Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 01:59 AM BST

PDB ID	:	6DHD
Title	:	Bovine glutamate dehydrogenase complexed with NADH, GTP, glutamate
Authors	:	Smith, T.J.
Deposited on	:	2018-05-19
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

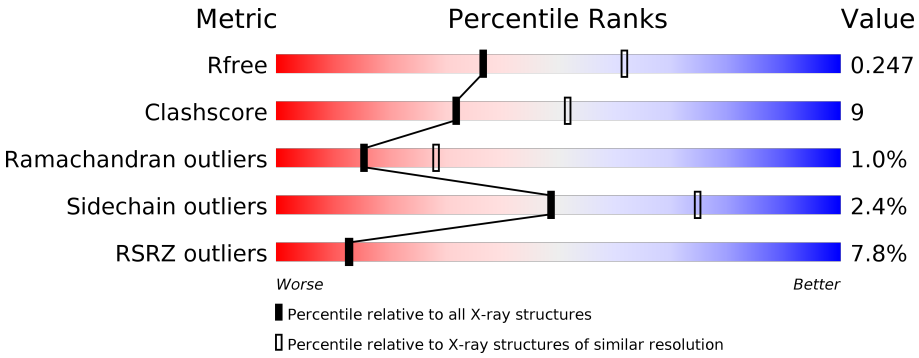
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	501	7% 78% 18%
1	B	501	5% 77% 19%
1	C	501	7% 79% 18%
1	D	501	9% 78% 20%
1	E	501	9% 76% 20%
1	F	501	9% 81% 16%

2 Entry composition

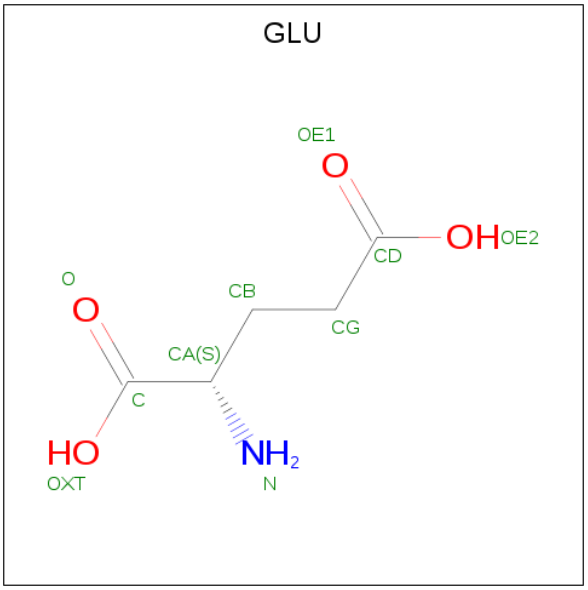
There are 5 unique types of molecules in this entry. The entry contains 24678 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

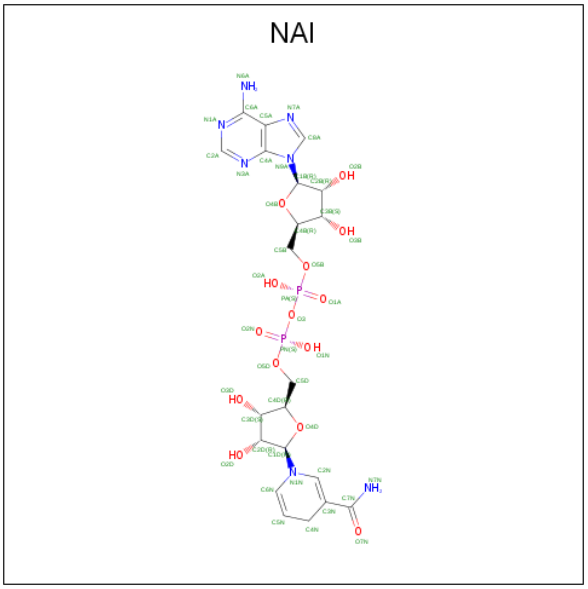
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	1	0
			3923	2478	689	737	19			
1	B	501	Total	C	N	O	S	0	1	0
			3923	2478	689	737	19			
1	C	501	Total	C	N	O	S	0	1	0
			3923	2478	689	737	19			
1	D	501	Total	C	N	O	S	0	1	0
			3923	2478	689	737	19			
1	E	501	Total	C	N	O	S	0	1	0
			3923	2478	689	737	19			
1	F	501	Total	C	N	O	S	0	1	0
			3923	2478	689	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 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
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	A	1	Total	C	N	O	P	10	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	10	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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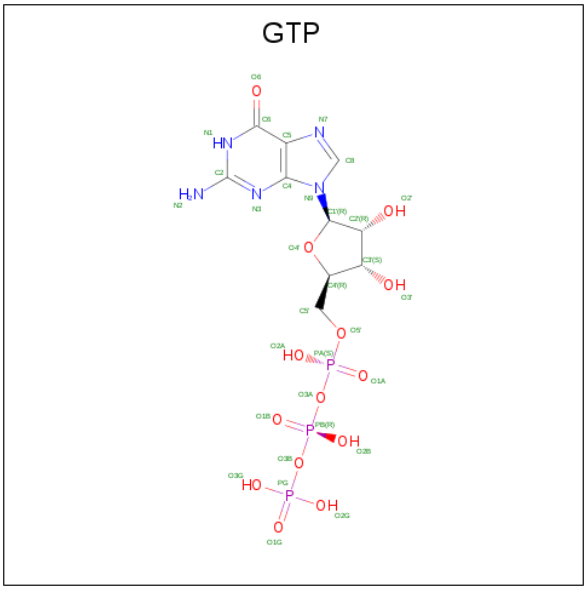
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	10	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	10	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	10	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	10	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

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

- Molecule 5 is water.

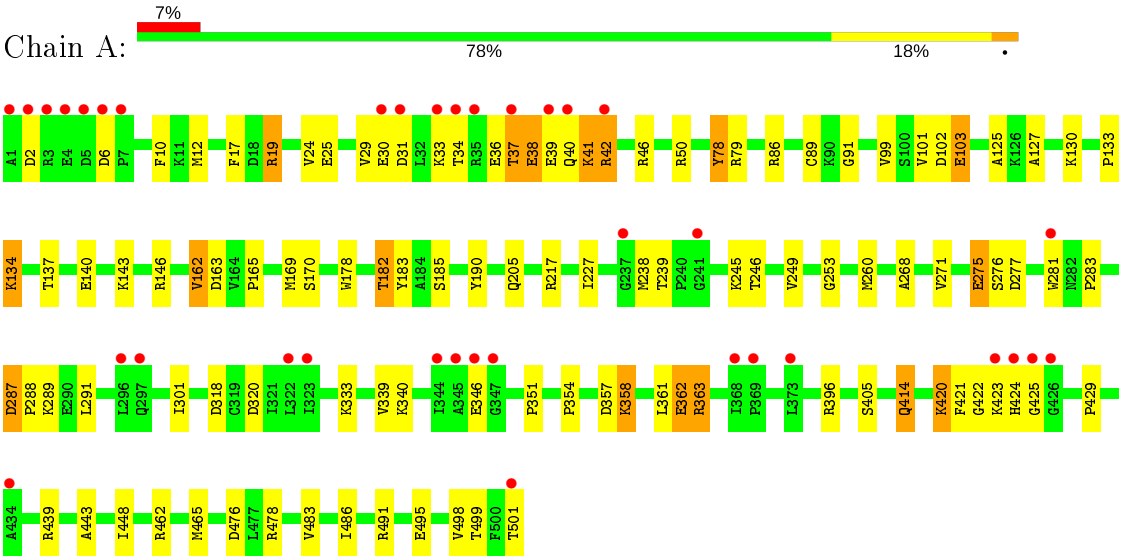
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	B	76	Total	O	0	0
			76	76		
5	C	67	Total	O	0	0
			67	67		
5	D	61	Total	O	0	0
			61	61		
5	E	43	Total	O	0	0
			43	43		
5	F	57	Total	O	0	0
			57	57		

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.

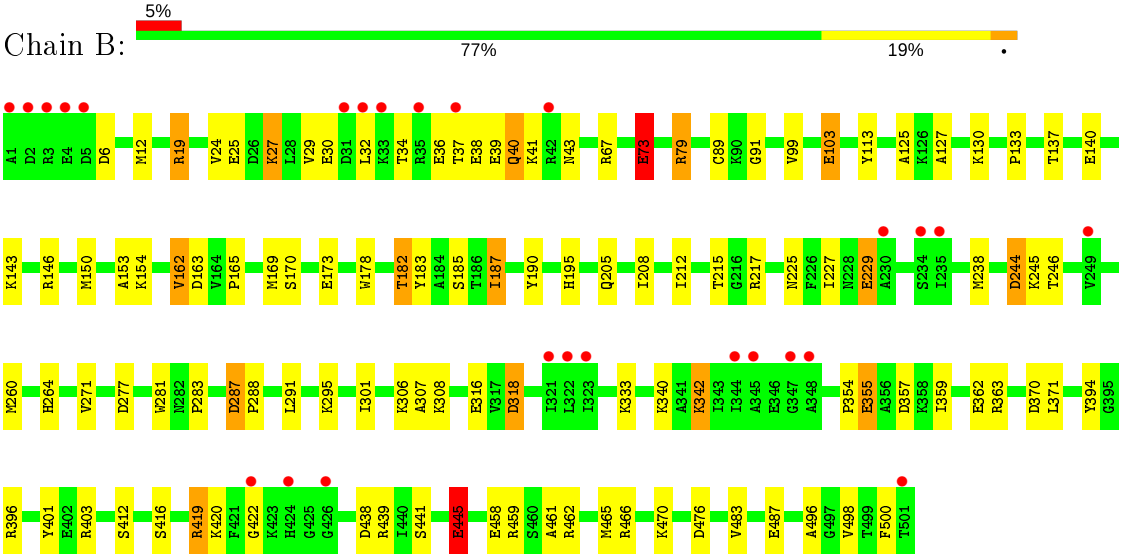
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain A:

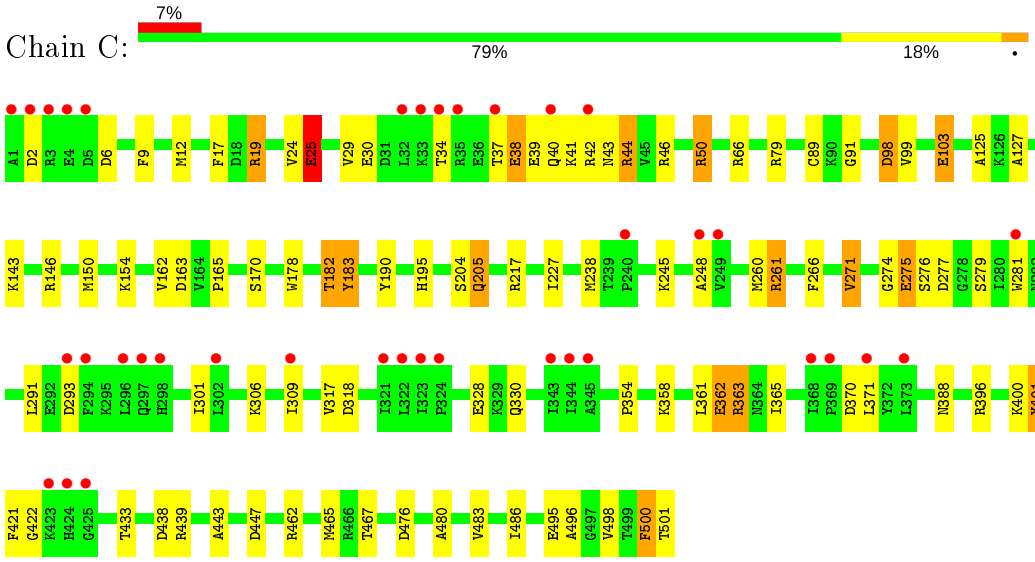


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

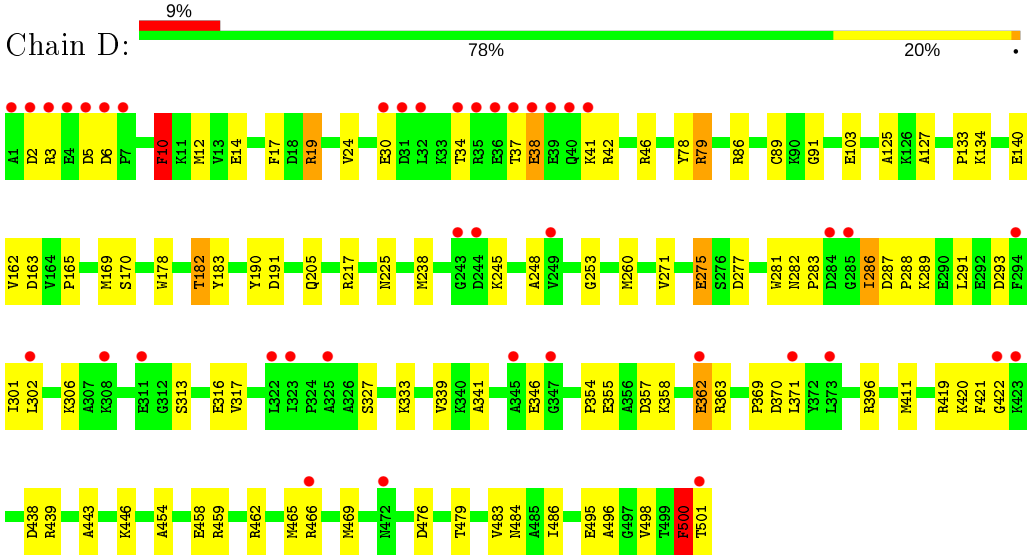
Chain B:



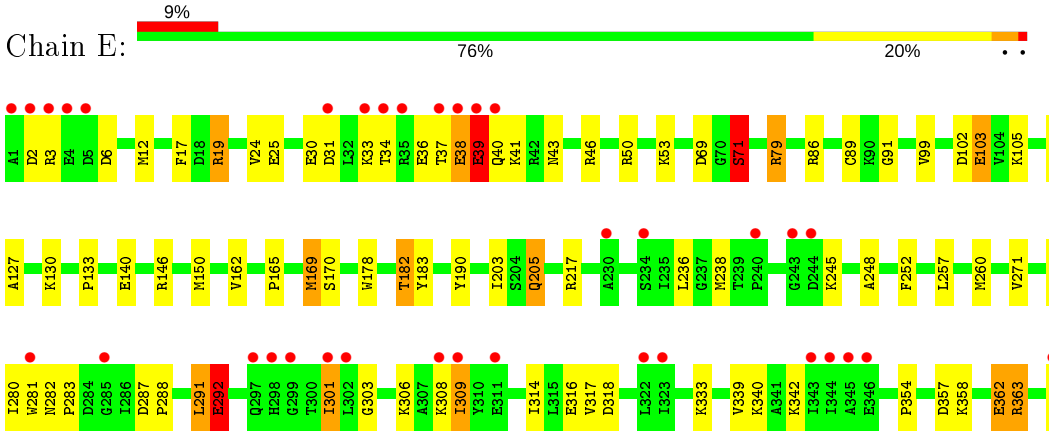
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

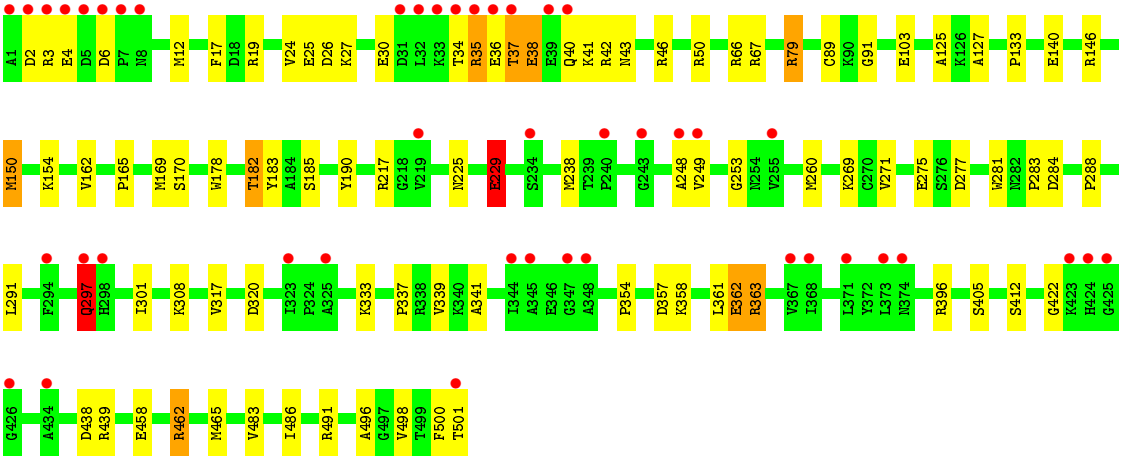


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	124.00Å 102.50Å 167.30Å 90.00° 101.64° 90.00°	Depositor
Resolution (Å)	28.59 – 2.50 28.59 – 2.28	Depositor EDS
% Data completeness (in resolution range)	87.8 (28.59-2.50) 69.4 (28.59-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.202 , 0.246 0.202 , 0.247	Depositor DCC
R_{free} test set	2000 reflections (1.53%)	wwPDB-VP
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24678	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: GTP, NAI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.05	24/4010 (0.6%)	1.02	32/5411 (0.6%)
1	B	0.80	24/4010 (0.6%)	1.12	43/5411 (0.8%)
1	C	0.92	25/4010 (0.6%)	1.12	41/5411 (0.8%)
1	D	0.90	21/4010 (0.5%)	1.07	40/5411 (0.7%)
1	E	0.77	20/4010 (0.5%)	1.02	38/5411 (0.7%)
1	F	0.74	17/4010 (0.4%)	0.85	21/5411 (0.4%)
All	All	0.87	131/24060 (0.5%)	1.04	215/32466 (0.7%)

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	3
1	B	0	6
1	C	0	4
1	D	0	2
1	E	0	5
1	F	0	3
All	All	0	23

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	GLU	CD-OE1	-25.49	0.97	1.25
1	A	78	TYR	CE1-CZ	-19.44	1.13	1.38
1	A	78	TYR	CG-CD2	-19.43	1.13	1.39
1	F	30	GLU	CD-OE1	-18.60	1.05	1.25
1	A	78	TYR	CG-CD1	-18.42	1.15	1.39
1	A	78	TYR	CE2-CZ	-18.36	1.14	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	183	TYR	CE2-CZ	-17.22	1.16	1.38
1	C	183	TYR	CE1-CZ	-17.20	1.16	1.38
1	C	183	TYR	CE2-CZ	-17.14	1.16	1.38
1	D	183	TYR	CE1-CZ	-17.03	1.16	1.38
1	B	30	GLU	CD-OE1	-16.58	1.07	1.25
1	D	103	GLU	CD-OE2	-16.20	1.07	1.25
1	D	183	TYR	CG-CD1	-15.10	1.19	1.39
1	D	183	TYR	CG-CD2	-15.02	1.19	1.39
1	C	183	TYR	CG-CD1	-14.99	1.19	1.39
1	C	183	TYR	CG-CD2	-14.90	1.19	1.39
1	A	86	ARG	CZ-NH1	-14.41	1.14	1.33
1	D	140	GLU	CD-OE2	-12.45	1.11	1.25
1	B	363	ARG	CB-CG	-12.20	1.19	1.52
1	E	30	GLU	CD-OE1	-11.76	1.12	1.25
1	E	301	ILE	CG1-CD1	-11.63	0.70	1.50
1	C	362	GLU	CD-OE1	-11.55	1.12	1.25
1	D	140	GLU	CD-OE1	-11.53	1.12	1.25
1	C	362	GLU	CD-OE2	-11.48	1.13	1.25
1	D	103	GLU	CD-OE1	-11.06	1.13	1.25
1	C	30	GLU	CD-OE1	-10.82	1.13	1.25
1	A	362	GLU	CD-OE1	-10.72	1.13	1.25
1	C	495	GLU	CD-OE2	-10.65	1.14	1.25
1	A	30	GLU	CD-OE1	-10.30	1.14	1.25
1	A	275	GLU	CG-CD	-10.25	1.36	1.51
1	A	414	GLN	CD-OE1	-10.09	1.01	1.24
1	F	275	GLU	CD-OE1	-9.52	1.15	1.25
1	B	6	ASP	CG-OD2	-9.34	1.03	1.25
1	B	183	TYR	CE1-CZ	-9.30	1.26	1.38
1	A	183	TYR	CE1-CZ	-9.21	1.26	1.38
1	E	140	GLU	CD-OE2	-9.16	1.15	1.25
1	F	183	TYR	CE1-CZ	-9.16	1.26	1.38
1	B	183	TYR	CE2-CZ	-9.16	1.26	1.38
1	A	362	GLU	CD-OE2	-9.15	1.15	1.25
1	E	183	TYR	CE2-CZ	-9.15	1.26	1.38
1	E	183	TYR	CE1-CZ	-9.06	1.26	1.38
1	E	363	ARG	CG-CD	-9.04	1.29	1.51
1	A	183	TYR	CE2-CZ	-8.98	1.26	1.38
1	F	183	TYR	CE2-CZ	-8.94	1.26	1.38
1	C	330	GLN	CD-NE2	-8.92	1.10	1.32
1	C	261	ARG	CZ-NH1	-8.87	1.21	1.33
1	A	414	GLN	CD-NE2	-8.60	1.11	1.32
1	E	140	GLU	CD-OE1	-8.58	1.16	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	495	GLU	CD-OE1	-8.46	1.16	1.25
1	F	229	GLU	CD-OE2	-8.44	1.16	1.25
1	F	103	GLU	CD-OE2	-8.38	1.16	1.25
1	D	275	GLU	CD-OE1	-8.25	1.16	1.25
1	C	330	GLN	CD-OE1	-8.25	1.05	1.24
1	F	103	GLU	CD-OE1	-8.24	1.16	1.25
1	F	30	GLU	CG-CD	-8.16	1.39	1.51
1	B	30	GLU	CG-CD	-8.15	1.39	1.51
1	E	183	TYR	CG-CD2	-7.92	1.28	1.39
1	A	183	TYR	CG-CD2	-7.91	1.28	1.39
1	F	183	TYR	CG-CD2	-7.84	1.28	1.39
1	B	183	TYR	CG-CD2	-7.79	1.29	1.39
1	C	25	GLU	CB-CG	-7.79	1.37	1.52
1	D	30	GLU	CG-CD	-7.69	1.40	1.51
1	D	30	GLU	CD-OE1	-7.67	1.17	1.25
1	B	183	TYR	CG-CD1	-7.65	1.29	1.39
1	E	275	GLU	CD-OE1	-7.64	1.17	1.25
1	D	306	LYS	CB-CG	-7.60	1.32	1.52
1	E	183	TYR	CG-CD1	-7.60	1.29	1.39
1	F	183	TYR	CG-CD1	-7.52	1.29	1.39
1	A	183	TYR	CG-CD1	-7.48	1.29	1.39
1	B	73	GLU	CD-OE2	-7.47	1.17	1.25
1	A	19	ARG	CB-CG	-7.38	1.32	1.52
1	D	30	GLU	CD-OE2	-7.32	1.17	1.25
1	C	275	GLU	CB-CG	-7.16	1.38	1.52
1	E	71	SER	CB-OG	-7.13	1.32	1.42
1	B	244	ASP	CB-CG	-7.11	1.36	1.51
1	F	19	ARG	CB-CG	-6.97	1.33	1.52
1	E	275	GLU	CB-CG	-6.93	1.39	1.52
1	B	73	GLU	CD-OE1	-6.76	1.18	1.25
1	D	275	GLU	CB-CG	-6.63	1.39	1.52
1	C	19	ARG	CB-CG	-6.63	1.34	1.52
1	D	484	ASN	CG-OD1	-6.39	1.09	1.24
1	D	30	GLU	CB-CG	-6.25	1.40	1.52
1	C	447	ASP	CG-OD2	-6.23	1.11	1.25
1	C	19	ARG	CG-CD	-6.22	1.36	1.51
1	E	205	GLN	CB-CG	-6.13	1.36	1.52
1	C	30	GLU	CG-CD	-6.11	1.42	1.51
1	B	287	ASP	CG-OD2	-5.98	1.11	1.25
1	B	162	VAL	CB-CG1	-5.86	1.40	1.52
1	A	162	VAL	CB-CG1	-5.75	1.40	1.52
1	C	447	ASP	CG-OD1	-5.75	1.12	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	362	GLU	CD-OE2	-5.72	1.19	1.25
1	C	287	ASP	CG-OD2	-5.71	1.12	1.25
1	E	19	ARG	CB-CG	-5.66	1.37	1.52
1	B	362	GLU	CD-OE2	-5.64	1.19	1.25
1	D	362	GLU	CD-OE2	-5.62	1.19	1.25
1	F	362	GLU	CD-OE2	-5.62	1.19	1.25
1	D	363	ARG	CB-CG	-5.59	1.37	1.52
1	E	306	LYS	CB-CG	-5.52	1.37	1.52
1	F	363	ARG	CB-CG	-5.51	1.37	1.52
1	F	362	GLU	CD-OE1	-5.47	1.19	1.25
1	B	363	ARG	CG-CD	-5.46	1.38	1.51
1	C	140	GLU	CD-OE1	-5.41	1.19	1.25
1	B	30	GLU	CD-OE2	-5.36	1.19	1.25
1	E	150	MET	SD-CE	-5.36	1.47	1.77
1	E	362	GLU	CD-OE1	-5.35	1.19	1.25
1	F	229	GLU	CD-OE1	-5.35	1.19	1.25
1	B	362	GLU	CD-OE1	-5.32	1.19	1.25
1	C	306	LYS	CB-CG	-5.31	1.38	1.52
1	D	362	GLU	CD-OE1	-5.30	1.19	1.25
1	B	140	GLU	CD-OE1	-5.29	1.19	1.25
1	C	103	GLU	CD-OE1	-5.29	1.19	1.25
1	F	140	GLU	CD-OE2	-5.28	1.19	1.25
1	F	140	GLU	CD-OE1	-5.23	1.19	1.25
1	A	30	GLU	CD-OE2	-5.21	1.20	1.25
1	B	140	GLU	CD-OE2	-5.20	1.20	1.25
1	A	30	GLU	CB-CG	-5.20	1.42	1.52
1	D	78	TYR	CG-CD2	-5.13	1.32	1.39
1	C	140	GLU	CD-OE2	-5.11	1.20	1.25
1	C	287	ASP	CG-OD1	-5.11	1.13	1.25
1	D	484	ASN	CG-ND2	-5.10	1.20	1.32
1	A	140	GLU	CD-OE1	-5.09	1.20	1.25
1	A	103	GLU	CD-OE2	-5.07	1.20	1.25
1	A	103	GLU	CD-OE1	-5.07	1.20	1.25
1	B	445	GLU	CD-OE1	-5.05	1.20	1.25
1	E	103	GLU	CD-OE2	-5.05	1.20	1.25
1	A	140	GLU	CD-OE2	-5.05	1.20	1.25
1	B	103	GLU	CD-OE2	-5.04	1.20	1.25
1	B	306	LYS	CB-CG	-5.03	1.39	1.52
1	B	103	GLU	CD-OE1	-5.03	1.20	1.25
1	B	229	GLU	CB-CG	-5.01	1.42	1.52
1	E	103	GLU	CD-OE1	-5.01	1.20	1.25

