Full wwPDB EM Validation Report

Sep 8, 2026 – 01:03 PM EDT

PDB ID	:	9ZQT / pdb_00009zqt
EMDB ID	:	EMD-74581
Title	:	Composite map of the bGDH di-hexamer in liganded form
Authors	:	Shan, Z.; Lyumkis, D.
Deposited on	:	2025-12-19
Resolution	:	3.50 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

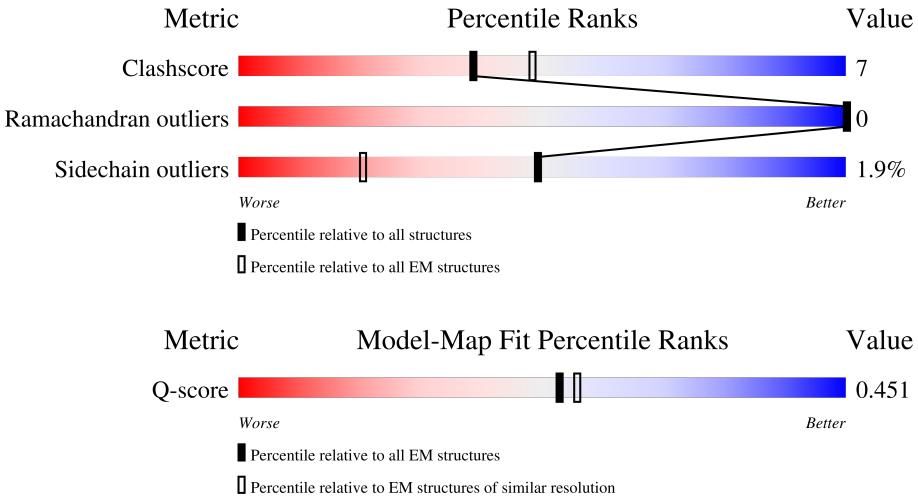
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	558	68% 20% 12%
1	B	558	72% 16% • 12%
1	C	558	73% 15% 12%
1	D	558	70% 18% 12%

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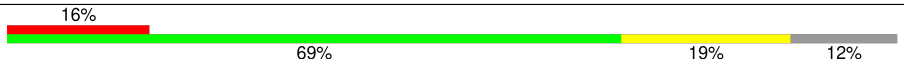
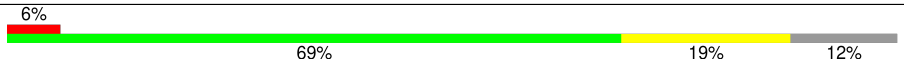
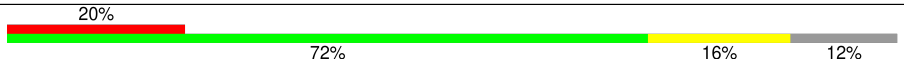
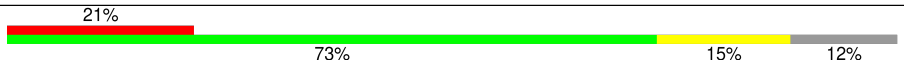
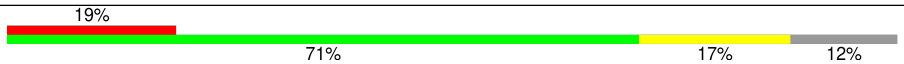
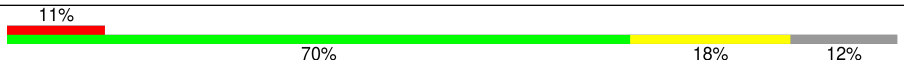
Mol	Chain	Length	Quality of chain
1	E	558	
1	F	558	
1	G	558	
1	H	558	
1	I	558	
1	J	558	
1	K	558	
1	L	558	

2 Entry composition (i)

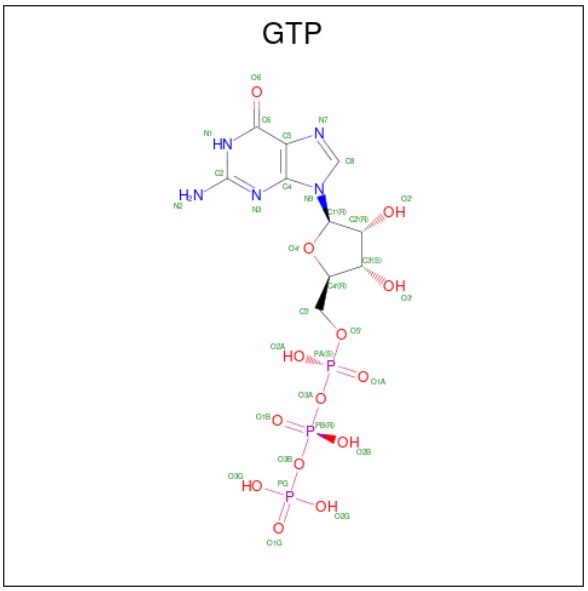
There are 4 unique types of molecules in this entry. The entry contains 47760 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Glutamate dehydrogenase 1, mitochondrial.

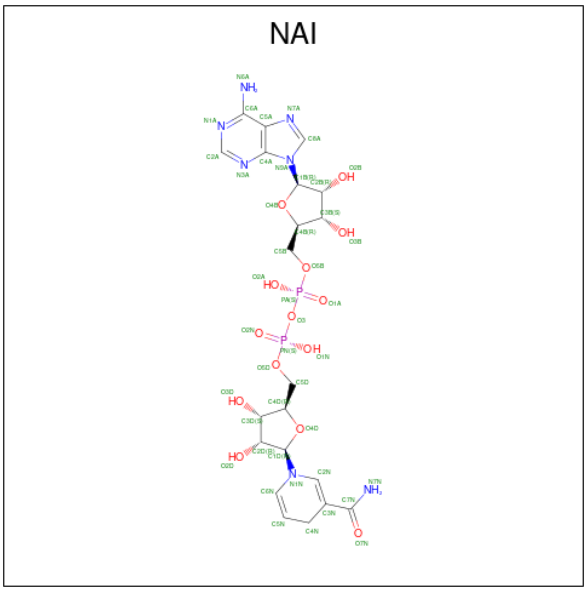
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	493	Total	C	N	O	S	0	0
			3855	2437	676	723	19		
1	B	493	Total	C	N	O	S	0	0
			3855	2437	676	723	19		
1	C	493	Total	C	N	O	S	0	0
			3855	2437	676	723	19		
1	D	493	Total	C	N	O	S	0	0
			3855	2437	676	723	19		
1	E	493	Total	C	N	O	S	0	0
			3855	2437	676	723	19		
1	F	493	Total	C	N	O	S	0	0
			3855	2437	676	723	19		
1	G	493	Total	C	N	O	S	0	0
			3855	2437	676	723	19		
1	H	493	Total	C	N	O	S	0	0
			3855	2437	676	723	19		
1	I	493	Total	C	N	O	S	0	0
			3855	2437	676	723	19		
1	J	493	Total	C	N	O	S	0	0
			3855	2437	676	723	19		
1	K	493	Total	C	N	O	S	0	0
			3855	2437	676	723	19		
1	L	493	Total	C	N	O	S	0	0
			3855	2437	676	723	19		

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	B	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	F	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	G	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	H	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	I	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	J	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	K	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	L	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	A	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	B	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	B	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	C	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	C	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	C	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	D	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	D	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	E	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	F	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	F	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	G	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	G	1	Total	C	N	O	P	0
			44	21	7	14	2	

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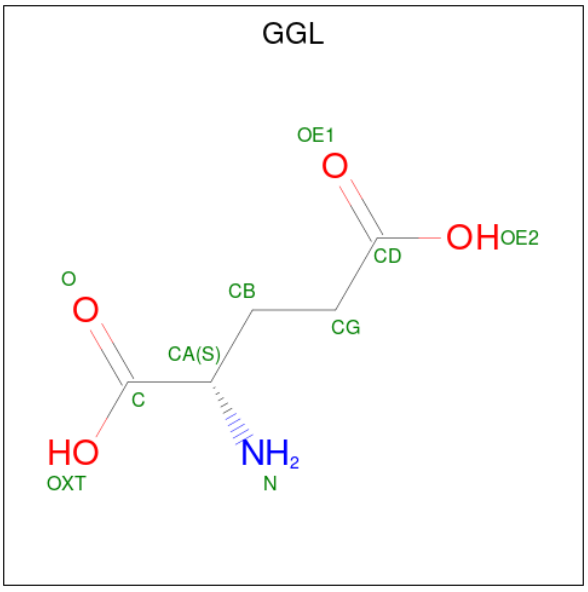
Mol	Chain	Residues	Atoms					AltConf
3	H	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	H	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	I	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	I	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	J	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	J	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	J	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	K	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	L	1	Total	C	N	O	P	0
			44	21	7	14	2	
3	L	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 4 is GAMMA-L-GLUTAMIC ACID (CCD ID: GGL) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			10	5	1	4	

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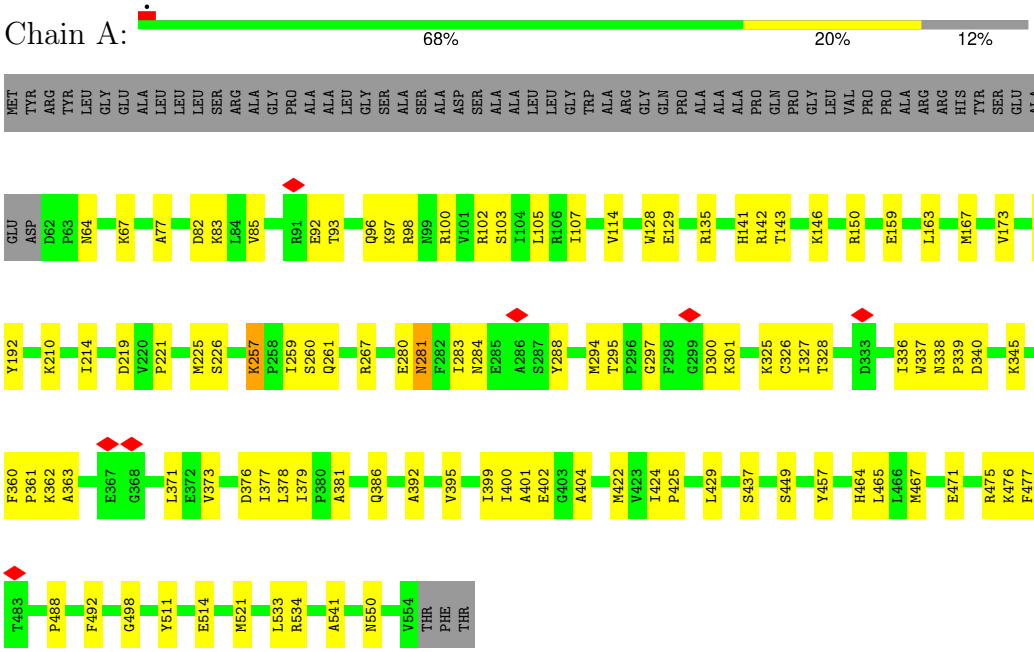
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			10	5	1	4	
4	C	1	Total	C	N	O	0
			10	5	1	4	
4	D	1	Total	C	N	O	0
			10	5	1	4	
4	E	1	Total	C	N	O	0
			10	5	1	4	
4	F	1	Total	C	N	O	0
			10	5	1	4	

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

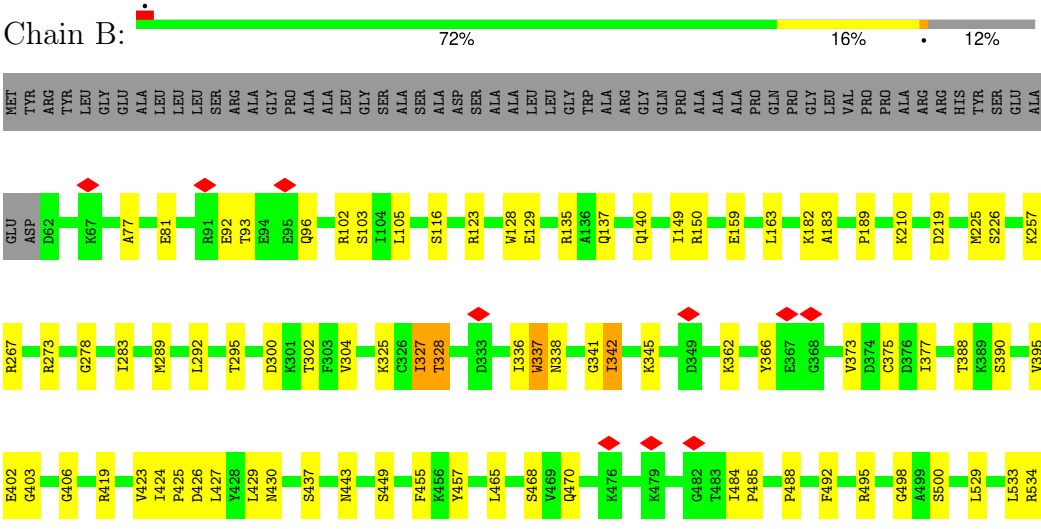
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

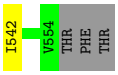
Chain A:



• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain B:

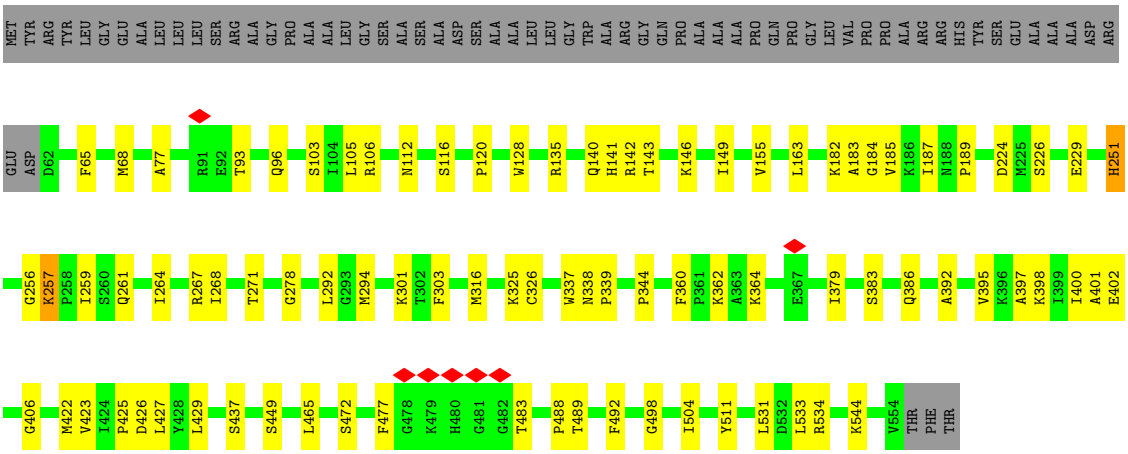




• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain C:

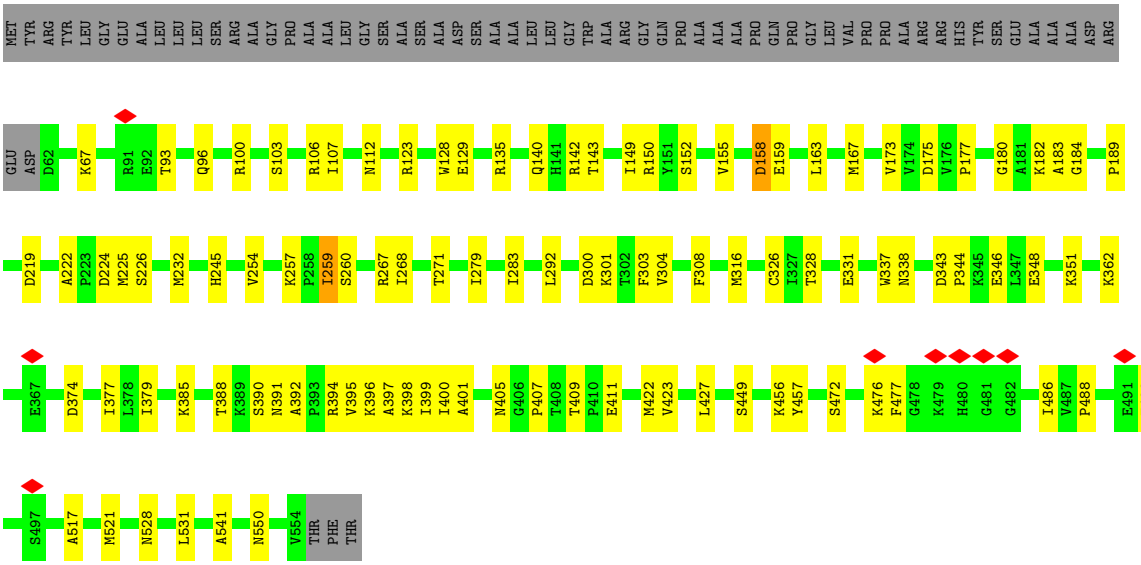




• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain D:

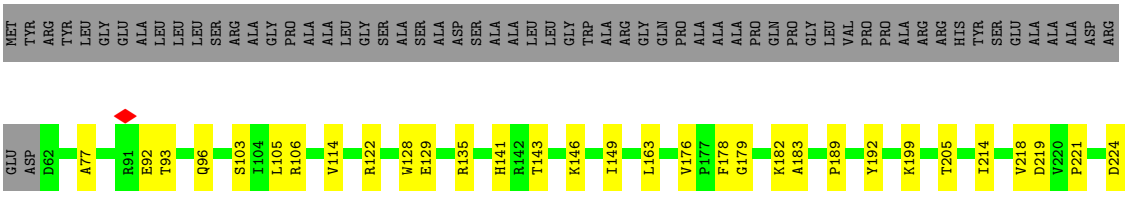


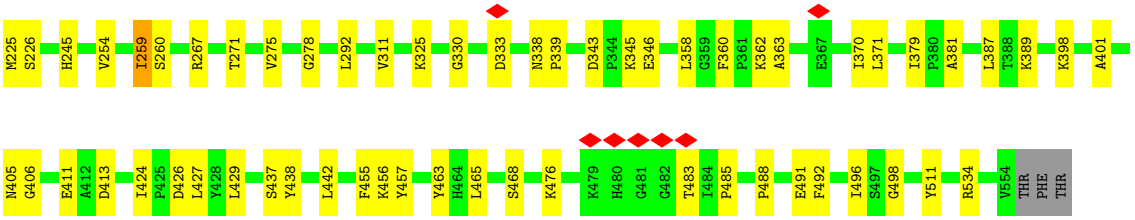


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain E:

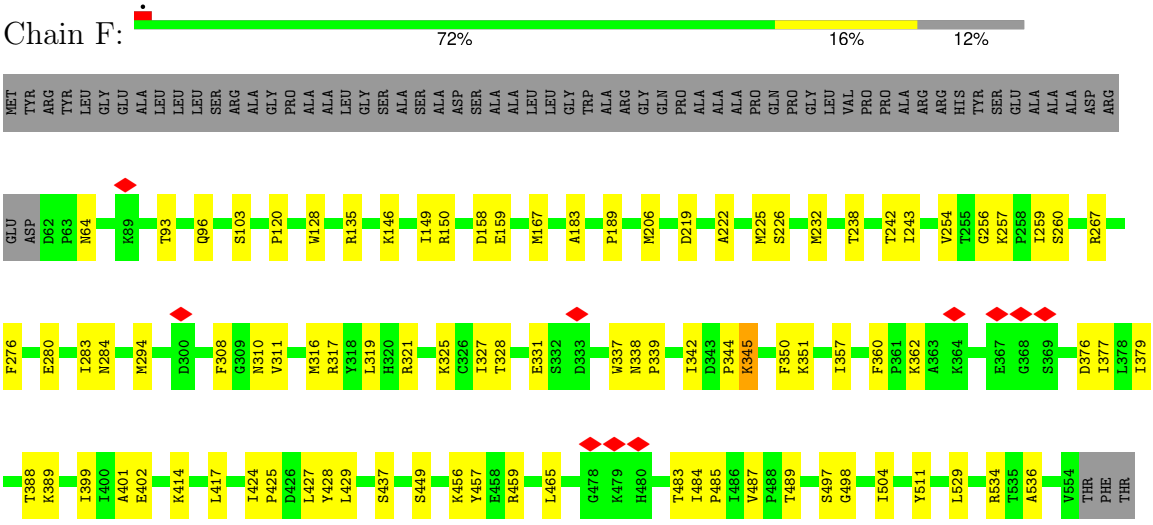






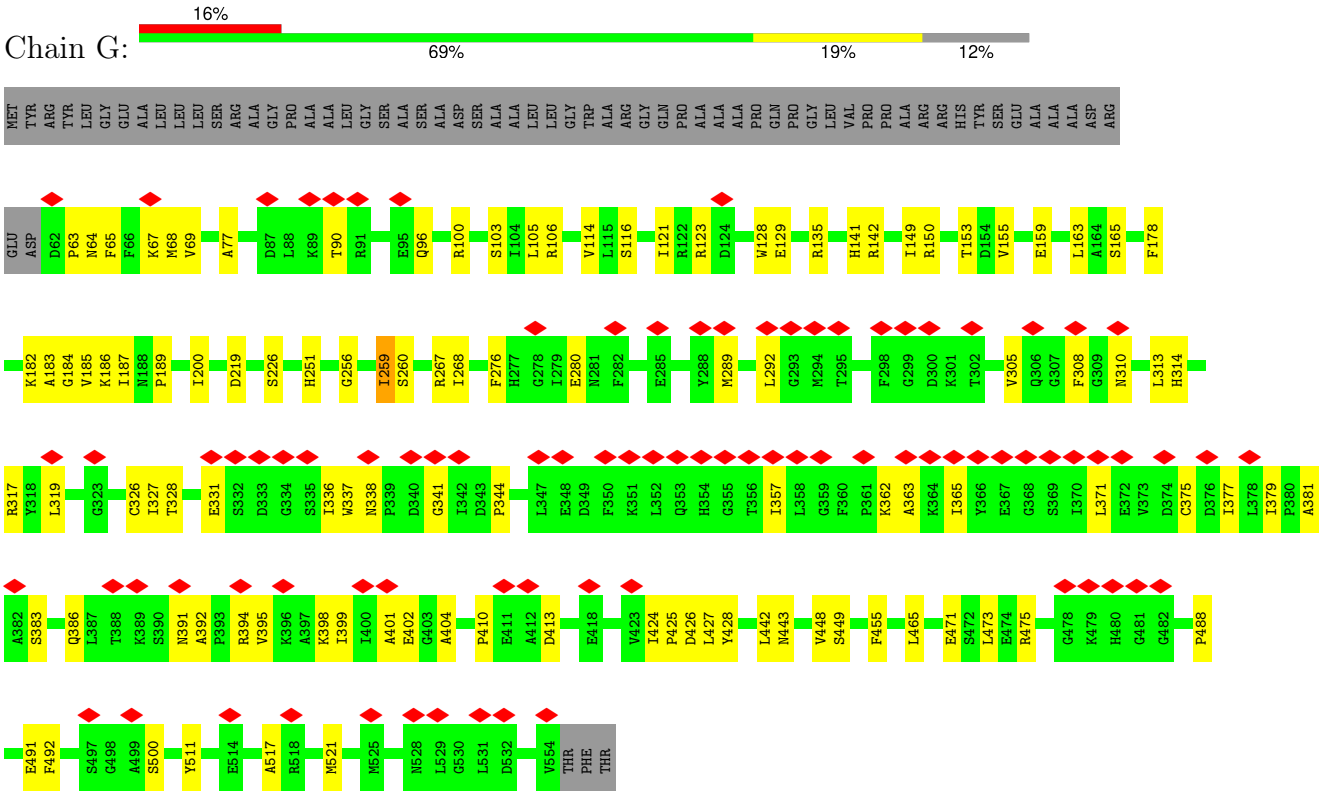
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain F:



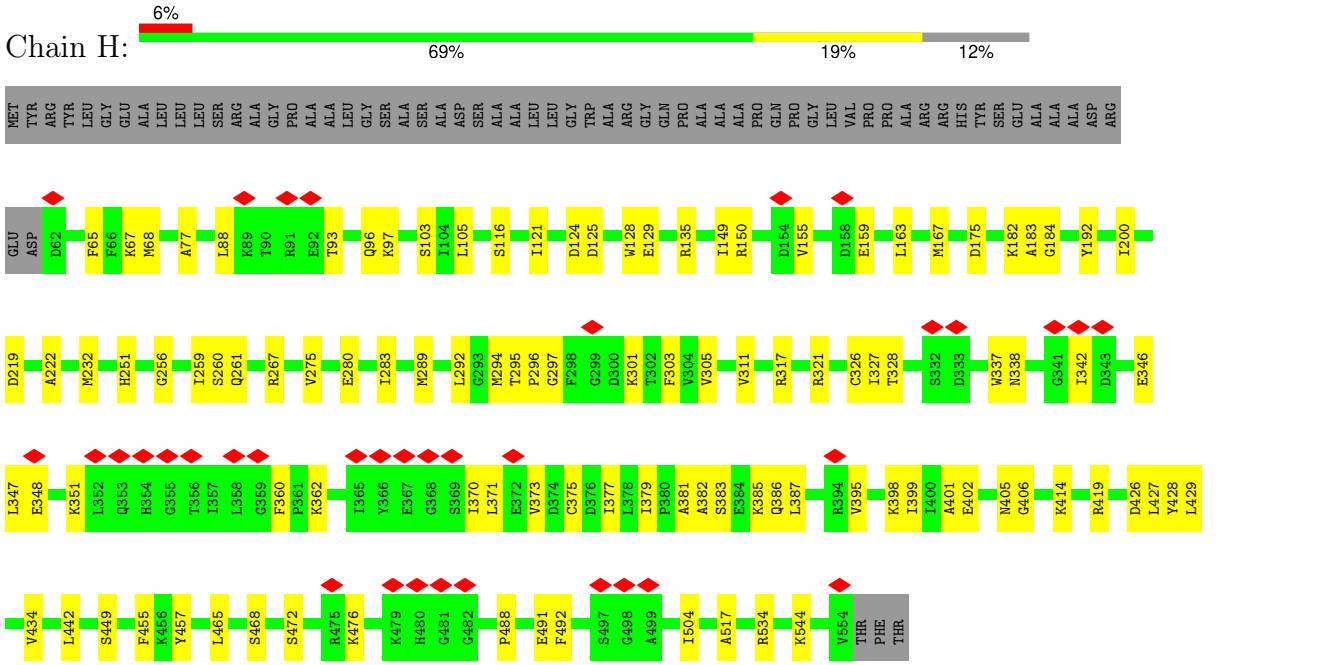
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain G:



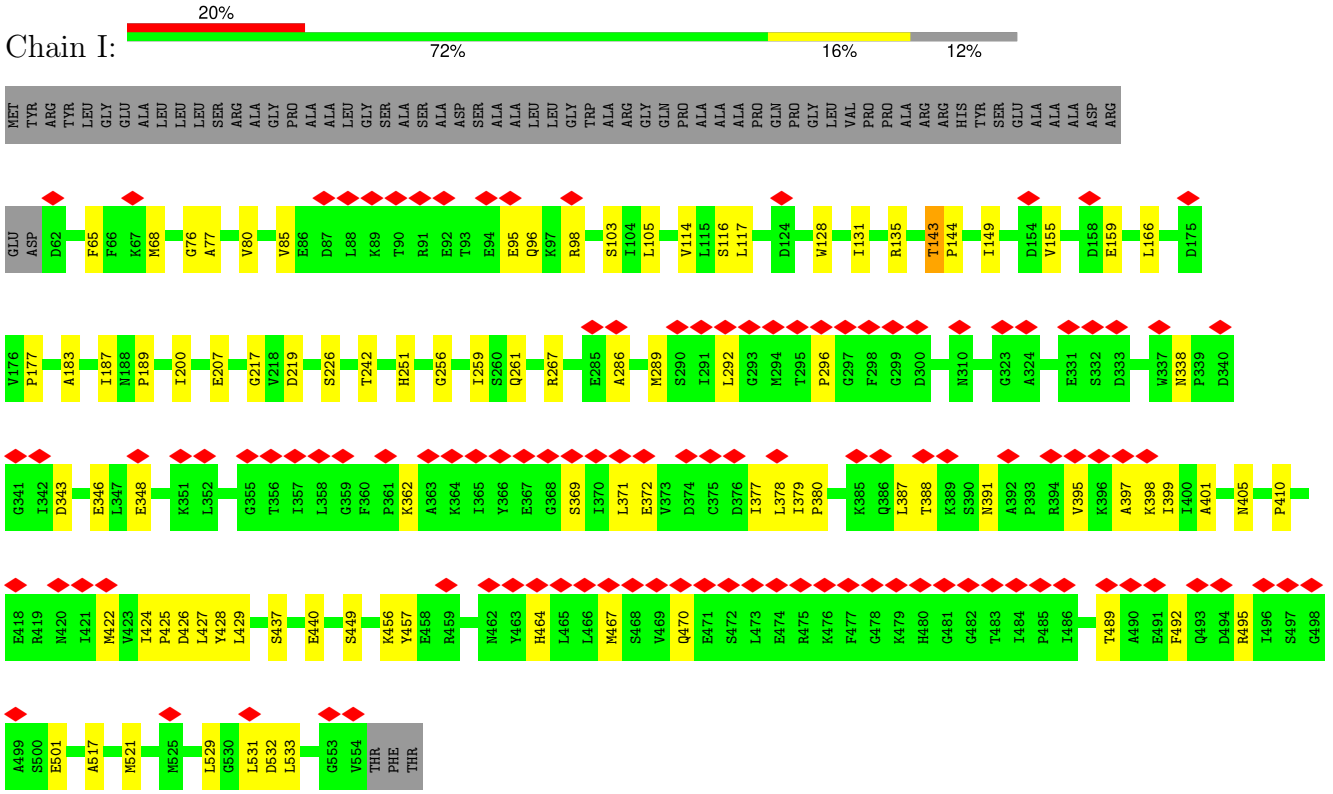
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain H:



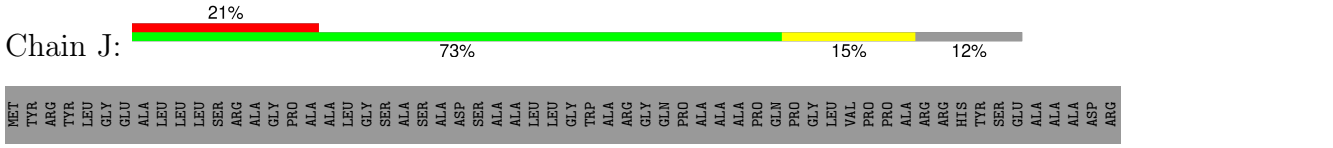
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

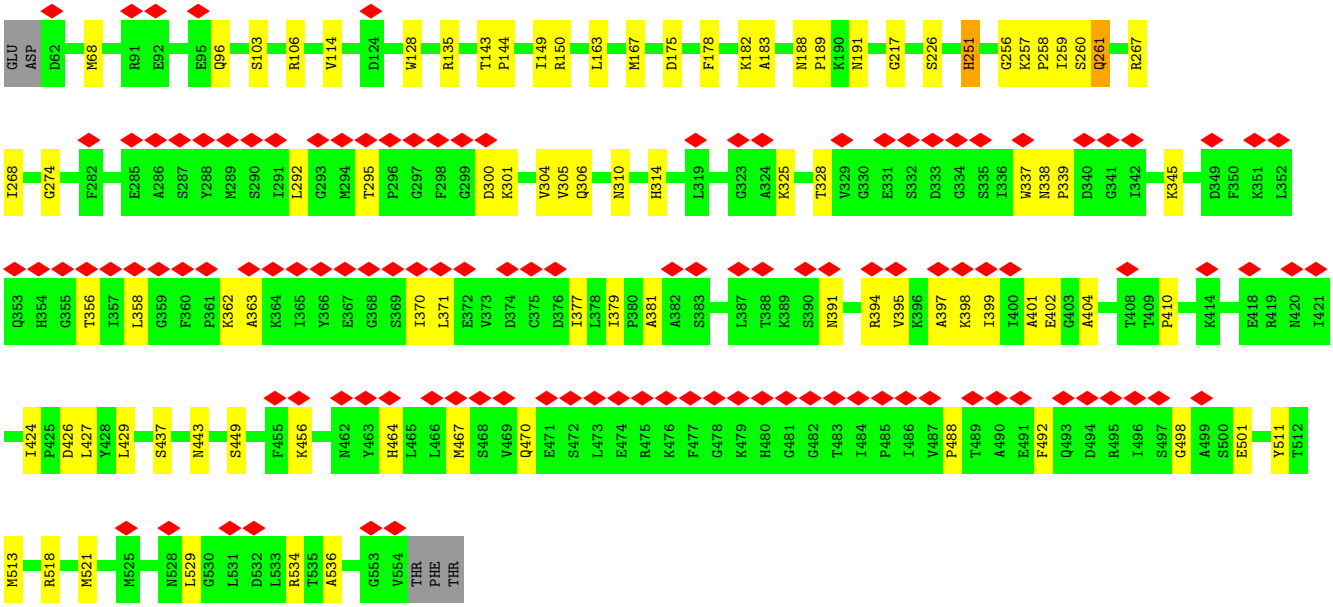
Chain I:



• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain J:

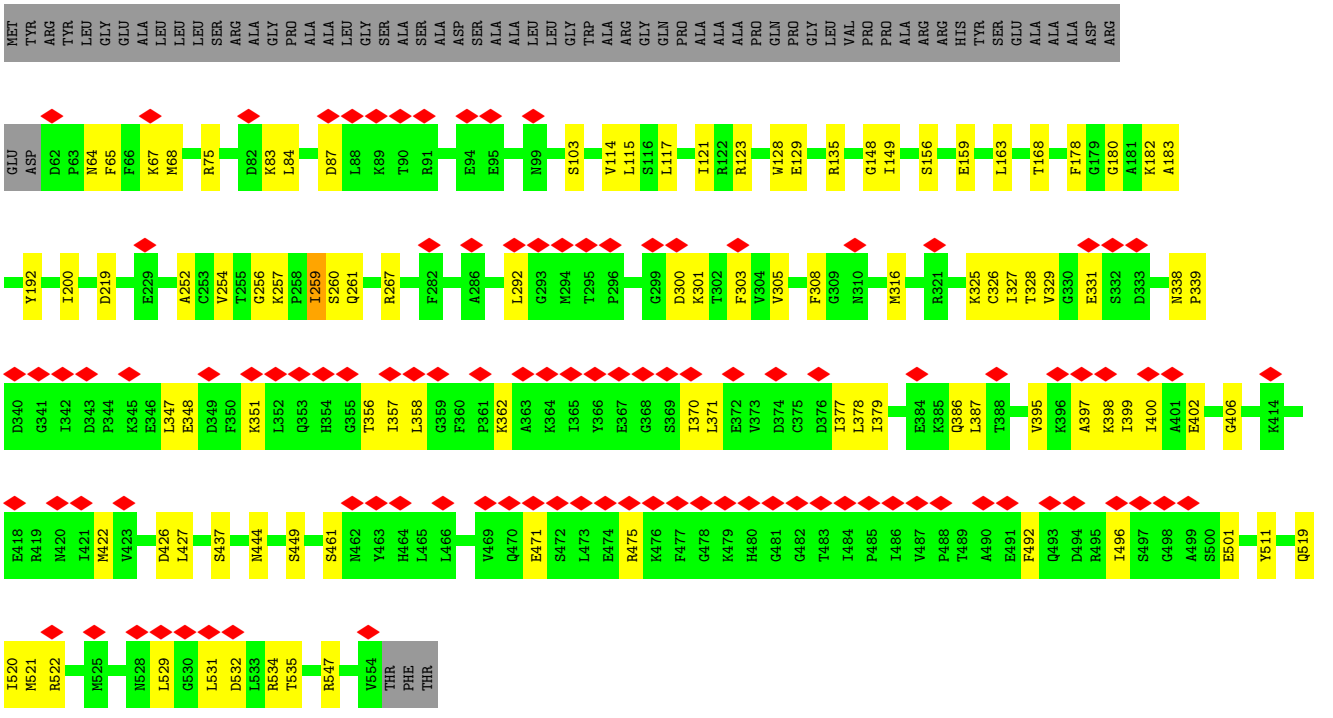




• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain K:

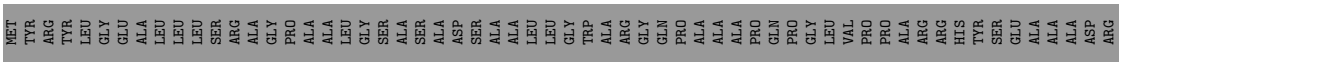


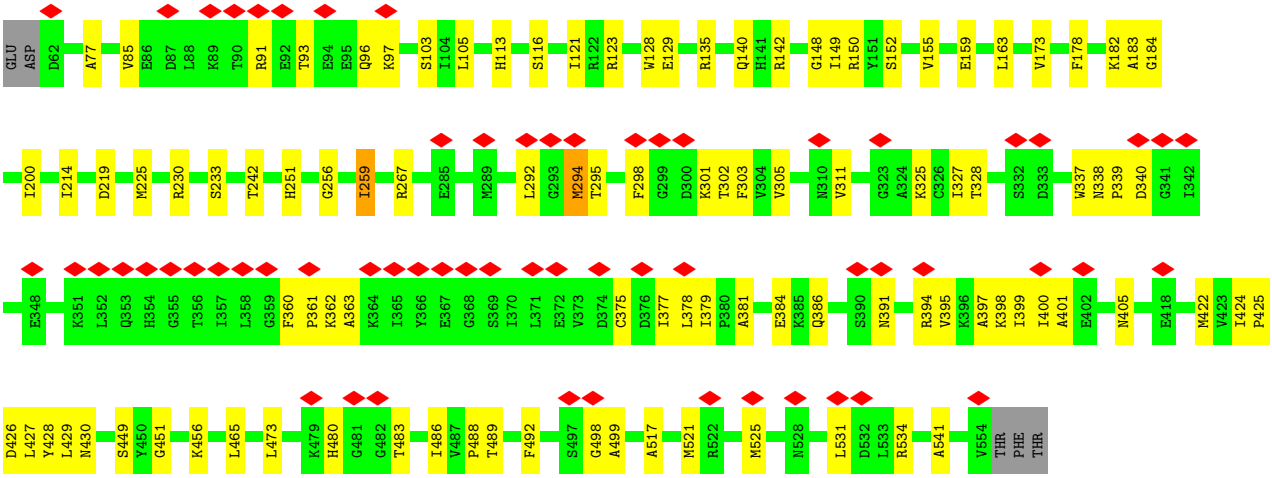


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain L:






GLU ASP D62 A77 V85 E86 D87 L88 K89 T90 R91 E92 T93 E94 E95 Q96 K97 S103 I104 L105 H113 S116 I121 R122 R123 W128 E129 R135 Q140 H141 R142 G148 I149 R150 Y151 S152 V155 E159 L163 V173 F178 K182 A183 G184
I200 I214 D219 M225 R230 S233 T242 H251 G256 I259 R267 E285 M289 L292 G293 M294 T295 F298 C299 D300 K301 T302 F303 V304 V305 N310 V311 G323 A324 K325 C326 I327 T328 S332 D333 W337 N338 P339 D340 G341 I342
E348 K351 L352 Q353 H354 G355 T356 I357 L358 G359 F360 P361 K362 A363 K364 I365 Y366 E367 G368 S369 I370 L371 E372 V373 D374 C375 D376 I377 L378 I379 P380 A381 E384 K385 Q386 S390 N391 R394 V395 K396 A397 K398 I399 I400 A401 E402 N405 E418 M422 V423 I424 P425
D426 L427 Y428 L429 N430 S449 Y450 G451 K456 L465 L473 K479 H480 G481 G482 T483 I486 V487 P488 T489 F492 S497 G498 A499 A517 M521 R522 M525 N528 L531 D532 L533 R534 A541 V554 THR PHE THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97554	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.677	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	420.86398, 420.86398, 420.86398	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3152, 1.3152, 1.3152	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GGL, NAI, GTP

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	0.08	0/3937	0.23	0/5315
1	B	0.09	0/3937	0.24	0/5315
1	C	0.08	0/3937	0.22	0/5315
1	D	0.08	0/3937	0.21	0/5315
1	E	0.08	0/3937	0.22	0/5315
1	F	0.08	0/3937	0.22	0/5315
1	G	0.07	0/3937	0.21	0/5315
1	H	0.08	0/3937	0.23	0/5315
1	I	0.07	0/3937	0.22	0/5315
1	J	0.07	0/3937	0.20	0/5315
1	K	0.07	0/3937	0.21	0/5315
1	L	0.07	0/3937	0.21	0/5315
All	All	0.08	0/47244	0.22	0/63780

