



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 12:49 AM EDT

PDB ID : 3ETD  
Title : Structure of glutamate dehydrogenase complexed with bithionol  
Authors : Li, M.; Smith, T.J.  
Deposited on : 2008-10-07  
Resolution : 2.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

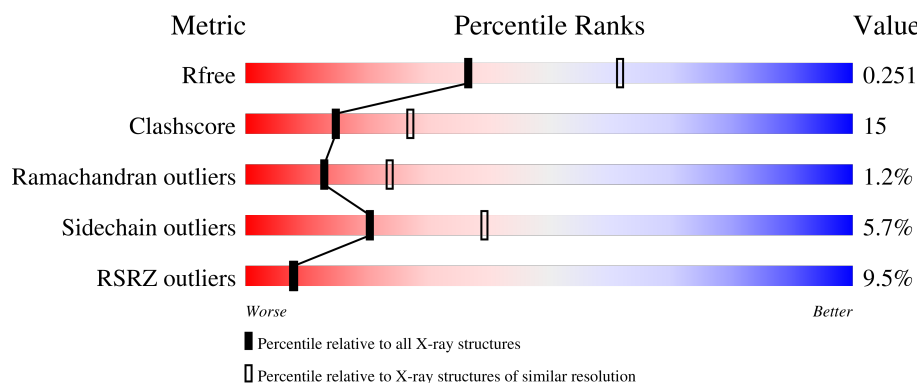
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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




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

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

Mol	Chain	Length	Quality of chain
1	A	501	<div> <div>11%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>.</div> </div> </div>
1	B	501	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>.</div> </div> </div>
1	C	501	<div> <div>7%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>.</div> </div> </div>
1	D	501	<div> <div>8%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>.</div> </div> </div>
1	E	501	<div> <div>8%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	501	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLU	D	550	-	-	X	-
2	GLU	E	550	-	-	X	-
4	GTP	A	553	-	-	-	X
4	GTP	B	553	-	-	-	X
4	GTP	E	553	X	-	-	-
4	GTP	F	553	-	-	-	X
5	B1T	A	552	-	-	-	X

## 2 Entry composition [i](#)

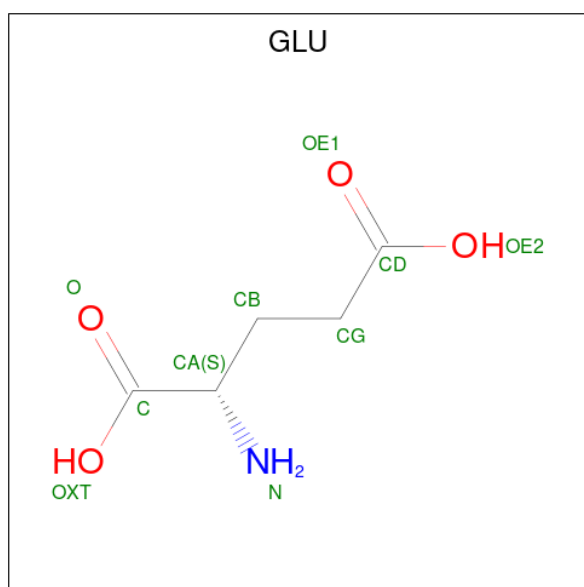
There are 6 unique types of molecules in this entry. The entry contains 24226 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUD1 protein.

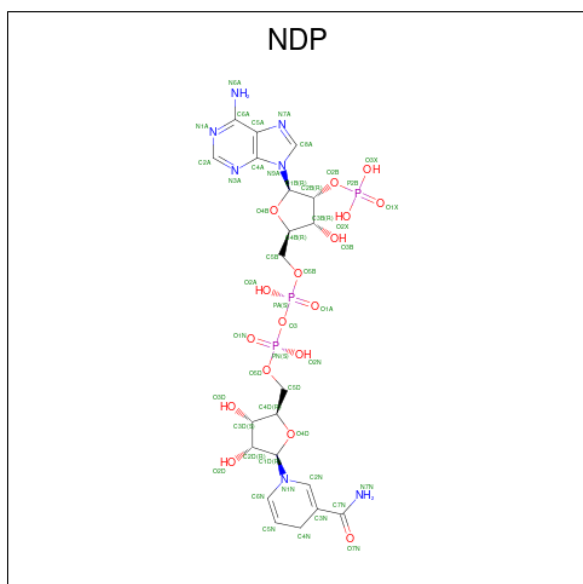
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			
1	B	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			
1	C	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			
1	D	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			
1	E	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			
1	F	501	Total	C	N	O	S	0	0	0
			3915	2473	687	736	19			

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 9	C 5	N 1	O 3	0	0
2	B	1	Total 9	C 5	N 1	O 3	0	0
2	C	1	Total 9	C 5	N 1	O 3	0	0
2	D	1	Total 9	C 5	N 1	O 3	0	0
2	E	1	Total 9	C 5	N 1	O 3	0	0
2	F	1	Total 9	C 5	N 1	O 3	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$ ).



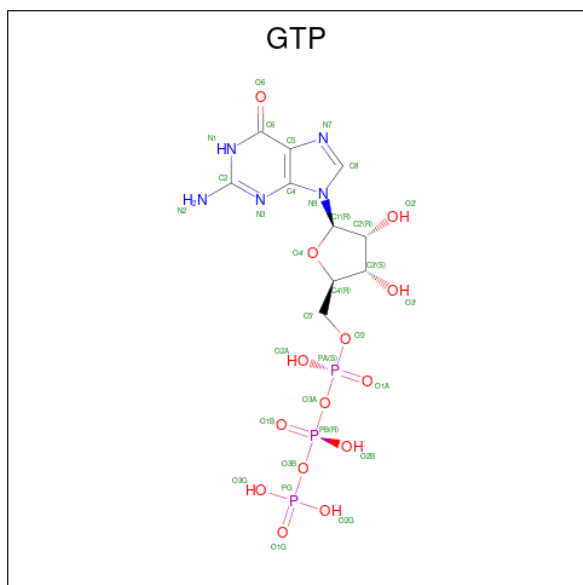
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	E	1	Total 48	C 21	N 7	O 17	P 3	0	0

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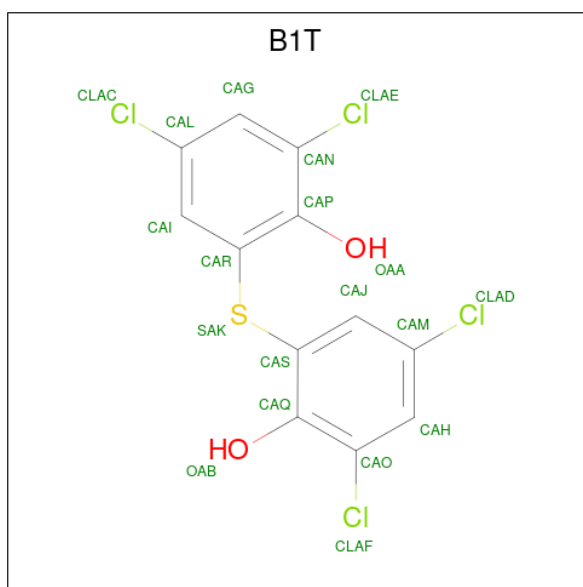
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- 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'-sulfanediylbis(4,6-dichlorophenol) (three-letter code: B1T) (formula:  $C_{12}H_6Cl_4O_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 19	C 12	Cl 4	O 2	S 1	0	0
5	B	1	Total 19	C 12	Cl 4	O 2	S 1	0	0
5	C	1	Total 19	C 12	Cl 4	O 2	S 1	0	0
5	D	1	Total 19	C 12	Cl 4	O 2	S 1	0	0
5	E	1	Total 19	C 12	Cl 4	O 2	S 1	0	0
5	F	1	Total 19	C 12	Cl 4	O 2	S 1	0	0

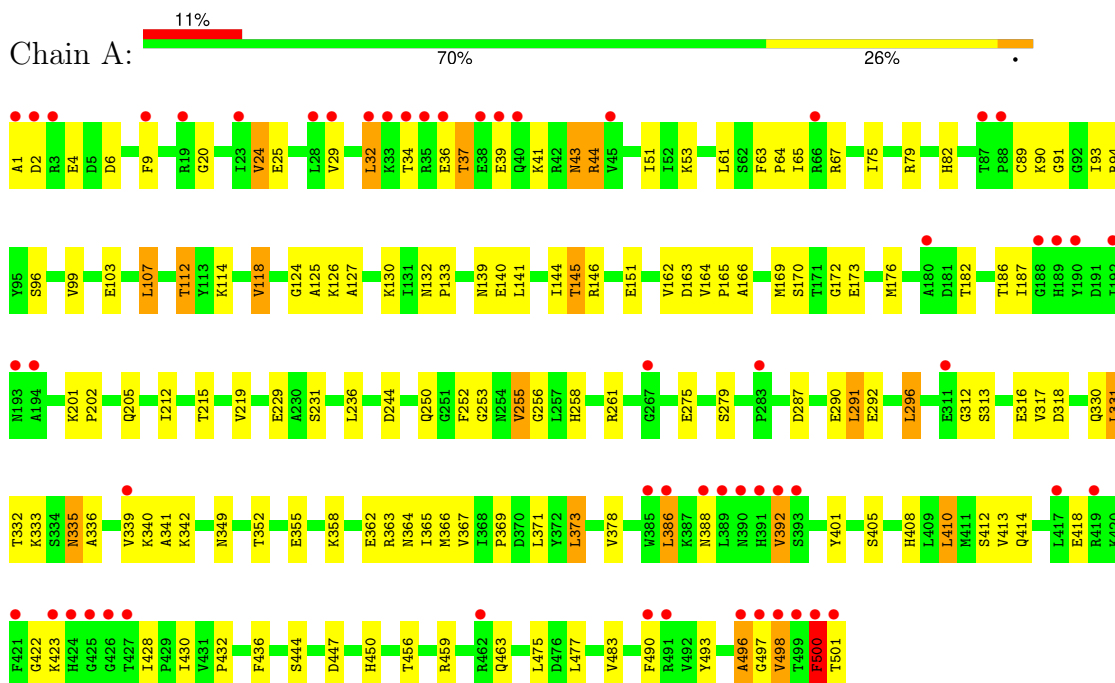
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	17	Total	O	0	0
			17	17		
6	C	19	Total	O	0	0
			19	19		
6	D	20	Total	O	0	0
			20	20		
6	E	13	Total	O	0	0
			13	13		
6	F	6	Total	O	0	0
			6	6		

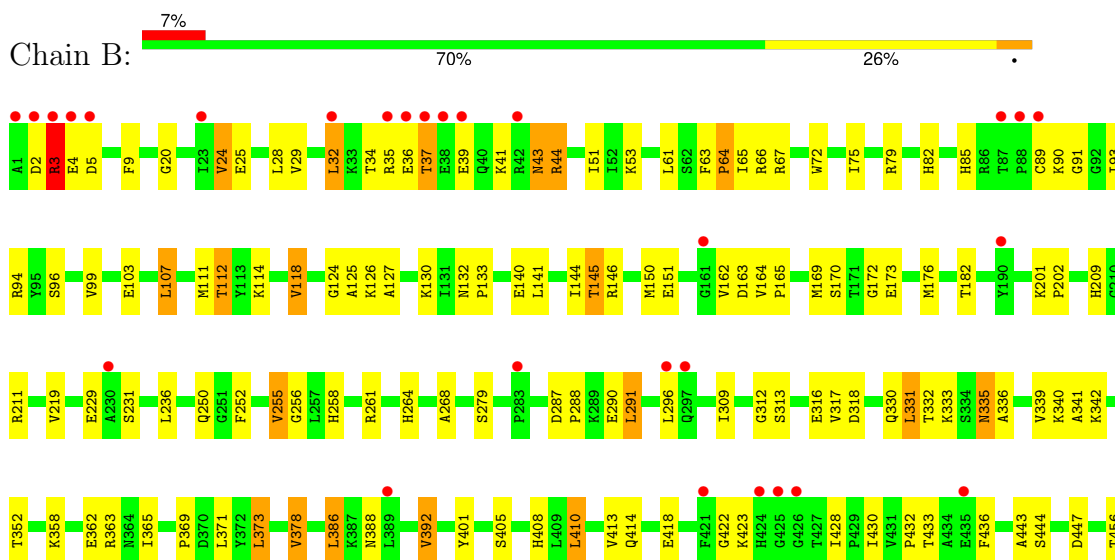
### 3 Residue-property plots

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

#### • Molecule 1: GLUD1 protein



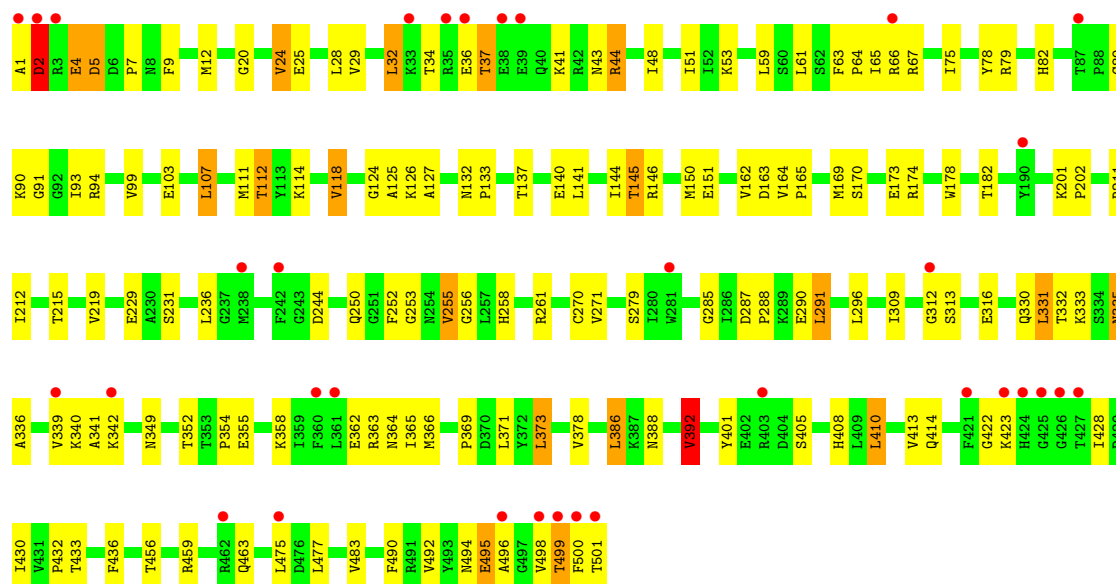
#### • Molecule 1: GLUD1 protein



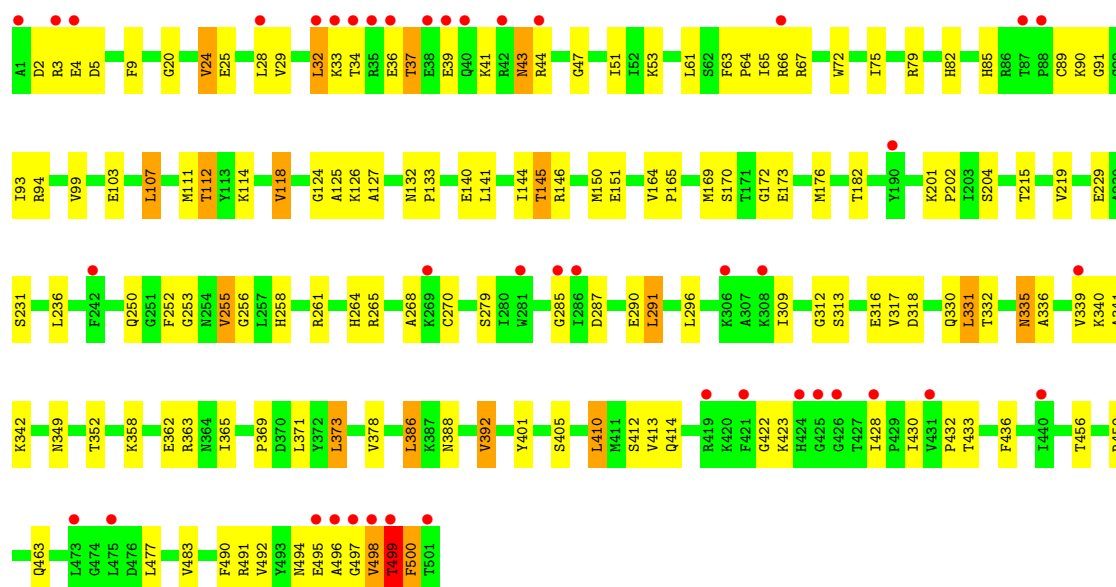




• Molecule 1: GLUD1 protein

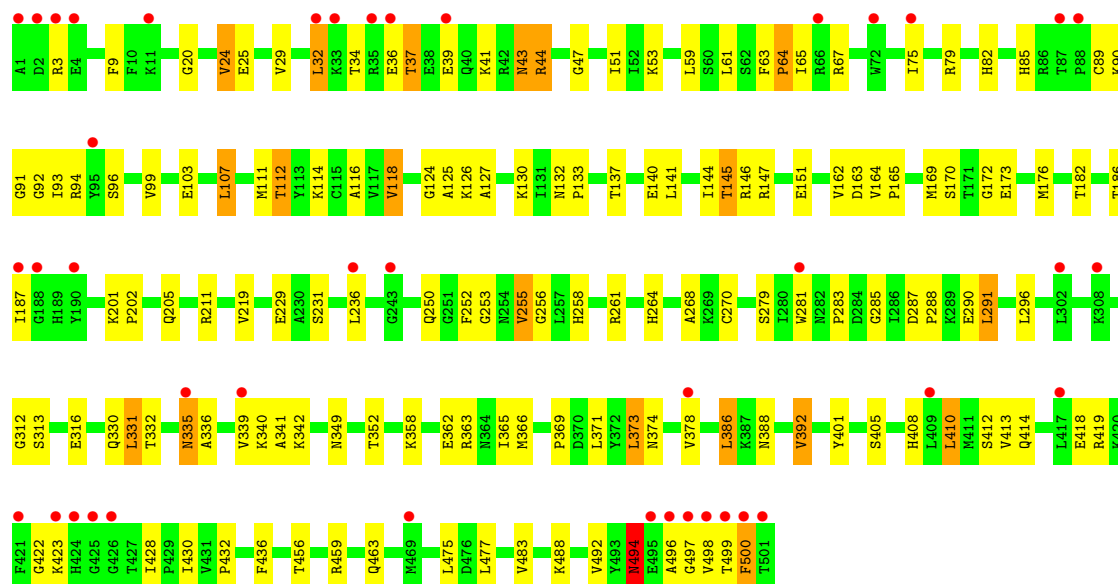


• Molecule 1: GLUD1 protein

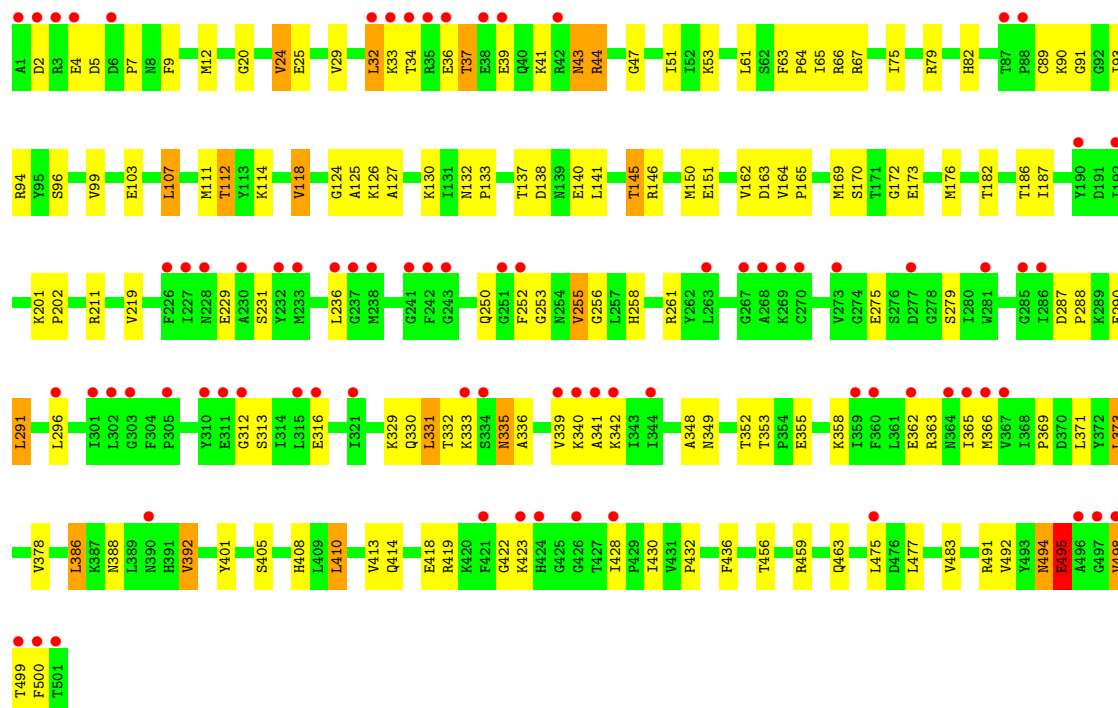


• Molecule 1: GLUD1 protein





• Molecule 1: GLUD1 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.38Å 101.30Å 166.59Å 90.00° 102.46° 90.00°	Depositor
Resolution (Å)	48.34 – 2.50 48.36 – 2.49	Depositor EDS
% Data completeness (in resolution range)	94.7 (48.34-2.50) 94.1 (48.36-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.239 , 0.257 0.230 , 0.251	Depositor DCC
$R_{free}$ test set	6984 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24226	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B1T, GTP, NDP

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	0/3998	0.74	3/5396 (0.1%)
1	B	0.44	0/3998	0.91	6/5396 (0.1%)
1	C	0.44	0/3998	0.73	4/5396 (0.1%)
1	D	0.43	0/3998	0.79	3/5396 (0.1%)
1	E	0.43	0/3998	0.73	4/5396 (0.1%)
1	F	0.43	0/3998	0.86	6/5396 (0.1%)
All	All	0.44	0/23988	0.80	26/32376 (0.1%)

