



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:28 PM UTC

PDB ID : 6DHN / pdb_00006dhn
Title : Bovine glutamate dehydrogenase complexed with Eu3+
Authors : Smith, T.J.
Deposited on : 2018-05-20
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

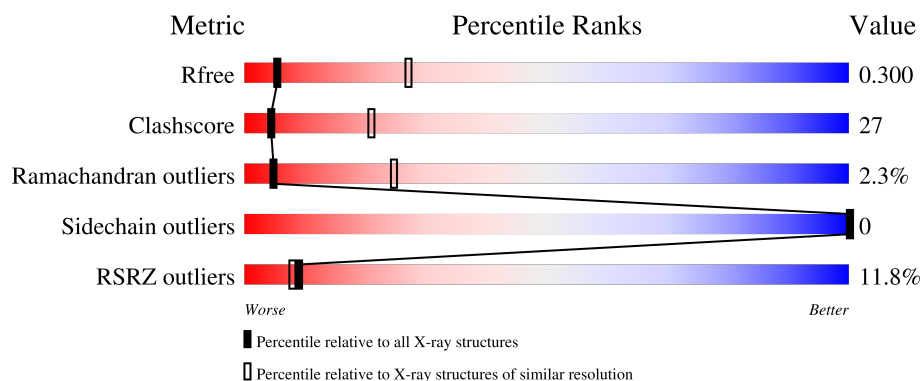
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	582	9% 46% 36% 14%
1	B	582	7% 46% 36% 14%
1	C	582	13% 46% 38% 14%
1	D	582	7% 49% 34% 14%
1	E	582	14% 45% 38% 14%

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Mol	Chain	Length	Quality of chain
1	F	582	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLU	A	601	-	-	X	-
2	GLU	B	601	-	-	X	-
2	GLU	E	601	-	-	X	-
2	GLU	F	602	-	-	X	-
3	GTP	A	602	-	-	X	-

2 Entry composition [i](#)

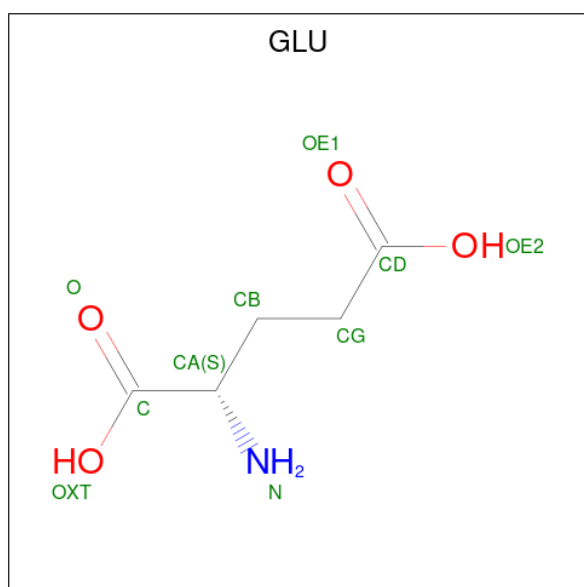
There are 4 unique types of molecules in this entry. The entry contains 24276 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate dehydrogenase 1, mitochondrial.

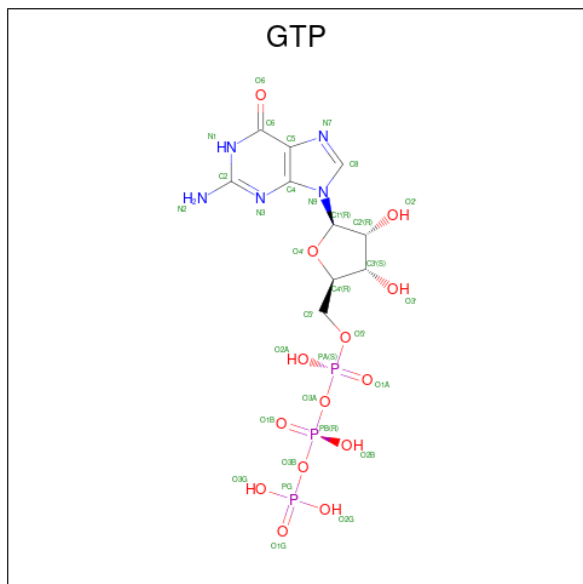
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	B	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	C	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	D	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	E	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	F	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



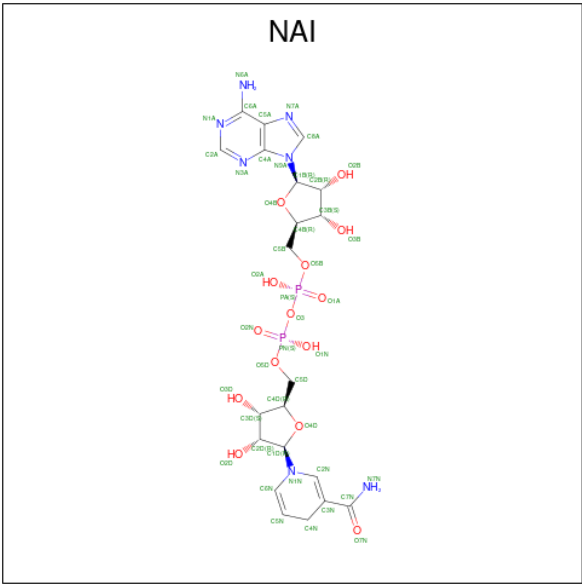
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

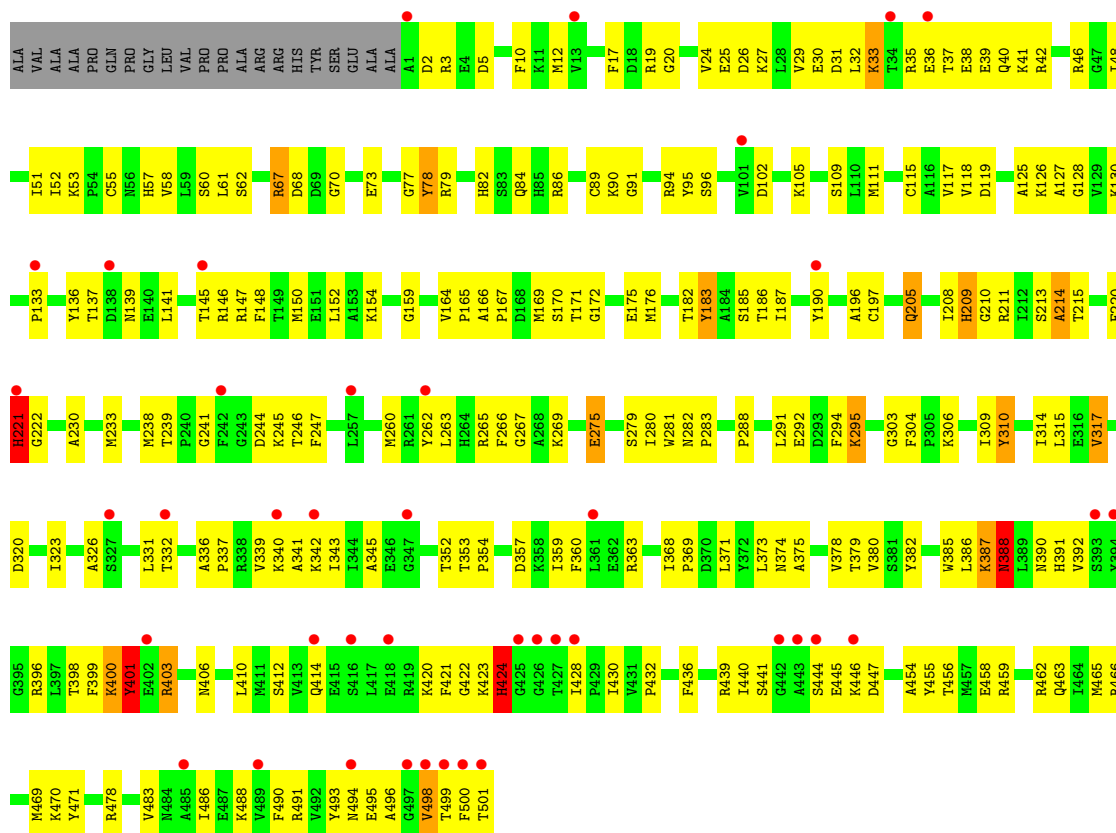


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

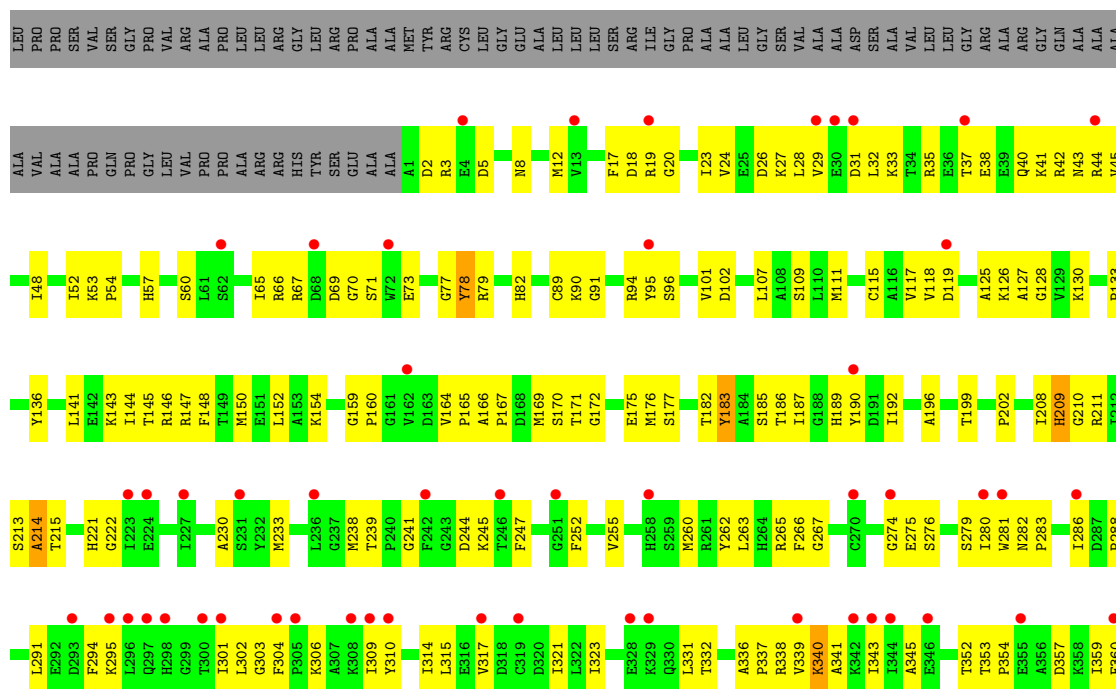
- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).

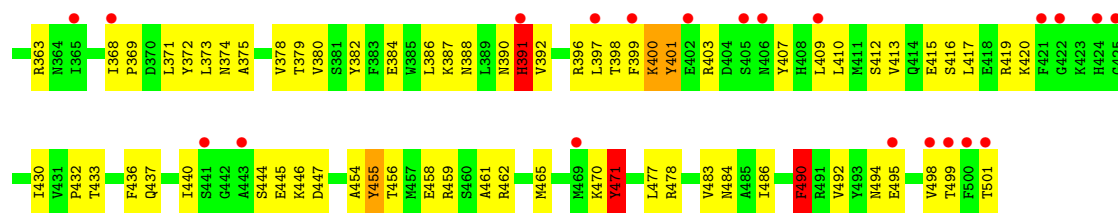


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	A	1	Total	C	N	O	P	12	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	11	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	16	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	10	0
			44	21	7	14	2		
4	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	13	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	16	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

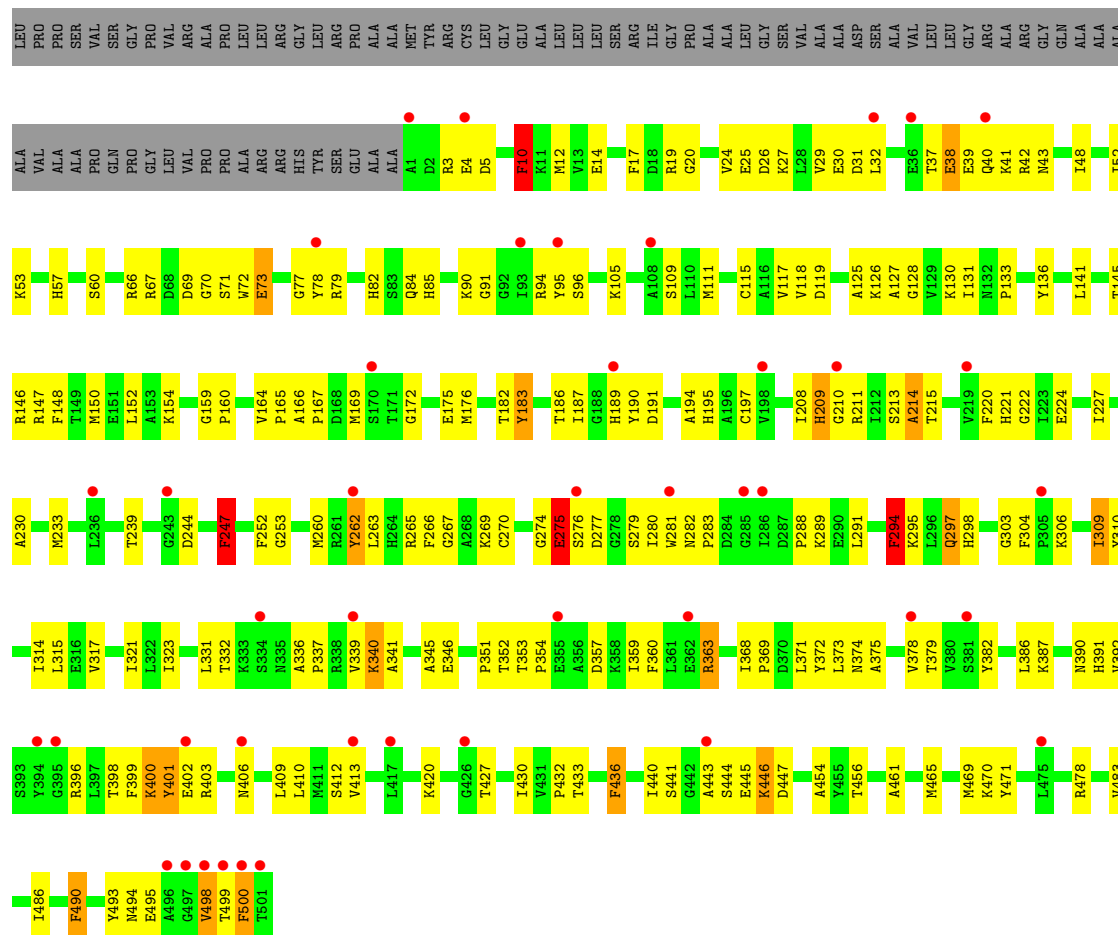


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

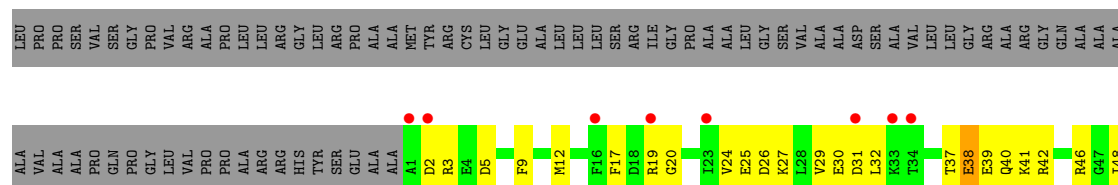
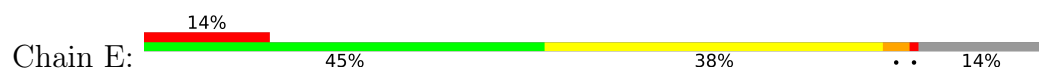


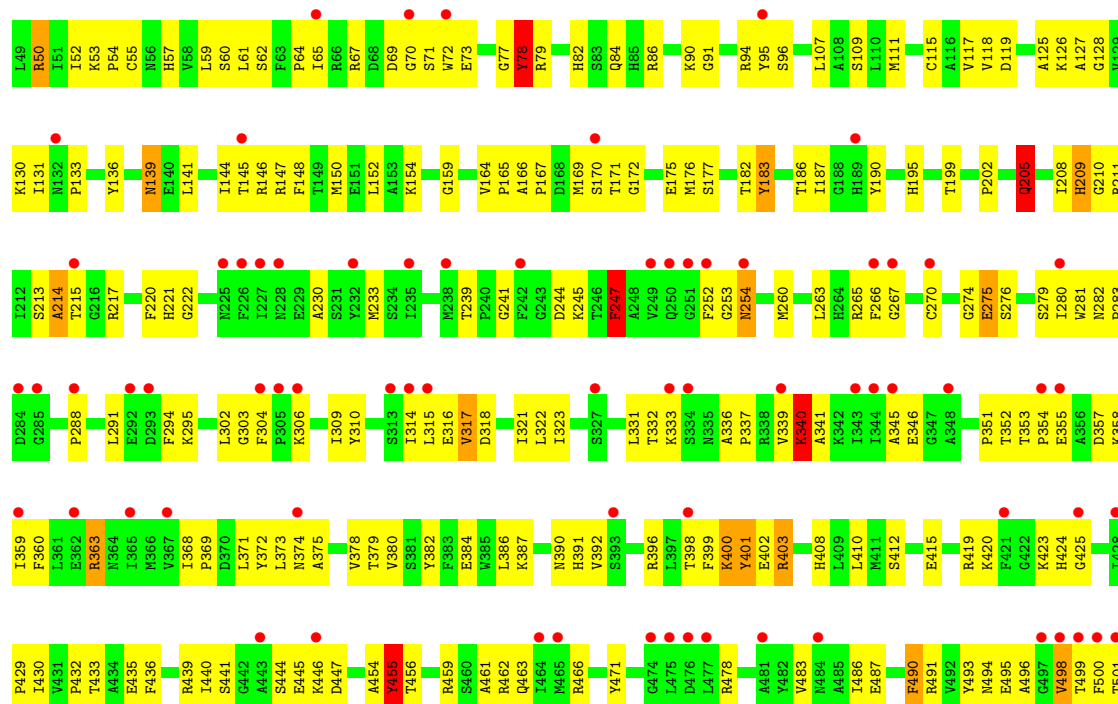


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

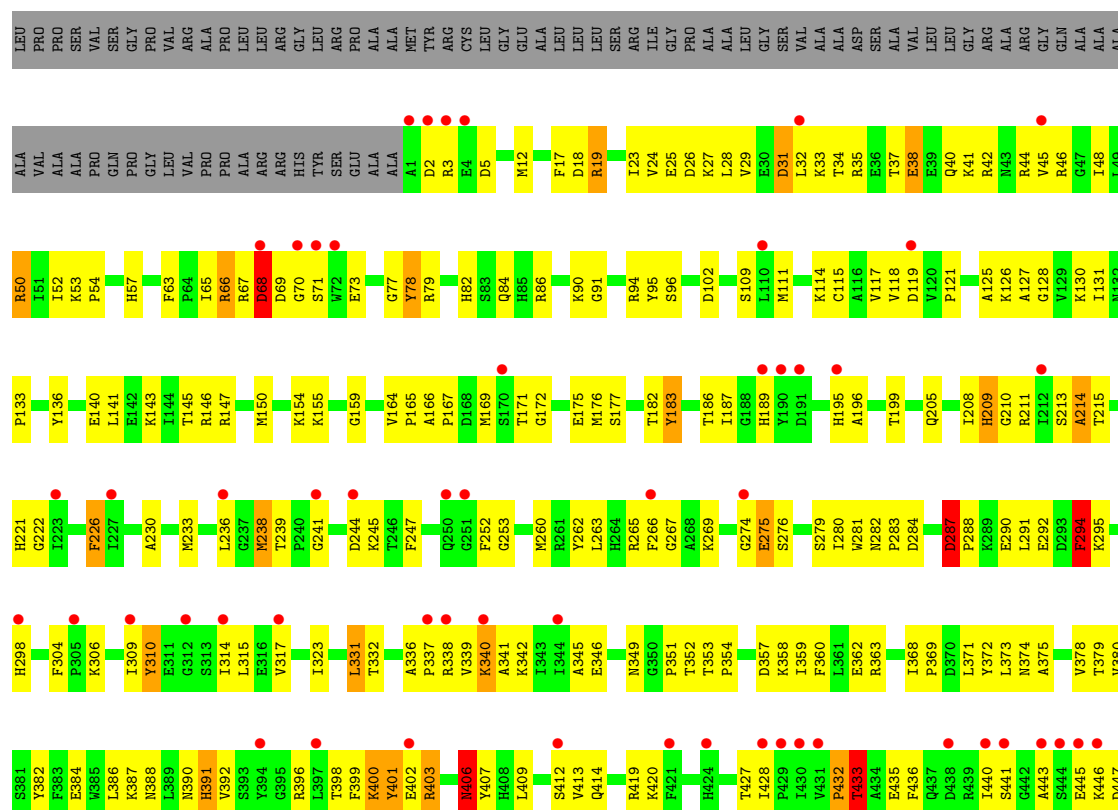
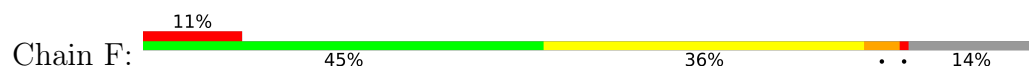


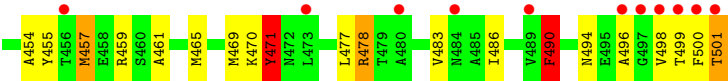
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial





- Molecule 1: Glutamate dehydrogenase 1, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.11Å 98.76Å 165.64Å 90.00° 101.55° 90.00°	Depositor
Resolution (Å)	43.89 – 3.30 43.89 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.3 (43.89-3.30) 92.3 (43.89-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.25Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.260 , 0.301 0.260 , 0.300	Depositor DCC
R_{free} test set	2842 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 17.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	24276	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.39	0/3999	0.90	17/5396 (0.3%)
1	B	0.41	3/3999 (0.1%)	0.91	18/5396 (0.3%)
1	C	0.37	0/3999	0.80	10/5396 (0.2%)
1	D	0.44	3/3999 (0.1%)	1.04	22/5396 (0.4%)
1	E	0.44	3/3999 (0.1%)	0.92	23/5396 (0.4%)
1	F	0.54	3/3999 (0.1%)	1.28	45/5396 (0.8%)
All	All	0.43	12/23994 (0.1%)	0.99	135/32376 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15
1	B	0	8
1	C	0	12
1	D	0	14
1	E	0	14
1	F	2	18
All	All	2	81

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	31	ASP	CG-OD1	-12.20	1.02	1.25
1	F	447	ASP	CG-OD1	-11.34	1.03	1.25
1	D	73	GLU	CD-OE1	-8.74	1.08	1.25
1	E	205	GLN	CD-OE1	-8.60	1.07	1.23
1	E	247	PHE	CG-CD1	-7.57	1.23	1.38
1	B	205	GLN	CD-OE1	-7.05	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	247	PHE	CG-CD1	-6.99	1.24	1.38
1	B	388	ASN	CG-OD1	-5.84	1.12	1.23
1	D	297	GLN	CB-CG	-5.82	1.35	1.52
1	B	19	ARG	CG-CD	-5.44	1.36	1.52
1	F	68	ASP	CG-OD1	-5.38	1.15	1.25
1	E	217	ARG	CD-NE	-5.07	1.39	1.46

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	PHE	CB-CG-CD1	31.81	174.77	120.70
1	F	63	PHE	CB-CG-CD2	-24.41	79.20	120.70
1	F	447	ASP	OD1-CG-OD2	-24.03	65.24	122.90
1	D	73	GLU	OE1-CD-OE2	-22.53	68.84	122.90
1	D	31	ASP	OD1-CG-OD2	-21.50	71.31	122.90
1	F	447	ASP	CB-CG-OD1	-18.50	75.86	118.40
1	A	261	ARG	CD-NE-CZ	17.51	148.92	124.40
1	D	31	ASP	CB-CG-OD1	17.39	158.39	118.40
1	B	19	ARG	CD-NE-CZ	17.12	148.36	124.40
1	D	73	GLU	CG-CD-OE1	-16.88	79.58	118.40
1	B	19	ARG	NE-CZ-NH1	-16.14	105.36	121.50
1	A	261	ARG	NE-CZ-NH1	-15.40	106.10	121.50
1	F	63	PHE	CD1-CG-CD2	-15.06	96.01	118.60
1	B	19	ARG	NE-CZ-NH2	14.74	132.47	119.20
1	A	261	ARG	NE-CZ-NH2	14.51	132.26	119.20
1	E	50	ARG	NE-CZ-NH2	13.22	131.10	119.20
1	F	478	ARG	NE-CZ-NH1	-12.88	108.61	121.50
1	B	275	GLU	CB-CG-CD	12.72	134.23	112.60
1	D	31	ASP	CB-CG-OD2	-12.47	89.72	118.40
1	E	217	ARG	NE-CZ-NH2	12.22	130.19	119.20
1	F	478	ARG	NE-CZ-NH2	12.19	130.17	119.20
1	E	50	ARG	NE-CZ-NH1	-11.79	109.71	121.50
1	E	217	ARG	NE-CZ-NH1	-11.70	109.80	121.50
1	F	478	ARG	CD-NE-CZ	11.01	139.81	124.40
1	D	73	GLU	CG-CD-OE2	10.96	143.62	118.40
1	A	195	HIS	CB-CG-CD2	-10.49	117.56	131.20
1	D	295	LYS	CD-CE-NZ	10.16	144.43	111.90
1	E	50	ARG	CD-NE-CZ	10.13	138.59	124.40
1	F	447	ASP	CB-CG-OD2	9.86	141.08	118.40
1	F	50	ARG	CD-NE-CZ	9.56	137.79	124.40
1	A	195	HIS	N-CA-CB	-9.53	94.39	110.49
1	D	297	GLN	CA-CB-CG	-9.49	95.12	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	457	MET	CA-CB-CG	-9.24	95.63	114.10
1	F	295	LYS	CD-CE-NZ	9.22	141.41	111.90
1	E	247	PHE	CD1-CG-CD2	-9.13	104.91	118.60
1	F	19	ARG	NE-CZ-NH1	-9.07	112.42	121.50
1	C	490	PHE	CB-CA-C	-8.92	96.53	110.81
1	F	238	MET	CA-CB-CG	8.89	131.88	114.10
1	E	247	PHE	N-CA-CB	-8.81	96.94	111.66
1	F	19	ARG	NE-CZ-NH2	8.62	126.96	119.20
1	F	63	PHE	CG-CD1-CE1	8.53	135.19	120.70
1	D	247	PHE	CD1-CG-CD2	-8.52	105.82	118.60
1	C	490	PHE	CB-CG-CD2	-8.52	106.22	120.70
1	F	490	PHE	CB-CG-CD2	-8.51	106.24	120.70
1	D	10	PHE	CB-CA-C	-8.34	97.47	110.81
1	E	455	TYR	CB-CA-C	-8.33	97.68	110.92
1	E	205	GLN	CB-CG-CD	8.27	126.66	112.60
1	D	247	PHE	N-CA-CB	-8.26	97.87	111.66
1	F	294	PHE	CB-CG-CD2	-8.26	106.66	120.70
1	F	501	THR	CA-CB-OG1	8.25	121.97	109.60
1	D	294	PHE	CB-CG-CD2	-8.23	106.71	120.70
1	A	455	TYR	CB-CA-C	-8.13	97.99	110.92
1	F	68	ASP	OD1-CG-OD2	-8.13	103.39	122.90
1	E	275	GLU	CB-CG-CD	8.08	126.33	112.60
1	F	490	PHE	CB-CA-C	-7.96	98.07	110.81
1	B	275	GLU	CG-CD-OE2	7.90	136.57	118.40
1	F	294	PHE	CB-CA-C	-7.83	98.53	110.90
1	E	217	ARG	CD-NE-CZ	7.82	135.34	124.40
1	D	294	PHE	CB-CA-C	-7.81	98.56	110.90
1	B	388	ASN	N-CA-CB	-7.73	97.92	110.14
1	E	455	TYR	CB-CG-CD2	-7.33	109.81	120.80
1	C	19	ARG	CD-NE-CZ	7.31	134.64	124.40
1	C	391	HIS	N-CA-CB	-7.31	101.08	112.41
1	F	31	ASP	CB-CA-C	-7.28	96.27	110.11
1	B	275	GLU	CG-CD-OE1	-7.26	101.71	118.40
1	E	247	PHE	CB-CA-C	7.22	125.97	110.45
1	F	31	ASP	CB-CG-OD2	7.17	134.89	118.40
1	F	19	ARG	CD-NE-CZ	7.08	134.31	124.40
1	A	402	GLU	CA-CB-CG	7.02	128.13	114.10
1	E	19	ARG	CD-NE-CZ	6.96	134.14	124.40
1	A	455	TYR	CB-CG-CD2	-6.88	110.48	120.80
1	F	471	TYR	CD1-CG-CD2	-6.82	107.86	118.10
1	D	247	PHE	CB-CA-C	6.82	125.11	110.45
1	F	331	LEU	CD1-CG-CD2	-6.81	95.81	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	297	GLN	CB-CG-CD	6.76	124.09	112.60
1	F	433	THR	CA-CB-OG1	6.63	119.54	109.60
1	C	490	PHE	CD1-CG-CD2	-6.54	108.80	118.60
1	E	139	ASN	CB-CA-C	-6.52	99.77	110.85
1	D	19	ARG	CD-NE-CZ	6.40	133.36	124.40
1	F	490	PHE	CD1-CG-CD2	-6.33	109.11	118.60
1	D	10	PHE	CD1-CG-CD2	-6.31	109.13	118.60
1	F	294	PHE	CD1-CG-CD2	-6.24	109.24	118.60
1	D	294	PHE	CD1-CG-CD2	-6.19	109.31	118.60
1	E	455	TYR	CD1-CG-CD2	-6.19	108.82	118.10
1	D	10	PHE	CB-CG-CD2	-6.12	110.30	120.70
1	F	275	GLU	CB-CG-CD	6.10	122.97	112.60
1	F	50	ARG	NE-CZ-NH1	-6.08	115.42	121.50
1	A	19	ARG	CD-NE-CZ	6.06	132.88	124.40
1	A	391	HIS	N-CA-CB	-6.06	103.02	112.41
1	B	387	LYS	CA-C-N	6.00	129.15	120.38
1	B	387	LYS	C-N-CA	6.00	129.15	120.38
1	C	391	HIS	CB-CG-CD2	-5.95	123.47	131.20
1	B	221	HIS	CB-CG-CD2	-5.93	123.49	131.20
1	A	295	LYS	CD-CE-NZ	5.89	130.74	111.90
1	B	424	HIS	CA-C-N	5.88	132.93	121.41
1	B	424	HIS	C-N-CA	5.88	132.93	121.41
1	B	295	LYS	CD-CE-NZ	5.86	130.65	111.90
1	C	295	LYS	CD-CE-NZ	5.84	130.60	111.90
1	E	295	LYS	CD-CE-NZ	5.82	130.53	111.90
1	A	455	TYR	CD1-CG-CD2	-5.78	109.42	118.10
1	A	195	HIS	ND1-CG-CD2	-5.73	100.37	106.10
1	E	247	PHE	CA-CB-CG	5.68	119.48	113.80
1	E	78	TYR	CA-CB-CG	5.65	124.06	113.90
1	F	68	ASP	CB-CG-OD1	5.64	131.37	118.40
1	A	406	ASN	N-CA-CB	-5.64	101.54	109.94
1	B	466	ARG	CA-CB-CG	5.64	125.37	114.10
1	F	433	THR	N-CA-CB	-5.61	101.01	110.49
1	A	78	TYR	CA-CB-CG	5.60	123.98	113.90
1	D	275	GLU	CA-CB-CG	-5.51	103.08	114.10
1	F	500	PHE	CA-C-N	5.50	131.60	121.70
1	F	500	PHE	C-N-CA	5.50	131.60	121.70
1	F	226	PHE	N-CA-CB	5.48	118.80	110.42
1	E	139	ASN	CB-CG-ND2	-5.38	108.33	116.40
1	E	139	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	D	446	LYS	CD-CE-NZ	5.34	128.99	111.90
1	C	19	ARG	NE-CZ-NH2	-5.33	114.41	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	287	ASP	CB-CA-C	-5.32	100.79	109.41
1	F	420	LYS	CG-CD-CE	5.30	123.49	111.30
1	A	275	GLU	CA-CB-CG	-5.29	103.53	114.10
1	B	388	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	F	420	LYS	CA-CB-CG	-5.22	103.66	114.10
1	E	217	ARG	CG-CD-NE	-5.21	100.53	112.00
1	F	317	VAL	N-CA-C	-5.17	102.91	109.58
1	A	195	HIS	CB-CA-C	5.16	120.68	110.42
1	B	317	VAL	CA-CB-CG1	5.16	119.16	110.40
1	F	471	TYR	N-CA-CB	5.13	118.34	110.70
1	C	471	TYR	CD1-CG-CD2	-5.13	110.41	118.10
1	B	401	TYR	CB-CA-C	-5.10	104.50	112.31
1	F	63	PHE	N-CA-C	5.07	117.31	110.31
1	F	406	ASN	N-CA-CB	-5.06	102.40	109.94
1	F	338	ARG	CG-CD-NE	5.06	123.13	112.00
1	C	391	HIS	ND1-CG-CD2	-5.04	101.06	106.10
1	B	221	HIS	N-CA-CB	5.04	118.75	110.39
1	E	19	ARG	NE-CZ-NH2	-5.04	114.67	119.20
1	D	247	PHE	CA-CB-CG	5.03	118.83	113.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	433	THR	CB
1	F	501	THR	CB

All (81) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	TYR	Sidechain
1	A	195	HIS	Sidechain
1	A	209	HIS	Sidechain
1	A	221	HIS	Sidechain
1	A	261	ARG	Sidechain
1	A	275	GLU	Sidechain
1	A	31	ASP	Sidechain
1	A	38	GLU	Peptide
1	A	391	HIS	Sidechain
1	A	401	TYR	Sidechain
1	A	402	GLU	Sidechain
1	A	406	ASN	Sidechain
1	A	455	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	490	PHE	Sidechain
1	A	78	TYR	Sidechain
1	B	102	ASP	Sidechain
1	B	139	ASN	Sidechain
1	B	183	TYR	Sidechain
1	B	209	HIS	Sidechain
1	B	221	HIS	Sidechain
1	B	388	ASN	Sidechain
1	B	401	TYR	Sidechain
1	B	78	TYR	Sidechain
1	C	183	TYR	Sidechain
1	C	209	HIS	Sidechain
1	C	35	ARG	Peptide
1	C	38	GLU	Sidechain
1	C	391	HIS	Sidechain
1	C	40	GLN	Peptide
1	C	401	TYR	Sidechain
1	C	455	TYR	Sidechain
1	C	471	TYR	Sidechain
1	C	484	ASN	Sidechain
1	C	490	PHE	Sidechain
1	C	78	TYR	Sidechain
1	D	10	PHE	Sidechain
1	D	183	TYR	Sidechain
1	D	209	HIS	Sidechain
1	D	247	PHE	Sidechain
1	D	262	TYR	Sidechain
1	D	275	GLU	Sidechain
1	D	294	PHE	Sidechain
1	D	297	GLN	Sidechain
1	D	38	GLU	Peptide
1	D	391	HIS	Sidechain
1	D	401	TYR	Sidechain
1	D	406	ASN	Sidechain
1	D	490	PHE	Sidechain
1	D	73	GLU	Sidechain
1	E	139	ASN	Sidechain
1	E	183	TYR	Sidechain
1	E	205	GLN	Sidechain
1	E	209	HIS	Sidechain
1	E	247	PHE	Sidechain
1	E	254	ASN	Sidechain

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Mol	Chain	Res	Type	Group
1	E	340	LYS	Peptide
1	E	38	GLU	Sidechain,Peptide
1	E	39	GLU	Peptide
1	E	401	TYR	Sidechain
1	E	455	TYR	Sidechain
1	E	490	PHE	Sidechain
1	E	78	TYR	Sidechain
1	F	102	ASP	Sidechain
1	F	183	TYR	Sidechain
1	F	19	ARG	Sidechain
1	F	195	HIS	Sidechain
1	F	209	HIS	Sidechain
1	F	226	PHE	Sidechain
1	F	287	ASP	Sidechain
1	F	294	PHE	Sidechain
1	F	310	TYR	Sidechain
1	F	38	GLU	Peptide
1	F	401	TYR	Sidechain
1	F	406	ASN	Sidechain
1	F	432	PRO	Peptide
1	F	471	TYR	Sidechain
1	F	490	PHE	Sidechain
1	F	50	ARG	Sidechain
1	F	68	ASP	Sidechain
1	F	78	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3916	0	3879	221	0
1	B	3916	0	3880	231	0
1	C	3916	0	3879	223	0
1	D	3916	0	3878	223	0
1	E	3916	0	3879	245	0
1	F	3916	0	3880	236	0
2	A	10	0	5	6	0
2	B	10	0	5	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10	0	5	3	0
2	D	10	0	5	3	0
2	E	10	0	5	6	0
2	F	10	0	5	4	0
3	A	32	0	12	13	0
3	B	32	0	12	2	0
3	C	32	0	12	0	0
3	D	32	0	12	1	0
3	E	32	0	12	1	0
3	F	32	0	12	4	0
4	A	88	0	51	12	0
4	B	88	0	51	15	0
4	C	88	0	50	10	0
4	D	88	0	50	10	0
4	E	44	0	25	10	0
4	F	132	0	75	24	0
All	All	24276	0	23679	1268	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 27.

