Full wwPDB X-ray Structure Validation Report (i)

Dec 15, 2024 – 09:26 AM EST

PDB ID	:	6DHN
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 (i) symbol.

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

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

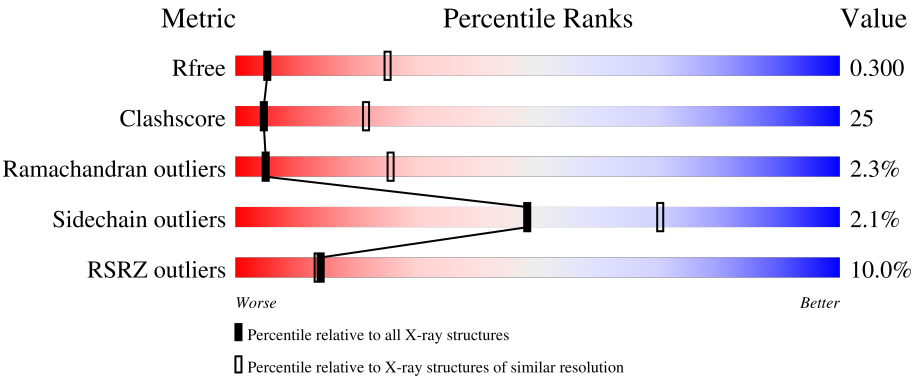
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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}	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (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 <=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% 47% 35% • • 14%
1	B	582	6% 47% 35% • • 14%
1	C	582	10% 46% 36% • • 14%
1	D	582	6% 48% 34% • • 14%
1	E	582	12% 45% 37% • • 14%

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Mol	Chain	Length	Quality of chain
1	F	582	9% 45% 36% 14%

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	C	601	-	-	X	-
2	GLU	D	601	-	-	X	-
2	GLU	E	601	-	-	X	-
2	GLU	F	602	-	-	X	-
3	GTP	A	602	-	-	X	-

2 Entry composition (i)

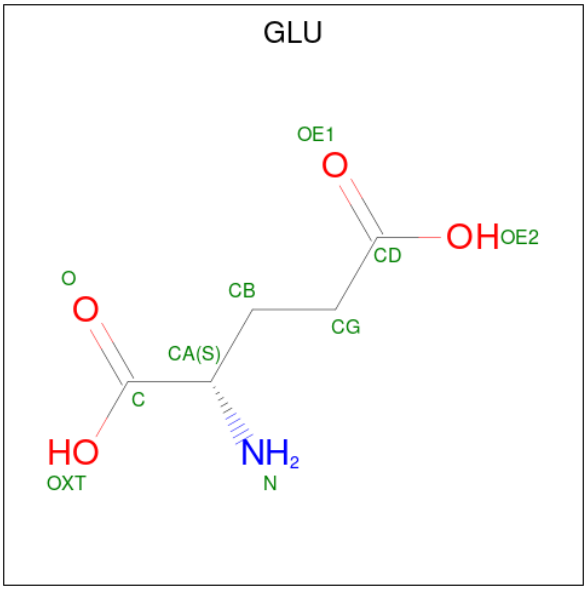
There are 4 unique types of molecules in this entry. The entry contains 24276 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

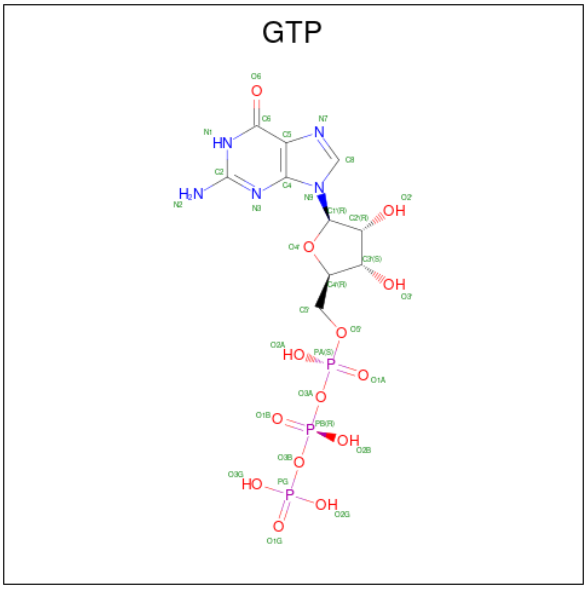
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	B	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	C	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	D	501	Total	C	N	O	S	0	0	0
			3916	2473	687	737	19			
1	E	501	Total	C	N	O	S	0	0	0
			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 (three-letter code: GLU) (formula: $C_5H_9NO_4$).



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 (three-letter code: 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		

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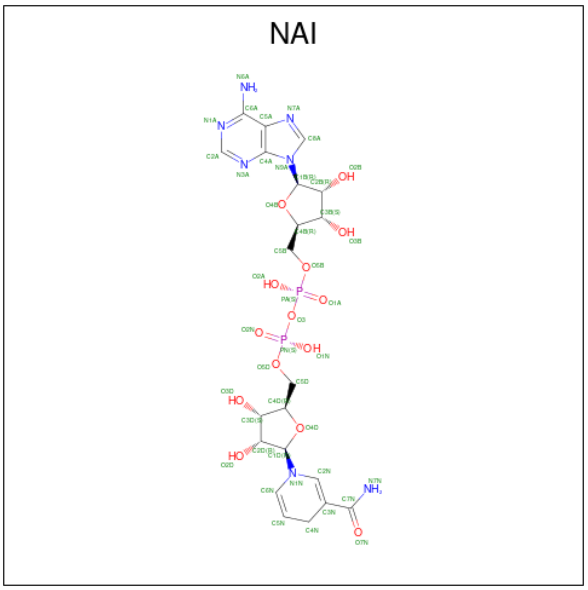
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



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		

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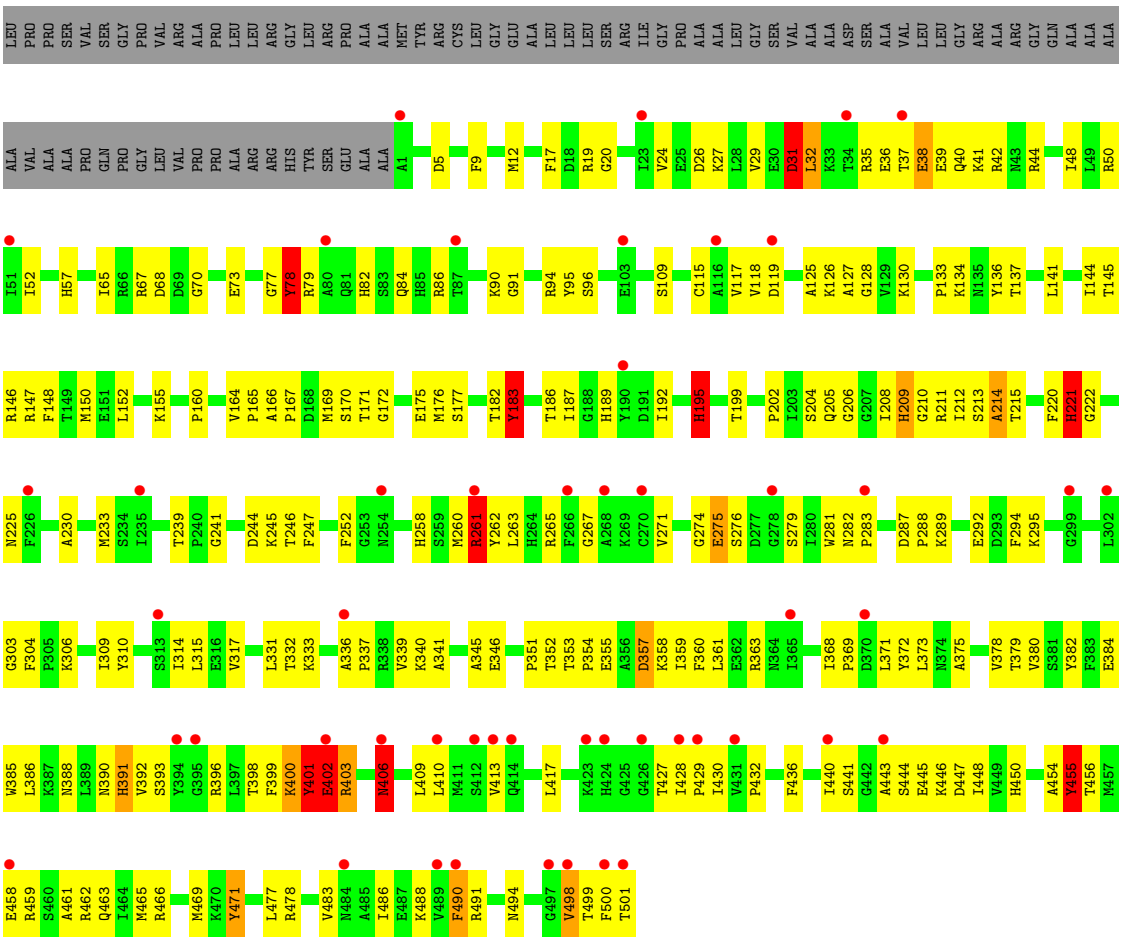
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	F	1	Total	C	N	O	P	16	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

3 Residue-property plots (i)

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

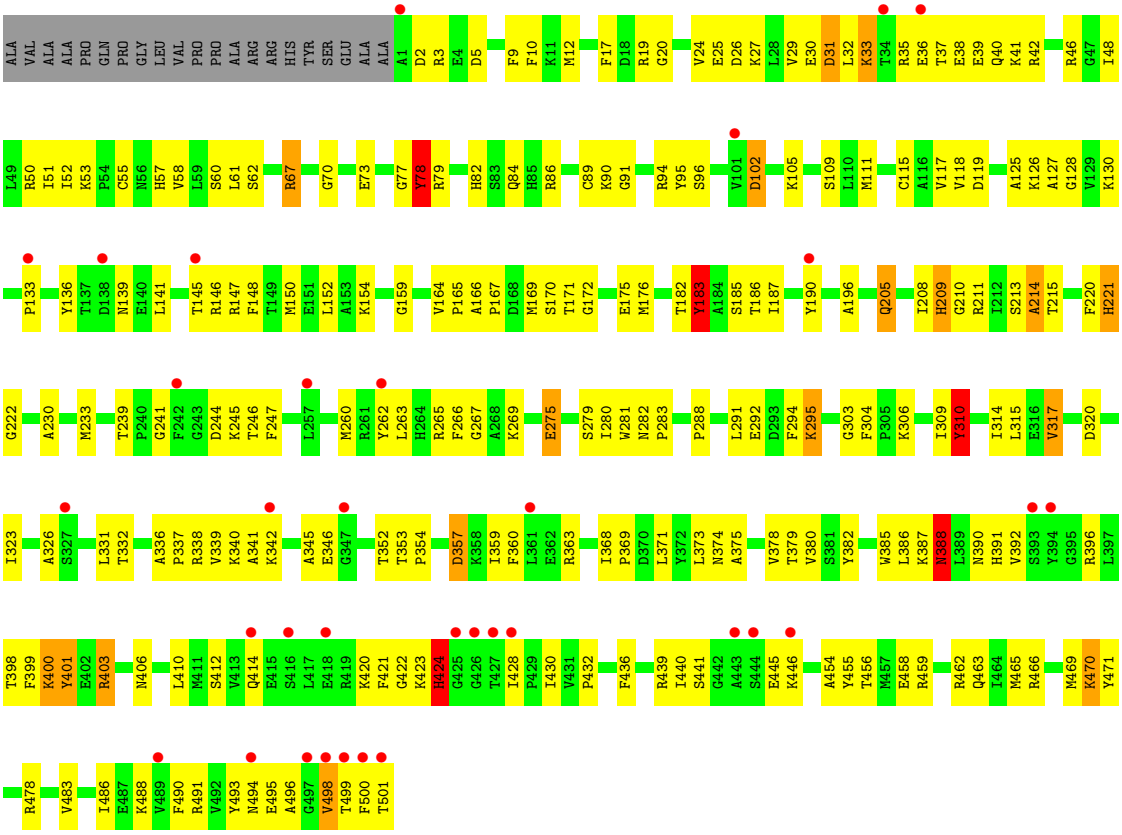
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain A:



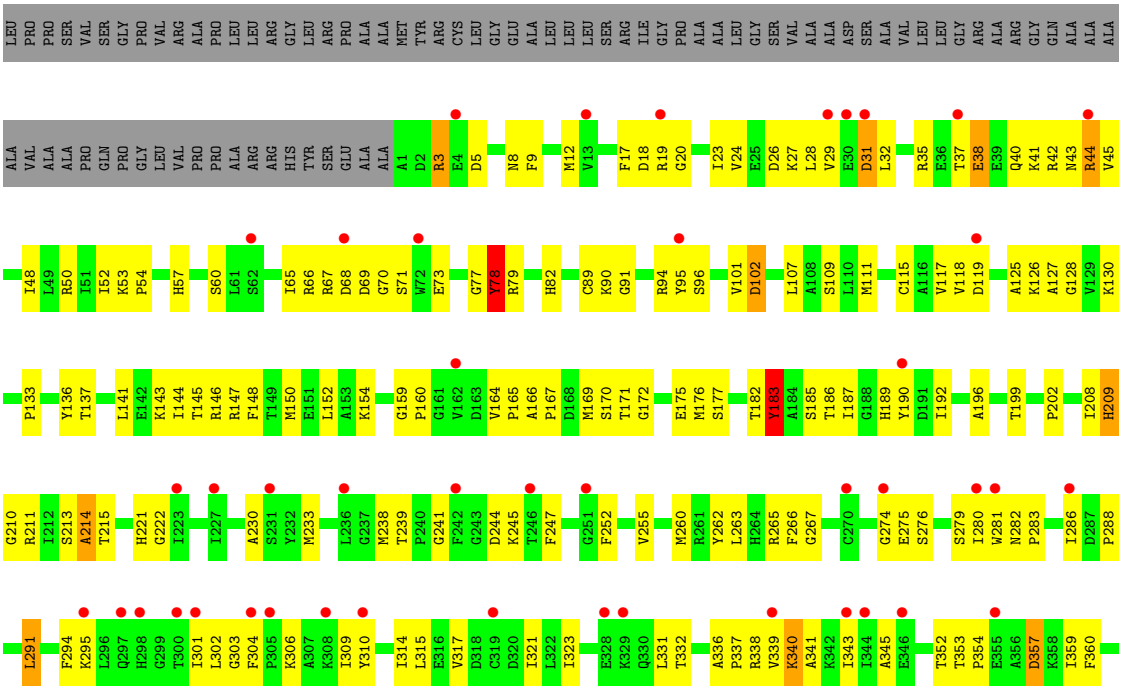
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

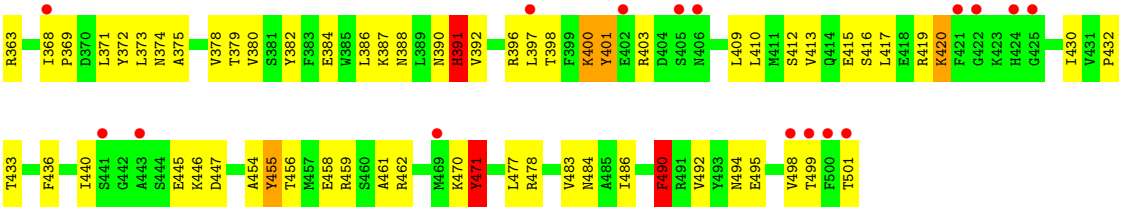
Chain B:



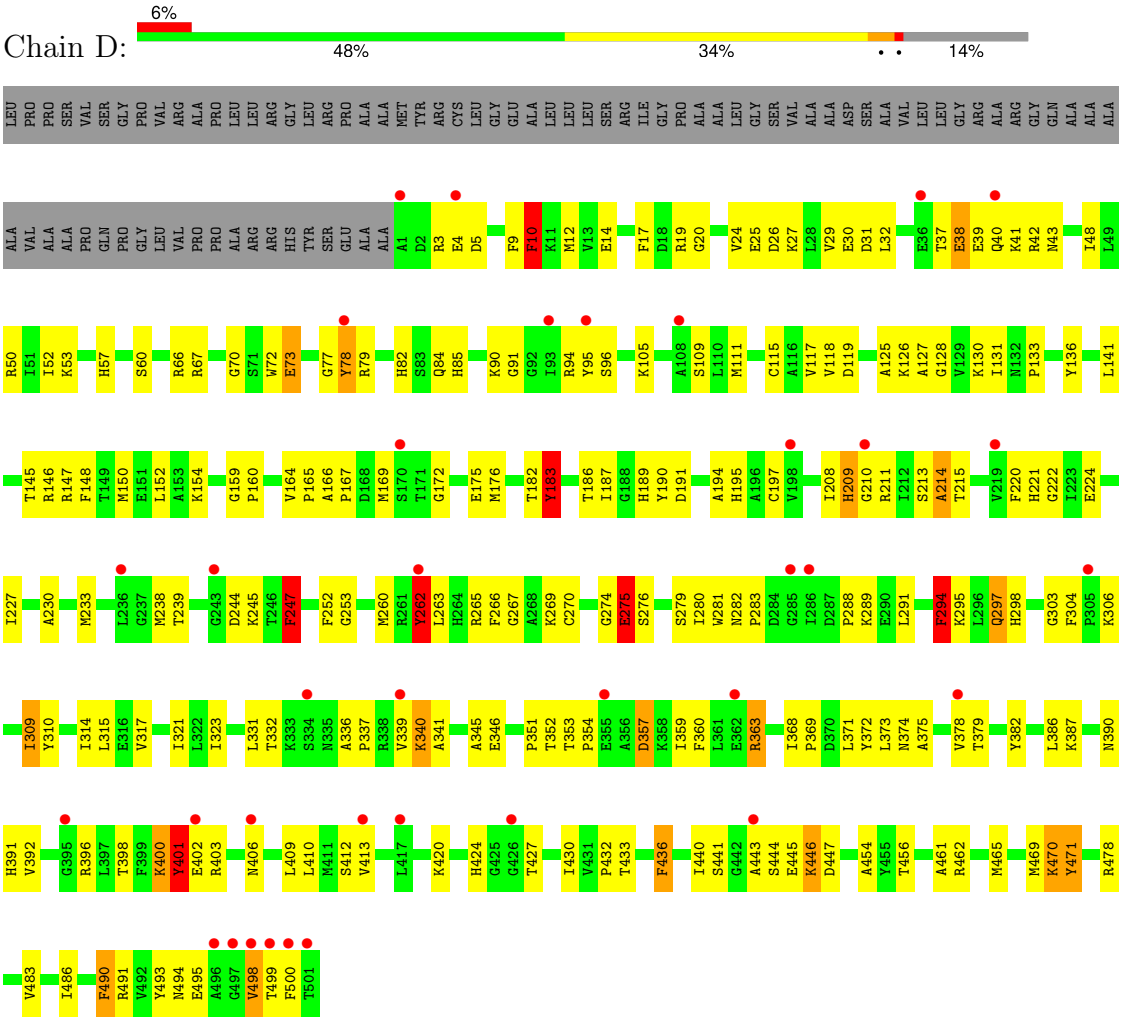
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain C:

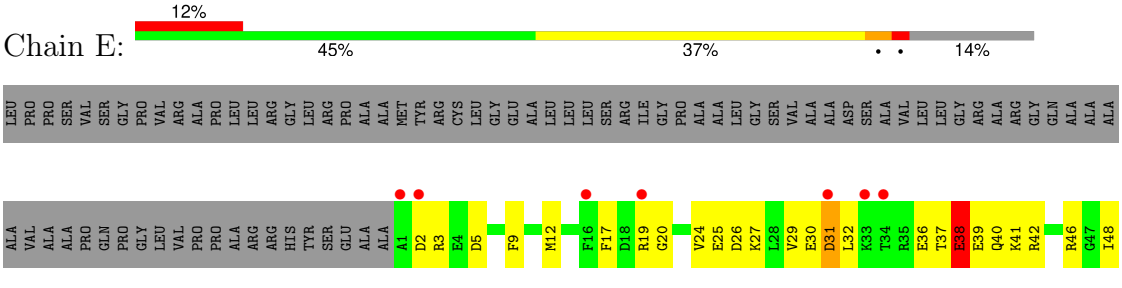


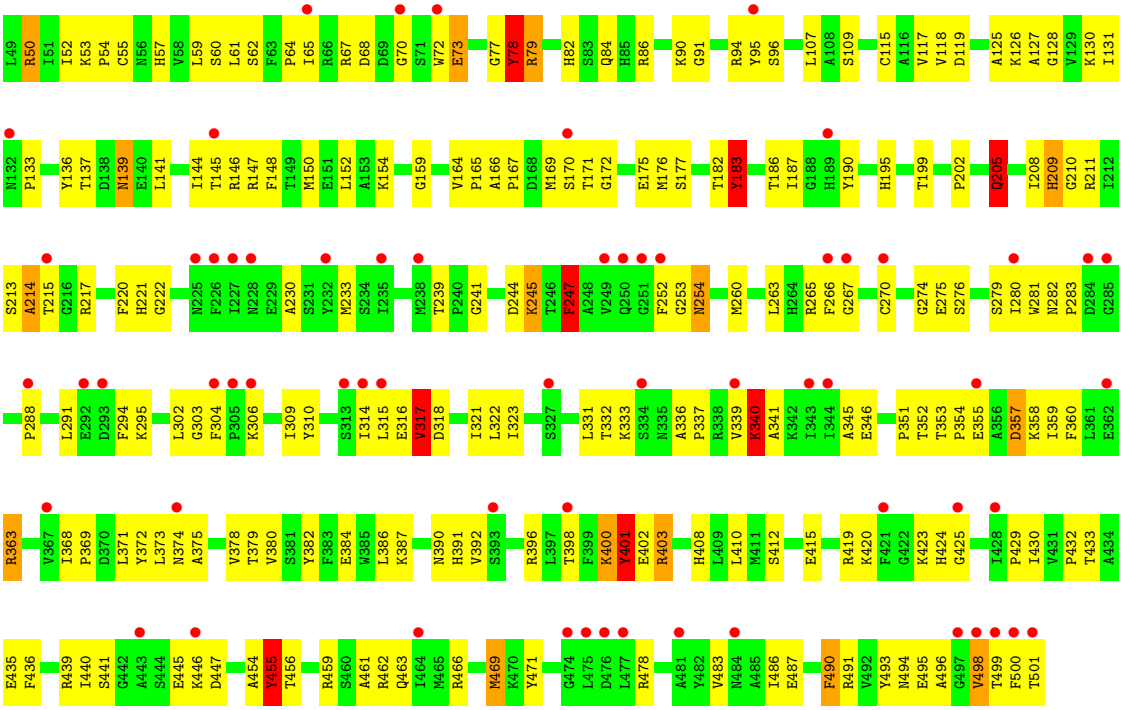


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial



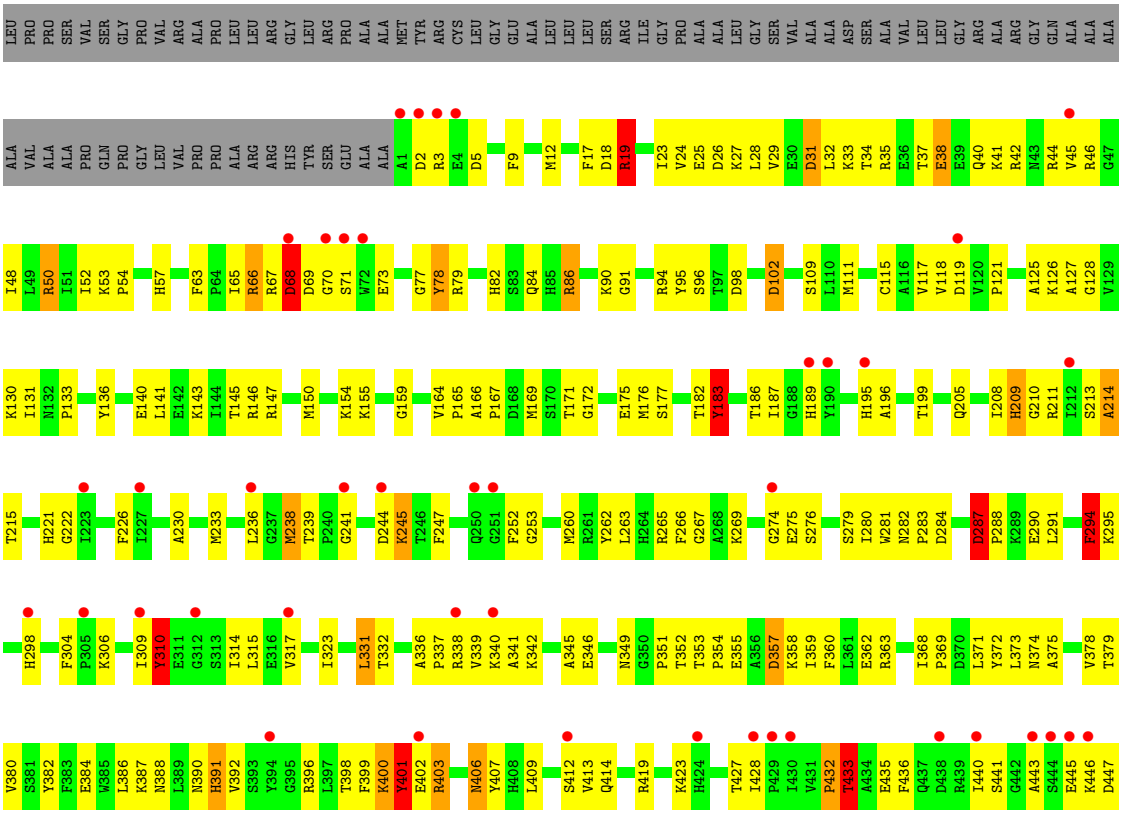
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