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	3855	0	3825	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3855	0	3825	59	0
1	C	3855	0	3825	55	0
1	D	3855	0	3825	68	0
1	E	3855	0	3825	62	0
1	F	3855	0	3825	62	0
1	G	3855	0	3825	69	0
1	H	3855	0	3825	65	0
1	I	3855	0	3825	61	0
1	J	3855	0	3825	55	0
1	K	3855	0	3825	54	0
1	L	3855	0	3825	67	0
2	A	32	0	12	0	0
2	B	32	0	12	1	0
2	C	32	0	12	0	0
2	D	32	0	12	1	0
2	E	32	0	12	0	0
2	F	32	0	12	1	0
2	G	32	0	12	0	0
2	H	32	0	12	3	0
2	I	32	0	12	1	0
2	J	32	0	12	1	0
2	K	32	0	12	1	0
2	L	32	0	12	0	0
3	A	88	0	54	0	0
3	B	88	0	54	1	0
3	C	132	0	81	4	0
3	D	88	0	54	2	0
3	E	44	0	27	3	0
3	F	88	0	54	2	0
3	G	88	0	54	2	0
3	H	88	0	54	4	0
3	I	88	0	54	3	0
3	J	132	0	81	3	0
3	K	44	0	27	1	0
3	L	88	0	54	3	0
4	A	10	0	7	2	0
4	B	10	0	7	1	0
4	C	10	0	7	2	0
4	D	10	0	7	2	0
4	E	10	0	7	2	0
4	F	10	0	7	1	0
All	All	47760	0	46734	686	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (686) 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:K:65:PHE:HA	1:K:68:MET:HE2	1.60	0.82
1:I:464:HIS:HA	1:I:467:MET:HE2	1.63	0.79
1:B:103:SER:HB3	1:E:128:TRP:HB2	1.65	0.78
1:D:103:SER:HB3	1:F:128:TRP:HB2	1.66	0.78
1:G:65:PHE:HA	1:G:68:MET:HE3	1.66	0.77
1:K:292:LEU:HD11	1:K:398:LYS:HB3	1.68	0.76
1:B:388:THR:HG22	1:B:390:SER:H	1.51	0.76
1:A:128:TRP:HB2	1:C:103:SER:HB3	1.68	0.76
1:F:338:ASN:ND2	1:F:362:LYS:O	2.20	0.74
1:G:114:VAL:HB	1:I:116:SER:HB2	1.70	0.73
1:A:325:LYS:NZ	1:A:339:PRO:O	2.22	0.72
1:H:128:TRP:HB2	1:K:103:SER:HB3	1.71	0.72
1:D:128:TRP:HB2	1:F:103:SER:HB3	1.69	0.71
1:C:292:LEU:HD11	1:C:398:LYS:HB3	1.72	0.71
1:A:103:SER:HB3	1:C:128:TRP:HB2	1.73	0.70
1:G:128:TRP:HB2	1:I:103:SER:HB3	1.71	0.70
1:L:426:ASP:O	1:L:430:ASN:ND2	2.24	0.70
1:A:379:ILE:HG12	1:A:401:ALA:HB3	1.74	0.70
1:D:476:LYS:NZ	1:E:483:THR:O	2.24	0.70
1:E:292:LEU:HD21	1:E:398:LYS:HB3	1.74	0.70
1:H:305:VAL:HG12	1:H:379:ILE:HB	1.73	0.70
1:B:128:TRP:HB2	1:E:103:SER:HB3	1.73	0.69
1:I:338:ASN:ND2	1:I:362:LYS:O	2.25	0.69
1:B:302:THR:HB	1:B:327:ILE:HG13	1.75	0.69
1:I:456:LYS:HB2	1:J:511:TYR:HB2	1.75	0.69
1:L:391:ASN:HA	1:L:394:ARG:HE	1.58	0.69
1:F:379:ILE:HG12	1:F:401:ALA:HB3	1.74	0.68
1:H:292:LEU:HD11	1:H:398:LYS:HG3	1.76	0.68
1:E:163:LEU:HB3	1:E:182:LYS:HD3	1.74	0.68
1:G:292:LEU:HD11	1:G:398:LYS:HB3	1.76	0.68
1:J:338:ASN:ND2	1:J:362:LYS:O	2.27	0.67
1:F:135:ARG:HH11	1:F:183:ALA:HB2	1.60	0.67
1:J:518:ARG:HA	1:J:521:MET:HE3	1.76	0.67
1:C:338:ASN:ND2	1:C:362:LYS:O	2.27	0.67
1:K:338:ASN:ND2	1:K:362:LYS:O	2.28	0.66
1:L:338:ASN:ND2	1:L:362:LYS:O	2.27	0.66
1:C:146:LYS:NZ	4:C:603:GGL:OE2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:371:LEU:HD11	1:H:386:GLN:HB3	1.77	0.66
1:C:483:THR:O	1:E:476:LYS:NZ	2.29	0.66
1:D:316:MET:HG2	1:D:344:PRO:HG3	1.77	0.66
1:G:402:GLU:HB3	1:G:426:ASP:HB3	1.78	0.66
1:H:103:SER:HB3	1:K:128:TRP:HB2	1.78	0.66
1:D:338:ASN:ND2	1:D:362:LYS:O	2.27	0.65
1:H:402:GLU:OE2	1:H:534:ARG:NH2	2.27	0.65
1:L:294:MET:HG2	1:L:301:LYS:HE3	1.78	0.65
1:B:402:GLU:OE2	1:B:534:ARG:NH2	2.27	0.65
1:H:135:ARG:HH11	1:H:183:ALA:HB2	1.62	0.65
1:J:103:SER:HB3	1:L:128:TRP:HB2	1.79	0.64
1:A:288:TYR:HE2	1:A:521:MET:HG2	1.61	0.64
1:B:457:TYR:OH	1:F:498:GLY:O	2.11	0.64
1:D:300:ASP:OD1	1:D:301:LYS:NZ	2.29	0.64
1:A:297:GLY:O	1:A:301:LYS:NZ	2.30	0.63
1:E:135:ARG:HH11	1:E:183:ALA:HB2	1.63	0.63
1:H:457:TYR:OH	1:L:498:GLY:O	2.16	0.63
1:H:88:LEU:O	1:H:97:LYS:NZ	2.31	0.63
1:K:135:ARG:HH11	1:K:183:ALA:HB2	1.63	0.63
1:G:135:ARG:HH11	1:G:183:ALA:HB2	1.64	0.63
1:A:477:PHE:HE2	1:H:296:PRO:HD3	1.64	0.63
1:I:95:GLU:OE1	1:I:95:GLU:N	2.30	0.63
1:L:379:ILE:HG12	1:L:401:ALA:HB3	1.81	0.63
1:L:488:PRO:HB3	1:L:492:PHE:HD2	1.63	0.63
1:D:472:SER:OG	1:E:485:PRO:O	2.13	0.63
1:F:377:ILE:HG12	1:F:399:ILE:HB	1.79	0.63
1:G:268:ILE:HG23	1:G:314:HIS:HE1	1.64	0.62
1:H:338:ASN:ND2	1:H:362:LYS:O	2.31	0.62
1:K:75:ARG:NH2	1:K:532:ASP:OD2	2.32	0.62
1:A:146:LYS:NZ	4:A:602:GGL:OE2	2.32	0.62
1:B:283:ILE:HG12	1:B:289:MET:HE2	1.79	0.62
1:H:476:LYS:NZ	1:L:483:THR:O	2.32	0.62
1:C:251:HIS:CE1	3:C:605:NAI:H42N	2.35	0.62
1:C:256:GLY:HA2	1:C:267:ARG:HG2	1.81	0.62
1:D:379:ILE:HG12	1:D:401:ALA:HB3	1.81	0.62
1:L:135:ARG:HH11	1:L:183:ALA:HB2	1.65	0.62
1:I:135:ARG:HH11	1:I:183:ALA:HB2	1.64	0.61
1:H:491:GLU:OE1	1:H:491:GLU:N	2.33	0.61
1:C:155:VAL:HG11	1:C:184:GLY:HA3	1.82	0.61
1:D:346:GLU:OE1	1:D:362:LYS:NZ	2.29	0.61
1:A:85:VAL:HG23	1:A:97:LYS:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:ILE:HG12	1:E:401:ALA:HB3	1.82	0.61
1:F:424:ILE:HG21	1:F:429:LEU:HD13	1.82	0.61
1:A:457:TYR:OH	1:B:498:GLY:O	2.17	0.61
1:C:498:GLY:O	1:E:457:TYR:OH	2.15	0.60
1:F:414:LYS:HE2	1:F:414:LYS:HA	1.82	0.60
1:J:149:ILE:HG12	1:J:183:ALA:HB3	1.83	0.60
1:D:135:ARG:HH11	1:D:183:ALA:HB2	1.66	0.60
1:F:280:GLU:O	1:F:284:ASN:ND2	2.34	0.60
1:C:135:ARG:HH11	1:C:183:ALA:HB2	1.66	0.60
1:J:128:TRP:HB2	1:L:103:SER:HB2	1.84	0.60
1:F:325:LYS:NZ	1:F:339:PRO:O	2.35	0.60
1:L:155:VAL:HG11	1:L:184:GLY:HA3	1.84	0.59
1:A:150:ARG:HG3	1:A:225:MET:HB2	1.82	0.59
1:B:149:ILE:HG12	1:B:183:ALA:HB3	1.82	0.59
1:C:379:ILE:HG12	1:C:401:ALA:HB3	1.84	0.59
1:E:189:PRO:HG3	1:E:226:SER:HB3	1.83	0.59
1:J:268:ILE:HG12	1:J:314:HIS:HE2	1.67	0.59
1:L:302:THR:HB	1:L:327:ILE:HD13	1.83	0.59
1:D:149:ILE:HG12	1:D:183:ALA:HB3	1.84	0.59
1:J:325:LYS:NZ	1:J:339:PRO:O	2.35	0.59
1:K:422:MET:HB3	1:K:531:LEU:HD22	1.85	0.59
1:L:377:ILE:HG12	1:L:399:ILE:HB	1.85	0.59
1:B:92:GLU:HB3	1:B:96:GLN:HB2	1.85	0.59
1:B:189:PRO:HG3	1:B:226:SER:HB3	1.83	0.59
1:F:308:PHE:HD2	1:F:351:LYS:HD2	1.68	0.59
1:L:395:VAL:HG22	1:L:397:ALA:H	1.67	0.59
1:G:338:ASN:ND2	1:G:362:LYS:O	2.37	0.58
1:A:377:ILE:HG12	1:A:399:ILE:HB	1.86	0.58
1:B:116:SER:HB2	1:E:114:VAL:HB	1.85	0.58
1:H:488:PRO:HB3	1:H:492:PHE:HD2	1.69	0.58
1:H:121:ILE:HG13	1:H:200:ILE:HG12	1.85	0.58
1:J:306:GLN:HG3	1:J:370:ILE:HG21	1.85	0.58
1:K:156:SER:H	1:K:159:GLU:HG2	1.68	0.58
1:H:256:GLY:HA2	1:H:267:ARG:HG2	1.86	0.57
1:I:149:ILE:HG12	1:I:183:ALA:HB3	1.86	0.57
1:I:242:THR:HB	1:L:242:THR:HB	1.86	0.57
1:A:267:ARG:NH2	4:A:602:GGL:OE1	2.37	0.57
1:D:422:MET:HB2	1:D:531:LEU:HD22	1.87	0.57
1:G:379:ILE:HG12	1:G:401:ALA:HB3	1.84	0.57
1:B:150:ARG:NH1	1:B:159:GLU:OE2	2.38	0.57
1:H:93:THR:HG22	1:H:96:GLN:HE22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:292:LEU:HD11	1:L:398:LYS:HB3	1.85	0.57
1:C:77:ALA:HB1	1:C:105:LEU:HD13	1.87	0.57
1:B:77:ALA:HB1	1:B:105:LEU:HD13	1.87	0.57
1:B:292:LEU:HD11	1:B:398:LYS:HB3	1.87	0.57
1:D:374:ASP:HA	1:D:396:LYS:HB2	1.87	0.57
1:G:90:THR:HG21	1:G:100:ARG:HH22	1.69	0.57
1:H:155:VAL:HG11	1:H:184:GLY:HA3	1.87	0.57
1:A:328:THR:HG21	1:A:373:VAL:HG11	1.86	0.57
1:B:425:PRO:HD3	1:B:533:LEU:HB2	1.87	0.57
1:B:135:ARG:HH11	1:B:183:ALA:HB2	1.69	0.57
1:J:114:VAL:HB	1:L:116:SER:HB2	1.87	0.57
1:L:149:ILE:HG12	1:L:183:ALA:HB3	1.86	0.57
1:A:498:GLY:O	1:F:457:TYR:OH	2.17	0.56
1:E:488:PRO:HB3	1:E:492:PHE:HD2	1.70	0.56
1:C:316:MET:HG2	1:C:344:PRO:HG3	1.86	0.56
1:J:467:MET:HA	1:J:470:GLN:HB3	1.86	0.56
1:A:267:ARG:NE	1:A:437:SER:OG	2.38	0.56
1:G:391:ASN:HB3	1:G:394:ARG:HH21	1.70	0.56
1:I:346:GLU:CD	1:I:346:GLU:H	2.13	0.56
1:K:149:ILE:HG12	1:K:183:ALA:HB3	1.86	0.56
1:K:371:LEU:HD21	1:K:386:GLN:HB3	1.86	0.56
1:A:422:MET:HE2	1:A:533:LEU:HD11	1.87	0.56
1:C:267:ARG:NE	1:C:437:SER:OG	2.38	0.56
1:E:224:ASP:OD1	4:E:602:GGL:N	2.35	0.56
1:E:389:LYS:HB3	1:E:411:GLU:HG3	1.88	0.56
1:E:405:ASN:ND2	3:E:601:NAI:O2D	2.38	0.56
1:G:103:SER:HB2	1:I:128:TRP:HB2	1.86	0.56
1:G:511:TYR:HB2	1:L:456:LYS:HB2	1.86	0.56
1:J:464:HIS:HA	1:J:467:MET:HE3	1.87	0.56
1:K:348:GLU:OE2	2:K:600:GTP:N2	2.36	0.56
3:C:602:NAI:N7N	3:C:602:NAI:O1N	2.38	0.56
1:G:377:ILE:HG12	1:G:399:ILE:HB	1.88	0.56
1:L:123:ARG:NH1	1:L:129:GLU:OE1	2.38	0.55
1:E:93:THR:HG22	1:E:96:GLN:HG2	1.87	0.55
1:I:68:MET:HE3	1:I:410:PRO:HD3	1.88	0.55
1:K:256:GLY:HA2	1:K:267:ARG:HG2	1.89	0.55
1:E:491:GLU:OE1	1:E:491:GLU:N	2.24	0.55
1:J:310:ASN:ND2	3:J:602:NAI:O1N	2.40	0.55
1:L:405:ASN:OD1	3:L:603:NAI:O2D	2.24	0.55
1:K:395:VAL:HG22	1:K:397:ALA:H	1.71	0.55
1:A:371:LEU:HD11	1:A:386:GLN:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:ILE:HB	1:C:423:VAL:HG22	1.88	0.55
1:I:378:LEU:HG	1:I:380:PRO:HD3	1.87	0.55
1:L:424:ILE:HG21	1:L:429:LEU:HD13	1.88	0.55
1:A:64:ASN:HB3	1:A:67:LYS:HG2	1.88	0.55
1:D:328:THR:HG23	1:D:337:TRP:HB2	1.87	0.55
1:J:391:ASN:HA	1:J:394:ARG:HE	1.72	0.55
1:E:424:ILE:HG21	1:E:429:LEU:HD13	1.87	0.55
1:G:289:MET:HE2	1:G:289:MET:HA	1.88	0.55
1:A:135:ARG:HH11	1:A:183:ALA:HB2	1.71	0.55
1:B:300:ASP:OD1	1:B:300:ASP:N	2.37	0.55
1:F:317:ARG:HG2	1:F:344:PRO:HB3	1.88	0.55
1:I:422:MET:HB2	1:I:531:LEU:HD22	1.88	0.55
1:F:402:GLU:OE2	1:F:534:ARG:NH2	2.28	0.54
1:K:121:ILE:HG21	1:K:200:ILE:HG12	1.89	0.54
1:D:150:ARG:NH1	1:D:159:GLU:OE2	2.40	0.54
1:E:338:ASN:ND2	1:E:362:LYS:O	2.41	0.54
1:G:150:ARG:NH1	1:G:159:GLU:OE2	2.40	0.54
1:B:93:THR:HG22	1:B:96:GLN:HG2	1.88	0.54
1:B:425:PRO:HB3	1:B:534:ARG:HA	1.90	0.54
1:G:116:SER:HB2	1:I:114:VAL:HB	1.88	0.54
1:F:150:ARG:HG3	1:F:225:MET:HB2	1.89	0.54
1:E:149:ILE:HG12	1:E:183:ALA:HB3	1.87	0.54
1:I:379:ILE:HG12	1:I:401:ALA:HB3	1.88	0.54
1:I:457:TYR:OH	1:J:498:GLY:O	2.25	0.54
1:J:456:LYS:HB2	1:K:511:TYR:HB2	1.88	0.54
1:G:64:ASN:HD22	1:G:67:LYS:NZ	2.06	0.54
1:G:189:PRO:HG3	1:G:226:SER:HB3	1.89	0.54
1:J:256:GLY:HA2	1:J:267:ARG:HG2	1.90	0.54
1:K:325:LYS:NZ	1:K:339:PRO:O	2.41	0.54
1:A:424:ILE:HG21	1:A:429:LEU:HD13	1.88	0.54
1:I:256:GLY:N	1:I:440:GLU:OE2	2.40	0.54
1:J:488:PRO:HB3	1:J:492:PHE:HD2	1.73	0.54
1:K:254:VAL:O	1:K:257:LYS:NZ	2.38	0.54
1:A:360:PHE:HB3	1:A:363:ALA:HB3	1.90	0.53
1:H:297:GLY:O	1:H:301:LYS:NZ	2.30	0.53
1:E:214:ILE:HD12	1:E:221:PRO:HG2	1.90	0.53
1:A:338:ASN:ND2	1:A:362:LYS:O	2.41	0.53
1:D:224:ASP:OD1	4:D:602:GGL:N	2.40	0.53
1:G:64:ASN:HB3	1:G:67:LYS:HG2	1.91	0.53
1:G:185:VAL:HG12	1:G:187:ILE:HG23	1.91	0.53
1:J:96:GLN:H	1:J:96:GLN:CD	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:HIS:HE1	1:E:179:GLY:HA2	1.73	0.53
1:F:222:ALA:HB3	4:F:602:GGL:HB3	1.91	0.53
1:G:488:PRO:HB3	1:G:492:PHE:HD2	1.73	0.53
1:J:106:ARG:NH2	1:L:128:TRP:O	2.42	0.53
1:K:356:THR:HG22	1:K:358:LEU:H	1.72	0.53
1:D:123:ARG:NH1	1:D:129:GLU:OE1	2.36	0.53
1:F:150:ARG:NH1	1:F:159:GLU:OE2	2.41	0.53
3:H:602:NAI:N7N	3:H:602:NAI:O1N	2.41	0.53
1:G:383:SER:HB2	1:G:386:GLN:HE21	1.74	0.53
1:J:135:ARG:HH11	1:J:183:ALA:HB2	1.73	0.53
1:B:465:LEU:HD21	1:F:465:LEU:HD23	1.90	0.53
1:D:189:PRO:HG3	1:D:226:SER:HB3	1.90	0.53
1:B:123:ARG:NH1	1:B:129:GLU:OE1	2.40	0.52
1:B:128:TRP:O	1:E:106:ARG:NH2	2.42	0.52
1:B:338:ASN:HD21	1:B:341:GLY:C	2.17	0.52
1:E:406:GLY:N	1:E:426:ASP:OD2	2.43	0.52
1:G:491:GLU:OE1	1:G:491:GLU:N	2.35	0.52
1:B:328:THR:HG22	1:B:337:TRP:HB2	1.91	0.52
1:E:267:ARG:NE	1:E:437:SER:OG	2.43	0.52
1:I:131:ILE:HG21	1:I:200:ILE:HD11	1.90	0.52
1:L:113:HIS:CE1	1:L:140:GLN:HE21	2.27	0.52
1:J:295:THR:OG1	1:J:300:ASP:OD2	2.27	0.52
1:B:468:SER:HA	1:F:489:THR:HG23	1.92	0.52
1:E:345:LYS:H	1:E:345:LYS:HD2	1.73	0.52
1:H:311:VAL:HG13	1:H:381:ALA:HB1	1.92	0.52
1:K:123:ARG:NH1	1:K:129:GLU:OE1	2.39	0.52
1:L:85:VAL:HG23	1:L:97:LYS:HB2	1.91	0.52
1:C:149:ILE:HG12	1:C:183:ALA:HB3	1.93	0.51
1:D:488:PRO:HB3	1:D:492:PHE:HD2	1.74	0.51
1:G:155:VAL:HG11	1:G:184:GLY:HA3	1.92	0.51
1:B:267:ARG:NH2	4:B:602:GGL:OE1	2.43	0.51
1:K:471:GLU:OE1	1:K:475:ARG:NH2	2.43	0.51
1:B:267:ARG:NE	1:B:437:SER:OG	2.42	0.51
1:J:188:ASN:ND2	1:J:191:ASN:OD1	2.43	0.51
1:J:189:PRO:HG3	1:J:226:SER:HB2	1.92	0.51
1:K:75:ARG:NH2	1:K:535:THR:OG1	2.43	0.51
1:F:321:ARG:NH1	2:F:600:GTP:O3G	2.40	0.51
1:G:448:VAL:HB	1:H:442:LEU:HD21	1.93	0.51
1:G:427:LEU:HD23	1:G:427:LEU:H	1.74	0.51
1:L:77:ALA:HB1	1:L:105:LEU:HD13	1.91	0.51
1:L:163:LEU:HD13	1:L:182:LYS:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:HD13	1:A:182:LYS:HE3	1.93	0.51
1:E:338:ASN:HD22	1:E:363:ALA:HA	1.76	0.51
1:F:267:ARG:NE	1:F:437:SER:OG	2.44	0.51
1:I:369:SER:HB3	1:I:372:GLU:HB2	1.93	0.51
1:B:304:VAL:HG22	1:B:328:THR:H	1.74	0.51
1:F:206:MET:HE1	1:F:243:ILE:HG12	1.92	0.51
1:A:465:LEU:HD21	1:B:465:LEU:HD23	1.92	0.51
1:B:395:VAL:O	1:B:419:ARG:NH2	2.39	0.51
1:D:254:VAL:O	1:D:257:LYS:NZ	2.44	0.51
1:F:189:PRO:HG3	1:F:226:SER:HB3	1.92	0.51
1:F:388:THR:HG22	1:F:389:LYS:H	1.75	0.51
1:I:85:VAL:HG21	1:I:98:ARG:HD2	1.92	0.51
1:I:399:ILE:HG12	1:I:422:MET:HE1	1.92	0.51
1:A:189:PRO:HG3	1:A:226:SER:HB3	1.91	0.50
1:H:468:SER:HA	1:L:489:THR:HG23	1.93	0.50
1:C:425:PRO:HD3	1:C:533:LEU:HB2	1.93	0.50
1:L:325:LYS:NZ	1:L:339:PRO:O	2.39	0.50
1:C:425:PRO:HB3	1:C:534:ARG:HA	1.93	0.50
1:C:488:PRO:HB3	1:C:492:PHE:HD2	1.76	0.50
1:F:310:ASN:OD1	1:F:311:VAL:N	2.45	0.50
1:I:187:ILE:HD13	1:I:200:ILE:HD13	1.94	0.50
1:D:100:ARG:NH2	1:D:550:ASN:OD1	2.35	0.50
1:E:325:LYS:NZ	1:E:339:PRO:O	2.45	0.50
1:F:93:THR:HG23	1:F:96:GLN:H	1.77	0.50
1:H:124:ASP:OD1	1:H:125:ASP:N	2.45	0.50
1:I:371:LEU:HD13	1:I:387:LEU:HD23	1.93	0.50
1:C:189:PRO:HG3	1:C:226:SER:HB3	1.94	0.49
1:I:177:PRO:HA	3:I:603:NAI:H61A	1.77	0.49
1:A:82:ASP:OD1	1:A:83:LYS:N	2.44	0.49
1:C:337:TRP:O	1:C:364:LYS:NZ	2.45	0.49
1:K:163:LEU:HD13	1:K:182:LYS:HE3	1.94	0.49
1:G:381:ALA:HA	1:G:404:ALA:HB2	1.94	0.49
1:H:348:GLU:OE2	2:H:601:GTP:N2	2.28	0.49
1:J:251:HIS:CD2	3:J:604:NAI:H42N	2.48	0.49
1:K:371:LEU:HD23	1:K:387:LEU:HD23	1.92	0.49
1:A:129:GLU:OE2	1:A:192:TYR:OH	2.30	0.49
1:I:65:PHE:HD2	1:I:159:GLU:HB2	1.77	0.49
1:F:316:MET:HG2	1:F:344:PRO:HG3	1.94	0.49
1:J:395:VAL:HG22	1:J:397:ALA:H	1.77	0.49
1:A:328:THR:HG23	1:A:337:TRP:HB2	1.94	0.49
1:G:336:ILE:HG22	1:G:365:ILE:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:405:ASN:OD1	3:H:602:NAI:O2D	2.26	0.49
1:H:377:ILE:HG12	1:H:399:ILE:HB	1.95	0.49
1:I:425:PRO:HD3	1:I:533:LEU:HB2	1.95	0.49
1:G:465:LEU:HD23	1:L:465:LEU:HD21	1.94	0.49
1:A:381:ALA:HA	1:A:404:ALA:HB2	1.95	0.49
1:A:480:HIS:O	1:A:480:HIS:ND1	2.43	0.49
1:D:155:VAL:HG11	1:D:184:GLY:HA3	1.95	0.49
1:H:427:LEU:H	1:H:427:LEU:HD23	1.78	0.49
1:H:294:MET:SD	1:H:295:THR:N	2.85	0.49
1:C:395:VAL:HG22	1:C:397:ALA:H	1.78	0.48
1:H:317:ARG:NH2	2:H:601:GTP:O1G	2.46	0.48
1:J:150:ARG:NH2	3:J:602:NAI:O2D	2.45	0.48
1:J:377:ILE:HG12	1:J:399:ILE:HB	1.95	0.48
1:A:100:ARG:NH1	1:A:550:ASN:OD1	2.46	0.48
1:F:310:ASN:HD21	3:F:601:NAI:H72N	1.61	0.48
1:G:276:PHE:O	1:G:280:GLU:N	2.31	0.48
1:I:388:THR:OG1	1:I:391:ASN:ND2	2.46	0.48
1:B:273:ARG:NH2	2:B:600:GTP:O3G	2.46	0.48
1:B:295:THR:OG1	1:B:300:ASP:OD2	2.31	0.48
1:F:256:GLY:HA2	1:F:267:ARG:HG2	1.94	0.48
1:F:350:PHE:HD2	1:F:360:PHE:HD1	1.61	0.48
1:G:276:PHE:CE1	1:G:319:LEU:HD22	2.48	0.48
1:L:93:THR:HG22	1:L:96:GLN:OE1	2.13	0.48
1:B:400:ILE:HB	1:B:423:VAL:HG22	1.95	0.48
1:E:122:ARG:O	1:E:199:LYS:NZ	2.35	0.48
1:G:338:ASN:HD22	1:G:363:ALA:HA	1.79	0.48
1:J:135:ARG:HD2	1:J:183:ALA:HB2	1.95	0.48
1:E:135:ARG:HH21	1:E:219:ASP:CG	2.22	0.48
1:E:271:THR:OG1	3:E:601:NAI:H42N	2.14	0.48
1:H:163:LEU:HD13	1:H:182:LYS:HE3	1.96	0.48
1:E:491:GLU:H	1:E:491:GLU:CD	2.18	0.48
1:K:83:LYS:NZ	1:K:87:ASP:HB2	2.29	0.48
1:A:338:ASN:HD22	1:A:363:ALA:HA	1.79	0.48
1:G:424:ILE:HG13	1:G:425:PRO:HD2	1.96	0.48
1:G:517:ALA:O	1:G:521:MET:HG3	2.14	0.48
1:H:346:GLU:HB3	1:H:360:PHE:HZ	1.78	0.48
1:H:395:VAL:O	1:H:419:ARG:NH2	2.45	0.48
1:J:267:ARG:NE	1:J:437:SER:OG	2.47	0.48
1:L:517:ALA:O	1:L:521:MET:HG2	2.14	0.48
1:B:455:PHE:HZ	1:B:500:SER:HA	1.78	0.48
1:E:360:PHE:CE2	1:E:362:LYS:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:327:ILE:HD11	1:G:375:CYS:HB3	1.96	0.48
1:L:399:ILE:HG12	1:L:422:MET:HB3	1.95	0.48
1:H:167:MET:HE1	1:H:434:VAL:HG21	1.96	0.48
1:J:305:VAL:HG12	1:J:379:ILE:HB	1.95	0.48
1:B:538:TYR:O	1:B:542:ILE:HG13	2.12	0.47
1:C:325:LYS:NZ	1:C:339:PRO:O	2.47	0.47
1:D:331:GLU:OE2	1:D:351:LYS:NZ	2.47	0.47
1:J:345:LYS:NZ	2:J:601:GTP:O6	2.42	0.47
1:L:338:ASN:HD22	1:L:363:ALA:HA	1.79	0.47
1:H:386:GLN:N	1:H:386:GLN:OE1	2.47	0.47
1:C:163:LEU:HB2	1:C:182:LYS:HG2	1.97	0.47
1:I:495:ARG:HH12	1:K:461:SER:HA	1.79	0.47
1:H:327:ILE:HD11	1:H:375:CYS:HB3	1.95	0.47
1:I:348:GLU:OE2	2:I:601:GTP:N2	2.43	0.47
1:D:400:ILE:HB	1:D:423:VAL:HG22	1.97	0.47
1:I:427:LEU:HD23	1:I:427:LEU:H	1.80	0.47
1:A:135:ARG:HH21	1:A:219:ASP:CG	2.22	0.47
1:D:135:ARG:HH21	1:D:219:ASP:CG	2.21	0.47
1:D:308:PHE:HD2	1:D:351:LYS:HD3	1.80	0.47
1:F:316:MET:HE3	1:F:344:PRO:HA	1.95	0.47
1:G:317:ARG:HG2	1:G:344:PRO:HB2	1.96	0.47
1:L:173:VAL:HG23	1:L:541:ALA:HB2	1.96	0.47
1:L:427:LEU:HD23	1:L:427:LEU:H	1.80	0.47
1:C:489:THR:HG23	1:E:468:SER:HA	1.96	0.47
1:H:303:PHE:CZ	1:H:326:CYS:HB2	2.50	0.47
1:A:214:ILE:HD12	1:A:221:PRO:HG2	1.96	0.47
1:F:238:THR:O	1:F:242:THR:OG1	2.32	0.47
1:H:472:SER:HB3	1:L:486:ILE:HA	1.96	0.47
1:J:427:LEU:H	1:J:427:LEU:HD23	1.80	0.47
1:C:229:GLU:HB3	1:C:268:ILE:HD11	1.96	0.47
1:E:259:ILE:H	1:E:259:ILE:HG12	1.37	0.47
1:F:427:LEU:HD23	1:F:427:LEU:H	1.80	0.47
1:G:308:PHE:CZ	1:G:313:LEU:HD13	2.50	0.47
1:C:294:MET:HG2	1:C:301:LYS:HE3	1.97	0.46
1:H:465:LEU:HD21	1:L:465:LEU:HD23	1.96	0.46
1:J:356:THR:HG22	1:J:358:LEU:H	1.80	0.46
1:D:106:ARG:NH2	1:F:128:TRP:O	2.47	0.46
1:A:288:TYR:CE2	1:A:521:MET:HG2	2.47	0.46
1:D:267:ARG:O	1:D:267:ARG:NH1	2.44	0.46
1:E:370:ILE:HG23	1:E:371:LEU:HG	1.98	0.46
1:G:410:PRO:HA	1:G:413:ASP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:289:MET:HB3	1:H:294:MET:O	2.15	0.46
1:K:64:ASN:HD22	1:K:67:LYS:HG2	1.81	0.46
1:K:492:PHE:O	1:K:496:ILE:N	2.48	0.46
1:D:385:LYS:H	1:D:407:PRO:HA	1.81	0.46
1:F:331:GLU:HB2	1:F:357:ILE:HD11	1.96	0.46
1:F:345:LYS:HB2	1:F:345:LYS:HE2	1.61	0.46
1:H:135:ARG:HH21	1:H:219:ASP:CG	2.24	0.46
1:A:378:LEU:HB3	1:A:400:ILE:HD13	1.96	0.46
1:D:225:MET:HE3	1:D:225:MET:HB2	1.86	0.46
1:K:148:GLY:H	1:K:182:LYS:HD2	1.81	0.46
1:G:149:ILE:HG12	1:G:183:ALA:HB3	1.96	0.46
1:L:214:ILE:HA	1:L:219:ASP:HB3	1.98	0.46
1:L:327:ILE:HD11	1:L:375:CYS:HB3	1.97	0.46
1:D:163:LEU:HB2	1:D:182:LYS:HG2	1.98	0.46
1:E:413:ASP:OD2	1:E:534:ARG:NE	2.46	0.46
1:H:150:ARG:NH1	1:H:159:GLU:OE2	2.48	0.46
1:L:121:ILE:HG21	1:L:200:ILE:HG12	1.97	0.46
1:C:303:PHE:CZ	1:C:326:CYS:HB2	2.51	0.46
1:I:286:ALA:O	1:I:289:MET:HG2	2.15	0.46
1:A:353:GLN:HG3	1:A:354:HIS:ND1	2.31	0.46
1:F:64:ASN:ND2	1:F:158:ASP:OD2	2.42	0.46
1:D:158:ASP:OD1	1:D:158:ASP:N	2.48	0.46
1:E:438:TYR:CZ	1:E:442:LEU:HD11	2.51	0.46
1:L:150:ARG:NH1	1:L:159:GLU:OE2	2.48	0.46
1:A:150:ARG:NH1	1:A:159:GLU:OE2	2.49	0.45
1:C:224:ASP:OD1	4:C:603:GGL:N	2.49	0.45
1:D:93:THR:HG23	1:D:96:GLN:H	1.80	0.45
1:D:150:ARG:HG3	1:D:225:MET:HB3	1.98	0.45
1:D:391:ASN:HA	1:D:394:ARG:HE	1.80	0.45
1:D:405:ASN:ND2	3:D:601:NAI:O2D	2.48	0.45
1:I:77:ALA:HB1	1:I:105:LEU:HD13	1.98	0.45
1:B:455:PHE:HD2	1:F:511:TYR:CE2	2.34	0.45
1:D:112:ASN:ND2	1:D:140:GLN:OE1	2.45	0.45
1:D:268:ILE:HD12	1:D:268:ILE:H	1.80	0.45
1:E:311:VAL:HG13	1:E:381:ALA:HB1	1.98	0.45
1:L:225:MET:HE2	3:L:603:NAI:H3D	1.98	0.45
1:D:259:ILE:H	1:D:259:ILE:HG12	1.36	0.45
1:E:275:VAL:HG23	1:E:429:LEU:HG	1.97	0.45
1:I:292:LEU:HD11	1:I:398:LYS:HB3	1.98	0.45
1:I:343:ASP:HB3	1:I:346:GLU:OE1	2.16	0.45
1:I:395:VAL:HG22	1:I:397:ALA:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:337:TRP:CE2	1:J:339:PRO:HD3	2.51	0.45
1:L:259:ILE:H	1:L:259:ILE:HG12	1.32	0.45
1:G:135:ARG:HH21	1:G:219:ASP:CG	2.23	0.45
1:J:258:PRO:HG2	1:J:261:GLN:HB2	1.98	0.45
1:A:92:GLU:HB3	1:A:96:GLN:HB2	1.98	0.45
1:F:254:VAL:O	1:F:257:LYS:NZ	2.40	0.45
1:G:106:ARG:NH2	1:I:128:TRP:O	2.47	0.45
1:I:135:ARG:HH21	1:I:219:ASP:CG	2.23	0.45
1:I:377:ILE:HG12	1:I:399:ILE:HB	1.97	0.45
1:D:142:ARG:HH21	1:D:177:PRO:HB3	1.81	0.45
1:G:123:ARG:NH1	1:G:129:GLU:OE1	2.48	0.45
1:J:144:PRO:HB3	1:J:217:GLY:C	2.42	0.45
1:J:424:ILE:HG21	1:J:429:LEU:HD13	1.98	0.45
1:C:93:THR:HG23	1:C:96:GLN:H	1.82	0.45
1:D:67:LYS:HA	1:D:67:LYS:HD2	1.76	0.45
1:D:395:VAL:HG22	1:D:397:ALA:H	1.81	0.45
1:L:328:THR:HG1	1:L:337:TRP:CD1	2.35	0.45
1:A:294:MET:HE1	1:A:376:ASP:HB3	1.99	0.45
1:B:137:GLN:OE1	1:B:140:GLN:NE2	2.50	0.45
1:H:347:LEU:O	1:H:351:LYS:N	2.36	0.45
1:L:480:HIS:HD1	1:L:480:HIS:H	1.64	0.45
1:A:173:VAL:HG23	1:A:541:ALA:HB2	1.98	0.45
1:C:402:GLU:OE2	1:C:534:ARG:NH2	2.29	0.45
1:F:135:ARG:NE	1:F:219:ASP:OD2	2.45	0.45
1:H:379:ILE:HA	1:H:401:ALA:O	2.17	0.45
1:I:166:LEU:HD12	1:I:166:LEU:HA	1.85	0.45
1:K:529:LEU:HD12	1:K:532:ASP:HB3	1.98	0.45
1:L:135:ARG:HH21	1:L:219:ASP:CG	2.25	0.45
1:L:425:PRO:HG2	1:L:428:TYR:HB3	1.98	0.45
1:F:225:MET:HE2	1:F:225:MET:HB3	1.83	0.45
1:G:276:PHE:CZ	1:G:319:LEU:HA	2.52	0.45
1:J:304:VAL:HG22	1:J:328:THR:HB	1.99	0.45
1:L:230:ARG:O	1:L:233:SER:OG	2.33	0.45
1:B:210:LYS:HG2	1:D:245:HIS:CG	2.52	0.44
1:D:152:SER:HB3	1:D:155:VAL:HG23	1.99	0.44
1:D:457:TYR:OH	1:E:498:GLY:O	2.24	0.44
1:G:276:PHE:HE1	1:G:319:LEU:HD22	1.81	0.44
1:G:331:GLU:HB2	1:G:357:ILE:HD11	1.98	0.44
1:G:425:PRO:HG2	1:G:428:TYR:HB3	1.99	0.44
1:H:275:VAL:HG23	1:H:429:LEU:HD21	1.99	0.44
1:H:342:ILE:HG22	1:H:347:LEU:HD21	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:256:GLY:HA2	1:I:267:ARG:HG2	1.98	0.44
1:J:295:THR:O	1:J:301:LYS:NZ	2.34	0.44
1:J:402:GLU:OE2	1:J:534:ARG:NH2	2.39	0.44
1:A:281:ASN:HD22	1:A:281:ASN:HA	1.57	0.44
1:D:167:MET:HB3	1:D:180:GLY:HA2	1.99	0.44
1:D:456:LYS:HB2	1:E:511:TYR:HB2	1.99	0.44
1:I:289:MET:HE1	1:I:296:PRO:HD3	1.98	0.44
1:J:68:MET:HG2	1:J:410:PRO:HD3	1.99	0.44
1:J:338:ASN:HD22	1:J:363:ALA:HA	1.82	0.44
1:D:222:ALA:HB3	4:D:602:GGL:HB3	2.00	0.44
1:E:427:LEU:H	1:E:427:LEU:HD23	1.82	0.44
1:G:153:THR:O	1:G:186:LYS:NZ	2.51	0.44
1:G:328:THR:HG23	1:G:337:TRP:HB2	1.99	0.44
1:K:331:GLU:HB2	1:K:357:ILE:HD11	1.98	0.44
1:A:128:TRP:O	1:C:106:ARG:NH2	2.50	0.44
1:A:511:TYR:HB2	1:F:456:LYS:HB2	2.00	0.44
1:B:257:LYS:HE2	1:B:257:LYS:HB2	1.59	0.44
1:C:465:LEU:HD23	1:E:465:LEU:HD11	1.98	0.44
1:L:256:GLY:HA2	1:L:267:ARG:HG2	1.98	0.44
1:C:472:SER:HB2	1:D:486:ILE:HD13	1.99	0.44
1:F:135:ARG:HH21	1:F:219:ASP:CG	2.25	0.44
1:C:278:GLY:HA3	1:C:429:LEU:HD12	1.99	0.44
1:C:406:GLY:N	1:C:426:ASP:OD2	2.51	0.44
1:H:77:ALA:HB1	1:H:105:LEU:HD13	2.00	0.44
1:H:280:GLU:HA	1:H:283:ILE:HG22	1.99	0.44
1:K:327:ILE:HG13	1:K:328:THR:N	2.33	0.44
1:L:521:MET:O	1:L:525:MET:HG2	2.17	0.44
1:A:107:ILE:HG12	1:C:120:PRO:HB3	1.99	0.44
1:B:488:PRO:HB3	1:B:492:PHE:HD2	1.83	0.44
1:H:149:ILE:HG12	1:H:183:ALA:HB3	2.00	0.44
1:B:470:GLN:NE2	1:B:484:ILE:O	2.38	0.44
1:E:205:THR:HG23	1:E:214:ILE:HD13	2.00	0.44
1:H:371:LEU:HD13	1:H:387:LEU:HD23	2.00	0.44
1:A:93:THR:HG22	1:A:96:GLN:HG3	2.00	0.43
1:D:377:ILE:HG12	1:D:399:ILE:HB	2.00	0.43
1:L:384:GLU:O	1:L:386:GLN:NE2	2.51	0.43
1:C:425:PRO:HB2	1:C:427:LEU:HD23	2.00	0.43
1:D:303:PHE:CZ	1:D:326:CYS:HB2	2.53	0.43
1:F:276:PHE:HD2	1:F:319:LEU:HD23	1.83	0.43
1:G:259:ILE:H	1:G:259:ILE:HG12	1.31	0.43
1:J:128:TRP:CD1	1:J:128:TRP:N	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:379:ILE:HG13	1:J:401:ALA:HB3	2.00	0.43
1:K:370:ILE:HG23	1:K:371:LEU:HD12	1.99	0.43
1:K:519:GLN:HG2	1:K:522:ARG:HH22	1.83	0.43
1:B:529:LEU:HD22	1:B:536:ALA:HB2	2.00	0.43
1:D:343:ASP:HB3	1:D:346:GLU:HG2	2.00	0.43
1:I:425:PRO:HG2	1:I:428:TYR:HB3	2.01	0.43
1:C:477:PHE:HZ	1:D:477:PHE:HE2	1.67	0.43
1:E:146:LYS:NZ	4:E:602:GGL:OE1	2.46	0.43
1:G:142:ARG:HD2	3:L:601:NAI:H4N	2.00	0.43
1:G:268:ILE:HG23	1:G:314:HIS:CE1	2.50	0.43
3:K:601:NAI:N7N	3:K:601:NAI:O1N	2.51	0.43
1:B:225:MET:HG3	3:B:601:NAI:H3D	2.00	0.43
1:D:308:PHE:CD2	1:D:351:LYS:HD3	2.53	0.43
1:D:409:THR:HG22	1:D:411:GLU:H	1.83	0.43
1:E:463:TYR:HE1	1:E:496:ILE:HG12	1.84	0.43
1:F:327:ILE:HD11	1:F:339:PRO:HA	2.00	0.43
1:G:471:GLU:OE2	1:G:475:ARG:NH2	2.52	0.43
1:I:85:VAL:HG21	1:I:98:ARG:HH11	1.83	0.43
1:A:98:ARG:HG2	1:A:102:ARG:HH21	1.83	0.43
1:G:326:CYS:O	1:G:341:GLY:HA2	2.19	0.43
1:J:167:MET:HE2	1:J:167:MET:HB2	1.86	0.43
1:K:135:ARG:HH21	1:K:219:ASP:CG	2.26	0.43
1:K:427:LEU:HD23	1:K:427:LEU:H	1.83	0.43
1:D:388:THR:HG23	1:D:390:SER:H	1.84	0.43
1:E:129:GLU:OE2	1:E:192:TYR:OH	2.37	0.43
1:G:163:LEU:HD13	1:G:182:LYS:HE3	2.01	0.43
1:G:256:GLY:HA2	1:G:267:ARG:HG2	2.00	0.43
1:I:529:LEU:HD12	1:I:532:ASP:HB3	2.01	0.43
1:L:311:VAL:HG13	1:L:381:ALA:HB1	2.00	0.43
1:A:295:THR:OG1	1:A:300:ASP:OD2	2.33	0.43
1:B:425:PRO:HB2	1:B:427:LEU:HD23	2.01	0.43
1:C:112:ASN:ND2	1:C:140:GLN:OE1	2.46	0.43
1:E:221:PRO:HB2	1:E:254:VAL:HG23	2.00	0.43
1:A:340:ASP:OD2	1:A:362:LYS:NZ	2.51	0.43
1:D:222:ALA:C	1:D:232:MET:HE2	2.43	0.43
1:E:225:MET:HG3	3:E:601:NAI:H3D	2.00	0.43
1:H:406:GLY:N	1:H:426:ASP:OD2	2.52	0.43
1:L:93:THR:N	1:L:96:GLN:OE1	2.45	0.43
1:L:152:SER:HB3	1:L:155:VAL:HG23	2.01	0.43
1:C:257:LYS:HB2	1:C:257:LYS:HE2	1.46	0.43
1:E:333:ASP:HB2	1:E:358:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:149:ILE:HG12	1:F:183:ALA:HB3	2.00	0.43
1:G:63:PRO:HB2	1:G:68:MET:HE2	2.00	0.43
1:H:428:TYR:OH	1:H:517:ALA:HB2	2.19	0.43
1:I:96:GLN:H	1:I:96:GLN:HG3	1.68	0.43
1:J:257:LYS:HE2	1:J:257:LYS:HB2	1.81	0.43
1:J:292:LEU:HD11	1:J:398:LYS:HB3	2.00	0.43
1:B:163:LEU:HB3	1:B:182:LYS:HD3	2.00	0.42
1:D:304:VAL:HG13	1:D:328:THR:HB	2.01	0.42
1:D:348:GLU:OE2	2:D:600:GTP:N2	2.41	0.42
1:D:173:VAL:HG23	1:D:541:ALA:HB2	2.01	0.42
1:E:92:GLU:HB2	1:E:96:GLN:HB2	2.01	0.42
1:F:417:LEU:HD12	1:F:417:LEU:HA	1.85	0.42
1:G:391:ASN:HA	1:G:394:ARG:HE	1.83	0.42
3:G:603:NAI:N3A	1:H:544:LYS:HB3	2.34	0.42
1:I:489:THR:HG23	1:I:492:PHE:H	1.84	0.42
1:B:337:TRP:HB3	1:B:366:TYR:HB2	2.01	0.42
1:B:401:ALA:HA	1:B:424:ILE:HD12	2.02	0.42
1:B:424:ILE:HG21	1:B:429:LEU:HD13	2.00	0.42
1:D:427:LEU:HD23	1:D:427:LEU:H	1.84	0.42
1:F:425:PRO:HG2	1:F:428:TYR:HB3	2.02	0.42
1:G:310:ASN:ND2	3:G:602:NAI:O1N	2.44	0.42
1:I:405:ASN:ND2	3:I:602:NAI:O2D	2.52	0.42
1:K:329:VAL:HG11	1:K:347:LEU:HD21	2.02	0.42
1:A:464:HIS:CE1	1:B:495:ARG:HH21	2.37	0.42
1:B:283:ILE:HD11	1:B:377:ILE:HD11	2.01	0.42
1:C:544:LYS:HB3	3:C:604:NAI:N3A	2.34	0.42
1:G:77:ALA:HB1	1:G:105:LEU:HD13	2.02	0.42
1:G:305:VAL:HG12	1:G:379:ILE:HB	2.01	0.42
1:J:274:GLY:O	1:J:513:MET:HE1	2.20	0.42
1:L:340:ASP:OD2	1:L:362:LYS:NZ	2.53	0.42
1:A:326:CYS:C	1:A:327:ILE:HD13	2.45	0.42
1:B:403:GLY:O	1:B:430:ASN:ND2	2.44	0.42
1:C:422:MET:HB2	1:C:531:LEU:HD22	2.02	0.42
1:C:504:ILE:HD13	1:C:504:ILE:HA	1.94	0.42
1:G:96:GLN:OE1	1:G:96:GLN:N	2.32	0.42
1:K:300:ASP:OD1	1:K:301:LYS:NZ	2.47	0.42
1:D:517:ALA:O	1:D:521:MET:HG3	2.19	0.42
1:E:77:ALA:HB1	1:E:105:LEU:HD13	2.02	0.42
1:I:143:THR:HG23	3:I:603:NAI:H72N	1.85	0.42
1:K:402:GLU:OE2	1:K:534:ARG:NH2	2.47	0.42
1:A:360:PHE:CD1	1:A:361:PRO:HD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:MET:HE3	3:F:601:NAI:H51A	2.02	0.42
1:G:473:LEU:HD13	1:L:473:LEU:HD21	2.01	0.42
1:H:382:ALA:HB1	3:H:602:NAI:C4A	2.50	0.42
1:A:141:HIS:CD2	1:A:142:ARG:HG2	2.55	0.42
1:A:467:MET:HA	1:A:467:MET:HE2	2.01	0.42
1:B:135:ARG:HH21	1:B:219:ASP:CG	2.27	0.42
1:B:406:GLY:N	1:B:426:ASP:OD2	2.52	0.42
1:F:222:ALA:C	1:F:232:MET:HE3	2.45	0.42
1:J:402:GLU:HB3	1:J:426:ASP:HB3	2.02	0.42
1:K:259:ILE:H	1:K:259:ILE:HG12	1.38	0.42
1:A:392:ALA:O	1:A:395:VAL:HG12	2.20	0.42
1:A:471:GLU:OE1	1:A:475:ARG:NH2	2.52	0.42
1:B:373:VAL:HG23	1:B:375:CYS:SG	2.60	0.42
1:C:185:VAL:HG12	1:C:187:ILE:HG23	2.02	0.42
1:D:107:ILE:HG12	1:F:120:PRO:HB3	2.02	0.42
1:E:278:GLY:HA3	1:E:429:LEU:HD12	2.02	0.42
1:H:321:ARG:HH22	2:H:601:GTP:PG	2.43	0.42
1:I:76:GLY:O	1:I:80:VAL:HG12	2.19	0.42
1:I:517:ALA:O	1:I:521:MET:HG3	2.20	0.42
1:J:529:LEU:HD12	1:J:536:ALA:HB2	2.02	0.42
1:K:252:ALA:HB2	1:K:444:ASN:HB2	2.02	0.42
1:K:267:ARG:NE	1:K:437:SER:OG	2.52	0.42
1:E:176:VAL:O	1:E:178:PHE:N	2.52	0.42
1:I:189:PRO:HG3	1:I:226:SER:HB2	2.01	0.42
1:H:370:ILE:O	1:H:373:VAL:HG12	2.20	0.41
1:H:383:SER:N	1:H:386:GLN:HE22	2.17	0.41
1:I:117:LEU:HD21	1:I:207:GLU:HB2	2.02	0.41
1:K:115:LEU:HG	1:K:117:LEU:HD12	2.02	0.41
1:A:257:LYS:HB2	1:A:257:LYS:HE2	1.54	0.41
1:I:267:ARG:NE	1:I:437:SER:OG	2.53	0.41
1:J:163:LEU:HD13	1:J:182:LYS:HZ2	1.85	0.41
1:L:91:ARG:H	1:L:91:ARG:HG2	1.72	0.41
1:A:210:LYS:HD2	1:E:245:HIS:CE1	2.55	0.41
1:C:141:HIS:CD2	1:C:142:ARG:HG2	2.56	0.41
1:E:225:MET:HE2	1:E:225:MET:HB3	1.73	0.41
1:F:308:PHE:CD2	1:F:351:LYS:HD2	2.53	0.41
1:G:371:LEU:HD11	1:G:386:GLN:HB3	2.02	0.41
1:I:467:MET:HA	1:I:470:GLN:HB3	2.02	0.41
1:L:360:PHE:CD1	1:L:361:PRO:HD2	2.55	0.41
1:A:288:TYR:HB3	1:A:422:MET:HE1	2.02	0.41
1:K:84:LEU:HD12	1:K:84:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLU:OE2	1:B:102:ARG:NE	2.53	0.41
1:C:392:ALA:O	1:C:395:VAL:HG12	2.21	0.41
1:E:330:GLY:HA3	1:E:370:ILE:HG12	2.02	0.41
1:G:69:VAL:HG11	1:G:165:SER:HB2	2.02	0.41
1:G:121:ILE:HG21	1:G:200:ILE:HG12	2.01	0.41
1:H:504:ILE:HD13	1:H:504:ILE:HA	1.91	0.41
1:K:168:THR:OG1	1:K:180:GLY:HA3	2.20	0.41
1:A:476:LYS:HD3	1:B:485:PRO:HD2	2.03	0.41
1:D:279:ILE:O	1:D:283:ILE:N	2.53	0.41
1:D:292:LEU:HD11	1:D:398:LYS:HB3	2.01	0.41
1:D:488:PRO:HB3	1:D:492:PHE:CD2	2.55	0.41
1:E:343:ASP:OD2	1:E:346:GLU:HG3	2.20	0.41
1:F:328:THR:HG1	1:F:337:TRP:CD1	2.38	0.41
1:K:303:PHE:CZ	1:K:326:CYS:HB2	2.56	0.41
1:L:378:LEU:HB3	1:L:400:ILE:HD13	2.03	0.41
1:C:65:PHE:CD1	1:C:68:MET:HE2	2.56	0.41
1:C:422:MET:HB2	1:C:531:LEU:HD13	2.02	0.41
1:E:371:LEU:HD13	1:E:387:LEU:HD23	2.02	0.41
1:F:459:ARG:HE	1:F:497:SER:HA	1.85	0.41
1:G:141:HIS:CD2	1:G:142:ARG:HG2	2.55	0.41
1:J:371:LEU:HD12	1:J:371:LEU:H	1.85	0.41
1:L:148:GLY:H	1:L:182:LYS:HD2	1.86	0.41
1:L:428:TYR:OH	1:L:517:ALA:HB2	2.21	0.41
1:A:77:ALA:HB1	1:A:105:LEU:HD13	2.02	0.41
1:F:504:ILE:HD13	1:F:504:ILE:HA	1.93	0.41
1:I:424:ILE:HG21	1:I:429:LEU:HD13	2.02	0.41
1:A:114:VAL:HB	1:C:116:SER:HB2	2.02	0.41
1:A:336:ILE:HG12	1:A:357:ILE:HD12	2.03	0.41
1:A:402:GLU:OE2	1:A:534:ARG:NH2	2.32	0.41
1:A:425:PRO:HD3	1:A:533:LEU:HB2	2.02	0.41
1:C:271:THR:OG1	3:C:602:NAI:H42N	2.21	0.41
1:D:271:THR:OG1	3:D:601:NAI:H42N	2.21	0.41
1:H:116:SER:HB2	1:K:114:VAL:HB	2.02	0.41
1:H:129:GLU:OE2	1:H:192:TYR:OH	2.36	0.41
1:H:414:LYS:HE2	1:H:414:LYS:HB2	1.84	0.41
1:I:144:PRO:HB3	1:I:217:GLY:C	2.46	0.41
1:I:267:ARG:O	1:I:267:ARG:NH1	2.50	0.41
1:I:426:ASP:OD1	1:I:426:ASP:N	2.53	0.41
1:F:146:LYS:O	1:F:167:MET:HG2	2.20	0.41
1:F:280:GLU:HA	1:F:283:ILE:HG22	2.04	0.41
1:G:455:PHE:CZ	1:G:500:SER:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:406:GLY:N	1:K:426:ASP:OD2	2.54	0.41
1:B:278:GLY:HA3	1:B:429:LEU:HD12	2.02	0.40
1:C:511:TYR:HB2	1:E:456:LYS:HB2	2.03	0.40
1:H:68:MET:HE1	1:H:385:LYS:HG2	2.03	0.40
1:J:370:ILE:HD12	1:J:370:ILE:HA	1.95	0.40
1:J:381:ALA:HA	1:J:404:ALA:HB2	2.02	0.40
1:K:305:VAL:HG22	1:K:379:ILE:HB	2.04	0.40
1:K:377:ILE:HG12	1:K:399:ILE:HD12	2.03	0.40
1:L:303:PHE:HE1	1:L:305:VAL:HG23	1.86	0.40
1:A:488:PRO:HB3	1:A:492:PHE:HD2	1.86	0.40
1:F:529:LEU:HD12	1:F:536:ALA:HB2	2.02	0.40
1:G:392:ALA:O	1:G:395:VAL:HG22	2.21	0.40
1:H:289:MET:SD	1:H:289:MET:N	2.95	0.40
1:H:328:THR:HG23	1:H:337:TRP:HB2	2.03	0.40
1:I:155:VAL:HA	1:I:159:GLU:OE2	2.21	0.40
1:B:327:ILE:O	1:B:342:ILE:HD11	2.21	0.40
1:K:520:ILE:HG23	1:K:521:MET:SD	2.61	0.40
1:A:146:LYS:O	1:A:167:MET:HG2	2.22	0.40
1:A:345:LYS:HE2	1:A:345:LYS:HB2	1.87	0.40
1:C:383:SER:HB2	1:C:386:GLN:NE2	2.35	0.40
1:F:360:PHE:CE2	1:F:362:LYS:HB3	2.57	0.40
1:H:222:ALA:C	1:H:232:MET:HE3	2.47	0.40
1:H:455:PHE:HD1	1:H:455:PHE:HA	1.81	0.40
1:K:308:PHE:HD2	1:K:351:LYS:HD2	1.86	0.40
1:K:378:LEU:HB3	1:K:400:ILE:HD13	2.04	0.40
1:C:360:PHE:CE2	1:C:362:LYS:HB3	2.56	0.40
1:D:392:ALA:O	1:D:395:VAL:HG12	2.22	0.40
1:F:294:MET:HE1	1:F:376:ASP:HB3	2.04	0.40
1:F:484:ILE:HA	1:F:485:PRO:HD3	1.96	0.40
3:H:603:NAI:H4N	1:L:142:ARG:HD3	2.02	0.40
1:I:429:LEU:HD12	1:I:429:LEU:HA	1.82	0.40
1:K:129:GLU:OE2	1:K:192:TYR:OH	2.36	0.40
1:L:425:PRO:HB3	1:L:534:ARG:HA	2.03	0.40
1:L:451:GLY:HA3	1:L:499:ALA:O	2.22	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 PDB entries followed by that with respect to all EM entries.

