Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:28 pm BST

PDB ID	:	3ETE
Title	:	Crystal structure of bovine glutamate dehydrogenase complexed with hexachlorophene
Authors	:	Li, M.; Smith, T.J.
Deposited on	:	2008-10-07
Resolution	:	3.00 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:

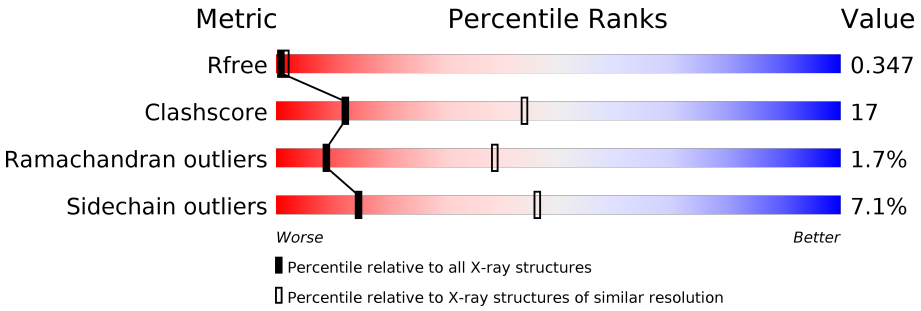
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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%

Mol	Chain	Length	Quality of chain
1	A	501	60% 34% 5% •
1	B	501	61% 34% • •
1	C	501	63% 32% • •
1	D	501	59% 36% • •
1	E	501	61% 34% • •
1	F	501	62% 33% • •

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLU	A	550	-	-	X	-
2	GLU	C	550	-	-	X	-
5	H3P	F	552	-	-	X	-

2 Entry composition

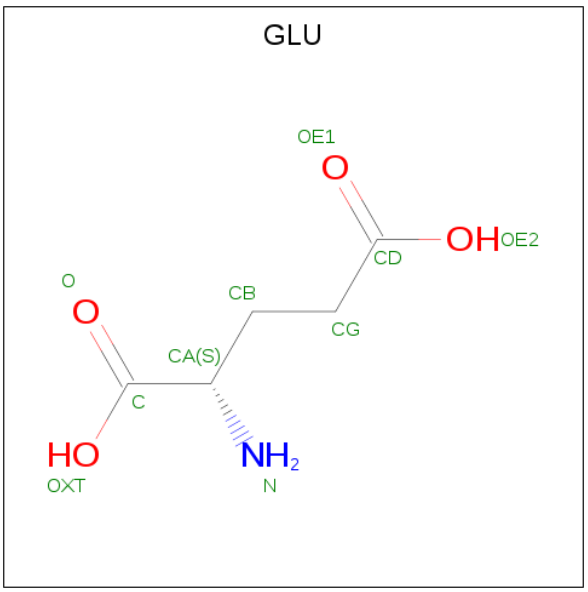
There are 6 unique types of molecules in this entry. The entry contains 24074 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

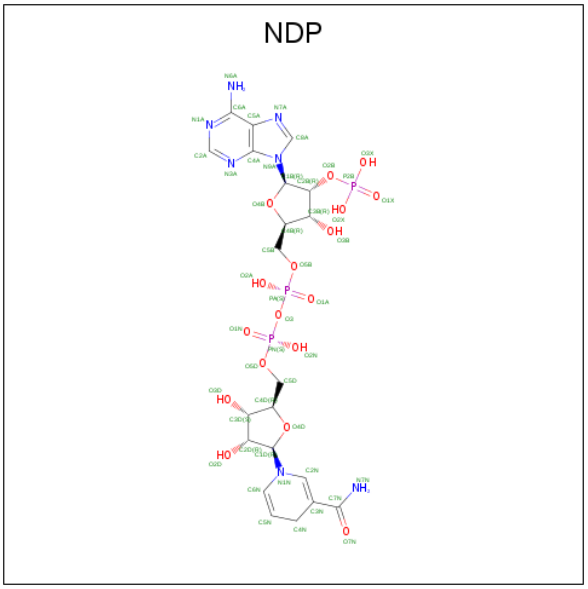
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3866	2443	678	726	19			
1	B	495	Total	C	N	O	S	0	0	0
			3866	2443	678	726	19			
1	C	495	Total	C	N	O	S	0	0	0
			3866	2443	678	726	19			
1	D	495	Total	C	N	O	S	0	0	0
			3866	2443	678	726	19			
1	E	495	Total	C	N	O	S	0	0	0
			3866	2443	678	726	19			
1	F	495	Total	C	N	O	S	0	0	0
			3866	2443	678	726	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
			9	5	1	3		
2	B	1	Total	C	N	O	0	0
			9	5	1	3		
2	C	1	Total	C	N	O	0	0
			9	5	1	3		
2	D	1	Total	C	N	O	0	0
			9	5	1	3		
2	E	1	Total	C	N	O	0	0
			9	5	1	3		
2	F	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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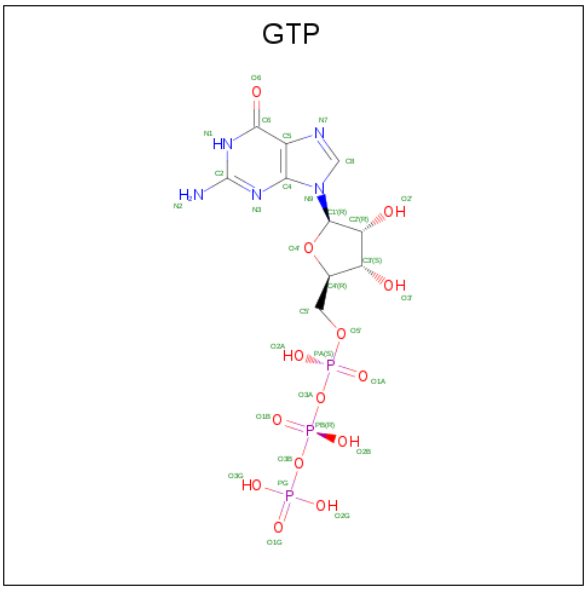
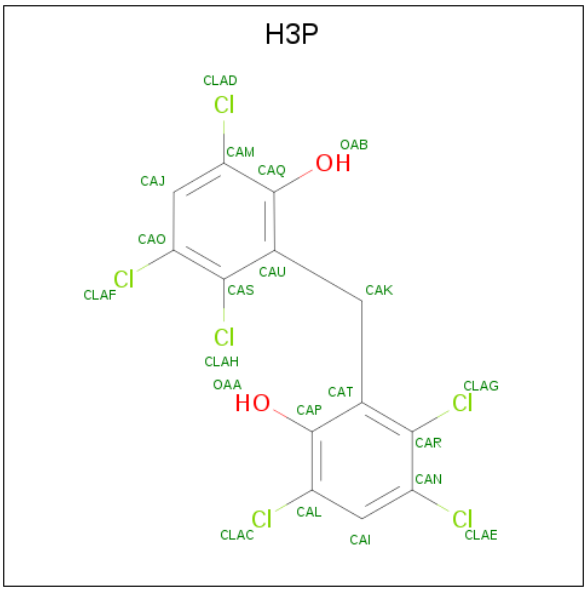
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- 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		
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 2,2'-methanediylbis(3,4,6-trichlorophenol) (three-letter code: H3P) (formula: $C_{13}H_6Cl_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C Cl O 21 13 6 2	0	0
5	B	1	Total C Cl O 21 13 6 2	0	0
5	C	1	Total C Cl O 21 13 6 2	0	0
5	C	1	Total C Cl O 21 13 6 2	0	0
5	D	1	Total C Cl O 21 13 6 2	0	0
5	F	1	Total C Cl O 21 13 6 2	0	0

- Molecule 6 is water.

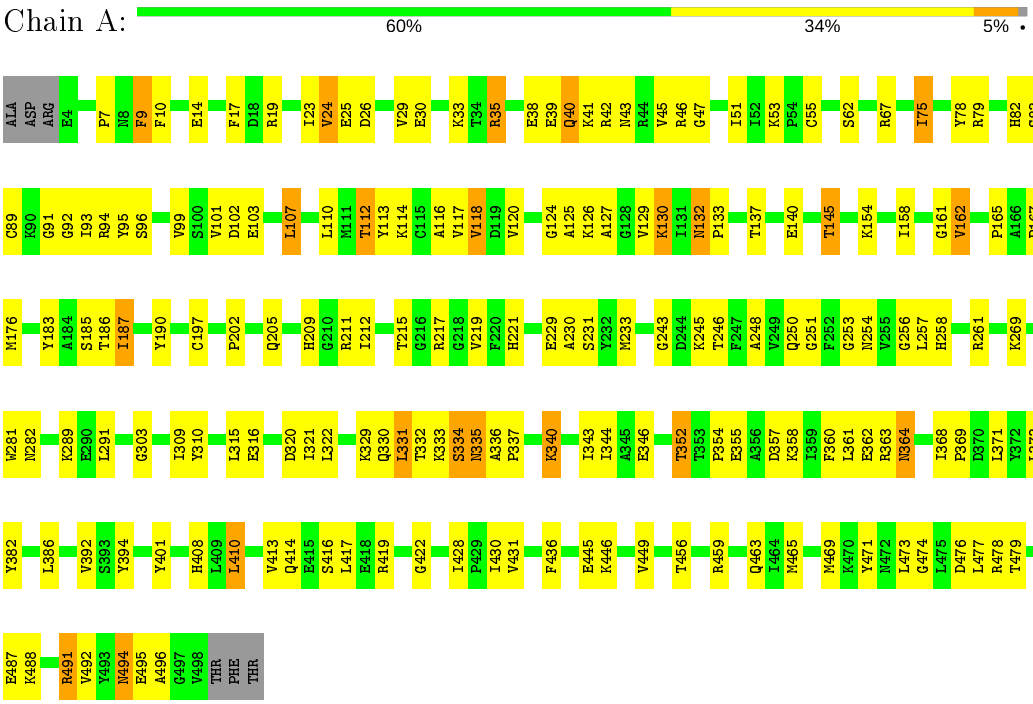
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	34	Total O 34 34	0	0
6	B	34	Total O 34 34	0	0
6	C	49	Total O 49 49	0	0
6	D	45	Total O 45 45	0	0
6	E	35	Total O 35 35	0	0
6	F	21	Total O 21 21	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

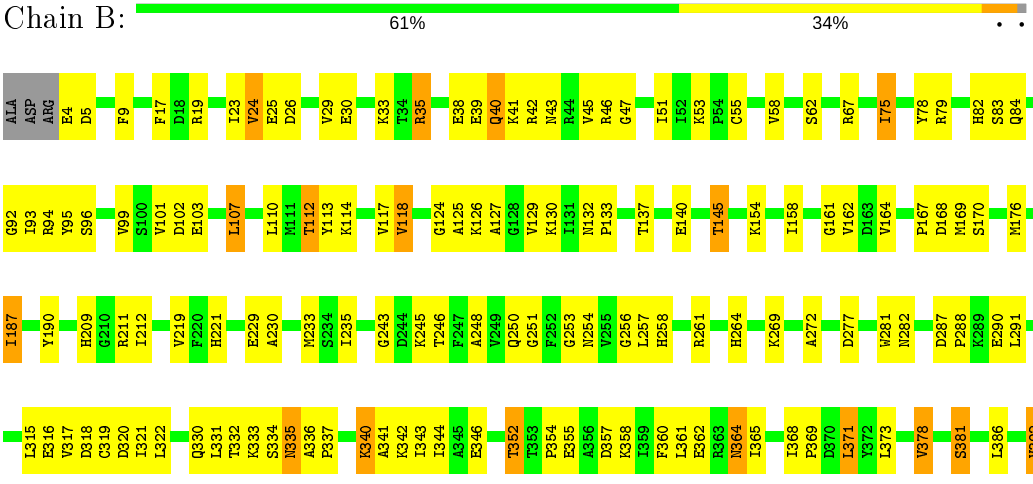
- Molecule 1: Glutamate dehydrogenase

Chain A:



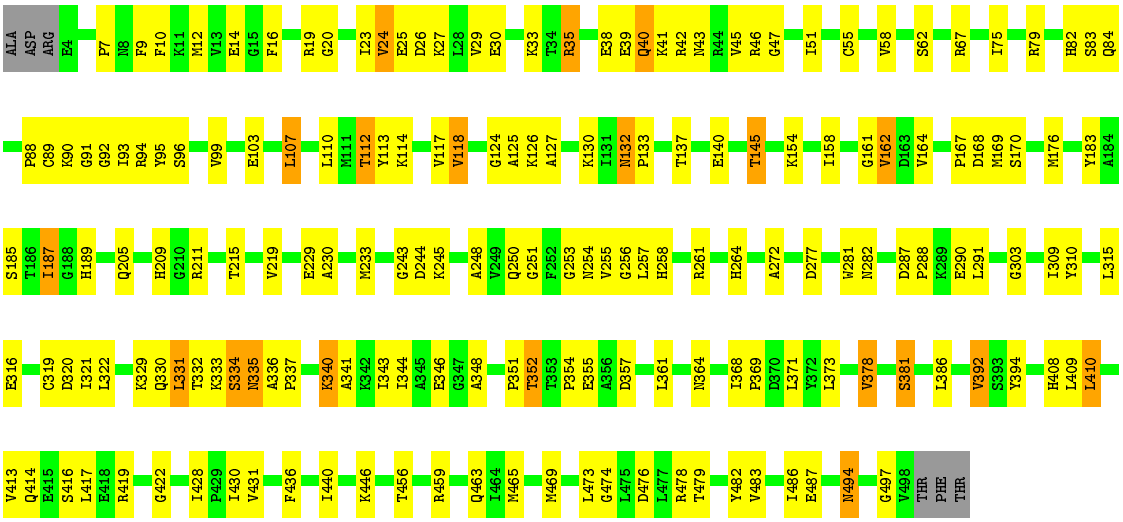
- Molecule 1: Glutamate dehydrogenase

Chain B:



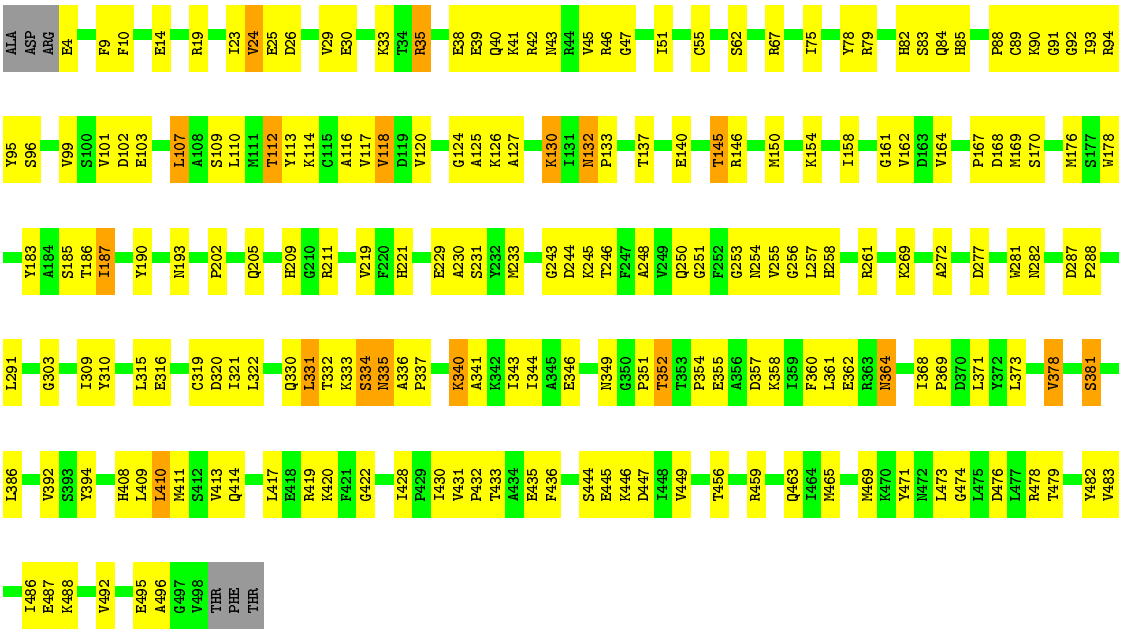
• Molecule 1: Glutamate dehydrogenase

Chain C:



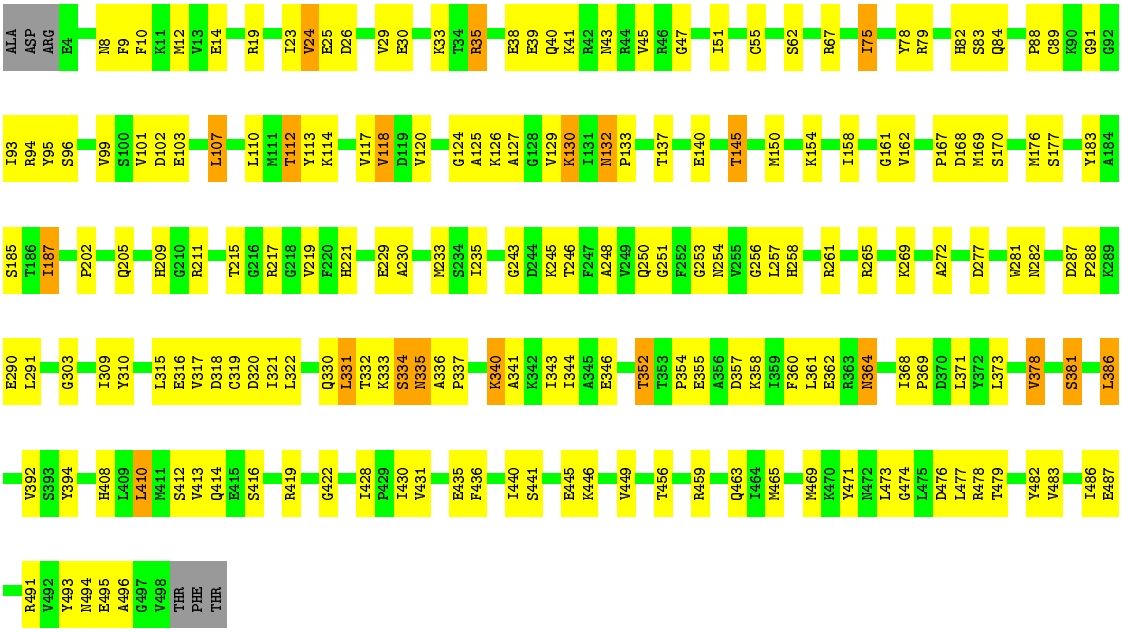
• Molecule 1: Glutamate dehydrogenase

Chain D:



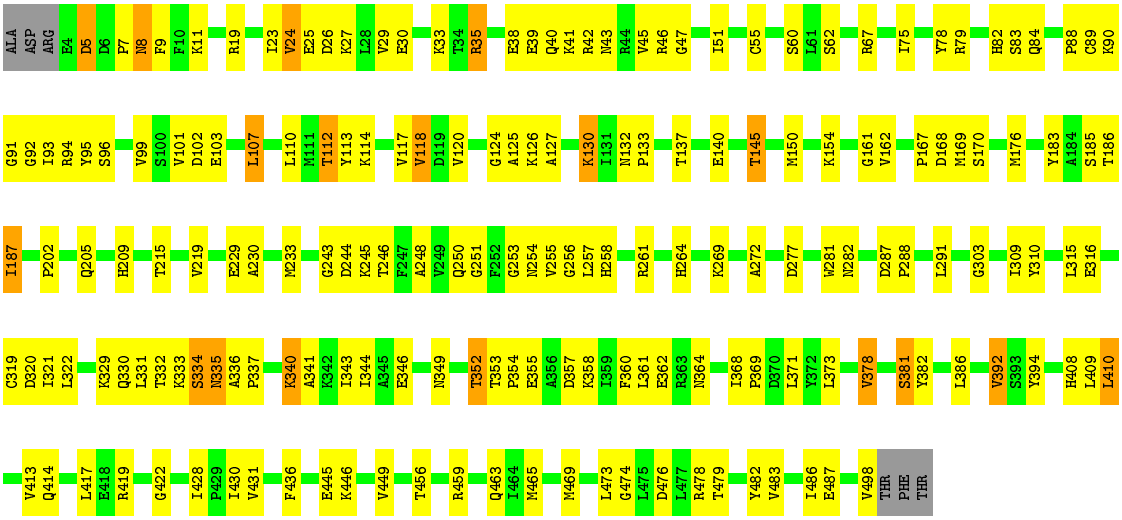
• Molecule 1: Glutamate dehydrogenase

Chain E:



- Molecule 1: Glutamate dehydrogenase

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	123.37Å 101.58Å 166.87Å 90.00° 102.34° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 48.49 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.00) 94.2 (48.49-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.266 0.329 , 0.347	Depositor DCC
R_{free} test set	6506 reflections (8.07%)	wwPDB-VP
Wilson B-factor (Å^2)	76.5	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 37.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	24074	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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, NDP, H3P

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.43	0/3948	0.71	1/5328 (0.0%)
1	B	0.43	0/3948	0.84	4/5328 (0.1%)
1	C	0.44	0/3948	0.71	1/5328 (0.0%)
1	D	0.44	0/3948	0.69	0/5328
1	E	0.46	0/3948	0.70	0/5328
1	F	0.46	0/3948	0.71	0/5328
All	All	0.45	0/23688	0.73	6/31968 (0.0%)

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	B	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	419	ARG	NE-CZ-NH1	-23.43	108.59	120.30
1	B	419	ARG	NE-CZ-NH2	23.09	131.85	120.30
1	B	419	ARG	CD-NE-CZ	11.18	139.25	123.60
1	C	40	GLN	N-CA-C	-5.19	96.99	111.00
1	A	40	GLN	N-CA-C	-5.12	97.18	111.00
1	B	40	GLN	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	493	TYR	Sidechain
1	E	493	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3866	0	3832	139	1
1	B	3866	0	3832	131	0
1	C	3866	0	3832	139	1
1	D	3866	0	3832	150	0
1	E	3866	0	3832	141	0
1	F	3866	0	3832	149	0
2	A	9	0	5	4	0
2	B	9	0	5	3	0
2	C	9	0	5	5	0
2	D	9	0	5	2	0
2	E	9	0	5	1	0
2	F	9	0	5	3	0
3	A	48	0	26	3	0
3	B	48	0	26	4	0
3	C	48	0	26	7	0
3	D	48	0	26	8	0
3	E	48	0	26	5	0
3	F	48	0	26	5	0
4	A	32	0	12	3	0
4	B	32	0	10	1	0
4	C	32	0	12	0	0
4	D	32	0	11	1	0
4	E	32	0	11	2	0
4	F	32	0	11	2	0
5	A	21	0	4	4	0
5	B	21	0	4	0	0
5	C	42	0	9	3	0
5	D	21	0	4	0	0
5	F	21	0	5	6	0
6	A	34	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	34	0	0	3	0
6	C	49	0	0	1	0
6	D	45	0	0	5	0
6	E	35	0	0	5	0
6	F	21	0	0	3	0
All	All	24074	0	23271	799	1

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 17.