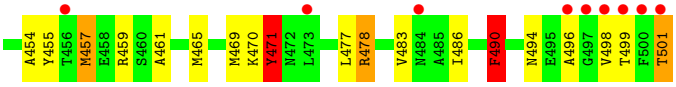




• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain F:




A454
Y455
T456
M457
E458
R459
S460
A461
M465
M469
K470
Y471
N472
L473
L477
R478
V483
N484
A485
I486
F490
N494
E495
A496
G497
V498
T499
F500
T501

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	7143 reflections (5.08%)	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]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.46	0/3999	1.06	26/5396 (0.5%)
1	B	0.48	3/3999 (0.1%)	1.01	21/5396 (0.4%)
1	C	0.46	2/3999 (0.1%)	0.89	16/5396 (0.3%)
1	D	0.57	3/3999 (0.1%)	1.45	32/5396 (0.6%)
1	E	0.55	6/3999 (0.2%)	1.08	31/5396 (0.6%)
1	F	0.60	6/3999 (0.2%)	2.03	52/5396 (1.0%)
All	All	0.52	20/23994 (0.1%)	1.31	178/32376 (0.5%)

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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	GLU	CD-OE1	-15.37	1.08	1.25
1	E	247	PHE	CG-CD1	-10.53	1.23	1.38
1	F	31	ASP	CG-OD1	-10.08	1.02	1.25
1	D	247	PHE	CG-CD1	-9.71	1.24	1.38
1	F	447	ASP	CG-OD1	-9.37	1.03	1.25
1	E	38	GLU	CD-OE1	-8.80	1.16	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	205	GLN	CD-OE1	-7.61	1.07	1.24
1	F	471	TYR	CG-CD1	-7.33	1.29	1.39
1	F	63	PHE	CE1-CZ	-6.95	1.24	1.37
1	D	297	GLN	CB-CG	-6.50	1.35	1.52
1	B	19	ARG	CG-CD	-6.33	1.36	1.51
1	B	205	GLN	CD-OE1	-6.27	1.10	1.24
1	E	38	GLU	CB-CG	-6.24	1.40	1.52
1	C	471	TYR	CG-CD1	-5.68	1.31	1.39
1	F	355	GLU	CB-CG	-5.44	1.41	1.52
1	E	36	GLU	CB-CG	-5.41	1.41	1.52
1	B	388	ASN	CG-OD1	-5.23	1.12	1.24
1	C	38	GLU	CD-OE1	-5.21	1.20	1.25
1	F	471	TYR	CE2-CZ	-5.18	1.31	1.38
1	E	73	GLU	CD-OE1	-5.17	1.20	1.25

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	63	PHE	CB-CG-CD1	77.11	174.77	120.80
1	F	63	PHE	CB-CG-CD2	-59.42	79.20	120.80
1	F	447	ASP	CB-CG-OD1	-47.16	75.86	118.30
1	D	73	GLU	OE1-CD-OE2	-45.39	68.84	123.30
1	D	31	ASP	CB-CG-OD1	44.55	158.39	118.30
1	D	31	ASP	CB-CG-OD2	-31.75	89.72	118.30
1	F	447	ASP	OD1-CG-OD2	-30.56	65.24	123.30
1	B	19	ARG	NE-CZ-NH1	-29.88	105.36	120.30
1	A	261	ARG	NE-CZ-NH1	-28.41	106.10	120.30
1	D	31	ASP	OD1-CG-OD2	-27.36	71.31	123.30
1	F	447	ASP	CB-CG-OD2	25.31	141.08	118.30
1	B	19	ARG	NE-CZ-NH2	24.34	132.47	120.30
1	A	261	ARG	NE-CZ-NH2	23.92	132.26	120.30
1	F	478	ARG	NE-CZ-NH1	-23.37	108.61	120.30
1	E	50	ARG	NE-CZ-NH2	21.60	131.10	120.30
1	E	50	ARG	NE-CZ-NH1	-21.18	109.71	120.30
1	E	217	ARG	NE-CZ-NH1	-21.00	109.80	120.30
1	C	490	PHE	CB-CG-CD2	-20.82	106.22	120.80
1	F	490	PHE	CB-CG-CD2	-20.80	106.24	120.80
1	F	294	PHE	CB-CG-CD2	-20.20	106.66	120.80
1	D	294	PHE	CB-CG-CD2	-20.13	106.71	120.80
1	E	217	ARG	NE-CZ-NH2	19.79	130.19	120.30
1	F	478	ARG	NE-CZ-NH2	19.74	130.17	120.30
1	D	73	GLU	CG-CD-OE1	-19.36	79.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	455	TYR	CB-CG-CD2	-18.65	109.81	121.00
1	F	31	ASP	CB-CG-OD2	18.44	134.89	118.30
1	A	261	ARG	CD-NE-CZ	18.08	148.92	123.60
1	B	19	ARG	CD-NE-CZ	17.69	148.36	123.60
1	A	455	TYR	CB-CG-CD2	-17.54	110.48	121.00
1	F	63	PHE	CD1-CG-CD2	-17.14	96.01	118.30
1	F	19	ARG	NE-CZ-NH1	-15.75	112.42	120.30
1	D	10	PHE	CB-CG-CD2	-15.00	110.30	120.80
1	F	68	ASP	CB-CG-OD1	14.53	131.37	118.30
1	D	295	LYS	CD-CE-NZ	14.23	144.43	111.70
1	F	19	ARG	NE-CZ-NH2	13.33	126.96	120.30
1	F	63	PHE	CG-CD1-CE1	13.08	135.19	120.80
1	F	295	LYS	CD-CE-NZ	12.92	141.41	111.70
1	D	73	GLU	CG-CD-OE2	12.66	143.62	118.30
1	C	19	ARG	NE-CZ-NH2	-11.78	114.41	120.30
1	F	478	ARG	CD-NE-CZ	11.58	139.81	123.60
1	C	19	ARG	NE-CZ-NH1	11.27	125.94	120.30
1	E	19	ARG	NE-CZ-NH2	-11.27	114.67	120.30
1	F	68	ASP	CB-CG-OD2	-11.09	108.32	118.30
1	F	238	MET	CA-CB-CG	10.93	131.88	113.30
1	A	19	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	E	19	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	D	401	TYR	CB-CG-CD2	-10.80	114.52	121.00
1	D	19	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	E	50	ARG	CD-NE-CZ	10.70	138.59	123.60
1	F	68	ASP	OD1-CG-OD2	-10.48	103.39	123.30
1	F	457	MET	CA-CB-CG	-10.39	95.63	113.30
1	D	19	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	A	19	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	E	247	PHE	CD1-CG-CD2	-10.30	104.91	118.30
1	F	50	ARG	CD-NE-CZ	10.14	137.79	123.60
1	F	50	ARG	NE-CZ-NH1	-9.75	115.42	120.30
1	D	247	PHE	CD1-CG-CD2	-9.60	105.82	118.30
1	F	401	TYR	CB-CG-CD2	-9.21	115.47	121.00
1	B	275	GLU	CG-CD-OE2	9.14	136.57	118.30
1	F	471	TYR	CD1-CG-CD2	-9.12	107.86	117.90
1	A	195	HIS	N-CA-CB	-9.00	94.39	110.60
1	A	401	TYR	CB-CG-CD2	-8.96	115.62	121.00
1	F	287	ASP	CB-CG-OD2	-8.96	110.23	118.30
1	F	287	ASP	CB-CG-OD1	8.96	126.36	118.30
1	F	310	TYR	CB-CG-CD2	-8.74	115.76	121.00
1	E	217	ARG	CD-NE-CZ	8.39	135.34	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	297	GLN	CA-CB-CG	-8.31	95.12	113.40
1	B	275	GLU	CG-CD-OE1	-8.30	101.71	118.30
1	A	295	LYS	CD-CE-NZ	8.28	130.74	111.70
1	E	455	TYR	CD1-CG-CD2	-8.25	108.82	117.90
1	B	295	LYS	CD-CE-NZ	8.24	130.65	111.70
1	C	295	LYS	CD-CE-NZ	8.22	130.60	111.70
1	E	295	LYS	CD-CE-NZ	8.19	130.53	111.70
1	C	19	ARG	CD-NE-CZ	7.88	134.64	123.60
1	F	471	TYR	CB-CG-CD2	-7.86	116.28	121.00
1	D	294	PHE	CB-CG-CD1	7.84	126.29	120.80
1	E	247	PHE	CB-CA-C	7.78	125.97	110.40
1	F	294	PHE	CB-CG-CD1	7.77	126.24	120.80
1	A	402	GLU	OE1-CD-OE2	-7.73	114.02	123.30
1	A	455	TYR	CD1-CG-CD2	-7.70	109.42	117.90
1	E	78	TYR	CB-CG-CD2	-7.70	116.38	121.00
1	D	262	TYR	CB-CG-CD2	-7.68	116.39	121.00
1	F	19	ARG	CD-NE-CZ	7.65	134.31	123.60
1	F	63	PHE	CG-CD2-CE2	7.63	129.19	120.80
1	E	247	PHE	N-CA-CB	-7.59	96.94	110.60
1	F	490	PHE	CB-CG-CD1	7.54	126.08	120.80
1	E	19	ARG	CD-NE-CZ	7.53	134.14	123.60
1	D	446	LYS	CD-CE-NZ	7.52	128.99	111.70
1	A	78	TYR	CB-CG-CD2	-7.52	116.49	121.00
1	B	275	GLU	CB-CG-CD	7.42	134.23	114.20
1	D	247	PHE	CB-CA-C	7.36	125.11	110.40
1	C	490	PHE	CD1-CG-CD2	-7.31	108.80	118.30
1	F	331	LEU	CB-CG-CD2	-7.18	98.80	111.00
1	E	38	GLU	OE1-CD-OE2	-7.12	114.76	123.30
1	D	247	PHE	N-CA-CB	-7.07	97.87	110.60
1	F	490	PHE	CD1-CG-CD2	-7.07	109.11	118.30
1	F	31	ASP	CB-CA-C	-7.06	96.27	110.40
1	F	31	ASP	CB-CG-OD1	-7.06	111.95	118.30
1	D	10	PHE	CD1-CG-CD2	-7.05	109.13	118.30
1	B	388	ASN	N-CA-CB	-7.04	97.92	110.60
1	D	19	ARG	CD-NE-CZ	6.97	133.36	123.60
1	F	294	PHE	CD1-CG-CD2	-6.97	109.24	118.30
1	C	490	PHE	CB-CA-C	-6.93	96.53	110.40
1	D	294	PHE	CD1-CG-CD2	-6.92	109.31	118.30
1	D	183	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	C	471	TYR	CD1-CG-CD2	-6.81	110.41	117.90
1	B	310	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	C	50	ARG	NE-CZ-NH2	-6.77	116.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	247	PHE	CB-CG-CD2	-6.76	116.07	120.80
1	C	490	PHE	CB-CG-CD1	6.75	125.52	120.80
1	A	402	GLU	CA-CB-CG	6.70	128.13	113.40
1	F	183	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	B	183	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	A	19	ARG	CD-NE-CZ	6.63	132.88	123.60
1	A	183	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	C	183	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	D	275	GLU	OE1-CD-OE2	-6.53	115.46	123.30
1	C	38	GLU	OE1-CD-OE2	-6.49	115.51	123.30
1	D	10	PHE	CB-CA-C	-6.47	97.47	110.40
1	B	50	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	E	183	TYR	CB-CG-CD2	-6.37	117.18	121.00
1	E	455	TYR	CB-CA-C	-6.36	97.68	110.40
1	A	50	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	E	78	TYR	CB-CG-CD1	6.32	124.79	121.00
1	B	317	VAL	CG1-CB-CG2	6.25	120.91	110.90
1	A	455	TYR	CB-CA-C	-6.20	97.99	110.40
1	F	501	THR	CA-CB-OG1	6.18	121.97	109.00
1	D	50	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	F	490	PHE	CB-CA-C	-6.17	98.07	110.40
1	B	470	LYS	CD-CE-NZ	6.13	125.81	111.70
1	A	31	ASP	CB-CG-OD1	6.08	123.77	118.30
1	C	50	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	F	317	VAL	CG1-CB-CG2	6.02	120.53	110.90
1	D	470	LYS	CD-CE-NZ	-6.00	97.90	111.70
1	F	31	ASP	OD1-CG-OD2	-5.97	111.96	123.30
1	F	294	PHE	CB-CA-C	-5.94	98.53	110.40
1	D	294	PHE	CB-CA-C	-5.92	98.56	110.40
1	A	471	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	A	78	TYR	CB-CG-CD1	5.84	124.50	121.00
1	F	287	ASP	OD1-CG-OD2	-5.80	112.28	123.30
1	B	102	ASP	CB-CG-OD1	5.80	123.52	118.30
1	E	205	GLN	CB-CG-CD	5.79	126.66	111.60
1	E	469	MET	CG-SD-CE	5.72	109.35	100.20
1	D	50	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	B	102	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	F	102	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	50	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	F	86	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	E	78	TYR	CA-CB-CG	5.61	124.06	113.40
1	C	291	LEU	CB-CG-CD2	5.60	120.52	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	78	TYR	CA-CB-CG	5.57	123.98	113.40
1	F	245	LYS	CD-CE-NZ	5.56	124.48	111.70
1	F	102	ASP	OD1-CG-OD2	-5.55	112.75	123.30
1	B	317	VAL	CA-CB-CG1	5.51	119.16	110.90
1	A	471	TYR	CB-CG-CD1	5.49	124.30	121.00
1	E	317	VAL	CG1-CB-CG2	-5.49	102.12	110.90
1	B	466	ARG	CA-CB-CG	5.44	125.37	113.40
1	F	338	ARG	CG-CD-NE	5.39	123.13	111.80
1	E	217	ARG	CG-CD-NE	-5.37	100.53	111.80
1	E	139	ASN	CB-CA-C	-5.31	99.77	110.40
1	E	447	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	391	HIS	N-CA-CB	-5.29	101.08	110.60
1	E	245	LYS	CD-CE-NZ	5.28	123.85	111.70
1	D	471	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	D	401	TYR	CD1-CG-CD2	-5.23	112.15	117.90
1	E	469	MET	CA-CB-CG	5.23	122.18	113.30
1	F	317	VAL	CA-CB-CG1	5.19	118.69	110.90
1	B	275	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	A	50	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	195	HIS	CB-CA-C	5.14	120.68	110.40
1	D	247	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	B	424	HIS	C-N-CA	5.06	132.93	122.30
1	A	32	LEU	CB-CG-CD1	-5.05	102.42	111.00
1	B	78	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	A	406	ASN	N-CA-CB	-5.03	101.54	110.60
1	F	433	THR	CA-CB-OG1	5.02	119.54	109.00
1	C	420	LYS	CD-CE-NZ	5.01	123.23	111.70
1	E	469	MET	CB-CG-SD	5.00	127.40	112.40

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
1	E	340	LYS	Peptide
1	E	38	GLU	Peptide,Sidechain
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	210	0
1	B	3916	0	3880	223	0
1	C	3916	0	3879	214	0
1	D	3916	0	3878	209	0
1	E	3916	0	3879	238	0
1	F	3916	0	3880	224	0
2	A	10	0	5	7	0
2	B	10	0	5	7	0
2	C	10	0	5	4	0
2	D	10	0	5	4	0
2	E	10	0	5	6	0
2	F	10	0	5	5	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	2	0
4	A	88	0	51	11	0
4	B	88	0	51	15	0
4	C	88	0	50	10	0
4	D	88	0	50	9	0
4	E	44	0	25	10	0
4	F	132	0	75	23	0
All	All	24276	0	23679	1210	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 25.