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	E	0	1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	419	ARG	NE-CZ-NH1	-22.85	108.87	120.30
1	F	419	ARG	NE-CZ-NH2	21.56	131.08	120.30
1	B	35	ARG	NE-CZ-NH1	-21.50	109.55	120.30
1	B	35	ARG	NE-CZ-NH2	21.09	130.85	120.30
1	B	44	ARG	NE-CZ-NH1	-19.57	110.51	120.30
1	D	44	ARG	NE-CZ-NH1	-18.97	110.81	120.30
1	B	44	ARG	NE-CZ-NH2	18.92	129.76	120.30
1	D	44	ARG	NE-CZ-NH2	18.54	129.57	120.30
1	A	44	ARG	NE-CZ-NH2	-11.39	114.60	120.30
1	F	44	ARG	NE-CZ-NH2	-11.11	114.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	F	419	ARG	CD-NE-CZ	10.70	138.58	123.60
1	C	44	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	C	44	ARG	NE-CZ-NH1	10.47	125.53	120.30
1	F	44	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	E	44	ARG	NE-CZ-NH2	-10.19	115.21	120.30
1	B	44	ARG	CD-NE-CZ	10.03	137.64	123.60
1	D	44	ARG	CD-NE-CZ	10.02	137.63	123.60
1	B	35	ARG	CD-NE-CZ	9.90	137.46	123.60
1	E	44	ARG	NE-CZ-NH1	9.59	125.10	120.30
1	F	44	ARG	CD-NE-CZ	5.79	131.70	123.60
1	A	44	ARG	CD-NE-CZ	5.68	131.55	123.60
1	C	44	ARG	CD-NE-CZ	5.57	131.40	123.60
1	E	44	ARG	CD-NE-CZ	5.37	131.12	123.60
1	C	392	VAL	CB-CA-C	-5.08	101.75	111.40
1	E	419	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	500	PHE	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3915	0	3880	124	0
1	B	3915	0	3880	127	0
1	C	3915	0	3880	125	0
1	D	3915	0	3880	124	0
1	E	3915	0	3880	131	0
1	F	3915	0	3880	123	0
2	A	9	0	5	1	0
2	B	9	0	5	3	0
2	C	9	0	5	0	0
2	D	9	0	5	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	9	0	5	5	0
2	F	9	0	5	2	0
3	A	48	0	26	8	0
3	B	48	0	26	5	0
3	C	48	0	26	6	0
3	D	48	0	26	8	0
3	E	48	0	26	8	0
3	F	48	0	26	9	0
4	A	32	0	12	2	0
4	B	32	0	10	1	0
4	C	32	0	12	1	0
4	D	32	0	12	1	0
4	E	32	0	12	0	0
4	F	32	0	12	0	0
5	A	19	0	4	2	0
5	B	19	0	4	2	0
5	C	19	0	4	3	0
5	D	19	0	4	4	0
5	E	19	0	4	1	0
5	F	19	0	4	2	0
6	A	13	0	0	1	0
6	B	17	0	0	0	0
6	C	19	0	0	0	0
6	D	20	0	0	2	0
6	E	13	0	0	1	0
6	F	6	0	0	1	0
All	All	24226	0	23560	724	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (724) 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:F:5:ASP:OD2	1:F:332:THR:HB	1.59	1.00
1:B:3:ARG:HG3	1:B:3:ARG:HH11	1.26	1.00
1:D:332:THR:H	1:D:335:ASN:HD21	1.12	0.98
1:C:150:MET:HG3	5:C:552:B1T:CLAE	2.03	0.95
1:B:150:MET:HG3	5:B:552:B1T:CLAE	2.04	0.94
1:E:332:THR:H	1:E:335:ASN:HD21	1.16	0.93
1:B:332:THR:H	1:B:335:ASN:HD21	1.17	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:THR:H	1:A:335:ASN:HD21	1.16	0.91
1:D:112:THR:HG22	1:D:124:GLY:HA3	1.52	0.91
1:F:150:MET:HG3	5:F:552:B1T:CLAE	2.08	0.90
1:C:332:THR:H	1:C:335:ASN:HD21	1.15	0.90
1:F:332:THR:H	1:F:335:ASN:HD21	1.16	0.90
1:F:112:THR:HG22	1:F:124:GLY:HA3	1.53	0.90
1:B:34:THR:HG22	1:B:36:GLU:H	1.38	0.89
1:B:112:THR:HG22	1:B:124:GLY:CA	2.03	0.88
1:B:112:THR:HG22	1:B:124:GLY:HA3	1.53	0.88
1:E:34:THR:HG22	1:E:36:GLU:H	1.39	0.88
1:C:112:THR:HG22	1:C:124:GLY:HA3	1.54	0.88
1:A:34:THR:HG22	1:A:36:GLU:H	1.38	0.88
1:F:250:GLN:HE22	1:F:330:GLN:HE21	1.22	0.87
1:C:250:GLN:HE22	1:C:330:GLN:HE21	1.22	0.87
1:D:250:GLN:HE22	1:D:330:GLN:HE21	1.22	0.87
1:D:34:THR:HG22	1:D:36:GLU:H	1.39	0.87
1:D:32:LEU:HD23	1:D:494:ASN:HD21	1.40	0.86
1:C:34:THR:HG22	1:C:36:GLU:H	1.37	0.86
1:F:34:THR:HG22	1:F:36:GLU:H	1.37	0.86
1:B:211:ARG:HH22	3:B:551:NDP:H71N	1.24	0.86
1:E:112:THR:HG22	1:E:124:GLY:CA	2.06	0.86
1:F:112:THR:HG22	1:F:124:GLY:CA	2.06	0.86
1:A:112:THR:HG22	1:A:124:GLY:HA3	1.57	0.86
1:E:126:LYS:HZ3	2:E:550:GLU:N	1.73	0.85
1:D:112:THR:HG22	1:D:124:GLY:CA	2.05	0.85
1:E:112:THR:HG22	1:E:124:GLY:HA3	1.57	0.85
1:A:250:GLN:HE22	1:A:330:GLN:HE21	1.24	0.85
1:A:112:THR:HG22	1:A:124:GLY:CA	2.07	0.84
1:C:112:THR:HG22	1:C:124:GLY:CA	2.06	0.84
1:E:250:GLN:HE22	1:E:330:GLN:HE21	1.21	0.84
3:D:551:NDP:H52N	3:D:551:NDP:H2N	1.58	0.83
1:B:250:GLN:HE22	1:B:330:GLN:HE21	1.26	0.83
1:C:48:ILE:HD11	1:C:499:THR:HG21	1.61	0.82
1:B:126:LYS:HZ3	2:B:550:GLU:N	1.78	0.82
1:B:112:THR:HG22	1:B:124:GLY:N	1.97	0.79
1:E:112:THR:HG22	1:E:124:GLY:N	1.98	0.79
1:F:32:LEU:HD23	1:F:494:ASN:HD21	1.46	0.79
1:B:51:ILE:HD12	1:E:64:PRO:HB3	1.65	0.79
1:B:112:THR:HG22	1:B:124:GLY:H	1.48	0.79
1:E:112:THR:HG22	1:E:124:GLY:H	1.48	0.79
1:A:205:GLN:HE22	1:B:496:ALA:HB2	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:THR:HG22	1:A:124:GLY:H	1.49	0.78
1:A:112:THR:HG22	1:A:124:GLY:N	1.99	0.78
1:E:211:ARG:HH22	3:E:551:NDP:H71N	1.31	0.76
1:B:72:TRP:HE1	1:E:499:THR:HG21	1.51	0.76
1:C:112:THR:HG22	1:C:124:GLY:N	2.01	0.76
1:C:91:GLY:HA3	1:C:125:ALA:O	1.86	0.75
1:E:173:GLU:HB3	1:E:202:PRO:HG3	1.68	0.75
1:C:112:THR:HG22	1:C:124:GLY:H	1.52	0.74
1:D:112:THR:HG22	1:D:124:GLY:N	2.01	0.74
3:A:551:NDP:H52N	3:A:551:NDP:H2N	1.69	0.74
1:F:107:LEU:HB3	1:F:126:LYS:HE3	1.69	0.74
1:B:64:PRO:HB3	1:E:51:ILE:HD12	1.70	0.73
3:F:551:NDP:H2N	3:F:551:NDP:H52N	1.70	0.73
1:D:255:VAL:HG23	6:D:557:HOH:O	1.88	0.73
1:F:112:THR:HG22	1:F:124:GLY:N	2.03	0.73
1:A:91:GLY:HA3	1:A:125:ALA:O	1.89	0.73
1:D:107:LEU:HB3	1:D:126:LYS:HE3	1.70	0.73
1:B:91:GLY:HA3	1:B:125:ALA:O	1.89	0.72
1:D:112:THR:HG22	1:D:124:GLY:H	1.52	0.72
1:F:112:THR:HG22	1:F:124:GLY:H	1.54	0.72
1:C:250:GLN:HE22	1:C:330:GLN:NE2	1.87	0.72
1:E:94:ARG:HG3	1:E:169:MET:HB2	1.72	0.72
1:F:91:GLY:HA3	1:F:125:ALA:O	1.89	0.72
1:A:107:LEU:HB3	1:A:126:LYS:HE3	1.72	0.72
1:C:107:LEU:HB3	1:C:126:LYS:HE3	1.71	0.71
1:D:250:GLN:HE22	1:D:330:GLN:NE2	1.88	0.71
1:C:212:ILE:HB	4:C:553:GTP:O3'	1.90	0.71
1:B:94:ARG:HG3	1:B:169:MET:HB2	1.72	0.71
1:F:94:ARG:HG3	1:F:169:MET:HB2	1.72	0.71
1:F:250:GLN:HE22	1:F:330:GLN:NE2	1.89	0.71
1:D:386:LEU:HD21	1:E:392:VAL:HG13	1.73	0.71
1:E:107:LEU:HB3	1:E:126:LYS:HE3	1.72	0.71
1:F:173:GLU:HB3	1:F:202:PRO:HG3	1.73	0.71
1:B:173:GLU:HB3	1:B:202:PRO:HG3	1.73	0.70
1:A:173:GLU:HB3	1:A:202:PRO:HG3	1.73	0.70
1:D:173:GLU:HB3	1:D:202:PRO:HG3	1.73	0.70
1:E:250:GLN:HE22	1:E:330:GLN:NE2	1.88	0.70
1:D:94:ARG:HG3	1:D:169:MET:HB2	1.74	0.69
1:B:107:LEU:HB3	1:B:126:LYS:HE3	1.73	0.69
1:C:51:ILE:HD12	1:F:64:PRO:HB3	1.74	0.69
1:C:173:GLU:HB3	1:C:202:PRO:HG3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ILE:HD12	1:D:64:PRO:HB3	1.73	0.69
1:A:94:ARG:HG3	1:A:169:MET:HB2	1.73	0.69
1:C:94:ARG:HG3	1:C:169:MET:HB2	1.74	0.68
1:D:91:GLY:HA3	1:D:125:ALA:O	1.93	0.68
1:A:250:GLN:HE22	1:A:330:GLN:NE2	1.90	0.68
1:B:250:GLN:HE22	1:B:330:GLN:NE2	1.91	0.68
1:E:91:GLY:HA3	1:E:125:ALA:O	1.92	0.68
3:C:551:NDP:H52N	3:C:551:NDP:H2N	1.74	0.68
1:B:34:THR:HG22	1:B:36:GLU:N	2.09	0.68
1:D:332:THR:N	1:D:335:ASN:HD21	1.90	0.68
1:C:501:THR:HA	1:F:66:ARG:NH2	2.08	0.67
1:C:258:HIS:HD2	1:C:261:ARG:HH11	1.42	0.67
1:F:332:THR:H	1:F:335:ASN:ND2	1.93	0.67
1:C:34:THR:HG22	1:C:36:GLU:N	2.09	0.66
1:E:34:THR:HG22	1:E:36:GLU:N	2.10	0.66
1:F:34:THR:HG22	1:F:36:GLU:N	2.09	0.66
1:C:1:ALA:O	1:C:2:ASP:HB2	1.93	0.66
1:D:34:THR:HG22	1:D:36:GLU:N	2.09	0.66
1:E:112:THR:CG2	1:E:124:GLY:H	2.09	0.66
1:B:112:THR:CG2	1:B:124:GLY:H	2.09	0.66
1:E:255:VAL:HG23	6:E:555:HOH:O	1.95	0.66
1:D:258:HIS:HD2	1:D:261:ARG:HH11	1.45	0.65
3:E:551:NDP:H52N	3:E:551:NDP:H2N	1.78	0.65
1:A:34:THR:HG22	1:A:36:GLU:N	2.10	0.65
1:E:258:HIS:HD2	1:E:261:ARG:HH11	1.43	0.65
1:F:258:HIS:HD2	1:F:261:ARG:HH11	1.44	0.65
1:C:64:PRO:HB3	1:F:51:ILE:HD12	1.78	0.65
1:D:332:THR:H	1:D:335:ASN:ND2	1.89	0.65
1:B:258:HIS:HD2	1:B:261:ARG:HH11	1.45	0.65
1:A:258:HIS:HD2	1:A:261:ARG:HH11	1.44	0.64
1:A:64:PRO:HB3	1:D:51:ILE:HD12	1.80	0.64
1:B:496:ALA:O	1:B:498:VAL:HG23	1.97	0.64
1:D:33:LYS:HD2	1:D:495:GLU:HB2	1.80	0.64
1:D:253:GLY:HA3	3:D:551:NDP:O1A	1.98	0.64
1:E:332:THR:H	1:E:335:ASN:ND2	1.93	0.64
1:C:253:GLY:HA3	3:C:551:NDP:O1A	1.97	0.64
1:F:253:GLY:HA3	3:F:551:NDP:O1A	1.98	0.64
1:B:44:ARG:HD3	1:B:499:THR:HA	1.79	0.64
1:E:496:ALA:HA	1:E:500:PHE:HB2	1.80	0.64
1:A:112:THR:CG2	1:A:124:GLY:H	2.10	0.63
1:E:253:GLY:HA3	3:E:551:NDP:O1A	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:THR:N	1:E:335:ASN:HD21	1.94	0.63
1:A:349:ASN:ND2	3:A:551:NDP:O2D	2.31	0.63
1:D:150:MET:HG3	5:D:552:B1T:CLAE	2.36	0.62
1:A:332:THR:H	1:A:335:ASN:ND2	1.94	0.62
1:C:112:THR:CG2	1:C:124:GLY:H	2.12	0.62
1:D:28:LEU:HD22	1:D:490:PHE:CD2	2.34	0.62
1:A:44:ARG:HH22	1:D:66:ARG:HH22	1.47	0.61
1:A:253:GLY:HA3	3:A:551:NDP:O1A	2.00	0.61
1:B:332:THR:H	1:B:335:ASN:ND2	1.94	0.61
1:B:332:THR:N	1:B:335:ASN:HD21	1.94	0.61
1:D:378:VAL:HG23	6:D:554:HOH:O	2.01	0.61
1:E:141:LEU:O	1:E:145:THR:HG23	2.01	0.61
1:D:112:THR:CG2	1:D:124:GLY:H	2.13	0.61
1:F:332:THR:N	1:F:335:ASN:HD21	1.93	0.61
1:D:141:LEU:O	1:D:145:THR:HG23	2.01	0.60
1:C:332:THR:H	1:C:335:ASN:ND2	1.93	0.60
1:F:7:PRO:HD2	1:F:329:LYS:HD2	1.82	0.60
1:C:141:LEU:O	1:C:145:THR:HG23	2.01	0.60
1:F:112:THR:CG2	1:F:124:GLY:H	2.14	0.60
1:A:141:LEU:O	1:A:145:THR:HG23	2.01	0.60
1:C:432:PRO:HB3	1:C:436:PHE:HD2	1.67	0.60
1:F:432:PRO:HB3	1:F:436:PHE:HD2	1.66	0.60
1:C:332:THR:N	1:C:335:ASN:HD21	1.93	0.60
1:E:53:LYS:O	1:E:82:HIS:HE1	1.84	0.60
1:F:53:LYS:O	1:F:82:HIS:HE1	1.85	0.59
1:F:141:LEU:O	1:F:145:THR:HG23	2.02	0.59
1:A:53:LYS:O	1:A:82:HIS:HE1	1.84	0.59
1:A:413:VAL:HG13	1:A:430:ILE:HG13	1.85	0.59
1:B:3:ARG:HH11	1:B:3:ARG:CG	2.08	0.59
1:D:410:LEU:HG	1:D:430:ILE:HG22	1.84	0.59
1:B:141:LEU:O	1:B:145:THR:HG23	2.03	0.58
1:F:410:LEU:HG	1:F:430:ILE:HG22	1.85	0.58
1:D:53:LYS:O	1:D:82:HIS:HE1	1.86	0.58
1:B:432:PRO:HB3	1:B:436:PHE:HD2	1.68	0.58
1:C:53:LYS:O	1:C:82:HIS:HE1	1.86	0.58
1:B:3:ARG:HG3	1:B:3:ARG:NH1	2.05	0.58
1:F:413:VAL:HG13	1:F:430:ILE:HG13	1.85	0.58
1:E:358:LYS:O	1:E:362:GLU:HG3	2.04	0.58
1:C:349:ASN:ND2	3:C:551:NDP:O2D	2.37	0.58
1:E:410:LEU:HG	1:E:430:ILE:HG22	1.84	0.58
1:F:114:LYS:HD2	1:F:378:VAL:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:THR:OG1	3:C:551:NDP:H42N	2.02	0.58
1:D:413:VAL:HG13	1:D:430:ILE:HG13	1.86	0.58
1:F:5:ASP:OD1	1:F:355:GLU:HB3	2.03	0.58
1:C:413:VAL:HG13	1:C:430:ILE:HG13	1.85	0.57
1:E:413:VAL:HG13	1:E:430:ILE:HG13	1.84	0.57
1:A:410:LEU:O	1:A:413:VAL:HG12	2.05	0.57
1:B:358:LYS:O	1:B:362:GLU:HG3	2.03	0.57
1:D:410:LEU:O	1:D:413:VAL:HG12	2.05	0.57
1:A:205:GLN:HE22	1:B:496:ALA:CB	2.16	0.57
1:A:332:THR:N	1:A:335:ASN:HD21	1.94	0.57
1:A:215:THR:OG1	3:A:551:NDP:H42N	2.04	0.57
1:D:498:VAL:HG22	1:E:146:ARG:NH2	2.19	0.57
1:B:63:PHE:CZ	1:B:75:ILE:HD11	2.40	0.57
1:A:201:LYS:NZ	1:A:388:ASN:HD21	2.03	0.56
1:D:114:LYS:HD2	1:D:378:VAL:HG21	1.87	0.56
1:E:494:ASN:O	1:E:498:VAL:HB	2.04	0.56
1:E:432:PRO:HB3	1:E:436:PHE:HD2	1.70	0.56
1:B:410:LEU:HG	1:B:430:ILE:HG22	1.86	0.56
1:D:358:LYS:O	1:D:362:GLU:HG3	2.06	0.56
1:A:392:VAL:HG13	1:B:386:LEU:HD21	1.88	0.56
1:A:432:PRO:HB3	1:A:436:PHE:HD2	1.71	0.56
2:B:550:GLU:HB3	3:B:551:NDP:H41N	1.88	0.56
1:C:20:GLY:O	1:C:24:VAL:HG23	2.06	0.56
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.70	0.56
1:F:82:HIS:HD2	1:F:112:THR:HG21	1.71	0.56
1:A:410:LEU:HG	1:A:430:ILE:HG22	1.86	0.56
1:B:53:LYS:O	1:B:82:HIS:HE1	1.88	0.56
1:E:92:GLY:HA3	2:E:550:GLU:N	2.21	0.56
1:B:413:VAL:HG13	1:B:430:ILE:HG13	1.87	0.56
1:F:82:HIS:CD2	1:F:112:THR:HG21	2.41	0.56
1:B:201:LYS:NZ	1:B:388:ASN:HD21	2.04	0.56
1:C:410:LEU:O	1:C:413:VAL:HG12	2.05	0.56
1:C:414:GLN:HG3	1:C:428:ILE:O	2.06	0.56
1:F:91:GLY:O	1:F:165:PRO:HA	2.06	0.56
1:A:91:GLY:O	1:A:165:PRO:HA	2.06	0.56
1:D:215:THR:OG1	3:D:551:NDP:H42N	2.06	0.56
1:B:392:VAL:HG13	1:F:386:LEU:HD21	1.88	0.55
1:A:44:ARG:NH2	1:D:66:ARG:HH22	2.03	0.55
1:C:82:HIS:CD2	1:C:112:THR:HG21	2.42	0.55
1:E:91:GLY:O	1:E:165:PRO:HA	2.07	0.55
1:B:209:HIS:HE1	4:B:553:GTP:O1A	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LYS:O	1:A:362:GLU:HG3	2.06	0.55
1:C:114:LYS:HD2	1:C:378:VAL:HG21	1.88	0.55
1:E:63:PHE:CZ	1:E:75:ILE:HD11	2.42	0.55
1:C:410:LEU:HG	1:C:430:ILE:HG22	1.89	0.55
1:B:414:GLN:HG3	1:B:428:ILE:O	2.06	0.55
1:C:358:LYS:O	1:C:362:GLU:HG3	2.06	0.55
1:E:349:ASN:CG	3:E:551:NDP:O2D	2.45	0.55
1:A:20:GLY:O	1:A:24:VAL:HG23	2.07	0.55
1:F:5:ASP:O	1:F:7:PRO:HD3	2.07	0.55
1:E:414:GLN:HG3	1:E:428:ILE:O	2.07	0.55
1:A:82:HIS:HD2	1:A:112:THR:HG21	1.72	0.55
1:D:20:GLY:O	1:D:24:VAL:HG23	2.07	0.55
1:E:410:LEU:O	1:E:413:VAL:HG12	2.07	0.55
1:C:63:PHE:CZ	1:C:75:ILE:HD11	2.42	0.54
1:D:63:PHE:CZ	1:D:75:ILE:HD11	2.42	0.54
1:A:205:GLN:NE2	1:B:496:ALA:HB2	2.20	0.54
1:B:20:GLY:O	1:B:24:VAL:HG23	2.08	0.54
1:C:91:GLY:O	1:C:165:PRO:HA	2.07	0.54
1:D:82:HIS:HD2	1:D:112:THR:HG21	1.73	0.54
1:A:63:PHE:CZ	1:A:75:ILE:HD11	2.42	0.54
1:C:82:HIS:HD2	1:C:112:THR:HG21	1.71	0.54
5:E:552:B1T:OAB	5:E:552:B1T:OAA	2.26	0.54
1:F:4:GLU:OE2	1:F:333:LYS:HB3	2.07	0.54
1:D:82:HIS:CD2	1:D:112:THR:HG21	2.42	0.54
1:E:79:ARG:HH11	1:E:127:ALA:HB2	1.73	0.54
1:E:82:HIS:CD2	1:E:112:THR:HG21	2.43	0.54
1:A:82:HIS:CD2	1:A:112:THR:HG21	2.43	0.54
1:D:91:GLY:O	1:D:165:PRO:HA	2.08	0.54
1:E:82:HIS:HD2	1:E:112:THR:HG21	1.72	0.54
5:B:552:B1T:OAA	5:B:552:B1T:OAB	2.25	0.54
1:D:459:ARG:NH1	1:D:463:GLN:HE22	2.05	0.54
1:A:386:LEU:HD21	1:F:392:VAL:HG13	1.90	0.54
1:B:66:ARG:HH22	1:E:44:ARG:HH22	1.56	0.54
1:F:20:GLY:O	1:F:24:VAL:HG23	2.07	0.54
1:F:358:LYS:O	1:F:362:GLU:HG3	2.08	0.54
1:B:410:LEU:O	1:B:413:VAL:HG12	2.08	0.53
1:C:366:MET:HB2	1:C:475:LEU:HD22	1.89	0.53
1:C:392:VAL:HG13	1:E:386:LEU:HD21	1.89	0.53
1:F:410:LEU:O	1:F:413:VAL:HG12	2.09	0.53
5:D:552:B1T:OAA	5:D:552:B1T:OAB	2.26	0.53
1:A:414:GLN:HG3	1:A:428:ILE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:PHE:CZ	1:F:75:ILE:HD11	2.43	0.53
1:A:79:ARG:HH11	1:A:127:ALA:HB2	1.73	0.53
1:C:99:VAL:HA	1:C:103:GLU:OE1	2.09	0.53
5:A:552:B1T:OAA	5:A:552:B1T:OAB	2.28	0.52
1:B:82:HIS:HD2	1:B:112:THR:HG21	1.74	0.52
1:B:85:HIS:HB2	1:B:492:VAL:HG11	1.91	0.52
1:B:82:HIS:CD2	1:B:112:THR:HG21	2.45	0.52
1:C:61:LEU:N	1:C:61:LEU:HD12	2.25	0.52
1:E:126:LYS:NZ	2:E:550:GLU:N	2.53	0.52
1:F:61:LEU:N	1:F:61:LEU:HD12	2.25	0.52
1:A:201:LYS:HZ1	1:A:388:ASN:HD21	1.58	0.52
5:A:552:B1T:SAK	1:E:147:ARG:HB2	2.49	0.52
1:C:24:VAL:HG22	1:C:483:VAL:HG22	1.92	0.52
1:B:91:GLY:O	1:B:165:PRO:HA	2.09	0.52
1:B:459:ARG:NH1	1:B:463:GLN:HE22	2.08	0.52
1:F:79:ARG:HH11	1:F:127:ALA:HB2	1.74	0.52
1:E:20:GLY:O	1:E:24:VAL:HG23	2.09	0.52
5:C:552:B1T:OAA	5:C:552:B1T:OAB	2.27	0.51
1:E:61:LEU:HD12	1:E:61:LEU:N	2.25	0.51
1:B:72:TRP:HE1	1:E:499:THR:CG2	2.23	0.51
1:D:499:THR:HG23	1:D:499:THR:O	2.11	0.51
1:A:498:VAL:HB	1:D:72:TRP:CH2	2.45	0.51
1:A:436:PHE:HB2	1:F:408:HIS:HB3	1.92	0.51
1:F:37:THR:HA	1:F:41:LYS:CD	2.40	0.51
1:C:201:LYS:NZ	1:C:388:ASN:HD21	2.09	0.51
1:F:316:GLU:O	1:F:340:LYS:HD3	2.10	0.51
5:F:552:B1T:OAA	5:F:552:B1T:OAB	2.28	0.51
1:B:37:THR:HA	1:B:41:LYS:CD	2.41	0.51
1:B:99:VAL:HA	1:B:103:GLU:OE1	2.10	0.51
1:D:79:ARG:HH11	1:D:127:ALA:HB2	1.75	0.51
1:F:99:VAL:HA	1:F:103:GLU:OE1	2.11	0.51
1:F:236:LEU:O	1:F:342:LYS:HE2	2.11	0.51
1:F:414:GLN:HG3	1:F:428:ILE:O	2.10	0.51
1:B:219:VAL:HG22	1:B:373:LEU:HD13	1.93	0.51
1:C:79:ARG:HH11	1:C:127:ALA:HB2	1.76	0.51
1:D:37:THR:HA	1:D:41:LYS:CD	2.41	0.51
1:E:89:CYS:HB3	1:E:125:ALA:HB2	1.93	0.51
1:F:7:PRO:HD2	1:F:329:LYS:CD	2.41	0.51
1:F:89:CYS:HB3	1:F:125:ALA:HB2	1.93	0.51
1:A:450:HIS:CE1	4:A:553:GTP:O3G	2.64	0.50
1:B:114:LYS:HD2	1:B:378:VAL:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:O	1:A:342:LYS:HE2	2.11	0.50
1:D:414:GLN:HG3	1:D:428:ILE:O	2.10	0.50
1:C:495:GLU:HG3	1:D:204:SER:OG	2.10	0.50
1:D:236:LEU:O	1:D:342:LYS:HE2	2.10	0.50
1:A:61:LEU:N	1:A:61:LEU:HD12	2.26	0.50
1:C:37:THR:HA	1:C:41:LYS:CD	2.41	0.50
1:D:61:LEU:N	1:D:61:LEU:HD12	2.26	0.50
1:C:37:THR:HA	1:C:41:LYS:HD2	1.94	0.50
1:C:174:ARG:HG3	1:E:497:GLY:N	2.27	0.50
1:B:126:LYS:NZ	2:B:550:GLU:N	2.57	0.50
1:B:236:LEU:O	1:B:342:LYS:HE2	2.11	0.50
1:C:236:LEU:O	1:C:342:LYS:HE2	2.12	0.50
1:E:37:THR:HA	1:E:41:LYS:CD	2.42	0.50
1:F:219:VAL:HG22	1:F:373:LEU:HD13	1.93	0.50
1:A:37:THR:HA	1:A:41:LYS:CD	2.42	0.49
1:A:99:VAL:HA	1:A:103:GLU:OE1	2.12	0.49
1:A:316:GLU:O	1:A:340:LYS:HD3	2.12	0.49
1:C:146:ARG:HG2	1:C:182:THR:OG1	2.12	0.49
1:A:367:VAL:HG23	6:A:555:HOH:O	2.12	0.49
1:E:236:LEU:O	1:E:342:LYS:HE2	2.12	0.49
1:A:498:VAL:HB	1:D:72:TRP:HH2	1.78	0.49
1:D:32:LEU:CD2	1:D:494:ASN:HD21	2.18	0.49
1:D:169:MET:HA	3:D:551:NDP:O1N	2.12	0.49
1:E:459:ARG:NH1	1:E:463:GLN:HE22	2.10	0.49
1:A:37:THR:HA	1:A:41:LYS:HD2	1.94	0.49
3:B:551:NDP:H52N	3:B:551:NDP:H2N	1.94	0.49
1:B:79:ARG:HH11	1:B:127:ALA:HB2	1.78	0.49
1:F:169:MET:HA	3:F:551:NDP:O1N	2.13	0.49
1:B:24:VAL:HG22	1:B:483:VAL:HG22	1.94	0.49
1:F:33:LYS:HG3	1:F:494:ASN:OD1	2.13	0.49
1:B:255:VAL:HG11	3:B:551:NDP:O4D	2.13	0.49
1:F:459:ARG:NH1	1:F:463:GLN:HE22	2.11	0.49
1:A:166:ALA:HB3	2:A:550:GLU:HG2	1.95	0.49
1:B:341:ALA:O	1:B:365:ILE:HD12	2.12	0.49
1:C:255:VAL:HG23	1:C:256:GLY:H	1.78	0.49
1:D:341:ALA:O	1:D:365:ILE:HD12	2.13	0.49
1:B:146:ARG:HG2	1:B:182:THR:OG1	2.13	0.49
1:F:255:VAL:HG23	1:F:256:GLY:H	1.78	0.49
1:E:341:ALA:O	1:E:365:ILE:HD12	2.13	0.48
1:D:61:LEU:HD23	1:D:151:GLU:HB3	1.95	0.48
1:D:24:VAL:HG22	1:D:483:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLU:O	1:A:107:LEU:HD22	2.13	0.48
1:D:99:VAL:HA	1:D:103:GLU:OE1	2.13	0.48
1:F:24:VAL:HG22	1:F:483:VAL:HG13	1.96	0.48
1:C:44:ARG:HH22	1:F:66:ARG:HH22	1.60	0.48
1:C:150:MET:CG	5:C:552:B1T:CLAE	2.89	0.48
1:F:5:ASP:O	1:F:353:THR:HG21	2.14	0.48