All (799) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:HIS:HD2	1:A:261:ARG:HH11	1.28	0.82
1:B:258:HIS:HD2	1:B:261:ARG:HH11	1.29	0.81
1:F:258:HIS:HD2	1:F:261:ARG:HH11	1.28	0.80
1:B:336:ALA:HB3	1:B:337:PRO:HD3	1.64	0.80
1:E:261:ARG:HD2	4:E:553:GTP:O6	1.82	0.79
1:C:336:ALA:HB3	1:C:337:PRO:HD3	1.62	0.79
1:C:258:HIS:HD2	1:C:261:ARG:HH11	1.29	0.79
1:E:258:HIS:HD2	1:E:261:ARG:HH11	1.30	0.79
3:E:551:NDP:H52N	3:E:551:NDP:H2N	1.65	0.78
1:D:258:HIS:HD2	1:D:261:ARG:HH11	1.31	0.78
1:F:336:ALA:HB3	1:F:337:PRO:HD3	1.66	0.78
1:E:336:ALA:HB3	1:E:337:PRO:HD3	1.65	0.77
1:A:212:ILE:HD12	4:A:553:GTP:O3'	1.84	0.77
1:A:336:ALA:HB3	1:A:337:PRO:HD3	1.66	0.76
1:C:332:THR:H	1:C:335:ASN:HD21	1.33	0.75
1:C:40:GLN:HA	1:C:43:ASN:HD22	1.52	0.74
1:B:332:THR:H	1:B:335:ASN:HD21	1.33	0.74
1:E:221:HIS:HE1	6:E:561:HOH:O	1.70	0.74
1:B:40:GLN:HA	1:B:43:ASN:HD22	1.52	0.74
1:D:336:ALA:HB3	1:D:337:PRO:HD3	1.68	0.74
1:C:118:VAL:HG22	1:C:456:THR:HG22	1.68	0.73
1:E:40:GLN:HA	1:E:43:ASN:HD22	1.53	0.73
1:F:40:GLN:HA	1:F:43:ASN:HD22	1.54	0.73
1:D:332:THR:H	1:D:335:ASN:HD21	1.35	0.73
1:A:40:GLN:HA	1:A:43:ASN:HD22	1.52	0.73
1:F:112:THR:HG22	1:F:124:GLY:HA3	1.69	0.73
1:F:91:GLY:HA3	1:F:125:ALA:O	1.89	0.73
1:E:332:THR:H	1:E:335:ASN:HD21	1.34	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:GLN:HA	1:D:43:ASN:HD22	1.54	0.71
1:B:118:VAL:HG22	1:B:456:THR:HG22	1.72	0.71
1:E:118:VAL:HG22	1:E:456:THR:HG22	1.72	0.71
1:B:315:LEU:HD13	1:B:331:LEU:HD12	1.73	0.71
1:F:332:THR:H	1:F:335:ASN:HD21	1.35	0.71
1:A:332:THR:H	1:A:335:ASN:HD21	1.37	0.71
1:D:91:GLY:HA3	1:D:125:ALA:O	1.91	0.70
1:F:7:PRO:HD2	1:F:329:LYS:HD2	1.73	0.70
1:A:118:VAL:HG22	1:A:456:THR:HG22	1.73	0.69
1:C:315:LEU:HD13	1:C:331:LEU:HD12	1.75	0.69
1:D:193:ASN:HB2	6:D:593:HOH:O	1.90	0.69
1:E:315:LEU:HD13	1:E:331:LEU:HD12	1.74	0.69
1:A:82:HIS:CD2	1:A:112:THR:HG21	2.28	0.69
1:A:126:LYS:NZ	2:A:550:GLU:N	2.40	0.68
1:F:209:HIS:HE1	4:F:553:GTP:O1A	1.76	0.68
1:C:91:GLY:HA3	1:C:125:ALA:O	1.92	0.68
1:B:112:THR:HG22	1:B:124:GLY:HA3	1.74	0.68
1:F:82:HIS:CD2	1:F:112:THR:HG21	2.28	0.68
1:B:107:LEU:HB3	1:B:126:LYS:HE3	1.74	0.68
1:C:24:VAL:HG22	1:C:483:VAL:HG22	1.76	0.68
1:D:250:GLN:NE2	1:D:330:GLN:HE21	1.91	0.68
1:C:55:CYS:O	1:F:62:SER:HB3	1.94	0.67
1:D:315:LEU:HD13	1:D:331:LEU:HD12	1.76	0.67
1:D:419:ARG:NH2	6:D:582:HOH:O	2.27	0.67
1:D:436:PHE:HB2	1:E:408:HIS:HB3	1.76	0.67
1:F:315:LEU:HD13	1:F:331:LEU:HD12	1.75	0.67
1:A:250:GLN:NE2	1:A:330:GLN:HE21	1.93	0.67
1:D:82:HIS:CD2	1:D:112:THR:HG21	2.30	0.67
1:E:82:HIS:CD2	1:E:112:THR:HG21	2.30	0.67
1:E:250:GLN:NE2	1:E:330:GLN:HE21	1.92	0.67
1:C:82:HIS:CD2	1:C:112:THR:HG21	2.30	0.67
1:A:91:GLY:HA3	1:A:125:ALA:O	1.96	0.66
1:C:92:GLY:H	2:C:550:GLU:HB3	1.60	0.66
1:F:118:VAL:HG22	1:F:456:THR:HG22	1.77	0.66
1:F:250:GLN:NE2	1:F:330:GLN:HE21	1.91	0.66
1:D:112:THR:HG22	1:D:124:GLY:HA3	1.77	0.66
1:D:85:HIS:HB2	1:D:492:VAL:HG11	1.78	0.66
1:E:211:ARG:HB3	6:E:578:HOH:O	1.95	0.66
1:E:217:ARG:HD3	6:E:561:HOH:O	1.95	0.66
1:D:107:LEU:HB3	1:D:126:LYS:HE3	1.77	0.66
1:A:315:LEU:HD13	1:A:331:LEU:HD12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:551:NDP:H2N	3:B:551:NDP:H52N	1.78	0.66
1:B:82:HIS:CD2	1:B:112:THR:HG21	2.31	0.66
1:C:250:GLN:NE2	1:C:330:GLN:HE21	1.95	0.65
1:C:118:VAL:HG22	1:C:456:THR:CG2	2.26	0.65
1:D:496:ALA:HB3	1:E:177:SER:OG	1.96	0.65
1:E:107:LEU:HB3	1:E:126:LYS:HE3	1.78	0.65
1:A:112:THR:HG22	1:A:124:GLY:HA3	1.77	0.65
1:D:118:VAL:HG22	1:D:456:THR:HG22	1.78	0.65
4:D:553:GTP:O1A	4:D:553:GTP:O1B	2.14	0.65
1:C:112:THR:HG22	1:C:124:GLY:HA3	1.79	0.65
1:D:255:VAL:HG11	3:D:551:NDP:O4D	1.97	0.65
1:D:95:TYR:OH	1:D:145:THR:HB	1.97	0.64
1:D:96:SER:O	1:D:130:LYS:HA	1.97	0.64
1:F:107:LEU:HB3	1:F:126:LYS:HE3	1.80	0.64
1:A:217:ARG:HD3	6:A:557:HOH:O	1.96	0.64
1:E:215:THR:OG1	3:E:551:NDP:H42N	1.97	0.64
1:F:414:GLN:HG3	1:F:428:ILE:O	1.97	0.64
1:A:7:PRO:HD2	1:A:329:LYS:HD2	1.80	0.64
1:B:250:GLN:NE2	1:B:330:GLN:HE21	1.96	0.64
1:F:95:TYR:OH	1:F:145:THR:HB	1.97	0.64
1:F:99:VAL:HA	1:F:103:GLU:OE1	1.98	0.64
1:A:107:LEU:HB3	1:A:126:LYS:HE3	1.78	0.64
1:C:99:VAL:HA	1:C:103:GLU:OE1	1.98	0.63
1:C:107:LEU:HB3	1:C:126:LYS:HE3	1.79	0.63
1:E:91:GLY:HA3	1:E:125:ALA:O	1.97	0.63
1:B:91:GLY:HA3	1:B:125:ALA:O	1.99	0.63
1:B:322:LEU:HB3	1:B:344:ILE:HD13	1.80	0.63
1:D:219:VAL:HG13	1:D:373:LEU:HD11	1.81	0.63
1:E:95:TYR:OH	1:E:145:THR:HB	1.99	0.63
1:C:414:GLN:HG3	1:C:428:ILE:O	1.99	0.62
1:C:95:TYR:OH	1:C:145:THR:HB	1.99	0.62
1:C:62:SER:HB3	1:F:55:CYS:O	1.99	0.62
1:A:414:GLN:HG3	1:A:428:ILE:O	1.98	0.62
1:F:169:MET:HG2	3:F:551:NDP:O1N	1.98	0.62
1:F:24:VAL:HG22	1:F:483:VAL:HG22	1.81	0.62
1:A:35:ARG:HH11	1:A:35:ARG:HA	1.64	0.62
1:A:95:TYR:OH	1:A:145:THR:HB	1.99	0.62
1:C:322:LEU:HB3	1:C:344:ILE:HD13	1.82	0.62
1:E:219:VAL:HG13	1:E:373:LEU:HD11	1.82	0.62
1:E:137:THR:OG1	1:E:140:GLU:HG3	1.99	0.62
1:E:322:LEU:HB3	1:E:344:ILE:HD13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:HA	1:A:103:GLU:OE1	1.99	0.62
1:D:322:LEU:HB3	1:D:344:ILE:HD13	1.82	0.62
1:E:112:THR:HG22	1:E:124:GLY:HA3	1.79	0.62
1:A:322:LEU:HB3	1:A:344:ILE:HD13	1.81	0.62
1:B:35:ARG:HA	1:B:35:ARG:HH11	1.65	0.61
1:D:99:VAL:HA	1:D:103:GLU:OE1	1.99	0.61
3:A:551:NDP:H52N	3:A:551:NDP:H2N	1.82	0.61
1:F:258:HIS:CD2	1:F:261:ARG:HH11	2.16	0.61
1:C:169:MET:HG2	3:C:551:NDP:O1N	1.99	0.61
1:E:35:ARG:HA	1:E:35:ARG:HH11	1.65	0.61
1:A:126:LYS:HZ3	2:A:550:GLU:N	1.99	0.61
1:A:219:VAL:HG13	1:A:373:LEU:HD11	1.81	0.61
1:A:40:GLN:HA	1:A:43:ASN:ND2	2.15	0.61
1:A:96:SER:O	1:A:130:LYS:HA	2.01	0.61
1:A:85:HIS:HB2	1:A:492:VAL:HG11	1.83	0.61
1:E:99:VAL:HA	1:E:103:GLU:OE1	2.00	0.61
1:C:40:GLN:HA	1:C:43:ASN:ND2	2.16	0.61
1:C:258:HIS:CD2	1:C:261:ARG:HH11	2.16	0.60
1:B:414:GLN:HG3	1:B:428:ILE:O	2.01	0.60
1:B:95:TYR:OH	1:B:145:THR:HB	2.01	0.60
1:D:40:GLN:HA	1:D:43:ASN:ND2	2.16	0.60
1:F:322:LEU:HB3	1:F:344:ILE:HD13	1.81	0.60
1:B:96:SER:O	1:B:130:LYS:HA	2.02	0.60
1:B:40:GLN:HA	1:B:43:ASN:ND2	2.16	0.60
1:D:35:ARG:HA	1:D:35:ARG:HH11	1.66	0.60
1:D:444:SER:H	1:D:447:ASP:HB2	1.66	0.60
1:E:93:ILE:HG12	1:E:127:ALA:HB3	1.84	0.60
1:B:419:ARG:HH12	1:F:431:VAL:HG12	1.67	0.60
1:A:137:THR:OG1	1:A:140:GLU:HG3	2.01	0.60
1:C:96:SER:O	1:C:130:LYS:HA	2.02	0.60
1:C:35:ARG:HH11	1:C:35:ARG:HA	1.67	0.60
1:E:96:SER:O	1:E:130:LYS:HA	2.02	0.59
1:A:258:HIS:CD2	1:A:261:ARG:HH11	2.16	0.59
1:A:335:ASN:N	1:A:335:ASN:HD22	2.01	0.59
1:A:41:LYS:O	1:A:45:VAL:HG23	2.02	0.59
1:C:27:LYS:HD3	1:C:487:GLU:OE2	2.02	0.59
1:F:35:ARG:HA	1:F:35:ARG:HH11	1.65	0.59
1:B:118:VAL:HG22	1:B:456:THR:CG2	2.33	0.59
3:F:551:NDP:H2N	3:F:551:NDP:H52N	1.83	0.59
1:B:99:VAL:HA	1:B:103:GLU:OE1	2.02	0.59
1:C:41:LYS:O	1:C:45:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:TYR:O	1:D:486:ILE:HG13	2.02	0.59
1:D:435:GLU:HB3	1:E:408:HIS:CE1	2.38	0.59
1:F:187:ILE:HG23	5:F:552:H3P:CAK	2.33	0.59
1:F:40:GLN:HA	1:F:43:ASN:ND2	2.16	0.59
1:C:333:LYS:HD2	1:C:355:GLU:OE1	2.03	0.59
1:D:41:LYS:O	1:D:45:VAL:HG23	2.02	0.59
1:D:93:ILE:HG12	1:D:127:ALA:HB3	1.84	0.58
1:B:229:GLU:O	1:B:230:ALA:HB3	2.03	0.58
1:C:93:ILE:HG12	1:C:127:ALA:HB3	1.85	0.58
1:D:137:THR:OG1	1:D:140:GLU:HG3	2.02	0.58
1:E:41:LYS:O	1:E:45:VAL:HG23	2.02	0.58
1:B:112:THR:HB	1:B:124:GLY:H	1.68	0.58
1:E:414:GLN:HG3	1:E:428:ILE:O	2.03	0.58
1:E:258:HIS:CD2	1:E:261:ARG:HH11	2.18	0.58
1:F:335:ASN:HD22	1:F:335:ASN:N	2.01	0.58
1:F:41:LYS:O	1:F:45:VAL:HG23	2.03	0.58
1:C:137:THR:OG1	1:C:140:GLU:HG3	2.03	0.58
1:C:219:VAL:HG13	1:C:373:LEU:HD11	1.85	0.58
1:F:112:THR:HB	1:F:124:GLY:H	1.69	0.58
1:B:219:VAL:HG13	1:B:373:LEU:HD11	1.84	0.58
1:C:478:ARG:HH11	1:C:478:ARG:HG3	1.68	0.58
1:D:459:ARG:O	1:D:463:GLN:HG3	2.03	0.58
1:E:482:TYR:O	1:E:486:ILE:HG13	2.04	0.58
1:F:219:VAL:HG13	1:F:373:LEU:HD11	1.85	0.58
1:B:335:ASN:HD22	1:B:335:ASN:N	2.02	0.57
1:C:392:VAL:HG13	1:E:386:LEU:HD21	1.84	0.57
1:B:258:HIS:CD2	1:B:261:ARG:HH11	2.16	0.57
1:B:482:TYR:O	1:B:486:ILE:HG13	2.04	0.57
1:D:414:GLN:HG3	1:D:428:ILE:O	2.03	0.57
1:E:335:ASN:HD22	1:E:335:ASN:N	2.02	0.57
1:F:229:GLU:O	1:F:230:ALA:HB3	2.05	0.57
1:B:93:ILE:HG12	1:B:127:ALA:HB3	1.86	0.57
1:E:478:ARG:HG3	1:E:478:ARG:HH11	1.69	0.57
1:F:133:PRO:HG2	1:F:170:SER:HB3	1.87	0.57
1:B:253:GLY:HA3	3:B:551:NDP:O1A	2.05	0.57
1:C:211:ARG:HH22	3:C:551:NDP:H72N	1.50	0.57
1:E:40:GLN:HA	1:E:43:ASN:ND2	2.17	0.57
1:E:459:ARG:O	1:E:463:GLN:HG3	2.04	0.57
1:C:335:ASN:N	1:C:335:ASN:HD22	2.03	0.57
1:C:7:PRO:HD2	1:C:329:LYS:HD2	1.85	0.57
1:F:96:SER:O	1:F:130:LYS:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LYS:HD3	1:C:185:SER:O	2.04	0.56
1:B:211:ARG:HH22	3:B:551:NDP:H71N	1.53	0.56
1:C:12:MET:HG3	1:C:354:PRO:HD3	1.87	0.56
1:D:133:PRO:HG2	1:D:170:SER:HB3	1.88	0.56
1:A:93:ILE:HG12	1:A:127:ALA:HB3	1.86	0.56
1:A:333:LYS:HD2	1:A:355:GLU:OE1	2.06	0.56
1:C:205:GLN:NE2	1:E:496:ALA:HB2	2.21	0.56
1:D:258:HIS:CD2	1:D:261:ARG:HH11	2.18	0.56
1:E:209:HIS:CD2	1:E:446:LYS:HG3	2.41	0.56
1:E:333:LYS:HD2	1:E:355:GLU:OE1	2.05	0.56
1:F:478:ARG:HH11	1:F:478:ARG:HG3	1.69	0.56
1:E:25:GLU:O	1:E:29:VAL:HG23	2.06	0.56
1:F:137:THR:OG1	1:F:140:GLU:HG3	2.05	0.56
1:A:118:VAL:HG22	1:A:456:THR:CG2	2.36	0.56
1:A:25:GLU:O	1:A:29:VAL:HG23	2.05	0.56
1:C:436:PHE:HB2	1:D:408:HIS:HB3	1.88	0.56
1:F:333:LYS:HD2	1:F:355:GLU:OE1	2.06	0.56
1:A:482:TYR:O	1:A:486:ILE:HG13	2.06	0.55
1:A:478:ARG:HG3	1:A:478:ARG:HH11	1.70	0.55
1:B:459:ARG:O	1:B:463:GLN:HG3	2.05	0.55
1:C:112:THR:HB	1:C:124:GLY:H	1.72	0.55
1:B:55:CYS:O	1:E:62:SER:HB3	2.07	0.55
1:D:335:ASN:N	1:D:335:ASN:HD22	2.02	0.55
1:F:187:ILE:HG23	5:F:552:H3P:HAKA	1.89	0.55
1:B:41:LYS:O	1:B:45:VAL:HG23	2.06	0.55
1:E:229:GLU:O	1:E:230:ALA:HB3	2.07	0.55
1:F:482:TYR:O	1:F:486:ILE:HG13	2.07	0.55
1:D:110:LEU:O	1:D:114:LYS:HB2	2.07	0.55
1:F:93:ILE:HG12	1:F:127:ALA:HB3	1.87	0.55
1:A:229:GLU:O	1:A:230:ALA:HB3	2.07	0.54
1:B:245:LYS:HA	1:B:320:ASP:OD1	2.07	0.54
1:D:303:GLY:H	1:D:309:ILE:HD11	1.72	0.54
1:F:25:GLU:O	1:F:29:VAL:HG23	2.07	0.54
1:C:459:ARG:O	1:C:463:GLN:HG3	2.06	0.54
1:A:169:MET:HA	3:A:551:NDP:O1N	2.06	0.54
1:C:133:PRO:HG2	1:C:170:SER:HB3	1.90	0.54
1:D:25:GLU:O	1:D:29:VAL:HG23	2.08	0.54
1:D:333:LYS:HD2	1:D:355:GLU:OE1	2.08	0.54
1:D:229:GLU:O	1:D:230:ALA:HB3	2.08	0.54
1:E:118:VAL:HG22	1:E:456:THR:CG2	2.38	0.54
1:A:245:LYS:HA	1:A:320:ASP:OD1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:HD21	4:A:553:GTP:HN21	1.72	0.54
1:E:19:ARG:O	1:E:23:ILE:HG12	2.07	0.54
1:B:133:PRO:HG2	1:B:170:SER:HB3	1.90	0.53
1:B:25:GLU:O	1:B:29:VAL:HG23	2.08	0.53
1:D:411:MET:HA	6:D:587:HOH:O	2.07	0.53
1:A:62:SER:HB3	1:D:55:CYS:O	2.07	0.53
1:F:459:ARG:O	1:F:463:GLN:HG3	2.08	0.53
1:C:431:VAL:HG12	1:D:419:ARG:HH12	1.74	0.53
1:D:478:ARG:HH11	1:D:478:ARG:HG3	1.72	0.53
1:E:303:GLY:H	1:E:309:ILE:HD11	1.73	0.53
1:A:459:ARG:O	1:A:463:GLN:HG3	2.07	0.53
1:E:473:LEU:HD22	1:E:479:THR:HB	1.90	0.53
1:F:19:ARG:O	1:F:23:ILE:HG12	2.08	0.53
1:F:354:PRO:O	1:F:357:ASP:HB2	2.09	0.53
1:A:112:THR:HB	1:A:124:GLY:H	1.74	0.53
1:B:303:GLY:H	1:B:309:ILE:HD11	1.73	0.53
1:A:368:ILE:HG22	1:A:373:LEU:HB2	1.91	0.53
1:C:497:GLY:HA3	1:D:178:TRP:HD1	1.74	0.53
1:F:187:ILE:HA	5:F:552:H3P:CAK	2.39	0.53
1:C:473:LEU:HD22	1:C:479:THR:HB	1.91	0.53
1:A:303:GLY:H	1:A:309:ILE:HD11	1.73	0.53
1:C:229:GLU:O	1:C:230:ALA:HB3	2.07	0.53
1:C:47:GLY:O	1:C:51:ILE:HG13	2.09	0.53
1:A:55:CYS:O	1:D:62:SER:HB3	2.09	0.53
1:E:133:PRO:HG2	1:E:170:SER:HB3	1.89	0.53
1:E:245:LYS:HA	1:E:320:ASP:OD1	2.08	0.53
1:A:133:PRO:HG2	1:A:170:SER:HB3	1.89	0.53
1:E:110:LEU:O	1:E:114:LYS:HB2	2.08	0.53
1:A:110:LEU:O	1:A:114:LYS:HB2	2.09	0.53
1:B:137:THR:OG1	1:B:140:GLU:HG3	2.08	0.53
1:E:248:ALA:HB1	1:E:272:ALA:HB3	1.91	0.53
1:B:110:LEU:O	1:B:114:LYS:HB2	2.10	0.52
1:B:67:ARG:HD2	1:B:140:GLU:OE2	2.09	0.52
1:C:110:LEU:O	1:C:114:LYS:HB2	2.08	0.52
1:F:316:GLU:O	1:F:340:LYS:HE2	2.09	0.52
1:F:368:ILE:HG22	1:F:373:LEU:HB2	1.91	0.52
1:A:113:TYR:O	1:A:117:VAL:HG23	2.08	0.52
1:C:19:ARG:O	1:C:23:ILE:HG12	2.09	0.52
1:D:154:LYS:HD3	1:F:185:SER:O	2.09	0.52
1:D:118:VAL:HG22	1:D:456:THR:CG2	2.39	0.52
1:C:245:LYS:HA	1:C:320:ASP:OD1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:TYR:O	1:C:486:ILE:HG13	2.10	0.52
1:B:478:ARG:HG3	1:B:478:ARG:HH11	1.73	0.52
1:C:113:TYR:O	1:C:117:VAL:HG23	2.10	0.52
1:C:303:GLY:H	1:C:309:ILE:HD11	1.75	0.52
1:E:368:ILE:HG22	1:E:373:LEU:HB2	1.91	0.52
1:B:473:LEU:HD22	1:B:479:THR:HB	1.91	0.52
1:C:25:GLU:O	1:C:29:VAL:HG23	2.09	0.52
1:D:410:LEU:O	1:D:413:VAL:HG22	2.10	0.52
1:F:245:LYS:HA	1:F:320:ASP:OD1	2.09	0.52
1:F:67:ARG:HD2	1:F:140:GLU:OE2	2.10	0.52
1:A:92:GLY:H	2:A:550:GLU:N	2.08	0.52
1:C:248:ALA:HB1	1:C:272:ALA:HB3	1.91	0.52
1:C:369:PRO:HB2	1:C:371:LEU:HD23	1.92	0.52
1:D:113:TYR:O	1:D:117:VAL:HG23	2.10	0.52
1:D:245:LYS:HA	1:D:320:ASP:OD1	2.10	0.52
1:E:113:TYR:O	1:E:117:VAL:HG23	2.09	0.52
1:A:209:HIS:CD2	1:A:446:LYS:HG3	2.45	0.52
1:B:315:LEU:HD13	1:B:331:LEU:CD1	2.40	0.52
1:A:289:LYS:HA	6:A:581:HOH:O	2.10	0.51
1:A:190:TYR:CD1	5:A:552:H3P:CLAE	3.00	0.51
1:C:413:VAL:HG23	1:C:430:ILE:HG13	1.92	0.51
1:D:103:GLU:HG2	1:D:107:LEU:CD2	2.40	0.51
1:F:8:ASN:HD22	1:F:9:PHE:N	2.08	0.51
1:D:473:LEU:HD22	1:D:479:THR:HB	1.93	0.51
1:E:315:LEU:HD13	1:E:331:LEU:CD1	2.39	0.51
1:F:114:LYS:NZ	2:F:550:GLU:O	2.43	0.51
1:F:255:VAL:HG11	3:F:551:NDP:O4D	2.10	0.51
1:B:333:LYS:HD2	1:B:355:GLU:OE1	2.09	0.51
1:D:26:ASP:O	1:D:30:GLU:HG3	2.11	0.51
1:D:85:HIS:HD2	1:D:492:VAL:HG21	1.74	0.51
1:F:118:VAL:HG22	1:F:456:THR:CG2	2.40	0.51
1:A:431:VAL:HG12	1:F:419:ARG:HH12	1.76	0.51
1:B:408:HIS:HB3	1:F:436:PHE:HB2	1.92	0.51
1:A:408:HIS:HB3	1:B:436:PHE:HB2	1.92	0.51
1:F:113:TYR:O	1:F:117:VAL:HG23	2.11	0.51
1:C:354:PRO:O	1:C:357:ASP:HB2	2.09	0.51
1:D:112:THR:HB	1:D:124:GLY:H	1.75	0.51
1:D:368:ILE:HG22	1:D:373:LEU:HB2	1.92	0.51
1:F:110:LEU:O	1:F:114:LYS:HB2	2.10	0.51
1:D:19:ARG:O	1:D:23:ILE:HG12	2.11	0.51
1:F:215:THR:OG1	3:F:551:NDP:H42N	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:ASP:O	1:F:30:GLU:HG3	2.11	0.51
1:A:19:ARG:O	1:A:23:ILE:HG12	2.11	0.51
1:A:473:LEU:HB3	1:A:476:ASP:HB3	1.93	0.51
1:A:79:ARG:HD3	1:A:127:ALA:HB2	1.93	0.51
1:C:368:ILE:HG22	1:C:373:LEU:HB2	1.92	0.51
1:D:354:PRO:O	1:D:357:ASP:HB2	2.11	0.51
1:B:19:ARG:O	1:B:23:ILE:HG12	2.11	0.51
1:C:409:LEU:HD22	1:D:409:LEU:HD21	1.93	0.51
1:D:378:VAL:HA	1:D:381:SER:HB2	1.93	0.51
1:A:419:ARG:HH12	1:B:431:VAL:HG12	1.75	0.51
1:B:126:LYS:NZ	2:B:550:GLU:N	2.59	0.50
1:D:316:GLU:O	1:D:340:LYS:HE2	2.10	0.50
1:D:413:VAL:HG23	1:D:430:ILE:HG13	1.93	0.50
1:B:190:TYR:HE2	1:F:162:VAL:HG11	1.75	0.50
1:B:62:SER:HB3	1:E:55:CYS:O	2.10	0.50
1:A:185:SER:O	1:E:154:LYS:HD3	2.11	0.50
1:B:316:GLU:O	1:B:340:LYS:HE2	2.10	0.50
1:A:410:LEU:O	1:A:413:VAL:HG22	2.12	0.50
1:B:103:GLU:HG2	1:B:107:LEU:CD2	2.42	0.50
1:C:26:ASP:O	1:C:30:GLU:HG3	2.11	0.50
1:E:378:VAL:HA	1:E:381:SER:HB2	1.94	0.50
1:E:413:VAL:HG23	1:E:430:ILE:HG13	1.93	0.50
1:F:5:ASP:OD2	1:F:353:THR:HG21	2.12	0.50
1:C:169:MET:HA	3:C:551:NDP:O1N	2.11	0.50
1:D:67:ARG:HD2	1:D:140:GLU:OE2	2.11	0.50
1:F:378:VAL:HA	1:F:381:SER:HB2	1.94	0.50
1:A:473:LEU:HD22	1:A:479:THR:HB	1.93	0.50
1:D:369:PRO:HB2	1:D:371:LEU:HD23	1.94	0.50
1:B:369:PRO:HB2	1:B:371:LEU:HD23	1.93	0.50
1:D:211:ARG:HH22	3:D:551:NDP:H71N	1.59	0.50
1:E:89:CYS:HB3	1:E:125:ALA:HB2	1.94	0.50
1:E:316:GLU:O	1:E:340:LYS:HE2	2.12	0.50
1:A:316:GLU:O	1:A:340:LYS:HE2	2.11	0.49
1:B:212:ILE:HG13	6:B:564:HOH:O	2.12	0.49
1:C:103:GLU:HG2	1:C:107:LEU:CD2	2.41	0.49
1:F:378:VAL:HG13	2:F:550:GLU:OE2	2.12	0.49
1:D:183:TYR:CD1	1:D:187:ILE:HD13	2.47	0.49
1:E:354:PRO:O	1:E:357:ASP:HB2	2.12	0.49
1:F:103:GLU:HG2	1:F:107:LEU:CD2	2.42	0.49
1:F:303:GLY:H	1:F:309:ILE:HD11	1.76	0.49
1:F:187:ILE:HA	5:F:552:H3P:CAT	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:HD13	1:A:331:LEU:CD1	2.43	0.49
1:B:354:PRO:O	1:B:357:ASP:HB2	2.11	0.49
1:C:230:ALA:HA	1:C:233:MET:HB2	1.94	0.49
1:A:154:LYS:HD3	1:E:185:SER:O	2.13	0.49
1:F:369:PRO:HB2	1:F:371:LEU:HD23	1.94	0.49
1:A:413:VAL:HG23	1:A:430:ILE:HG13	1.93	0.49
1:E:112:THR:HB	1:E:124:GLY:H	1.76	0.49
1:E:26:ASP:O	1:E:30:GLU:HG3	2.12	0.49
1:A:26:ASP:O	1:A:30:GLU:HG3	2.13	0.49
1:B:368:ILE:HG22	1:B:373:LEU:HB2	1.94	0.49
1:C:321:ILE:HG12	1:C:343:ILE:HB	1.94	0.49
1:C:410:LEU:O	1:C:413:VAL:HG22	2.13	0.49
1:F:315:LEU:HD13	1:F:331:LEU:CD1	2.43	0.49
1:A:321:ILE:HG12	1:A:343:ILE:HB	1.93	0.49
1:C:497:GLY:HA3	1:D:178:TRP:CD1	2.48	0.49
1:A:230:ALA:HA	1:A:233:MET:HB2	1.95	0.49
1:A:7:PRO:HD2	1:A:329:LYS:CD	2.43	0.49
1:C:417:LEU:CD1	1:D:417:LEU:HD21	2.43	0.49
1:E:230:ALA:HA	1:E:233:MET:HB2	1.94	0.49
1:E:321:ILE:HG12	1:E:343:ILE:HB	1.95	0.49
1:C:315:LEU:HD13	1:C:331:LEU:CD1	2.41	0.49
1:D:321:ILE:HG12	1:D:343:ILE:HB	1.94	0.49
1:C:408:HIS:HB3	1:E:436:PHE:HB2	1.94	0.49
1:F:183:TYR:CD1	1:F:187:ILE:HD13	2.48	0.49
1:B:410:LEU:O	1:B:413:VAL:HG22	2.13	0.49
1:F:89:CYS:HB3	1:F:125:ALA:HB2	1.94	0.49
1:B:113:TYR:O	1:B:117:VAL:HG23	2.12	0.49
1:C:183:TYR:CD1	1:C:187:ILE:HD13	2.48	0.48
2:C:550:GLU:HA	3:C:551:NDP:H41N	1.94	0.48
1:D:465:MET:O	1:D:469:MET:HG2	2.13	0.48
1:F:107:LEU:CB	1:F:126:LYS:HG2	2.42	0.48
1:F:321:ILE:HG12	1:F:343:ILE:HB	1.94	0.48
1:F:473:LEU:HD22	1:F:479:THR:HB	1.95	0.48
1:B:230:ALA:HA	1:B:233:MET:HB2	1.96	0.48
1:C:162:VAL:HG11	1:D:190:TYR:HE2	1.77	0.48
1:D:248:ALA:HB1	1:D:272:ALA:HB3	1.94	0.48
1:B:321:ILE:HG12	1:B:343:ILE:HB	1.95	0.48
1:E:79:ARG:HD3	1:E:127:ALA:HB2	1.96	0.48
1:F:114:LYS:NZ	1:F:349:ASN:HD21	2.11	0.48
1:B:209:HIS:HE1	4:B:553:GTP:O1A	1.97	0.48
1:B:88:PRO:HB3	1:B:161:GLY:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:473:LEU:HB3	1:F:476:ASP:HB3	1.95	0.48
