



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 10:32 AM UTC

PDB ID : 3ETE / pdb_00003ete
Title : Crystal structure of bovine glutamate dehydrogenase complexed with hexachlorophene
Authors : Li, M.; Smith, T.J.
Deposited on : 2008-10-07
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

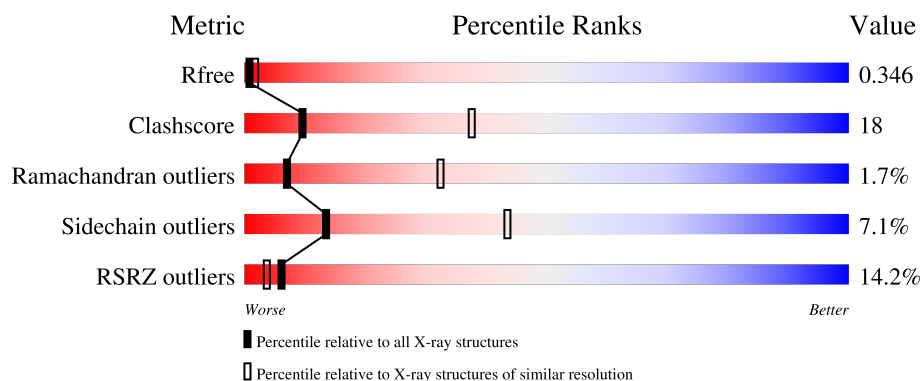
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	501	19% 58% 36% 5%
1	B	501	11% 58% 36% 5%
1	C	501	13% 59% 34% 5%
1	D	501	16% 57% 36% 5%
1	E	501	14% 58% 36% 5%

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Mol	Chain	Length	Quality of chain
1	F	501	12% 60% 34% 5% **

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

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

2 Entry composition [i](#)

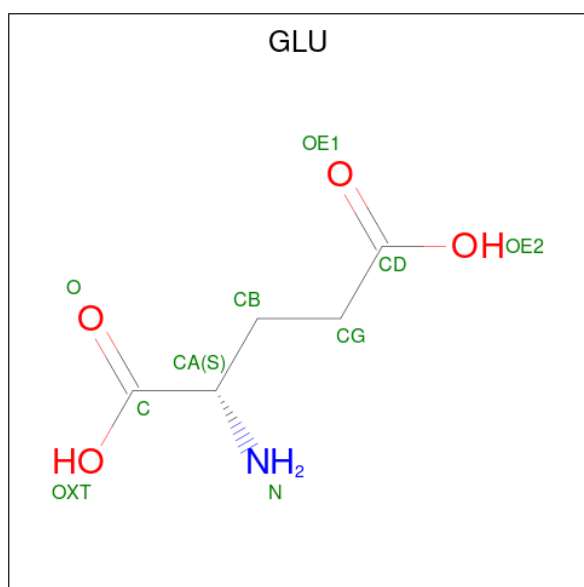
There are 6 unique types of molecules in this entry. The entry contains 24074 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Glutamate dehydrogenase.

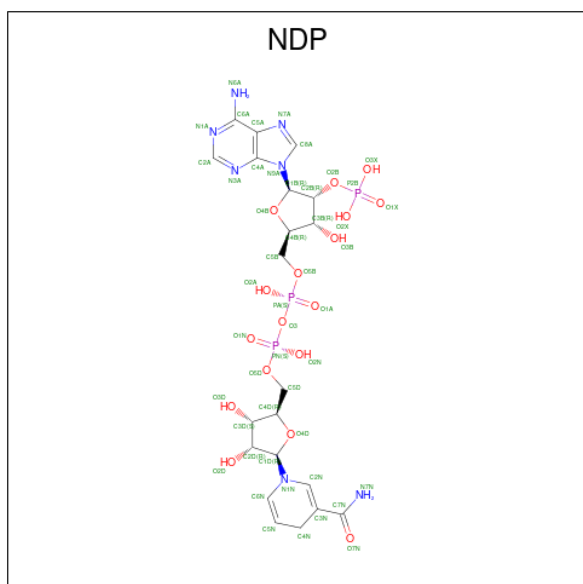
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3866	2443	678	726	19			
1	B	495	Total	C	N	O	S	0	0	0
			3866	2443	678	726	19			
1	C	495	Total	C	N	O	S	0	0	0
			3866	2443	678	726	19			
1	D	495	Total	C	N	O	S	0	0	0
			3866	2443	678	726	19			
1	E	495	Total	C	N	O	S	0	0	0
	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

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



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 (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



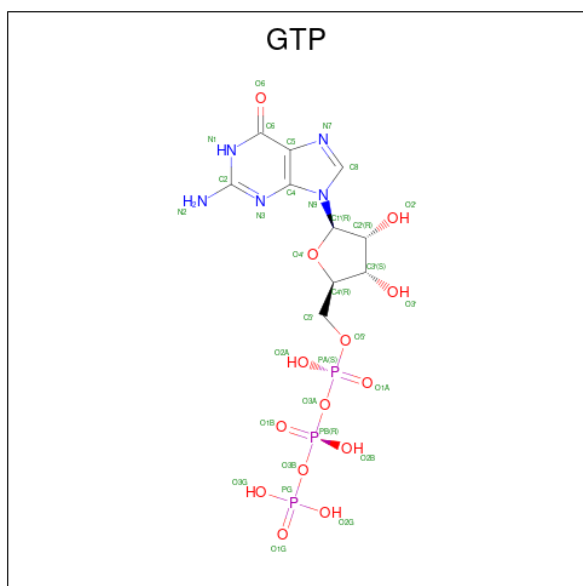
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	E	1	Total 48	C 21	N 7	O 17	P 3	0	0