1:A:459:ARG:NH1	1:A:463:GLN:HE22	2.11	0.48
1:B:61:LEU:HD12	1:B:61:LEU:N	2.28	0.48
1:C:341:ALA:O	1:C:365:ILE:HD12	2.14	0.48
1:D:316:GLU:O	1:D:340:LYS:HD3	2.12	0.48
1:E:255:VAL:HG23	1:E:256:GLY:H	1.78	0.48
1:E:349:ASN:ND2	3:E:551:NDP:O2D	2.46	0.48
1:B:37:THR:HA	1:B:41:LYS:HD2	1.96	0.48
1:B:423:LYS:HE2	1:B:423:LYS:HA	1.95	0.48
1:E:401:TYR:O	1:E:405:SER:HB2	2.13	0.48
1:E:499:THR:O	1:E:499:THR:HG22	2.14	0.48
1:A:255:VAL:HG23	1:A:256:GLY:H	1.78	0.48
1:C:219:VAL:HG22	1:C:373:LEU:HD13	1.95	0.48
1:D:67:ARG:HD2	1:D:140:GLU:OE2	2.14	0.48
1:D:423:LYS:HA	1:D:423:LYS:HE2	1.96	0.48
1:B:103:GLU:O	1:B:107:LEU:HD22	2.14	0.48
1:C:459:ARG:NH1	1:C:463:GLN:HE22	2.11	0.48
2:D:550:GLU:HA	3:D:551:NDP:H41N	1.95	0.48
1:E:114:LYS:HD2	1:E:378:VAL:HG21	1.94	0.48
1:F:341:ALA:O	1:F:365:ILE:HD12	2.14	0.48
1:D:369:PRO:HD3	1:D:477:LEU:HB2	1.96	0.48
1:E:252:PHE:CZ	1:E:291:LEU:HD13	2.49	0.48
1:A:366:MET:HB2	1:A:475:LEU:HD22	1.95	0.47
1:B:89:CYS:HB3	1:B:125:ALA:HB2	1.95	0.47
1:F:348:ALA:HA	3:F:551:NDP:H1D	1.96	0.47
1:D:255:VAL:HG23	1:D:256:GLY:H	1.77	0.47
1:E:99:VAL:HA	1:E:103:GLU:OE1	2.14	0.47
1:E:146:ARG:HG2	1:E:182:THR:OG1	2.14	0.47
1:C:118:VAL:HG13	1:C:118:VAL:O	2.14	0.47
1:A:212:ILE:HB	4:A:553:GTP:O2'	2.14	0.47
1:B:252:PHE:CZ	1:B:291:LEU:HD13	2.49	0.47
1:B:255:VAL:HG23	1:B:256:GLY:H	1.79	0.47
1:C:252:PHE:CZ	1:C:291:LEU:HD13	2.49	0.47
1:D:436:PHE:HB2	1:E:408:HIS:HB3	1.96	0.47
1:D:497:GLY:O	1:D:498:VAL:C	2.52	0.47
1:A:275:GLU:HG2	3:A:551:NDP:O3B	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:SER:H	1:A:447:ASP:HB2	1.78	0.47
1:B:111:MET:SD	1:B:114:LYS:HE3	2.55	0.47
1:C:89:CYS:HB3	1:C:125:ALA:HB2	1.96	0.47
1:D:118:VAL:O	1:D:118:VAL:HG13	2.14	0.47
1:D:219:VAL:HG22	1:D:373:LEU:HD13	1.96	0.47
1:E:201:LYS:NZ	1:E:388:ASN:HD21	2.12	0.47
1:A:24:VAL:CG2	1:A:483:VAL:HG13	2.45	0.47
1:A:349:ASN:HB2	3:A:551:NDP:O2D	2.15	0.47
1:A:401:TYR:O	1:A:405:SER:HB2	2.14	0.47
1:A:423:LYS:HA	1:A:423:LYS:HE2	1.97	0.47
1:C:423:LYS:HE2	1:C:423:LYS:HA	1.96	0.47
1:E:219:VAL:HG22	1:E:373:LEU:HD13	1.97	0.47
1:F:201:LYS:NZ	1:F:388:ASN:HD21	2.13	0.47
1:F:369:PRO:HB2	1:F:371:LEU:HD23	1.97	0.47
1:A:114:LYS:HD2	1:A:378:VAL:HG21	1.95	0.47
1:D:37:THR:HA	1:D:41:LYS:HD2	1.95	0.47
1:E:118:VAL:O	1:E:118:VAL:HG13	2.15	0.47
1:B:316:GLU:O	1:B:340:LYS:HD3	2.15	0.47
1:E:37:THR:HA	1:E:41:LYS:HD2	1.96	0.47
1:E:423:LYS:HE2	1:E:423:LYS:HA	1.96	0.47
1:F:335:ASN:HD22	1:F:336:ALA:N	2.13	0.47
1:A:93:ILE:HG12	1:A:127:ALA:HB3	1.97	0.47
1:A:341:ALA:O	1:A:365:ILE:HD12	2.14	0.47
1:B:201:LYS:HZ1	1:B:388:ASN:HD21	1.62	0.47
1:C:316:GLU:O	1:C:340:LYS:HD3	2.14	0.47
1:D:265:ARG:NH1	4:D:553:GTP:O2G	2.45	0.47
1:F:67:ARG:HD2	1:F:140:GLU:OE2	2.15	0.47
1:F:275:GLU:HG2	3:F:551:NDP:O3B	2.15	0.47
1:A:89:CYS:HB3	1:A:125:ALA:HB2	1.96	0.46
1:B:229:GLU:C	1:B:231:SER:H	2.18	0.46
1:C:24:VAL:CG2	1:C:483:VAL:HG13	2.46	0.46
1:C:61:LEU:HD23	1:C:151:GLU:HB3	1.98	0.46
1:F:126:LYS:HZ3	2:F:550:GLU:N	2.12	0.46
1:F:494:ASN:O	1:F:499:THR:HG22	2.15	0.46
1:A:219:VAL:HG22	1:A:373:LEU:HD13	1.97	0.46
1:C:103:GLU:O	1:C:107:LEU:HD22	2.16	0.46
1:F:37:THR:HA	1:F:41:LYS:HD2	1.96	0.46
1:A:118:VAL:HG13	1:A:118:VAL:O	2.14	0.46
1:B:4:GLU:OE1	1:B:333:LYS:HB3	2.16	0.46
1:B:401:TYR:O	1:B:405:SER:HB2	2.15	0.46
1:D:229:GLU:C	1:D:231:SER:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:THR:HG22	1:C:501:THR:O	2.15	0.46
1:E:335:ASN:N	1:E:335:ASN:HD22	2.13	0.46
1:E:369:PRO:HB2	1:E:371:LEU:HD23	1.96	0.46
1:E:369:PRO:HD3	1:E:477:LEU:HB2	1.98	0.46
1:A:369:PRO:HD3	1:A:477:LEU:HB2	1.97	0.46
1:B:496:ALA:C	1:B:498:VAL:H	2.19	0.46
1:D:252:PHE:CZ	1:D:291:LEU:HD13	2.51	0.46
1:F:103:GLU:O	1:F:107:LEU:HD22	2.15	0.46
1:C:369:PRO:HD3	1:C:477:LEU:HB2	1.97	0.46
1:C:401:TYR:O	1:C:405:SER:HB2	2.15	0.46
1:D:93:ILE:HG12	1:D:127:ALA:HB3	1.97	0.46
1:F:24:VAL:HG22	1:F:483:VAL:HG22	1.96	0.46
1:B:335:ASN:N	1:B:335:ASN:HD22	2.14	0.46
1:E:316:GLU:O	1:E:340:LYS:HD3	2.16	0.46
1:F:252:PHE:CZ	1:F:291:LEU:HD13	2.51	0.46
1:A:65:ILE:HG13	1:A:65:ILE:O	2.16	0.46
1:A:335:ASN:N	1:A:335:ASN:HD22	2.14	0.46
1:E:118:VAL:HG22	1:E:456:THR:HG22	1.97	0.46
1:F:339:VAL:O	1:F:340:LYS:HB2	2.16	0.46
1:A:90:LYS:HD2	1:A:164:VAL:HB	1.98	0.46
1:D:401:TYR:O	1:D:405:SER:HB2	2.15	0.46
2:D:550:GLU:HA	3:D:551:NDP:C5N	2.46	0.46
1:E:67:ARG:HD2	1:E:140:GLU:OE2	2.16	0.46
1:F:118:VAL:HG22	1:F:456:THR:HG22	1.97	0.46
1:F:495:GLU:O	1:F:498:VAL:HB	2.16	0.46
1:A:146:ARG:HG2	1:A:182:THR:OG1	2.15	0.45
1:D:201:LYS:NZ	1:D:388:ASN:HD21	2.14	0.45
1:E:103:GLU:O	1:E:107:LEU:HD22	2.17	0.45
1:A:412:SER:HA	1:B:433:THR:HG23	1.97	0.45
1:B:5:ASP:OD2	1:B:332:THR:HB	2.17	0.45
1:E:374:ASN:HB2	3:E:551:NDP:H6N	1.98	0.45
1:F:423:LYS:HA	1:F:423:LYS:HE2	1.98	0.45
1:C:66:ARG:HH22	1:F:44:ARG:HH22	1.65	0.45
1:D:335:ASN:HD22	1:D:336:ALA:N	2.15	0.45
1:A:369:PRO:HB2	1:A:371:LEU:HD23	1.99	0.45
1:C:118:VAL:HG22	1:C:456:THR:HG22	1.97	0.45
1:E:331:LEU:HB2	1:E:352:THR:HG22	1.98	0.45
1:A:4:GLU:HA	1:A:4:GLU:OE1	2.16	0.45
1:A:252:PHE:CZ	1:A:291:LEU:HD13	2.52	0.45
1:B:65:ILE:O	1:B:65:ILE:HG13	2.16	0.45
1:C:5:ASP:OD1	1:C:7:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:VAL:HG22	1:E:456:THR:CG2	2.46	0.45
1:F:61:LEU:HD23	1:F:151:GLU:HB3	1.98	0.45
1:F:492:VAL:O	1:F:498:VAL:HG11	2.17	0.45
1:A:2:ASP:O	1:A:6:ASP:HB2	2.16	0.45
1:A:67:ARG:HD2	1:A:140:GLU:OE2	2.17	0.45
2:D:550:GLU:HA	3:D:551:NDP:C4N	2.47	0.45
1:E:32:LEU:HD22	1:E:34:THR:OG1	2.17	0.45
1:F:287:ASP:HB3	1:F:290:GLU:HG3	1.99	0.45
1:F:401:TYR:O	1:F:405:SER:HB2	2.17	0.45
1:C:67:ARG:HD2	1:C:140:GLU:OE2	2.17	0.45
1:D:85:HIS:HD2	1:D:492:VAL:HG21	1.82	0.45
1:F:32:LEU:HD22	1:F:34:THR:OG1	2.16	0.45
1:F:118:VAL:O	1:F:118:VAL:HG13	2.16	0.45
1:B:93:ILE:HG12	1:B:127:ALA:HB3	1.99	0.45
1:C:93:ILE:HG12	1:C:127:ALA:HB3	1.98	0.45
1:C:229:GLU:C	1:C:231:SER:H	2.20	0.45
1:C:433:THR:HG23	1:D:412:SER:HA	1.98	0.45
1:D:32:LEU:HD22	1:D:34:THR:OG1	2.17	0.45
1:D:433:THR:HG23	1:E:412:SER:HA	1.99	0.45
1:A:229:GLU:O	1:A:231:SER:N	2.44	0.45
1:C:331:LEU:HD23	1:C:352:THR:HG22	1.99	0.45
1:A:331:LEU:HD23	1:A:352:THR:HG22	1.99	0.44
1:D:118:VAL:HG22	1:D:456:THR:HG22	1.98	0.44
1:D:146:ARG:HD3	5:D:552:B1T:HA1	1.99	0.44
1:E:331:LEU:HD23	1:E:352:THR:HG22	1.98	0.44
1:E:366:MET:HB2	1:E:475:LEU:HD22	1.99	0.44
1:F:4:GLU:OE2	1:F:5:ASP:N	2.50	0.44
1:A:24:VAL:HG22	1:A:483:VAL:HG13	1.98	0.44
1:A:496:ALA:HA	1:A:500:PHE:CG	2.52	0.44
1:C:118:VAL:HG22	1:C:456:THR:CG2	2.47	0.44
1:C:169:MET:HA	3:C:551:NDP:O1N	2.17	0.44
1:F:24:VAL:CG2	1:F:483:VAL:HG13	2.47	0.44
1:A:75:ILE:CD1	1:A:144:ILE:HG23	2.48	0.44
1:B:118:VAL:HG13	1:B:118:VAL:O	2.16	0.44
1:B:369:PRO:HB2	1:B:371:LEU:HD23	1.99	0.44
1:E:24:VAL:HG22	1:E:483:VAL:HG22	2.00	0.44
1:F:331:LEU:HB2	1:F:352:THR:HG22	2.00	0.44
1:B:32:LEU:HD22	1:B:34:THR:OG1	2.17	0.44
1:B:496:ALA:C	1:B:498:VAL:N	2.70	0.44
1:D:89:CYS:HB3	1:D:125:ALA:HB2	1.98	0.44
1:F:335:ASN:HD22	1:F:335:ASN:N	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:HG22	1:A:483:VAL:HG22	1.98	0.44
1:C:335:ASN:N	1:C:335:ASN:HD22	2.14	0.44
1:D:65:ILE:O	1:D:65:ILE:HG13	2.17	0.44
1:D:270:CYS:O	1:D:285:GLY:HA2	2.17	0.44
1:E:92:GLY:H	2:E:550:GLU:N	2.15	0.44
1:C:24:VAL:HG22	1:C:483:VAL:HG13	1.99	0.44
1:C:32:LEU:HD22	1:C:34:THR:OG1	2.18	0.44
1:C:369:PRO:HB2	1:C:371:LEU:HD23	1.99	0.44
1:D:103:GLU:O	1:D:107:LEU:HD22	2.17	0.44
1:D:369:PRO:HB2	1:D:371:LEU:HD23	2.00	0.44
1:F:65:ILE:O	1:F:65:ILE:HG13	2.17	0.44
1:B:335:ASN:HD22	1:B:336:ALA:N	2.15	0.44
1:C:111:MET:SD	1:C:114:LYS:HE3	2.58	0.44
1:E:186:THR:OG1	1:E:187:ILE:N	2.50	0.44
1:E:229:GLU:C	1:E:231:SER:H	2.21	0.44
1:F:111:MET:SD	1:F:114:LYS:HE3	2.58	0.44
1:B:287:ASP:HB3	1:B:290:GLU:HG3	2.00	0.44
1:C:211:ARG:HH22	3:C:551:NDP:H71N	1.65	0.44
1:C:270:CYS:O	1:C:285:GLY:HA2	2.18	0.44
1:C:335:ASN:HD22	1:C:336:ALA:N	2.16	0.44
1:D:5:ASP:OD2	1:D:332:THR:HB	2.18	0.44
1:D:335:ASN:HD22	1:D:335:ASN:N	2.15	0.44
1:D:496:ALA:HB2	1:E:202:PRO:CB	2.48	0.44
1:B:331:LEU:HB2	1:B:352:THR:HG22	2.00	0.43
1:B:487:GLU:OE2	1:B:491:ARG:NH2	2.51	0.43
1:D:339:VAL:O	1:D:340:LYS:HB2	2.18	0.43
1:B:67:ARG:HD2	1:B:140:GLU:OE2	2.17	0.43
1:B:414:GLN:O	1:B:418:GLU:HG3	2.19	0.43
1:B:493:TYR:C	1:B:495:GLU:H	2.20	0.43
1:C:12:MET:HG3	1:C:354:PRO:HD3	1.99	0.43
1:E:93:ILE:HG12	1:E:127:ALA:HB3	1.99	0.43
1:E:339:VAL:O	1:E:340:LYS:HB2	2.19	0.43
1:B:28:LEU:HD22	1:B:490:PHE:CD2	2.53	0.43
1:C:65:ILE:O	1:C:65:ILE:HG13	2.18	0.43
1:D:90:LYS:HG3	2:D:550:GLU:OE1	2.18	0.43
1:D:349:ASN:ND2	3:D:551:NDP:O2D	2.52	0.43
1:E:116:ALA:O	1:E:488:LYS:HD2	2.18	0.43
1:E:270:CYS:O	1:E:285:GLY:HA2	2.18	0.43
1:F:25:GLU:O	1:F:29:VAL:HG23	2.19	0.43
1:A:349:ASN:CB	3:A:551:NDP:O2D	2.66	0.43
1:B:118:VAL:HG22	1:B:456:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:HIS:HB3	1:E:436:PHE:HB2	1.99	0.43
1:D:90:LYS:HD2	1:D:164:VAL:HB	1.99	0.43
1:D:496:ALA:HB1	1:E:205:GLN:CG	2.48	0.43
1:E:287:ASP:HB3	1:E:290:GLU:HG3	2.01	0.43
1:F:287:ASP:HA	1:F:288:PRO:HD3	1.92	0.43
1:B:491:ARG:HH11	1:B:491:ARG:HG3	1.84	0.43
1:D:146:ARG:HG2	1:D:182:THR:OG1	2.18	0.43
1:E:335:ASN:HD22	1:E:336:ALA:N	2.16	0.43
1:A:32:LEU:HD22	1:A:34:THR:OG1	2.18	0.43
1:E:65:ILE:O	1:E:65:ILE:HG13	2.18	0.43
1:F:9:PHE:O	1:F:12:MET:HB3	2.18	0.43
1:A:335:ASN:HD22	1:A:336:ALA:N	2.16	0.43
1:B:90:LYS:HD2	1:B:164:VAL:HB	2.01	0.43
1:C:44:ARG:NH2	1:F:66:ARG:HH22	2.17	0.43
1:E:85:HIS:HD2	1:E:492:VAL:HG21	1.83	0.43
1:E:287:ASP:HA	1:E:288:PRO:HD3	1.91	0.43
1:A:501:THR:C	1:F:138:ASP:OD2	2.57	0.43
1:D:111:MET:SD	1:D:114:LYS:HE3	2.59	0.43
1:D:201:LYS:HZ1	1:D:388:ASN:HD21	1.67	0.43
1:D:287:ASP:HB3	1:D:290:GLU:HG3	2.00	0.43
1:F:96:SER:O	1:F:130:LYS:HA	2.18	0.43
1:F:186:THR:OG1	1:F:187:ILE:N	2.52	0.43
1:A:25:GLU:O	1:A:29:VAL:HG23	2.19	0.43
1:B:61:LEU:HD23	1:B:151:GLU:HB3	2.00	0.43
1:B:369:PRO:HD3	1:B:477:LEU:HB2	1.99	0.43
1:C:287:ASP:HA	1:C:288:PRO:HD3	1.91	0.43
1:D:24:VAL:CG2	1:D:483:VAL:HG13	2.49	0.43
1:E:90:LYS:HD2	1:E:164:VAL:HB	2.00	0.43
1:F:331:LEU:HD23	1:F:352:THR:HG22	2.00	0.43
1:B:118:VAL:HG22	1:B:456:THR:HG22	2.01	0.43
1:B:172:GLY:O	1:B:176:MET:HG2	2.19	0.43
1:C:178:TRP:NE1	1:E:497:GLY:O	2.51	0.43
1:C:229:GLU:O	1:C:231:SER:N	2.45	0.43
1:C:339:VAL:O	1:C:340:LYS:HB2	2.19	0.42
1:C:496:ALA:C	1:C:498:VAL:H	2.21	0.42
1:C:496:ALA:H	1:C:500:PHE:HE1	1.66	0.42
2:E:550:GLU:HB3	3:E:551:NDP:H41N	2.00	0.42
1:A:229:GLU:C	1:A:231:SER:H	2.19	0.42
1:A:162:VAL:HG23	1:A:163:ASP:N	2.34	0.42
1:B:408:HIS:HB3	1:F:436:PHE:HB2	2.01	0.42
1:C:287:ASP:HB3	1:C:290:GLU:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:MET:HG2	3:E:551:NDP:O1N	2.20	0.42
1:C:386:LEU:HD21	1:D:392:VAL:HG13	2.00	0.42
1:D:118:VAL:HG22	1:D:456:THR:CG2	2.49	0.42
1:E:61:LEU:HD23	1:E:151:GLU:HB3	2.02	0.42
1:E:172:GLY:O	1:E:176:MET:HG2	2.19	0.42
1:F:229:GLU:C	1:F:231:SER:H	2.21	0.42
1:F:498:VAL:C	1:F:500:PHE:H	2.23	0.42
1:B:32:LEU:HD23	1:B:494:ASN:OD1	2.19	0.42
1:B:339:VAL:O	1:B:340:LYS:HB2	2.19	0.42
1:C:78:TYR:O	1:C:127:ALA:HA	2.18	0.42
1:C:174:ARG:HG3	1:E:497:GLY:HA2	2.00	0.42
1:C:364:ASN:HD22	1:C:364:ASN:HA	1.62	0.42
1:E:201:LYS:HZ1	1:E:388:ASN:HD21	1.66	0.42
1:F:369:PRO:HD3	1:F:477:LEU:HB2	2.01	0.42
1:A:61:LEU:HD23	1:A:151:GLU:HB3	2.01	0.42
1:A:408:HIS:HB3	1:B:436:PHE:HB2	2.01	0.42
1:C:137:THR:OG1	1:C:140:GLU:HG3	2.19	0.42
1:D:33:LYS:HD2	1:D:495:GLU:CB	2.48	0.42
1:D:498:VAL:HA	1:D:500:PHE:CE1	2.54	0.42
1:A:172:GLY:O	1:A:176:MET:HG2	2.19	0.42
1:A:186:THR:OG1	1:A:187:ILE:N	2.49	0.42
1:A:490:PHE:O	1:A:493:TYR:N	2.48	0.42
1:D:309:ILE:HD12	1:D:309:ILE:N	2.35	0.42
1:D:335:ASN:ND2	1:D:335:ASN:H	2.18	0.42
1:F:118:VAL:HG22	1:F:456:THR:CG2	2.49	0.42
1:F:172:GLY:O	1:F:176:MET:HG2	2.20	0.42
1:A:331:LEU:HB2	1:A:352:THR:HG22	2.01	0.42
1:B:444:SER:H	1:B:447:ASP:HB2	1.84	0.42
1:C:28:LEU:HD22	1:C:490:PHE:CD2	2.54	0.42
1:C:331:LEU:HB2	1:C:352:THR:HG22	2.01	0.42
1:E:75:ILE:CD1	1:E:144:ILE:HG23	2.50	0.42
1:A:335:ASN:ND2	1:A:335:ASN:H	2.17	0.42
1:B:229:GLU:O	1:B:231:SER:N	2.44	0.42
1:D:386:LEU:HD21	1:E:392:VAL:CG1	2.46	0.42
1:F:90:LYS:HD2	1:F:164:VAL:HB	2.02	0.42
1:F:146:ARG:HG2	1:F:182:THR:OG1	2.19	0.42
1:A:244:ASP:OD2	1:A:244:ASP:N	2.51	0.42
1:B:79:ARG:HA	1:B:126:LYS:O	2.20	0.42
1:D:378:VAL:HG22	2:D:550:GLU:HB2	2.02	0.42
1:A:287:ASP:HB3	1:A:290:GLU:HG3	2.01	0.41
1:D:331:LEU:HD23	1:D:352:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:ILE:HG12	1:F:127:ALA:HB3	2.02	0.41
1:F:366:MET:HB2	1:F:475:LEU:HD22	2.01	0.41
1:A:79:ARG:HA	1:A:126:LYS:O	2.20	0.41
1:A:292:GLU:O	1:A:296:LEU:HB2	2.21	0.41
1:B:309:ILE:HD12	1:B:309:ILE:N	2.35	0.41
1:C:174:ARG:HG3	1:E:497:GLY:CA	2.50	0.41
1:C:333:LYS:HD2	1:C:355:GLU:HG2	2.02	0.41
1:D:75:ILE:CD1	1:D:144:ILE:HG23	2.50	0.41
1:E:281:TRP:CZ2	1:E:283:PRO:HD3	2.54	0.41
1:F:39:GLU:O	1:F:43:ASN:HB2	2.20	0.41
1:B:413:VAL:CG1	1:B:430:ILE:HG21	2.51	0.41
1:C:90:LYS:HD2	1:C:164:VAL:HB	2.02	0.41
1:D:24:VAL:HG22	1:D:483:VAL:HG13	2.01	0.41
1:E:47:GLY:O	1:E:51:ILE:HG12	2.20	0.41
1:E:111:MET:SD	1:E:114:LYS:HE3	2.60	0.41
1:E:133:PRO:HG2	1:E:170:SER:HB3	2.02	0.41
1:F:114:LYS:HD2	1:F:378:VAL:CG2	2.50	0.41
1:B:133:PRO:HG2	1:B:170:SER:HB3	2.03	0.41
1:C:44:ARG:HE	1:C:499:THR:HG22	1.85	0.41
1:D:79:ARG:HA	1:D:126:LYS:O	2.21	0.41
1:D:146:ARG:HD3	5:D:552:B1T:CAI	2.49	0.41
1:F:414:GLN:O	1:F:418:GLU:HG3	2.20	0.41
1:A:1:ALA:N	1:A:6:ASP:OD1	2.50	0.41
1:A:75:ILE:HD11	1:A:144:ILE:HG23	2.02	0.41
1:B:169:MET:HG2	3:B:551:NDP:O1N	2.21	0.41
1:C:201:LYS:HZ1	1:C:388:ASN:HD21	1.68	0.41
1:D:172:GLY:O	1:D:176:MET:HG2	2.20	0.41
1:E:335:ASN:ND2	1:E:335:ASN:H	2.18	0.41
1:F:4:GLU:CD	1:F:5:ASP:N	2.74	0.41
1:F:137:THR:OG1	1:F:140:GLU:HG3	2.21	0.41
1:F:371:LEU:HD23	1:F:371:LEU:H	1.86	0.41
1:A:317:VAL:HG22	1:A:318:ASP:N	2.36	0.41
1:B:317:VAL:HG22	1:B:318:ASP:N	2.36	0.41
1:C:4:GLU:O	1:C:5:ASP:HB3	2.19	0.41
1:E:25:GLU:O	1:E:29:VAL:HG23	2.20	0.41
1:E:79:ARG:HA	1:E:126:LYS:O	2.20	0.41
1:E:413:VAL:CG1	1:E:430:ILE:HG21	2.51	0.41
1:E:496:ALA:O	1:E:500:PHE:HB2	2.21	0.41
1:A:339:VAL:O	1:A:340:LYS:HB2	2.19	0.41
1:B:39:GLU:O	1:B:43:ASN:HB2	2.21	0.41
1:C:492:VAL:O	1:C:496:ALA:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ASN:ND2	1:C:335:ASN:H	2.19	0.41
1:E:414:GLN:O	1:E:418:GLU:HG3	2.21	0.41
1:F:211:ARG:HB3	6:F:557:HOH:O	2.21	0.41
1:A:118:VAL:HG22	1:A:456:THR:HG22	2.02	0.41
1:A:169:MET:HA	3:A:551:NDP:O1N	2.21	0.41
1:A:414:GLN:O	1:A:418:GLU:HG3	2.21	0.41
1:B:66:ARG:HH22	1:E:44:ARG:NH2	2.19	0.41
1:B:335:ASN:ND2	1:B:335:ASN:H	2.18	0.41
1:C:114:LYS:HD2	1:C:378:VAL:CG2	2.51	0.41
1:C:133:PRO:HG2	1:C:170:SER:HB3	2.03	0.41
1:D:317:VAL:HG22	1:D:318:ASP:N	2.36	0.41
1:E:24:VAL:CG2	1:E:483:VAL:HG13	2.51	0.41
1:E:162:VAL:HG23	1:E:163:ASP:N	2.36	0.41
1:F:349:ASN:N	3:F:551:NDP:O2D	2.54	0.41
2:F:550:GLU:HB2	3:F:551:NDP:H41N	2.02	0.41
1:A:333:LYS:HD2	1:A:355:GLU:HG2	2.02	0.41
1:B:25:GLU:O	1:B:29:VAL:HG23	2.21	0.41
1:E:39:GLU:O	1:E:43:ASN:HB2	2.20	0.41
1:A:139:ASN:HD22	1:B:501:THR:CG2	2.34	0.40
1:A:401:TYR:CD2	1:B:443:ALA:HB2	2.55	0.40
1:C:25:GLU:O	1:C:29:VAL:HG23	2.21	0.40
1:C:59:LEU:HG	1:C:61:LEU:HD11	2.03	0.40
1:C:162:VAL:HG23	1:C:163:ASP:N	2.36	0.40
1:C:309:ILE:HD12	1:C:309:ILE:N	2.36	0.40
1:D:2:ASP:CG	1:D:3:ARG:H	2.25	0.40
1:E:107:LEU:CB	1:E:126:LYS:HG2	2.52	0.40
1:E:137:THR:OG1	1:E:140:GLU:HG3	2.21	0.40
1:F:47:GLY:O	1:F:51:ILE:HG12	2.22	0.40
1:F:79:ARG:HA	1:F:126:LYS:O	2.21	0.40
1:F:133:PRO:HG2	1:F:170:SER:HB3	2.02	0.40
1:A:401:TYR:CE2	1:B:443:ALA:HB2	2.57	0.40
1:B:96:SER:O	1:B:130:LYS:HA	2.21	0.40
1:C:75:ILE:CD1	1:C:144:ILE:HG23	2.51	0.40
1:D:39:GLU:O	1:D:43:ASN:HB2	2.21	0.40
1:D:47:GLY:O	1:D:51:ILE:HG12	2.21	0.40
1:A:96:SER:O	1:A:130:LYS:HA	2.20	0.40
1:B:75:ILE:CD1	1:B:144:ILE:HG23	2.51	0.40
1:B:162:VAL:HG23	1:B:163:ASP:N	2.36	0.40
1:B:264:HIS:HA	1:B:268:ALA:O	2.22	0.40
1:C:107:LEU:HB3	1:C:126:LYS:HG2	2.03	0.40
1:D:33:LYS:HD2	1:D:495:GLU:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:ARG:HH11	1:D:491:ARG:HG3	1.86	0.40
1:E:107:LEU:HB3	1:E:126:LYS:HG2	2.02	0.40
1:E:264:HIS:HA	1:E:268:ALA:O	2.21	0.40
1:A:133:PRO:HG2	1:A:170:SER:HB3	2.02	0.40
1:A:413:VAL:CG1	1:A:430:ILE:HG21	2.52	0.40
1:B:287:ASP:HA	1:B:288:PRO:HD3	1.90	0.40
1:B:371:LEU:HD23	1:B:371:LEU:H	1.86	0.40
1:C:498:VAL:O	1:C:499:THR:CB	2.69	0.40
1:E:59:LEU:HG	1:E:61:LEU:HD11	2.02	0.40
1:A:39:GLU:O	1:A:43:ASN:HB2	2.22	0.40
1:B:331:LEU:HD23	1:B:352:THR:HG22	2.02	0.40
1:C:244:ASP:OD2	1:C:244:ASP:N	2.51	0.40
1:D:25:GLU:O	1:D:29:VAL:HG23	2.21	0.40
1:D:133:PRO:HG2	1:D:170:SER:HB3	2.04	0.40
1:D:264:HIS:HA	1:D:268:ALA:O	2.22	0.40
1:E:24:VAL:HG22	1:E:483:VAL:HG13	2.03	0.40
1:E:96:SER:O	1:E:130:LYS:HA	2.21	0.40
1:F:162:VAL:HG23	1:F:163:ASP:N	2.36	0.40
1:F:349:ASN:N	3:F:551:NDP:HO2N	2.19	0.40
1:F:349:ASN:HB2	3:F:551:NDP:O2D	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/501 (100%)	464 (93%)	28 (6%)	7 (1%)	11	20
1	B	499/501 (100%)	463 (93%)	30 (6%)	6 (1%)	13	24
1	C	499/501 (100%)	459 (92%)	33 (7%)	7 (1%)	11	20
1	D	499/501 (100%)	462 (93%)	32 (6%)	5 (1%)	15	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	499/501 (100%)	462 (93%)	33 (7%)	4 (1%)	19	35
1	F	499/501 (100%)	462 (93%)	30 (6%)	7 (1%)	11	20
All	All	2994/3006 (100%)	2772 (93%)	186 (6%)	36 (1%)	13	24