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	491/558 (88%)	483 (98%)	8 (2%)	0	100	100
1	B	491/558 (88%)	478 (97%)	13 (3%)	0	100	100
1	C	491/558 (88%)	480 (98%)	11 (2%)	0	100	100
1	D	491/558 (88%)	479 (98%)	12 (2%)	0	100	100
1	E	491/558 (88%)	480 (98%)	11 (2%)	0	100	100
1	F	491/558 (88%)	474 (96%)	17 (4%)	0	100	100
1	G	491/558 (88%)	478 (97%)	13 (3%)	0	100	100
1	H	491/558 (88%)	481 (98%)	10 (2%)	0	100	100
1	I	491/558 (88%)	485 (99%)	6 (1%)	0	100	100
1	J	491/558 (88%)	481 (98%)	10 (2%)	0	100	100
1	K	491/558 (88%)	479 (98%)	12 (2%)	0	100	100
1	L	491/558 (88%)	481 (98%)	10 (2%)	0	100	100
All	All	5892/6696 (88%)	5759 (98%)	133 (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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	413/456 (91%)	402 (97%)	11 (3%)	39	62
1	B	413/456 (91%)	401 (97%)	12 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	413/456 (91%)	406 (98%)	7 (2%)	53	70
1	D	413/456 (91%)	406 (98%)	7 (2%)	53	70
1	E	413/456 (91%)	408 (99%)	5 (1%)	63	73
1	F	413/456 (91%)	406 (98%)	7 (2%)	53	70
1	G	413/456 (91%)	406 (98%)	7 (2%)	53	70
1	H	413/456 (91%)	405 (98%)	8 (2%)	50	68
1	I	413/456 (91%)	407 (98%)	6 (2%)	57	71
1	J	413/456 (91%)	403 (98%)	10 (2%)	43	64
1	K	413/456 (91%)	405 (98%)	8 (2%)	50	68
1	L	413/456 (91%)	405 (98%)	8 (2%)	50	68
All	All	4956/5472 (91%)	4860 (98%)	96 (2%)	49	68

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	THR
1	A	257	LYS
1	A	259	ILE
1	A	260	SER
1	A	261	GLN
1	A	280	GLU
1	A	281	ASN
1	A	283	ILE
1	A	284	ASN
1	A	449	SER
1	A	514	GLU
1	B	259	ILE
1	B	261	GLN
1	B	325	LYS
1	B	327	ILE
1	B	328	THR
1	B	336	ILE
1	B	337	TRP
1	B	342	ILE
1	B	345	LYS
1	B	362	LYS
1	B	443	ASN
1	B	449	SER

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Mol	Chain	Res	Type
1	C	143	THR
1	C	251	HIS
1	C	257	LYS
1	C	259	ILE
1	C	261	GLN
1	C	264	ILE
1	C	449	SER
1	D	143	THR
1	D	158	ASP
1	D	175	ASP
1	D	259	ILE
1	D	260	SER
1	D	449	SER
1	D	528	ASN
1	E	143	THR
1	E	218	VAL
1	E	259	ILE
1	E	260	SER
1	E	455	PHE
1	F	259	ILE
1	F	260	SER
1	F	342	ILE
1	F	345	LYS
1	F	449	SER
1	F	483	THR
1	F	487	VAL
1	G	178	PHE
1	G	251	HIS
1	G	259	ILE
1	G	260	SER
1	G	442	LEU
1	G	443	ASN
1	G	449	SER
1	H	65	PHE
1	H	67	LYS
1	H	175	ASP
1	H	251	HIS
1	H	259	ILE
1	H	260	SER
1	H	261	GLN
1	H	449	SER
1	I	143	THR

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Mol	Chain	Res	Type
1	I	251	HIS
1	I	259	ILE
1	I	261	GLN
1	I	449	SER
1	I	501	GLU
1	J	143	THR
1	J	175	ASP
1	J	178	PHE
1	J	251	HIS
1	J	259	ILE
1	J	260	SER
1	J	261	GLN
1	J	443	ASN
1	J	449	SER
1	J	501	GLU
1	K	178	PHE
1	K	259	ILE
1	K	260	SER
1	K	261	GLN
1	K	316	MET
1	K	449	SER
1	K	501	GLU
1	K	547	ARG
1	L	178	PHE
1	L	251	HIS
1	L	259	ILE
1	L	294	MET
1	L	295	THR
1	L	298	PHE
1	L	449	SER
1	L	531	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	HIS
1	A	284	ASN
1	A	447	HIS
1	A	493	GLN
1	B	251	HIS
1	B	265	HIS
1	B	338	ASN

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Mol	Chain	Res	Type
1	C	96	GLN
1	C	249	ASN
1	C	284	ASN
1	C	447	HIS
1	C	480	HIS
1	C	540	ASN
1	D	284	ASN
1	D	353	GLN
1	D	420	ASN
1	D	443	ASN
1	D	447	HIS
1	E	265	HIS
1	E	284	ASN
1	E	338	ASN
1	E	447	HIS
1	F	140	GLN
1	F	245	HIS
1	F	443	ASN
1	F	444	ASN
1	F	447	HIS
1	F	493	GLN
1	F	550	ASN
1	G	64	ASN
1	G	137	GLN
1	G	265	HIS
1	G	443	ASN
1	H	405	ASN
1	H	420	ASN
1	H	447	HIS
1	H	550	ASN
1	I	284	ASN
1	I	354	HIS
1	I	443	ASN
1	I	462	ASN
1	J	261	GLN
1	J	284	ASN
1	J	310	ASN
1	J	443	ASN
1	J	550	ASN
1	K	284	ASN
1	K	405	ASN
1	K	444	ASN

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Mol	Chain	Res	Type
1	K	447	HIS
1	K	519	GLN
1	K	528	ASN
1	L	137	GLN
1	L	140	GLN
1	L	261	GLN
1	L	265	HIS
1	L	443	ASN
1	L	444	ASN
1	L	447	HIS
1	L	470	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 oligosaccharides in this entry.

5.6 Ligand geometry

42 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAI	A	603	-	47,48,48	1.31	5 (10%)	64,73,73	1.04	3 (4%)
3	NAI	J	602	-	47,48,48	1.32	6 (12%)	64,73,73	1.03	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GGL	A	602	-	8,9,9	1.12	0	8,11,11	0.69	0
3	NAI	C	605	-	47,48,48	1.32	5 (10%)	64,73,73	1.06	3 (4%)
2	GTP	G	601	-	33,34,34	2.39	9 (27%)	50,54,54	1.75	10 (20%)
3	NAI	D	601	-	47,48,48	1.32	5 (10%)	64,73,73	1.03	3 (4%)
2	GTP	F	600	-	33,34,34	2.40	9 (27%)	50,54,54	1.76	11 (22%)
2	GTP	E	600	-	33,34,34	2.38	9 (27%)	50,54,54	1.77	12 (24%)
2	GTP	I	601	-	33,34,34	2.39	9 (27%)	50,54,54	1.77	11 (22%)
3	NAI	C	602	-	47,48,48	1.30	5 (10%)	64,73,73	1.03	2 (3%)
2	GTP	L	602	-	33,34,34	2.40	9 (27%)	50,54,54	1.76	11 (22%)
2	GTP	D	600	-	33,34,34	2.42	9 (27%)	50,54,54	1.77	11 (22%)
3	NAI	F	601	-	47,48,48	1.33	6 (12%)	64,73,73	1.03	2 (3%)
3	NAI	H	603	-	47,48,48	1.33	6 (12%)	64,73,73	1.03	3 (4%)
3	NAI	L	603	-	47,48,48	1.32	6 (12%)	64,73,73	1.05	3 (4%)
3	NAI	B	603	-	47,48,48	1.33	5 (10%)	64,73,73	1.06	3 (4%)
3	NAI	J	604	-	47,48,48	1.34	6 (12%)	64,73,73	1.03	3 (4%)
3	NAI	A	601	-	47,48,48	1.31	6 (12%)	64,73,73	1.03	2 (3%)
3	NAI	D	603	-	47,48,48	1.31	4 (8%)	64,73,73	1.05	3 (4%)
3	NAI	F	603	-	47,48,48	1.33	6 (12%)	64,73,73	1.03	3 (4%)
2	GTP	H	601	-	33,34,34	2.40	9 (27%)	50,54,54	1.76	10 (20%)
2	GTP	B	600	-	33,34,34	2.37	9 (27%)	50,54,54	1.76	11 (22%)
3	NAI	I	603	-	47,48,48	1.32	6 (12%)	64,73,73	1.07	3 (4%)
4	GGL	E	602	-	8,9,9	1.11	0	8,11,11	0.67	0
3	NAI	H	602	-	47,48,48	1.32	6 (12%)	64,73,73	1.03	2 (3%)
3	NAI	C	604	-	47,48,48	1.36	5 (10%)	64,73,73	1.03	3 (4%)
2	GTP	A	600	-	33,34,34	2.38	9 (27%)	50,54,54	1.76	11 (22%)
4	GGL	D	602	-	8,9,9	1.17	0	8,11,11	0.66	0
4	GGL	B	602	-	8,9,9	1.12	0	8,11,11	0.68	0
3	NAI	L	601	-	47,48,48	1.33	6 (12%)	64,73,73	1.04	3 (4%)
3	NAI	G	602	-	47,48,48	1.33	6 (12%)	64,73,73	1.02	2 (3%)
3	NAI	K	601	-	47,48,48	1.30	6 (12%)	64,73,73	1.02	2 (3%)
4	GGL	F	602	-	8,9,9	1.14	0	8,11,11	0.66	0
2	GTP	J	601	-	33,34,34	2.40	9 (27%)	50,54,54	1.76	10 (20%)
2	GTP	C	601	-	33,34,34	2.39	9 (27%)	50,54,54	1.77	11 (22%)
4	GGL	C	603	-	8,9,9	1.15	0	8,11,11	0.64	0
3	NAI	I	602	-	47,48,48	1.31	6 (12%)	64,73,73	1.04	2 (3%)
3	NAI	B	601	-	47,48,48	1.31	6 (12%)	64,73,73	1.03	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAI	G	603	-	47,48,48	1.30	4 (8%)	64,73,73	1.03	2 (3%)
2	GTP	K	600	-	33,34,34	2.38	9 (27%)	50,54,54	1.77	11 (22%)
3	NAI	J	603	-	47,48,48	1.35	6 (12%)	64,73,73	1.05	3 (4%)
3	NAI	E	601	-	47,48,48	1.30	6 (12%)	64,73,73	1.06	3 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAI	A	603	-	-	7/29/72/72	0/5/5/5
3	NAI	J	602	-	-	11/29/72/72	0/5/5/5
4	GGL	A	602	-	-	6/9/9/9	-
3	NAI	C	605	-	-	13/29/72/72	0/5/5/5
2	GTP	G	601	-	-	4/22/38/38	0/3/3/3
3	NAI	D	601	-	-	7/29/72/72	0/5/5/5
2	GTP	F	600	-	-	1/22/38/38	0/3/3/3
2	GTP	E	600	-	-	6/22/38/38	0/3/3/3
2	GTP	I	601	-	-	3/22/38/38	0/3/3/3
3	NAI	C	602	-	-	9/29/72/72	0/5/5/5
2	GTP	L	602	-	-	3/22/38/38	0/3/3/3
2	GTP	D	600	-	-	6/22/38/38	0/3/3/3
3	NAI	F	601	-	-	1/29/72/72	0/5/5/5
3	NAI	H	603	-	-	10/29/72/72	0/5/5/5
3	NAI	L	603	-	-	9/29/72/72	0/5/5/5
3	NAI	B	603	-	-	18/29/72/72	0/5/5/5
3	NAI	J	604	-	-	7/29/72/72	0/5/5/5
3	NAI	A	601	-	-	5/29/72/72	0/5/5/5
3	NAI	D	603	-	-	11/29/72/72	0/5/5/5
3	NAI	F	603	-	-	16/29/72/72	0/5/5/5
2	GTP	H	601	-	-	2/22/38/38	0/3/3/3
2	GTP	B	600	-	-	6/22/38/38	0/3/3/3
3	NAI	I	603	-	-	12/29/72/72	0/5/5/5
4	GGL	E	602	-	-	3/9/9/9	-
3	NAI	H	602	-	-	8/29/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAI	C	604	-	-	13/29/72/72	0/5/5/5
2	GTP	A	600	-	-	4/22/38/38	0/3/3/3
4	GGL	D	602	-	-	3/9/9/9	-
4	GGL	B	602	-	-	4/9/9/9	-
3	NAI	L	601	-	-	9/29/72/72	0/5/5/5
3	NAI	G	602	-	-	11/29/72/72	0/5/5/5
3	NAI	K	601	-	-	12/29/72/72	0/5/5/5
4	GGL	F	602	-	-	2/9/9/9	-
2	GTP	J	601	-	-	4/22/38/38	0/3/3/3
2	GTP	C	601	-	-	4/22/38/38	0/3/3/3
4	GGL	C	603	-	-	3/9/9/9	-
3	NAI	I	602	-	-	9/29/72/72	0/5/5/5
3	NAI	B	601	-	-	6/29/72/72	0/5/5/5
3	NAI	G	603	-	-	9/29/72/72	0/5/5/5
2	GTP	K	600	-	-	5/22/38/38	0/3/3/3
3	NAI	J	603	-	-	11/29/72/72	0/5/5/5
3	NAI	E	601	-	-	7/29/72/72	0/5/5/5

All (242) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	GTP	PB-O3A	8.51	1.68	1.59
2	J	601	GTP	PB-O3A	8.32	1.68	1.59
2	F	600	GTP	PB-O3A	8.31	1.68	1.59
2	C	601	GTP	PB-O3A	8.29	1.68	1.59
2	A	600	GTP	PB-O3A	8.28	1.68	1.59
2	E	600	GTP	PB-O3A	8.27	1.68	1.59
2	K	600	GTP	PB-O3A	8.23	1.68	1.59
2	H	601	GTP	PB-O3A	8.23	1.68	1.59
2	I	601	GTP	PB-O3A	8.23	1.68	1.59
2	L	602	GTP	PB-O3A	8.22	1.68	1.59
2	G	601	GTP	PB-O3A	8.04	1.68	1.59
2	B	600	GTP	PB-O3A	7.91	1.68	1.59
2	G	601	GTP	PA-O5'	6.36	1.84	1.59
2	J	601	GTP	PA-O5'	6.33	1.84	1.59
2	D	600	GTP	PA-O5'	6.32	1.84	1.59
2	I	601	GTP	PA-O5'	6.31	1.84	1.59
2	L	602	GTP	PA-O5'	6.30	1.84	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	600	GTP	PA-O5'	6.28	1.84	1.59
2	K	600	GTP	PA-O5'	6.28	1.84	1.59
2	B	600	GTP	PA-O5'	6.26	1.83	1.59
2	H	601	GTP	PA-O5'	6.26	1.83	1.59
2	C	601	GTP	PA-O5'	6.26	1.83	1.59
2	E	600	GTP	PA-O5'	6.25	1.83	1.59
2	A	600	GTP	PA-O5'	6.25	1.83	1.59
2	B	600	GTP	PA-O3A	-4.09	1.55	1.59
2	H	601	GTP	PB-O3B	-4.05	1.55	1.59
2	G	601	GTP	PA-O3A	-4.05	1.55	1.59
2	L	602	GTP	PA-O3A	-4.01	1.55	1.59
2	H	601	GTP	PA-O3A	-4.00	1.55	1.59
2	I	601	GTP	PB-O3B	-3.99	1.55	1.59
2	C	601	GTP	PA-O3A	-3.98	1.55	1.59
2	E	600	GTP	PA-O3A	-3.97	1.55	1.59
2	B	600	GTP	PB-O3B	-3.96	1.55	1.59
2	F	600	GTP	PA-O3A	-3.96	1.55	1.59
2	A	600	GTP	PA-O3A	-3.94	1.55	1.59
2	L	602	GTP	PB-O3B	-3.94	1.55	1.59
2	J	601	GTP	PB-O3B	-3.91	1.55	1.59
2	F	600	GTP	PB-O3B	-3.90	1.55	1.59
2	K	600	GTP	PA-O3A	-3.88	1.55	1.59
2	I	601	GTP	PA-O3A	-3.88	1.55	1.59
2	K	600	GTP	PB-O3B	-3.88	1.55	1.59
2	G	601	GTP	PB-O3B	-3.88	1.55	1.59
2	D	600	GTP	PB-O3B	-3.87	1.55	1.59
2	J	601	GTP	PA-O3A	-3.85	1.55	1.59
2	C	601	GTP	PB-O3B	-3.83	1.55	1.59
2	E	600	GTP	PB-O3B	-3.83	1.55	1.59
2	D	600	GTP	PA-O3A	-3.81	1.55	1.59
2	A	600	GTP	PB-O3B	-3.75	1.55	1.59
3	F	601	NAI	PN-O5D	3.29	1.72	1.59
3	I	603	NAI	PN-O5D	3.25	1.72	1.59
3	D	603	NAI	PN-O5D	3.21	1.72	1.59
3	K	601	NAI	PN-O5D	3.20	1.71	1.59
3	L	603	NAI	PN-O5D	3.19	1.71	1.59
3	J	604	NAI	PN-O5D	3.19	1.71	1.59
3	C	604	NAI	PN-O5D	3.18	1.71	1.59
3	B	603	NAI	PN-O5D	3.18	1.71	1.59
3	A	601	NAI	PN-O5D	3.18	1.71	1.59
3	I	602	NAI	PN-O5D	3.18	1.71	1.59
3	J	603	NAI	PN-O5D	3.18	1.71	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	603	NAI	PN-O5D	3.17	1.71	1.59
3	A	603	NAI	PN-O5D	3.16	1.71	1.59
3	D	601	NAI	PN-O5D	3.16	1.71	1.59
3	L	601	NAI	PN-O5D	3.16	1.71	1.59
3	J	602	NAI	PN-O5D	3.16	1.71	1.59
3	C	605	NAI	PN-O5D	3.15	1.71	1.59
3	H	603	NAI	PN-O5D	3.15	1.71	1.59
3	B	601	NAI	PN-O5D	3.15	1.71	1.59
3	G	602	NAI	PN-O5D	3.15	1.71	1.59
3	H	602	NAI	PN-O5D	3.13	1.71	1.59
3	C	602	NAI	PN-O5D	3.13	1.71	1.59
3	G	603	NAI	PN-O5D	3.13	1.71	1.59
3	E	601	NAI	PN-O5D	3.12	1.71	1.59
3	F	603	NAI	PA-O5B	2.94	1.70	1.59
3	B	603	NAI	PA-O5B	2.90	1.70	1.59
3	A	603	NAI	PA-O5B	2.89	1.70	1.59
3	G	602	NAI	PA-O5B	2.89	1.70	1.59
3	C	605	NAI	PA-O5B	2.87	1.70	1.59
3	H	602	NAI	PA-O5B	2.87	1.70	1.59
3	C	604	NAI	PA-O5B	2.87	1.70	1.59
3	J	603	NAI	PA-O5B	2.86	1.70	1.59
3	A	601	NAI	PA-O5B	2.86	1.70	1.59
3	L	603	NAI	PA-O5B	2.85	1.70	1.59
3	G	603	NAI	PA-O5B	2.85	1.70	1.59
3	I	603	NAI	PA-O5B	2.85	1.70	1.59
3	H	603	NAI	PA-O5B	2.84	1.70	1.59
3	I	602	NAI	PA-O5B	2.84	1.70	1.59
3	L	601	NAI	PA-O5B	2.84	1.70	1.59
3	J	604	NAI	PA-O5B	2.84	1.70	1.59
3	D	603	NAI	PA-O5B	2.84	1.70	1.59
3	D	601	NAI	PA-O5B	2.83	1.70	1.59
3	B	601	NAI	PA-O5B	2.82	1.70	1.59
3	K	601	NAI	PA-O5B	2.82	1.70	1.59
3	C	602	NAI	PA-O5B	2.81	1.70	1.59
3	E	601	NAI	PA-O5B	2.81	1.70	1.59
3	J	602	NAI	PA-O5B	2.81	1.70	1.59
3	F	601	NAI	PA-O5B	2.79	1.70	1.59
2	A	600	GTP	C4-N3	2.59	1.40	1.34
2	G	601	GTP	C4-N3	2.59	1.40	1.34
2	B	600	GTP	C4-N3	2.59	1.40	1.34
2	D	600	GTP	C4-N3	2.57	1.40	1.34
2	J	601	GTP	C4-N3	2.56	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	GTP	C4-N3	2.56	1.40	1.34
2	K	600	GTP	C4-N3	2.55	1.40	1.34
2	E	600	GTP	C4-N3	2.55	1.40	1.34
2	F	600	GTP	C4-N3	2.54	1.40	1.34
2	I	601	GTP	C4-N3	2.54	1.40	1.34
2	L	602	GTP	C4-N3	2.54	1.40	1.34
3	G	602	NAI	C8A-N9A	2.50	1.41	1.37
3	K	601	NAI	C8A-N9A	2.50	1.41	1.37
3	F	601	NAI	C8A-N9A	2.48	1.41	1.37
2	H	601	GTP	C4-N3	2.47	1.39	1.34
3	L	603	NAI	C8A-N9A	2.47	1.41	1.37
3	A	601	NAI	C8A-N9A	2.47	1.41	1.37
3	J	604	NAI	C8A-N9A	2.46	1.41	1.37
3	H	602	NAI	C8A-N9A	2.45	1.41	1.37
3	I	602	NAI	C8A-N9A	2.44	1.41	1.37
3	E	601	NAI	C8A-N9A	2.44	1.41	1.37
2	E	600	GTP	C6-N1	2.44	1.43	1.38
2	K	600	GTP	C2-N2	2.44	1.39	1.34
2	H	601	GTP	C6-N1	2.43	1.43	1.38
2	I	601	GTP	C2-N2	2.43	1.39	1.34
3	B	601	NAI	C8A-N9A	2.43	1.41	1.37
2	F	600	GTP	C2-N2	2.43	1.39	1.34
2	G	601	GTP	O5'-C5'	-2.42	1.35	1.44
2	H	601	GTP	O5'-C5'	-2.42	1.35	1.44
2	F	600	GTP	O5'-C5'	-2.42	1.35	1.44
2	A	600	GTP	C2-N2	2.42	1.39	1.34
3	C	602	NAI	C8A-N9A	2.42	1.41	1.37
2	E	600	GTP	O5'-C5'	-2.41	1.35	1.44
2	K	600	GTP	O5'-C5'	-2.41	1.35	1.44
2	B	600	GTP	O5'-C5'	-2.41	1.35	1.44
2	I	601	GTP	C6-N1	2.41	1.43	1.38
3	J	602	NAI	C8A-N9A	2.41	1.41	1.37
2	A	600	GTP	O5'-C5'	-2.41	1.35	1.44
2	L	602	GTP	C2-N2	2.41	1.39	1.34
3	H	603	NAI	C8A-N9A	2.40	1.41	1.37
2	C	601	GTP	C2-N2	2.40	1.39	1.34
2	G	601	GTP	C2-N2	2.40	1.39	1.34
2	J	601	GTP	O5'-C5'	-2.40	1.35	1.44
2	F	600	GTP	C6-N1	2.40	1.43	1.38
2	G	601	GTP	C6-N1	2.40	1.43	1.38
2	B	600	GTP	C6-N1	2.40	1.43	1.38
2	D	600	GTP	C2-N2	2.40	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	GTP	C2-N2	2.40	1.39	1.34
2	D	600	GTP	C6-N1	2.40	1.43	1.38
3	D	601	NAI	C8A-N9A	2.39	1.41	1.37
2	L	602	GTP	O5'-C5'	-2.39	1.35	1.44
2	C	601	GTP	O5'-C5'	-2.38	1.35	1.44
2	I	601	GTP	O5'-C5'	-2.38	1.35	1.44
2	E	600	GTP	C2-N2	2.38	1.39	1.34
2	K	600	GTP	C6-N1	2.38	1.43	1.38
3	L	601	NAI	C8A-N9A	2.38	1.41	1.37
2	D	600	GTP	O5'-C5'	-2.38	1.35	1.44
3	I	603	NAI	C8A-N9A	2.38	1.41	1.37
2	J	601	GTP	C6-N1	2.37	1.43	1.38
2	J	601	GTP	C2-N2	2.37	1.39	1.34
2	H	601	GTP	C2-N2	2.36	1.39	1.34
2	L	602	GTP	C6-N1	2.36	1.43	1.38
2	A	600	GTP	C6-N1	2.36	1.43	1.38
3	J	603	NAI	C8A-N9A	2.36	1.41	1.37
3	G	603	NAI	C8A-N9A	2.35	1.41	1.37
2	C	601	GTP	C6-N1	2.35	1.43	1.38
3	C	604	NAI	C8A-N9A	2.34	1.41	1.37
3	A	603	NAI	C8A-N9A	2.30	1.41	1.37
3	F	603	NAI	C8A-N9A	2.29	1.41	1.37
3	D	603	NAI	C8A-N9A	2.29	1.41	1.37
3	B	603	NAI	C8A-N9A	2.28	1.41	1.37
2	H	601	GTP	C8-N9	2.26	1.42	1.37
2	G	601	GTP	C8-N9	2.24	1.42	1.37
3	C	605	NAI	C8A-N9A	2.24	1.41	1.37
2	D	600	GTP	C8-N9	2.23	1.42	1.37
2	I	601	GTP	C8-N9	2.22	1.42	1.37
2	K	600	GTP	C8-N9	2.22	1.42	1.37
2	A	600	GTP	C8-N9	2.22	1.42	1.37
2	E	600	GTP	C8-N9	2.22	1.42	1.37
2	J	601	GTP	C8-N9	2.22	1.42	1.37
2	F	600	GTP	C8-N9	2.22	1.42	1.37
2	L	602	GTP	C8-N9	2.21	1.42	1.37
2	B	600	GTP	C8-N9	2.20	1.42	1.37
3	H	602	NAI	C2A-N1A	2.18	1.37	1.33
3	I	602	NAI	C5A-C4A	2.15	1.42	1.39
3	G	602	NAI	C5A-C4A	2.14	1.42	1.39
2	C	601	GTP	C8-N9	2.14	1.42	1.37
3	F	601	NAI	C5A-C4A	2.14	1.42	1.39
3	J	602	NAI	C2A-N1A	2.13	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	601	NAI	O5B-C5B	-2.13	1.36	1.44
3	G	602	NAI	C2A-N1A	2.12	1.37	1.33
3	H	602	NAI	C5A-C4A	2.12	1.42	1.39
3	K	601	NAI	C5A-C4A	2.12	1.42	1.39
3	B	601	NAI	C5A-C4A	2.12	1.42	1.39
3	C	602	NAI	C5A-C4A	2.12	1.42	1.39
3	J	602	NAI	C5A-C4A	2.12	1.42	1.39
3	B	601	NAI	O5B-C5B	-2.11	1.36	1.44
3	J	602	NAI	O5B-C5B	-2.11	1.36	1.44
3	A	601	NAI	C5A-C4A	2.11	1.42	1.39
3	E	601	NAI	O5B-C5B	-2.11	1.36	1.44
3	J	603	NAI	C2A-N1A	2.11	1.37	1.33
3	J	603	NAI	C5A-C4A	2.10	1.42	1.39
3	J	604	NAI	C2A-N1A	2.10	1.37	1.33
3	L	601	NAI	C2A-N1A	2.10	1.37	1.33
3	D	601	NAI	O5B-C5B	-2.10	1.36	1.44
3	I	602	NAI	C2A-N1A	2.09	1.37	1.33
3	L	603	NAI	O5B-C5B	-2.09	1.36	1.44
3	F	601	NAI	C2A-N1A	2.09	1.37	1.33
3	G	603	NAI	O5B-C5B	-2.09	1.36	1.44
3	L	601	NAI	C5A-C4A	2.09	1.42	1.39
3	L	603	NAI	C2A-N1A	2.09	1.37	1.33
3	L	601	NAI	O5B-C5B	-2.09	1.36	1.44
3	A	601	NAI	O5B-C5B	-2.09	1.36	1.44
3	K	601	NAI	O5B-C5B	-2.09	1.36	1.44
3	E	601	NAI	C5A-C4A	2.08	1.42	1.39
3	C	604	NAI	O5B-C5B	-2.08	1.36	1.44
3	H	603	NAI	C2A-N1A	2.08	1.37	1.33
3	H	603	NAI	O5B-C5B	-2.08	1.36	1.44
3	G	602	NAI	O5B-C5B	-2.08	1.36	1.44
3	C	602	NAI	O5B-C5B	-2.08	1.36	1.44
3	A	603	NAI	O5B-C5B	-2.07	1.36	1.44
3	H	602	NAI	O5B-C5B	-2.07	1.36	1.44
3	I	602	NAI	O5B-C5B	-2.07	1.36	1.44
3	I	603	NAI	O5B-C5B	-2.07	1.36	1.44
3	J	604	NAI	O5B-C5B	-2.07	1.36	1.44
3	K	601	NAI	C2A-N1A	2.07	1.37	1.33
3	D	603	NAI	O5B-C5B	-2.06	1.36	1.44
3	C	605	NAI	O5B-C5B	-2.06	1.36	1.44
3	D	601	NAI	C5A-C4A	2.06	1.42	1.39
3	L	603	NAI	C5A-C4A	2.06	1.42	1.39
3	J	603	NAI	O5B-C5B	-2.06	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	603	NAI	C5A-C4A	2.06	1.42	1.39
3	I	603	NAI	C2A-N1A	2.05	1.37	1.33
3	I	603	NAI	C5A-C4A	2.05	1.42	1.39
3	B	603	NAI	O5B-C5B	-2.05	1.36	1.44
3	A	601	NAI	C2A-N1A	2.05	1.37	1.33
3	J	604	NAI	C5A-C4A	2.05	1.42	1.39
3	B	601	NAI	C2A-N1A	2.04	1.37	1.33
3	E	601	NAI	C2A-N1A	2.04	1.37	1.33
3	F	603	NAI	O5B-C5B	-2.04	1.36	1.44
3	C	604	NAI	C2A-N1A	2.03	1.37	1.33
3	B	603	NAI	C2A-N1A	2.02	1.37	1.33
3	C	605	NAI	C2A-N1A	2.02	1.37	1.33
3	F	603	NAI	C5A-C4A	2.01	1.42	1.39
3	A	603	NAI	C2A-N1A	2.01	1.37	1.33
3	F	603	NAI	C2A-N1A	2.00	1.37	1.33