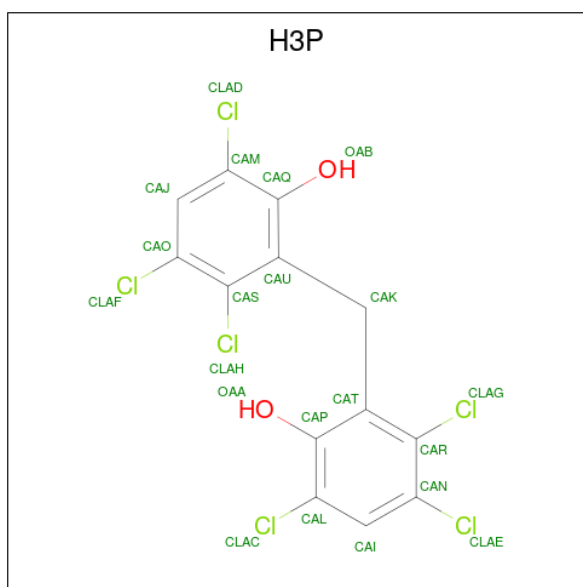
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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





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

- Molecule 6 is water.

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

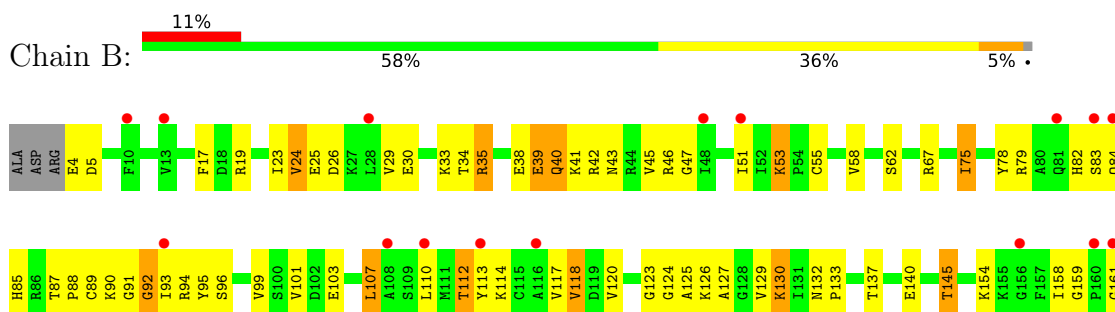
3 Residue-property plots [i](#)

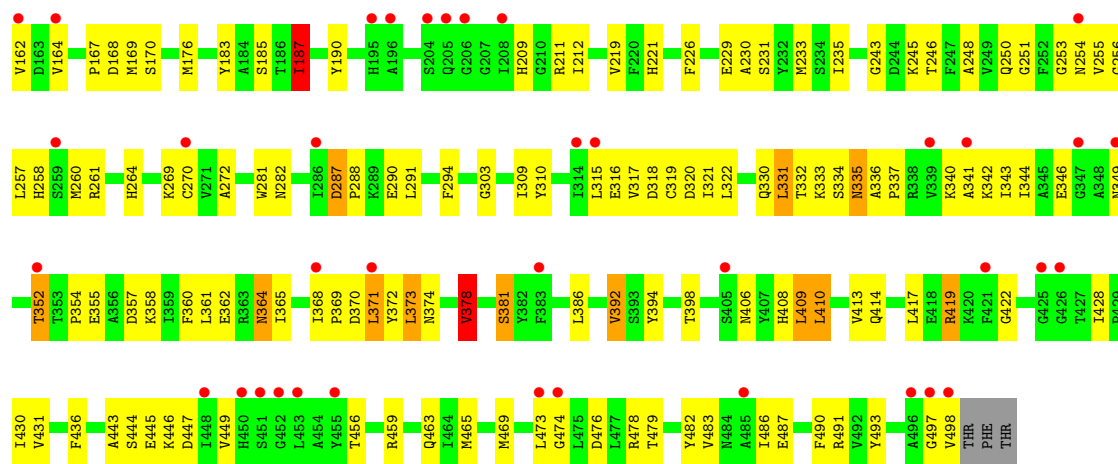
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Glutamate dehydrogenase