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	SER
1	A	496	ALA
1	B	3	ARG
1	B	313	SER
1	C	2	ASP
1	C	5	ASP
1	C	313	SER
1	C	494	ASN
1	C	495	GLU
1	D	313	SER
1	D	498	VAL
1	E	313	SER
1	F	313	SER
1	F	495	GLU
1	A	312	GLY
1	A	422	GLY
1	A	497	GLY
1	B	312	GLY
1	B	422	GLY
1	B	495	GLU
1	C	312	GLY
1	C	422	GLY
1	D	312	GLY
1	D	422	GLY
1	D	499	THR
1	E	312	GLY
1	E	422	GLY
1	E	494	ASN
1	F	312	GLY
1	F	422	GLY
1	F	494	ASN
1	A	500	PHE
1	B	2	ASP
1	F	2	ASP

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Mol	Chain	Res	Type
1	F	498	VAL
1	A	498	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	417/417 (100%)	394 (94%)	23 (6%)	21	41
1	B	417/417 (100%)	393 (94%)	24 (6%)	20	38
1	C	417/417 (100%)	392 (94%)	25 (6%)	19	37
1	D	417/417 (100%)	393 (94%)	24 (6%)	20	38
1	E	417/417 (100%)	393 (94%)	24 (6%)	20	38
1	F	417/417 (100%)	395 (95%)	22 (5%)	22	43
All	All	2502/2502 (100%)	2360 (94%)	142 (6%)	20	39

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	24	VAL
1	A	32	LEU
1	A	37	THR
1	A	43	ASN
1	A	107	LEU
1	A	112	THR
1	A	118	VAL
1	A	132	ASN
1	A	145	THR
1	A	255	VAL
1	A	279	SER
1	A	291	LEU
1	A	296	LEU
1	A	331	LEU
1	A	335	ASN

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Mol	Chain	Res	Type
1	A	363	ARG
1	A	364	ASN
1	A	373	LEU
1	A	386	LEU
1	A	392	VAL
1	A	410	LEU
1	A	500	PHE
1	B	3	ARG
1	B	9	PHE
1	B	24	VAL
1	B	32	LEU
1	B	37	THR
1	B	43	ASN
1	B	64	PRO
1	B	107	LEU
1	B	112	THR
1	B	118	VAL
1	B	132	ASN
1	B	145	THR
1	B	255	VAL
1	B	279	SER
1	B	291	LEU
1	B	296	LEU
1	B	331	LEU
1	B	335	ASN
1	B	363	ARG
1	B	373	LEU
1	B	378	VAL
1	B	386	LEU
1	B	392	VAL
1	B	410	LEU
1	C	2	ASP
1	C	4	GLU
1	C	9	PHE
1	C	24	VAL
1	C	32	LEU
1	C	37	THR
1	C	43	ASN
1	C	107	LEU
1	C	112	THR
1	C	118	VAL
1	C	132	ASN

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Mol	Chain	Res	Type
1	C	145	THR
1	C	255	VAL
1	C	271	VAL
1	C	279	SER
1	C	291	LEU
1	C	296	LEU
1	C	331	LEU
1	C	335	ASN
1	C	363	ARG
1	C	373	LEU
1	C	386	LEU
1	C	392	VAL
1	C	410	LEU
1	C	499	THR
1	D	4	GLU
1	D	9	PHE
1	D	24	VAL
1	D	32	LEU
1	D	37	THR
1	D	43	ASN
1	D	107	LEU
1	D	112	THR
1	D	118	VAL
1	D	132	ASN
1	D	145	THR
1	D	255	VAL
1	D	279	SER
1	D	291	LEU
1	D	296	LEU
1	D	331	LEU
1	D	335	ASN
1	D	363	ARG
1	D	373	LEU
1	D	386	LEU
1	D	392	VAL
1	D	410	LEU
1	D	499	THR
1	D	500	PHE
1	E	3	ARG
1	E	9	PHE
1	E	24	VAL
1	E	32	LEU

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Mol	Chain	Res	Type
1	E	37	THR
1	E	43	ASN
1	E	64	PRO
1	E	107	LEU
1	E	112	THR
1	E	118	VAL
1	E	132	ASN
1	E	145	THR
1	E	255	VAL
1	E	279	SER
1	E	291	LEU
1	E	296	LEU
1	E	331	LEU
1	E	335	ASN
1	E	363	ARG
1	E	373	LEU
1	E	386	LEU
1	E	392	VAL
1	E	410	LEU
1	E	494	ASN
1	F	24	VAL
1	F	32	LEU
1	F	37	THR
1	F	43	ASN
1	F	107	LEU
1	F	112	THR
1	F	118	VAL
1	F	132	ASN
1	F	145	THR
1	F	255	VAL
1	F	279	SER
1	F	291	LEU
1	F	296	LEU
1	F	331	LEU
1	F	335	ASN
1	F	363	ARG
1	F	373	LEU
1	F	386	LEU
1	F	392	VAL
1	F	410	LEU
1	F	491	ARG
1	F	495	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	82	HIS
1	A	132	ASN
1	A	195	HIS
1	A	205	GLN
1	A	254	ASN
1	A	258	HIS
1	A	330	GLN
1	A	335	ASN
1	A	364	ASN
1	A	388	ASN
1	A	406	ASN
1	A	450	HIS
1	B	56	ASN
1	B	82	HIS
1	B	132	ASN
1	B	195	HIS
1	B	205	GLN
1	B	209	HIS
1	B	254	ASN
1	B	258	HIS
1	B	330	GLN
1	B	335	ASN
1	B	364	ASN
1	B	388	ASN
1	B	406	ASN
1	C	56	ASN
1	C	82	HIS
1	C	132	ASN
1	C	195	HIS
1	C	254	ASN
1	C	258	HIS
1	C	330	GLN
1	C	335	ASN
1	C	364	ASN
1	C	388	ASN
1	C	406	ASN
1	C	494	ASN
1	D	56	ASN
1	D	82	HIS
1	D	132	ASN

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Mol	Chain	Res	Type
1	D	195	HIS
1	D	254	ASN
1	D	258	HIS
1	D	330	GLN
1	D	335	ASN
1	D	364	ASN
1	D	388	ASN
1	D	406	ASN
1	D	494	ASN
1	E	56	ASN
1	E	82	HIS
1	E	132	ASN
1	E	195	HIS
1	E	254	ASN
1	E	258	HIS
1	E	330	GLN
1	E	335	ASN
1	E	364	ASN
1	E	388	ASN
1	E	390	ASN
1	E	406	ASN
1	E	494	ASN
1	F	56	ASN
1	F	82	HIS
1	F	132	ASN
1	F	195	HIS
1	F	254	ASN
1	F	258	HIS
1	F	330	GLN
1	F	335	ASN
1	F	364	ASN
1	F	388	ASN
1	F	406	ASN
1	F	450	HIS
1	F	494	ASN

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NDP	F	551	-	47,52,52	1.66	8 (17%)	61,80,80	2.63	22 (36%)
3	NDP	E	551	-	47,52,52	1.54	7 (14%)	61,80,80	2.61	18 (29%)
4	GTP	B	553	-	29,34,34	1.96	7 (24%)	35,54,54	5.40	13 (37%)
2	GLU	A	550	-	7,8,9	0.89	0	4,9,11	1.33	0
4	GTP	E	553	-	29,34,34	1.52	7 (24%)	35,54,54	4.27	15 (42%)
2	GLU	F	550	-	7,8,9	1.71	2 (28%)	4,9,11	1.65	1 (25%)
5	B1T	B	552	-	20,20,20	0.76	0	29,29,29	0.85	0
5	B1T	A	552	-	20,20,20	0.78	0	29,29,29	0.99	0
2	GLU	E	550	-	7,8,9	0.99	0	4,9,11	0.88	0
5	B1T	D	552	-	20,20,20	0.82	0	29,29,29	0.86	0
2	GLU	D	550	-	7,8,9	0.98	0	4,9,11	0.79	0
4	GTP	F	553	-	29,34,34	2.87	5 (17%)	35,54,54	4.55	14 (40%)
3	NDP	B	551	-	47,52,52	1.89	7 (14%)	61,80,80	2.68	22 (36%)
3	NDP	A	551	-	47,52,52	1.89	9 (19%)	61,80,80	2.79	27 (44%)
3	NDP	D	551	-	47,52,52	1.92	9 (19%)	61,80,80	2.71	23 (37%)
4	GTP	C	553	-	29,34,34	2.24	6 (20%)	35,54,54	1.50	7 (20%)
5	B1T	F	552	-	20,20,20	0.83	1 (5%)	29,29,29	0.96	0
4	GTP	D	553	-	29,34,34	2.51	6 (20%)	35,54,54	3.13	13 (37%)
2	GLU	B	550	-	7,8,9	0.98	0	4,9,11	1.08	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NDP	C	551	-	47,52,52	2.04	8 (17%)	61,80,80	2.67	22 (36%)
5	B1T	C	552	-	20,20,20	0.76	0	29,29,29	0.86	0
5	B1T	E	552	-	20,20,20	0.79	0	29,29,29	0.95	0
2	GLU	C	550	-	7,8,9	1.03	0	4,9,11	1.33	0
4	GTP	A	553	-	29,34,34	1.87	4 (13%)	35,54,54	3.15	14 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	F	551	-	-	2/30/77/77	0/5/5/5
3	NDP	E	551	-	-	2/30/77/77	0/5/5/5
4	GTP	B	553	-	-	2/18/38/38	0/3/3/3
2	GLU	A	550	-	-	2/6/7/9	-
4	GTP	E	553	-	1/1/7/7	2/18/38/38	0/3/3/3
2	GLU	F	550	-	-	2/6/7/9	-
5	B1T	B	552	-	-	0/4/4/4	0/2/2/2
5	B1T	A	552	-	-	0/4/4/4	0/2/2/2
2	GLU	E	550	-	-	2/6/7/9	-
5	B1T	D	552	-	-	0/4/4/4	0/2/2/2
2	GLU	D	550	-	-	5/6/7/9	-
4	GTP	F	553	-	-	1/18/38/38	0/3/3/3
3	NDP	B	551	-	-	2/30/77/77	0/5/5/5
3	NDP	A	551	-	-	5/30/77/77	0/5/5/5
3	NDP	D	551	-	-	3/30/77/77	0/5/5/5
4	GTP	C	553	-	-	1/18/38/38	0/3/3/3
5	B1T	F	552	-	-	0/4/4/4	0/2/2/2
4	GTP	D	553	-	-	4/18/38/38	0/3/3/3
2	GLU	B	550	-	-	3/6/7/9	-
3	NDP	C	551	-	-	5/30/77/77	0/5/5/5
5	B1T	C	552	-	-	0/4/4/4	0/2/2/2
5	B1T	E	552	-	-	0/4/4/4	0/2/2/2
2	GLU	C	550	-	-	1/6/7/9	-
4	GTP	A	553	-	-	3/18/38/38	0/3/3/3

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	553	GTP	O4'-C1'	12.07	1.56	1.40
3	C	551	NDP	PN-O3	-9.56	1.49	1.59
4	D	553	GTP	PB-O3A	9.12	1.69	1.59
3	D	551	NDP	PN-O3	-7.86	1.51	1.59
3	A	551	NDP	PN-O3	-7.47	1.51	1.59
3	B	551	NDP	PN-O3	-7.36	1.51	1.59
4	D	553	GTP	O4'-C1'	7.17	1.50	1.40
4	C	553	GTP	O4'-C1'	7.01	1.50	1.40
4	C	553	GTP	PB-O3B	6.65	1.66	1.59
3	D	551	NDP	O4B-C1B	5.98	1.48	1.40
3	F	551	NDP	O4B-C1B	5.92	1.48	1.40
4	B	553	GTP	PB-O3B	5.84	1.65	1.59
3	B	551	NDP	O4B-C1B	5.76	1.48	1.40
4	A	553	GTP	O4'-C1'	5.56	1.48	1.40
3	A	551	NDP	O4B-C1B	5.35	1.47	1.40
3	C	551	NDP	O4B-C1B	5.14	1.47	1.40
4	F	553	GTP	C3'-C4'	5.02	1.65	1.53
4	A	553	GTP	PB-O3A	4.94	1.64	1.59
3	E	551	NDP	O4B-C1B	4.23	1.46	1.40
4	B	553	GTP	PA-O3A	4.20	1.64	1.59
4	F	553	GTP	PB-O3B	3.74	1.63	1.59
3	E	551	NDP	O4D-C1D	3.69	1.50	1.42
4	A	553	GTP	PB-O3B	3.60	1.63	1.59
4	D	553	GTP	PA-O3A	3.59	1.63	1.59
3	F	551	NDP	PN-O3	-3.56	1.55	1.59
3	C	551	NDP	O4D-C1D	3.56	1.50	1.42
3	A	551	NDP	O4D-C1D	3.50	1.50	1.42
4	E	553	GTP	PB-O3B	3.45	1.63	1.59
3	D	551	NDP	O4D-C1D	3.33	1.49	1.42
3	F	551	NDP	O4D-C1D	3.30	1.49	1.42
4	F	553	GTP	C1'-N9	3.23	1.59	1.50
3	B	551	NDP	O4D-C1D	3.20	1.49	1.42
4	E	553	GTP	O4'-C1'	3.13	1.45	1.40
3	A	551	NDP	P2B-O2B	3.12	1.65	1.59
2	F	550	GLU	CG-CD	3.10	1.57	1.50
4	C	553	GTP	PB-O3A	3.04	1.62	1.59
3	E	551	NDP	PN-O3	-2.99	1.56	1.59
4	B	553	GTP	C8-N7	-2.99	1.30	1.34
4	B	553	GTP	C2'-C3'	2.94	1.61	1.53
4	C	553	GTP	PA-O3A	2.94	1.62	1.59
4	F	553	GTP	PA-O3A	2.84	1.62	1.59
4	E	553	GTP	O4'-C4'	2.68	1.51	1.45
4	A	553	GTP	C8-N7	-2.68	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	553	GTP	C8-N7	-2.66	1.30	1.34
4	D	553	GTP	PB-O3B	2.64	1.62	1.59
4	B	553	GTP	C5-C6	-2.59	1.42	1.47
3	B	551	NDP	C7N-C3N	-2.54	1.43	1.48
4	B	553	GTP	PB-O3A	2.53	1.62	1.59
3	D	551	NDP	P2B-O2B	2.48	1.63	1.59
3	F	551	NDP	P2B-O2B	2.44	1.63	1.59
3	D	551	NDP	C1D-N1N	2.42	1.53	1.46
4	E	553	GTP	C3'-C4'	2.40	1.59	1.53
3	D	551	NDP	C7N-C3N	-2.38	1.43	1.48
3	C	551	NDP	C2N-C3N	2.38	1.41	1.35
3	E	551	NDP	P2B-O3X	2.37	1.63	1.54
3	E	551	NDP	C7N-C3N	-2.36	1.43	1.48
3	B	551	NDP	P2B-O2B	2.35	1.63	1.59
3	A	551	NDP	PA-O5B	2.33	1.68	1.59
4	B	553	GTP	O4'-C1'	2.32	1.43	1.40
3	C	551	NDP	PA-O3	-2.29	1.57	1.59
5	F	552	B1T	CAR-SAK	-2.23	1.75	1.78
3	C	551	NDP	C7N-C3N	-2.21	1.44	1.48
3	F	551	NDP	P2B-O2X	2.20	1.63	1.54
4	E	553	GTP	C5-C6	-2.20	1.43	1.47
3	C	551	NDP	C8A-N7A	-2.16	1.30	1.34
3	F	551	NDP	P2B-O3X	2.15	1.62	1.54
4	E	553	GTP	C8-N7	-2.15	1.31	1.34
4	C	553	GTP	PG-O2G	2.14	1.62	1.54
3	B	551	NDP	O4D-C4D	2.14	1.49	1.45
4	D	553	GTP	C8-N7	-2.13	1.31	1.34
3	B	551	NDP	C8A-N7A	-2.13	1.30	1.34
3	E	551	NDP	P2B-O2X	2.13	1.62	1.54
4	E	553	GTP	PG-O2G	2.12	1.62	1.54
3	E	551	NDP	PA-O5B	2.12	1.67	1.59
3	A	551	NDP	C8A-N7A	-2.11	1.30	1.34
3	A	551	NDP	P2B-O2X	2.10	1.62	1.54
3	C	551	NDP	P2B-O2X	2.10	1.62	1.54
3	A	551	NDP	P2B-O3X	2.09	1.62	1.54
3	F	551	NDP	C1B-N9A	2.09	1.55	1.49
3	D	551	NDP	PA-O5B	2.07	1.67	1.59
3	D	551	NDP	P2B-O3X	2.06	1.62	1.54
3	A	551	NDP	C2N-C3N	2.05	1.40	1.35
3	F	551	NDP	C2N-C3N	2.04	1.40	1.35
4	D	553	GTP	PG-O2G	2.01	1.62	1.54
2	F	550	GLU	CB-CA	2.01	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	551	NDP	C8A-N7A	-2.00	1.31	1.34