All (1268) 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)
4:C:604:NAI:O4B	4:C:604:NAI:C1B	1.63	1.23
1:B:458:GLU:OE2	1:B:462:ARG:NH1	1.80	1.12
1:A:463:GLN:HG2	1:A:466:ARG:HH12	1.18	1.09
1:F:38:GLU:HB2	1:F:40:GLN:H	1.19	1.07
1:C:303:GLY:H	1:C:309:ILE:HD11	1.21	1.04
1:A:38:GLU:HB2	1:A:40:GLN:H	1.29	0.97
1:E:339:VAL:O	1:E:340:LYS:HD3	1.66	0.96
1:E:315:LEU:O	1:E:340:LYS:NZ	2.00	0.94
1:C:337:PRO:O	1:C:363:ARG:NH1	2.00	0.94
1:B:30:GLU:O	1:B:33:LYS:NZ	2.02	0.93
1:F:337:PRO:O	1:F:363:ARG:NH1	2.02	0.93
1:B:337:PRO:O	1:B:363:ARG:NH1	2.02	0.92
1:A:261:ARG:NH2	3:A:602:GTP:O2G	2.02	0.92
1:D:396:ARG:NH1	1:F:119:ASP:O	2.03	0.92
1:D:337:PRO:O	1:D:363:ARG:NH1	2.05	0.90
1:D:3:ARG:NH1	1:D:4:GLU:HG3	1.87	0.90
1:A:463:GLN:HG2	1:A:466:ARG:NH1	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:PRO:O	1:E:363:ARG:NH1	2.04	0.90
1:E:339:VAL:O	1:E:341:ALA:N	2.04	0.89
1:A:337:PRO:O	1:A:363:ARG:NH1	2.06	0.89
1:B:221:HIS:CD2	1:B:454:ALA:HA	2.09	0.88
1:D:374:ASN:HB2	4:D:603:NAI:H5N	1.55	0.86
2:A:601:GLU:HA	4:A:603:NAI:H4N	1.57	0.85
1:C:183:TYR:HD1	1:C:187:ILE:HG23	1.40	0.85
1:E:303:GLY:H	1:E:309:ILE:HD11	1.40	0.85
1:B:29:VAL:HG21	1:B:42:ARG:HG3	1.58	0.85
1:A:183:TYR:HD1	1:A:187:ILE:HG23	1.41	0.84
1:A:29:VAL:HG21	1:A:42:ARG:HG3	1.60	0.83
1:C:147:ARG:NH1	1:F:499:THR:OG1	2.12	0.83
1:A:119:ASP:O	1:C:396:ARG:NH1	2.10	0.82
1:B:488:LYS:HA	1:B:491:ARG:HH12	1.45	0.82
1:C:29:VAL:HG21	1:C:42:ARG:HG3	1.61	0.82
1:D:183:TYR:HD1	1:D:187:ILE:HG23	1.41	0.82
1:B:499:THR:OG1	1:E:147:ARG:NH1	2.12	0.81
1:E:487:GLU:HG2	1:E:491:ARG:HH12	1.46	0.81
1:F:28:LEU:HB3	1:F:490:PHE:HE2	1.47	0.80
1:B:459:ARG:HH21	1:B:463:GLN:NE2	1.79	0.80
1:A:499:THR:OG1	1:D:147:ARG:NH1	2.14	0.80
1:B:221:HIS:HD2	1:B:454:ALA:HA	1.44	0.80
1:C:458:GLU:HG2	1:C:462:ARG:NH1	1.97	0.80
1:E:339:VAL:C	1:E:340:LYS:HD3	2.07	0.80
1:E:462:ARG:NH1	1:E:466:ARG:HH22	1.81	0.79
1:A:333:LYS:NZ	1:A:355:GLU:OE1	2.13	0.79
1:E:435:GLU:OE2	1:E:435:GLU:N	2.17	0.78
1:E:27:LYS:NZ	1:E:31:ASP:OD2	2.16	0.77
1:E:29:VAL:HG21	1:E:42:ARG:HG3	1.64	0.77
1:E:322:LEU:HD22	1:E:340:LYS:NZ	2.00	0.77
1:B:387:LYS:HE2	4:B:604:NAI:H3D	1.67	0.77
1:B:488:LYS:HA	1:B:491:ARG:NH1	1.99	0.77
1:A:413:VAL:HG11	1:C:413:VAL:HG13	1.67	0.77
1:C:146:ARG:HH11	1:C:182:THR:HG22	1.50	0.77
1:A:146:ARG:HH11	1:A:182:THR:HG22	1.50	0.76
1:A:147:ARG:NH1	1:D:499:THR:OG1	2.18	0.76
4:D:604:NAI:H4N	1:E:195:HIS:CD2	2.21	0.76
1:A:443:ALA:HA	1:C:401:TYR:CE2	2.20	0.76
1:B:90:LYS:NZ	2:B:601:GLU:OE2	2.19	0.76
1:F:146:ARG:HH11	1:F:182:THR:HG22	1.50	0.76
1:E:318:ASP:HA	1:E:340:LYS:HG3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ARG:NH1	1:E:499:THR:OG1	2.18	0.76
1:F:5:ASP:HB3	1:F:332:THR:HB	1.68	0.76
4:F:601:NAI:H52N	4:F:601:NAI:H6N	1.68	0.76
1:D:5:ASP:HB3	1:D:332:THR:HB	1.67	0.75
1:E:119:ASP:O	1:F:396:ARG:NH1	2.20	0.75
1:F:34:THR:HG21	1:F:44:ARG:HH22	1.52	0.75
1:E:403:ARG:HH11	1:E:441:SER:HG	1.34	0.75
1:A:262:TYR:OH	3:A:602:GTP:O1G	2.03	0.75
1:C:141:LEU:O	1:C:145:THR:HG23	1.87	0.74
1:C:190:TYR:OH	1:E:190:TYR:OH	2.06	0.74
1:A:409:LEU:HD22	1:C:409:LEU:HD21	1.68	0.74
1:D:146:ARG:HH11	1:D:182:THR:HG22	1.51	0.74
1:C:183:TYR:CD1	1:C:187:ILE:HG23	2.22	0.73
1:F:29:VAL:HG21	1:F:42:ARG:HG3	1.70	0.73
1:B:146:ARG:HH11	1:B:182:THR:HG22	1.51	0.73
1:A:303:GLY:H	1:A:309:ILE:HD11	1.54	0.73
1:D:38:GLU:HB2	1:D:40:GLN:H	1.53	0.73
1:E:247:PHE:CE2	1:E:270:CYS:HA	2.24	0.73
1:A:5:ASP:HB3	1:A:332:THR:HB	1.68	0.73
1:C:90:LYS:NZ	2:C:601:GLU:OE1	2.21	0.73
1:D:183:TYR:CD1	1:D:187:ILE:HG23	2.24	0.73
1:D:141:LEU:O	1:D:145:THR:HG23	1.87	0.73
1:D:3:ARG:HH12	1:D:4:GLU:HG3	1.50	0.72
1:B:141:LEU:O	1:B:145:THR:HG23	1.88	0.72
1:F:90:LYS:NZ	2:F:602:GLU:OE2	2.21	0.72
1:F:387:LYS:HE2	4:F:603:NAI:H52N	1.70	0.72
1:E:239:THR:O	1:E:245:LYS:NZ	2.22	0.72
1:F:38:GLU:HB2	1:F:40:GLN:N	2.01	0.72
1:F:294:PHE:CE2	1:F:304:PHE:HA	2.25	0.72
1:C:27:LYS:NZ	1:C:31:ASP:OD2	2.22	0.72
1:E:141:LEU:O	1:E:145:THR:HG23	1.90	0.72
1:E:247:PHE:CD2	1:E:270:CYS:HA	2.24	0.72
1:E:146:ARG:HH11	1:E:182:THR:HG22	1.53	0.72
1:F:141:LEU:O	1:F:145:THR:HG23	1.90	0.72
1:D:401:TYR:CE2	1:F:443:ALA:HA	2.25	0.72
1:E:38:GLU:OE2	1:E:40:GLN:OE1	2.07	0.72
1:A:221:HIS:CD2	1:A:454:ALA:HA	2.24	0.72
1:D:294:PHE:CE2	1:D:304:PHE:HA	2.24	0.71
1:A:428:ILE:HG12	1:C:420:LYS:NZ	2.05	0.71
1:F:239:THR:O	1:F:245:LYS:NZ	2.22	0.71
1:A:141:LEU:O	1:A:145:THR:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:401:TYR:HE2	1:F:443:ALA:HA	1.54	0.71
1:E:12:MET:HG3	1:E:354:PRO:HD3	1.72	0.71
1:A:183:TYR:CD1	1:A:187:ILE:HG23	2.24	0.71
1:F:18:ASP:OD1	1:F:53:LYS:NZ	2.23	0.71
1:A:265:ARG:NH2	3:A:602:GTP:O3G	2.23	0.71
1:D:247:PHE:CE2	1:D:270:CYS:HA	2.26	0.71
1:C:415:GLU:O	1:C:419:ARG:HG2	1.91	0.70
1:E:322:LEU:HD13	1:E:340:LYS:HZ1	1.56	0.70
1:A:499:THR:HG1	1:D:147:ARG:HH12	1.36	0.70
1:B:77:GLY:C	1:B:78:TYR:HD2	2.00	0.70
1:B:337:PRO:HD3	1:B:359:ILE:HD13	1.72	0.70
1:F:280:ILE:HD11	1:F:291:LEU:HD11	1.73	0.70
1:A:265:ARG:HH22	3:A:602:GTP:PG	2.15	0.70
2:A:601:GLU:HA	4:A:603:NAI:C4N	2.21	0.70
1:E:5:ASP:HB3	1:E:332:THR:HB	1.74	0.70
1:B:38:GLU:HG3	1:B:40:GLN:HB3	1.74	0.69
1:A:206:GLY:HA2	4:A:604:NAI:H3D	1.74	0.69
1:B:12:MET:HG3	1:B:354:PRO:HD3	1.75	0.69
1:A:428:ILE:HG12	1:C:420:LYS:HZ2	1.57	0.69
1:B:459:ARG:HH21	1:B:463:GLN:HE21	1.38	0.69
1:E:463:GLN:HA	1:E:466:ARG:HH11	1.58	0.69
1:A:65:ILE:HG21	1:A:144:ILE:HG12	1.75	0.69
1:E:247:PHE:HE2	1:E:270:CYS:CB	2.06	0.69
1:C:458:GLU:CD	1:C:462:ARG:HH12	2.00	0.69
1:D:12:MET:HG3	1:D:354:PRO:HD3	1.74	0.69
1:D:90:LYS:NZ	2:D:601:GLU:OE2	2.24	0.69
1:E:280:ILE:HD11	1:E:291:LEU:HD11	1.74	0.69
1:D:247:PHE:CD2	1:D:270:CYS:HA	2.27	0.69
1:B:27:LYS:NZ	1:B:31:ASP:OD2	2.26	0.68
1:E:317:VAL:O	1:E:340:LYS:HG3	1.93	0.68
1:E:95:TYR:HB3	1:E:133:PRO:HG3	1.75	0.68
1:E:274:GLY:O	1:E:275:GLU:HG2	1.94	0.68
1:A:126:LYS:NZ	2:A:601:GLU:OXT	2.27	0.67
1:C:126:LYS:NZ	2:C:601:GLU:O	2.27	0.67
1:F:77:GLY:C	1:F:78:TYR:HD2	2.02	0.67
1:C:77:GLY:C	1:C:78:TYR:HD2	2.02	0.67
1:D:280:ILE:HD11	1:D:291:LEU:HD11	1.76	0.67
1:A:26:ASP:OD1	1:A:42:ARG:NH2	2.28	0.67
1:C:12:MET:HG3	1:C:354:PRO:HD3	1.75	0.67
1:E:77:GLY:C	1:E:78:TYR:HD2	2.02	0.67
1:A:12:MET:HG3	1:A:354:PRO:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:HIS:O	4:D:604:NAI:N7N	2.28	0.67
1:D:126:LYS:NZ	2:D:601:GLU:OXT	2.28	0.67
1:C:28:LEU:HB3	1:C:490:PHE:HE2	1.59	0.67
1:E:439:ARG:NH1	1:F:401:TYR:CD1	2.63	0.67
1:E:252:PHE:HB3	1:E:275:GLU:OE2	1.94	0.67
1:F:349:ASN:N	4:F:605:NAI:O2D	2.26	0.67
1:C:5:ASP:HB3	1:C:332:THR:HB	1.77	0.67
1:E:439:ARG:NH1	1:F:401:TYR:CE1	2.62	0.67
1:C:26:ASP:OD1	1:C:42:ARG:NH2	2.28	0.66
1:C:303:GLY:N	1:C:309:ILE:HD11	2.04	0.66
1:F:346:GLU:OE2	1:F:478:ARG:NH1	2.28	0.66
1:F:68:ASP:OD1	1:F:140:GLU:HG3	1.94	0.66
1:A:90:LYS:NZ	2:A:601:GLU:OE1	2.23	0.66
1:A:95:TYR:HB3	1:A:133:PRO:HG3	1.76	0.66
1:F:95:TYR:HB3	1:F:133:PRO:HG3	1.77	0.66
1:D:77:GLY:C	1:D:78:TYR:HD2	2.04	0.66
1:B:339:VAL:O	1:B:341:ALA:N	2.29	0.66
1:C:57:HIS:HD2	1:F:155:LYS:HG3	1.61	0.66
1:A:37:THR:HA	1:A:41:LYS:HE3	1.77	0.66
1:A:261:ARG:NH1	3:A:602:GTP:O2G	2.29	0.66
1:E:126:LYS:NZ	2:E:601:GLU:OXT	2.28	0.66
1:D:37:THR:HA	1:D:41:LYS:HE3	1.77	0.66
1:C:3:ARG:HB2	1:C:3:ARG:NH1	2.11	0.66
1:F:126:LYS:NZ	2:F:602:GLU:O	2.28	0.66
1:B:95:TYR:HB3	1:B:133:PRO:HG3	1.77	0.66
1:D:339:VAL:O	1:D:341:ALA:N	2.29	0.65
1:E:95:TYR:OH	1:E:145:THR:HG22	1.96	0.65
1:C:455:TYR:O	1:C:459:ARG:N	2.28	0.65
1:D:29:VAL:HG21	1:D:42:ARG:HG3	1.77	0.65
1:F:12:MET:HG3	1:F:354:PRO:HD3	1.76	0.65
1:A:95:TYR:OH	1:A:145:THR:HG22	1.97	0.65
1:D:95:TYR:HB3	1:D:133:PRO:HG3	1.79	0.65
1:B:190:TYR:OH	1:D:190:TYR:OH	2.15	0.64
1:E:37:THR:HA	1:E:41:LYS:HE3	1.79	0.64
1:E:90:LYS:NZ	2:E:601:GLU:OE1	2.27	0.64
1:E:374:ASN:HB2	4:E:603:NAI:H5N	1.79	0.64
1:F:28:LEU:HB3	1:F:490:PHE:CE2	2.31	0.64
1:B:126:LYS:NZ	2:B:601:GLU:O	2.30	0.64
1:A:339:VAL:O	1:A:341:ALA:N	2.31	0.64
1:B:2:ASP:O	1:B:3:ARG:HD3	1.98	0.64
1:B:5:ASP:HB3	1:B:332:THR:HB	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:THR:HG22	1:B:269:LYS:HE3	1.78	0.64
1:A:396:ARG:NH1	1:B:119:ASP:O	2.30	0.64
1:D:420:LYS:CE	1:F:428:ILE:HG12	2.28	0.64
1:E:316:GLU:C	1:E:340:LYS:HD2	2.23	0.64
2:E:601:GLU:HA	4:E:603:NAI:H4N	1.80	0.64
1:B:211:ARG:O	1:B:211:ARG:NH1	2.29	0.63
1:B:396:ARG:NH1	1:C:119:ASP:O	2.31	0.63
1:C:499:THR:OG1	1:F:147:ARG:NH1	2.31	0.63
1:E:26:ASP:OD1	1:E:42:ARG:NH2	2.31	0.63
1:F:95:TYR:OH	1:F:145:THR:HG22	1.99	0.63
1:A:287:ASP:OD2	1:A:289:LYS:HG2	1.97	0.63
1:F:25:GLU:OE1	1:F:46:ARG:NH1	2.32	0.63
1:F:372:TYR:O	1:F:457:MET:HE1	1.99	0.63
1:A:38:GLU:OE2	1:A:40:GLN:HB2	1.99	0.63
1:C:95:TYR:HB3	1:C:133:PRO:HG3	1.79	0.63
1:E:260:MET:HG2	1:E:288:PRO:HG3	1.80	0.63
1:E:46:ARG:O	1:E:50:ARG:HG3	1.97	0.63
1:D:66:ARG:HG2	1:D:67:ARG:O	1.98	0.63
1:F:339:VAL:O	1:F:341:ALA:N	2.31	0.63
1:B:95:TYR:OH	1:B:145:THR:HG22	1.99	0.63
1:E:302:LEU:HD22	1:E:309:ILE:HD12	1.81	0.63
1:A:221:HIS:HD2	1:A:454:ALA:HA	1.62	0.63
1:D:215:THR:OG1	4:D:603:NAI:H42N	1.97	0.63
1:B:26:ASP:OD1	1:B:42:ARG:NH2	2.32	0.62
1:A:261:ARG:CZ	3:A:602:GTP:O2G	2.47	0.62
1:D:247:PHE:HE2	1:D:270:CYS:CB	2.11	0.62
1:E:282:ASN:ND2	1:E:306:LYS:O	2.31	0.62
1:F:260:MET:HG2	1:F:288:PRO:HG3	1.82	0.62
1:C:209:HIS:CD2	1:C:446:LYS:HB2	2.33	0.62
1:A:456:THR:HA	1:A:459:ARG:HB3	1.81	0.62
1:D:26:ASP:OD1	1:D:42:ARG:NH2	2.33	0.62
1:C:37:THR:HA	1:C:41:LYS:HE3	1.80	0.62
1:A:77:GLY:C	1:A:78:TYR:HD2	2.08	0.61
1:D:95:TYR:OH	1:D:145:THR:HG22	2.00	0.61
1:E:317:VAL:O	1:E:340:LYS:HE3	1.99	0.61
1:A:260:MET:HG2	1:A:288:PRO:HG3	1.81	0.61
1:F:86:ARG:HE	4:F:601:NAI:H62A	1.47	0.61
1:B:196:ALA:HB2	1:B:388:ASN:HB3	1.81	0.61
1:C:458:GLU:OE1	1:C:462:ARG:NH1	2.26	0.61
1:F:26:ASP:OD1	1:F:42:ARG:NH2	2.33	0.61
1:D:470:LYS:HB3	1:D:471:TYR:CD2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:MET:HG2	1:B:288:PRO:HG3	1.82	0.61
1:B:392:VAL:HG22	1:C:386:LEU:HD13	1.82	0.61
1:D:470:LYS:HB3	1:D:471:TYR:HD2	1.63	0.61
4:B:604:NAI:H2A	1:C:492:VAL:CG2	2.31	0.61
1:D:456:THR:HG21	1:E:396:ARG:NH2	2.15	0.61
1:F:282:ASN:ND2	1:F:306:LYS:O	2.33	0.61
1:A:315:LEU:HD13	1:A:331:LEU:HD12	1.83	0.60
1:B:280:ILE:HD11	1:B:291:LEU:HD11	1.83	0.60
1:D:387:LYS:HE2	4:F:601:NAI:H51N	1.82	0.60
1:A:396:ARG:HH21	1:B:456:THR:HG21	1.66	0.60
1:C:95:TYR:OH	1:C:145:THR:HG22	2.01	0.60
1:B:91:GLY:HA2	1:B:111:MET:HE2	1.83	0.60
1:D:294:PHE:HD1	1:D:298:HIS:HD1	1.50	0.60
1:C:339:VAL:O	1:C:341:ALA:N	2.35	0.60
1:C:387:LYS:HE2	4:C:603:NAI:H3D	1.84	0.60
1:E:455:TYR:CE2	1:F:399:PHE:HD2	2.18	0.60
1:B:117:VAL:HG21	1:B:371:LEU:HB3	1.84	0.60
1:B:412:SER:HA	1:C:433:THR:HG23	1.84	0.60
1:E:2:ASP:O	1:E:3:ARG:HD2	2.02	0.60
1:E:322:LEU:HD22	1:E:340:LYS:HZ3	1.66	0.60
1:E:340:LYS:HE2	1:E:341:ALA:HB2	1.84	0.59
1:C:117:VAL:HG21	1:C:371:LEU:HB3	1.84	0.59
1:E:403:ARG:NH1	1:E:441:SER:OG	2.29	0.59
1:F:331:LEU:HD23	1:F:360:PHE:HZ	1.66	0.59
1:C:230:ALA:HA	1:C:233:MET:HB2	1.83	0.59
1:E:415:GLU:O	1:E:419:ARG:HB2	2.02	0.59
1:F:471:TYR:HD2	1:F:471:TYR:N	1.99	0.59
1:D:315:LEU:HD13	1:D:331:LEU:HD12	1.84	0.59
1:A:209:HIS:CD2	1:A:446:LYS:HB2	2.37	0.59
1:A:428:ILE:HA	1:C:420:LYS:HE3	1.85	0.59
1:C:91:GLY:HA2	1:C:111:MET:HE2	1.85	0.59
1:D:247:PHE:CD2	1:D:247:PHE:C	2.81	0.59
1:F:209:HIS:CD2	1:F:446:LYS:HB2	2.38	0.59
1:A:211:ARG:O	1:A:211:ARG:NH1	2.33	0.59
1:B:55:CYS:O	1:E:62:SER:HB2	2.03	0.59
1:D:211:ARG:O	1:D:211:ARG:NH1	2.30	0.59
1:D:247:PHE:HE1	1:D:263:LEU:HB2	1.67	0.59
1:E:211:ARG:O	1:E:211:ARG:NH1	2.30	0.59
1:E:315:LEU:HD13	1:E:331:LEU:HD12	1.85	0.59
1:A:91:GLY:HA2	1:A:111:MET:HE2	1.85	0.59
1:C:57:HIS:CD2	1:F:155:LYS:HG3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:ARG:O	1:F:211:ARG:NH1	2.29	0.59
1:F:331:LEU:HB2	1:F:352:THR:HG22	1.85	0.59
1:A:44:ARG:NH1	1:A:494:ASN:OD1	2.34	0.58
1:E:209:HIS:CD2	1:E:446:LYS:HB2	2.38	0.58
1:B:79:ARG:HH11	1:B:127:ALA:HB2	1.69	0.58
1:B:154:LYS:HB3	1:F:189:HIS:NE2	2.18	0.58
1:D:260:MET:HG2	1:D:288:PRO:HG3	1.86	0.58
1:F:79:ARG:HH11	1:F:127:ALA:HB2	1.69	0.58
1:A:333:LYS:HE3	1:A:355:GLU:HB3	1.84	0.58
1:B:190:TYR:HH	1:D:190:TYR:HH	1.48	0.58
1:B:238:MET:HE1	1:B:343:ILE:HG13	1.85	0.58
1:E:339:VAL:O	1:E:339:VAL:HG12	2.03	0.58
1:D:375:ALA:O	1:D:379:THR:OG1	2.19	0.58
1:A:79:ARG:HH11	1:A:127:ALA:HB2	1.68	0.58
1:E:230:ALA:HA	1:E:233:MET:HB2	1.84	0.58
1:F:169:MET:HA	4:F:605:NAI:O1N	2.04	0.58
1:A:386:LEU:HD22	1:C:392:VAL:HG22	1.86	0.58
1:C:211:ARG:O	1:C:211:ARG:NH1	2.30	0.58
1:A:117:VAL:HG21	1:A:371:LEU:HB3	1.86	0.58
1:A:500:PHE:CZ	1:D:150:MET:HG3	2.38	0.58
1:B:150:MET:HG3	1:E:500:PHE:CE2	2.38	0.58
1:A:500:PHE:HZ	1:D:150:MET:HG3	1.69	0.57
1:B:154:LYS:HD2	1:F:189:HIS:ND1	2.18	0.57
1:D:91:GLY:HA2	1:D:111:MET:HE2	1.85	0.57
1:D:117:VAL:HG21	1:D:371:LEU:HB3	1.86	0.57
1:E:462:ARG:NH1	1:E:466:ARG:NH2	2.51	0.57
1:E:463:GLN:HA	1:E:466:ARG:NH1	2.19	0.57
1:B:241:GLY:O	1:B:245:LYS:NZ	2.37	0.57
1:D:247:PHE:HE2	1:D:270:CYS:SG	2.28	0.57
1:D:386:LEU:HD13	1:E:392:VAL:HG22	1.86	0.57
1:C:208:ILE:HG13	1:C:445:GLU:OE2	2.04	0.57
1:D:244:ASP:HA	1:D:269:LYS:HZ3	1.68	0.57
1:A:393:SER:HB3	4:A:604:NAI:O3	2.05	0.57
1:B:500:PHE:HE2	1:E:150:MET:HG3	1.69	0.57
1:D:289:LYS:NZ	3:D:602:GTP:O6	2.37	0.57
1:D:282:ASN:ND2	1:D:306:LYS:O	2.36	0.57
1:F:253:GLY:HA3	4:F:605:NAI:PA	2.44	0.57
1:A:391:HIS:HD1	1:B:385:TRP:HH2	1.51	0.57
1:E:423:LYS:O	1:E:425:GLY:N	2.38	0.57
1:F:86:ARG:HD2	4:F:601:NAI:C3N	2.35	0.57
2:A:601:GLU:CA	4:A:603:NAI:H4N	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:LEU:HD23	1:B:360:PHE:CZ	2.39	0.57
1:A:401:TYR:CE1	1:B:439:ARG:NH1	2.71	0.57
1:A:396:ARG:NH2	1:B:456:THR:HG21	2.18	0.56
1:D:303:GLY:H	1:D:309:ILE:HD11	1.69	0.56
1:A:282:ASN:ND2	1:A:306:LYS:O	2.37	0.56
4:C:604:NAI:H2N	4:C:604:NAI:O1N	2.05	0.56
1:B:37:THR:HA	1:B:41:LYS:HE3	1.86	0.56
1:B:208:ILE:HG13	1:B:445:GLU:OE2	2.04	0.56
1:C:79:ARG:HH11	1:C:127:ALA:HB2	1.70	0.56
1:C:331:LEU:HD23	1:C:360:PHE:CZ	2.40	0.56
1:D:167:PRO:HA	1:D:176:MET:HE3	1.87	0.56
1:C:3:ARG:HB2	1:C:3:ARG:CZ	2.34	0.56
1:D:167:PRO:HD3	1:D:176:MET:HG3	1.87	0.56
1:E:171:THR:HG22	1:E:175:GLU:HG2	1.86	0.56
1:E:247:PHE:CD2	1:E:247:PHE:C	2.84	0.56
1:C:171:THR:HG22	1:C:175:GLU:HG2	1.87	0.56
1:C:260:MET:HG2	1:C:288:PRO:HG3	1.87	0.56
1:D:331:LEU:HB2	1:D:352:THR:HG22	1.88	0.56
1:D:409:LEU:HD21	1:F:409:LEU:HD22	1.88	0.56
1:E:331:LEU:HD23	1:E:360:PHE:CZ	2.40	0.56
1:F:117:VAL:HG21	1:F:371:LEU:HB3	1.87	0.56
1:F:331:LEU:HD23	1:F:360:PHE:CZ	2.40	0.56
1:F:403:ARG:NH1	1:F:407:TYR:HE2	2.02	0.56
1:A:401:TYR:CD1	1:B:439:ARG:NH1	2.74	0.56
1:B:150:MET:CE	1:B:186:THR:HG21	2.36	0.56
1:B:281:TRP:HB2	1:B:310:TYR:HB2	1.87	0.56
1:D:390:ASN:O	1:D:392:VAL:HG23	2.05	0.56
1:E:169:MET:HG2	4:E:603:NAI:H52N	1.88	0.56
1:F:390:ASN:O	1:F:392:VAL:HG23	2.06	0.56
1:C:444:SER:OG	1:C:447:ASP:OD1	2.24	0.56
1:D:230:ALA:HA	1:D:233:MET:HB2	1.87	0.56
1:E:247:PHE:HE1	1:E:263:LEU:HB2	1.70	0.56
1:B:331:LEU:HB2	1:B:352:THR:HG22	1.87	0.56
1:B:392:VAL:CG2	1:C:386:LEU:HD13	2.36	0.56
1:E:499:THR:HG23	1:E:501:THR:HB	1.88	0.56
1:F:455:TYR:CE1	1:F:459:ARG:HD2	2.41	0.56
1:D:444:SER:OG	1:D:447:ASP:OD1	2.23	0.56
1:B:185:SER:O	1:F:154:LYS:HD3	2.07	0.55
1:E:167:PRO:HD3	1:E:176:MET:HG3	1.88	0.55
1:F:252:PHE:HB3	1:F:275:GLU:OE2	2.06	0.55
1:B:499:THR:HG23	1:B:501:THR:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:169:MET:HG2	4:F:605:NAI:H52N	1.87	0.55
1:F:221:HIS:CD2	1:F:454:ALA:HA	2.42	0.55
1:A:331:LEU:HB2	1:A:352:THR:HG22	1.89	0.55
1:D:3:ARG:HH12	1:D:4:GLU:CG	2.18	0.55
1:F:34:THR:HG21	1:F:44:ARG:NH2	2.22	0.55
1:A:331:LEU:HD23	1:A:360:PHE:CZ	2.41	0.55
1:D:221:HIS:CD2	1:D:454:ALA:HA	2.42	0.55
4:B:604:NAI:H2A	1:C:492:VAL:HG23	1.89	0.55
1:C:331:LEU:HB2	1:C:352:THR:HG22	1.88	0.55
1:E:117:VAL:HG21	1:E:371:LEU:HB3	1.87	0.55
1:A:220:PHE:HD2	1:A:221:HIS:HD1	1.55	0.55
1:B:62:SER:HB2	1:E:55:CYS:O	2.06	0.55
1:D:79:ARG:HH11	1:D:127:ALA:HB2	1.70	0.55
1:E:459:ARG:HA	1:E:462:ARG:HD3	1.87	0.55
1:F:37:THR:HA	1:F:41:LYS:HE3	1.89	0.55
1:B:167:PRO:HD3	1:B:176:MET:HG3	1.88	0.55
1:B:169:MET:HG2	4:B:603:NAI:H52N	1.88	0.55
1:E:91:GLY:HA2	1:E:111:MET:HE2	1.88	0.55
2:E:601:GLU:HA	4:E:603:NAI:C4N	2.37	0.55
1:A:91:GLY:HA3	1:A:125:ALA:O	2.06	0.55
1:E:390:ASN:O	1:E:392:VAL:HG23	2.07	0.55
1:F:167:PRO:HD3	1:F:176:MET:HG3	1.88	0.55
1:A:413:VAL:HG11	1:C:413:VAL:CG1	2.35	0.55
1:E:150:MET:CE	1:E:186:THR:HG21	2.37	0.55
1:C:282:ASN:ND2	1:C:306:LYS:O	2.36	0.55
1:C:471:TYR:N	1:C:471:TYR:HD2	2.04	0.55
1:E:79:ARG:HH11	1:E:127:ALA:HB2	1.71	0.55
1:F:402:GLU:HG3	1:F:406:ASN:OD1	2.06	0.55
1:D:247:PHE:C	1:D:247:PHE:HD2	2.14	0.54
1:E:331:LEU:HB2	1:E:352:THR:HG22	1.90	0.54
1:C:150:MET:CE	1:C:186:THR:HG21	2.37	0.54
1:C:462:ARG:HG2	1:C:465:MET:HE2	1.90	0.54
1:D:91:GLY:HA3	1:D:125:ALA:O	2.07	0.54
1:D:150:MET:CE	1:D:186:THR:HG21	2.37	0.54
1:E:455:TYR:CZ	1:F:399:PHE:HD2	2.26	0.54
1:F:126:LYS:HZ1	2:F:602:GLU:N	2.05	0.54
1:F:406:ASN:ND2	1:F:436:PHE:HZ	2.05	0.54
1:A:406:ASN:ND2	1:A:436:PHE:HZ	2.06	0.54
1:B:230:ALA:HA	1:B:233:MET:HB2	1.89	0.54
1:E:279:SER:OG	1:E:314:ILE:HB	2.06	0.54
1:E:375:ALA:O	1:E:379:THR:OG1	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:SER:HA	1:A:258:HIS:ND1	2.22	0.54
1:C:91:GLY:HA3	1:C:125:ALA:O	2.07	0.54
1:C:390:ASN:O	1:C:392:VAL:HG23	2.08	0.54
1:E:53:LYS:HB2	1:E:54:PRO:HD3	1.89	0.54
1:E:254:ASN:HB2	4:E:603:NAI:O2N	2.07	0.54
1:F:209:HIS:HD2	1:F:446:LYS:HB2	1.72	0.54
1:B:24:VAL:HG13	1:B:483:VAL:HG13	1.88	0.54
1:C:470:LYS:HG3	1:C:471:TYR:CD2	2.42	0.54
1:F:281:TRP:HB2	1:F:310:TYR:HB2	1.89	0.54
1:F:345:ALA:HB1	1:F:373:LEU:HD21	1.89	0.54
1:C:252:PHE:HB3	1:C:275:GLU:OE2	2.08	0.54
1:D:331:LEU:HD23	1:D:360:PHE:CZ	2.42	0.54
1:F:34:THR:HG21	1:F:44:ARG:HH12	1.73	0.54
1:B:150:MET:HG3	1:E:500:PHE:HE2	1.71	0.54
1:B:375:ALA:O	1:B:379:THR:OG1	2.20	0.54
1:B:414:GLN:HG3	1:B:428:ILE:O	2.08	0.54
1:D:119:ASP:O	1:E:396:ARG:NH1	2.41	0.54
1:F:171:THR:HG22	1:F:175:GLU:HG2	1.89	0.54
1:C:167:PRO:HD3	1:C:176:MET:HG3	1.90	0.54
1:F:23:ILE:HG22	1:F:471:TYR:HD1	1.73	0.54
1:A:27:LYS:NZ	1:A:31:ASP:OD2	2.38	0.54
1:C:501:THR:OG1	1:F:66:ARG:NH1	2.40	0.54
1:D:32:LEU:HD11	1:D:494:ASN:OD1	2.07	0.54
1:E:247:PHE:CE2	1:E:270:CYS:CA	2.90	0.54
1:F:471:TYR:N	1:F:471:TYR:CD2	2.75	0.53
1:A:390:ASN:O	1:A:392:VAL:HG23	2.06	0.53
1:F:42:ARG:O	1:F:46:ARG:HG3	2.09	0.53
1:F:274:GLY:O	1:F:275:GLU:HG2	2.08	0.53
1:B:91:GLY:HA3	1:B:125:ALA:O	2.07	0.53
1:B:357:ASP:OD2	1:B:478:ARG:NE	2.36	0.53
1:E:91:GLY:HA3	1:E:125:ALA:O	2.08	0.53
1:B:90:LYS:HD2	1:B:164:VAL:O	2.09	0.53
1:F:24:VAL:HG13	1:F:483:VAL:HG13	1.91	0.53
1:A:167:PRO:HD3	1:A:176:MET:HG3	1.89	0.53
1:A:230:ALA:HA	1:A:233:MET:HB2	1.91	0.53
1:C:275:GLU:HG3	1:C:301:ILE:HD13	1.90	0.53
1:C:315:LEU:HD13	1:C:331:LEU:HD12	1.90	0.53
1:E:79:ARG:HD2	1:E:127:ALA:HB2	1.88	0.53
1:E:221:HIS:CD2	1:E:454:ALA:HA	2.43	0.53
1:F:27:LYS:NZ	1:F:31:ASP:OD2	2.42	0.53
1:F:358:LYS:O	1:F:362:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PHE:HB3	1:A:275:GLU:OE2	2.09	0.53
1:C:388:ASN:O	1:C:391:HIS:CD2	2.62	0.53
1:A:368:ILE:HG21	1:A:373:LEU:HD13	1.91	0.53
1:B:169:MET:HA	4:B:603:NAI:O1N	2.09	0.53
1:B:279:SER:OG	1:B:314:ILE:HB	2.08	0.53
1:C:221:HIS:CD2	1:C:454:ALA:HA	2.44	0.53
1:E:345:ALA:HB1	1:E:373:LEU:HD21	1.91	0.53
1:F:32:LEU:HD11	1:F:494:ASN:OD1	2.08	0.53
1:A:24:VAL:HG13	1:A:483:VAL:HG13	1.90	0.53
1:B:282:ASN:ND2	1:B:306:LYS:O	2.37	0.53
1:C:345:ALA:HB1	1:C:373:LEU:HD21	1.91	0.53
1:C:471:TYR:N	1:C:471:TYR:CD2	2.77	0.53
1:D:279:SER:OG	1:D:314:ILE:HB	2.09	0.53
1:E:150:MET:HE1	1:E:186:THR:HG21	1.91	0.53
1:D:10:PHE:HE1	1:D:53:LYS:NZ	2.07	0.53
1:D:244:ASP:HA	1:D:269:LYS:NZ	2.23	0.53
1:F:406:ASN:HD22	1:F:436:PHE:HZ	1.57	0.53
1:D:10:PHE:CD2	1:D:105:LYS:HE2	2.44	0.52
1:F:91:GLY:HA3	1:F:125:ALA:O	2.09	0.52
1:A:499:THR:HG23	1:A:501:THR:HB	1.91	0.52
1:C:458:GLU:CG	1:C:462:ARG:NH1	2.71	0.52
1:B:35:ARG:O	1:B:37:THR:N	2.36	0.52
1:E:368:ILE:HG21	1:E:373:LEU:HD13	1.92	0.52
1:B:345:ALA:HB1	1:B:373:LEU:HD21	1.90	0.52
1:D:247:PHE:CE2	1:D:270:CYS:CA	2.91	0.52
1:A:488:LYS:HG2	1:A:491:ARG:NH2	2.23	0.52
1:B:315:LEU:HD22	1:B:331:LEU:HD11	1.92	0.52
1:C:53:LYS:HB2	1:C:54:PRO:HD3	1.91	0.52
1:C:279:SER:OG	1:C:314:ILE:HB	2.09	0.52
1:C:458:GLU:CG	1:C:462:ARG:HH12	2.22	0.52
1:C:499:THR:HG23	1:C:501:THR:HB	1.91	0.52
1:D:398:THR:O	1:D:401:TYR:N	2.42	0.52
1:F:346:GLU:CD	1:F:478:ARG:HH12	2.17	0.52
1:F:382:TYR:CZ	1:F:386:LEU:HD11	2.45	0.52
1:B:396:ARG:NH2	1:C:456:THR:HG21	2.25	0.52
1:D:24:VAL:CG1	1:D:483:VAL:HG13	2.39	0.52
1:E:24:VAL:HG13	1:E:483:VAL:HG13	1.91	0.52
1:A:115:CYS:SG	1:A:378:VAL:HG11	2.50	0.52
1:A:292:GLU:CD	3:A:602:GTP:HN1	2.17	0.52
1:A:444:SER:OG	1:A:447:ASP:OD1	2.25	0.52
1:B:33:LYS:HD3	1:B:41:LYS:NZ	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:THR:HB	4:B:603:NAI:H42N	1.91	0.52
1:B:390:ASN:O	1:B:392:VAL:HG23	2.09	0.52
1:F:91:GLY:HA2	1:F:111:MET:HE2	1.90	0.52
1:F:239:THR:HG21	1:F:244:ASP:OD2	2.10	0.52
1:C:458:GLU:HG2	1:C:462:ARG:HH11	1.73	0.52
1:E:25:GLU:OE1	1:E:46:ARG:NH1	2.43	0.52
1:F:186:THR:OG1	1:F:187:ILE:N	2.43	0.52
1:A:279:SER:OG	1:A:314:ILE:HB	2.10	0.52
1:A:388:ASN:O	1:A:391:HIS:CD2	2.63	0.52
1:C:458:GLU:HG2	1:C:462:ARG:HH12	1.74	0.52
1:D:294:PHE:CD2	1:D:304:PHE:HD1	2.28	0.52
1:F:368:ILE:HG21	1:F:373:LEU:HD13	1.91	0.52
1:B:24:VAL:CG1	1:B:483:VAL:HG13	2.40	0.52
1:C:28:LEU:HB3	1:C:490:PHE:CE2	2.42	0.52
1:E:126:LYS:HZ1	2:E:601:GLU:N	2.08	0.52
1:A:345:ALA:HB1	1:A:373:LEU:HD21	1.91	0.51
1:E:280:ILE:HG22	1:E:309:ILE:HD13	1.93	0.51
1:A:427:THR:O	1:C:420:LYS:HE3	2.11	0.51
1:B:150:MET:HE1	1:B:186:THR:HG21	1.91	0.51
1:B:159:GLY:HA2	1:B:183:TYR:HE2	1.75	0.51
1:C:24:VAL:HG13	1:C:483:VAL:HG13	1.93	0.51
1:C:280:ILE:HD11	1:C:291:LEU:HD11	1.92	0.51
1:D:77:GLY:C	1:D:78:TYR:CD2	2.88	0.51
1:D:427:THR:O	1:E:420:LYS:HE2	2.10	0.51
1:B:403:ARG:HA	1:B:440:ILE:O	2.10	0.51
1:C:78:TYR:HD1	1:C:101:VAL:HG23	1.75	0.51
1:F:236:LEU:HD22	1:F:342:LYS:HD2	1.92	0.51
1:F:294:PHE:HD1	1:F:298:HIS:HD1	1.57	0.51
1:A:24:VAL:CG1	1:A:483:VAL:HG13	2.40	0.51
1:A:186:THR:OG1	1:A:187:ILE:N	2.43	0.51
1:B:115:CYS:SG	1:B:378:VAL:HG11	2.50	0.51
1:E:172:GLY:N	1:E:175:GLU:OE2	2.42	0.51
1:F:159:GLY:HA2	1:F:183:TYR:HE2	1.76	0.51
1:F:294:PHE:CD2	1:F:304:PHE:HD1	2.28	0.51
1:A:192:ILE:HG12	1:A:391:HIS:HE1	1.75	0.51
1:A:406:ASN:HD22	1:A:436:PHE:HZ	1.56	0.51
1:D:269:LYS:N	1:D:269:LYS:HD2	2.25	0.51
1:F:222:GLY:HA3	1:F:373:LEU:HD12	1.92	0.51
1:F:279:SER:OG	1:F:314:ILE:HB	2.11	0.51
1:A:155:LYS:HG3	1:D:57:HIS:CD2	2.46	0.51
1:D:345:ALA:HB1	1:D:373:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:VAL:HG13	1:F:413:VAL:HG11	1.93	0.51
1:E:5:ASP:HB2	1:E:333:LYS:HG2	1.93	0.51
1:E:247:PHE:HE2	1:E:270:CYS:SG	2.32	0.51
1:F:115:CYS:SG	1:F:378:VAL:HG11	2.50	0.51
1:A:336:ALA:HB3	1:A:359:ILE:HD12	1.92	0.51
1:B:399:PHE:HD2	1:C:455:TYR:CE2	2.29	0.51
1:C:115:CYS:SG	1:C:378:VAL:HG11	2.51	0.51
1:F:238:MET:HE1	1:F:342:LYS:HB3	1.93	0.51
1:F:287:ASP:HB3	1:F:290:GLU:HG3	1.93	0.51
1:A:459:ARG:NH1	1:A:459:ARG:HG3	2.24	0.51
1:D:402:GLU:OE2	1:E:402:GLU:OE2	2.29	0.51
1:E:487:GLU:HG2	1:E:491:ARG:NH1	2.21	0.51
1:B:39:GLU:OE2	1:B:42:ARG:HD2	2.11	0.51
1:C:118:VAL:HG21	1:C:375:ALA:HB1	1.93	0.51
1:C:382:TYR:CZ	1:C:386:LEU:HD11	2.46	0.51
1:D:209:HIS:CD2	1:D:446:LYS:HB2	2.45	0.51
1:C:375:ALA:O	1:C:379:THR:OG1	2.22	0.51
1:F:269:LYS:HD2	1:F:284:ASP:O	2.11	0.51
1:A:36:GLU:HB3	1:A:40:GLN:HG2	1.91	0.50
1:A:357:ASP:OD2	1:A:478:ARG:NE	2.35	0.50
1:B:32:LEU:HD11	1:B:494:ASN:OD1	2.11	0.50
1:B:51:ILE:HG12	1:E:64:PRO:HB3	1.93	0.50
1:C:222:GLY:HA3	1:C:373:LEU:HD12	1.93	0.50
1:B:292:GLU:OE1	3:B:602:GTP:N2	2.32	0.50
1:C:150:MET:HE1	1:C:186:THR:HG21	1.92	0.50
1:D:336:ALA:HB3	1:D:359:ILE:HD12	1.93	0.50
1:D:403:ARG:HA	1:D:440:ILE:O	2.12	0.50
1:E:222:GLY:HA3	1:E:373:LEU:HD12	1.93	0.50
1:F:24:VAL:CG1	1:F:483:VAL:HG13	2.42	0.50
1:A:118:VAL:HG21	1:A:375:ALA:HB1	1.94	0.50
1:A:463:GLN:HA	1:A:466:ARG:NH1	2.26	0.50
1:D:436:PHE:HB2	1:E:408:HIS:HB3	1.93	0.50
1:D:495:GLU:O	1:E:205:GLN:OE1	2.28	0.50
1:E:159:GLY:HA2	1:E:183:TYR:HE2	1.75	0.50
1:E:213:SER:O	1:E:215:THR:N	2.45	0.50
1:F:213:SER:O	1:F:215:THR:N	2.45	0.50
1:D:24:VAL:HG13	1:D:483:VAL:HG13	1.92	0.50
1:B:396:ARG:CZ	1:C:456:THR:HG21	2.42	0.50
1:C:23:ILE:HG22	1:C:471:TYR:HD1	1.77	0.50
1:E:118:VAL:HG21	1:E:375:ALA:HB1	1.92	0.50
1:A:90:LYS:HD2	1:A:164:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:GLY:HA3	1:B:373:LEU:HD12	1.93	0.50
1:D:382:TYR:CZ	1:D:386:LEU:HD11	2.47	0.50
1:F:398:THR:O	1:F:401:TYR:N	2.42	0.50
1:C:32:LEU:HD11	1:C:494:ASN:OD1	2.11	0.50
1:C:43:ASN:O	1:C:44:ARG:NH1	2.45	0.50
1:D:118:VAL:HG21	1:D:375:ALA:HB1	1.93	0.50
1:F:375:ALA:O	1:F:379:THR:OG1	2.24	0.50
1:F:403:ARG:HA	1:F:440:ILE:O	2.11	0.50
1:A:77:GLY:C	1:A:78:TYR:CD2	2.90	0.50
1:A:205:GLN:CD	1:B:495:GLU:O	2.55	0.50
1:A:315:LEU:HD22	1:A:331:LEU:HD11	1.94	0.50
4:A:604:NAI:H71N	1:B:86:ARG:HD3	1.76	0.50
1:B:500:PHE:CE2	1:E:150:MET:HG3	2.46	0.50
1:C:368:ILE:HG21	1:C:373:LEU:HD13	1.92	0.50
1:F:241:GLY:O	1:F:245:LYS:NZ	2.45	0.50
1:A:213:SER:O	1:A:215:THR:N	2.45	0.50
1:B:213:SER:O	1:B:215:THR:N	2.45	0.50
1:B:239:THR:HG21	1:B:244:ASP:OD2	2.12	0.50
1:B:368:ILE:HG21	1:B:373:LEU:HD13	1.93	0.50
1:C:65:ILE:HD13	1:C:144:ILE:HG12	1.93	0.50
1:D:213:SER:O	1:D:215:THR:N	2.45	0.50
1:D:432:PRO:HA	1:E:412:SER:OG	2.12	0.50
1:E:303:GLY:N	1:E:309:ILE:HD11	2.19	0.50
1:E:315:LEU:HD22	1:E:331:LEU:HD11	1.92	0.50
1:E:318:ASP:CA	1:E:340:LYS:HG3	2.40	0.50
1:E:496:ALA:HA	1:F:177:SER:OG	2.12	0.50
1:A:209:HIS:HD2	1:A:446:LYS:HB2	1.76	0.49
1:C:66:ARG:HG2	1:C:71:SER:O	2.12	0.49
1:E:94:ARG:HG3	1:E:169:MET:HB2	1.94	0.49
1:E:209:HIS:HD2	1:E:446:LYS:HB2	1.75	0.49
1:C:67:ARG:HD3	1:C:73:GLU:OE1	2.12	0.49
1:B:396:ARG:NE	1:C:456:THR:HG21	2.28	0.49
1:B:465:MET:O	1:B:469:MET:HG2	2.12	0.49
1:E:171:THR:HA	1:E:175:GLU:OE2	2.12	0.49
1:E:247:PHE:C	1:E:247:PHE:HD2	2.19	0.49
1:E:382:TYR:CZ	1:E:386:LEU:HD11	2.47	0.49
1:A:403:ARG:HA	1:A:440:ILE:O	2.12	0.49
1:C:470:LYS:HG3	1:C:471:TYR:CE2	2.47	0.49
1:D:386:LEU:HD13	1:E:392:VAL:CG2	2.43	0.49
1:A:155:LYS:HG3	1:D:57:HIS:HD2	1.77	0.49
1:E:32:LEU:HD11	1:E:494:ASN:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:PHE:CE2	1:E:270:CYS:CB	2.92	0.49
1:F:391:HIS:HA	4:F:603:NAI:H4D	1.95	0.49
1:A:32:LEU:HD11	1:A:494:ASN:OD1	2.11	0.49
1:A:57:HIS:HA	1:D:60:SER:O	2.11	0.49
1:A:67:ARG:NH1	1:A:136:TYR:CE2	2.81	0.49
1:C:24:VAL:CG1	1:C:483:VAL:HG13	2.43	0.49
1:D:357:ASP:OD2	1:D:478:ARG:NE	2.39	0.49
1:C:213:SER:O	1:C:215:THR:N	2.46	0.49
1:D:315:LEU:HD22	1:D:331:LEU:HD11	1.94	0.49
1:F:23:ILE:HG22	1:F:471:TYR:CD1	2.48	0.49
1:C:315:LEU:HD22	1:C:331:LEU:HD11	1.94	0.49
1:D:247:PHE:CD1	1:D:263:LEU:HD12	2.48	0.49
1:F:34:THR:OG1	1:F:35:ARG:N	2.46	0.49
1:A:177:SER:OG	1:B:496:ALA:HA	2.13	0.49
1:C:403:ARG:HA	1:C:440:ILE:O	2.13	0.49
1:D:339:VAL:O	1:D:340:LYS:C	2.55	0.49
1:D:443:ALA:HA	1:E:401:TYR:CE2	2.48	0.49
1:B:33:LYS:HD3	1:B:41:LYS:HZ3	1.77	0.49
1:B:388:ASN:N	1:B:388:ASN:HD22	2.11	0.49
1:D:247:PHE:HD2	1:D:247:PHE:O	1.96	0.49
1:E:24:VAL:CG1	1:E:483:VAL:HG13	2.42	0.49
1:E:403:ARG:HA	1:E:440:ILE:O	2.12	0.49
1:F:118:VAL:HG21	1:F:375:ALA:HB1	1.94	0.49
1:F:230:ALA:HA	1:F:233:MET:HB2	1.95	0.49
1:F:247:PHE:CE1	1:F:263:LEU:HB2	2.48	0.49
1:F:336:ALA:HB3	1:F:359:ILE:HD12	1.94	0.49
1:A:150:MET:HE2	1:A:186:THR:HG21	1.95	0.48
1:B:60:SER:O	1:E:57:HIS:HA	2.13	0.48
1:B:167:PRO:HA	1:B:176:MET:HE3	1.95	0.48
1:B:337:PRO:HD3	1:B:359:ILE:CD1	2.41	0.48
1:D:456:THR:HG21	1:E:396:ARG:CZ	2.43	0.48
1:B:331:LEU:HD23	1:B:360:PHE:HZ	1.77	0.48
1:F:372:TYR:O	1:F:457:MET:CE	2.60	0.48
1:B:118:VAL:HG21	1:B:375:ALA:HB1	1.95	0.48
1:D:289:LYS:HD2	1:D:289:LYS:HA	1.59	0.48
1:E:239:THR:HG21	1:E:244:ASP:OD2	2.13	0.48
1:A:382:TYR:CZ	1:A:386:LEU:HD11	2.47	0.48
1:A:417:LEU:CD1	1:C:417:LEU:HD21	2.43	0.48
1:B:247:PHE:C	1:B:247:PHE:CD2	2.92	0.48
1:D:209:HIS:HD2	1:D:446:LYS:HB2	1.78	0.48
1:F:146:ARG:NH1	1:F:182:THR:HG22	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ARG:HD2	1:A:465:MET:CE	2.43	0.48
1:C:65:ILE:O	1:C:65:ILE:HG13	2.13	0.48
1:C:239:THR:HG21	1:C:244:ASP:OD2	2.14	0.48
