%)	69	76
1	B	155/165 (94%)	152 (98%)	3 (2%)	57	64
1	C	156/165 (94%)	155 (99%)	1 (1%)	86	90
1	D	157/165 (95%)	156 (99%)	1 (1%)	86	90
1	E	150/165 (91%)	149 (99%)	1 (1%)	84	88
1	F	155/165 (94%)	154 (99%)	1 (1%)	86	90
1	G	155/165 (94%)	153 (99%)	2 (1%)	69	76
1	H	156/165 (94%)	154 (99%)	2 (1%)	69	76
1	I	154/165 (93%)	153 (99%)	1 (1%)	86	90
1	J	157/165 (95%)	155 (99%)	2 (1%)	69	76
1	K	153/165 (93%)	151 (99%)	2 (1%)	69	76
1	L	157/165 (95%)	156 (99%)	1 (1%)	86	90
1	M	151/165 (92%)	150 (99%)	1 (1%)	84	88
1	N	153/165 (93%)	151 (99%)	2 (1%)	69	76
1	O	149/165 (90%)	148 (99%)	1 (1%)	84	88
1	P	149/165 (90%)	148 (99%)	1 (1%)	84	88
All	All	2462/2640 (93%)	2438 (99%)	24 (1%)	76	82

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	442	MET
1	A	457	ASP
1	B	457	ASP
1	B	625	ARG
1	B	626	LYS
1	C	457	ASP
1	D	457	ASP
1	E	457	ASP
1	F	457	ASP
1	G	457	ASP
1	G	499	ILE
1	H	457	ASP
1	H	499	ILE
1	I	560	ASP
1	J	457	ASP
1	J	579	GLU

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Mol	Chain	Res	Type
1	K	499	ILE
1	K	579	GLU
1	L	457	ASP
1	M	457	ASP
1	N	499	ILE
1	N	579	GLU
1	O	579	GLU
1	P	457	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	618	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 47 ligands modelled in this entry, 16 are monoatomic - leaving 31 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	G	703	-	5,5,5	0.39	0	5,5,5	0.44	0
4	GOL	C	704	-	5,5,5	0.42	0	5,5,5	0.46	0
2	T99	C	702	3	24,33,33	0.81	0	29,52,52	1.07	2 (6%)
2	T99	K	701	3	24,33,33	0.78	0	29,52,52	0.94	2 (6%)
4	GOL	O	703	-	5,5,5	0.38	0	5,5,5	0.28	0
2	T99	F	702	3	24,33,33	0.81	1 (4%)	29,52,52	0.98	2 (6%)
4	GOL	I	701	-	5,5,5	0.31	0	5,5,5	0.39	0
4	GOL	E	703	-	5,5,5	0.41	0	5,5,5	0.38	0
2	T99	G	701	3	24,33,33	0.93	1 (4%)	29,52,52	1.15	2 (6%)
4	GOL	D	702	-	5,5,5	0.39	0	5,5,5	0.53	0
2	T99	O	701	3	24,33,33	0.83	0	29,52,52	1.02	2 (6%)
2	T99	P	701	3	24,33,33	0.89	2 (8%)	29,52,52	1.04	2 (6%)
2	T99	H	701	3	24,33,33	0.94	1 (4%)	29,52,52	0.95	2 (6%)
4	GOL	J	702	-	5,5,5	0.40	0	5,5,5	0.42	0
2	T99	J	703	3	24,33,33	0.82	0	29,52,52	1.12	3 (10%)
2	T99	B	701	3	24,33,33	1.11	1 (4%)	29,52,52	0.98	2 (6%)
2	T99	D	701	3	24,33,33	0.94	1 (4%)	29,52,52	0.99	2 (6%)
4	GOL	A	704	-	5,5,5	0.36	0	5,5,5	0.32	0
2	T99	N	701	3	24,33,33	0.85	1 (4%)	29,52,52	1.03	2 (6%)
2	T99	A	701	3	24,33,33	0.92	1 (4%)	29,52,52	1.04	2 (6%)
4	GOL	F	701	-	5,5,5	0.43	0	5,5,5	0.47	0
4	GOL	L	701	-	5,5,5	0.40	0	5,5,5	0.48	0
2	T99	I	702	3	24,33,33	0.79	0	29,52,52	0.95	2 (6%)
4	GOL	J	701	-	5,5,5	0.36	0	5,5,5	0.38	0
2	T99	E	701	3	24,33,33	1.02	1 (4%)	29,52,52	0.96	2 (6%)
4	GOL	F	703	-	5,5,5	0.34	0	5,5,5	0.44	0
2	T99	L	702	3	24,33,33	1.08	1 (4%)	29,52,52	0.93	2 (6%)
2	T99	M	701	3	24,33,33	0.80	0	29,52,52	1.03	2 (6%)
4	GOL	K	703	-	5,5,5	0.36	0	5,5,5	0.43	0
4	GOL	C	701	-	5,5,5	0.41	0	5,5,5	0.34	0
4	GOL	A	703	-	5,5,5	0.47	0	5,5,5	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	G	703	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	704	-	-	0/4/4/4	-
2	T99	C	702	3	-	3/14/38/38	0/3/3/3
2	T99	K	701	3	-	3/14/38/38	0/3/3/3
4	GOL	O	703	-	-	1/4/4/4	-
2	T99	F	702	3	-	7/14/38/38	0/3/3/3
4	GOL	I	701	-	-	0/4/4/4	-
4	GOL	E	703	-	-	0/4/4/4	-
2	T99	G	701	3	-	5/14/38/38	0/3/3/3
4	GOL	D	702	-	-	0/4/4/4	-
2	T99	O	701	3	-	3/14/38/38	0/3/3/3
2	T99	P	701	3	-	4/14/38/38	0/3/3/3
2	T99	H	701	3	-	4/14/38/38	0/3/3/3
4	GOL	J	702	-	-	2/4/4/4	-
2	T99	J	703	3	-	8/14/38/38	0/3/3/3
2	T99	B	701	3	-	2/14/38/38	0/3/3/3
2	T99	D	701	3	-	5/14/38/38	0/3/3/3
4	GOL	A	704	-	-	0/4/4/4	-
2	T99	N	701	3	-	6/14/38/38	0/3/3/3
2	T99	A	701	3	-	4/14/38/38	0/3/3/3
4	GOL	F	701	-	-	0/4/4/4	-
4	GOL	L	701	-	-	0/4/4/4	-
2	T99	I	702	3	-	5/14/38/38	0/3/3/3
4	GOL	J	701	-	-	0/4/4/4	-
2	T99	E	701	3	-	3/14/38/38	0/3/3/3
4	GOL	F	703	-	-	0/4/4/4	-
2	T99	L	702	3	-	3/14/38/38	0/3/3/3
2	T99	M	701	3	-	5/14/38/38	0/3/3/3
4	GOL	K	703	-	-	1/4/4/4	-
4	GOL	C	701	-	-	0/4/4/4	-
4	GOL	A	703	-	-	0/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	T99	PA-O5'	4.50	1.65	1.57
2	L	702	T99	PA-O5'	4.18	1.64	1.57
2	E	701	T99	PA-O5'	3.85	1.64	1.57
2	D	701	T99	PA-O5'	3.23	1.63	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	701	T99	PA-O5'	2.64	1.62	1.57
2	N	701	T99	PB-O2B	-2.37	1.44	1.55
2	A	701	T99	PA-O5'	2.31	1.61	1.57
2	G	701	T99	PB-O2B	-2.20	1.45	1.55
2	F	702	T99	PB-O2B	-2.11	1.45	1.55
2	P	701	T99	PB-O2B	-2.04	1.45	1.55
2	P	701	T99	PG-O1A	2.03	1.57	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	T99	PA-O5'-C5'	3.59	131.51	120.16
2	M	701	T99	PA-O5'-C5'	3.56	131.41	120.16
2	O	701	T99	PA-O5'-C5'	3.36	130.78	120.16
2	G	701	T99	PA-O5'-C5'	3.32	130.65	120.16
2	P	701	T99	PA-O5'-C5'	3.20	130.26	120.16
2	F	702	T99	PA-O5'-C5'	3.10	129.97	120.16
2	C	702	T99	PA-O5'-C5'	3.10	129.94	120.16
2	L	702	T99	PA-O5'-C5'	2.98	129.59	120.16
2	E	701	T99	PA-O5'-C5'	2.92	129.40	120.16
2	N	701	T99	PA-O5'-C5'	2.79	128.98	120.16
2	A	701	T99	C5-C6-N6	2.71	124.47	120.35
2	A	701	T99	PA-O5'-C5'	2.66	128.56	120.16
2	E	701	T99	C5-C6-N6	2.64	124.36	120.35
2	H	701	T99	PA-O5'-C5'	2.62	128.43	120.16
2	H	701	T99	C5-C6-N6	2.52	124.18	120.35
2	I	702	T99	PA-O5'-C5'	2.52	128.12	120.16
2	M	701	T99	C5-C6-N6	2.52	124.18	120.35
2	L	702	T99	C5-C6-N6	2.49	124.14	120.35
2	D	701	T99	C5-C6-N6	2.46	124.10	120.35
2	K	701	T99	C5-C6-N6	2.43	124.05	120.35
2	B	701	T99	C5-C6-N6	2.41	124.02	120.35
2	F	702	T99	C5-C6-N6	2.38	123.98	120.35
2	C	702	T99	C5-C6-N6	2.35	123.92	120.35
2	K	701	T99	PA-O5'-C5'	2.34	127.55	120.16
2	P	701	T99	C5-C6-N6	2.32	123.88	120.35
2	J	703	T99	PA-O5'-C5'	2.32	127.50	120.16
2	I	702	T99	C5-C6-N6	2.31	123.86	120.35
2	J	703	T99	C5-C6-N6	2.30	123.85	120.35
2	N	701	T99	C5-C6-N6	2.27	123.80	120.35
2	O	701	T99	C5-C6-N6	2.24	123.75	120.35
2	G	701	T99	C5-C6-N6	2.22	123.73	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	701	T99	PA-O5'-C5'	2.05	126.65	120.16
2	J	703	T99	C3'-C2'-C1'	-2.01	97.96	100.98

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	701	T99	C4'-C5'-O5'-PA
2	F	702	T99	PB-O3B-PG-O3G
2	B	701	T99	C4'-C5'-O5'-PA
2	D	701	T99	C4'-C5'-O5'-PA
2	H	701	T99	C4'-C5'-O5'-PA
2	N	701	T99	PB-O3B-PG-O3G
2	A	701	T99	C4'-C5'-O5'-PA
2	I	702	T99	PB-O3B-PG-O3G
2	J	703	T99	PB-O3B-PG-O3G
2	E	701	T99	C4'-C5'-O5'-PA
2	L	702	T99	C4'-C5'-O5'-PA
2	M	701	T99	PB-O3B-PG-O3G
2	M	701	T99	C4'-C5'-O5'-PA
2	F	702	T99	C4'-C5'-O5'-PA
2	J	703	T99	C4'-C5'-O5'-PA
2	I	702	T99	C5'-O5'-PA-O2A
2	O	701	T99	C5'-O5'-PA-O2A
2	D	701	T99	PA-O3A-PB-O1B
2	G	701	T99	C5'-O5'-PA-O2A
2	P	701	T99	C5'-O5'-PA-O2A
2	N	701	T99	C5'-O5'-PA-O2A
2	O	701	T99	C4'-C5'-O5'-PA
2	N	701	T99	C4'-C5'-O5'-PA
2	C	702	T99	C5'-O5'-PA-O2A
2	I	702	T99	PB-O3B-PG-O1A
2	M	701	T99	PB-O3B-PG-O1A
2	M	701	T99	C5'-O5'-PA-O2A
2	P	701	T99	C4'-C5'-O5'-PA
2	J	703	T99	C5'-O5'-PA-O2A
2	F	702	T99	C5'-O5'-PA-O2A
2	D	701	T99	C5'-O5'-PA-O2A
2	I	702	T99	O4'-C4'-C5'-O5'
2	F	702	T99	PG-O3B-PB-O2B
2	K	701	T99	C5'-O5'-PA-O2A
2	C	702	T99	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
2	G	701	T99	C4'-C5'-O5'-PA
2	F	702	T99	PA-O3A-PB-O1B
2	J	703	T99	PA-O3A-PB-O2B
2	I	702	T99	C4'-C5'-O5'-PA
2	P	701	T99	PG-O3B-PB-O2B
2	J	703	T99	PG-O3B-PB-O1B
4	J	702	GOL	C1-C2-C3-O3
2	A	701	T99	C5'-O5'-PA-O2A
2	E	701	T99	C5'-O5'-PA-O2A
2	P	701	T99	O4'-C4'-C5'-O5'
2	L	702	T99	C5'-O5'-PA-O2A
2	D	701	T99	PG-O3B-PB-O2B
4	J	702	GOL	O1-C1-C2-C3
2	D	701	T99	O4'-C4'-C5'-O5'
2	A	701	T99	O4'-C4'-C5'-O5'
2	E	701	T99	O4'-C4'-C5'-O5'
2	N	701	T99	PB-O3B-PG-O2G
2	J	703	T99	PB-O3B-PG-O2G
2	K	701	T99	O4'-C4'-C5'-O5'
2	F	702	T99	O4'-C4'-C5'-O5'
2	O	701	T99	O4'-C4'-C5'-O5'
2	B	701	T99	O4'-C4'-C5'-O5'
2	H	701	T99	O4'-C4'-C5'-O5'
2	J	703	T99	O4'-C4'-C5'-O5'
2	L	702	T99	O4'-C4'-C5'-O5'
2	M	701	T99	O4'-C4'-C5'-O5'
2	F	702	T99	PG-O3B-PB-O1B
2	G	701	T99	PG-O3B-PB-O1B
2	G	701	T99	PG-O3B-PB-O2B
2	H	701	T99	PG-O3B-PB-O2B
2	N	701	T99	PG-O3B-PB-O1B
2	A	701	T99	PG-O3B-PB-O2B
4	O	703	GOL	O1-C1-C2-C3
4	K	703	GOL	O1-C1-C2-C3
2	H	701	T99	C5'-O5'-PA-O2A
2	C	702	T99	O4'-C4'-C5'-O5'
2	G	701	T99	O4'-C4'-C5'-O5'
2	N	701	T99	O4'-C4'-C5'-O5'
2	J	703	T99	PB-O3B-PG-O1A