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	50	ARG	NE-CZ-NH1	-24.96	107.82	120.30
1	A	86	ARG	NE-CZ-NH1	-24.36	108.12	120.30
1	B	6	ASP	CB-CG-OD1	24.32	140.19	118.30
1	A	86	ARG	NE-CZ-NH2	24.10	132.35	120.30
1	C	50	ARG	NE-CZ-NH2	22.71	131.66	120.30
1	B	187	ILE	CG1-CB-CG2	-19.63	68.22	111.40
1	D	103	GLU	OE1-CD-OE2	-18.16	101.51	123.30
1	B	244	ASP	CB-CG-OD2	17.38	133.94	118.30
1	C	439	ARG	NE-CZ-NH1	-16.98	111.81	120.30
1	E	217	ARG	NE-CZ-NH1	-16.44	112.08	120.30
1	D	439	ARG	NE-CZ-NH1	-16.41	112.09	120.30
1	B	217	ARG	NE-CZ-NH1	-16.34	112.13	120.30
1	C	439	ARG	NE-CZ-NH2	16.03	128.31	120.30
1	D	439	ARG	NE-CZ-NH2	15.73	128.17	120.30
1	E	217	ARG	NE-CZ-NH2	15.06	127.83	120.30
1	B	217	ARG	NE-CZ-NH2	14.95	127.78	120.30
1	E	150	MET	CG-SD-CE	-14.69	76.70	100.20
1	D	446	LYS	CD-CE-NZ	14.27	144.53	111.70
1	C	261	ARG	NE-CZ-NH2	13.89	127.24	120.30
1	D	140	GLU	OE1-CD-OE2	-13.55	107.03	123.30
1	B	420	LYS	CD-CE-NZ	13.53	142.82	111.70
1	E	363	ARG	CG-CD-NE	13.16	139.43	111.80
1	C	362	GLU	OE1-CD-OE2	-12.99	107.71	123.30
1	B	244	ASP	CB-CG-OD1	-12.80	106.78	118.30
1	D	301	ILE	CG1-CB-CG2	-12.57	83.75	111.40
1	D	469	MET	CB-CG-SD	12.01	148.44	112.40
1	C	50	ARG	CD-NE-CZ	11.91	140.28	123.60
1	B	73	GLU	OE1-CD-OE2	-11.82	109.11	123.30
1	B	306	LYS	CD-CE-NZ	11.81	138.86	111.70
1	E	438	ASP	CB-CG-OD1	-11.74	107.74	118.30
1	D	363	ARG	NE-CZ-NH1	-11.63	114.49	120.30
1	E	438	ASP	CB-CG-OD2	11.56	128.71	118.30
1	C	261	ARG	NE-CZ-NH1	-11.22	114.69	120.30
1	D	302	LEU	CB-CG-CD1	11.00	129.69	111.00
1	A	78	TYR	CD1-CG-CD2	-10.86	105.95	117.90
1	A	363	ARG	NE-CZ-NH1	-10.82	114.89	120.30
1	A	362	GLU	OE1-CD-OE2	-10.78	110.37	123.30
1	F	363	ARG	NE-CZ-NH1	-10.74	114.93	120.30
1	F	229	GLU	OE1-CD-OE2	-10.68	110.48	123.30
1	B	27	LYS	CB-CG-CD	10.59	139.12	111.60
1	D	363	ARG	NE-CZ-NH2	10.44	125.52	120.30
1	B	6	ASP	OD1-CG-OD2	-10.38	103.57	123.30
1	E	363	ARG	CA-CB-CG	10.30	136.07	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	411	MET	CG-SD-CE	10.16	116.46	100.20
1	C	495	GLU	OE1-CD-OE2	-10.13	111.15	123.30
1	F	363	ARG	NE-CZ-NH2	9.91	125.25	120.30
1	C	420	LYS	CD-CE-NZ	9.88	134.42	111.70
1	F	103	GLU	OE1-CD-OE2	-9.83	111.51	123.30
1	D	286	ILE	CG1-CB-CG2	-9.73	90.00	111.40
1	E	439	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	C	447	ASP	CB-CG-OD1	9.53	126.88	118.30
1	E	140	GLU	OE1-CD-OE2	-9.52	111.87	123.30
1	B	287	ASP	CB-CG-OD1	9.47	126.83	118.30
1	E	420	LYS	CD-CE-NZ	9.47	133.48	111.70
1	A	78	TYR	CE1-CZ-CE2	-9.36	104.83	119.80
1	B	439	ARG	NE-CZ-NH2	-9.35	115.63	120.30
1	C	287	ASP	CB-CG-OD1	9.32	126.69	118.30
1	A	318	ASP	CB-CG-OD1	9.31	126.68	118.30
1	C	447	ASP	CB-CG-OD2	9.25	126.63	118.30
1	A	78	TYR	CZ-CE2-CD2	9.24	128.12	119.80
1	E	363	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	A	363	ARG	NE-CZ-NH2	9.12	124.86	120.30
1	E	428	ILE	CG1-CB-CG2	-9.06	91.46	111.40
1	B	287	ASP	OD1-CG-OD2	-9.02	106.17	123.30
1	C	447	ASP	OD1-CG-OD2	-8.97	106.25	123.30
1	F	217	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	F	275	GLU	CA-CB-CG	8.81	132.78	113.40
1	D	306	LYS	CA-CB-CG	8.70	132.54	113.40
1	D	217	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	F	439	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	E	439	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	C	217	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	E	287	ASP	CB-CG-OD1	8.60	126.04	118.30
1	C	287	ASP	OD1-CG-OD2	-8.59	106.99	123.30
1	A	287	ASP	CB-CG-OD1	8.58	126.02	118.30
1	B	439	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	A	217	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	E	53	LYS	CD-CE-NZ	8.50	131.25	111.70
1	C	287	ASP	CB-CG-OD2	8.44	125.90	118.30
1	B	187	ILE	CA-CB-CG1	8.41	126.97	111.00
1	B	363	ARG	CG-CD-NE	-8.40	94.16	111.80
1	C	275	GLU	CA-CB-CG	8.38	131.84	113.40
1	E	205	GLN	CB-CG-CD	8.37	133.36	111.60
1	B	287	ASP	CB-CG-OD2	8.31	125.78	118.30
1	A	30	GLU	CG-CD-OE2	8.30	134.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	302	LEU	CA-CB-CG	8.29	134.38	115.30
1	B	318	ASP	CB-CG-OD1	8.25	125.72	118.30
1	F	217	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	C	439	ARG	CD-NE-CZ	8.22	135.10	123.60
1	A	275	GLU	CG-CD-OE2	8.20	134.69	118.30
1	D	439	ARG	CD-NE-CZ	8.14	134.99	123.60
1	A	78	TYR	CD1-CE1-CZ	8.09	127.08	119.80
1	A	217	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	D	297	GLN	CA-CB-CG	8.05	131.12	113.40
1	D	217	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	E	30	GLU	OE1-CD-OE2	-7.93	113.78	123.30
1	C	261	ARG	CG-CD-NE	7.91	128.41	111.80
1	C	217	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	D	306	LYS	CB-CG-CD	-7.88	91.12	111.60
1	A	439	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	E	318	ASP	CB-CG-OD1	7.75	125.27	118.30
1	F	439	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	D	183	TYR	CZ-CE2-CD2	7.74	126.76	119.80
1	C	183	TYR	CD1-CG-CD2	-7.73	109.40	117.90
1	B	187	ILE	CB-CG1-CD1	7.67	135.38	113.90
1	C	183	TYR	CZ-CE2-CD2	7.67	126.70	119.80
1	E	363	ARG	CD-NE-CZ	7.64	134.29	123.60
1	B	295	LYS	CD-CE-NZ	7.59	129.17	111.70
1	E	366	MET	CG-SD-CE	7.59	112.34	100.20
1	D	183	TYR	CD1-CG-CD2	-7.56	109.58	117.90
1	E	363	ARG	CB-CG-CD	-7.53	92.02	111.60
1	A	78	TYR	CB-CG-CD1	7.52	125.51	121.00
1	C	183	TYR	CB-CG-CD1	7.52	125.51	121.00
1	D	302	LEU	CB-CG-CD2	-7.50	98.24	111.00
1	B	438	ASP	CB-CG-OD2	7.47	125.02	118.30
1	D	183	TYR	CD1-CE1-CZ	7.46	126.51	119.80
1	C	183	TYR	CD1-CE1-CZ	7.44	126.49	119.80
1	A	420	LYS	CD-CE-NZ	7.40	128.73	111.70
1	B	217	ARG	CD-NE-CZ	7.35	133.89	123.60
1	D	183	TYR	CB-CG-CD1	7.35	125.41	121.00
1	A	162	VAL	CG1-CB-CG2	-7.33	99.17	110.90
1	D	19	ARG	CG-CD-NE	7.28	127.08	111.80
1	E	217	ARG	CD-NE-CZ	7.27	133.78	123.60
1	C	19	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	30	GLU	OE1-CD-OE2	-7.07	114.81	123.30
1	E	292	GLU	CG-CD-OE2	-7.05	104.21	118.30
1	B	363	ARG	NE-CZ-NH1	-7.03	116.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	162	VAL	CG1-CB-CG2	-6.94	99.80	110.90
1	F	19	ARG	NE-CZ-NH1	-6.88	116.86	120.30
1	E	86	ARG	CD-NE-CZ	-6.88	113.97	123.60
1	E	292	GLU	CG-CD-OE1	6.75	131.79	118.30
1	D	183	TYR	CE1-CZ-CE2	-6.67	109.12	119.80
1	C	271	VAL	CG1-CB-CG2	-6.66	100.24	110.90
1	C	183	TYR	CE1-CZ-CE2	-6.61	109.22	119.80
1	E	363	ARG	N-CA-CB	-6.58	98.76	110.60
1	B	27	LYS	CA-CB-CG	6.58	127.86	113.40
1	E	71	SER	CA-CB-OG	6.57	128.95	111.20
1	B	30	GLU	OE1-CD-OE2	-6.57	115.42	123.30
1	A	275	GLU	CG-CD-OE1	-6.55	105.20	118.30
1	D	327	SER	N-CA-CB	-6.54	100.69	110.50
1	B	445	GLU	OE1-CD-OE2	-6.52	115.48	123.30
1	C	261	ARG	NH1-CZ-NH2	-6.48	112.28	119.40
1	C	183	TYR	CB-CG-CD2	6.47	124.88	121.00
1	D	183	TYR	CB-CG-CD2	6.44	124.86	121.00
1	D	275	GLU	OE1-CD-OE2	-6.44	115.58	123.30
1	B	229	GLU	CG-CD-OE1	6.36	131.03	118.30
1	B	355	GLU	CG-CD-OE1	-6.30	105.69	118.30
1	C	25	GLU	CG-CD-OE2	-6.27	105.75	118.30
1	B	244	ASP	N-CA-CB	-6.25	99.34	110.60
1	C	363	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	B	229	GLU	OE1-CD-OE2	-6.19	115.87	123.30
1	F	462	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	A	287	ASP	OD1-CG-OD2	-6.12	111.67	123.30
1	F	297	GLN	CA-CB-CG	-6.11	99.97	113.40
1	C	25	GLU	CG-CD-OE1	6.10	130.50	118.30
1	E	362	GLU	OE1-CD-OE2	-6.01	116.08	123.30
1	F	362	GLU	OE1-CD-OE2	-5.99	116.12	123.30
1	D	362	GLU	OE1-CD-OE2	-5.96	116.15	123.30
1	A	19	ARG	CG-CD-NE	-5.95	99.30	111.80
1	B	355	GLU	CG-CD-OE2	5.94	130.18	118.30
1	B	103	GLU	OE1-CD-OE2	-5.92	116.19	123.30
1	A	130	LYS	CD-CE-NZ	5.89	125.25	111.70
1	C	98	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	D	103	GLU	CG-CD-OE1	5.86	130.03	118.30
1	A	103	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	F	30	GLU	OE1-CD-OE2	-5.83	116.30	123.30
1	A	499	THR	OG1-CB-CG2	5.83	123.41	110.00
1	D	306	LYS	N-CA-CB	-5.81	100.14	110.60
1	A	439	ARG	NE-CZ-NH1	5.80	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	140	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	F	50	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	F	50	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	C	103	GLU	OE1-CD-OE2	-5.72	116.44	123.30
1	C	140	GLU	OE1-CD-OE2	-5.71	116.44	123.30
1	E	103	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	B	187	ILE	CA-CB-CG2	-5.71	99.49	110.90
1	B	229	GLU	CG-CD-OE2	-5.70	106.89	118.30
1	B	362	GLU	OE1-CD-OE2	-5.68	116.49	123.30
1	C	275	GLU	CB-CA-C	-5.67	99.06	110.40
1	D	287	ASP	CB-CG-OD1	5.66	123.40	118.30
1	C	291	LEU	CA-CB-CG	5.66	128.31	115.30
1	E	339	VAL	CG1-CB-CG2	5.65	119.94	110.90
1	B	363	ARG	CB-CA-C	5.63	121.67	110.40
1	B	30	GLU	CG-CD-OE2	5.62	129.53	118.30
1	F	140	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	E	102	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	140	GLU	OE1-CD-OE2	-5.57	116.62	123.30
1	E	50	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	E	50	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	446	LYS	CB-CG-CD	-5.50	97.30	111.60
1	F	249	VAL	CG1-CB-CG2	5.47	119.65	110.90
1	D	411	MET	CB-CG-SD	-5.47	96.00	112.40
1	D	306	LYS	CB-CA-C	5.46	121.32	110.40
1	D	275	GLU	CB-CA-C	5.44	121.27	110.40
1	F	30	GLU	N-CA-CB	-5.43	100.82	110.60
1	C	363	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	A	249	VAL	CG1-CB-CG2	5.37	119.50	110.90
1	E	19	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	F	462	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	F	4	GLU	CA-CB-CG	5.29	125.04	113.40
1	B	355	GLU	CB-CG-CD	5.29	128.48	114.20
1	E	205	GLN	CA-CB-CG	-5.28	101.79	113.40
1	B	229	GLU	CA-CB-CG	-5.24	101.87	113.40
1	D	30	GLU	OE1-CD-OE2	-5.23	117.02	123.30
1	D	446	LYS	CG-CD-CE	5.23	127.60	111.90
1	C	291	LEU	CB-CG-CD1	5.19	119.82	111.00
1	B	363	ARG	N-CA-CB	-5.18	101.27	110.60
1	E	438	ASP	OD1-CG-OD2	-5.18	113.46	123.30
1	A	137	THR	OG1-CB-CG2	5.16	121.87	110.00
1	A	19	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	E	130	LYS	CB-CG-CD	-5.12	98.28	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	50	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	D	140	GLU	CG-CD-OE1	5.08	128.45	118.30
1	C	401	TYR	CG-CD1-CE1	-5.01	117.29	121.30
1	E	169	MET	CG-SD-CE	5.00	108.20	100.20

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ASP	Sidechain
1	A	39	GLU	Peptide
1	A	41	LYS	Peptide
1	B	229	GLU	Sidechain
1	B	244	ASP	Sidechain
1	B	357	ASP	Sidechain
1	B	40	GLN	Peptide
1	B	445	GLU	Sidechain
1	B	73	GLU	Sidechain
1	C	25	GLU	Sidechain
1	C	293	ASP	Sidechain
1	C	39	GLU	Peptide
1	C	98	ASP	Sidechain
1	D	10	PHE	Sidechain
1	D	275	GLU	Sidechain
1	E	282	ASN	Sidechain
1	E	292	GLU	Sidechain
1	E	39	GLU	Peptide
1	E	424	HIS	Peptide
1	E	438	ASP	Sidechain
1	F	229	GLU	Sidechain
1	F	277	ASP	Sidechain
1	F	297	GLN	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	3923	0	3887	75	0
1	B	3923	0	3887	82	0
1	C	3923	0	3887	73	0
1	D	3923	0	3887	79	0
1	E	3923	0	3887	80	0
1	F	3923	0	3887	64	0
2	A	10	0	5	1	0
2	B	10	0	5	1	0
2	C	10	0	5	1	0
2	D	10	0	5	1	0
2	E	10	0	5	1	0
2	F	10	0	5	1	0
3	A	88	0	54	3	0
3	B	88	0	54	2	0
3	C	88	0	53	2	0
3	D	88	0	53	5	0
3	E	88	0	54	1	0
3	F	88	0	54	3	0
4	A	32	0	12	0	0
4	B	32	0	12	0	0
4	C	32	0	12	3	0
4	D	32	0	12	0	0
4	E	32	0	12	0	0
4	F	32	0	12	0	0
5	A	56	0	0	4	0
5	B	76	0	0	12	0
5	C	67	0	0	4	0
5	D	61	0	0	5	0
5	E	43	0	0	4	0
5	F	57	0	0	0	0
All	All	24678	0	23746	425	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 9.