1:E:473:LEU:HB3	1:E:476:ASP:HB3	1.94	0.48
1:A:248:ALA:HB1	1:A:272:ALA:HB3	1.95	0.48
1:B:26:ASP:O	1:B:30:GLU:HG3	2.13	0.48
1:C:209:HIS:CD2	1:C:446:LYS:HG3	2.48	0.48
1:D:185:SER:O	1:F:154:LYS:HD3	2.14	0.48
1:E:94:ARG:HB2	1:E:168:ASP:OD2	2.13	0.48
1:F:413:VAL:HG23	1:F:430:ILE:HG13	1.96	0.48
1:A:354:PRO:O	1:A:357:ASP:HB2	2.13	0.48
2:C:550:GLU:O	2:C:550:GLU:HG3	2.14	0.48
1:C:94:ARG:HB2	1:C:168:ASP:OD2	2.14	0.48
1:B:79:ARG:HD3	1:B:127:ALA:HB2	1.95	0.48
1:D:89:CYS:HB3	1:D:125:ALA:HB2	1.95	0.48
1:D:150:MET:CE	1:F:186:THR:HG22	2.44	0.48
1:B:209:HIS:CD2	1:B:446:LYS:HG3	2.49	0.48
1:A:369:PRO:HB2	1:A:371:LEU:HD23	1.95	0.48
1:A:47:GLY:O	1:A:51:ILE:HG13	2.14	0.47
1:B:413:VAL:HG23	1:B:430:ILE:HG13	1.95	0.47
1:B:47:GLY:O	1:B:51:ILE:HG13	2.13	0.47
1:E:183:TYR:CD1	1:E:187:ILE:HD13	2.49	0.47
1:A:23:ILE:HG22	1:A:471:TYR:CD2	2.49	0.47
1:A:67:ARG:HD2	1:A:140:GLU:OE2	2.14	0.47
1:B:221:HIS:HE1	6:B:565:HOH:O	1.96	0.47
1:B:248:ALA:HB1	1:B:272:ALA:HB3	1.97	0.47
1:D:47:GLY:O	1:D:51:ILE:HG13	2.15	0.47
1:E:103:GLU:HG2	1:E:107:LEU:CD2	2.44	0.47
1:F:248:ALA:HB1	1:F:272:ALA:HB3	1.96	0.47
1:B:392:VAL:HG13	1:F:382:TYR:OH	2.14	0.47
1:B:419:ARG:HH12	1:F:431:VAL:CG1	2.28	0.47
1:E:410:LEU:O	1:E:413:VAL:HG22	2.14	0.47
1:F:253:GLY:HA3	3:F:551:NDP:O1A	2.14	0.47
1:F:209:HIS:CE1	4:F:553:GTP:O1A	2.64	0.47
1:D:92:GLY:HA3	2:D:550:GLU:N	2.30	0.47
1:E:369:PRO:HB2	1:E:371:LEU:HD23	1.97	0.47
1:F:88:PRO:HB3	1:F:161:GLY:C	2.35	0.47
1:D:150:MET:HE2	1:F:186:THR:HG22	1.96	0.47
1:D:230:ALA:HA	1:D:233:MET:HB2	1.96	0.47
1:D:315:LEU:HD13	1:D:331:LEU:CD1	2.43	0.47
1:E:107:LEU:CB	1:E:126:LYS:HG2	2.45	0.47
1:E:265:ARG:NH1	4:E:553:GTP:O3G	2.46	0.47
1:C:378:VAL:HA	1:C:381:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:THR:HG1	1:E:140:GLU:HG3	1.79	0.47
1:E:317:VAL:HG22	1:E:318:ASP:N	2.30	0.47
1:B:89:CYS:HB3	1:B:125:ALA:HB2	1.97	0.47
1:F:250:GLN:NE2	1:F:330:GLN:NE2	2.63	0.47
1:E:169:MET:HG2	3:E:551:NDP:O1N	2.15	0.47
1:F:334:SER:O	1:F:337:PRO:HD2	2.15	0.47
5:C:552:H3P:HAI	6:F:572:HOH:O	2.14	0.46
1:E:38:GLU:O	1:E:40:GLN:N	2.47	0.46
1:A:378:VAL:HA	1:A:381:SER:HB2	1.96	0.46
1:E:47:GLY:O	1:E:51:ILE:HG13	2.16	0.46
1:A:382:TYR:OH	1:F:392:VAL:HG13	2.16	0.46
1:B:183:TYR:CD1	1:B:187:ILE:HD13	2.50	0.46
1:A:183:TYR:CD1	1:A:187:ILE:HD13	2.50	0.46
1:C:162:VAL:HG22	1:D:190:TYR:HD2	1.81	0.46
1:B:126:LYS:HZ3	2:B:550:GLU:N	2.12	0.46
1:C:88:PRO:HB3	1:C:161:GLY:C	2.36	0.46
1:D:79:ARG:HD3	1:D:127:ALA:HB2	1.98	0.46
1:D:83:SER:O	1:D:84:GLN:HG3	2.15	0.46
1:E:346:GLU:OE1	1:E:352:THR:HG23	2.16	0.46
1:F:378:VAL:HG22	6:F:555:HOH:O	2.15	0.46
1:B:378:VAL:HA	1:B:381:SER:HB2	1.96	0.46
1:C:473:LEU:HB3	1:C:476:ASP:HB3	1.97	0.46
1:B:483:VAL:O	1:B:487:GLU:HB2	2.16	0.46
1:C:67:ARG:HD2	1:C:140:GLU:OE2	2.15	0.46
1:E:169:MET:HA	3:E:551:NDP:O1N	2.15	0.46
1:A:107:LEU:CB	1:A:126:LYS:HG2	2.45	0.46
1:A:187:ILE:HG23	5:A:552:H3P:HAKA	1.98	0.46
1:D:169:MET:HG2	3:D:551:NDP:O1N	2.15	0.46
1:F:410:LEU:O	1:F:413:VAL:HG22	2.16	0.46
1:A:258:HIS:CD2	1:A:261:ARG:HD3	2.51	0.46
1:C:346:GLU:OE1	1:C:352:THR:HG23	2.15	0.46
1:E:67:ARG:HD2	1:E:140:GLU:OE2	2.16	0.46
1:B:187:ILE:HG23	5:C:554:H3P:HAKA	1.97	0.46
1:B:346:GLU:OE1	1:B:352:THR:HG23	2.15	0.46
1:B:94:ARG:HB2	1:B:168:ASP:OD2	2.16	0.46
1:A:89:CYS:HB3	1:A:125:ALA:HB2	1.97	0.45
1:C:316:GLU:O	1:C:340:LYS:HE2	2.15	0.45
1:C:409:LEU:HD13	1:D:409:LEU:HD11	1.97	0.45
1:A:335:ASN:N	1:A:335:ASN:ND2	2.64	0.45
1:C:465:MET:O	1:C:469:MET:HG2	2.16	0.45
1:D:78:TYR:CE2	1:D:101:VAL:HG22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:LEU:CD1	1:F:417:LEU:HD21	2.46	0.45
1:A:88:PRO:HB3	1:A:161:GLY:C	2.36	0.45
1:C:255:VAL:HG11	3:C:551:NDP:O4D	2.16	0.45
1:E:24:VAL:HG22	1:E:483:VAL:HG22	1.99	0.45
1:E:209:HIS:NE2	1:E:446:LYS:HG3	2.31	0.45
1:A:103:GLU:HG2	1:A:107:LEU:CD2	2.46	0.45
1:B:444:SER:H	1:B:447:ASP:HB2	1.82	0.45
1:B:473:LEU:HB3	1:B:476:ASP:HB3	1.98	0.45
1:C:118:VAL:HG13	1:C:118:VAL:O	2.16	0.45
1:C:287:ASP:HA	1:C:288:PRO:HD3	1.78	0.45
1:E:23:ILE:HG22	1:E:471:TYR:CD2	2.52	0.45
1:F:230:ALA:HA	1:F:233:MET:HB2	1.99	0.45
1:F:258:HIS:CD2	1:F:261:ARG:HD3	2.52	0.45
1:F:7:PRO:HD2	1:F:329:LYS:CD	2.44	0.45
1:A:483:VAL:O	1:A:487:GLU:HB2	2.17	0.45
1:D:346:GLU:OE1	1:D:352:THR:HG23	2.17	0.45
1:F:94:ARG:HB2	1:F:168:ASP:OD2	2.16	0.45
1:A:38:GLU:O	1:A:40:GLN:N	2.49	0.45
1:C:79:ARG:HD3	1:C:127:ALA:HB2	1.99	0.45
1:E:88:PRO:HB3	1:E:161:GLY:C	2.37	0.45
1:F:483:VAL:O	1:F:487:GLU:HB2	2.16	0.45
1:A:364:ASN:HD22	1:A:364:ASN:HA	1.48	0.45
1:E:281:TRP:CB	1:E:310:TYR:HB2	2.47	0.45
1:A:331:LEU:HD23	1:A:360:PHE:HE1	1.81	0.45
1:F:107:LEU:HB2	1:F:126:LYS:HG2	1.97	0.45
1:F:90:LYS:NZ	2:F:550:GLU:OE1	2.39	0.45
1:A:369:PRO:HD3	1:A:477:LEU:HB2	1.99	0.45
1:D:251:GLY:O	1:D:256:GLY:HA3	2.16	0.45
1:E:167:PRO:HG3	1:E:176:MET:CG	2.47	0.45
1:C:258:HIS:CD2	1:C:261:ARG:HD3	2.52	0.44
1:D:107:LEU:CB	1:D:126:LYS:HG2	2.47	0.44
1:D:349:ASN:N	3:D:551:NDP:O2D	2.50	0.44
1:C:126:LYS:NZ	2:C:550:GLU:N	2.65	0.44
1:C:42:ARG:O	1:C:46:ARG:HG3	2.16	0.44
1:B:107:LEU:CB	1:B:126:LYS:HG2	2.47	0.44
1:B:417:LEU:HD21	1:F:417:LEU:CD1	2.47	0.44
1:C:253:GLY:O	1:C:257:LEU:HB3	2.18	0.44
1:D:88:PRO:HB3	1:D:161:GLY:C	2.37	0.44
1:D:255:VAL:HG12	3:D:551:NDP:O2N	2.17	0.44
1:E:246:THR:HG22	1:E:269:LYS:HB3	1.98	0.44
1:A:281:TRP:CB	1:A:310:TYR:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:SER:O	1:A:84:GLN:HG3	2.18	0.44
1:B:258:HIS:CD2	1:B:261:ARG:HD3	2.52	0.44
1:A:478:ARG:HG3	1:A:478:ARG:NH1	2.32	0.44
1:B:364:ASN:HA	1:B:364:ASN:HD22	1.49	0.44
1:D:107:LEU:HB2	1:D:126:LYS:HG2	2.00	0.44
1:D:473:LEU:HB3	1:D:476:ASP:HB3	1.98	0.44
1:F:281:TRP:CB	1:F:310:TYR:HB2	2.47	0.44
1:F:346:GLU:OE1	1:F:352:THR:HG23	2.17	0.44
1:C:162:VAL:CG2	1:D:190:TYR:HD2	2.30	0.44
1:C:24:VAL:O	1:C:25:GLU:C	2.56	0.44
1:D:42:ARG:O	1:D:46:ARG:HG3	2.18	0.44
1:E:24:VAL:O	1:E:25:GLU:C	2.56	0.44
1:E:358:LYS:O	1:E:362:GLU:HG3	2.17	0.44
1:E:331:LEU:HD23	1:E:360:PHE:HE1	1.82	0.44
1:F:187:ILE:HG23	5:F:552:H3P:HAK	1.98	0.44
1:B:281:TRP:CG	1:B:282:ASN:N	2.85	0.44
1:B:92:GLY:H	2:B:550:GLU:N	2.15	0.44
1:D:431:VAL:HG12	1:E:419:ARG:HH12	1.83	0.44
1:C:281:TRP:CG	1:C:282:ASN:N	2.86	0.44
1:D:55:CYS:HA	1:D:82:HIS:HA	2.00	0.44
1:E:12:MET:HG3	1:E:354:PRO:HD3	2.00	0.44
1:A:436:PHE:HB2	1:F:408:HIS:HB3	2.00	0.44
1:B:24:VAL:O	1:B:25:GLU:C	2.56	0.44
1:C:167:PRO:HG3	1:C:176:MET:CG	2.48	0.44
1:C:334:SER:O	1:C:337:PRO:HD2	2.17	0.44
1:C:55:CYS:HA	1:C:82:HIS:HA	2.00	0.44
1:F:253:GLY:O	1:F:257:LEU:HB3	2.18	0.44
1:F:42:ARG:O	1:F:46:ARG:HG3	2.17	0.44
1:A:107:LEU:HB2	1:A:126:LYS:HG2	1.99	0.43
1:A:99:VAL:O	1:A:130:LYS:HE3	2.17	0.43
1:A:211:ARG:NH2	2:A:550:GLU:OE2	2.51	0.43
1:B:409:LEU:HD21	1:F:409:LEU:HD22	1.99	0.43
1:C:215:THR:O	1:C:219:VAL:HG23	2.18	0.43
1:C:244:ASP:OD2	1:C:245:LYS:NZ	2.50	0.43
1:C:7:PRO:O	1:C:329:LYS:NZ	2.51	0.43
1:D:38:GLU:O	1:D:40:GLN:N	2.47	0.43
1:E:334:SER:O	1:E:337:PRO:HD2	2.17	0.43
1:E:55:CYS:HA	1:E:82:HIS:HA	2.00	0.43
1:B:190:TYR:CE2	1:F:162:VAL:HG11	2.52	0.43
1:C:189:HIS:HB3	5:C:554:H3P:CLAF	2.55	0.43
1:E:335:ASN:ND2	1:E:335:ASN:N	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:PRO:HA	6:F:574:HOH:O	2.17	0.43
1:F:335:ASN:ND2	1:F:335:ASN:N	2.65	0.43
1:A:118:VAL:O	1:A:118:VAL:HG13	2.17	0.43
1:A:253:GLY:O	1:A:257:LEU:HB3	2.18	0.43
1:A:334:SER:O	1:A:337:PRO:HD2	2.19	0.43
1:C:251:GLY:O	1:C:256:GLY:HA3	2.18	0.43
1:D:118:VAL:CG1	1:D:120:VAL:HG23	2.48	0.43
1:E:258:HIS:CD2	1:E:261:ARG:HD3	2.52	0.43
1:F:478:ARG:NH1	1:F:478:ARG:HG3	2.33	0.43
1:A:116:ALA:O	1:A:488:LYS:HD2	2.19	0.43
1:A:186:THR:HG22	1:E:150:MET:HE2	2.00	0.43
1:A:246:THR:HG22	1:A:269:LYS:HB3	2.01	0.43
4:A:553:GTP:H2'	4:A:553:GTP:N3	2.33	0.43
1:D:118:VAL:O	1:D:118:VAL:HG13	2.17	0.43
1:D:319:CYS:O	1:D:341:ALA:HA	2.18	0.43
1:D:332:THR:O	1:D:336:ALA:HB2	2.18	0.43
1:E:99:VAL:O	1:E:130:LYS:HE3	2.17	0.43
1:E:250:GLN:NE2	1:E:330:GLN:NE2	2.64	0.43
1:F:281:TRP:CG	1:F:282:ASN:N	2.87	0.43
1:F:281:TRP:HB3	1:F:310:TYR:HB2	2.00	0.43
1:A:221:HIS:HE1	6:A:557:HOH:O	2.01	0.43
1:C:408:HIS:CE1	1:E:435:GLU:HB3	2.53	0.43
1:F:202:PRO:HB2	1:F:205:GLN:HG2	1.99	0.43
1:A:491:ARG:HH11	1:A:491:ARG:CG	2.31	0.43
1:A:55:CYS:HA	1:A:82:HIS:HA	1.99	0.43
1:B:118:VAL:O	1:B:118:VAL:HG13	2.18	0.43
1:B:79:ARG:CD	1:B:127:ALA:HB2	2.49	0.43
1:A:401:TYR:CD2	1:B:443:ALA:HB2	2.53	0.43
1:C:38:GLU:O	1:C:40:GLN:N	2.49	0.43
1:C:478:ARG:HG3	1:C:478:ARG:NH1	2.32	0.43
1:D:410:LEU:HG	1:D:430:ILE:HG22	2.00	0.43
6:C:592:HOH:O	1:D:420:LYS:HB2	2.18	0.43
1:D:483:VAL:O	1:D:487:GLU:HB2	2.18	0.43
1:E:281:TRP:HB3	1:E:310:TYR:HB2	2.01	0.43
1:A:42:ARG:O	1:A:46:ARG:HG3	2.19	0.43
1:B:465:MET:O	1:B:469:MET:HG2	2.18	0.43
1:D:281:TRP:CG	1:D:282:ASN:N	2.87	0.43
1:D:334:SER:O	1:D:337:PRO:HD2	2.19	0.43
1:D:335:ASN:N	1:D:335:ASN:ND2	2.65	0.43
1:A:187:ILE:HA	5:A:552:H3P:CAK	2.49	0.43
1:B:78:TYR:CE2	1:B:101:VAL:HG22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:GLY:HA3	3:D:551:NDP:O1A	2.19	0.43
1:F:250:GLN:HE22	1:F:330:GLN:NE2	2.17	0.43
1:A:118:VAL:CG1	1:A:120:VAL:HG23	2.49	0.43
1:A:202:PRO:HB2	1:A:205:GLN:HG2	2.01	0.43
1:B:253:GLY:O	1:B:257:LEU:HB3	2.18	0.43
1:B:410:LEU:HD12	1:B:410:LEU:HA	1.90	0.43
1:B:58:VAL:O	6:B:570:HOH:O	2.22	0.43
1:D:186:THR:HG22	1:F:150:MET:CE	2.49	0.43
1:E:10:PHE:O	1:E:14:GLU:HG3	2.19	0.43
1:E:79:ARG:CD	1:E:127:ALA:HB2	2.48	0.43
1:A:24:VAL:O	1:A:25:GLU:C	2.57	0.43
1:C:89:CYS:HB3	1:C:125:ALA:HB2	2.01	0.43
1:C:132:ASN:C	1:C:132:ASN:HD22	2.22	0.43
1:C:335:ASN:N	1:C:335:ASN:ND2	2.66	0.43
1:D:94:ARG:HB2	1:D:168:ASP:OD2	2.19	0.43
1:A:17:PHE:CE1	1:A:486:ILE:HG12	2.54	0.42
1:A:78:TYR:CE2	1:A:101:VAL:HG22	2.54	0.42
1:B:99:VAL:O	1:B:130:LYS:HE3	2.19	0.42
1:D:90:LYS:HD2	1:D:164:VAL:HB	2.01	0.42
1:E:253:GLY:O	1:E:257:LEU:HB3	2.19	0.42
1:F:167:PRO:HG3	1:F:176:MET:CG	2.49	0.42
1:F:336:ALA:CB	1:F:337:PRO:HD3	2.45	0.42
1:F:83:SER:O	1:F:84:GLN:HG3	2.19	0.42
1:B:342:LYS:O	1:B:365:ILE:HG23	2.19	0.42
1:B:358:LYS:O	1:B:362:GLU:HG3	2.19	0.42
1:B:38:GLU:O	1:B:40:GLN:N	2.50	0.42
1:C:392:VAL:HG22	1:E:386:LEU:HG	2.00	0.42
1:E:364:ASN:HD22	1:E:364:ASN:HA	1.47	0.42
1:E:478:ARG:HG3	1:E:478:ARG:NH1	2.33	0.42
1:F:465:MET:O	1:F:469:MET:HG2	2.19	0.42
1:A:346:GLU:OE1	1:A:352:THR:HG23	2.18	0.42
1:D:10:PHE:O	1:D:14:GLU:HG3	2.19	0.42
1:D:445:GLU:O	1:D:449:VAL:HG23	2.20	0.42
1:D:495:GLU:O	1:D:496:ALA:HB3	2.18	0.42
1:A:250:GLN:NE2	1:A:330:GLN:NE2	2.65	0.42
1:B:319:CYS:O	1:B:341:ALA:HA	2.19	0.42
1:D:167:PRO:HG3	1:D:176:MET:CG	2.49	0.42
1:D:253:GLY:O	1:D:257:LEU:HB3	2.19	0.42
1:D:99:VAL:O	1:D:130:LYS:HE3	2.20	0.42
1:E:83:SER:HB2	6:E:559:HOH:O	2.18	0.42
1:F:287:ASP:HA	1:F:288:PRO:HD3	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:CYS:HA	1:F:82:HIS:HA	2.01	0.42
1:A:419:ARG:HH12	1:B:431:VAL:CG1	2.33	0.42
1:B:42:ARG:O	1:B:46:ARG:HG3	2.20	0.42
1:F:79:ARG:HD3	1:F:127:ALA:HB2	2.01	0.42
1:F:244:ASP:OD2	1:F:245:LYS:NZ	2.53	0.42
1:F:331:LEU:HD23	1:F:360:PHE:HE1	1.84	0.42
1:F:38:GLU:O	1:F:40:GLN:N	2.48	0.42
1:A:75:ILE:HD13	1:A:129:VAL:HG13	2.01	0.42
1:D:250:GLN:NE2	1:D:330:GLN:NE2	2.64	0.42
1:E:114:LYS:NZ	2:E:550:GLU:O	2.53	0.42
1:F:264:HIS:CD2	1:F:288:PRO:HD3	2.55	0.42
1:A:10:PHE:O	1:A:14:GLU:HG3	2.18	0.42
1:A:445:GLU:O	1:A:449:VAL:HG23	2.19	0.42
1:B:167:PRO:HG3	1:B:176:MET:CG	2.49	0.42
1:B:331:LEU:HD23	1:B:360:PHE:HE1	1.85	0.42
1:B:55:CYS:HA	1:B:82:HIS:HA	2.01	0.42
1:E:410:LEU:HG	1:E:430:ILE:HG22	2.02	0.42
1:B:246:THR:HG22	1:B:269:LYS:HB3	2.02	0.42
1:C:264:HIS:CD2	1:C:288:PRO:HD3	2.55	0.42
1:D:258:HIS:CD2	1:D:261:ARG:HD3	2.54	0.42
1:D:250:GLN:HE22	1:D:330:GLN:HE21	1.63	0.42
3:D:551:NDP:H52N	3:D:551:NDP:H2N	2.02	0.42
1:B:335:ASN:N	1:B:335:ASN:ND2	2.66	0.42
1:B:83:SER:O	1:B:84:GLN:HG3	2.20	0.42
1:C:107:LEU:CB	1:C:126:LYS:HG2	2.50	0.42
1:C:281:TRP:CB	1:C:310:TYR:HB2	2.50	0.42
1:D:202:PRO:HB2	1:D:205:GLN:HG2	2.02	0.42
1:D:24:VAL:O	1:D:25:GLU:C	2.58	0.42
1:D:281:TRP:CB	1:D:310:TYR:HB2	2.49	0.42
1:E:118:VAL:O	1:E:118:VAL:HG13	2.20	0.42
1:E:319:CYS:O	1:E:341:ALA:HA	2.19	0.42
1:E:369:PRO:HD3	1:E:477:LEU:HB2	2.02	0.42
1:F:251:GLY:O	1:F:256:GLY:HA3	2.20	0.42
1:A:79:ARG:CD	1:A:127:ALA:HB2	2.50	0.42
1:B:107:LEU:HB2	1:B:126:LYS:HG2	2.01	0.42
1:C:79:ARG:CD	1:C:127:ALA:HB2	2.50	0.42
1:D:250:GLN:HE22	1:D:330:GLN:NE2	2.17	0.42
1:E:107:LEU:HB2	1:E:126:LYS:HG2	2.01	0.42
1:E:281:TRP:CG	1:E:282:ASN:N	2.88	0.42
1:F:99:VAL:O	1:F:130:LYS:HE3	2.19	0.42
1:F:51:ILE:HD13	1:F:498:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:GLY:O	1:F:51:ILE:HG13	2.19	0.42
1:B:190:TYR:HD2	1:F:162:VAL:HG22	1.85	0.41
1:B:287:ASP:OD1	1:B:290:GLU:HG2	2.20	0.41
1:B:445:GLU:O	1:B:449:VAL:HG23	2.19	0.41
1:D:364:ASN:HA	1:D:364:ASN:HD22	1.51	0.41
1:E:78:TYR:CE2	1:E:101:VAL:HG22	2.55	0.41
1:A:165:PRO:HD2	1:A:197:CYS:O	2.21	0.41
1:A:215:THR:O	1:A:219:VAL:HG23	2.20	0.41
1:C:483:VAL:O	1:C:487:GLU:HB2	2.20	0.41
1:C:90:LYS:HD2	1:C:164:VAL:HB	2.02	0.41
1:E:118:VAL:CG1	1:E:120:VAL:HG23	2.50	0.41
1:E:465:MET:O	1:E:469:MET:HG2	2.20	0.41
1:A:281:TRP:HB3	1:A:310:TYR:HB2	2.02	0.41
1:A:465:MET:O	1:A:469:MET:HG2	2.20	0.41
1:B:75:ILE:HD13	1:B:129:VAL:HG13	2.02	0.41
1:C:369:PRO:HB2	1:C:371:LEU:CD2	2.50	0.41
1:E:202:PRO:HB2	1:E:205:GLN:HG2	2.02	0.41
1:B:251:GLY:O	1:B:256:GLY:HA3	2.21	0.41
1:B:185:SER:O	1:C:154:LYS:HD3	2.19	0.41
1:E:441:SER:HB2	6:E:587:HOH:O	2.21	0.41
1:B:409:LEU:HD11	1:F:409:LEU:HD13	2.02	0.41
1:F:27:LYS:HD3	1:F:487:GLU:OE2	2.20	0.41
1:F:92:GLY:O	1:F:126:LYS:HD3	2.20	0.41
1:B:281:TRP:CB	1:B:310:TYR:HB2	2.50	0.41
1:B:4:GLU:HA	1:B:4:GLU:OE1	2.20	0.41
1:C:250:GLN:HE22	1:C:330:GLN:HE21	1.65	0.41
1:C:497:GLY:HA3	1:D:146:ARG:NH2	2.36	0.41
1:D:287:ASP:HA	1:D:288:PRO:HD3	1.76	0.41
1:B:419:ARG:NH1	1:F:431:VAL:HG12	2.35	0.41
1:F:445:GLU:O	1:F:449:VAL:HG23	2.19	0.41
1:F:209:HIS:CD2	1:F:446:LYS:HG3	2.55	0.41
1:F:78:TYR:CE2	1:F:101:VAL:HG22	2.56	0.41
1:A:132:ASN:C	1:A:132:ASN:HD22	2.22	0.41
1:A:94:ARG:HB2	1:A:168:ASP:OD2	2.20	0.41
1:A:186:THR:HG22	1:E:150:MET:CE	2.49	0.41
1:A:253:GLY:HA3	3:A:551:NDP:O1A	2.21	0.41
1:C:248:ALA:CB	1:C:272:ALA:HB3	2.51	0.41
1:C:92:GLY:N	2:C:550:GLU:HB3	2.33	0.41
1:E:287:ASP:HA	1:E:288:PRO:HD3	1.79	0.41
1:E:287:ASP:OD1	1:E:290:GLU:HG2	2.21	0.41
1:F:187:ILE:HA	5:F:552:H3P:HAKA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:VAL:O	1:F:25:GLU:C	2.58	0.41
1:C:255:VAL:HG12	3:C:551:NDP:O2N	2.20	0.41
1:C:319:CYS:O	1:C:341:ALA:HA	2.20	0.41
1:C:410:LEU:HG	1:C:430:ILE:HG22	2.02	0.41
1:D:23:ILE:HG22	1:D:471:TYR:CD2	2.56	0.41
1:D:246:THR:HG22	1:D:269:LYS:HB3	2.02	0.41
2:D:550:GLU:CB	3:D:551:NDP:H41N	2.50	0.41
1:B:190:TYR:HD2	1:F:162:VAL:CG2	2.33	0.41
1:F:332:THR:O	1:F:336:ALA:HB2	2.20	0.41
1:A:358:LYS:O	1:A:362:GLU:HG3	2.21	0.41
1:B:90:LYS:HD2	1:B:164:VAL:HB	2.02	0.41
1:C:162:VAL:HG11	1:D:190:TYR:CE2	2.56	0.41
1:D:132:ASN:C	1:D:132:ASN:HD22	2.24	0.41
1:D:209:HIS:CD2	1:D:446:LYS:HG3	2.56	0.41
1:D:244:ASP:OD2	1:D:245:LYS:NZ	2.54	0.41
1:A:251:GLY:O	1:A:256:GLY:HA3	2.21	0.41
1:B:264:HIS:CD2	1:B:288:PRO:HD3	2.56	0.41
1:C:83:SER:O	1:C:84:GLN:HG3	2.21	0.41
1:D:331:LEU:HD23	1:D:360:PHE:HE1	1.84	0.41
1:D:346:GLU:HG2	1:D:351:PRO:CG	2.51	0.41
1:D:92:GLY:O	1:D:126:LYS:HD3	2.21	0.41
1:E:253:GLY:HA3	3:E:551:NDP:O1A	2.21	0.41
1:D:433:THR:HG23	1:E:412:SER:HA	2.03	0.41
1:E:445:GLU:O	1:E:449:VAL:HG23	2.21	0.41
1:E:83:SER:O	1:E:84:GLN:HG3	2.20	0.41
1:B:169:MET:HA	3:B:551:NDP:O1N	2.20	0.41
1:B:17:PHE:CE2	1:B:53:LYS:HG3	2.56	0.41
1:B:94:ARG:HE	1:B:169:MET:HG3	1.86	0.41
1:C:346:GLU:HG2	1:C:351:PRO:HG2	2.02	0.41
1:C:16:PHE:CG	1:C:478:ARG:HD3	2.55	0.41
1:E:251:GLY:O	1:E:256:GLY:HA3	2.21	0.41
1:E:332:THR:O	1:E:336:ALA:HB2	2.21	0.41
1:A:281:TRP:CG	1:A:282:ASN:N	2.89	0.41
1:B:235:ILE:HG13	1:B:235:ILE:H	1.72	0.41
1:B:317:VAL:HG22	1:B:318:ASP:N	2.36	0.41
1:C:99:VAL:O	1:C:130:LYS:HE3	2.21	0.41
1:C:20:GLY:O	1:C:24:VAL:HG23	2.21	0.41
1:E:75:ILE:HD13	1:E:129:VAL:HG13	2.03	0.41
1:F:358:LYS:O	1:F:362:GLU:HG3	2.20	0.41
1:A:332:THR:O	1:A:336:ALA:HB2	2.21	0.40
1:A:187:ILE:HG23	5:A:552:H3P:CAK	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:VAL:HG22	6:D:559:HOH:O	2.21	0.40
1:E:183:TYR:HA	1:E:187:ILE:HD12	2.03	0.40
1:E:483:VAL:O	1:E:487:GLU:HB2	2.20	0.40
1:C:250:GLN:HE22	1:C:330:GLN:NE2	2.19	0.40
1:C:250:GLN:NE2	1:C:330:GLN:NE2	2.66	0.40
1:C:419:ARG:HH12	1:E:431:VAL:HG12	1.86	0.40
1:D:221:HIS:HE1	6:D:562:HOH:O	2.03	0.40
1:E:94:ARG:HG3	1:E:169:MET:HB2	2.03	0.40
1:E:410:LEU:HA	1:E:410:LEU:HD12	1.91	0.40
1:F:319:CYS:O	1:F:341:ALA:HA	2.22	0.40
1:A:229:GLU:C	1:A:231:SER:H	2.24	0.40
1:A:53:LYS:O	1:A:82:HIS:HE1	2.04	0.40
1:C:10:PHE:O	1:C:14:GLU:HG3	2.22	0.40
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.86	0.40
1:E:235:ILE:H	1:E:235:ILE:HG13	1.71	0.40
1:F:118:VAL:CG1	1:F:120:VAL:HG23	2.51	0.40
1:F:8:ASN:OD1	1:F:11:LYS:HE3	2.21	0.40
1:A:167:PRO:HG3	1:A:176:MET:CG	2.52	0.40
1:D:281:TRP:HB3	1:D:310:TYR:HB2	2.03	0.40
1:D:358:LYS:O	1:D:362:GLU:HG3	2.22	0.40
1:E:132:ASN:HD22	1:E:132:ASN:C	2.25	0.40
1:E:9:PHE:O	1:E:12:MET:HB3	2.20	0.40
1:F:215:THR:O	1:F:219:VAL:HG23	2.21	0.40
1:C:58:VAL:HB	1:F:60:SER:HB2	2.02	0.40
1:A:162:VAL:HA	6:A:582:HOH:O	2.20	0.40
1:C:281:TRP:HB3	1:C:310:TYR:HB2	2.03	0.40
1:C:287:ASP:OD1	1:C:290:GLU:HG2	2.22	0.40
1:C:348:ALA:HA	3:C:551:NDP:H1D	2.04	0.40
1:D:109:SER:O	1:D:112:THR:HG23	2.21	0.40
1:D:229:GLU:C	1:D:231:SER:H	2.25	0.40
1:D:346:GLU:HG2	1:D:351:PRO:HG2	2.04	0.40
1:D:116:ALA:O	1:D:488:LYS:HD2	2.21	0.40
1:F:246:THR:HG22	1:F:269:LYS:HB3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ARG:CG	1:C:38:GLU:OE2[2_657]	2.06	0.14