All (1210) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:339:VAL:C	1:E:340:LYS:HD3	2.07	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:E:403:ARG:HH11	1:E:441:SER:HG	1.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:A:90:LYS:NZ	2:A:601:GLU:OE1	2.23	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:499:THR:HG1	1:D:147:ARG:HH12	1.39	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: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:D:280:ILE:HD11	1:D:291:LEU:HD11	1.76	0.67
1:E:322:LEU:HD13	1:E:340:LYS:HZ1	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:MET:HG3	1:A:354:PRO:HD3	1.76	0.67
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: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: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:F:18:ASP:OD1	1:F:53:LYS:NZ	2.23	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:B:77:GLY:C	1:B:78:TYR:HD2	2.00	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:C:458:GLU:CD	1:C:462:ARG:HH12	2.00	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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:F:77:GLY:C	1:F:78:TYR:HD2	2.02	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:C:77:GLY:C	1:C:78:TYR:HD2	2.02	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:E:77:GLY:C	1:E:78:TYR:HD2	2.02	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: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:D:77:GLY:C	1:D:78:TYR:HD2	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:E:316:GLU:C	1:E:340:LYS:HD2	2.23	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:C:57:HIS:CD2	1:F:155:LYS:HG3	2.37	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:322:LEU:HD22	1:E:340:LYS:HZ3	1.68	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:E:126:LYS:HZ1	2:E:601:GLU:N	2.01	0.58
1:E:339:VAL:O	1:E:339:VAL:HG12	2.03	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:F:126:LYS:HZ1	2:F:602:GLU:N	2.00	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: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: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
1:A:77:GLY:C	1:A:78:TYR:HD2	2.08	0.57
2:A:601:GLU:CA	4:A:603:NAI:H4N	2.32	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:3:ARG:HB2	1:C:3:ARG:CZ	2.34	0.56
1:D:150:MET:HE1	1:D:186:THR:HG21	1.86	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:B:126:LYS:HZ1	2:B:601:GLU:N	2.03	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:A:428:ILE:HG12	1:C:420:LYS:HZ2	1.71	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: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:C:126:LYS:HZ1	2:C:601:GLU:N	2.04	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:126:LYS:HZ1	2:A:601:GLU:N	2.05	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
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:126:LYS:HZ1	2:D:601:GLU:N	2.05	0.54
1:D:247:PHE:CD2	1:D:247:PHE:C	2.81	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:150:MET:HE1	1:C:186:THR:HG21	1.90	0.53
1:D:244:ASP:HA	1:D:269:LYS:NZ	2.23	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
1:A:252:PHE:HB3	1:A:275:GLU:OE2	2.09	0.53
1:A:399:PHE:HD2	1:B:455:TYR:HH	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:10:PHE:HE1	1:D:53:LYS:NZ	2.07	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: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:B:33:LYS:HD3	1:B:41:LYS:NZ	2.25	0.52
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:372:TYR:O	1:F:457:MET:HE3	2.10	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:A:345:ALA:HB1	1:A:373:LEU:HD21	1.91	0.51
1:E:247:PHE:CD2	1:E:247:PHE:C	2.84	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:238:MET:HE1	1:C:343:ILE:HG13	1.92	0.51
1:C:280:ILE:HD11	1:C:291:LEU:HD11	1.92	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:68:ASP:OD2	1:C:137:THR:OG1	2.27	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
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:403:ARG:HA	1:F:440:ILE:O	2.11	0.50
1:A:315:LEU:HD22	1:A:331:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:247:PHE:C	1:D:247:PHE:HD2	2.14	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:A:241:GLY:O	1:A:245:LYS:NZ	2.44	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:F:372:TYR:O	1:F:457:MET:CE	2.60	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: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:D:375:ALA:O	1:D:379:THR:OG1	2.19	0.49
1:E:32:LEU:HD11	1:E:494:ASN:OD1	2.12	0.49
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:C:186:THR:OG1	1:C:187:ILE:N	2.44	0.49
1:D:357:ASP:OD2	1:D:478:ARG:NE	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:443:ALA:HA	1:E:401:TYR:CE2	2.48	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:B:60:SER:O	1:E:57:HIS:HA	2.13	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:E:150:MET:HE1	1:E:186:THR:HG21	1.95	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: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
1:A:462:ARG:HD2	1:A:465:MET:CE	2.43	0.48
1:C:65:ILE:HG13	1:C:65:ILE:O	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:346:GLU:OE1	1:D:352:THR:OG1	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ILE:O	1:E:52:ILE:HG13	2.14	0.48
1:F:53:LYS:HB2	1:F:54:PRO:HD3	1.95	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:E:68:ASP:OD2	1:E:137:THR:OG1	2.28	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:D:294:PHE:HD1	1:D:298:HIS:ND1	2.11	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:F:294:PHE:HD1	1:F:298:HIS:ND1	2.12	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
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:F:346:GLU:CD	1:F:478:ARG:HH12	2.17	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:A:292:GLU:CD	3:A:602:GTP:HN1	2.17	0.47
1:B:38:GLU:HG3	1:B:40:GLN:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:GLU:HA	1:D:53:LYS:HE3	1.96	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: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: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: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:D:77:GLY:C	1:D:78:TYR:CD2	2.88	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: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:111:MET:HE1	2:B:601:GLU:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:SER:OG	1:A:447:ASP:OD1	2.25	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: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:B:33:LYS:HD3	1:B:41:LYS:HZ3	1.80	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: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:346:GLU:OE1	1:B:352:THR:OG1	2.24	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: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:C	1:E:247:PHE:HD2	2.19	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:A:205:GLN:CD	1:B:495:GLU:O	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:TRP:HH2	1:C:391:HIS:HD1	1.62	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: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: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
1:A:166:ALA:HB1	1:A:167:PRO:HD2	1.98	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
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: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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95:TYR:HH	1:E:145:THR:HG22	1.81	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
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:375:ALA:O	1:E:379:THR:OG1	2.24	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:339:VAL:O	1:D:340:LYS:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:247:PHE:C	1:B:247:PHE:CD2	2.92	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: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: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:E:423:LYS:C	1:E:425:GLY:H	2.22	0.43
1:F:269:LYS:HD2	1:F:284:ASP:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:E:316:GLU:O	1:E:340:LYS:HD2	2.19	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:77:GLY:C	1:A:78:TYR:CD2	2.90	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:E:133:PRO:HG2	1:E:170:SER:HB3	2.00	0.43
1:E:150:MET:HE2	1:E:186:THR:HG21	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
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: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:68:ASP:OD2	1:A:137:THR:OG1	2.26	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:E:119:ASP:C	1:F:396:ARG:HH12	2.21	0.42
1:F:247:PHE:C	1:F:247:PHE:CD2	2.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:8:ASN:ND2	1:C:102:ASP:OD2	2.45	0.42
1:C:111:MET:HE1	2:C:601:GLU:HG3	2.01	0.42
1:D:10:PHE:CE2	1:D:105:LYS:HE2	2.54	0.42
1:E:48:ILE:HG21	1:E:490:PHE:HD1	1.83	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:A:150:MET:HE1	1:A:186:THR:HG21	2.00	0.42
1:B:295:LYS:O	1:B:295:LYS:HG3	2.19	0.42
1:C:60:SER:O	1:F:57:HIS:HA	2.20	0.42
1:C:247:PHE:C	1:C:247:PHE:CD2	2.93	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:E:495:GLU:O	1:F:205:GLN:CD	2.58	0.42
1:A:133:PRO:HG2	1:A:170:SER:HB3	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:210:GLY:O	1:C:214:ALA:HB2	2.20	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:F:238:MET:HE1	1:F:342:LYS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:444:SER:OG	1:D:447:ASP:OD1	2.23	0.42
1:E:400:LYS:O	1:E:400:LYS:HG2	2.20	0.42
1:F:77:GLY:C	1:F:78:TYR:CD2	2.88	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:B:78:TYR:N	1:B:78:TYR:CD2	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: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: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: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:317:VAL:C	1:E:340:LYS:HG3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:422:GLY:C	1:B:424:HIS:H	2.23	0.41
1:C:244:ASP:OD1	1:C:244:ASP:N	2.54	0.41
1:C:265:ARG:C	1:C:267:GLY:H	2.24	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: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: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: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:111:MET:HE1	2:D:601:GLU:HG3	2.01	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:C:69:ASP:OD1	1:C:71:SER:OG	2.25	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:F:375:ALA:O	1:F:379:THR:OG1	2.24	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:B:20:GLY:O	1:B:24:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:VAL:O	1:B:27:LYS:N	2.54	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
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: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: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: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: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:247:PHE:C	1:A:247:PHE:CD2	2.94	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:77:GLY:C	1:B:78:TYR:CD2	2.88	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:374:ASN:HB2	4:C:604:NAI:C5N	2.51	0.41
1:D:25:GLU:O	1:D:29:VAL:HG23	2.21	0.41
1:D:265:ARG:C	1:D:267:GLY:H	2.24	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: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
1:D:164:VAL:HA	1:D:197:CYS:O	2.21	0.41
1:D:239:THR:O	1:D:245:LYS:NZ	2.39	0.41
1:D:339:VAL:O	1:D:339:VAL:HG12	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ARG:HH11	1:B:182:THR:CG2	2.30	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: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: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
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
1:F:432:PRO:HB3	1:F:436:PHE:HD2	1.86	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:F:86:ARG:HB3	1:F:121:PRO:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:MET:HE1	2:F:602:GLU:HG3	2.03	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: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%)	7	30
1	B	499/582 (86%)	444 (89%)	41 (8%)	14 (3%)	4	22
1	C	499/582 (86%)	448 (90%)	43 (9%)	8 (2%)	8	32
1	D	499/582 (86%)	447 (90%)	40 (8%)	12 (2%)	5	25
1	E	499/582 (86%)	444 (89%)	43 (9%)	12 (2%)	5	25
1	F	499/582 (86%)	446 (89%)	38 (8%)	15 (3%)	3	21
All	All	2994/3492 (86%)	2677 (89%)	247 (8%)	70 (2%)	5	26

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	HIS

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	417/471 (88%)	409 (98%)	8 (2%)	52 72
1	B	417/471 (88%)	410 (98%)	7 (2%)	56 74
1	C	417/471 (88%)	409 (98%)	8 (2%)	52 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	417/471 (88%)	407 (98%)	10 (2%)	44 68
1	E	417/471 (88%)	407 (98%)	10 (2%)	44 68
1	F	417/471 (88%)	408 (98%)	9 (2%)	47 69
All	All	2502/2826 (88%)	2450 (98%)	52 (2%)	48 70

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	35	ARG
1	A	78	TYR
1	A	195	HIS
1	A	221	HIS
1	A	357	ASP
1	A	450	HIS
1	A	455	TYR
1	B	9	PHE
1	B	31	ASP
1	B	78	TYR
1	B	183	TYR
1	B	310	TYR
1	B	338	ARG
1	B	357	ASP
1	C	3	ARG
1	C	9	PHE
1	C	31	ASP
1	C	44	ARG
1	C	78	TYR
1	C	102	ASP
1	C	357	ASP
1	C	490	PHE
1	D	9	PHE
1	D	10	PHE
1	D	78	TYR
1	D	238	MET
1	D	247	PHE
1	D	294	PHE
1	D	357	ASP
1	D	424	HIS
1	D	462	ARG
1	D	491	ARG

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Mol	Chain	Res	Type
1	E	9	PHE
1	E	31	ASP
1	E	79	ARG
1	E	183	TYR
1	E	247	PHE
1	E	340	LYS
1	E	357	ASP
1	E	401	TYR
1	E	455	TYR
1	E	469	MET
1	F	9	PHE
1	F	19	ARG
1	F	98	ASP
1	F	183	TYR
1	F	294	PHE
1	F	310	TYR
1	F	357	ASP
1	F	423	LYS
1	F	490	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	205	GLN
1	B	209	HIS
1	D	209	HIS
1	D	391	HIS
1	E	195	HIS
1	F	195	HIS
1	F	209	HIS
1	F	391	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	GTP	C	602	-	29,34,34	1.45	5 (17%)	35,54,54	1.34	3 (8%)
4	NAI	E	603	-	43,48,48	4.19	20 (46%)	50,73,73	1.90	8 (16%)
4	NAI	A	604	-	43,48,48	4.30	20 (46%)	50,73,73	2.23	11 (22%)
3	GTP	A	602	-	29,34,34	1.39	3 (10%)	35,54,54	1.74	11 (31%)
3	GTP	F	604	-	29,34,34	1.25	3 (10%)	35,54,54	1.37	5 (14%)
3	GTP	B	602	-	29,34,34	1.29	4 (13%)	35,54,54	1.64	6 (17%)
3	GTP	E	602	-	29,34,34	1.34	5 (17%)	35,54,54	1.34	5 (14%)
4	NAI	F	603	-	43,48,48	4.19	21 (48%)	50,73,73	1.90	9 (18%)
4	NAI	C	603	-	43,48,48	4.23	19 (44%)	50,73,73	1.92	4 (8%)
2	GLU	D	601	-	8,9,9	1.13	1 (12%)	8,11,11	1.11	1 (12%)
2	GLU	A	601	-	8,9,9	1.16	1 (12%)	8,11,11	1.11	1 (12%)
4	NAI	C	604	-	43,48,48	4.22	22 (51%)	50,73,73	1.81	8 (16%)
4	NAI	D	603	-	43,48,48	4.12	20 (46%)	50,73,73	1.81	5 (10%)
4	NAI	D	604	-	43,48,48	4.24	20 (46%)	50,73,73	1.91	9 (18%)
2	GLU	B	601	-	8,9,9	1.07	1 (12%)	8,11,11	1.34	1 (12%)
2	GLU	F	602	-	8,9,9	1.09	1 (12%)	8,11,11	1.31	1 (12%)
4	NAI	F	605	-	43,48,48	4.18	21 (48%)	50,73,73	1.93	9 (18%)
2	GLU	E	601	-	8,9,9	1.14	1 (12%)	8,11,11	1.17	1 (12%)
2	GLU	C	601	-	8,9,9	1.07	1 (12%)	8,11,11	1.22	1 (12%)
4	NAI	B	603	-	43,48,48	4.18	20 (46%)	50,73,73	2.03	8 (16%)
4	NAI	F	601	-	43,48,48	4.26	19 (44%)	50,73,73	2.10	10 (20%)
3	GTP	D	602	-	29,34,34	1.28	3 (10%)	35,54,54	1.35	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAI	A	603	-	43,48,48	4.13	19 (44%)	50,73,73	2.16	9 (18%)
4	NAI	B	604	-	43,48,48	4.16	18 (41%)	50,73,73	1.87	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	C	602	-	-	5/18/38/38	0/3/3/3
4	NAI	E	603	-	-	9/25/72/72	0/5/5/5
4	NAI	A	604	-	-	13/25/72/72	0/5/5/5
3	GTP	A	602	-	-	5/18/38/38	0/3/3/3
3	GTP	F	604	-	-	2/18/38/38	0/3/3/3
3	GTP	B	602	-	-	3/18/38/38	0/3/3/3
3	GTP	E	602	-	-	2/18/38/38	0/3/3/3
4	NAI	F	603	-	-	10/25/72/72	0/5/5/5
4	NAI	C	603	-	-	12/25/72/72	0/5/5/5
2	GLU	D	601	-	-	1/9/9/9	-
2	GLU	A	601	-	-	3/9/9/9	-
4	NAI	C	604	-	-	15/25/72/72	0/5/5/5
4	NAI	D	603	-	-	12/25/72/72	0/5/5/5
4	NAI	D	604	-	-	11/25/72/72	0/5/5/5
2	GLU	B	601	-	-	0/9/9/9	-
2	GLU	F	602	-	-	0/9/9/9	-
4	NAI	F	605	-	-	14/25/72/72	0/5/5/5
2	GLU	E	601	-	-	0/9/9/9	-
2	GLU	C	601	-	-	1/9/9/9	-
4	NAI	B	603	-	-	9/25/72/72	0/5/5/5
4	NAI	F	601	-	-	8/25/72/72	0/5/5/5
3	GTP	D	602	-	-	3/18/38/38	0/3/3/3
4	NAI	A	603	-	-	8/25/72/72	0/5/5/5
4	NAI	B	604	-	-	11/25/72/72	0/5/5/5

All (268) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	604	NAI	O4B-C1B	17.31	1.63	1.40
4	F	605	NAI	O4B-C1B	16.97	1.63	1.40
4	A	603	NAI	O4B-C1B	16.86	1.63	1.40
4	A	604	NAI	O4B-C1B	16.76	1.62	1.40
4	B	604	NAI	O4B-C1B	16.72	1.62	1.40
4	B	603	NAI	O4B-C1B	16.62	1.62	1.40
4	E	603	NAI	O4B-C1B	16.53	1.62	1.40
4	D	603	NAI	O4B-C1B	16.51	1.62	1.40
4	C	603	NAI	O4B-C1B	16.48	1.62	1.40
4	D	604	NAI	O4B-C1B	16.44	1.62	1.40
4	F	603	NAI	O4B-C1B	16.40	1.62	1.40
4	F	601	NAI	O4B-C1B	16.27	1.62	1.40
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	O4D-C1D	9.04	1.62	1.42
4	A	603	NAI	O4D-C1D	8.95	1.62	1.42
4	C	604	NAI	O4D-C1D	8.90	1.62	1.42
4	A	604	NAI	O4D-C1D	8.89	1.62	1.42
4	D	603	NAI	O4D-C1D	8.87	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
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	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	A	604	NAI	C2D-C1D	-7.08	1.31	1.53
4	B	603	NAI	C2N-C3N	7.06	1.54	1.35
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	C	604	NAI	C2N-C3N	6.80	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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	F	605	NAI	PN-O3	4.53	1.64	1.59
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	B	604	NAI	C7N-N7N	4.24	1.45	1.33
4	F	601	NAI	C7N-N7N	4.23	1.45	1.33
3	A	602	GTP	C5-C6	-4.23	1.39	1.47
3	D	602	GTP	C5-C6	-4.22	1.39	1.47
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	F	604	GTP	C5-C6	-3.98	1.39	1.47
3	E	602	GTP	C5-C6	-3.94	1.39	1.47
3	B	602	GTP	C5-C6	-3.89	1.39	1.47
3	C	602	GTP	C5-C6	-3.84	1.39	1.47
3	C	602	GTP	PA-O3A	3.53	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	GTP	PB-O3A	3.44	1.63	1.59
4	E	603	NAI	C6N-N1N	3.39	1.45	1.37
4	A	604	NAI	C6A-N6A	3.30	1.45	1.34
4	A	603	NAI	C6A-N6A	3.29	1.45	1.34
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	C	604	NAI	C6A-N6A	3.28	1.45	1.34
4	E	603	NAI	C6A-N6A	3.27	1.45	1.34
4	B	604	NAI	C6A-N6A	3.25	1.45	1.34
4	F	603	NAI	C6A-N6A	3.25	1.45	1.34
4	B	603	NAI	C6A-N6A	3.24	1.45	1.34
4	F	601	NAI	O3D-C3D	-3.24	1.34	1.43
4	D	603	NAI	C6A-N6A	3.24	1.45	1.34
4	F	605	NAI	C6A-N6A	3.22	1.45	1.34
4	D	604	NAI	C6N-N1N	3.21	1.45	1.37
4	D	604	NAI	C6A-N6A	3.20	1.45	1.34
4	C	603	NAI	C6A-N6A	3.20	1.45	1.34
4	F	603	NAI	C6N-N1N	3.19	1.45	1.37
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	F	603	NAI	O2B-C2B	3.08	1.50	1.43
4	F	601	NAI	C6A-N6A	3.08	1.45	1.34
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	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	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	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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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	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	E	603	NAI	O3B-C3B	-2.69	1.36	1.43
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	601	NAI	C2A-N3A	2.66	1.36	1.32
4	A	603	NAI	O2B-C2B	2.65	1.49	1.43
4	A	604	NAI	C2A-N3A	2.65	1.36	1.32
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	F	605	NAI	C2A-N3A	2.60	1.36	1.32
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
3	E	602	GTP	C2-N3	2.54	1.39	1.33
4	D	604	NAI	O3B-C3B	-2.54	1.36	1.43
4	F	603	NAI	C1B-N9A	-2.54	1.43	1.49
4	D	604	NAI	C2A-N3A	2.53	1.36	1.32
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
3	E	602	GTP	PA-O3A	2.51	1.62	1.59
3	D	602	GTP	C2-N3	2.51	1.39	1.33
4	B	603	NAI	O3D-C3D	-2.50	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	GTP	C2-N3	2.47	1.39	1.33
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
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
4	B	603	NAI	C2A-N3A	2.37	1.35	1.32
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
4	C	604	NAI	C2A-N3A	2.32	1.35	1.32
4	E	603	NAI	C2A-N3A	2.31	1.35	1.32
4	F	605	NAI	PA-O5B	2.30	1.68	1.59
3	C	602	GTP	C2-N3	2.30	1.38	1.33
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	604	NAI	C2A-N3A	2.25	1.35	1.32
4	D	603	NAI	C1B-N9A	-2.24	1.44	1.49
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	D	603	NAI	C2A-N3A	2.23	1.35	1.32
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	C1B-N9A	-2.20	1.44	1.49
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
4	C	603	NAI	C2A-N3A	2.18	1.35	1.32
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	F	603	NAI	C2A-N3A	2.14	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	603	NAI	PA-O5B	2.09	1.67	1.59
4	F	603	NAI	C5B-C4B	2.09	1.57	1.51
4	A	603	NAI	C2A-N3A	2.09	1.35	1.32
4	C	604	NAI	C5B-C4B	2.05	1.57	1.51
4	F	605	NAI	C1B-N9A	-2.05	1.44	1.49
4	F	605	NAI	C5B-C4B	2.04	1.57	1.51
4	C	604	NAI	C1B-N9A	-2.03	1.44	1.49
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

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	601	NAI	C3N-C2N-N1N	-9.23	109.65	123.20
4	B	604	NAI	C5A-C6A-N6A	7.44	131.64	120.31
4	C	603	NAI	C5A-C6A-N6A	7.37	131.54	120.31
4	B	603	NAI	C5A-C6A-N6A	7.29	131.41	120.31
4	E	603	NAI	C5A-C6A-N6A	7.23	131.32	120.31
4	A	603	NAI	C5A-C6A-N6A	7.19	131.26	120.31
4	A	604	NAI	C5A-C6A-N6A	7.05	131.06	120.31
4	A	603	NAI	N3A-C2A-N1A	-7.01	119.16	128.67
4	D	603	NAI	C5A-C6A-N6A	6.97	130.93	120.31
4	C	604	NAI	C5A-C6A-N6A	6.94	130.88	120.31
4	A	604	NAI	C3N-C2N-N1N	-6.94	113.02	123.20
4	B	603	NAI	N3A-C2A-N1A	-6.80	119.44	128.67
4	C	603	NAI	N3A-C2A-N1A	-6.68	119.61	128.67
4	D	604	NAI	C5A-C6A-N6A	6.67	130.47	120.31
4	F	605	NAI	C5A-C6A-N6A	6.60	130.36	120.31
4	C	604	NAI	N3A-C2A-N1A	-6.57	119.75	128.67
4	E	603	NAI	N3A-C2A-N1A	-6.50	119.84	128.67
4	D	603	NAI	N3A-C2A-N1A	-6.49	119.86	128.67
4	F	603	NAI	C5A-C6A-N6A	6.07	129.56	120.31
4	D	604	NAI	N3A-C2A-N1A	-6.00	120.53	128.67
4	F	605	NAI	N3A-C2A-N1A	-5.98	120.56	128.67
4	F	603	NAI	N3A-C2A-N1A	-5.91	120.64	128.67
4	F	601	NAI	N3A-C2A-N1A	-5.87	120.70	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	604	NAI	N3A-C2A-N1A	-5.87	120.71	128.67
3	A	602	GTP	O2G-PG-O3B	5.44	122.89	104.64
4	B	604	NAI	N3A-C2A-N1A	-5.30	121.48	128.67
4	D	604	NAI	C4D-O4D-C1D	-5.21	97.96	109.47
4	B	603	NAI	N6A-C6A-N1A	-4.92	107.82	118.33
4	C	603	NAI	N6A-C6A-N1A	-4.86	107.95	118.33
4	A	603	NAI	N6A-C6A-N1A	-4.74	108.21	118.33
4	B	604	NAI	N6A-C6A-N1A	-4.62	108.45	118.33
4	A	603	NAI	O4B-C1B-N9A	4.58	114.81	108.75
4	E	603	NAI	N6A-C6A-N1A	-4.55	108.61	118.33
4	F	601	NAI	C5A-C6A-N6A	4.51	127.18	120.31
4	A	604	NAI	C2D-C1D-N1N	-4.44	102.40	113.31
4	A	604	NAI	N6A-C6A-N1A	-4.41	108.91	118.33
4	C	604	NAI	N6A-C6A-N1A	-4.34	109.07	118.33
4	D	603	NAI	N6A-C6A-N1A	-4.34	109.07	118.33
4	C	603	NAI	C3N-C2N-N1N	-4.27	116.93	123.20
4	F	605	NAI	O4D-C1D-N1N	4.24	116.16	108.08
4	D	604	NAI	N6A-C6A-N1A	-4.18	109.40	118.33
4	F	605	NAI	N6A-C6A-N1A	-4.15	109.47	118.33
4	B	604	NAI	C4D-O4D-C1D	-4.08	100.45	109.47
3	B	602	GTP	C4'-O4'-C1'	4.06	113.64	109.92
4	F	603	NAI	C3N-C2N-N1N	-3.90	117.48	123.20
3	B	602	GTP	C8-N7-C5	3.85	109.10	102.55
4	F	603	NAI	N6A-C6A-N1A	-3.78	110.27	118.33
4	A	603	NAI	C1D-N1N-C2N	3.77	127.35	121.14
3	C	602	GTP	C8-N7-C5	3.70	108.85	102.55
4	F	603	NAI	O4B-C1B-N9A	-3.64	103.92	108.75
3	F	604	GTP	C8-N7-C5	3.62	108.71	102.55
4	A	603	NAI	C3N-C7N-N7N	3.60	124.07	117.67
4	F	603	NAI	O4D-C1D-N1N	3.55	114.86	108.08
3	E	602	GTP	C8-N7-C5	3.54	108.57	102.55
4	B	603	NAI	O4D-C1D-N1N	3.51	114.78	108.08
3	A	602	GTP	C8-N7-C5	3.45	108.42	102.55
4	A	604	NAI	C3D-C2D-C1D	3.44	107.96	101.46
4	A	604	NAI	C4B-O4B-C1B	-3.41	106.80	109.92
3	D	602	GTP	C8-N7-C5	3.40	108.33	102.55
4	B	603	NAI	C3N-C7N-N7N	3.36	123.64	117.67
3	E	602	GTP	C4'-O4'-C1'	3.36	113.00	109.92
3	B	602	GTP	O4'-C1'-N9	-3.32	104.34	108.75
4	D	603	NAI	C4B-O4B-C1B	-3.29	106.92	109.92
3	B	602	GTP	C2-N1-C6	-3.14	119.36	125.11
4	B	604	NAI	C4B-O4B-C1B	-3.13	107.06	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	604	NAI	C3N-C2N-N1N	-3.13	118.61	123.20
4	F	601	NAI	C2D-C1D-N1N	-3.10	105.69	113.31
3	D	602	GTP	C2-N1-C6	-3.09	119.45	125.11
3	F	604	GTP	O4'-C1'-N9	2.99	112.71	108.75
4	F	601	NAI	C6N-N1N-C2N	-2.98	116.13	119.32
3	A	602	GTP	C4'-O4'-C1'	-2.97	107.21	109.92
3	E	602	GTP	C2-N1-C6	-2.96	119.69	125.11
4	E	603	NAI	O4D-C1D-C2D	-2.94	100.33	106.62
3	C	602	GTP	C2-N1-C6	-2.92	119.77	125.11
3	B	602	GTP	C5-C6-N1	2.91	119.62	114.07
2	B	601	GLU	OXT-C-O	-2.90	117.50	124.08
3	E	602	GTP	C5-C6-N1	2.90	119.59	114.07
2	F	602	GLU	OXT-C-O	-2.88	117.54	124.08
3	D	602	GTP	C5-C6-N1	2.85	119.51	114.07
4	F	603	NAI	C4B-O4B-C1B	-2.83	107.34	109.92
4	B	603	NAI	C1D-N1N-C2N	2.80	125.75	121.14
3	C	602	GTP	C5-C6-N1	2.80	119.41	114.07
2	C	601	GLU	OXT-C-O	-2.76	117.81	124.08
3	A	602	GTP	C5-C6-N1	2.74	119.30	114.07
4	F	603	NAI	C2D-C1D-N1N	-2.72	106.61	113.31
4	F	605	NAI	C2D-C1D-N1N	-2.72	106.62	113.31
4	F	601	NAI	N6A-C6A-N1A	-2.65	112.68	118.33
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
3	D	602	GTP	C4'-O4'-C1'	2.61	112.32	109.92
4	A	604	NAI	C6N-N1N-C2N	-2.60	116.54	119.32
4	C	604	NAI	C4B-O4B-C1B	-2.59	107.56	109.92
4	A	603	NAI	C1D-N1N-C6N	-2.58	115.32	120.77
4	D	603	NAI	O5D-C5D-C4D	2.53	117.61	108.99
3	F	604	GTP	C2-N1-C6	-2.53	120.48	125.11
3	F	604	GTP	C5-C6-N1	2.52	118.88	114.07
3	A	602	GTP	C2-N1-C6	-2.51	120.52	125.11
4	F	605	NAI	C1D-N1N-C2N	2.50	125.26	121.14
2	E	601	GLU	OXT-C-O	-2.49	118.42	124.08
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	B	602	GTP	O3G-PG-O3B	2.44	112.82	104.64
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
4	D	604	NAI	O4D-C1D-N1N	2.42	112.71	108.08
2	D	601	GLU	OXT-C-O	-2.39	118.66	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	603	NAI	C3D-C2D-C1D	-2.39	96.95	101.46
4	B	603	NAI	C3N-C2N-N1N	-2.36	119.73	123.20
4	A	604	NAI	O4B-C1B-N9A	2.31	111.81	108.75
4	A	603	NAI	C3N-C2N-N1N	-2.31	119.82	123.20
4	F	605	NAI	C4D-O4D-C1D	-2.30	104.39	109.47
3	A	602	GTP	O6-C6-C5	-2.28	119.80	124.32
4	F	601	NAI	C3N-C7N-N7N	2.28	121.71	117.67
3	D	602	GTP	O6-C6-C5	-2.27	119.83	124.32
2	A	601	GLU	OXT-C-O	-2.25	118.97	124.08
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	A	603	NAI	C4B-O4B-C1B	-2.22	107.89	109.92
4	F	605	NAI	O4D-C4D-C3D	-2.22	100.76	105.15
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
4	D	604	NAI	C3N-C2N-N1N	-2.18	120.00	123.20
4	E	603	NAI	O4B-C1B-N9A	-2.16	105.88	108.75
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	D	604	NAI	O4D-C4D-C3D	-2.11	100.96	105.15
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
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	B	604	NAI	O4B-C1B-N9A	2.06	111.47	108.75
4	C	604	NAI	O4D-C1D-N1N	2.05	112.00	108.08
3	E	602	GTP	O6-C6-C5	-2.05	120.25	124.32
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 (157) 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'