All (425) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:ILE:CB	1:E:301:ILE:CD1	1.88	1.52
1:D:205:GLN:HE22	1:F:496:ALA:HB2	1.18	1.08
1:B:205:GLN:HE22	1:C:496:ALA:HB2	0.94	1.07
1:D:454:ALA:O	1:D:458:GLU:OE1	1.70	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLN:NE2	1:C:496:ALA:HB2	1.73	1.02
1:F:462:ARG:HH11	1:F:465:MET:HE1	1.26	1.00
1:C:29:VAL:HG21	1:C:42:ARG:HG2	1.47	0.97
1:F:229:GLU:OE2	1:F:462:ARG:NH1	1.96	0.96
1:D:24:VAL:CG1	1:D:483:VAL:HG13	1.96	0.95
1:B:205:GLN:OE1	5:B:701:HOH:O	1.84	0.94
1:A:501:THR:HG23	1:D:143:LYS:NZ	1.82	0.92
1:C:363:ARG:NH2	1:C:365:ILE:HD11	1.85	0.92
1:C:363:ARG:HH21	1:C:365:ILE:HD11	1.36	0.91
1:B:225:ASN:HD21	1:B:458:GLU:HA	1.35	0.91
1:E:301:ILE:HB	1:E:301:ILE:CD1	1.99	0.90
1:E:301:ILE:HD13	1:E:301:ILE:CG1	1.37	0.88
1:F:462:ARG:HD3	1:F:465:MET:HE1	1.53	0.88
1:E:301:ILE:HD12	1:E:301:ILE:CG1	1.37	0.88
1:E:301:ILE:CD1	1:E:301:ILE:HG12	1.36	0.88
1:E:301:ILE:CG1	1:E:301:ILE:HD11	1.37	0.87
1:E:301:ILE:CD1	1:E:301:ILE:HG13	1.36	0.87
3:C:604:NAI:O2A	5:C:701:HOH:O	1.93	0.84
1:D:5:ASP:HB2	1:D:333:LYS:HE2	1.58	0.84
1:D:205:GLN:NE2	1:F:496:ALA:HB2	1.92	0.84
1:E:25:GLU:CD	1:E:46:ARG:HE	1.80	0.83
1:A:363:ARG:NH2	5:A:702:HOH:O	2.10	0.82
1:F:462:ARG:HD3	1:F:465:MET:CE	2.09	0.82
1:D:205:GLN:OE1	5:D:701:HOH:O	1.96	0.82
1:A:501:THR:HG23	1:D:143:LYS:HZ3	1.44	0.81
1:B:466:ARG:O	1:B:470:LYS:HD3	1.80	0.81
1:E:105:LYS:NZ	5:E:702:HOH:O	2.13	0.80
1:B:225:ASN:ND2	1:B:458:GLU:HA	1.98	0.79
1:B:394:TYR:OH	5:B:702:HOH:O	1.99	0.79
1:D:496:ALA:HB2	1:E:205:GLN:OE1	1.83	0.78
1:F:36:GLU:O	1:F:38:GLU:N	2.16	0.78
1:B:459:ARG:NH1	5:B:703:HOH:O	2.13	0.77
1:B:27:LYS:HD2	1:B:487:GLU:OE2	1.84	0.77
1:B:333:LYS:HD3	1:B:355:GLU:HB3	1.66	0.77
1:D:479:THR:O	1:D:483:VAL:HG23	1.84	0.77
1:C:261:ARG:HB3	1:C:261:ARG:HH11	1.52	0.75
1:B:208:ILE:HG13	1:B:445:GLU:OE2	1.87	0.74
1:D:454:ALA:O	1:D:458:GLU:CD	2.25	0.74
1:D:24:VAL:HG11	1:D:483:VAL:HG13	1.70	0.73
1:D:190:TYR:CD1	1:F:162:VAL:HG11	2.24	0.73
1:C:467:THR:CG2	1:C:480:ALA:HB1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:ARG:NH2	5:D:702:HOH:O	2.13	0.71
1:D:458:GLU:N	1:D:458:GLU:OE1	2.23	0.71
1:B:190:TYR:CD1	1:C:162:VAL:HG11	2.25	0.71
1:D:19:ARG:NH2	1:D:476:ASP:OD2	2.24	0.71
1:E:34:THR:HG21	1:E:36:GLU:OE1	1.91	0.71
1:E:112:THR:O	5:E:701:HOH:O	2.07	0.71
1:E:162:VAL:HG11	1:F:190:TYR:CD1	2.26	0.70
1:B:19:ARG:NH2	1:B:476:ASP:OD2	2.24	0.70
1:B:137:THR:HB	5:B:764:HOH:O	1.90	0.70
3:D:603:NAI:O3B	1:F:491:ARG:NH2	2.24	0.70
2:D:601:GLU:HA	3:D:602:NAI:H4N	1.74	0.70
1:E:301:ILE:CD1	1:E:301:ILE:CG1	0.70	0.69
1:A:190:TYR:CD1	1:B:162:VAL:HG11	2.28	0.69
1:C:25:GLU:OE1	1:C:42:ARG:NH2	2.24	0.69
1:E:257:LEU:HD21	1:E:292:GLU:OE2	1.93	0.69
1:C:19:ARG:NH2	1:C:476:ASP:OD2	2.25	0.69
1:D:162:VAL:HG11	1:E:190:TYR:CD1	2.28	0.69
1:A:162:VAL:HG11	1:C:190:TYR:CD1	2.28	0.69
1:A:78:TYR:CE2	1:A:101:VAL:HG22	2.29	0.68
1:F:24:VAL:CG1	1:F:483:VAL:HG13	2.23	0.68
1:A:462:ARG:HA	1:A:465:MET:HE2	1.76	0.67
1:A:24:VAL:CG1	1:A:483:VAL:HG13	2.24	0.67
2:F:601:GLU:HA	3:F:603:NAI:H4N	1.77	0.67
1:A:346:GLU:OE1	1:A:478:ARG:NH2	2.22	0.67
1:D:282:ASN:HB3	1:D:286:ILE:HD12	1.77	0.67
1:E:423:LYS:N	1:E:423:LYS:HD3	2.11	0.66
1:B:287:ASP:OD1	5:B:704:HOH:O	2.14	0.66
1:A:501:THR:HG23	1:D:143:LYS:HZ1	1.61	0.66
1:B:153:ALA:HB1	1:B:187:ILE:CD1	2.26	0.65
1:E:69:ASP:OD1	1:E:71:SER:HB2	1.96	0.65
1:A:501:THR:CG2	1:D:143:LYS:HZ1	2.09	0.65
1:A:205:GLN:HE22	1:B:496:ALA:HB2	1.63	0.64
1:C:467:THR:HG22	1:C:480:ALA:HB1	1.79	0.64
1:E:236:LEU:O	1:E:342:LYS:NZ	2.30	0.64
1:A:275:GLU:HG3	1:A:276:SER:H	1.63	0.64
1:D:79:ARG:NH2	1:D:163:ASP:OD1	2.23	0.64
1:B:318:ASP:HB3	1:B:340:LYS:HE3	1.79	0.64
1:D:10:PHE:HE1	1:D:14:GLU:HG3	1.63	0.64
1:B:153:ALA:HB1	1:B:187:ILE:HD13	1.80	0.63
1:E:19:ARG:NH2	1:E:476:ASP:OD2	2.32	0.63
1:E:25:GLU:OE2	1:E:46:ARG:NE	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:VAL:CG1	1:B:483:VAL:HG13	2.29	0.62
2:B:601:GLU:HA	3:B:602:NAI:H4N	1.81	0.62
1:C:261:ARG:NH2	4:C:602:GTP:C8	2.68	0.61
1:E:462:ARG:HA	1:E:465:MET:HE2	1.82	0.61
1:B:113:TYR:OH	5:B:705:HOH:O	2.16	0.61
1:E:252:PHE:CZ	1:E:257:LEU:HD13	2.36	0.61
1:E:40:GLN:HA	1:E:43:ASN:HB2	1.81	0.61
1:C:261:ARG:NH2	4:C:602:GTP:N7	2.49	0.61
1:F:26:ASP:OD1	1:F:42:ARG:NH2	2.32	0.61
1:A:268:ALA:O	5:A:703:HOH:O	2.16	0.60
1:B:281:TRP:CZ2	1:B:283:PRO:HG3	2.36	0.60
1:B:271:VAL:HG13	1:B:283:PRO:HA	1.83	0.60
2:E:601:GLU:HA	3:E:602:NAI:H4N	1.83	0.60
1:E:301:ILE:HD13	1:E:301:ILE:HB	1.73	0.60
1:B:462:ARG:HA	1:B:465:MET:HE2	1.84	0.60
1:C:281:TRP:CZ2	1:C:283:PRO:HG3	2.36	0.60
1:E:91:GLY:HA3	1:E:125:ALA:O	2.02	0.60
1:B:195[A]:HIS:CE1	5:B:710:HOH:O	2.55	0.59
1:E:34:THR:HG23	1:E:36:GLU:HG2	1.84	0.59
1:E:133:PRO:HG2	1:E:170:SER:HB3	1.85	0.59
1:A:281:TRP:CZ2	1:A:283:PRO:HG3	2.37	0.59
1:C:238:MET:HE1	1:C:245:LYS:HE3	1.83	0.59
1:D:225:ASN:ND2	1:D:458:GLU:HA	2.17	0.59
1:B:67:ARG:HD2	1:B:73:GLU:OE1	2.02	0.59
1:A:339:VAL:N	5:A:702:HOH:O	2.35	0.59
2:A:601:GLU:HA	3:A:602:NAI:H4N	1.83	0.59
1:C:266:PHE:O	5:C:703:HOH:O	2.17	0.58
1:D:281:TRP:CZ2	1:D:283:PRO:HG3	2.38	0.58
1:E:79:ARG:HD2	1:E:127:ALA:HB2	1.85	0.58
1:B:308:LYS:HD3	1:B:308:LYS:N	2.17	0.58
2:C:601:GLU:HA	3:C:603:NAI:H4N	1.85	0.58
1:B:316:GLU:O	1:B:340:LYS:HD3	2.04	0.58
1:B:91:GLY:HA3	1:B:125:ALA:O	2.04	0.58
1:C:133:PRO:HG2	1:C:170:SER:HB3	1.85	0.58
1:D:133:PRO:HG2	1:D:170:SER:HB3	1.86	0.58
1:D:459:ARG:NH2	5:D:708:HOH:O	2.35	0.58
1:D:79:ARG:HD2	1:D:127:ALA:HB2	1.84	0.58
1:E:281:TRP:CZ2	1:E:283:PRO:HG3	2.38	0.58
1:F:281:TRP:CZ2	1:F:283:PRO:HG3	2.38	0.58
1:C:91:GLY:HA3	1:C:125:ALA:O	2.04	0.58
1:F:462:ARG:HA	1:F:465:MET:HE2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LYS:HD3	1:E:501:THR:HG23	1.85	0.58
1:B:133:PRO:HG2	1:B:170:SER:HB3	1.86	0.58
3:D:603:NAI:O1N	5:D:703:HOH:O	2.17	0.58
1:E:31:ASP:O	1:E:33:LYS:HG2	2.04	0.57
1:A:91:GLY:HA3	1:A:125:ALA:O	2.04	0.57
1:B:333:LYS:HD2	1:B:359:ILE:HD11	1.86	0.57
1:F:91:GLY:HA3	1:F:125:ALA:O	2.04	0.57
1:C:363:ARG:CZ	1:C:365:ILE:HD11	2.35	0.57
1:D:91:GLY:HA3	1:D:125:ALA:O	2.04	0.57
1:F:79:ARG:HD2	1:F:127:ALA:HB2	1.86	0.57
1:B:79:ARG:HD2	1:B:127:ALA:HB2	1.87	0.56
1:A:78:TYR:HE2	1:A:101:VAL:HG22	1.69	0.56
1:B:441:SER:HB2	5:B:736:HOH:O	2.05	0.56
1:A:133:PRO:HG2	1:A:170:SER:HB3	1.85	0.56
1:B:307:ALA:C	1:B:308:LYS:HD3	2.25	0.56
1:A:19:ARG:NH2	1:A:476:ASP:OD2	2.34	0.56
1:D:146:ARG:HH11	1:D:182:THR:HG22	1.71	0.56
1:C:183:TYR:OH	5:C:702:HOH:O	1.98	0.56
1:C:37:THR:HA	1:C:41:LYS:HE3	1.87	0.56
1:A:146:ARG:HH11	1:A:182:THR:HG22	1.71	0.55
1:C:146:ARG:HH11	1:C:182:THR:HG22	1.72	0.55
1:F:146:ARG:HH11	1:F:182:THR:HG22	1.71	0.55
1:F:37:THR:HA	1:F:41:LYS:HE3	1.88	0.55
1:A:275:GLU:CG	1:A:276:SER:H	2.17	0.55
1:C:38:GLU:HG3	1:C:40:GLN:H	1.72	0.55
1:D:495:GLU:C	1:E:205:GLN:HE22	2.10	0.55
1:D:10:PHE:C	1:D:10:PHE:CD1	2.80	0.55
1:E:37:THR:HA	1:E:41:LYS:HE3	1.88	0.55
1:F:133:PRO:HG2	1:F:170:SER:HB3	1.86	0.55
1:F:462:ARG:HH11	1:F:465:MET:CE	2.11	0.55
1:D:277:ASP:OD1	1:D:277:ASP:N	2.40	0.55
1:D:225:ASN:HD21	1:D:458:GLU:HA	1.70	0.55
1:B:146:ARG:HH11	1:B:182:THR:HG22	1.72	0.54
1:B:37:THR:HA	1:B:41:LYS:HE3	1.90	0.54
1:E:146:ARG:HH11	1:E:182:THR:HG22	1.71	0.54
1:A:238:MET:HG2	1:A:245:LYS:NZ	2.22	0.54
1:E:280:ILE:HD13	1:E:301:ILE:CG2	2.37	0.54
1:A:260:MET:HG2	1:A:288:PRO:HG3	1.89	0.54
1:A:37:THR:HA	1:A:41:LYS:HE3	1.90	0.54
1:E:34:THR:CG2	1:E:36:GLU:HG2	2.37	0.54
1:D:37:THR:HA	1:D:41:LYS:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:MET:HG2	1:E:288:PRO:HG3	1.89	0.54
1:A:271:VAL:HG12	1:A:283:PRO:HA	1.90	0.54
1:A:414:GLN:NE2	1:A:429:PRO:HA	2.23	0.54
1:A:238:MET:HG3	1:A:239:THR:H	1.72	0.53
1:F:260:MET:HG2	1:F:288:PRO:HG3	1.90	0.53
1:F:24:VAL:HG11	1:F:483:VAL:HG13	1.90	0.53
1:C:143:LYS:HE3	1:F:501:THR:HA	1.90	0.53
1:C:260:MET:HG2	1:C:288:PRO:HG3	1.90	0.53
1:F:358:LYS:O	1:F:362:GLU:HG3	2.09	0.53
1:F:40:GLN:HA	1:F:43:ASN:HB2	1.89	0.53
1:A:425:GLY:O	1:C:420:LYS:NZ	2.31	0.53
1:A:24:VAL:HG11	1:A:483:VAL:HG13	1.90	0.53
1:D:253:GLY:HA3	3:D:602:NAI:O5B	2.08	0.53
1:A:79:ARG:HD2	1:A:127:ALA:HB2	1.89	0.53
1:C:43:ASN:HB3	1:C:44:ARG:CZ	2.39	0.53
1:B:401:TYR:OH	5:B:706:HOH:O	2.19	0.53
1:B:277:ASP:OD1	1:B:277:ASP:N	2.40	0.52
1:C:46:ARG:HG3	1:C:50:ARG:NH1	2.24	0.52
1:E:301:ILE:HD12	1:E:301:ILE:N	2.25	0.52
1:F:169:MET:HG2	3:F:603:NAI:O1N	2.09	0.52
1:B:238:MET:HE1	1:B:342:LYS:HB2	1.91	0.52
1:A:275:GLU:CG	1:A:276:SER:N	2.73	0.52
1:C:271:VAL:HG12	1:C:283:PRO:HA	1.91	0.52
1:C:25:GLU:OE1	1:C:42:ARG:CZ	2.58	0.51
1:D:260:MET:HG2	1:D:288:PRO:HG3	1.91	0.51
1:A:501:THR:CG2	1:D:143:LYS:NZ	2.59	0.51
1:D:24:VAL:HG13	1:D:483:VAL:HG13	1.89	0.51
1:D:462:ARG:HA	1:D:465:MET:HE2	1.91	0.51
1:C:24:VAL:HG13	1:C:483:VAL:HG22	1.92	0.51
1:A:253:GLY:HA3	3:A:602:NAI:O5B	2.11	0.51
1:C:261:ARG:CB	1:C:261:ARG:HH11	2.21	0.51
1:E:24:VAL:HG13	1:E:483:VAL:HG22	1.91	0.51
1:A:238:MET:HG3	1:A:245:LYS:HZ1	1.76	0.51
1:D:10:PHE:CE1	1:D:14:GLU:HG3	2.44	0.51
1:D:282:ASN:HB3	1:D:286:ILE:CD1	2.40	0.51
1:D:2:ASP:O	1:D:6:ASP:HB2	2.10	0.51
1:D:433:THR:HG23	1:E:412:SER:HA	1.91	0.51
1:A:38:GLU:HB3	1:A:40:GLN:HG2	1.93	0.51
1:B:150:MET:SD	1:E:500:PHE:HE1	2.34	0.51
1:F:3:ARG:HG2	1:F:3:ARG:O	2.10	0.51
1:A:358:LYS:O	1:A:362:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:LYS:HG3	1:D:295:LYS:O	2.11	0.51
1:F:337:PRO:C	1:F:363:ARG:HH12	2.15	0.51
1:C:79:ARG:HH11	1:C:127:ALA:HB2	1.75	0.51
1:A:238:MET:CG	1:A:245:LYS:NZ	2.75	0.51
1:C:34:THR:HG22	1:C:41:LYS:HE2	1.93	0.50
1:E:271:VAL:HG13	1:E:283:PRO:HA	1.93	0.50
1:B:173:GLU:OE2	1:B:212:ILE:HD11	2.12	0.50
1:C:501:THR:HG22	1:F:66:ARG:HG2	1.93	0.50
1:E:291:LEU:HD21	1:E:301:ILE:HG23	1.94	0.50
1:B:99:VAL:HA	1:B:103:GLU:OE1	2.12	0.50
1:A:42:ARG:HH11	1:A:46:ARG:NH1	2.09	0.50
1:C:358:LYS:O	1:C:362:GLU:HG3	2.12	0.50
1:B:260:MET:HG2	1:B:288:PRO:HG3	1.93	0.49
1:E:99:VAL:HA	1:E:103:GLU:OE1	2.11	0.49
1:E:314:ILE:HG13	1:E:314:ILE:O	2.13	0.49
1:B:318:ASP:CB	1:B:340:LYS:HE3	2.43	0.49
1:D:169:MET:HG2	3:D:602:NAI:O1N	2.13	0.49
1:D:191:ASP:OD2	5:D:704:HOH:O	2.18	0.49
1:C:99:VAL:HA	1:C:103:GLU:OE1	2.12	0.48
1:F:308:LYS:HE3	1:F:308:LYS:HB3	1.50	0.48
1:A:287:ASP:OD1	1:A:289:LYS:NZ	2.42	0.48
1:B:146:ARG:NH1	1:B:182:THR:HG22	2.28	0.48
1:E:277:ASP:N	1:E:277:ASP:OD1	2.40	0.48
1:A:99:VAL:HA	1:A:103:GLU:OE1	2.13	0.48
1:C:29:VAL:HG21	1:C:42:ARG:CG	2.30	0.48
1:E:146:ARG:NH1	1:E:182:THR:HG22	2.28	0.48
1:E:358:LYS:O	1:E:362:GLU:HG3	2.13	0.48
1:F:38:GLU:CB	1:F:40:GLN:H	2.26	0.48
1:F:34:THR:HG22	1:F:41:LYS:HE2	1.95	0.48
1:F:2:ASP:O	1:F:6:ASP:HB2	2.13	0.48
1:B:34:THR:HG22	1:B:41:LYS:HE2	1.94	0.48
1:C:146:ARG:NH1	1:C:182:THR:HG22	2.29	0.48
1:A:36:GLU:O	1:A:38:GLU:N	2.47	0.47
1:D:146:ARG:NH1	1:D:182:THR:HG22	2.28	0.47
1:D:271:VAL:HG13	1:D:283:PRO:HA	1.96	0.47
1:B:24:VAL:HG11	1:B:483:VAL:HG13	1.95	0.47
1:D:10:PHE:HE1	1:D:14:GLU:CG	2.27	0.47
1:F:146:ARG:NH1	1:F:182:THR:HG22	2.29	0.47
1:F:36:GLU:HG3	1:F:38:GLU:HG3	1.96	0.47
1:C:195[B]:HIS:CE1	1:C:388:ASN:ND2	2.82	0.47
1:B:238:MET:SD	1:B:245:LYS:HE2	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:HH11	1:A:127:ALA:HB2	1.80	0.47
1:B:215:THR:HG23	5:B:711:HOH:O	2.15	0.47
1:D:443:ALA:HB2	1:E:401:TYR:CD2	2.49	0.47
1:A:346:GLU:HB3	1:A:351:PRO:HG3	1.96	0.47
1:D:238:MET:HE2	1:D:245:LYS:HE3	1.97	0.47
1:B:416:SER:HA	1:B:419:ARG:NH2	2.30	0.47
1:A:205:GLN:NE2	1:B:496:ALA:HB2	2.29	0.47
1:B:79:ARG:HH11	1:B:127:ALA:HB2	1.80	0.47
1:F:79:ARG:HH11	1:F:127:ALA:HB2	1.80	0.47
1:B:227:ILE:HD11	1:B:245:LYS:HD3	1.97	0.47
1:D:38:GLU:CD	1:D:38:GLU:H	2.18	0.47
1:B:130:LYS:O	5:B:707:HOH:O	2.20	0.47
1:C:204:SER:C	1:C:205:GLN:HG2	2.33	0.47
1:E:403:ARG:NH1	1:E:441:SER:OG	2.48	0.47
1:A:227:ILE:HD11	1:A:245:LYS:HD2	1.95	0.46
1:A:423:LYS:C	1:A:425:GLY:H	2.19	0.46
1:A:462:ARG:CZ	1:A:465:MET:HE1	2.45	0.46
1:D:34:THR:HG22	1:D:41:LYS:HE2	1.96	0.46
1:E:303:GLY:H	1:E:309:ILE:HD11	1.80	0.46
1:A:146:ARG:NH1	1:A:182:THR:HG22	2.29	0.46
1:E:36:GLU:O	1:E:38:GLU:N	2.48	0.46
1:B:38:GLU:C	1:B:40:GLN:H	2.18	0.46
1:D:333:LYS:HG3	1:D:355:GLU:CB	2.46	0.46
1:E:470:LYS:HD3	1:E:471:TYR:CE2	2.51	0.46
1:A:339:VAL:O	1:A:340:LYS:HB2	2.15	0.46
1:A:491:ARG:O	1:A:495:GLU:HG3	2.16	0.46
1:E:38:GLU:HG2	1:E:39:GLU:N	2.29	0.46
1:E:316:GLU:O	1:E:340:LYS:HD3	2.16	0.46
1:A:277:ASP:OD1	1:A:277:ASP:N	2.40	0.46
1:B:40:GLN:HA	1:B:43:ASN:HB2	1.98	0.46
1:F:301:ILE:HG23	1:F:301:ILE:HD12	1.71	0.46
1:D:42:ARG:O	1:D:46:ARG:HG3	2.16	0.46
1:E:333:LYS:HB2	1:E:333:LYS:HE2	1.78	0.46
1:A:31:ASP:O	1:A:33:LYS:HG2	2.17	0.45
1:C:462:ARG:HA	1:C:465:MET:HE2	1.98	0.45
1:D:289:LYS:HD2	1:D:289:LYS:HA	1.70	0.45
1:E:79:ARG:HH11	1:E:127:ALA:HB2	1.80	0.45
1:A:169:MET:HG2	3:A:602:NAI:O1N	2.17	0.45
1:B:169:MET:HG2	3:B:602:NAI:O1N	2.16	0.45
1:B:412:SER:HA	1:C:433:THR:HG23	1.98	0.45
1:E:91:GLY:O	1:E:165:PRO:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:PHE:C	1:D:10:PHE:HD1	2.18	0.45
1:D:79:ARG:HH11	1:D:127:ALA:HB2	1.80	0.45
1:F:89:CYS:HB3	1:F:125:ALA:HB2	1.99	0.45
1:F:91:GLY:O	1:F:165:PRO:HA	2.17	0.45
1:B:89:CYS:HB3	1:B:125:ALA:HB2	1.99	0.45
1:D:313:SER:HB3	1:D:316:GLU:HG3	1.97	0.45
1:D:339:VAL:HG12	1:D:341:ALA:H	1.81	0.45
1:E:24:VAL:CG1	1:E:483:VAL:HG13	2.46	0.45
1:A:134:LYS:HD2	1:A:134:LYS:HA	1.72	0.45
1:C:227:ILE:HD11	1:C:245:LYS:HD3	1.99	0.45
1:C:40:GLN:NE2	1:C:44:ARG:HE	2.14	0.45
1:C:9:PHE:CE2	1:C:328:GLU:HG3	2.51	0.45
1:B:500:PHE:HD1	1:B:500:PHE:H	1.60	0.45
1:E:34:THR:HG23	1:E:36:GLU:CG	2.46	0.45
1:F:238:MET:HE3	1:F:320:ASP:HB3	1.98	0.45
1:F:38:GLU:HB2	1:F:40:GLN:HB3	1.98	0.45
1:A:246:THR:OG1	1:A:320:ASP:OD1	2.35	0.45
1:C:274:GLY:HA2	1:C:279:SER:HB3	1.97	0.45
1:D:12:MET:HG3	1:D:354:PRO:HD3	1.99	0.45
1:F:465:MET:HB2	1:F:465:MET:HE2	1.79	0.45
1:F:339:VAL:HG12	1:F:341:ALA:H	1.82	0.45
1:B:466:ARG:HG2	1:B:470:LYS:NZ	2.32	0.44
1:C:261:ARG:NH2	4:C:602:GTP:C5	2.85	0.44
1:A:89:CYS:HB3	1:A:125:ALA:HB2	1.99	0.44
1:A:301:ILE:HD12	1:A:301:ILE:HG23	1.71	0.44
1:B:91:GLY:O	1:B:165:PRO:HA	2.17	0.44
1:C:12:MET:HG3	1:C:354:PRO:HD3	1.99	0.44
1:D:443:ALA:HB2	1:E:401:TYR:CE2	2.52	0.44
1:E:178:TRP:O	1:E:182:THR:HG23	2.18	0.44
1:A:42:ARG:HH11	1:A:46:ARG:HH12	1.64	0.44
1:B:401:TYR:CD2	1:C:443:ALA:HB2	2.52	0.44
1:D:10:PHE:CD1	1:D:10:PHE:O	2.70	0.44
1:A:79:ARG:NH2	1:A:163:ASP:OD1	2.33	0.44
1:E:370:ASP:OD1	1:E:371:LEU:N	2.50	0.44
1:C:361:LEU:HA	1:C:361:LEU:HD23	1.88	0.44
1:C:89:CYS:HB3	1:C:125:ALA:HB2	1.99	0.44
1:D:420:LYS:HG3	1:D:421:PHE:CD1	2.53	0.44
1:F:297:GLN:HG3	1:F:297:GLN:O	2.17	0.44
1:A:34:THR:HG22	1:A:41:LYS:HE2	1.99	0.44
1:A:91:GLY:O	1:A:165:PRO:HA	2.18	0.44
1:C:277:ASP:OD1	1:C:277:ASP:N	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:TRP:O	1:B:182:THR:HG23	2.18	0.43
1:B:185:SER:O	1:F:154:LYS:HD3	2.18	0.43
1:D:91:GLY:O	1:D:165:PRO:HA	2.18	0.43
1:F:38:GLU:HB2	1:F:40:GLN:H	1.83	0.43
1:B:301:ILE:HD13	1:B:301:ILE:HA	1.73	0.43
1:C:275:GLU:HB3	1:C:276:SER:H	1.54	0.43
1:D:462:ARG:CZ	1:D:465:MET:HE1	2.47	0.43
1:E:17:PHE:CE2	1:E:486:ILE:HG12	2.54	0.43
1:E:89:CYS:HB3	1:E:125:ALA:HB2	2.00	0.43
1:A:361:LEU:HA	1:A:361:LEU:HD23	1.89	0.43
1:D:89:CYS:HB3	1:D:125:ALA:HB2	2.00	0.43
1:C:24:VAL:CG1	1:C:483:VAL:HG13	2.49	0.43
1:C:91:GLY:O	1:C:165:PRO:HA	2.18	0.43
1:D:500:PHE:C	1:D:500:PHE:CD2	2.92	0.43
1:E:435:GLU:OE1	1:E:435:GLU:N	2.49	0.43
1:A:178:TRP:O	1:A:182:THR:HG23	2.19	0.43
1:B:143:LYS:HD3	1:E:501:THR:CG2	2.47	0.43
1:C:25:GLU:O	1:C:29:VAL:HG23	2.18	0.43
1:F:337:PRO:HA	1:F:363:ARG:NH1	2.34	0.43
1:C:261:ARG:CG	1:C:261:ARG:HH11	2.31	0.43
1:D:333:LYS:HG3	1:D:355:GLU:HB3	2.01	0.43
1:F:17:PHE:CE2	1:F:486:ILE:HG12	2.54	0.43
1:B:264:HIS:HD2	5:B:724:HOH:O	2.02	0.43
1:D:178:TRP:O	1:D:182:THR:HG23	2.18	0.43
1:F:25:GLU:OE2	1:F:46:ARG:NH1	2.52	0.42
1:A:185:SER:HB3	1:B:500:PHE:CE1	2.54	0.42
1:D:370:ASP:OD1	1:D:371:LEU:N	2.51	0.42
1:D:500:PHE:C	1:D:500:PHE:HD2	2.22	0.42
1:F:253:GLY:HA3	3:F:603:NAI:O5B	2.19	0.42
1:A:275:GLU:HG3	1:A:276:SER:N	2.31	0.42
1:E:203:ILE:HG12	5:E:729:HOH:O	2.19	0.42
1:A:17:PHE:CE2	1:A:486:ILE:HG12	2.54	0.42
1:C:178:TRP:O	1:C:182:THR:HG23	2.19	0.42
1:F:178:TRP:O	1:F:182:THR:HG23	2.20	0.42
1:F:271:VAL:HG12	1:F:283:PRO:HA	2.01	0.42
1:B:12:MET:HG3	1:B:354:PRO:HD3	2.02	0.42
1:A:2:ASP:O	1:A:6:ASP:HB2	2.19	0.42
1:C:2:ASP:O	1:C:6:ASP:HB2	2.20	0.42
1:E:433:THR:HG23	1:F:412:SER:HA	2.00	0.42
1:B:154:LYS:HD3	1:F:185:SER:O	2.19	0.42
1:E:238:MET:SD	1:E:245:LYS:NZ	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:ASP:OD1	1:C:371:LEU:N	2.51	0.42
1:A:443:ALA:HB2	1:C:401:TYR:CD2	2.55	0.42
1:D:346:GLU:OE1	1:D:369:PRO:HA	2.19	0.42
1:E:236:LEU:O	1:E:342:LYS:CE	2.68	0.42
1:F:150:MET:HE2	1:F:150:MET:HB3	1.73	0.42
1:C:79:ARG:HE	1:C:163:ASP:CG	2.24	0.41
1:D:17:PHE:CE2	1:D:486:ILE:HG12	2.54	0.41
1:F:361:LEU:HD23	1:F:361:LEU:HA	1.88	0.41
1:A:12:MET:HG3	1:A:354:PRO:HD3	2.02	0.41
1:C:38:GLU:HB3	1:C:40:GLN:HB3	2.02	0.41
1:E:2:ASP:O	1:E:6:ASP:HB2	2.21	0.41
1:A:448:ILE:HA	1:A:448:ILE:HD13	1.90	0.41
1:C:420:LYS:HG2	1:C:421:PHE:CD1	2.55	0.41
1:E:248:ALA:HB2	1:E:317:VAL:HG11	2.02	0.41
1:F:12:MET:HG3	1:F:354:PRO:HD3	2.01	0.41
1:F:225:ASN:HD21	1:F:458:GLU:HA	1.86	0.41
1:B:301:ILE:HG23	1:B:301:ILE:HD12	1.70	0.41
1:C:400:LYS:HB3	5:C:744:HOH:O	2.20	0.41
1:B:370:ASP:OD1	1:B:371:LEU:N	2.51	0.41
1:E:12:MET:HG3	1:E:354:PRO:HD3	2.02	0.41
1:E:458:GLU:OE1	1:E:462:ARG:HD2	2.21	0.41
1:F:67:ARG:HE	1:F:67:ARG:HB3	1.75	0.41
1:D:358:LYS:O	1:D:362:GLU:HG3	2.21	0.41
1:B:79:ARG:NH2	1:B:163:ASP:OD1	2.33	0.41
1:B:36:GLU:HB3	1:B:38:GLU:OE1	2.20	0.41
1:C:38:GLU:O	1:C:41:LYS:HB2	2.20	0.41
1:E:308:LYS:HE2	1:E:308:LYS:HB3	1.91	0.41
1:F:35:ARG:HB3	1:F:36:GLU:H	1.76	0.41
1:C:301:ILE:HG23	1:C:301:ILE:HD12	1.72	0.41
1:D:134:LYS:HA	1:D:134:LYS:HD3	1.53	0.41
1:A:143:LYS:HE2	1:D:501:THR:HG23	2.03	0.41
1:A:10:PHE:HE1	5:A:734:HOH:O	2.04	0.41
1:C:248:ALA:HB2	1:C:317:VAL:HG11	2.03	0.41
1:E:238:MET:HG2	1:E:245:LYS:HZ1	1.86	0.41
1:F:248:ALA:HB2	1:F:317:VAL:HG11	2.03	0.41
1:F:333:LYS:HE3	1:F:333:LYS:HB2	1.96	0.41
1:A:420:LYS:HG3	1:A:421:PHE:CD1	2.56	0.40
1:C:17:PHE:CE2	1:C:486:ILE:HG12	2.55	0.40
1:E:495:GLU:OE1	5:E:703:HOH:O	2.22	0.40
1:A:25:GLU:O	1:A:29:VAL:HG23	2.21	0.40
1:B:25:GLU:O	1:B:29:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ASN:O	1:C:46:ARG:HG2	2.21	0.40
1:D:86:ARG:HD3	1:D:86:ARG:HH11	1.72	0.40
1:B:246:THR:HB	1:B:271:VAL:HG21	2.03	0.40
1:B:333:LYS:HD2	1:B:359:ILE:CD1	2.49	0.40
1:B:225:ASN:HD22	1:B:461:ALA:HB3	1.87	0.40
1:F:269:LYS:HD2	1:F:284:ASP:O	2.21	0.40
1:B:225:ASN:HD21	1:B:458:GLU:CA	2.20	0.40
1:C:150:MET:O	1:C:154:LYS:HG3	2.22	0.40
1:D:248:ALA:HB2	1:D:317:VAL:HG11	2.04	0.40
1:E:301:ILE:HD12	1:E:301:ILE:CA	2.51	0.40
1:F:27:LYS:HG2	1:F:27:LYS:O	2.21	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	500/501 (100%)	470 (94%)	24 (5%)	6 (1%)	13	24
1	B	500/501 (100%)	476 (95%)	21 (4%)	3 (1%)	25	43
1	C	500/501 (100%)	473 (95%)	22 (4%)	5 (1%)	15	28
1	D	500/501 (100%)	477 (95%)	18 (4%)	5 (1%)	15	28
1	E	500/501 (100%)	473 (95%)	22 (4%)	5 (1%)	15	28
1	F	500/501 (100%)	475 (95%)	20 (4%)	5 (1%)	15	28
All	All	3000/3006 (100%)	2844 (95%)	127 (4%)	29 (1%)	15	28

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	GLU

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Mol	Chain	Res	Type
1	A	42	ARG
1	A	422	GLY
1	B	422	GLY
1	C	422	GLY
1	D	422	GLY
1	D	500	PHE
1	E	38	GLU
1	E	422	GLY
1	E	500	PHE
1	F	35	ARG
1	F	37	THR
1	F	422	GLY
1	A	37	THR
1	B	498	VAL
1	C	498	VAL
1	D	498	VAL
1	E	498	VAL
1	F	498	VAL
1	A	498	VAL
1	B	32	LEU
1	A	424	HIS
1	D	38	GLU
1	D	425	GLY
1	C	38	GLU
1	C	309	ILE
1	F	38	GLU
1	C	500	PHE
1	E	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	418/417 (100%)	410 (98%)	8 (2%)	57 80
1	B	418/417 (100%)	409 (98%)	9 (2%)	52 77
1	C	418/417 (100%)	409 (98%)	9 (2%)	52 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	418/417 (100%)	407 (97%)	11 (3%)	46 72
1	E	418/417 (100%)	405 (97%)	13 (3%)	40 67
1	F	418/417 (100%)	409 (98%)	9 (2%)	52 77
All	All	2508/2502 (100%)	2449 (98%)	59 (2%)	49 74

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	LYS
1	A	182	THR
1	A	291	LEU
1	A	333	LYS
1	A	357	ASP
1	A	358	LYS
1	A	396	ARG
1	A	405	SER
1	B	19	ARG
1	B	39	GLU
1	B	79	ARG
1	B	182	THR
1	B	291	LEU
1	B	342	LYS
1	B	396	ARG
1	B	403	ARG
1	B	419	ARG
1	C	44	ARG
1	C	66	ARG
1	C	182	THR
1	C	205	GLN
1	C	318	ASP
1	C	396	ARG
1	C	405	SER
1	C	438	ASP
1	C	500	PHE
1	D	3	ARG
1	D	10	PHE
1	D	79	ARG
1	D	182	THR
1	D	291	LEU
1	D	293	ASP
1	D	357	ASP