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	493/501 (98%)	444 (90%)	39 (8%)	10 (2%)	7 34
1	B	493/501 (98%)	442 (90%)	43 (9%)	8 (2%)	9 40
1	C	493/501 (98%)	441 (90%)	44 (9%)	8 (2%)	9 40
1	D	493/501 (98%)	441 (90%)	45 (9%)	7 (1%)	11 43
1	E	493/501 (98%)	435 (88%)	48 (10%)	10 (2%)	7 34
1	F	493/501 (98%)	444 (90%)	42 (8%)	7 (1%)	11 43
All	All	2958/3006 (98%)	2647 (90%)	261 (9%)	50 (2%)	9 39

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	474	GLY
1	A	496	ALA
1	B	39	GLU
1	B	474	GLY
1	C	39	GLU
1	C	474	GLY
1	C	494	ASN
1	D	39	GLU
1	D	474	GLY
1	E	39	GLU
1	E	474	GLY
1	F	39	GLU
1	F	474	GLY
1	A	334	SER
1	A	494	ASN
1	B	5	ASP
1	B	334	SER
1	C	334	SER
1	C	422	GLY

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Mol	Chain	Res	Type
1	D	334	SER
1	D	422	GLY
1	E	334	SER
1	E	495	GLU
1	F	334	SER
1	F	422	GLY
1	A	130	LYS
1	A	422	GLY
1	B	422	GLY
1	E	422	GLY
1	A	9	PHE
1	B	371	LEU
1	D	130	LYS
1	E	8	ASN
1	E	130	LYS
1	F	5	ASP
1	F	130	LYS
1	C	243	GLY
1	F	243	GLY
1	A	243	GLY
1	B	243	GLY
1	C	158	ILE
1	D	243	GLY
1	E	243	GLY
1	A	158	ILE
1	C	440	ILE
1	D	158	ILE
1	E	440	ILE
1	B	158	ILE
1	E	158	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	412/417 (99%)	380 (92%)	32 (8%)	12 42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	412/417 (99%)	385 (93%)	27 (7%)	16 49
1	C	412/417 (99%)	383 (93%)	29 (7%)	15 47
1	D	412/417 (99%)	383 (93%)	29 (7%)	15 47
1	E	412/417 (99%)	382 (93%)	30 (7%)	14 44
1	F	412/417 (99%)	386 (94%)	26 (6%)	18 51
All	All	2472/2502 (99%)	2299 (93%)	173 (7%)	14 47

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	24	VAL
1	A	33	LYS
1	A	35	ARG
1	A	75	ILE
1	A	102	ASP
1	A	107	LEU
1	A	112	THR
1	A	118	VAL
1	A	132	ASN
1	A	145	THR
1	A	162	VAL
1	A	187	ILE
1	A	254	ASN
1	A	277	ASP
1	A	291	LEU
1	A	331	LEU
1	A	335	ASN
1	A	340	LYS
1	A	352	THR
1	A	361	LEU
1	A	364	ASN
1	A	378	VAL
1	A	381	SER
1	A	386	LEU
1	A	392	VAL
1	A	394	TYR
1	A	410	LEU
1	A	416	SER
1	A	491	ARG

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Mol	Chain	Res	Type
1	A	494	ASN
1	A	495	GLU
1	B	9	PHE
1	B	24	VAL
1	B	33	LYS
1	B	35	ARG
1	B	75	ILE
1	B	102	ASP
1	B	107	LEU
1	B	112	THR
1	B	118	VAL
1	B	132	ASN
1	B	145	THR
1	B	162	VAL
1	B	187	ILE
1	B	254	ASN
1	B	277	ASP
1	B	291	LEU
1	B	335	ASN
1	B	340	LYS
1	B	352	THR
1	B	361	LEU
1	B	364	ASN
1	B	378	VAL
1	B	381	SER
1	B	386	LEU
1	B	392	VAL
1	B	394	TYR
1	B	410	LEU
1	C	9	PHE
1	C	24	VAL
1	C	33	LYS
1	C	35	ARG
1	C	75	ILE
1	C	107	LEU
1	C	112	THR
1	C	118	VAL
1	C	132	ASN
1	C	145	THR
1	C	162	VAL
1	C	187	ILE
1	C	254	ASN

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Mol	Chain	Res	Type
1	C	277	ASP
1	C	291	LEU
1	C	331	LEU
1	C	335	ASN
1	C	340	LYS
1	C	352	THR
1	C	361	LEU
1	C	364	ASN
1	C	378	VAL
1	C	381	SER
1	C	386	LEU
1	C	392	VAL
1	C	394	TYR
1	C	410	LEU
1	C	416	SER
1	C	494	ASN
1	D	4	GLU
1	D	9	PHE
1	D	24	VAL
1	D	33	LYS
1	D	35	ARG
1	D	75	ILE
1	D	102	ASP
1	D	107	LEU
1	D	112	THR
1	D	118	VAL
1	D	132	ASN
1	D	145	THR
1	D	162	VAL
1	D	187	ILE
1	D	254	ASN
1	D	277	ASP
1	D	291	LEU
1	D	331	LEU
1	D	335	ASN
1	D	340	LYS
1	D	352	THR
1	D	361	LEU
1	D	364	ASN
1	D	378	VAL
1	D	381	SER
1	D	386	LEU

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Mol	Chain	Res	Type
1	D	392	VAL
1	D	394	TYR
1	D	410	LEU
1	E	24	VAL
1	E	33	LYS
1	E	35	ARG
1	E	75	ILE
1	E	102	ASP
1	E	107	LEU
1	E	112	THR
1	E	118	VAL
1	E	132	ASN
1	E	145	THR
1	E	162	VAL
1	E	187	ILE
1	E	254	ASN
1	E	277	ASP
1	E	291	LEU
1	E	331	LEU
1	E	335	ASN
1	E	340	LYS
1	E	352	THR
1	E	361	LEU
1	E	364	ASN
1	E	378	VAL
1	E	381	SER
1	E	386	LEU
1	E	392	VAL
1	E	394	TYR
1	E	410	LEU
1	E	416	SER
1	E	491	ARG
1	E	494	ASN
1	F	8	ASN
1	F	24	VAL
1	F	33	LYS
1	F	35	ARG
1	F	75	ILE
1	F	102	ASP
1	F	107	LEU
1	F	112	THR
1	F	118	VAL

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Mol	Chain	Res	Type
1	F	132	ASN
1	F	145	THR
1	F	187	ILE
1	F	254	ASN
1	F	277	ASP
1	F	291	LEU
1	F	335	ASN
1	F	340	LYS
1	F	352	THR
1	F	361	LEU
1	F	364	ASN
1	F	378	VAL
1	F	381	SER
1	F	386	LEU
1	F	392	VAL
1	F	394	TYR
1	F	410	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	56	ASN
1	A	82	HIS
1	A	132	ASN
1	A	250	GLN
1	A	254	ASN
1	A	258	HIS
1	A	298	HIS
1	A	335	ASN
1	A	364	ASN
1	A	388	ASN
1	A	390	ASN
1	A	406	ASN
1	A	408	HIS
1	B	43	ASN
1	B	56	ASN
1	B	82	HIS
1	B	132	ASN
1	B	209	HIS
1	B	250	GLN
1	B	254	ASN

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Mol	Chain	Res	Type
1	B	258	HIS
1	B	298	HIS
1	B	335	ASN
1	B	364	ASN
1	B	388	ASN
1	B	390	ASN
1	B	406	ASN
1	B	494	ASN
1	C	43	ASN
1	C	56	ASN
1	C	82	HIS
1	C	132	ASN
1	C	205	GLN
1	C	250	GLN
1	C	254	ASN
1	C	258	HIS
1	C	298	HIS
1	C	335	ASN
1	C	364	ASN
1	C	388	ASN
1	C	390	ASN
1	C	406	ASN
1	C	408	HIS
1	C	494	ASN
1	D	43	ASN
1	D	56	ASN
1	D	82	HIS
1	D	132	ASN
1	D	250	GLN
1	D	254	ASN
1	D	258	HIS
1	D	298	HIS
1	D	335	ASN
1	D	364	ASN
1	D	388	ASN
1	D	390	ASN
1	D	406	ASN
1	D	408	HIS
1	D	484	ASN
1	E	43	ASN
1	E	56	ASN
1	E	82	HIS

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Mol	Chain	Res	Type
1	E	132	ASN
1	E	209	HIS
1	E	250	GLN
1	E	254	ASN
1	E	258	HIS
1	E	298	HIS
1	E	335	ASN
1	E	364	ASN
1	E	388	ASN
1	E	390	ASN
1	E	406	ASN
1	F	43	ASN
1	F	56	ASN
1	F	82	HIS
1	F	132	ASN
1	F	209	HIS
1	F	250	GLN
1	F	254	ASN
1	F	258	HIS
1	F	298	HIS
1	F	335	ASN
1	F	364	ASN
1	F	388	ASN
1	F	390	ASN
1	F	406	ASN
1	F	408	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	H3P	C	554	-	22,22,22	0.37	0	27,33,33	0.78	0
4	GTP	B	553	-	26,34,34	1.69	6 (23%)	33,54,54	3.16	19 (57%)
3	NDP	E	551	-	45,52,52	1.56	8 (17%)	53,80,80	2.45	15 (28%)
3	NDP	B	551	-	45,52,52	1.65	6 (13%)	53,80,80	2.45	15 (28%)
4	GTP	F	553	-	26,34,34	1.69	6 (23%)	33,54,54	2.42	13 (39%)
3	NDP	D	551	-	45,52,52	1.60	8 (17%)	53,80,80	2.41	15 (28%)
5	H3P	C	552	-	22,22,22	0.38	0	27,33,33	1.31	2 (7%)
4	GTP	A	553	-	26,34,34	1.47	4 (15%)	33,54,54	2.15	11 (33%)
4	GTP	C	553	-	26,34,34	1.78	6 (23%)	33,54,54	2.17	9 (27%)
5	H3P	A	552	-	22,22,22	0.37	0	27,33,33	0.82	0
3	NDP	C	551	-	45,52,52	1.40	6 (13%)	53,80,80	2.51	20 (37%)
3	NDP	F	551	-	45,52,52	1.57	6 (13%)	53,80,80	2.45	15 (28%)
5	H3P	B	552	-	22,22,22	0.50	0	27,33,33	1.16	2 (7%)
5	H3P	D	552	-	22,22,22	0.69	0	27,33,33	1.24	2 (7%)
4	GTP	D	553	-	26,34,34	1.68	6 (23%)	33,54,54	2.84	14 (42%)
5	H3P	F	552	-	22,22,22	0.57	0	27,33,33	0.79	0
3	NDP	A	551	-	45,52,52	1.68	6 (13%)	53,80,80	2.46	14 (26%)
4	GTP	E	553	-	26,34,34	1.58	4 (15%)	33,54,54	2.67	13 (39%)

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
5	H3P	C	554	-	-	0/4/4/4	0/2/2/2
4	GTP	B	553	-	-	2/18/38/38	0/3/3/3
3	NDP	E	551	-	-	3/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	B	551	-	-	3/30/77/77	0/5/5/5
4	GTP	F	553	-	-	2/18/38/38	0/3/3/3
3	NDP	D	551	-	-	3/30/77/77	0/5/5/5
5	H3P	C	552	-	-	0/4/4/4	0/2/2/2
4	GTP	A	553	-	-	0/18/38/38	0/3/3/3
4	GTP	C	553	-	-	0/18/38/38	0/3/3/3
5	H3P	A	552	-	-	0/4/4/4	0/2/2/2
3	NDP	C	551	-	-	2/30/77/77	0/5/5/5
3	NDP	F	551	-	-	2/30/77/77	0/5/5/5
5	H3P	B	552	-	-	0/4/4/4	0/2/2/2
5	H3P	D	552	-	-	0/4/4/4	0/2/2/2
4	GTP	D	553	-	-	2/18/38/38	0/3/3/3
5	H3P	F	552	-	-	0/4/4/4	0/2/2/2
3	NDP	A	551	-	-	4/30/77/77	0/5/5/5
4	GTP	E	553	-	-	3/18/38/38	0/3/3/3

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	551	NDP	O4B-C1B	6.30	1.49	1.41
3	A	551	NDP	O4B-C1B	5.90	1.49	1.41
4	C	553	GTP	C2'-C1'	5.00	1.61	1.53
3	E	551	NDP	O4B-C1B	4.97	1.48	1.41
3	D	551	NDP	O4B-C1B	4.85	1.47	1.41
4	F	553	GTP	C2'-C1'	4.30	1.60	1.53
4	A	553	GTP	O4'-C1'	4.26	1.47	1.41
4	E	553	GTP	O4'-C1'	4.20	1.46	1.41
3	F	551	NDP	O4D-C1D	4.14	1.51	1.42
3	C	551	NDP	O4B-C1B	4.14	1.46	1.41
3	D	551	NDP	O4D-C1D	3.96	1.51	1.42
3	B	551	NDP	O4D-C1D	3.73	1.50	1.42
3	A	551	NDP	O4D-C1D	3.64	1.50	1.42
3	E	551	NDP	O4D-C1D	3.62	1.50	1.42
4	B	553	GTP	C2'-C3'	3.54	1.63	1.53
3	F	551	NDP	P2B-O2B	3.52	1.66	1.59
4	C	553	GTP	O4'-C1'	3.51	1.46	1.41
3	F	551	NDP	O4B-C1B	3.48	1.45	1.41
4	B	553	GTP	C8-N7	-3.44	1.28	1.34
4	D	553	GTP	C3'-C4'	3.34	1.61	1.53
4	B	553	GTP	C2'-C1'	3.32	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	553	GTP	C8-N7	-3.18	1.29	1.34
3	F	551	NDP	C7N-C3N	-3.15	1.41	1.48
4	D	553	GTP	C8-N7	-3.12	1.29	1.34
3	A	551	NDP	P2B-O2B	2.96	1.64	1.59
4	F	553	GTP	O4'-C1'	2.94	1.45	1.41
3	C	551	NDP	O4D-C1D	2.93	1.48	1.42
4	E	553	GTP	C2'-C1'	2.88	1.58	1.53
4	C	553	GTP	C2'-C3'	2.88	1.61	1.53
3	E	551	NDP	C3B-C2B	2.82	1.59	1.52
4	B	553	GTP	C3'-C4'	2.75	1.60	1.53
3	D	551	NDP	P2B-O2B	2.75	1.64	1.59
3	D	551	NDP	C7N-C3N	-2.75	1.42	1.48
4	F	553	GTP	C8-N7	-2.74	1.29	1.34
4	D	553	GTP	C2'-C1'	2.71	1.57	1.53
4	E	553	GTP	C8-N7	-2.68	1.29	1.34
3	A	551	NDP	PA-O5B	2.59	1.69	1.59
4	D	553	GTP	O4'-C1'	2.58	1.44	1.41
4	C	553	GTP	C6-C5	2.56	1.45	1.41
3	E	551	NDP	P2B-O2B	2.53	1.64	1.59
3	E	551	NDP	P2B-O2X	2.48	1.64	1.54
4	F	553	GTP	C2'-C3'	2.46	1.60	1.53
3	C	551	NDP	C7N-C3N	-2.39	1.43	1.48
3	C	551	NDP	P2B-O2X	2.37	1.64	1.54
4	D	553	GTP	C6-N1	2.36	1.37	1.33
3	A	551	NDP	C5B-C4B	2.32	1.58	1.51
3	A	551	NDP	P2B-O2X	2.31	1.63	1.54
3	B	551	NDP	C5B-C4B	2.31	1.58	1.51
3	B	551	NDP	PA-O5B	2.30	1.68	1.59
3	C	551	NDP	PA-O5B	2.28	1.68	1.59
4	F	553	GTP	C6-N1	2.28	1.37	1.33
3	D	551	NDP	C1D-N1N	2.25	1.52	1.46
4	C	553	GTP	C6-N1	2.20	1.36	1.33
4	D	553	GTP	C2'-C3'	2.20	1.59	1.53
3	F	551	NDP	C1D-N1N	2.20	1.52	1.46
3	B	551	NDP	C7N-C3N	-2.17	1.44	1.48
3	E	551	NDP	PA-O5B	2.16	1.68	1.59
3	F	551	NDP	P2B-O2X	2.15	1.63	1.54
4	A	553	GTP	PG-O3G	2.14	1.63	1.54
4	B	553	GTP	C6-N1	2.13	1.36	1.33
4	E	553	GTP	PA-O2A	2.13	1.65	1.55
3	D	551	NDP	PA-O5B	2.11	1.67	1.59
3	E	551	NDP	P2B-O3X	2.10	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	553	GTP	C3'-C4'	2.10	1.58	1.53
4	C	553	GTP	PG-O3G	2.09	1.62	1.54
4	B	553	GTP	PG-O2G	2.09	1.62	1.54
3	B	551	NDP	P2B-O2X	2.09	1.62	1.54
3	C	551	NDP	C8A-N7A	-2.06	1.31	1.34
3	D	551	NDP	P2B-O3X	2.06	1.62	1.54
3	E	551	NDP	PN-O2N	2.05	1.64	1.55
3	D	551	NDP	P2B-O2X	2.05	1.62	1.54
4	A	553	GTP	PG-O2G	2.04	1.62	1.54