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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	603	NAI	O4B-C4B-C5B-O5B
4	C	603	NAI	O4D-C4D-C5D-O5D
4	E	603	NAI	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	E	603	NAI	C3B-C4B-C5B-O5B
4	D	604	NAI	O4D-C4D-C5D-O5D
3	D	602	GTP	PB-O3A-PA-O5'
4	C	604	NAI	PN-O3-PA-O5B
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	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
3	A	602	GTP	PA-O3A-PB-O3B
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
4	E	603	NAI	O4D-C1D-N1N-C6N
2	A	601	GLU	OE2-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
3	E	602	GTP	PA-O3A-PB-O1B
3	F	604	GTP	PA-O3A-PB-O1B
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
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
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	E	603	NAI	10	0
4	A	604	NAI	7	0
3	A	602	GTP	13	0
3	F	604	GTP	2	0
3	B	602	GTP	2	0
3	E	602	GTP	1	0
4	F	603	NAI	3	0
4	C	603	NAI	4	0
2	D	601	GLU	4	0
2	A	601	GLU	7	0
4	C	604	NAI	6	0

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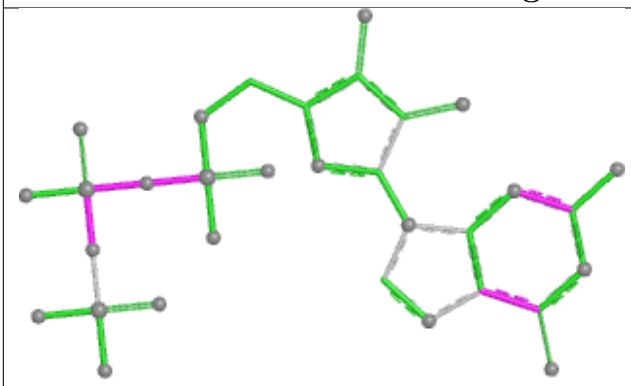
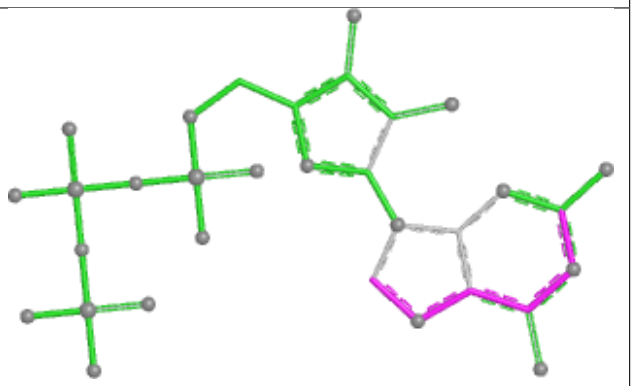
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	603	NAI	5	0
4	D	604	NAI	4	0
2	B	601	GLU	7	0
2	F	602	GLU	5	0
4	F	605	NAI	9	0
2	E	601	GLU	6	0
2	C	601	GLU	4	0
4	B	603	NAI	12	0
4	F	601	NAI	11	0
3	D	602	GTP	1	0
4	A	603	NAI	4	0
4	B	604	NAI	3	0

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

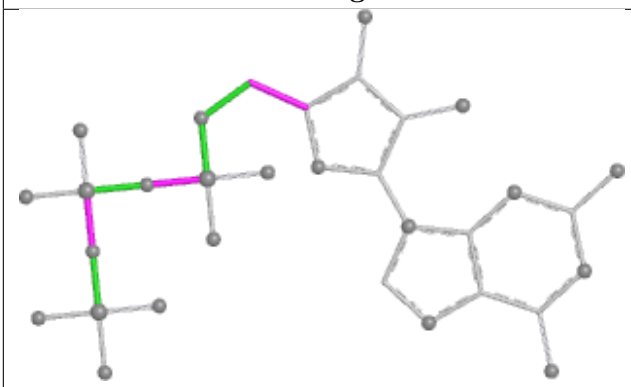
Ligand GTP C 602



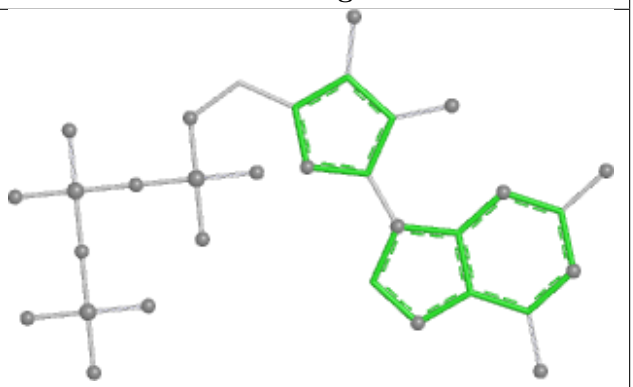
Bond lengths



Bond angles

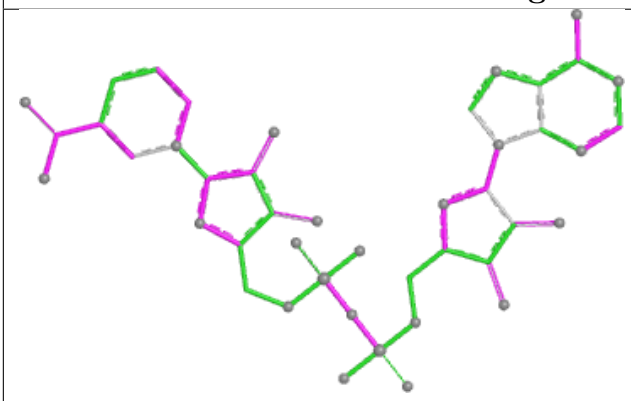


Torsions

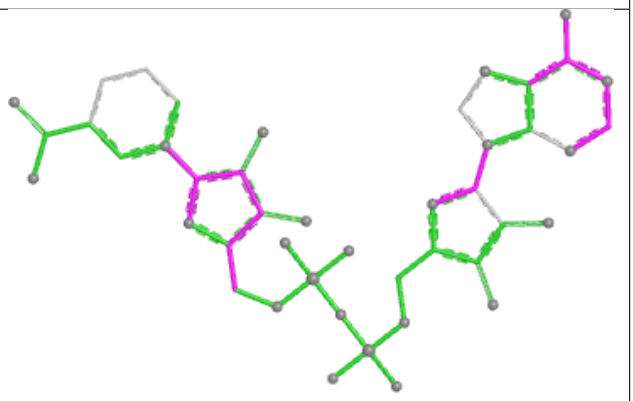


Rings

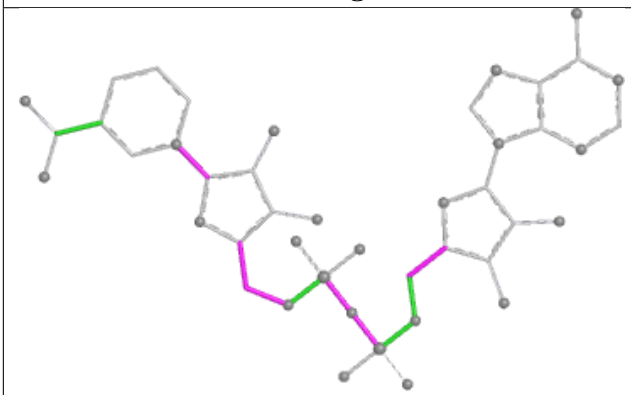
Ligand NAI E 603



Bond lengths



Bond angles



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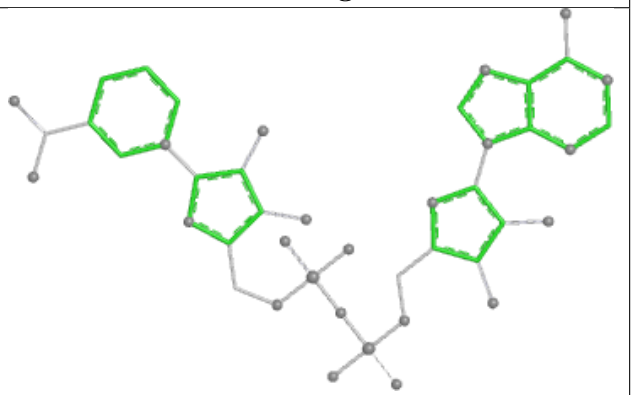
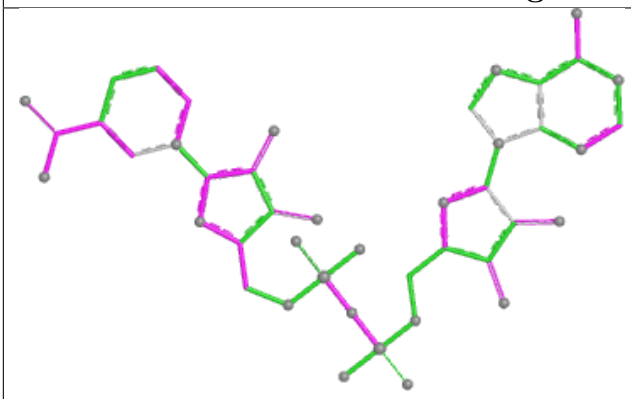


Rings

Ligand NAI A 604



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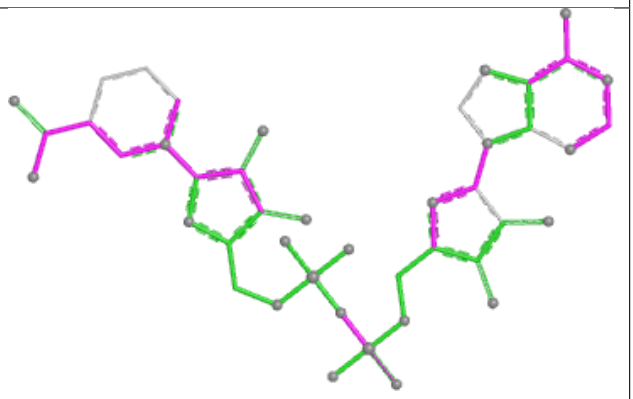
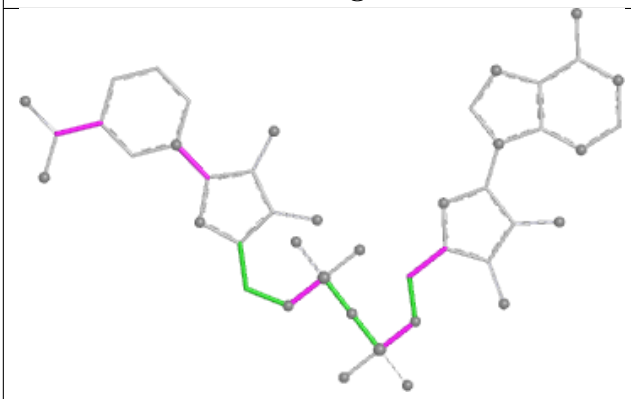
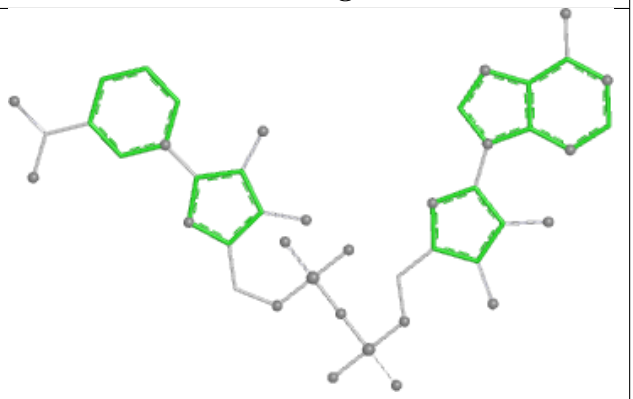


Bond angles

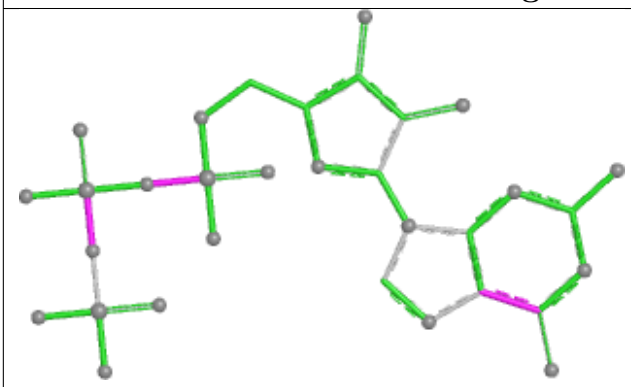


Torsions



Rings

Ligand GTP A 602



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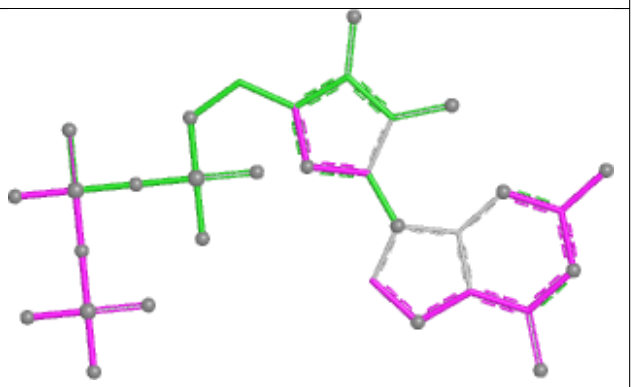
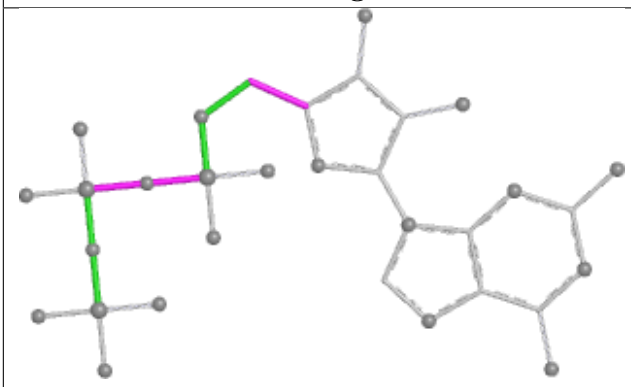
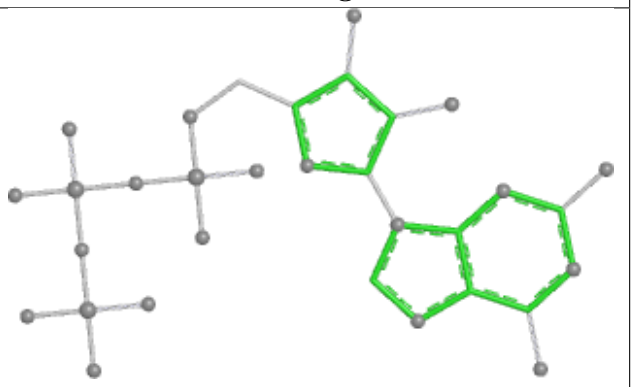


Bond angles

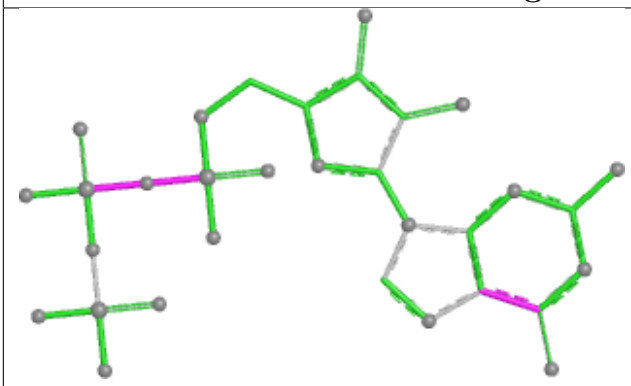


Torsions

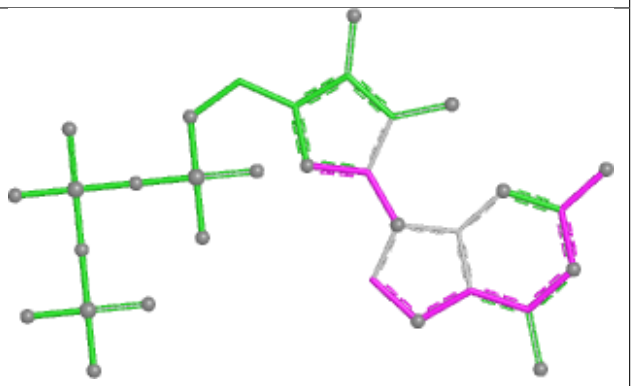


Rings

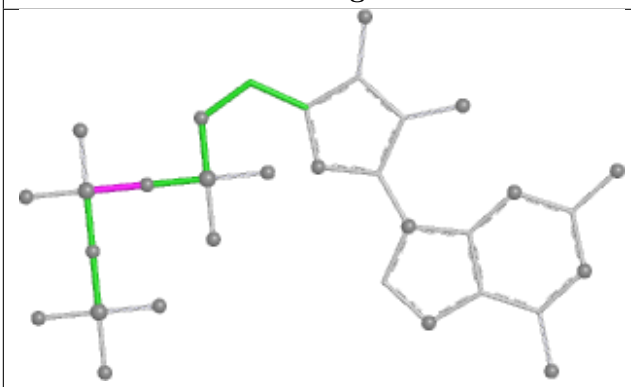
Ligand GTP F 604



Bond lengths



Bond angles



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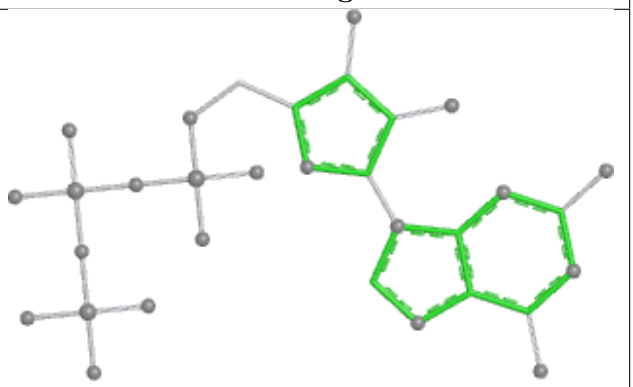
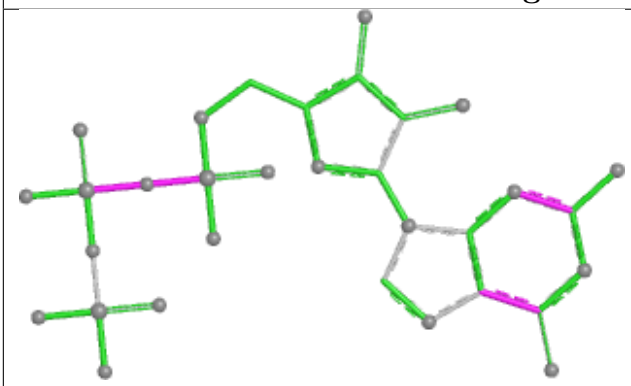


Rings

Ligand GTP B 602



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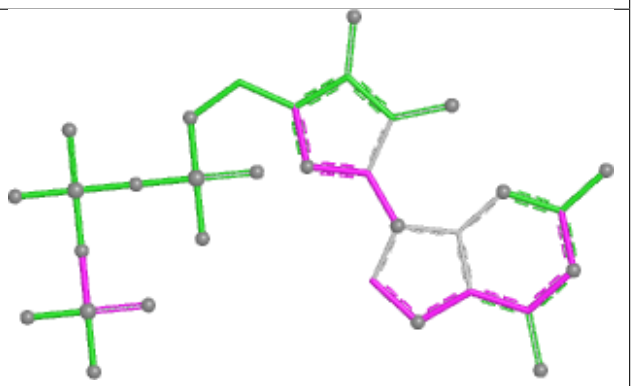