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	553	GTP	C4'-O4'-C1'	-25.78	86.32	109.92
4	E	553	GTP	C5'-C4'-C3'	14.60	167.75	115.21
4	F	553	GTP	O4'-C1'-N9	13.54	126.70	108.75
4	F	553	GTP	O4'-C4'-C3'	-12.04	81.25	105.15
4	F	553	GTP	O4'-C4'-C5'	-10.91	74.38	109.33
4	A	553	GTP	O3A-PA-O1A	-10.82	78.15	110.70
4	B	553	GTP	O4'-C1'-N9	10.16	122.21	108.75
4	D	553	GTP	O2A-PA-O3A	-9.36	81.98	107.27
4	E	553	GTP	O4'-C4'-C5'	-9.31	79.52	109.33
4	E	553	GTP	O4'-C1'-N9	8.89	120.53	108.75
3	A	551	NDP	C4B-O4B-C1B	-8.79	101.88	109.92
4	F	553	GTP	C5'-C4'-C3'	8.62	146.23	115.21
4	D	553	GTP	O3A-PA-O1A	-8.27	85.83	110.70
4	B	553	GTP	O3A-PB-O1B	-7.81	87.21	110.70
3	C	551	NDP	C4B-O4B-C1B	-7.74	102.84	109.92
4	A	553	GTP	O5'-PA-O1A	-7.65	78.63	108.94
4	A	553	GTP	O2A-PA-O3A	-7.47	87.09	107.27
3	E	551	NDP	P2B-O2B-C2B	-7.21	104.18	123.43
4	F	553	GTP	C2'-C3'-C4'	7.20	116.52	102.61
3	B	551	NDP	C4B-O4B-C1B	-7.13	103.39	109.92
3	D	551	NDP	C4B-O4B-C1B	-7.13	103.39	109.92
4	E	553	GTP	O4'-C4'-C3'	-6.90	91.46	105.15
3	F	551	NDP	P2B-O2B-C2B	-6.88	105.05	123.43
4	E	553	GTP	O3A-PB-O1B	-6.87	90.05	110.70
3	E	551	NDP	C4B-O4B-C1B	-6.87	103.64	109.92
3	C	551	NDP	P2B-O2B-C2B	-6.86	105.12	123.43
3	D	551	NDP	P2B-O2B-C2B	-6.57	105.89	123.43
3	B	551	NDP	P2B-O2B-C2B	-6.39	106.38	123.43
3	D	551	NDP	O4B-C1B-C2B	-6.32	95.83	106.61
4	E	553	GTP	O2B-PB-O3A	-6.27	90.31	107.27
3	A	551	NDP	O3-PA-O1A	5.82	128.20	110.70
3	E	551	NDP	O5D-PN-O1N	-5.80	85.95	108.94
3	D	551	NDP	O4D-C1D-N1N	5.78	119.11	108.08
4	D	553	GTP	O2A-PA-O5'	-5.77	81.43	107.57
3	D	551	NDP	O2N-PN-O5D	-5.75	81.49	107.57
3	F	551	NDP	C4B-O4B-C1B	-5.75	104.66	109.92
4	B	553	GTP	O2B-PB-O3A	-5.74	91.75	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	551	NDP	O4B-C1B-C2B	-5.68	96.92	106.61
4	D	553	GTP	PA-O5'-C5'	-5.60	89.26	121.35
3	B	551	NDP	O2N-PN-O5D	-5.58	82.28	107.57
3	A	551	NDP	P2B-O2B-C2B	-5.51	108.72	123.43
4	E	553	GTP	O3B-PB-O1B	5.51	127.27	110.70
3	F	551	NDP	O4B-C1B-C2B	-5.41	97.38	106.61
3	C	551	NDP	O2N-PN-O5D	-5.37	83.22	107.57
3	A	551	NDP	O2N-PN-O5D	-5.37	83.22	107.57
3	C	551	NDP	O3-PA-O1A	5.35	126.80	110.70
3	F	551	NDP	O2N-PN-O5D	-5.34	83.35	107.57
3	B	551	NDP	O4D-C1D-N1N	5.32	118.23	108.08
4	D	553	GTP	O5'-PA-O1A	-5.30	87.91	108.94
4	B	553	GTP	O3B-PB-O1B	5.29	126.62	110.70
3	B	551	NDP	O4B-C1B-C2B	-5.29	97.58	106.61
3	B	551	NDP	O5B-PA-O1A	-5.27	88.04	108.94
3	A	551	NDP	O4D-C1D-N1N	5.25	118.09	108.08
3	E	551	NDP	O5B-PA-O1A	-5.21	88.30	108.94
3	E	551	NDP	O2N-PN-O5D	-5.19	84.03	107.57
4	B	553	GTP	O5'-C5'-C4'	-5.19	91.34	108.99
3	F	551	NDP	O3-PA-O1A	5.15	126.20	110.70
3	C	551	NDP	O5B-PA-O1A	-5.08	88.81	108.94
3	E	551	NDP	N3A-C2A-N1A	-4.98	121.91	128.67
3	F	551	NDP	O5B-PA-O1A	-4.98	89.21	108.94
4	D	553	GTP	O5'-C5'-C4'	4.97	125.90	108.99
3	C	551	NDP	O4B-C1B-C2B	-4.95	98.16	106.61
3	B	551	NDP	O3-PA-O1A	4.93	125.55	110.70
3	F	551	NDP	O5D-PN-O1N	-4.93	89.40	108.94
3	C	551	NDP	O4D-C1D-N1N	4.92	117.46	108.08
3	D	551	NDP	N3A-C2A-N1A	-4.89	122.04	128.67
3	B	551	NDP	O5D-PN-O1N	-4.88	89.59	108.94
4	F	553	GTP	O5'-PA-O1A	-4.87	89.63	108.94
3	A	551	NDP	N3A-C2A-N1A	-4.86	122.07	128.67
3	C	551	NDP	N3A-C2A-N1A	-4.85	122.08	128.67
3	B	551	NDP	N3A-C2A-N1A	-4.80	122.16	128.67
3	A	551	NDP	O4B-C1B-N9A	4.77	115.07	108.75
3	A	551	NDP	O5B-PA-O1A	-4.71	90.26	108.94
3	C	551	NDP	O5D-PN-O1N	-4.71	90.26	108.94
3	F	551	NDP	O4D-C1D-N1N	4.71	117.06	108.08
3	F	551	NDP	O4B-C1B-N9A	4.68	114.95	108.75
3	F	551	NDP	N3A-C2A-N1A	-4.65	122.36	128.67
3	A	551	NDP	O5D-PN-O1N	-4.63	90.59	108.94
3	E	551	NDP	O3-PA-O1A	4.61	124.57	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	551	NDP	O4B-C1B-C2B	-4.58	98.80	106.61
3	D	551	NDP	O5D-PN-O1N	-4.57	90.81	108.94
3	D	551	NDP	O3-PA-O1A	4.53	124.34	110.70
4	A	553	GTP	O2A-PA-O5'	-4.45	87.38	107.57
4	C	553	GTP	C8-N7-C5	4.45	110.13	102.55
3	C	551	NDP	C2D-C3D-C4D	4.45	111.21	102.61
4	E	553	GTP	C2'-C3'-C4'	4.43	111.17	102.61
3	F	551	NDP	O2A-PA-O5B	-4.42	87.54	107.57
4	B	553	GTP	O4'-C4'-C5'	4.40	123.42	109.33
3	D	551	NDP	O5B-PA-O1A	-4.39	91.54	108.94
4	F	553	GTP	O5'-C5'-C4'	-4.38	94.08	108.99
4	A	553	GTP	PA-O5'-C5'	-4.36	96.34	121.35
4	F	553	GTP	C8-N7-C5	4.34	109.94	102.55
3	E	551	NDP	C2D-C3D-C4D	4.34	110.99	102.61
4	F	553	GTP	O3A-PA-O1A	4.26	123.51	110.70
3	A	551	NDP	C2D-C3D-C4D	4.24	110.80	102.61
3	F	551	NDP	C2D-C3D-C4D	4.18	110.68	102.61
4	F	553	GTP	O2A-PA-O3A	4.17	118.53	107.27
3	F	551	NDP	O3-PN-O1N	4.16	123.21	110.70
3	E	551	NDP	O2A-PA-O5B	-4.15	88.75	107.57
4	B	553	GTP	C8-N7-C5	4.09	109.52	102.55
3	D	551	NDP	O2A-PA-O5B	-4.05	89.21	107.57
3	D	551	NDP	C2D-C3D-C4D	4.05	110.43	102.61
4	D	553	GTP	C8-N7-C5	4.01	109.37	102.55
3	D	551	NDP	O4B-C1B-N9A	3.98	114.02	108.75
3	D	551	NDP	O2A-PA-O3	3.96	117.99	107.27
3	B	551	NDP	C2D-C3D-C4D	3.96	110.27	102.61
3	E	551	NDP	O4D-C1D-N1N	3.94	115.61	108.08
4	E	553	GTP	C8-N7-C5	3.90	109.20	102.55
3	E	551	NDP	O3-PN-O1N	3.82	122.21	110.70
4	E	553	GTP	C4'-O4'-C1'	3.81	113.42	109.92
3	E	551	NDP	O2A-PA-O3	3.80	117.56	107.27
4	A	553	GTP	C8-N7-C5	3.75	108.93	102.55
3	B	551	NDP	O4B-C1B-N9A	3.74	113.71	108.75
4	F	553	GTP	O2A-PA-O5'	-3.74	90.60	107.57
3	D	551	NDP	O3-PN-O1N	3.71	121.88	110.70
3	B	551	NDP	C2D-C1D-N1N	-3.67	104.28	113.31
3	A	551	NDP	O3-PN-O1N	3.66	121.72	110.70
3	C	551	NDP	O2N-PN-O3	3.56	116.91	107.27
3	A	551	NDP	O2A-PA-O5B	-3.55	91.50	107.57
3	B	551	NDP	O2A-PA-O5B	-3.52	91.63	107.57
3	D	551	NDP	O4D-C4D-C5D	-3.49	98.16	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	551	NDP	O2A-PA-O5B	-3.45	91.95	107.57
3	B	551	NDP	O2N-PN-O3	3.42	116.52	107.27
3	B	551	NDP	O3-PN-O1N	3.41	120.97	110.70
3	D	551	NDP	O2N-PN-O3	3.38	116.42	107.27
4	B	553	GTP	C2'-C3'-C4'	-3.36	96.11	102.61
3	F	551	NDP	O2N-PN-O3	3.31	116.22	107.27
4	A	553	GTP	O5'-C5'-C4'	3.30	120.22	108.99
3	B	551	NDP	O2A-PA-O3	3.27	116.12	107.27
4	C	553	GTP	O4'-C1'-N9	3.24	113.04	108.75
3	E	551	NDP	O4B-C1B-N9A	3.21	113.00	108.75
3	A	551	NDP	O2N-PN-O3	3.20	115.92	107.27
3	A	551	NDP	C2D-C1D-N1N	-3.17	105.52	113.31
4	D	553	GTP	O4'-C1'-N9	3.11	112.87	108.75
3	C	551	NDP	O3-PN-O1N	3.05	119.87	110.70
4	F	553	GTP	O2B-PB-O3A	2.96	115.27	107.27
3	B	551	NDP	O4D-C4D-C5D	-2.95	99.89	109.33
4	E	553	GTP	O2B-PB-O3B	2.92	115.16	107.27
3	F	551	NDP	O2A-PA-O3	2.90	115.12	107.27
3	E	551	NDP	O2N-PN-O3	2.89	115.08	107.27
4	B	553	GTP	C5'-C4'-C3'	2.82	125.37	115.21
4	B	553	GTP	C5-C6-N1	2.80	119.41	114.07
3	F	551	NDP	C2D-C1D-N1N	-2.76	106.52	113.31
4	B	553	GTP	C2-N1-C6	-2.75	120.07	125.11
3	C	551	NDP	C2D-C1D-N1N	-2.75	106.55	113.31
4	F	553	GTP	C2-N1-C6	-2.73	120.10	125.11
3	F	551	NDP	C4A-C5A-N7A	-2.66	106.52	109.34
4	B	553	GTP	O2B-PB-O3B	2.65	114.45	107.27
4	C	553	GTP	C2-N1-C6	-2.63	120.29	125.11
3	C	551	NDP	C5D-C4D-C3D	-2.63	105.73	115.21
3	C	551	NDP	O4B-C1B-N9A	2.63	112.24	108.75
4	E	553	GTP	C5-C6-N1	2.62	119.08	114.07
3	C	551	NDP	PN-O5D-C5D	-2.62	106.32	121.35
3	C	551	NDP	O2A-PA-O3	2.61	114.32	107.27
3	A	551	NDP	C1D-N1N-C6N	-2.55	115.39	120.77
4	E	553	GTP	C2-N1-C6	-2.52	120.49	125.11
4	D	553	GTP	C2-N1-C6	-2.52	120.49	125.11
4	A	553	GTP	C5-C6-N1	2.51	118.86	114.07
3	A	551	NDP	O2A-PA-O3	2.51	114.06	107.27
3	F	551	NDP	C1D-N1N-C6N	-2.49	115.51	120.77
4	A	553	GTP	C2-N1-C6	-2.47	120.58	125.11
4	D	553	GTP	C5'-C4'-C3'	-2.46	106.35	115.21
4	D	553	GTP	C2'-C3'-C4'	2.45	107.33	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	553	GTP	C5-C6-N1	2.43	118.71	114.07
2	F	550	GLU	OE2-CD-CG	2.43	121.67	114.00
4	F	553	GTP	C5-C6-N1	2.42	118.69	114.07
3	A	551	NDP	PN-O5D-C5D	-2.40	107.62	121.35
3	E	551	NDP	C2D-C1D-N1N	-2.39	107.42	113.31
4	D	553	GTP	C5-C6-N1	2.38	118.62	114.07
4	A	553	GTP	C5'-C4'-C3'	-2.38	106.64	115.21
3	D	551	NDP	C1D-N1N-C6N	-2.38	115.75	120.77
4	A	553	GTP	O4'-C1'-N9	2.37	111.89	108.75
3	D	551	NDP	C2D-C1D-N1N	-2.35	107.52	113.31
3	C	551	NDP	C1D-N1N-C6N	-2.32	115.88	120.77
3	F	551	NDP	O2B-C2B-C1B	2.30	118.14	110.05
4	A	553	GTP	C2'-C3'-C4'	2.28	107.02	102.61
4	E	553	GTP	O5'-C5'-C4'	-2.28	101.25	108.99
3	D	551	NDP	C1D-N1N-C2N	2.26	124.86	121.14
3	A	551	NDP	C5B-C4B-C3B	-2.24	107.14	115.21
3	B	551	NDP	C1D-N1N-C6N	-2.24	116.03	120.77
3	B	551	NDP	PN-O5D-C5D	-2.24	108.52	121.35
3	A	551	NDP	C5D-C4D-C3D	-2.24	107.15	115.21
4	E	553	GTP	O6-C6-C5	-2.24	119.88	124.32
3	C	551	NDP	C5B-C4B-C3B	-2.24	107.16	115.21
4	C	553	GTP	C2'-C3'-C4'	2.23	106.92	102.61
3	A	551	NDP	C4A-C5A-N7A	-2.22	106.99	109.34
3	A	551	NDP	O5D-C5D-C4D	2.22	116.54	108.99
4	A	553	GTP	O3G-PG-O3B	2.19	111.97	104.64
3	B	551	NDP	C3D-C2D-C1D	2.17	105.56	101.46
3	A	551	NDP	O2B-C2B-C3B	2.17	119.45	111.68
3	F	551	NDP	C1D-N1N-C2N	2.17	124.71	121.14
3	A	551	NDP	C3N-C2N-N1N	-2.16	120.03	123.20
3	A	551	NDP	C3N-C7N-N7N	2.16	121.50	117.67
3	D	551	NDP	C5B-C4B-C3B	-2.16	107.45	115.21
4	D	553	GTP	O3G-PG-O3B	2.15	111.86	104.64
4	A	553	GTP	O2A-PA-O1A	2.15	122.44	112.44
3	D	551	NDP	PN-O5D-C5D	-2.15	109.05	121.35
4	C	553	GTP	C4'-O4'-C1'	-2.12	107.98	109.92
3	E	551	NDP	C5B-C4B-C3B	-2.10	107.64	115.21
3	D	551	NDP	O2B-C2B-C1B	2.09	117.40	110.05
3	B	551	NDP	C3N-C7N-N7N	2.09	121.38	117.67
3	F	551	NDP	C3N-C2N-N1N	-2.08	120.15	123.20
3	C	551	NDP	O5D-C5D-C4D	2.07	116.04	108.99
3	A	551	NDP	O4D-C4D-C5D	-2.07	102.71	109.33
3	F	551	NDP	PN-O5D-C5D	-2.07	109.50	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	551	NDP	C4A-C5A-N7A	-2.06	107.16	109.34
3	C	551	NDP	C3N-C2N-N1N	-2.05	120.19	123.20
3	A	551	NDP	C1D-N1N-C2N	2.05	124.51	121.14
3	D	551	NDP	C4A-C5A-N7A	-2.03	107.19	109.34
3	E	551	NDP	C4A-C5A-N7A	-2.02	107.20	109.34
4	C	553	GTP	O3G-PG-O3B	2.01	111.36	104.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	553	GTP	C4'

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	550	GLU	N-CA-CB-CG
2	A	550	GLU	C-CA-CB-CG
2	C	550	GLU	O-C-CA-CB
2	D	550	GLU	O-C-CA-CB
2	D	550	GLU	N-CA-CB-CG
2	D	550	GLU	C-CA-CB-CG
3	A	551	NDP	C5D-O5D-PN-O3
3	B	551	NDP	O4D-C1D-N1N-C6N
3	C	551	NDP	C5D-O5D-PN-O3
3	D	551	NDP	O4D-C1D-N1N-C6N
3	E	551	NDP	O4D-C1D-N1N-C6N
3	F	551	NDP	O4D-C1D-N1N-C6N
4	A	553	GTP	C5'-O5'-PA-O1A
4	A	553	GTP	C5'-O5'-PA-O2A
4	B	553	GTP	O4'-C4'-C5'-O5'
3	A	551	NDP	O4D-C1D-N1N-C6N
3	C	551	NDP	O4D-C1D-N1N-C6N
4	E	553	GTP	O4'-C4'-C5'-O5'
4	F	553	GTP	O4'-C4'-C5'-O5'
4	A	553	GTP	PB-O3A-PA-O1A
4	C	553	GTP	C5'-O5'-PA-O1A
4	D	553	GTP	C5'-O5'-PA-O1A
4	D	553	GTP	C5'-O5'-PA-O2A
2	E	550	GLU	OE1-CD-CG-CB
2	B	550	GLU	OE2-CD-CG-CB
3	A	551	NDP	PN-O3-PA-O1A
2	E	550	GLU	OE2-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
2	B	550	GLU	OE1-CD-CG-CB
3	B	551	NDP	PN-O3-PA-O1A
3	C	551	NDP	PA-O3-PN-O2N
3	E	551	NDP	PN-O3-PA-O1A
3	F	551	NDP	PA-O3-PN-O2N
4	B	553	GTP	PG-O3B-PB-O1B
4	D	553	GTP	PB-O3A-PA-O1A
4	D	553	GTP	PB-O3A-PA-O2A
4	E	553	GTP	PG-O3B-PB-O1B
3	D	551	NDP	O4D-C4D-C5D-O5D
2	D	550	GLU	OE1-CD-CG-CB
2	F	550	GLU	OE1-CD-CG-CB
2	F	550	GLU	OE2-CD-CG-CB
3	C	551	NDP	O4D-C4D-C5D-O5D
2	D	550	GLU	OE2-CD-CG-CB
2	B	550	GLU	N-CA-CB-CG
3	A	551	NDP	PA-O3-PN-O2N
3	C	551	NDP	PN-O3-PA-O1A
3	D	551	NDP	PN-O3-PA-O1A
3	A	551	NDP	O4D-C4D-C5D-O5D

There are no ring outliers.

21 monomers are involved in 73 short contacts:

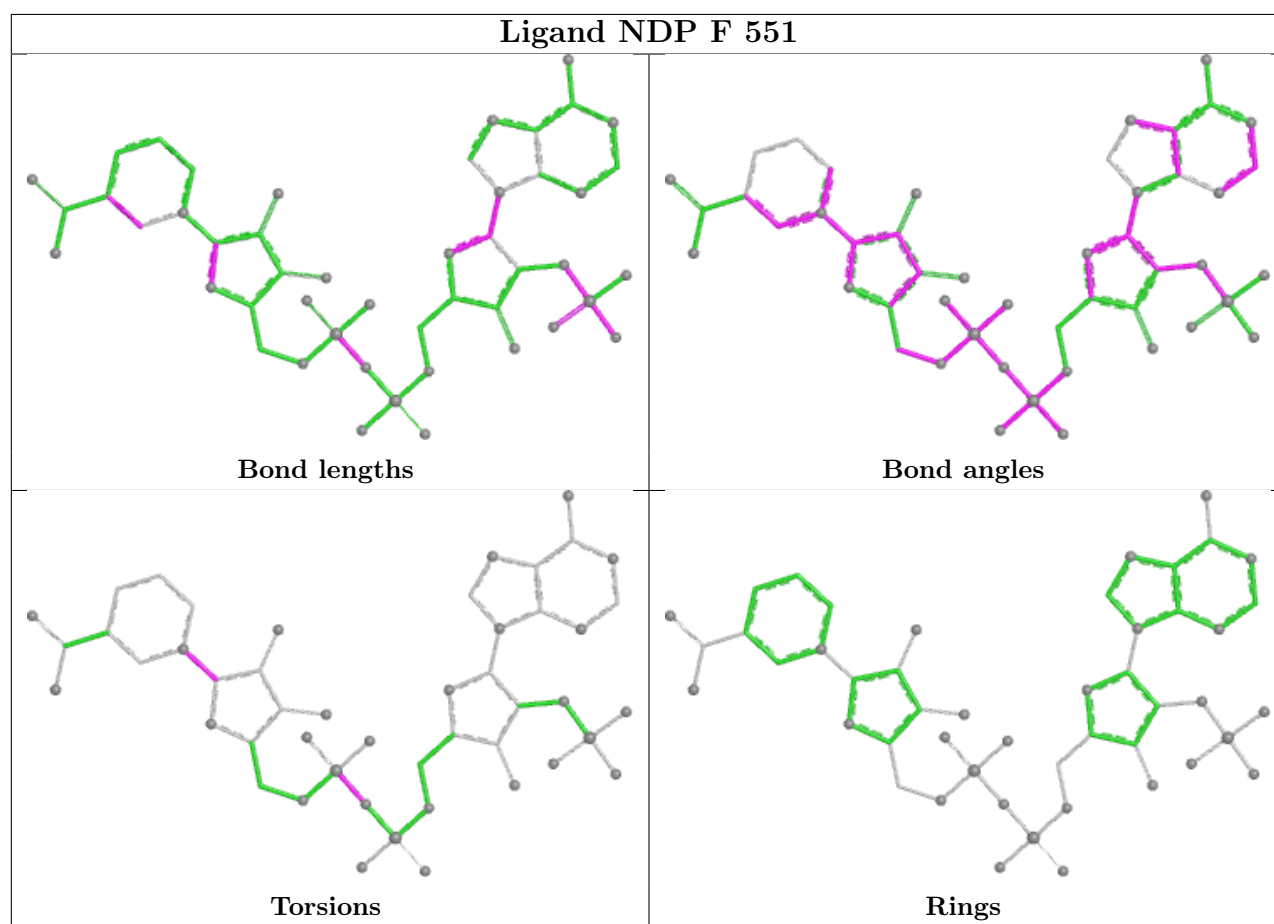
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	551	NDP	9	0
3	E	551	NDP	8	0
4	B	553	GTP	1	0
2	A	550	GLU	1	0
2	F	550	GLU	2	0
5	B	552	B1T	2	0
5	A	552	B1T	2	0
2	E	550	GLU	5	0
5	D	552	B1T	4	0
2	D	550	GLU	5	0
3	B	551	NDP	5	0
3	A	551	NDP	8	0
3	D	551	NDP	8	0
4	C	553	GTP	1	0
5	F	552	B1T	2	0
4	D	553	GTP	1	0
2	B	550	GLU	3	0

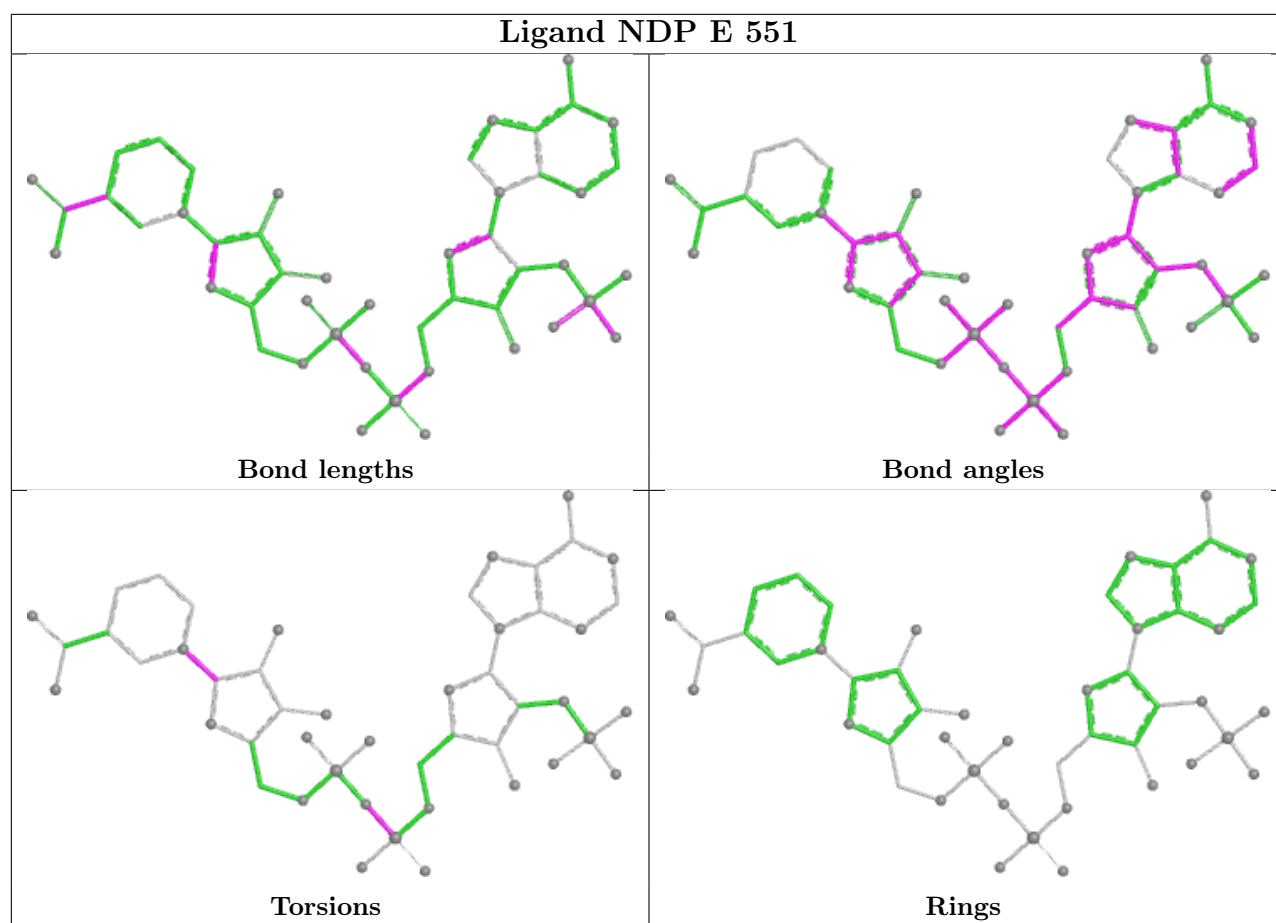
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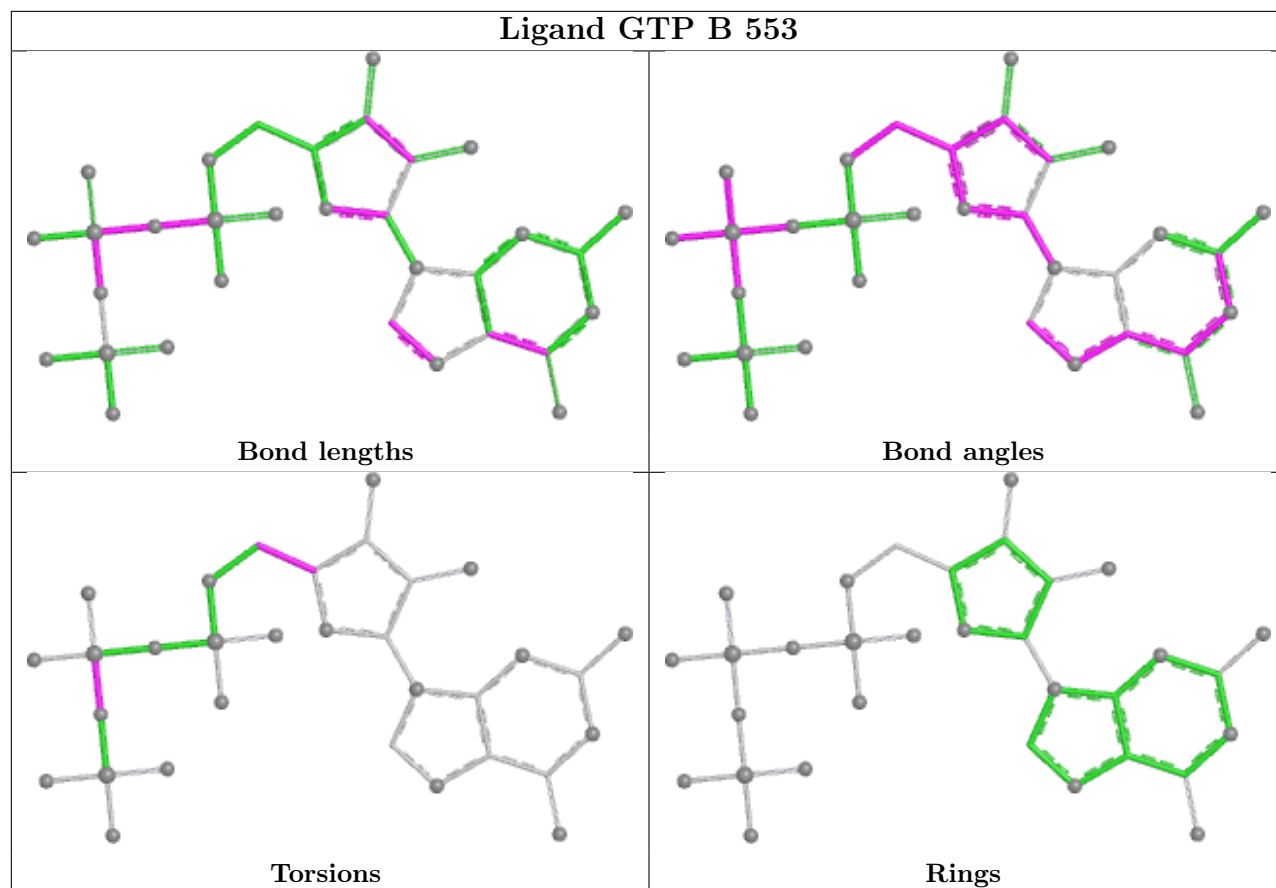
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	551	NDP	6	0
5	C	552	B1T	3	0
5	E	552	B1T	1	0
4	A	553	GTP	2	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