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	551	NDP	PN-O3-PA	-8.86	102.43	132.83
3	E	551	NDP	PN-O3-PA	-8.85	102.47	132.83
3	C	551	NDP	PN-O3-PA	-8.34	104.21	132.83
3	D	551	NDP	PN-O3-PA	-8.04	105.23	132.83
3	B	551	NDP	PN-O3-PA	-7.80	106.05	132.83
3	F	551	NDP	PN-O3-PA	-7.75	106.24	132.83
4	B	553	GTP	O2G-PG-O3B	-6.89	81.53	104.64
4	D	553	GTP	O2A-PA-O1A	-6.18	81.68	112.24
4	D	553	GTP	O5'-PA-O1A	6.17	133.18	109.07
4	D	553	GTP	O2A-PA-O5'	-5.98	79.97	107.75
4	B	553	GTP	O3G-PG-O3B	-5.88	84.91	104.64
3	E	551	NDP	O5B-PA-O1A	-5.84	86.23	109.07
3	C	551	NDP	O2N-PN-O5D	-5.80	80.83	107.75
4	C	553	GTP	C2-N3-C4	5.77	121.95	115.36
3	D	551	NDP	O5D-PN-O1N	-5.72	86.72	109.07
3	B	551	NDP	O5B-PA-O1A	-5.70	86.80	109.07
3	F	551	NDP	O2N-PN-O5D	-5.60	81.72	107.75
3	E	551	NDP	O2N-PN-O5D	-5.57	81.87	107.75
4	E	553	GTP	PB-O3B-PG	-5.56	113.74	132.83
3	B	551	NDP	O5D-PN-O1N	-5.54	87.40	109.07
4	E	553	GTP	O5'-PA-O1A	5.54	130.70	109.07
3	C	551	NDP	O5B-PA-O1A	-5.53	87.47	109.07
3	A	551	NDP	O2N-PN-O5D	-5.41	82.62	107.75
3	F	551	NDP	O5D-PN-O1N	-5.31	88.32	109.07
3	D	551	NDP	O2N-PN-O5D	-5.30	83.13	107.75
4	F	553	GTP	PB-O3B-PG	-5.27	114.74	132.83
3	F	551	NDP	O5B-PA-O1A	-5.26	88.52	109.07
4	B	553	GTP	O5'-C5'-C4'	-5.20	91.10	108.99
4	E	553	GTP	O2A-PA-O5'	-5.18	83.67	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	551	NDP	O5D-PN-O1N	-5.14	88.99	109.07
3	E	551	NDP	O5D-PN-O1N	-5.13	89.01	109.07
3	D	551	NDP	O4B-C1B-C2B	-5.09	97.76	106.59
4	A	553	GTP	PA-O3A-PB	-5.09	115.37	132.83
3	A	551	NDP	C2D-C3D-C4D	5.07	112.50	102.64
4	E	553	GTP	C2-N3-C4	5.07	121.14	115.36
3	A	551	NDP	O5B-PA-O1A	-5.05	89.35	109.07
3	B	551	NDP	O2N-PN-O5D	-4.98	84.61	107.75
4	C	553	GTP	O4'-C1'-C2'	-4.86	99.82	106.93
3	F	551	NDP	O4D-C1D-N1N	4.85	117.54	108.06
3	A	551	NDP	O4B-C1B-C2B	-4.85	98.18	106.59
4	D	553	GTP	PB-O3B-PG	-4.83	116.26	132.83
4	A	553	GTP	C2-N3-C4	4.82	120.87	115.36
3	B	551	NDP	O4B-C1B-C2B	-4.79	98.28	106.59
4	B	553	GTP	O3B-PG-O1G	-4.78	84.70	111.19
3	D	551	NDP	C2D-C3D-C4D	4.76	111.88	102.64
4	E	553	GTP	O2A-PA-O1A	-4.74	88.80	112.24
4	F	553	GTP	C2-N3-C4	4.72	120.75	115.36
3	B	551	NDP	C2D-C3D-C4D	4.72	111.81	102.64
4	B	553	GTP	C2-N3-C4	4.71	120.73	115.36
4	D	553	GTP	C2-N3-C4	4.69	120.72	115.36
3	B	551	NDP	O4D-C1D-N1N	4.67	117.19	108.06
3	D	551	NDP	O5B-PA-O1A	-4.58	91.17	109.07
4	F	553	GTP	O5'-C5'-C4'	-4.56	93.31	108.99
3	A	551	NDP	O5D-PN-O1N	-4.56	91.27	109.07
3	D	551	NDP	N3A-C2A-N1A	-4.54	121.58	128.68
3	C	551	NDP	O4D-C1D-N1N	4.43	116.72	108.06
3	C	551	NDP	O4B-C1B-C2B	-4.41	98.95	106.59
4	A	553	GTP	PB-O3B-PG	-4.41	117.71	132.83
4	D	553	GTP	C1'-N9-C4	4.32	134.23	126.64
4	C	553	GTP	PB-O3B-PG	-4.30	118.09	132.83
4	B	553	GTP	C3'-C2'-C1'	-4.28	94.53	100.98
3	B	551	NDP	N3A-C2A-N1A	-4.25	122.03	128.68
3	E	551	NDP	O4B-C1B-C2B	-4.21	99.28	106.59
3	F	551	NDP	N3A-C2A-N1A	-4.21	122.09	128.68
3	E	551	NDP	N3A-C2A-N1A	-4.16	122.17	128.68
5	C	552	H3P	CAU-CAK-CAT	-4.16	108.27	117.85
4	F	553	GTP	O4'-C4'-C5'	4.14	122.98	109.37
3	C	551	NDP	C2D-C3D-C4D	4.09	110.59	102.64
3	A	551	NDP	O4D-C1D-N1N	4.09	116.04	108.06
3	A	551	NDP	N3A-C2A-N1A	-4.07	122.31	128.68
3	D	551	NDP	O2A-PA-O5B	-4.05	88.95	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	553	GTP	O4'-C1'-C2'	-4.03	101.04	106.93
4	B	553	GTP	O4'-C4'-C5'	4.00	122.52	109.37
4	B	553	GTP	N3-C2-N1	-3.98	121.92	127.22
4	E	553	GTP	O4'-C4'-C5'	3.96	122.42	109.37
3	F	551	NDP	O4B-C1B-C2B	-3.96	99.72	106.59
3	F	551	NDP	C2D-C3D-C4D	3.95	110.31	102.64
5	D	552	H3P	CAU-CAK-CAT	-3.94	108.76	117.85
3	C	551	NDP	N3A-C2A-N1A	-3.94	122.52	128.68
3	E	551	NDP	C2D-C3D-C4D	3.93	110.29	102.64
4	A	553	GTP	C5-C6-N1	-3.86	118.15	123.43
4	C	553	GTP	N3-C2-N1	-3.81	122.14	127.22
5	B	552	H3P	CAU-CAK-CAT	-3.78	109.13	117.85
4	F	553	GTP	N3-C2-N1	-3.78	122.18	127.22
3	F	551	NDP	O2A-PA-O5B	-3.75	90.34	107.75
4	F	553	GTP	O4'-C1'-C2'	-3.72	101.48	106.93
4	A	553	GTP	N3-C2-N1	-3.70	122.28	127.22
3	B	551	NDP	O2A-PA-O5B	-3.67	90.70	107.75
3	A	551	NDP	O2A-PA-O5B	-3.67	90.71	107.75
4	B	553	GTP	C5-C6-N1	-3.66	118.42	123.43
4	E	553	GTP	N3-C2-N1	-3.64	122.37	127.22
4	C	553	GTP	C5-C6-N1	-3.57	118.55	123.43
4	F	553	GTP	C5-C6-N1	-3.53	118.61	123.43
4	D	553	GTP	N3-C2-N1	-3.50	122.55	127.22
4	E	553	GTP	C5-C6-N1	-3.45	118.71	123.43
4	D	553	GTP	O4'-C4'-C5'	3.40	120.57	109.37
4	D	553	GTP	C5-C6-N1	-3.36	118.83	123.43
4	B	553	GTP	C1'-N9-C4	3.33	132.49	126.64
4	B	553	GTP	O2G-PG-O1G	3.27	123.49	110.68
3	E	551	NDP	O4D-C1D-N1N	3.24	114.40	108.06
4	F	553	GTP	C1'-N9-C4	3.22	132.30	126.64
4	B	553	GTP	C2'-C3'-C4'	-3.20	96.43	102.64
4	F	553	GTP	C2'-C3'-C4'	-3.14	96.53	102.64
4	E	553	GTP	O4'-C1'-C2'	-3.13	102.34	106.93
3	D	551	NDP	O4D-C1D-N1N	3.13	114.17	108.06
4	B	553	GTP	C5'-C4'-C3'	3.08	126.73	115.18
4	E	553	GTP	C1'-N9-C4	3.06	132.01	126.64
4	D	553	GTP	C3'-C2'-C1'	-3.02	96.43	100.98
3	C	551	NDP	O2A-PA-O5B	-3.02	93.74	107.75
3	F	551	NDP	C2D-C1D-N1N	-2.99	105.82	113.30
3	C	551	NDP	C2D-C1D-N1N	-2.91	106.00	113.30
3	E	551	NDP	O5D-C5D-C4D	2.90	118.97	108.99
4	B	553	GTP	PB-O3B-PG	-2.89	122.90	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	553	GTP	C6-C5-C4	-2.89	118.04	120.80
4	C	553	GTP	C6-N1-C2	2.88	120.51	115.93
4	B	553	GTP	C6-N1-C2	2.87	120.50	115.93
4	A	553	GTP	C6-N1-C2	2.85	120.46	115.93
4	A	553	GTP	O3G-PG-O3B	2.85	114.19	104.64
3	F	551	NDP	C4A-C5A-N7A	-2.84	106.44	109.40
3	B	551	NDP	O4D-C4D-C5D	-2.83	100.06	109.37
3	E	551	NDP	O2A-PA-O5B	-2.80	94.72	107.75
4	A	553	GTP	C3'-C2'-C1'	2.76	105.13	100.98
3	C	551	NDP	C3N-C2N-N1N	-2.75	119.17	123.10
3	E	551	NDP	C4A-C5A-N7A	-2.75	106.53	109.40
4	C	553	GTP	O5'-C5'-C4'	-2.72	99.63	108.99
3	C	551	NDP	O5D-C5D-C4D	2.71	118.31	108.99
3	A	551	NDP	C2D-C1D-N1N	-2.69	106.56	113.30
3	C	551	NDP	PN-O5D-C5D	-2.66	106.09	121.68
3	E	551	NDP	PN-O5D-C5D	-2.66	106.10	121.68
4	D	553	GTP	O4'-C1'-C2'	-2.62	103.10	106.93
4	C	553	GTP	C4-C5-N7	-2.62	106.67	109.40
4	F	553	GTP	C6-N1-C2	2.60	120.07	115.93
4	E	553	GTP	C6-N1-C2	2.59	120.05	115.93
4	A	553	GTP	O5'-C5'-C4'	-2.53	100.27	108.99
4	D	553	GTP	C6-N1-C2	2.52	119.93	115.93
3	C	551	NDP	C1D-N1N-C6N	-2.51	115.42	120.83
3	D	551	NDP	PN-O5D-C5D	-2.48	107.13	121.68
5	C	552	H3P	CAT-CAR-CLAG	-2.47	116.11	119.87
3	F	551	NDP	PN-O5D-C5D	-2.45	107.31	121.68
3	A	551	NDP	PN-O5D-C5D	-2.42	107.46	121.68
3	C	551	NDP	C5D-C4D-C3D	-2.40	106.20	115.18
4	B	553	GTP	C6-C5-C4	-2.39	118.51	120.80
4	E	553	GTP	O5'-C5'-C4'	-2.39	100.77	108.99
3	B	551	NDP	C2D-C1D-N1N	-2.38	107.33	113.30
3	F	551	NDP	O5D-C5D-C4D	2.38	117.20	108.99
3	C	551	NDP	C5B-C4B-C3B	-2.38	106.27	115.18
3	F	551	NDP	C5D-C4D-C3D	-2.36	106.33	115.18
4	D	553	GTP	PA-O3A-PB	-2.36	124.72	132.83
3	D	551	NDP	O2B-C2B-C1B	2.35	118.56	110.10
4	A	553	GTP	C6-C5-C4	-2.33	118.57	120.80
5	D	552	H3P	CAI-CAL-CAP	-2.31	118.65	121.78
3	B	551	NDP	C1D-N1N-C6N	-2.30	115.88	120.83
3	C	551	NDP	C4A-C5A-N7A	-2.29	107.01	109.40
4	E	553	GTP	PA-O3A-PB	-2.29	124.97	132.83
3	A	551	NDP	O4D-C4D-C5D	-2.29	101.85	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	553	GTP	C3'-C2'-C1'	-2.28	97.55	100.98
3	F	551	NDP	C3B-C2B-C1B	-2.19	98.76	102.89
4	B	553	GTP	O3G-PG-O2G	2.17	115.94	107.64
3	D	551	NDP	O5D-C5D-C4D	2.17	116.45	108.99
3	D	551	NDP	C4A-C5A-N7A	-2.16	107.15	109.40
4	F	553	GTP	C5'-C4'-C3'	2.15	123.24	115.18
3	D	551	NDP	O2N-PN-O1N	2.15	122.85	112.24
3	D	551	NDP	C5D-C4D-C3D	-2.13	107.21	115.18
3	E	551	NDP	C1D-N1N-C6N	-2.12	116.27	120.83
3	A	551	NDP	O2B-C2B-C1B	2.11	117.69	110.10
3	C	551	NDP	O2N-PN-O1N	2.10	122.62	112.24
4	F	553	GTP	C6-C5-C4	-2.07	118.82	120.80
3	C	551	NDP	O4D-C1D-C2D	2.07	111.14	106.64
3	B	551	NDP	C5B-C4B-C3B	-2.06	107.45	115.18
5	B	552	H3P	CAP-CAL-CLAC	2.05	121.36	118.78
4	B	553	GTP	O5'-PA-O1A	2.05	117.07	109.07
3	A	551	NDP	C4A-C5A-N7A	-2.03	107.28	109.40
3	B	551	NDP	PN-O5D-C5D	-2.03	109.76	121.68
4	D	553	GTP	C2'-C3'-C4'	-2.03	98.70	102.64
3	E	551	NDP	C5B-C4B-C3B	-2.01	107.65	115.18
3	C	551	NDP	C3N-C7N-N7N	2.01	121.23	117.67
3	E	551	NDP	C5D-C4D-C3D	-2.00	107.67	115.18
3	B	551	NDP	C3N-C7N-N7N	2.00	121.22	117.67
4	A	553	GTP	C1'-N9-C4	2.00	130.16	126.64

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	551	NDP	O4D-C1D-N1N-C6N
4	E	553	GTP	C5'-O5'-PA-O1A
4	D	553	GTP	C5'-O5'-PA-O1A
3	F	551	NDP	O4D-C1D-N1N-C6N
3	B	551	NDP	O4D-C1D-N1N-C6N
3	A	551	NDP	O4D-C1D-N1N-C6N
4	B	553	GTP	O4'-C4'-C5'-O5'
3	E	551	NDP	O4D-C1D-N1N-C6N
4	F	553	GTP	O4'-C4'-C5'-O5'
3	C	551	NDP	O4D-C1D-N1N-C6N
4	B	553	GTP	C5'-O5'-PA-O2A
3	D	551	NDP	PN-O3-PA-O1A
3	B	551	NDP	PN-O3-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	E	553	GTP	O4'-C4'-C5'-O5'
4	D	553	GTP	O4'-C4'-C5'-O5'
3	E	551	NDP	C5D-O5D-PN-O3
3	D	551	NDP	C5D-O5D-PN-O3
3	C	551	NDP	C5D-O5D-PN-O3
3	B	551	NDP	C5D-O5D-PN-O3
3	A	551	NDP	C5D-O5D-PN-O3
3	E	551	NDP	PN-O3-PA-O1A
4	F	553	GTP	PG-O3B-PB-O1B
4	E	553	GTP	PB-O3A-PA-O2A
3	F	551	NDP	PN-O3-PA-O1A
3	A	551	NDP	PN-O3-PA-O1A
3	A	551	NDP	PA-O3-PN-O2N

There are no ring outliers.

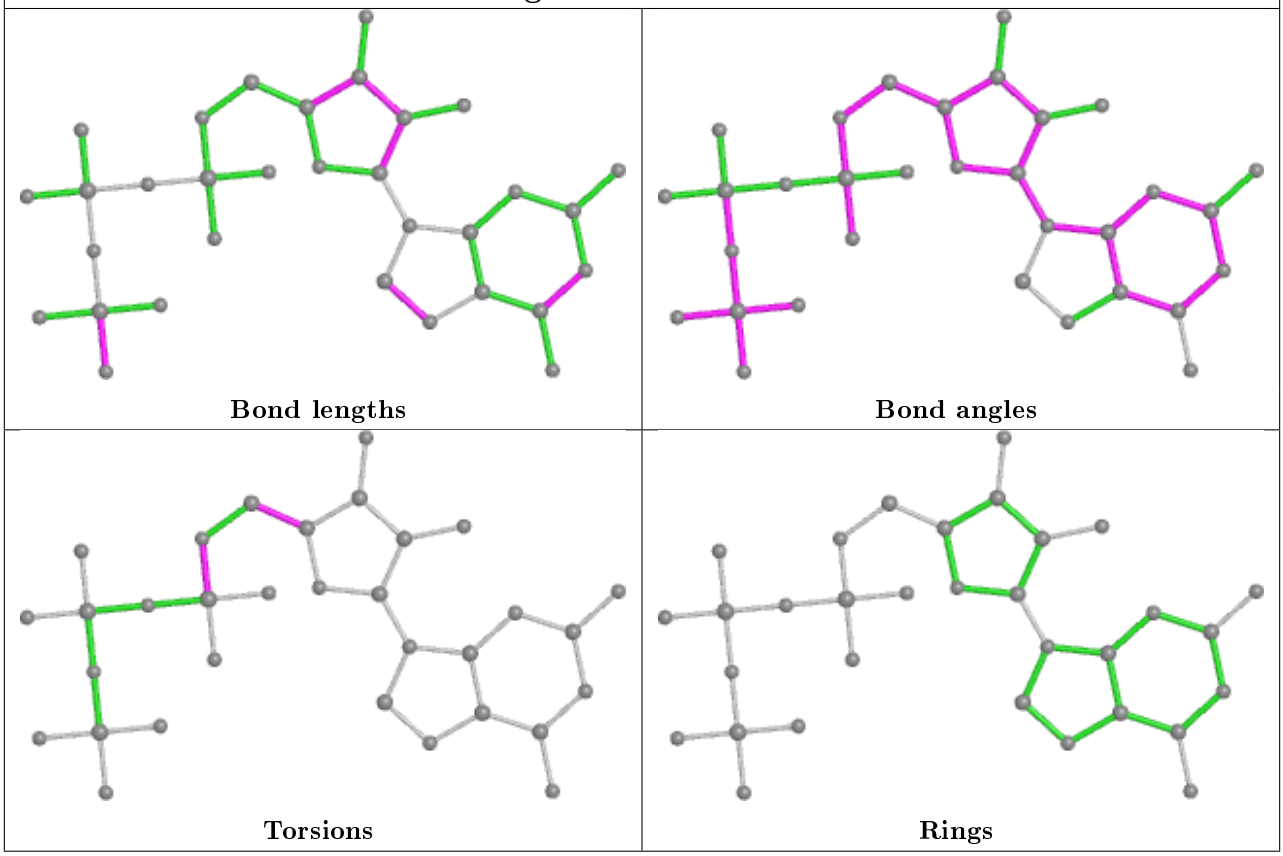
15 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	554	H3P	2	0
4	B	553	GTP	1	0
3	E	551	NDP	5	0
3	B	551	NDP	4	0
4	F	553	GTP	2	0
3	D	551	NDP	8	0
5	C	552	H3P	1	0
4	A	553	GTP	3	0
5	A	552	H3P	4	0
3	C	551	NDP	7	0
3	F	551	NDP	5	0
4	D	553	GTP	1	0
5	F	552	H3P	6	0
3	A	551	NDP	3	0
4	E	553	GTP	2	0

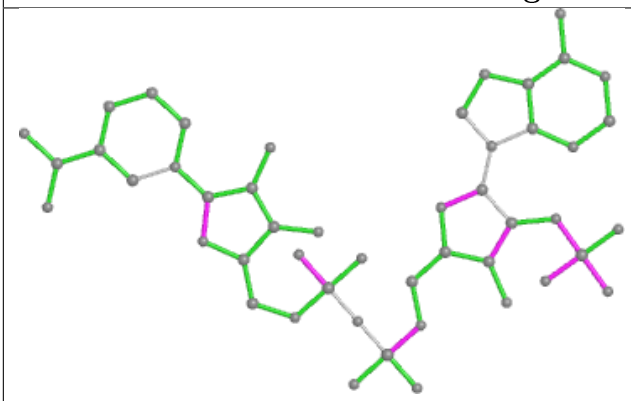
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

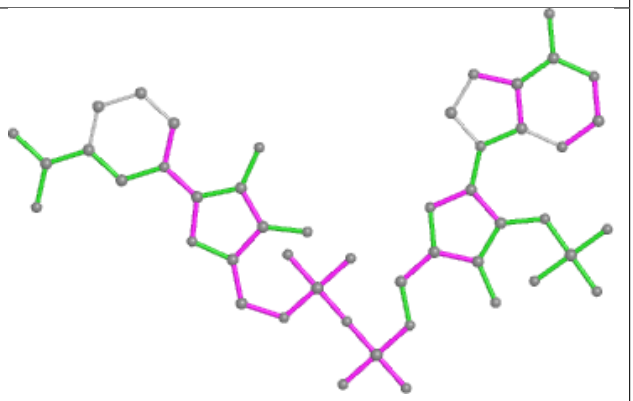
Ligand GTP B 553



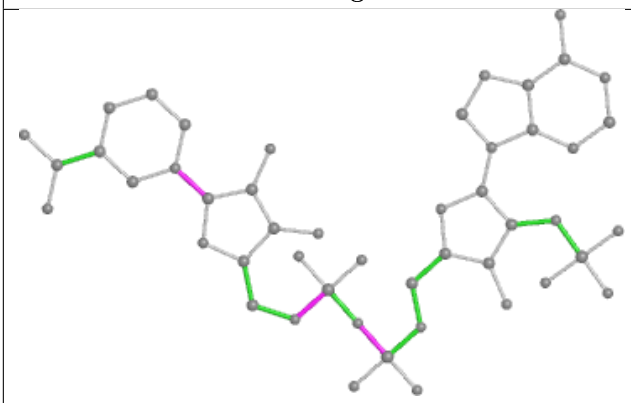
Ligand NDP E 551



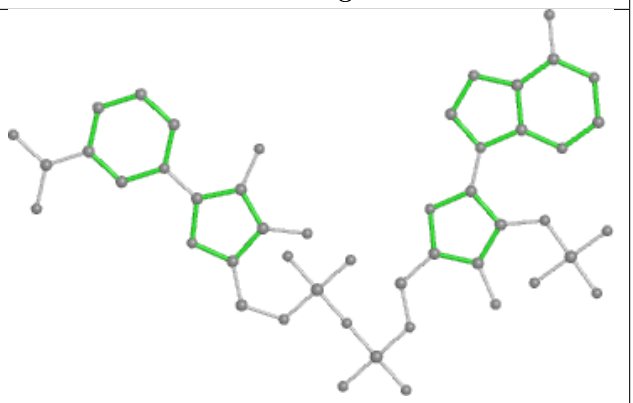
Bond lengths



Bond angles

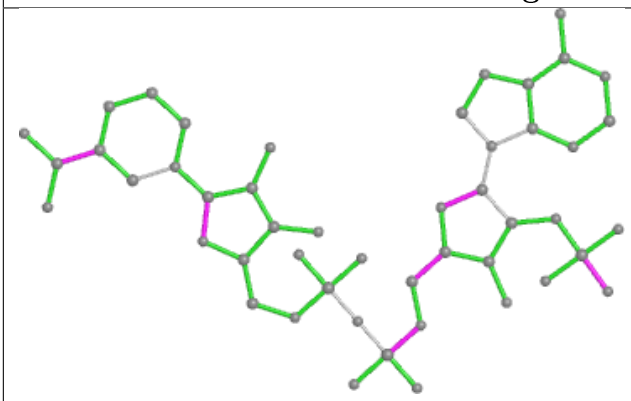


Torsions

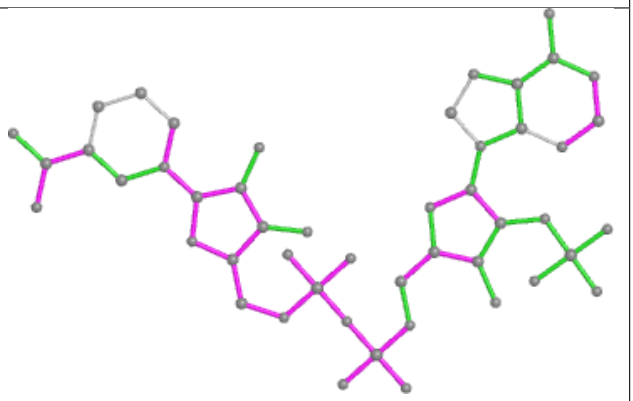


Rings

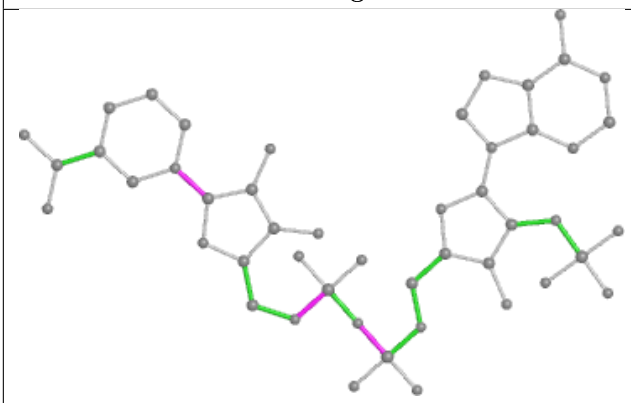
Ligand NDP B 551



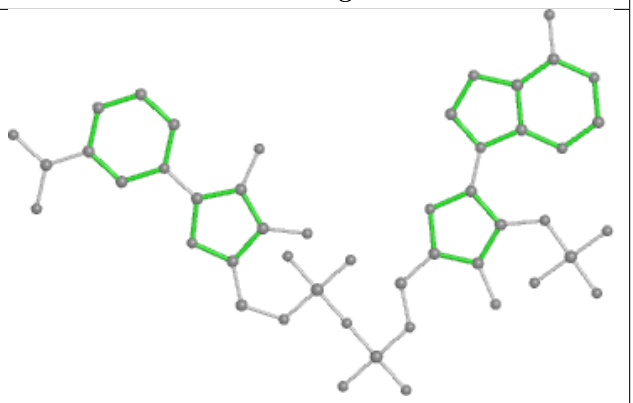
Bond lengths



Bond angles

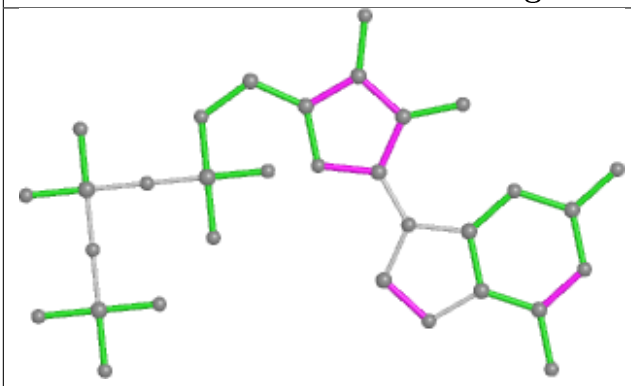


Torsions



Rings

Ligand GTP F 553



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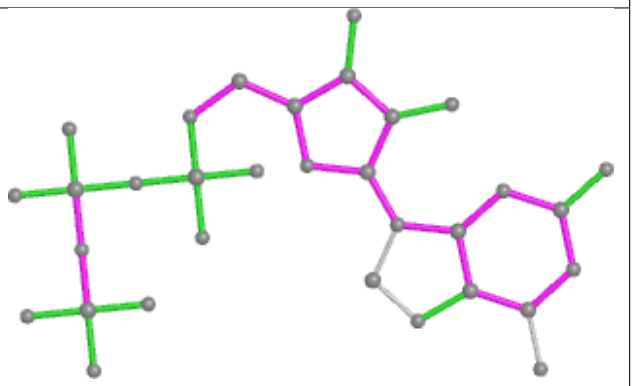
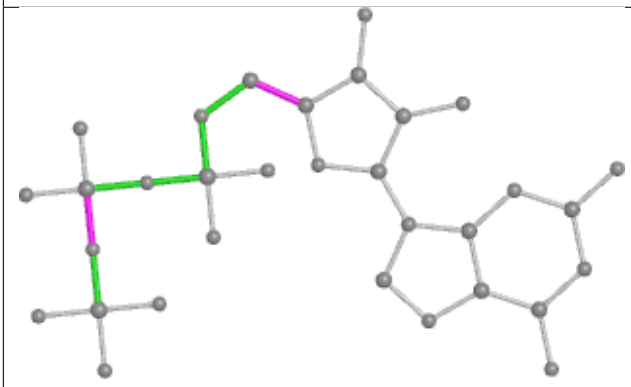