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	GTP	O2B-PB-O3A	-5.25	93.07	107.27
2	C	601	GTP	O2B-PB-O3A	-5.24	93.12	107.27
2	A	600	GTP	O2B-PB-O3A	-5.23	93.13	107.27
2	I	601	GTP	O2B-PB-O3A	-5.23	93.15	107.27
2	D	600	GTP	O2B-PB-O3A	-5.22	93.16	107.27
2	E	600	GTP	O2B-PB-O3A	-5.22	93.17	107.27
2	L	602	GTP	O2B-PB-O3A	-5.21	93.19	107.27
2	H	601	GTP	O2B-PB-O3A	-5.20	93.22	107.27
2	F	600	GTP	O2B-PB-O3A	-5.20	93.23	107.27
2	K	600	GTP	O2B-PB-O3A	-5.19	93.23	107.27
2	G	601	GTP	O2B-PB-O3A	-5.19	93.24	107.27
2	J	601	GTP	O2B-PB-O3A	-5.08	93.54	107.27
2	D	600	GTP	O5'-PA-O1A	-4.07	92.82	108.94
2	C	601	GTP	O5'-PA-O1A	-4.05	92.88	108.94
2	I	601	GTP	O5'-PA-O1A	-4.03	92.95	108.94
2	J	601	GTP	O5'-PA-O1A	-3.99	93.14	108.94
2	A	600	GTP	O5'-PA-O1A	-3.97	93.18	108.94
2	E	600	GTP	O5'-PA-O1A	-3.97	93.20	108.94
2	H	601	GTP	O5'-PA-O1A	-3.96	93.25	108.94
2	L	602	GTP	O5'-PA-O1A	-3.95	93.27	108.94
2	K	600	GTP	O5'-PA-O1A	-3.95	93.29	108.94
2	F	600	GTP	O5'-PA-O1A	-3.90	93.46	108.94
2	G	601	GTP	O5'-PA-O1A	-3.86	93.62	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	GTP	O5'-PA-O1A	-3.81	93.85	108.94
2	E	600	GTP	O3A-PA-O1A	3.64	121.66	110.70
2	L	602	GTP	O3A-PA-O1A	3.63	121.62	110.70
2	B	600	GTP	O3A-PA-O1A	3.62	121.61	110.70
2	C	601	GTP	O3A-PA-O1A	3.62	121.60	110.70
2	G	601	GTP	O3A-PA-O1A	3.62	121.59	110.70
2	I	601	GTP	O3A-PA-O1A	3.61	121.55	110.70
2	A	600	GTP	O3A-PA-O1A	3.61	121.55	110.70
2	D	600	GTP	O3A-PA-O1A	3.59	121.52	110.70
2	K	600	GTP	O3A-PA-O1A	3.59	121.50	110.70
2	F	600	GTP	O3A-PA-O1A	3.59	121.49	110.70
2	H	601	GTP	O3A-PA-O1A	3.59	121.49	110.70
2	J	601	GTP	O3A-PA-O1A	3.54	121.35	110.70
2	J	601	GTP	O2A-PA-O3A	3.49	116.70	107.27
2	H	601	GTP	O2A-PA-O3A	3.45	116.60	107.27
2	K	600	GTP	O2A-PA-O3A	3.45	116.59	107.27
2	F	600	GTP	O2A-PA-O3A	3.42	116.53	107.27
2	D	600	GTP	O2A-PA-O3A	3.41	116.50	107.27
2	C	601	GTP	O2A-PA-O3A	3.40	116.48	107.27
2	A	600	GTP	O2A-PA-O3A	3.39	116.42	107.27
2	E	600	GTP	O2A-PA-O3A	3.37	116.39	107.27
2	I	601	GTP	O2A-PA-O3A	3.37	116.37	107.27
2	L	602	GTP	O2A-PA-O3A	3.34	116.30	107.27
2	G	601	GTP	O2A-PA-O3A	3.33	116.28	107.27
2	B	600	GTP	O2A-PA-O3A	3.32	116.25	107.27
2	F	600	GTP	O2B-PB-O3B	3.27	116.12	107.27
2	K	600	GTP	O2B-PB-O3B	3.26	116.08	107.27
2	L	602	GTP	O2B-PB-O3B	3.25	116.06	107.27
2	J	601	GTP	O2B-PB-O3B	3.25	116.06	107.27
2	B	600	GTP	O2B-PB-O3B	3.24	116.03	107.27
2	G	601	GTP	O2B-PB-O3B	3.24	116.02	107.27
2	E	600	GTP	O2B-PB-O3B	3.23	116.02	107.27
2	I	601	GTP	O2B-PB-O3B	3.23	116.00	107.27
2	A	600	GTP	O2B-PB-O3B	3.22	115.99	107.27
2	D	600	GTP	O2B-PB-O3B	3.22	115.97	107.27
2	C	601	GTP	O2B-PB-O3B	3.21	115.96	107.27
2	H	601	GTP	O2B-PB-O3B	3.21	115.94	107.27
3	C	605	NAI	C3N-C2N-N1N	-3.09	118.66	123.20
3	I	603	NAI	C3N-C2N-N1N	-2.95	118.87	123.20
3	D	601	NAI	O1N-PN-O2N	2.90	125.95	112.44
3	F	601	NAI	O1N-PN-O2N	2.90	125.95	112.44
3	C	602	NAI	O1N-PN-O2N	2.90	125.92	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	601	NAI	O1N-PN-O2N	2.90	125.92	112.44
3	J	602	NAI	O1N-PN-O2N	2.89	125.87	112.44
3	B	601	NAI	O1N-PN-O2N	2.88	125.86	112.44
3	A	601	NAI	O1N-PN-O2N	2.88	125.84	112.44
3	L	603	NAI	O1N-PN-O2N	2.88	125.83	112.44
3	H	602	NAI	O1N-PN-O2N	2.88	125.83	112.44
3	I	602	NAI	O1N-PN-O2N	2.88	125.82	112.44
3	F	603	NAI	O1N-PN-O2N	2.87	125.77	112.44
3	H	603	NAI	O1N-PN-O2N	2.86	125.77	112.44
3	J	603	NAI	O1N-PN-O2N	2.86	125.76	112.44
3	A	603	NAI	O1N-PN-O2N	2.86	125.76	112.44
3	K	601	NAI	O1N-PN-O2N	2.86	125.75	112.44
3	L	601	NAI	O1N-PN-O2N	2.86	125.73	112.44
3	G	602	NAI	O1N-PN-O2N	2.85	125.72	112.44
3	C	604	NAI	O1N-PN-O2N	2.85	125.71	112.44
3	B	603	NAI	O1N-PN-O2N	2.84	125.67	112.44
3	C	605	NAI	O1N-PN-O2N	2.84	125.67	112.44
3	D	603	NAI	O1N-PN-O2N	2.84	125.67	112.44
3	I	603	NAI	O1N-PN-O2N	2.84	125.66	112.44
3	G	603	NAI	O1N-PN-O2N	2.84	125.64	112.44
3	J	604	NAI	O1N-PN-O2N	2.78	125.35	112.44
3	J	603	NAI	C3N-C2N-N1N	-2.75	119.17	123.20
3	B	603	NAI	C3N-C2N-N1N	-2.68	119.27	123.20
3	L	601	NAI	C3N-C2N-N1N	-2.67	119.29	123.20
3	A	603	NAI	C3N-C2N-N1N	-2.51	119.52	123.20
2	I	601	GTP	C2-N1-C6	-2.45	120.66	125.11
2	K	600	GTP	C2-N1-C6	-2.44	120.69	125.11
3	C	604	NAI	C3N-C2N-N1N	-2.44	119.62	123.20
2	H	601	GTP	C2-N1-C6	-2.44	120.69	125.11
2	A	600	GTP	C2-N1-C6	-2.42	120.71	125.11
2	D	600	GTP	C2-N1-C6	-2.42	120.72	125.11
2	G	601	GTP	O6-C6-N1	-2.42	115.56	120.11
2	F	600	GTP	C2-N1-C6	-2.42	120.73	125.11
2	B	600	GTP	C2-N1-C6	-2.42	120.73	125.11
2	C	601	GTP	C2-N1-C6	-2.42	120.73	125.11
2	G	601	GTP	C2-N1-C6	-2.41	120.73	125.11
2	E	600	GTP	C2-N1-C6	-2.41	120.74	125.11
2	J	601	GTP	C2-N1-C6	-2.41	120.74	125.11
2	J	601	GTP	O6-C6-N1	-2.41	115.59	120.11
2	A	600	GTP	O6-C6-N1	-2.40	115.59	120.11
3	B	601	NAI	O2A-PA-O1A	2.40	123.60	112.44
2	I	601	GTP	O6-C6-N1	-2.40	115.61	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	601	GTP	O6-C6-N1	-2.40	115.61	120.11
3	E	601	NAI	O2A-PA-O1A	2.39	123.58	112.44
3	D	603	NAI	O2A-PA-O1A	2.39	123.58	112.44
2	D	600	GTP	O6-C6-N1	-2.39	115.61	120.11
2	L	602	GTP	C2-N1-C6	-2.39	120.78	125.11
3	A	601	NAI	O2A-PA-O1A	2.39	123.56	112.44
3	D	601	NAI	O2A-PA-O1A	2.39	123.55	112.44
3	G	603	NAI	O2A-PA-O1A	2.39	123.55	112.44
3	H	603	NAI	O2A-PA-O1A	2.39	123.55	112.44
3	L	601	NAI	O2A-PA-O1A	2.39	123.55	112.44
2	K	600	GTP	O6-C6-N1	-2.39	115.63	120.11
2	B	600	GTP	O6-C6-N1	-2.38	115.63	120.11
3	F	601	NAI	O2A-PA-O1A	2.38	123.53	112.44
3	H	602	NAI	O2A-PA-O1A	2.38	123.53	112.44
3	I	602	NAI	O2A-PA-O1A	2.38	123.52	112.44
3	J	602	NAI	O2A-PA-O1A	2.38	123.52	112.44
2	F	600	GTP	O6-C6-N1	-2.38	115.64	120.11
3	A	603	NAI	O2A-PA-O1A	2.38	123.50	112.44
3	J	603	NAI	O2A-PA-O1A	2.38	123.50	112.44
3	L	603	NAI	O2A-PA-O1A	2.38	123.50	112.44
3	C	605	NAI	O2A-PA-O1A	2.38	123.50	112.44
3	C	604	NAI	O2A-PA-O1A	2.37	123.49	112.44
3	I	603	NAI	O2A-PA-O1A	2.37	123.49	112.44
2	E	600	GTP	O6-C6-N1	-2.37	115.66	120.11
2	C	601	GTP	O6-C6-N1	-2.37	115.66	120.11
3	C	602	NAI	O2A-PA-O1A	2.37	123.46	112.44
3	B	603	NAI	O2A-PA-O1A	2.37	123.45	112.44
2	L	602	GTP	O6-C6-N1	-2.37	115.67	120.11
3	G	602	NAI	O2A-PA-O1A	2.36	123.43	112.44
3	J	604	NAI	O2A-PA-O1A	2.36	123.43	112.44
3	F	603	NAI	O2A-PA-O1A	2.36	123.43	112.44
3	H	603	NAI	C3N-C2N-N1N	-2.34	119.77	123.20
2	J	601	GTP	O2A-PA-O5'	-2.33	97.00	107.57
3	K	601	NAI	O2A-PA-O1A	2.33	123.28	112.44
2	A	600	GTP	O2A-PA-O5'	-2.31	97.09	107.57
2	G	601	GTP	O2A-PA-O5'	-2.30	97.16	107.57
2	I	601	GTP	O2A-PA-O5'	-2.29	97.17	107.57
2	E	600	GTP	O2A-PA-O5'	-2.29	97.18	107.57
2	L	602	GTP	O2A-PA-O5'	-2.29	97.19	107.57
2	K	600	GTP	O2A-PA-O5'	-2.29	97.19	107.57
2	K	600	GTP	N1-C2-N3	2.28	127.50	123.32
2	F	600	GTP	O2A-PA-O5'	-2.28	97.22	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	601	GTP	N1-C2-N3	2.28	127.49	123.32
2	D	600	GTP	N1-C2-N3	2.28	127.49	123.32
2	B	600	GTP	N1-C2-N3	2.28	127.49	123.32
2	D	600	GTP	O2A-PA-O5'	-2.28	97.25	107.57
2	B	600	GTP	O2A-PA-O5'	-2.28	97.25	107.57
2	C	601	GTP	N1-C2-N3	2.28	127.49	123.32
2	E	600	GTP	N1-C2-N3	2.27	127.48	123.32
2	A	600	GTP	N1-C2-N3	2.27	127.48	123.32
2	H	601	GTP	N1-C2-N3	2.27	127.47	123.32
2	H	601	GTP	O2A-PA-O5'	-2.26	97.32	107.57
2	G	601	GTP	N1-C2-N3	2.26	127.46	123.32
2	C	601	GTP	O2A-PA-O5'	-2.26	97.32	107.57
2	L	602	GTP	N1-C2-N3	2.26	127.45	123.32
2	F	600	GTP	N1-C2-N3	2.25	127.44	123.32
2	J	601	GTP	N1-C2-N3	2.24	127.43	123.32
3	F	603	NAI	C3N-C2N-N1N	-2.20	119.97	123.20
3	D	603	NAI	C3N-C2N-N1N	-2.17	120.02	123.20
2	F	600	GTP	O3'-C3'-C4'	-2.14	104.94	111.08
2	C	601	GTP	C2'-C1'-N9	-2.14	107.31	113.25
2	K	600	GTP	C3'-C2'-C1'	-2.13	97.43	101.46
2	C	601	GTP	O3'-C3'-C4'	-2.13	104.97	111.08
2	F	600	GTP	C3'-C2'-C1'	-2.13	97.44	101.46
2	D	600	GTP	O3'-C3'-C4'	-2.11	105.01	111.08
2	L	602	GTP	O3'-C3'-C4'	-2.11	105.01	111.08
2	B	600	GTP	O3'-C3'-C4'	-2.10	105.06	111.08
2	J	601	GTP	O3'-C3'-C4'	-2.09	105.06	111.08
2	I	601	GTP	O3'-C3'-C4'	-2.09	105.07	111.08
2	K	600	GTP	O3'-C3'-C4'	-2.09	105.08	111.08
2	G	601	GTP	O3'-C3'-C4'	-2.09	105.08	111.08
2	H	601	GTP	O3'-C3'-C4'	-2.09	105.08	111.08
2	A	600	GTP	O3'-C3'-C4'	-2.09	105.09	111.08
2	E	600	GTP	O3'-C3'-C4'	-2.07	105.12	111.08
2	D	600	GTP	C2'-C1'-N9	-2.05	107.53	113.25
2	B	600	GTP	C3'-C2'-C1'	-2.04	97.61	101.46
3	E	601	NAI	C3N-C2N-N1N	-2.03	120.22	123.20
3	J	604	NAI	C3N-C2N-N1N	-2.03	120.23	123.20
3	L	603	NAI	C3N-C2N-N1N	-2.02	120.23	123.20
2	I	601	GTP	C2'-C1'-N9	-2.02	107.62	113.25
2	A	600	GTP	C2'-C1'-N9	-2.02	107.62	113.25
3	D	601	NAI	C3N-C2N-N1N	-2.01	120.25	123.20
2	E	600	GTP	C3'-C2'-C1'	-2.00	97.67	101.46
2	E	600	GTP	C2'-C1'-N9	-2.00	107.68	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	602	GTP	C2'-C1'-N9	-2.00	107.68	113.25

There are no chirality outliers.

All (300) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	GTP	PB-O3B-PG-O3G
2	B	600	GTP	C5'-O5'-PA-O1A
2	B	600	GTP	O4'-C4'-C5'-O5'
2	C	601	GTP	PB-O3B-PG-O3G
2	D	600	GTP	C5'-O5'-PA-O3A
2	D	600	GTP	C5'-O5'-PA-O1A
2	E	600	GTP	PB-O3B-PG-O3G
2	G	601	GTP	PB-O3B-PG-O3G
2	I	601	GTP	PB-O3B-PG-O3G
2	K	600	GTP	C5'-O5'-PA-O1A
2	L	602	GTP	PB-O3B-PG-O3G
3	A	601	NAI	C5D-O5D-PN-O2N
3	B	601	NAI	PN-O3-PA-O5B
3	B	601	NAI	C5D-O5D-PN-O2N
3	B	603	NAI	C5B-O5B-PA-O1A
3	B	603	NAI	C5B-O5B-PA-O2A
3	B	603	NAI	C5B-O5B-PA-O3
3	B	603	NAI	C5D-O5D-PN-O3
3	B	603	NAI	C5D-O5D-PN-O1N
3	B	603	NAI	C5D-O5D-PN-O2N
3	C	602	NAI	C5B-O5B-PA-O1A
3	C	602	NAI	C5D-O5D-PN-O2N
3	C	604	NAI	C5B-O5B-PA-O1A
3	C	604	NAI	C5B-O5B-PA-O2A
3	C	604	NAI	C5B-O5B-PA-O3
3	C	604	NAI	C5D-O5D-PN-O3
3	C	604	NAI	C5D-O5D-PN-O1N
3	C	604	NAI	C5D-O5D-PN-O2N
3	C	604	NAI	C2N-C3N-C7N-O7N
3	C	605	NAI	C5B-O5B-PA-O2A
3	C	605	NAI	C2N-C3N-C7N-O7N
3	D	601	NAI	PN-O3-PA-O5B
3	D	601	NAI	C5D-O5D-PN-O3
3	D	601	NAI	C5D-O5D-PN-O2N
3	D	603	NAI	C5B-O5B-PA-O1A
3	D	603	NAI	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
3	D	603	NAI	C5D-O5D-PN-O1N
3	D	603	NAI	C5D-O5D-PN-O2N
3	E	601	NAI	PN-O3-PA-O5B
3	E	601	NAI	C5D-O5D-PN-O3
3	E	601	NAI	C5D-O5D-PN-O2N
3	F	603	NAI	C5B-O5B-PA-O1A
3	F	603	NAI	C5B-O5B-PA-O2A
3	F	603	NAI	C5D-O5D-PN-O3
3	F	603	NAI	C5D-O5D-PN-O1N
3	F	603	NAI	C5D-O5D-PN-O2N
3	F	603	NAI	C2N-C3N-C7N-O7N
3	F	603	NAI	C2N-C3N-C7N-N7N
3	G	602	NAI	C5B-O5B-PA-O1A
3	G	602	NAI	C5B-O5B-PA-O3
3	G	602	NAI	PN-O3-PA-O5B
3	G	602	NAI	O4D-C1D-N1N-C6N
3	G	603	NAI	C5D-O5D-PN-O3
3	G	603	NAI	C5D-O5D-PN-O2N
3	H	602	NAI	C5B-O5B-PA-O1A
3	H	602	NAI	C5D-O5D-PN-O2N
3	H	602	NAI	O4D-C1D-N1N-C6N
3	H	603	NAI	O4D-C4D-C5D-O5D
3	I	602	NAI	C5B-O5B-PA-O1A
3	I	602	NAI	C5B-O5B-PA-O3
3	I	602	NAI	O4D-C1D-N1N-C6N
3	I	603	NAI	C5B-O5B-PA-O1A
3	I	603	NAI	C5B-O5B-PA-O3
3	I	603	NAI	PA-O3-PN-O5D
3	I	603	NAI	C5D-O5D-PN-O1N
3	I	603	NAI	C2N-C3N-C7N-O7N
3	J	602	NAI	C5B-O5B-PA-O1A
3	J	602	NAI	C5D-O5D-PN-O3
3	J	602	NAI	C5D-O5D-PN-O2N
3	J	603	NAI	PA-O3-PN-O5D
3	J	603	NAI	C5D-O5D-PN-O3
3	J	603	NAI	C5D-O5D-PN-O1N
3	J	603	NAI	C5D-O5D-PN-O2N
3	J	604	NAI	C2N-C3N-C7N-O7N
3	K	601	NAI	C5B-O5B-PA-O1A
3	K	601	NAI	C5D-O5D-PN-O3
3	K	601	NAI	C5D-O5D-PN-O2N
3	L	601	NAI	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
3	L	603	NAI	C5B-O5B-PA-O1A
4	A	602	GGL	N-CA-CB-CG
4	A	602	GGL	C-CA-CB-CG
3	A	601	NAI	O4D-C1D-N1N-C6N
3	L	603	NAI	O4D-C1D-N1N-C6N
3	C	605	NAI	O4B-C4B-C5B-O5B
3	G	602	NAI	O4D-C4D-C5D-O5D
3	L	603	NAI	O4D-C4D-C5D-O5D
3	B	601	NAI	O4D-C1D-N1N-C6N
3	E	601	NAI	O4D-C1D-N1N-C6N
3	H	603	NAI	O4D-C1D-N1N-C2N
3	J	603	NAI	O4D-C1D-N1N-C2N
2	A	600	GTP	O4'-C4'-C5'-O5'
2	E	600	GTP	O4'-C4'-C5'-O5'
2	K	600	GTP	O4'-C4'-C5'-O5'
3	B	603	NAI	C3B-C4B-C5B-O5B
3	C	604	NAI	O4D-C4D-C5D-O5D
3	C	605	NAI	C3B-C4B-C5B-O5B
3	F	603	NAI	O4D-C4D-C5D-O5D
3	G	603	NAI	O4D-C4D-C5D-O5D
3	H	603	NAI	C3D-C4D-C5D-O5D
3	J	603	NAI	O4B-C4B-C5B-O5B
3	J	603	NAI	C3B-C4B-C5B-O5B
3	J	604	NAI	O4B-C4B-C5B-O5B
3	J	604	NAI	C3B-C4B-C5B-O5B
3	L	601	NAI	O4D-C4D-C5D-O5D
4	B	602	GGL	OXT-C-CA-N
3	K	601	NAI	C3B-C4B-C5B-O5B
2	B	600	GTP	C3'-C4'-C5'-O5'
3	B	603	NAI	O4B-C4B-C5B-O5B
3	G	602	NAI	C3D-C4D-C5D-O5D
3	K	601	NAI	O4B-C4B-C5B-O5B
3	L	603	NAI	C3D-C4D-C5D-O5D
3	A	603	NAI	O4B-C4B-C5B-O5B
3	G	603	NAI	C3D-C4D-C5D-O5D
3	I	603	NAI	O4B-C4B-C5B-O5B
4	B	602	GGL	CA-CB-CG-CD
3	J	602	NAI	O4D-C1D-N1N-C6N
3	J	604	NAI	O4D-C1D-N1N-C2N
3	L	601	NAI	O4D-C1D-N1N-C2N
2	A	600	GTP	C3'-C4'-C5'-O5'
3	G	602	NAI	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	G	603	NAI	O4B-C4B-C5B-O5B
3	H	602	NAI	O4B-C4B-C5B-O5B
3	I	602	NAI	O4B-C4B-C5B-O5B
3	I	603	NAI	C3B-C4B-C5B-O5B
3	J	602	NAI	O4B-C4B-C5B-O5B
3	F	601	NAI	O4D-C1D-N1N-C6N
2	J	601	GTP	PB-O3B-PG-O1G
2	K	600	GTP	C3'-C4'-C5'-O5'
2	B	600	GTP	PA-O3A-PB-O1B
3	D	601	NAI	O4D-C1D-N1N-C6N
2	E	600	GTP	C3'-C4'-C5'-O5'
3	C	602	NAI	O4B-C4B-C5B-O5B
3	F	603	NAI	C3D-C4D-C5D-O5D
3	G	602	NAI	C3B-C4B-C5B-O5B
3	H	602	NAI	C3B-C4B-C5B-O5B
3	I	602	NAI	O4D-C4D-C5D-O5D
3	J	602	NAI	C3B-C4B-C5B-O5B
3	B	603	NAI	C2N-C3N-C7N-N7N
3	C	604	NAI	C3D-C4D-C5D-O5D
3	C	604	NAI	C2N-C3N-C7N-N7N
3	C	605	NAI	C2N-C3N-C7N-N7N
3	I	602	NAI	C3B-C4B-C5B-O5B
3	I	603	NAI	C2N-C3N-C7N-N7N
3	J	604	NAI	C2N-C3N-C7N-N7N
3	L	601	NAI	C3D-C4D-C5D-O5D
3	C	602	NAI	PN-O3-PA-O5B
3	C	602	NAI	C3B-C4B-C5B-O5B
2	C	601	GTP	PB-O3B-PG-O2G
2	D	600	GTP	PB-O3B-PG-O2G
2	H	601	GTP	PB-O3B-PG-O2G
2	I	601	GTP	PB-O3B-PG-O2G
4	C	603	GGL	OXT-C-CA-N
3	B	603	NAI	C2D-C1D-N1N-C6N
3	C	604	NAI	C4D-C5D-O5D-PN
3	F	603	NAI	C4D-C5D-O5D-PN
3	A	601	NAI	C2B-C1B-N9A-C8A
3	A	603	NAI	C2B-C1B-N9A-C8A
3	B	601	NAI	C2B-C1B-N9A-C8A
3	C	605	NAI	C2B-C1B-N9A-C8A
3	G	603	NAI	C2B-C1B-N9A-C8A
3	H	603	NAI	C2B-C1B-N9A-C8A
3	J	602	NAI	C2B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
3	K	601	NAI	C2B-C1B-N9A-C8A
3	L	601	NAI	C2B-C1B-N9A-C8A
2	C	601	GTP	PB-O3A-PA-O2A
2	E	600	GTP	PB-O3A-PA-O2A
2	F	600	GTP	PB-O3A-PA-O2A
2	J	601	GTP	PB-O3A-PA-O2A
2	K	600	GTP	PB-O3A-PA-O2A
3	C	605	NAI	PN-O3-PA-O2A
3	F	603	NAI	PN-O3-PA-O2A
3	D	603	NAI	O4D-C1D-N1N-C2N
3	G	603	NAI	O4D-C1D-N1N-C2N
3	I	603	NAI	O4D-C1D-N1N-C2N
3	B	603	NAI	C2D-C1D-N1N-C2N
3	B	603	NAI	C2N-C3N-C7N-O7N
4	E	602	GGL	N-CA-CB-CG
3	A	603	NAI	O4D-C1D-N1N-C2N
3	C	602	NAI	O4D-C1D-N1N-C6N
2	D	600	GTP	C5'-O5'-PA-O2A
2	E	600	GTP	C5'-O5'-PA-O1A
2	J	601	GTP	C5'-O5'-PA-O3A
2	J	601	GTP	C5'-O5'-PA-O2A
3	C	602	NAI	C5D-O5D-PN-O3
3	C	605	NAI	C5B-O5B-PA-O1A
3	C	605	NAI	C5B-O5B-PA-O3
3	D	601	NAI	C5D-O5D-PN-O1N
3	D	603	NAI	C5B-O5B-PA-O2A
3	D	603	NAI	C5B-O5B-PA-O3
3	E	601	NAI	C5D-O5D-PN-O1N
3	F	603	NAI	C5B-O5B-PA-O3
3	G	602	NAI	C5B-O5B-PA-O2A
3	G	603	NAI	C5D-O5D-PN-O1N
3	H	602	NAI	C5B-O5B-PA-O3
3	H	602	NAI	C5D-O5D-PN-O3
3	H	603	NAI	C5D-O5D-PN-O3
3	H	603	NAI	C5D-O5D-PN-O1N
3	H	603	NAI	C5D-O5D-PN-O2N
3	I	602	NAI	C5B-O5B-PA-O2A
3	I	603	NAI	C5B-O5B-PA-O2A
3	I	603	NAI	C5D-O5D-PN-O3
3	J	602	NAI	C5D-O5D-PN-O1N
3	J	603	NAI	C5B-O5B-PA-O1A
3	J	604	NAI	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	K	601	NAI	C5B-O5B-PA-O2A
3	K	601	NAI	C5B-O5B-PA-O3
3	K	601	NAI	C5D-O5D-PN-O1N
3	L	601	NAI	C5D-O5D-PN-O3
3	L	601	NAI	C5D-O5D-PN-O1N
3	L	603	NAI	C5B-O5B-PA-O3
3	D	603	NAI	C4D-C5D-O5D-PN
4	A	602	GGL	CA-CB-CG-CD
3	D	601	NAI	O4B-C4B-C5B-O5B
2	D	600	GTP	PA-O3A-PB-O1B
2	G	601	GTP	PB-O3A-PA-O2A
2	H	601	GTP	PB-O3A-PA-O2A
2	I	601	GTP	PB-O3A-PA-O2A
2	L	602	GTP	PB-O3A-PA-O2A
3	C	605	NAI	PN-O3-PA-O1A
3	F	603	NAI	PN-O3-PA-O1A
3	F	603	NAI	PA-O3-PN-O1N
3	I	602	NAI	C3D-C4D-C5D-O5D
3	B	603	NAI	C4D-C5D-O5D-PN
3	B	603	NAI	O4D-C1D-N1N-C6N
3	C	605	NAI	O4D-C1D-N1N-C2N
3	F	603	NAI	O4D-C1D-N1N-C2N
3	H	603	NAI	O4B-C4B-C5B-O5B
3	L	601	NAI	O4B-C4B-C5B-O5B
3	B	603	NAI	O4D-C1D-N1N-C2N
3	C	604	NAI	O4D-C1D-N1N-C2N
4	E	602	GGL	CA-CB-CG-CD
3	H	603	NAI	C2B-C1B-N9A-C4A
4	D	602	GGL	OE2-CD-CG-CB
4	D	602	GGL	OE1-CD-CG-CB
3	A	603	NAI	C2N-C3N-C7N-N7N
3	B	601	NAI	C2N-C3N-C7N-N7N
3	G	602	NAI	C2N-C3N-C7N-N7N
3	J	603	NAI	C2N-C3N-C7N-N7N
3	K	601	NAI	O4D-C1D-N1N-C6N
3	L	603	NAI	C2N-C3N-C7N-N7N
4	F	602	GGL	OE2-CD-CG-CB
3	B	603	NAI	PA-O3-PN-O1N
4	F	602	GGL	OE1-CD-CG-CB
3	L	603	NAI	PN-O3-PA-O5B
4	D	602	GGL	CA-CB-CG-CD
3	A	601	NAI	O4B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
3	A	603	NAI	O4B-C1B-N9A-C8A
3	J	602	NAI	O4B-C1B-N9A-C8A
3	A	601	NAI	C2B-C1B-N9A-C4A
3	F	603	NAI	C4B-C5B-O5B-PA
3	I	603	NAI	C4D-C5D-O5D-PN
4	C	603	GGL	OE2-CD-CG-CB
3	C	605	NAI	O4B-C1B-N9A-C8A
2	E	600	GTP	PB-O3B-PG-O1G
2	G	601	GTP	PB-O3B-PG-O1G
2	D	600	GTP	PB-O3B-PG-O3G
2	G	601	GTP	PB-O3B-PG-O2G
2	K	600	GTP	PB-O3B-PG-O2G
2	L	602	GTP	PB-O3B-PG-O2G
3	C	602	NAI	C2B-C1B-N9A-C8A
4	C	603	GGL	OE1-CD-CG-CB
4	E	602	GGL	C-CA-CB-CG
3	B	601	NAI	O4B-C1B-N9A-C8A
3	G	603	NAI	O4B-C1B-N9A-C8A
3	K	601	NAI	O4B-C1B-N9A-C8A
3	L	601	NAI	O4B-C1B-N9A-C8A
3	K	601	NAI	C2D-C1D-N1N-C6N
3	B	603	NAI	C2B-C1B-N9A-C8A
2	A	600	GTP	PB-O3A-PA-O2A
2	B	600	GTP	PA-O3A-PB-O2B
2	B	600	GTP	PB-O3A-PA-O1A
3	H	603	NAI	O4B-C1B-N9A-C8A
3	L	603	NAI	O4B-C4B-C5B-O5B
4	A	602	GGL	OE2-CD-CG-CB
4	A	602	GGL	OE1-CD-CG-CB
3	E	601	NAI	C2B-C1B-N9A-C8A
3	J	603	NAI	C2B-C1B-N9A-C8A
3	A	603	NAI	C2B-C1B-N9A-C4A
3	C	605	NAI	C2B-C1B-N9A-C4A
3	J	602	NAI	C2B-C1B-N9A-C4A
2	C	601	GTP	PB-O3B-PG-O1G
3	D	601	NAI	C3B-C4B-C5B-O5B
3	D	603	NAI	O4B-C4B-C5B-O5B
3	A	603	NAI	C2N-C3N-C7N-O7N
3	D	603	NAI	C2B-C1B-N9A-C8A
3	J	603	NAI	C2N-C3N-C7N-O7N
3	J	604	NAI	C2B-C1B-N9A-C8A
4	A	602	GGL	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
3	C	604	NAI	C2D-C1D-N1N-C2N
4	B	602	GGL	O-C-CA-N
4	B	602	GGL	OE2-CD-CG-CB
3	C	602	NAI	PA-O3-PN-O1N
3	E	601	NAI	PA-O3-PN-O1N
3	G	602	NAI	PA-O3-PN-O1N
3	H	602	NAI	PA-O3-PN-O1N
3	I	602	NAI	PA-O3-PN-O1N
3	J	602	NAI	PA-O3-PN-O1N
3	L	603	NAI	PA-O3-PN-O1N
3	B	603	NAI	O4D-C4D-C5D-O5D
3	D	603	NAI	C3B-C4B-C5B-O5B

There are no ring outliers.