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Mol	Chain	Res	Type
1	D	396	ARG
1	D	438	ASP
1	D	466	ARG
1	D	500	PHE
1	E	3	ARG
1	E	39	GLU
1	E	71	SER
1	E	79	ARG
1	E	169	MET
1	E	182	THR
1	E	291	LEU
1	E	357	ASP
1	E	363	ARG
1	E	396	ARG
1	E	403	ARG
1	E	405	SER
1	E	419	ARG
1	F	79	ARG
1	F	150	MET
1	F	182	THR
1	F	291	LEU
1	F	357	ASP
1	F	396	ARG
1	F	405	SER
1	F	438	ASP
1	F	500	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	GLN
1	B	205	GLN
1	B	225	ASN
1	C	225	ASN
1	C	330	GLN
1	D	205	GLN
1	D	484	ASN
1	E	205	GLN
1	E	225	ASN
1	F	225	ASN
1	F	364	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
2	GLU	F	601	-	2,9,9	0.47	0	2,11,11	0.32	0
3	NAI	C	603	-	42,48,48	1.00	2 (4%)	47,73,73	1.23	5 (10%)
2	GLU	E	601	-	2,9,9	0.44	0	2,11,11	0.53	0
3	NAI	D	603	1	42,48,48	1.02	2 (4%)	47,73,73	1.52	7 (14%)
3	NAI	A	602	-	42,48,48	0.99	2 (4%)	47,73,73	1.38	6 (12%)
4	GTP	D	604	-	26,34,34	1.01	1 (3%)	33,54,54	1.64	6 (18%)
3	NAI	D	602	-	42,48,48	0.99	2 (4%)	47,73,73	1.22	4 (8%)
4	GTP	A	604	-	26,34,34	1.02	1 (3%)	33,54,54	1.71	7 (21%)
2	GLU	D	601	-	2,9,9	0.53	0	2,11,11	0.35	0
4	GTP	C	602	-	26,34,34	1.00	1 (3%)	33,54,54	1.66	6 (18%)
3	NAI	C	604	1	42,48,48	1.02	2 (4%)	47,73,73	1.68	7 (14%)
4	GTP	B	603	-	26,34,34	1.00	1 (3%)	33,54,54	1.72	6 (18%)
2	GLU	C	601	-	2,9,9	0.47	0	2,11,11	0.29	0
4	GTP	F	604	-	26,34,34	1.02	1 (3%)	33,54,54	1.78	10 (30%)
3	NAI	E	602	-	42,48,48	0.99	2 (4%)	47,73,73	1.23	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAI	B	604	-	42,48,48	0.98	2 (4%)	47,73,73	1.29	5 (10%)
3	NAI	F	602	-	42,48,48	1.07	3 (7%)	47,73,73	1.70	8 (17%)
3	NAI	F	603	-	42,48,48	1.01	2 (4%)	47,73,73	1.20	3 (6%)
4	GTP	E	604	-	26,34,34	0.98	1 (3%)	33,54,54	1.72	5 (15%)
3	NAI	B	602	-	42,48,48	0.99	2 (4%)	47,73,73	1.26	3 (6%)
3	NAI	A	603	-	42,48,48	1.02	2 (4%)	47,73,73	1.53	6 (12%)
2	GLU	B	601	-	2,9,9	0.40	0	2,11,11	0.46	0
3	NAI	E	603	-	42,48,48	1.01	2 (4%)	47,73,73	1.45	6 (12%)
2	GLU	A	601	-	2,9,9	0.36	0	2,11,11	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	F	601	-	-	1/3/9/9	-
3	NAI	C	603	-	-	9/25/72/72	0/5/5/5
2	GLU	E	601	-	-	2/3/9/9	-
3	NAI	D	603	1	-	4/25/72/72	0/5/5/5
3	NAI	A	602	-	-	9/25/72/72	0/5/5/5
4	GTP	D	604	-	-	0/18/38/38	0/3/3/3
3	NAI	D	602	-	-	6/25/72/72	0/5/5/5
4	GTP	A	604	-	-	1/18/38/38	0/3/3/3
2	GLU	D	601	-	-	1/3/9/9	-
4	GTP	C	602	-	-	6/18/38/38	0/3/3/3
3	NAI	C	604	1	-	6/25/72/72	0/5/5/5
4	GTP	B	603	-	-	1/18/38/38	0/3/3/3
2	GLU	C	601	-	-	1/3/9/9	-
4	GTP	F	604	-	-	0/18/38/38	0/3/3/3
3	NAI	E	602	-	-	7/25/72/72	0/5/5/5
3	NAI	B	604	-	-	4/25/72/72	0/5/5/5
3	NAI	F	602	-	-	8/25/72/72	0/5/5/5
3	NAI	F	603	-	-	9/25/72/72	0/5/5/5
4	GTP	E	604	-	-	2/18/38/38	0/3/3/3
3	NAI	B	602	-	-	5/25/72/72	0/5/5/5
3	NAI	A	603	-	-	4/25/72/72	0/5/5/5
2	GLU	B	601	-	-	2/3/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAI	E	603	-	-	8/25/72/72	0/5/5/5
2	GLU	A	601	-	-	2/3/9/9	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	NAI	C6N-C5N	3.63	1.39	1.33
3	D	603	NAI	C6N-C5N	3.61	1.39	1.33
3	E	603	NAI	C6N-C5N	3.52	1.39	1.33
3	B	604	NAI	C6N-C5N	3.52	1.39	1.33
3	C	604	NAI	C6N-C5N	3.45	1.39	1.33
3	F	602	NAI	C6N-C5N	3.44	1.39	1.33
3	B	602	NAI	C6N-C5N	3.41	1.39	1.33
3	E	602	NAI	C6N-C5N	3.36	1.39	1.33
3	F	603	NAI	C6N-C5N	3.31	1.39	1.33
4	A	604	GTP	C6-N1	3.28	1.38	1.33
4	F	604	GTP	C6-N1	3.24	1.38	1.33
3	A	602	NAI	C6N-C5N	3.22	1.39	1.33
3	C	603	NAI	C6N-C5N	3.20	1.39	1.33
4	D	604	GTP	C6-N1	3.19	1.38	1.33
4	B	603	GTP	C6-N1	3.17	1.38	1.33
4	E	604	GTP	C6-N1	3.14	1.38	1.33
3	D	602	NAI	C6N-C5N	3.13	1.38	1.33
4	C	602	GTP	C6-N1	3.10	1.38	1.33
3	F	602	NAI	C5A-C4A	2.68	1.48	1.40
3	D	603	NAI	C5A-C4A	2.61	1.47	1.40
3	A	603	NAI	C5A-C4A	2.51	1.47	1.40
3	E	603	NAI	C5A-C4A	2.48	1.47	1.40
3	C	604	NAI	C5A-C4A	2.44	1.47	1.40
3	F	603	NAI	C5A-C4A	2.37	1.47	1.40
3	C	603	NAI	C5A-C4A	2.34	1.47	1.40
3	D	602	NAI	C5A-C4A	2.34	1.47	1.40
3	B	604	NAI	C5A-C4A	2.33	1.47	1.40
3	F	602	NAI	O4B-C1B	2.29	1.44	1.41
3	E	602	NAI	C5A-C4A	2.28	1.47	1.40
3	B	602	NAI	C5A-C4A	2.27	1.46	1.40
3	A	602	NAI	C5A-C4A	2.25	1.46	1.40

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	604	NAI	C2D-C1D-N1N	-5.73	98.96	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	604	GTP	N3-C2-N1	-5.48	119.91	127.22
4	A	604	GTP	N3-C2-N1	-5.40	120.02	127.22
4	E	604	GTP	N3-C2-N1	-5.39	120.03	127.22
4	C	602	GTP	N3-C2-N1	-5.28	120.18	127.22
4	B	603	GTP	N3-C2-N1	-5.24	120.23	127.22
3	F	602	NAI	PN-O3-PA	-5.20	115.00	132.83
4	D	604	GTP	N3-C2-N1	-5.12	120.39	127.22
3	E	603	NAI	PN-O3-PA	-5.07	115.43	132.83
3	D	603	NAI	C1D-N1N-C2N	-4.59	113.47	121.11
3	A	603	NAI	C2D-C1D-N1N	-4.58	101.83	113.30
3	C	604	NAI	PN-O3-PA	-4.57	117.14	132.83
3	F	602	NAI	O4B-C1B-C2B	-4.52	100.33	106.93
4	E	604	GTP	C2-N3-C4	4.26	120.22	115.36
3	B	604	NAI	PN-O3-PA	-4.22	118.34	132.83
3	A	603	NAI	PN-O3-PA	-4.14	118.63	132.83
4	C	602	GTP	C2-N3-C4	4.04	119.97	115.36
4	B	603	GTP	C2-N3-C4	4.03	119.97	115.36
4	A	604	GTP	C2-N3-C4	4.03	119.95	115.36
4	F	604	GTP	C2-N3-C4	4.02	119.95	115.36
4	D	604	GTP	C2-N3-C4	3.86	119.76	115.36
3	D	603	NAI	PN-O3-PA	-3.80	119.79	132.83
3	F	602	NAI	C2D-C1D-N1N	-3.78	103.83	113.30
4	E	604	GTP	PB-O3B-PG	-3.67	120.22	132.83
3	A	603	NAI	C1D-N1N-C2N	-3.65	115.04	121.11
3	A	602	NAI	N3A-C2A-N1A	-3.57	123.10	128.68
3	D	603	NAI	C2D-C1D-N1N	-3.55	104.40	113.30
3	C	604	NAI	C1D-N1N-C2N	-3.48	115.31	121.11
3	F	603	NAI	N3A-C2A-N1A	-3.47	123.25	128.68
3	B	604	NAI	N3A-C2A-N1A	-3.47	123.25	128.68
3	E	602	NAI	N3A-C2A-N1A	-3.44	123.31	128.68
3	C	603	NAI	N3A-C2A-N1A	-3.42	123.33	128.68
3	D	602	NAI	N3A-C2A-N1A	-3.39	123.38	128.68
3	B	602	NAI	N3A-C2A-N1A	-3.37	123.41	128.68
3	D	602	NAI	PN-O3-PA	-3.31	121.46	132.83
3	B	602	NAI	PN-O3-PA	-3.26	121.63	132.83
3	C	604	NAI	N3A-C2A-N1A	-3.26	123.59	128.68
3	A	603	NAI	O4D-C1D-N1N	3.22	114.34	108.06
3	A	602	NAI	PN-O3-PA	-3.20	121.83	132.83
3	A	602	NAI	C1B-N9A-C4A	-3.19	121.04	126.64
3	A	603	NAI	C4A-C5A-N7A	-3.12	106.15	109.40
3	C	604	NAI	O2D-C2D-C3D	3.11	121.88	111.82
3	A	603	NAI	N3A-C2A-N1A	-3.10	123.84	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	602	NAI	C1D-N1N-C2N	-3.08	115.98	121.11
4	B	603	GTP	PB-O3B-PG	-3.03	122.42	132.83
3	D	603	NAI	N3A-C2A-N1A	-3.02	123.96	128.68
3	E	602	NAI	PN-O3-PA	-3.02	122.47	132.83
3	A	602	NAI	C4A-C5A-N7A	-3.02	106.25	109.40
3	E	603	NAI	N3A-C2A-N1A	-3.00	123.99	128.68
3	E	603	NAI	C4A-C5A-N7A	-2.95	106.33	109.40
4	D	604	GTP	PB-O3B-PG	-2.92	122.79	132.83
3	F	602	NAI	N3A-C2A-N1A	-2.92	124.11	128.68
3	F	602	NAI	C5B-C4B-C3B	-2.91	104.28	115.18
4	D	604	GTP	PA-O3A-PB	-2.89	122.89	132.83
3	D	603	NAI	C4A-C5A-N7A	-2.89	106.39	109.40
3	E	603	NAI	C1D-N1N-C2N	-2.87	116.33	121.11
4	F	604	GTP	C5-C6-N1	-2.86	119.52	123.43
4	E	604	GTP	C5-C6-N1	-2.86	119.53	123.43
3	F	602	NAI	O4D-C1D-N1N	2.85	113.62	108.06
4	A	604	GTP	C5-C6-N1	-2.84	119.55	123.43
4	C	602	GTP	C5-C6-N1	-2.84	119.55	123.43
3	E	602	NAI	C1B-N9A-C4A	-2.83	121.67	126.64
4	B	603	GTP	C5-C6-N1	-2.82	119.58	123.43
4	B	603	GTP	PA-O3A-PB	-2.82	123.16	132.83
3	F	603	NAI	PN-O3-PA	-2.82	123.17	132.83
4	C	602	GTP	PB-O3B-PG	-2.81	123.17	132.83
3	D	602	NAI	C4A-C5A-N7A	-2.79	106.49	109.40
4	D	604	GTP	C5-C6-N1	-2.79	119.62	123.43
3	B	604	NAI	C4A-C5A-N7A	-2.76	106.52	109.40
3	C	603	NAI	C4A-C5A-N7A	-2.75	106.53	109.40
3	F	602	NAI	C4A-C5A-N7A	-2.72	106.57	109.40
3	C	604	NAI	C4A-C5A-N7A	-2.70	106.59	109.40
4	F	604	GTP	C6-N1-C2	2.69	120.20	115.93
4	A	604	GTP	PB-O3B-PG	-2.69	123.61	132.83
3	E	602	NAI	C4A-C5A-N7A	-2.67	106.61	109.40
3	D	603	NAI	O4D-C1D-N1N	2.66	113.26	108.06
4	A	604	GTP	C6-N1-C2	2.63	120.11	115.93
4	F	604	GTP	PB-O3B-PG	-2.62	123.84	132.83
4	F	604	GTP	PA-O3A-PB	-2.60	123.91	132.83
4	E	604	GTP	C6-N1-C2	2.57	120.00	115.93
4	C	602	GTP	C6-N1-C2	2.54	119.96	115.93
4	B	603	GTP	C6-N1-C2	2.52	119.93	115.93
3	A	602	NAI	O5D-C5D-C4D	2.50	117.61	108.99
4	D	604	GTP	C6-N1-C2	2.49	119.88	115.93
3	B	602	NAI	C4A-C5A-N7A	-2.48	106.81	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	603	NAI	PN-O3-PA	-2.46	124.37	132.83
3	F	603	NAI	C4A-C5A-N7A	-2.38	106.92	109.40
4	A	604	GTP	PA-O3A-PB	-2.38	124.66	132.83
4	F	604	GTP	N2-C2-N1	2.37	120.94	117.25
3	C	603	NAI	C1D-N1N-C6N	-2.33	115.81	120.83
3	E	603	NAI	O4B-C1B-C2B	-2.28	103.60	106.93
3	C	604	NAI	C3B-C2B-C1B	2.26	104.38	100.98
4	A	604	GTP	N2-C2-N1	2.17	120.63	117.25
4	F	604	GTP	C1'-N9-C4	-2.15	122.86	126.64
4	F	604	GTP	O3G-PG-O3B	2.14	111.80	104.64
4	F	604	GTP	C6-C5-C4	-2.06	118.83	120.80
3	A	602	NAI	C2A-N1A-C6A	2.06	122.28	118.75
3	C	603	NAI	C1B-N9A-C4A	-2.06	123.02	126.64
3	B	604	NAI	C3D-C2D-C1D	2.05	105.32	101.43
3	B	604	NAI	C1D-N1N-C2N	-2.02	117.75	121.11
3	D	602	NAI	C1D-N1N-C6N	-2.01	116.50	120.83
4	C	602	GTP	O3G-PG-O3B	2.01	111.38	104.64
3	D	603	NAI	O4B-C1B-C2B	-2.01	103.99	106.93
3	E	603	NAI	PN-O5D-C5D	-2.00	109.93	121.68

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	601	GLU	N-CA-CB-CG
3	C	603	NAI	O4B-C4B-C5B-O5B
3	C	603	NAI	C5D-O5D-PN-O2N
2	E	601	GLU	C-CA-CB-CG
3	D	603	NAI	C5D-O5D-PN-O1N
3	D	603	NAI	C5D-O5D-PN-O2N
3	A	602	NAI	C5D-O5D-PN-O1N
3	A	602	NAI	O4D-C4D-C5D-O5D
3	A	602	NAI	C3D-C4D-C5D-O5D
3	D	602	NAI	O4D-C4D-C5D-O5D
4	A	604	GTP	PB-O3B-PG-O3G
2	D	601	GLU	N-CA-CB-CG
4	C	602	GTP	C5'-O5'-PA-O1A
4	C	602	GTP	C5'-O5'-PA-O2A
3	C	604	NAI	C5B-O5B-PA-O1A
3	C	604	NAI	C5D-O5D-PN-O1N
3	C	604	NAI	C5D-O5D-PN-O2N
3	C	604	NAI	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	C	601	GLU	N-CA-CB-CG
3	E	602	NAI	O4D-C4D-C5D-O5D
3	B	604	NAI	C5D-O5D-PN-O1N
3	B	604	NAI	C5D-O5D-PN-O2N
3	F	602	NAI	C5B-O5B-PA-O1A
3	F	602	NAI	C5D-O5D-PN-O2N
3	F	602	NAI	O4D-C1D-N1N-C2N
3	F	603	NAI	C5D-O5D-PN-O1N
3	F	603	NAI	O4D-C4D-C5D-O5D
3	B	602	NAI	O4D-C4D-C5D-O5D
3	B	602	NAI	C3D-C4D-C5D-O5D
3	A	603	NAI	C5D-O5D-PN-O2N
3	A	603	NAI	O4D-C1D-N1N-C2N
2	B	601	GLU	N-CA-CB-CG
2	B	601	GLU	C-CA-CB-CG
3	E	603	NAI	C5B-O5B-PA-O1A
3	E	603	NAI	C5D-O5D-PN-O3
3	E	603	NAI	C5D-O5D-PN-O1N
2	A	601	GLU	N-CA-CB-CG
2	A	601	GLU	C-CA-CB-CG
3	D	602	NAI	C3D-C4D-C5D-O5D
3	E	602	NAI	C3D-C4D-C5D-O5D
3	F	603	NAI	C3D-C4D-C5D-O5D
3	E	603	NAI	O4B-C4B-C5B-O5B
3	C	603	NAI	C3B-C4B-C5B-O5B
3	B	604	NAI	O4D-C1D-N1N-C2N
3	E	603	NAI	C3B-C4B-C5B-O5B
4	C	602	GTP	O4'-C4'-C5'-O5'
3	D	603	NAI	O4D-C1D-N1N-C2N
4	C	602	GTP	PA-O3A-PB-O1B
3	C	603	NAI	C2D-C1D-N1N-C6N
4	C	602	GTP	C3'-C4'-C5'-O5'
4	E	604	GTP	PA-O3A-PB-O3B
3	A	602	NAI	C5D-O5D-PN-O3
4	C	602	GTP	C5'-O5'-PA-O3A
3	F	602	NAI	C5D-O5D-PN-O3
3	F	603	NAI	C5D-O5D-PN-O3
3	E	603	NAI	C5B-O5B-PA-O3
3	F	602	NAI	C3B-C4B-C5B-O5B
4	B	603	GTP	PB-O3A-PA-O1A
3	C	603	NAI	O4D-C1D-N1N-C6N
3	E	603	NAI	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	E	602	NAI	C2D-C1D-N1N-C6N
3	C	603	NAI	C5D-O5D-PN-O1N
3	A	602	NAI	C5D-O5D-PN-O2N
3	F	603	NAI	C5D-O5D-PN-O2N
3	A	603	NAI	C5D-O5D-PN-O1N
3	E	603	NAI	C5B-O5B-PA-O2A
2	E	601	GLU	N-CA-CB-CG
3	E	602	NAI	O4D-C1D-N1N-C6N
3	A	602	NAI	O4D-C1D-N1N-C6N
3	F	603	NAI	O4D-C1D-N1N-C6N
3	F	602	NAI	PN-O3-PA-O1A
3	D	602	NAI	O4D-C1D-N1N-C6N
3	B	602	NAI	O4D-C1D-N1N-C6N
3	A	602	NAI	C2D-C1D-N1N-C6N
3	F	603	NAI	C2D-C1D-N1N-C6N
3	F	603	NAI	O4B-C4B-C5B-O5B
3	C	603	NAI	O4D-C1D-N1N-C2N
3	C	603	NAI	C2D-C1D-N1N-C2N
3	D	602	NAI	C2D-C1D-N1N-C6N
3	E	602	NAI	C2D-C1D-N1N-C2N
3	B	602	NAI	C2D-C1D-N1N-C6N
3	E	602	NAI	O4D-C1D-N1N-C2N
3	E	602	NAI	O4B-C4B-C5B-O5B
3	B	602	NAI	O4B-C4B-C5B-O5B
3	C	603	NAI	C5D-O5D-PN-O3
3	D	603	NAI	C5D-O5D-PN-O3
3	C	604	NAI	C5B-O5B-PA-O3
3	C	604	NAI	C5D-O5D-PN-O3
3	B	604	NAI	C5D-O5D-PN-O3
3	A	603	NAI	C5D-O5D-PN-O3
3	A	602	NAI	O4B-C4B-C5B-O5B
3	D	602	NAI	O4B-C4B-C5B-O5B
3	F	602	NAI	O4B-C4B-C5B-O5B
3	F	602	NAI	PN-O3-PA-O2A
3	F	603	NAI	PN-O3-PA-O2A
4	E	604	GTP	PA-O3A-PB-O1B
3	A	602	NAI	C2N-C3N-C7N-N7N
3	D	602	NAI	C5D-O5D-PN-O2N

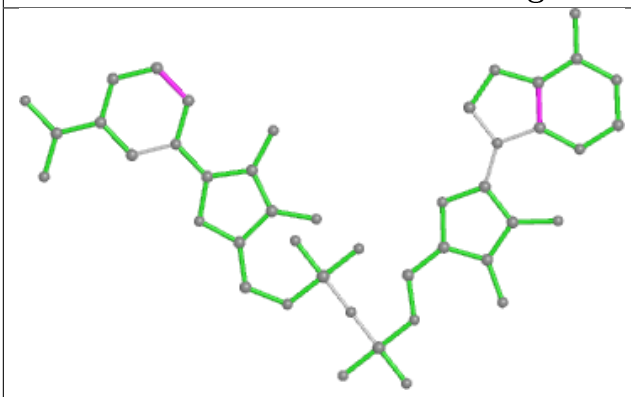
There are no ring outliers.

15 monomers are involved in 19 short contacts:

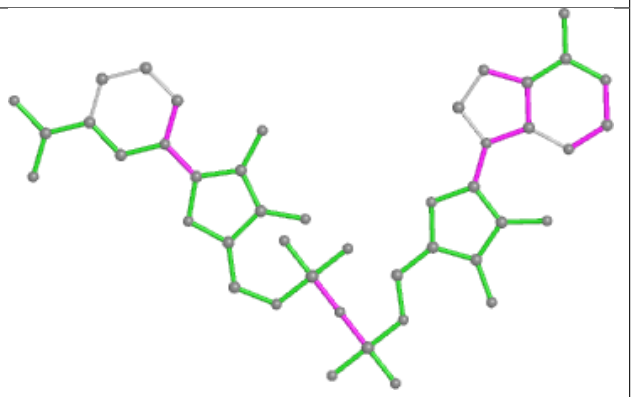
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	GLU	1	0
3	C	603	NAI	1	0
2	E	601	GLU	1	0
3	D	603	NAI	2	0
3	A	602	NAI	3	0
3	D	602	NAI	3	0
2	D	601	GLU	1	0
4	C	602	GTP	3	0
3	C	604	NAI	1	0
2	C	601	GLU	1	0
3	E	602	NAI	1	0
3	F	603	NAI	3	0
3	B	602	NAI	2	0
2	B	601	GLU	1	0
2	A	601	GLU	1	0

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

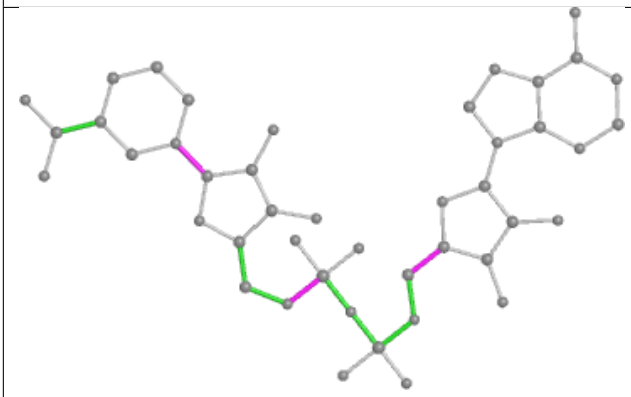
Ligand NAI C 603



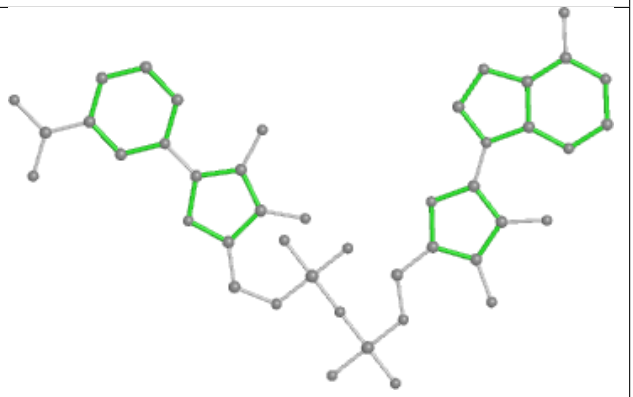
Bond lengths



Bond angles

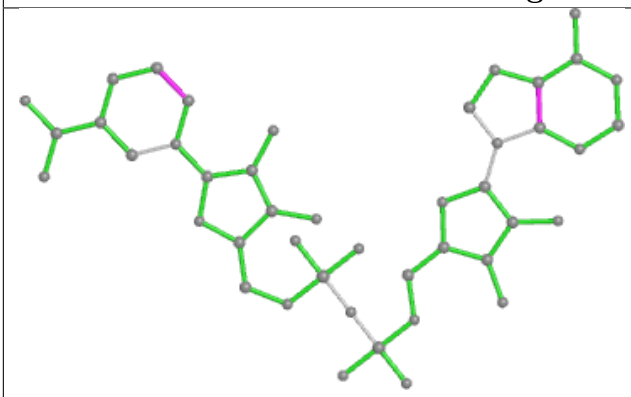


Torsions



Rings

Ligand NAI D 603



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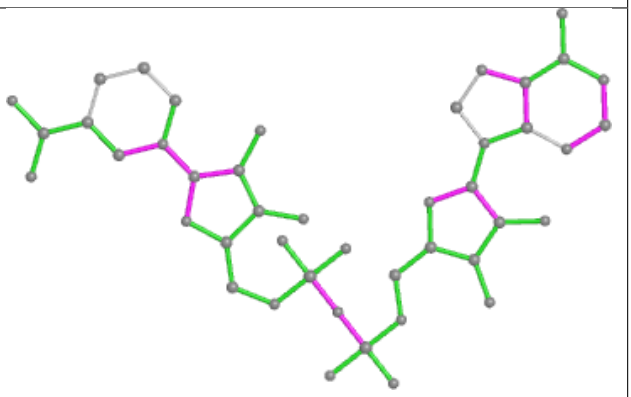

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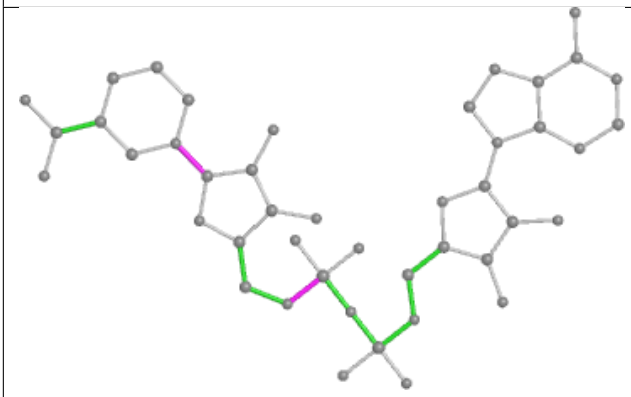

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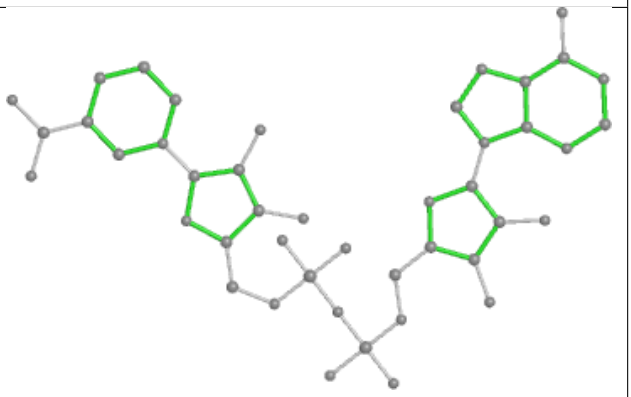
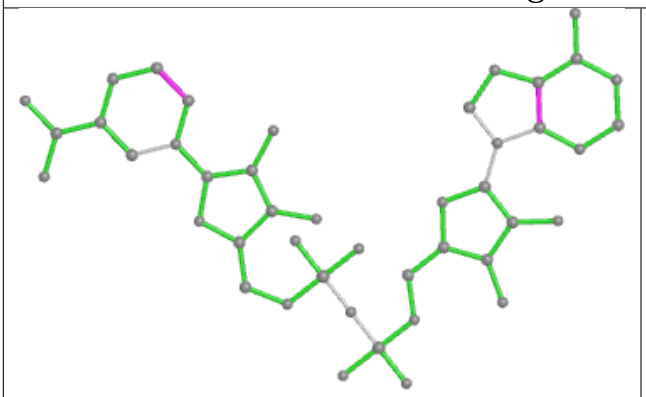