Bond angles



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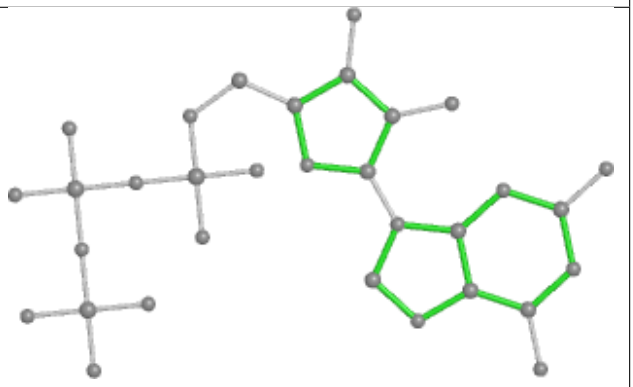
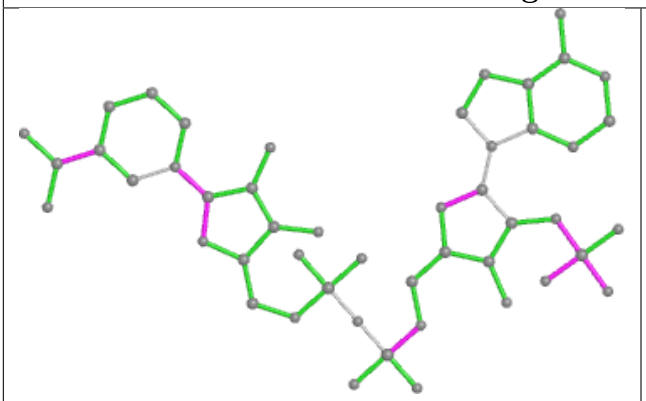
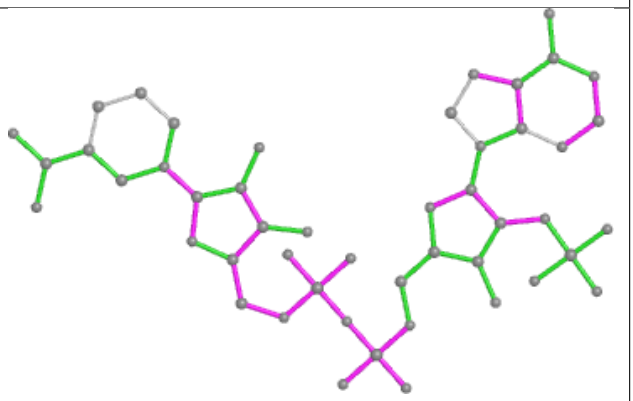


Rings

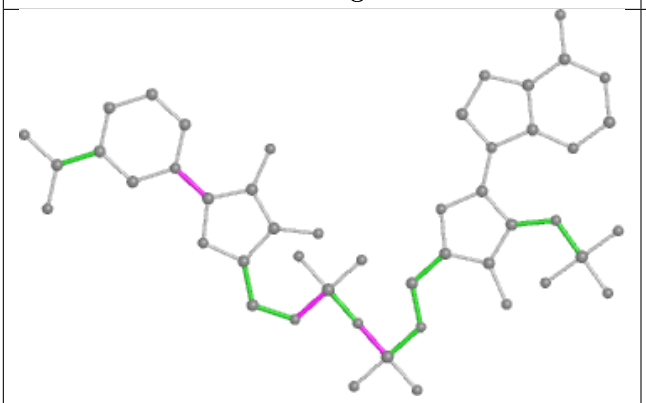
Ligand NDP D 551



Bond lengths



Bond angles



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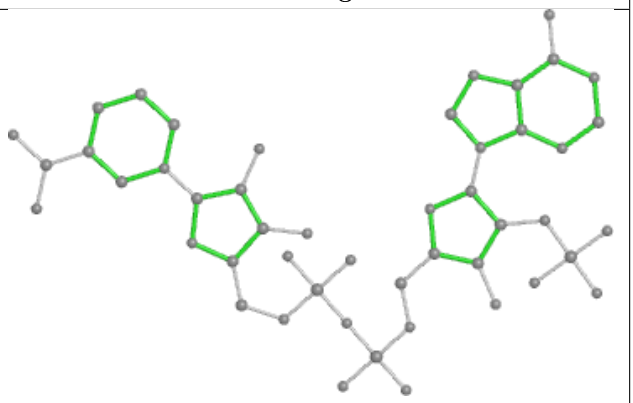
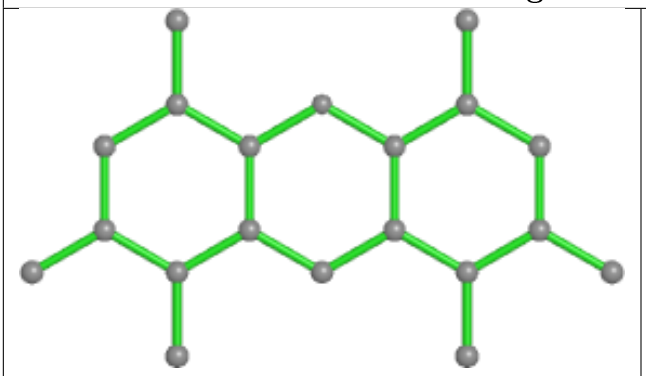


Rings

Ligand H3P C 552



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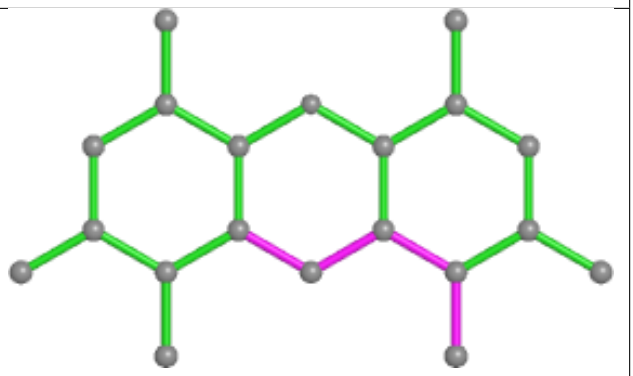
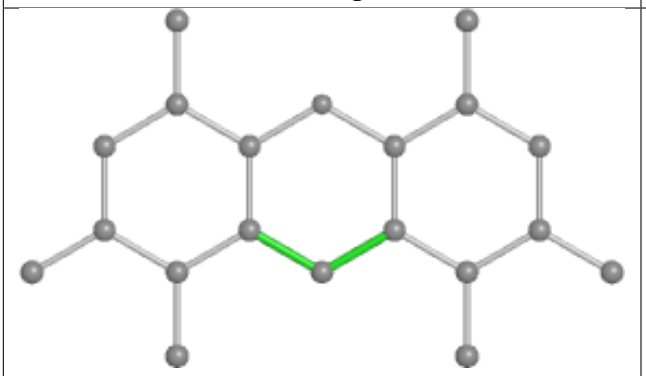


Bond angles



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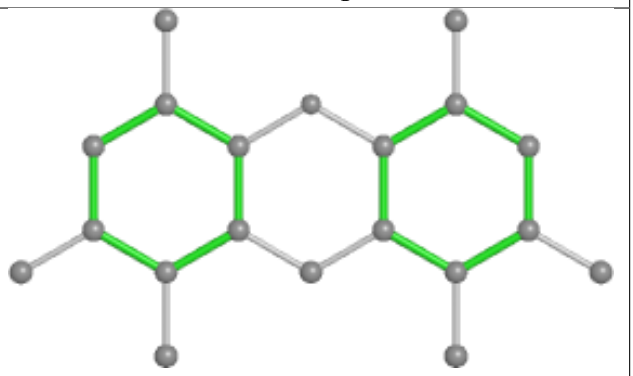
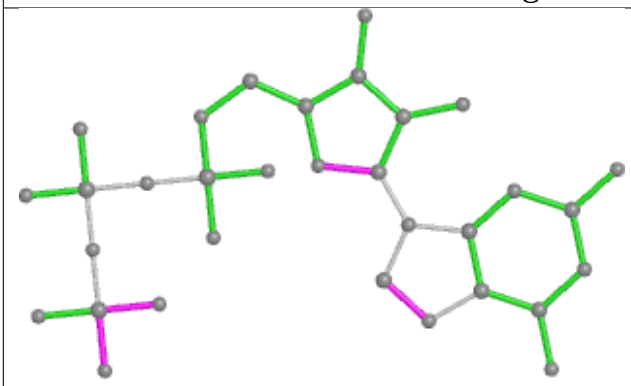
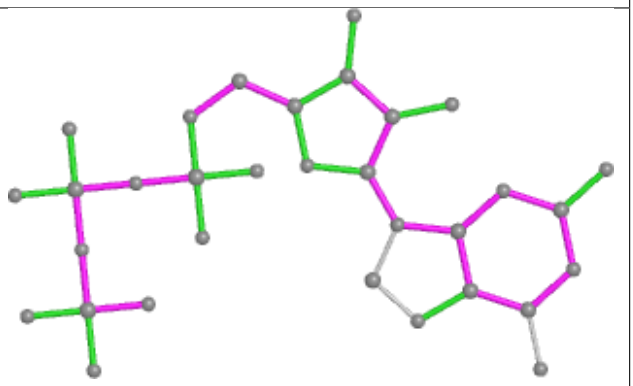


Rings

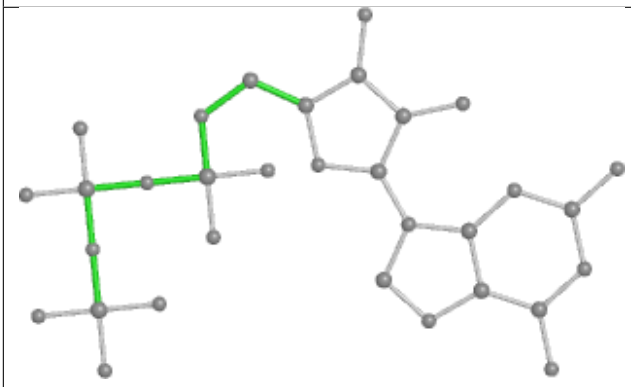
Ligand GTP A 553



Bond lengths



Bond angles



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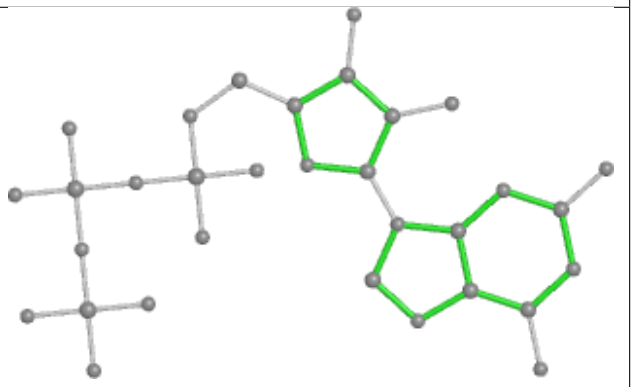
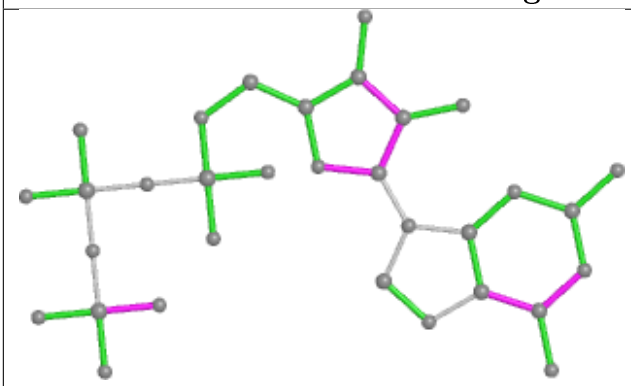


Rings

Ligand GTP C 553



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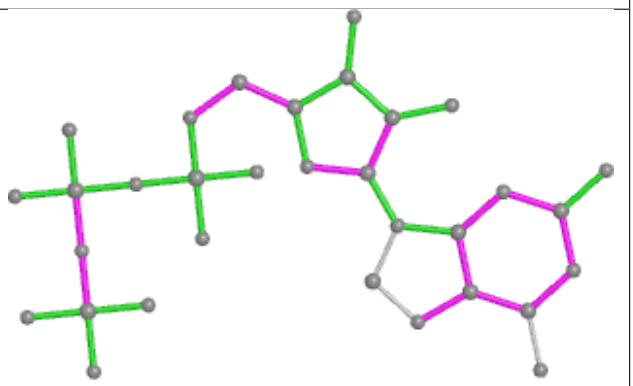

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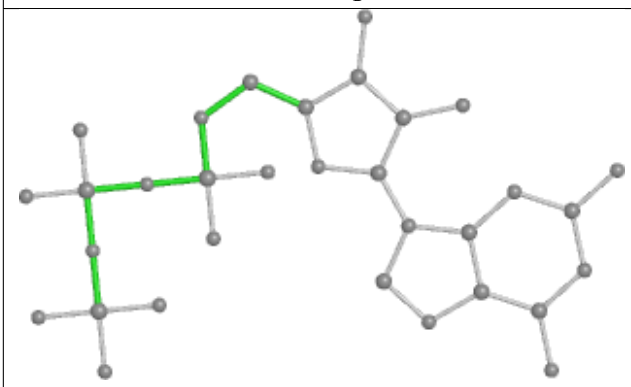

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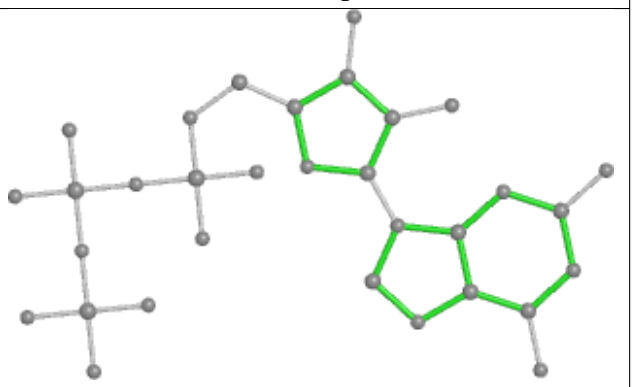
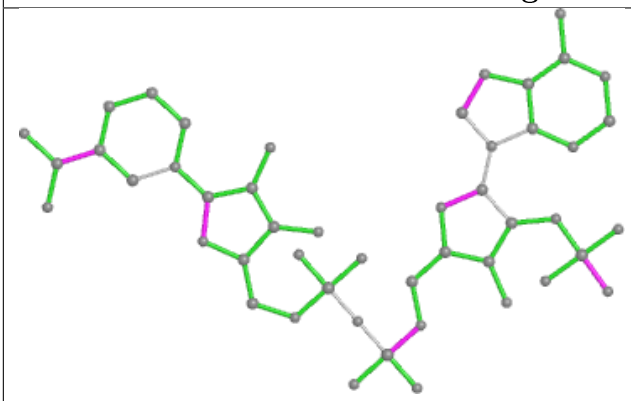


Rings

Ligand NDP C 551



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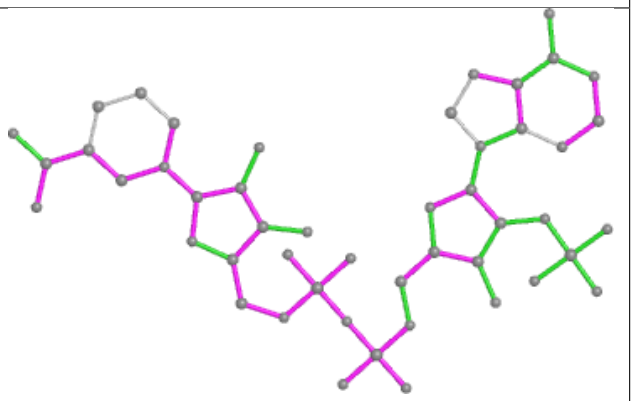
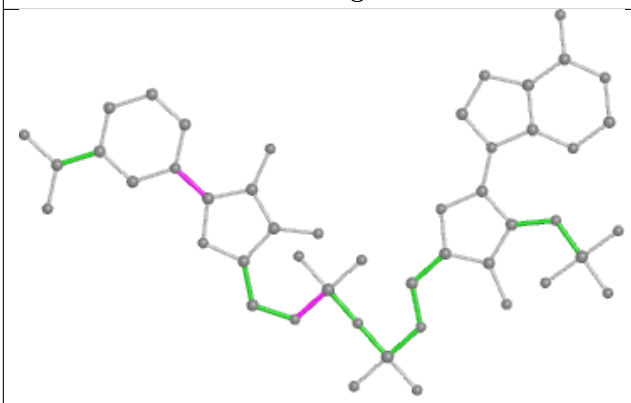


Bond angles



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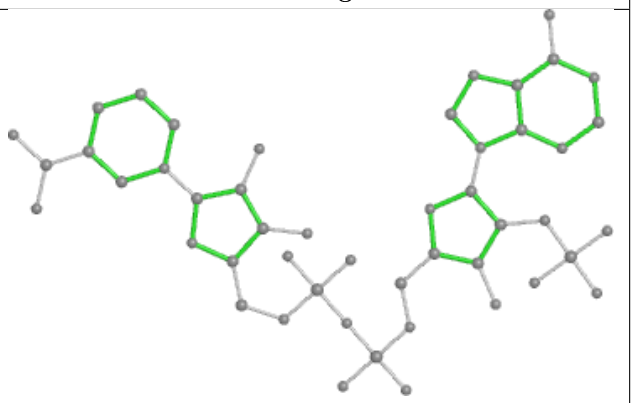
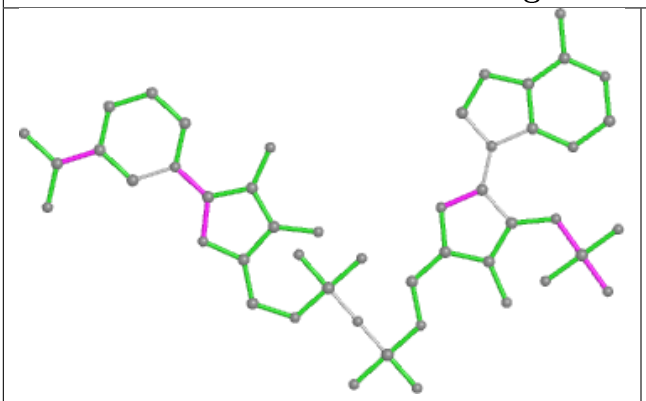
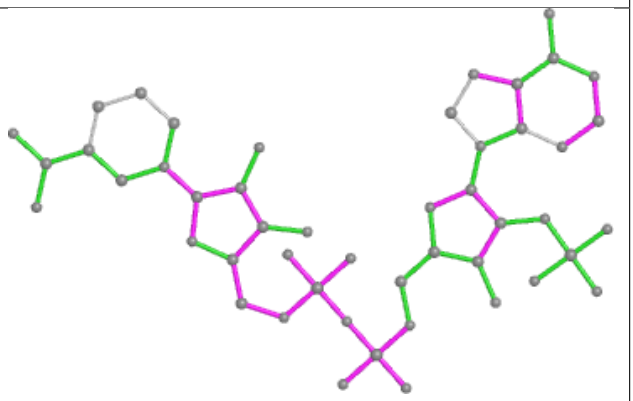


Rings

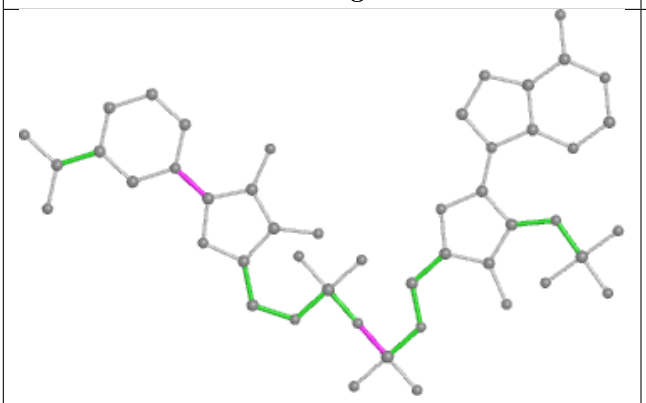
Ligand NDP F 551



Bond lengths



Bond angles



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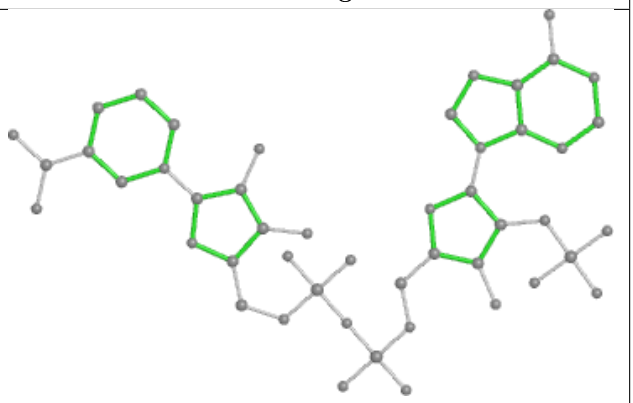
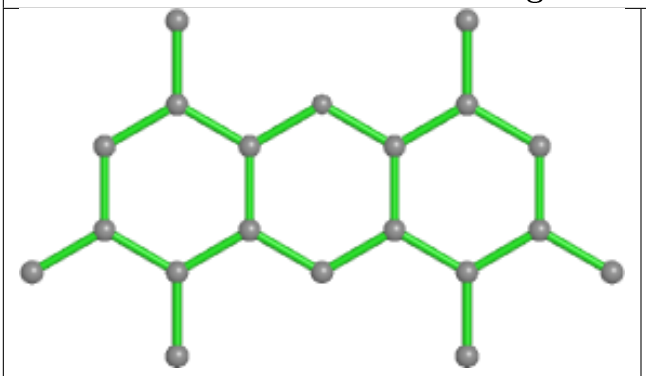