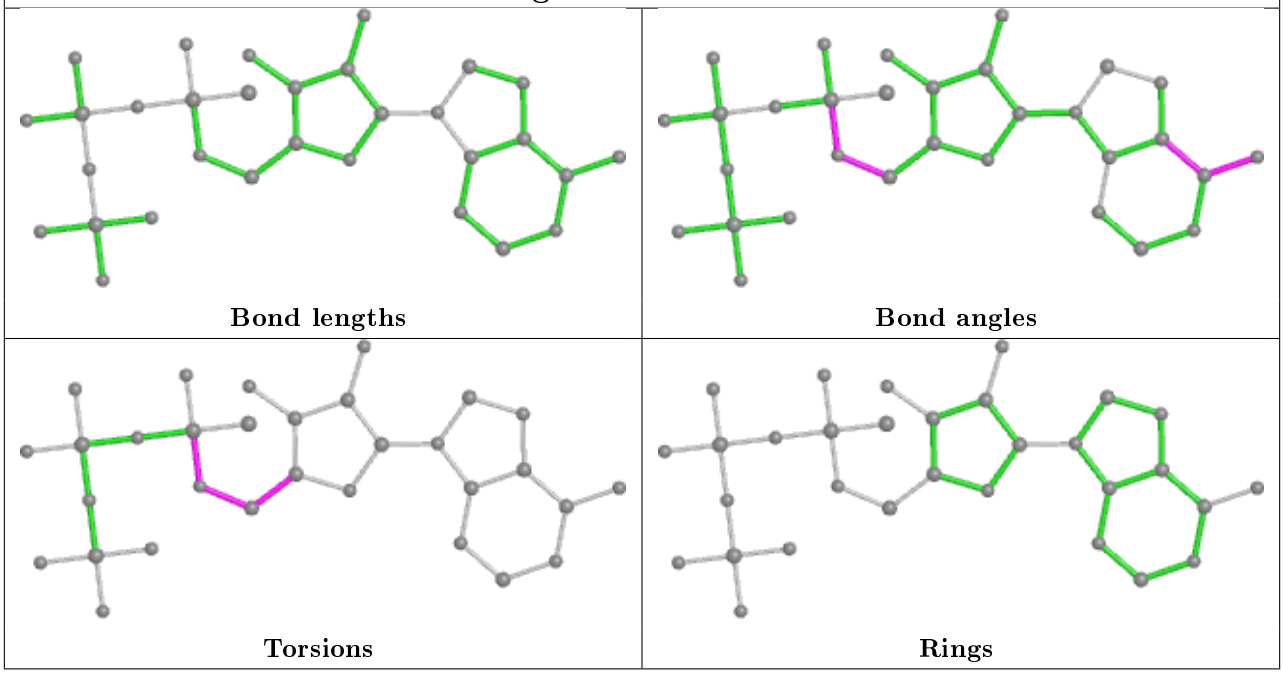
There are no ring outliers.

5 monomers are involved in 5 short contacts:

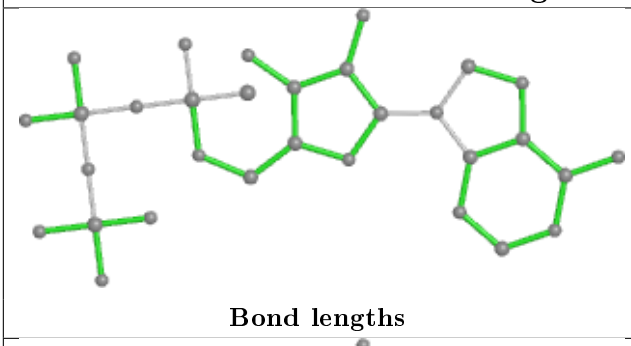
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	702	T99	1	0
2	F	702	T99	1	0
2	O	701	T99	1	0
2	J	703	T99	1	0
2	D	701	T99	1	0

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.