1:D:53:LYS:O	1:D:82:HIS:NE2	2.46	0.48
1:D:208:ILE:HG13	1:D:445:GLU:OE2	2.13	0.48
1:D:222:GLY:HA3	1:D:373:LEU:HD12	1.94	0.48
1:D:368:ILE:HG21	1:D:373:LEU:HD13	1.96	0.48
4:E:603:NAI:H2N	4:E:603:NAI:O1N	2.14	0.48
1:F:400:LYS:O	1:F:400:LYS:HG2	2.13	0.48
1:A:208:ILE:HG13	1:A:445:GLU:OE2	2.14	0.48
1:D:209:HIS:HD2	1:D:446:LYS:HA	1.78	0.48
1:E:48:ILE:O	1:E:52:ILE:HG13	2.14	0.48
1:E:423:LYS:C	1:E:425:GLY:H	2.22	0.48
1:F:53:LYS:HB2	1:F:54:PRO:HD3	1.95	0.48
1:F:269:LYS:HD2	1:F:284:ASP:C	2.38	0.48
1:A:171:THR:HG22	1:A:175:GLU:HG2	1.96	0.48
1:B:213:SER:HB3	3:B:602:GTP:O2'	2.14	0.48
1:C:209:HIS:HD2	1:C:446:LYS:HB2	1.74	0.48
1:C:286:ILE:HG21	1:C:291:LEU:HD12	1.94	0.48
1:E:107:LEU:HB2	1:E:126:LYS:HG2	1.95	0.48
1:F:77:GLY:C	1:F:78:TYR:CD2	2.88	0.48
1:E:265:ARG:O	1:E:267:GLY:N	2.47	0.48
1:E:398:THR:O	1:E:401:TYR:N	2.45	0.48
4:F:605:NAI:O1N	4:F:605:NAI:O1A	2.32	0.48
1:E:456:THR:HG21	1:F:396:ARG:NE	2.29	0.48
1:F:374:ASN:HB2	4:F:605:NAI:H5N	1.95	0.48
1:A:346:GLU:OE1	1:A:351:PRO:HD2	2.14	0.48
4:A:604:NAI:N7N	1:B:86:ARG:NH1	2.61	0.48
2:B:601:GLU:HA	4:B:603:NAI:C4N	2.43	0.48
1:D:3:ARG:NH1	1:D:4:GLU:CG	2.70	0.48
1:D:115:CYS:SG	1:D:378:VAL:HG11	2.54	0.48
1:A:82:HIS:CG	1:A:109:SER:HA	2.49	0.47
1:A:222:GLY:HA3	1:A:373:LEU:HD12	1.95	0.47
1:D:420:LYS:NZ	1:F:428:ILE:HG12	2.29	0.47
1:E:115:CYS:SG	1:E:378:VAL:HG11	2.54	0.47
1:A:432:PRO:HB3	1:A:436:PHE:CD2	2.49	0.47
4:A:604:NAI:H8A	4:A:604:NAI:H2B	1.64	0.47
1:A:148:PHE:CE2	1:A:152:LEU:HD11	2.50	0.47
1:A:247:PHE:CE1	1:A:263:LEU:HB2	2.49	0.47
1:A:398:THR:O	1:A:401:TYR:N	2.43	0.47
1:B:382:TYR:CZ	1:B:386:LEU:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:TYR:CE1	1:B:459:ARG:HG3	2.49	0.47
1:E:86:ARG:HG3	4:F:603:NAI:H62A	1.80	0.47
1:E:247:PHE:HA	1:E:321:ILE:O	2.14	0.47
1:E:77:GLY:C	1:E:78:TYR:CD2	2.89	0.47
1:E:90:LYS:HD2	1:E:164:VAL:O	2.15	0.47
1:E:159:GLY:HA2	1:E:183:TYR:CE2	2.50	0.47
1:E:186:THR:OG1	1:E:187:ILE:N	2.45	0.47
1:F:172:GLY:N	1:F:175:GLU:OE2	2.42	0.47
1:A:239:THR:HG21	1:A:244:ASP:OD2	2.14	0.47
1:B:38:GLU:HG3	1:B:40:GLN:CB	2.44	0.47
1:D:14:GLU:HA	1:D:53:LYS:HE3	1.96	0.47
1:D:294:PHE:HD1	1:D:298:HIS:ND1	2.11	0.47
1:E:119:ASP:C	1:F:396:ARG:HH12	2.21	0.47
1:F:247:PHE:C	1:F:247:PHE:CD2	2.92	0.47
1:A:177:SER:HB2	1:A:202:PRO:HG2	1.96	0.47
1:B:169:MET:HA	4:B:603:NAI:O1A	2.15	0.47
1:B:246:THR:HG22	1:B:269:LYS:CE	2.45	0.47
1:C:166:ALA:HB1	1:C:167:PRO:HD2	1.95	0.47
1:E:38:GLU:HB3	1:E:40:GLN:H	1.78	0.47
1:A:67:ARG:HD3	1:A:73:GLU:OE1	2.15	0.47
1:A:265:ARG:O	1:A:267:GLY:N	2.46	0.47
1:A:274:GLY:O	1:A:275:GLU:HG3	2.14	0.47
1:B:126:LYS:HZ1	2:B:601:GLU:N	2.13	0.47
1:B:159:GLY:HA2	1:B:183:TYR:CE2	2.49	0.47
1:B:303:GLY:H	1:B:309:ILE:HD12	1.80	0.47
1:B:432:PRO:HB3	1:B:436:PHE:CD2	2.49	0.47
1:D:172:GLY:N	1:D:175:GLU:OE2	2.40	0.47
1:D:213:SER:HB2	1:D:262:TYR:HE2	1.80	0.47
1:D:239:THR:HG21	1:D:244:ASP:OD2	2.15	0.47
1:D:247:PHE:HA	1:D:321:ILE:O	2.15	0.47
1:E:167:PRO:HA	1:E:176:MET:HE3	1.95	0.47
1:E:471:TYR:CD2	1:E:471:TYR:N	2.83	0.47
1:F:23:ILE:CG2	1:F:471:TYR:HD1	2.27	0.47
1:F:369:PRO:HB3	1:F:478:ARG:HA	1.97	0.47
1:F:470:LYS:HG3	1:F:471:TYR:CD2	2.50	0.47
1:A:429:PRO:O	1:C:416:SER:HB3	2.15	0.47
1:C:67:ARG:NH1	1:C:136:TYR:CE2	2.83	0.47
1:C:186:THR:HG22	1:D:150:MET:HE1	1.96	0.47
1:E:353:THR:HB	1:E:354:PRO:HD2	1.97	0.47
1:E:456:THR:HG21	1:F:396:ARG:NH2	2.30	0.47
1:C:247:PHE:C	1:C:247:PHE:CD2	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:495:GLU:O	1:F:205:GLN:CD	2.58	0.47
4:E:603:NAI:O1N	4:E:603:NAI:H2D	2.15	0.47
1:F:159:GLY:HA2	1:F:183:TYR:CE2	2.50	0.47
1:F:465:MET:O	1:F:469:MET:HG2	2.15	0.47
1:A:57:HIS:CE1	1:A:84:GLN:HE22	2.33	0.47
1:B:183:TYR:HD1	1:B:183:TYR:O	1.98	0.47
1:C:331:LEU:HD23	1:C:360:PHE:HZ	1.80	0.47
1:D:67:ARG:NH1	1:D:136:TYR:CE2	2.83	0.47
1:F:294:PHE:HD1	1:F:298:HIS:ND1	2.12	0.47
1:B:209:HIS:CD2	1:B:446:LYS:HB2	2.50	0.46
1:C:78:TYR:HE1	1:C:101:VAL:HB	1.79	0.46
1:C:432:PRO:HB3	1:C:436:PHE:CD2	2.50	0.46
1:D:39:GLU:O	1:D:43:ASN:ND2	2.48	0.46
1:D:471:TYR:CD2	1:D:471:TYR:N	2.83	0.46
1:E:177:SER:HB2	1:E:202:PRO:HG2	1.97	0.46
1:B:172:GLY:N	1:B:175:GLU:OE2	2.39	0.46
1:B:401:TYR:HE2	1:C:447:ASP:CB	2.28	0.46
1:B:77:GLY:C	1:B:78:TYR:CD2	2.88	0.46
1:C:196:ALA:HB2	1:C:388:ASN:HB2	1.97	0.46
1:C:357:ASP:OD2	1:C:478:ARG:NE	2.34	0.46
1:C:398:THR:O	1:C:401:TYR:N	2.46	0.46
1:D:150:MET:HE1	1:D:186:THR:HG21	1.97	0.46
1:D:432:PRO:HB3	1:D:436:PHE:CD2	2.50	0.46
1:F:209:HIS:HE1	3:F:604:GTP:H5"	1.80	0.46
1:A:146:ARG:NH1	1:A:182:THR:HG22	2.25	0.46
1:C:44:ARG:HA	1:C:44:ARG:HD3	1.37	0.46
1:C:78:TYR:CE1	1:C:101:VAL:HB	2.50	0.46
1:C:265:ARG:O	1:C:267:GLY:N	2.46	0.46
1:D:353:THR:HB	1:D:354:PRO:HD2	1.98	0.46
1:E:317:VAL:C	1:E:340:LYS:HG3	2.40	0.46
1:F:67:ARG:NH1	1:F:136:TYR:CE2	2.83	0.46
1:A:432:PRO:HB3	1:A:436:PHE:HD2	1.81	0.46
1:B:67:ARG:HD3	1:B:73:GLU:OE1	2.15	0.46
1:B:470:LYS:HB3	1:B:471:TYR:HD2	1.79	0.46
1:C:146:ARG:HH11	1:C:182:THR:CG2	2.26	0.46
1:C:265:ARG:C	1:C:267:GLY:H	2.24	0.46
1:D:10:PHE:HE1	1:D:53:LYS:HZ2	1.58	0.46
1:D:294:PHE:CD1	1:D:298:HIS:ND1	2.84	0.46
1:D:369:PRO:HB3	1:D:478:ARG:HA	1.98	0.46
1:E:247:PHE:CE1	1:E:263:LEU:HD12	2.50	0.46
1:E:318:ASP:HA	1:E:340:LYS:CG	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:TRP:CG	1:F:310:TYR:HD2	2.33	0.46
1:B:281:TRP:CG	1:B:310:TYR:HD2	2.33	0.46
1:C:255:VAL:HG23	4:C:604:NAI:O2N	2.15	0.46
1:C:336:ALA:HB3	1:C:359:ILE:HD12	1.97	0.46
1:D:82:HIS:CG	1:D:109:SER:HA	2.50	0.46
1:E:67:ARG:NH1	1:E:136:TYR:CE2	2.83	0.46
1:E:455:TYR:HH	1:F:399:PHE:HD2	1.64	0.46
1:B:303:GLY:H	1:B:309:ILE:CD1	2.28	0.46
1:C:172:GLY:N	1:C:175:GLU:OE2	2.42	0.46
1:C:280:ILE:HG22	1:C:309:ILE:HD13	1.97	0.46
1:D:400:LYS:O	1:D:400:LYS:HG2	2.15	0.46
1:D:433:THR:HG23	1:E:412:SER:HA	1.97	0.46
1:F:323:ILE:HG12	1:F:345:ALA:HB3	1.97	0.46
1:C:107:LEU:HB2	1:C:126:LYS:HG2	1.97	0.46
1:D:167:PRO:CA	1:D:176:MET:HE3	2.46	0.46
1:A:24:VAL:O	1:A:27:LYS:N	2.49	0.46
1:B:275:GLU:HG3	4:B:603:NAI:H1B	1.97	0.46
1:B:353:THR:HB	1:B:354:PRO:HD2	1.97	0.46
1:B:420:LYS:HG2	1:B:421:PHE:CE1	2.51	0.46
1:C:28:LEU:HD13	1:C:490:PHE:CD2	2.50	0.46
1:E:82:HIS:CG	1:E:109:SER:HA	2.50	0.46
1:E:336:ALA:HB3	1:E:359:ILE:HD12	1.98	0.46
1:A:150:MET:CE	1:A:186:THR:HG21	2.46	0.46
1:A:375:ALA:O	1:A:379:THR:OG1	2.24	0.46
1:B:422:GLY:C	1:B:424:HIS:H	2.23	0.46
1:B:432:PRO:HB3	1:B:436:PHE:HD2	1.81	0.46
1:C:23:ILE:HG22	1:C:471:TYR:CD1	2.51	0.46
1:F:48:ILE:O	1:F:52:ILE:HG13	2.16	0.46
1:F:166:ALA:HB1	1:F:167:PRO:HD2	1.98	0.46
1:A:77:GLY:O	1:A:78:TYR:HD2	1.99	0.45
1:A:471:TYR:N	1:A:471:TYR:CD2	2.84	0.45
1:C:82:HIS:CG	1:C:109:SER:HA	2.51	0.45
1:D:53:LYS:O	1:D:53:LYS:HD3	2.16	0.45
1:D:265:ARG:C	1:D:267:GLY:H	2.24	0.45
1:D:420:LYS:HE2	1:F:427:THR:O	2.16	0.45
1:E:241:GLY:O	1:E:245:LYS:NZ	2.48	0.45
1:E:294:PHE:CE2	1:E:304:PHE:HA	2.51	0.45
1:B:67:ARG:NH1	1:B:136:TYR:CE2	2.84	0.45
1:B:336:ALA:HB3	1:B:359:ILE:HD12	1.98	0.45
1:C:17:PHE:CE2	1:C:486:ILE:HG12	2.50	0.45
1:C:302:LEU:HD22	1:C:309:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:ILE:HG12	1:E:345:ALA:HB3	1.99	0.45
1:E:369:PRO:HB3	1:E:478:ARG:HA	1.98	0.45
1:A:96:SER:O	1:A:130:LYS:HA	2.17	0.45
1:A:247:PHE:C	1:A:247:PHE:CD2	2.94	0.45
1:B:154:LYS:HD2	1:F:189:HIS:CG	2.51	0.45
1:E:67:ARG:HD3	1:E:73:GLU:OE1	2.16	0.45
1:E:247:PHE:HD2	1:E:247:PHE:O	1.99	0.45
1:F:208:ILE:HG13	1:F:445:GLU:OE2	2.16	0.45
1:A:192:ILE:CG1	1:A:391:HIS:HE1	2.29	0.45
1:C:323:ILE:HG12	1:C:345:ALA:HB3	1.99	0.45
1:D:191:ASP:HB3	1:D:194:ALA:HB2	1.98	0.45
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.81	0.45
1:E:247:PHE:CD1	1:E:263:LEU:HD12	2.52	0.45
1:F:183:TYR:HD1	1:F:183:TYR:O	2.00	0.45
1:F:353:THR:HB	1:F:354:PRO:HD2	1.98	0.45
2:F:602:GLU:HA	4:F:605:NAI:H4N	1.99	0.45
1:A:382:TYR:O	1:A:386:LEU:HG	2.17	0.45
1:B:57:HIS:HA	1:E:60:SER:O	2.17	0.45
1:B:209:HIS:HD2	1:B:446:LYS:HA	1.82	0.45
1:D:166:ALA:HB1	1:D:167:PRO:HD2	1.99	0.45
1:D:281:TRP:HB2	1:D:310:TYR:HB2	1.98	0.45
1:A:396:ARG:NE	1:B:456:THR:HG21	2.32	0.45
1:B:48:ILE:O	1:B:52:ILE:HG13	2.17	0.45
1:C:150:MET:CE	1:D:186:THR:HG22	2.47	0.45
1:C:167:PRO:HA	1:C:176:MET:HE3	1.97	0.45
1:C:185:SER:O	1:D:154:LYS:HD3	2.17	0.45
1:C:432:PRO:HB3	1:C:436:PHE:HD2	1.82	0.45
1:D:323:ILE:HG12	1:D:345:ALA:HB3	1.98	0.45
1:D:403:ARG:HB2	1:D:441:SER:HA	1.99	0.45
1:D:456:THR:HG21	1:E:396:ARG:HH21	1.82	0.45
1:F:82:HIS:CG	1:F:109:SER:HA	2.52	0.45
1:F:90:LYS:HD2	1:F:164:VAL:O	2.17	0.45
1:A:241:GLY:O	1:A:245:LYS:NZ	2.44	0.45
1:A:491:ARG:HE	4:C:603:NAI:H2B	1.82	0.45
1:D:24:VAL:O	1:D:27:LYS:N	2.50	0.45
1:D:252:PHE:HB3	1:D:275:GLU:OE2	2.16	0.45
1:E:166:ALA:HB1	1:E:167:PRO:HD2	1.99	0.45
1:E:253:GLY:HA3	4:E:603:NAI:O5B	2.17	0.45
1:E:500:PHE:HA	1:F:146:ARG:CZ	2.47	0.45
3:E:602:GTP:O5'	3:E:602:GTP:H8	2.00	0.45
1:A:48:ILE:HG21	1:A:490:PHE:HD1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ALA:HB1	1:A:167:PRO:HD2	1.98	0.45
1:A:276:SER:OG	4:A:603:NAI:O2B	2.22	0.45
1:A:369:PRO:HB3	1:A:478:ARG:HA	1.98	0.45
1:D:281:TRP:CG	1:D:310:TYR:HD2	2.35	0.45
1:E:444:SER:OG	1:E:447:ASP:OD1	2.26	0.45
1:F:65:ILE:HG22	1:F:66:ARG:C	2.42	0.45
3:A:602:GTP:O1G	3:A:602:GTP:H2'	2.16	0.45
1:B:205:GLN:OE1	1:C:495:GLU:O	2.35	0.45
1:D:57:HIS:CE1	1:D:84:GLN:HE22	2.35	0.45
1:E:57:HIS:CE1	1:E:84:GLN:HE22	2.35	0.45
1:F:262:TYR:OH	3:F:604:GTP:O2G	2.28	0.45
1:F:399:PHE:C	1:F:401:TYR:H	2.24	0.45
1:A:294:PHE:CE2	1:A:304:PHE:HA	2.52	0.44
1:B:209:HIS:CD2	1:B:446:LYS:HA	2.52	0.44
1:B:444:SER:OG	1:B:447:ASP:OD1	2.24	0.44
1:B:498:VAL:HB	1:E:72:TRP:CH2	2.53	0.44
1:C:18:ASP:OD1	1:C:53:LYS:HD3	2.17	0.44
1:E:265:ARG:C	1:E:267:GLY:H	2.25	0.44
1:F:69:ASP:OD1	1:F:71:SER:OG	2.25	0.44
1:F:244:ASP:OD1	1:F:244:ASP:N	2.50	0.44
1:A:36:GLU:O	1:A:40:GLN:HB3	2.18	0.44
1:A:292:GLU:OE2	3:A:602:GTP:N1	2.48	0.44
1:F:265:ARG:O	1:F:267:GLY:N	2.46	0.44
1:A:213:SER:HB3	3:A:602:GTP:O2'	2.17	0.44
1:A:399:PHE:C	1:A:401:TYR:H	2.25	0.44
1:C:199:THR:HA	1:C:384:GLU:OE1	2.16	0.44
1:C:294:PHE:CE2	1:C:304:PHE:HA	2.52	0.44
1:F:236:LEU:O	1:F:342:LYS:HE2	2.17	0.44
1:F:265:ARG:C	1:F:267:GLY:H	2.26	0.44
1:F:346:GLU:OE1	1:F:351:PRO:HD2	2.17	0.44
1:A:204:SER:HB3	1:B:491:ARG:HG2	1.99	0.44
1:A:209:HIS:HE1	3:A:602:GTP:H5''	1.82	0.44
1:A:281:TRP:CZ2	1:A:283:PRO:HG3	2.52	0.44
1:A:396:ARG:HE	1:B:456:THR:HG21	1.81	0.44
1:B:186:THR:OG1	1:B:187:ILE:N	2.44	0.44
1:B:215:THR:CB	4:B:603:NAI:H42N	2.46	0.44
1:B:388:ASN:N	1:B:388:ASN:ND2	2.66	0.44
1:B:388:ASN:HD22	1:B:388:ASN:H	1.66	0.44
1:B:471:TYR:N	1:B:471:TYR:CD2	2.84	0.44
1:E:183:TYR:HD1	1:E:183:TYR:O	1.99	0.44
1:E:317:VAL:O	1:E:340:LYS:CE	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:ARG:NH1	1:F:143:LYS:HE2	2.32	0.44
1:F:126:LYS:HG3	1:F:127:ALA:H	1.82	0.44
1:F:315:LEU:HD22	1:F:331:LEU:HD11	1.98	0.44
1:A:39:GLU:OE1	1:A:42:ARG:HD2	2.17	0.44
1:A:213:SER:HB2	1:A:262:TYR:HE2	1.83	0.44
1:A:261:ARG:HH12	3:A:602:GTP:PG	2.40	0.44
1:A:455:TYR:O	1:A:459:ARG:N	2.36	0.44
1:B:244:ASP:OD1	1:B:244:ASP:N	2.51	0.44
1:B:369:PRO:HB3	1:B:478:ARG:HA	1.98	0.44
1:E:456:THR:HG21	1:F:396:ARG:HE	1.81	0.44
1:F:94:ARG:HG3	1:F:169:MET:HB2	2.00	0.44
1:F:150:MET:CE	1:F:186:THR:HG21	2.48	0.44
1:B:82:HIS:CG	1:B:109:SER:HA	2.52	0.44
2:B:601:GLU:HA	4:B:603:NAI:C3N	2.48	0.44
1:D:17:PHE:CE2	1:D:486:ILE:HG12	2.52	0.44
1:D:210:GLY:O	1:D:214:ALA:HB2	2.17	0.44
1:D:401:TYR:CE2	1:F:443:ALA:CA	2.99	0.44
4:A:604:NAI:H71N	1:B:86:ARG:HH11	1.65	0.44
1:B:86:ARG:HD3	1:B:86:ARG:HH11	1.64	0.44
1:B:171:THR:HG22	1:B:175:GLU:HG2	2.00	0.44
1:B:208:ILE:HA	1:B:445:GLU:OE2	2.18	0.44
1:B:247:PHE:CE1	1:B:263:LEU:HB2	2.53	0.44
1:B:400:LYS:O	1:B:400:LYS:HG2	2.17	0.44
1:B:410:LEU:HG	1:B:430:ILE:HG22	2.00	0.44
1:E:172:GLY:O	1:E:176:MET:HG2	2.18	0.44
1:E:429:PRO:HG2	1:F:419:ARG:NH2	2.33	0.44
2:E:601:GLU:HA	4:E:603:NAI:C3N	2.48	0.44
1:F:209:HIS:CD2	1:F:446:LYS:HA	2.52	0.44
1:F:215:THR:HG21	4:F:605:NAI:N7N	2.32	0.44
1:A:86:ARG:NH2	4:C:603:NAI:N3A	2.66	0.44
1:A:358:LYS:NZ	1:A:361:LEU:HD13	2.33	0.44
1:A:402:GLU:O	1:A:406:ASN:OD1	2.36	0.44
1:B:146:ARG:NH1	1:B:182:THR:HG22	2.27	0.44
1:B:326:ALA:HB1	4:B:603:NAI:C6A	2.48	0.44
1:C:208:ILE:HA	1:C:445:GLU:OE2	2.18	0.44
1:C:215:THR:OG1	4:C:604:NAI:H42N	2.18	0.44
1:C:353:THR:HB	1:C:354:PRO:HD2	1.99	0.44
1:D:195:HIS:CD2	4:F:601:NAI:O7N	2.71	0.44
1:E:252:PHE:CB	1:E:275:GLU:OE2	2.65	0.44
1:F:199:THR:HA	1:F:384:GLU:OE1	2.18	0.44
1:A:498:VAL:HB	1:D:72:TRP:CZ2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LYS:HZ1	2:C:601:GLU:N	2.16	0.44
1:C:281:TRP:CG	1:C:310:TYR:HD2	2.36	0.44
1:D:48:ILE:HG21	1:D:490:PHE:HD1	1.83	0.44
1:D:172:GLY:O	1:D:176:MET:HG2	2.18	0.44
1:F:339:VAL:O	1:F:339:VAL:HG12	2.17	0.44
1:B:209:HIS:HD2	1:B:446:LYS:HB2	1.82	0.43
1:B:323:ILE:HG12	1:B:345:ALA:HB3	1.99	0.43
1:C:90:LYS:HD2	1:C:164:VAL:O	2.18	0.43
1:D:48:ILE:O	1:D:52:ILE:HG13	2.17	0.43
1:D:150:MET:HE2	1:D:186:THR:HG21	1.99	0.43
1:E:346:GLU:OE1	1:E:351:PRO:HD2	2.18	0.43
1:E:456:THR:HG21	1:F:396:ARG:HH21	1.83	0.43
1:F:209:HIS:HD2	1:F:446:LYS:HA	1.82	0.43
1:A:244:ASP:OD1	1:A:244:ASP:N	2.51	0.43
1:A:432:PRO:HA	1:C:412:SER:OG	2.18	0.43
1:B:58:VAL:O	1:E:59:LEU:HA	2.18	0.43
2:B:601:GLU:HA	4:B:603:NAI:H4N	1.99	0.43
1:D:69:ASP:OD1	1:D:71:SER:OG	2.25	0.43
1:D:372:TYR:OH	1:D:461:ALA:HB2	2.18	0.43
1:E:17:PHE:CE2	1:E:486:ILE:HG12	2.53	0.43
1:A:369:PRO:HD3	1:A:477:LEU:HB2	2.00	0.43
1:C:369:PRO:HB3	1:C:478:ARG:HA	1.99	0.43
1:B:57:HIS:CE1	1:B:84:GLN:HE22	2.36	0.43
1:B:61:LEU:HD21	1:E:57:HIS:CD2	2.53	0.43
1:B:126:LYS:HG3	1:B:127:ALA:H	1.83	0.43
1:B:148:PHE:CE2	1:B:152:LEU:HD11	2.53	0.43
1:C:281:TRP:CZ2	1:C:283:PRO:HG3	2.54	0.43
1:E:432:PRO:HB3	1:E:436:PHE:CD2	2.54	0.43
1:F:403:ARG:HB2	1:F:441:SER:HA	2.00	0.43
1:A:208:ILE:HA	1:A:445:GLU:OE2	2.19	0.43
1:B:91:GLY:O	1:B:165:PRO:HA	2.19	0.43
1:C:274:GLY:O	1:C:275:GLU:HG2	2.18	0.43
1:C:372:TYR:OH	1:C:461:ALA:HB2	2.18	0.43
1:D:90:LYS:HD2	1:D:164:VAL:O	2.19	0.43
1:D:96:SER:O	1:D:130:LYS:HA	2.18	0.43
1:D:275:GLU:C	1:D:277:ASP:H	2.27	0.43
4:D:604:NAI:H3D	1:E:387:LYS:HE2	2.01	0.43
1:E:148:PHE:CE2	1:E:152:LEU:HD11	2.54	0.43
1:F:146:ARG:HH11	1:F:182:THR:CG2	2.27	0.43
1:A:409:LEU:CD2	1:C:409:LEU:HD21	2.44	0.43
1:B:294:PHE:CE2	1:B:304:PHE:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ASP:HA	1:B:342:LYS:CD	2.48	0.43
1:B:470:LYS:HG2	1:B:471:TYR:CE2	2.54	0.43
1:D:169:MET:HA	4:D:603:NAI:O1A	2.18	0.43
1:E:220:PHE:HD1	1:E:263:LEU:HD23	1.83	0.43
1:B:392:VAL:HG22	1:C:386:LEU:CD1	2.47	0.43
1:C:27:LYS:HD2	1:C:471:TYR:OH	2.19	0.43
1:D:412:SER:HA	1:F:433:THR:HG23	2.00	0.43
1:E:244:ASP:OD1	1:E:244:ASP:N	2.49	0.43
1:E:357:ASP:OD2	1:E:478:ARG:NE	2.39	0.43
1:F:28:LEU:HD13	1:F:490:PHE:CD2	2.54	0.43
1:F:67:ARG:HD3	1:F:73:GLU:OE1	2.18	0.43
1:F:196:ALA:HB2	1:F:388:ASN:HB2	2.01	0.43
1:A:17:PHE:CE2	1:A:486:ILE:HG12	2.54	0.43
1:A:206:GLY:CA	4:A:604:NAI:H3D	2.47	0.43
1:A:491:ARG:HG2	4:C:603:NAI:O2B	2.18	0.43
1:B:48:ILE:HG21	1:B:490:PHE:HD1	1.83	0.43
1:B:96:SER:O	1:B:130:LYS:HA	2.19	0.43
1:B:265:ARG:O	1:B:267:GLY:N	2.47	0.43
1:C:48:ILE:O	1:C:52:ILE:HG13	2.19	0.43
1:C:401:TYR:C	1:C:403:ARG:N	2.76	0.43
1:C:410:LEU:HG	1:C:430:ILE:HG22	2.00	0.43
1:D:10:PHE:CE1	1:D:53:LYS:NZ	2.84	0.43
1:F:402:GLU:O	1:F:406:ASN:OD1	2.36	0.43
1:A:172:GLY:N	1:A:175:GLU:OE2	2.40	0.43
1:A:465:MET:O	1:A:469:MET:HG2	2.19	0.43
1:B:78:TYR:HD2	1:B:78:TYR:N	2.16	0.43
1:C:154:LYS:HB3	1:D:189:HIS:NE2	2.34	0.43
1:C:382:TYR:O	1:C:386:LEU:HG	2.19	0.43
1:D:94:ARG:O	1:D:128:GLY:HA2	2.19	0.43
1:D:433:THR:N	1:E:412:SER:OG	2.48	0.43
1:E:210:GLY:O	1:E:214:ALA:HB2	2.19	0.43
1:B:68:ASP:OD2	1:B:137:THR:OG1	2.26	0.43
1:B:315:LEU:HD13	1:B:331:LEU:HD12	2.01	0.43
1:B:398:THR:O	1:B:401:TYR:N	2.46	0.43
1:C:213:SER:HB2	1:C:262:TYR:HE2	1.84	0.43
1:D:29:VAL:HG13	1:D:41:LYS:HB2	2.00	0.43
1:D:160:PRO:HD3	1:D:183:TYR:CE2	2.54	0.43
1:D:399:PHE:C	1:D:401:TYR:H	2.26	0.43
1:E:133:PRO:HG2	1:E:170:SER:HB3	2.00	0.43
1:E:355:GLU:OE1	1:E:358:LYS:HD2	2.19	0.43
1:F:57:HIS:CE1	1:F:84:GLN:HE22	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:SER:HB2	1:F:262:TYR:HE2	1.84	0.43
1:F:294:PHE:CD1	1:F:298:HIS:ND1	2.86	0.43
1:A:353:THR:HB	1:A:354:PRO:HD2	2.00	0.42
1:B:57:HIS:CD2	1:E:61:LEU:HD21	2.54	0.42
1:B:166:ALA:HB1	1:B:167:PRO:HD2	2.01	0.42
1:B:422:GLY:C	1:B:424:HIS:N	2.75	0.42
1:C:96:SER:O	1:C:130:LYS:HA	2.19	0.42
1:D:247:PHE:CE1	1:D:263:LEU:HD12	2.54	0.42
1:D:281:TRP:CZ2	1:D:283:PRO:HG3	2.54	0.42
4:D:604:NAI:H4N	1:E:195:HIS:NE2	2.33	0.42
1:E:199:THR:HA	1:E:384:GLU:OE1	2.19	0.42
1:E:211:ARG:HA	1:E:380:VAL:HG11	2.01	0.42
1:F:213:SER:HB3	3:F:604:GTP:O2'	2.20	0.42
1:F:281:TRP:CG	1:F:310:TYR:CD2	3.07	0.42
1:A:32:LEU:O	1:A:33:LYS:C	2.62	0.42
1:C:247:PHE:CE1	1:C:263:LEU:HB2	2.54	0.42
1:C:281:TRP:HB2	1:C:310:TYR:HB2	2.00	0.42
1:D:209:HIS:CD2	1:D:446:LYS:HA	2.54	0.42
1:D:410:LEU:HG	1:D:430:ILE:HG22	1.99	0.42
1:D:465:MET:O	1:D:469:MET:HG2	2.18	0.42
1:E:65:ILE:HD13	1:E:144:ILE:CG1	2.50	0.42
1:F:292:GLU:CD	3:F:604:GTP:HN21	2.28	0.42
1:F:339:VAL:O	1:F:340:LYS:C	2.62	0.42
1:A:212:ILE:HG22	1:A:258:HIS:HE1	1.85	0.42
1:B:363:ARG:HE	1:B:363:ARG:HB3	1.69	0.42
1:C:32:LEU:O	1:C:33:LYS:C	2.62	0.42
1:C:154:LYS:HD2	1:D:189:HIS:ND1	2.35	0.42
1:C:369:PRO:HD3	1:C:477:LEU:HB2	2.01	0.42
1:D:215:THR:CB	4:D:603:NAI:H42N	2.48	0.42
1:E:208:ILE:HA	1:E:445:GLU:OE2	2.19	0.42
1:F:34:THR:CG2	1:F:44:ARG:HH22	2.25	0.42
1:A:265:ARG:C	1:A:267:GLY:H	2.26	0.42
1:B:401:TYR:CE2	1:C:447:ASP:HB3	2.54	0.42
1:D:247:PHE:CE2	1:D:270:CYS:CB	2.97	0.42
1:E:281:TRP:CG	1:E:310:TYR:HD2	2.37	0.42
1:F:96:SER:O	1:F:130:LYS:HA	2.20	0.42
1:A:126:LYS:HG3	1:A:127:ALA:H	1.84	0.42
1:A:407:TYR:HH	1:A:437:GLN:HE22	1.59	0.42
1:C:8:ASN:ND2	1:C:102:ASP:OD2	2.45	0.42
1:D:10:PHE:CE2	1:D:105:LYS:HE2	2.54	0.42
1:D:119:ASP:CG	4:D:604:NAI:H2B	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ILE:HG21	1:E:490:PHE:HD1	1.83	0.42
1:E:69:ASP:OD1	1:E:71:SER:OG	2.23	0.42
1:E:94:ARG:O	1:E:128:GLY:HA2	2.19	0.42
1:E:247:PHE:HE2	1:E:270:CYS:HB2	1.82	0.42
1:E:433:THR:HG23	1:F:412:SER:HA	2.01	0.42
1:F:17:PHE:CE2	1:F:486:ILE:HG12	2.54	0.42
1:F:209:HIS:HD2	1:F:446:LYS:CA	2.33	0.42
1:F:247:PHE:HE1	1:F:263:LEU:HB2	1.84	0.42
1:F:294:PHE:HE2	1:F:304:PHE:HA	1.81	0.42
1:F:372:TYR:OH	1:F:461:ALA:HB2	2.19	0.42
1:A:281:TRP:CG	1:A:310:TYR:HD2	2.37	0.42
1:B:213:SER:HB2	1:B:262:TYR:HE2	1.83	0.42
1:C:94:ARG:O	1:C:128:GLY:HA2	2.20	0.42
1:C:159:GLY:HA2	1:C:183:TYR:CE2	2.55	0.42
1:C:241:GLY:O	1:C:245:LYS:NZ	2.45	0.42
1:E:208:ILE:HG13	1:E:445:GLU:OE2	2.20	0.42
1:B:295:LYS:O	1:B:295:LYS:HG3	2.19	0.42
1:C:2:ASP:CG	1:C:3:ARG:H	2.26	0.42
1:C:60:SER:O	1:F:57:HIS:HA	2.20	0.42
1:D:159:GLY:HA2	1:D:183:TYR:CE2	2.55	0.42
1:D:265:ARG:O	1:D:267:GLY:N	2.46	0.42
1:E:24:VAL:O	1:E:27:LYS:N	2.52	0.42
1:E:331:LEU:HD23	1:E:360:PHE:HZ	1.82	0.42
1:A:133:PRO:HG2	1:A:170:SER:HB3	2.01	0.42
1:A:169:MET:HE2	1:A:169:MET:HB3	1.98	0.42
1:A:238:MET:HE1	1:A:343:ILE:HG13	2.01	0.42
1:A:403:ARG:HD2	1:A:441:SER:OG	2.19	0.42
1:A:462:ARG:O	1:A:465:MET:N	2.53	0.42
1:B:10:PHE:CD2	1:B:105:LYS:HE2	2.54	0.42
1:B:403:ARG:O	1:B:406:ASN:N	2.53	0.42
1:C:186:THR:OG1	1:C:187:ILE:N	2.44	0.42
1:C:210:GLY:O	1:C:214:ALA:HB2	2.20	0.42
1:D:126:LYS:HZ1	2:D:601:GLU:N	2.17	0.42
1:D:209:HIS:HD2	1:D:446:LYS:CA	2.31	0.42
1:F:2:ASP:OD1	1:F:3:ARG:N	2.42	0.42
1:A:160:PRO:HD3	1:A:183:TYR:CE2	2.55	0.42
1:A:337:PRO:HG3	1:A:359:ILE:HD13	2.00	0.42
1:A:396:ARG:CZ	1:B:456:THR:HG21	2.50	0.42
1:A:409:LEU:HD13	1:C:409:LEU:HD11	2.01	0.42
1:B:210:GLY:O	1:B:214:ALA:HB2	2.20	0.42
1:C:247:PHE:HB3	1:C:321:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:GLY:O	1:D:275:GLU:HG3	2.20	0.42
1:D:382:TYR:O	1:D:386:LEU:HG	2.20	0.42
1:E:400:LYS:O	1:E:400:LYS:HG2	2.20	0.42
1:F:281:TRP:CZ2	1:F:283:PRO:HG3	2.54	0.42
1:A:281:TRP:HB2	1:A:310:TYR:HB2	2.02	0.42
1:A:391:HIS:O	1:B:382:TYR:OH	2.38	0.42
1:B:78:TYR:CD2	1:B:78:TYR:N	2.88	0.42
1:B:281:TRP:CZ2	1:B:283:PRO:HG3	2.55	0.42
1:C:89:CYS:HB3	1:C:125:ALA:HB2	2.02	0.42
1:C:172:GLY:O	1:C:176:MET:HG2	2.19	0.42
1:D:208:ILE:HA	1:D:445:GLU:OE2	2.20	0.42
1:D:493:TYR:O	1:D:498:VAL:HG22	2.20	0.42
1:E:316:GLU:O	1:E:340:LYS:HD2	2.19	0.42
1:F:86:ARG:HD2	4:F:601:NAI:C2N	2.50	0.42
1:F:91:GLY:O	1:F:165:PRO:HA	2.20	0.42
1:F:210:GLY:O	1:F:214:ALA:HB2	2.20	0.42
1:F:363:ARG:HE	1:F:363:ARG:HB3	1.72	0.42
1:F:432:PRO:HB3	1:F:436:PHE:CD2	2.55	0.42
1:A:199:THR:HA	1:A:384:GLU:OE1	2.19	0.41
1:B:172:GLY:O	1:B:176:MET:HG2	2.20	0.41
1:B:265:ARG:C	1:B:267:GLY:H	2.27	0.41
1:B:336:ALA:N	1:B:337:PRO:HD2	2.35	0.41
1:C:148:PHE:CE2	1:C:152:LEU:HD11	2.55	0.41
1:C:338:ARG:O	1:C:340:LYS:HG2	2.20	0.41
1:D:32:LEU:HA	1:D:32:LEU:HD12	1.80	0.41
1:D:346:GLU:OE1	1:D:351:PRO:HD2	2.20	0.41
1:E:27:LYS:O	1:E:30:GLU:HB3	2.20	0.41
1:F:86:ARG:HG3	4:F:601:NAI:H62A	1.84	0.41
1:F:211:ARG:HA	1:F:380:VAL:HG11	2.01	0.41
1:A:20:GLY:O	1:A:24:VAL:HG22	2.20	0.41
1:B:337:PRO:C	1:B:363:ARG:NH1	2.76	0.41
1:B:493:TYR:O	1:B:498:VAL:HG22	2.19	0.41
1:C:143:LYS:HE3	1:F:501:THR:HA	2.02	0.41
1:D:209:HIS:HD2	1:D:446:LYS:CB	2.32	0.41
1:E:91:GLY:O	1:E:165:PRO:HA	2.19	0.41
1:E:281:TRP:CZ2	1:E:283:PRO:HG3	2.54	0.41
1:E:339:VAL:O	1:E:340:LYS:CD	2.52	0.41
1:E:340:LYS:HG2	1:E:341:ALA:HB2	2.02	0.41
1:E:372:TYR:OH	1:E:461:ALA:HB2	2.19	0.41
1:E:403:ARG:NH1	1:E:440:ILE:HG23	2.34	0.41
1:F:78:TYR:CD2	1:F:78:TYR:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ILE:O	1:A:52:ILE:HG13	2.20	0.41
1:A:189:HIS:ND1	1:E:154:LYS:HD2	2.35	0.41
1:B:211:ARG:HA	1:B:380:VAL:HG11	2.02	0.41
1:B:310:TYR:CE2	1:B:317:VAL:HG22	2.54	0.41
1:B:374:ASN:HB2	4:B:603:NAI:H5N	2.02	0.41
1:C:77:GLY:C	1:C:78:TYR:CD2	2.92	0.41
1:C:244:ASP:OD1	1:C:244:ASP:N	2.54	0.41
1:C:400:LYS:HG2	1:C:400:LYS:O	2.20	0.41
1:D:148:PHE:CE2	1:D:152:LEU:HD11	2.55	0.41
1:E:9:PHE:CD1	1:E:12:MET:HE2	2.56	0.41
1:E:459:ARG:NH1	1:E:459:ARG:HG3	2.35	0.41
1:F:65:ILE:HG22	1:F:66:ARG:O	2.19	0.41
1:F:209:HIS:HD2	1:F:446:LYS:CB	2.34	0.41
1:A:94:ARG:HG3	1:A:169:MET:HB2	2.03	0.41
1:A:146:ARG:HH11	1:A:182:THR:CG2	2.26	0.41
1:A:150:MET:HE1	1:E:186:THR:HG22	2.02	0.41
1:A:210:GLY:O	1:A:214:ALA:HB2	2.20	0.41
1:C:91:GLY:O	1:C:165:PRO:HA	2.20	0.41
1:C:150:MET:HE1	1:D:186:THR:HG22	2.01	0.41
1:C:177:SER:HB2	1:C:202:PRO:HG2	2.02	0.41
1:C:211:ARG:HA	1:C:380:VAL:HG11	2.03	0.41
1:D:77:GLY:O	1:D:78:TYR:HD2	2.03	0.41
1:D:387:LYS:HE2	4:F:601:NAI:C5D	2.50	0.41
1:E:5:ASP:HB2	1:E:333:LYS:HE3	2.02	0.41
1:E:382:TYR:O	1:E:386:LEU:HG	2.20	0.41
1:F:41:LYS:O	1:F:45:VAL:HG23	2.20	0.41
1:A:94:ARG:O	1:A:128:GLY:HA2	2.20	0.41
1:B:150:MET:HE2	1:B:186:THR:HG21	2.02	0.41
1:B:211:ARG:NH2	4:B:603:NAI:O7N	2.36	0.41
1:C:65:ILE:HG21	1:C:144:ILE:HG12	2.03	0.41
1:D:37:THR:HG23	1:D:41:LYS:HE3	2.03	0.41
1:D:146:ARG:HH11	1:D:182:THR:CG2	2.25	0.41
1:A:211:ARG:O	1:A:214:ALA:HB3	2.20	0.41
1:A:220:PHE:HD1	1:A:263:LEU:HD23	1.86	0.41
1:A:275:GLU:C	1:A:277:ASP:H	2.28	0.41
1:B:20:GLY:O	1:B:24:VAL:HG22	2.20	0.41
1:B:24:VAL:O	1:B:27:LYS:N	2.54	0.41
1:C:69:ASP:C	1:C:71:SER:H	2.29	0.41
1:D:401:TYR:C	1:D:403:ARG:N	2.75	0.41
1:F:86:ARG:NE	4:F:601:NAI:H62A	2.17	0.41
1:F:337:PRO:HG3	1:F:359:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:433:THR:HG23	1:F:433:THR:H	1.61	0.41
1:A:29:VAL:HG13	1:A:41:LYS:HB2	2.02	0.41
1:B:94:ARG:O	1:B:128:GLY:HA2	2.21	0.41
1:D:20:GLY:O	1:D:24:VAL:HG22	2.21	0.41
1:D:164:VAL:HG13	1:D:197:CYS:C	2.46	0.41
1:E:410:LEU:HG	1:E:430:ILE:HG22	2.03	0.41
1:F:24:VAL:O	1:F:27:LYS:N	2.53	0.41
1:F:69:ASP:C	1:F:71:SER:H	2.29	0.41
1:A:265:ARG:NH2	3:A:602:GTP:PG	2.89	0.41
1:A:448:ILE:HD12	1:C:397:LEU:O	2.21	0.41
1:B:17:PHE:CE2	1:B:486:ILE:HG12	2.55	0.41
1:B:164:VAL:HG13	1:B:197:CYS:C	2.46	0.41
1:B:491:ARG:CZ	1:B:491:ARG:HB2	2.50	0.41
1:C:20:GLY:O	1:C:24:VAL:HG22	2.21	0.41
1:C:169:MET:CG	4:C:604:NAI:H3D	2.51	0.41
1:C:211:ARG:O	1:C:214:ALA:HB3	2.21	0.41
1:D:346:GLU:OE1	1:D:352:THR:OG1	2.24	0.41
1:F:121:PRO:HA	4:F:601:NAI:N6A	2.36	0.41
1:F:406:ASN:ND2	1:F:436:PHE:CZ	2.88	0.41
4:F:601:NAI:H52N	4:F:601:NAI:C6N	2.44	0.41
1:A:91:GLY:O	1:A:165:PRO:HA	2.20	0.41
1:A:150:MET:HE3	1:D:500:PHE:CE2	2.56	0.41
1:A:410:LEU:HG	1:A:430:ILE:HG22	2.02	0.41
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.91	0.41
1:B:133:PRO:HG2	1:B:170:SER:HB3	2.03	0.41
1:B:154:LYS:HB3	1:F:189:HIS:CE1	2.56	0.41
1:B:211:ARG:O	1:B:214:ALA:HB3	2.21	0.41
1:B:320:ASP:HA	1:B:342:LYS:HD2	2.03	0.41
1:C:238:MET:HE1	1:C:343:ILE:HG13	2.03	0.41
1:C:374:ASN:HB2	4:C:604:NAI:C5N	2.51	0.41
1:C:399:PHE:C	1:C:401:TYR:H	2.29	0.41
1:C:407:TYR:HH	1:C:437:GLN:HE22	1.61	0.41
1:D:25:GLU:O	1:D:29:VAL:HG23	2.21	0.41
1:E:96:SER:O	1:E:130:LYS:HA	2.20	0.41
1:E:493:TYR:O	1:E:498:VAL:HG22	2.21	0.41
1:F:25:GLU:CD	1:F:46:ARG:NH1	2.78	0.41
1:F:119:ASP:CG	4:F:601:NAI:H2B	2.46	0.41
1:F:337:PRO:C	1:F:363:ARG:NH1	2.78	0.41
1:F:374:ASN:HB2	4:F:605:NAI:C5N	2.51	0.41
1:B:38:GLU:HB2	1:B:39:GLU:H	1.74	0.41
1:D:27:LYS:O	1:D:30:GLU:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:VAL:HA	1:D:197:CYS:O	2.21	0.41
1:F:211:ARG:O	1:F:214:ALA:HB3	2.21	0.41
1:A:406:ASN:ND2	1:C:409:LEU:HD12	2.37	0.40
1:B:146:ARG:HH11	1:B:182:THR:CG2	2.30	0.40
1:B:339:VAL:C	1:B:341:ALA:H	2.29	0.40
1:B:403:ARG:NH1	1:B:441:SER:OG	2.54	0.40
1:C:29:VAL:HG13	1:C:41:LYS:HB2	2.03	0.40
1:C:43:ASN:HB3	1:C:44:ARG:CZ	2.51	0.40
1:C:189:HIS:CE1	1:D:154:LYS:HB3	2.56	0.40
1:D:91:GLY:O	1:D:165:PRO:HA	2.21	0.40
1:D:253:GLY:HA3	4:D:603:NAI:PA	2.60	0.40
1:D:339:VAL:O	1:D:339:VAL:HG12	2.19	0.40
1:E:20:GLY:O	1:E:24:VAL:HG22	2.21	0.40
1:A:211:ARG:HA	1:A:380:VAL:HG11	2.03	0.40
1:A:246:THR:HB	1:A:271:VAL:CG2	2.51	0.40
1:A:372:TYR:OH	1:A:461:ALA:HB2	2.21	0.40
1:C:45:VAL:HG22	1:C:490:PHE:CZ	2.56	0.40
1:C:154:LYS:HB3	1:D:189:HIS:CE1	2.56	0.40
1:D:131:ILE:HB	1:D:136:TYR:CE1	2.56	0.40
1:D:220:PHE:HD1	1:D:263:LEU:HD23	1.86	0.40
1:D:224:GLU:HA	1:D:227:ILE:HG22	2.03	0.40
1:D:331:LEU:HD23	1:D:360:PHE:HZ	1.85	0.40
1:E:27:LYS:HD2	1:E:471:TYR:OH	2.21	0.40
1:E:61:LEU:N	1:E:77:GLY:O	2.54	0.40
1:E:78:TYR:HD2	1:E:78:TYR:N	2.20	0.40
1:E:211:ARG:O	1:E:214:ALA:HB3	2.21	0.40
1:E:281:TRP:HB2	1:E:310:TYR:HB2	2.02	0.40
1:F:69:ASP:O	1:F:71:SER:N	2.54	0.40
1:F:114:LYS:NZ	1:F:349:ASN:OD1	2.53	0.40
1:F:357:ASP:OD2	1:F:478:ARG:HD2	2.21	0.40
1:F:369:PRO:HD3	1:F:477:LEU:HB2	2.03	0.40
1:A:69:ASP:C	1:A:71:SER:H	2.29	0.40
2:A:601:GLU:CB	4:A:603:NAI:H4N	2.52	0.40
1:B:17:PHE:CD1	1:B:53:LYS:HG2	2.57	0.40
1:B:25:GLU:OE1	1:B:46:ARG:NE	2.54	0.40
1:B:220:PHE:HD1	1:B:263:LEU:HD23	1.86	0.40
1:C:65:ILE:HD13	1:C:144:ILE:CG1	2.52	0.40
1:C:133:PRO:HG2	1:C:170:SER:HB3	2.03	0.40
1:C:339:VAL:O	1:C:339:VAL:HG12	2.21	0.40
1:E:247:PHE:CE1	1:E:263:LEU:HB2	2.53	0.40
1:F:94:ARG:O	1:F:128:GLY:HA2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:432:PRO:HB3	1:F:436:PHE:HD2	1.86	0.40
1:A:111:MET:HE3	1:A:111:MET:HB3	1.95	0.40
1:A:269:LYS:HD2	1:A:284:ASP:C	2.46	0.40
1:A:400:LYS:HG2	1:A:400:LYS:O	2.20	0.40
1:B:89:CYS:HB3	1:B:125:ALA:HB2	2.03	0.40
1:C:470:LYS:CG	1:C:471:TYR:CE2	3.04	0.40
1:D:27:LYS:HD2	1:D:471:TYR:OH	2.21	0.40
1:E:131:ILE:HB	1:E:136:TYR:CE1	2.56	0.40
1:E:455:TYR:CD1	1:E:455:TYR:C	2.99	0.40
1:F:86:ARG:HB3	1:F:121:PRO:O	2.22	0.40
1:F:172:GLY:O	1:F:176:MET:HG2	2.20	0.40
1:F:414:GLN:HG3	1:F:428:ILE:O	2.22	0.40
1:A:134:LYS:HD3	1:A:134:LYS:HA	1.64	0.40
1:A:225:ASN:OD1	1:A:458:GLU:HG2	2.20	0.40
1:B:27:LYS:HD2	1:B:471:TYR:OH	2.22	0.40
1:C:69:ASP:O	1:C:71:SER:N	2.54	0.40
1:C:160:PRO:HD3	1:C:183:TYR:CE2	2.56	0.40
1:C:192:ILE:HG12	1:C:391:HIS:HE1	1.85	0.40
1:E:215:THR:HB	4:E:603:NAI:H42N	2.02	0.40
1:E:399:PHE:C	1:E:401:TYR:H	2.30	0.40
1:F:131:ILE:HB	1:F:136:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/582 (86%)	448 (90%)	42 (8%)	9 (2%)	6	29
1	B	499/582 (86%)	444 (89%)	41 (8%)	14 (3%)	4	21
1	C	499/582 (86%)	448 (90%)	43 (9%)	8 (2%)	7	31
1	D	499/582 (86%)	447 (90%)	40 (8%)	12 (2%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	499/582 (86%)	444 (89%)	43 (9%)	12 (2%)	4	24
1	F	499/582 (86%)	446 (89%)	38 (8%)	15 (3%)	3	20
All	All	2994/3492 (86%)	2677 (89%)	247 (8%)	70 (2%)	5	25