Rings

Ligand H3P B 552



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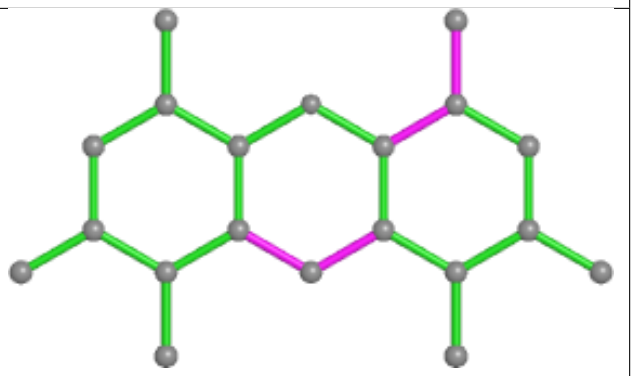
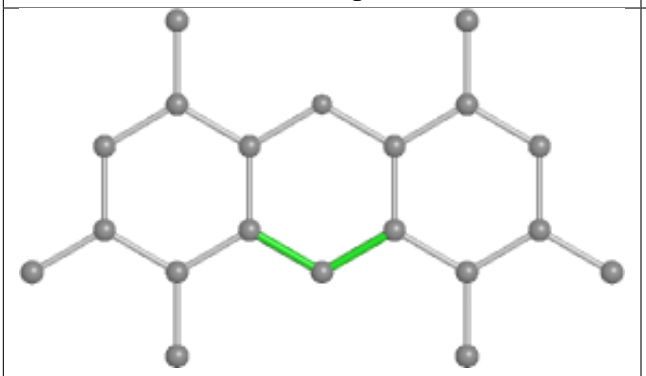
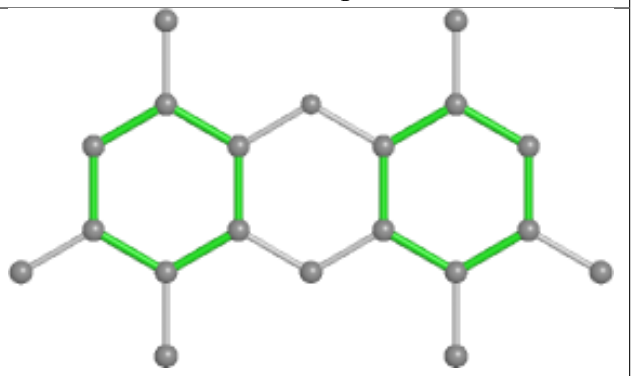


Bond angles

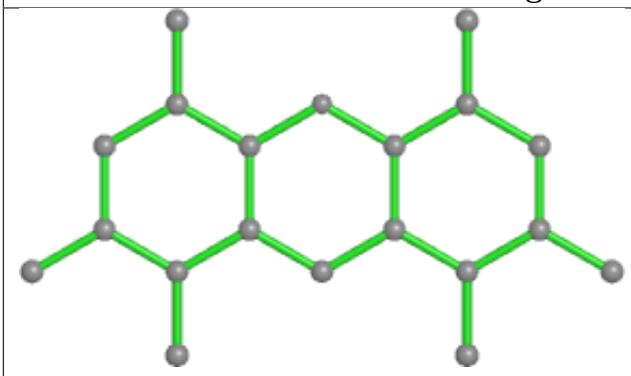


Torsions



Rings

Ligand H3P D 552



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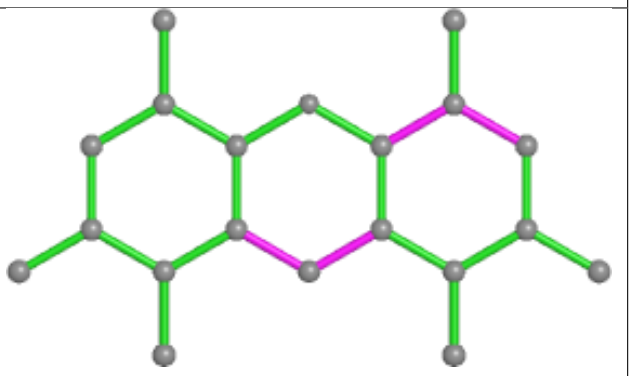
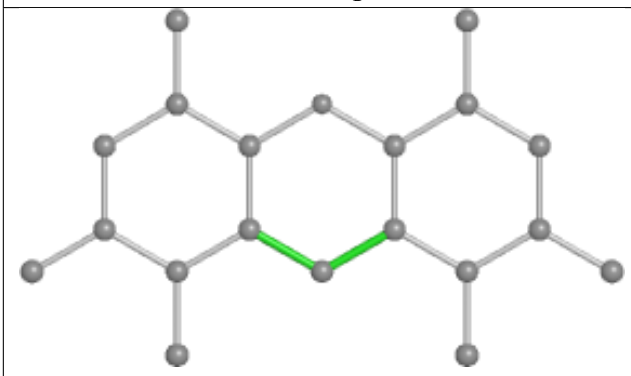
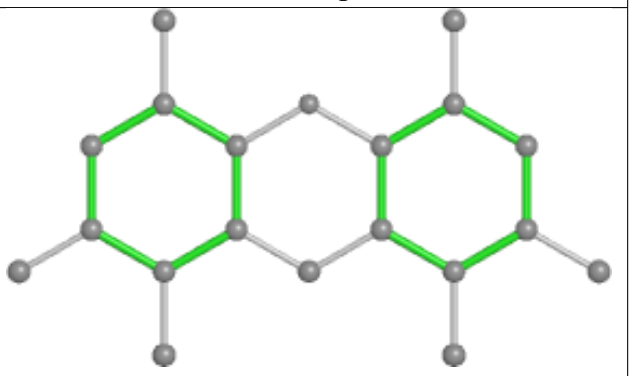


Bond angles

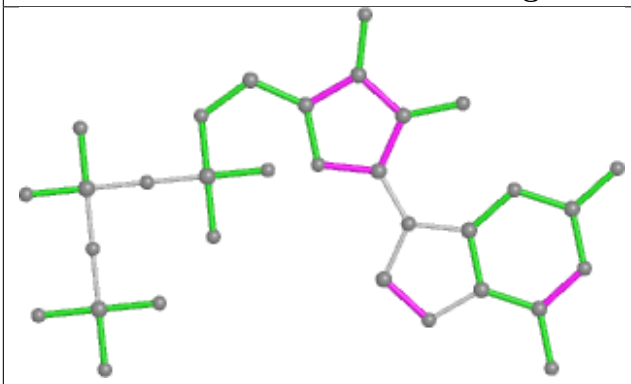


Torsions



Rings

Ligand GTP D 553



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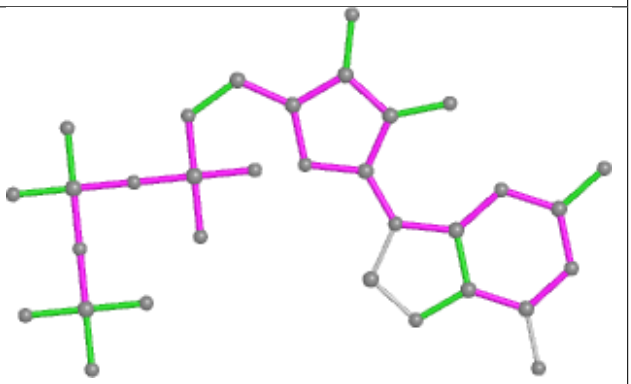
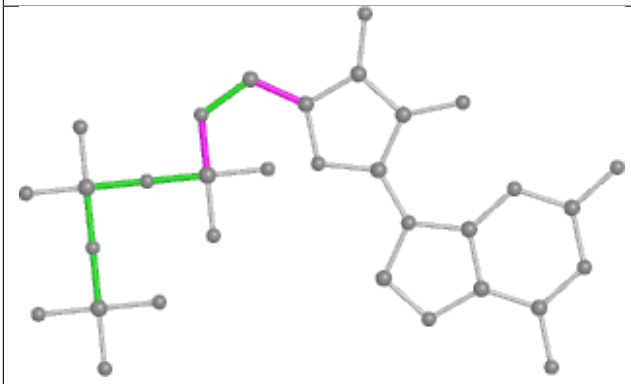


Bond angles



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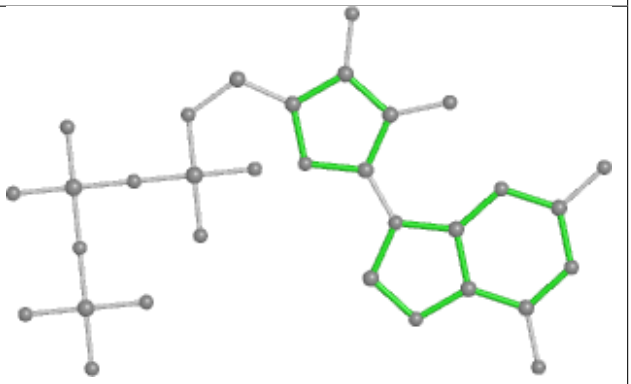
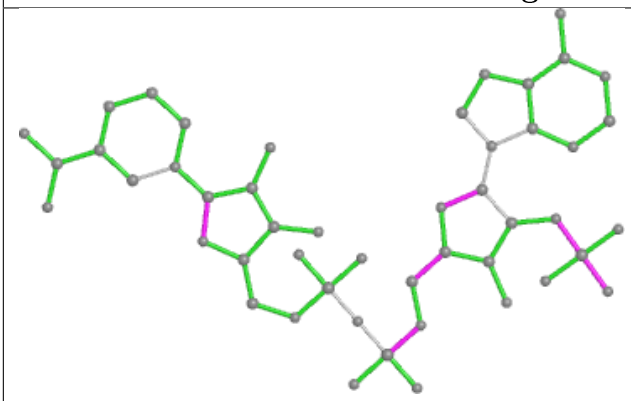
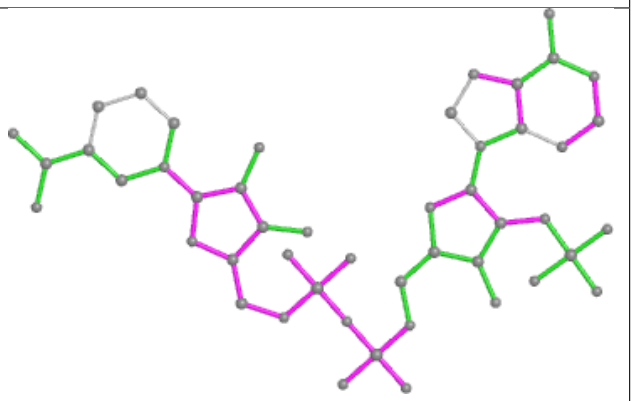


Rings

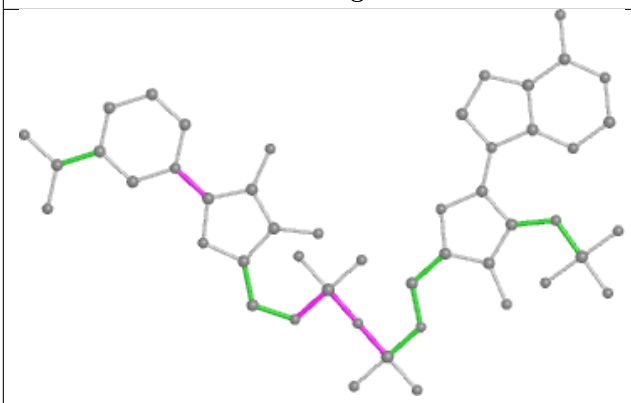
Ligand NDP A 551



Bond lengths



Bond angles



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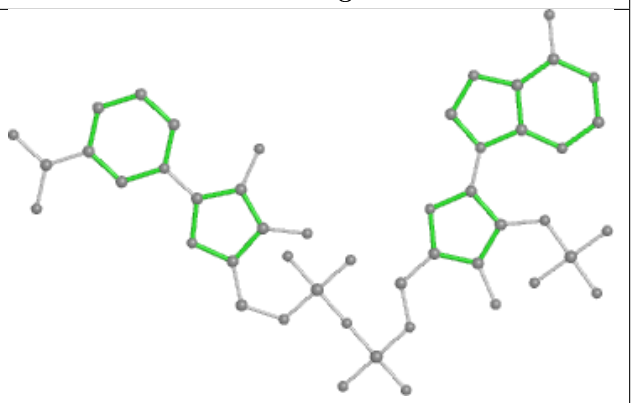
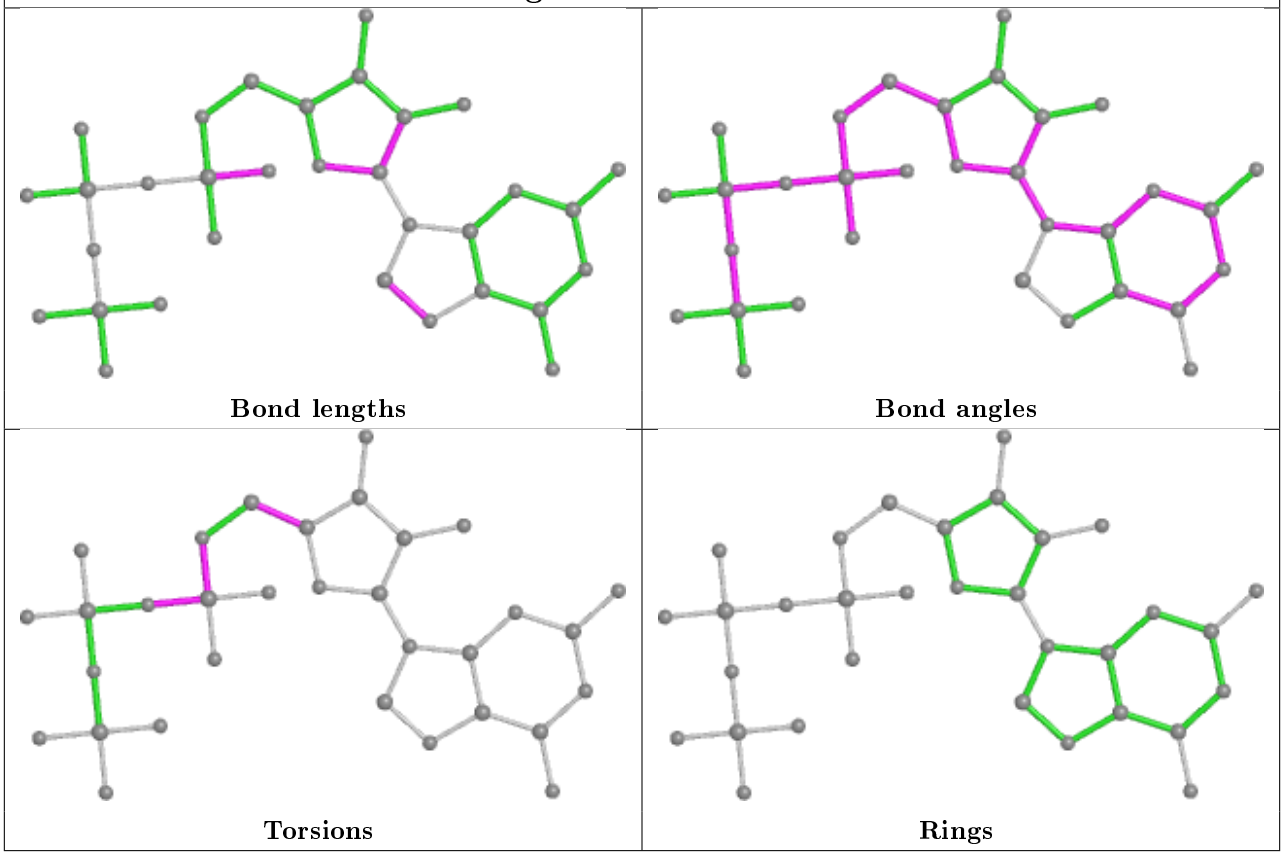


Rings

Ligand GTP E 553



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

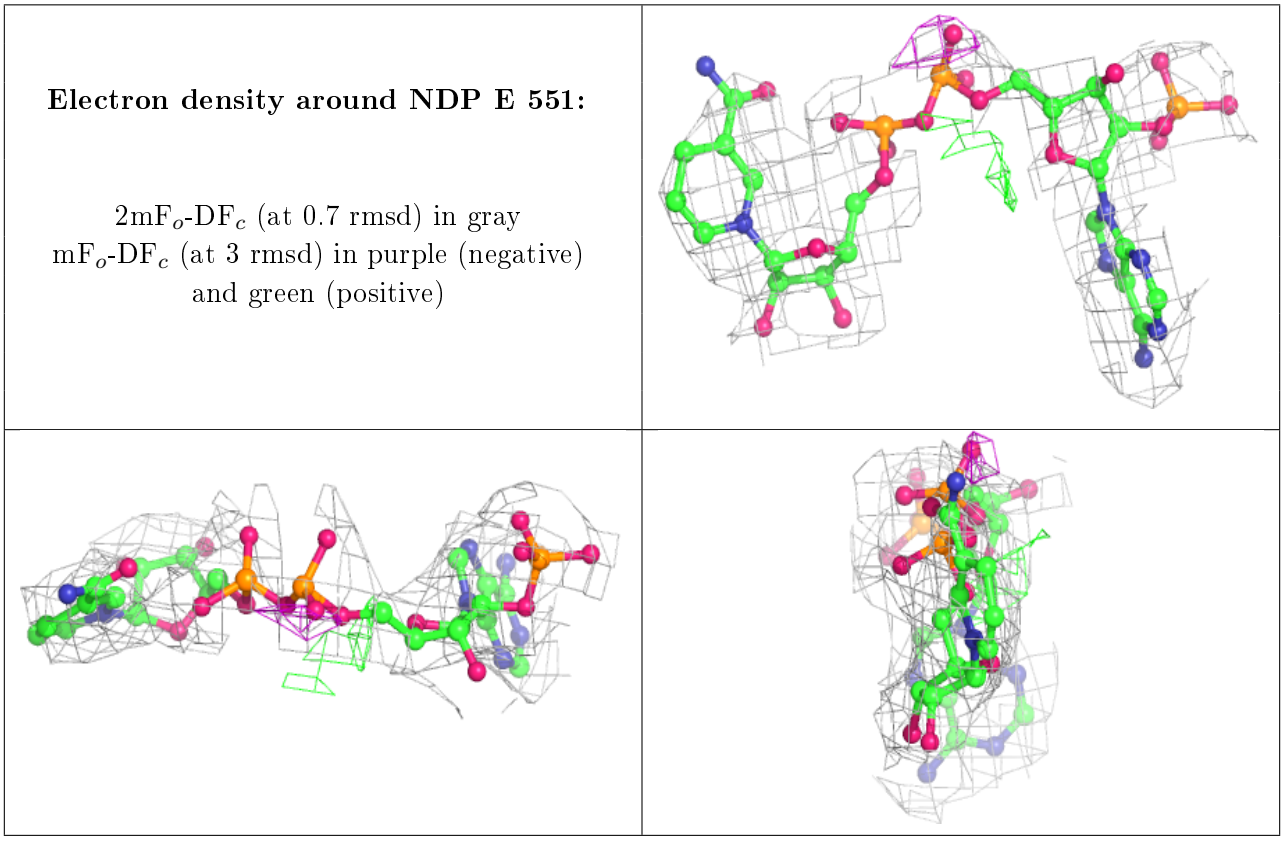
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

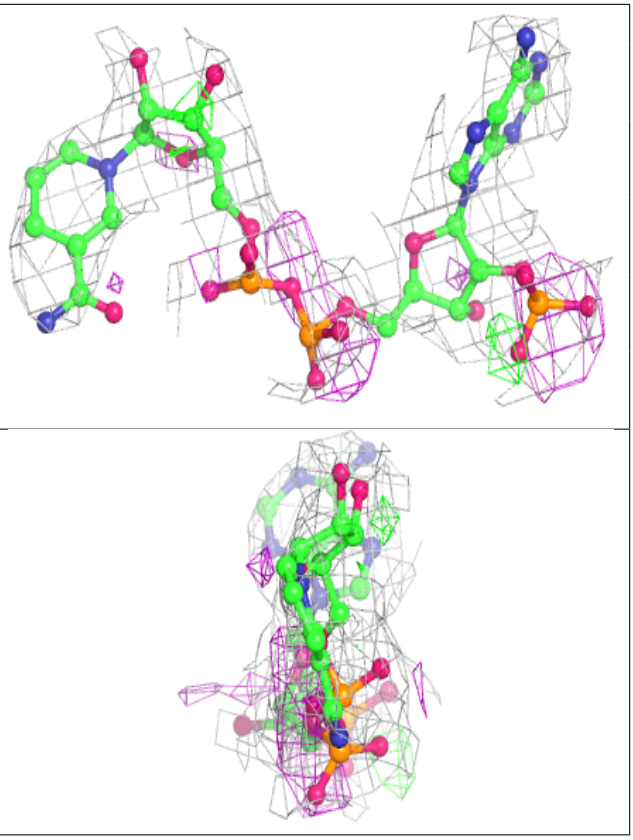
Electron density around NDP E 551:

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



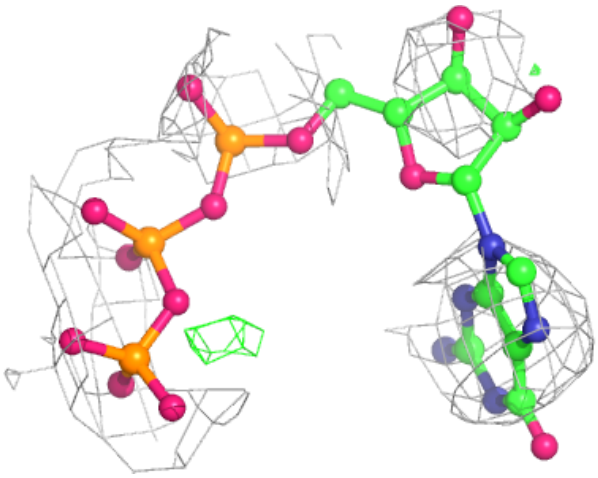
Electron density around NDP D 551:

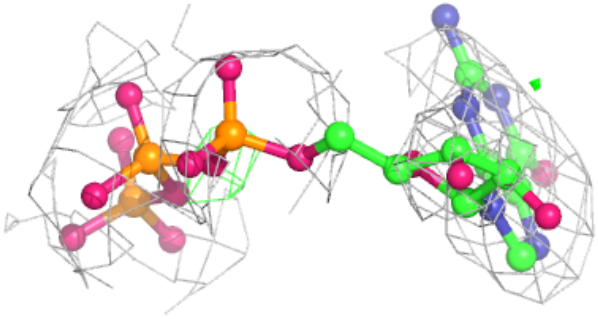
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

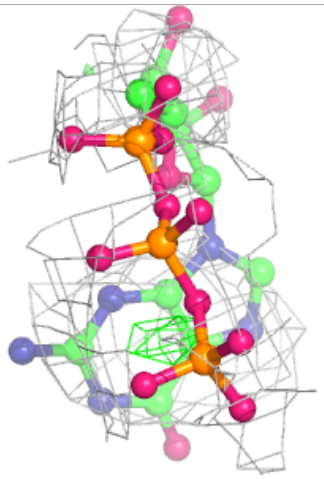


Electron density around GTP C 553:

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

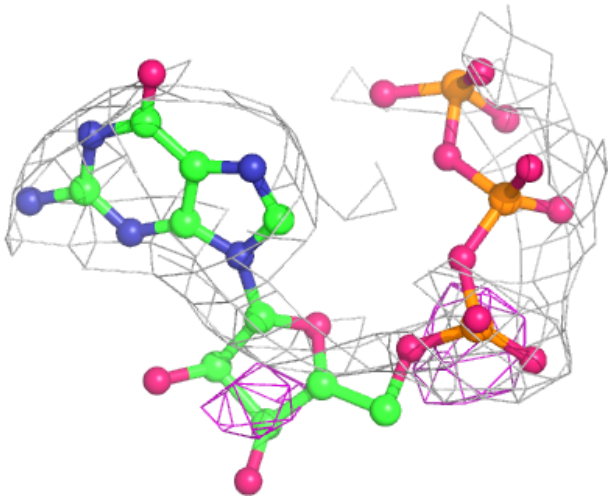


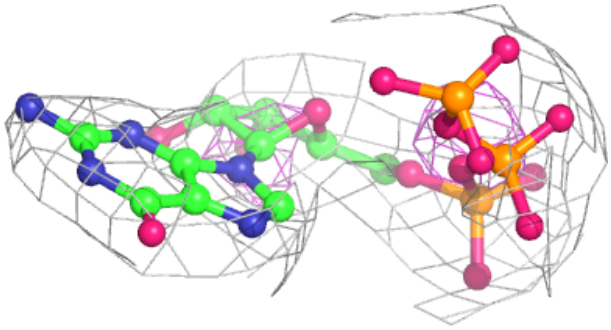


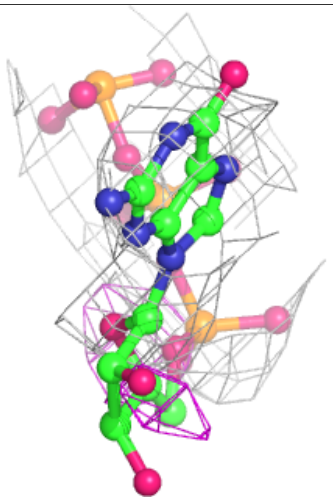


Electron density around GTP B 553:

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

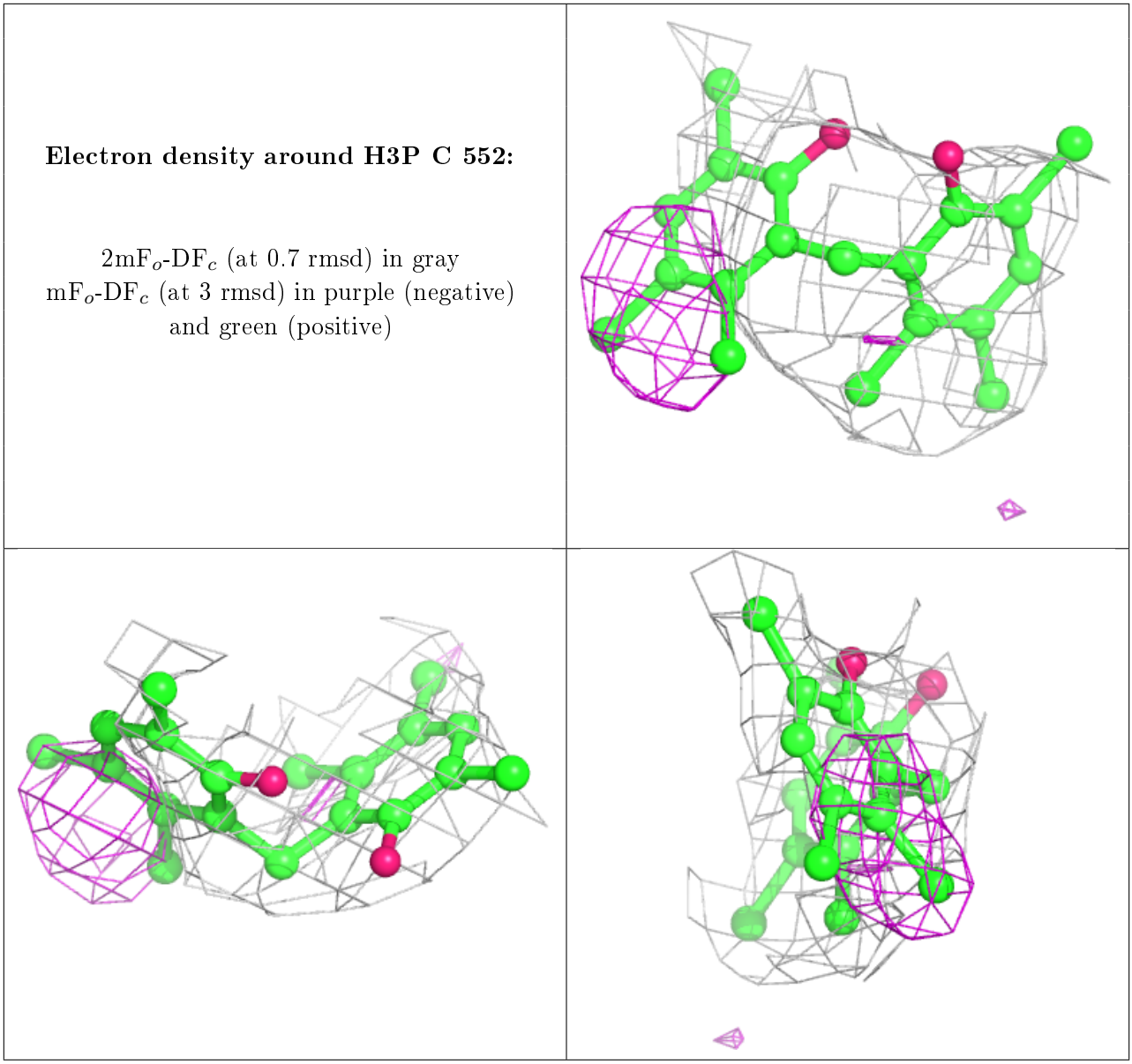






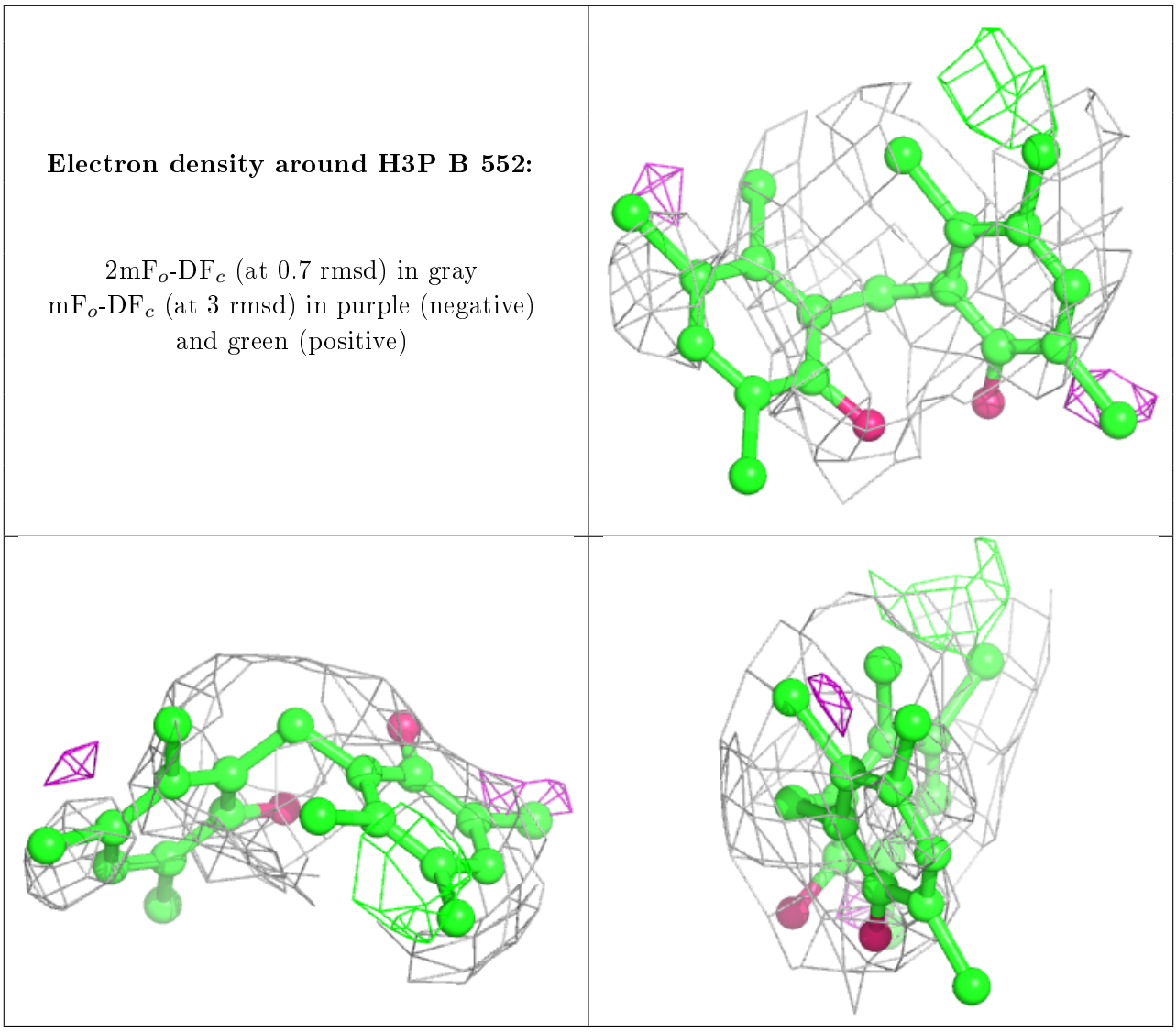
Electron density around H3P C 552:

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



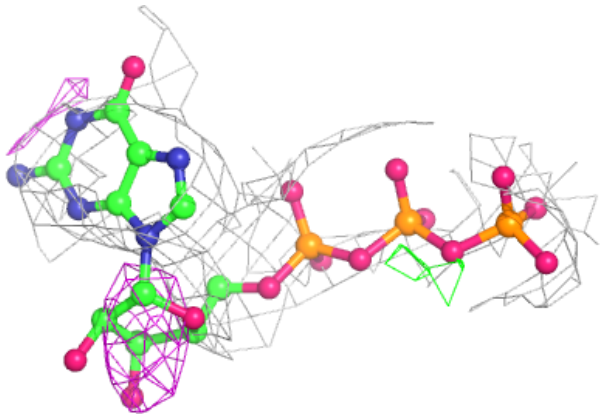
Electron density around H3P B 552:

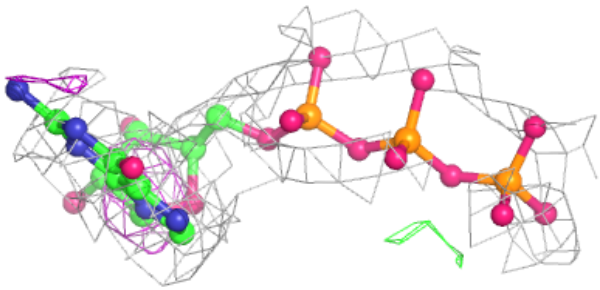
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

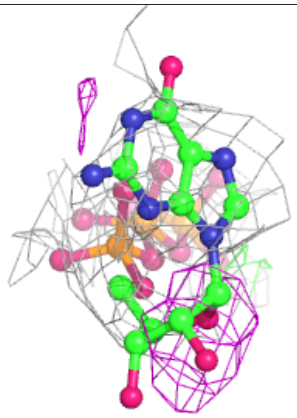


Electron density around GTP A 553:

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

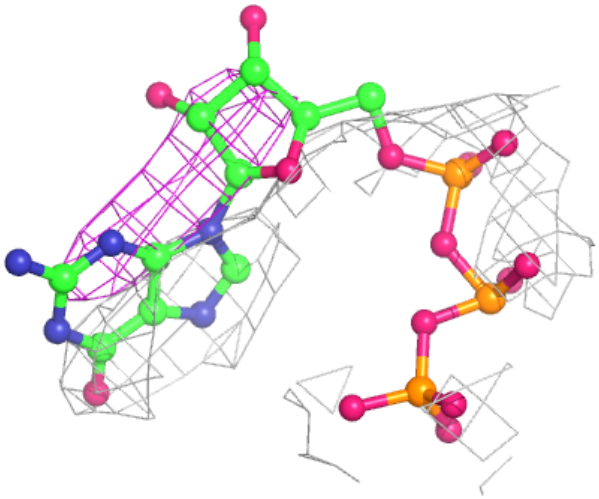


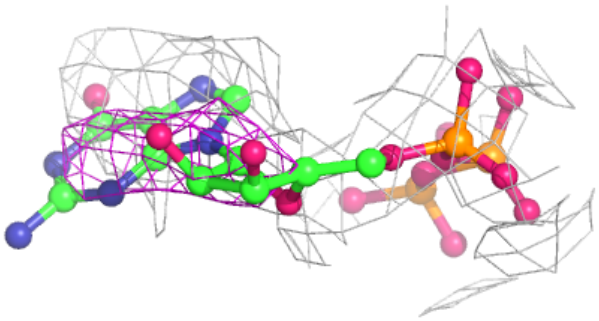


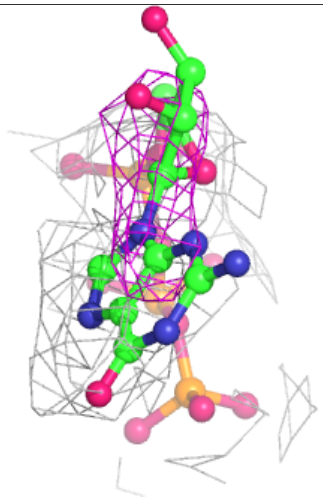


Electron density around GTP F 553:

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

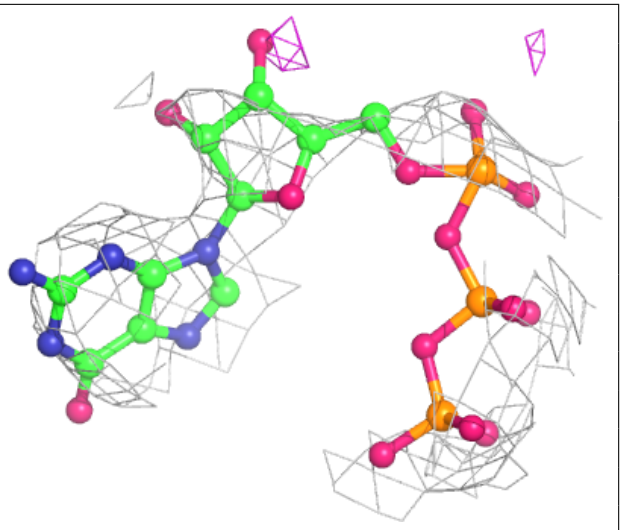


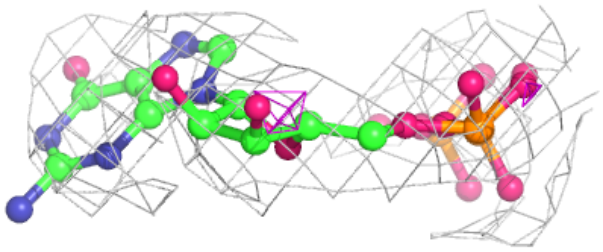


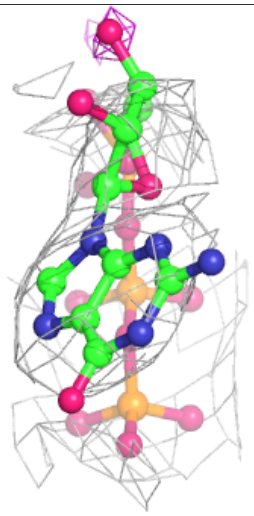


Electron density around GTP E 553:

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

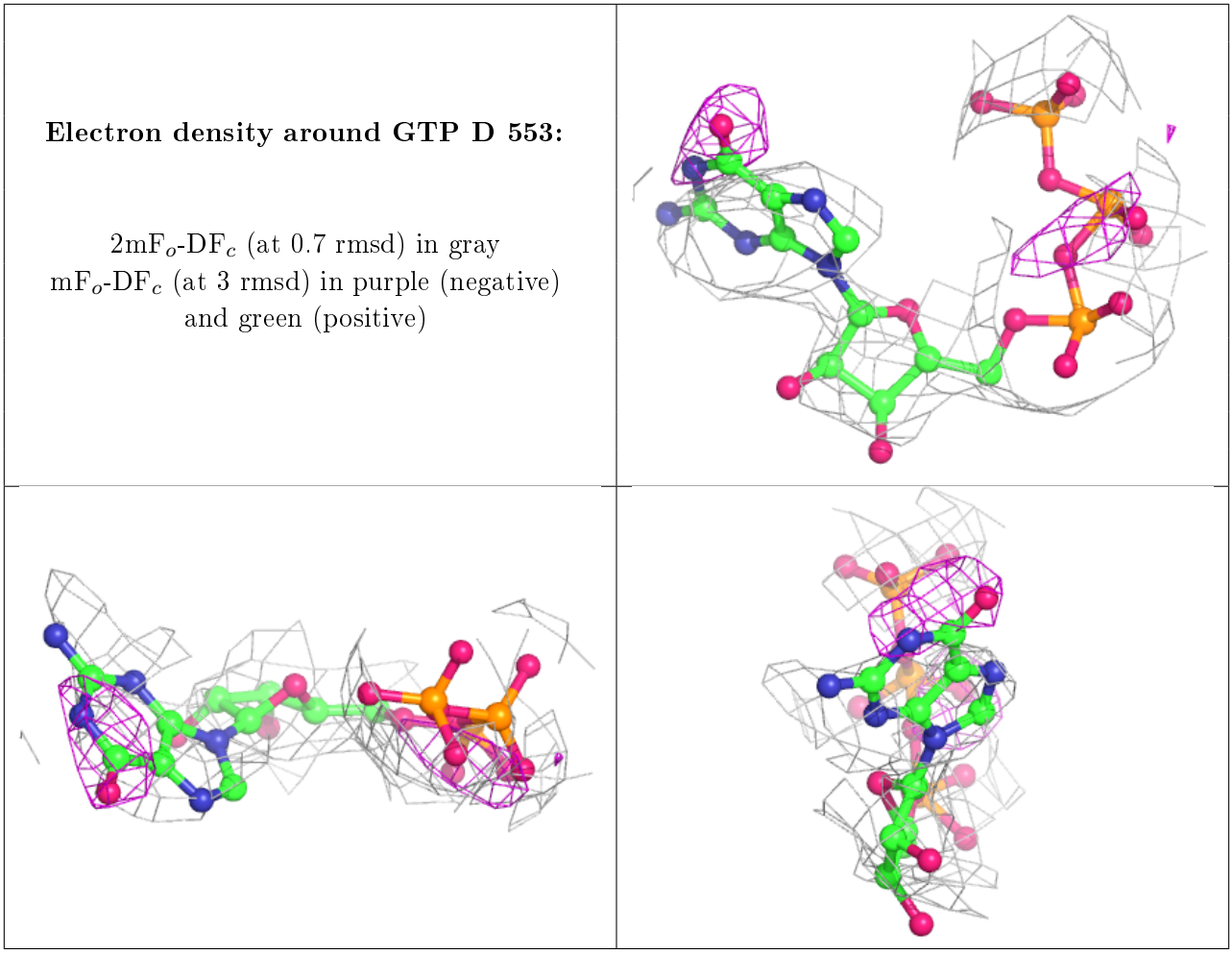






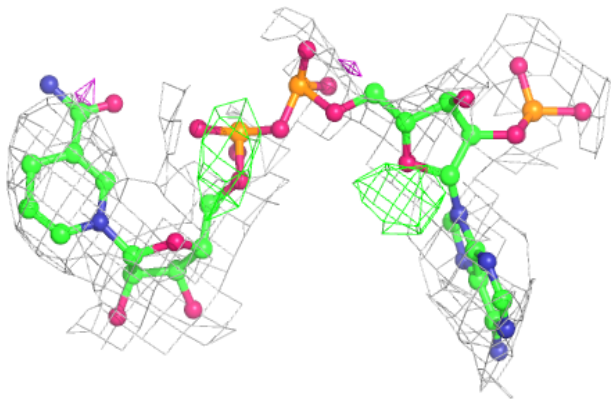
Electron density around GTP D 553:

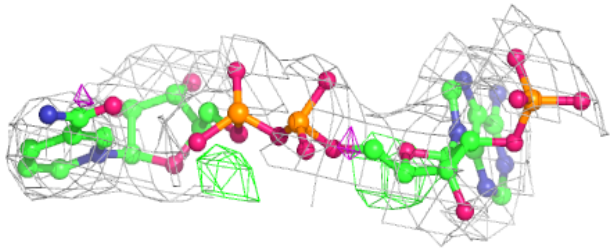
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

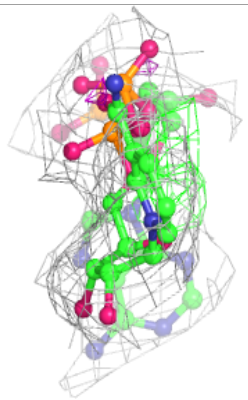


Electron density around NDP F 551:

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

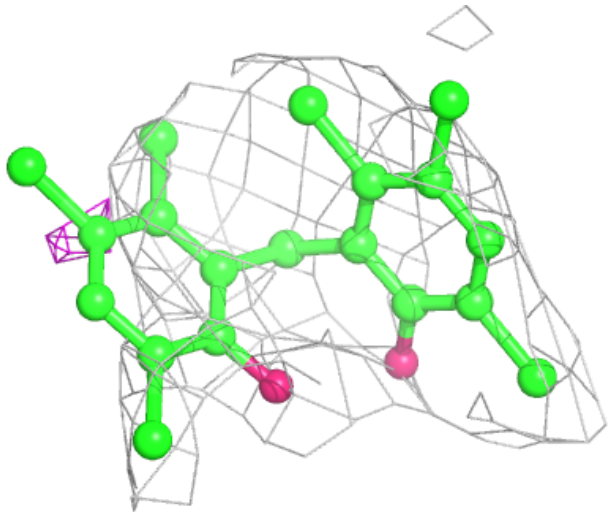


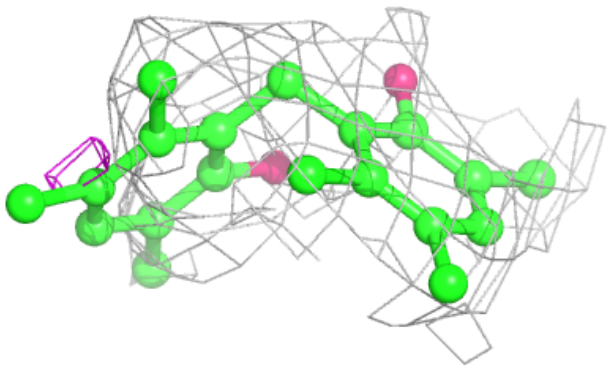


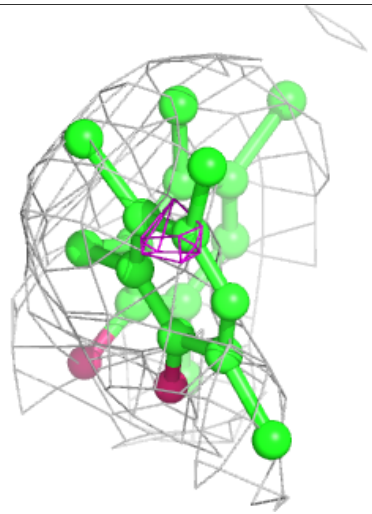


Electron density around H3P D 552:

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

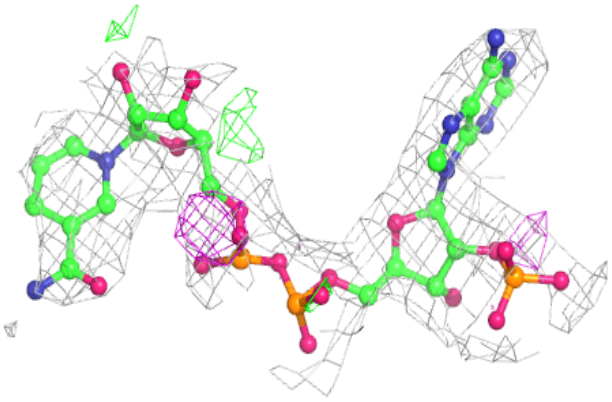


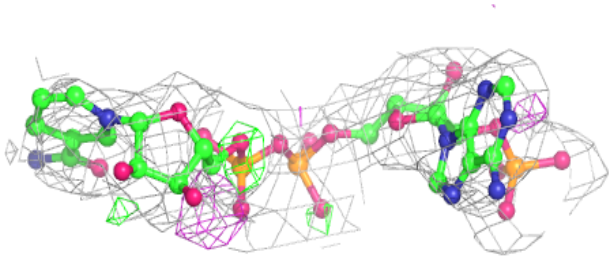


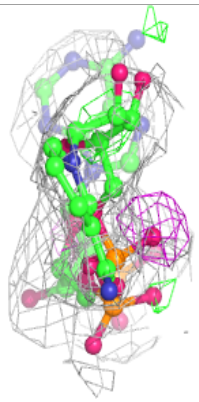


Electron density around NDP C 551:

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

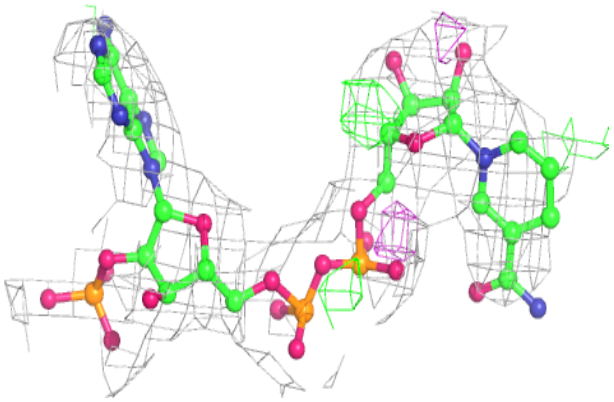


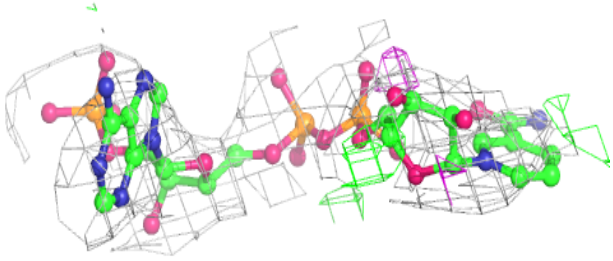


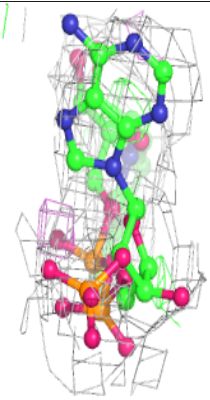


Electron density around NDP B 551:

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

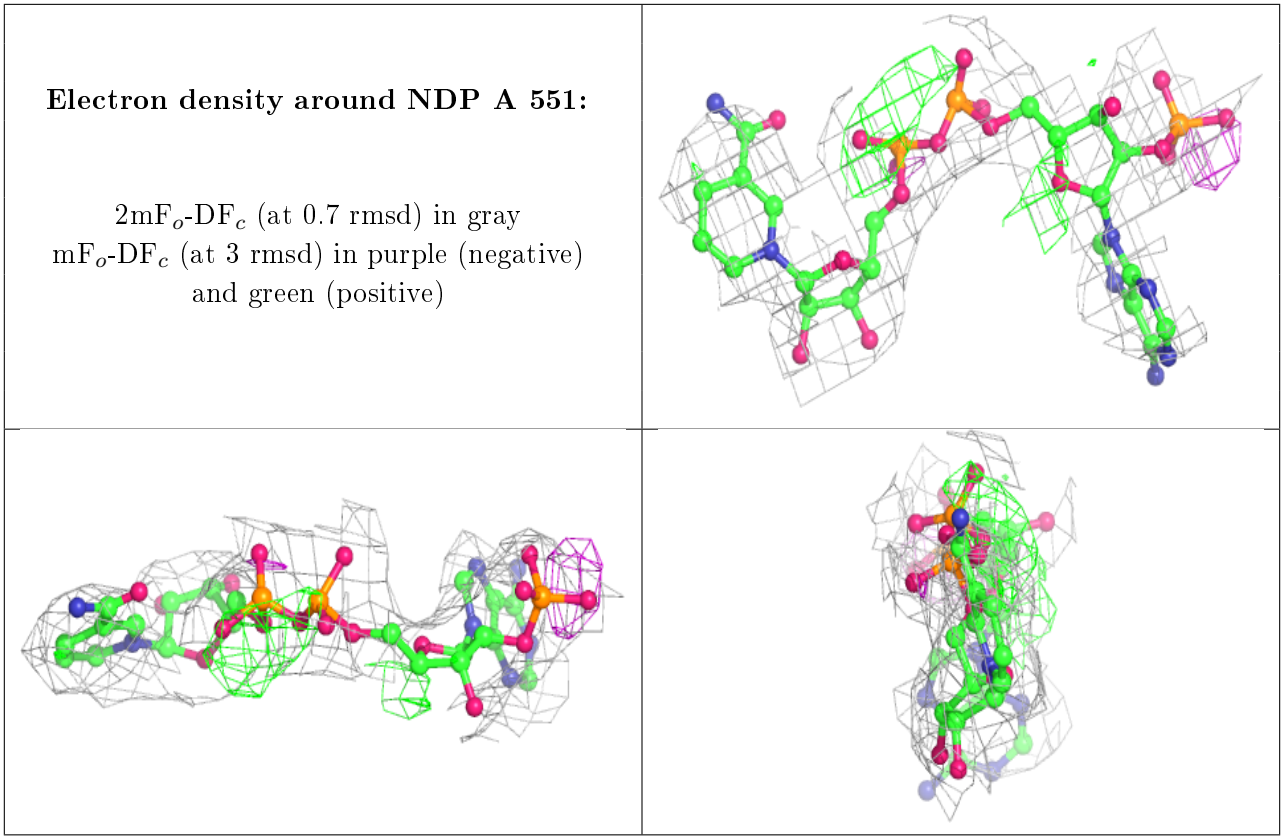






Electron density around NDP A 551:

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



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.