Rings

Ligand NAI A 602



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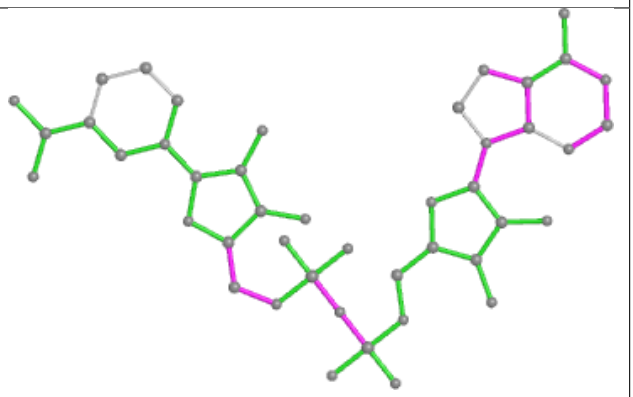

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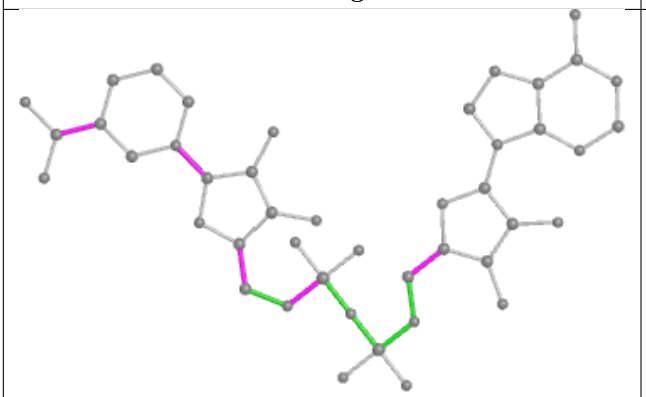

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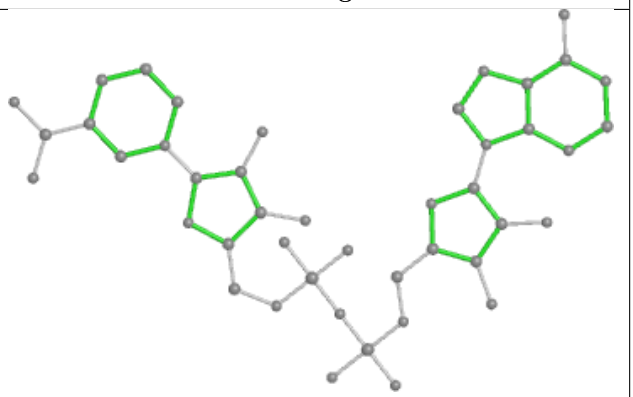
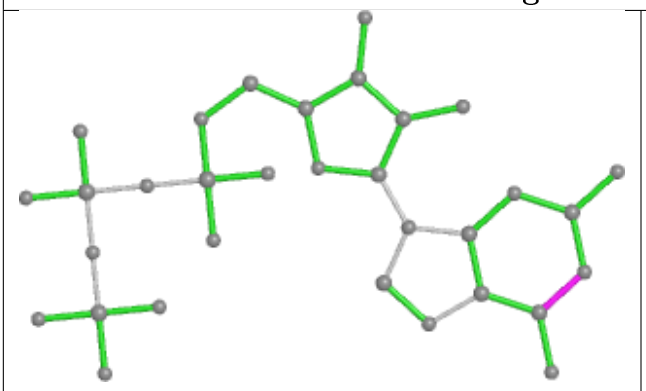


Rings

Ligand GTP D 604



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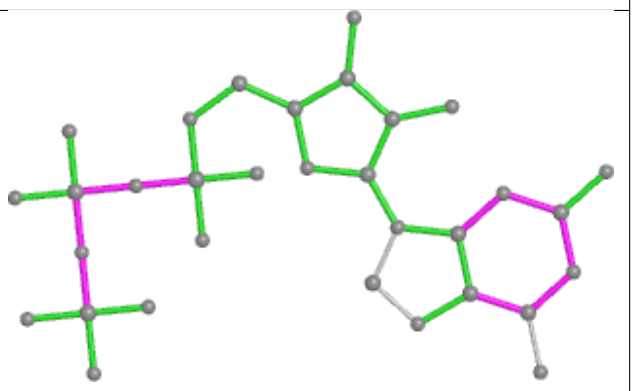

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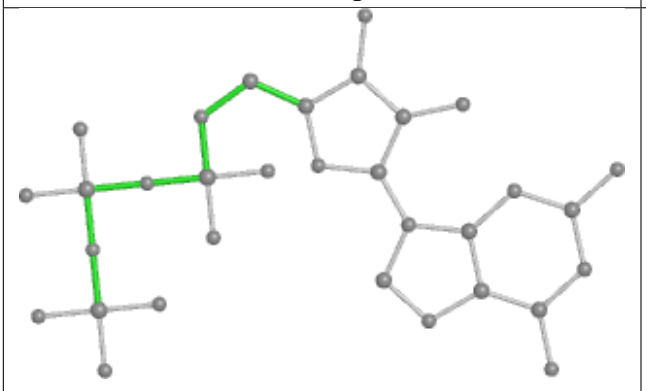

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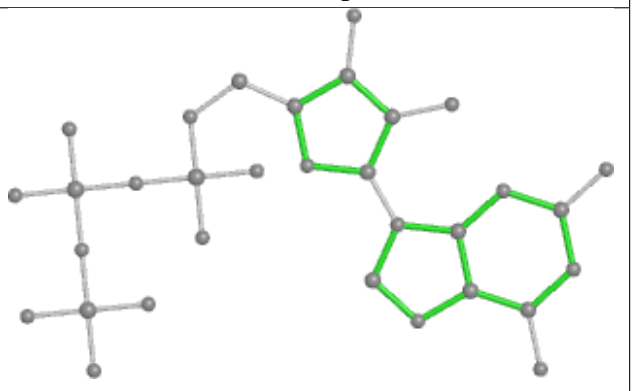
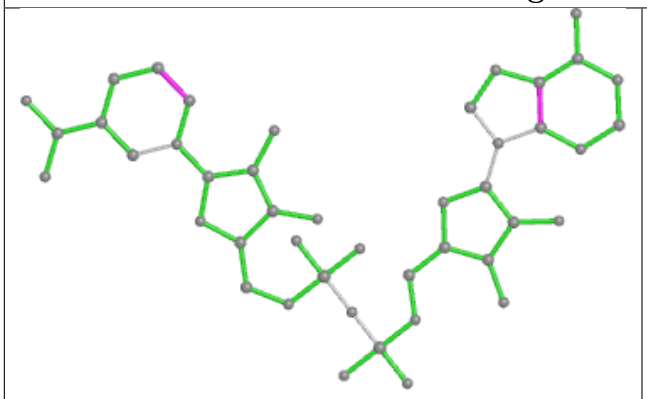


Rings

Ligand NAI D 602



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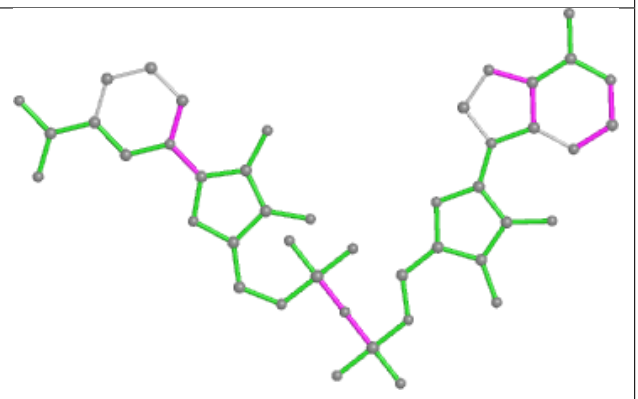

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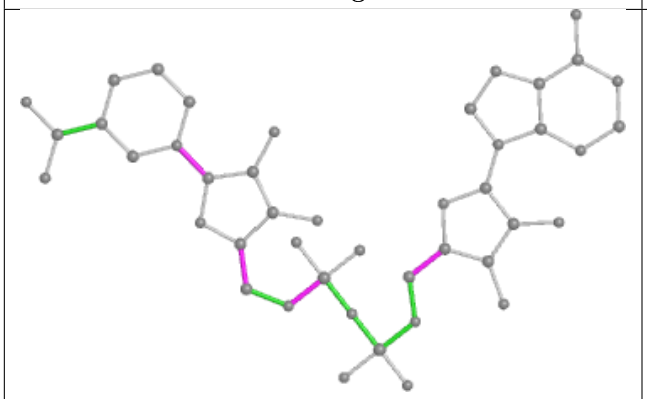

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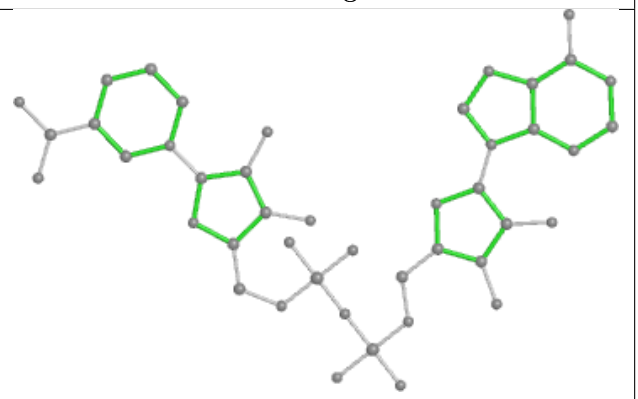
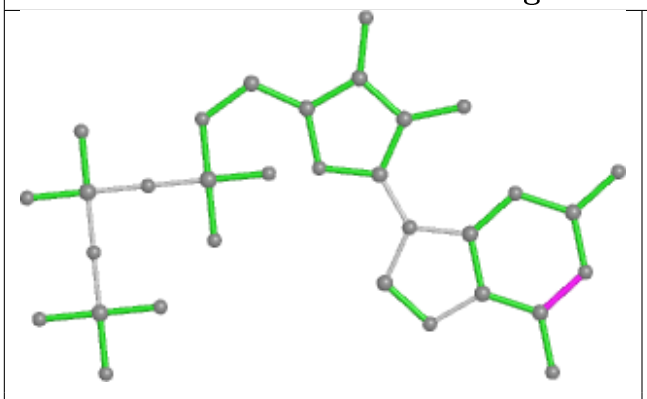


Rings

Ligand GTP A 604



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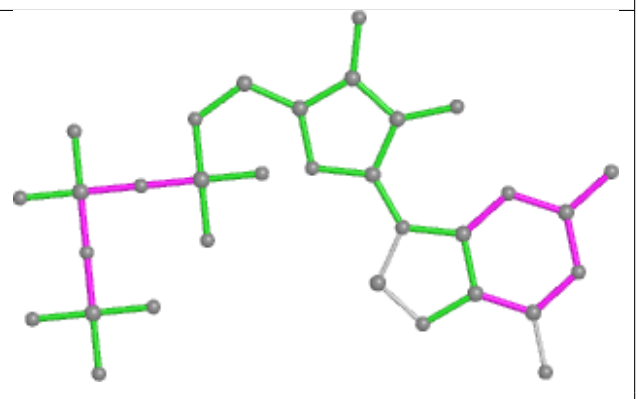

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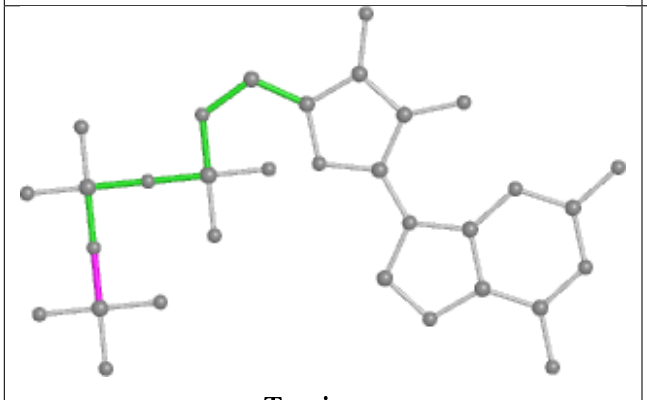

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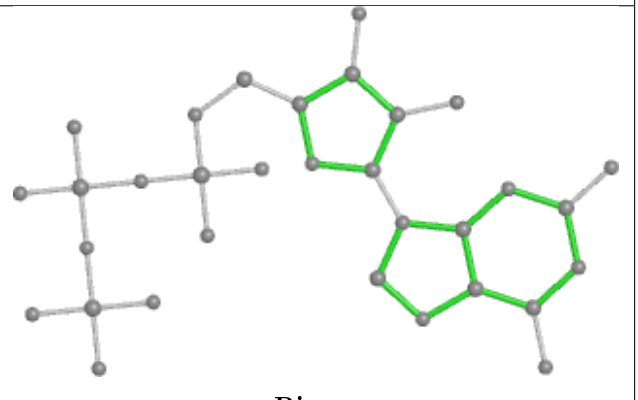
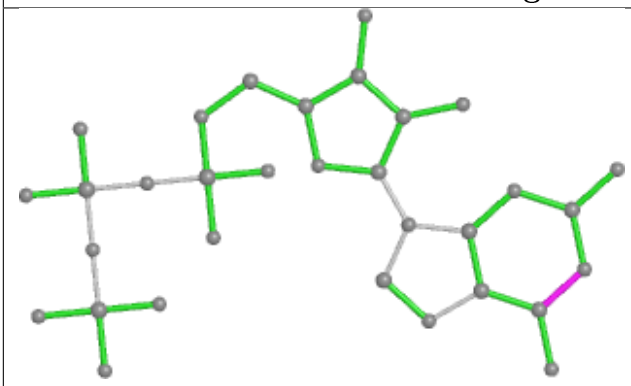


Rings

Ligand GTP C 602



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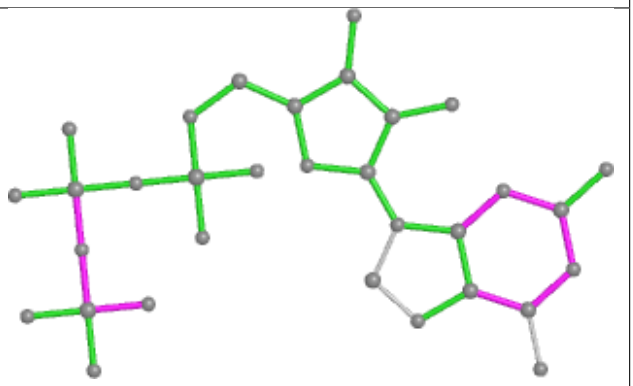

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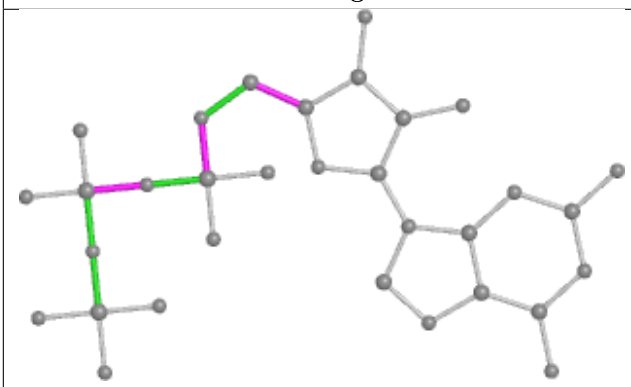

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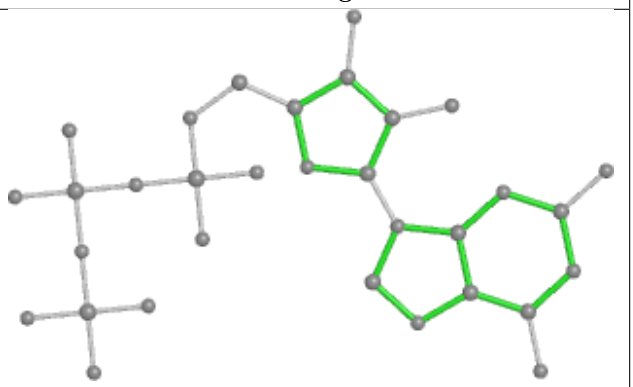
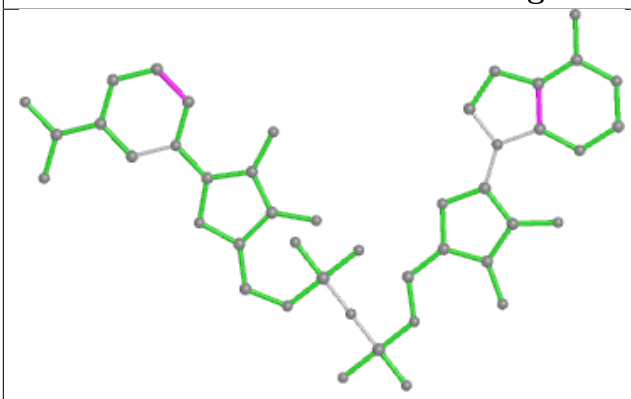


Rings

Ligand NAI C 604



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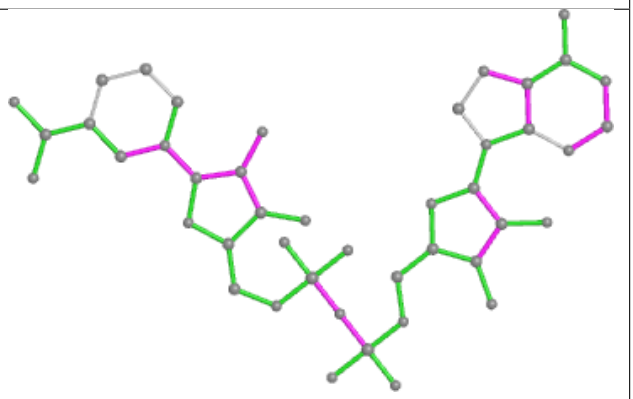

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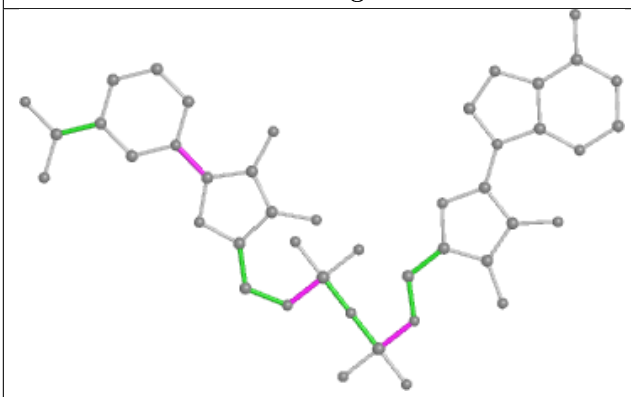

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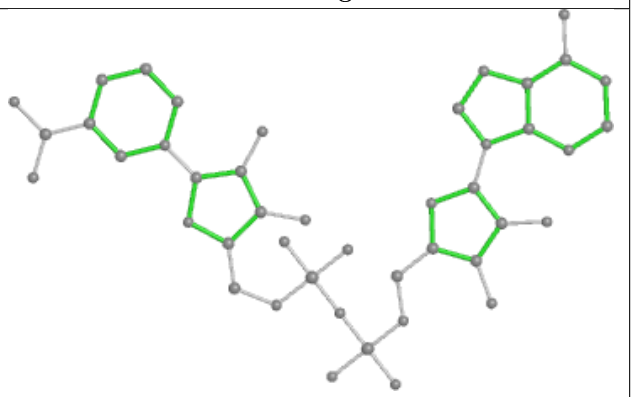
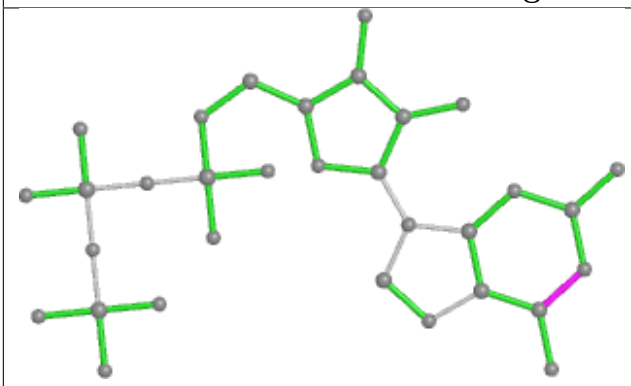


Rings

Ligand GTP B 603



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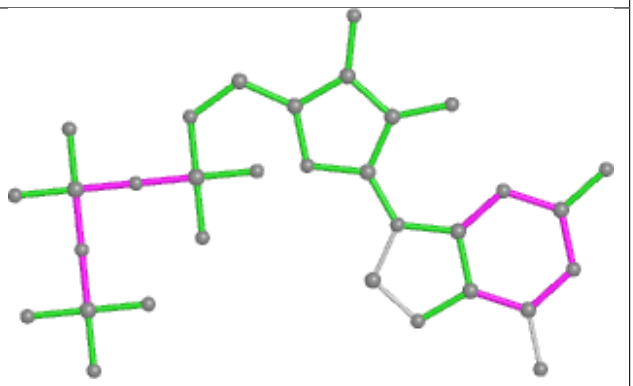

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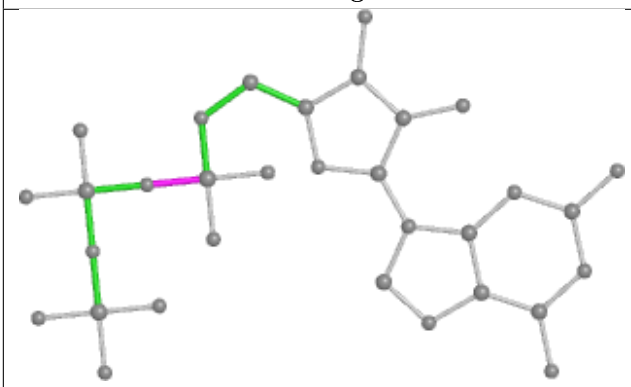

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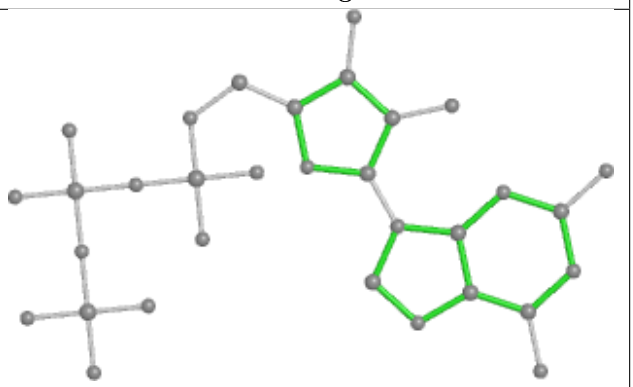
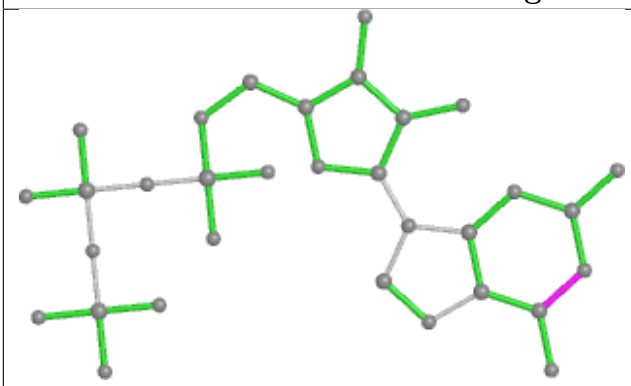


Rings

Ligand GTP F 604



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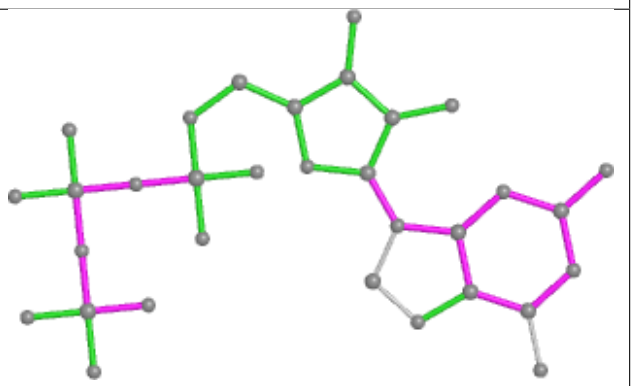

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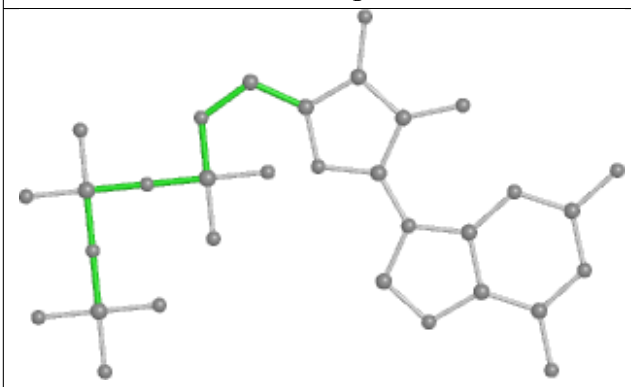

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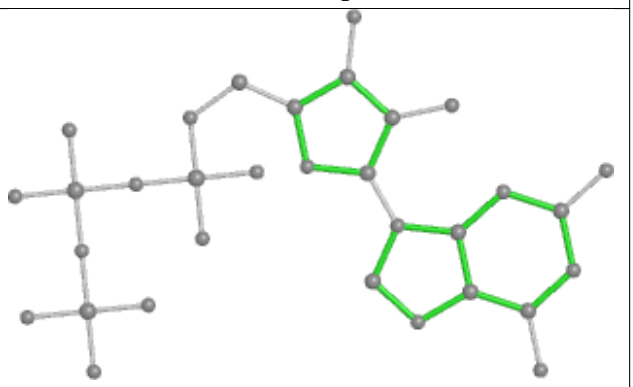
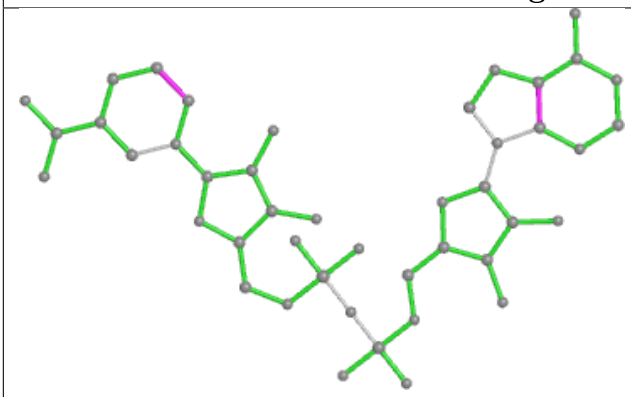


Rings

Ligand NAI E 602



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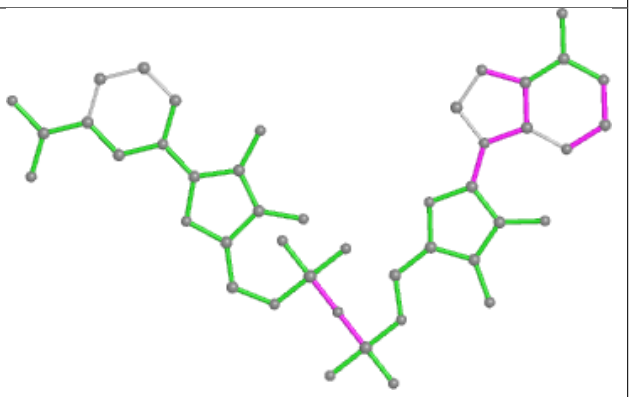