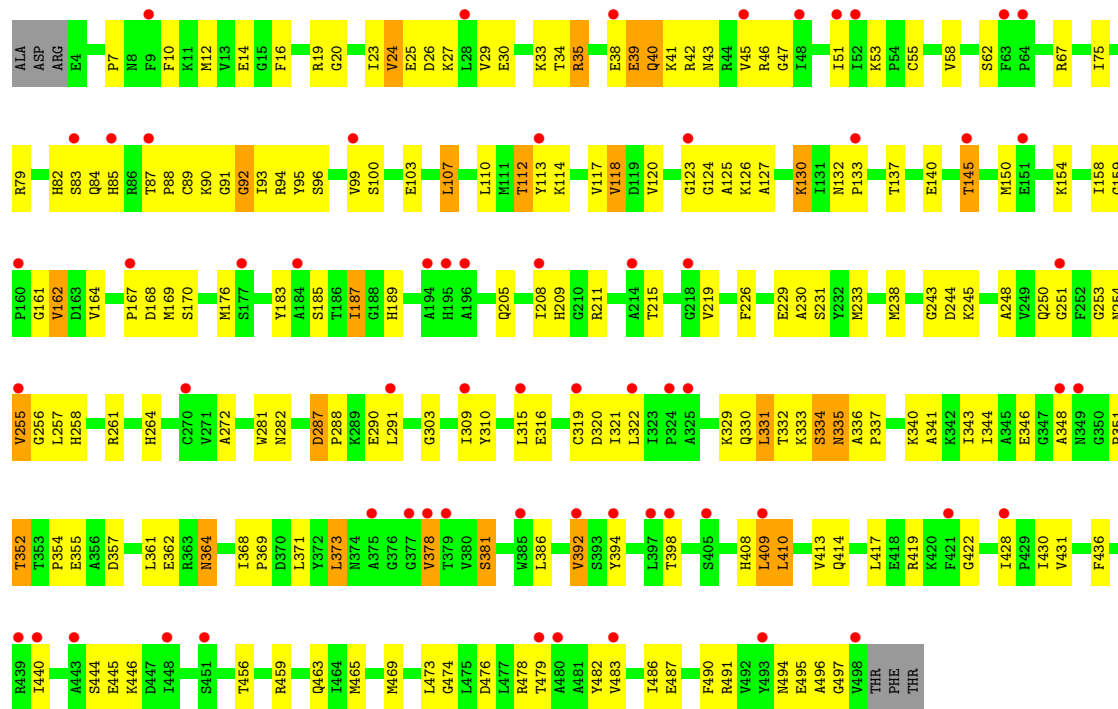


• Molecule 1: Glutamate dehydrogenase

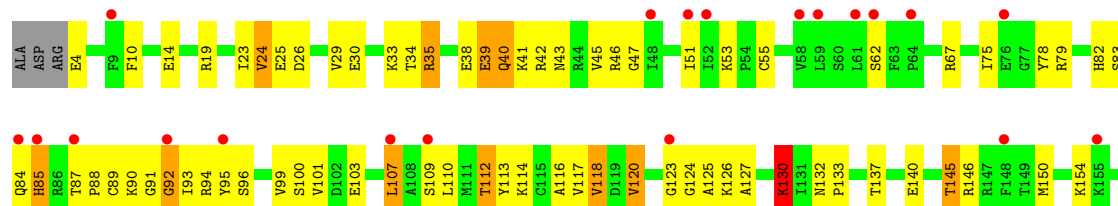


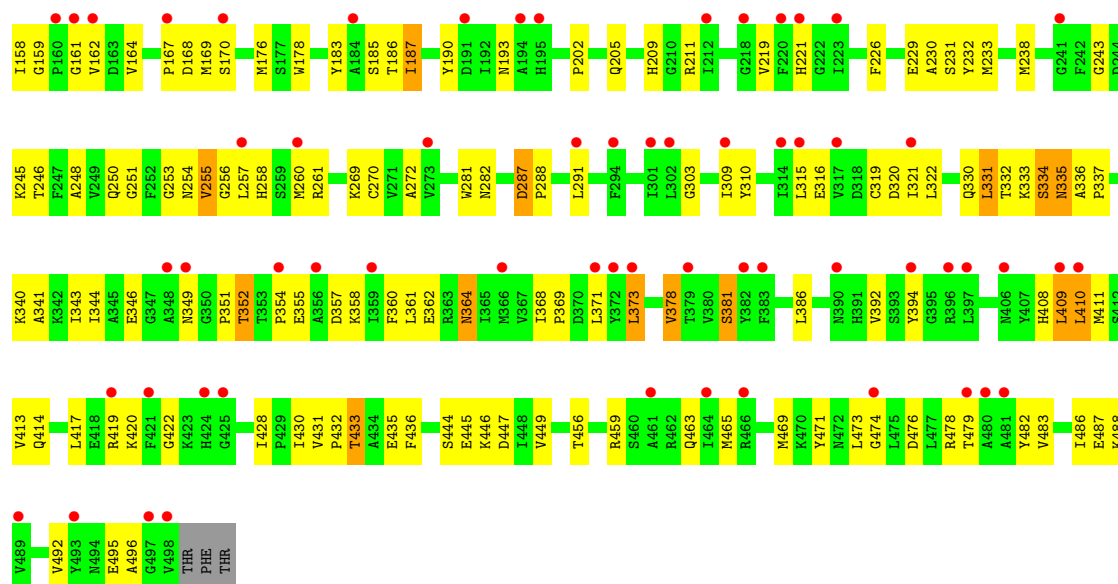


• Molecule 1: Glutamate dehydrogenase



• Molecule 1: Glutamate dehydrogenase



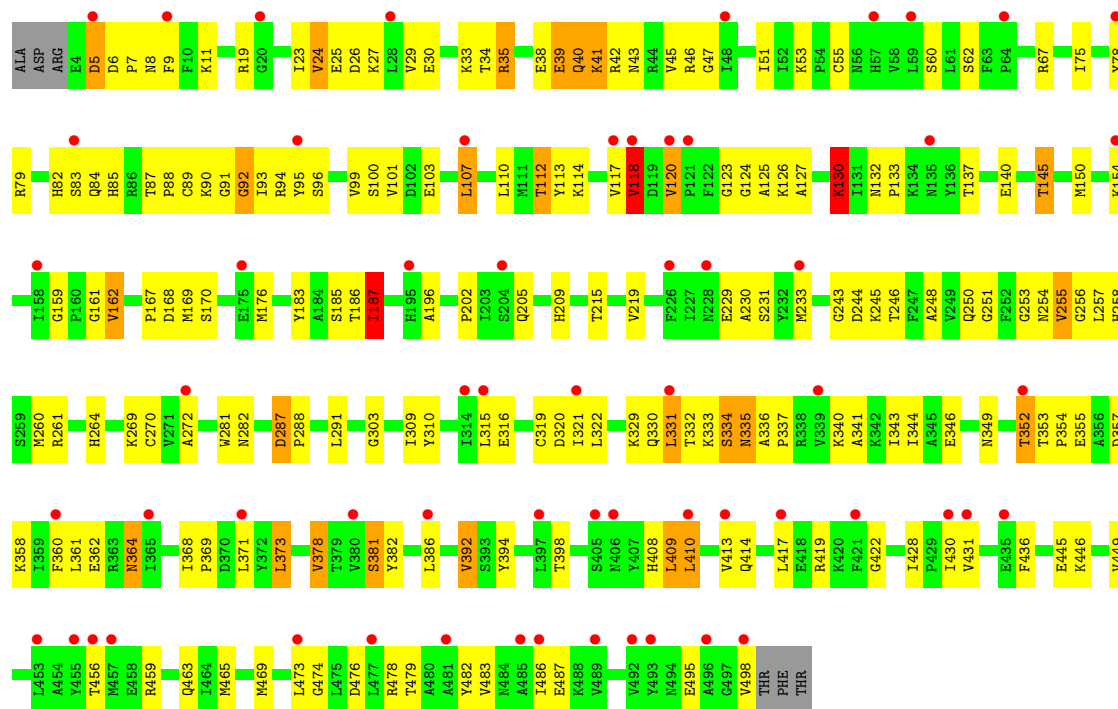


• Molecule 1: Glutamate dehydrogenase



• Molecule 1: Glutamate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.37Å 101.58Å 166.87Å 90.00° 102.34° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.00) 94.2 (50.00-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.266 0.328 , 0.346	Depositor DCC
R_{free} test set	6506 reflections (8.07%)	wwPDB-VP
Wilson B-factor (Å ²)	76.5	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	24074	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H3P, 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	0.56	0/3948	1.04	12/5328 (0.2%)
1	B	0.56	0/3948	1.08	19/5328 (0.4%)
1	C	0.57	0/3948	1.06	17/5328 (0.3%)
1	D	0.57	0/3948	1.04	16/5328 (0.3%)
1	E	0.57	0/3948	1.04	16/5328 (0.3%)
1	F	0.57	0/3948	1.05	19/5328 (0.4%)
All	All	0.57	0/23688	1.05	99/31968 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	ARG	NE-CZ-NH2	14.05	131.85	119.20
1	C	40	GLN	N-CA-C	-13.09	96.99	113.23
1	A	40	GLN	N-CA-C	-12.95	97.18	113.23
1	B	419	ARG	NE-CZ-NH1	-12.91	108.59	121.50
1	B	40	GLN	N-CA-C	-12.74	97.43	113.23
1	D	40	GLN	N-CA-C	-12.36	97.91	113.23
1	E	40	GLN	N-CA-C	-12.29	97.99	113.23
1	F	40	GLN	N-CA-C	-12.08	97.91	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	ARG	CD-NE-CZ	10.61	139.25	124.40
1	A	120	VAL	N-CA-C	-7.15	99.58	107.73
1	F	6	ASP	N-CA-C	-7.05	98.60	108.76
1	E	120	VAL	N-CA-C	-6.95	99.81	107.73
1	B	120	VAL	N-CA-C	-6.93	99.83	107.73