31 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	602	NAI	2	0
4	A	602	GGL	2	0
3	C	605	NAI	1	0
3	D	601	NAI	2	0
2	F	600	GTP	1	0
2	I	601	GTP	1	0
3	C	602	NAI	2	0
2	D	600	GTP	1	0
3	F	601	NAI	2	0
3	H	603	NAI	1	0
3	L	603	NAI	2	0
3	J	604	NAI	1	0
2	H	601	GTP	3	0
2	B	600	GTP	1	0
3	I	603	NAI	2	0
4	E	602	GGL	2	0
3	H	602	NAI	3	0
3	C	604	NAI	1	0
4	D	602	GGL	2	0
4	B	602	GGL	1	0
3	L	601	NAI	1	0
3	G	602	NAI	1	0
3	K	601	NAI	1	0
4	F	602	GGL	1	0
2	J	601	GTP	1	0

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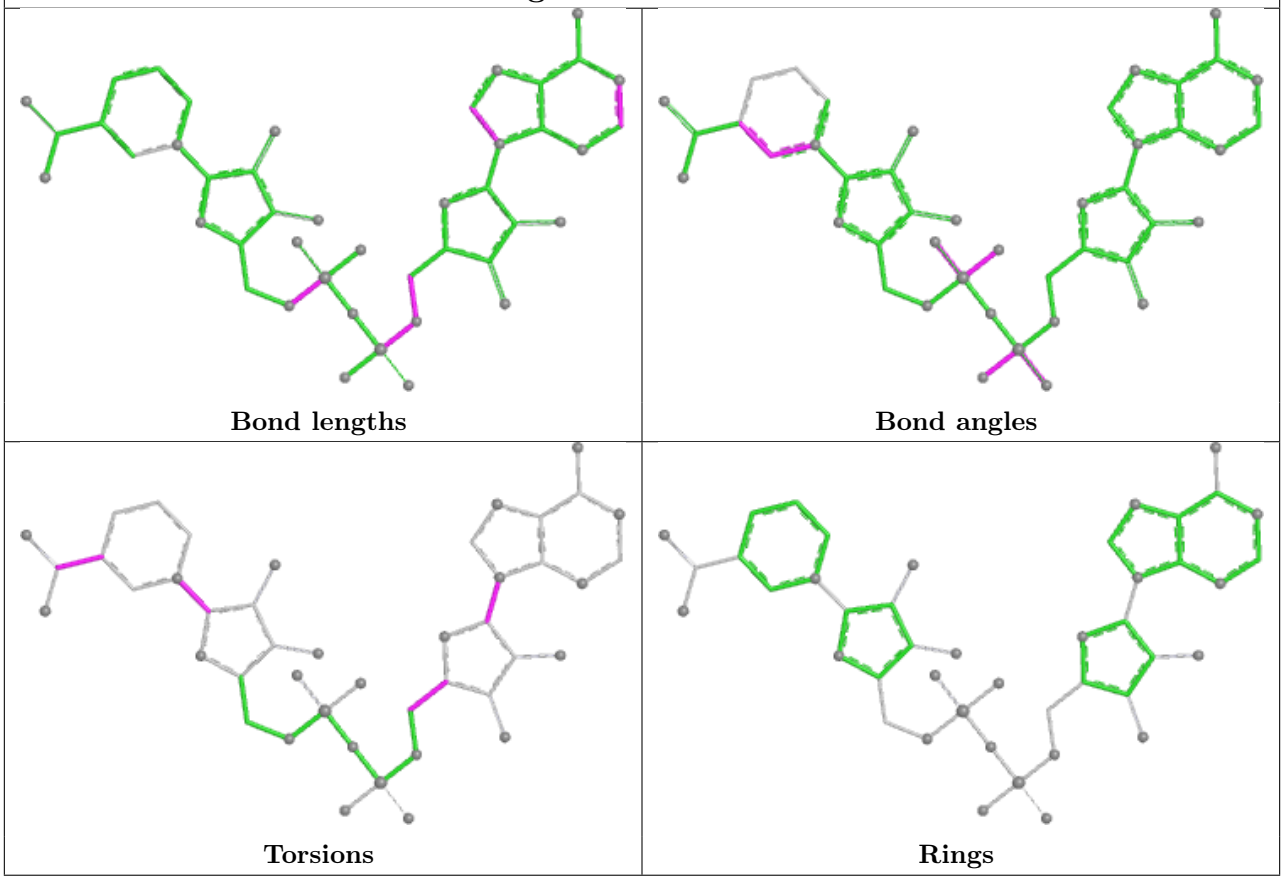
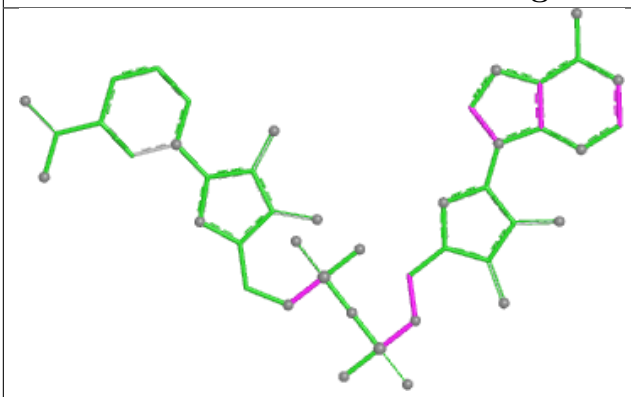
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	603	GGL	2	0
3	I	602	NAI	1	0
3	B	601	NAI	1	0
3	G	603	NAI	1	0
2	K	600	GTP	1	0
3	E	601	NAI	3	0

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.

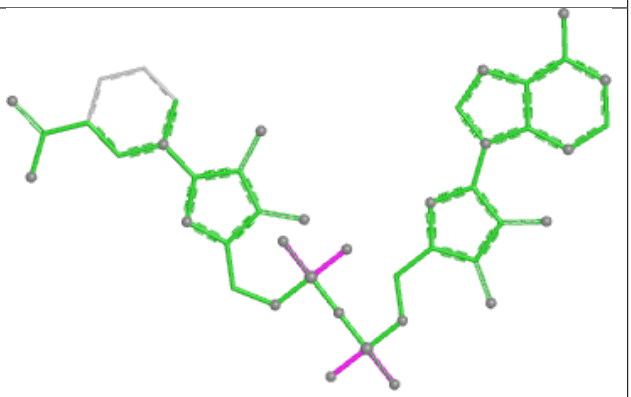
Ligand NAI A 603



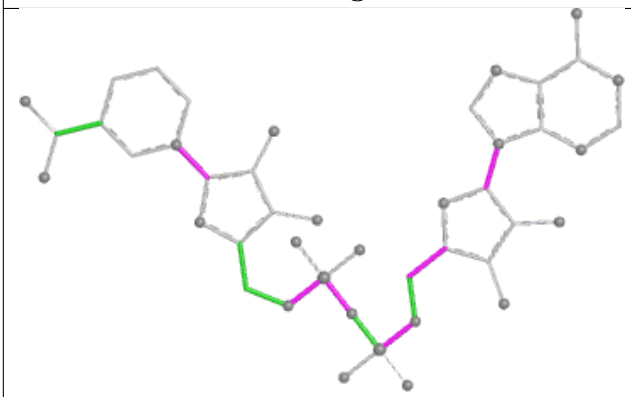
Ligand NAI J 602



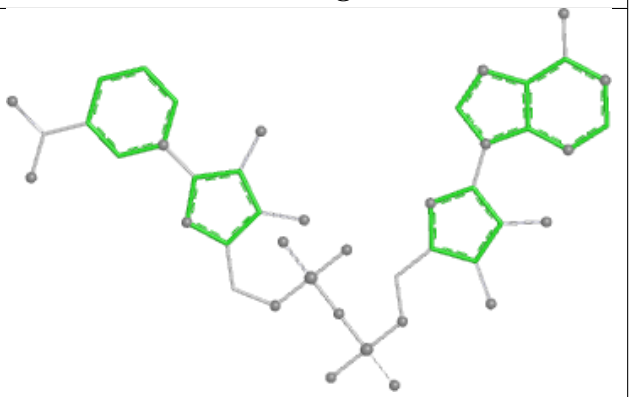
Bond lengths



Bond angles

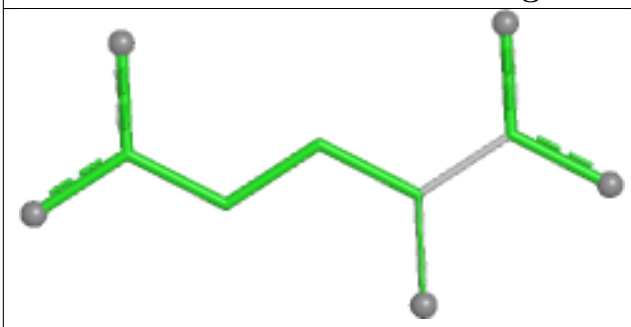


Torsions



Rings

Ligand GGL A 602



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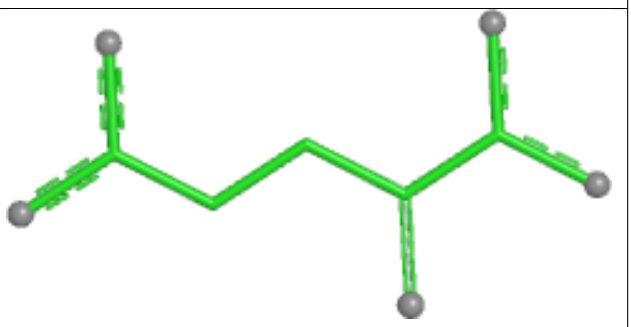

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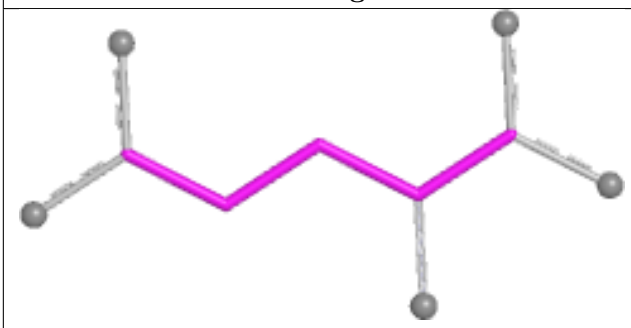

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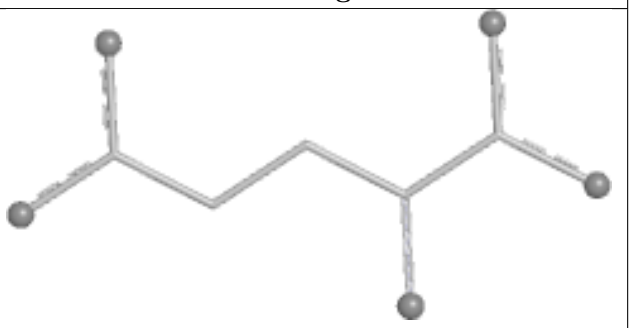
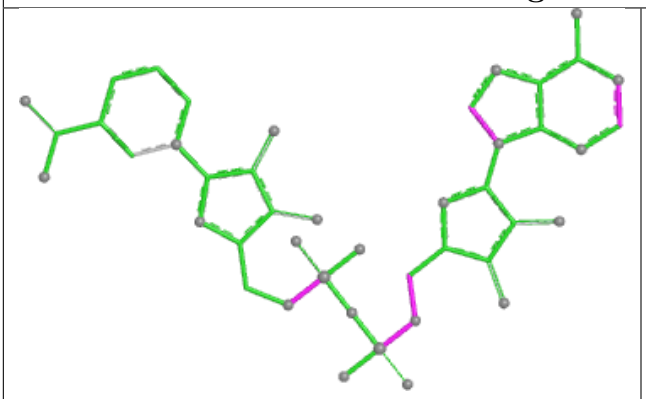


Rings

Ligand NAI C 605



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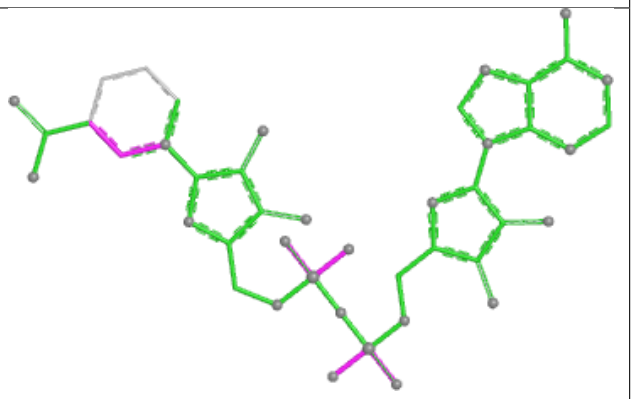
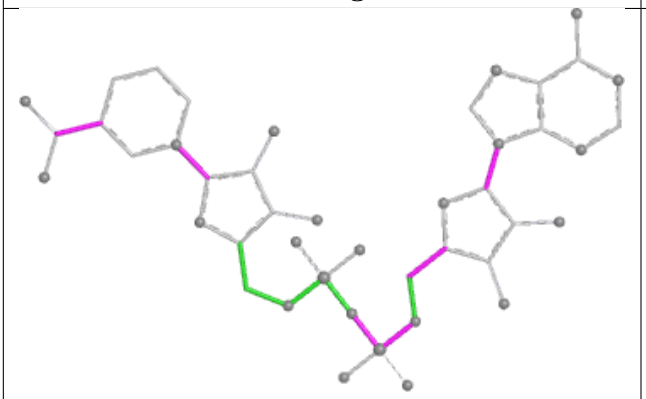


Bond angles



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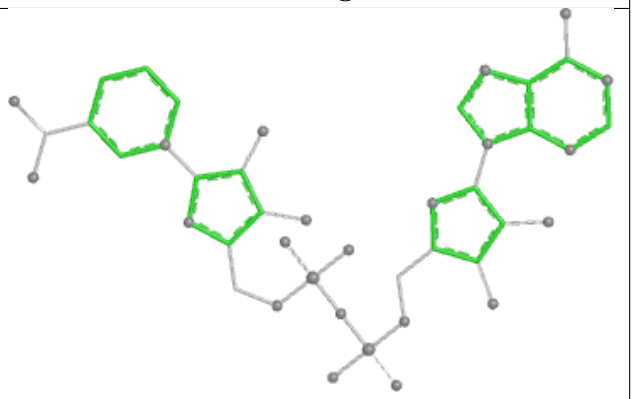
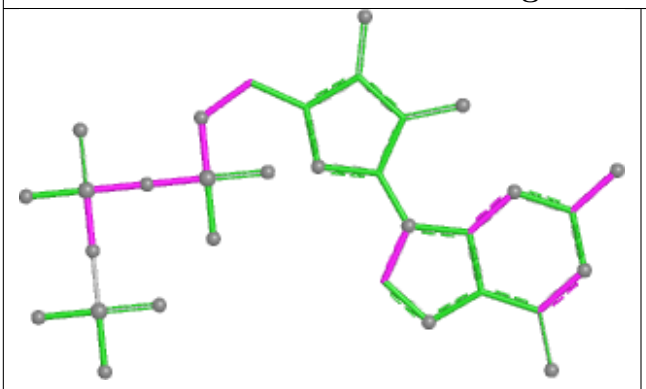


Rings

Ligand GTP G 601



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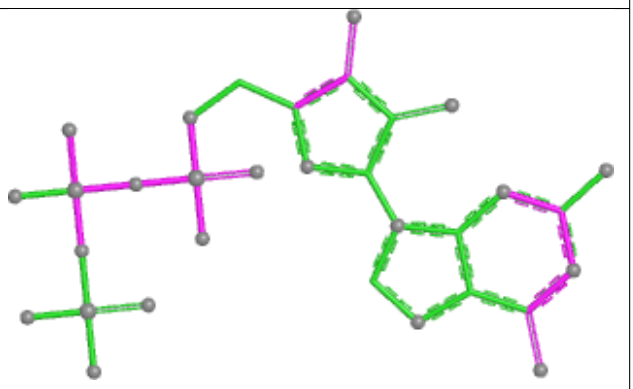

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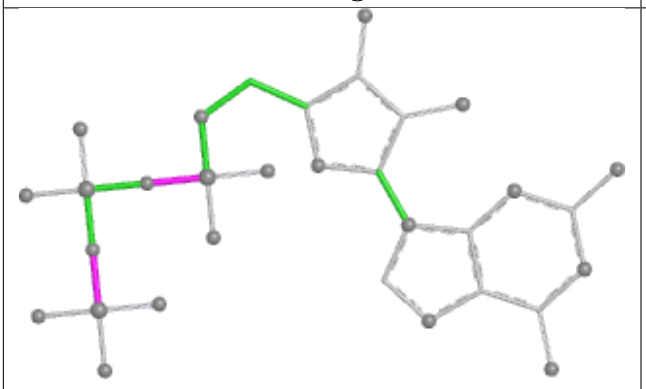

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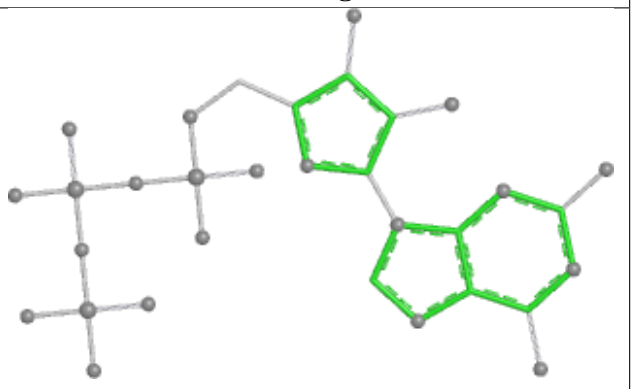
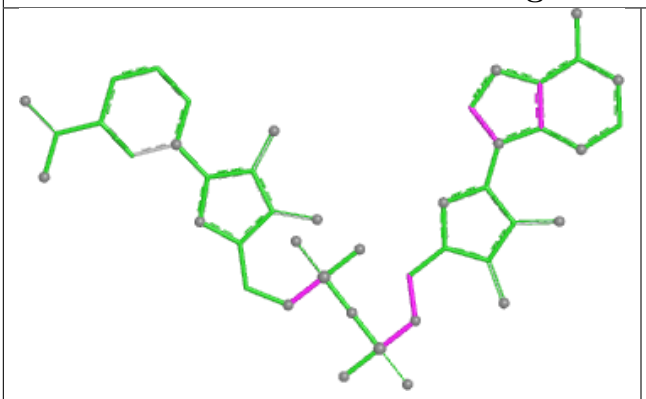


Rings

Ligand NAI D 601



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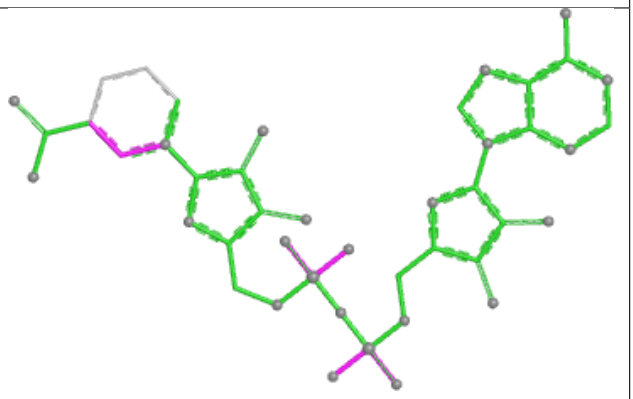

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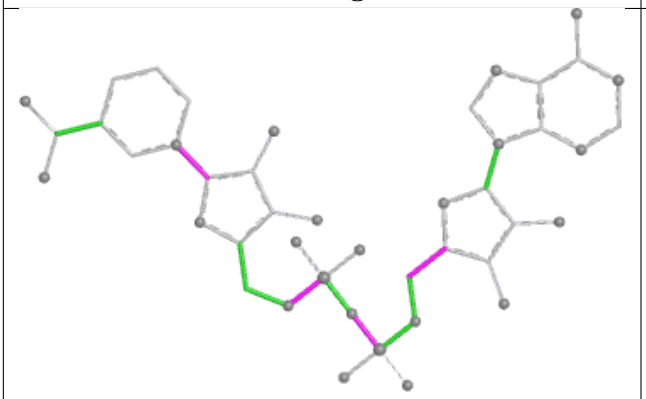

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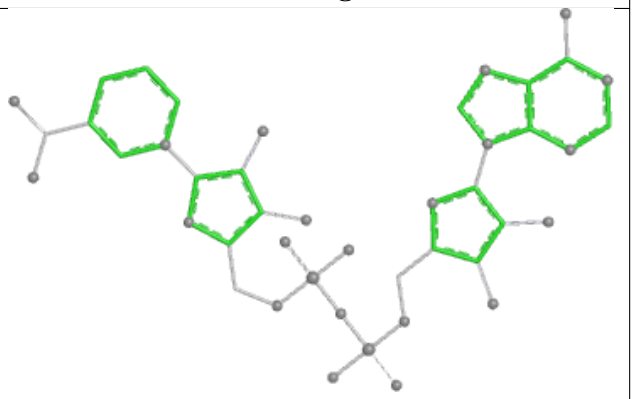
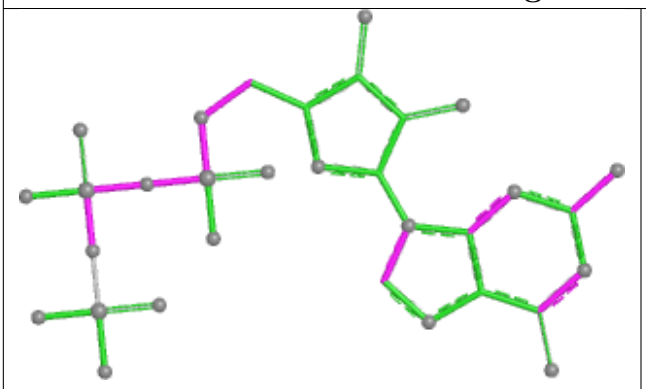


Rings

Ligand GTP F 600



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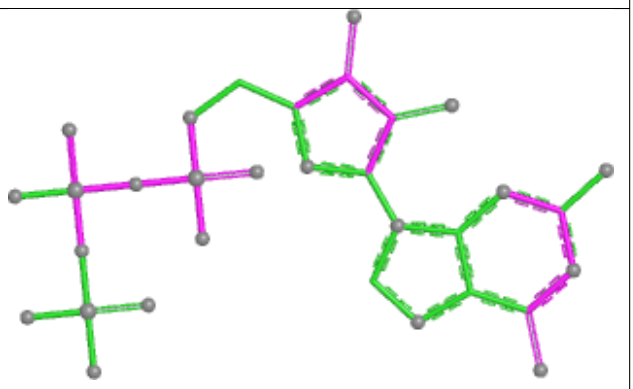

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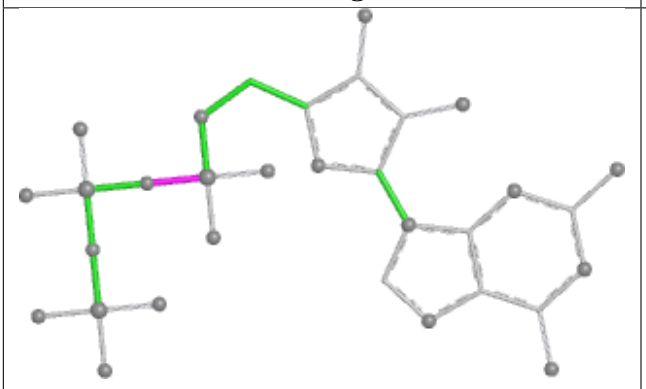

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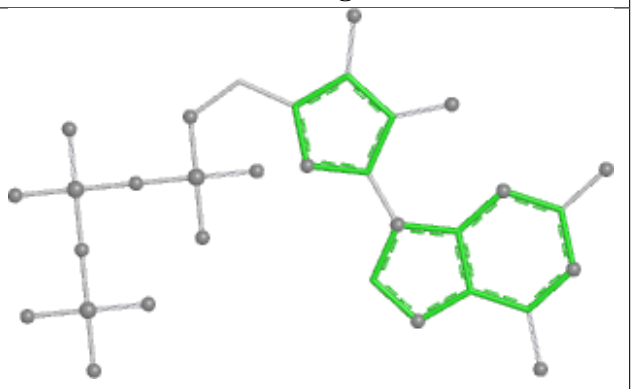

Rings

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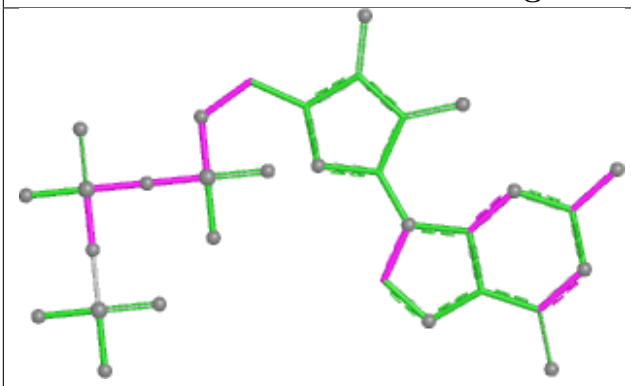

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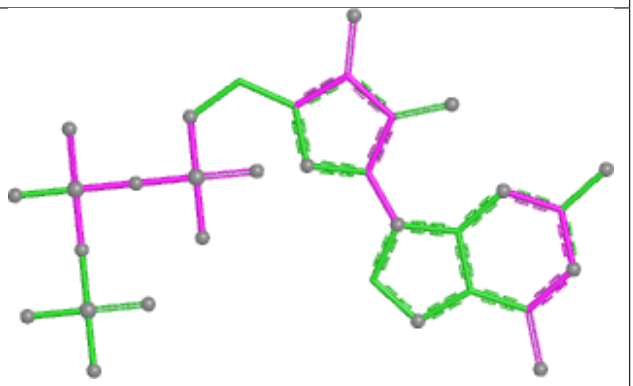

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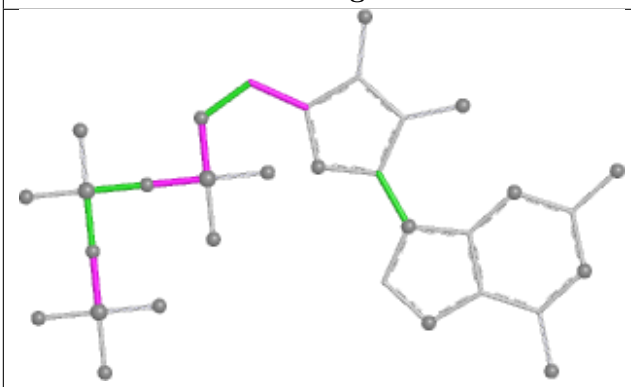

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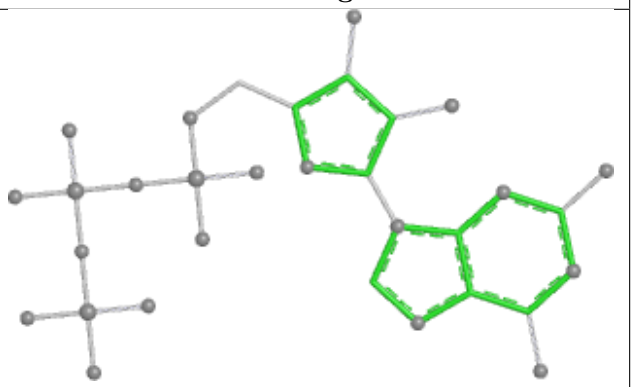

Rings

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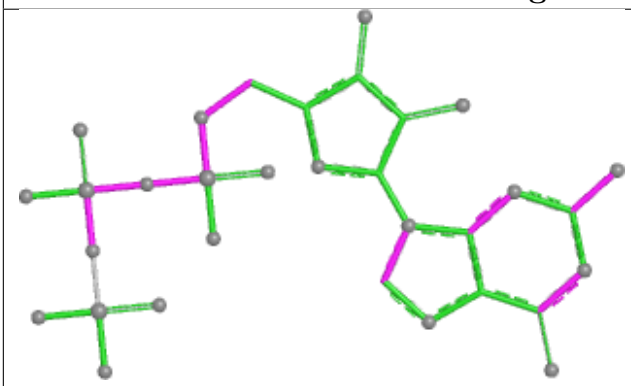

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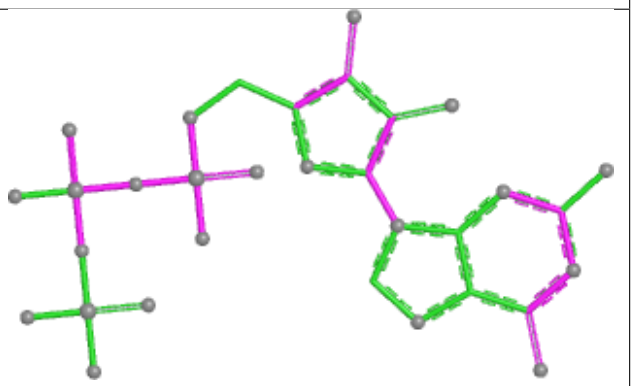

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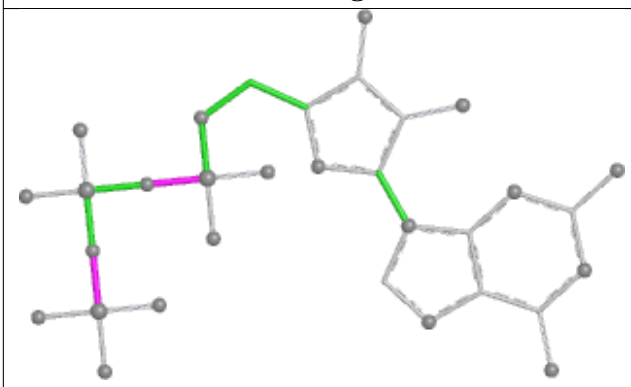

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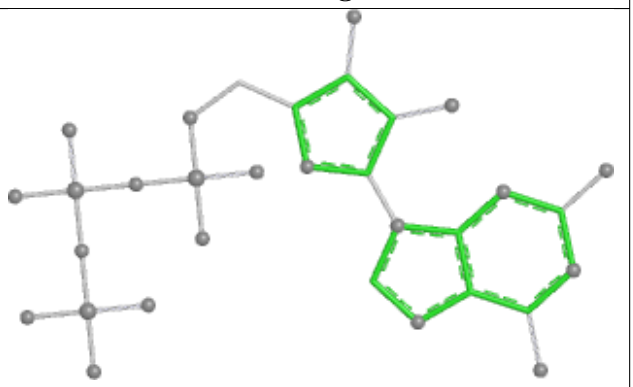
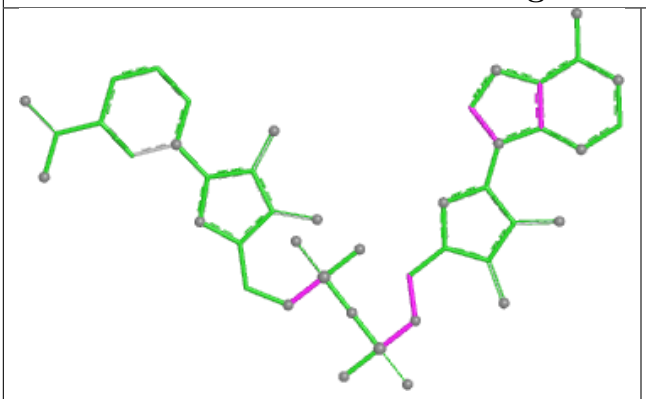


Rings

Ligand NAI C 602



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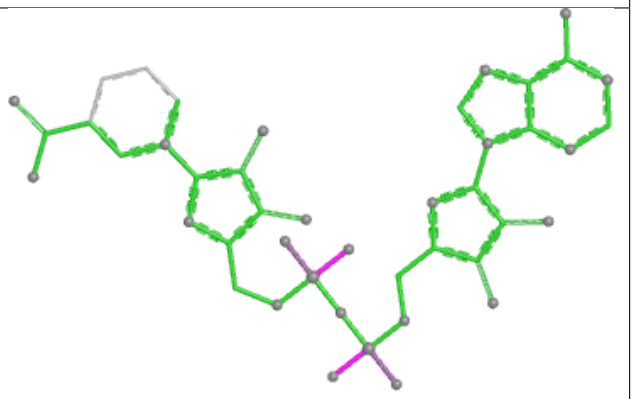
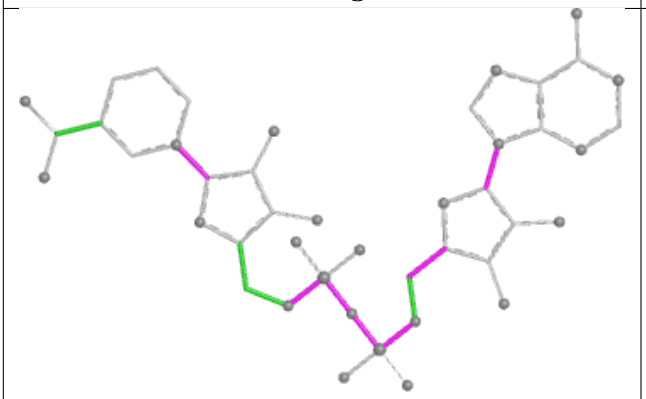


Bond angles



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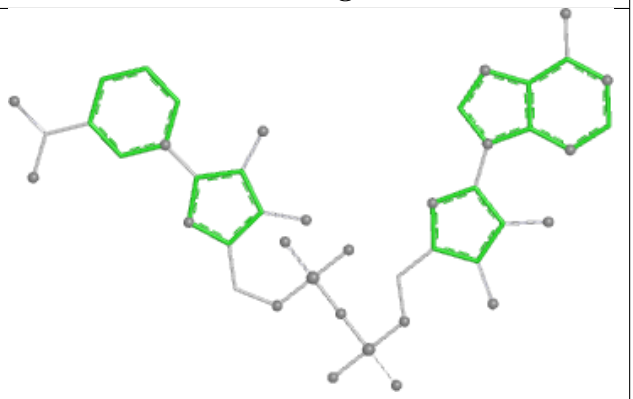
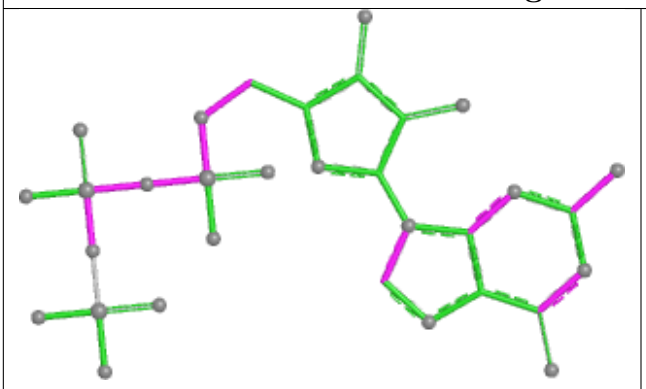


Rings

Ligand GTP L 602



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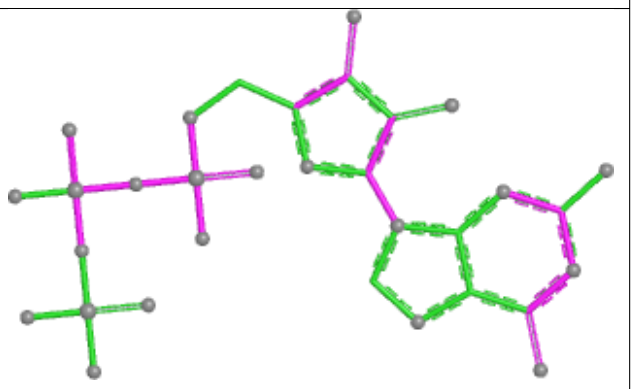
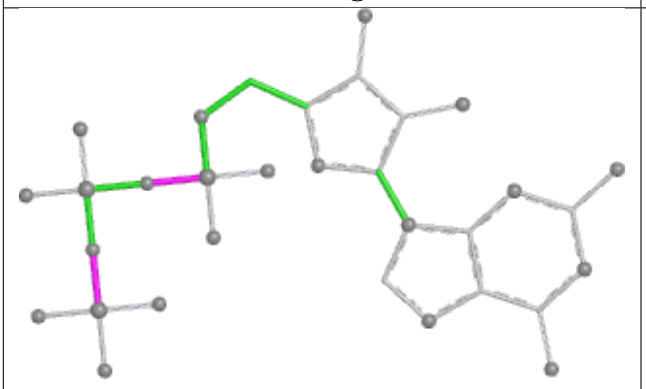


Bond angles



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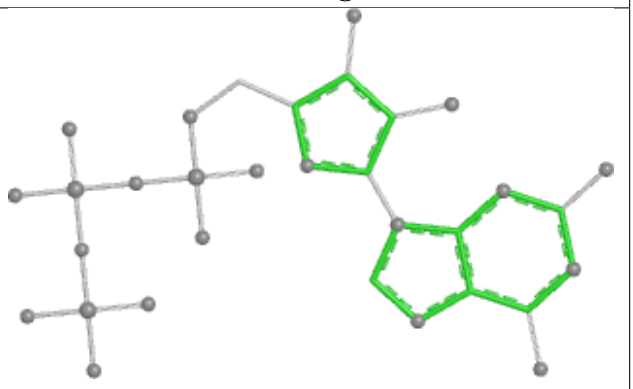

Rings

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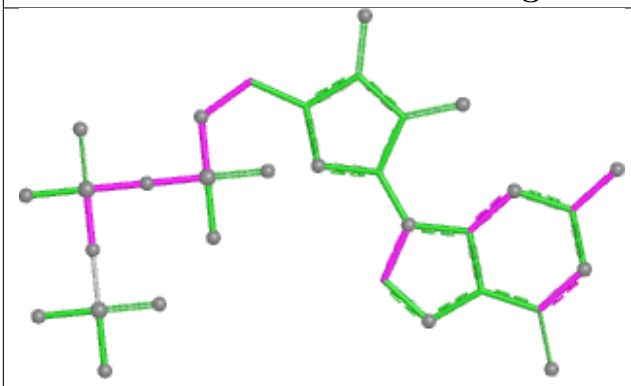

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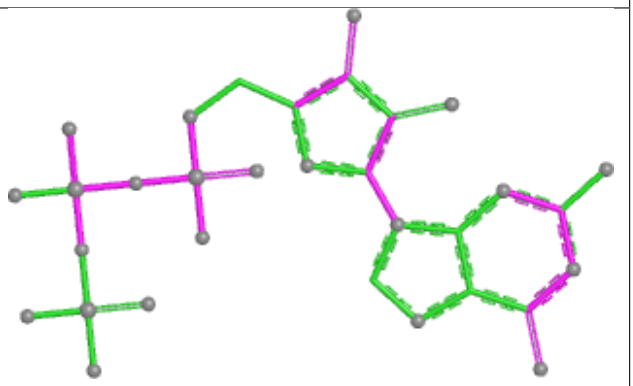

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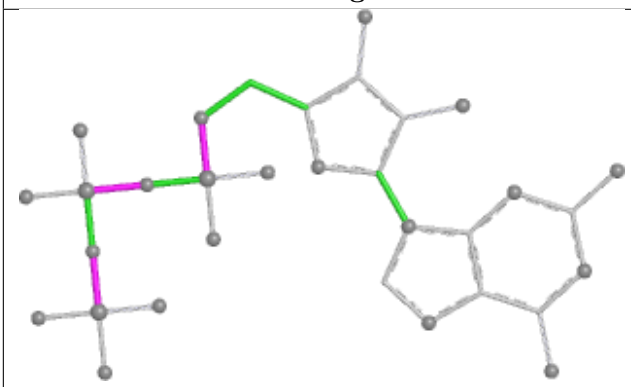

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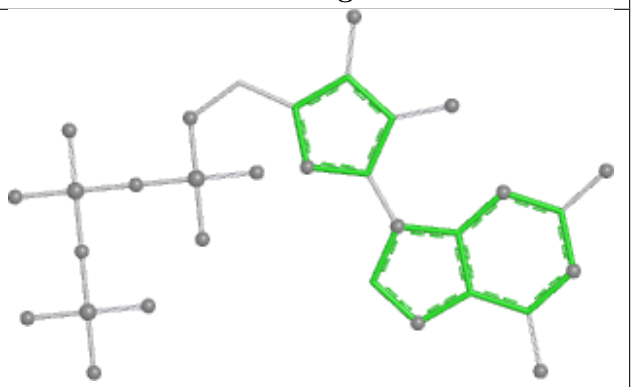

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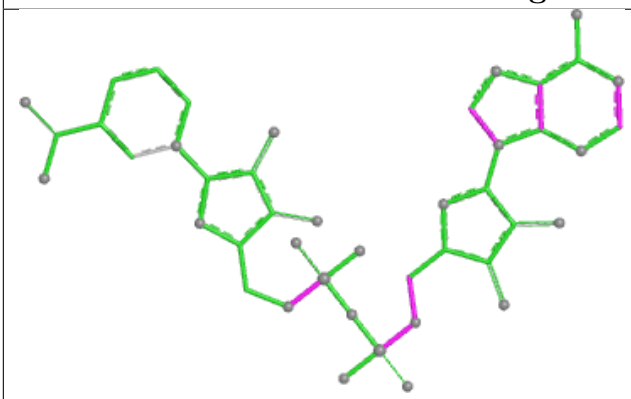

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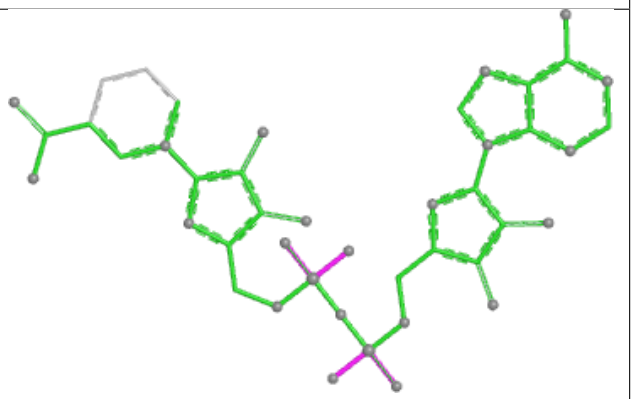