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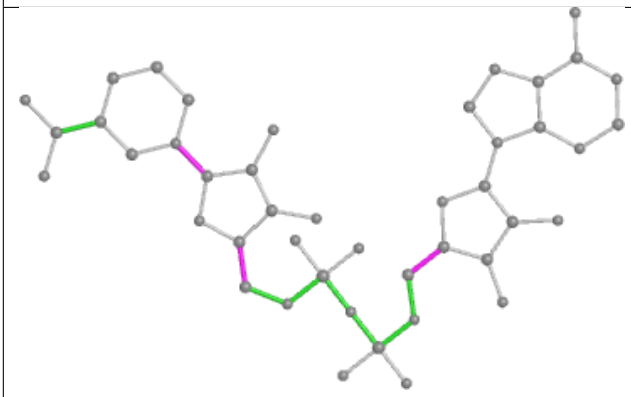

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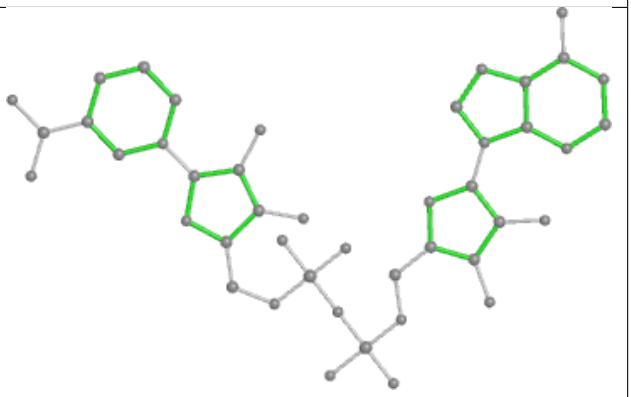
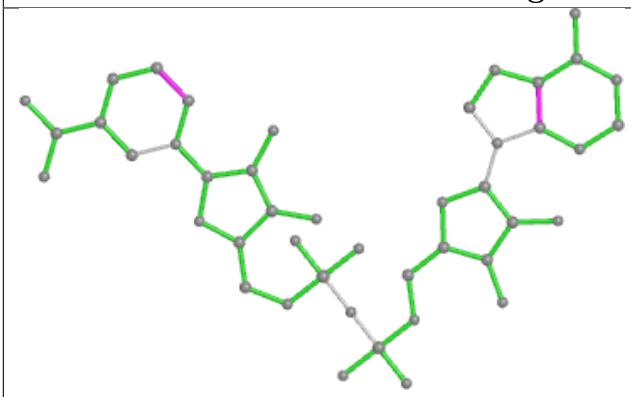


Rings

Ligand NAI B 604



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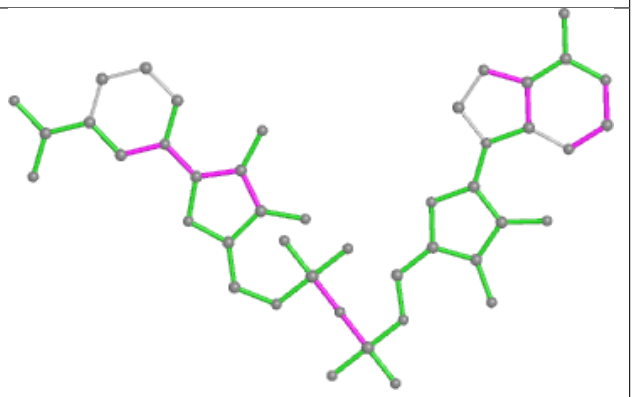
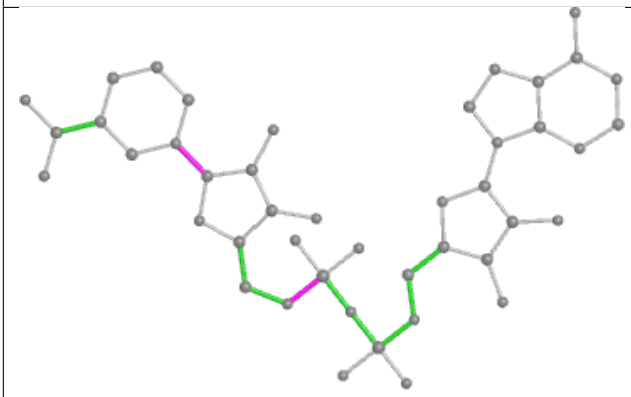


Bond angles



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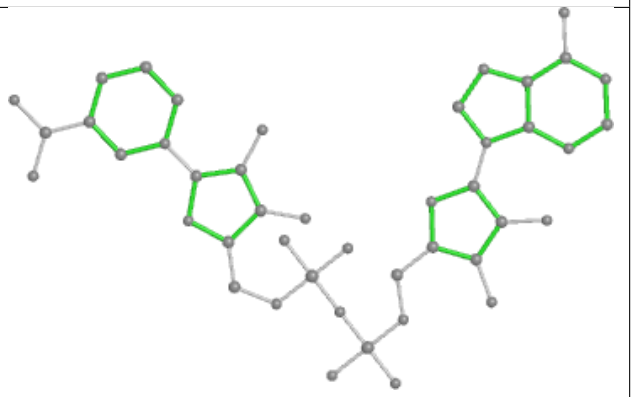
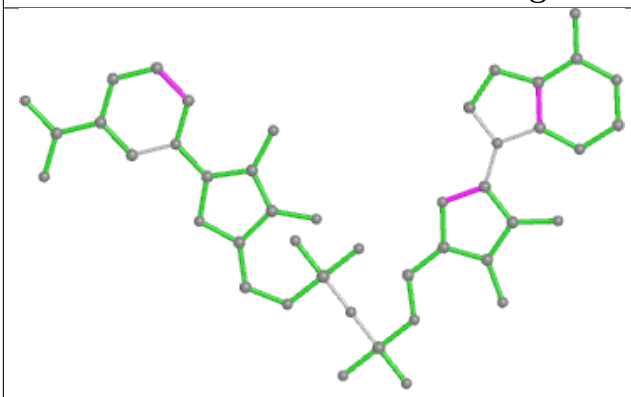


Rings

Ligand NAI F 602



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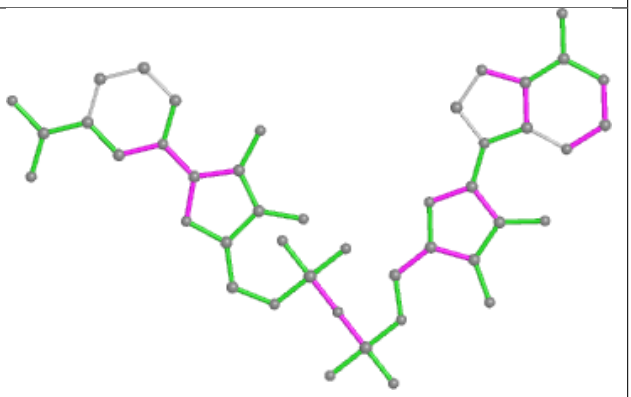
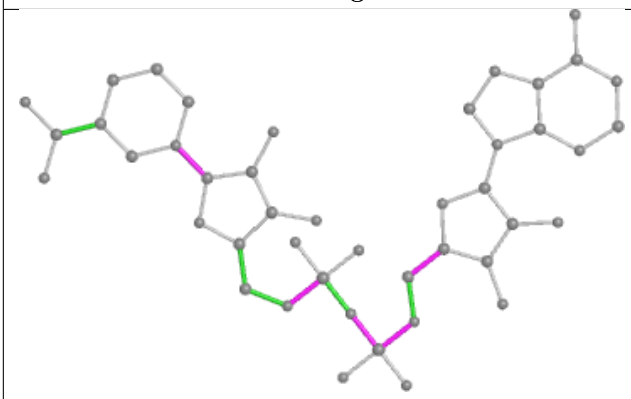
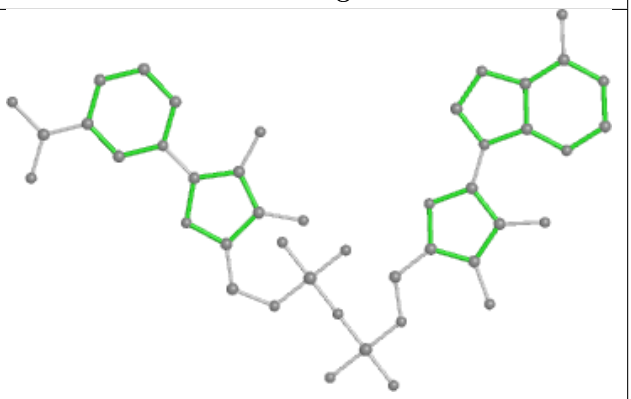