1	C	120	VAL	N-CA-C	-6.87	99.90	107.73
1	F	120	VAL	N-CA-C	-6.83	99.95	107.73
1	D	120	VAL	N-CA-C	-6.69	100.11	107.73
1	F	85	HIS	N-CA-C	-6.61	105.18	113.18
1	C	34	THR	N-CA-C	6.49	118.70	110.33
1	B	85	HIS	N-CA-C	-6.45	105.38	113.18
1	D	92	GLY	N-CA-C	6.37	122.36	111.98
1	E	123	GLY	N-CA-C	-6.24	104.21	112.82
1	E	34	THR	N-CA-C	6.24	118.38	110.33
1	E	159	GLY	CA-C-N	6.23	126.42	119.32
1	E	159	GLY	C-N-CA	6.23	126.42	119.32
1	A	287	ASP	CA-C-N	6.22	125.96	119.05
1	A	287	ASP	C-N-CA	6.22	125.96	119.05
1	A	409	LEU	N-CA-C	-6.22	104.41	111.07
1	D	85	HIS	N-CA-C	-6.19	105.69	113.18
1	B	92	GLY	N-CA-C	6.15	122.64	112.30
1	D	123	GLY	N-CA-C	-6.11	103.30	113.02
1	A	123	GLY	N-CA-C	-6.09	103.33	113.02
1	A	85	HIS	N-CA-C	-6.09	105.81	113.18
1	B	287	ASP	CA-C-N	6.06	125.78	119.05
1	B	287	ASP	C-N-CA	6.06	125.78	119.05
1	E	287	ASP	CA-C-N	6.06	125.78	119.05
1	E	287	ASP	C-N-CA	6.06	125.78	119.05
1	C	287	ASP	CA-C-N	6.06	125.78	119.05
1	C	287	ASP	C-N-CA	6.06	125.78	119.05
1	F	287	ASP	CA-C-N	6.04	125.76	119.05
1	F	287	ASP	C-N-CA	6.04	125.76	119.05
1	D	287	ASP	CA-C-N	6.03	125.74	119.05
1	D	287	ASP	C-N-CA	6.03	125.74	119.05
1	C	159	GLY	CA-C-N	6.01	126.17	119.32
1	C	159	GLY	C-N-CA	6.01	126.17	119.32
1	E	92	GLY	N-CA-C	5.98	121.73	111.98
1	E	85	HIS	N-CA-C	-5.96	105.96	113.18
1	B	34	THR	N-CA-C	5.88	117.91	110.33
1	B	123	GLY	N-CA-C	-5.85	103.71	113.02
1	C	92	GLY	N-CA-C	5.84	122.12	112.30
1	C	409	LEU	N-CA-C	-5.81	104.85	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	34	THR	N-CA-C	5.80	117.82	110.33
1	C	123	GLY	N-CA-C	-5.78	104.84	112.82
1	A	92	GLY	N-CA-C	5.76	121.47	112.31
1	F	92	GLY	N-CA-C	5.68	121.83	112.30
1	E	409	LEU	N-CA-C	-5.67	105.00	111.07
1	A	34	THR	N-CA-C	5.66	117.63	110.33