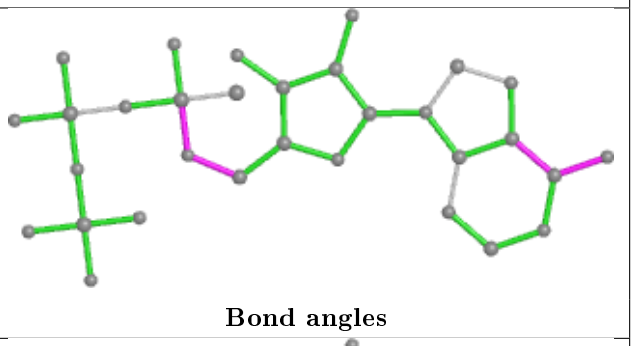
Ligand T99 C 702



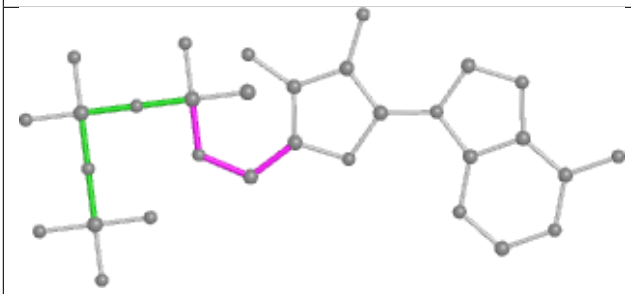
Ligand T99 K 701



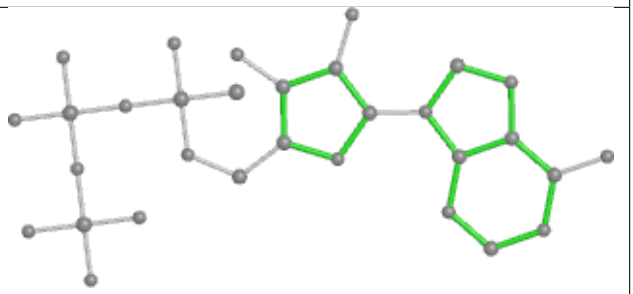
Bond lengths



Bond angles

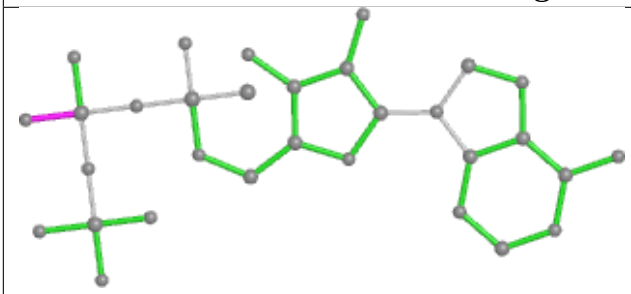


Torsions

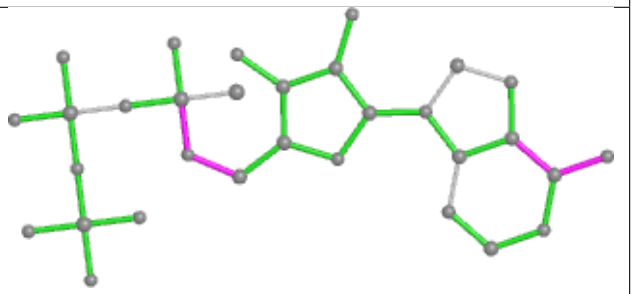


Rings

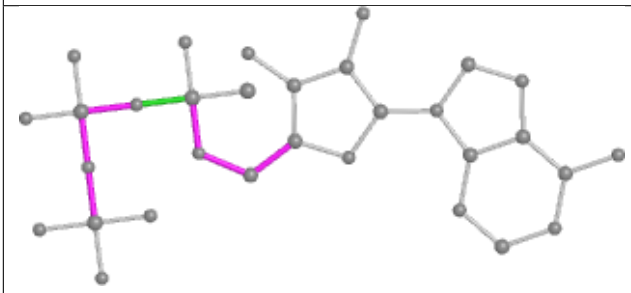
Ligand T99 F 702



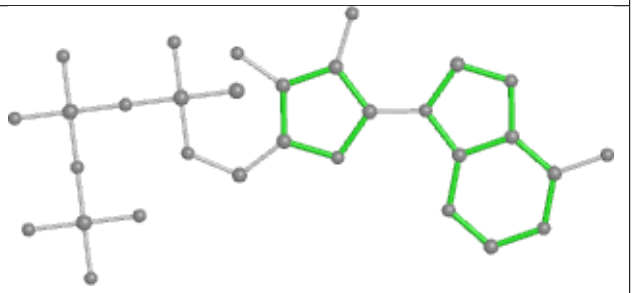
Bond lengths



Bond angles

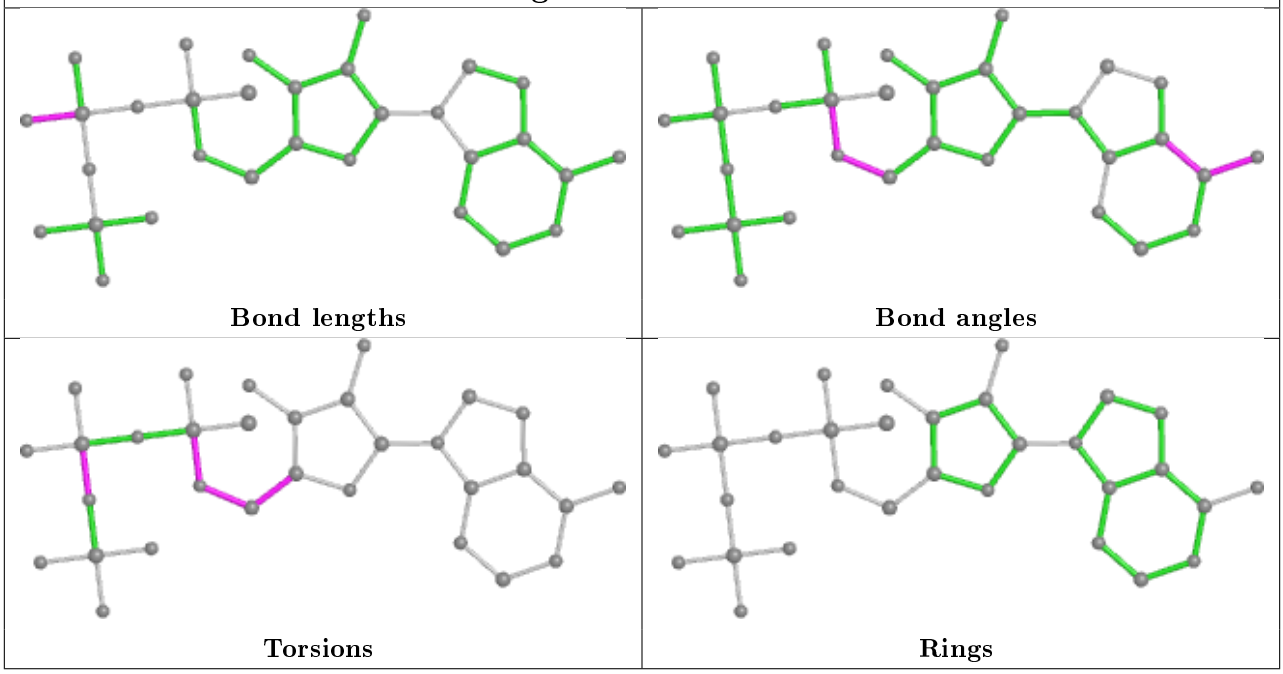


Torsions

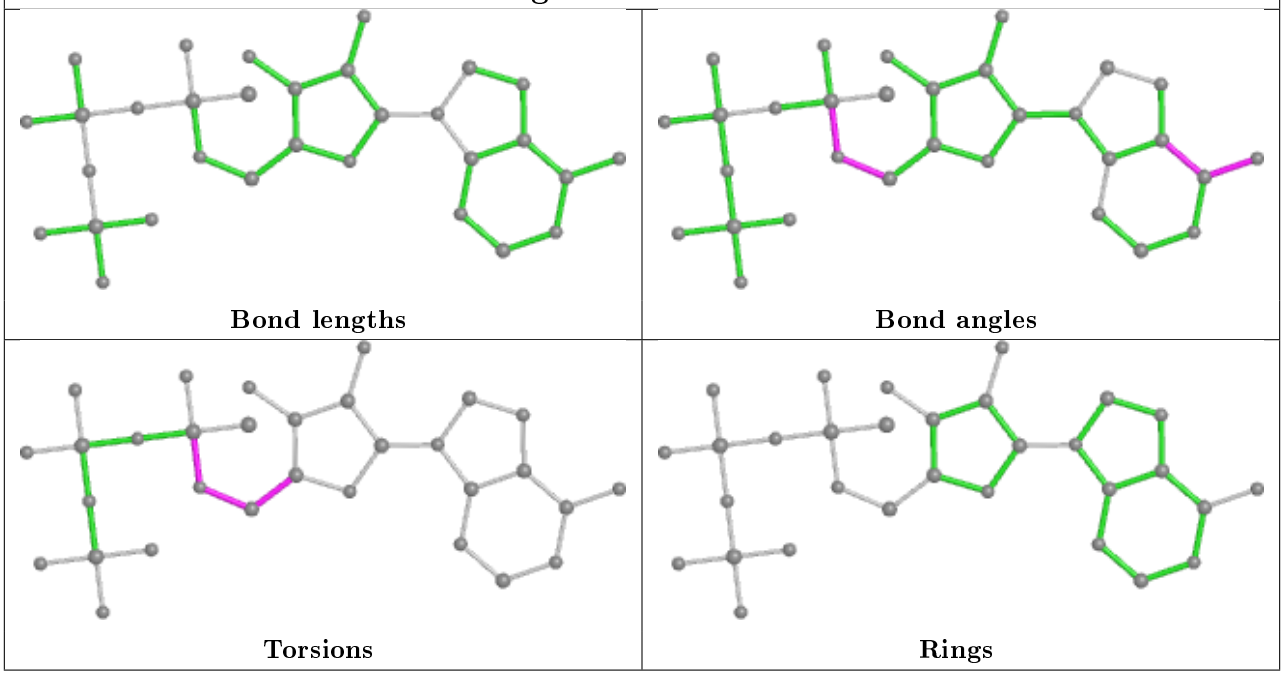


Rings

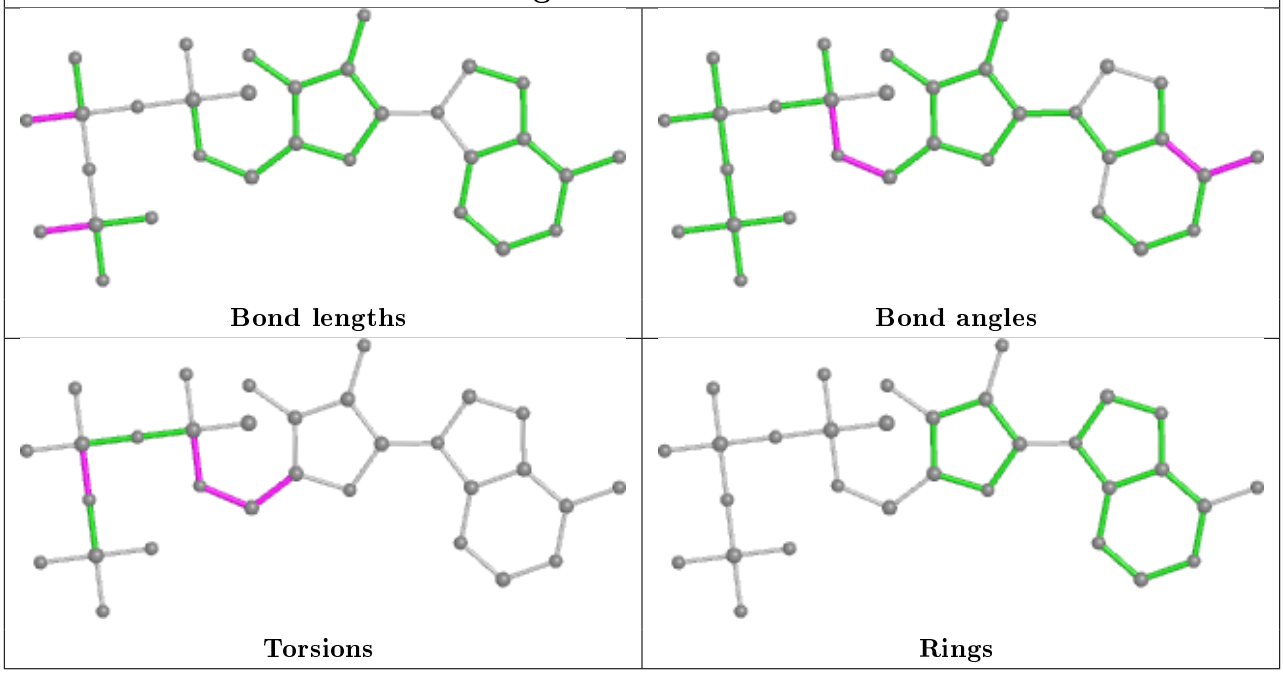
Ligand T99 G 701



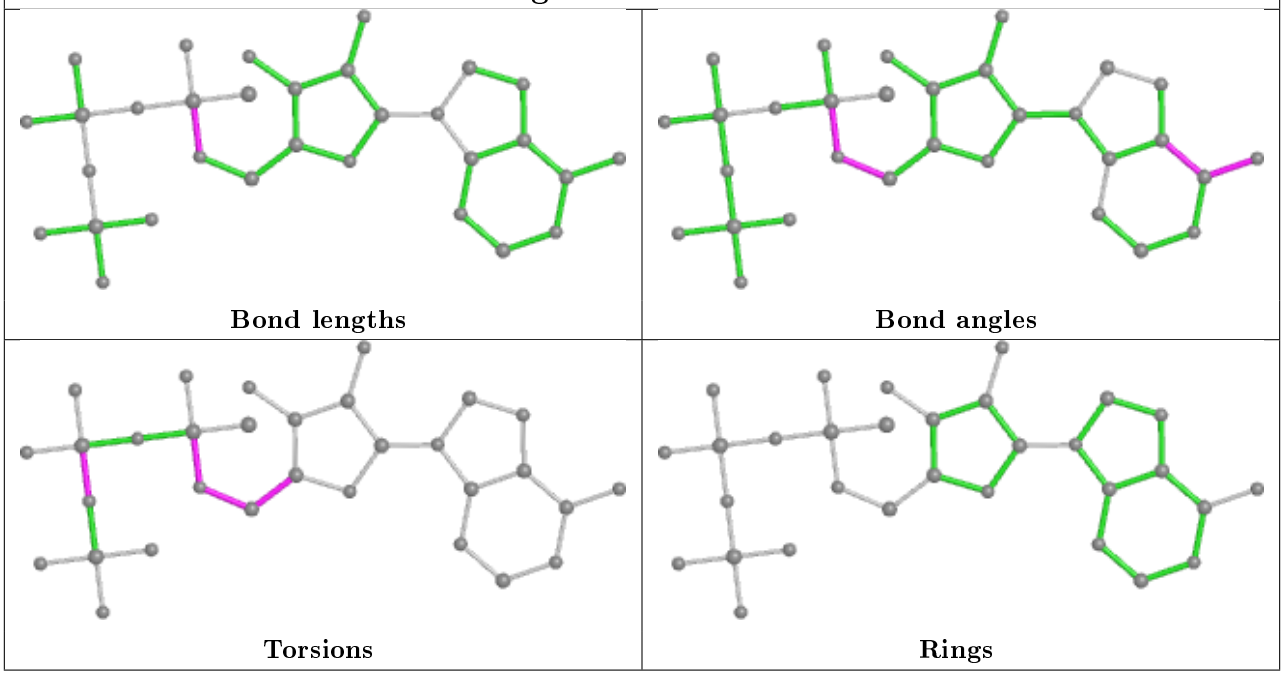
Ligand T99 O 701



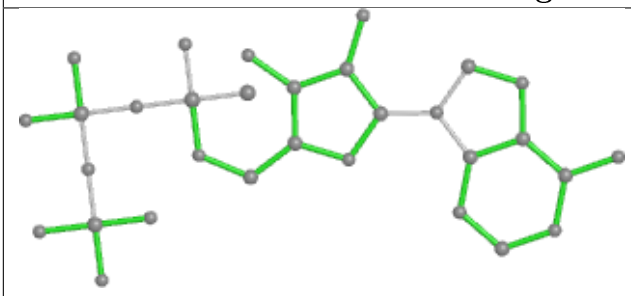
Ligand T99 P 701



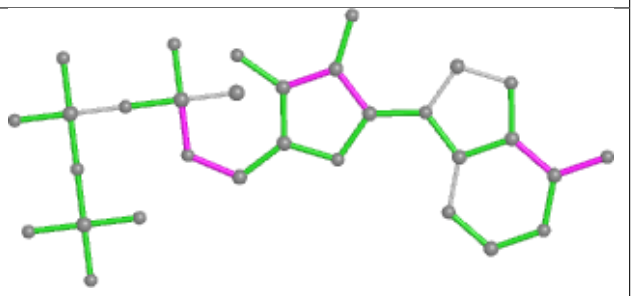
Ligand T99 H 701



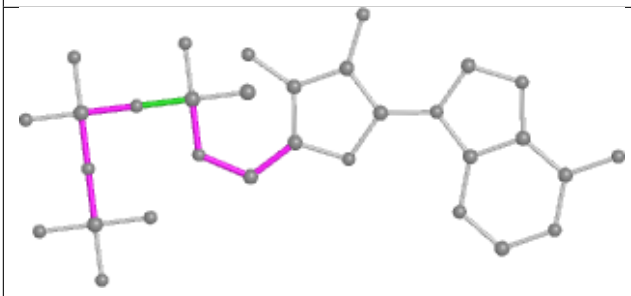
Ligand T99 J 703



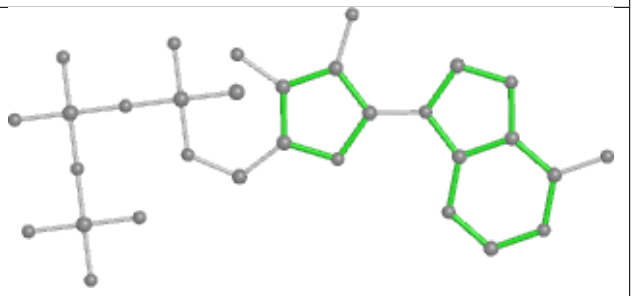
Bond lengths



Bond angles

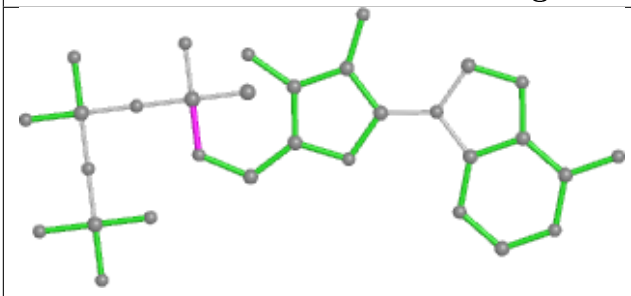


Torsions

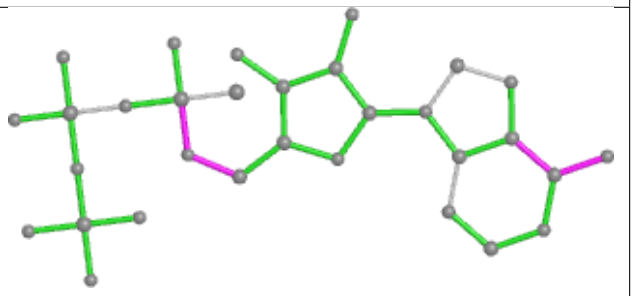


Rings

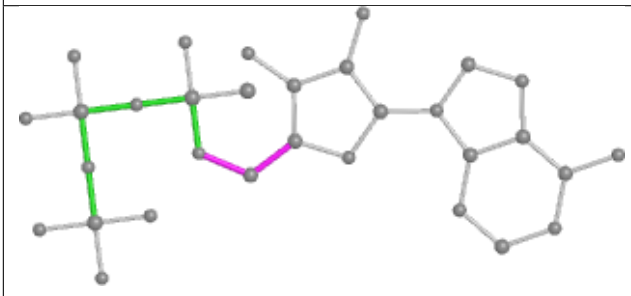
Ligand T99 B 701



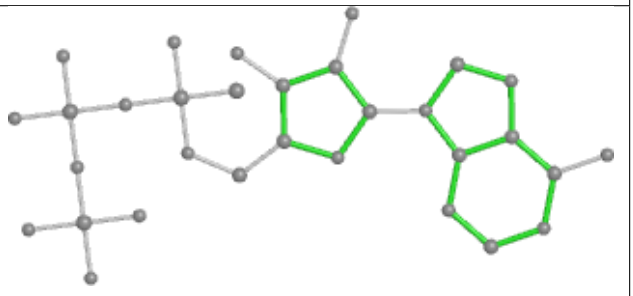
Bond lengths



Bond angles

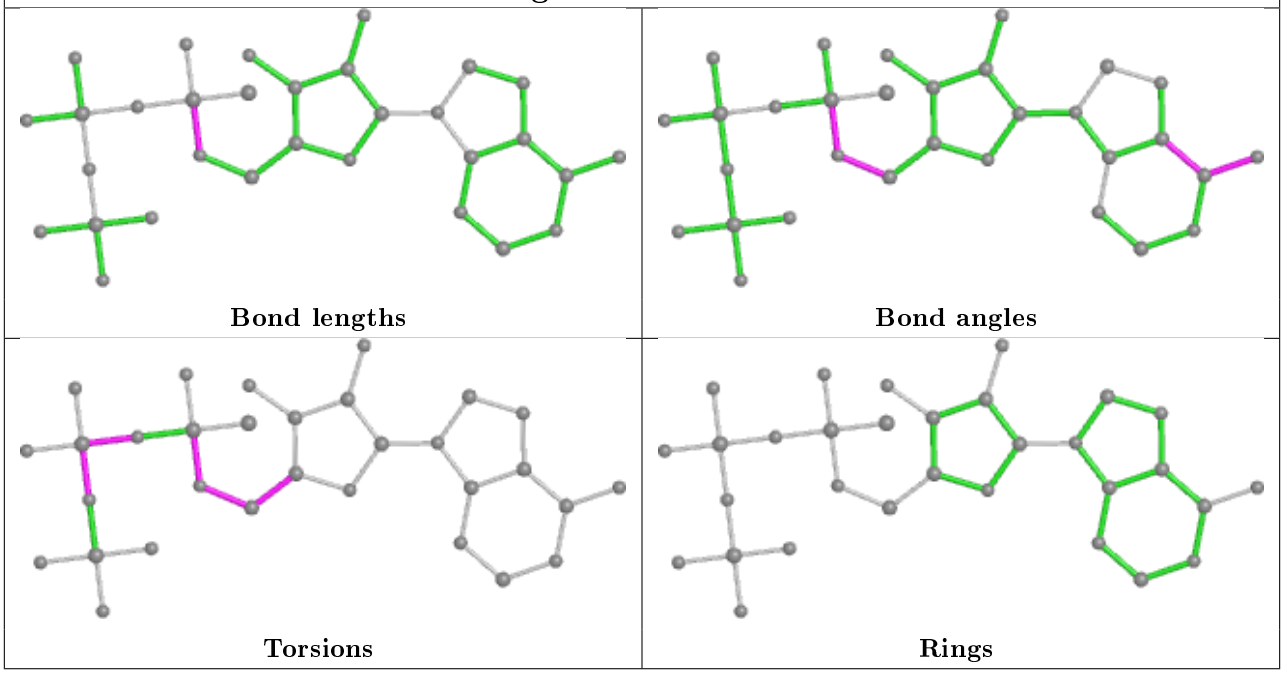


Torsions

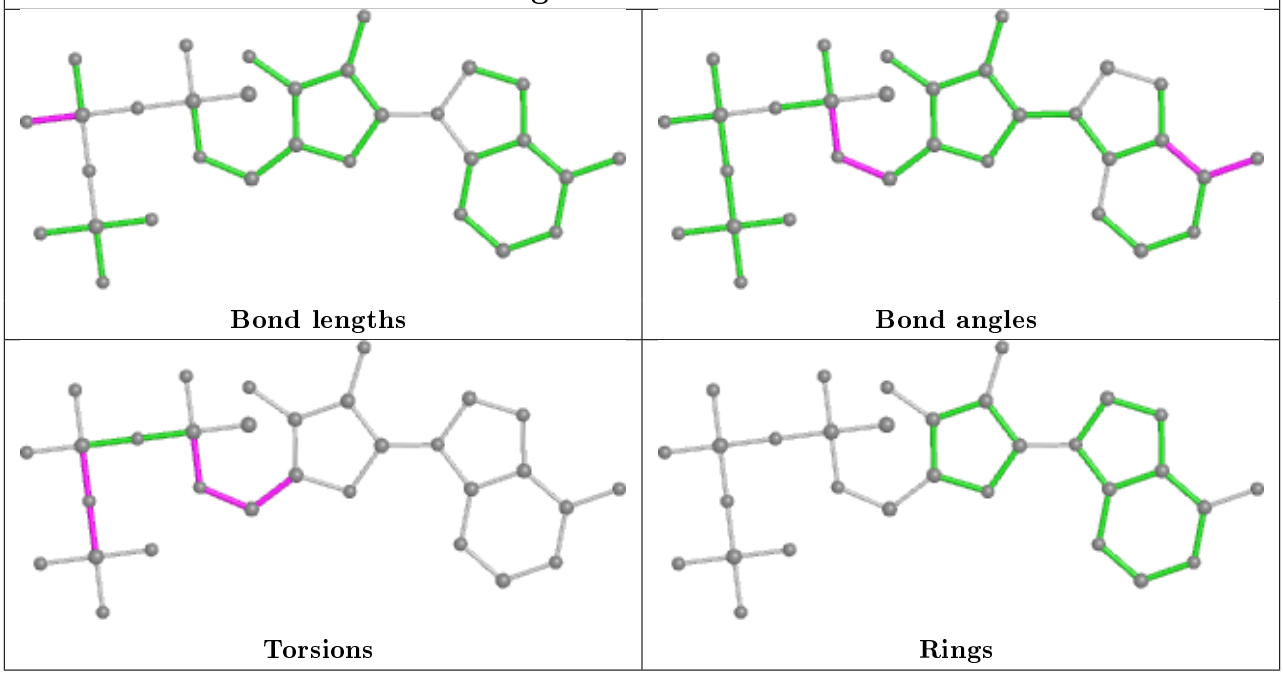


Rings

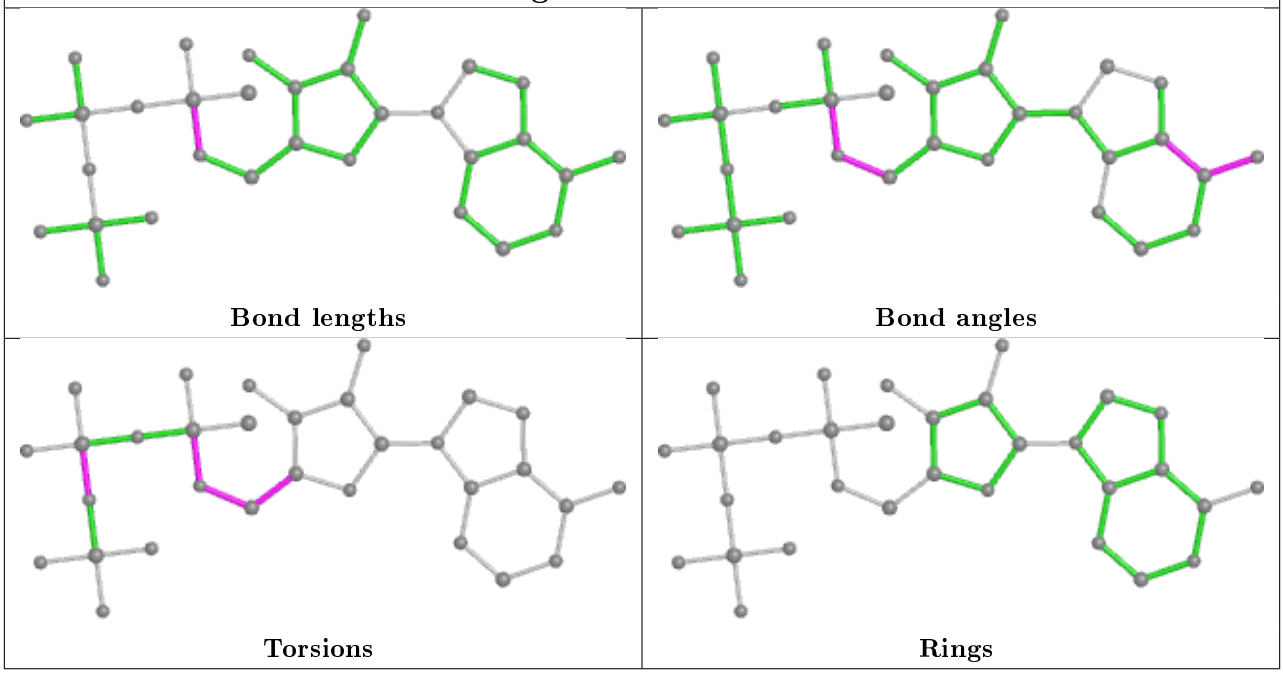
Ligand T99 D 701



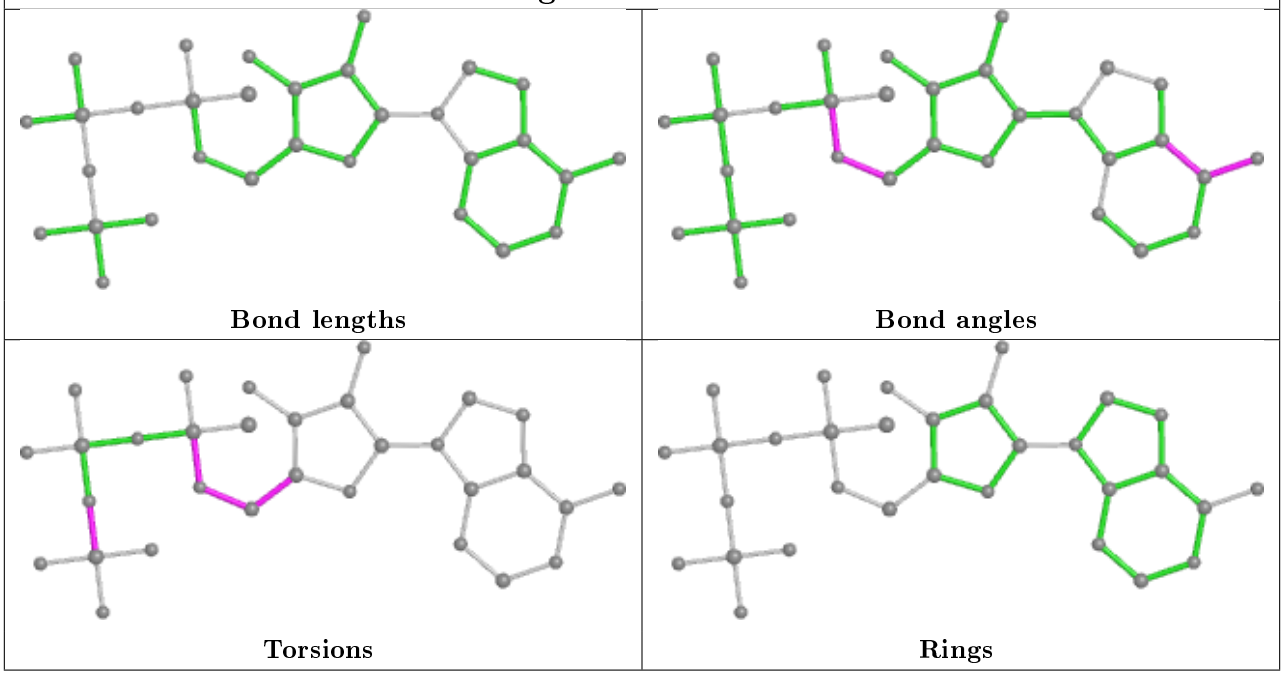
Ligand T99 N 701



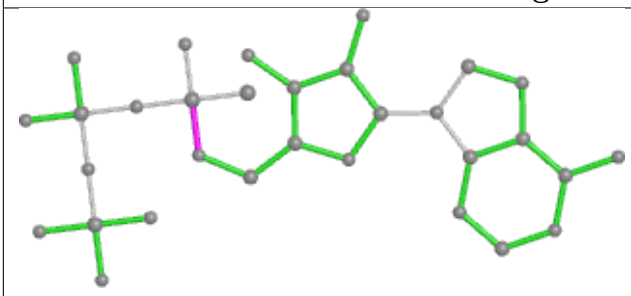
Ligand T99 A 701



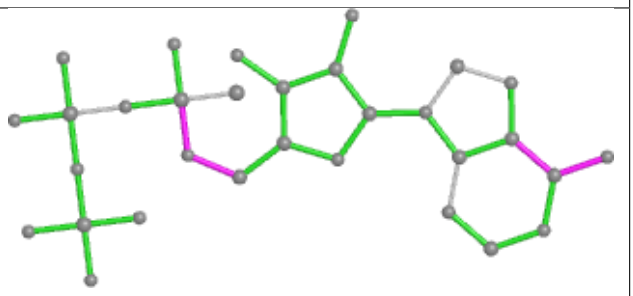
Ligand T99 I 702



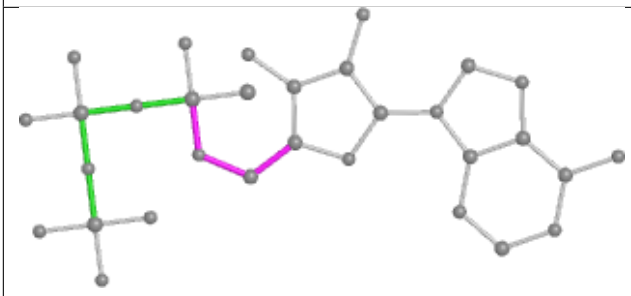
Ligand T99 E 701



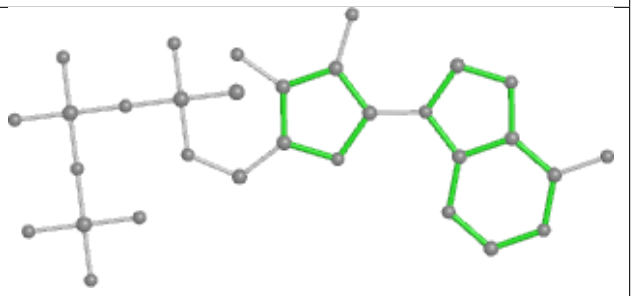
Bond lengths



Bond angles

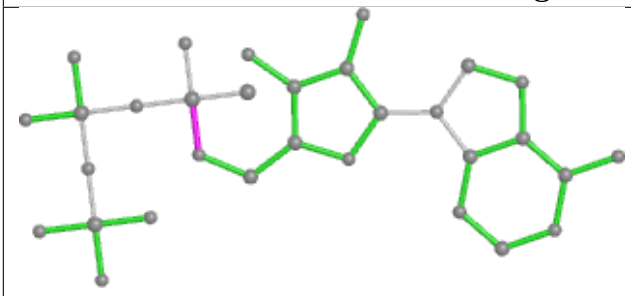


Torsions

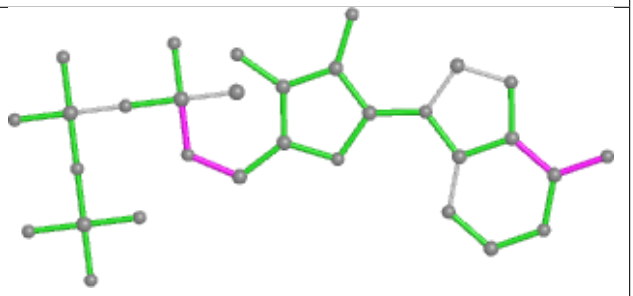