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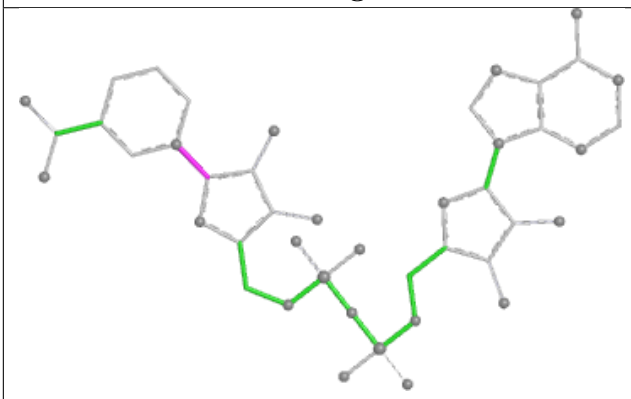

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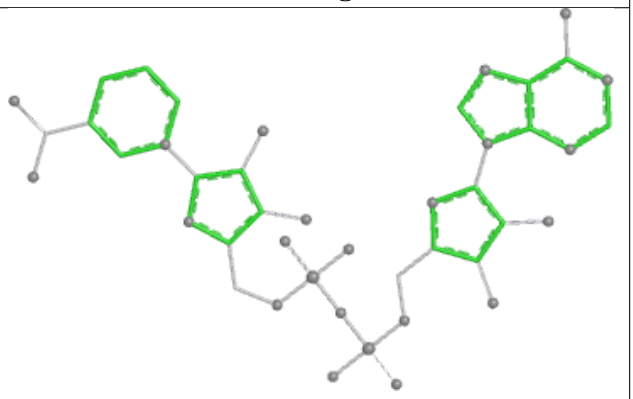

Rings

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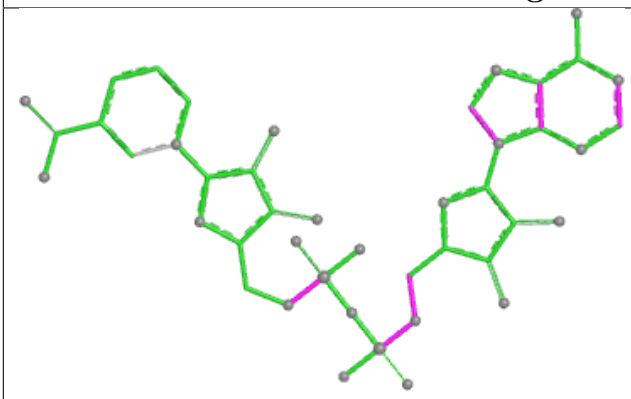

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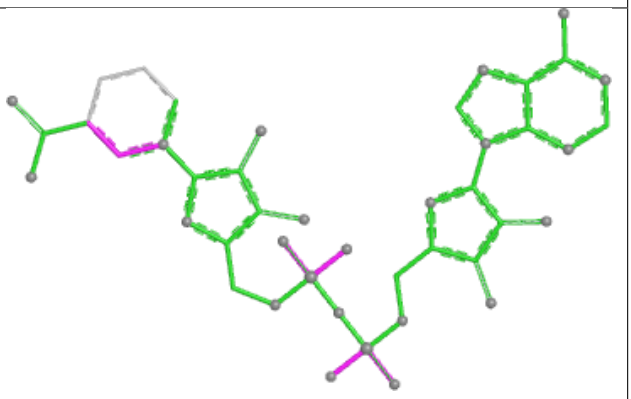

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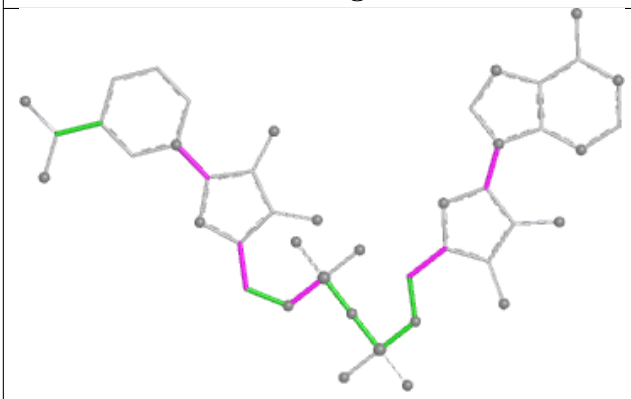

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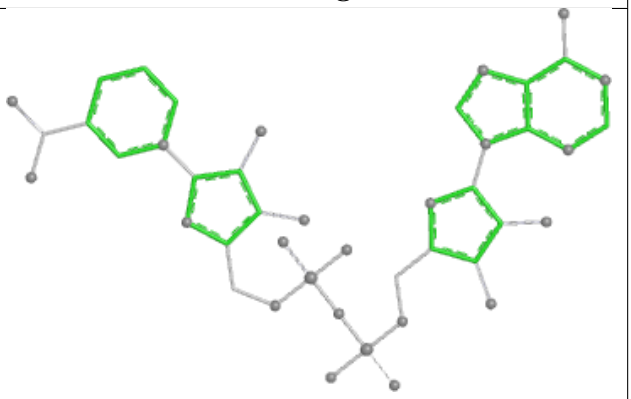

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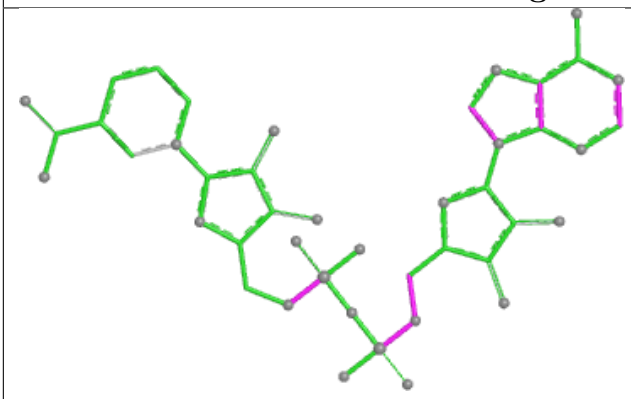

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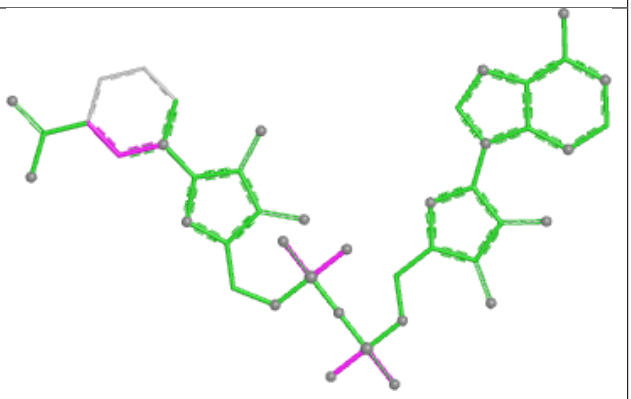

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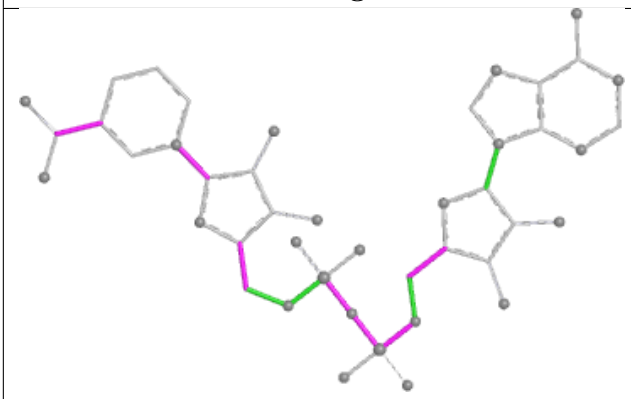

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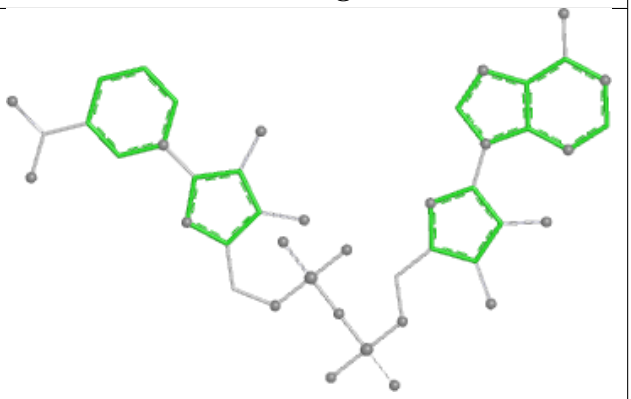

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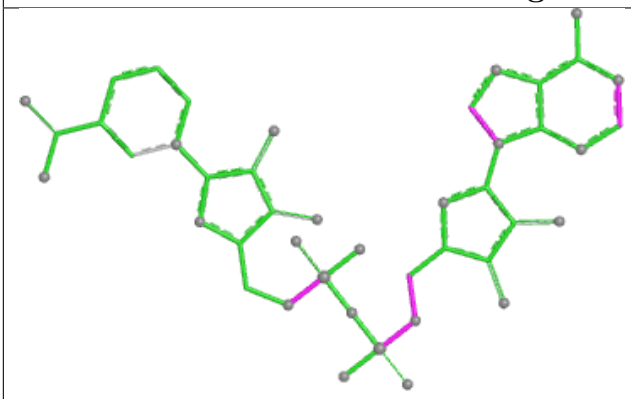

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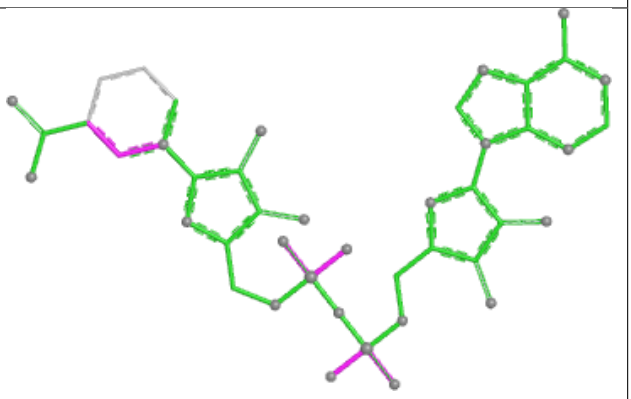

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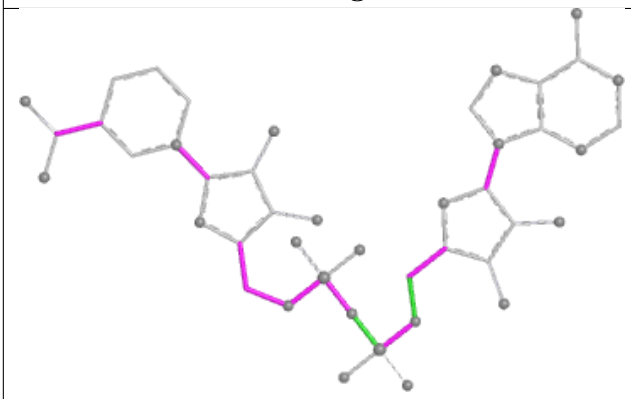

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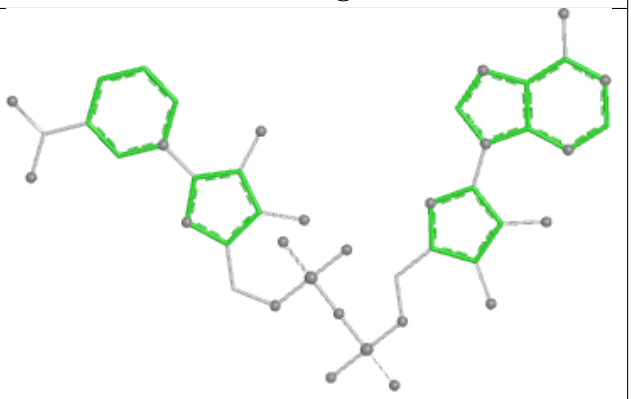

Rings

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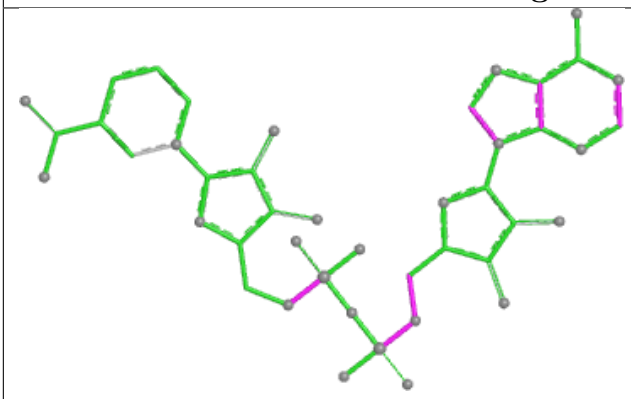

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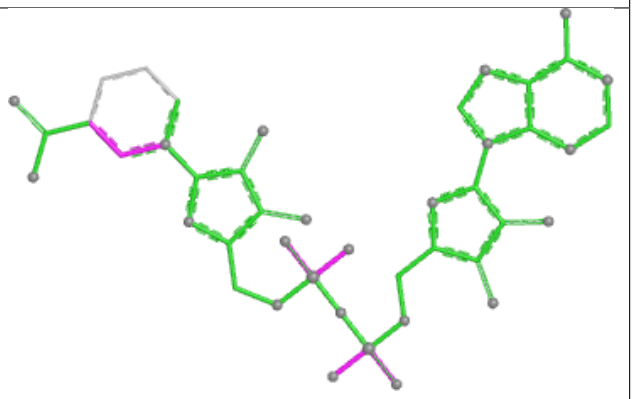

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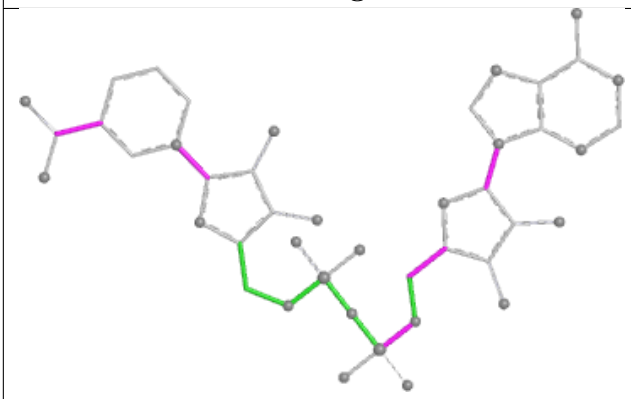

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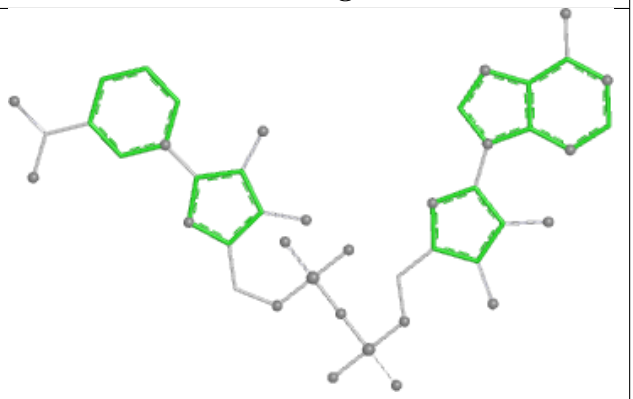

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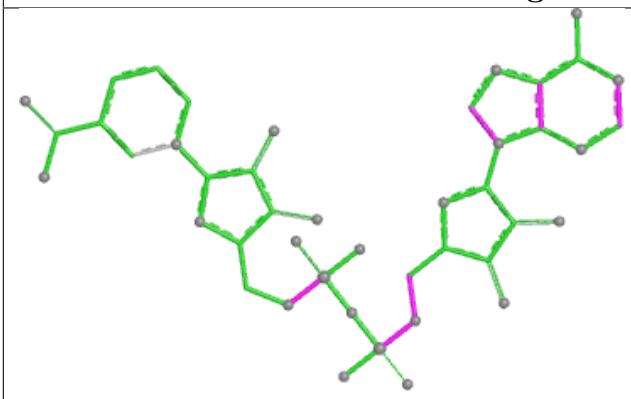

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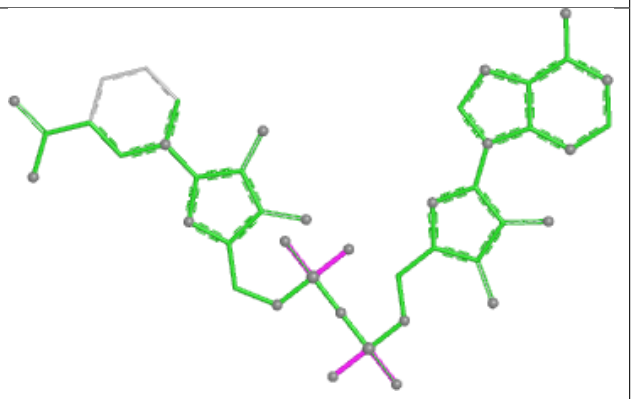

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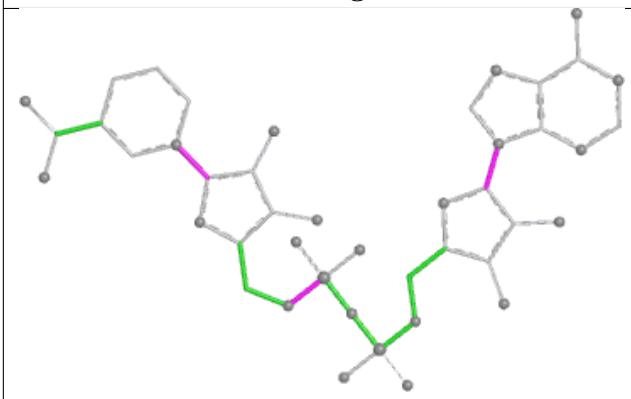

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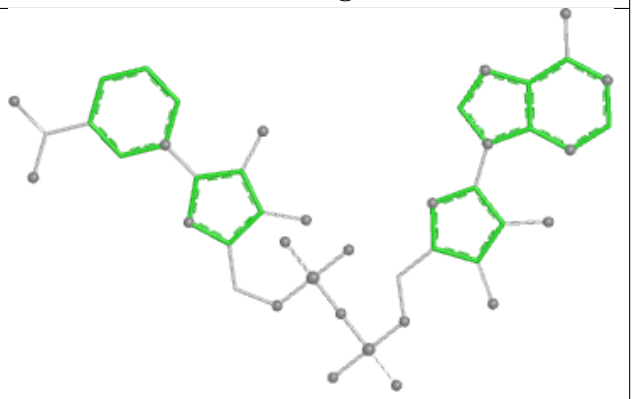

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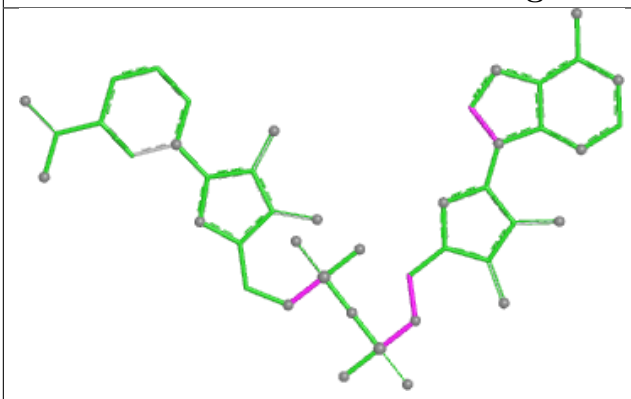

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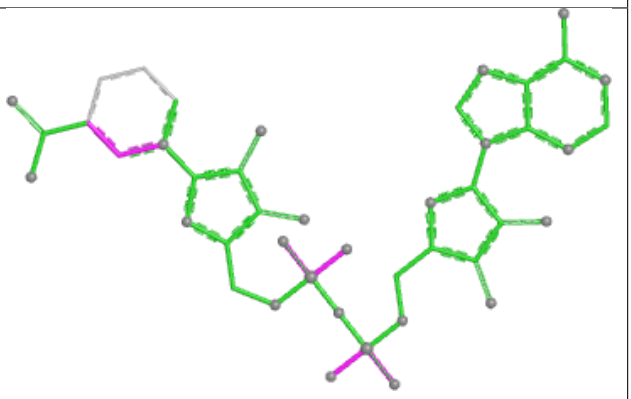

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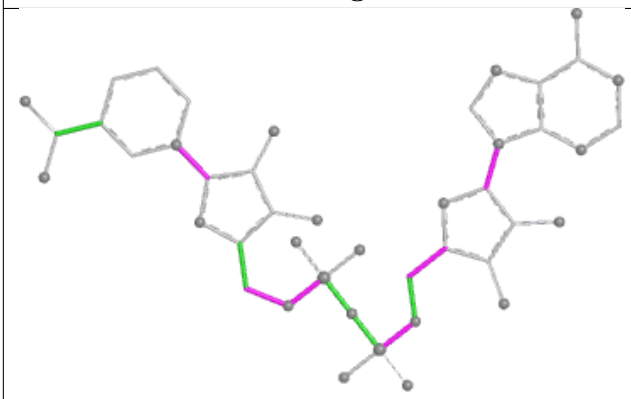

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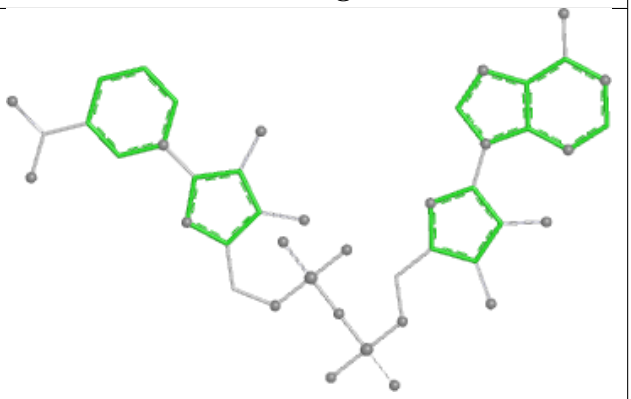

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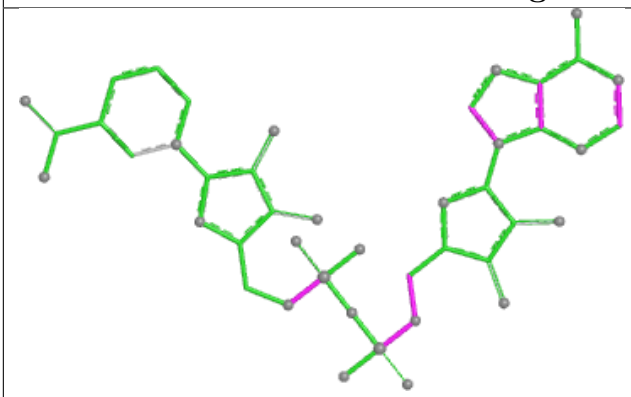

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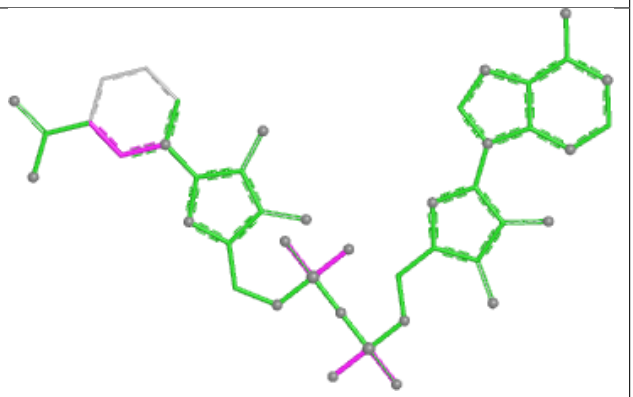

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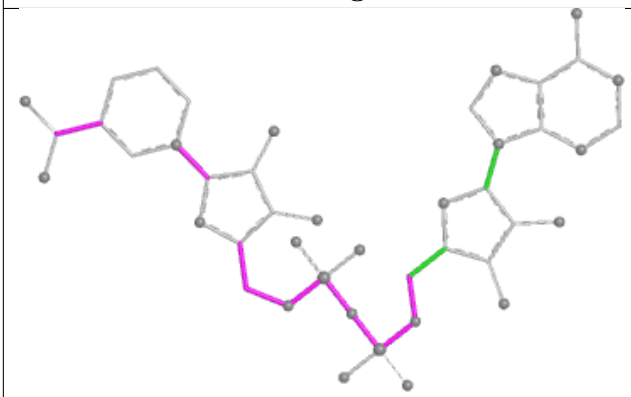

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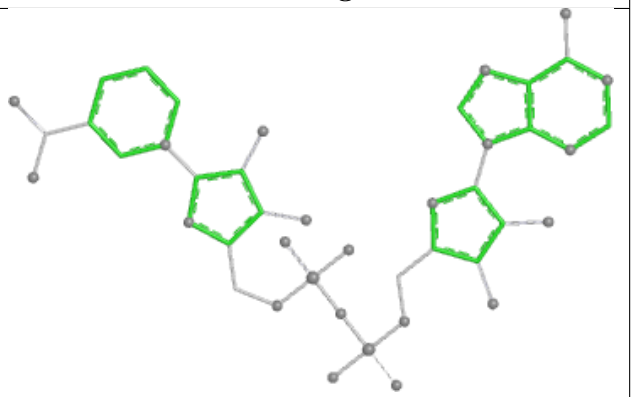

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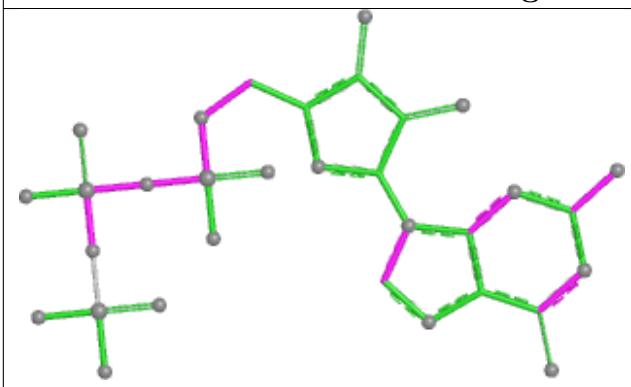

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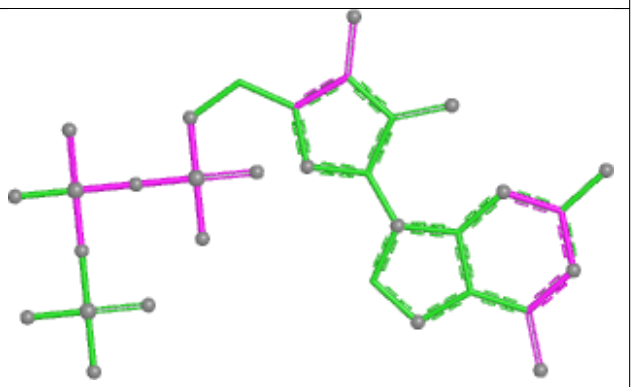

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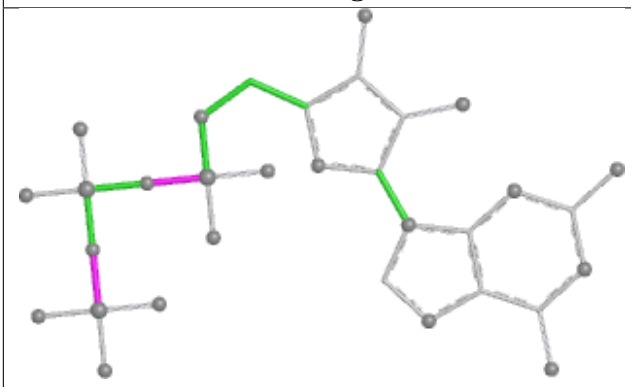

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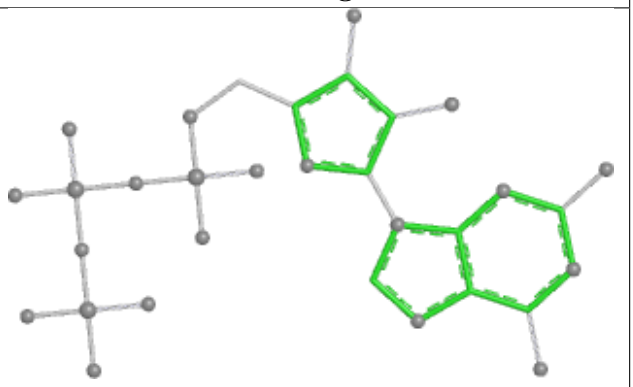

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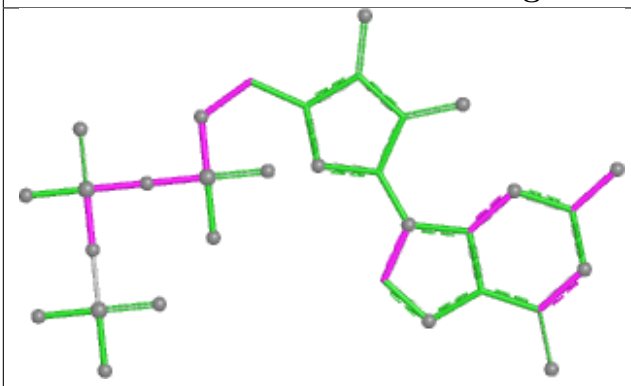

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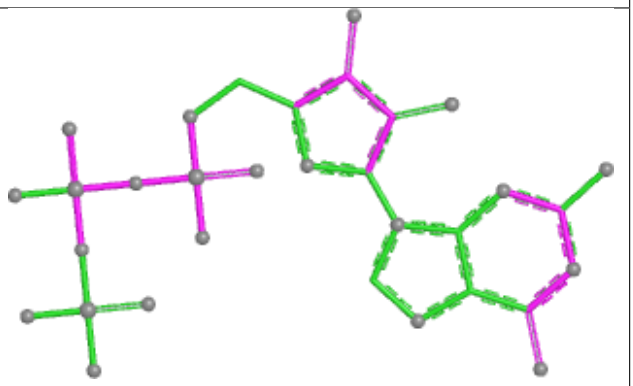

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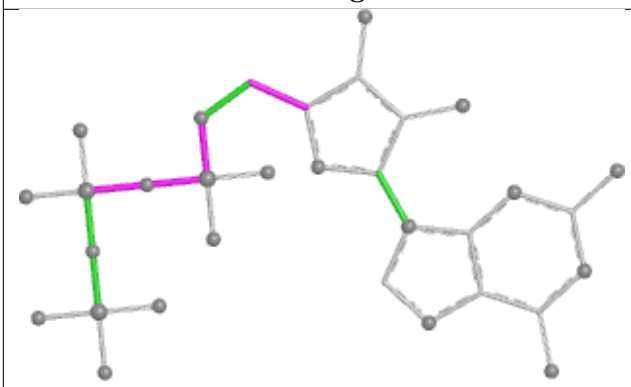

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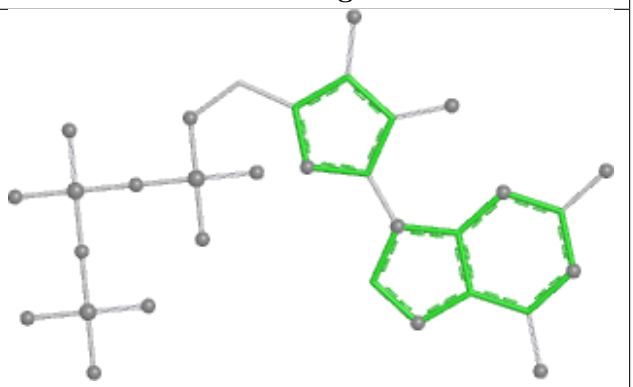

Rings

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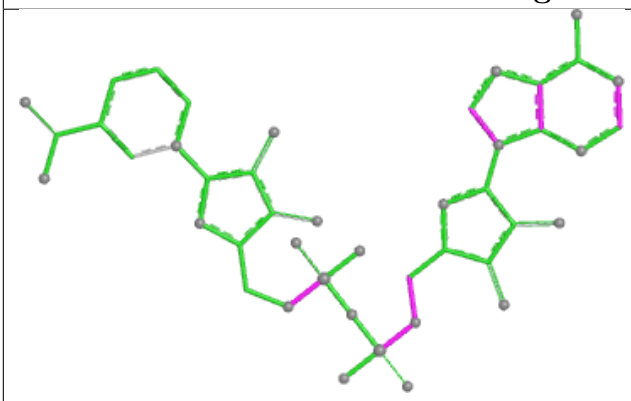

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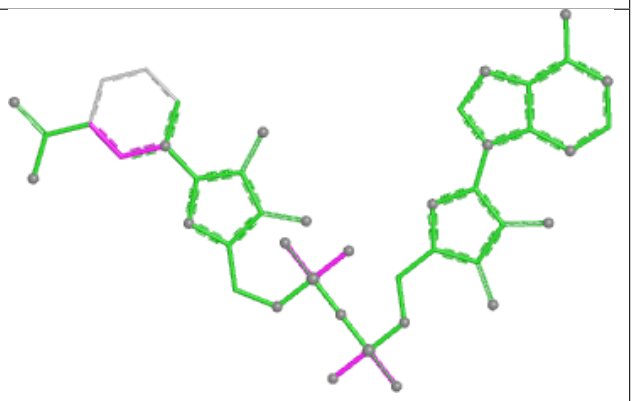

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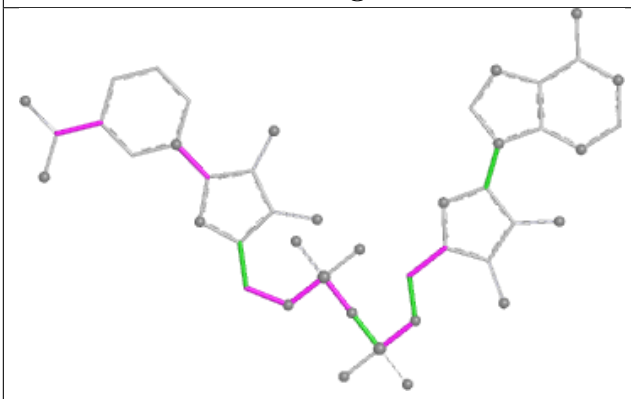

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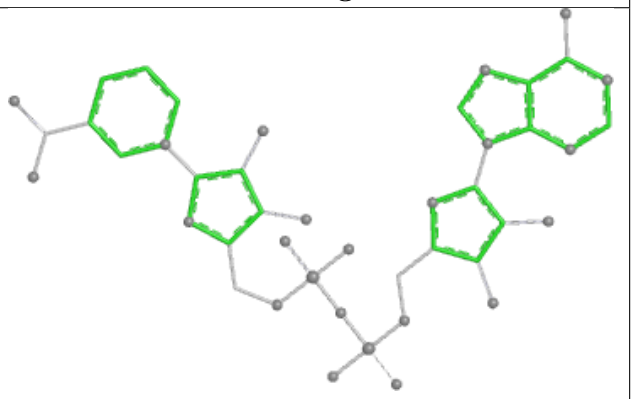
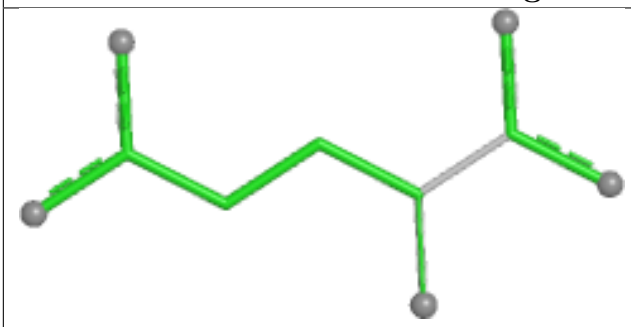


Rings

Ligand GGL E 602



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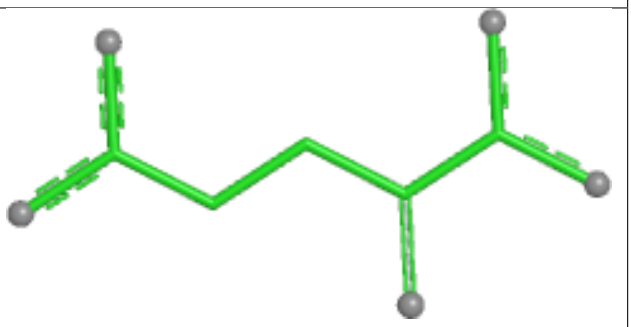

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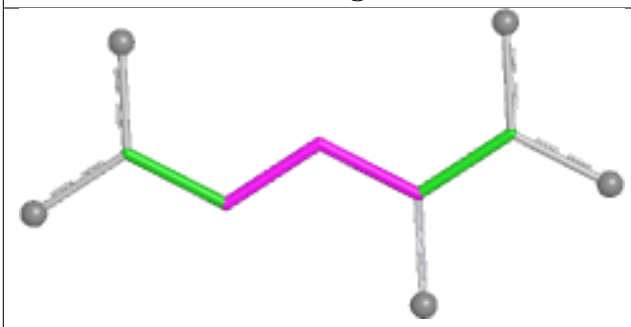

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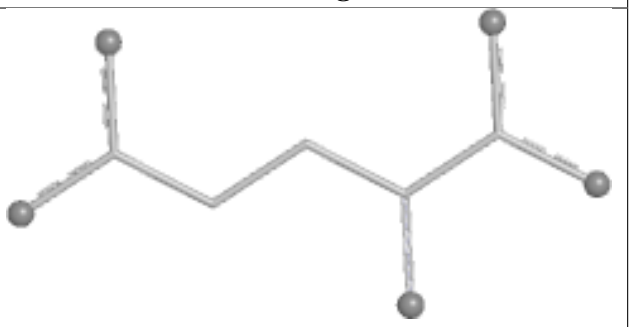

Rings

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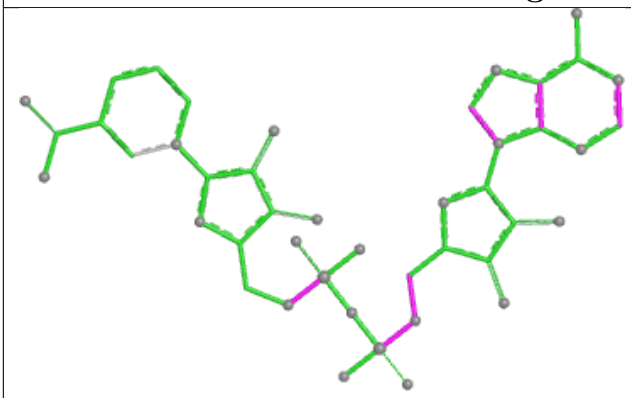

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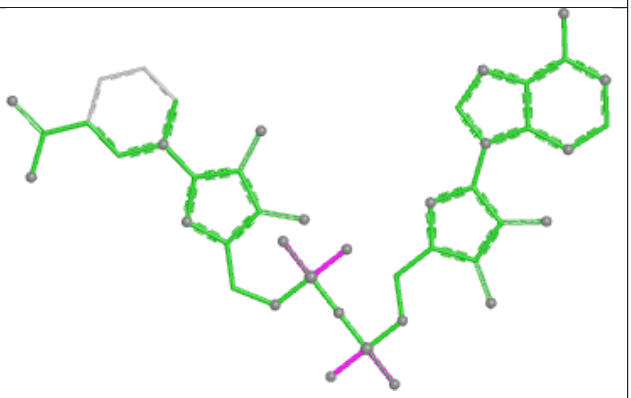

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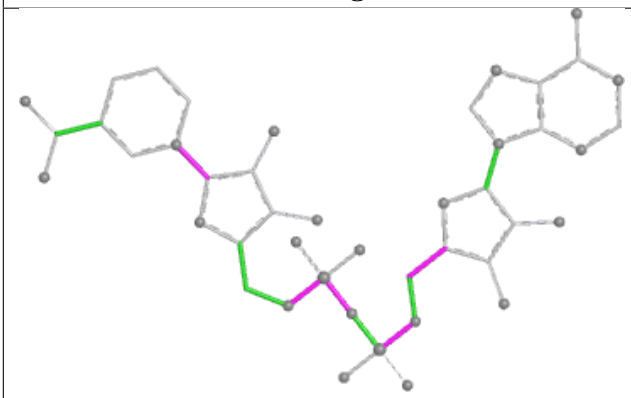