1	B	409	LEU	N-CA-C	-5.63	105.04	111.07
1	F	53	LYS	N-CA-C	5.61	122.20	109.81
1	C	85	HIS	N-CA-C	-5.60	106.41	113.18
1	F	159	GLY	CA-C-N	5.58	125.68	119.32
1	F	159	GLY	C-N-CA	5.58	125.68	119.32
1	B	53	LYS	N-CA-C	5.55	122.07	109.81
1	C	100	SER	N-CA-C	-5.49	100.96	109.14
1	F	187	ILE	CB-CA-C	-5.45	104.91	111.88
1	D	409	LEU	N-CA-C	-5.44	105.25	111.07
1	F	409	LEU	N-CA-C	-5.43	105.26	111.07
1	C	53	LYS	N-CA-C	5.42	121.78	109.81
1	F	123	GLY	N-CA-C	-5.40	104.43	113.02
1	E	40	GLN	CA-C-N	5.39	127.51	120.28
1	E	40	GLN	C-N-CA	5.39	127.51	120.28
1	D	34	THR	N-CA-C	5.37	117.26	110.33
1	C	444	SER	N-CA-C	-5.35	102.24	109.95
1	E	53	LYS	N-CA-C	5.33	121.58	109.81
1	D	53	LYS	N-CA-C	5.32	121.56	109.81
1	B	187	ILE	CB-CA-C	-5.31	105.09	111.88
1	A	53	LYS	N-CA-C	5.30	121.53	109.81
1	B	378	VAL	CB-CA-C	-5.28	103.70	112.26
1	E	100	SER	N-CA-C	-5.28	101.27	109.14
1	D	100	SER	N-CA-C	-5.27	101.28	109.14
1	E	41	LYS	N-CA-C	-5.27	105.53	111.28
1	B	398	THR	N-CA-C	5.24	121.40	114.12
1	F	41	LYS	N-CA-C	-5.22	105.59	111.28
1	A	187	ILE	CB-CA-C	-5.20	105.23	112.04
1	D	433	THR	N-CA-C	-5.19	103.19	110.35
1	C	398	THR	N-CA-C	5.15	121.34	113.61
1	F	100	SER	N-CA-C	-5.15	101.46	109.14
1	F	118	VAL	N-CA-C	5.10	118.67	112.80
1	F	398	THR	N-CA-C	5.10	121.21	114.12
1	A	398	THR	N-CA-C	5.06	121.15	114.12
1	B	294	PHE	N-CA-C	-5.04	105.68	111.07
1	C	40	GLN	CA-C-N	5.04	127.03	120.28
1	C	40	GLN	C-N-CA	5.04	127.03	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	GLY	CA-C-N	5.03	125.06	119.32
1	B	159	GLY	C-N-CA	5.03	125.06	119.32
1	D	40	GLN	CA-C-N	5.03	127.02	120.28
1	D	40	GLN	C-N-CA	5.03	127.02	120.28
1	F	196	ALA	N-CA-C	-5.02	107.00	112.72
1	D	159	GLY	CA-C-N	5.01	125.04	119.32
1	D	159	GLY	C-N-CA	5.01	125.04	119.32