Rings

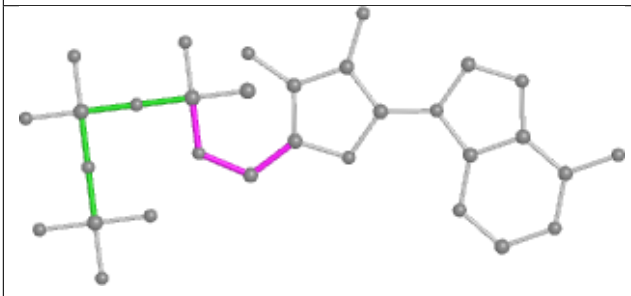
Ligand T99 L 702



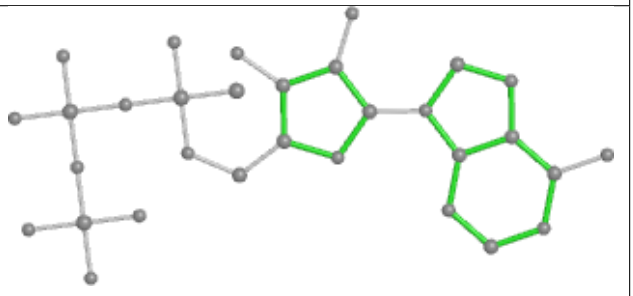
Bond lengths



Bond angles

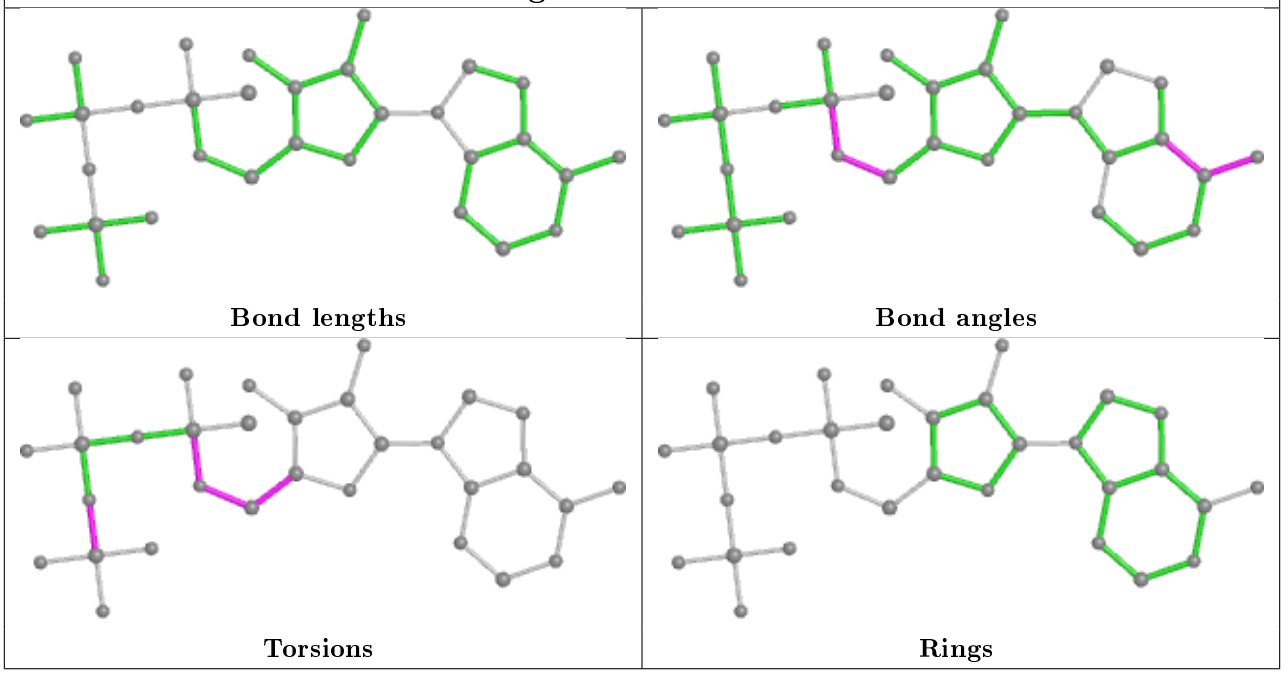


Torsions



Rings

Ligand T99 M 701



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	184/193 (95%)	-0.32	1 (0%) 91 91	19, 36, 73, 100	0
1	B	184/193 (95%)	-0.50	1 (0%) 91 91	15, 28, 47, 78	0
1	C	184/193 (95%)	-0.49	0 100 100	20, 33, 66, 97	0
1	D	185/193 (95%)	-0.63	2 (1%) 80 81	13, 23, 45, 92	0
1	E	182/193 (94%)	-0.35	2 (1%) 80 81	21, 37, 71, 96	0
1	F	185/193 (95%)	-0.54	2 (1%) 80 81	19, 32, 51, 97	0
1	G	185/193 (95%)	-0.37	5 (2%) 54 55	19, 34, 64, 98	0
1	H	185/193 (95%)	-0.45	1 (0%) 91 91	13, 22, 43, 77	0
1	I	182/193 (94%)	-0.20	2 (1%) 80 81	27, 43, 73, 94	0
1	J	185/193 (95%)	-0.42	0 100 100	19, 32, 56, 82	0
1	K	183/193 (94%)	0.04	4 (2%) 62 63	21, 56, 89, 104	0
1	L	185/193 (95%)	-0.50	1 (0%) 91 91	13, 26, 48, 80	0
1	M	180/193 (93%)	-0.56	2 (1%) 80 81	20, 36, 66, 93	0
1	N	181/193 (93%)	-0.13	5 (2%) 53 53	30, 47, 75, 104	0
1	O	179/193 (92%)	-0.28	1 (0%) 89 89	26, 45, 73, 83	0
1	P	179/193 (92%)	-0.02	5 (2%) 53 53	30, 54, 86, 111	0
All	All	2928/3088 (94%)	-0.36	34 (1%) 79 80	13, 36, 73, 111	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	442	MET	5.9
1	N	443	THR	5.5
1	D	443	THR	4.7
1	F	443	THR	4.5
1	P	443	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	K	443	THR	3.6
1	B	443	THR	3.6
1	G	442	MET	3.2
1	O	626	LYS	3.2
1	K	444	GLU	3.1
1	A	443	THR	3.1
1	E	444	GLU	3.0
1	P	555	ALA	3.0
1	I	613	GLY	2.8
1	G	561	LEU	2.7
1	G	444	GLU	2.7
1	M	443	THR	2.7
1	N	444	GLU	2.6
1	L	443	THR	2.5
1	K	561	LEU	2.5
1	F	442	MET	2.5
1	H	442	MET	2.4
1	E	613	GLY	2.4
1	P	533	THR	2.4
1	D	442	MET	2.3