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	HIS
1	A	214	ALA
1	A	340	LYS
1	B	33	LYS
1	B	214	ALA
1	C	214	ALA
1	D	214	ALA
1	D	340	LYS
1	E	214	ALA
1	E	340	LYS
1	F	214	ALA
1	F	340	LYS
1	F	433	THR
1	A	498	VAL
1	B	67	ARG
1	B	340	LYS
1	B	403	ARG
1	B	424	HIS
1	B	498	VAL
1	C	340	LYS
1	C	498	VAL
1	D	276	SER
1	D	436	PHE
1	D	498	VAL
1	E	317	VAL
1	E	498	VAL
1	F	33	LYS
1	F	498	VAL
1	B	391	HIS
1	C	266	PHE
1	D	266	PHE
1	D	500	PHE
1	E	266	PHE
1	E	391	HIS

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Mol	Chain	Res	Type
1	E	424	HIS
1	F	66	ARG
1	F	309	ILE
1	F	403	ARG
1	A	70	GLY
1	A	276	SER
1	A	400	LYS
1	A	403	ARG
1	B	70	GLY
1	B	310	TYR
1	B	423	LYS
1	C	70	GLY
1	C	276	SER
1	C	400	LYS
1	D	70	GLY
1	D	400	LYS
1	E	70	GLY
1	E	276	SER
1	E	400	LYS
1	E	403	ARG
1	F	70	GLY
1	F	266	PHE
1	F	391	HIS
1	F	400	LYS
1	F	435	GLU
1	B	36	GLU
1	B	400	LYS
1	D	363	ARG
1	F	276	SER
1	B	266	PHE
1	E	363	ARG
1	F	496	ALA
1	D	317	VAL
1	A	317	VAL
1	C	317	VAL
1	D	309	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	417/471 (88%)	417 (100%)	0	100	100
1	B	417/471 (88%)	417 (100%)	0	100	100
1	C	417/471 (88%)	417 (100%)	0	100	100
1	D	417/471 (88%)	417 (100%)	0	100	100
1	E	417/471 (88%)	417 (100%)	0	100	100
1	F	417/471 (88%)	417 (100%)	0	100	100
All	All	2502/2826 (88%)	2502 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	84	GLN
1	A	406	ASN
1	A	450	HIS
1	B	56	ASN
1	B	84	GLN
1	B	139	ASN
1	B	193	ASN
1	B	205	GLN
1	B	209	HIS
1	B	406	ASN
1	B	450	HIS
1	C	225	ASN
1	C	450	HIS
1	D	56	ASN
1	D	84	GLN
1	D	193	ASN
1	D	209	HIS
1	D	391	HIS
1	D	406	ASN
1	E	43	ASN
1	E	56	ASN
1	E	84	GLN
1	E	193	ASN
1	E	406	ASN

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Mol	Chain	Res	Type
1	E	450	HIS
1	F	56	ASN
1	F	84	GLN
1	F	193	ASN
1	F	195	HIS
1	F	209	HIS
1	F	264	HIS
1	F	408	HIS
1	F	450	HIS

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 ⓘ

24 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	$\# Z > 2$
4	NAI	D	604	-	47,48,48	3.71	23 (48%)	64,73,73	1.93	17 (26%)
4	NAI	C	604	-	47,48,48	3.65	24 (51%)	64,73,73	1.81	16 (25%)
3	GTP	A	602	-	33,34,34	1.10	2 (6%)	50,54,54	1.80	15 (30%)
2	GLU	D	601	-	8,9,9	1.13	1 (12%)	8,11,11	1.11	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GTP	D	602	-	33,34,34	1.01	3 (9%)	50,54,54	1.70	8 (16%)
2	GLU	B	601	-	8,9,9	1.07	1 (12%)	8,11,11	1.34	1 (12%)
4	NAI	A	603	-	47,48,48	3.59	22 (46%)	64,73,73	2.09	16 (25%)
2	GLU	C	601	-	8,9,9	1.07	1 (12%)	8,11,11	1.22	1 (12%)
3	GTP	B	602	-	33,34,34	1.07	3 (9%)	50,54,54	1.80	10 (20%)
4	NAI	E	603	-	47,48,48	3.66	22 (46%)	64,73,73	1.80	15 (23%)
4	NAI	B	603	-	47,48,48	3.63	23 (48%)	64,73,73	2.08	17 (26%)
4	NAI	C	603	-	47,48,48	3.72	21 (44%)	64,73,73	1.84	12 (18%)
3	GTP	C	602	-	33,34,34	1.22	4 (12%)	50,54,54	1.65	8 (16%)
4	NAI	A	604	-	47,48,48	3.75	22 (46%)	64,73,73	2.16	18 (28%)
4	NAI	F	603	-	47,48,48	3.67	23 (48%)	64,73,73	1.89	17 (26%)
4	NAI	D	603	-	47,48,48	3.60	22 (46%)	64,73,73	1.71	11 (17%)
3	GTP	F	604	-	33,34,34	0.96	2 (6%)	50,54,54	1.57	10 (20%)
2	GLU	E	601	-	8,9,9	1.14	1 (12%)	8,11,11	1.17	1 (12%)
4	NAI	F	601	-	47,48,48	3.74	22 (46%)	64,73,73	2.13	15 (23%)
4	NAI	B	604	-	47,48,48	3.63	21 (44%)	64,73,73	1.74	14 (21%)
3	GTP	E	602	-	33,34,34	1.12	4 (12%)	50,54,54	1.65	8 (16%)
2	GLU	A	601	-	8,9,9	1.16	1 (12%)	8,11,11	1.11	1 (12%)
4	NAI	F	605	-	47,48,48	3.61	23 (48%)	64,73,73	1.97	17 (26%)
2	GLU	F	602	-	8,9,9	1.09	1 (12%)	8,11,11	1.31	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAI	D	604	-	-	11/29/72/72	0/5/5/5
4	NAI	C	604	-	-	16/29/72/72	0/5/5/5
3	GTP	A	602	-	-	5/22/38/38	0/3/3/3
2	GLU	D	601	-	-	1/9/9/9	-
3	GTP	D	602	-	-	3/22/38/38	0/3/3/3
2	GLU	B	601	-	-	0/9/9/9	-
4	NAI	A	603	-	-	8/29/72/72	0/5/5/5
2	GLU	C	601	-	-	1/9/9/9	-
3	GTP	B	602	-	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAI	E	603	-	-	9/29/72/72	0/5/5/5
4	NAI	B	603	-	-	9/29/72/72	0/5/5/5
4	NAI	C	603	-	-	13/29/72/72	0/5/5/5
3	GTP	C	602	-	-	5/22/38/38	0/3/3/3
4	NAI	A	604	-	-	16/29/72/72	0/5/5/5
4	NAI	F	603	-	-	13/29/72/72	0/5/5/5
4	NAI	D	603	-	-	13/29/72/72	0/5/5/5
3	GTP	F	604	-	-	2/22/38/38	0/3/3/3
2	GLU	E	601	-	-	0/9/9/9	-
4	NAI	F	601	-	-	11/29/72/72	0/5/5/5
4	NAI	B	604	-	-	13/29/72/72	0/5/5/5
3	GTP	E	602	-	-	2/22/38/38	0/3/3/3
2	GLU	A	601	-	-	3/9/9/9	-
4	NAI	F	605	-	-	17/29/72/72	0/5/5/5
2	GLU	F	602	-	-	0/9/9/9	-