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3866	0	3832	145	1
1	B	3866	0	3832	142	0
1	C	3866	0	3832	146	1
1	D	3866	0	3832	156	0
1	E	3866	0	3832	147	0
1	F	3866	0	3832	155	0
2	A	9	0	5	4	0
2	B	9	0	5	4	0
2	C	9	0	5	5	0
2	D	9	0	5	2	0
2	E	9	0	5	1	0
2	F	9	0	5	4	0
3	A	48	0	26	3	0
3	B	48	0	26	5	0
3	C	48	0	26	7	0
3	D	48	0	26	8	0
3	E	48	0	26	5	0
3	F	48	0	26	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	32	0	12	3	0
4	B	32	0	10	1	0
4	C	32	0	12	0	0
4	D	32	0	11	1	0
4	E	32	0	11	2	0
4	F	32	0	11	2	0
5	A	21	0	4	4	0
5	B	21	0	4	0	0
5	C	42	0	9	4	0
5	D	21	0	4	0	0
5	F	21	0	5	7	0
6	A	34	0	0	5	0
6	B	34	0	0	3	0
6	C	49	0	0	1	0
6	D	45	0	0	5	0
6	E	35	0	0	5	0
6	F	21	0	0	3	0
All	All	24074	0	23271	840	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (840) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:HIS:HD2	1:A:261:ARG:HH11	1.28	0.82
1:B:258:HIS:HD2	1:B:261:ARG:HH11	1.29	0.81
1:F:258:HIS:HD2	1:F:261:ARG:HH11	1.28	0.80
1:B:336:ALA:HB3	1:B:337:PRO:HD3	1.64	0.80
1:E:261:ARG:HD2	4:E:553:GTP:O6	1.82	0.79
1:C:336:ALA:HB3	1:C:337:PRO:HD3	1.62	0.79
1:C:258:HIS:HD2	1:C:261:ARG:HH11	1.29	0.79
1:E:258:HIS:HD2	1:E:261:ARG:HH11	1.30	0.79
3:E:551:NDP:H52N	3:E:551:NDP:H2N	1.65	0.78
1:D:258:HIS:HD2	1:D:261:ARG:HH11	1.31	0.78
1:F:336:ALA:HB3	1:F:337:PRO:HD3	1.66	0.78
1:E:336:ALA:HB3	1:E:337:PRO:HD3	1.65	0.77
1:A:212:ILE:HD12	4:A:553:GTP:O3'	1.84	0.77
1:A:336:ALA:HB3	1:A:337:PRO:HD3	1.66	0.76
1:C:332:THR:H	1:C:335:ASN:HD21	1.33	0.75
1:C:40:GLN:HA	1:C:43:ASN:HD22	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:THR:H	1:B:335:ASN:HD21	1.33	0.74
1:E:221:HIS:HE1	6:E:561:HOH:O	1.70	0.74
1:B:40:GLN:HA	1:B:43:ASN:HD22	1.52	0.74
1:D:336:ALA:HB3	1:D:337:PRO:HD3	1.68	0.74
1:C:118:VAL:HG22	1:C:456:THR:HG22	1.68	0.73
1:E:40:GLN:HA	1:E:43:ASN:HD22	1.53	0.73
1:F:40:GLN:HA	1:F:43:ASN:HD22	1.54	0.73
1:D:332:THR:H	1:D:335:ASN:HD21	1.35	0.73
1:A:40:GLN:HA	1:A:43:ASN:HD22	1.52	0.73
1:F:112:THR:HG22	1:F:124:GLY:HA3	1.69	0.73
1:F:91:GLY:HA3	1:F:125:ALA:O	1.89	0.73
1:E:332:THR:H	1:E:335:ASN:HD21	1.34	0.71
1:D:40:GLN:HA	1:D:43:ASN:HD22	1.54	0.71
1:B:118:VAL:HG22	1:B:456:THR:HG22	1.72	0.71
1:E:118:VAL:HG22	1:E:456:THR:HG22	1.72	0.71
1:B:315:LEU:HD13	1:B:331:LEU:HD12	1.73	0.71
1:F:332:THR:H	1:F:335:ASN:HD21	1.35	0.71
1:A:332:THR:H	1:A:335:ASN:HD21	1.37	0.71
1:D:91:GLY:HA3	1:D:125:ALA:O	1.91	0.70
1:F:7:PRO:HD2	1:F:329:LYS:HD2	1.73	0.70
1:A:118:VAL:HG22	1:A:456:THR:HG22	1.73	0.69
1:C:315:LEU:HD13	1:C:331:LEU:HD12	1.75	0.69
1:D:193:ASN:HB2	6:D:593:HOH:O	1.90	0.69
1:E:315:LEU:HD13	1:E:331:LEU:HD12	1.74	0.69
1:A:82:HIS:CD2	1:A:112:THR:HG21	2.28	0.69
1:A:126:LYS:NZ	2:A:550:GLU:N	2.40	0.68
1:F:209:HIS:HE1	4:F:553:GTP:O1A	1.76	0.68
1:C:91:GLY:HA3	1:C:125:ALA:O	1.92	0.68
1:B:112:THR:HG22	1:B:124:GLY:HA3	1.74	0.68
1:F:82:HIS:CD2	1:F:112:THR:HG21	2.28	0.68
1:B:107:LEU:HB3	1:B:126:LYS:HE3	1.74	0.68
1:C:24:VAL:HG22	1:C:483:VAL:HG22	1.76	0.68
1:D:250:GLN:NE2	1:D:330:GLN:HE21	1.91	0.68
1:C:55:CYS:O	1:F:62:SER:HB3	1.94	0.67
1:D:315:LEU:HD13	1:D:331:LEU:HD12	1.76	0.67
1:D:419:ARG:NH2	6:D:582:HOH:O	2.27	0.67
1:D:436:PHE:HB2	1:E:408:HIS:HB3	1.76	0.67
1:F:315:LEU:HD13	1:F:331:LEU:HD12	1.75	0.67
1:A:250:GLN:NE2	1:A:330:GLN:HE21	1.93	0.67
1:D:82:HIS:CD2	1:D:112:THR:HG21	2.30	0.67
1:E:82:HIS:CD2	1:E:112:THR:HG21	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:GLN:NE2	1:E:330:GLN:HE21	1.92	0.67
1:C:82:HIS:CD2	1:C:112:THR:HG21	2.30	0.67
1:A:91:GLY:HA3	1:A:125:ALA:O	1.96	0.66
1:C:92:GLY:H	2:C:550:GLU:HB3	1.60	0.66
1:F:118:VAL:HG22	1:F:456:THR:HG22	1.77	0.66