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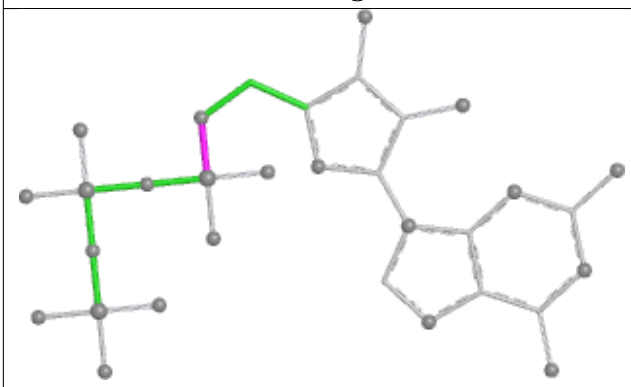

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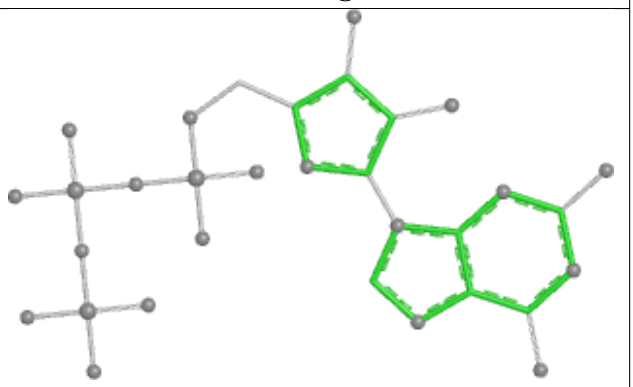
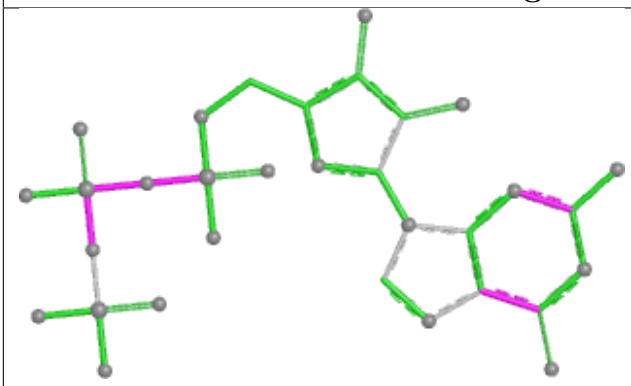


Rings

Ligand GTP E 602



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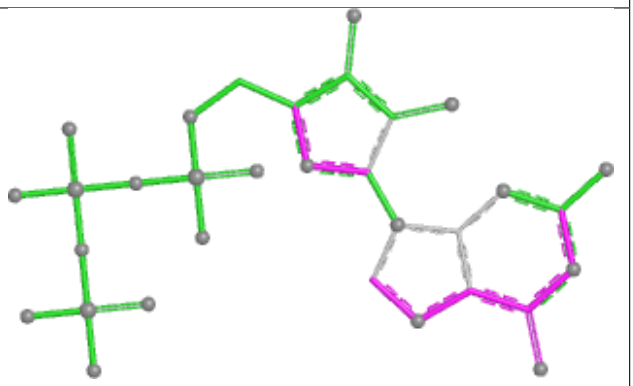

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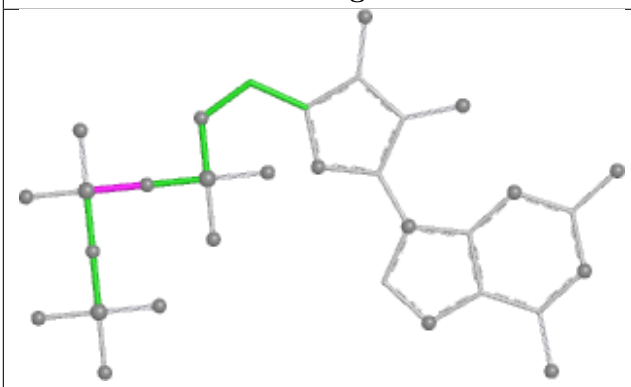

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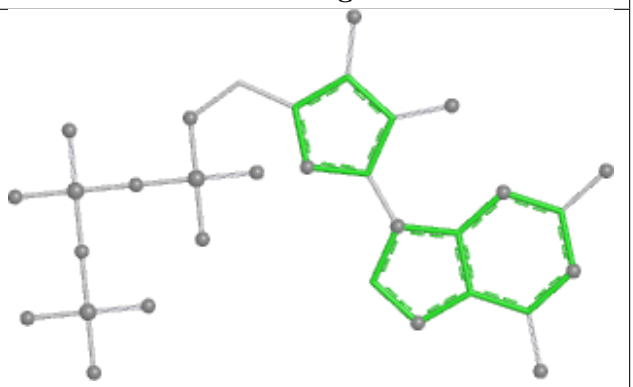
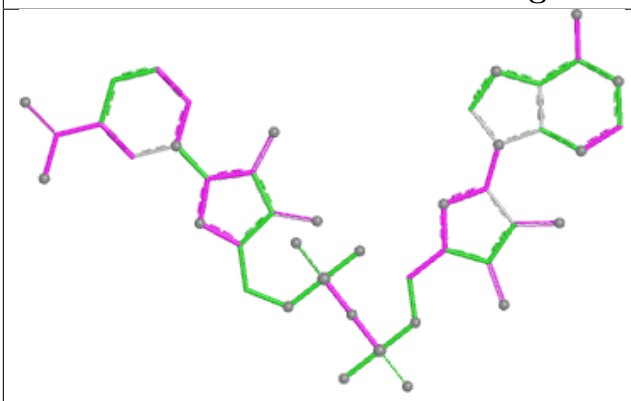


Rings

Ligand NAI F 603



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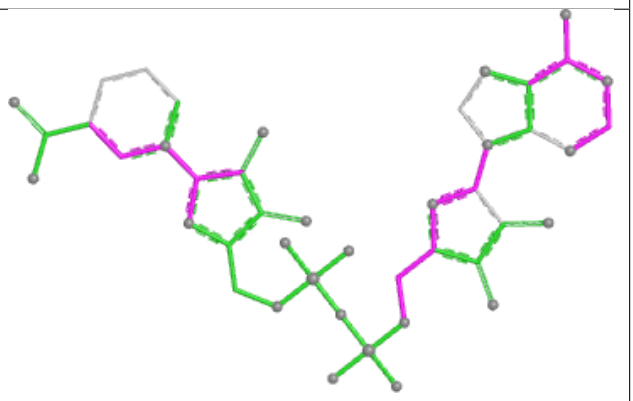

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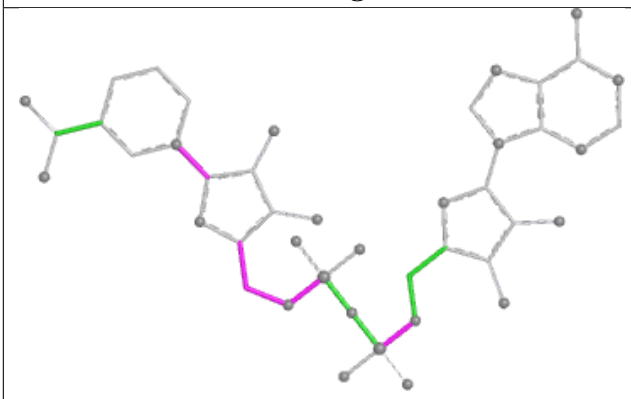

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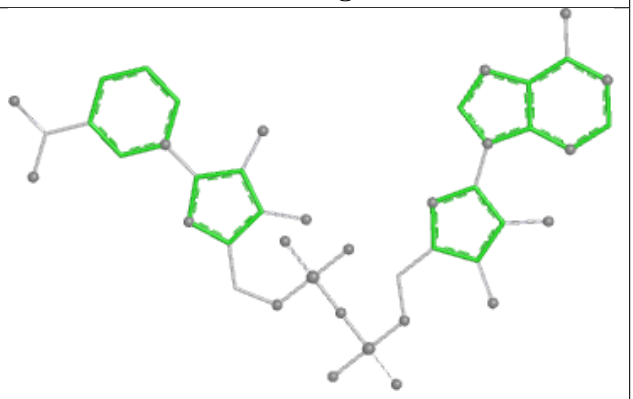
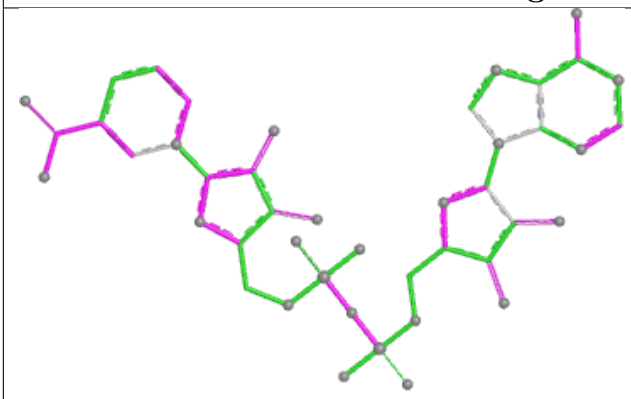


Rings

Ligand NAI C 603



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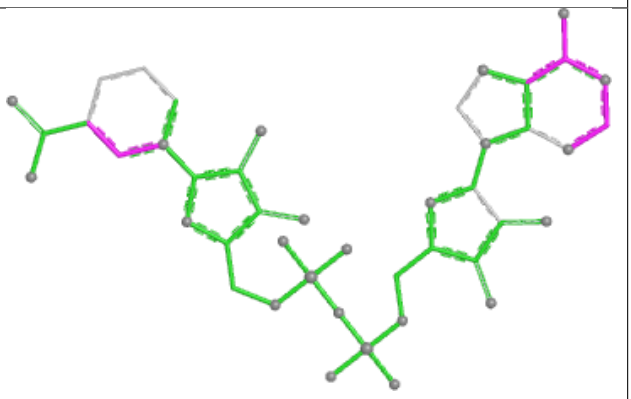

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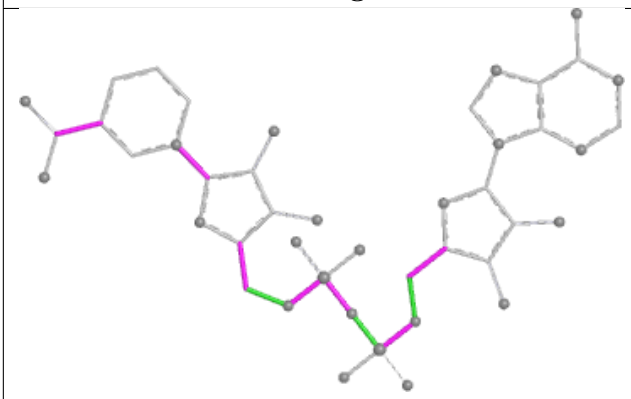

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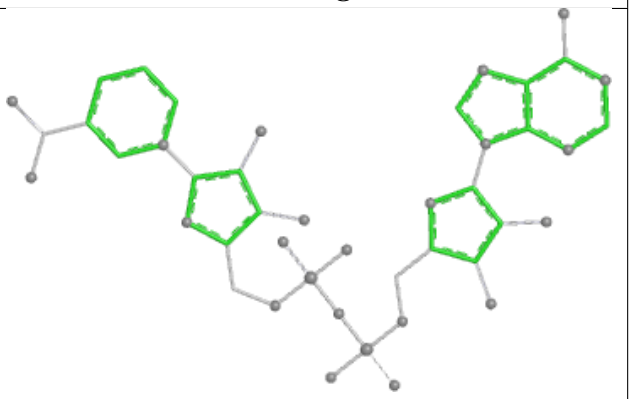
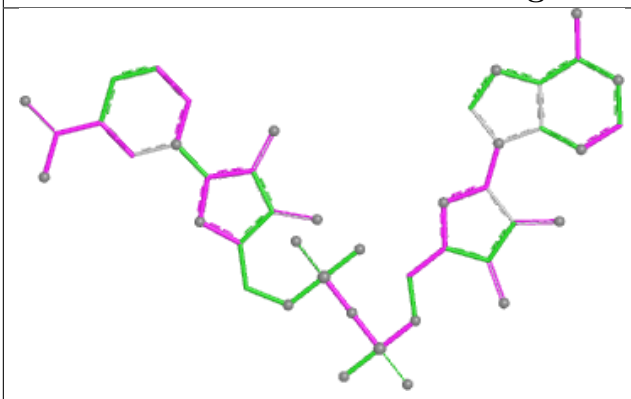
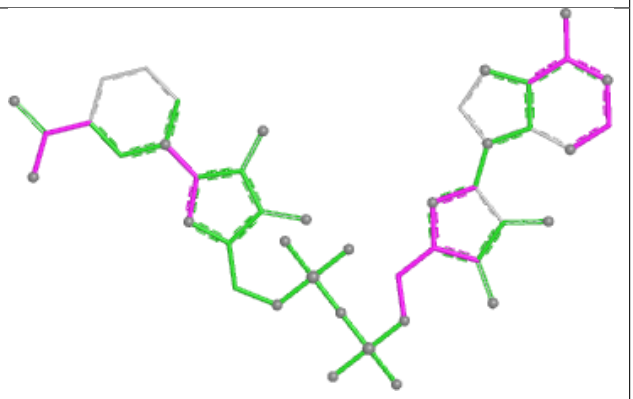


Rings

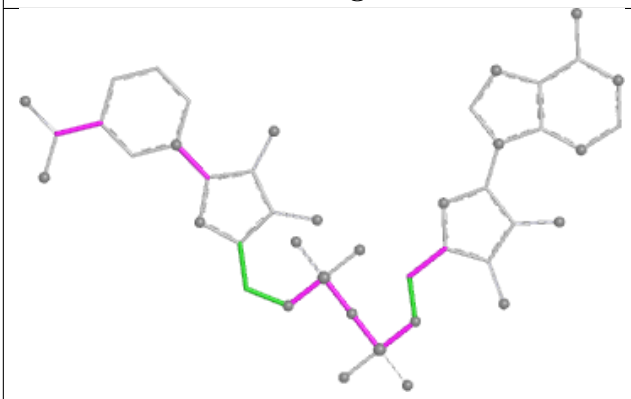
Ligand NAI C 604



Bond lengths



Bond angles



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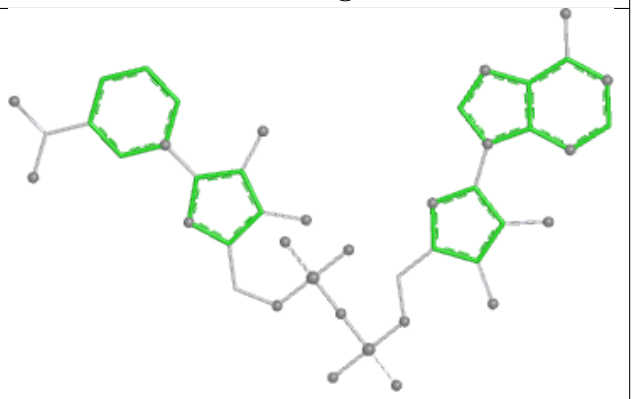
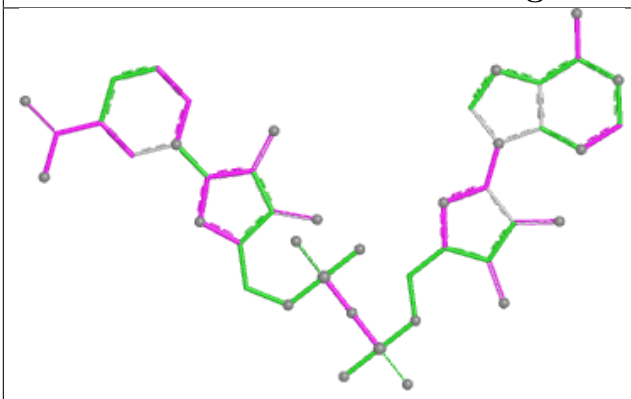


Rings

Ligand NAI D 603



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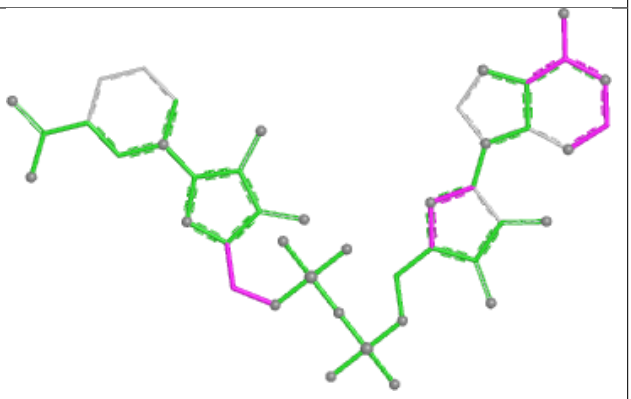
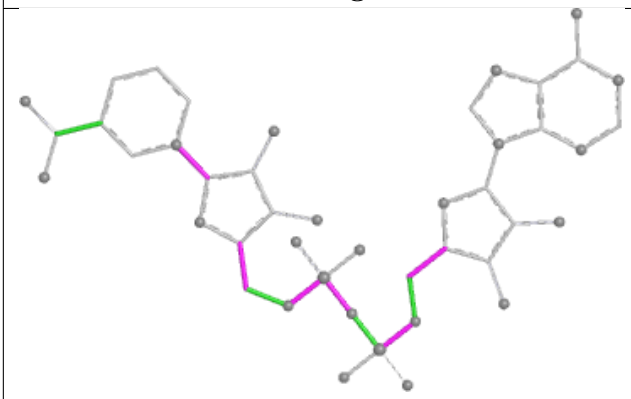
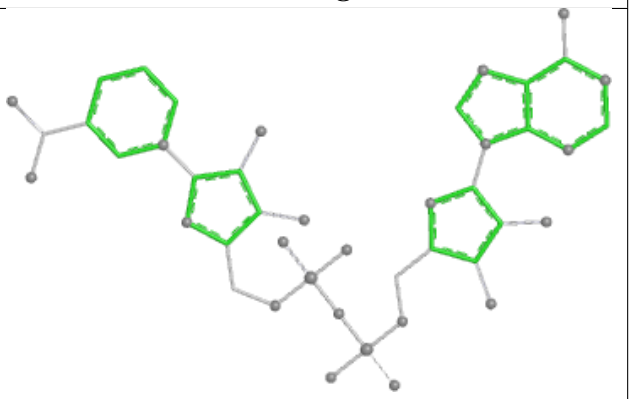