All (292) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	604	NAI	O4B-C1B	9.35	1.63	1.42
4	C	603	NAI	O4D-C1D	9.27	1.63	1.42
4	F	603	NAI	O4D-C1D	9.26	1.63	1.42
4	F	605	NAI	O4B-C1B	9.16	1.63	1.42
4	A	603	NAI	O4B-C1B	9.09	1.63	1.42
4	F	605	NAI	O4D-C1D	9.04	1.62	1.42
4	A	604	NAI	O4B-C1B	9.04	1.62	1.42
4	B	604	NAI	O4B-C1B	9.01	1.62	1.42
4	B	603	NAI	O4B-C1B	8.96	1.62	1.42
4	A	603	NAI	O4D-C1D	8.95	1.62	1.42
4	E	603	NAI	O4B-C1B	8.91	1.62	1.42
4	C	604	NAI	O4D-C1D	8.90	1.62	1.42
4	D	603	NAI	O4B-C1B	8.90	1.62	1.42
4	A	604	NAI	O4D-C1D	8.89	1.62	1.42
4	C	603	NAI	O4B-C1B	8.88	1.62	1.42
4	D	603	NAI	O4D-C1D	8.87	1.62	1.42
4	D	604	NAI	O4B-C1B	8.86	1.62	1.42
4	F	603	NAI	O4B-C1B	8.83	1.62	1.42
4	E	603	NAI	O4D-C1D	8.82	1.62	1.42
4	F	601	NAI	O4D-C1D	8.76	1.62	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	601	NAI	O4B-C1B	8.76	1.62	1.42
4	D	604	NAI	O4D-C1D	8.73	1.62	1.42
4	B	603	NAI	O4D-C1D	8.65	1.62	1.42
4	B	604	NAI	O4D-C1D	8.50	1.61	1.42
4	A	604	NAI	PA-O3	7.62	1.67	1.59
4	B	603	NAI	C2D-C1D	-7.47	1.30	1.53
4	F	601	NAI	PA-O3	7.41	1.67	1.59
4	E	603	NAI	C2D-C1D	-7.30	1.30	1.53
4	F	603	NAI	C2D-C1D	-7.28	1.30	1.53
4	F	605	NAI	C2D-C1D	-7.28	1.30	1.53
4	C	603	NAI	C2D-C1D	-7.27	1.30	1.53
4	C	604	NAI	C2B-C1B	-7.18	1.30	1.53
4	F	601	NAI	C2D-C1D	-7.18	1.30	1.53
4	C	604	NAI	C2D-C1D	-7.15	1.31	1.53
4	B	604	NAI	C2D-C1D	-7.13	1.31	1.53
4	D	603	NAI	C2D-C1D	-7.12	1.31	1.53
4	A	603	NAI	C2N-C3N	7.11	1.54	1.35
4	A	604	NAI	PN-O3	7.09	1.67	1.59
4	C	603	NAI	C2B-C1B	-7.08	1.31	1.53
4	A	604	NAI	C2D-C1D	-7.08	1.31	1.53
4	B	604	NAI	C2B-C1B	-7.07	1.31	1.53
4	D	603	NAI	C2B-C1B	-7.06	1.31	1.53
4	B	603	NAI	C2N-C3N	7.06	1.54	1.35
4	E	603	NAI	C2B-C1B	-7.03	1.31	1.53
4	D	604	NAI	PA-O3	6.94	1.67	1.59
4	A	603	NAI	C2D-C1D	-6.93	1.31	1.53
4	D	604	NAI	C2D-C1D	-6.93	1.31	1.53
4	A	603	NAI	C2B-C1B	-6.91	1.31	1.53
4	F	601	NAI	C2B-C1B	-6.90	1.31	1.53
4	D	604	NAI	C2B-C1B	-6.90	1.31	1.53
4	F	605	NAI	C2B-C1B	-6.90	1.31	1.53
4	F	603	NAI	C2B-C1B	-6.90	1.31	1.53
4	C	604	NAI	C2N-C3N	6.80	1.53	1.35
4	F	601	NAI	PN-O3	6.78	1.66	1.59
4	E	603	NAI	C2N-C3N	6.76	1.53	1.35
4	D	604	NAI	C2N-C3N	6.72	1.53	1.35
4	A	604	NAI	C2B-C1B	-6.71	1.32	1.53
4	D	604	NAI	PN-O3	6.68	1.66	1.59
4	C	603	NAI	C6N-C5N	6.66	1.53	1.33
4	F	605	NAI	C2N-C3N	6.66	1.53	1.35
4	C	603	NAI	PN-O3	6.65	1.66	1.59
4	B	603	NAI	C2B-C1B	-6.62	1.32	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	NAI	C2N-C3N	6.60	1.53	1.35
4	B	604	NAI	C2N-C3N	6.58	1.53	1.35
4	A	604	NAI	C6N-C5N	6.55	1.53	1.33
4	C	603	NAI	PA-O3	6.53	1.66	1.59
4	F	603	NAI	C6N-C5N	6.50	1.53	1.33
4	E	603	NAI	C6N-C5N	6.50	1.53	1.33
4	B	604	NAI	O4D-C4D	-6.48	1.30	1.45
4	D	603	NAI	C6N-C5N	6.44	1.52	1.33
4	D	604	NAI	C6N-C5N	6.43	1.52	1.33
4	F	605	NAI	O4D-C4D	-6.42	1.30	1.45
4	F	601	NAI	C6N-C5N	6.40	1.52	1.33
4	C	604	NAI	C6N-C5N	6.36	1.52	1.33
4	C	603	NAI	C2N-C3N	6.36	1.52	1.35
4	F	605	NAI	C6N-C5N	6.34	1.52	1.33
4	A	604	NAI	C2N-C3N	6.32	1.52	1.35
4	D	603	NAI	O4B-C4B	-6.32	1.30	1.45
4	F	603	NAI	C2N-C3N	6.31	1.52	1.35
4	E	603	NAI	O4B-C4B	-6.27	1.31	1.45
4	B	603	NAI	C6N-C5N	6.25	1.52	1.33
4	A	603	NAI	C6N-C5N	6.24	1.52	1.33
4	A	603	NAI	O4D-C4D	-6.24	1.31	1.45
4	F	601	NAI	O4D-C4D	-6.24	1.31	1.45
4	F	601	NAI	C2N-C3N	6.24	1.52	1.35
4	D	604	NAI	O4D-C4D	-6.22	1.31	1.45
4	A	604	NAI	O4B-C4B	-6.18	1.31	1.45
4	A	604	NAI	O4D-C4D	-6.16	1.31	1.45
4	F	603	NAI	O4D-C4D	-6.16	1.31	1.45
4	B	603	NAI	O4D-C4D	-6.10	1.31	1.45
4	D	604	NAI	O4B-C4B	-6.09	1.31	1.45
4	F	603	NAI	O4B-C4B	-6.08	1.31	1.45
4	C	604	NAI	O4D-C4D	-6.05	1.31	1.45
4	E	603	NAI	O4D-C4D	-6.05	1.31	1.45
4	B	604	NAI	C6N-C5N	6.04	1.51	1.33
4	B	604	NAI	PN-O3	6.04	1.66	1.59
4	F	601	NAI	O4B-C4B	-6.03	1.31	1.45
4	C	603	NAI	O4B-C4B	-6.02	1.31	1.45
4	D	603	NAI	O4D-C4D	-6.01	1.31	1.45
4	B	604	NAI	O4B-C4B	-6.01	1.31	1.45
4	A	603	NAI	O4B-C4B	-6.00	1.31	1.45
4	B	603	NAI	O4B-C4B	-5.99	1.31	1.45
4	C	603	NAI	O4D-C4D	-5.97	1.31	1.45
4	F	603	NAI	PA-O3	5.91	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	604	NAI	O4B-C4B	-5.90	1.31	1.45
4	F	603	NAI	PN-O3	5.83	1.65	1.59
4	F	605	NAI	O4B-C4B	-5.79	1.32	1.45
4	E	603	NAI	PN-O3	5.73	1.65	1.59
4	B	604	NAI	PA-O3	5.72	1.65	1.59
4	C	604	NAI	PA-O3	5.71	1.65	1.59
4	B	603	NAI	PA-O3	5.57	1.65	1.59
4	B	603	NAI	PN-O3	5.54	1.65	1.59
4	E	603	NAI	PA-O3	5.48	1.65	1.59
4	F	605	NAI	PA-O3	5.35	1.65	1.59
4	D	603	NAI	PA-O3	5.17	1.65	1.59
4	A	603	NAI	PN-O3	5.10	1.65	1.59
4	C	604	NAI	PN-O3	4.91	1.64	1.59
4	D	603	NAI	PN-O3	4.89	1.64	1.59
4	A	603	NAI	PA-O3	4.82	1.64	1.59
4	A	604	NAI	C6A-N6A	4.58	1.45	1.34
4	A	603	NAI	C6A-N6A	4.56	1.45	1.34
4	C	604	NAI	C6A-N6A	4.55	1.45	1.34
4	E	603	NAI	C6A-N6A	4.54	1.45	1.34
4	F	605	NAI	PN-O3	4.53	1.64	1.59
4	B	604	NAI	C6A-N6A	4.51	1.45	1.34
4	F	603	NAI	C6A-N6A	4.50	1.45	1.34
4	B	603	NAI	C6A-N6A	4.50	1.45	1.34
4	D	603	NAI	C6A-N6A	4.49	1.45	1.34
4	F	605	NAI	C6A-N6A	4.47	1.45	1.34
4	D	604	NAI	C6A-N6A	4.43	1.45	1.34
4	C	603	NAI	C6A-N6A	4.43	1.45	1.34
4	B	603	NAI	C7N-N7N	4.41	1.46	1.33
4	F	603	NAI	C7N-N7N	4.32	1.45	1.33
4	A	603	NAI	C7N-N7N	4.31	1.45	1.33
4	E	603	NAI	C7N-N7N	4.31	1.45	1.33
4	C	603	NAI	C7N-N7N	4.30	1.45	1.33
4	D	603	NAI	C7N-N7N	4.30	1.45	1.33
4	D	604	NAI	C7N-N7N	4.29	1.45	1.33
4	F	601	NAI	C6A-N6A	4.26	1.45	1.34
4	B	604	NAI	C7N-N7N	4.24	1.45	1.33
4	F	601	NAI	C7N-N7N	4.23	1.45	1.33
4	A	604	NAI	C7N-N7N	4.21	1.45	1.33
4	C	604	NAI	C7N-N7N	4.19	1.45	1.33
4	F	605	NAI	C7N-N7N	4.17	1.45	1.33
3	C	602	GTP	PA-O3A	3.53	1.63	1.59
3	C	602	GTP	PB-O3A	3.44	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	603	NAI	C6N-N1N	3.39	1.45	1.37
3	A	602	GTP	PB-O3B	3.29	1.63	1.59
4	C	603	NAI	C6N-N1N	3.29	1.45	1.37
4	F	601	NAI	O3D-C3D	-3.24	1.34	1.43
4	D	604	NAI	C6N-N1N	3.21	1.45	1.37
4	F	603	NAI	C6N-N1N	3.19	1.45	1.37
4	F	601	NAI	C5A-N7A	-3.16	1.33	1.39
4	C	604	NAI	C6N-N1N	3.13	1.44	1.37
4	D	603	NAI	C6N-N1N	3.13	1.44	1.37
4	F	605	NAI	O3D-C3D	-3.11	1.35	1.43
4	B	603	NAI	O2B-C2B	3.10	1.50	1.43
4	B	603	NAI	C5A-C4A	-3.10	1.33	1.39
4	F	603	NAI	O2B-C2B	3.08	1.50	1.43
4	B	604	NAI	O2D-C2D	3.06	1.50	1.43
4	F	605	NAI	C6N-N1N	3.04	1.44	1.37
4	F	603	NAI	C5A-C4A	-3.04	1.33	1.39
4	C	604	NAI	O2B-C2B	3.03	1.50	1.43
4	A	603	NAI	C6N-N1N	3.03	1.44	1.37
4	F	601	NAI	C6N-N1N	3.02	1.44	1.37
4	D	603	NAI	O2B-C2B	3.02	1.50	1.43
4	E	603	NAI	O2B-C2B	3.02	1.50	1.43
4	D	604	NAI	O2B-C2B	3.02	1.50	1.43
4	D	603	NAI	C5A-C4A	-3.01	1.33	1.39
4	A	604	NAI	O2B-C2B	3.00	1.50	1.43
4	F	601	NAI	O2B-C2B	3.00	1.50	1.43
4	E	603	NAI	O3D-C3D	-2.99	1.35	1.43
4	C	603	NAI	C5A-C4A	-2.97	1.33	1.39
4	A	603	NAI	C5A-C4A	-2.95	1.33	1.39
4	B	603	NAI	C6N-N1N	2.94	1.44	1.37
4	B	604	NAI	O2B-C2B	2.93	1.50	1.43
4	D	604	NAI	C7N-C3N	2.93	1.55	1.48
4	C	604	NAI	C5A-C4A	-2.92	1.33	1.39
4	E	603	NAI	C5A-C4A	-2.92	1.33	1.39
4	F	601	NAI	O2D-C2D	2.92	1.50	1.43
4	D	603	NAI	O2D-C2D	2.90	1.50	1.43
4	A	604	NAI	O2D-C2D	2.89	1.50	1.43
4	D	604	NAI	O3D-C3D	-2.87	1.35	1.43
4	F	605	NAI	C5A-N7A	-2.87	1.33	1.39
4	F	601	NAI	O7N-C7N	-2.84	1.17	1.24
4	F	603	NAI	O3D-C3D	-2.83	1.35	1.43
4	F	605	NAI	O2B-C2B	2.83	1.50	1.43
4	C	603	NAI	O2B-C2B	2.83	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	601	NAI	C5A-C4A	-2.82	1.34	1.39
4	B	603	NAI	O2D-C2D	2.80	1.49	1.43
4	C	604	NAI	O2D-C2D	2.80	1.49	1.43
4	C	603	NAI	O2D-C2D	2.80	1.49	1.43
4	F	603	NAI	O3B-C3B	-2.79	1.36	1.43
4	A	604	NAI	C5A-N7A	-2.77	1.34	1.39
4	A	603	NAI	O3D-C3D	-2.77	1.36	1.43
4	C	604	NAI	O3B-C3B	-2.76	1.36	1.43
4	C	603	NAI	O3D-C3D	-2.76	1.36	1.43
4	A	603	NAI	O2D-C2D	2.76	1.49	1.43
4	E	603	NAI	O2D-C2D	2.76	1.49	1.43
4	C	603	NAI	O3B-C3B	-2.75	1.36	1.43
4	B	604	NAI	C6N-N1N	2.73	1.43	1.37
4	D	603	NAI	O3D-C3D	-2.72	1.36	1.43
4	A	604	NAI	C6N-N1N	2.71	1.43	1.37
4	D	603	NAI	O3B-C3B	-2.71	1.36	1.43
4	D	604	NAI	C5A-N7A	-2.71	1.34	1.39
4	B	603	NAI	C5A-N7A	-2.70	1.34	1.39
4	E	603	NAI	O3B-C3B	-2.69	1.36	1.43
4	F	605	NAI	C5A-C4A	-2.67	1.34	1.39
4	B	604	NAI	O3B-C3B	-2.67	1.36	1.43
4	B	604	NAI	O3D-C3D	-2.67	1.36	1.43
4	F	603	NAI	C5A-N7A	-2.67	1.34	1.39
4	A	603	NAI	O2B-C2B	2.65	1.49	1.43
4	F	605	NAI	O3B-C3B	-2.65	1.36	1.43
4	F	605	NAI	O2D-C2D	2.62	1.49	1.43
4	A	604	NAI	O3B-C3B	-2.61	1.36	1.43
4	F	601	NAI	O3B-C3B	-2.61	1.36	1.43
4	B	604	NAI	C5A-C4A	-2.60	1.34	1.39
4	D	603	NAI	C5A-N7A	-2.60	1.34	1.39
4	D	604	NAI	O2D-C2D	2.60	1.49	1.43
3	E	602	GTP	PB-O3B	2.60	1.62	1.59
4	F	603	NAI	O7N-C7N	-2.58	1.18	1.24
4	C	604	NAI	C5A-N7A	-2.57	1.34	1.39
3	E	602	GTP	C2-N3	2.56	1.39	1.33
4	D	604	NAI	O3B-C3B	-2.54	1.36	1.43
4	E	603	NAI	C5A-N7A	-2.54	1.34	1.39
3	D	602	GTP	C2-N3	2.53	1.39	1.33
4	D	604	NAI	C5A-C4A	-2.53	1.34	1.39
4	A	603	NAI	C7N-C3N	2.52	1.54	1.48
4	C	604	NAI	O3D-C3D	-2.52	1.36	1.43
3	B	602	GTP	PA-O3A	2.51	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	GTP	PA-O3A	2.51	1.62	1.59
4	A	604	NAI	C5A-C4A	-2.51	1.34	1.39
4	B	603	NAI	O3D-C3D	-2.50	1.36	1.43
3	B	602	GTP	C2-N3	2.50	1.39	1.33
4	A	603	NAI	C5A-N7A	-2.49	1.34	1.39
4	B	604	NAI	C5A-N7A	-2.49	1.34	1.39
4	A	604	NAI	O7N-C7N	-2.47	1.18	1.24
4	B	604	NAI	O7N-C7N	-2.46	1.18	1.24
4	F	605	NAI	O7N-C7N	-2.46	1.18	1.24
4	A	603	NAI	O3B-C3B	-2.44	1.36	1.43
4	C	603	NAI	C5A-N7A	-2.43	1.34	1.39
3	E	602	GTP	PB-O3A	2.43	1.62	1.59
4	B	603	NAI	C7N-C3N	2.42	1.53	1.48
3	B	602	GTP	PB-O3A	2.42	1.62	1.59
4	B	603	NAI	O3B-C3B	-2.40	1.37	1.43
2	A	601	GLU	OXT-C	-2.37	1.23	1.30
4	A	604	NAI	O3D-C3D	-2.35	1.37	1.43
3	F	604	GTP	PB-O3A	2.35	1.62	1.59
2	D	601	GLU	OXT-C	-2.35	1.23	1.30
2	E	601	GLU	OXT-C	-2.34	1.23	1.30
4	F	603	NAI	O2D-C2D	2.34	1.48	1.43
4	C	604	NAI	O7N-C7N	-2.34	1.19	1.24
4	C	603	NAI	O7N-C7N	-2.33	1.19	1.24
3	C	602	GTP	C2-N3	2.32	1.38	1.33
4	F	605	NAI	PA-O5B	2.30	1.68	1.59
4	A	604	NAI	C7N-C3N	2.29	1.53	1.48
4	E	603	NAI	O7N-C7N	-2.27	1.19	1.24
4	B	603	NAI	C8A-N9A	-2.26	1.33	1.37
4	E	603	NAI	C8A-N9A	-2.25	1.33	1.37
3	D	602	GTP	PA-O3A	2.24	1.61	1.59
2	F	602	GLU	OXT-C	-2.23	1.23	1.30
4	C	603	NAI	C7N-C3N	2.23	1.53	1.48
4	A	603	NAI	O7N-C7N	-2.21	1.19	1.24
4	B	603	NAI	O7N-C7N	-2.20	1.19	1.24
4	C	604	NAI	C7N-C3N	2.20	1.53	1.48
4	E	603	NAI	C7N-C3N	2.20	1.53	1.48
4	D	603	NAI	O7N-C7N	-2.20	1.19	1.24
3	C	602	GTP	PB-O3B	2.19	1.61	1.59
4	F	601	NAI	C4N-C3N	2.18	1.54	1.50
3	F	604	GTP	PA-O3A	2.18	1.61	1.59
4	C	604	NAI	PA-O5B	2.17	1.67	1.59
4	D	603	NAI	C8A-N9A	-2.17	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	604	NAI	C8A-N9A	-2.14	1.33	1.37
2	B	601	GLU	OXT-C	-2.14	1.23	1.30
2	C	601	GLU	OXT-C	-2.13	1.23	1.30
4	D	604	NAI	C4N-C3N	2.12	1.54	1.50
3	A	602	GTP	PA-O3A	2.12	1.61	1.59
4	F	603	NAI	C7N-C3N	2.11	1.53	1.48
4	B	604	NAI	C8A-N9A	-2.11	1.34	1.37
4	F	603	NAI	C8A-N9A	-2.11	1.34	1.37
4	B	603	NAI	PA-O5B	2.09	1.67	1.59
4	F	603	NAI	C5B-C4B	2.09	1.57	1.51
4	F	601	NAI	C8A-N9A	-2.07	1.34	1.37
4	C	604	NAI	C5B-C4B	2.05	1.57	1.51
3	D	602	GTP	C5-N7	-2.05	1.35	1.39
4	D	604	NAI	C8A-N9A	-2.04	1.34	1.37
4	F	605	NAI	C5B-C4B	2.04	1.57	1.51
4	F	605	NAI	C8A-N9A	-2.04	1.34	1.37
4	A	604	NAI	C5D-C4D	2.02	1.57	1.51
4	D	604	NAI	PA-O5B	2.01	1.67	1.59
4	D	603	NAI	C7N-C3N	2.01	1.53	1.48
4	A	603	NAI	C8A-N9A	-2.01	1.34	1.37

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	601	NAI	C3N-C2N-N1N	-9.23	109.65	123.20
4	A	604	NAI	C3N-C2N-N1N	-6.94	113.02	123.20
4	A	603	NAI	N3A-C2A-N1A	-6.23	119.16	128.58
4	B	603	NAI	C5A-C4A-N3A	-6.13	118.28	126.72
4	B	603	NAI	N3A-C2A-N1A	-6.04	119.44	128.58
3	B	602	GTP	C5-C4-N3	-6.00	118.84	128.39
4	C	603	NAI	N3A-C2A-N1A	-5.93	119.61	128.58
3	D	602	GTP	C5-C4-N3	-5.93	118.96	128.39
3	E	602	GTP	C5-C4-N3	-5.89	119.02	128.39
4	C	604	NAI	N3A-C2A-N1A	-5.84	119.75	128.58
4	E	603	NAI	N3A-C2A-N1A	-5.77	119.84	128.58
4	D	603	NAI	N3A-C2A-N1A	-5.76	119.86	128.58
4	A	604	NAI	C5A-C4A-N3A	-5.73	118.82	126.72
4	F	601	NAI	C5A-C4A-N3A	-5.68	118.89	126.72
4	D	604	NAI	C5A-C4A-N3A	-5.58	119.03	126.72
4	F	605	NAI	C5A-C4A-N3A	-5.58	119.04	126.72
4	A	603	NAI	C5A-C4A-N3A	-5.53	119.11	126.72
3	C	602	GTP	C5-C4-N3	-5.52	119.60	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	GTP	O2G-PG-O3B	5.44	122.89	104.64
4	D	604	NAI	N3A-C2A-N1A	-5.32	120.53	128.58
4	F	605	NAI	N3A-C2A-N1A	-5.30	120.56	128.58
4	F	603	NAI	N3A-C2A-N1A	-5.24	120.64	128.58
4	D	604	NAI	C4D-O4D-C1D	-5.21	97.96	109.47
4	F	601	NAI	N3A-C2A-N1A	-5.21	120.70	128.58
4	A	604	NAI	N3A-C2A-N1A	-5.20	120.71	128.58
4	C	603	NAI	C5A-C4A-N3A	-4.94	119.91	126.72
4	C	604	NAI	C5A-C4A-N3A	-4.90	119.97	126.72
4	F	603	NAI	C5A-C4A-N3A	-4.90	119.97	126.72
3	B	602	GTP	C2-N3-C4	4.88	120.71	112.30
4	B	604	NAI	C5A-C4A-N3A	-4.87	120.02	126.72
3	E	602	GTP	C2-N3-C4	4.86	120.67	112.30
3	C	602	GTP	C2-N3-C4	4.80	120.56	112.30
4	B	603	NAI	N6A-C6A-N1A	-4.74	107.82	118.38
3	D	602	GTP	C2-N3-C4	4.73	120.44	112.30
4	D	603	NAI	C5A-C4A-N3A	-4.72	120.22	126.72
4	E	603	NAI	C5A-C4A-N3A	-4.71	120.23	126.72
4	B	604	NAI	N3A-C2A-N1A	-4.69	121.48	128.58
4	C	603	NAI	N6A-C6A-N1A	-4.68	107.95	118.38
3	F	604	GTP	C2-N3-C4	4.64	120.30	112.30
3	A	602	GTP	C2-N3-C4	4.64	120.29	112.30
4	A	603	NAI	N6A-C6A-N1A	-4.56	108.21	118.38
4	B	604	NAI	N6A-C6A-N1A	-4.46	108.45	118.38
4	A	604	NAI	C2D-C1D-N1N	-4.44	102.40	113.31
4	F	603	NAI	N9A-C8A-N7A	-4.43	107.64	113.94
4	E	603	NAI	N6A-C6A-N1A	-4.39	108.61	118.38
3	F	604	GTP	C5-C4-N3	-4.34	121.48	128.39
3	A	602	GTP	C5-C4-N3	-4.28	121.58	128.39
4	C	603	NAI	C3N-C2N-N1N	-4.27	116.93	123.20
4	A	604	NAI	N6A-C6A-N1A	-4.25	108.91	118.38
4	F	605	NAI	O4D-C1D-N1N	4.24	116.16	108.08
4	F	601	NAI	N3A-C4A-N9A	4.22	134.35	127.17
4	D	603	NAI	N9A-C8A-N7A	-4.21	107.96	113.94
4	B	603	NAI	C2A-N3A-C4A	4.21	122.11	111.83
4	C	604	NAI	N9A-C8A-N7A	-4.21	107.97	113.94
4	C	604	NAI	N6A-C6A-N1A	-4.18	109.07	118.38
4	D	603	NAI	N6A-C6A-N1A	-4.18	109.07	118.38
3	D	602	GTP	N9-C4-N3	4.15	134.26	125.95
4	E	603	NAI	N9A-C8A-N7A	-4.12	108.09	113.94
4	B	604	NAI	C4D-O4D-C1D	-4.08	100.45	109.47
4	D	604	NAI	N6A-C6A-N1A	-4.03	109.40	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	NAI	C2A-N3A-C4A	4.03	121.67	111.83
3	E	602	GTP	N9-C4-N3	4.02	133.99	125.95
4	F	605	NAI	N6A-C6A-N1A	-4.00	109.47	118.38
3	B	602	GTP	N9-C4-N3	3.92	133.80	125.95
4	B	603	NAI	N9A-C8A-N7A	-3.92	108.38	113.94
4	A	603	NAI	N9A-C8A-N7A	-3.91	108.39	113.94
4	F	603	NAI	C3N-C2N-N1N	-3.90	117.48	123.20
4	A	604	NAI	N9A-C8A-N7A	-3.79	108.56	113.94
4	C	603	NAI	N9A-C8A-N7A	-3.78	108.57	113.94
4	A	603	NAI	C1D-N1N-C2N	3.77	127.35	121.14
4	C	603	NAI	C2A-N3A-C4A	3.69	120.84	111.83
4	F	605	NAI	N3A-C4A-N9A	3.68	133.43	127.17
4	B	604	NAI	N9A-C8A-N7A	-3.68	108.72	113.94
4	F	603	NAI	N6A-C6A-N1A	-3.64	110.27	118.38
4	A	603	NAI	C3N-C7N-N7N	3.60	124.07	117.67
3	C	602	GTP	N9-C4-N3	3.56	133.08	125.95
4	F	603	NAI	O4D-C1D-N1N	3.55	114.86	108.08
4	D	604	NAI	N9A-C8A-N7A	-3.53	108.92	113.94
4	F	605	NAI	N9A-C8A-N7A	-3.52	108.94	113.94
4	B	603	NAI	O4D-C1D-N1N	3.51	114.78	108.08
4	B	603	NAI	N3A-C4A-N9A	3.50	133.13	127.17
4	A	603	NAI	O4B-C1B-N9A	3.50	114.81	108.09
4	A	604	NAI	N3A-C4A-N9A	3.50	133.12	127.17
4	D	604	NAI	N3A-C4A-N9A	3.46	133.05	127.17
4	C	604	NAI	C2A-N3A-C4A	3.45	120.27	111.83
4	A	604	NAI	C3D-C2D-C1D	3.44	107.96	101.46
4	D	604	NAI	C2A-N3A-C4A	3.43	120.22	111.83
4	A	604	NAI	C2A-N3A-C4A	3.42	120.19	111.83
4	E	603	NAI	C2A-N3A-C4A	3.40	120.14	111.83
4	F	605	NAI	C2A-N3A-C4A	3.39	120.11	111.83
4	B	604	NAI	C5A-C6A-N6A	3.37	131.64	123.29
4	D	603	NAI	C2A-N3A-C4A	3.36	120.05	111.83
4	B	603	NAI	C3N-C7N-N7N	3.36	123.64	117.67
4	F	603	NAI	N3A-C4A-N9A	3.33	132.84	127.17
4	C	603	NAI	C5A-C6A-N6A	3.33	131.54	123.29
4	B	603	NAI	C5A-C6A-N6A	3.28	131.41	123.29
4	D	604	NAI	C3B-C2B-C1B	3.28	107.67	101.46
4	E	603	NAI	C5A-C6A-N6A	3.25	131.32	123.29
4	F	603	NAI	C2A-N3A-C4A	3.22	119.70	111.83
4	A	603	NAI	C5A-C6A-N6A	3.22	131.26	123.29
4	F	601	NAI	C2A-N3A-C4A	3.22	119.69	111.83
4	A	604	NAI	C3B-C2B-C1B	3.19	107.50	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	GTP	C2-N1-C6	-3.17	119.36	125.11
4	B	603	NAI	C5A-N7A-C8A	3.16	108.41	103.45
4	A	604	NAI	C5A-C6A-N6A	3.14	131.06	123.29
4	B	604	NAI	C3N-C2N-N1N	-3.13	118.61	123.20
3	D	602	GTP	C2-N1-C6	-3.12	119.45	125.11
4	F	601	NAI	C6A-C5A-C4A	3.12	121.43	117.18
4	A	603	NAI	C3B-C2B-C1B	3.11	107.34	101.46
4	F	601	NAI	C2D-C1D-N1N	-3.10	105.69	113.31
4	A	604	NAI	C5A-N7A-C8A	3.09	108.31	103.45
4	D	603	NAI	C5A-C6A-N6A	3.09	130.93	123.29
4	C	604	NAI	C5A-C6A-N6A	3.07	130.88	123.29
4	B	603	NAI	C3B-C2B-C1B	3.04	107.22	101.46
4	B	604	NAI	C2A-N3A-C4A	3.02	119.22	111.83
4	C	604	NAI	C5A-N7A-C8A	2.99	108.15	103.45
3	E	602	GTP	C2-N1-C6	-2.99	119.69	125.11
4	F	601	NAI	C6N-N1N-C2N	-2.98	116.13	119.32
4	A	603	NAI	C5A-N7A-C8A	2.96	108.10	103.45
4	A	603	NAI	N3A-C4A-N9A	2.96	132.19	127.17
3	C	602	GTP	C2-N1-C6	-2.95	119.77	125.11
4	E	603	NAI	O4D-C1D-C2D	-2.94	100.33	106.62
4	C	604	NAI	C3B-C2B-C1B	-2.94	95.90	101.46
4	C	603	NAI	C5A-C4A-N9A	2.92	108.99	105.81
2	B	601	GLU	OXT-C-O	-2.90	117.50	124.08
4	D	604	NAI	C5A-C6A-N6A	2.90	130.47	123.29
4	F	601	NAI	N9A-C8A-N7A	-2.89	109.83	113.94
2	F	602	GLU	OXT-C-O	-2.88	117.54	124.08
4	D	603	NAI	C5A-N7A-C8A	2.86	107.94	103.45
4	F	605	NAI	C5A-C6A-N6A	2.86	130.36	123.29
4	E	603	NAI	C5A-N7A-C8A	2.85	107.93	103.45
4	F	605	NAI	C3B-C2B-C1B	2.84	106.83	101.46
4	F	603	NAI	C5A-N7A-C8A	2.84	107.91	103.45
3	B	602	GTP	C3'-C2'-C1'	2.83	106.82	101.46
4	B	603	NAI	C1D-N1N-C2N	2.80	125.75	121.14
4	F	603	NAI	C4A-N9A-C8A	2.80	108.67	105.74
4	C	604	NAI	N3A-C4A-N9A	2.79	131.92	127.17
2	C	601	GLU	OXT-C-O	-2.76	117.81	124.08
4	B	603	NAI	C4A-C5A-N7A	-2.74	107.45	110.58
3	A	602	GTP	N9-C8-N7	-2.74	108.32	113.40
4	D	603	NAI	N3A-C4A-N9A	2.74	131.82	127.17
4	F	603	NAI	C2D-C1D-N1N	-2.72	106.61	113.31
4	D	604	NAI	C5A-N7A-C8A	2.72	107.73	103.45
4	F	605	NAI	C2D-C1D-N1N	-2.72	106.62	113.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	GTP	C8-N7-C5	2.72	109.10	104.26
4	C	603	NAI	C5A-N7A-C8A	2.67	107.65	103.45
4	B	604	NAI	C5A-N7A-C8A	2.67	107.65	103.45
4	A	603	NAI	C5A-C4A-N9A	2.65	108.69	105.81
4	E	603	NAI	N3A-C4A-N9A	2.64	131.65	127.17
4	A	604	NAI	C6A-C5A-C4A	2.63	120.77	117.18
4	F	605	NAI	C5A-N7A-C8A	2.63	107.58	103.45
4	A	604	NAI	O2A-PA-O3	2.62	114.36	107.27
4	F	601	NAI	C3D-C2D-C1D	2.62	106.42	101.46
4	A	603	NAI	C4A-C5A-N7A	-2.62	107.59	110.58
4	A	604	NAI	C6N-N1N-C2N	-2.60	116.54	119.32
3	F	604	GTP	N9-C8-N7	-2.59	108.61	113.40
4	A	603	NAI	C1D-N1N-C6N	-2.58	115.32	120.77
3	C	602	GTP	C8-N7-C5	2.57	108.85	104.26
4	B	604	NAI	N3A-C4A-N9A	2.57	131.54	127.17
4	F	605	NAI	C6A-C5A-C4A	2.57	120.69	117.18
4	F	601	NAI	C3B-C2B-C1B	2.56	106.31	101.46
4	F	601	NAI	N6A-C6A-N1A	-2.56	112.68	118.38
4	C	603	NAI	C3B-C2B-C1B	2.55	106.29	101.46
3	F	604	GTP	C2-N1-C6	-2.55	120.48	125.11
3	A	602	GTP	O6-C6-C5	-2.55	119.80	126.53
4	C	603	NAI	C4A-C5A-N7A	-2.55	107.67	110.58
4	B	603	NAI	C5A-C4A-N9A	2.55	108.59	105.81
3	D	602	GTP	O6-C6-C5	-2.54	119.83	126.53
4	F	603	NAI	C5A-C6A-N6A	2.54	129.56	123.29
4	D	603	NAI	O5D-C5D-C4D	2.53	117.61	108.99
3	A	602	GTP	C2-N1-C6	-2.53	120.52	125.11
4	F	605	NAI	C1D-N1N-C2N	2.50	125.26	121.14
3	B	602	GTP	C5-C6-N1	2.50	119.62	113.25
3	F	604	GTP	C8-N7-C5	2.50	108.71	104.26
2	E	601	GLU	OXT-C-O	-2.49	118.42	124.08
3	E	602	GTP	C5-C6-N1	2.49	119.59	113.25
4	D	604	NAI	C6A-C5A-C4A	2.48	120.57	117.18
4	B	604	NAI	C4A-C5A-N7A	-2.48	107.75	110.58
4	E	603	NAI	O4D-C1D-N1N	2.47	112.80	108.08
4	F	601	NAI	C2D-C3D-C4D	2.47	107.39	102.61
4	F	601	NAI	O7N-C7N-C3N	-2.47	116.25	120.90
3	D	602	GTP	C5-C6-N1	2.46	119.51	113.25
3	B	602	GTP	O3G-PG-O3B	2.44	112.82	104.64
4	F	603	NAI	C3B-C2B-C1B	2.44	106.07	101.46
3	F	604	GTP	N2-C2-N1	2.43	121.90	116.76
4	F	605	NAI	C3N-C2N-N1N	-2.43	119.64	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	604	NAI	O4D-C1D-N1N	2.42	112.71	108.08
3	E	602	GTP	C8-N7-C5	2.42	108.57	104.26
3	C	602	GTP	C5-C6-N1	2.42	119.41	113.25
4	B	604	NAI	C5A-C4A-N9A	2.41	108.44	105.81
3	D	602	GTP	C2'-C1'-N9	-2.41	106.55	113.25
3	C	602	GTP	N9-C8-N7	-2.39	108.97	113.40
2	D	601	GLU	OXT-C-O	-2.39	118.66	124.08
4	E	603	NAI	C3D-C2D-C1D	-2.39	96.95	101.46
4	C	604	NAI	C4A-C5A-N7A	-2.39	107.85	110.58
3	E	602	GTP	O6-C6-C5	-2.38	120.25	126.53
4	F	605	NAI	C2B-C1B-N9A	-2.38	107.39	113.30
4	E	603	NAI	C4A-C5A-N7A	-2.38	107.86	110.58
3	A	602	GTP	C5-C6-N1	2.38	119.30	113.25
3	B	602	GTP	N9-C8-N7	-2.37	109.01	113.40
4	B	603	NAI	C3N-C2N-N1N	-2.36	119.73	123.20
4	A	604	NAI	C4A-C5A-N7A	-2.34	107.90	110.58
3	A	602	GTP	C8-N7-C5	2.34	108.42	104.26
4	A	603	NAI	C3N-C2N-N1N	-2.31	119.82	123.20
4	C	603	NAI	N3A-C4A-N9A	2.31	131.09	127.17
4	F	605	NAI	C4D-O4D-C1D	-2.30	104.39	109.47
3	A	602	GTP	N9-C4-N3	2.29	130.54	125.95
3	D	602	GTP	C8-N7-C5	2.29	108.33	104.26
3	B	602	GTP	O6-C6-C5	-2.28	120.51	126.53
4	F	601	NAI	C3N-C7N-N7N	2.28	121.71	117.67
2	A	601	GLU	OXT-C-O	-2.25	118.97	124.08
4	D	603	NAI	C4A-N9A-C8A	2.24	108.09	105.74
4	B	603	NAI	C1D-N1N-C6N	-2.23	116.05	120.77
4	A	604	NAI	C3N-C7N-N7N	2.22	121.61	117.67
4	F	605	NAI	O4D-C4D-C3D	-2.22	100.76	105.15
4	D	603	NAI	C4A-C5A-N7A	-2.21	108.05	110.58
3	F	604	GTP	C5-C6-N1	2.21	118.88	113.25
3	A	602	GTP	C2'-C1'-N9	2.21	119.39	113.25
4	C	604	NAI	O5B-C5B-C4B	2.20	116.50	108.99
4	E	603	NAI	C5D-C4D-C3D	-2.19	107.33	115.21
3	F	604	GTP	C3'-C2'-C1'	2.19	105.60	101.46
3	C	602	GTP	O6-C6-C5	-2.18	120.77	126.53
4	D	604	NAI	C3N-C2N-N1N	-2.18	120.00	123.20
3	F	604	GTP	C4-C5-N7	-2.18	107.22	110.67
4	F	603	NAI	O4B-C1B-N9A	-2.17	103.92	108.09
4	F	603	NAI	C2B-C1B-N9A	-2.16	107.93	113.30
3	F	604	GTP	O6-C6-C5	-2.16	120.83	126.53
4	B	603	NAI	C6A-C5A-C4A	2.16	120.13	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	603	NAI	C4A-N9A-C8A	2.15	108.00	105.74
4	F	603	NAI	C6A-C5A-C4A	2.13	120.09	117.18
3	A	602	GTP	N1-C2-N3	-2.13	119.42	123.32
3	A	602	GTP	O2B-PB-O3B	2.12	113.02	107.27
4	B	604	NAI	C6A-C5A-C4A	2.12	120.07	117.18
4	E	603	NAI	C5A-C4A-N9A	2.11	108.12	105.81
4	D	604	NAI	O4D-C4D-C3D	-2.11	100.96	105.15
4	C	604	NAI	C5A-C4A-N9A	2.11	108.11	105.81
4	D	604	NAI	C2B-C3B-C4B	2.10	106.68	102.61
4	D	604	NAI	O7N-C7N-N7N	-2.08	118.23	122.89
4	D	604	NAI	C4A-C5A-N7A	-2.08	108.20	110.58
3	A	602	GTP	N2-C2-N1	2.07	121.14	116.76
4	B	604	NAI	O5D-C5D-C4D	2.07	116.05	108.99
4	C	604	NAI	C4A-N9A-C8A	2.07	107.91	105.74
4	A	604	NAI	C5A-C4A-N9A	2.06	108.06	105.81
3	E	602	GTP	N9-C8-N7	-2.06	109.58	113.40
4	C	604	NAI	O4D-C1D-N1N	2.05	112.00	108.08
4	C	604	NAI	C3N-C7N-N7N	2.05	121.31	117.67
4	C	604	NAI	O4B-C4B-C3B	-2.04	101.10	105.15
3	A	602	GTP	O3G-PG-O1G	-2.02	102.97	110.83
3	A	602	GTP	O3B-PB-O1B	2.01	116.76	110.70
4	F	603	NAI	O5B-C5B-C4B	2.01	115.84	108.99

There are no chirality outliers.

All (174) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GTP	PB-O3A-PA-O5'
3	B	602	GTP	C5'-O5'-PA-O3A
3	B	602	GTP	C5'-O5'-PA-O1A
3	C	602	GTP	O4'-C4'-C5'-O5'
3	C	602	GTP	C3'-C4'-C5'-O5'
4	A	604	NAI	C5B-O5B-PA-O1A
4	A	604	NAI	C5B-O5B-PA-O3
4	A	604	NAI	C5D-O5D-PN-O3
4	A	604	NAI	C5D-O5D-PN-O1N
4	A	604	NAI	O4D-C1D-N1N-C2N
4	A	604	NAI	C2N-C3N-C7N-N7N
4	B	603	NAI	C5D-O5D-PN-O3
4	B	603	NAI	C5D-O5D-PN-O1N
4	B	603	NAI	C5D-O5D-PN-O2N
4	B	603	NAI	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
4	B	603	NAI	C3D-C4D-C5D-O5D
4	B	604	NAI	C5D-O5D-PN-O3
4	B	604	NAI	C5D-O5D-PN-O1N
4	B	604	NAI	C5D-O5D-PN-O2N
4	B	604	NAI	C4D-C5D-O5D-PN
4	B	604	NAI	O4D-C1D-N1N-C2N
4	C	603	NAI	O4D-C1D-N1N-C2N
4	C	603	NAI	C2N-C3N-C7N-N7N
4	C	604	NAI	C5B-O5B-PA-O1A
4	C	604	NAI	C5B-O5B-PA-O2A
4	C	604	NAI	C5B-O5B-PA-O3
4	C	604	NAI	C5D-O5D-PN-O3
4	C	604	NAI	C5D-O5D-PN-O1N
4	C	604	NAI	C5D-O5D-PN-O2N
4	C	604	NAI	C2N-C3N-C7N-N7N
4	D	603	NAI	C5B-O5B-PA-O3
4	D	603	NAI	O4B-C4B-C5B-O5B
4	D	603	NAI	C3B-C4B-C5B-O5B
4	D	603	NAI	C5D-O5D-PN-O3
4	D	603	NAI	C5D-O5D-PN-O1N
4	D	603	NAI	C5D-O5D-PN-O2N
4	D	603	NAI	O4D-C4D-C5D-O5D
4	D	603	NAI	C3D-C4D-C5D-O5D
4	D	604	NAI	C5B-O5B-PA-O3
4	D	604	NAI	C4B-C5B-O5B-PA
4	D	604	NAI	O4B-C4B-C5B-O5B
4	D	604	NAI	C5D-O5D-PN-O3
4	D	604	NAI	C5D-O5D-PN-O1N
4	E	603	NAI	PA-O3-PN-O5D
4	E	603	NAI	O4D-C4D-C5D-O5D
4	F	601	NAI	C5B-O5B-PA-O1A
4	F	601	NAI	C5B-O5B-PA-O2A
4	F	601	NAI	C5B-O5B-PA-O3
4	F	601	NAI	C5D-O5D-PN-O3
4	F	601	NAI	C5D-O5D-PN-O1N
4	F	601	NAI	C5D-O5D-PN-O2N
4	F	603	NAI	C5B-O5B-PA-O1A
4	F	603	NAI	C5B-O5B-PA-O2A
4	F	603	NAI	C5B-O5B-PA-O3
4	F	603	NAI	C5D-O5D-PN-O3
4	F	603	NAI	C5D-O5D-PN-O1N
4	F	603	NAI	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
4	F	605	NAI	O4B-C4B-C5B-O5B
4	F	605	NAI	C3B-C4B-C5B-O5B
4	F	605	NAI	C5D-O5D-PN-O3
4	F	605	NAI	C5D-O5D-PN-O1N
4	F	605	NAI	C5D-O5D-PN-O2N
4	F	605	NAI	O4D-C4D-C5D-O5D
4	F	605	NAI	O4D-C1D-N1N-C6N
4	F	605	NAI	C2N-C3N-C7N-N7N
4	F	603	NAI	O4D-C1D-N1N-C2N
3	A	602	GTP	O4'-C4'-C5'-O5'
4	A	603	NAI	O4B-C4B-C5B-O5B
4	A	603	NAI	C3B-C4B-C5B-O5B
4	B	603	NAI	C3B-C4B-C5B-O5B
4	B	604	NAI	O4B-C4B-C5B-O5B
4	C	604	NAI	O4B-C4B-C5B-O5B
4	C	604	NAI	C3B-C4B-C5B-O5B
4	D	604	NAI	C3B-C4B-C5B-O5B
4	E	603	NAI	C3D-C4D-C5D-O5D
4	F	603	NAI	C3D-C4D-C5D-O5D
4	D	604	NAI	O4D-C1D-N1N-C6N
3	D	602	GTP	O4'-C4'-C5'-O5'
3	D	602	GTP	C3'-C4'-C5'-O5'
4	A	604	NAI	O4B-C4B-C5B-O5B
4	A	604	NAI	C3B-C4B-C5B-O5B
4	B	604	NAI	C3B-C4B-C5B-O5B
3	A	602	GTP	C3'-C4'-C5'-O5'
4	C	603	NAI	C3D-C4D-C5D-O5D
4	D	604	NAI	C3D-C4D-C5D-O5D
4	F	605	NAI	C3D-C4D-C5D-O5D
4	B	604	NAI	C2B-C1B-N9A-C8A
4	F	601	NAI	C2B-C1B-N9A-C8A
4	B	603	NAI	O4B-C4B-C5B-O5B
4	C	603	NAI	O4D-C4D-C5D-O5D
4	E	603	NAI	O4B-C4B-C5B-O5B
4	E	603	NAI	C3B-C4B-C5B-O5B
4	D	604	NAI	O4D-C4D-C5D-O5D
4	B	604	NAI	C2B-C1B-N9A-C4A
4	A	604	NAI	C2B-C1B-N9A-C8A
4	F	605	NAI	C2B-C1B-N9A-C8A
4	F	601	NAI	C2B-C1B-N9A-C4A
3	D	602	GTP	PB-O3A-PA-O5'
4	C	604	NAI	PN-O3-PA-O5B

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Mol	Chain	Res	Type	Atoms
4	C	604	NAI	PA-O3-PN-O5D
4	D	604	NAI	PN-O3-PA-O5B
4	E	603	NAI	PN-O3-PA-O5B
4	C	603	NAI	C2D-C1D-N1N-C6N
3	C	602	GTP	PG-O3B-PB-O3A
4	C	603	NAI	C2D-C1D-N1N-C2N
4	B	603	NAI	O4D-C1D-N1N-C6N
4	F	603	NAI	C2B-C1B-N9A-C8A
4	C	603	NAI	PA-O3-PN-O2N
4	F	601	NAI	O4D-C1D-N1N-C2N
4	A	603	NAI	C2D-C1D-N1N-C2N
4	A	603	NAI	C2D-C1D-N1N-C6N
4	A	604	NAI	C2N-C3N-C7N-O7N
4	C	603	NAI	C2N-C3N-C7N-O7N
4	A	603	NAI	O4D-C4D-C5D-O5D
3	B	602	GTP	C5'-O5'-PA-O2A
4	A	604	NAI	C5B-O5B-PA-O2A
4	A	604	NAI	C5D-O5D-PN-O2N
4	B	604	NAI	C5B-O5B-PA-O1A
4	B	604	NAI	C5B-O5B-PA-O2A
4	B	604	NAI	C5B-O5B-PA-O3
4	C	603	NAI	C5B-O5B-PA-O1A
4	C	603	NAI	C5D-O5D-PN-O2N
4	F	603	NAI	C5D-O5D-PN-O2N
4	F	605	NAI	C5B-O5B-PA-O2A
4	F	605	NAI	C5B-O5B-PA-O3
4	E	603	NAI	C4D-C5D-O5D-PN
4	A	603	NAI	O4D-C1D-N1N-C2N
4	A	603	NAI	O4D-C1D-N1N-C6N
4	F	603	NAI	C4D-C5D-O5D-PN
4	D	603	NAI	PA-O3-PN-O2N
4	F	605	NAI	PA-O3-PN-O2N
4	A	604	NAI	C2B-C1B-N9A-C4A
4	F	605	NAI	C2B-C1B-N9A-C4A
4	C	603	NAI	C2B-C1B-N9A-C8A
4	C	604	NAI	C2B-C1B-N9A-C8A
3	A	602	GTP	PA-O3A-PB-O3B
4	F	603	NAI	O4B-C1B-N9A-C4A
4	C	604	NAI	O4D-C1D-N1N-C6N
2	A	601	GLU	O-C-CA-N
2	D	601	GLU	O-C-CA-N
4	D	603	NAI	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
4	E	603	NAI	O4D-C1D-N1N-C6N
2	A	601	GLU	OE2-CD-CG-CB
3	E	602	GTP	PA-O3A-PB-O1B
3	F	604	GTP	PA-O3A-PB-O1B
4	F	603	NAI	O4B-C1B-N9A-C8A
4	C	603	NAI	O4B-C4B-C5B-O5B
4	D	603	NAI	C2D-C1D-N1N-C6N
4	F	601	NAI	C4B-C5B-O5B-PA
4	C	604	NAI	C2D-C1D-N1N-C6N
4	A	604	NAI	C2D-C1D-N1N-C6N
4	B	603	NAI	C4B-C5B-O5B-PA
4	E	603	NAI	C2D-C1D-N1N-C6N
4	D	603	NAI	C2B-C1B-N9A-C8A
3	C	602	GTP	PG-O3B-PB-O1B
3	C	602	GTP	PB-O3A-PA-O2A
4	B	604	NAI	PN-O3-PA-O2A
4	C	604	NAI	PN-O3-PA-O1A
4	C	604	NAI	PN-O3-PA-O2A
4	D	603	NAI	PA-O3-PN-O1N
4	F	605	NAI	PA-O3-PN-O1N
4	A	604	NAI	O4B-C1B-N9A-C8A
4	F	601	NAI	O4B-C1B-N9A-C8A
4	F	605	NAI	O4B-C1B-N9A-C8A
3	E	602	GTP	PA-O3A-PB-O3B
4	A	604	NAI	C2D-C1D-N1N-C2N
2	A	601	GLU	OE1-CD-CG-CB
2	C	601	GLU	OE2-CD-CG-CB
3	A	602	GTP	PA-O3A-PB-O1B
3	F	604	GTP	PA-O3A-PB-O2B
4	A	603	NAI	PN-O3-PA-O1A
4	C	603	NAI	PA-O3-PN-O1N
4	D	604	NAI	PN-O3-PA-O2A
4	F	605	NAI	PN-O3-PA-O2A

There are no ring outliers.