1	N	482	LEU	2.2
1	P	511	GLU	2.2
1	G	626	LYS	2.2
1	K	514	PRO	2.2
1	M	444	GLU	2.2
1	G	443	THR	2.2
1	P	444	GLU	2.1
1	I	544	ILE	2.0
1	N	557	VAL	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
4	GOL	J	701	6/6	0.85	0.17	57,63,64,64	0
4	GOL	J	702	6/6	0.87	0.19	49,53,61,62	0
4	GOL	K	703	6/6	0.89	0.15	53,63,73,76	0
3	CA	O	702	1/1	0.91	0.12	50,50,50,50	0
4	GOL	F	701	6/6	0.91	0.13	46,47,51,53	0
4	GOL	D	702	6/6	0.91	0.13	45,52,53,53	0
2	T99	I	702	31/31	0.92	0.13	38,63,88,91	0
3	CA	N	702	1/1	0.92	0.09	46,46,46,46	0
4	GOL	C	704	6/6	0.92	0.13	37,48,49,51	0
2	T99	K	701	31/31	0.94	0.14	34,44,67,75	0
2	T99	D	701	31/31	0.94	0.13	31,43,63,69	0
2	T99	H	701	31/31	0.94	0.17	32,49,74,85	0
2	T99	N	701	31/31	0.94	0.12	51,57,80,83	0
4	GOL	O	703	6/6	0.94	0.12	50,53,54,55	0
2	T99	J	703	31/31	0.94	0.14	48,77,94,99	0
4	GOL	G	703	6/6	0.94	0.13	36,41,45,46	0
4	GOL	L	701	6/6	0.94	0.10	33,37,38,40	0
2	T99	C	702	31/31	0.94	0.13	34,53,78,84	0
4	GOL	F	703	6/6	0.94	0.15	40,52,55,57	0
2	T99	G	701	31/31	0.94	0.15	40,51,78,83	0
4	GOL	C	701	6/6	0.94	0.15	47,52,55,57	0
2	T99	P	701	31/31	0.94	0.11	50,73,83,88	0
4	GOL	A	703	6/6	0.94	0.12	40,44,46,46	0
4	GOL	E	703	6/6	0.95	0.10	42,48,56,57	0
2	T99	E	701	31/31	0.95	0.12	34,46,67,76	0
4	GOL	A	704	6/6	0.95	0.11	56,56,59,59	0
2	T99	L	702	31/31	0.95	0.13	42,51,64,71	0
2	T99	M	701	31/31	0.95	0.11	45,52,79,84	0
3	CA	K	702	1/1	0.95	0.12	38,38,38,38	0
3	CA	C	703	1/1	0.95	0.10	37,37,37,37	0
4	GOL	I	701	6/6	0.95	0.12	59,68,72,76	0
2	T99	O	701	31/31	0.95	0.12	54,74,84,88	0
3	CA	P	702	1/1	0.95	0.13	52,52,52,52	0
2	T99	F	702	31/31	0.96	0.12	46,56,71,77	0
3	CA	G	702	1/1	0.96	0.12	35,35,35,35	0
2	T99	B	701	31/31	0.96	0.11	39,49,67,72	0
3	CA	J	704	1/1	0.96	0.12	38,38,38,38	0