1:F:250:GLN:NE2	1:F:330:GLN:HE21	1.91	0.66
1:D:85:HIS:HB2	1:D:492:VAL:HG11	1.78	0.66
1:D:112:THR:HG22	1:D:124:GLY:HA3	1.77	0.66
1:E:211:ARG:HB3	6:E:578:HOH:O	1.95	0.66
1:E:217:ARG:HD3	6:E:561:HOH:O	1.95	0.66
1:D:107:LEU:HB3	1:D:126:LYS:HE3	1.77	0.66
1:A:315:LEU:HD13	1:A:331:LEU:HD12	1.76	0.66
3:B:551:NDP:H52N	3:B:551:NDP:H2N	1.78	0.66
1:B:82:HIS:CD2	1:B:112:THR:HG21	2.31	0.66
1:C:250:GLN:NE2	1:C:330:GLN:HE21	1.95	0.65
1:C:118:VAL:HG22	1:C:456:THR:CG2	2.26	0.65
1:D:496:ALA:HB3	1:E:177:SER:OG	1.96	0.65
1:E:107:LEU:HB3	1:E:126:LYS:HE3	1.78	0.65
1:A:112:THR:HG22	1:A:124:GLY:HA3	1.77	0.65
1:D:118:VAL:HG22	1:D:456:THR:HG22	1.78	0.65
4:D:553:GTP:O1A	4:D:553:GTP:O1B	2.14	0.65
1:C:112:THR:HG22	1:C:124:GLY:HA3	1.79	0.65
1:D:255:VAL:HG11	3:D:551:NDP:O4D	1.97	0.65
1:D:95:TYR:OH	1:D:145:THR:HB	1.97	0.64
1:D:96:SER:O	1:D:130:LYS:HA	1.97	0.64
1:F:107:LEU:HB3	1:F:126:LYS:HE3	1.80	0.64
1:A:217:ARG:HD3	6:A:557:HOH:O	1.96	0.64
1:E:215:THR:OG1	3:E:551:NDP:H42N	1.97	0.64
1:F:414:GLN:HG3	1:F:428:ILE:O	1.97	0.64
1:A:7:PRO:HD2	1:A:329:LYS:HD2	1.80	0.64
1:B:250:GLN:NE2	1:B:330:GLN:HE21	1.96	0.64
1:F:95:TYR:OH	1:F:145:THR:HB	1.97	0.64
1:F:99:VAL:HA	1:F:103:GLU:OE1	1.98	0.64
1:A:107:LEU:HB3	1:A:126:LYS:HE3	1.78	0.64
1:C:99:VAL:HA	1:C:103:GLU:OE1	1.98	0.63
1:C:107:LEU:HB3	1:C:126:LYS:HE3	1.79	0.63
1:E:91:GLY:HA3	1:E:125:ALA:O	1.97	0.63
1:B:91:GLY:HA3	1:B:125:ALA:O	1.99	0.63
1:B:322:LEU:HB3	1:B:344:ILE:HD13	1.80	0.63
1:D:219:VAL:HG13	1:D:373:LEU:HD11	1.81	0.63
1:E:95:TYR:OH	1:E:145:THR:HB	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:SER:HB3	1:F:55:CYS:O	1.99	0.62
1:C:95:TYR:OH	1:C:145:THR:HB	1.99	0.62
1:C:414:GLN:HG3	1:C:428:ILE:O	1.99	0.62
1:A:414:GLN:HG3	1:A:428:ILE:O	1.98	0.62
1:F:24:VAL:HG22	1:F:483:VAL:HG22	1.81	0.62
1:F:169:MET:HG2	3:F:551:NDP:O1N	1.98	0.62
1:A:35:ARG:HH11	1:A:35:ARG:HA	1.64	0.62
1:A:95:TYR:OH	1:A:145:THR:HB	1.99	0.62
1:C:322:LEU:HB3	1:C:344:ILE:HD13	1.82	0.62
1:E:219:VAL:HG13	1:E:373:LEU:HD11	1.82	0.62
1:E:137:THR:OG1	1:E:140:GLU:HG3	1.99	0.62
1:E:322:LEU:HB3	1:E:344:ILE:HD13	1.82	0.62
1:A:99:VAL:HA	1:A:103:GLU:OE1	1.99	0.62
1:D:322:LEU:HB3	1:D:344:ILE:HD13	1.82	0.62
1:E:112:THR:HG22	1:E:124:GLY:HA3	1.79	0.62
1:A:322:LEU:HB3	1:A:344:ILE:HD13	1.81	0.62
1:B:35:ARG:HA	1:B:35:ARG:HH11	1.65	0.61
1:D:99:VAL:HA	1:D:103:GLU:OE1	1.99	0.61
3:A:551:NDP:H52N	3:A:551:NDP:H2N	1.82	0.61
1:F:258:HIS:CD2	1:F:261:ARG:HH11	2.16	0.61
1:C:169:MET:HG2	3:C:551:NDP:O1N	1.99	0.61
1:E:35:ARG:HA	1:E:35:ARG:HH11	1.65	0.61
1:A:126:LYS:HZ3	2:A:550:GLU:N	1.99	0.61
1:A:40:GLN:HA	1:A:43:ASN:ND2	2.15	0.61
1:A:219:VAL:HG13	1:A:373:LEU:HD11	1.81	0.61
1:A:85:HIS:HB2	1:A:492:VAL:HG11	1.83	0.61
1:A:96:SER:O	1:A:130:LYS:HA	2.01	0.61
1:E:99:VAL:HA	1:E:103:GLU:OE1	2.00	0.61
1:C:40:GLN:HA	1:C:43:ASN:ND2	2.16	0.61
1:C:258:HIS:CD2	1:C:261:ARG:HH11	2.16	0.60
1:B:414:GLN:HG3	1:B:428:ILE:O	2.01	0.60
1:B:95:TYR:OH	1:B:145:THR:HB	2.01	0.60
1:D:40:GLN:HA	1:D:43:ASN:ND2	2.16	0.60
1:F:322:LEU:HB3	1:F:344:ILE:HD13	1.81	0.60
1:B:96:SER:O	1:B:130:LYS:HA	2.02	0.60
1:B:40:GLN:HA	1:B:43:ASN:ND2	2.16	0.60
1:D:35:ARG:HA	1:D:35:ARG:HH11	1.66	0.60
1:D:444:SER:H	1:D:447:ASP:HB2	1.66	0.60
1:E:93:ILE:HG12	1:E:127:ALA:HB3	1.84	0.60
1:B:419:ARG:HH12	1:F:431:VAL:HG12	1.67	0.60
1:A:137:THR:OG1	1:A:140:GLU:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ARG:HH11	1:C:35:ARG:HA	1.67	0.60
1:C:96:SER:O	1:C:130:LYS:HA	2.02	0.60
1:E:96:SER:O	1:E:130:LYS:HA	2.02	0.59
1:A:258:HIS:CD2	1:A:261:ARG:HH11	2.16	0.59
1:A:41:LYS:O	1:A:45:VAL:HG23	2.02	0.59