23 monomers are involved in 119 short contacts:

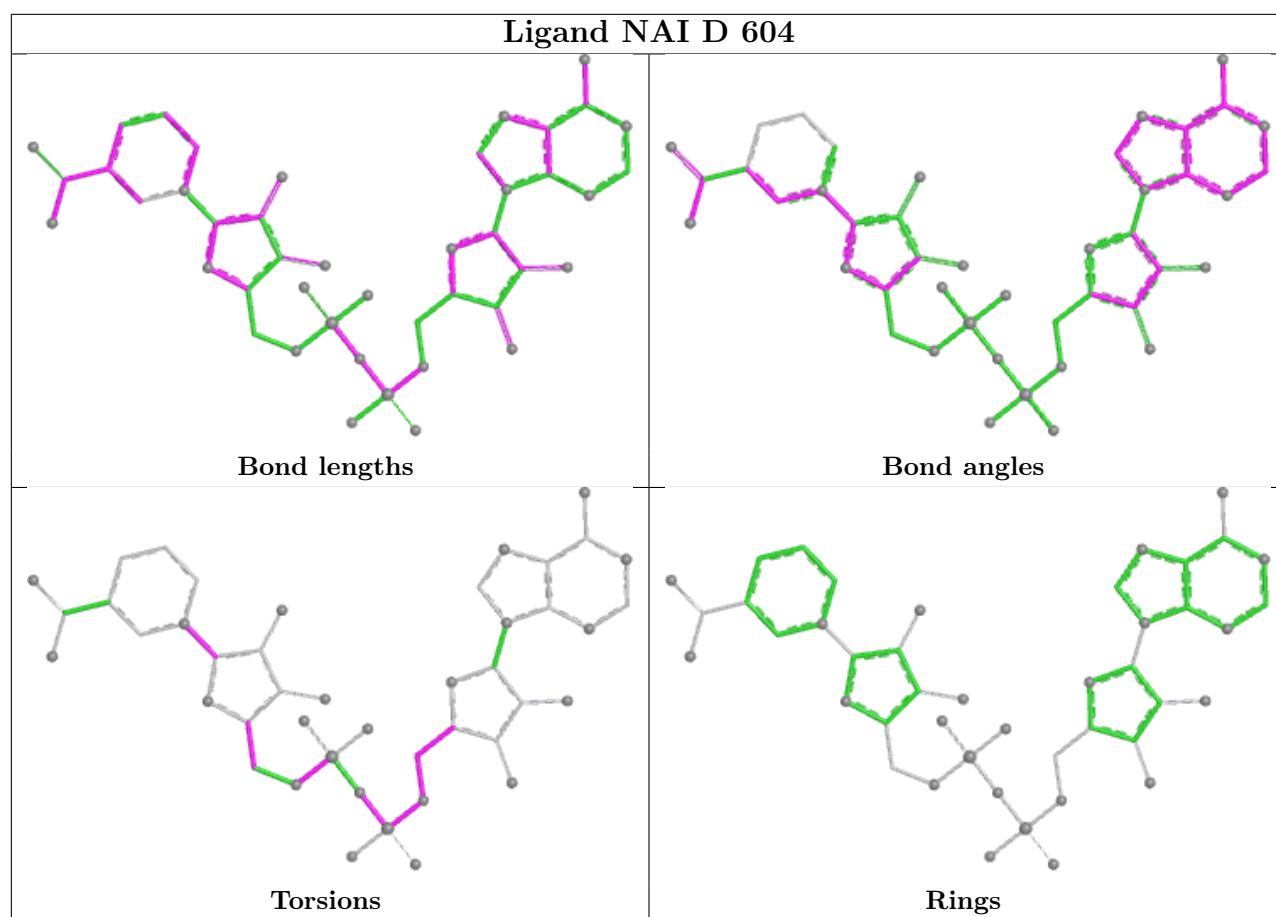
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	604	NAI	5	0
4	C	604	NAI	6	0
3	A	602	GTP	13	0
2	D	601	GLU	3	0

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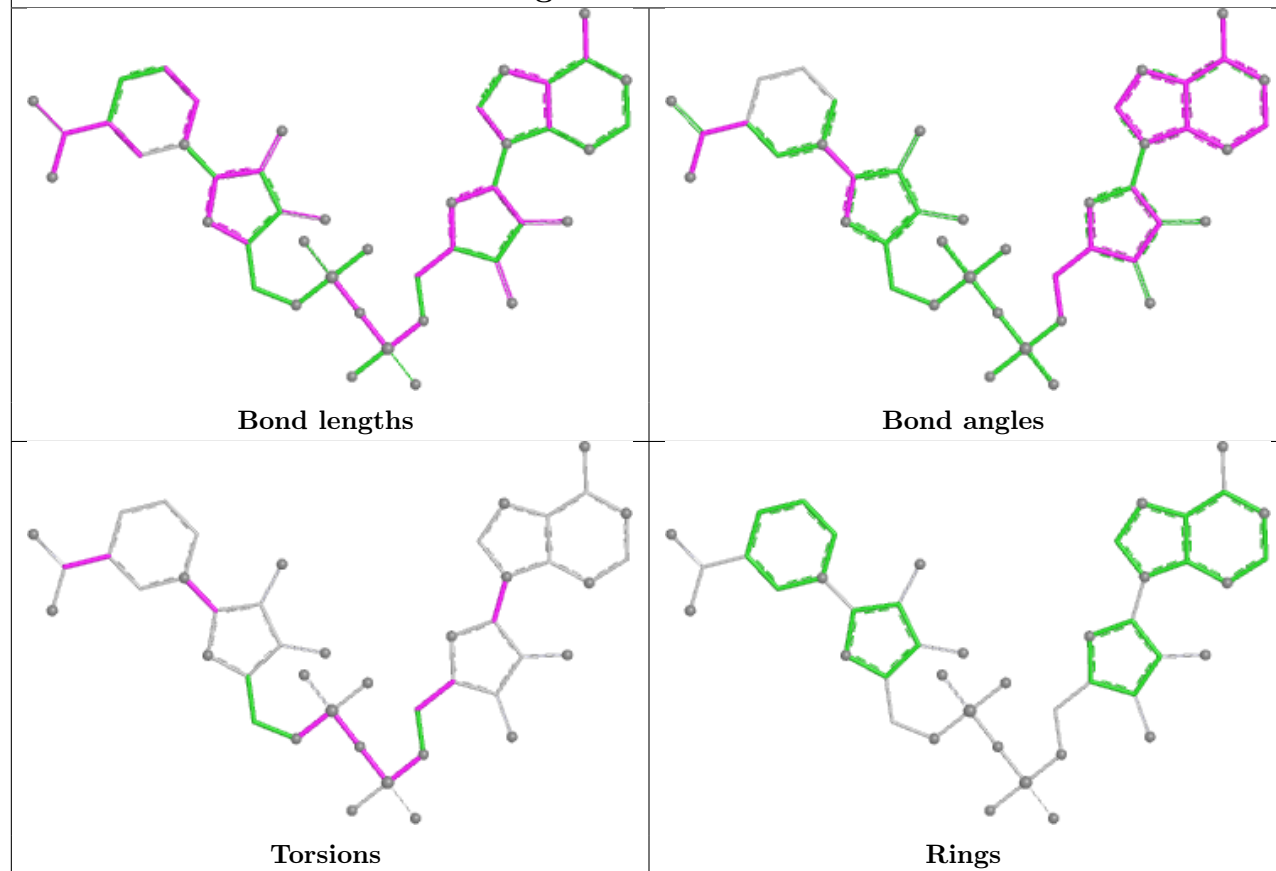
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	GTP	1	0
2	B	601	GLU	6	0
4	A	603	NAI	5	0
2	C	601	GLU	3	0
3	B	602	GTP	2	0
4	E	603	NAI	10	0
4	B	603	NAI	12	0
4	C	603	NAI	4	0
4	A	604	NAI	7	0
4	F	603	NAI	3	0
4	D	603	NAI	5	0
3	F	604	GTP	4	0
2	E	601	GLU	6	0
4	F	601	NAI	12	0
4	B	604	NAI	3	0
3	E	602	GTP	1	0
2	A	601	GLU	6	0
4	F	605	NAI	9	0
2	F	602	GLU	4	0

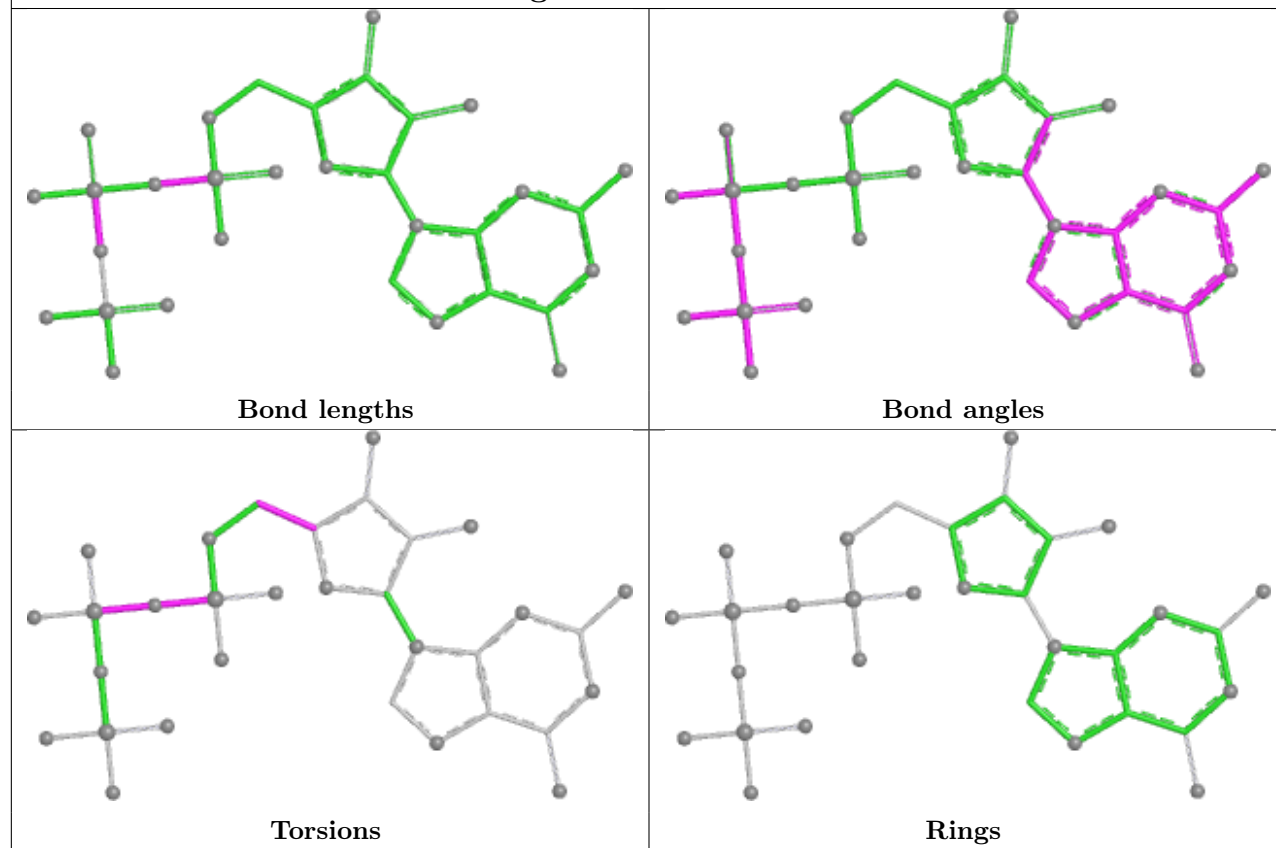
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

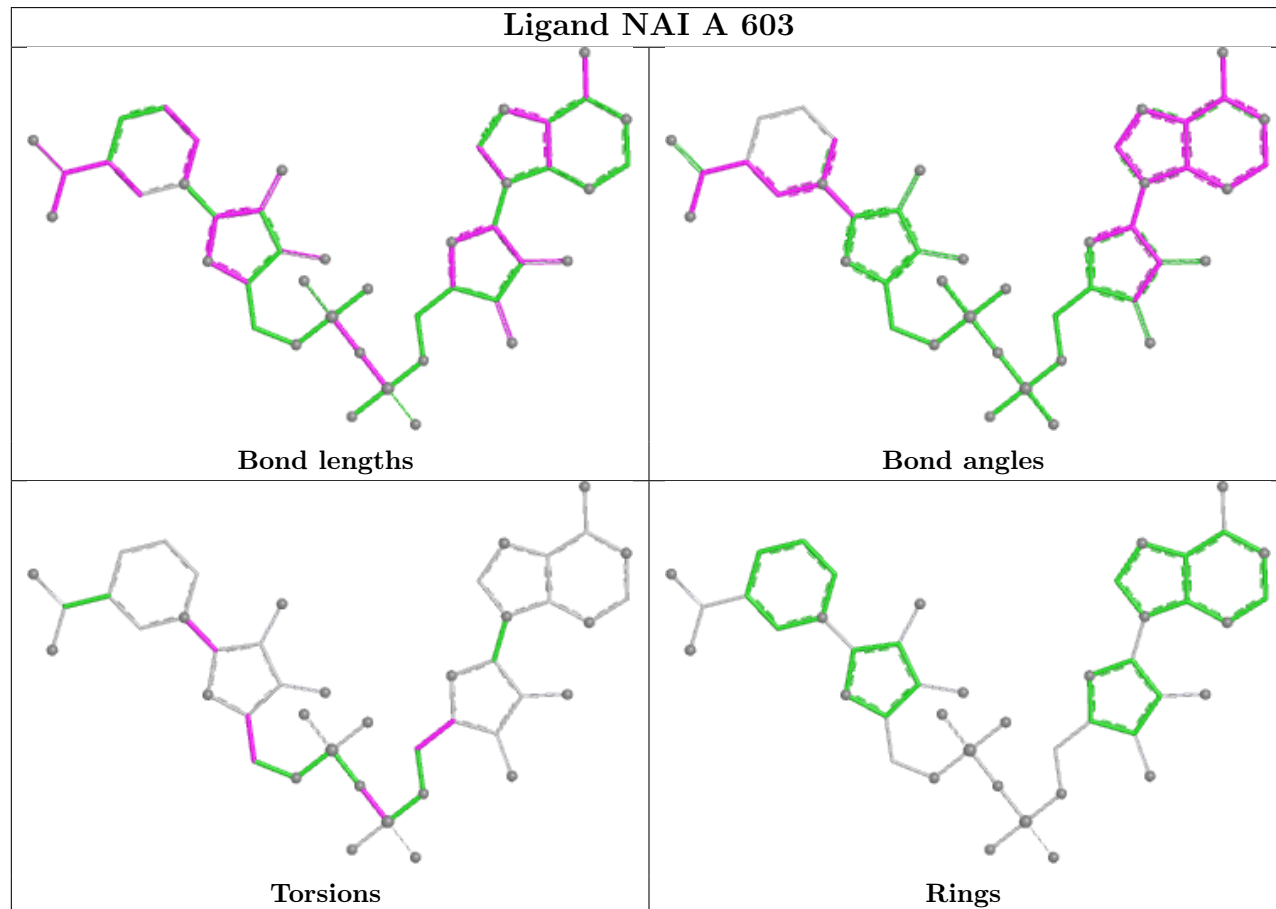
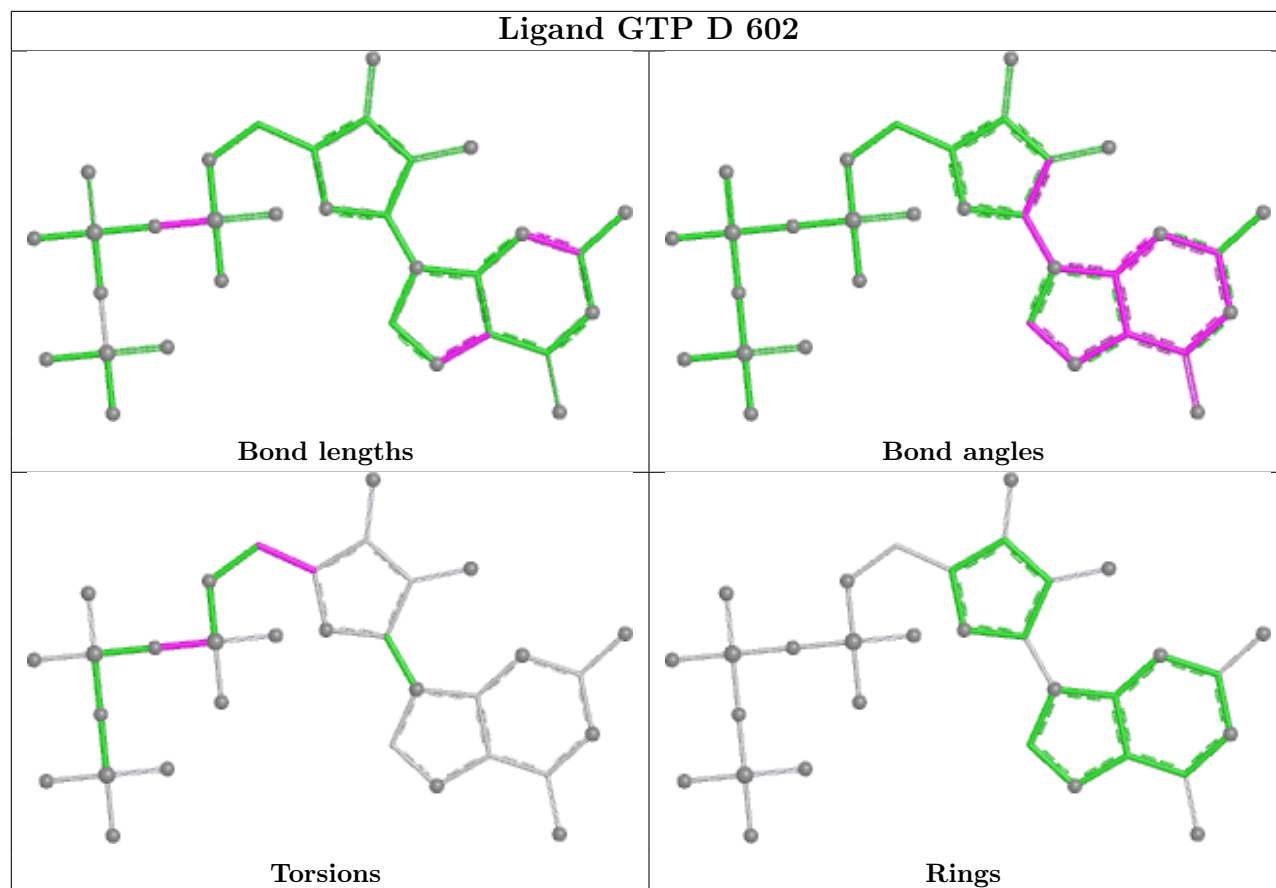


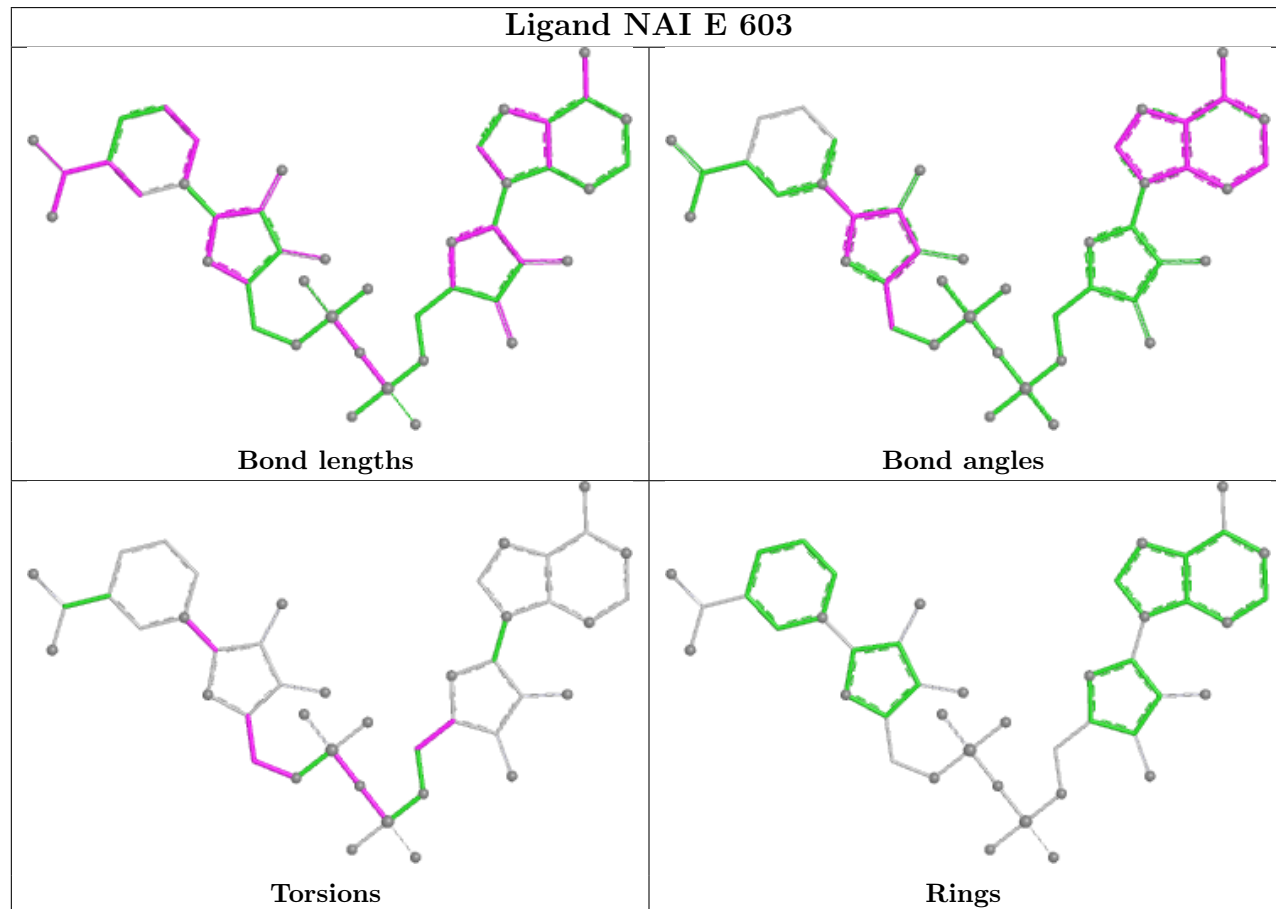
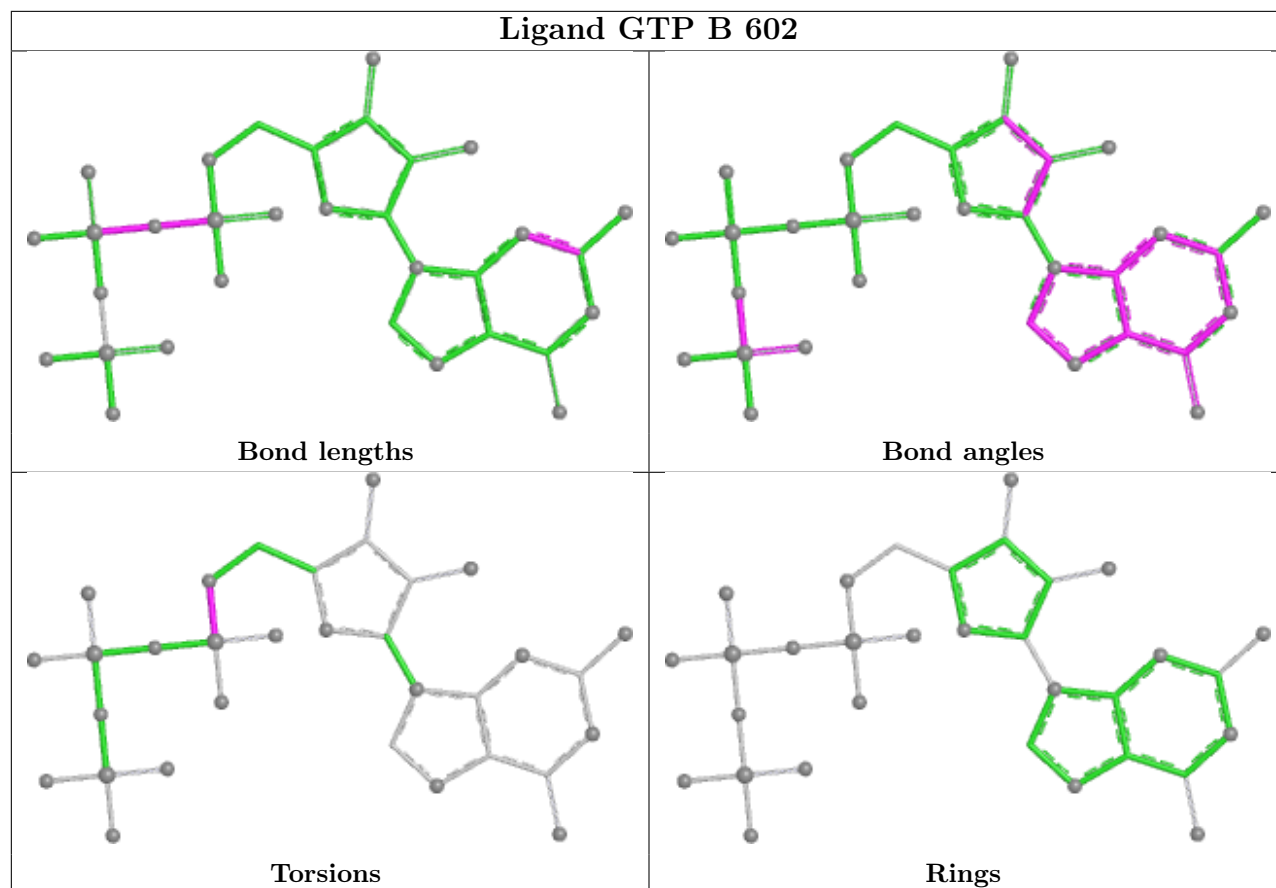
Ligand NAI C 604