Bond angles

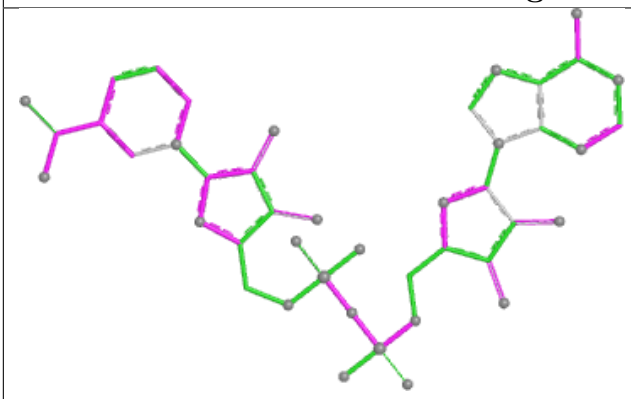


Torsions

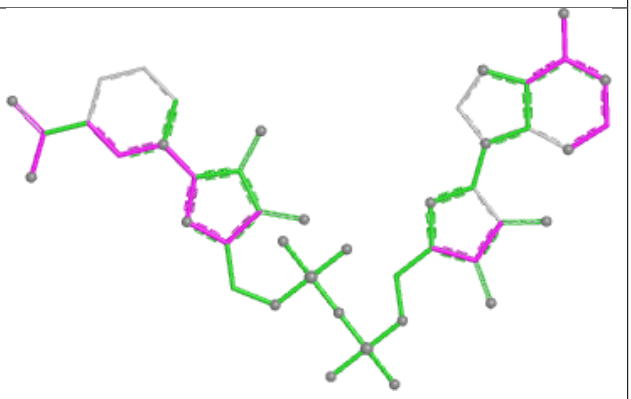


Rings

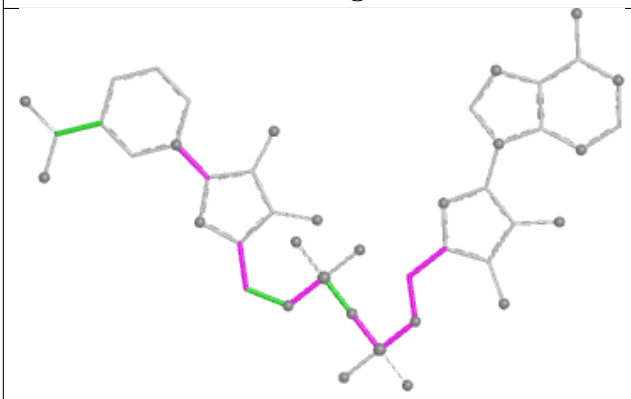
Ligand NAI D 604



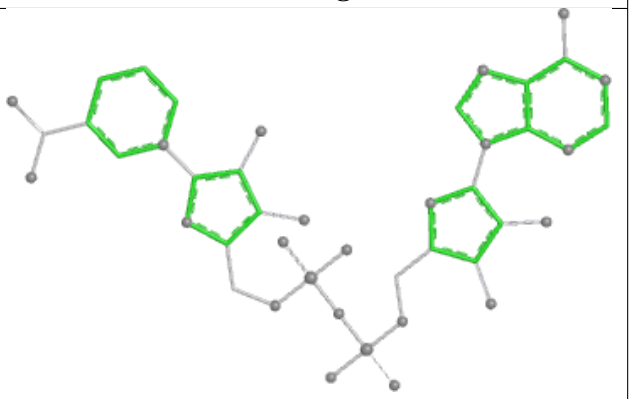
Bond lengths



Bond angles

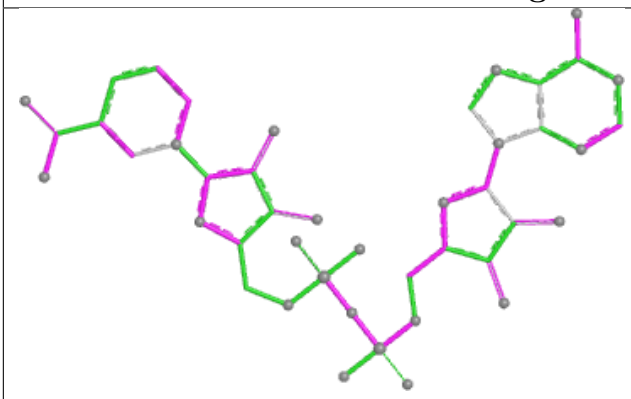


Torsions

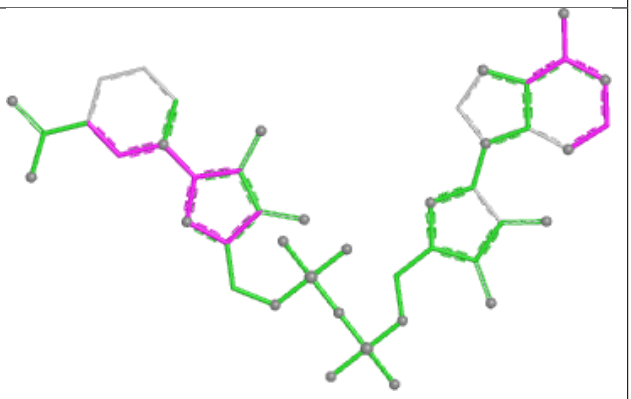


Rings

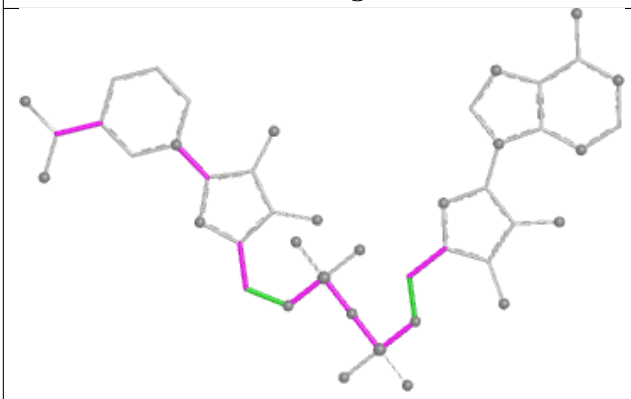
Ligand NAI F 605



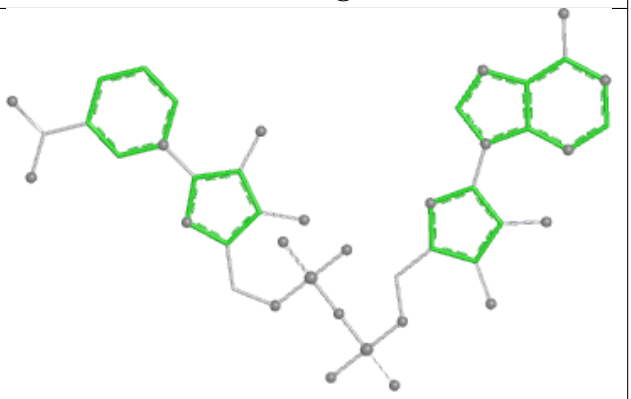
Bond lengths



Bond angles

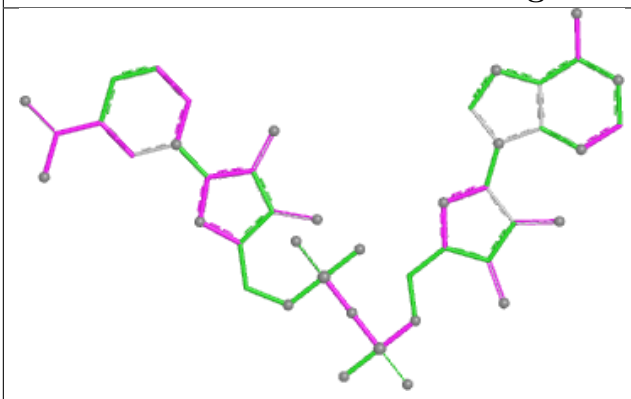


Torsions

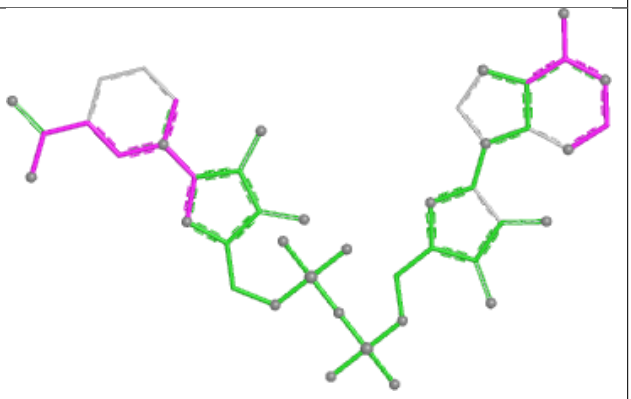


Rings

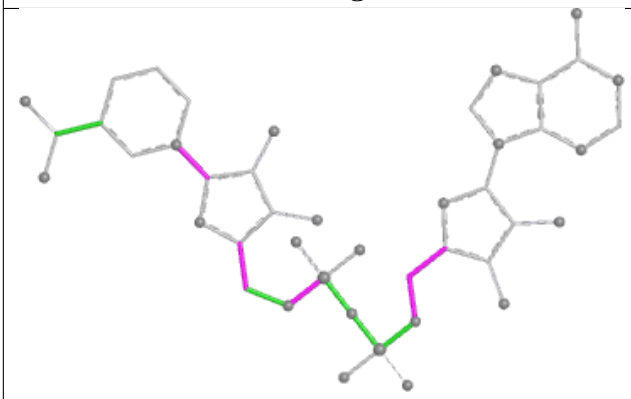
Ligand NAI B 603



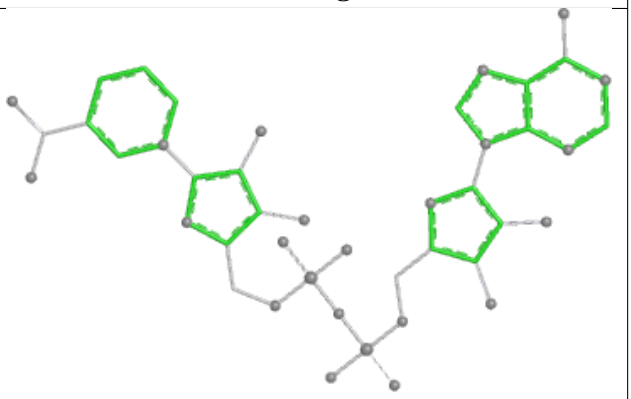
Bond lengths



Bond angles

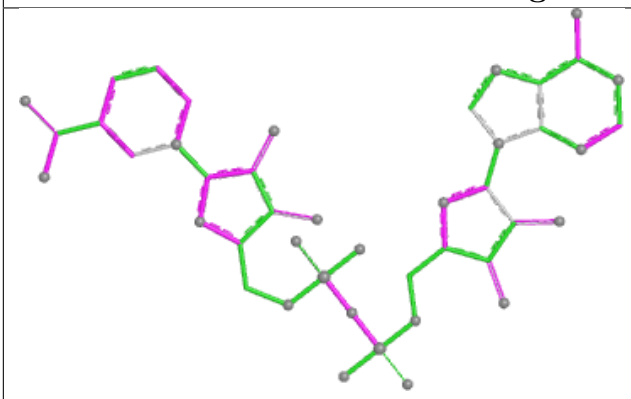


Torsions

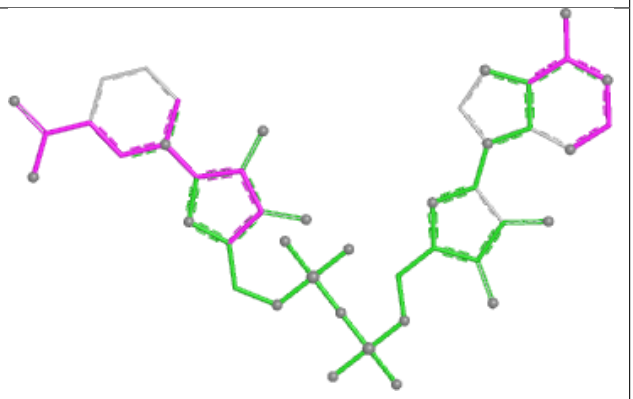


Rings

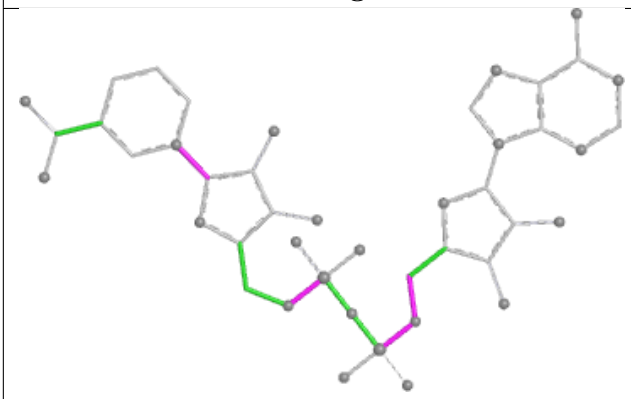
Ligand NAI F 601



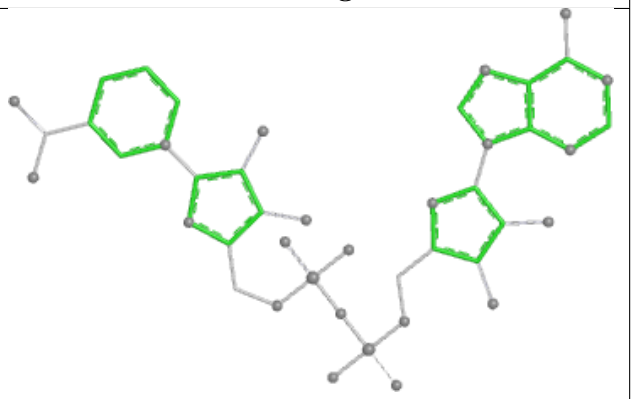
Bond lengths



Bond angles

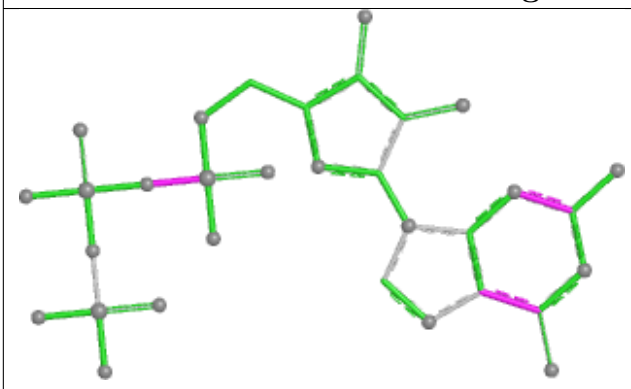


Torsions

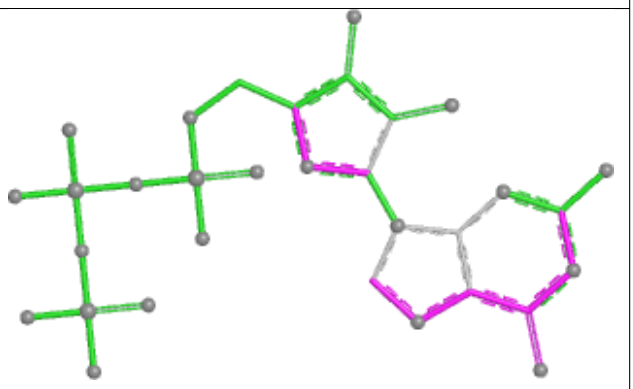


Rings

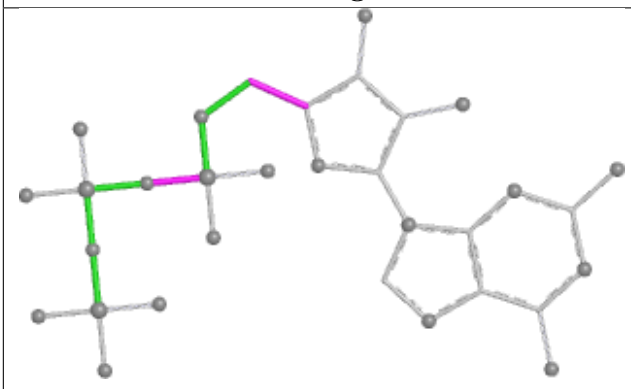
Ligand GTP D 602



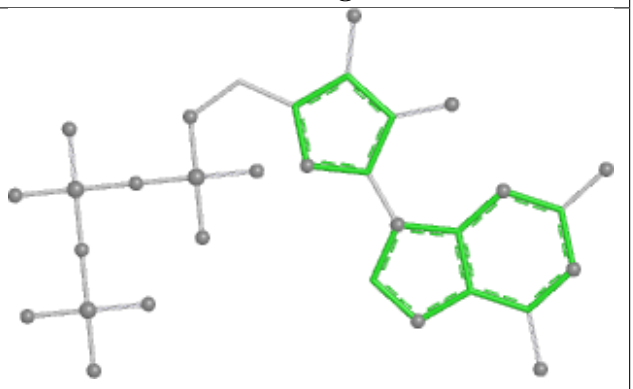
Bond lengths



Bond angles

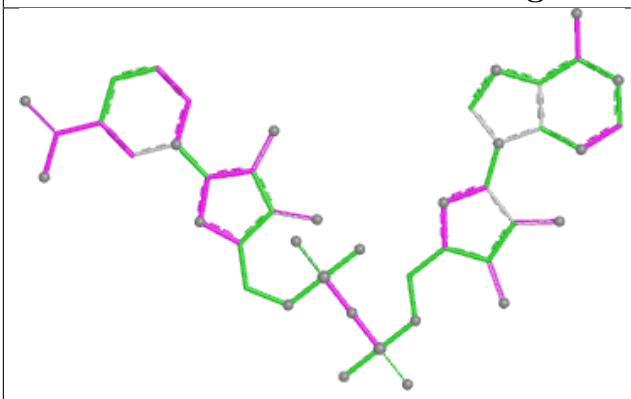


Torsions

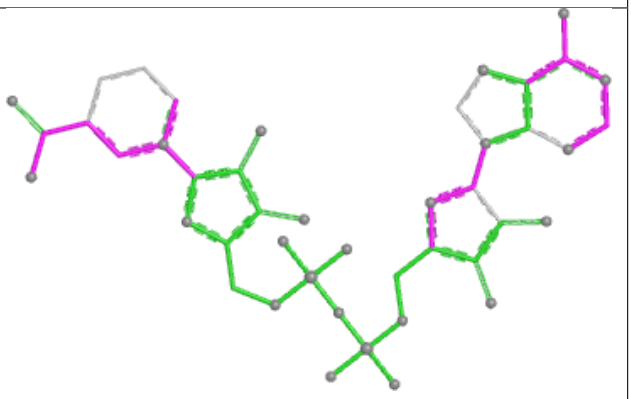


Rings

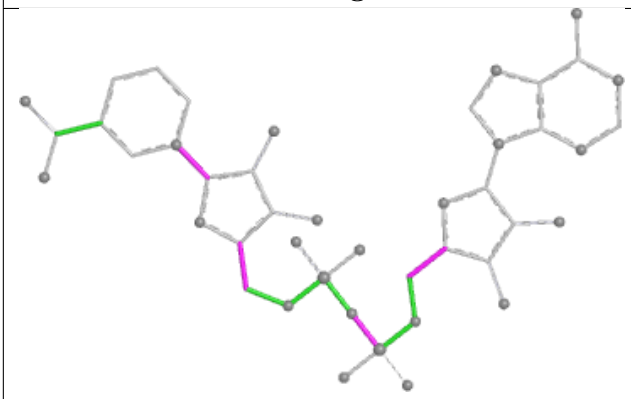
Ligand NAI A 603



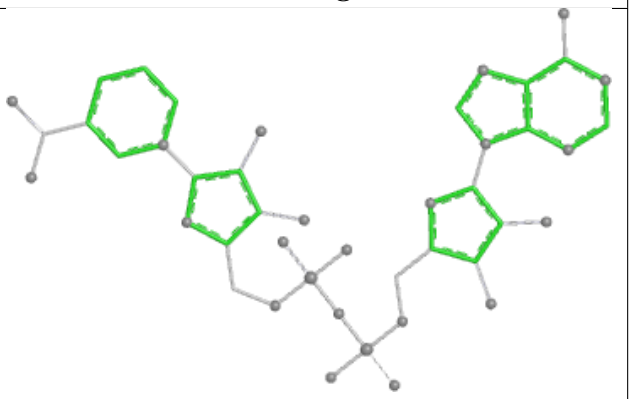
Bond lengths



Bond angles

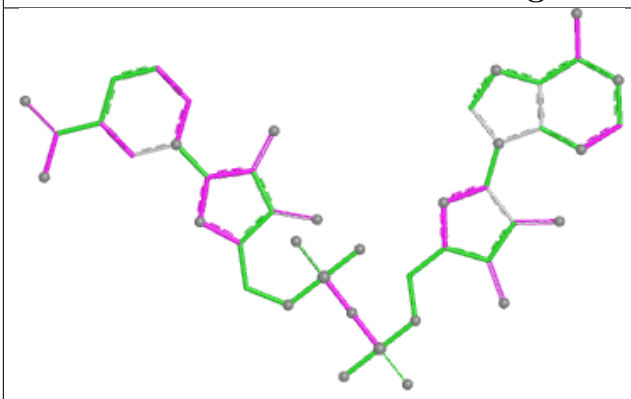


Torsions

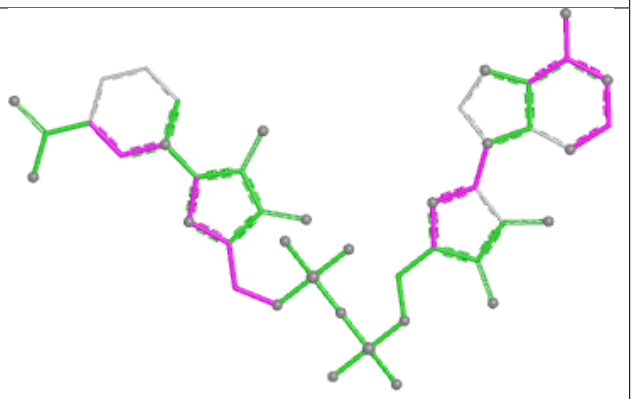


Rings

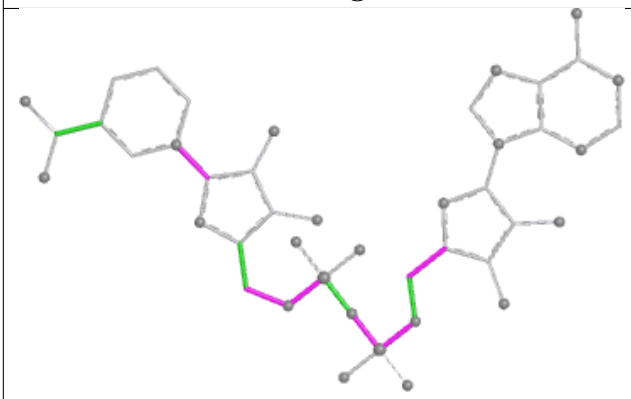
Ligand NAI B 604



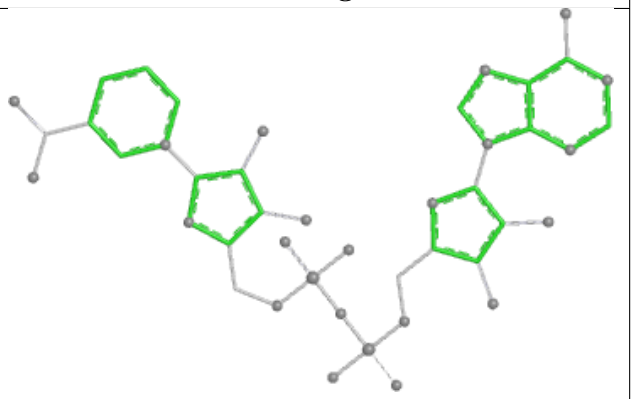
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	501/582 (86%)	0.86	50 (9%) 14 13	8, 34, 69, 101	0
1	B	501/582 (86%)	0.78	34 (6%) 25 20	7, 29, 65, 94	0
1	C	501/582 (86%)	0.99	60 (11%) 10 10	12, 37, 72, 99	0
1	D	501/582 (86%)	0.81	36 (7%) 23 19	8, 30, 62, 89	0
1	E	501/582 (86%)	1.06	70 (13%) 7 8	7, 41, 78, 95	0
1	F	501/582 (86%)	0.92	51 (10%) 13 13	9, 34, 66, 95	0
All	All	3006/3492 (86%)	0.90	301 (10%) 14 13	7, 34, 73, 101	0