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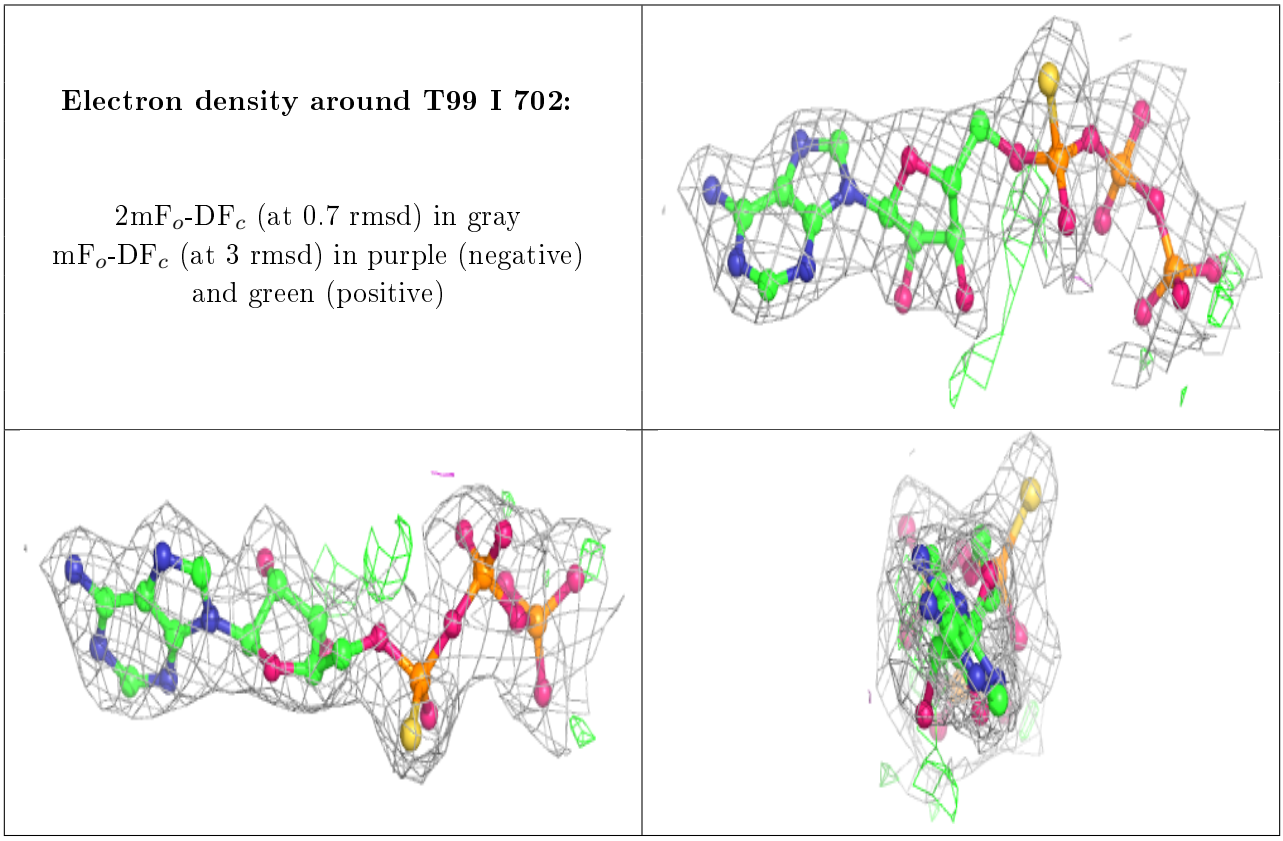
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	E	702	1/1	0.97	0.12	38,38,38,38	0
3	CA	I	703	1/1	0.97	0.07	46,46,46,46	0
2	T99	A	701	31/31	0.97	0.11	28,38,58,59	0
3	CA	B	702	1/1	0.98	0.11	38,38,38,38	0
3	CA	L	703	1/1	0.98	0.10	32,32,32,32	0
3	CA	F	704	1/1	0.98	0.08	40,40,40,40	0
3	CA	A	702	1/1	0.98	0.08	34,34,34,34	0
3	CA	M	702	1/1	0.99	0.08	42,42,42,42	0
3	CA	D	703	1/1	0.99	0.10	27,27,27,27	0
3	CA	H	702	1/1	0.99	0.12	29,29,29,29	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.

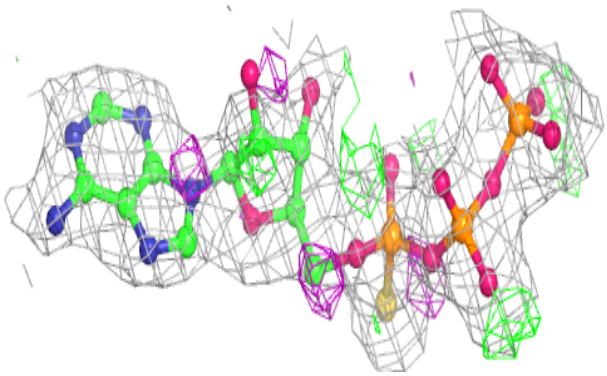
Electron density around T99 I 702:

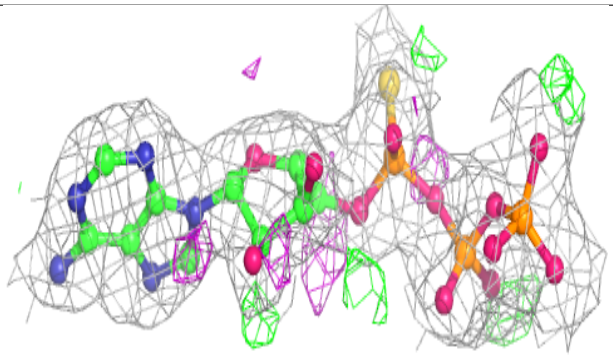
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

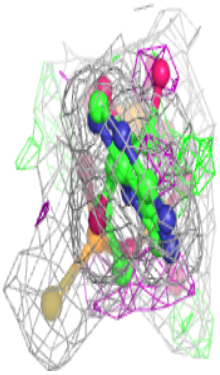


Electron density around T99 K 701:

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

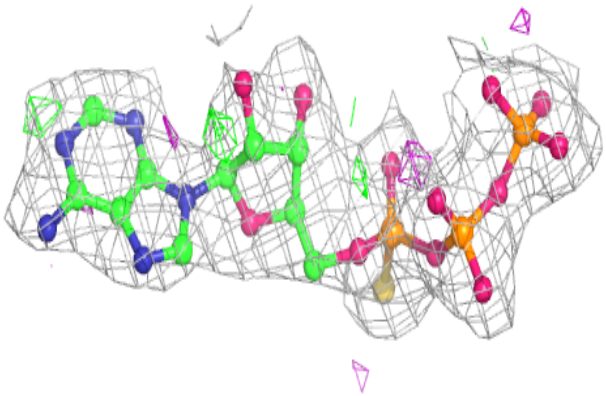


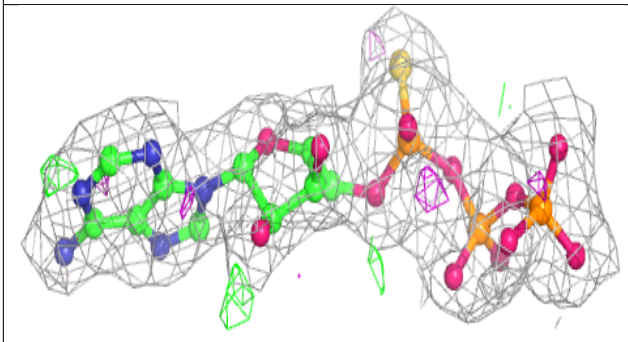


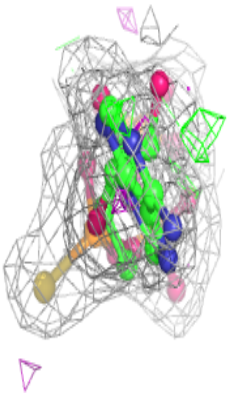


Electron density around T99 D 701:

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

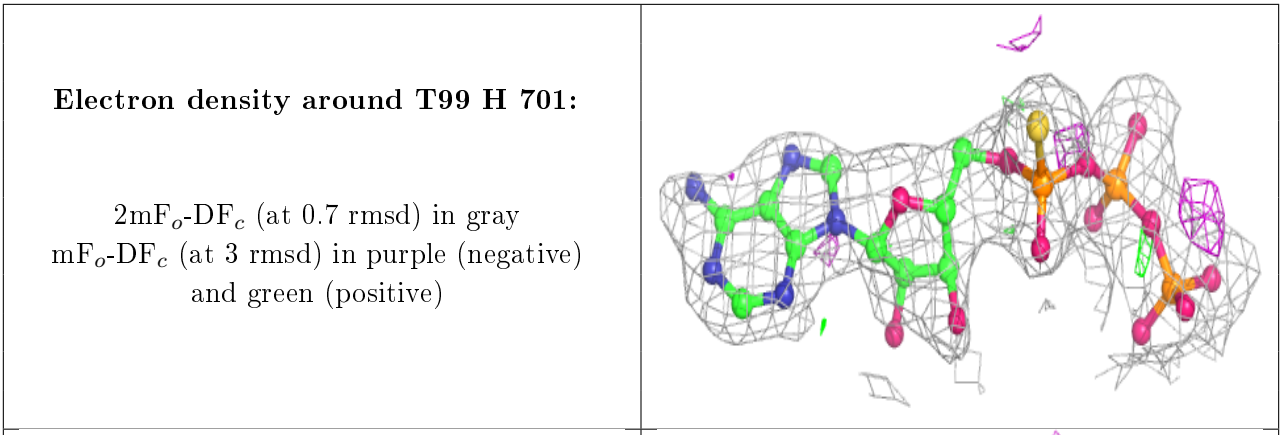






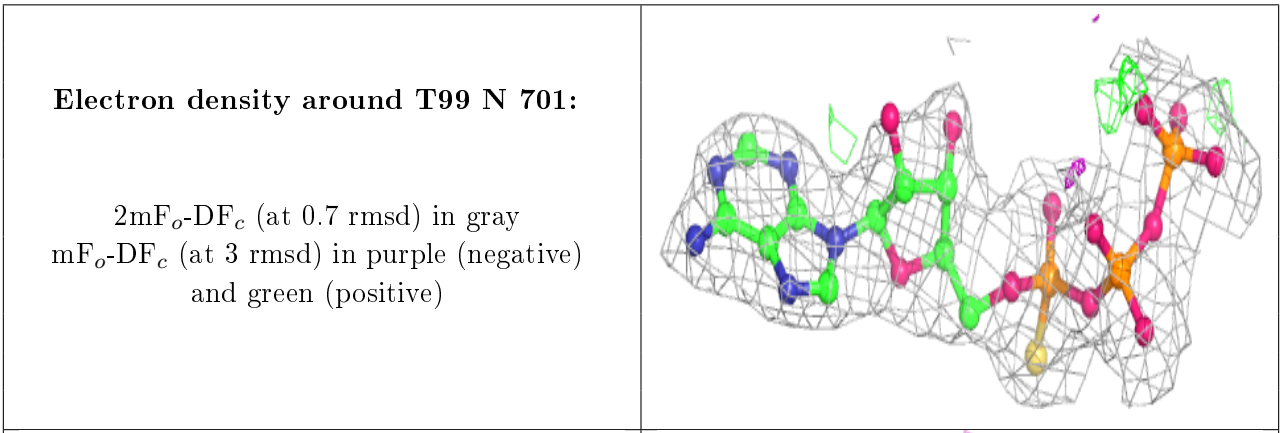
Electron density around T99 H 701:

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



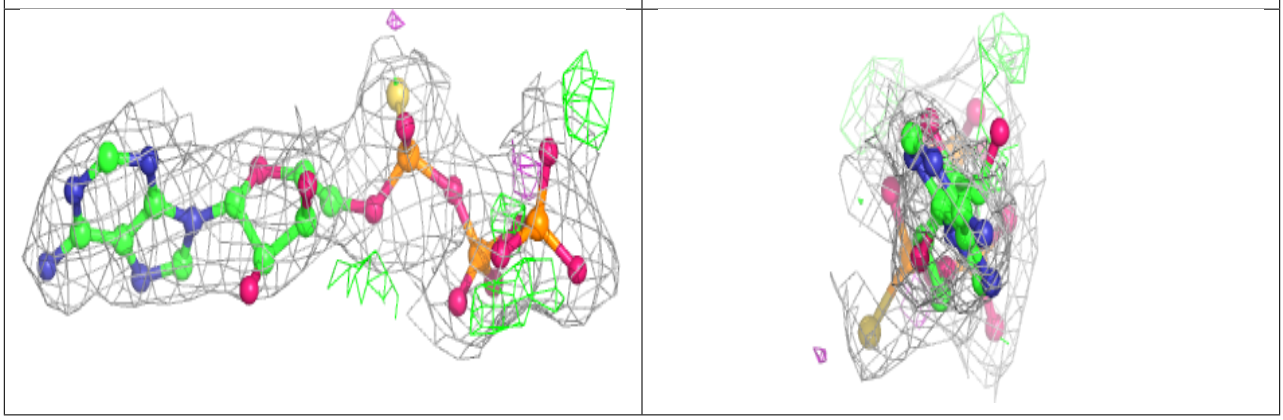
Electron density around T99 N 701:

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



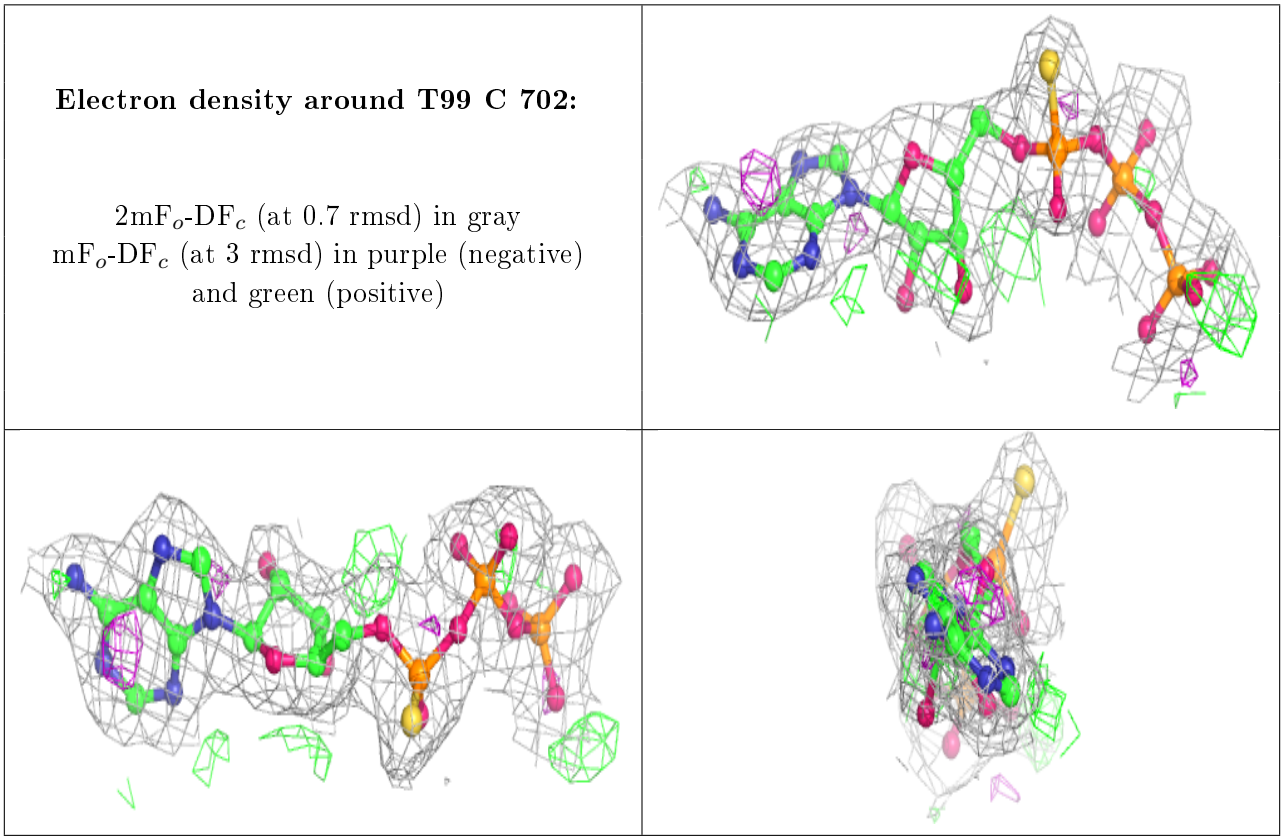
Electron density around T99 J 703:

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



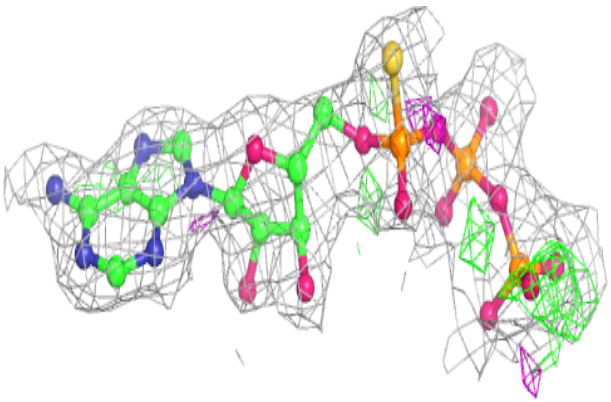
Electron density around T99 C 702:

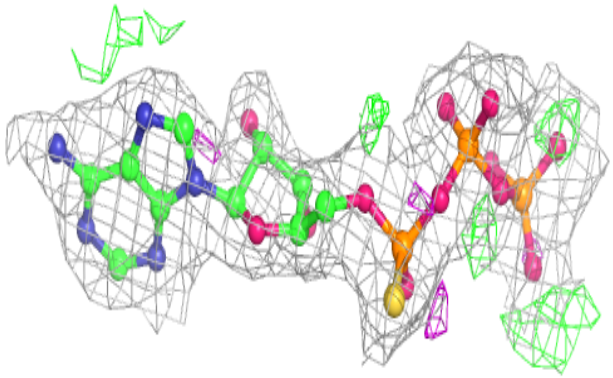
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

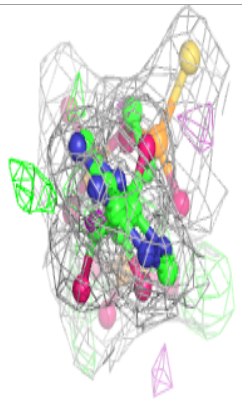


Electron density around T99 G 701:

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

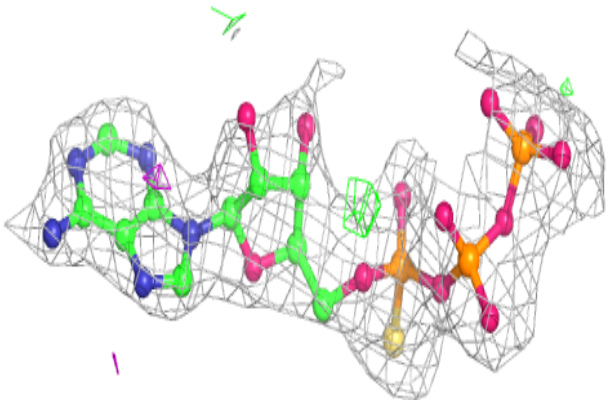


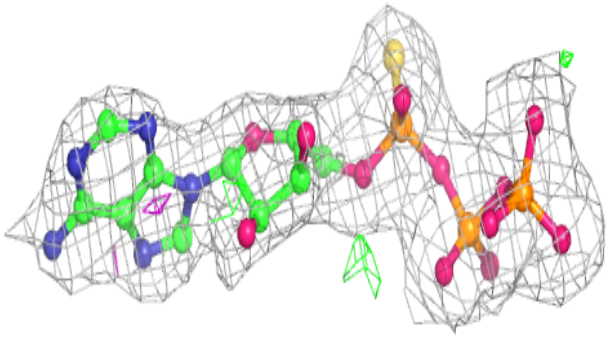


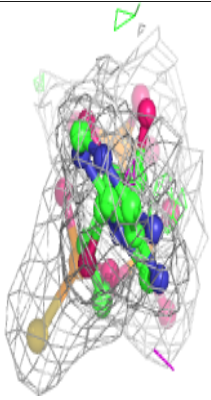


Electron density around T99 P 701:

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

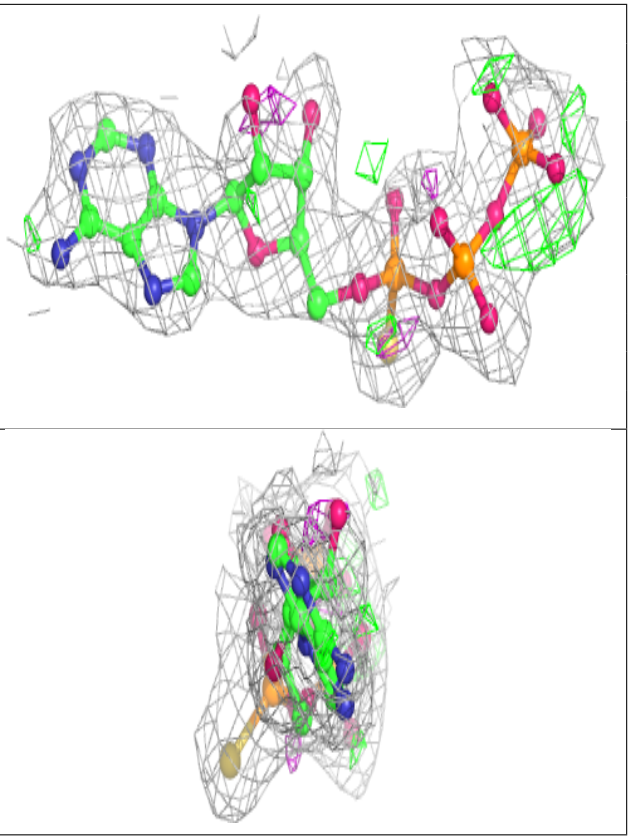






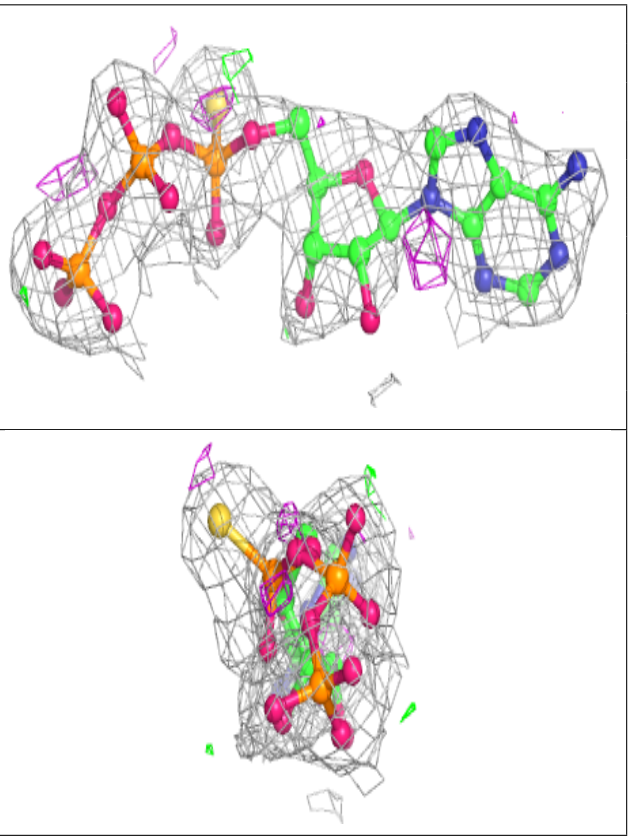
Electron density around T99 E 701:

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



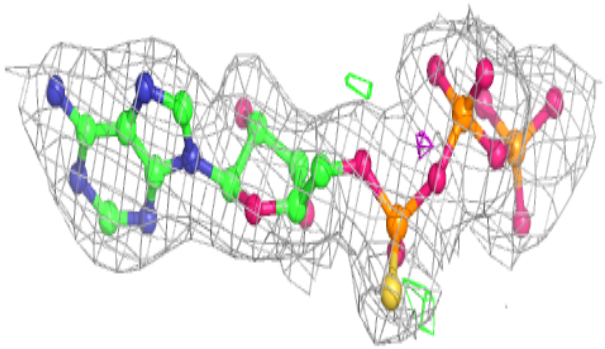
Electron density around T99 L 702:

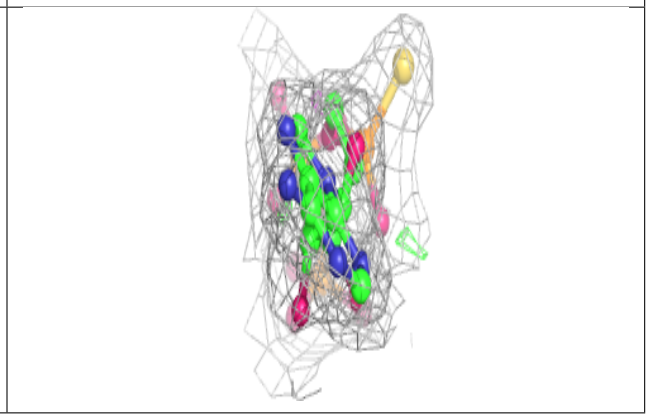
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around T99 M 701:

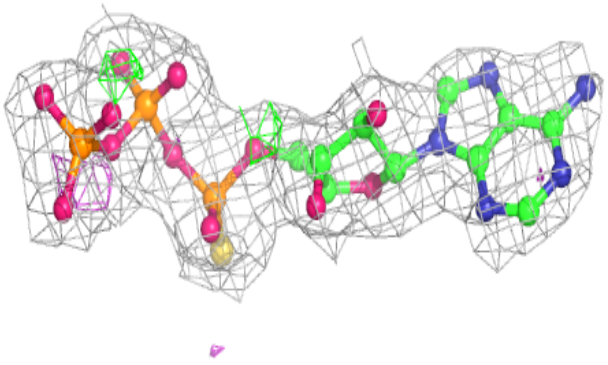
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

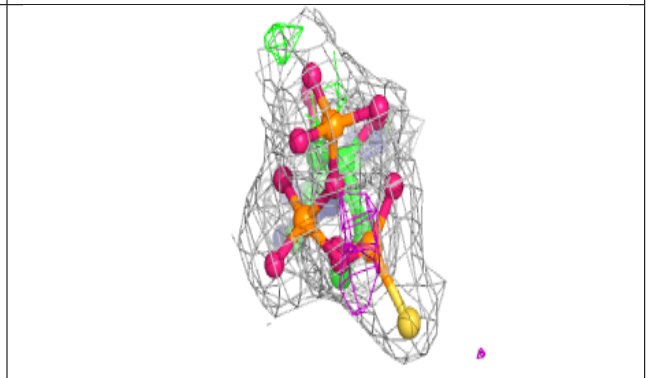




Electron density around T99 O 701:

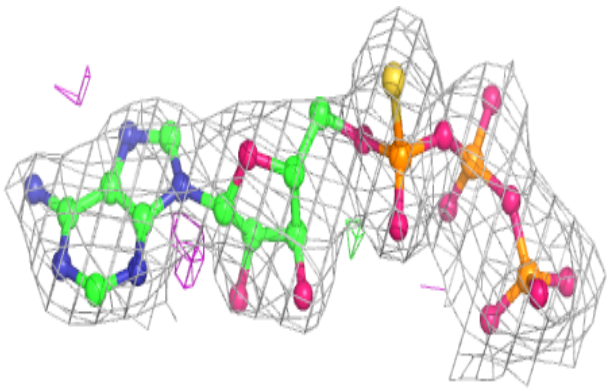
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

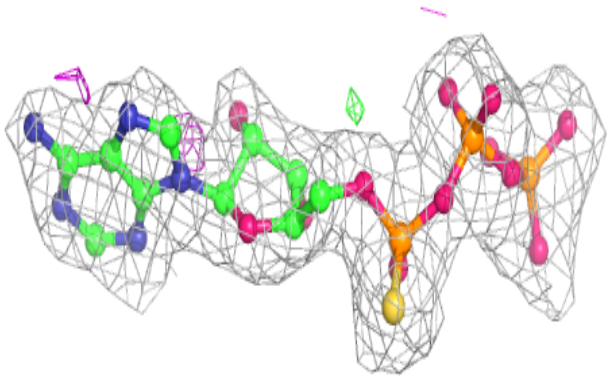


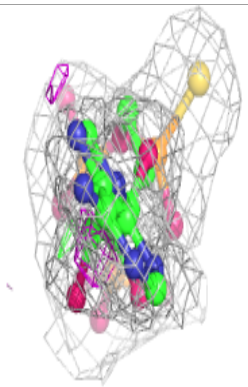


Electron density around T99 F 702:

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

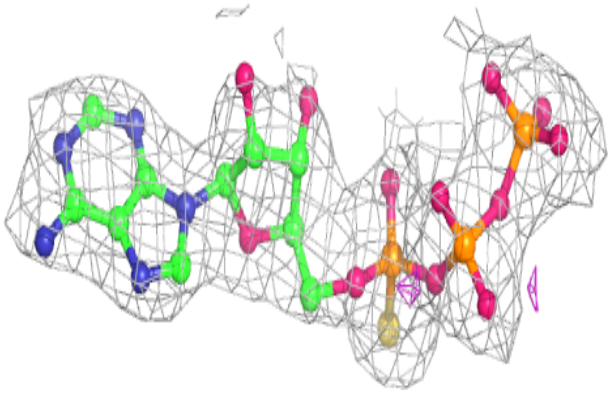


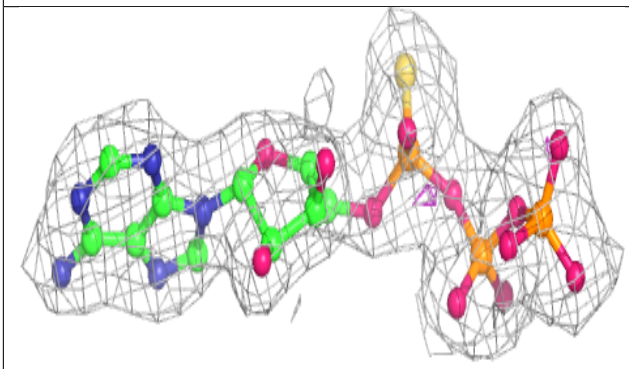


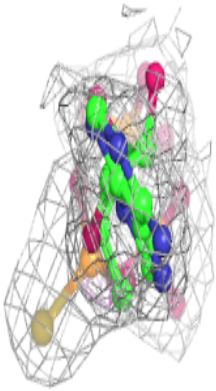


Electron density around T99 B 701:

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

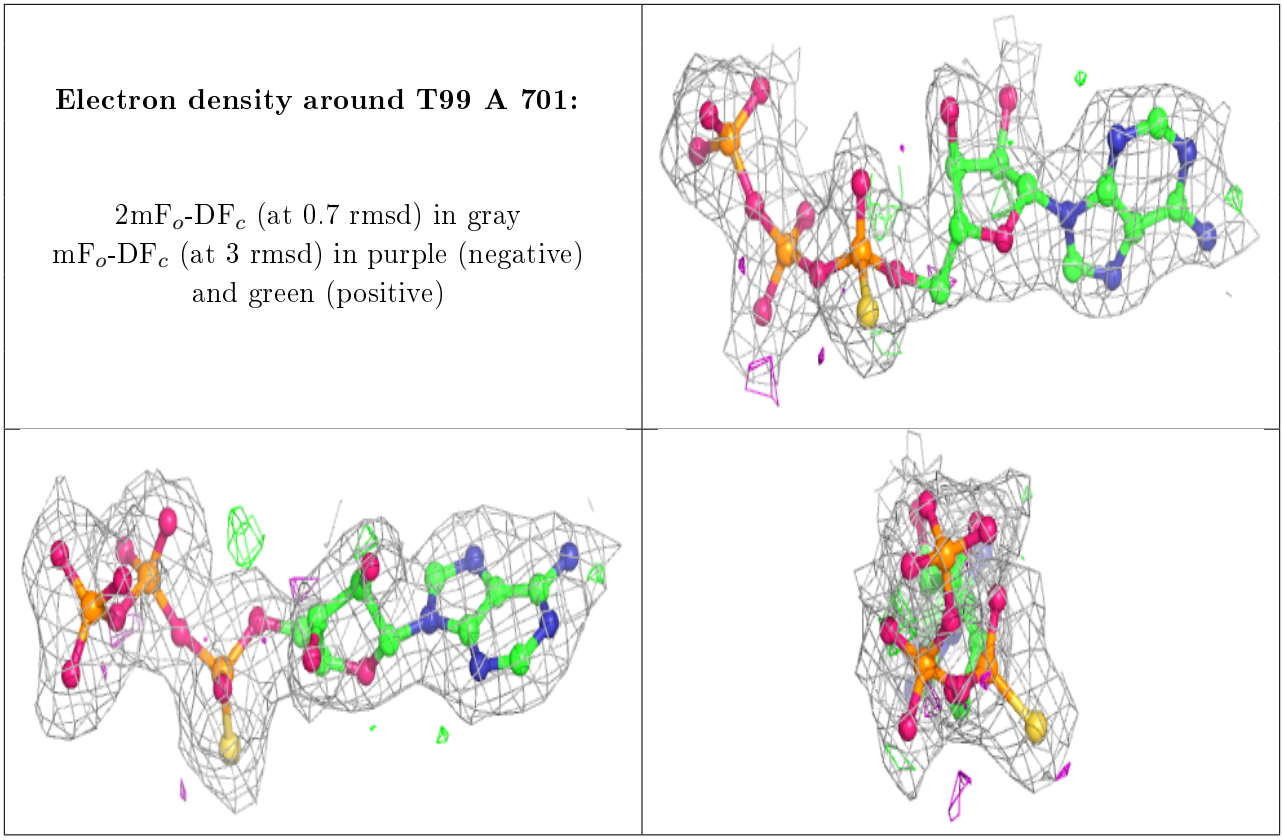






Electron density around T99 A 701:

$2mF_o$-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.