Bond angles

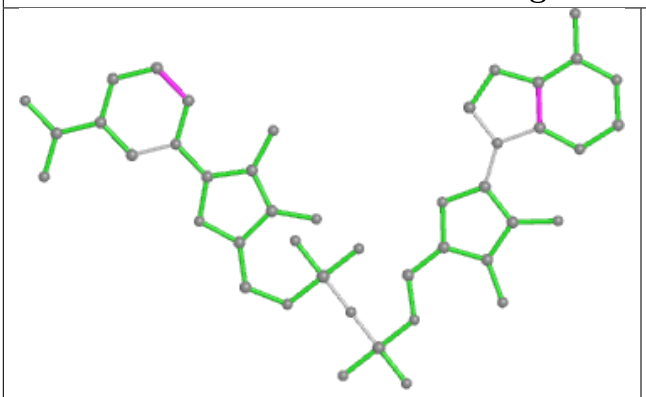


Torsions

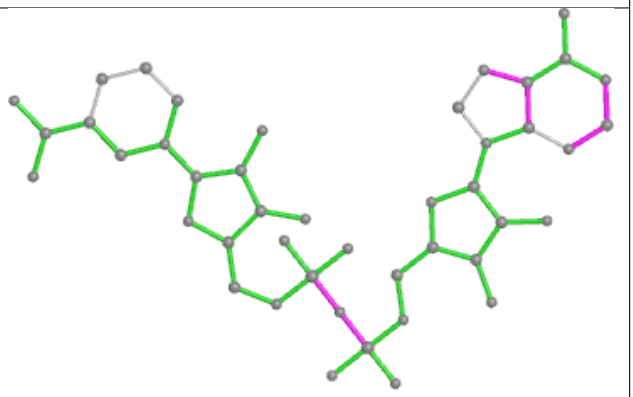


Rings

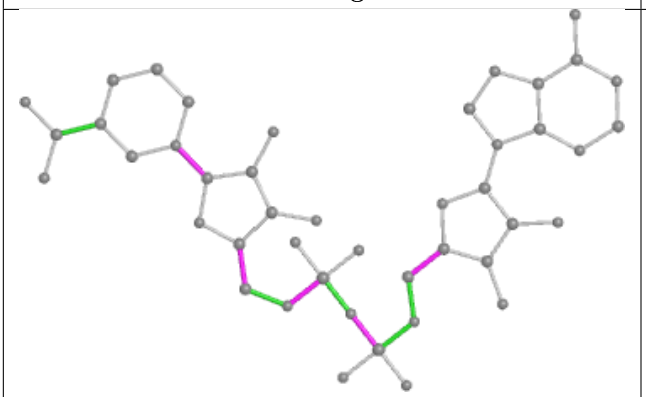
Ligand NAI F 603



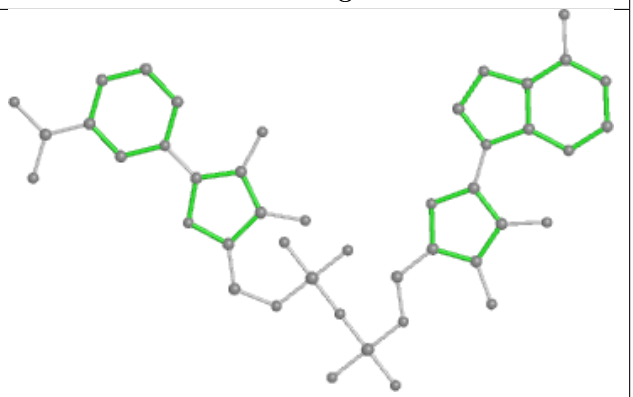
Bond lengths



Bond angles

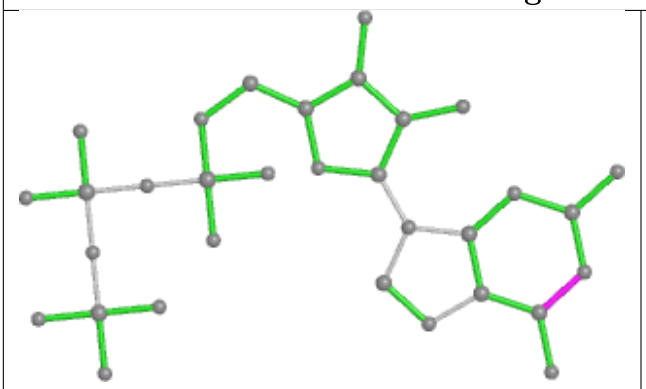


Torsions

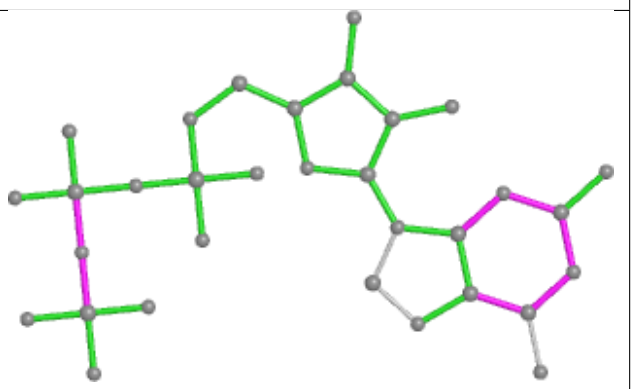


Rings

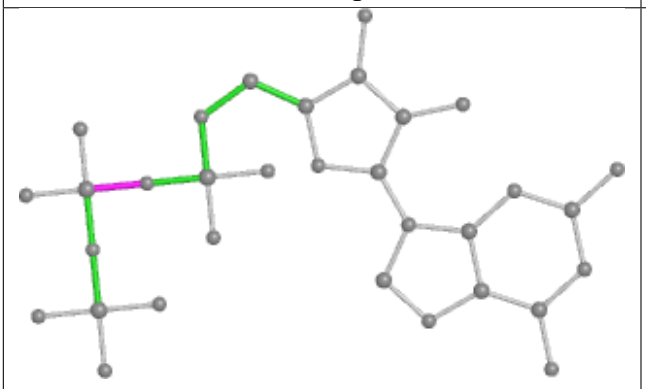
Ligand GTP E 604



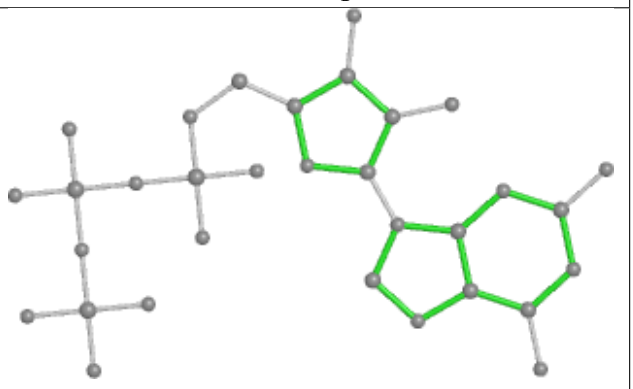
Bond lengths



Bond angles

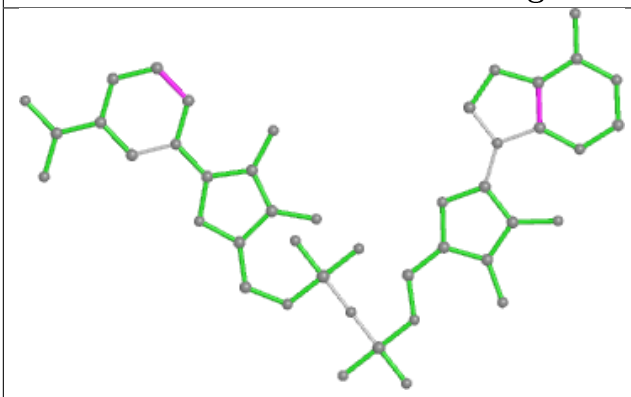


Torsions

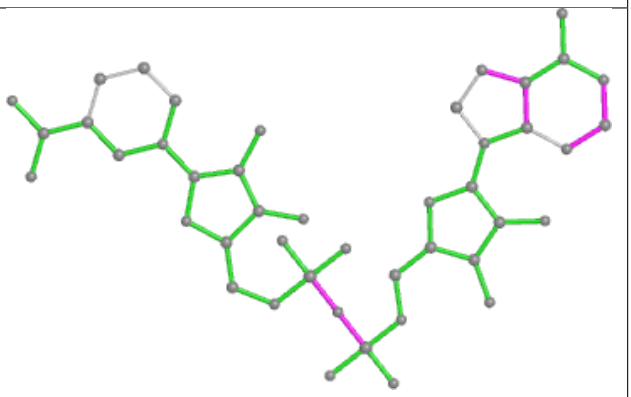


Rings

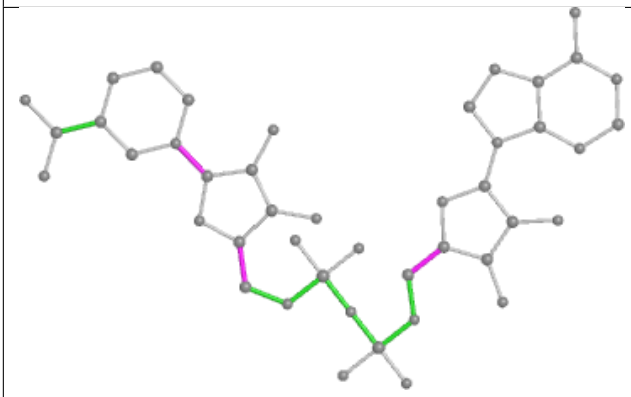
Ligand NAI B 602



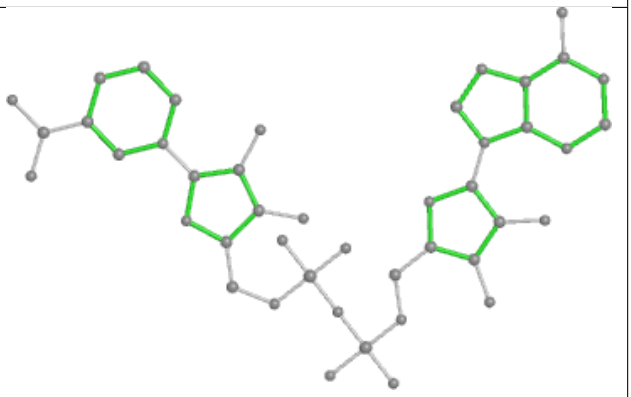
Bond lengths



Bond angles

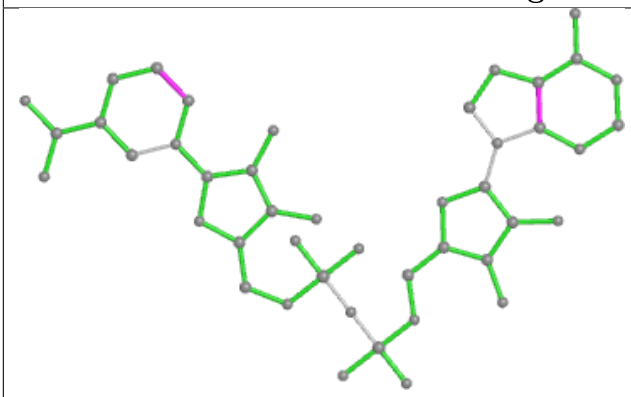


Torsions

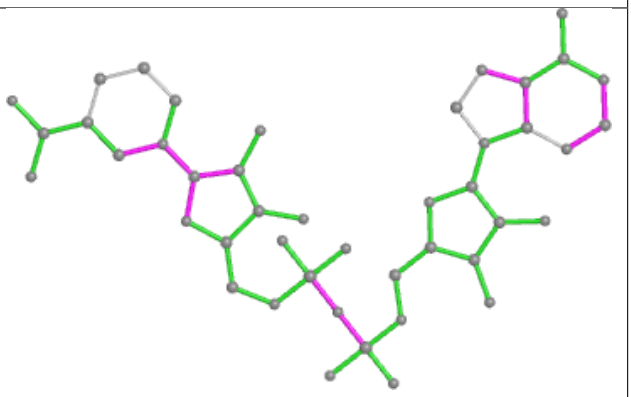


Rings

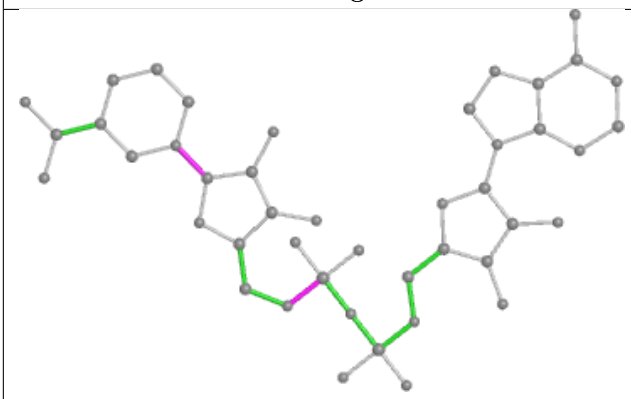
Ligand NAI A 603



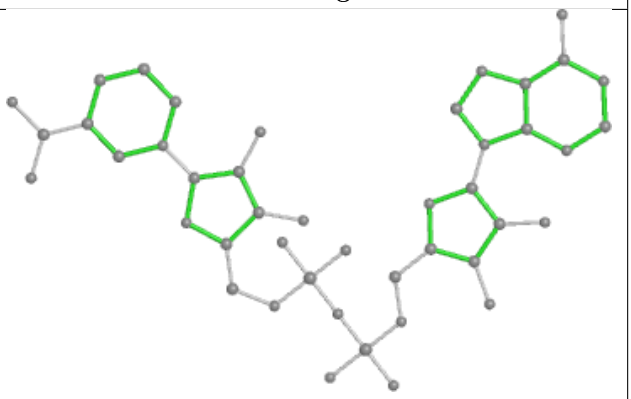
Bond lengths



Bond angles

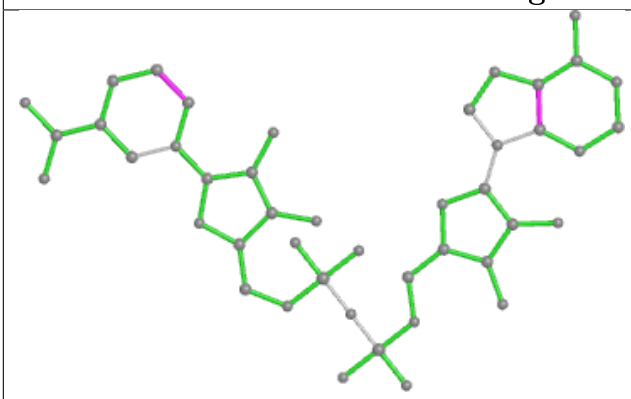


Torsions

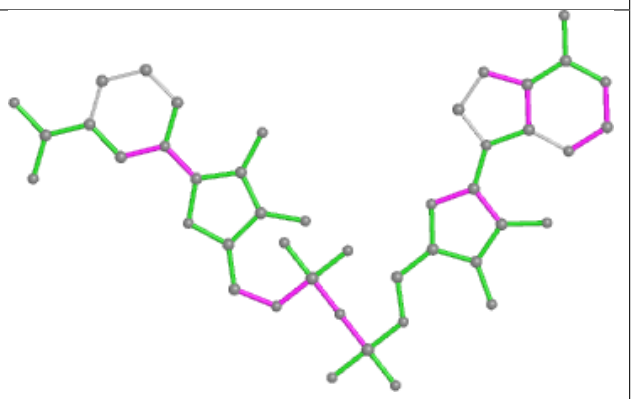


Rings

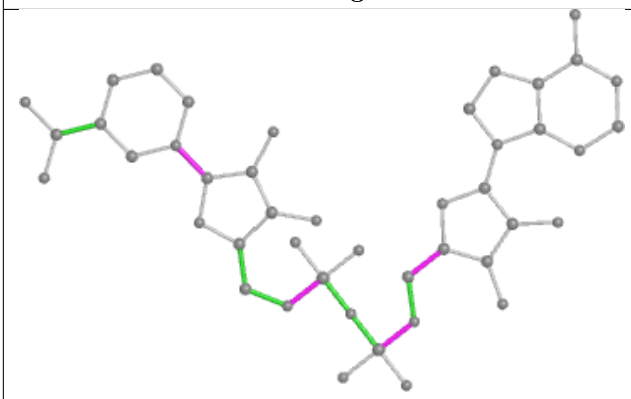
Ligand NAI E 603



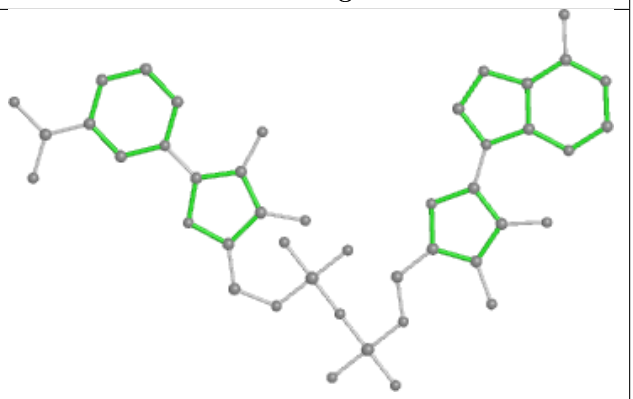
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	501/501 (100%)	0.22	36 (7%) 15 16	37, 61, 98, 132	0
1	B	501/501 (100%)	0.17	26 (5%) 27 29	35, 58, 98, 124	0
1	C	501/501 (100%)	0.27	37 (7%) 14 15	36, 61, 100, 132	0
1	D	501/501 (100%)	0.33	46 (9%) 9 9	36, 63, 105, 129	0
1	E	501/501 (100%)	0.33	46 (9%) 9 9	35, 66, 107, 123	0
1	F	501/501 (100%)	0.22	44 (8%) 10 10	34, 58, 99, 127	0
All	All	3006/3006 (100%)	0.26	235 (7%) 13 13	34, 61, 104, 132	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	13.5
1	D	1	ALA	11.1
1	C	1	ALA	10.5
1	A	1	ALA	10.4
1	E	1	ALA	8.1
1	F	1	ALA	7.1
1	A	424	HIS	7.1
1	C	3	ARG	5.9
1	F	424	HIS	5.8
1	D	3	ARG	5.8
1	D	424	HIS	5.6
1	D	425	GLY	5.5
1	E	309	ILE	5.5
1	B	424	HIS	5.5
1	F	425	GLY	5.4
1	D	37	THR	5.4
1	A	4	GLU	5.3
1	F	37	THR	5.3
1	C	423	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	426	GLY	5.2
1	E	424	HIS	5.2
1	E	243	GLY	5.1
1	B	501	THR	5.0
1	D	2	ASP	5.0
1	B	2	ASP	4.9
1	E	345	ALA	4.9
1	A	425	GLY	4.8
1	E	37	THR	4.7
1	D	35	ARG	4.7
1	A	37	THR	4.6
1	C	4	GLU	4.6
1	A	2	ASP	4.6
1	B	3	ARG	4.6
1	B	4	GLU	4.6
1	B	426	GLY	4.5
1	D	423	LYS	4.5
1	F	2	ASP	4.5
1	B	230	ALA	4.5
1	E	501	THR	4.4
1	A	423	LYS	4.3
1	E	3	ARG	4.3
1	A	345	ALA	4.3
1	B	33	LYS	4.2
1	A	35	ARG	4.2
1	B	35	ARG	4.2
1	B	37	THR	4.2
1	F	423	LYS	4.1
1	D	4	GLU	4.1
1	D	422	GLY	4.1
1	D	36	GLU	4.0
1	F	33	LYS	4.0
1	C	345	ALA	4.0
1	E	344	ILE	3.9
1	C	2	ASP	3.9
1	E	302	LEU	3.9
1	E	35	ARG	3.9
1	B	323	ILE	3.8
1	B	42	ARG	3.8
1	E	367	VAL	3.8
1	E	368	ILE	3.8
1	C	298	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	3	ARG	3.7
1	E	281	TRP	3.7
1	C	37	THR	3.7
1	E	500	PHE	3.7
1	E	323	ILE	3.7
1	D	302	LEU	3.7
1	C	425	GLY	3.7
1	D	323	ILE	3.6
1	B	32	LEU	3.6
1	D	297	GLN	3.6
1	F	4	GLU	3.5
1	C	40	GLN	3.5
1	E	371	LEU	3.5
1	A	501	THR	3.5
1	E	373	LEU	3.4
1	C	323	ILE	3.4
1	F	34	THR	3.4
1	E	2	ASP	3.4
1	E	5	ASP	3.4
1	E	285	GLY	3.3
1	A	323	ILE	3.3
1	D	244	ASP	3.3
1	C	424	HIS	3.3
1	D	243	GLY	3.2
1	F	35	ARG	3.2
1	E	423	LYS	3.2
1	F	323	ILE	3.2
1	C	34	THR	3.2
1	E	297	GLN	3.1
1	F	368	ILE	3.1
1	D	6	ASP	3.1
1	C	281	TRP	3.1
1	D	41	LYS	3.1
1	D	39	GLU	3.1
1	E	38	GLU	3.1
1	B	234	SER	3.0
1	C	32	LEU	3.0
1	D	31	ASP	3.0
1	A	322	LEU	3.0
1	C	373	LEU	3.0
1	B	31	ASP	3.0
1	A	33	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	501	THR	3.0
1	A	42	ARG	3.0
1	F	297	GLN	2.9
1	C	294	PHE	2.9
1	A	281	TRP	2.9
1	A	3	ARG	2.9
1	F	240	PRO	2.8
1	D	40	GLN	2.8
1	F	298	HIS	2.8
1	D	294	PHE	2.8
1	F	294	PHE	2.8
1	F	348	ALA	2.8
1	C	369	PRO	2.8
1	F	219	VAL	2.8
1	D	30	GLU	2.8
1	B	345	ALA	2.8
1	F	234	SER	2.8
1	D	5	ASP	2.8
1	A	346	GLU	2.7
1	F	345	ALA	2.7
1	F	374	ASN	2.7
1	B	5	ASP	2.7
1	E	33	LYS	2.7
1	F	8	ASN	2.7
1	E	4	GLU	2.7
1	A	368	ILE	2.7
1	E	308	LYS	2.7
1	F	249	VAL	2.7
1	D	472	ASN	2.7
1	C	368	ILE	2.7
1	C	240	PRO	2.7
1	A	297	GLN	2.7
1	D	373	LEU	2.6
1	C	297	GLN	2.6
1	F	36	GLU	2.6
1	A	34	THR	2.6
1	F	347	GLY	2.6
1	C	309	ILE	2.6
1	C	296	LEU	2.6
1	F	371	LEU	2.6
1	A	373	LEU	2.6
1	C	321	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	346	GLU	2.6
1	A	241	GLY	2.6
1	A	5	ASP	2.6
1	D	284	ASP	2.6
1	D	298	HIS	2.5
1	E	298	HIS	2.5
1	A	434	ALA	2.5
1	C	35	ARG	2.5
1	E	31	ASP	2.5
1	E	322	LEU	2.5
1	B	322	LEU	2.5
1	E	40	GLN	2.5
1	C	5	ASP	2.5
1	A	296	LEU	2.5
1	F	40	GLN	2.5
1	E	234	SER	2.5
1	B	347	GLY	2.5
1	A	39	GLU	2.4
1	A	344	ILE	2.4
1	F	39	GLU	2.4
1	C	249	VAL	2.4
1	E	374	ASN	2.4
1	A	7	PRO	2.4
1	F	248	ALA	2.4
1	D	311	GLU	2.4
1	C	293	ASP	2.4
1	F	7	PRO	2.4
1	C	344	ILE	2.4
1	F	325	ALA	2.4
1	A	40	GLN	2.4
1	A	347	GLY	2.4
1	F	367	VAL	2.4
1	C	302	LEU	2.4
1	D	347	GLY	2.3
1	C	324	PRO	2.3
1	B	348	ALA	2.3
1	C	33	LYS	2.3
1	C	322	LEU	2.3
1	F	32	LEU	2.3
1	E	299	GLY	2.3
1	D	38	GLU	2.3
1	F	5	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	30	GLU	2.3
1	D	249	VAL	2.3
1	F	255	VAL	2.3
1	E	230	ALA	2.3
1	B	235	ILE	2.2
1	A	31	ASP	2.2
1	B	344	ILE	2.2
1	D	296	LEU	2.2
1	F	373	LEU	2.2
1	F	6	ASP	2.2
1	E	369	PRO	2.2
1	C	42	ARG	2.2
1	A	369	PRO	2.2
1	E	366	MET	2.2
1	E	39	GLU	2.2
1	D	501	THR	2.2
1	E	34	THR	2.2
1	B	321	ILE	2.2
1	B	422	GLY	2.2
1	D	32	LEU	2.2
1	D	345	ALA	2.1
1	E	426	GLY	2.1
1	C	248	ALA	2.1
1	D	34	THR	2.1
1	E	343	ILE	2.1
1	E	244	ASP	2.1
1	D	285	GLY	2.1
1	F	344	ILE	2.1
1	B	249	VAL	2.1
1	F	434	ALA	2.1
1	C	371	LEU	2.1
1	D	371	LEU	2.1
1	E	311	GLU	2.1
1	C	343	ILE	2.1
1	D	362	GLU	2.1
1	A	426	GLY	2.1
1	D	426	GLY	2.1
1	D	7	PRO	2.0
1	A	237	GLY	2.0
1	F	243	GLY	2.0
1	D	466	ARG	2.0
1	E	240	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	6	ASP	2.0
1	F	31	ASP	2.0
1	D	308	LYS	2.0
1	D	325	ALA	2.0
1	D	322	LEU	2.0
1	E	301	ILE	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
2	GLU	C	601	10/10	0.92	0.21	47,56,69,69	0
3	NAI	A	603	44/44	0.92	0.15	46,57,77,93	14
2	GLU	B	601	10/10	0.92	0.21	53,61,63,66	0
2	GLU	A	601	10/10	0.92	0.26	55,65,76,76	0
3	NAI	B	604	44/44	0.93	0.14	34,59,77,95	12
3	NAI	E	603	44/44	0.93	0.14	35,55,86,101	12
2	GLU	E	601	10/10	0.93	0.19	53,61,69,72	0
3	NAI	A	602	44/44	0.94	0.15	45,59,72,78	0
3	NAI	F	602	44/44	0.94	0.15	44,59,81,89	13
2	GLU	D	601	10/10	0.94	0.15	59,69,77,78	0
3	NAI	C	604	44/44	0.94	0.13	34,57,79,99	13
3	NAI	D	603	44/44	0.94	0.15	43,60,75,98	16
3	NAI	E	602	44/44	0.94	0.14	51,71,89,93	0
3	NAI	C	603	44/44	0.95	0.14	48,64,78,86	0
2	GLU	F	601	10/10	0.95	0.17	51,62,74,74	0
3	NAI	D	602	44/44	0.95	0.16	52,70,91,97	0
3	NAI	B	602	44/44	0.95	0.15	36,52,65,90	0

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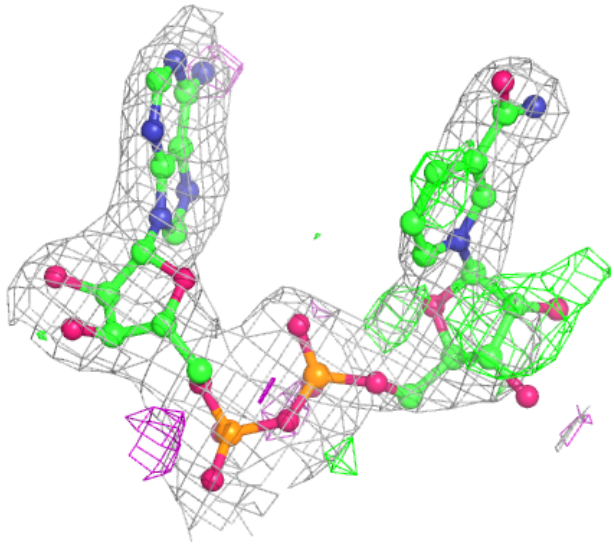
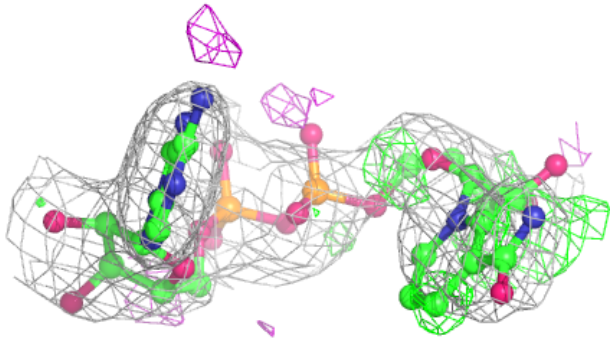
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAI	F	603	44/44	0.96	0.15	43,56,69,72	0
4	GTP	D	604	32/32	0.96	0.14	47,66,91,92	0
4	GTP	F	604	32/32	0.98	0.11	40,59,68,75	0
4	GTP	A	604	32/32	0.98	0.14	53,68,79,80	0
4	GTP	E	604	32/32	0.98	0.14	55,69,82,90	0
4	GTP	C	602	32/32	0.98	0.12	49,68,81,88	0
4	GTP	B	603	32/32	0.99	0.10	44,54,67,71	0

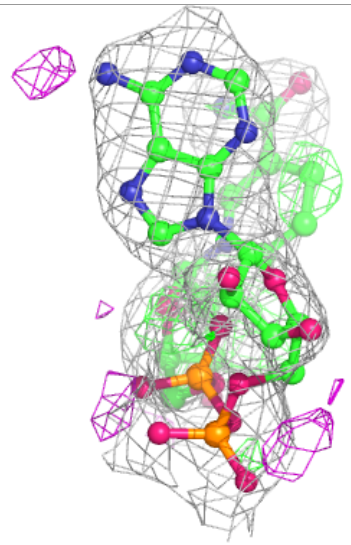
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI 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)

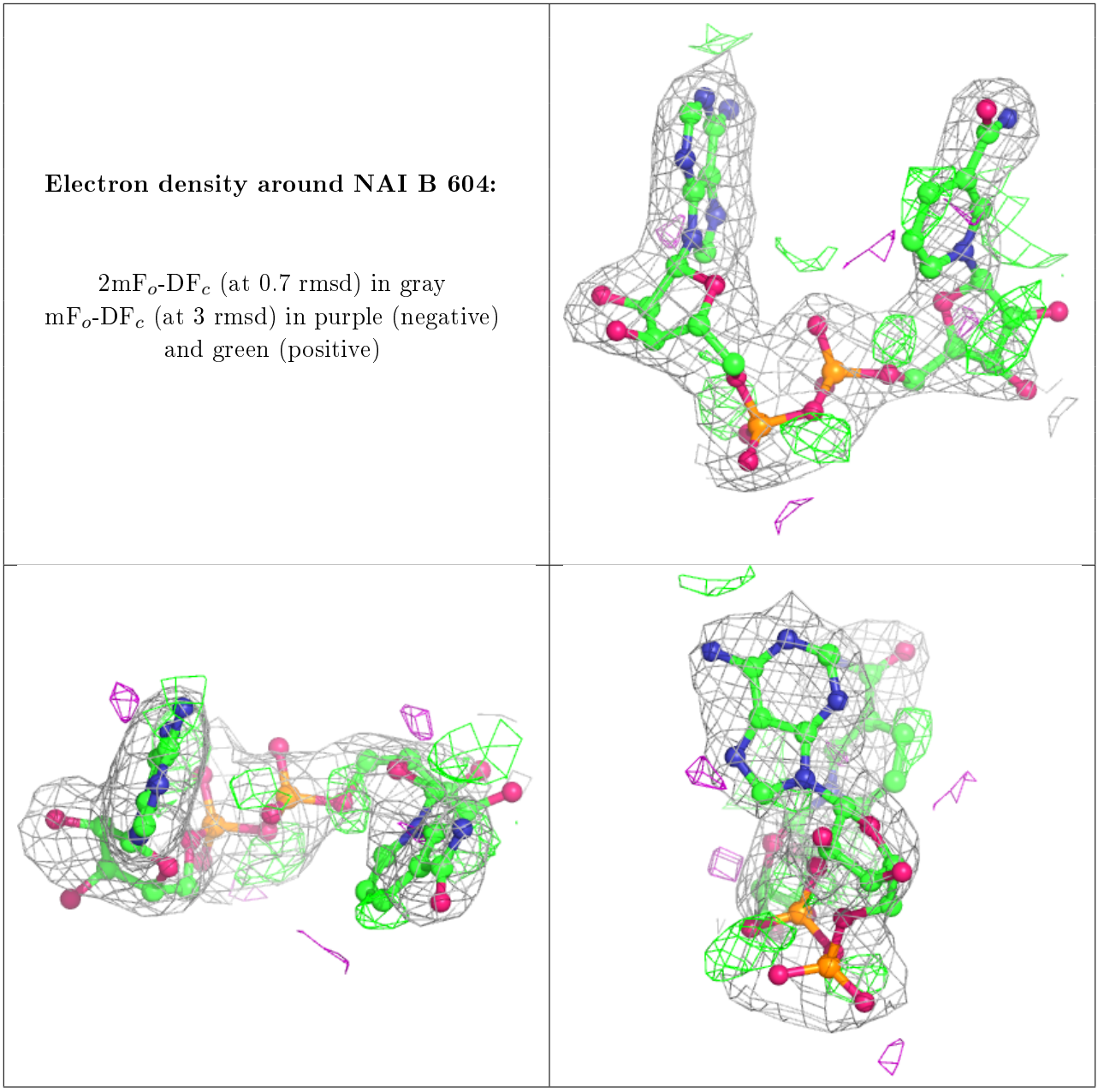






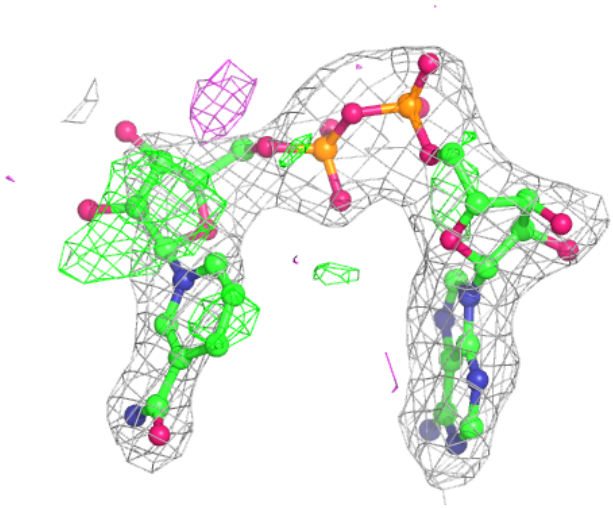
Electron density around NAI B 604:

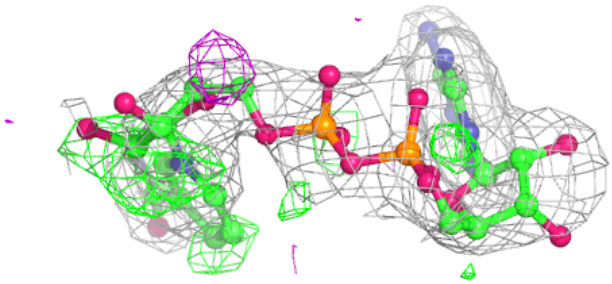
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

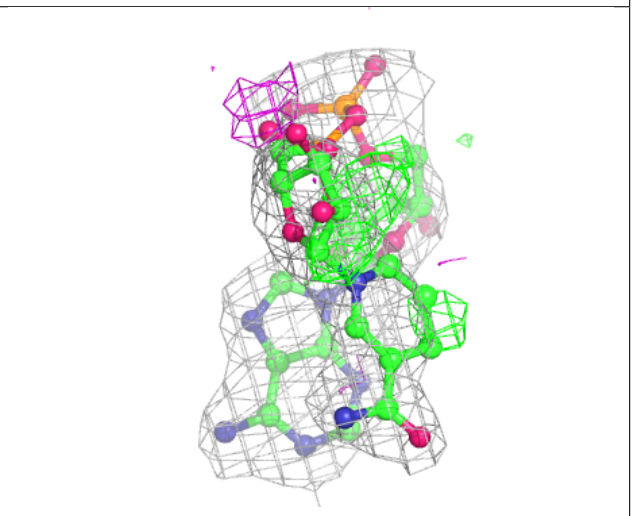


Electron density around NAI E 603:

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

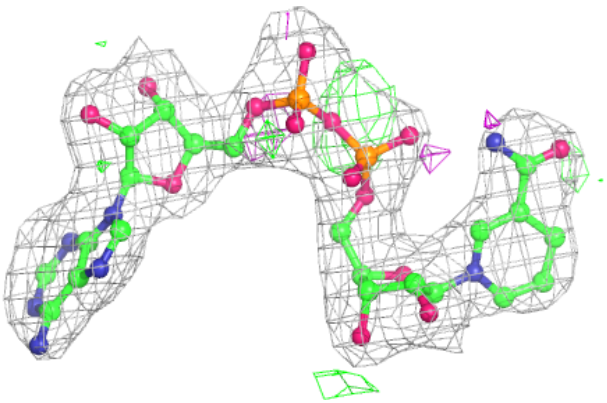


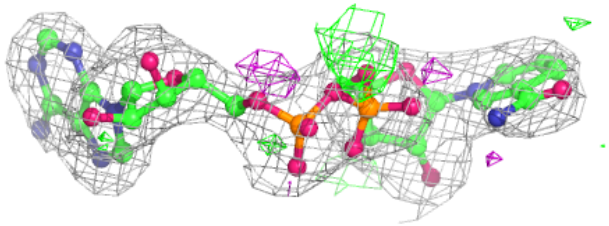


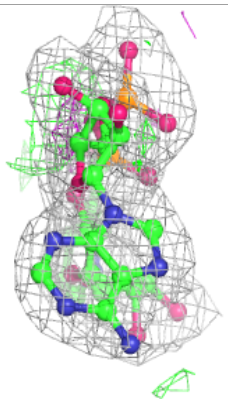


Electron density around NAI A 602:

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

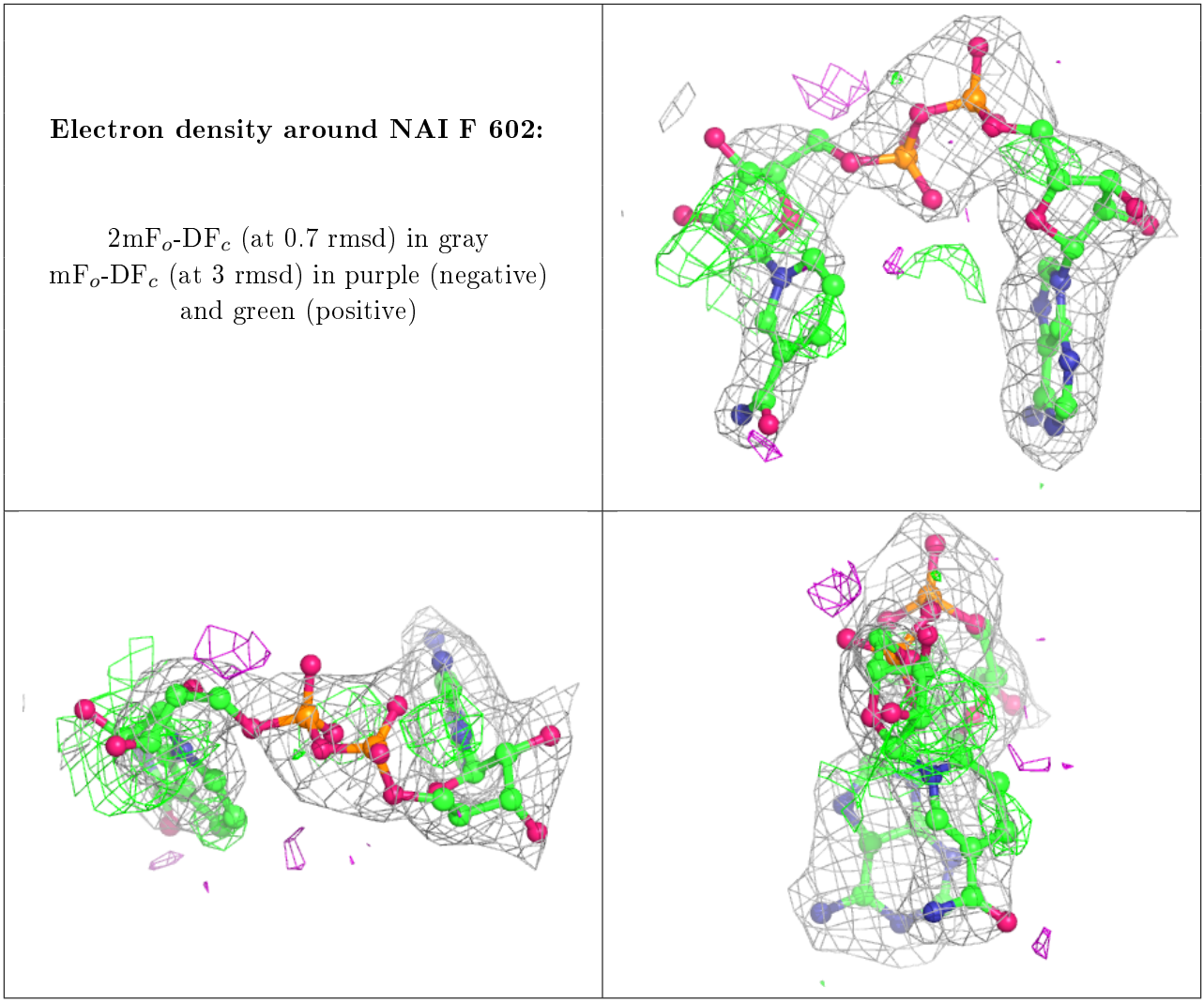






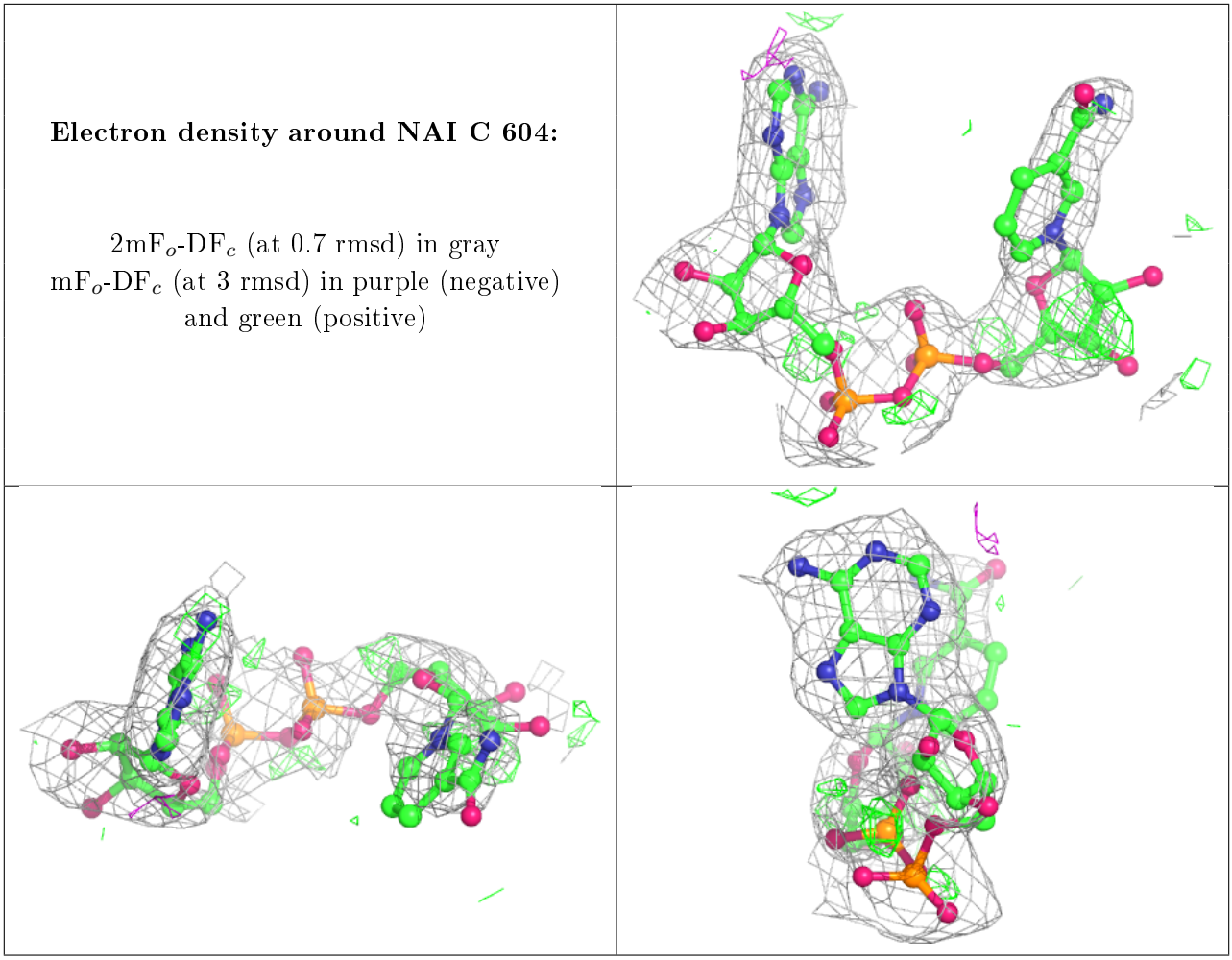
Electron density around NAI F 602:

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



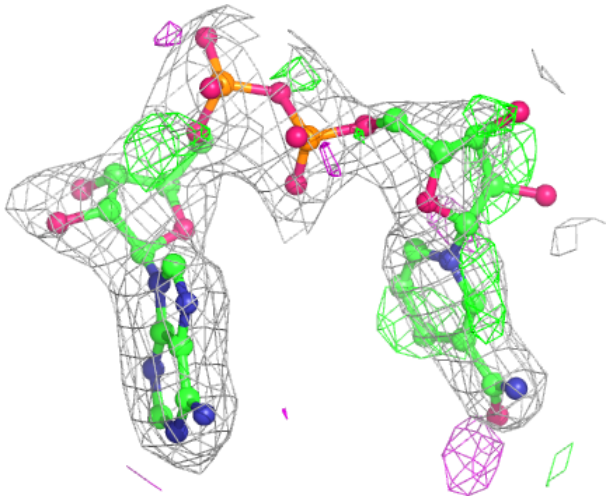
Electron density around NAI C 604:

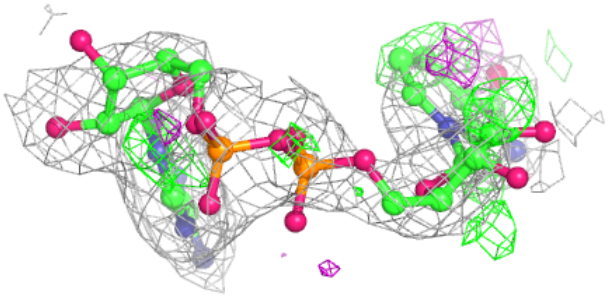
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