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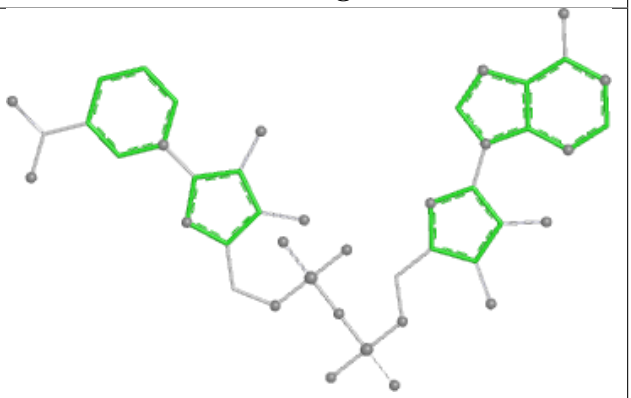
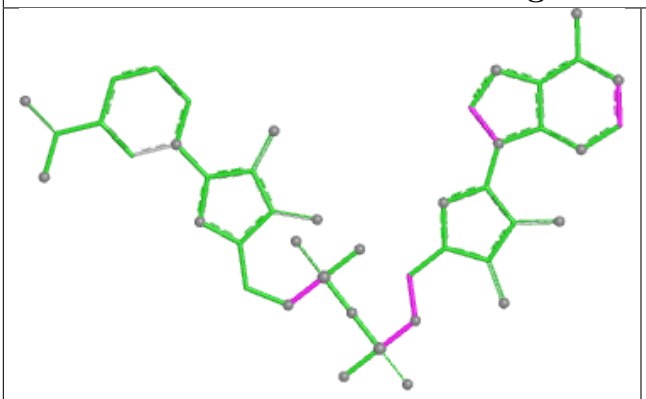


Rings

Ligand NAI C 604



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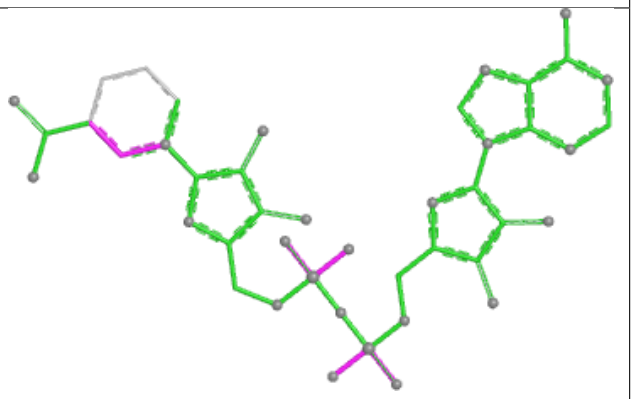

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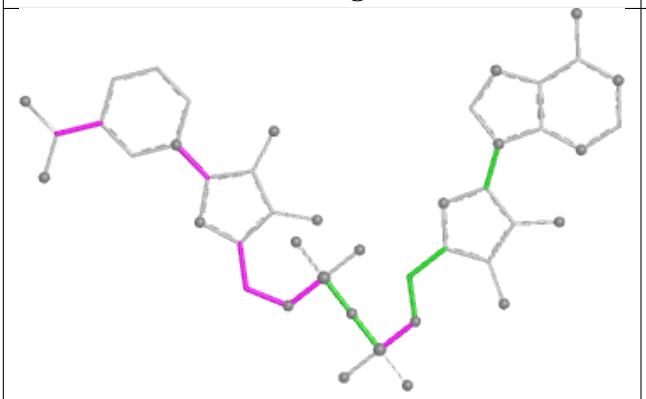

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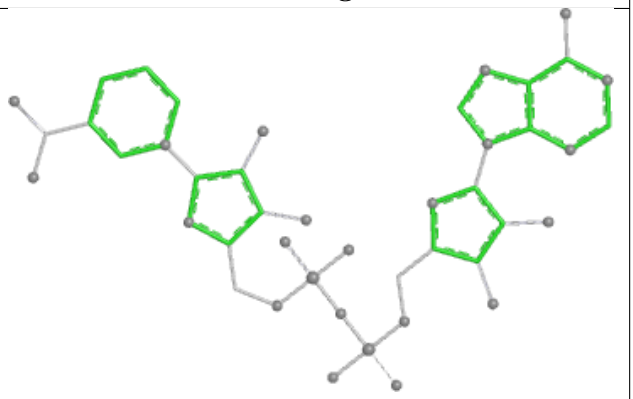
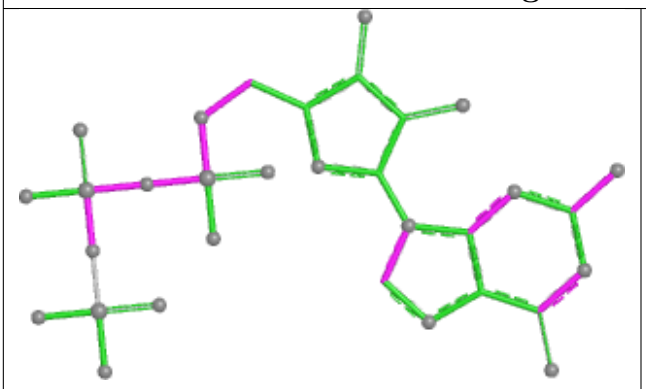


Rings

Ligand GTP A 600



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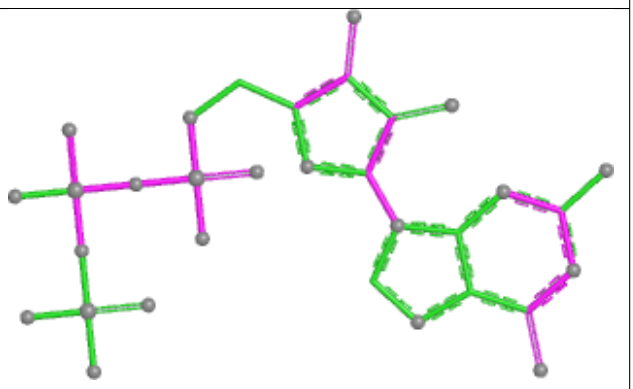

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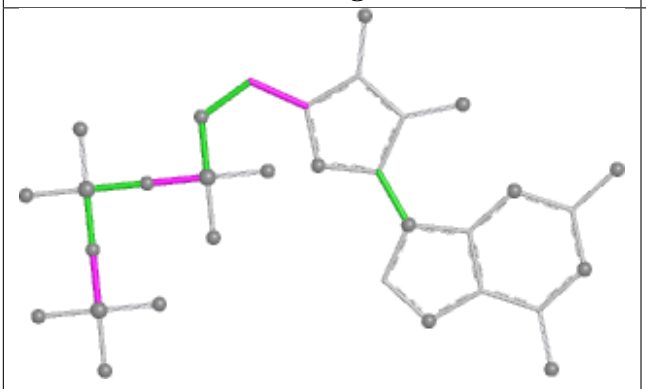

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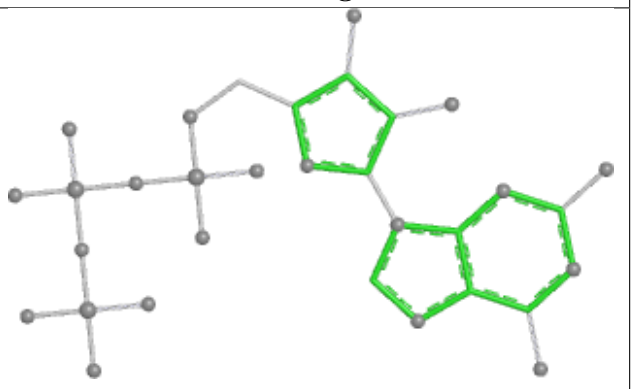

Rings

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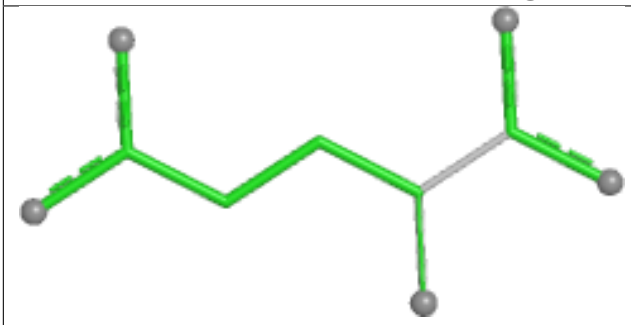
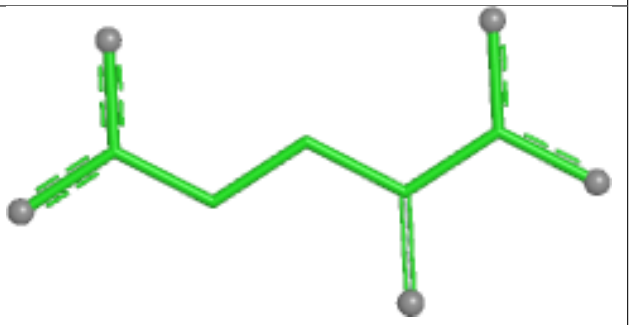
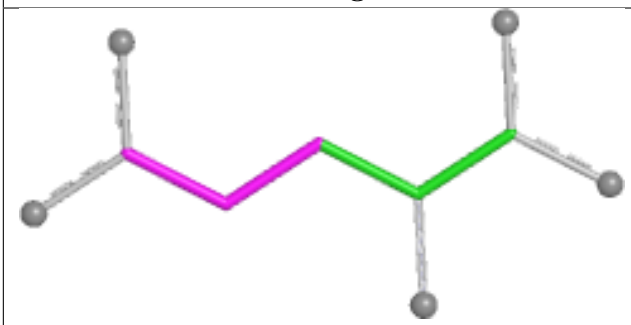
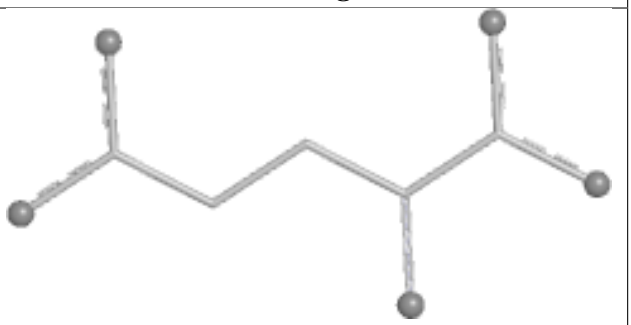
 Bond lengths	 Bond angles
 Torsions	 Rings

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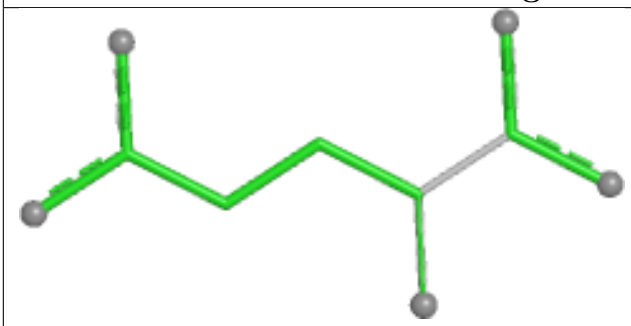
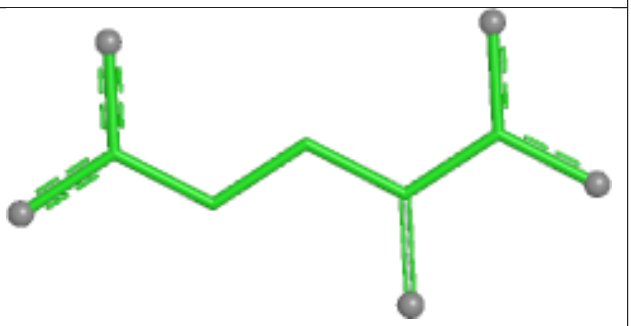
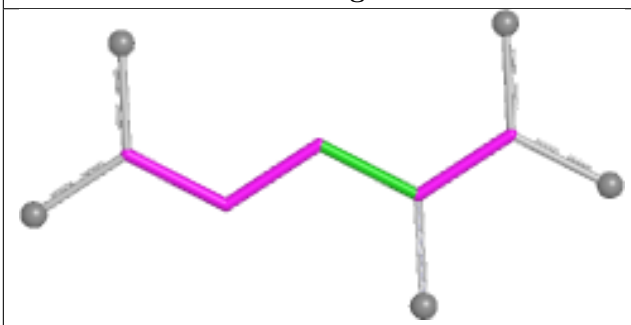
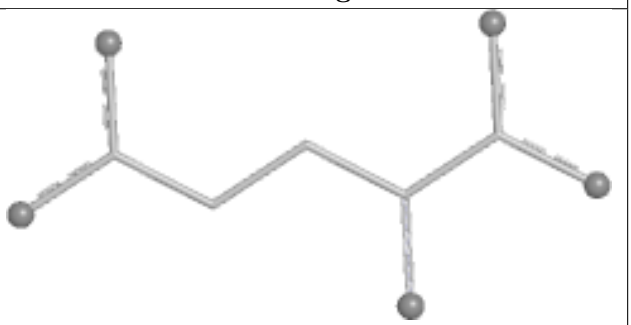
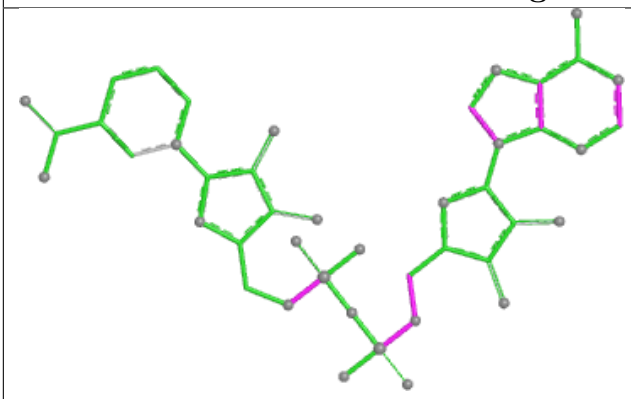
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAI L 601



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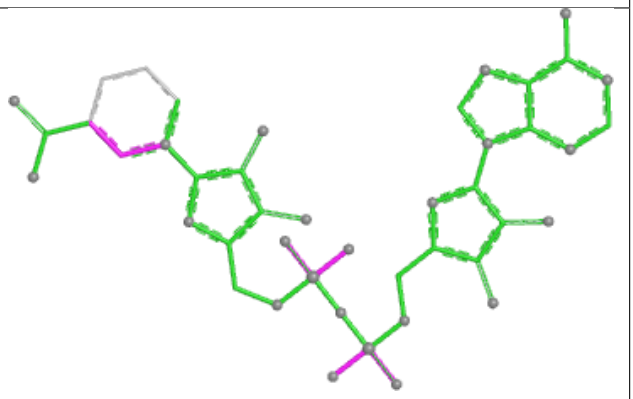

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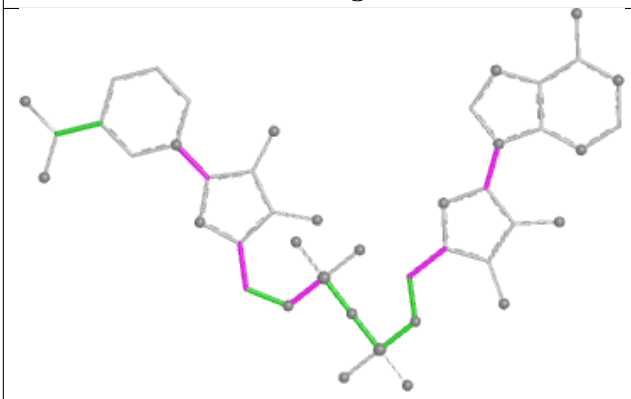

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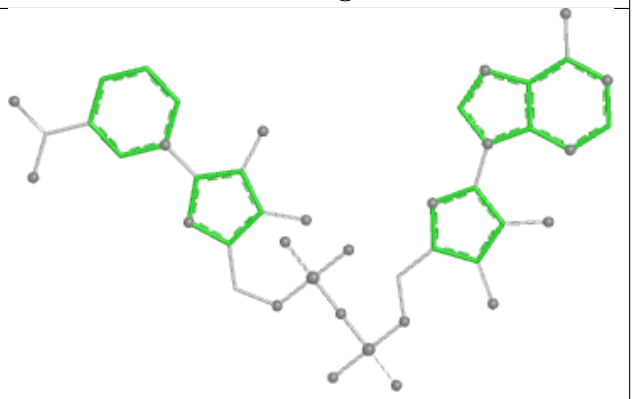
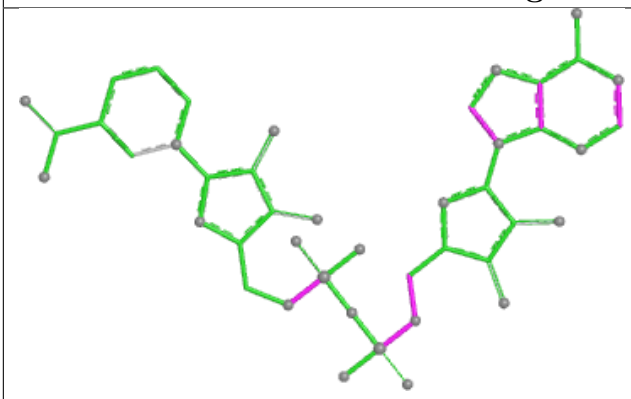


Rings

Ligand NAI G 602



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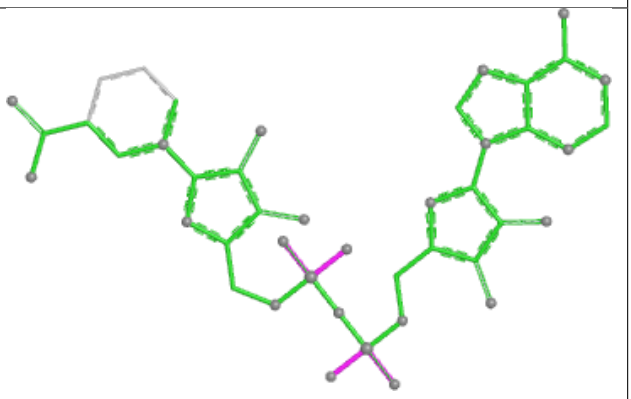

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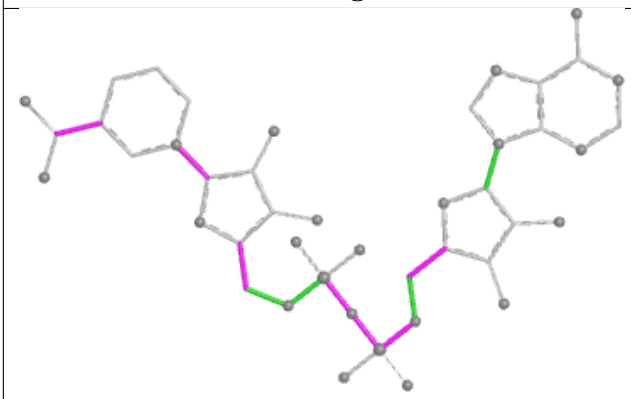

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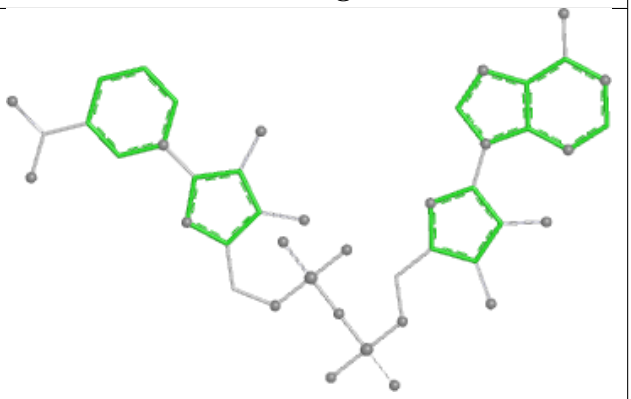
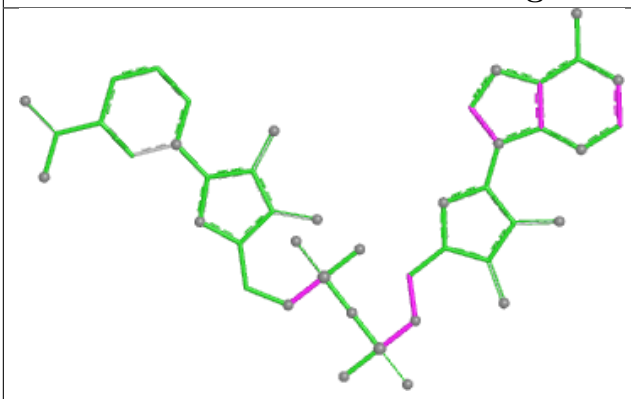


Rings

Ligand NAI K 601



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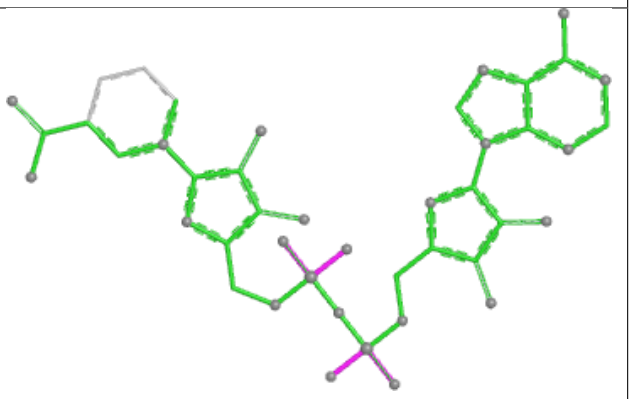

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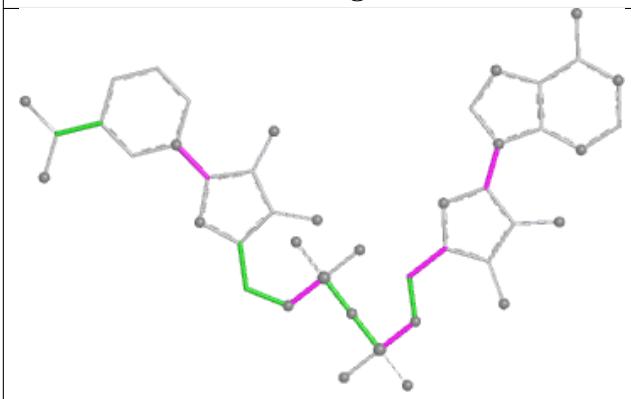

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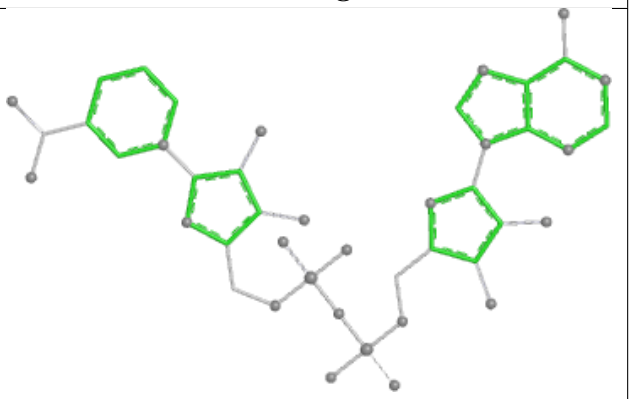
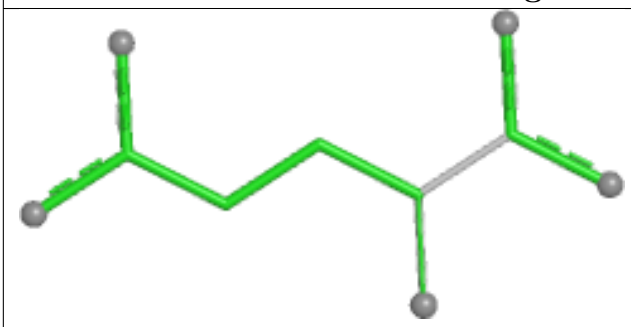


Rings

Ligand GGL F 602



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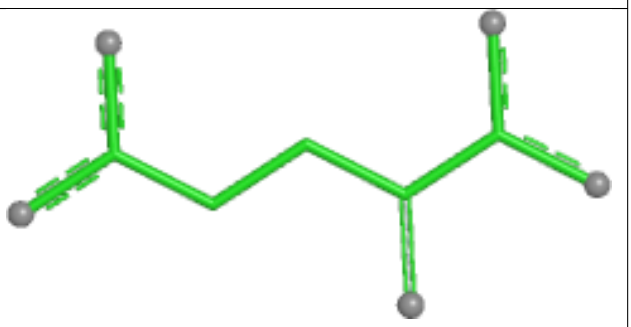

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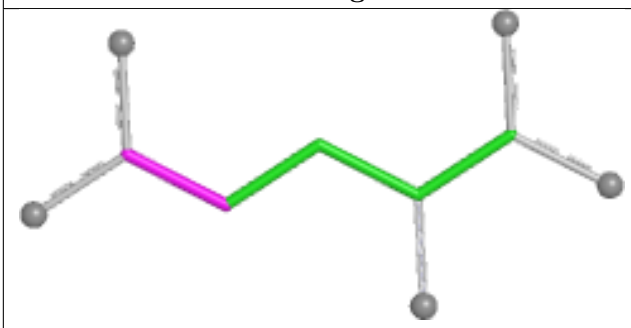

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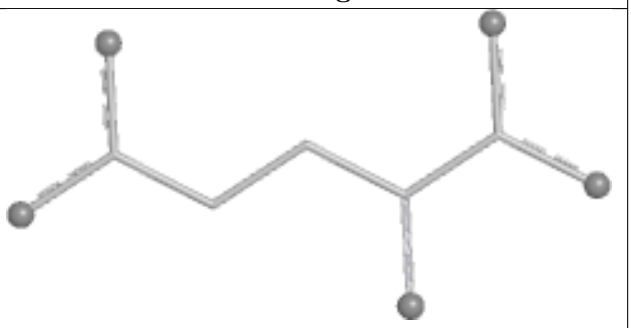
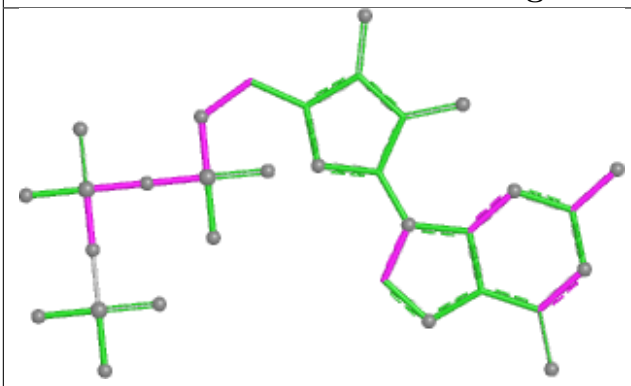


Rings

Ligand GTP J 601



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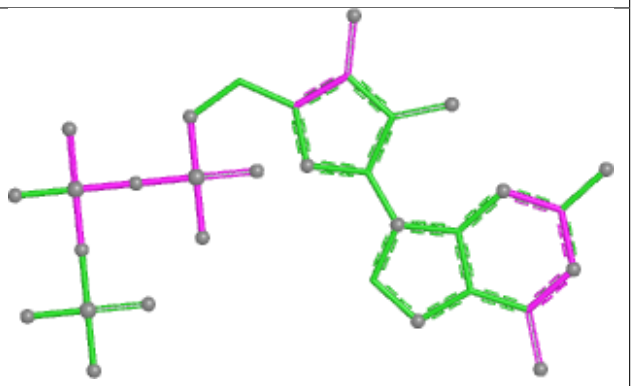

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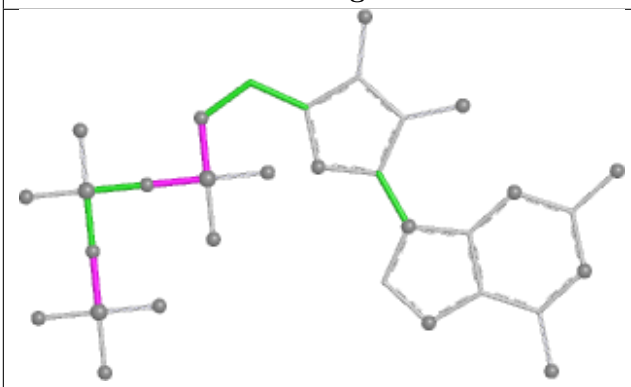

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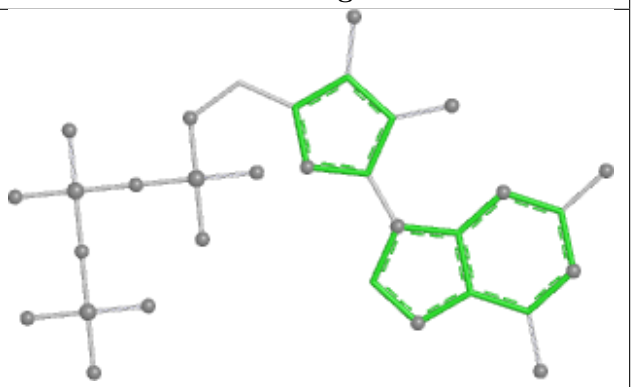

Rings

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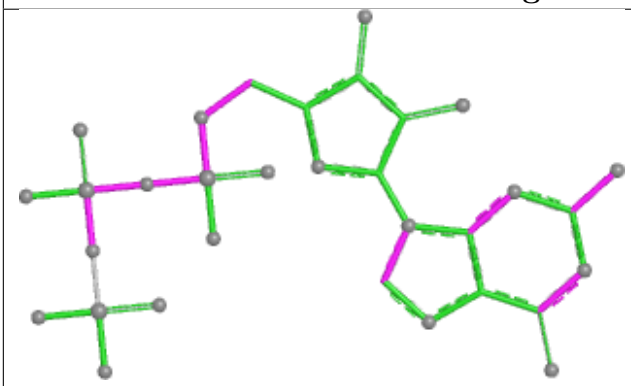

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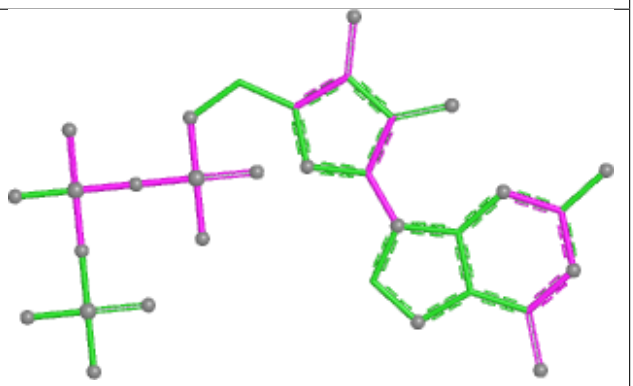

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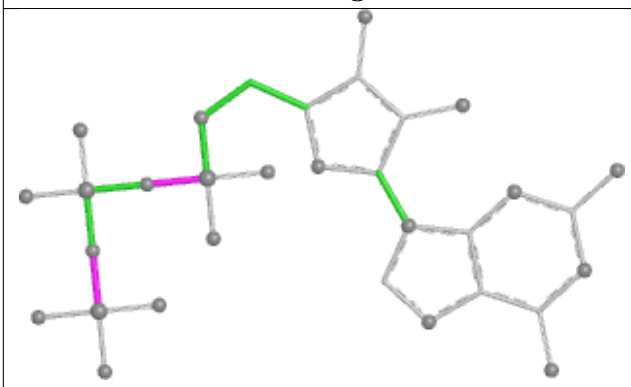

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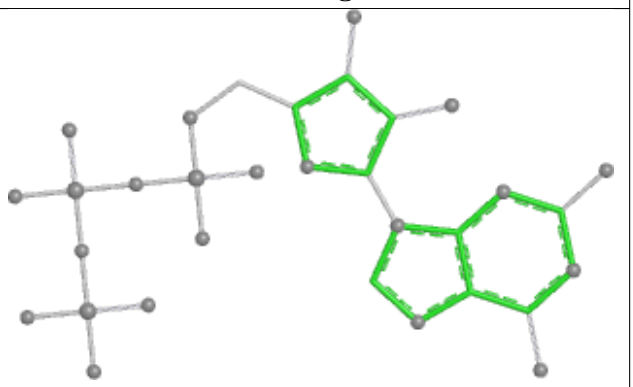
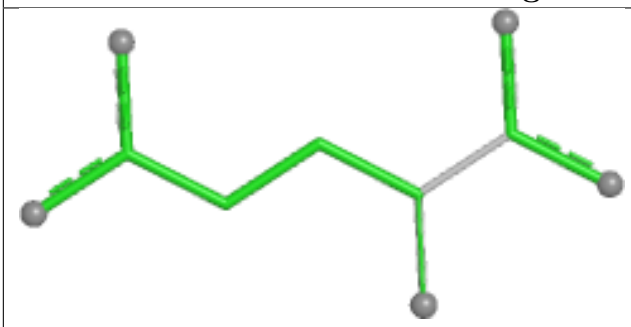


Rings

Ligand GGL C 603



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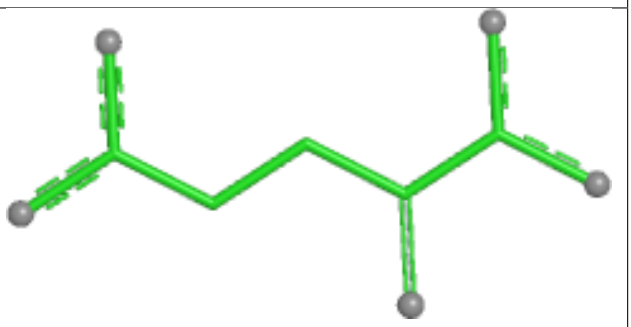

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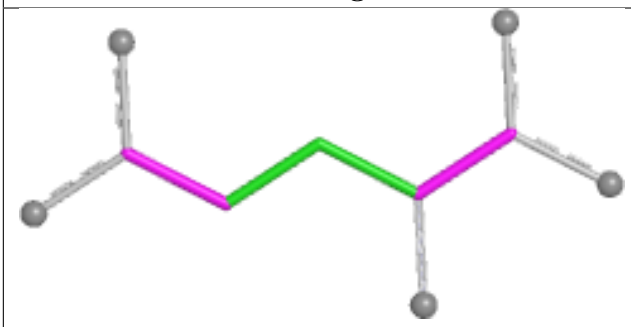

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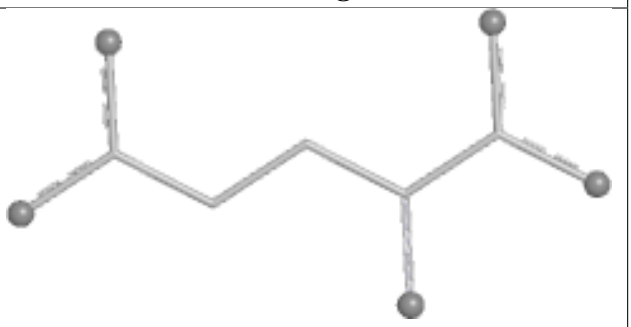
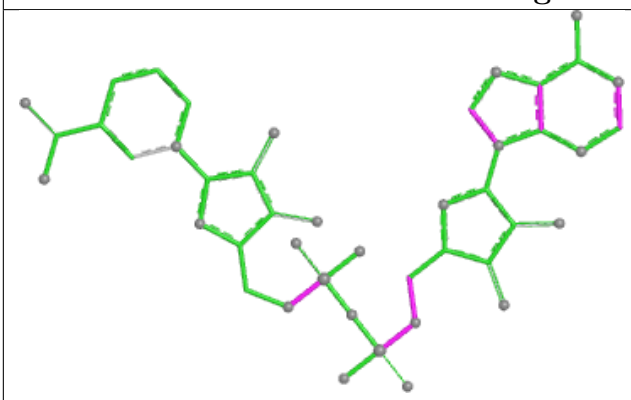


Rings

Ligand NAI I 602



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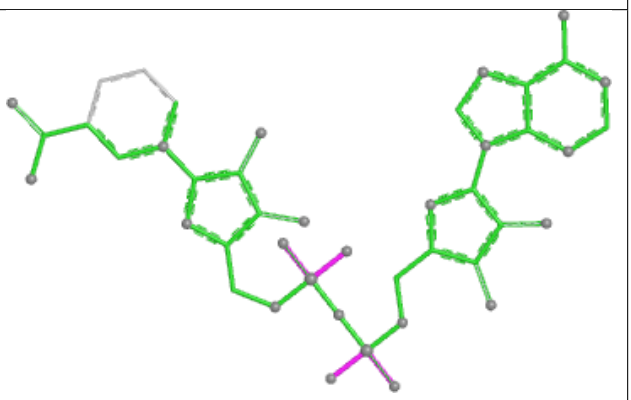

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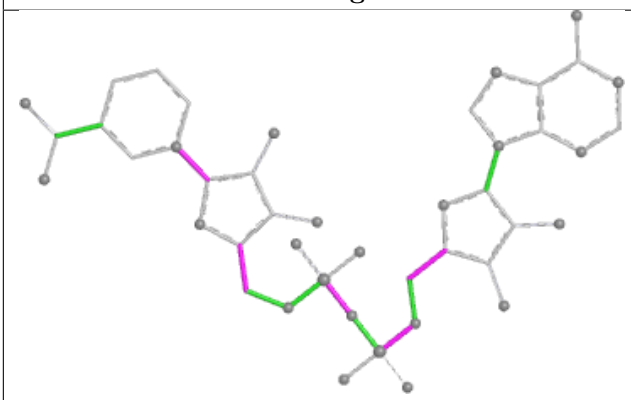

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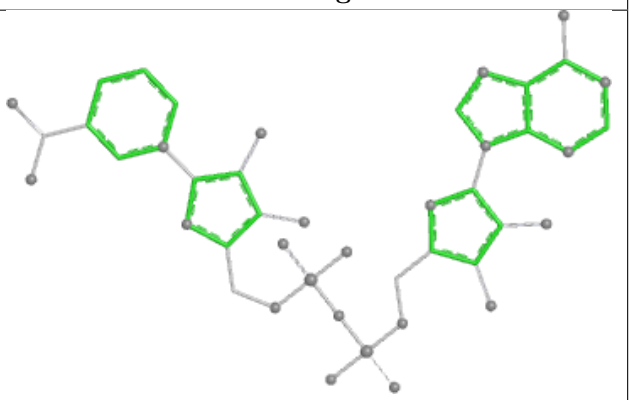
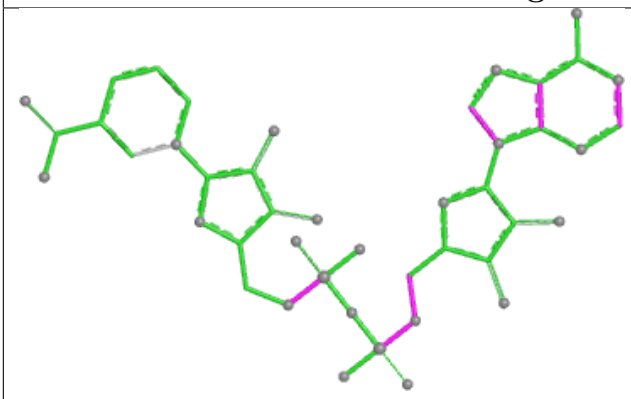


Rings

Ligand NAI B 601



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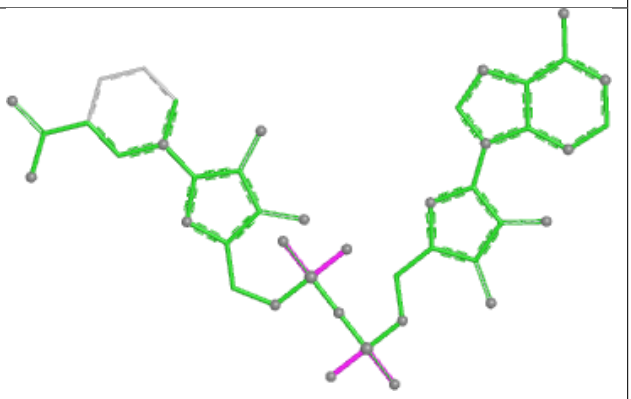

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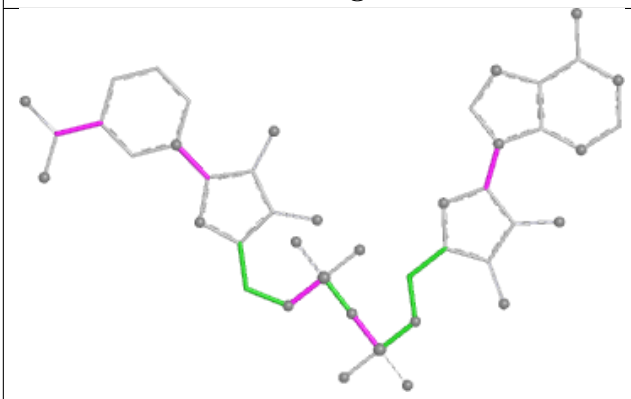