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	THR	6.0
1	D	500	PHE	5.2
1	B	499	THR	5.0
1	F	223	ILE	5.0
1	B	498	VAL	4.9
1	C	500	PHE	4.6
1	A	413	VAL	4.5
1	D	499	THR	4.4
1	C	319	CYS	4.4
1	B	497	GLY	4.3
1	F	443	ALA	4.3
1	F	498	VAL	4.2
1	F	501	THR	4.2
1	F	500	PHE	4.1
1	D	498	VAL	4.1
1	A	37	THR	4.1
1	A	119	ASP	4.0
1	C	286	ILE	4.0
1	F	4	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	424	HIS	4.0
1	E	250	GLN	4.0
1	B	428	ILE	4.0
1	A	490	PHE	3.9
1	E	305	PRO	3.8
1	B	426	GLY	3.8
1	A	395	GLY	3.8
1	E	474	GLY	3.8
1	B	501	THR	3.8
1	C	31	ASP	3.7
1	E	267	GLY	3.7
1	E	249	VAL	3.7
1	B	393	SER	3.7
1	B	257	LEU	3.7
1	F	251	GLY	3.6
1	F	2	ASP	3.6
1	E	393	SER	3.6
1	B	500	PHE	3.6
1	F	190	TYR	3.5
1	A	410	LEU	3.5
1	F	71	SER	3.5
1	E	498	VAL	3.5
1	D	402	GLU	3.5
1	D	210	GLY	3.5
1	E	266	PHE	3.5
1	C	301	ILE	3.5
1	D	501	THR	3.4
1	E	288	PRO	3.4
1	E	315	LEU	3.3
1	A	484	ASN	3.3
1	C	280	ILE	3.3
1	D	285	GLY	3.3
1	D	286	ILE	3.3
1	F	499	THR	3.3
1	F	298	HIS	3.3
1	E	475	LEU	3.3
1	E	464	ILE	3.3
1	E	497	GLY	3.2
1	E	1	ALA	3.2
1	C	251	GLY	3.2
1	E	425	GLY	3.2
1	C	242	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	430	ILE	3.2
1	D	497	GLY	3.1
1	C	298	HIS	3.1
1	F	189	HIS	3.1
1	F	412	SER	3.1
1	E	443	ALA	3.1
1	E	252	PHE	3.1
1	A	440	ILE	3.1
1	C	501	THR	3.0
1	E	215	THR	3.0
1	E	421	PHE	3.0
1	A	23	ILE	3.0
1	D	4	GLU	3.0
1	F	241	GLY	3.0
1	F	1	ALA	3.0
1	D	355	GLU	3.0
1	B	133	PRO	3.0
1	C	339	VAL	3.0
1	E	313	SER	3.0
1	F	440	ILE	3.0
1	C	499	THR	2.9
1	C	62	SER	2.9
1	A	254	ASN	2.9
1	E	251	GLY	2.9
1	B	394	TYR	2.9
1	C	300	THR	2.9
1	E	2	ASP	2.9
1	E	270	CYS	2.9
1	E	227	ILE	2.9
1	E	501	THR	2.8
1	E	284	ASP	2.8
1	C	405	SER	2.8
1	A	190	TYR	2.8
1	E	304	PHE	2.8
1	F	317	VAL	2.8
1	C	441	SER	2.8
1	E	16	PHE	2.8
1	B	347	GLY	2.8
1	C	270	CYS	2.8
1	E	226	PHE	2.8
1	D	362	GLU	2.8
1	E	477	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	243	GLY	2.7
1	E	500	PHE	2.7
1	C	443	ALA	2.7
1	E	481	ALA	2.7
1	F	340	LYS	2.7
1	E	292	GLU	2.7
1	E	339	VAL	2.7
1	B	425	GLY	2.7
1	E	446	LYS	2.7
1	F	424	HIS	2.7
1	F	394	TYR	2.7
1	A	431	VAL	2.7
1	C	343	ILE	2.7
1	C	425	GLY	2.7
1	C	68	ASP	2.6
1	F	484	ASN	2.6
1	A	336	ALA	2.6
1	E	499	THR	2.6
1	D	426	GLY	2.6
1	B	414	GLN	2.6
1	F	70	GLY	2.6
1	F	445	GLU	2.6
1	C	236	LEU	2.6
1	E	327	SER	2.6
1	D	413	VAL	2.6
1	F	312	GLY	2.6
1	D	1	ALA	2.6
1	B	36	GLU	2.6
1	F	402	GLU	2.6
1	D	78	TYR	2.5
1	A	299	GLY	2.5
1	A	497	GLY	2.5
1	C	308	LYS	2.5
1	A	428	ILE	2.5
1	F	227	ILE	2.5
1	E	72	TRP	2.5
1	F	72	TRP	2.5
1	A	426	GLY	2.5
1	E	19	ARG	2.5
1	D	443	ALA	2.5
1	A	103	GLU	2.5
1	E	355	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	339	VAL	2.5
1	B	416	SER	2.5
1	E	334	SER	2.5
1	E	398	THR	2.5
1	B	242	PHE	2.5
1	B	443	ALA	2.5
1	C	162	VAL	2.5
1	E	293	ASP	2.5
1	F	338	ARG	2.5
1	A	402	GLU	2.5
1	A	302	LEU	2.5
1	A	226	PHE	2.5
1	A	394	TYR	2.5
1	C	29	VAL	2.5
1	C	4	GLU	2.5
1	A	278	GLY	2.4
1	E	65	ILE	2.4
1	F	3	ARG	2.4
1	D	334	SER	2.4
1	E	476	ASP	2.4
1	C	44	ARG	2.4
1	D	108	ALA	2.4
1	F	45	VAL	2.4
1	A	429	PRO	2.4
1	E	428	ILE	2.4
1	C	469	MET	2.4
1	A	498	VAL	2.4
1	F	444	SER	2.4
1	B	418	GLU	2.4
1	B	489	VAL	2.4
1	A	51	ILE	2.3
1	D	305	PRO	2.3
1	E	343	ILE	2.3
1	A	266	PHE	2.3
1	F	119	ASP	2.3
1	E	285	GLY	2.3
1	A	489	VAL	2.3
1	C	19	ARG	2.3
1	A	414	GLN	2.3
1	C	368	ILE	2.3
1	F	429	PRO	2.3
1	A	313	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	327	SER	2.3
1	C	30	GLU	2.3
1	D	170	SER	2.3
1	C	355	GLU	2.3
1	F	438	ASP	2.3
1	B	101	VAL	2.3
1	C	72	TRP	2.3
1	F	212	ILE	2.3
1	C	421	PHE	2.3
1	C	328	GLU	2.3
1	D	198	VAL	2.3
1	D	236	LEU	2.3
1	B	262	TYR	2.3
1	D	95	TYR	2.3
1	F	236	LEU	2.3
1	F	244	ASP	2.2
1	A	270	CYS	2.2
1	D	219	VAL	2.2
1	A	1	ALA	2.2
1	A	80	ALA	2.2
1	A	235	ILE	2.2
1	D	93	ILE	2.2
1	E	314	ILE	2.2
1	F	428	ILE	2.2
1	C	304	PHE	2.2
1	C	305	PRO	2.2
1	C	498	VAL	2.2
1	F	496	ALA	2.2
1	C	223	ILE	2.2
1	C	119	ASP	2.2
1	C	406	ASN	2.2
1	A	34	THR	2.2
1	A	87	THR	2.2
1	E	232	TYR	2.2
1	F	250	GLN	2.2
1	C	346	GLU	2.2
1	B	444	SER	2.2
1	C	281	TRP	2.2
1	B	446	LYS	2.2
1	B	138	ASP	2.2
1	A	424	HIS	2.2
1	E	362	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	423	LYS	2.2
1	B	342	LYS	2.2
1	D	406	ASN	2.2
1	E	132	ASN	2.2
1	E	484	ASN	2.2
1	A	443	ALA	2.1
1	D	40	GLN	2.2
1	E	235	ILE	2.1
1	E	33	LYS	2.1
1	A	412	SER	2.1
1	E	367	VAL	2.1
1	F	473	LEU	2.1
1	E	306	LYS	2.1
1	A	501	THR	2.1
1	E	145	THR	2.1
1	B	494	ASN	2.1
1	E	225	ASN	2.1
1	F	68	ASP	2.1
1	A	283	PRO	2.1
1	F	195	HIS	2.1
1	D	417	LEU	2.1
1	A	268	ALA	2.1
1	B	427	THR	2.1
1	C	246	THR	2.1
1	F	456	THR	2.1
1	C	297	GLN	2.1
1	C	329	LYS	2.1
1	F	305	PRO	2.1
1	C	295	LYS	2.1
1	C	190	TYR	2.1
1	E	70	GLY	2.1
1	C	231	SER	2.1
1	E	95	TYR	2.1
1	E	170	SER	2.1
1	E	31	ASP	2.1
1	D	36	GLU	2.1
1	A	261	ARG	2.0
1	D	496	ALA	2.0
1	F	309	ILE	2.0
1	F	446	LYS	2.0
1	D	395	GLY	2.0
1	F	497	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	34	THR	2.0
1	B	190	TYR	2.0
1	E	34	THR	2.0
1	A	406	ASN	2.0
1	A	370	ASP	2.0
1	B	361	LEU	2.0
1	E	238	MET	2.0
1	A	116	ALA	2.0
1	A	365	ILE	2.0
1	C	344	ILE	2.0
1	C	274	GLY	2.0
1	F	274	GLY	2.0
1	B	145	THR	2.0
1	C	95	TYR	2.0
1	C	310	TYR	2.0
1	D	262	TYR	2.0
1	A	500	PHE	2.0
1	C	397	LEU	2.0
1	E	228	ASN	2.0
1	E	374	ASN	2.0
1	C	13	VAL	2.0
1	D	378	VAL	2.0
1	E	189	HIS	2.0
1	A	458	GLU	2.0
1	B	1	ALA	2.0
1	C	227	ILE	2.0
1	C	402	GLU	2.0
1	E	280	ILE	2.0
1	E	344	ILE	2.0
1	C	422	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

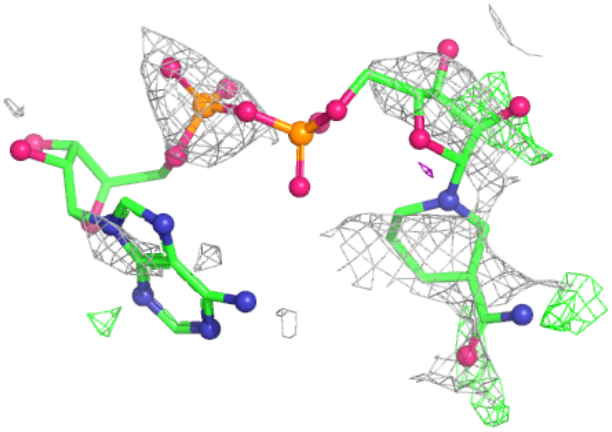
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

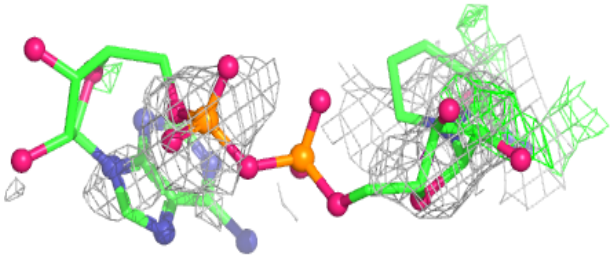
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAI	F	603	44/44	0.61	0.27	16,43,66,71	17
3	GTP	E	602	32/32	0.62	0.17	56,83,98,104	0
4	NAI	D	604	44/44	0.63	0.21	10,32,61,93	11
4	NAI	B	604	44/44	0.67	0.20	19,37,52,71	14
4	NAI	C	603	44/44	0.68	0.23	7,46,62,83	18
3	GTP	D	602	32/32	0.69	0.15	34,65,87,94	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
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

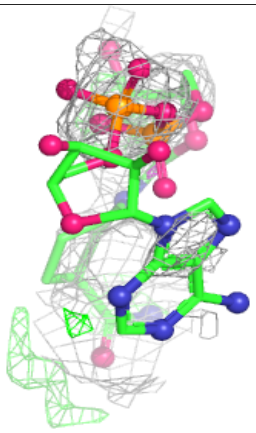
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

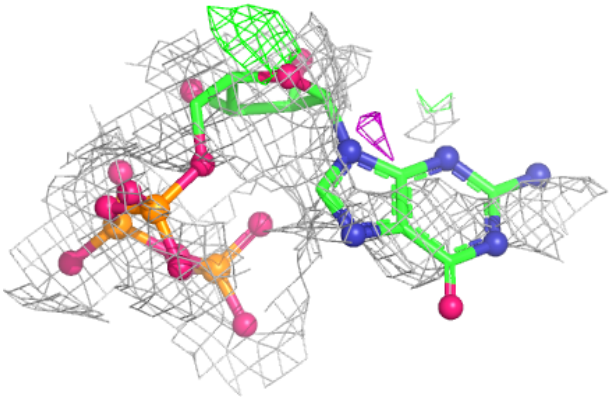


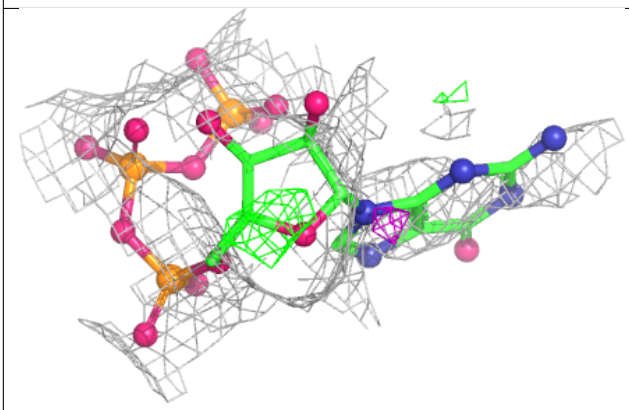


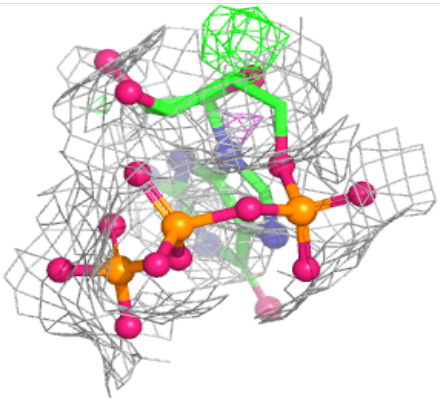


Electron density around GTP E 602:

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

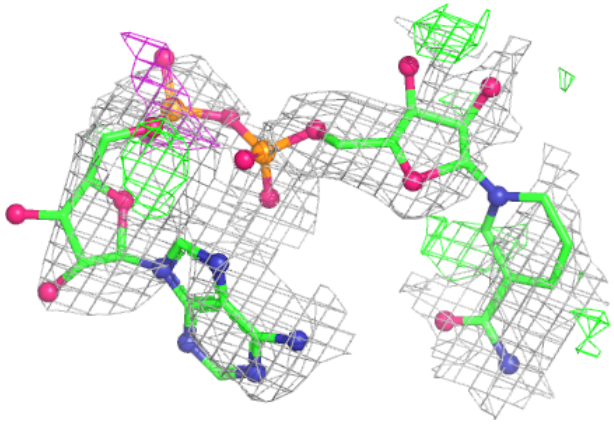


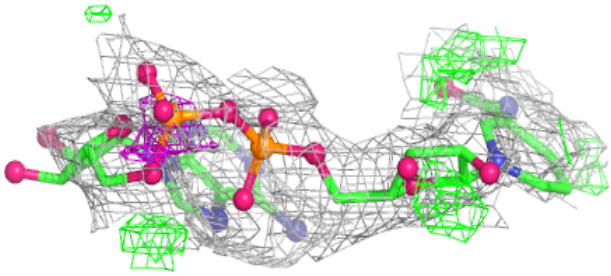


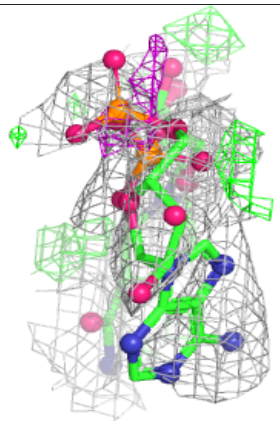


Electron density around NAI D 604:

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

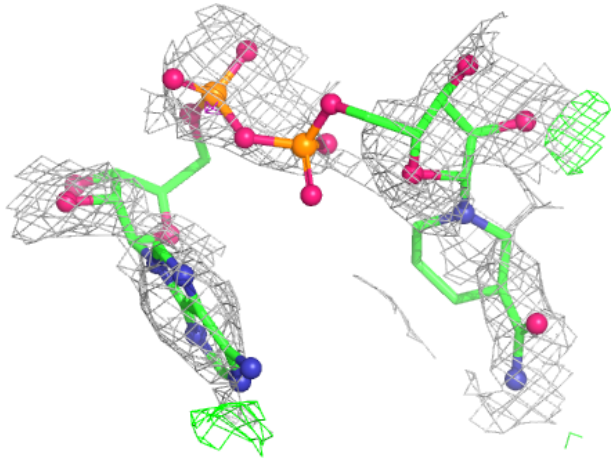


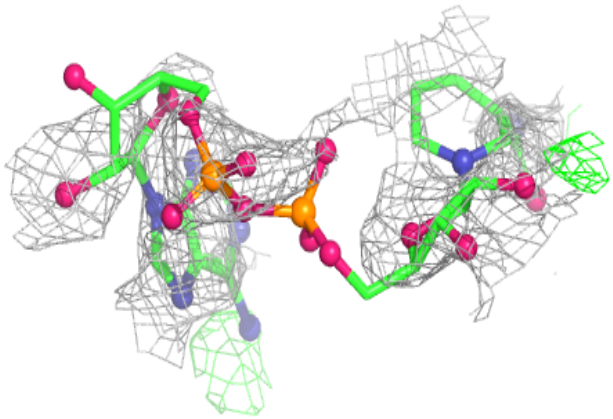


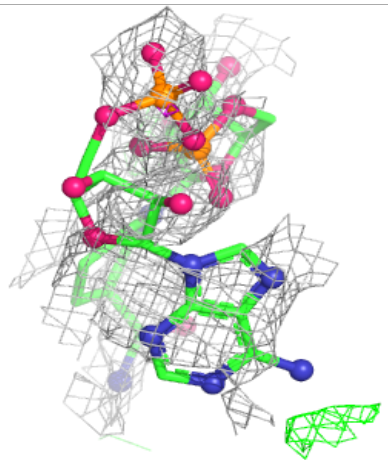


Electron density around NAI B 604:

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

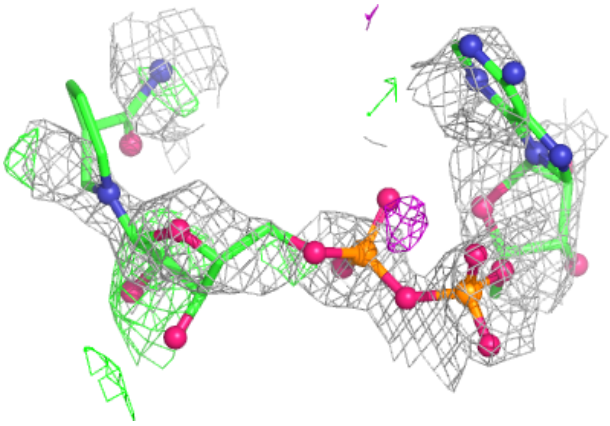


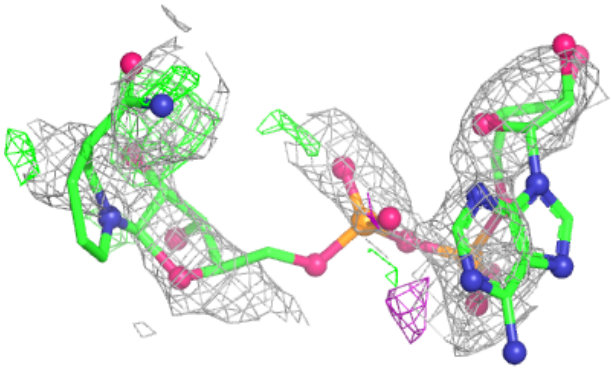


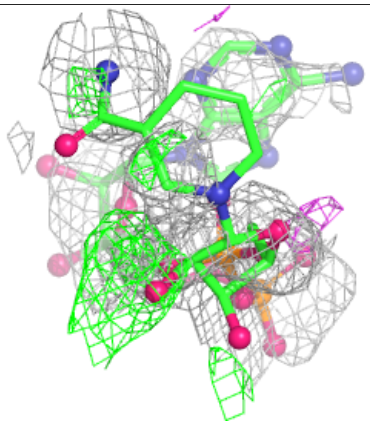


Electron density around NAI C 603:

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

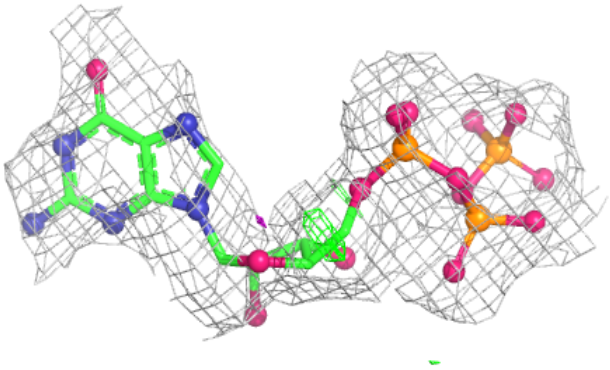


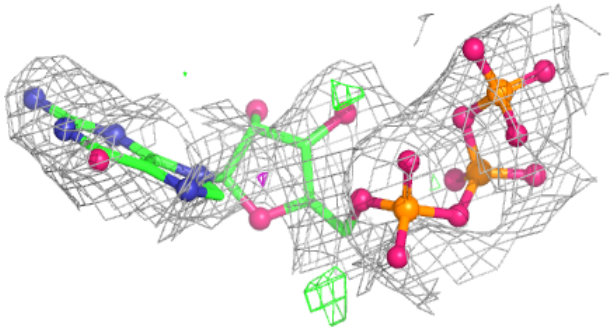


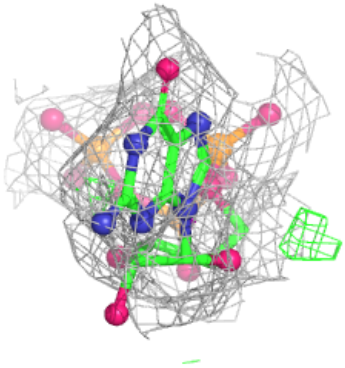


Electron density around GTP D 602:

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

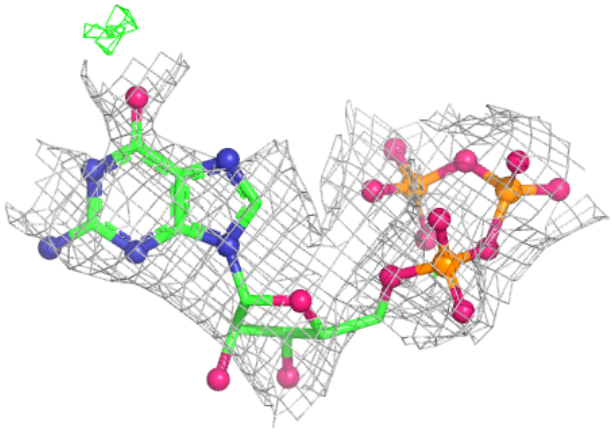


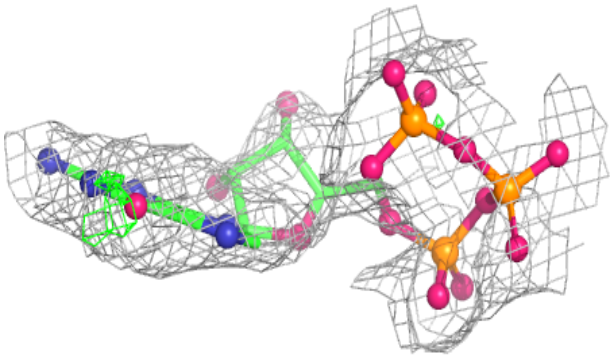


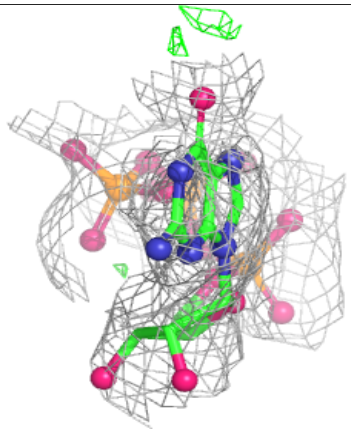


Electron density around GTP C 602:

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

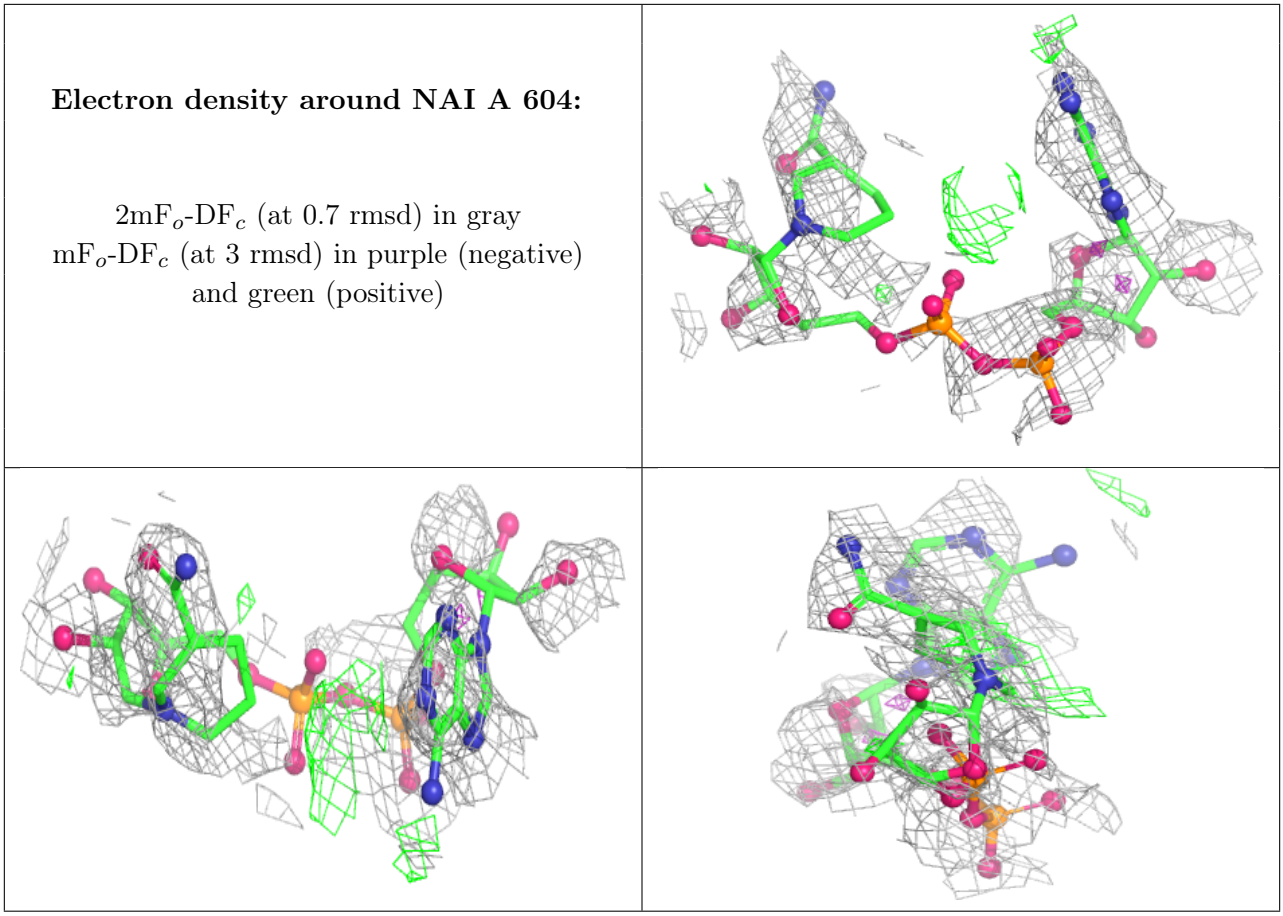






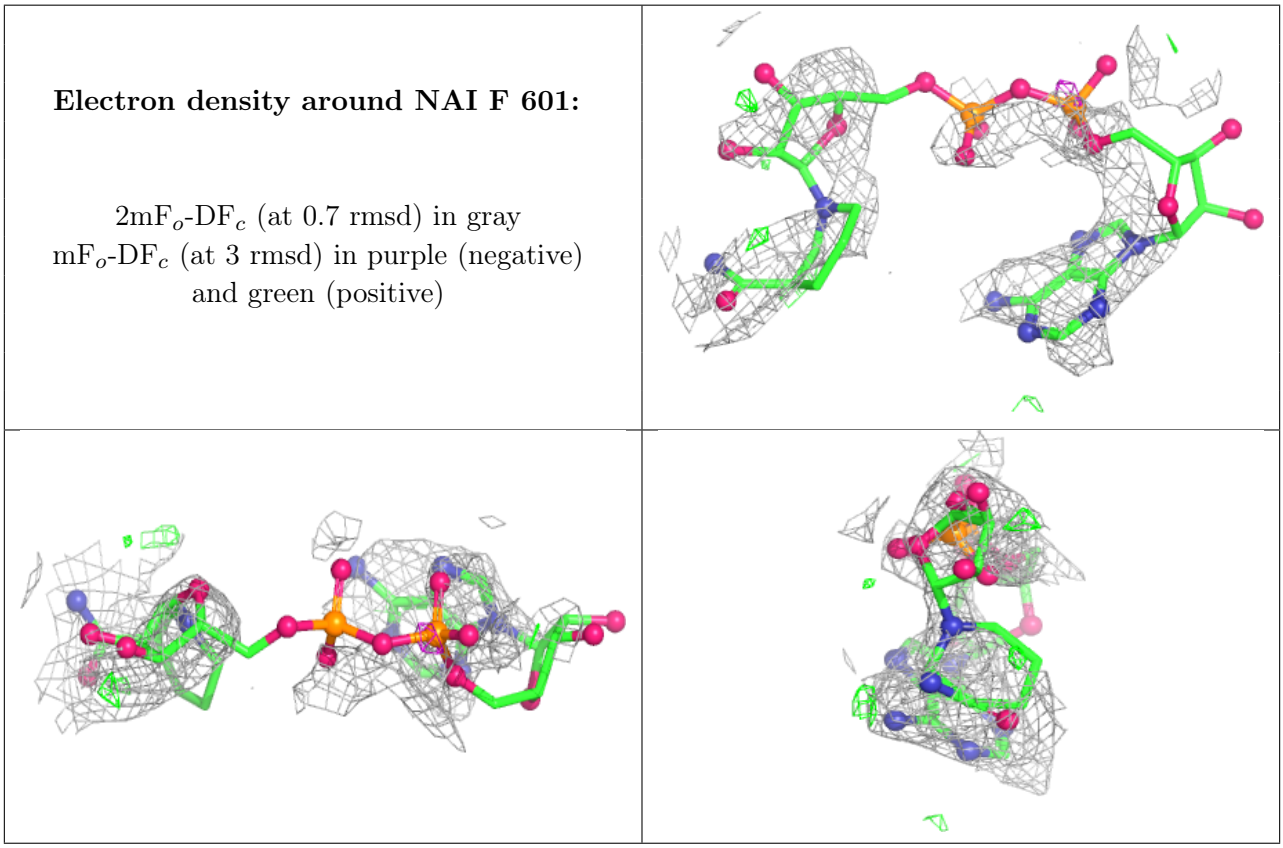
Electron density around NAI A 604:

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



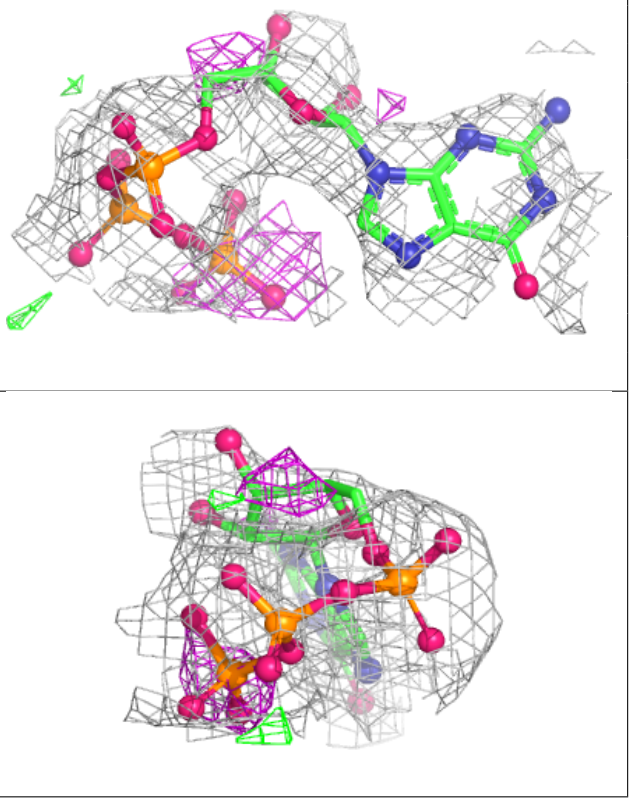
Electron density around NAI F 601:

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



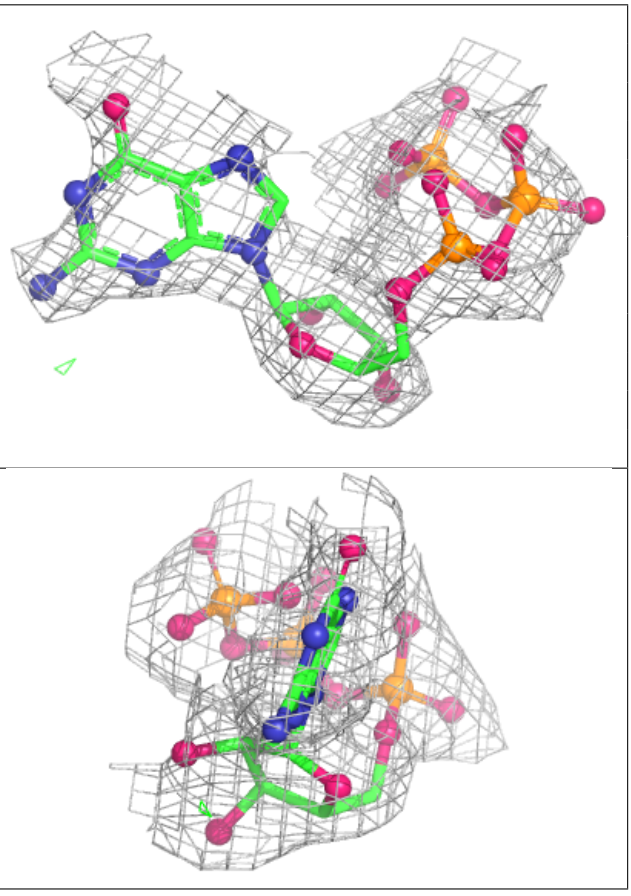
Electron density around GTP A 602:

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



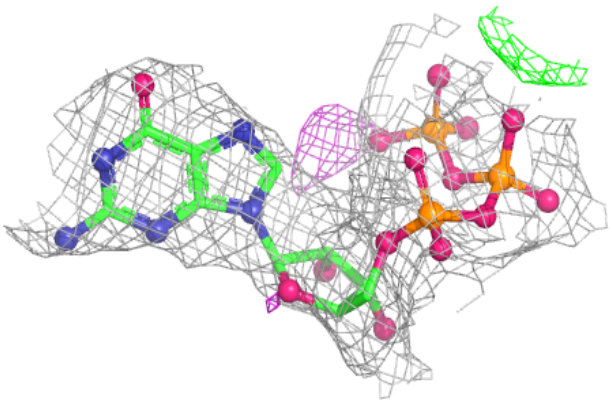
Electron density around GTP F 604:

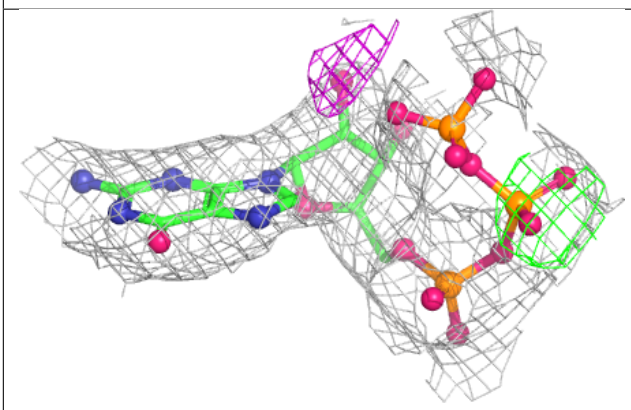
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

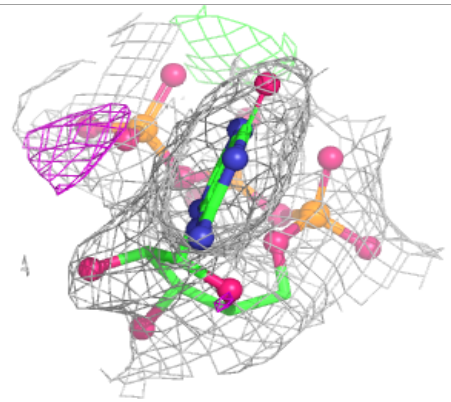


Electron density around GTP B 602:

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

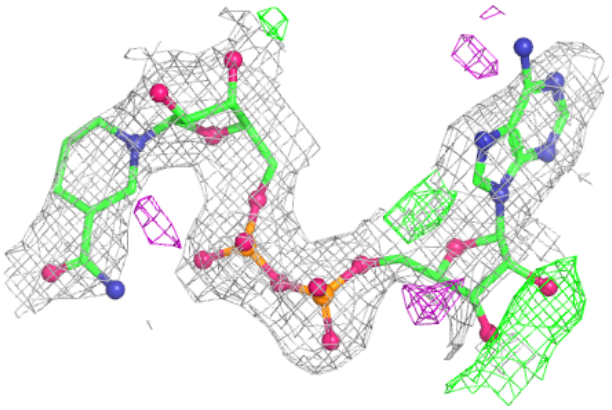


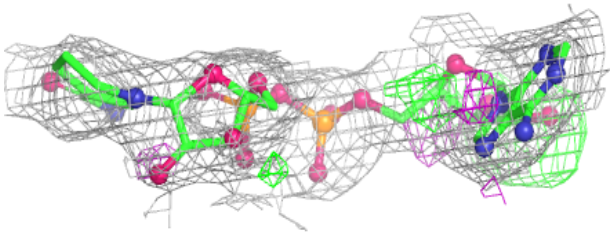


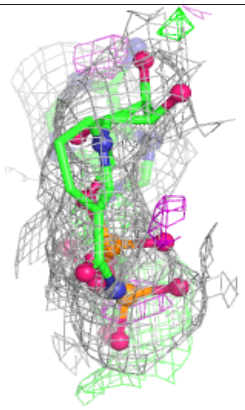


Electron density around NAI B 603:

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

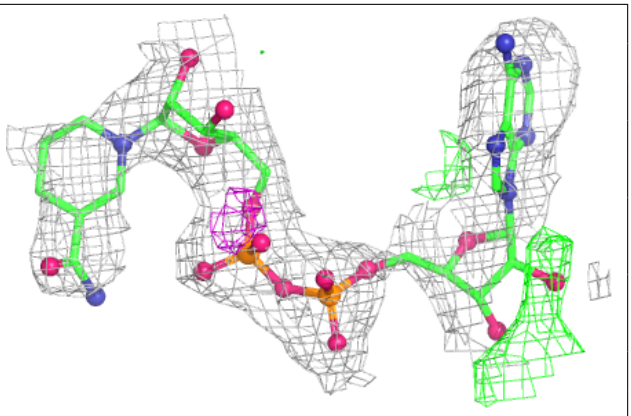


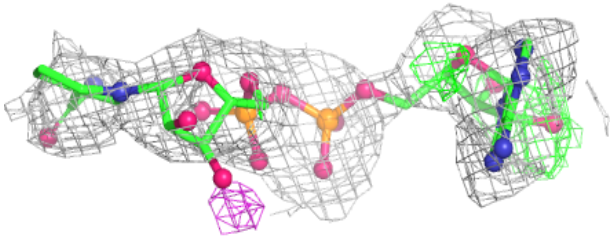


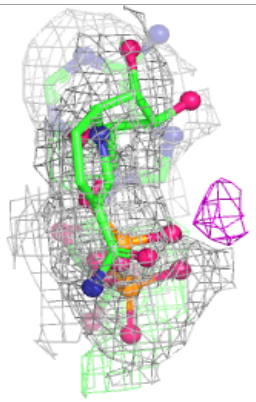


Electron density around NAI F 605:

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

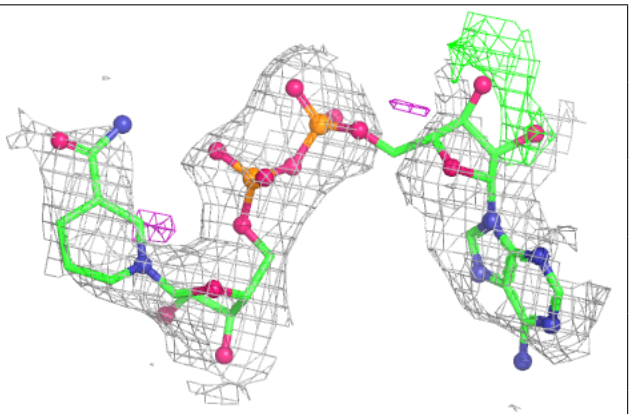


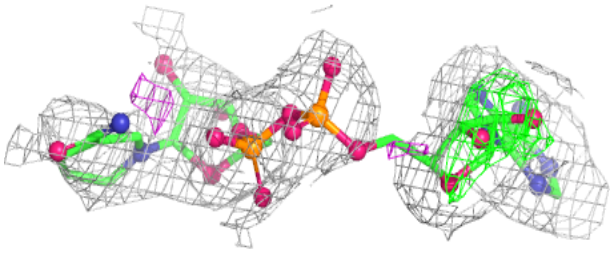


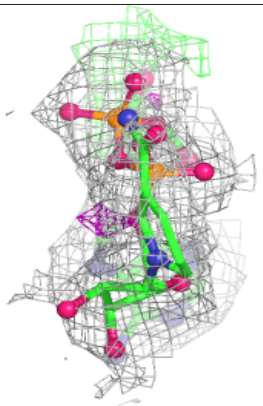


Electron density around NAI A 603:

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

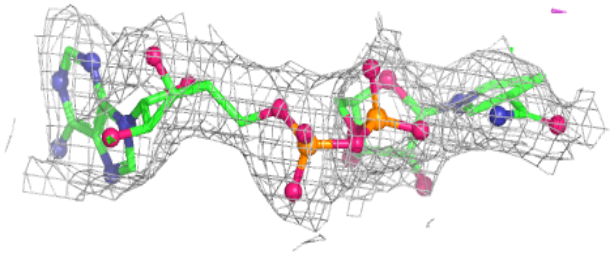


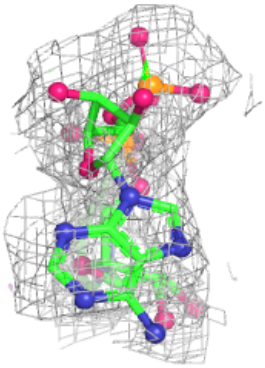




Electron density around NAI C 604:

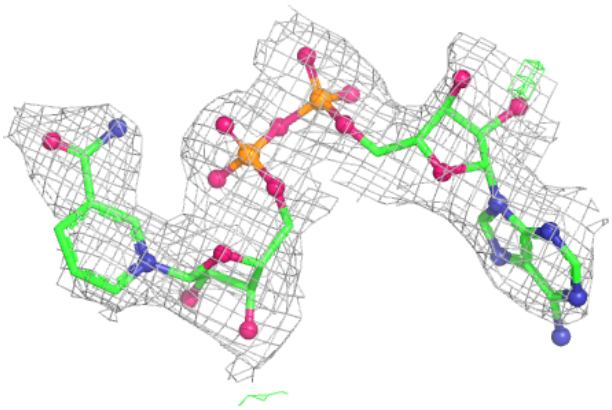
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

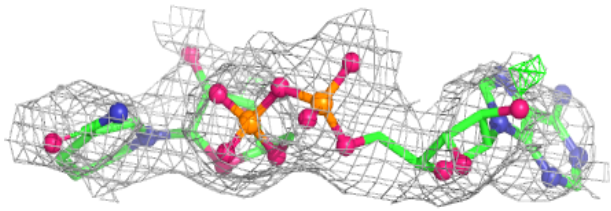


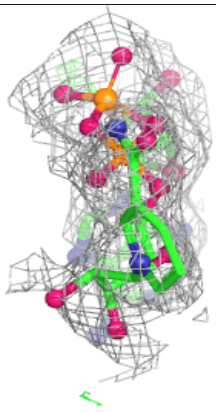


Electron density around NAI E 603:

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

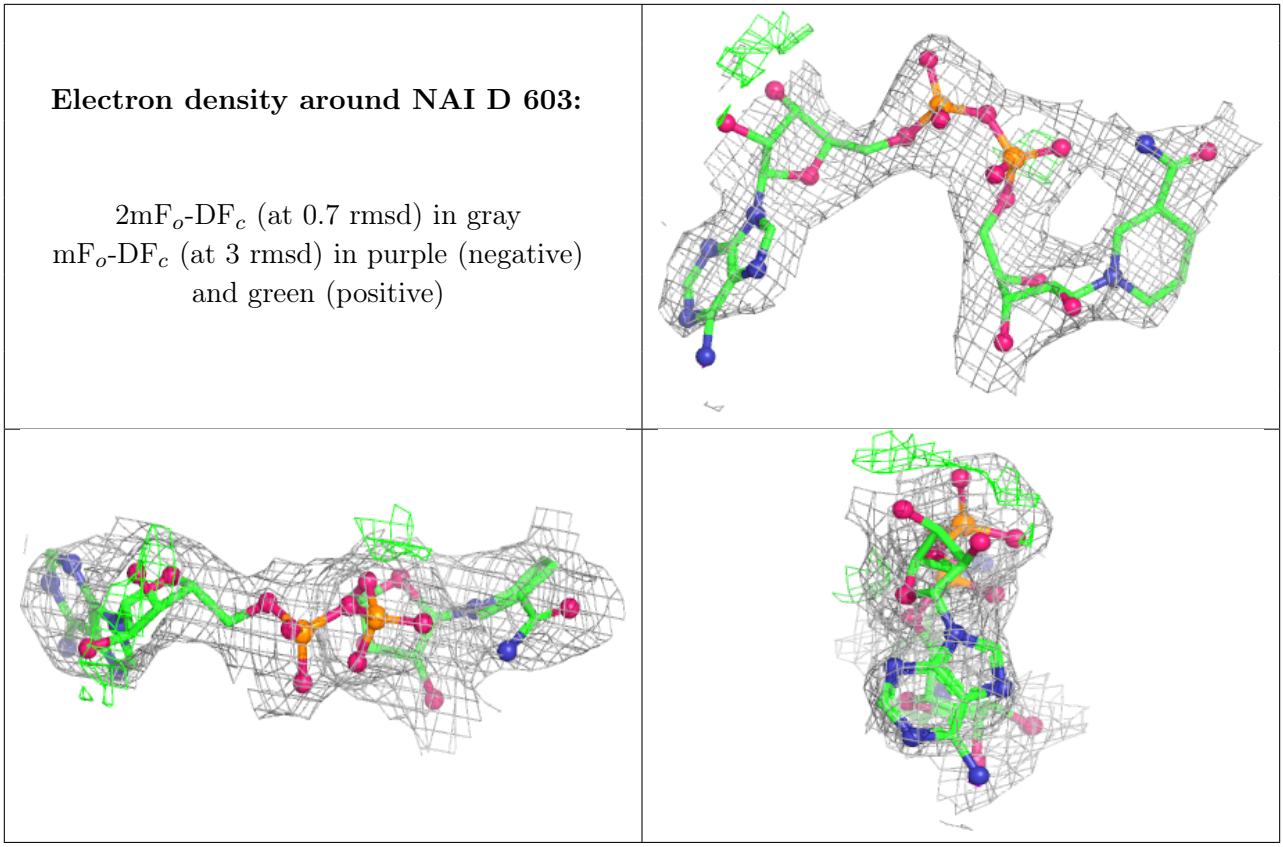






Electron density around NAI D 603:

$2mF_o$-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

There are no such residues in this entry.