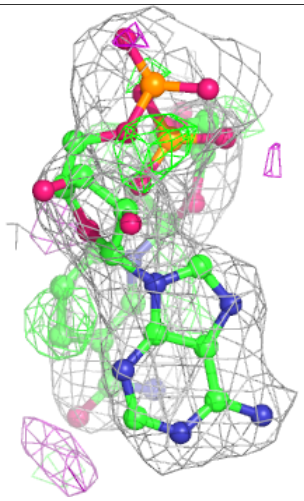


Electron density around NAI D 603:

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

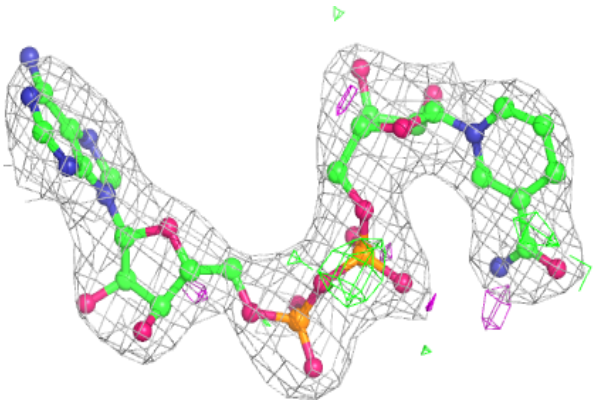


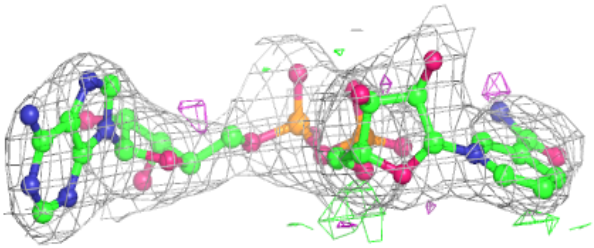


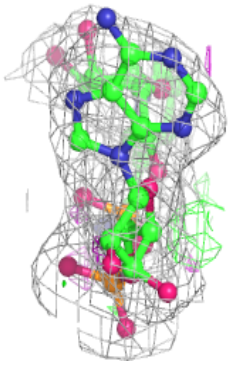


Electron density around NAI E 602:

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

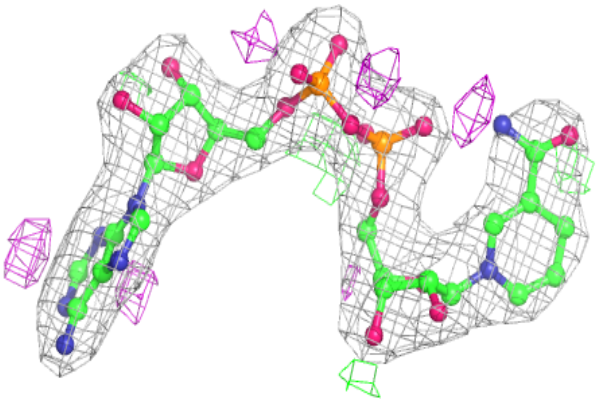


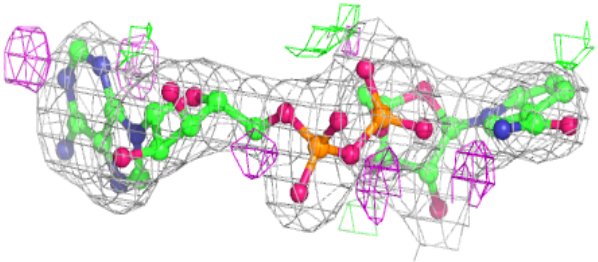


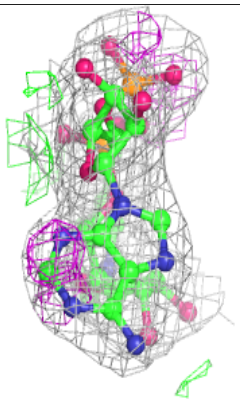


Electron density around NAI C 603:

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

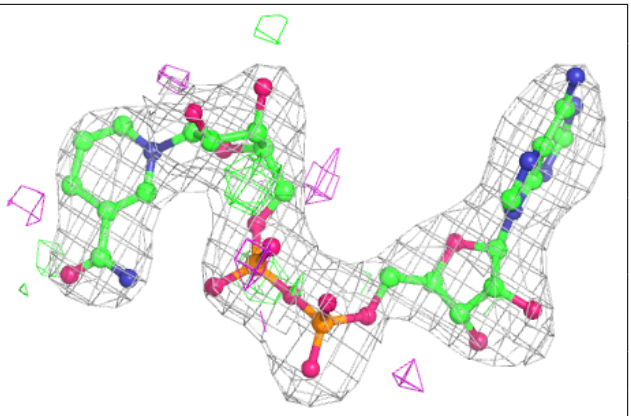


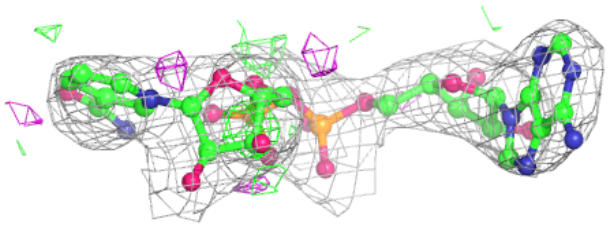


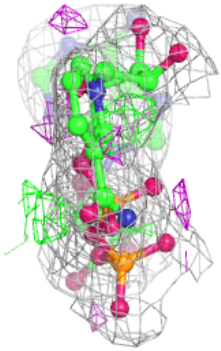


Electron density around NAI D 602:

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

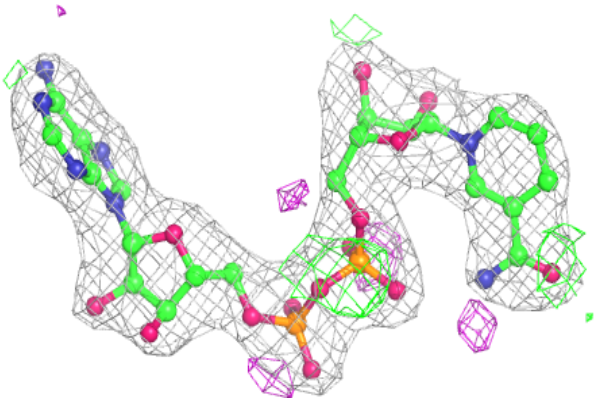


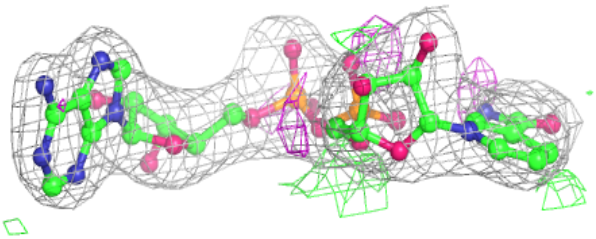


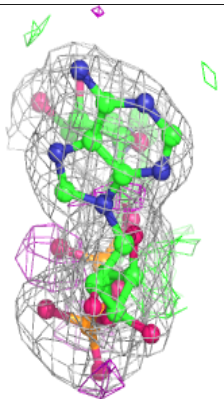


Electron density around NAI B 602:

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

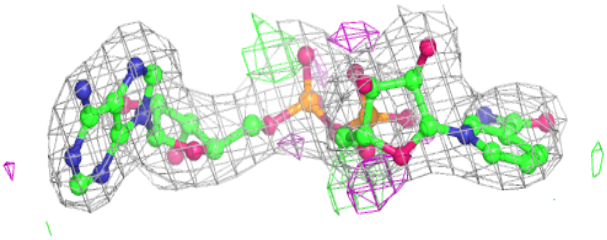


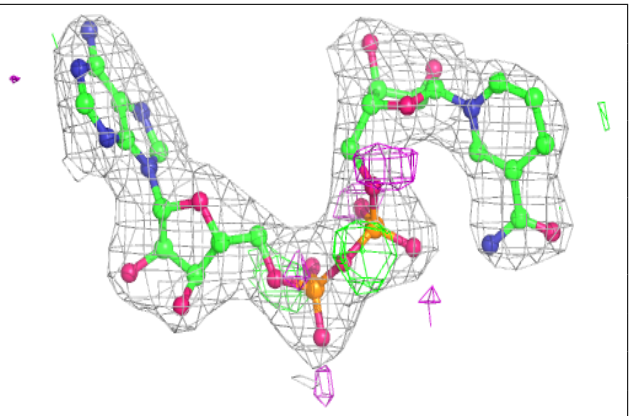


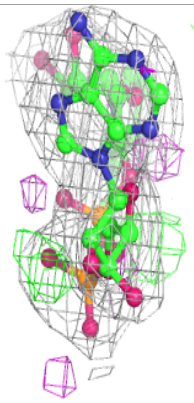


Electron density around NAI F 603:

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

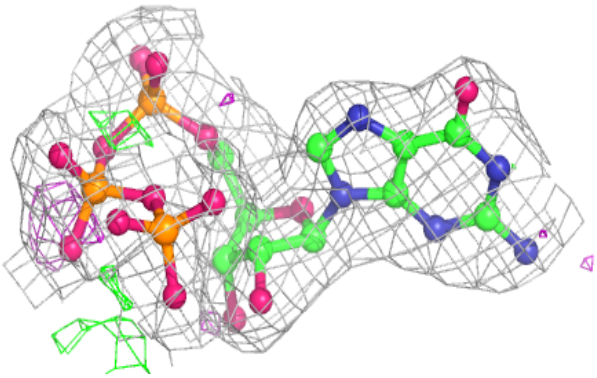


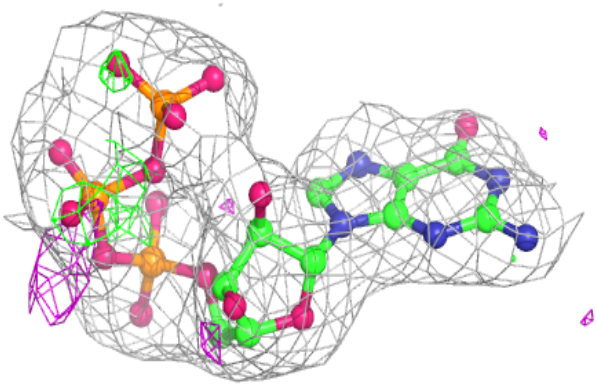


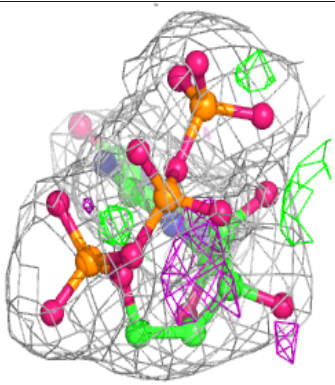


Electron density around GTP D 604:

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

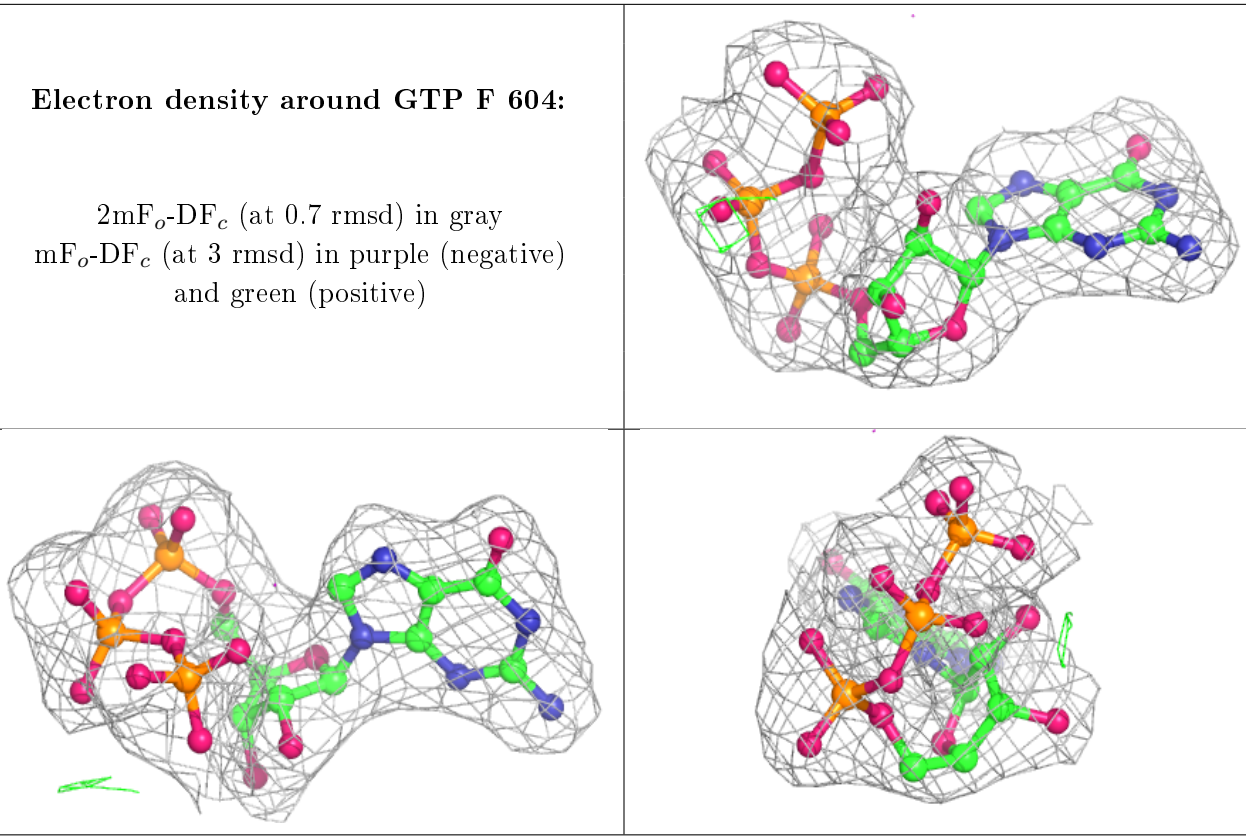






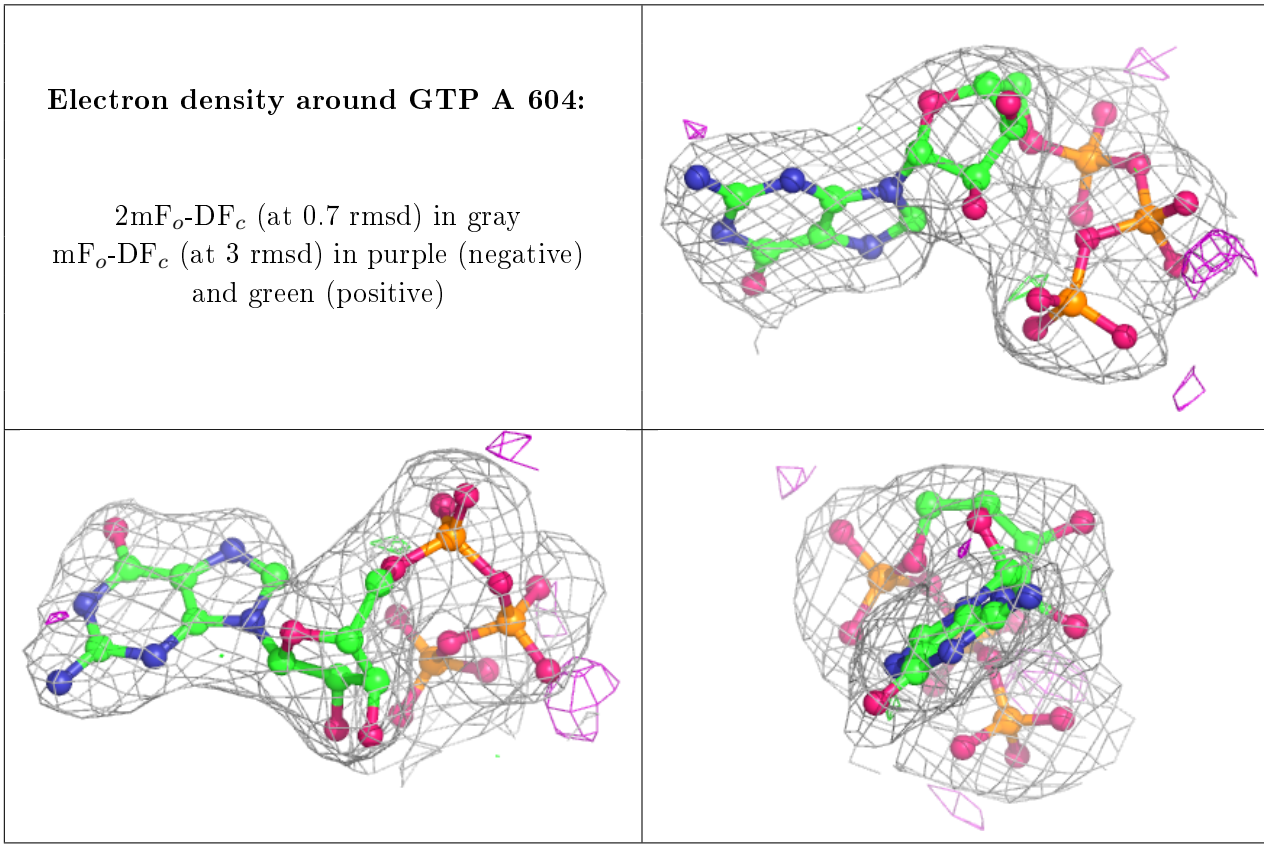
Electron density around GTP F 604:

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



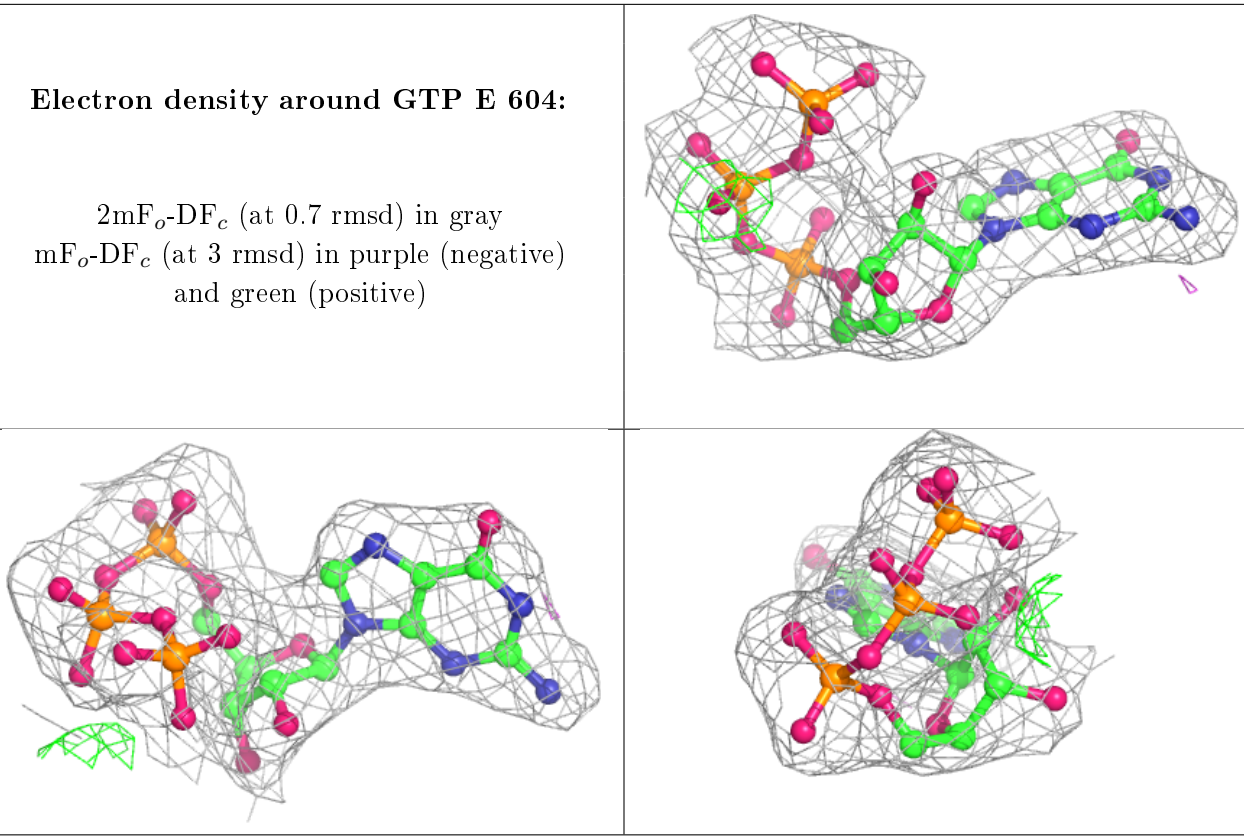
Electron density around GTP A 604:

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



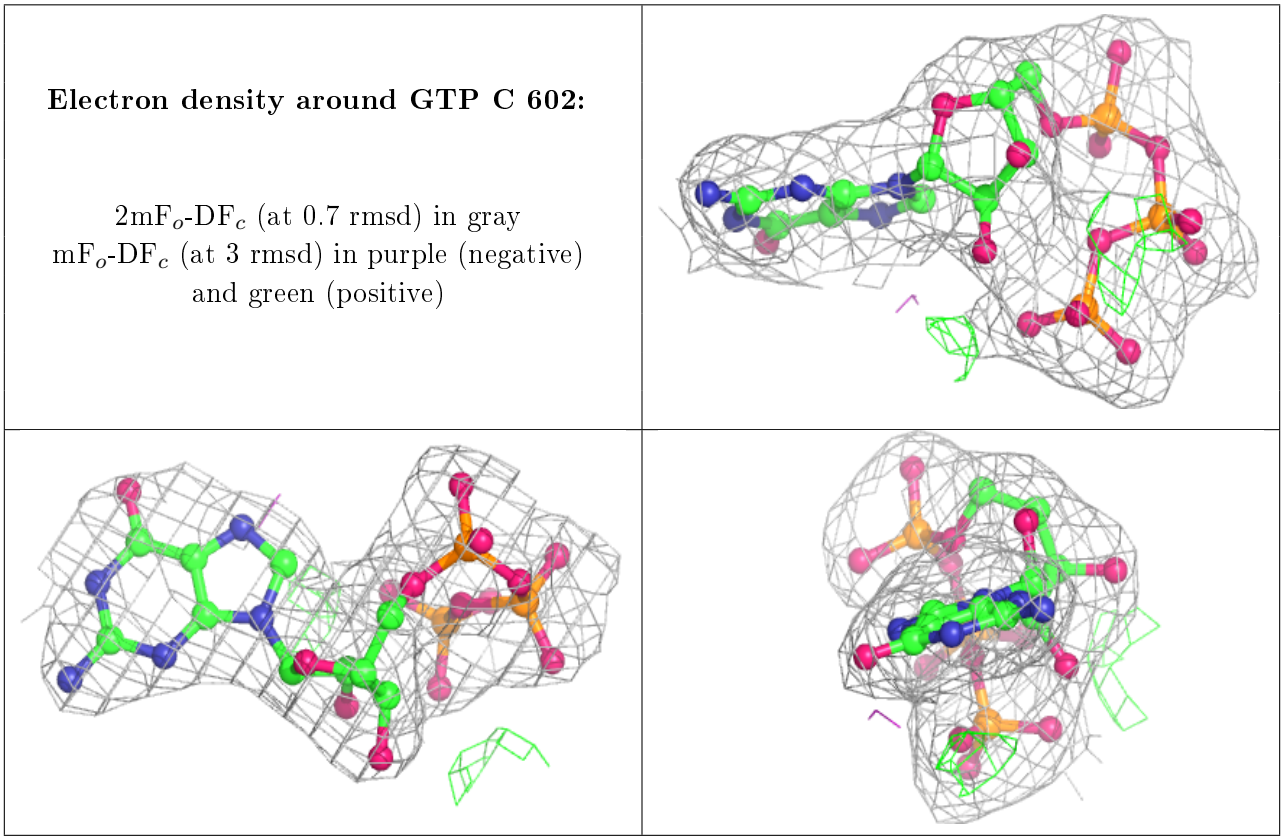
Electron density around GTP E 604:

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



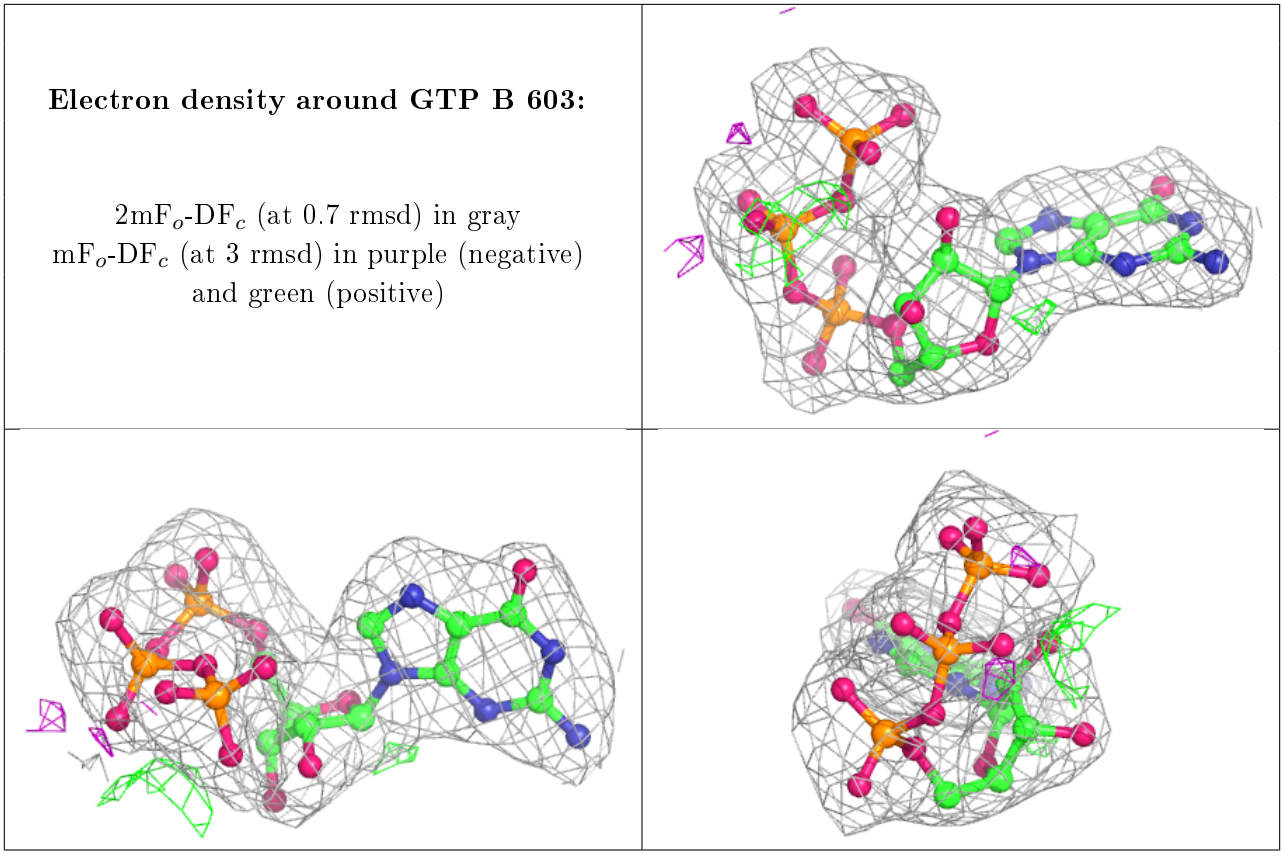
Electron density around GTP C 602:

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



Electron density around GTP 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)



6.5 Other polymers

There are no such residues in this entry.