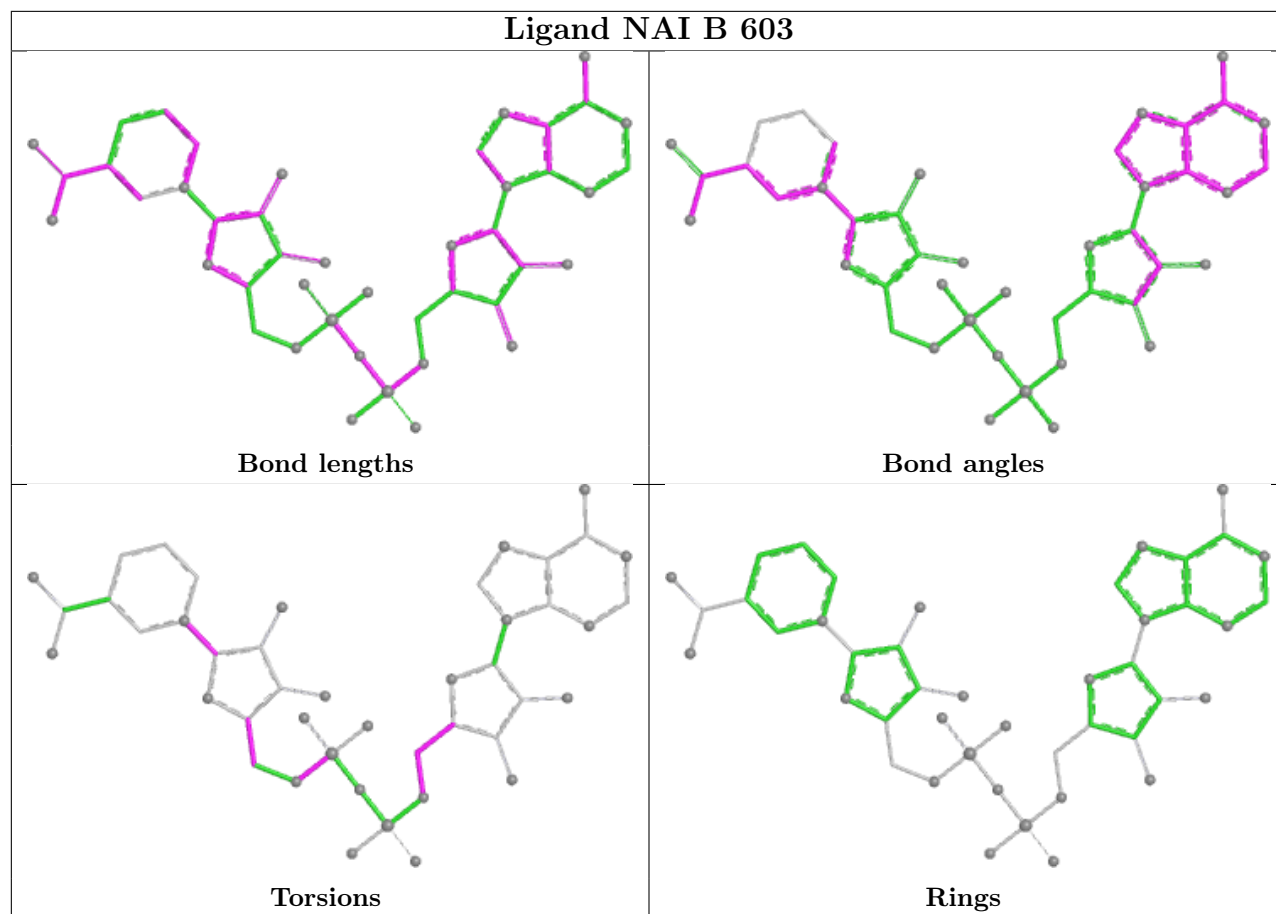
Ligand GTP A 602



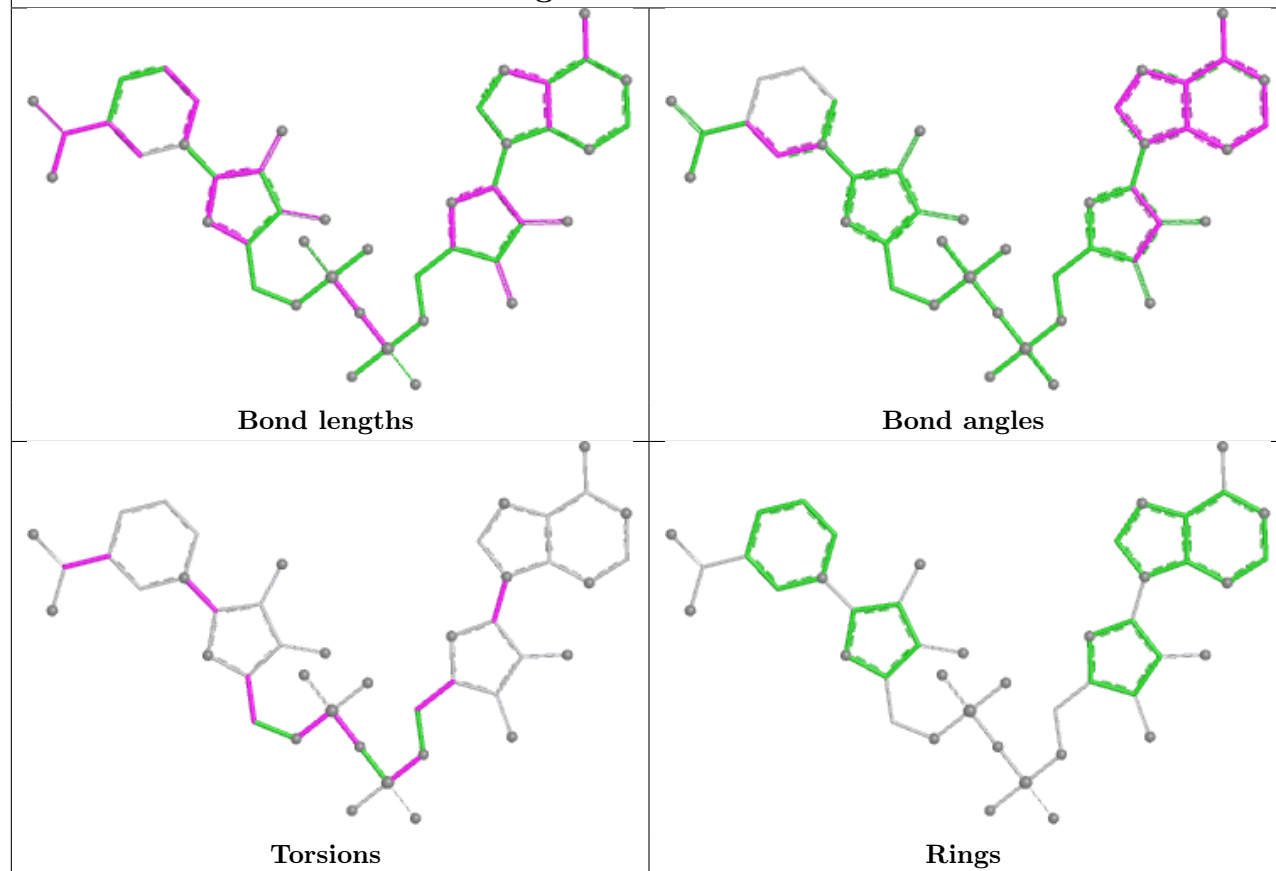




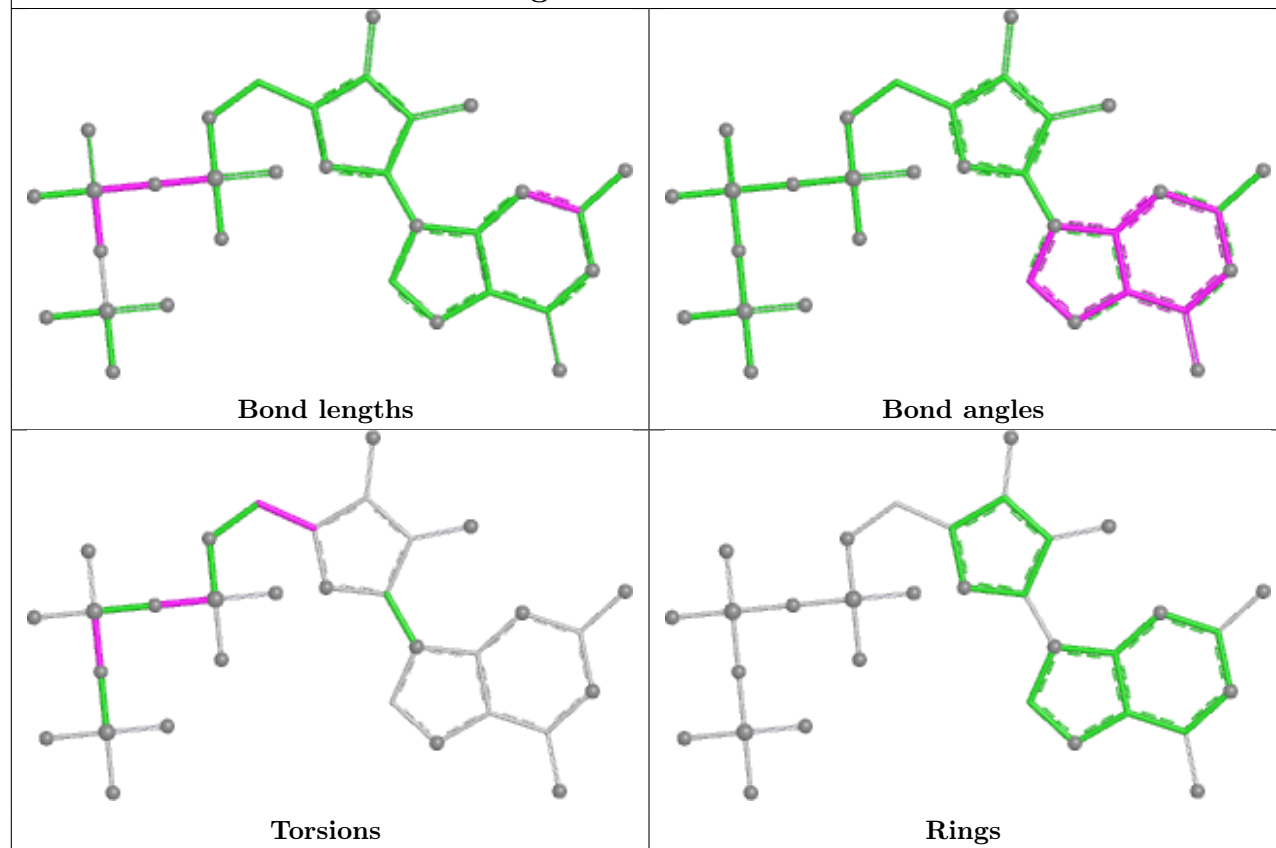
Ligand NAI B 603

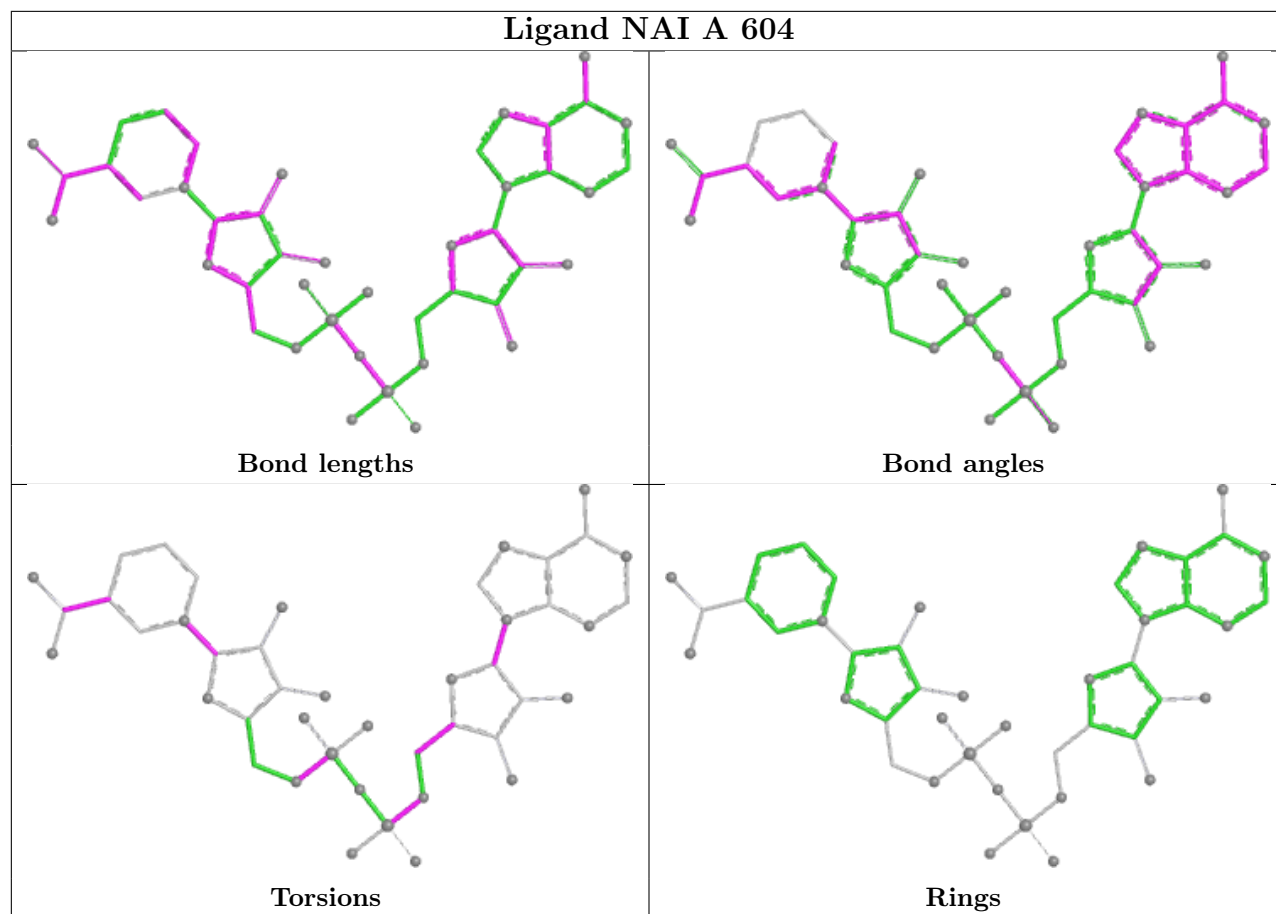


Ligand NAI C 603

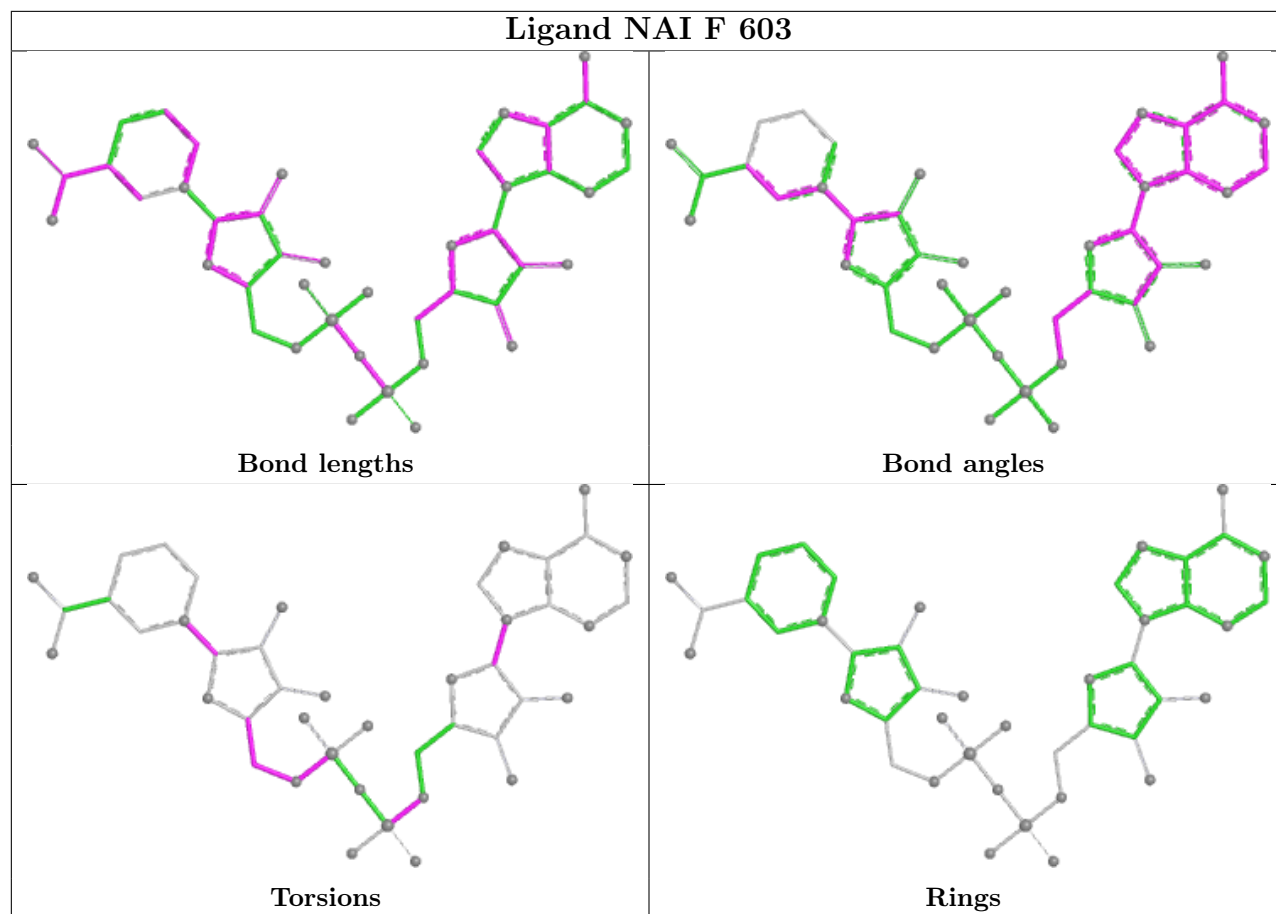


Ligand GTP C 602

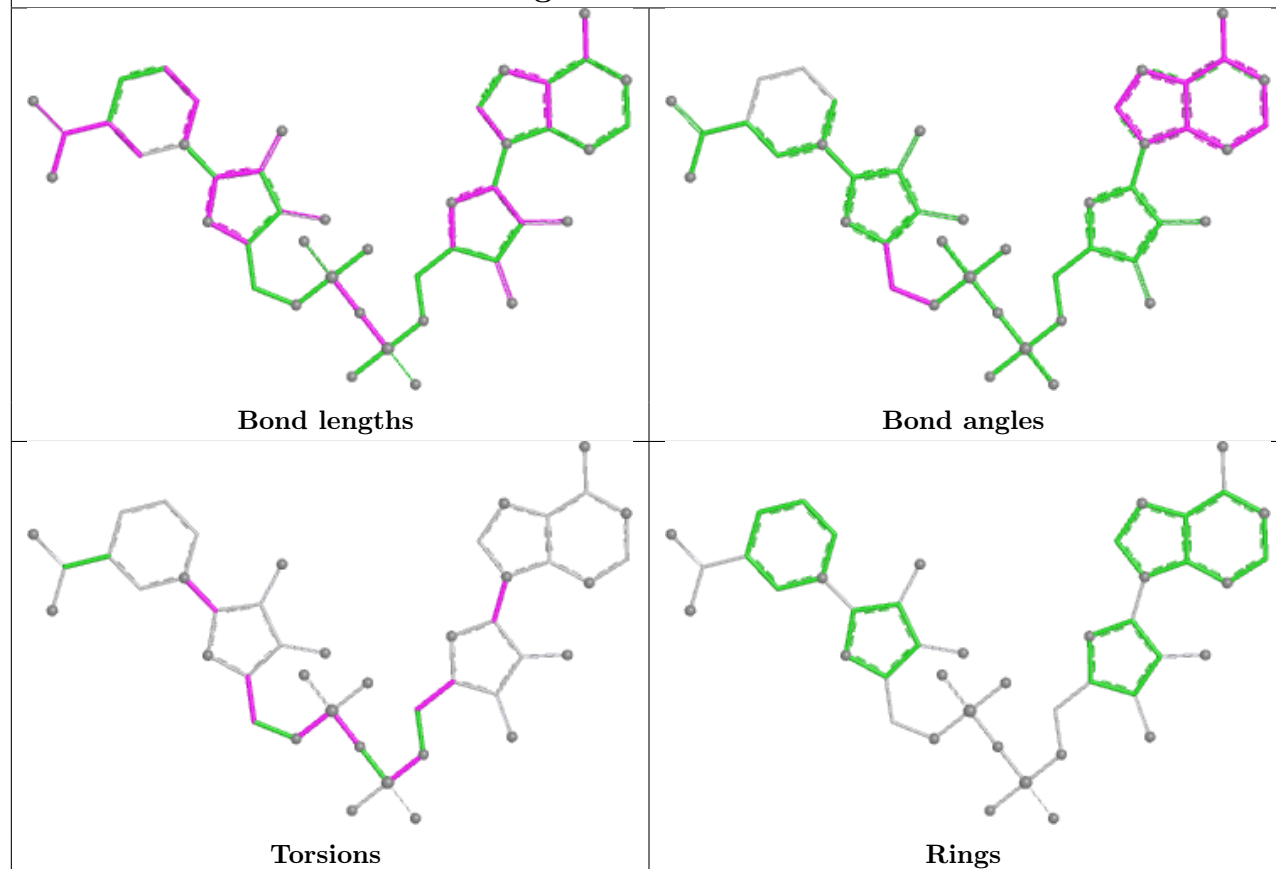




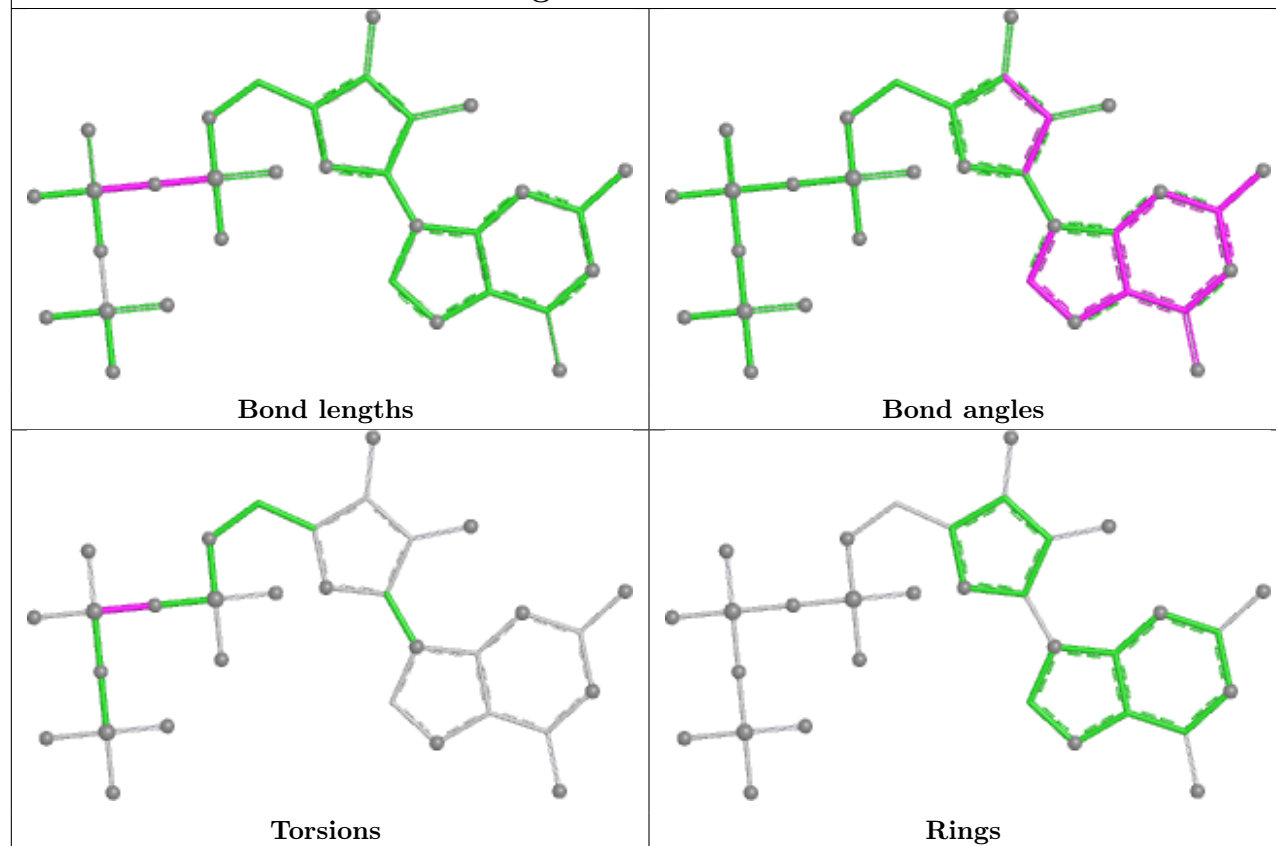
Ligand NAI F 603



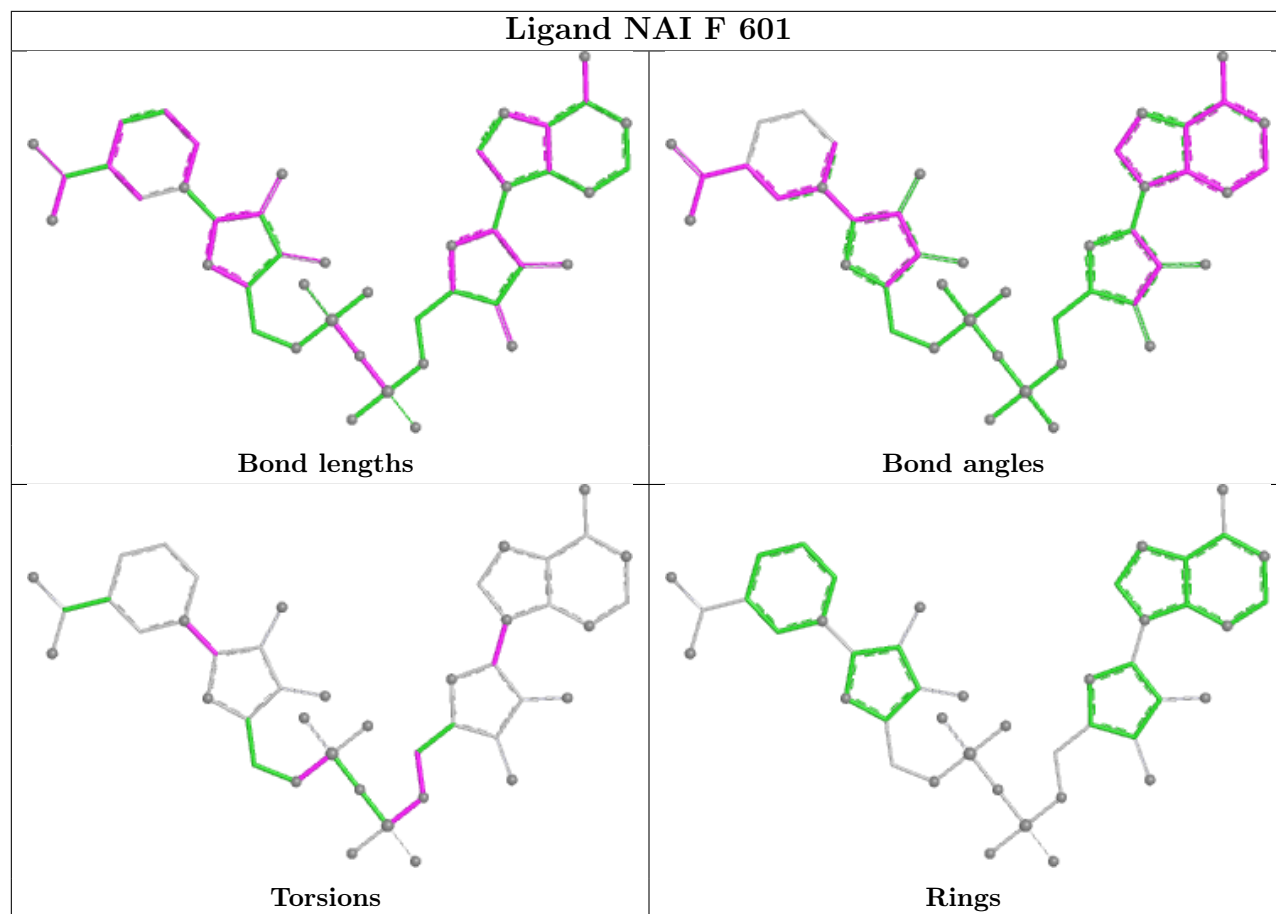
Ligand NAI D 603



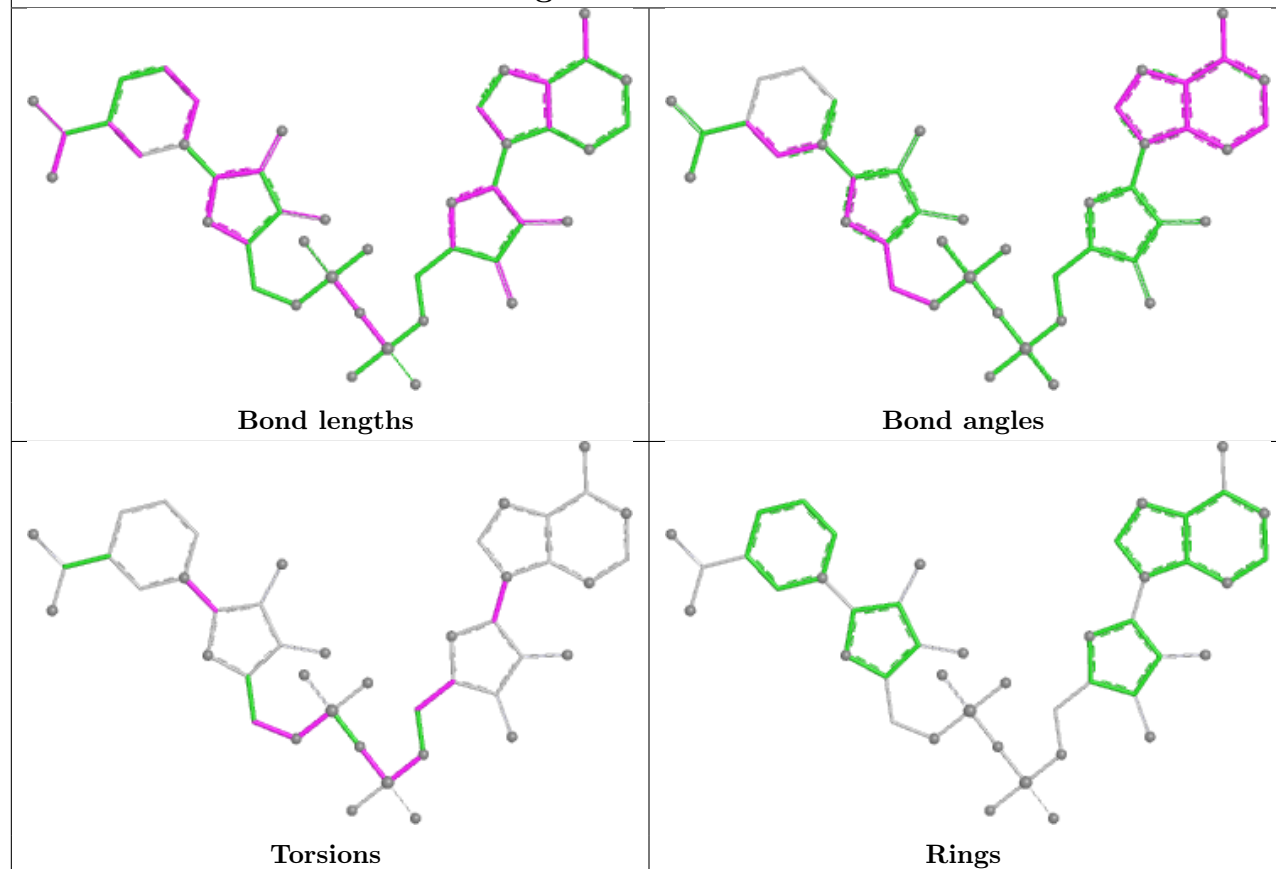
Ligand GTP F 604



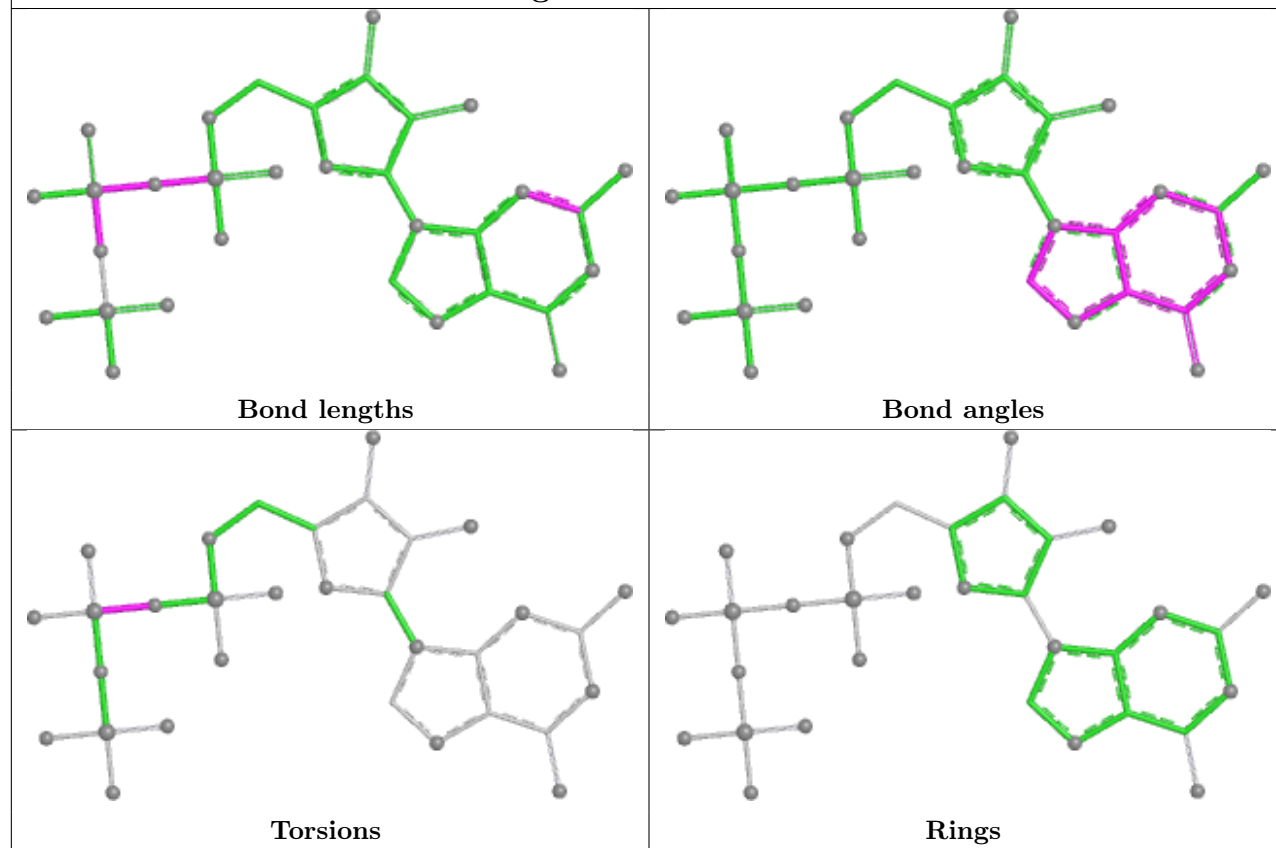
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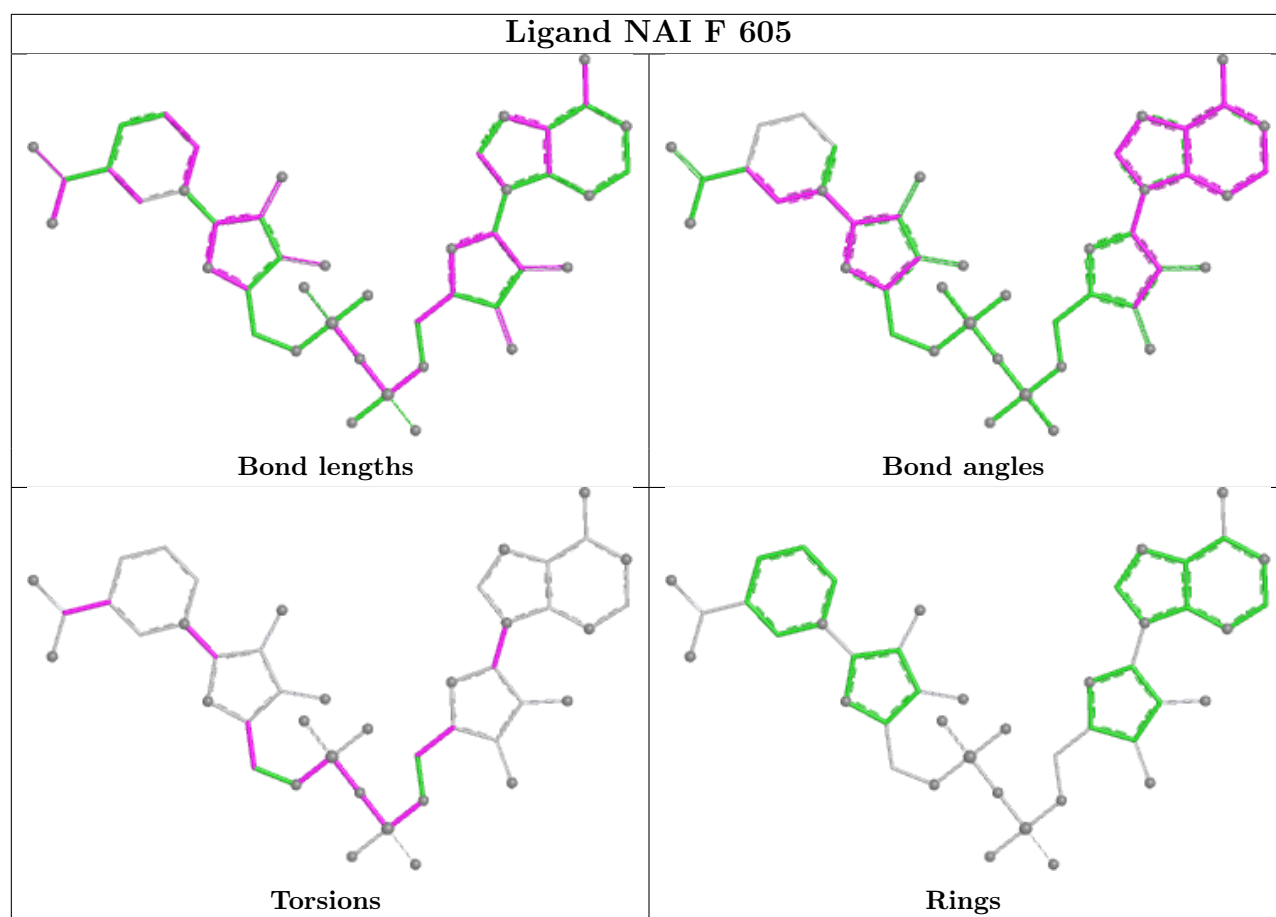


Ligand NAI B 604



Ligand GTP E 602





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	501/582 (86%)	1.01	54 (10%) 11 9	8, 34, 69, 101	0
1	B	501/582 (86%)	0.93	41 (8%) 17 13	7, 29, 65, 94	0
1	C	501/582 (86%)	1.14	73 (14%) 6 5	12, 37, 72, 99	0
1	D	501/582 (86%)	0.96	43 (8%) 16 12	8, 30, 62, 89	0
1	E	501/582 (86%)	1.21	80 (15%) 5 4	7, 41, 78, 95	0
1	F	501/582 (86%)	1.06	65 (12%) 7 6	9, 34, 66, 95	0
All	All	3006/3492 (86%)	1.05	356 (11%) 9 8	7, 34, 73, 101	0

All (356) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	THR	6.2
1	D	500	PHE	5.4
1	B	499	THR	5.1
1	F	223	ILE	5.1
1	B	498	VAL	5.1
1	C	500	PHE	4.8
1	A	413	VAL	4.7
1	D	499	THR	4.6
1	C	319	CYS	4.6
1	B	497	GLY	4.5
1	F	443	ALA	4.4
1	F	498	VAL	4.4
1	F	501	THR	4.3
1	F	500	PHE	4.3
1	D	498	VAL	4.2
1	A	37	THR	4.2
1	A	119	ASP	4.2
1	C	286	ILE	4.2
1	C	424	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	4	GLU	4.1
1	A	490	PHE	4.1
1	B	428	ILE	4.1
1	E	250	GLN	4.1
1	E	305	PRO	4.0
1	B	426	GLY	4.0
1	A	395	GLY	3.9
1	E	474	GLY	3.9
1	B	501	THR	3.9
1	C	31	ASP	3.9
1	E	267	GLY	3.9
1	B	393	SER	3.9
1	E	249	VAL	3.8
1	F	251	GLY	3.8
1	B	257	LEU	3.8
1	E	393	SER	3.8
1	F	2	ASP	3.8
1	B	500	PHE	3.8
1	F	190	TYR	3.7
1	F	71	SER	3.7
1	A	410	LEU	3.7
1	E	266	PHE	3.7
1	E	498	VAL	3.6
1	D	210	GLY	3.6
1	D	402	GLU	3.6
1	C	301	ILE	3.6
1	D	501	THR	3.6
1	E	288	PRO	3.5
1	E	315	LEU	3.5
1	D	285	GLY	3.5
1	A	484	ASN	3.5
1	F	499	THR	3.5
1	F	298	HIS	3.5
1	C	280	ILE	3.5
1	D	286	ILE	3.5
1	E	475	LEU	3.4
1	E	497	GLY	3.4
1	E	464	ILE	3.4
1	C	242	PHE	3.4
1	C	251	GLY	3.4
1	E	425	GLY	3.4
1	E	1	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	412	SER	3.3
1	D	497	GLY	3.3
1	C	298	HIS	3.3
1	F	189	HIS	3.3
1	F	430	ILE	3.3
1	E	443	ALA	3.3
1	E	252	PHE	3.3
1	E	421	PHE	3.2
1	C	501	THR	3.2
1	E	215	THR	3.2
1	A	440	ILE	3.2
1	F	241	GLY	3.2
1	B	133	PRO	3.2
1	A	23	ILE	3.2
1	E	313	SER	3.1
1	F	1	ALA	3.1
1	D	4	GLU	3.1
1	C	339	VAL	3.1
1	C	62	SER	3.1
1	D	355	GLU	3.1
1	F	440	ILE	3.1
1	C	499	THR	3.1
1	E	251	GLY	3.1
1	B	394	TYR	3.1
1	A	254	ASN	3.1
1	E	2	ASP	3.1
1	E	270	CYS	3.1
1	C	300	THR	3.0
1	E	304	PHE	3.0
1	C	405	SER	3.0
1	A	190	TYR	3.0
1	E	284	ASP	3.0
1	E	501	THR	3.0
1	E	227	ILE	3.0
1	C	441	SER	3.0
1	E	16	PHE	3.0
1	F	317	VAL	3.0
1	C	270	CYS	3.0
1	E	226	PHE	3.0
1	B	347	GLY	2.9
1	E	500	PHE	2.9
1	D	243	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	477	LEU	2.9
1	D	362	GLU	2.9
1	B	425	GLY	2.9
1	F	394	TYR	2.9
1	F	424	HIS	2.9
1	C	443	ALA	2.9
1	E	481	ALA	2.9
1	E	339	VAL	2.9
1	E	292	GLU	2.8
1	C	425	GLY	2.8
1	F	340	LYS	2.8
1	C	68	ASP	2.8
1	A	431	VAL	2.8
1	E	446	LYS	2.8
1	C	343	ILE	2.8
1	E	499	THR	2.8
1	D	426	GLY	2.8
1	F	484	ASN	2.8
1	A	336	ALA	2.8
1	E	327	SER	2.8
1	F	70	GLY	2.8
1	B	414	GLN	2.8
1	C	236	LEU	2.8
1	E	72	TRP	2.7
1	F	72	TRP	2.7
1	F	312	GLY	2.7
1	D	413	VAL	2.7
1	F	445	GLU	2.7
1	D	78	TYR	2.7
1	D	1	ALA	2.7
1	A	299	GLY	2.7
1	A	497	GLY	2.7
1	B	242	PHE	2.7
1	A	426	GLY	2.7
1	B	36	GLU	2.7
1	F	402	GLU	2.7
1	B	416	SER	2.7
1	E	334	SER	2.7
1	A	428	ILE	2.7
1	F	227	ILE	2.7
1	E	398	THR	2.7
1	D	443	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	339	VAL	2.7
1	E	293	ASP	2.7
1	A	226	PHE	2.6
1	C	308	LYS	2.6
1	A	103	GLU	2.6
1	E	355	GLU	2.6
1	B	443	ALA	2.6
1	C	162	VAL	2.6
1	A	394	TYR	2.6
1	E	19	ARG	2.6
1	A	302	LEU	2.6
1	A	278	GLY	2.6
1	A	402	GLU	2.6
1	C	29	VAL	2.6
1	F	338	ARG	2.6
1	D	334	SER	2.6
1	E	476	ASP	2.6
1	C	4	GLU	2.6
1	E	65	ILE	2.6
1	A	429	PRO	2.6
1	C	469	MET	2.5
1	F	444	SER	2.5
1	F	3	ARG	2.5
1	F	45	VAL	2.5
1	D	108	ALA	2.5
1	E	428	ILE	2.5
1	A	266	PHE	2.5
1	D	305	PRO	2.5
1	C	44	ARG	2.5
1	A	498	VAL	2.5
1	F	119	ASP	2.5
1	C	72	TRP	2.5
1	F	429	PRO	2.5
1	E	285	GLY	2.5
1	A	313	SER	2.5
1	B	327	SER	2.5
1	B	489	VAL	2.5
1	B	418	GLU	2.5
1	A	51	ILE	2.5
1	E	343	ILE	2.5
1	A	414	GLN	2.5
1	A	489	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	170	SER	2.5
1	C	368	ILE	2.5
1	C	421	PHE	2.5
1	F	438	ASP	2.5
1	C	30	GLU	2.4
1	C	19	ARG	2.4
1	B	262	TYR	2.4
1	D	95	TYR	2.4
1	B	101	VAL	2.4
1	F	212	ILE	2.4
1	A	270	CYS	2.4
1	C	355	GLU	2.4
1	D	236	LEU	2.4
1	F	244	ASP	2.4
1	D	198	VAL	2.4
1	C	304	PHE	2.4
1	C	328	GLU	2.4
1	F	236	LEU	2.4
1	C	281	TRP	2.4
1	C	305	PRO	2.4
1	D	219	VAL	2.4
1	C	119	ASP	2.4
1	A	1	ALA	2.4
1	A	80	ALA	2.4
1	A	235	ILE	2.4
1	D	93	ILE	2.4
1	E	232	TYR	2.4
1	E	314	ILE	2.4
1	F	428	ILE	2.4
1	B	444	SER	2.4
1	C	498	VAL	2.4
1	A	34	THR	2.3
1	A	87	THR	2.3
1	C	223	ILE	2.3
1	C	406	ASN	2.3
1	F	496	ALA	2.3
1	B	138	ASP	2.3
1	F	250	GLN	2.3
1	A	424	HIS	2.3
1	C	346	GLU	2.3
1	A	412	SER	2.3
1	D	406	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	132	ASN	2.3
1	E	484	ASN	2.3
1	D	40	GLN	2.3
1	E	362	GLU	2.3
1	B	446	LYS	2.3
1	E	235	ILE	2.3
1	A	443	ALA	2.3
1	F	473	LEU	2.3
1	F	68	ASP	2.3
1	A	423	LYS	2.3
1	B	342	LYS	2.3
1	E	367	VAL	2.3
1	A	283	PRO	2.3
1	A	501	THR	2.3
1	E	145	THR	2.3
1	F	195	HIS	2.3
1	B	494	ASN	2.3
1	E	33	LYS	2.3
1	E	225	ASN	2.3
1	F	305	PRO	2.2
1	D	417	LEU	2.2
1	B	427	THR	2.2
1	C	246	THR	2.2
1	F	456	THR	2.2
1	C	190	TYR	2.2
1	C	231	SER	2.2
1	E	95	TYR	2.2
1	E	170	SER	2.2
1	E	306	LYS	2.2
1	C	297	GLN	2.2
1	E	31	ASP	2.2
1	A	268	ALA	2.2
1	E	70	GLY	2.2
1	B	190	TYR	2.2
1	A	370	ASP	2.2
1	D	395	GLY	2.2
1	E	238	MET	2.2
1	F	497	GLY	2.2
1	C	329	LYS	2.2
1	A	500	PHE	2.2
1	B	34	THR	2.2
1	E	34	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	95	TYR	2.2
1	C	310	TYR	2.2
1	D	262	TYR	2.2
1	F	309	ILE	2.2
1	A	406	ASN	2.2
1	B	361	LEU	2.2
1	D	36	GLU	2.2
1	C	274	GLY	2.2
1	D	496	ALA	2.2
1	F	274	GLY	2.2
1	C	295	LYS	2.2
1	F	266	PHE	2.2
1	B	145	THR	2.2
1	E	189	HIS	2.2
1	A	365	ILE	2.2
1	C	344	ILE	2.2
1	F	170	SER	2.2
1	C	397	LEU	2.2
1	E	465	MET	2.2
1	A	116	ALA	2.2
1	E	228	ASN	2.2
1	E	374	ASN	2.2
1	C	422	GLY	2.2
1	F	446	LYS	2.2
1	A	261	ARG	2.2
1	D	189	HIS	2.2
1	B	332	THR	2.1
1	C	13	VAL	2.1
1	D	378	VAL	2.1
1	C	227	ILE	2.1
1	E	280	ILE	2.1
1	E	344	ILE	2.1
1	D	475	LEU	2.1
1	A	458	GLU	2.1
1	B	1	ALA	2.1
1	D	381	SER	2.1
1	C	402	GLU	2.1
1	E	254	ASN	2.1
1	E	354	PRO	2.1
1	A	215	THR	2.1
1	A	286	ILE	2.1
1	F	344	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	485	ALA	2.1
1	E	348	ALA	2.1
1	C	224	GLU	2.1
1	F	441	SER	2.1
1	C	399	PHE	2.1
1	D	281	TRP	2.1
1	F	489	VAL	2.1
1	C	342	LYS	2.1
1	C	365	ILE	2.1
1	F	110	LEU	2.1
1	B	402	GLU	2.1
1	B	442	GLY	2.1
1	C	495	GLU	2.1
1	A	22	SER	2.1
1	A	399	PHE	2.1
1	C	360	PHE	2.1
1	D	276	SER	2.1
1	C	293	ASP	2.1
1	F	314	ILE	2.1
1	F	397	LEU	2.1
1	D	394	TYR	2.1
1	E	333	LYS	2.1
1	C	296	LEU	2.1
1	C	309	ILE	2.1
1	D	32	LEU	2.1
1	C	391	HIS	2.1
1	F	191	ASP	2.1
1	E	345	ALA	2.1
1	E	359	ILE	2.0
1	C	258	HIS	2.0
1	F	480	ALA	2.0
1	E	242	PHE	2.0
1	F	421	PHE	2.0
1	B	340	LYS	2.0
1	B	13	VAL	2.0
1	F	431	VAL	2.0
1	C	409	LEU	2.0
1	E	23	ILE	2.0
1	E	365	ILE	2.0
1	B	221	HIS	2.0
1	F	337	PRO	2.0
1	C	317	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	32	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAI	F	603	44/44	0.61	0.27	16,43,66,71	17
3	GTP	E	602	32/32	0.62	0.17	56,83,98,104	0
4	NAI	D	604	44/44	0.63	0.21	10,32,61,93	11
4	NAI	B	604	44/44	0.67	0.20	19,37,52,71	14
4	NAI	C	603	44/44	0.68	0.23	7,46,62,83	18
3	GTP	D	602	32/32	0.69	0.15	34,65,87,94	0
3	GTP	C	602	32/32	0.69	0.16	41,73,95,108	0
4	NAI	A	604	44/44	0.70	0.21	12,33,59,76	13
4	NAI	F	601	44/44	0.71	0.20	11,31,69,97	14
3	GTP	A	602	32/32	0.75	0.14	30,51,81,91	0
3	GTP	F	604	32/32	0.75	0.13	34,50,77,85	0
2	GLU	E	601	10/10	0.81	0.18	21,22,26,36	0
3	GTP	B	602	32/32	0.83	0.10	23,37,48,50	0
4	NAI	B	603	44/44	0.85	0.15	9,17,36,44	0
2	GLU	B	601	10/10	0.85	0.16	9,15,19,21	0
2	GLU	C	601	10/10	0.85	0.14	15,19,25,25	0
4	NAI	F	605	44/44	0.86	0.16	12,27,44,47	0
4	NAI	A	603	44/44	0.87	0.15	10,23,37,44	0
4	NAI	C	604	44/44	0.87	0.13	18,31,53,66	0
4	NAI	E	603	44/44	0.88	0.12	25,41,72,75	0
2	GLU	A	601	10/10	0.88	0.18	16,20,25,30	0
4	NAI	D	603	44/44	0.89	0.12	15,24,45,55	0