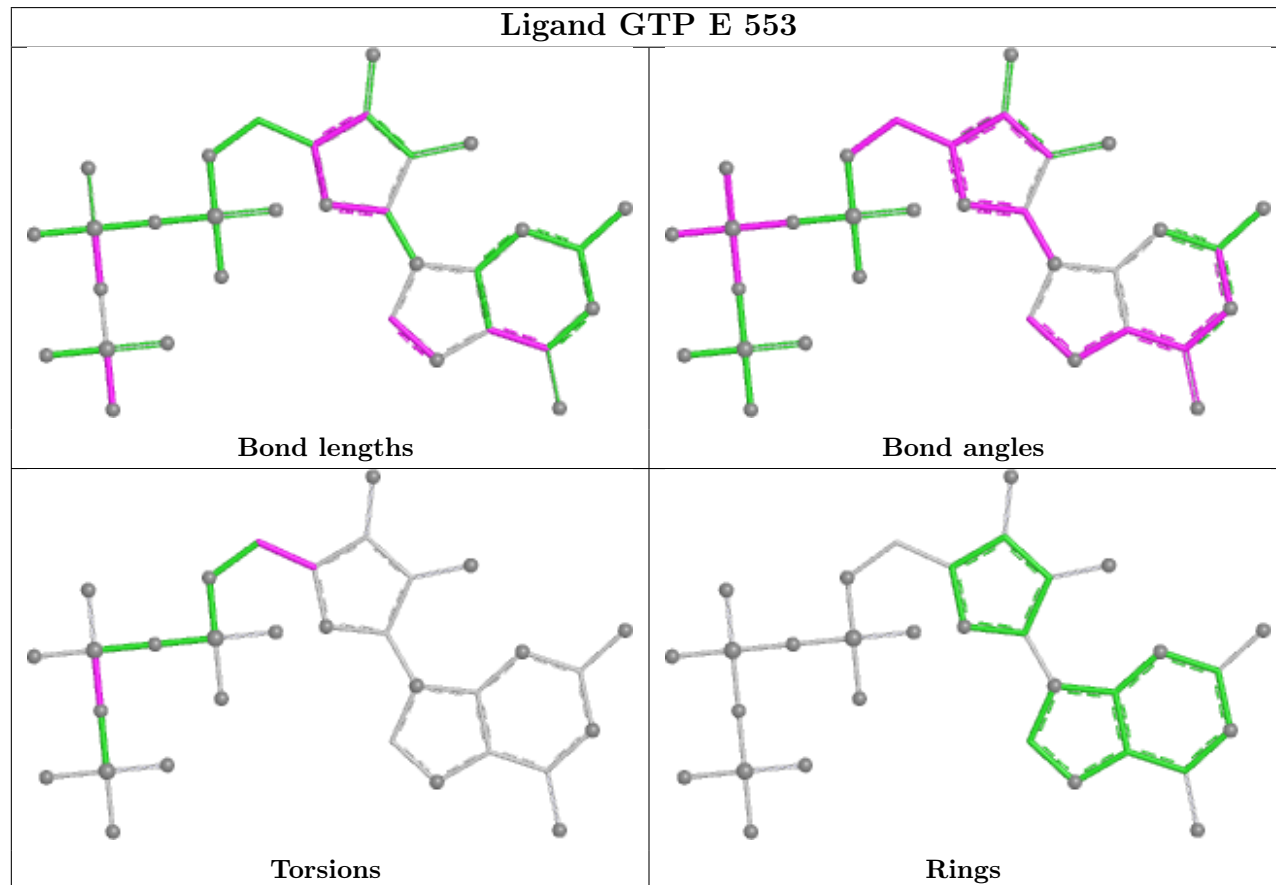




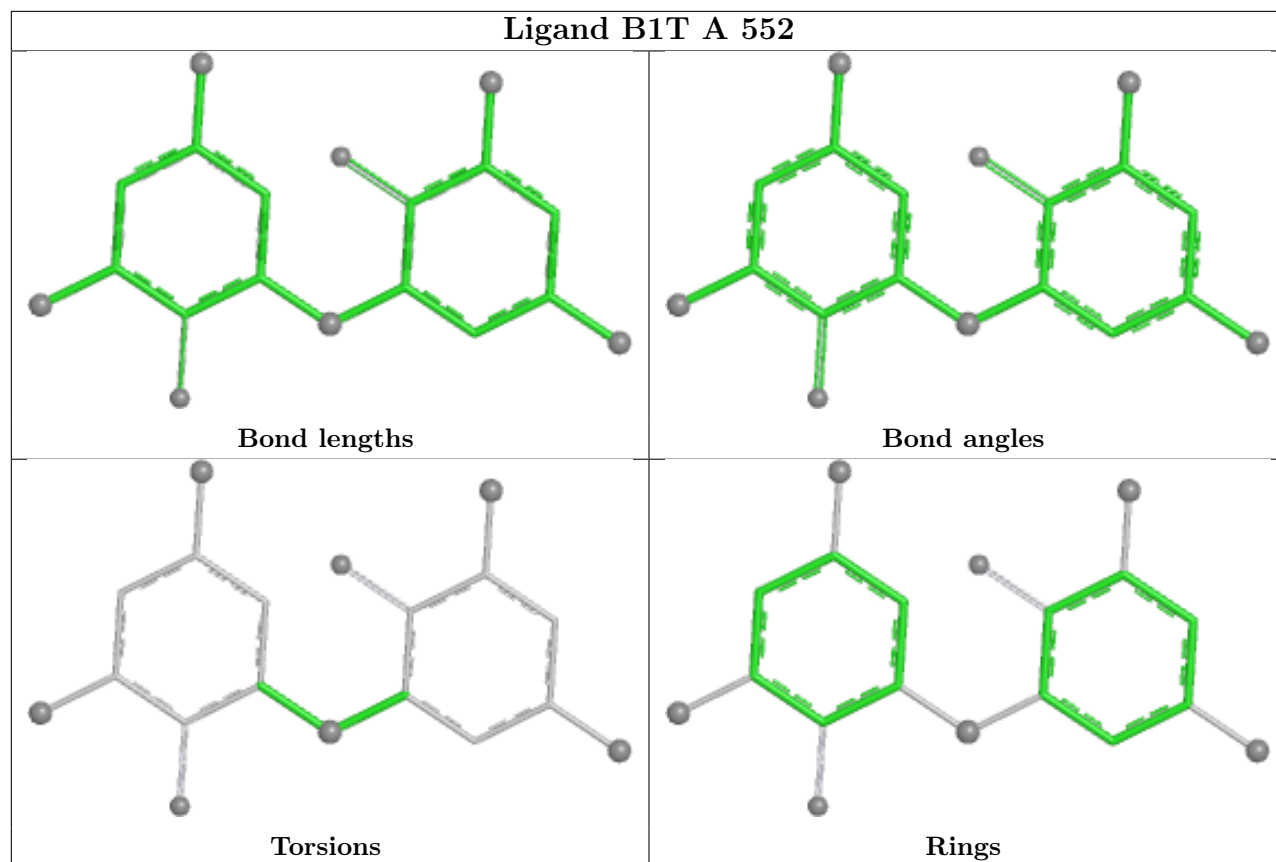
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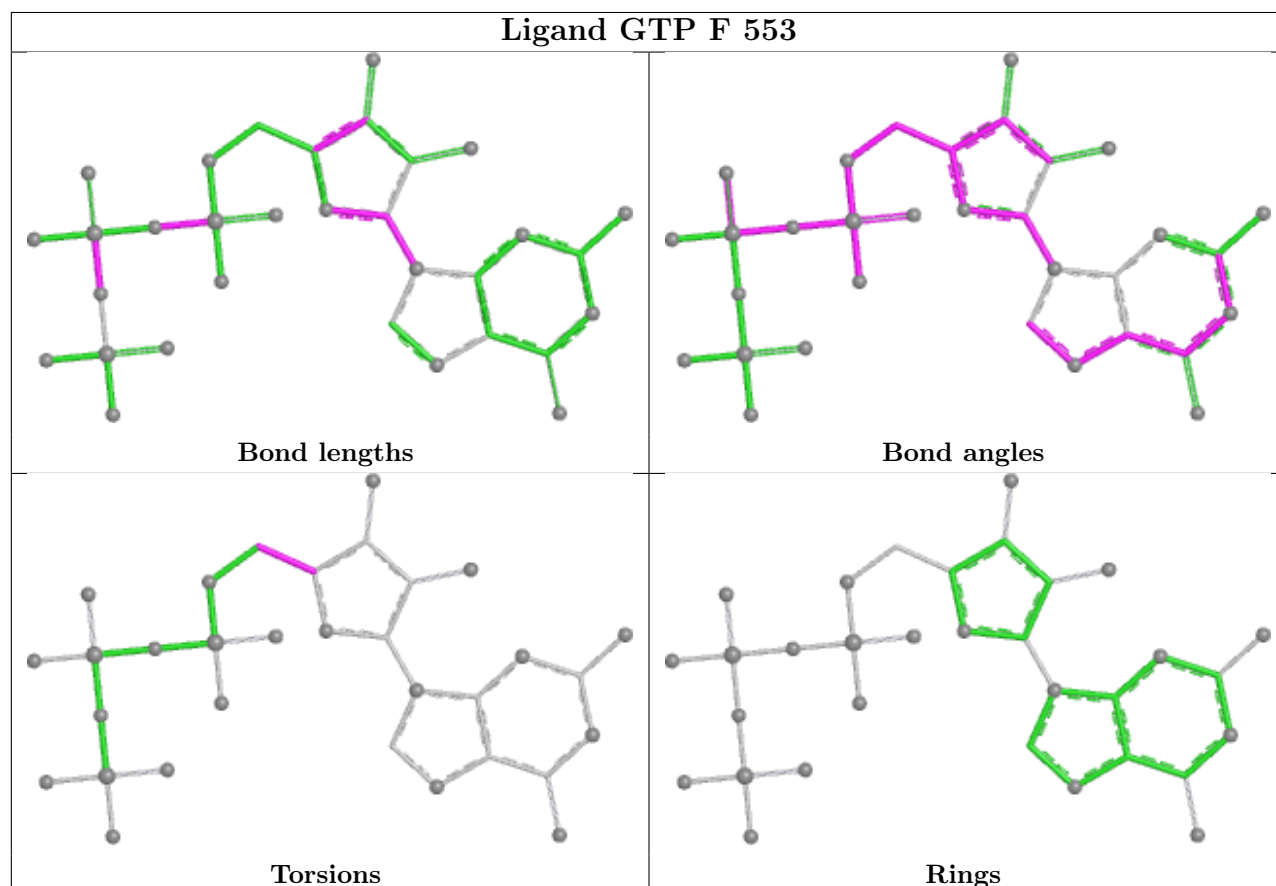
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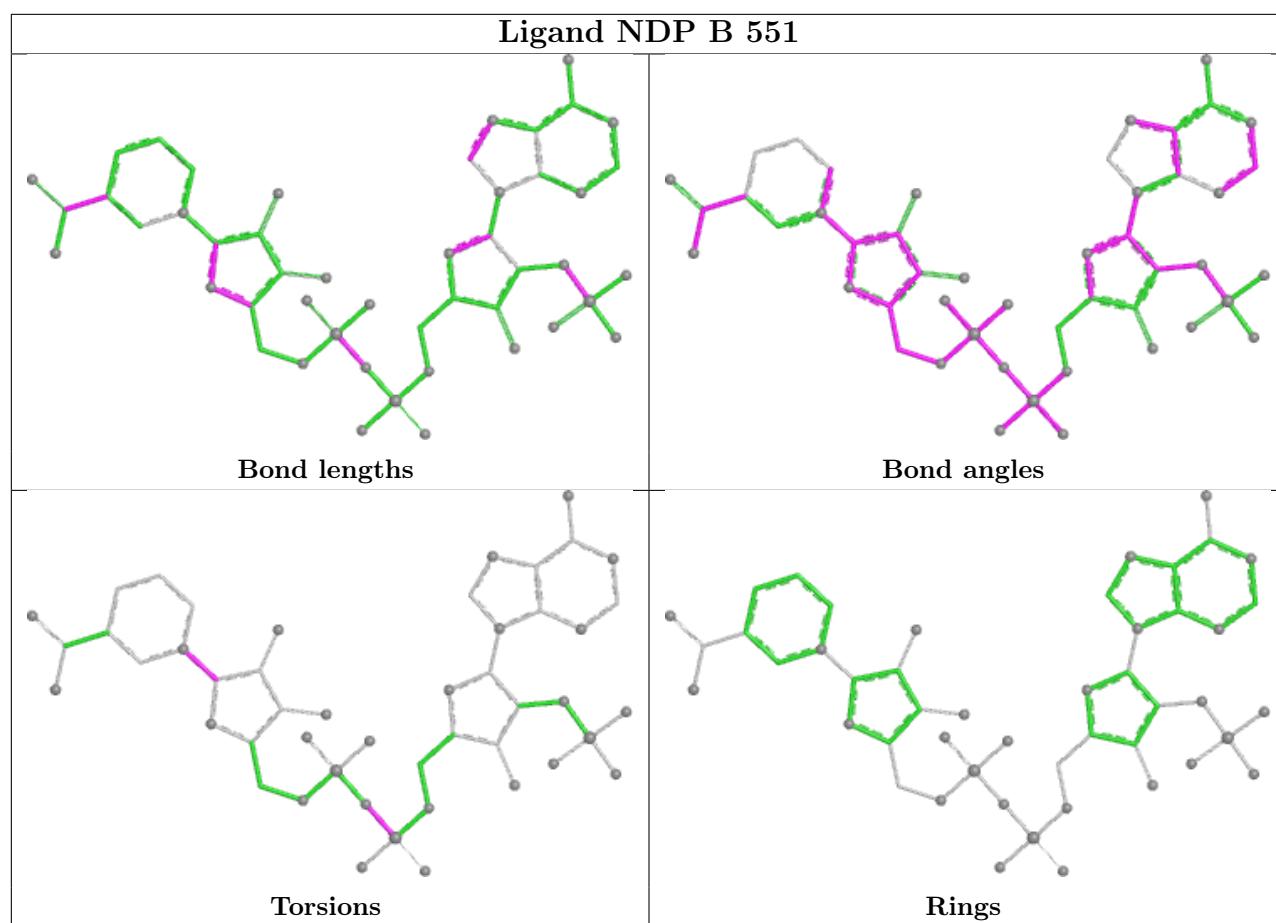


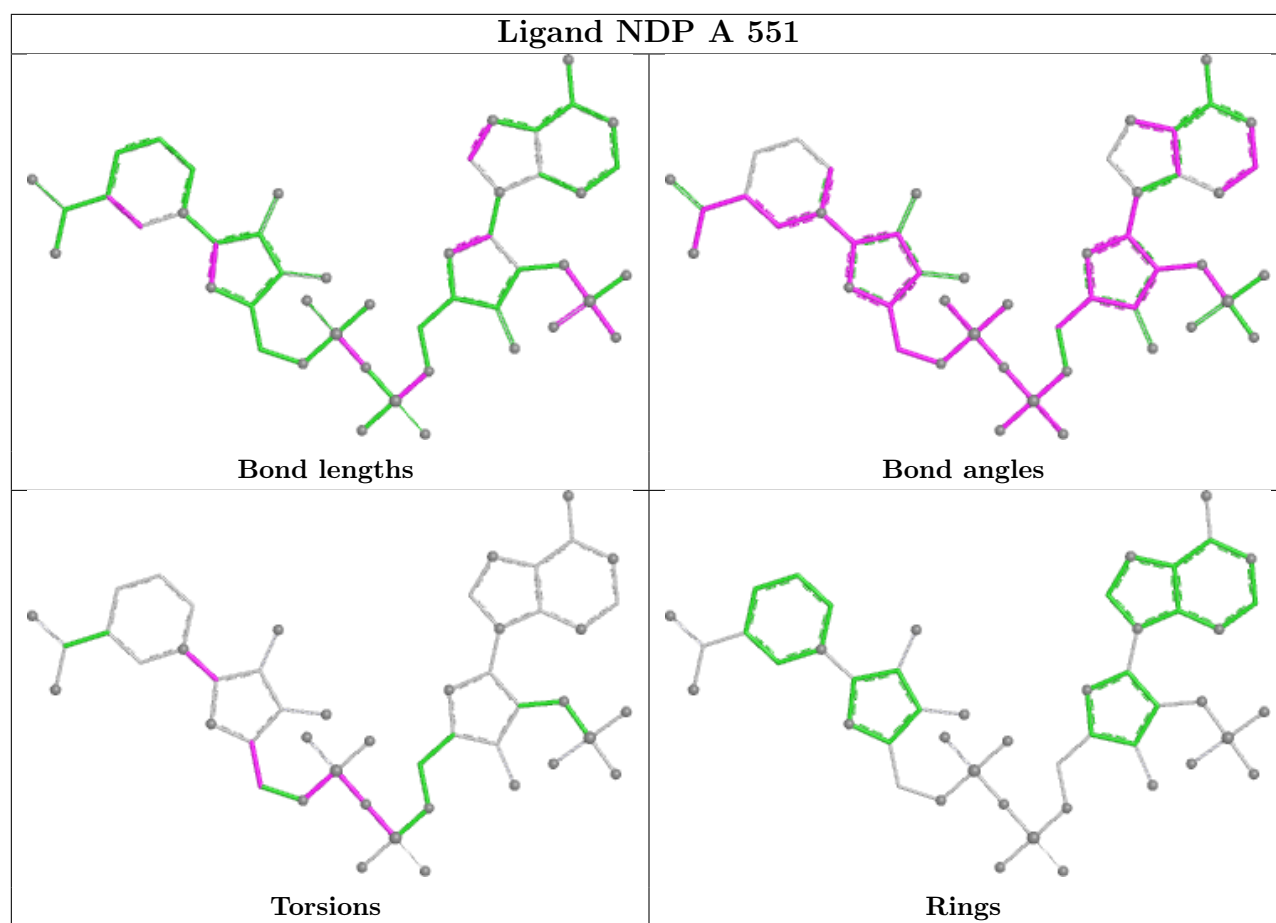
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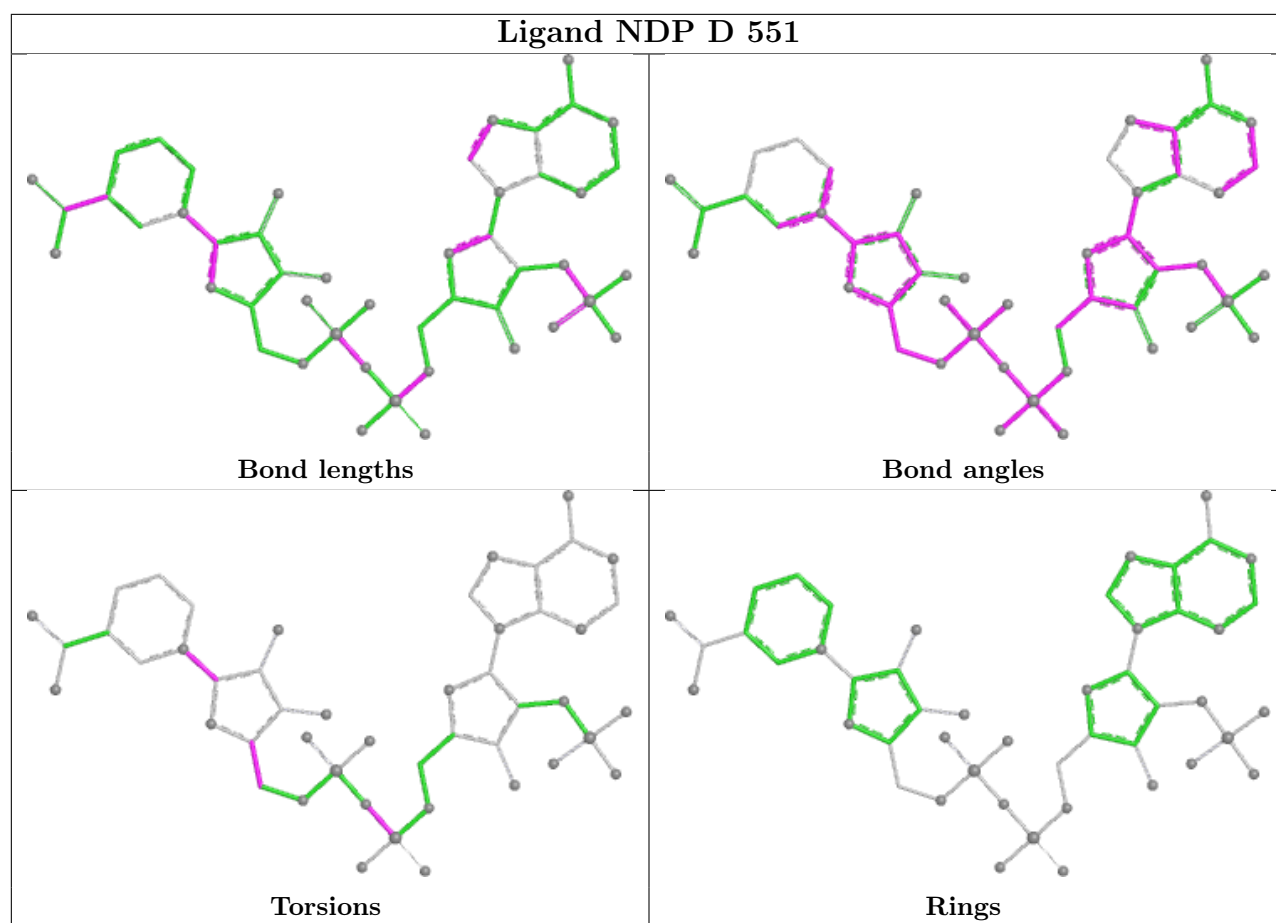
## Ligand GTP F 553