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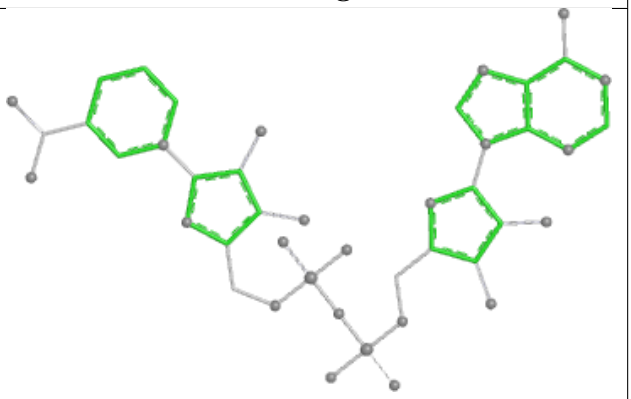
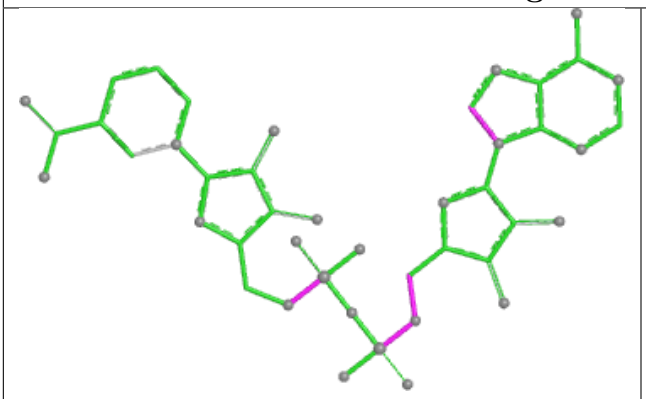


Rings

Ligand NAI G 603



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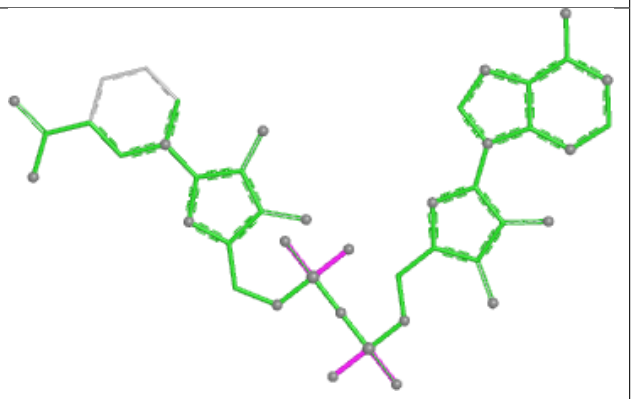

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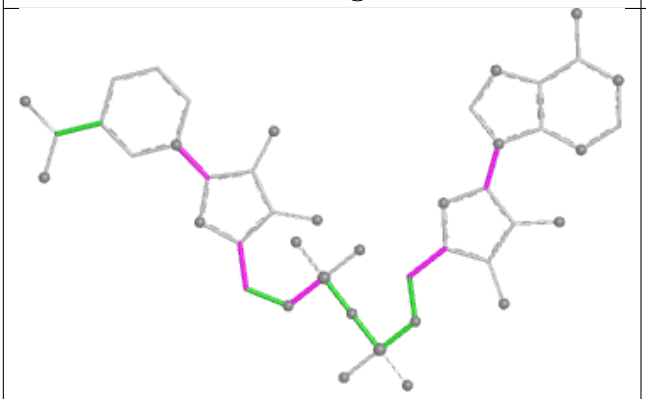

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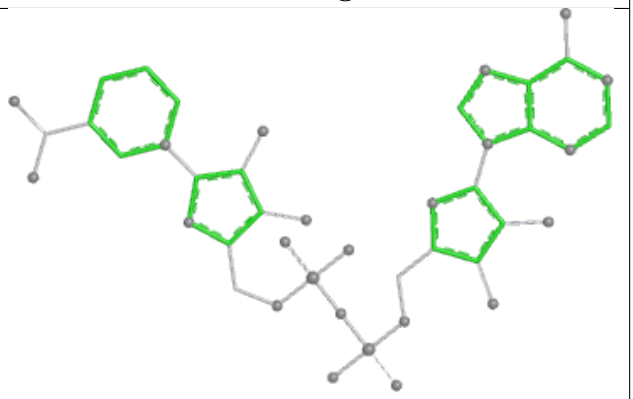
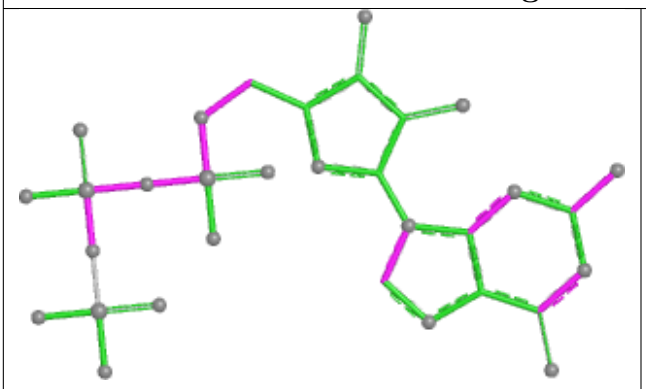


Rings

Ligand GTP K 600



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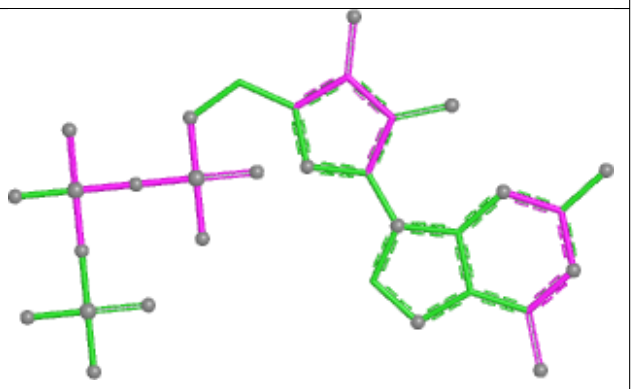

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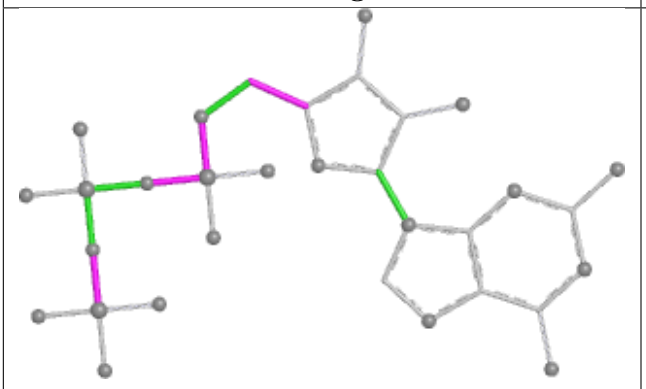
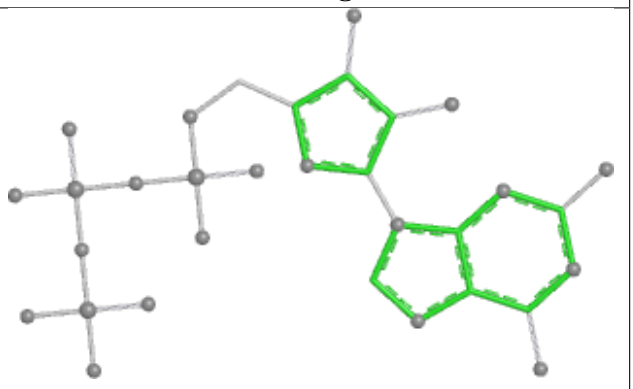
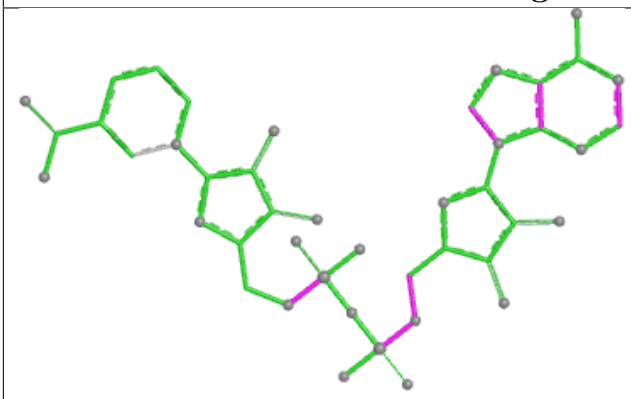


Torsions

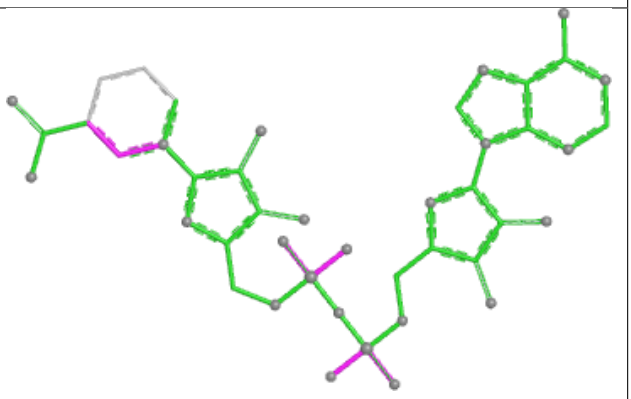


Rings

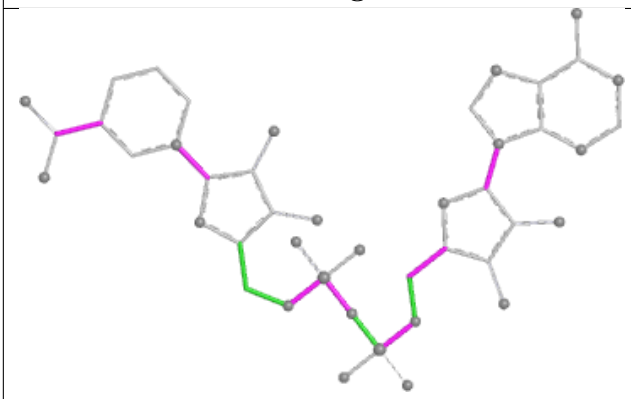
Ligand NAI J 603



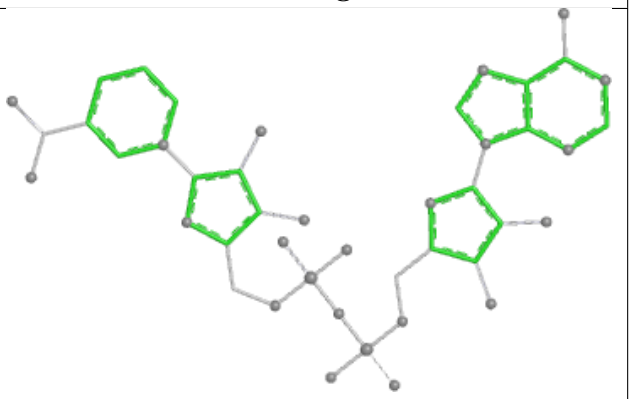
Bond lengths



Bond angles

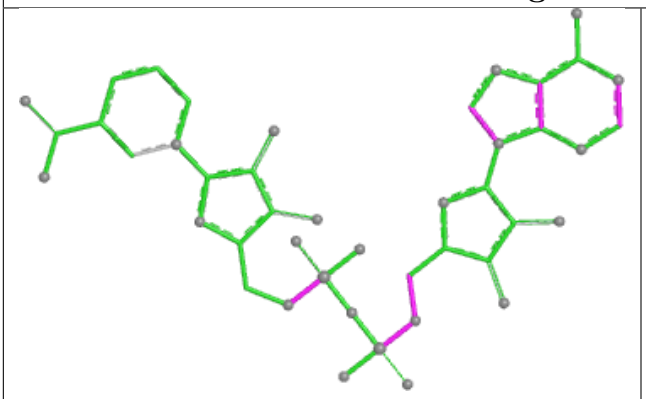


Torsions

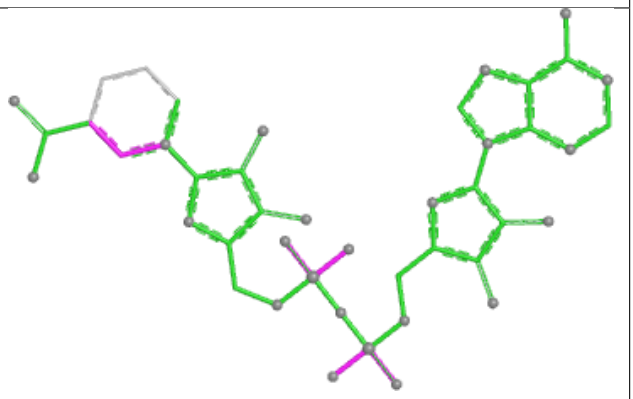


Rings

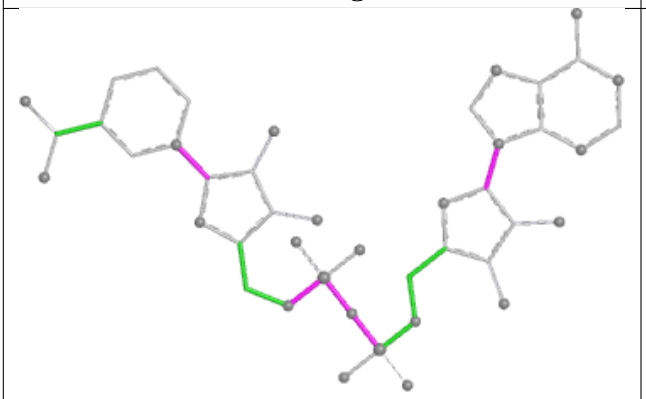
Ligand NAI E 601



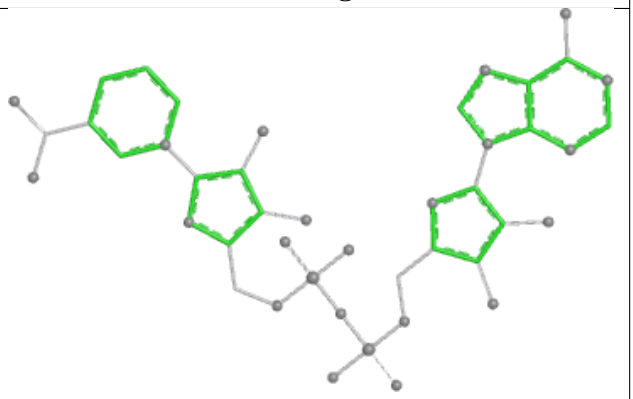
Bond lengths



Bond angles



Torsions



Rings

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.

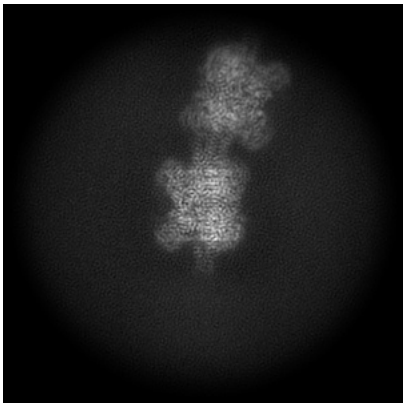
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-74581. These allow visual inspection of the internal detail of the map and identification of artifacts.

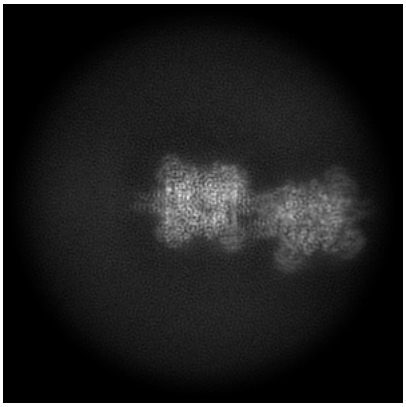
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

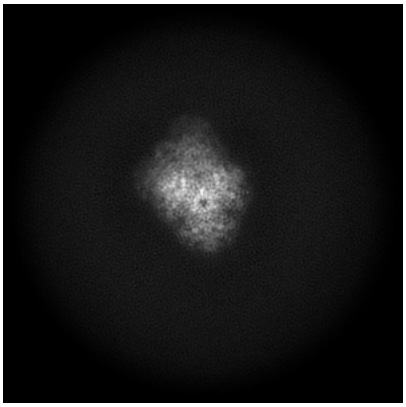
6.1.1 Primary map



X



Y

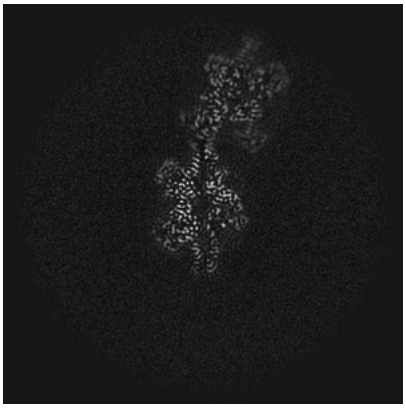


Z

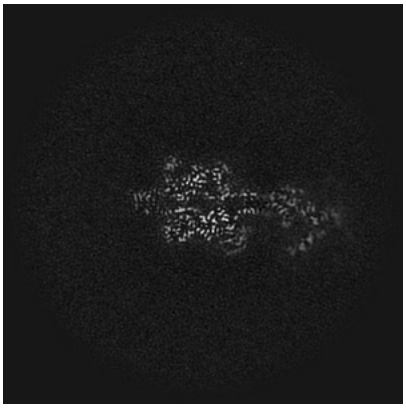
The images above show the map projected in three orthogonal directions.

6.2 Central slices

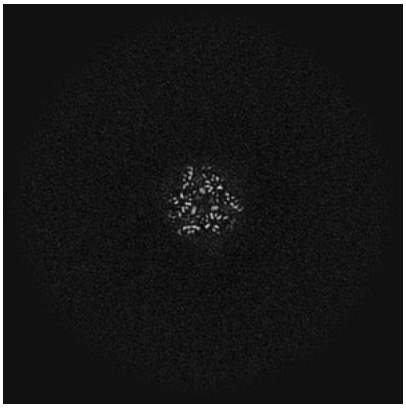
6.2.1 Primary map



X Index: 160



Y Index: 160

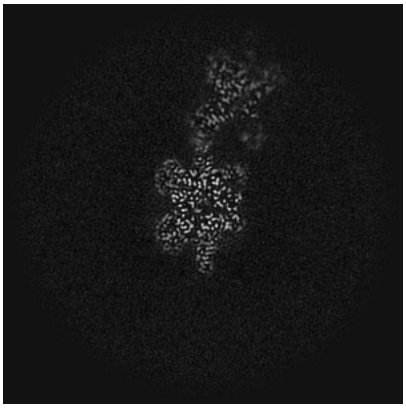


Z Index: 160

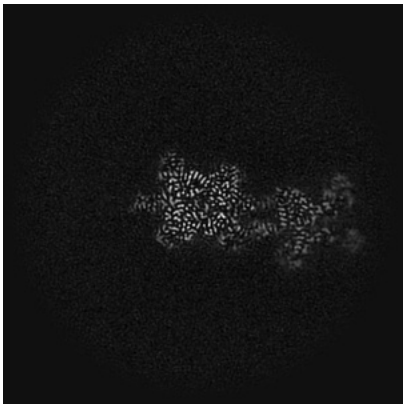
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

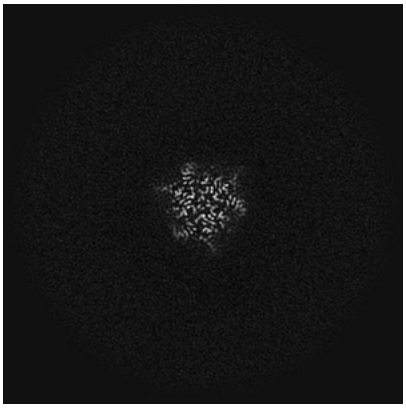
6.3.1 Primary map



X Index: 166



Y Index: 167

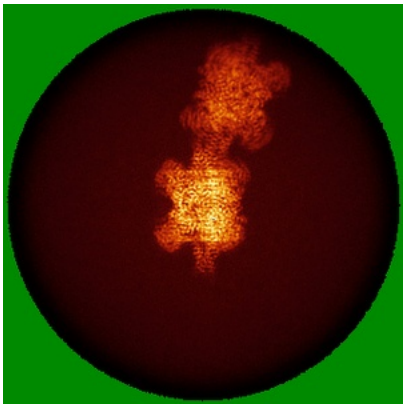


Z Index: 169

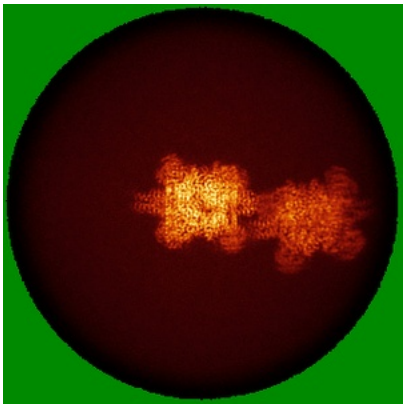
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

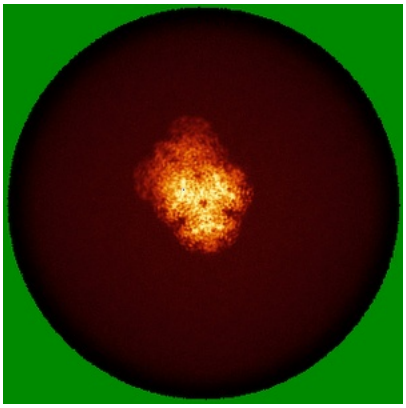
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

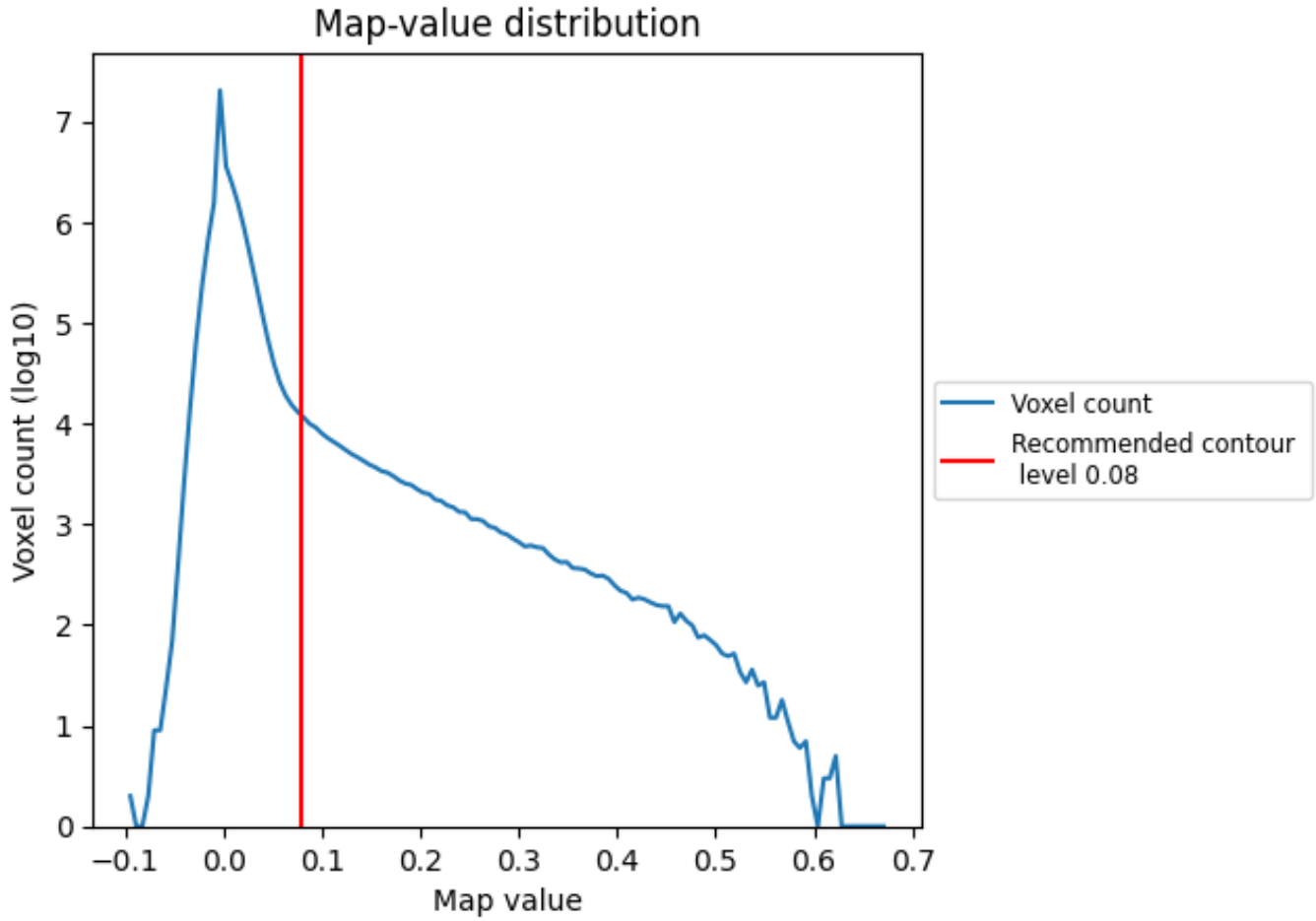
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

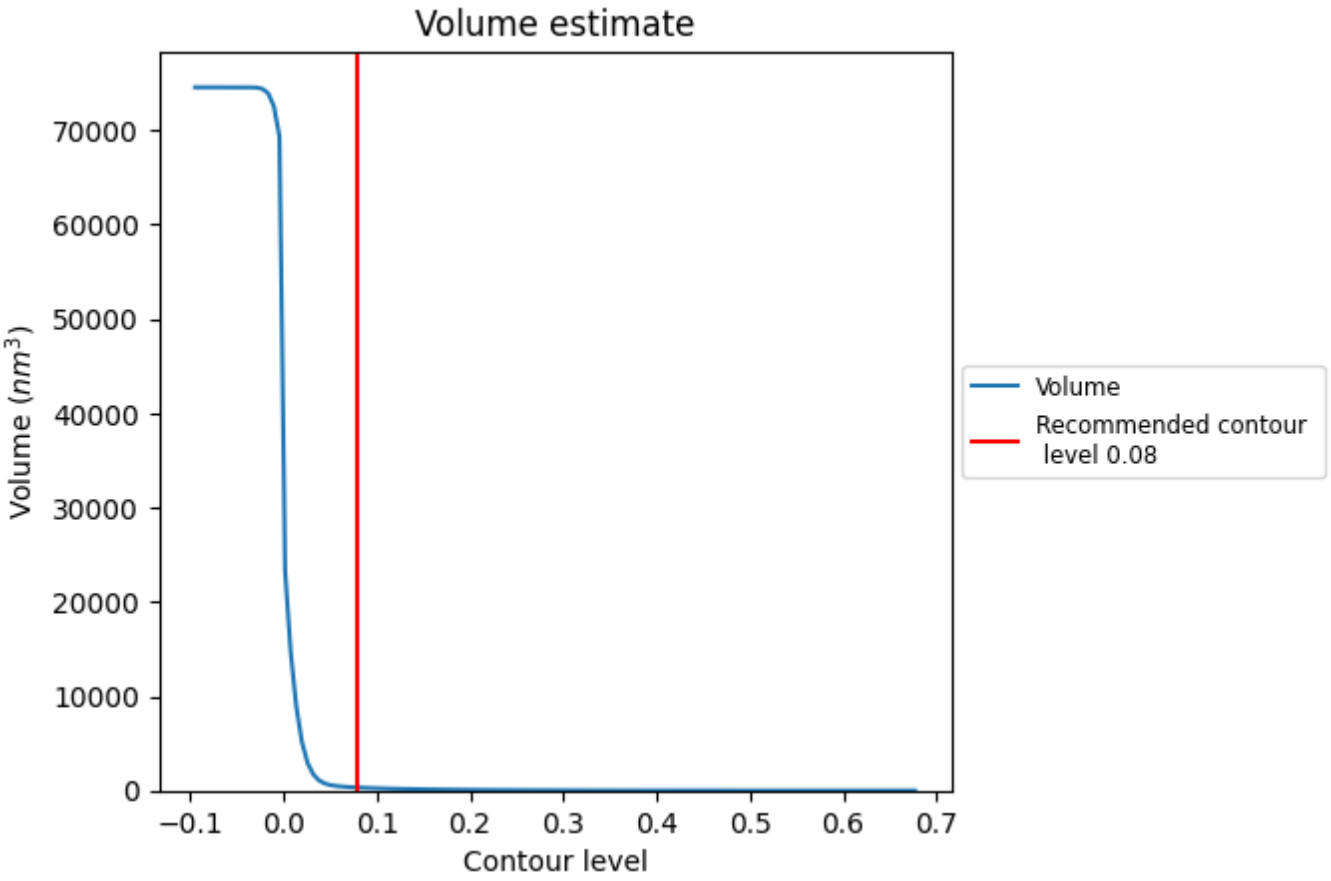
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

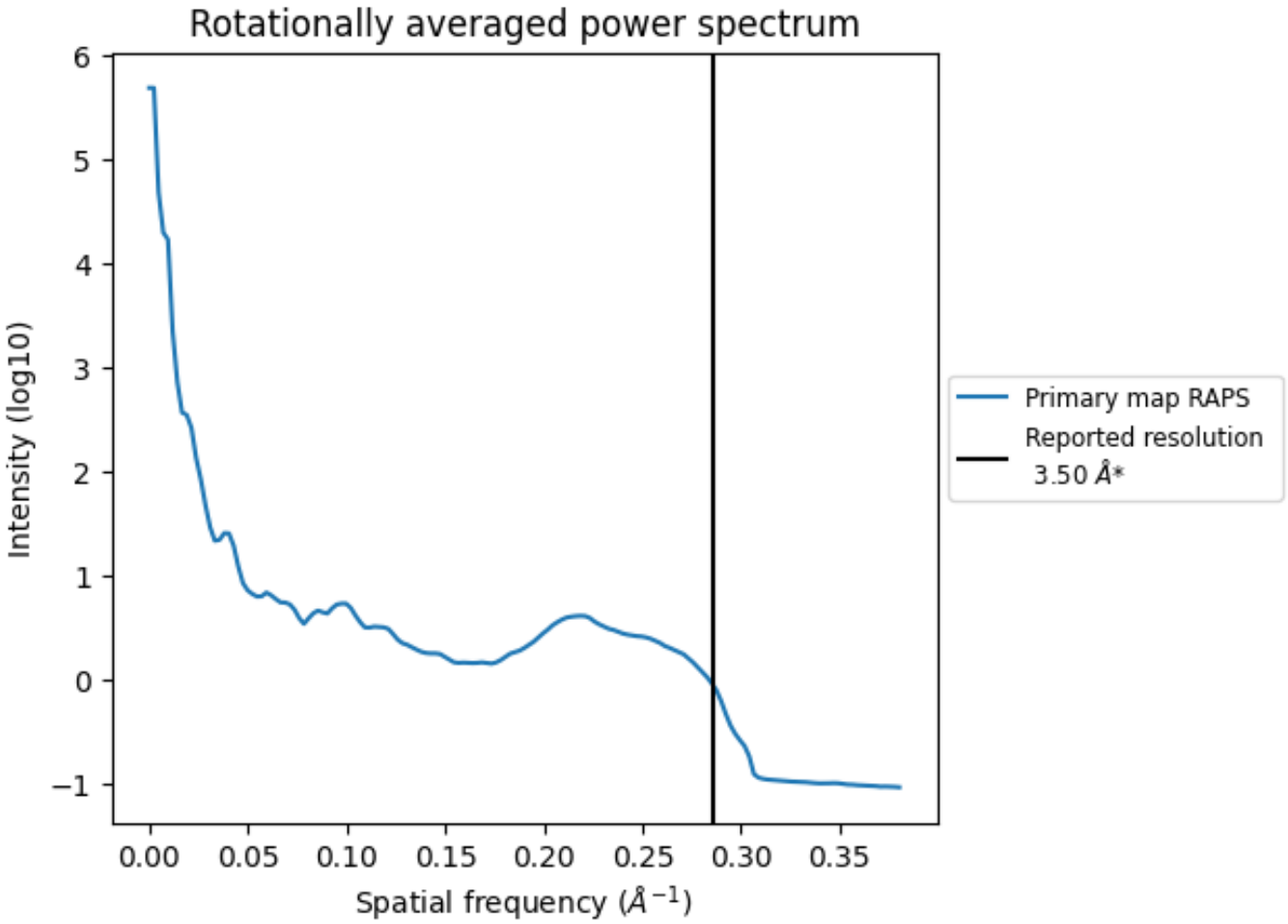
7.2 Volume estimate



The volume at the recommended contour level is 318 nm^3; this corresponds to an approximate mass of 287 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

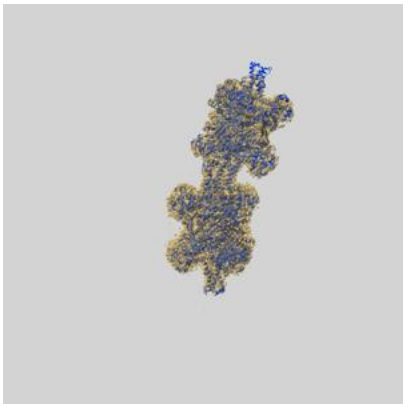
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

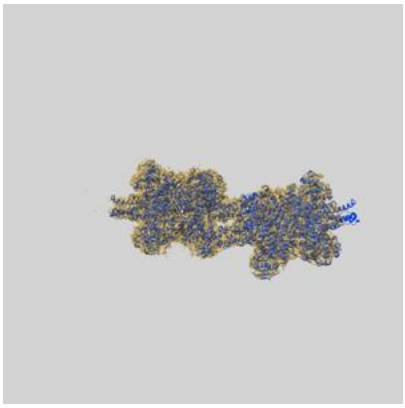
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-74581 and PDB model 9ZQT. Per-residue inclusion information can be found in section 3 on page 9.

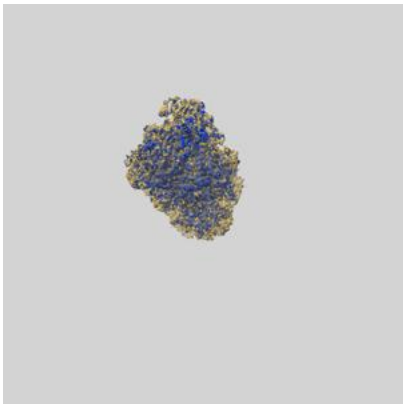
9.1 Map-model overlay



X



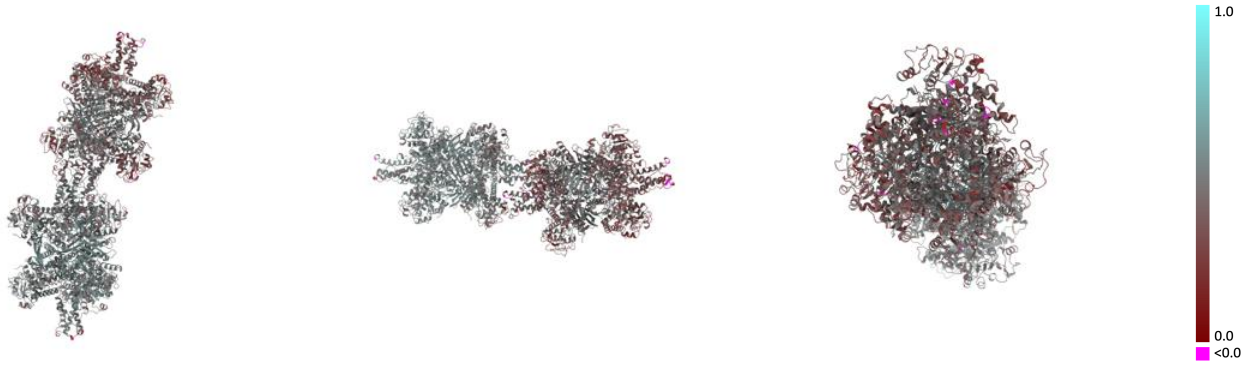
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

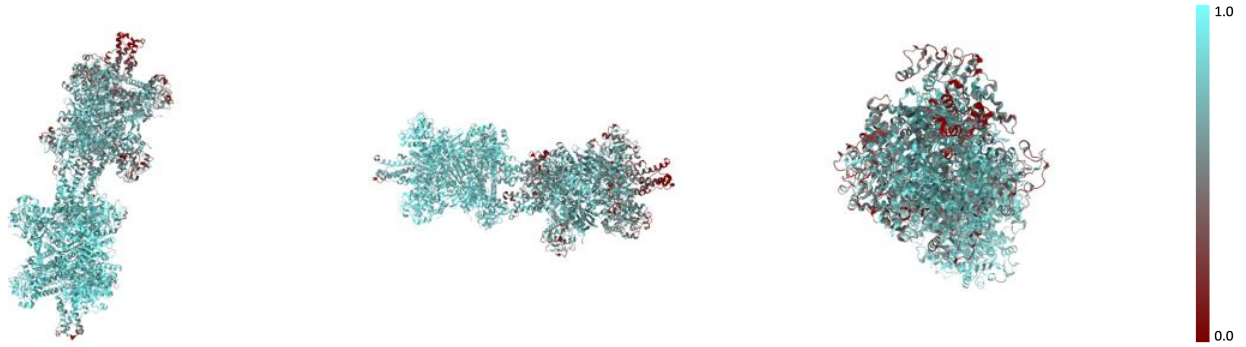
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

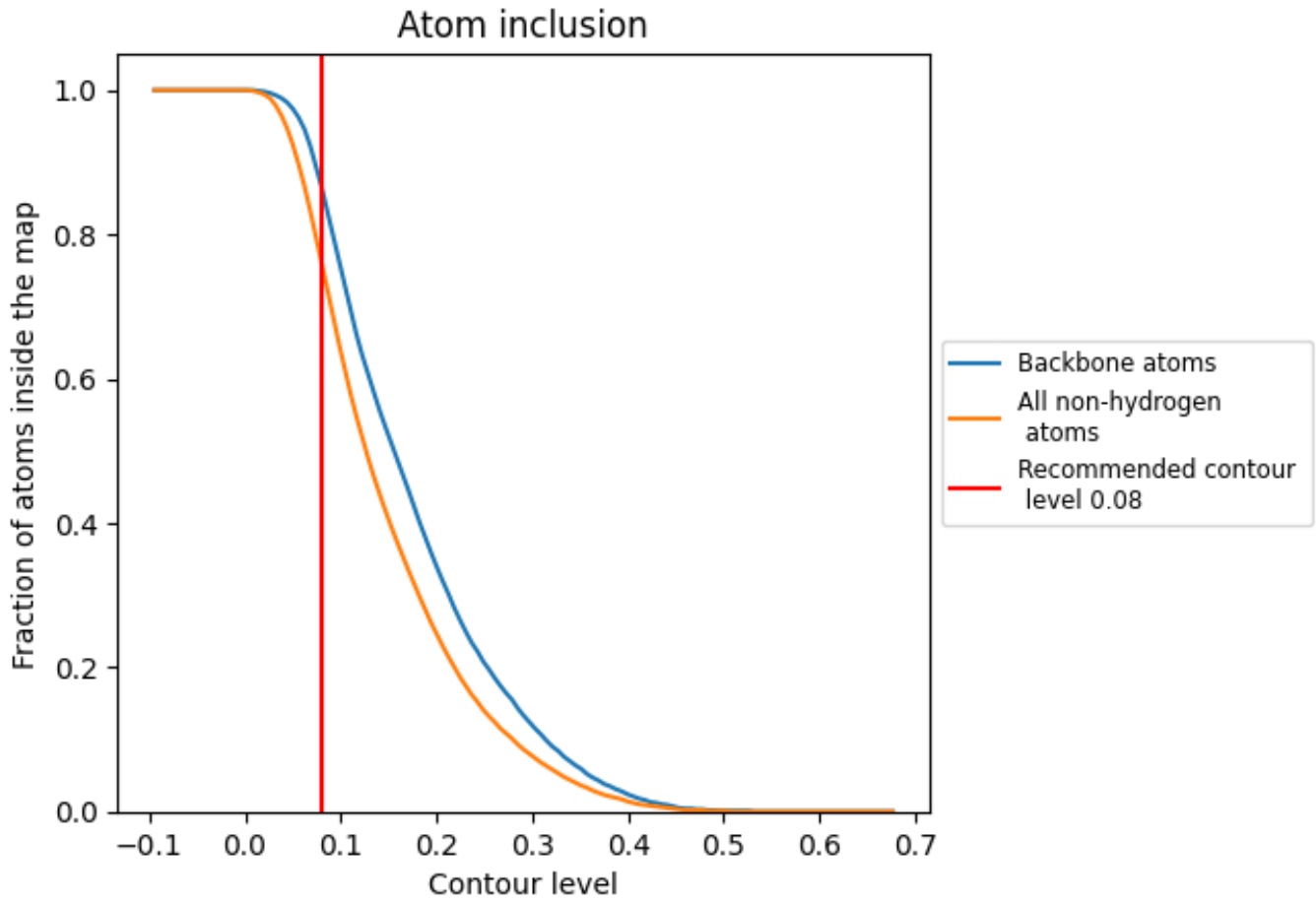
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7620	0.4510
A	0.8650	0.4860
B	0.8720	0.4950
C	0.8830	0.5140
D	0.8870	0.5110
E	0.8800	0.5100
F	0.8580	0.4870
G	0.6580	0.3960
H	0.7380	0.4250
I	0.6100	0.3990
J	0.5810	0.3760
K	0.6260	0.4000
L	0.6910	0.4170