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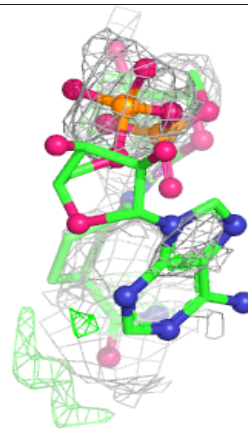
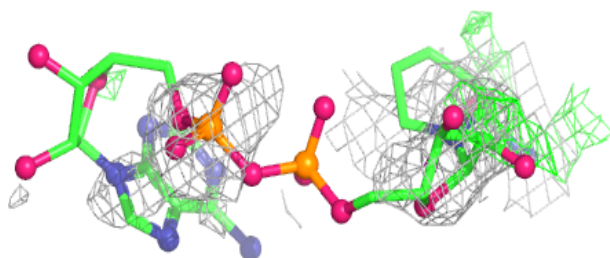
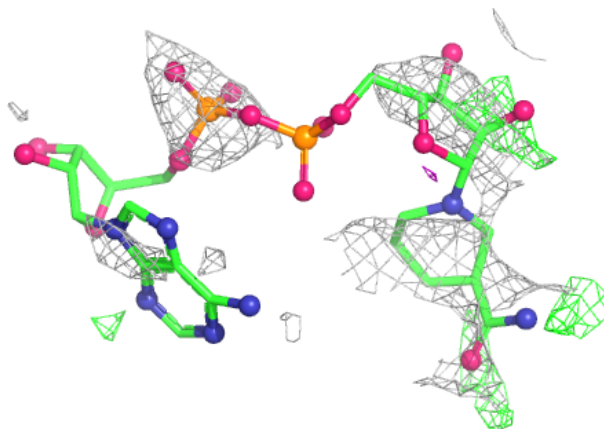
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLU	D	601	10/10	0.92	0.15	10,15,21,27	0
2	GLU	F	602	10/10	0.92	0.11	11,14,18,24	0

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

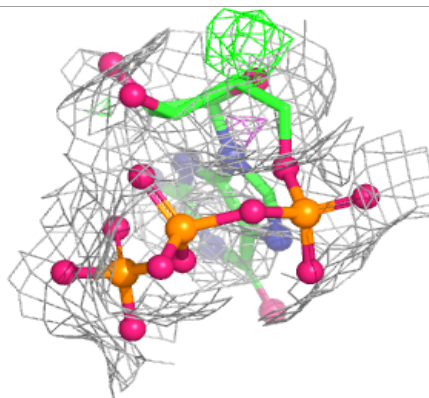
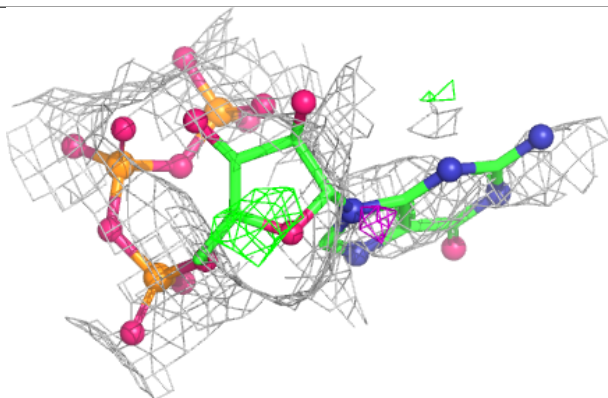
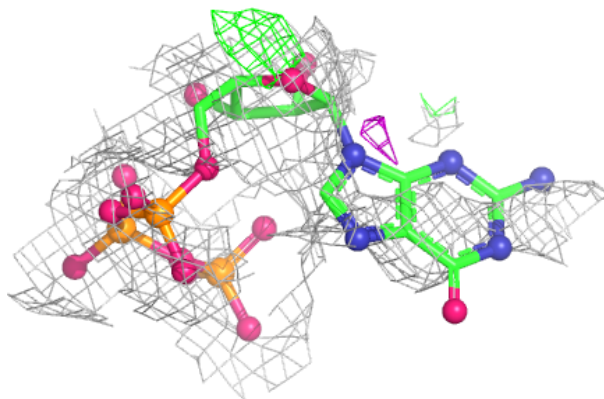
Electron density around NAI F 603:

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

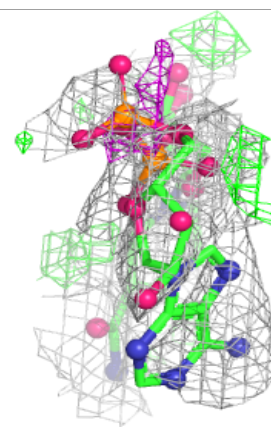
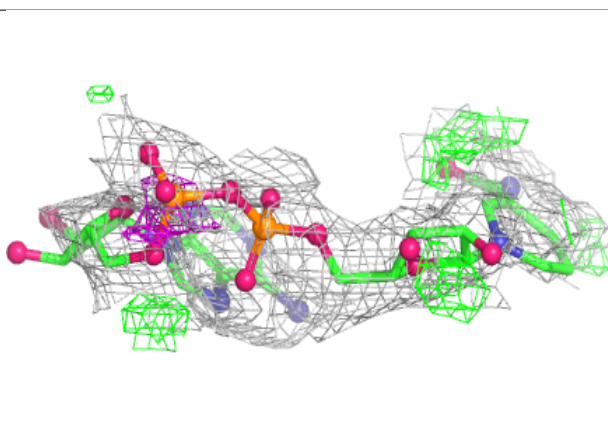
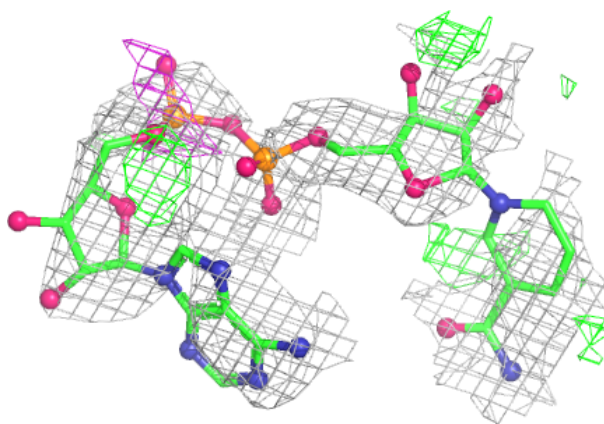


Electron density around GTP E 602:

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

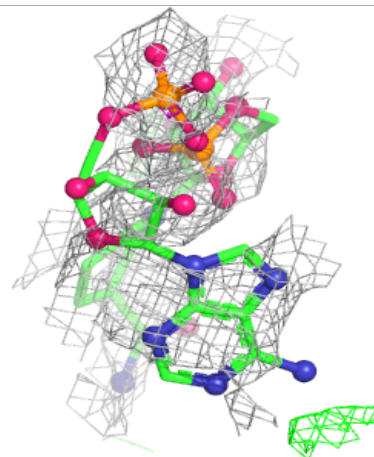
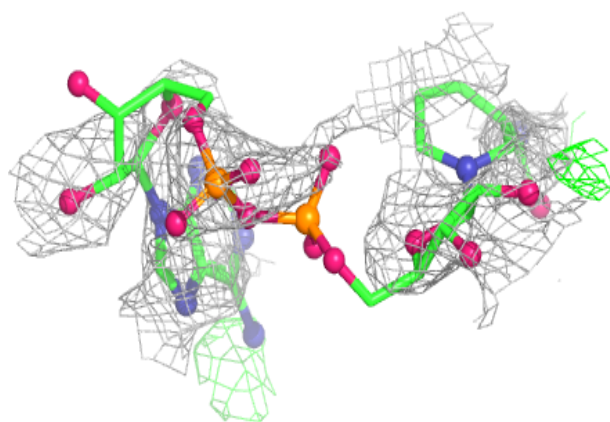
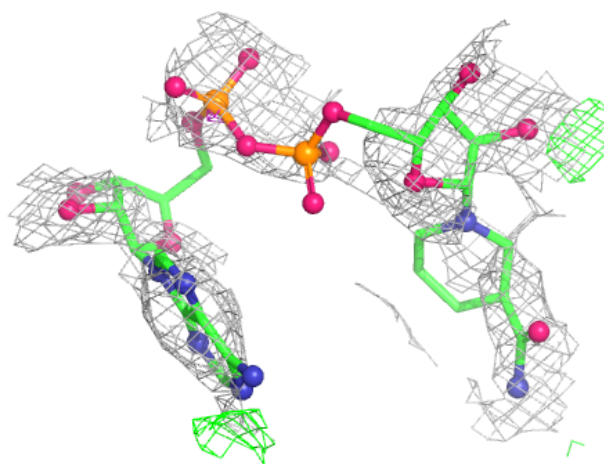
**Electron density around NAI D 604:**

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



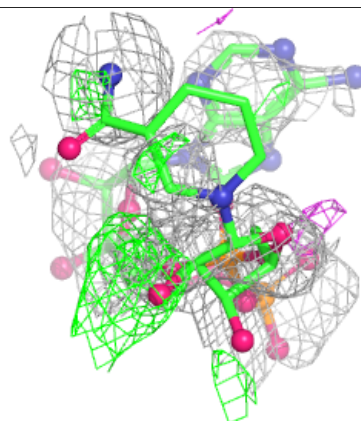
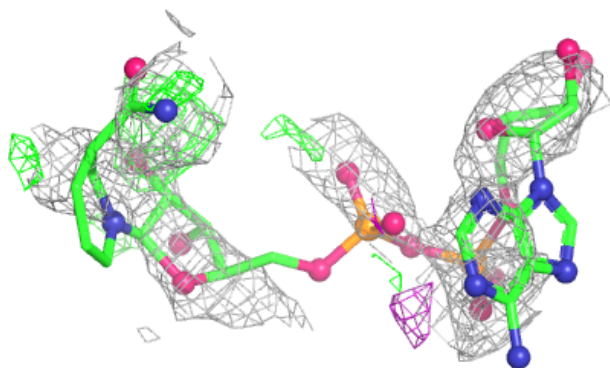
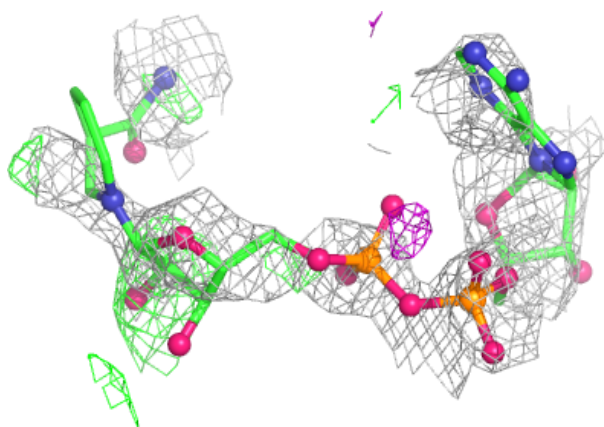
Electron density around NAI B 604:

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

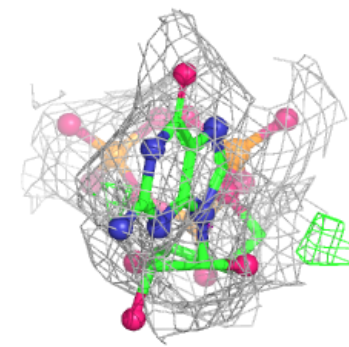
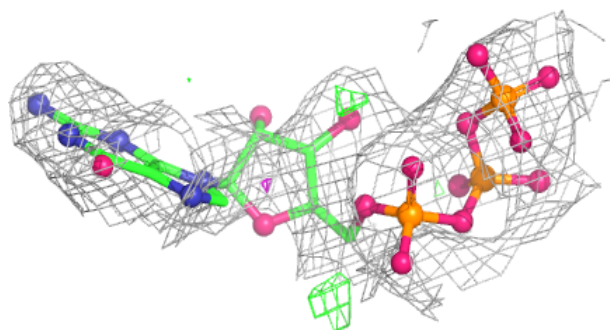
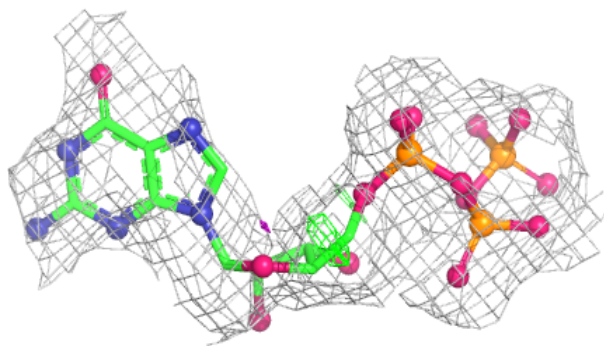


Electron density around NAI C 603:

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

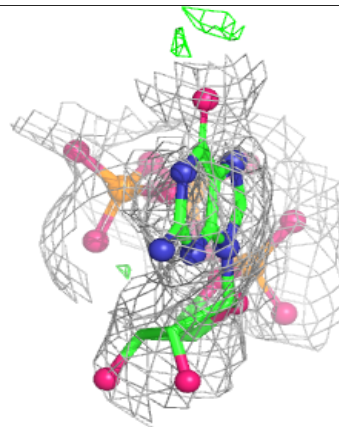
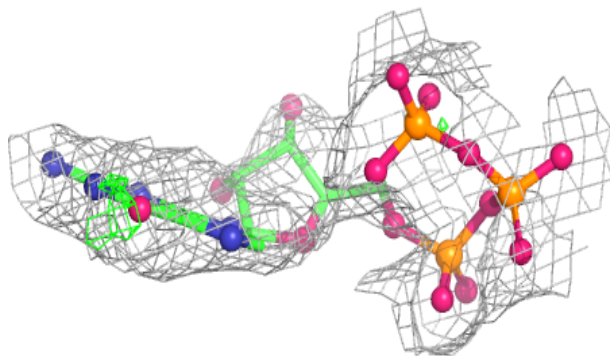
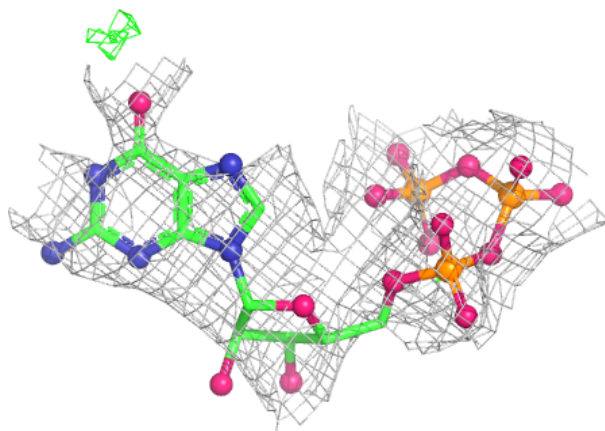
**Electron density around GTP D 602:**

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



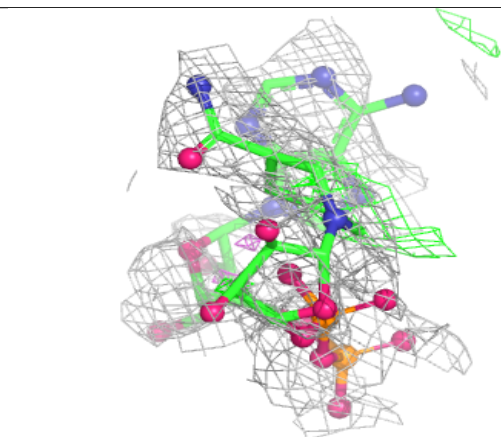
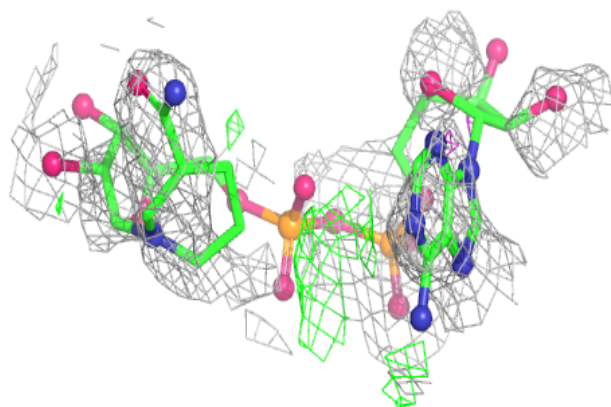
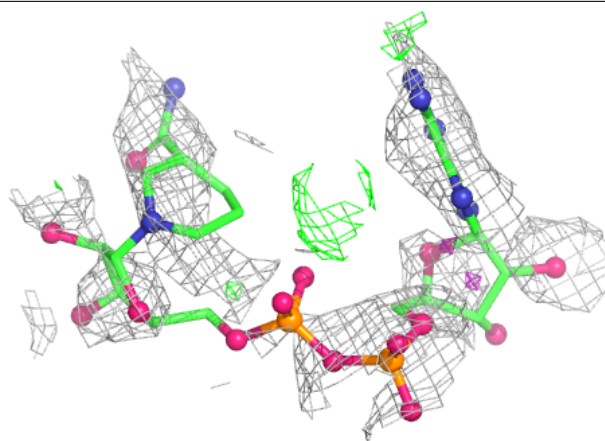
Electron density around GTP C 602:

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

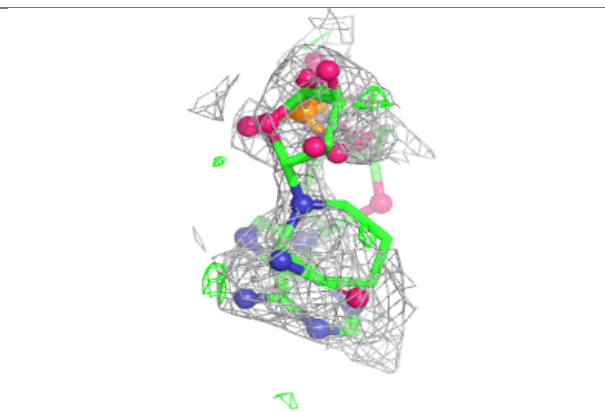
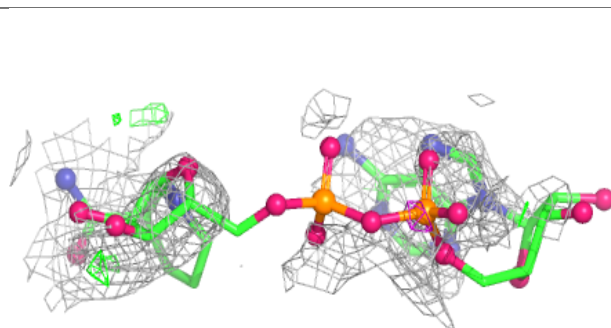
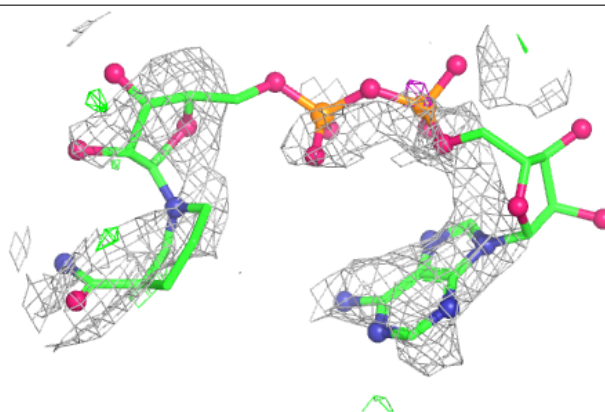


Electron density around NAI A 604:

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

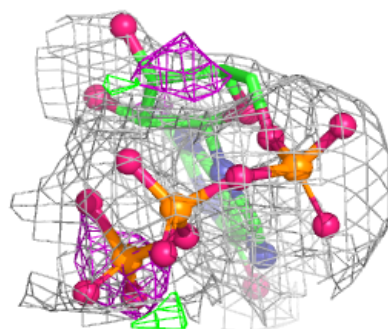
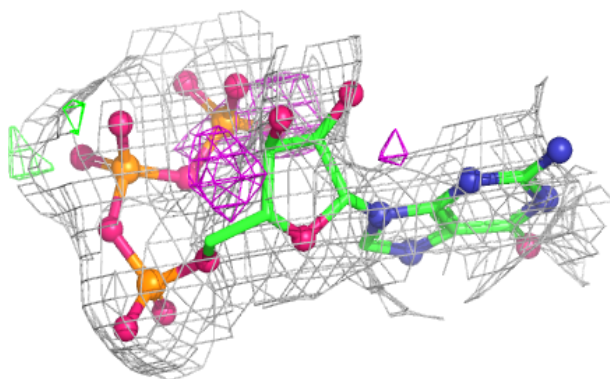
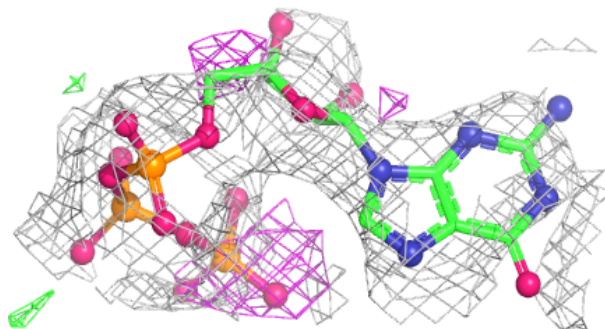
**Electron density around NAI F 601:**

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

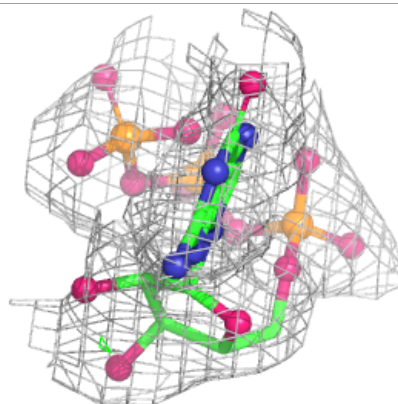
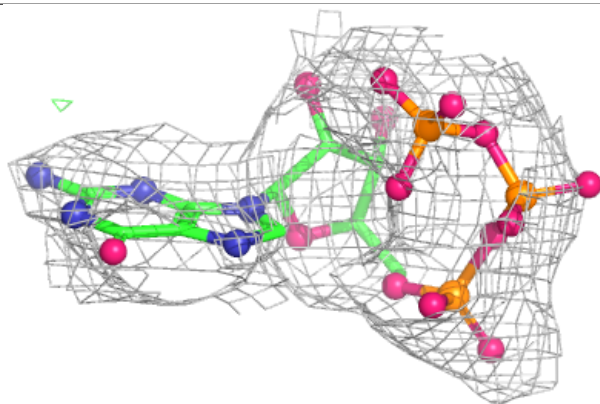
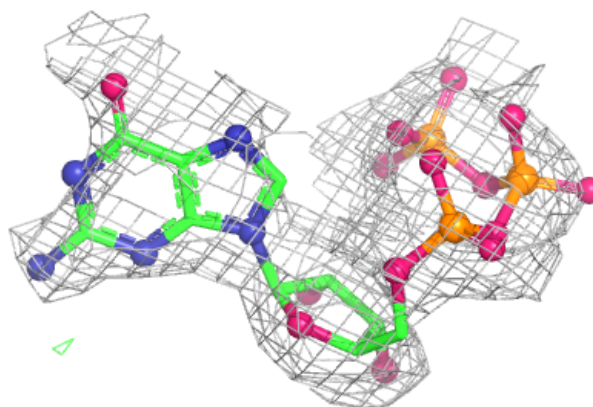


Electron density around GTP A 602:

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

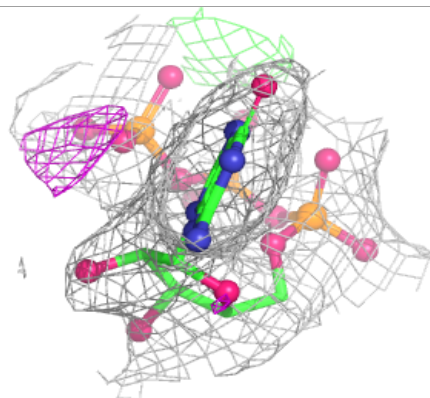
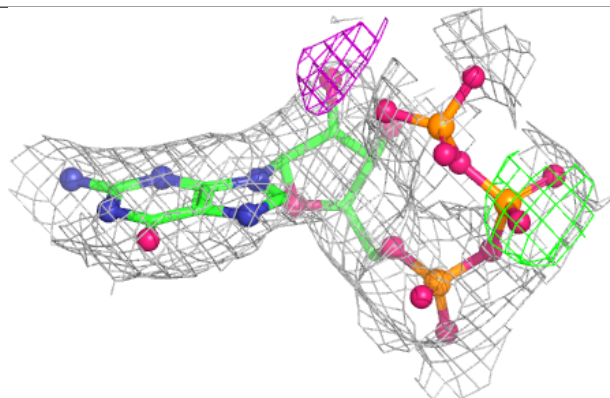
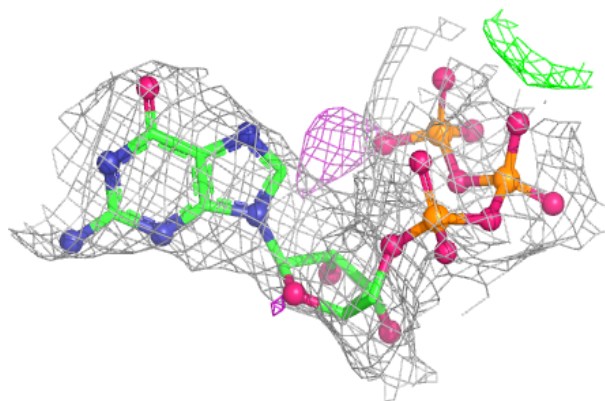
**Electron density around GTP F 604:**

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

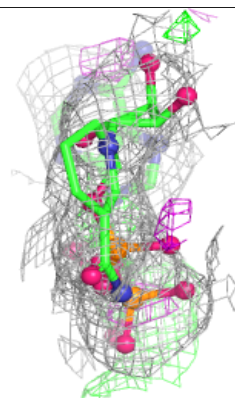
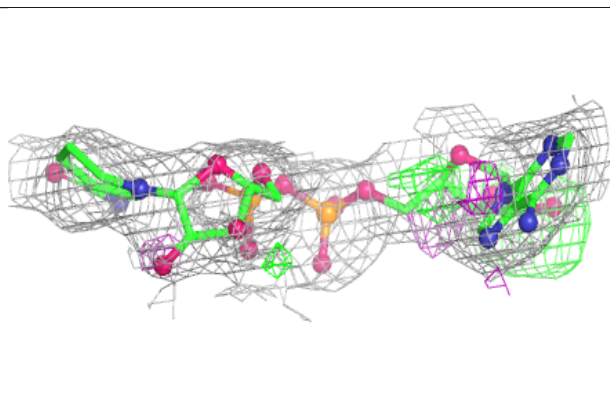
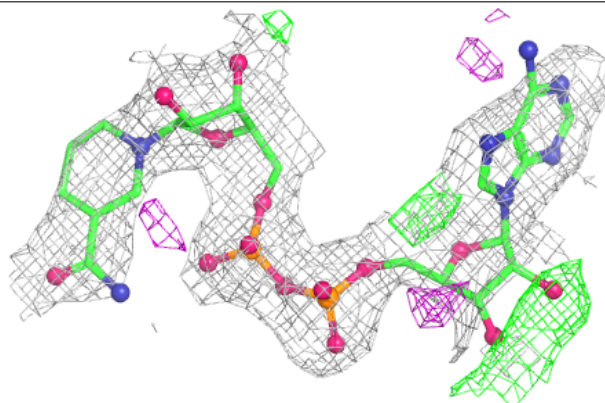


Electron density around GTP B 602:

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

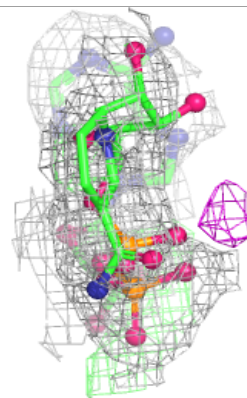
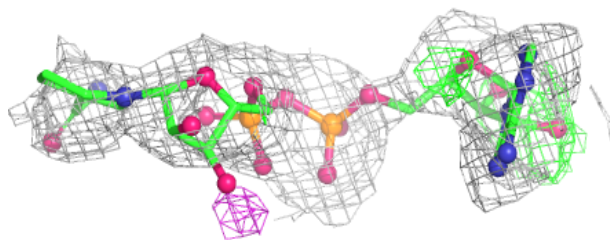
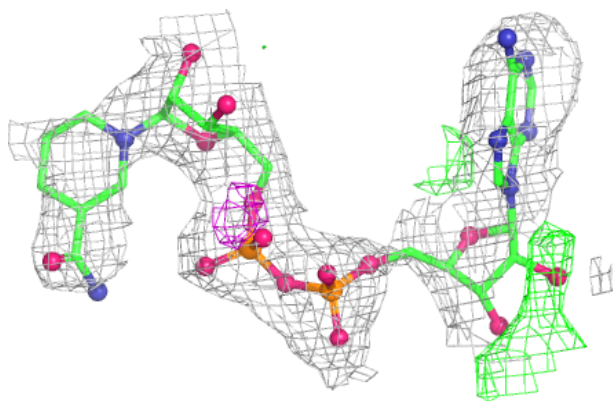
**Electron density around NAI B 603:**

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

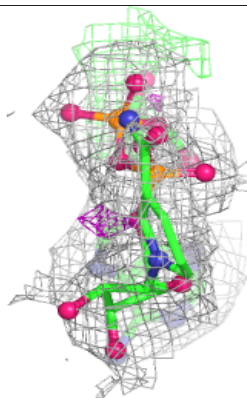
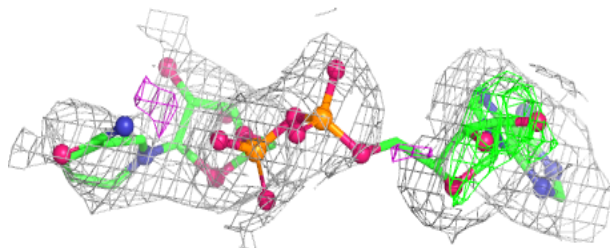
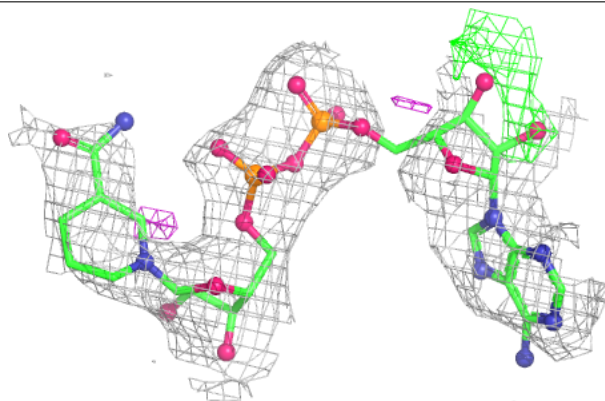


Electron density around NAI F 605:

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

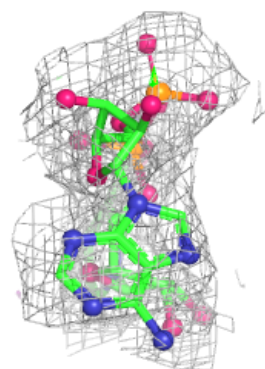
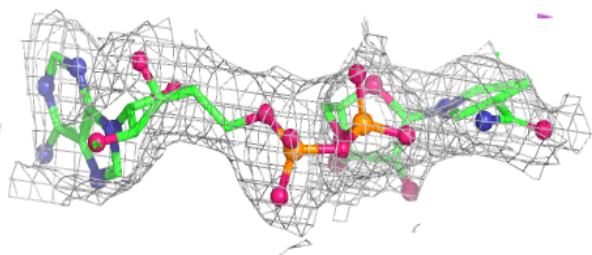
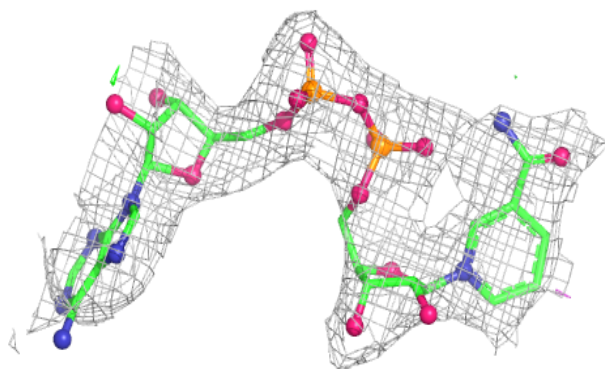
**Electron density around NAI A 603:**

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

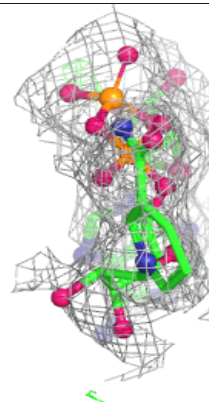
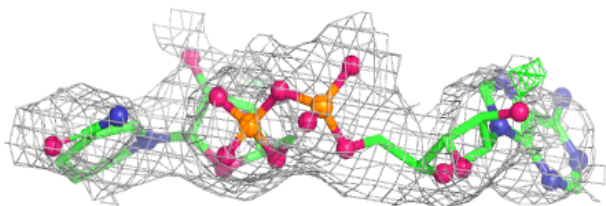
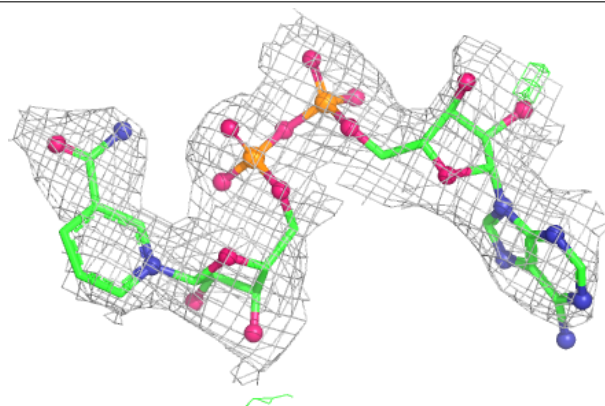


Electron density around NAI C 604:

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

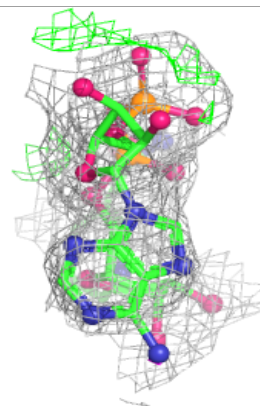
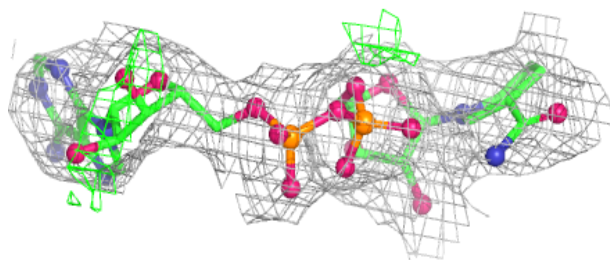
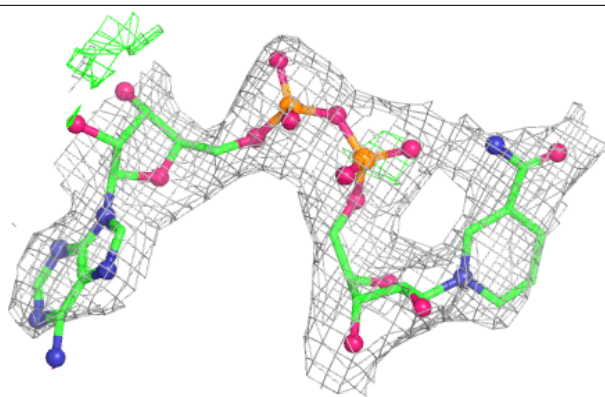
**Electron density around NAI E 603:**

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



Electron density around NAI D 603:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.