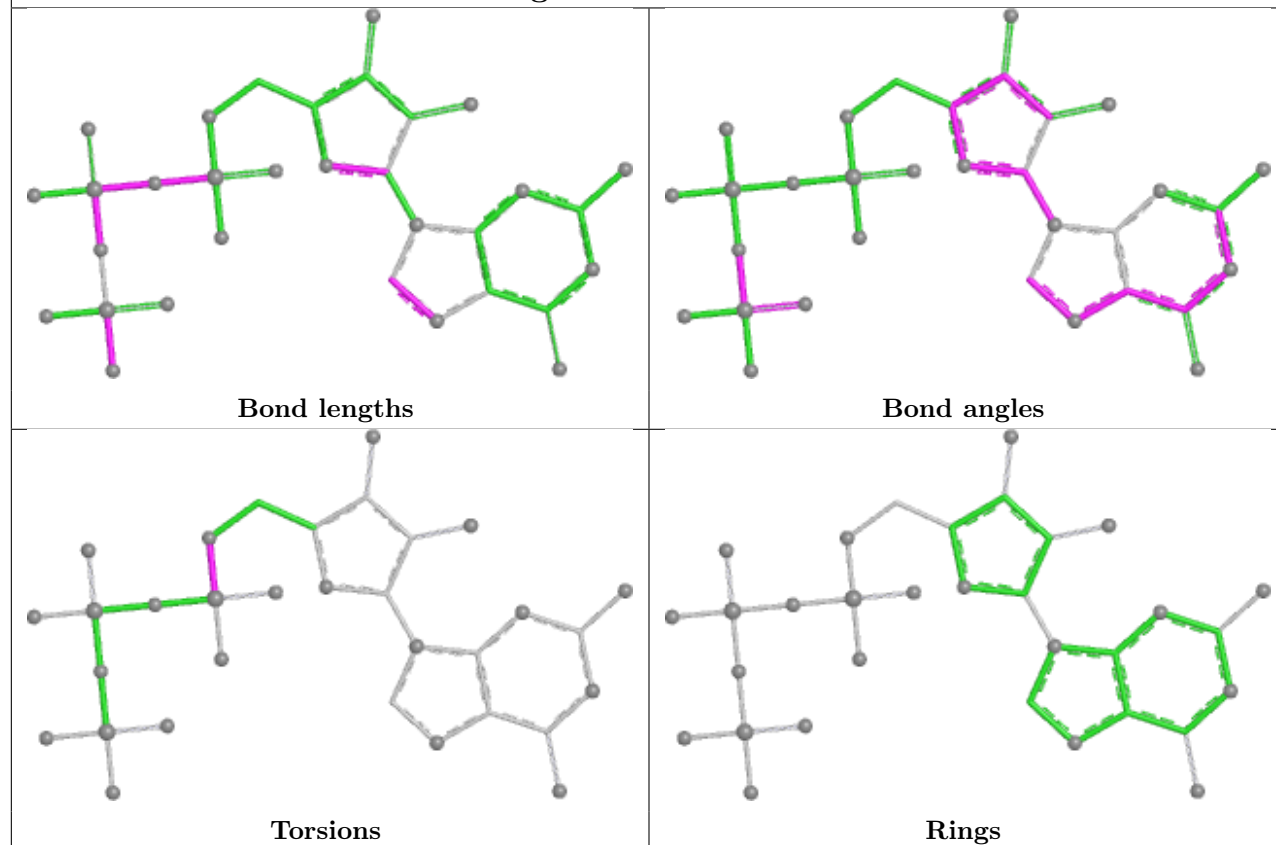




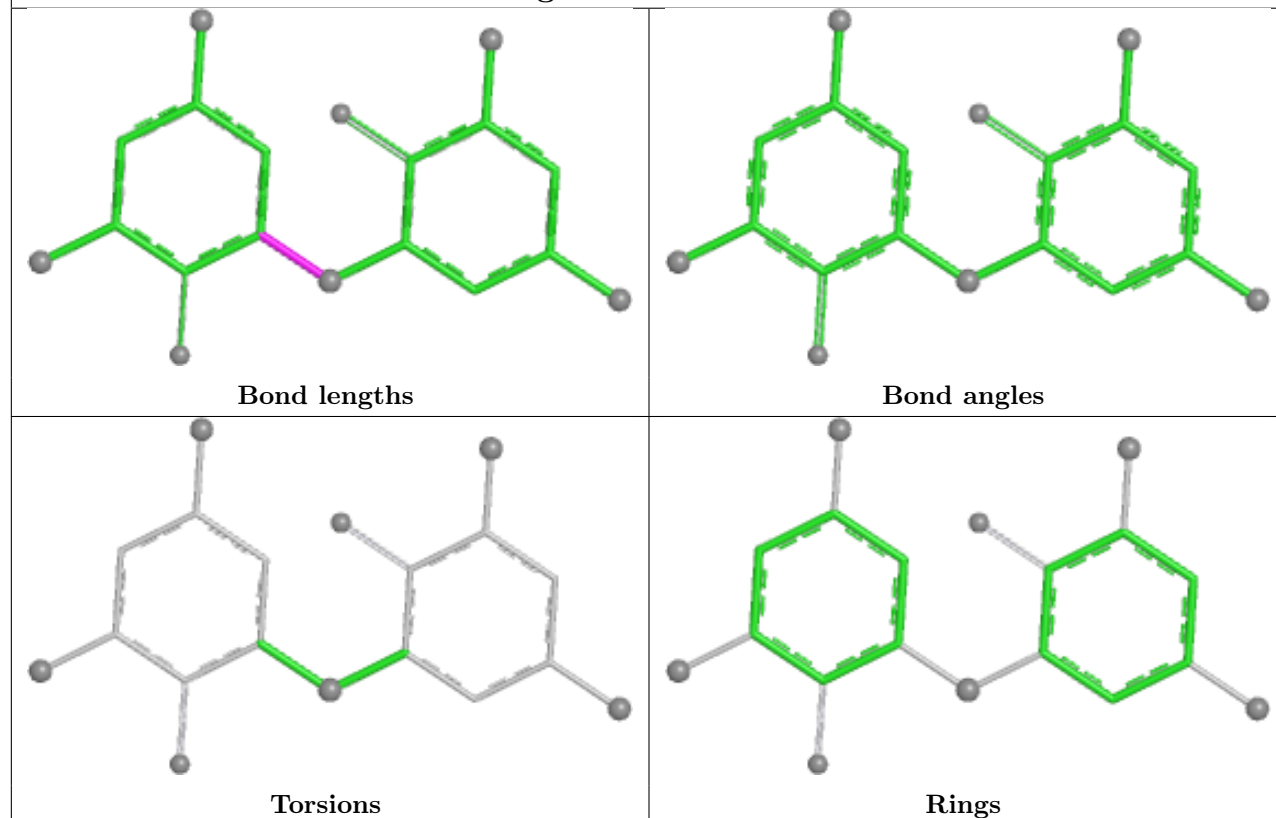


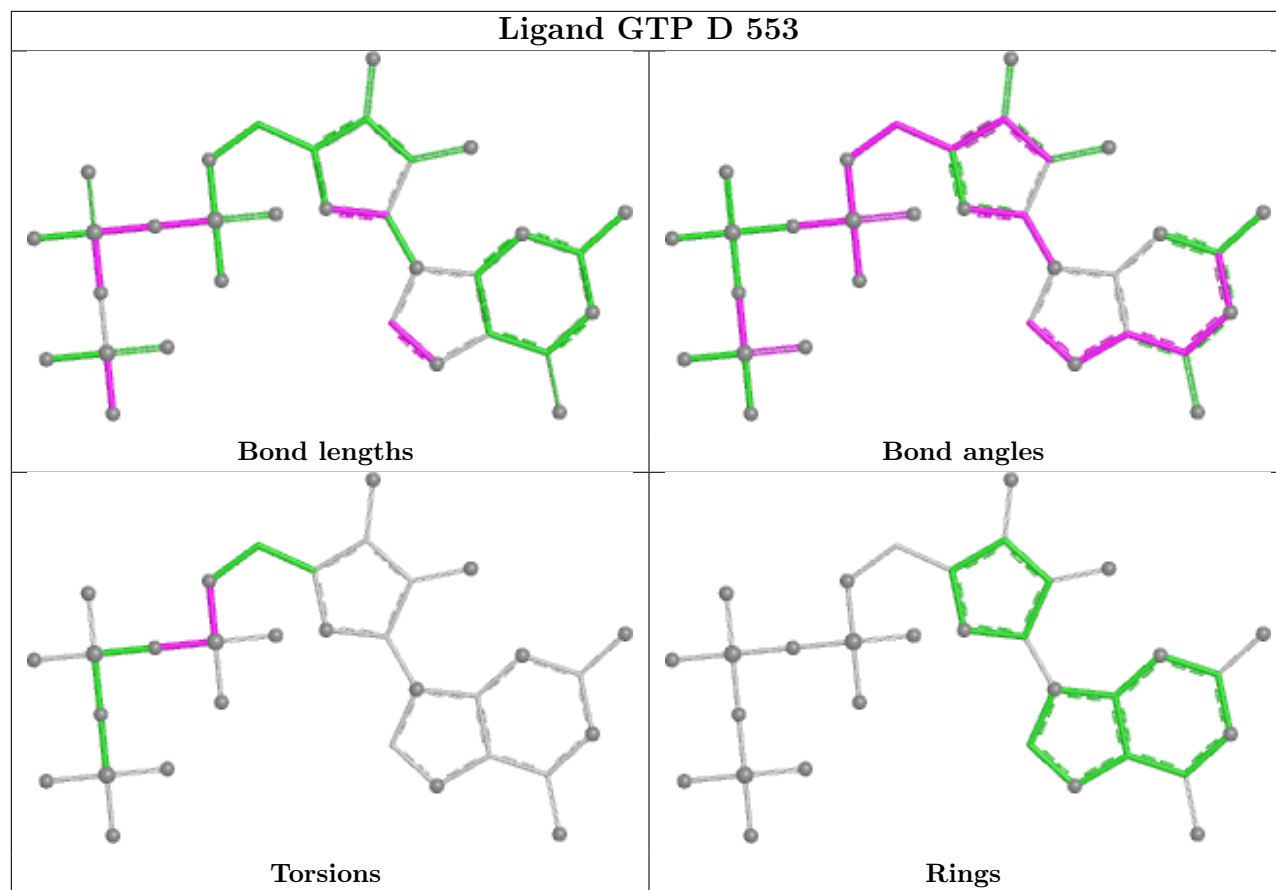


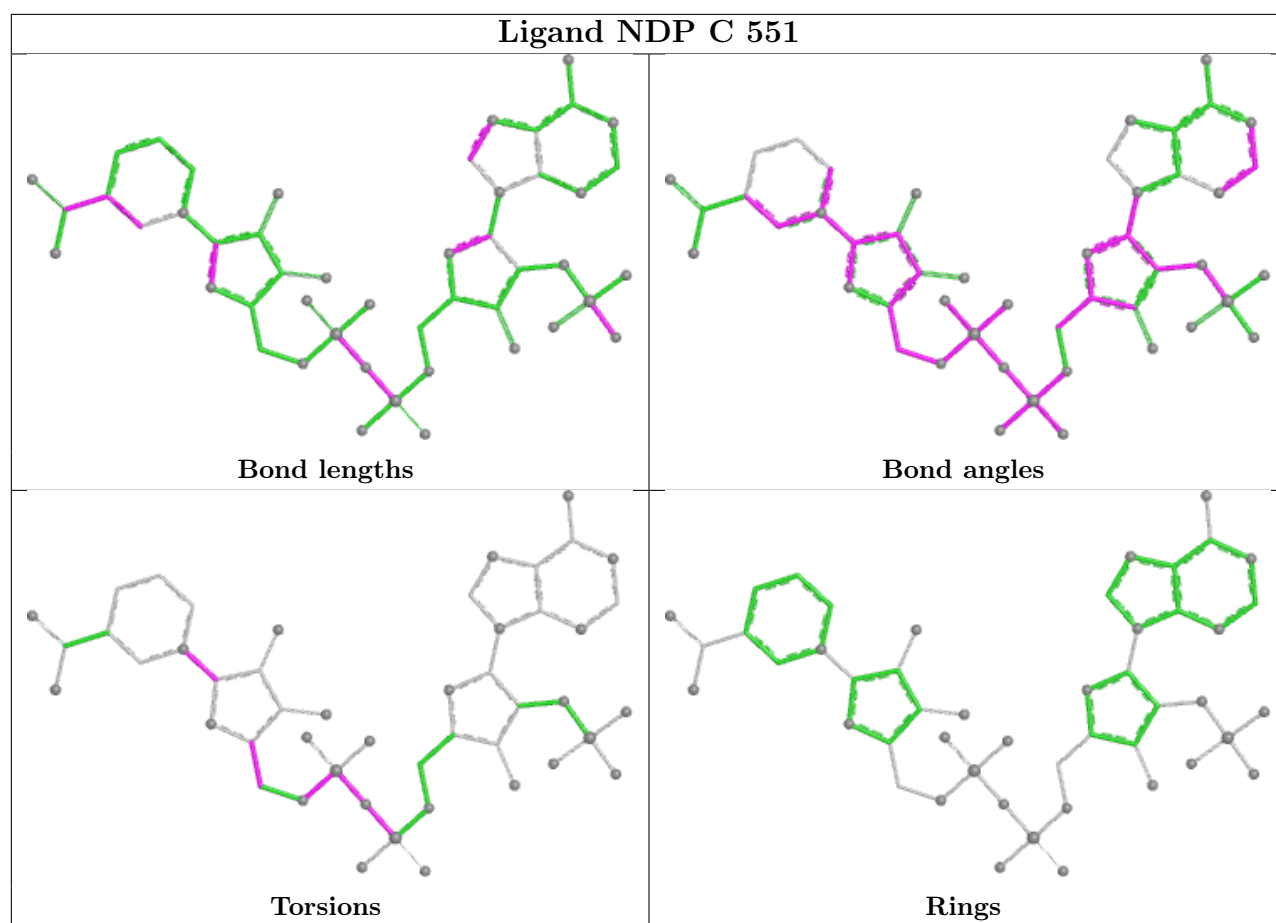
## Ligand GTP C 553

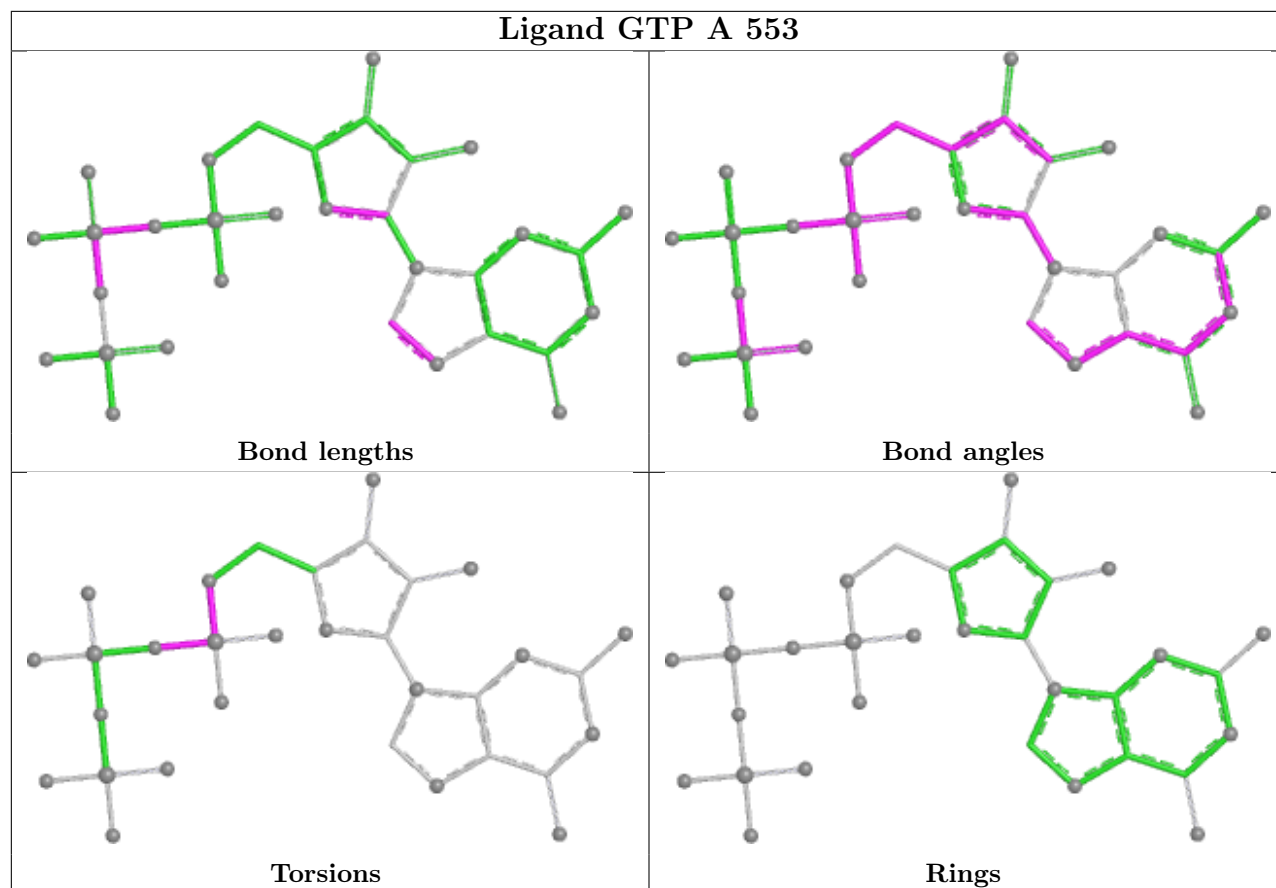


## Ligand B1T F 552









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	501/501 (100%)	0.74	56 (11%) 5 4	36, 60, 90, 105	0
1	B	501/501 (100%)	0.57	34 (6%) 17 17	36, 61, 90, 104	0
1	C	501/501 (100%)	0.51	33 (6%) 18 19	34, 59, 90, 107	0
1	D	501/501 (100%)	0.63	42 (8%) 11 11	36, 60, 91, 105	0
1	E	501/501 (100%)	0.66	42 (8%) 11 11	36, 60, 90, 105	0
1	F	501/501 (100%)	0.79	79 (15%) 2 1	37, 61, 90, 105	0
All	All	3006/3006 (100%)	0.65	286 (9%) 8 8	34, 60, 91, 107	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	11.8
1	C	1	ALA	11.1
1	E	1	ALA	10.1
1	D	1	ALA	9.4
1	D	424	HIS	9.4
1	F	1	ALA	9.3
1	A	501	THR	9.2
1	A	498	VAL	8.7
1	B	499	THR	8.0
1	A	500	PHE	7.9
1	A	424	HIS	7.7
1	F	339	VAL	7.4
1	C	501	THR	7.4
1	D	498	VAL	7.1
1	A	497	GLY	6.9
1	B	424	HIS	6.8
1	A	499	THR	6.4
1	E	4	GLU	6.1
1	A	1	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	35	ARG	5.9
1	D	39	GLU	5.7
1	E	501	THR	5.6
1	F	3	ARG	5.5
1	E	424	HIS	5.5
1	F	32	LEU	5.5
1	B	501	THR	5.4
1	C	424	HIS	5.4
1	A	425	GLY	5.4
1	A	421	PHE	5.2
1	D	499	THR	5.1
1	B	425	GLY	5.1
1	C	426	GLY	5.1
1	F	2	ASP	5.1
1	E	3	ARG	5.0
1	F	227	ILE	5.0
1	B	500	PHE	5.0
1	F	242	PHE	5.0
1	F	500	PHE	5.0
1	E	425	GLY	5.0
1	F	499	THR	4.9
1	A	423	LYS	4.9
1	F	501	THR	4.8
1	D	496	ALA	4.8
1	F	426	GLY	4.8
1	B	32	LEU	4.7
1	E	496	ALA	4.7
1	F	365	ILE	4.6
1	F	496	ALA	4.5
1	E	35	ARG	4.5
1	D	497	GLY	4.5
1	A	190	TYR	4.4
1	C	190	TYR	4.3
1	E	190	TYR	4.3
1	A	32	LEU	4.3
1	C	2	ASP	4.3
1	B	498	VAL	4.2
1	A	426	GLY	4.2
1	F	286	ILE	4.2
1	B	426	GLY	4.2
1	F	190	TYR	4.2
1	A	3	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	190	TYR	4.1
1	F	33	LYS	4.1
1	E	72	TRP	4.0
1	A	40	GLN	4.0
1	D	425	GLY	4.0
1	D	281	TRP	3.9
1	C	425	GLY	3.9
1	B	190	TYR	3.9
1	F	34	THR	3.9
1	B	497	GLY	3.9
1	F	475	LEU	3.8
1	F	4	GLU	3.8
1	A	35	ARG	3.8
1	B	88	PRO	3.8
1	F	35	ARG	3.8
1	D	32	LEU	3.8
1	E	426	GLY	3.8
1	B	39	GLU	3.7
1	C	339	VAL	3.7
1	F	310	TYR	3.7
1	F	302	LEU	3.7
1	E	421	PHE	3.6
1	E	499	THR	3.6
1	E	500	PHE	3.6
1	B	3	ARG	3.5
1	F	243	GLY	3.5
1	D	87	THR	3.5
1	D	88	PRO	3.5
1	F	285	GLY	3.5
1	A	389	LEU	3.5
1	A	417	LEU	3.5
1	F	232	TYR	3.5
1	E	87	THR	3.5
1	F	366	MET	3.4
1	D	36	GLU	3.4
1	C	35	ARG	3.4
1	E	497	GLY	3.3
1	F	315	LEU	3.3
1	A	33	LYS	3.3
1	F	230	ALA	3.3
1	A	29	VAL	3.3
1	B	2	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	281	TRP	3.3
1	F	312	GLY	3.3
1	C	3	ARG	3.3
1	D	3	ARG	3.3
1	C	87	THR	3.2
1	A	36	GLU	3.2
1	E	2	ASP	3.2
1	B	389	LEU	3.2
1	D	308	LYS	3.2
1	F	238	MET	3.1
1	D	44	ARG	3.1
1	B	23	ILE	3.1
1	D	40	GLN	3.1
1	F	237	GLY	3.1
1	B	35	ARG	3.1
1	D	4	GLU	3.1
1	F	424	HIS	3.1
1	A	496	ALA	3.1
1	E	32	LEU	3.1
1	F	270	CYS	3.1
1	B	297	GLN	3.0
1	F	236	LEU	3.0
1	D	501	THR	3.0
1	D	306	LYS	3.0
1	B	87	THR	3.0
1	A	38	GLU	3.0
1	E	302	LEU	3.0
1	F	303	GLY	3.0
1	A	390	ASN	2.9
1	A	88	PRO	2.9
1	C	66	ARG	2.9
1	A	39	GLU	2.9
1	E	417	LEU	2.9
1	F	228	ASN	2.9
1	F	359	ILE	2.9
1	A	2	ASP	2.8
1	B	36	GLU	2.8
1	E	423	LYS	2.8
1	F	241	GLY	2.8
1	C	421	PHE	2.8
1	F	39	GLU	2.8
1	A	34	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	236	LEU	2.8
1	D	426	GLY	2.8
1	F	263	LEU	2.8
1	B	496	ALA	2.8
1	A	87	THR	2.7
1	C	500	PHE	2.7
1	C	498	VAL	2.7
1	D	431	VAL	2.7
1	C	39	GLU	2.7
1	C	496	ALA	2.7
1	C	360	PHE	2.7
1	F	252	PHE	2.7
1	F	301	ILE	2.7
1	A	339	VAL	2.6
1	D	339	VAL	2.6
1	F	268	ALA	2.6
1	F	277	ASP	2.6
1	E	33	LYS	2.6
1	A	45	VAL	2.6
1	C	361	LEU	2.6
1	F	362	GLU	2.6
1	A	189	HIS	2.6
1	F	334	SER	2.6
1	A	188	GLY	2.6
1	F	226	PHE	2.6
1	E	339	VAL	2.6
1	D	28	LEU	2.6
1	E	308	LYS	2.6
1	A	66	ARG	2.6
1	F	87	THR	2.6
1	F	305	PRO	2.5
1	B	38	GLU	2.5
1	A	388	ASN	2.5
1	D	34	THR	2.5
1	F	321	ILE	2.5
1	F	333	LYS	2.5
1	F	316	GLU	2.5
1	A	391	HIS	2.5
1	F	38	GLU	2.5
1	F	498	VAL	2.5
1	F	364	ASN	2.5
1	F	281	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	421	PHE	2.5
1	C	423	LYS	2.4
1	A	385	TRP	2.4
1	A	311	GLU	2.4
1	A	427	THR	2.4
1	D	42	ARG	2.4
1	C	499	THR	2.4
1	B	4	GLU	2.4
1	D	33	LYS	2.4
1	F	340	LYS	2.4
1	C	238	MET	2.4
1	D	440	ILE	2.4
1	F	269	LYS	2.4
1	A	28	LEU	2.4
1	B	89	CYS	2.4
1	A	19	ARG	2.4
1	E	66	ARG	2.4
1	E	243	GLY	2.3
1	F	267	GLY	2.3
1	C	38	GLU	2.3
1	C	281	TRP	2.3
1	D	38	GLU	2.3
1	A	267	GLY	2.3
1	F	497	GLY	2.3
1	F	36	GLU	2.3
1	E	88	PRO	2.3
1	F	251	GLY	2.3
1	D	495	GLU	2.3
1	A	386	LEU	2.3
1	F	423	LYS	2.3
1	A	180	ALA	2.3
1	A	392	VAL	2.3
1	E	378	VAL	2.3
1	E	498	VAL	2.3
1	F	342	LYS	2.3
1	D	66	ARG	2.2
1	F	88	PRO	2.2
1	B	161	GLY	2.2
1	F	390	ASN	2.2
1	A	9	PHE	2.2
1	B	283	PRO	2.2
1	C	36	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	6	ASP	2.2
1	C	33	LYS	2.2
1	F	311	GLU	2.2
1	A	491	ARG	2.2
1	B	435	GLU	2.2
1	F	192	ILE	2.2
1	B	421	PHE	2.2
1	D	285	GLY	2.2
1	A	462	ARG	2.2
1	C	462	ARG	2.2
1	E	95	TYR	2.2
1	F	273	VAL	2.2
1	F	341	ALA	2.2
1	A	23	ILE	2.2
1	C	312	GLY	2.1
1	E	187	ILE	2.1
1	B	296	LEU	2.1
1	C	475	LEU	2.1
1	E	335	ASN	2.1
1	E	495	GLU	2.1
1	C	427	THR	2.1
1	E	36	GLU	2.1
1	F	344	ILE	2.1
1	F	360	PHE	2.1
1	B	42	ARG	2.1
1	D	269	LYS	2.1
1	E	11	LYS	2.1
1	E	188	GLY	2.1
1	E	469	MET	2.1
1	B	37	THR	2.1
1	A	419	ARG	2.1
1	A	490	PHE	2.1
1	C	242	PHE	2.1
1	A	393	SER	2.1
1	F	367	VAL	2.1
1	B	5	ASP	2.1
1	E	75	ILE	2.1
1	E	409	LEU	2.1
1	C	342	LYS	2.1
1	D	419	ARG	2.1
1	A	192	ILE	2.1
1	D	475	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	283	PRO	2.0
1	D	242	PHE	2.0
1	E	39	GLU	2.0
1	F	42	ARG	2.0
1	F	233	MET	2.0
1	C	403	ARG	2.0
1	F	296	LEU	2.0
1	A	194	ALA	2.0
1	B	230	ALA	2.0
1	A	193	ASN	2.0
1	D	286	ILE	2.0
1	D	428	ILE	2.0
1	D	473	LEU	2.0
1	F	428	ILE	2.0
1	D	421	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

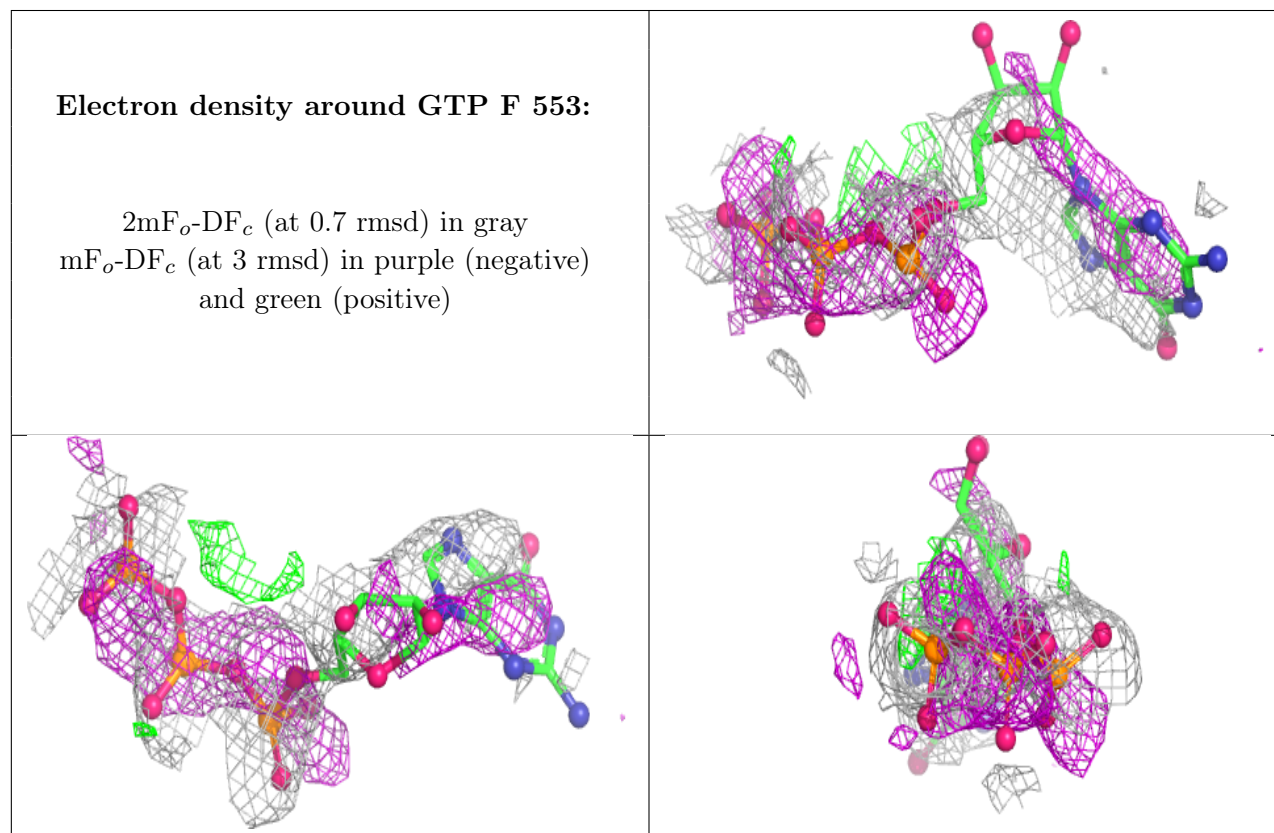
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GTP	F	553	32/32	0.52	0.54	116,119,134,135	0
4	GTP	B	553	32/32	0.53	0.48	105,112,119,119	0
5	B1T	E	552	19/19	0.56	0.38	105,108,114,116	0
5	B1T	B	552	19/19	0.58	0.37	103,109,112,113	0
5	B1T	A	552	19/19	0.58	0.49	106,110,114,117	0
4	GTP	D	553	32/32	0.64	0.31	105,111,117,118	0
4	GTP	E	553	32/32	0.64	0.30	100,110,124,125	0
4	GTP	A	553	32/32	0.65	0.42	111,116,125,126	0

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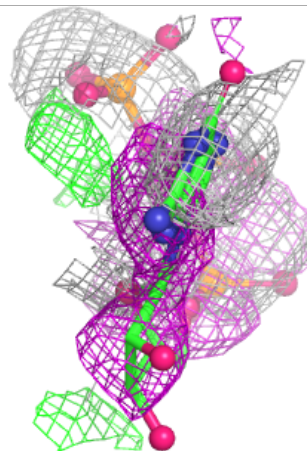
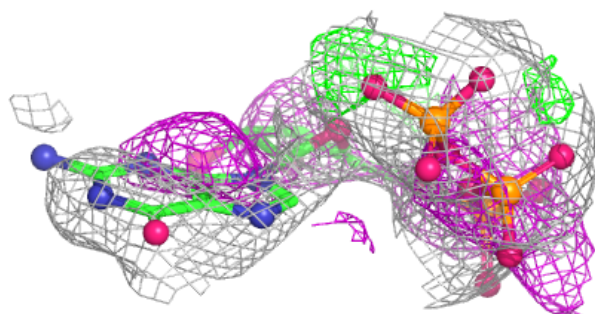
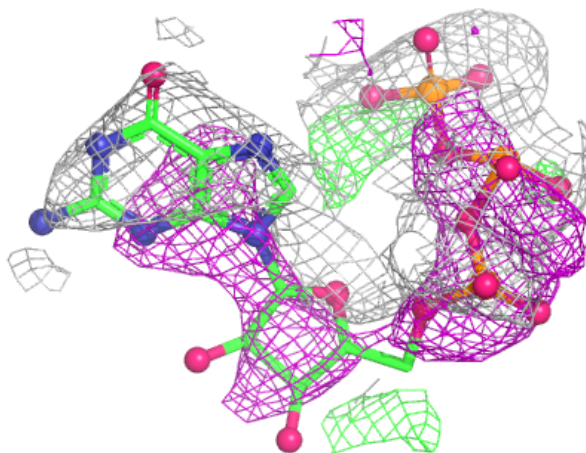
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GTP	C	553	32/32	0.66	0.33	104,113,129,131	0
5	B1T	C	552	19/19	0.67	0.33	104,108,114,115	0
5	B1T	D	552	19/19	0.69	0.32	104,107,112,113	0
2	GLU	E	550	9/10	0.78	0.39	68,73,74,75	0
5	B1T	F	552	19/19	0.80	0.24	93,95,99,100	0
3	NDP	B	551	48/48	0.84	0.22	64,71,80,85	0
3	NDP	E	551	48/48	0.84	0.23	67,81,86,87	0
3	NDP	D	551	48/48	0.85	0.26	52,63,74,79	0
3	NDP	F	551	48/48	0.85	0.22	74,83,85,87	0
3	NDP	A	551	48/48	0.87	0.20	59,66,73,77	0
2	GLU	A	550	9/10	0.88	0.27	58,61,62,63	0
3	NDP	C	551	48/48	0.90	0.21	43,55,66,72	0
2	GLU	F	550	9/10	0.91	0.20	67,68,70,71	0
2	GLU	B	550	9/10	0.92	0.24	54,58,60,60	0
2	GLU	D	550	9/10	0.93	0.21	41,46,50,51	0
2	GLU	C	550	9/10	0.94	0.19	52,55,56,57	0

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



**Electron density around GTP B 553:**

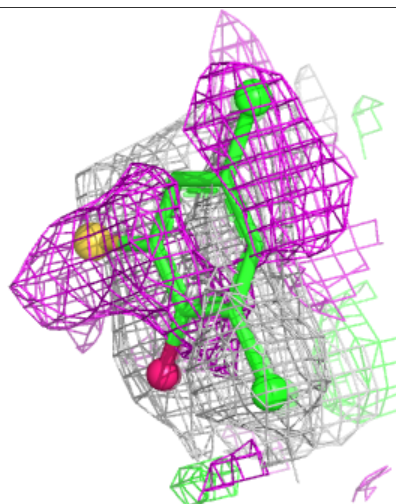
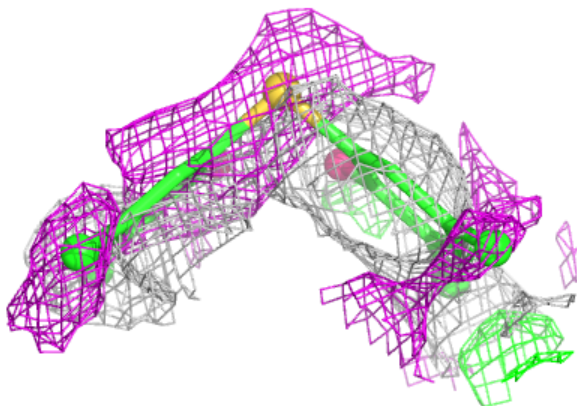
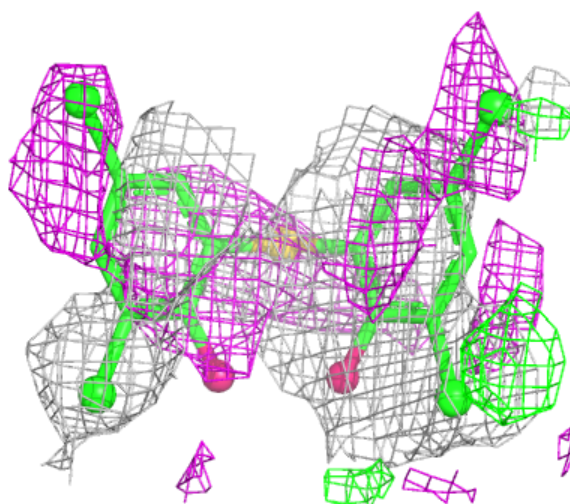
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around B1T A 552:**

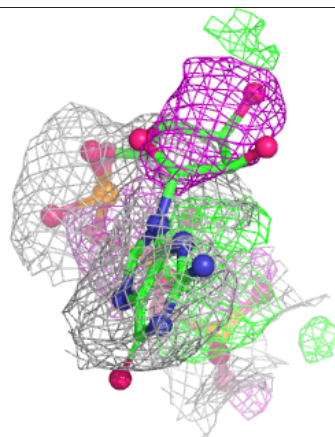
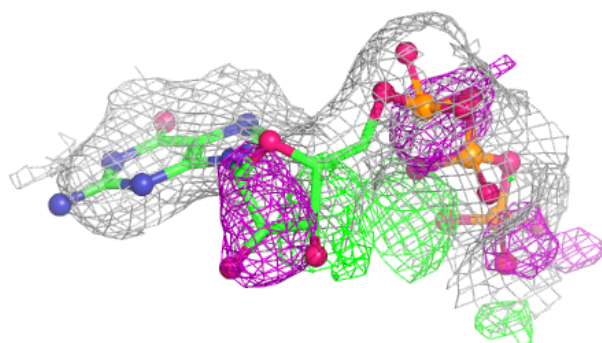
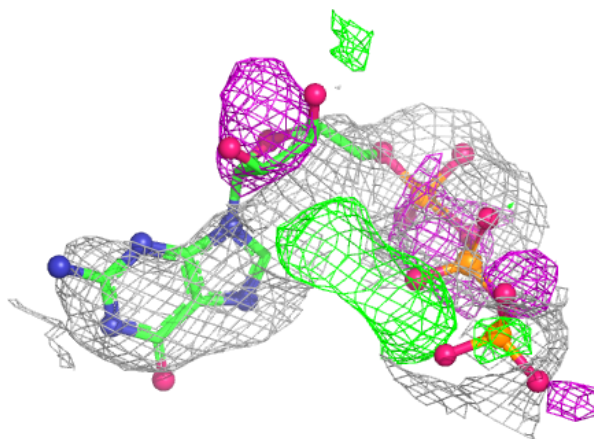
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





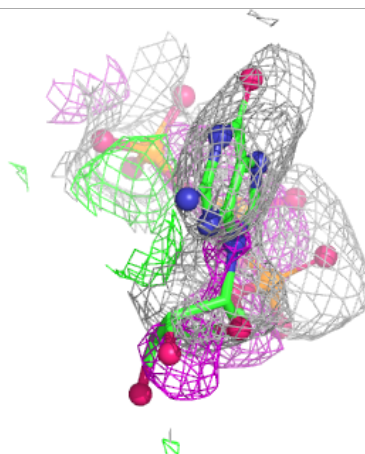
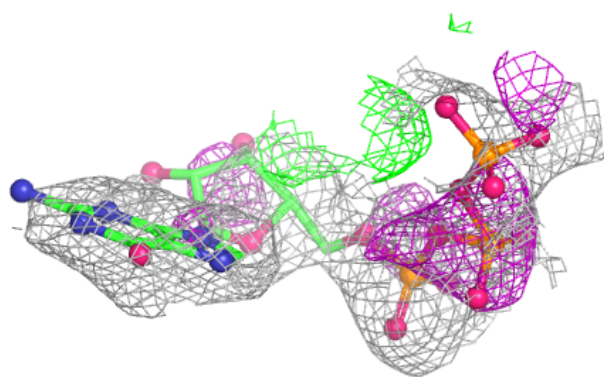
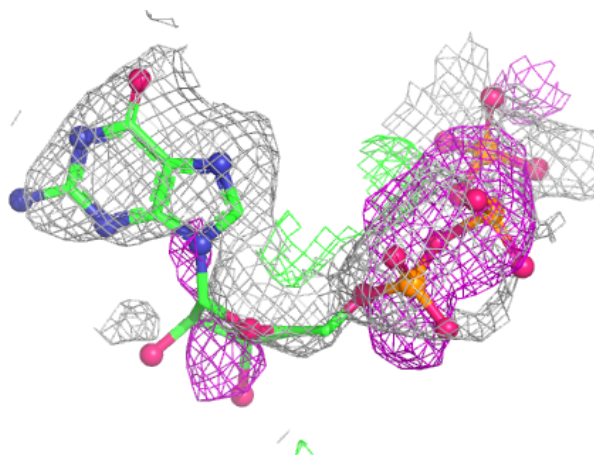
**Electron density around GTP D 553:**

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



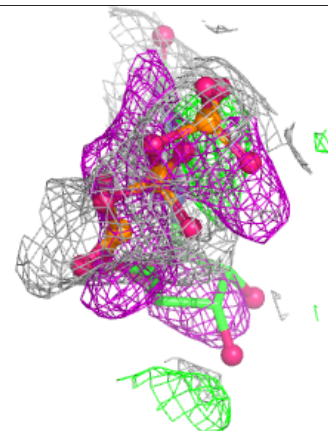
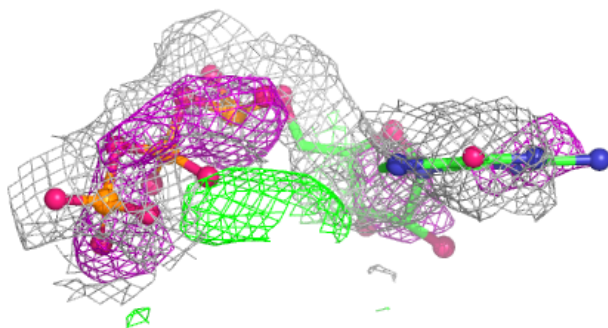
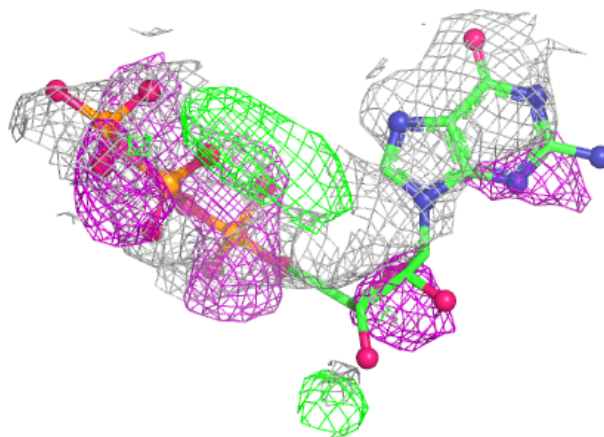
**Electron density around GTP E 553:**

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

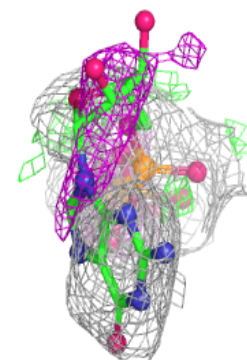
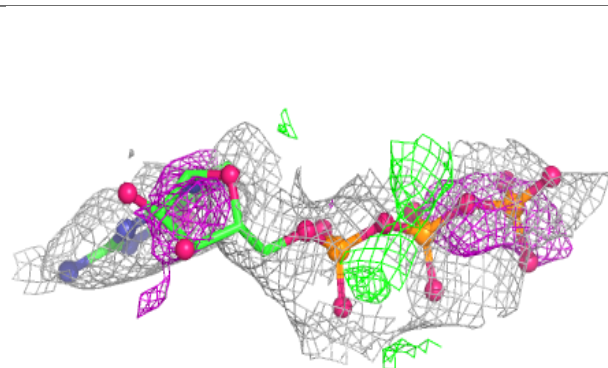
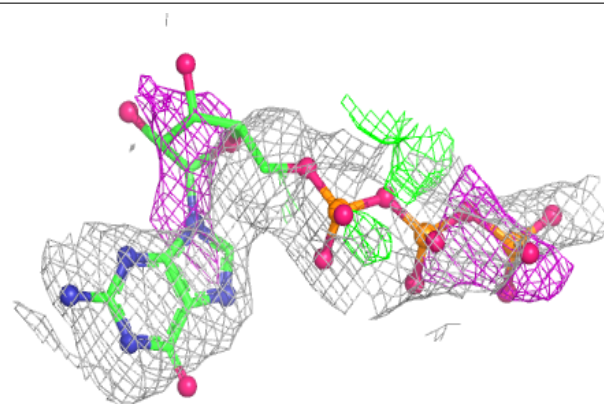


**Electron density around GTP A 553:**

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

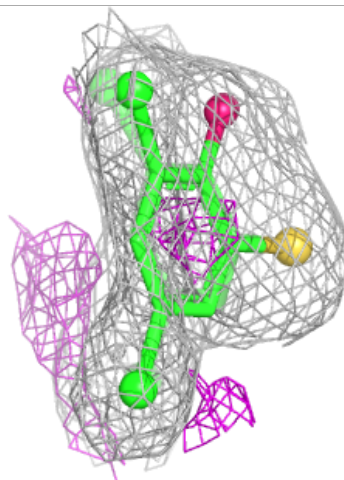
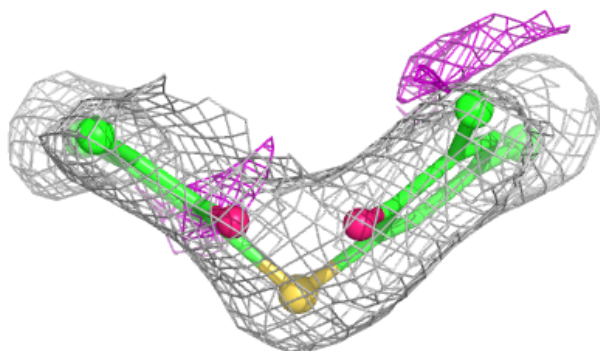
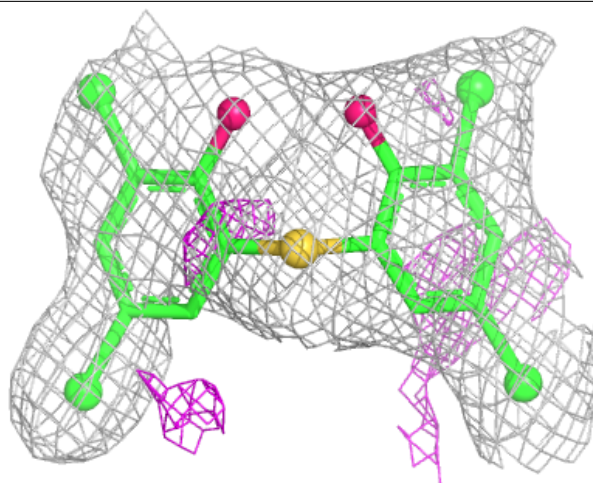
**Electron density around GTP C 553:**

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



**Electron density around B1T F 552:**

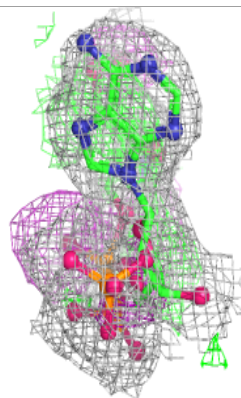
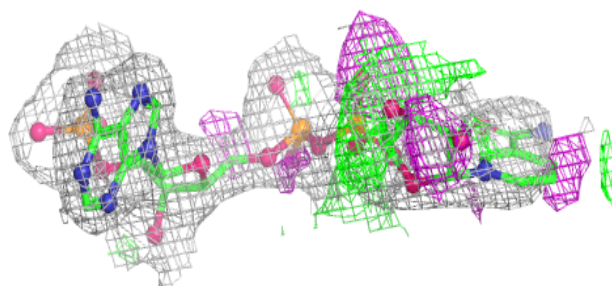
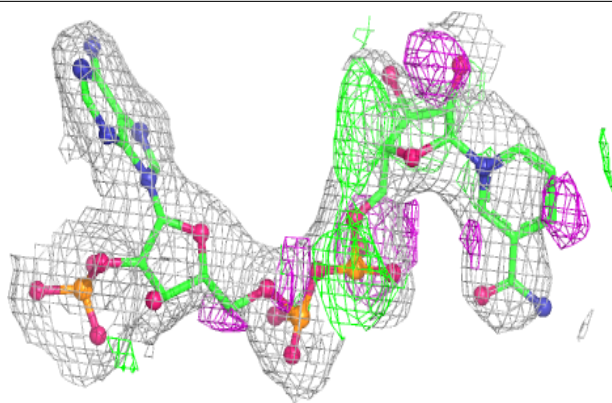
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



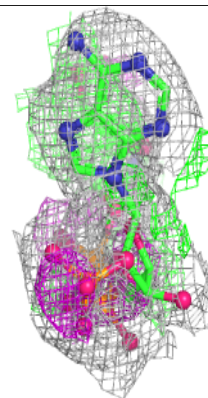
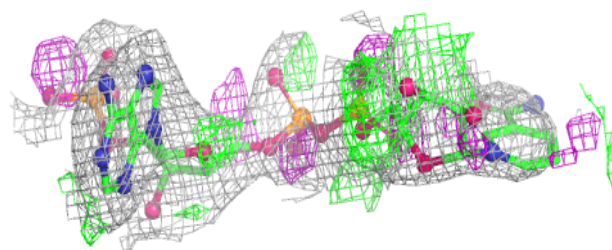
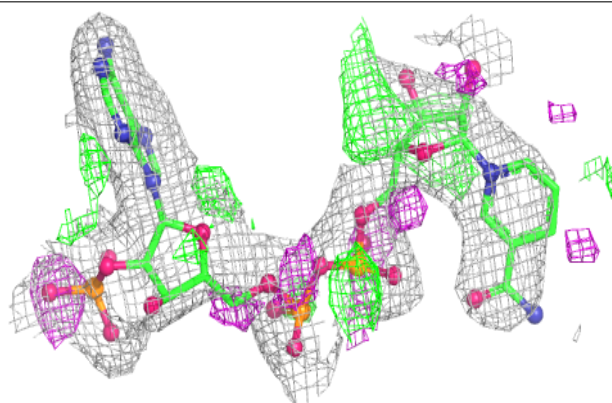


**Electron density around NDP B 551:**

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

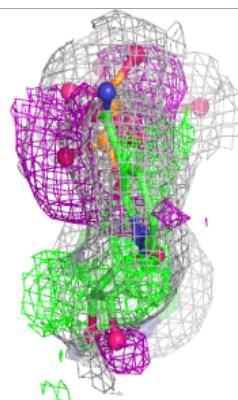
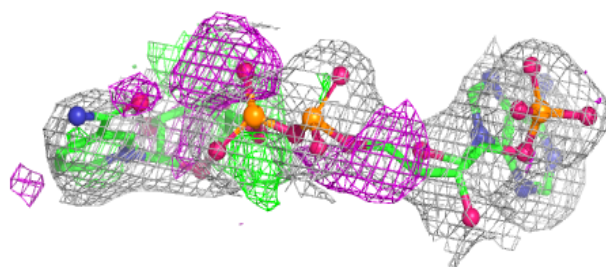
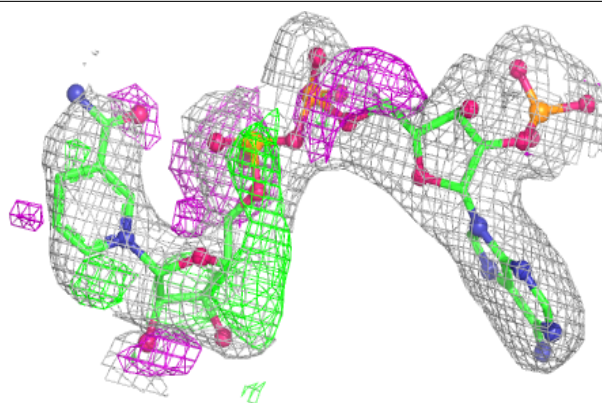
**Electron density around NDP E 551:**

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

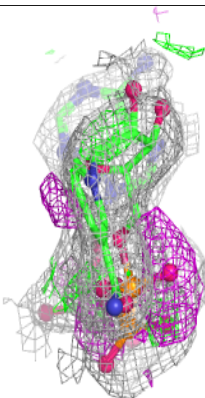
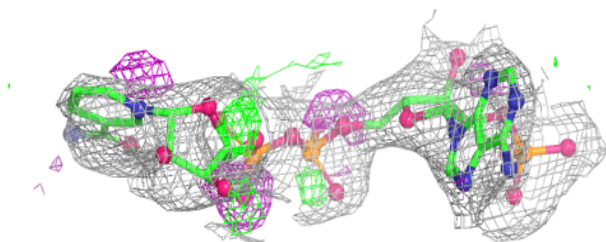
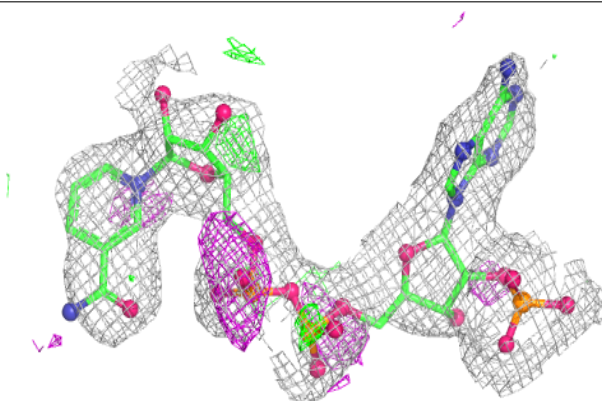


**Electron density around NDP D 551:**

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

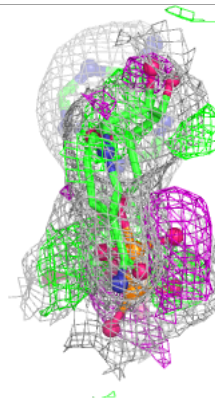
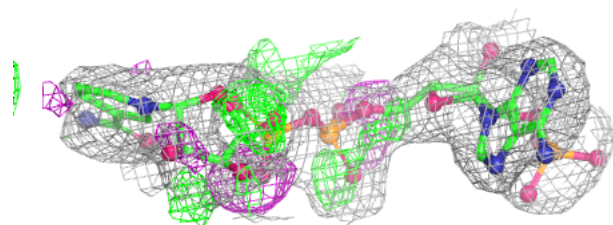
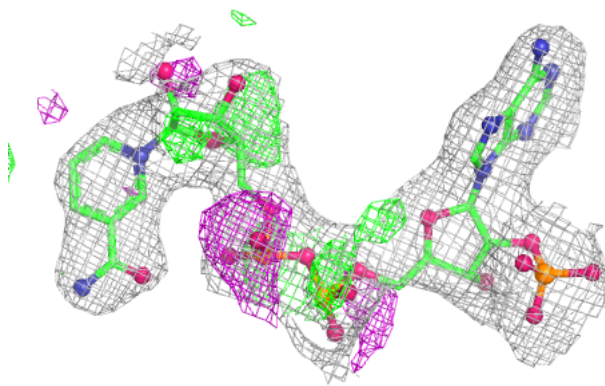
**Electron density around NDP F 551:**

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

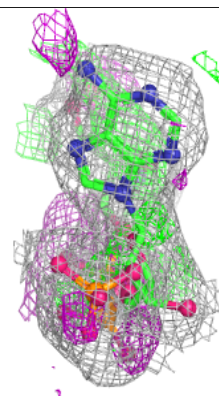
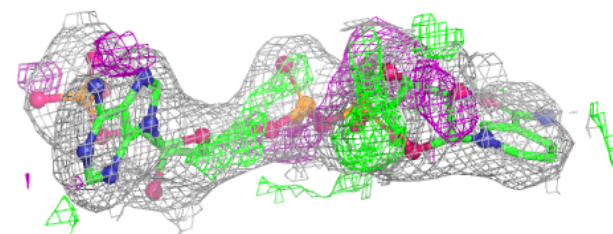
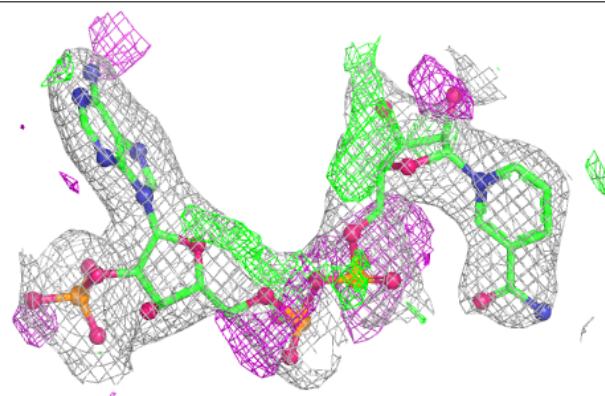


**Electron density around NDP A 551:**

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

**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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.