1:A:335:ASN:N	1:A:335:ASN:HD22	2.01	0.59
1:C:27:LYS:HD3	1:C:487:GLU:OE2	2.02	0.59
1:F:35:ARG:HH11	1:F:35:ARG:HA	1.65	0.59
1:B:118:VAL:HG22	1:B:456:THR:CG2	2.33	0.59
3:F:551:NDP:H2N	3:F:551:NDP:H52N	1.83	0.59
1:B:99:VAL:HA	1:B:103:GLU:OE1	2.02	0.59
1:C:41:LYS:O	1:C:45:VAL:HG23	2.02	0.59
1:D:435:GLU:HB3	1:E:408:HIS:CE1	2.38	0.59
1:D:482:TYR:O	1:D:486:ILE:HG13	2.02	0.59
1:F:40:GLN:HA	1:F:43:ASN:ND2	2.16	0.59
1:F:187:ILE:HG23	5:F:552:H3P:CAK	2.33	0.59
1:C:333:LYS:HD2	1:C:355:GLU:OE1	2.03	0.59
1:D:41:LYS:O	1:D:45:VAL:HG23	2.02	0.59
1:C:150:MET:HE1	5:C:554:H3P:CLAC	2.40	0.58
1:D:93:ILE:HG12	1:D:127:ALA:HB3	1.84	0.58
1:C:93:ILE:HG12	1:C:127:ALA:HB3	1.85	0.58
1:D:137:THR:OG1	1:D:140:GLU:HG3	2.02	0.58
1:E:41:LYS:O	1:E:45:VAL:HG23	2.02	0.58
1:B:112:THR:HB	1:B:124:GLY:H	1.68	0.58
1:E:414:GLN:HG3	1:E:428:ILE:O	2.03	0.58
1:E:258:HIS:CD2	1:E:261:ARG:HH11	2.18	0.58
1:F:41:LYS:O	1:F:45:VAL:HG23	2.03	0.58
1:F:335:ASN:HD22	1:F:335:ASN:N	2.01	0.58
1:C:137:THR:OG1	1:C:140:GLU:HG3	2.03	0.58
1:C:219:VAL:HG13	1:C:373:LEU:HD11	1.85	0.58
1:F:112:THR:HB	1:F:124:GLY:H	1.69	0.58
1:B:219:VAL:HG13	1:B:373:LEU:HD11	1.84	0.58
1:C:478:ARG:HH11	1:C:478:ARG:HG3	1.68	0.58
1:D:459:ARG:O	1:D:463:GLN:HG3	2.03	0.58
1:E:482:TYR:O	1:E:486:ILE:HG13	2.04	0.58
1:B:229:GLU:O	1:B:230:ALA:HB3	2.03	0.58
1:F:219:VAL:HG13	1:F:373:LEU:HD11	1.85	0.58
1:B:335:ASN:N	1:B:335:ASN:HD22	2.02	0.57
1:C:392:VAL:HG13	1:E:386:LEU:HD21	1.84	0.57
1:B:258:HIS:CD2	1:B:261:ARG:HH11	2.16	0.57
1:B:482:TYR:O	1:B:486:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:GLN:HG3	1:D:428:ILE:O	2.03	0.57
1:E:335:ASN:N	1:E:335:ASN:HD22	2.02	0.57
1:F:229:GLU:O	1:F:230:ALA:HB3	2.05	0.57
1:B:93:ILE:HG12	1:B:127:ALA:HB3	1.86	0.57
1:E:478:ARG:HG3	1:E:478:ARG:HH11	1.69	0.57
1:F:133:PRO:HG2	1:F:170:SER:HB3	1.87	0.57
1:B:253:GLY:HA3	3:B:551:NDP:O1A	2.05	0.57
1:C:211:ARG:HH22	3:C:551:NDP:H72N	1.50	0.57
1:E:40:GLN:HA	1:E:43:ASN:ND2	2.17	0.57
1:E:459:ARG:O	1:E:463:GLN:HG3	2.04	0.57
1:C:335:ASN:N	1:C:335:ASN:HD22	2.03	0.57
1:C:7:PRO:HD2	1:C:329:LYS:HD2	1.85	0.57
1:F:96:SER:O	1:F:130:LYS:HA	2.04	0.57
1:B:154:LYS:HD3	1:C:185:SER:O	2.04	0.56
1:B:211:ARG:HH22	3:B:551:NDP:H71N	1.53	0.56
1:A:93:ILE:HG12	1:A:127:ALA:HB3	1.86	0.56
1:C:12:MET:HG3	1:C:354:PRO:HD3	1.87	0.56
1:D:133:PRO:HG2	1:D:170:SER:HB3	1.88	0.56
1:A:333:LYS:HD2	1:A:355:GLU:OE1	2.06	0.56
1:C:205:GLN:NE2	1:E:496:ALA:HB2	2.21	0.56
1:D:258:HIS:CD2	1:D:261:ARG:HH11	2.18	0.56
1:E:209:HIS:CD2	1:E:446:LYS:HG3	2.41	0.56
1:E:333:LYS:HD2	1:E:355:GLU:OE1	2.05	0.56
1:F:478:ARG:HG3	1:F:478:ARG:HH11	1.69	0.56
1:E:25:GLU:O	1:E:29:VAL:HG23	2.06	0.56
1:F:137:THR:OG1	1:F:140:GLU:HG3	2.05	0.56
1:A:25:GLU:O	1:A:29:VAL:HG23	2.05	0.56
1:A:118:VAL:HG22	1:A:456:THR:CG2	2.36	0.56
1:C:436:PHE:HB2	1:D:408:HIS:HB3	1.88	0.56
1:F:333:LYS:HD2	1:F:355:GLU:OE1	2.06	0.56
1:A:482:TYR:O	1:A:486:ILE:HG13	2.06	0.55
1:A:478:ARG:HG3	1:A:478:ARG:HH11	1.70	0.55
1:B:459:ARG:O	1:B:463:GLN:HG3	2.05	0.55
1:C:112:THR:HB	1:C:124:GLY:H	1.72	0.55
1:B:55:CYS:O	1:E:62:SER:HB3	2.07	0.55
1:D:335:ASN:N	1:D:335:ASN:HD22	2.02	0.55
1:F:187:ILE:HG23	5:F:552:H3P:HAKA	1.89	0.55
1:B:41:LYS:O	1:B:45:VAL:HG23	2.06	0.55
1:E:229:GLU:O	1:E:230:ALA:HB3	2.07	0.55
1:F:482:TYR:O	1:F:486:ILE:HG13	2.07	0.55
1:D:110:LEU:O	1:D:114:LYS:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:MET:HE1	5:F:552:H3P:CLAC	2.43	0.55
1:F:93:ILE:HG12	1:F:127:ALA:HB3	1.87	0.55
1:A:229:GLU:O	1:A:230:ALA:HB3	2.07	0.54
1:B:245:LYS:HA	1:B:320:ASP:OD1	2.07	0.54
1:D:303:GLY:H	1:D:309:ILE:HD11	1.72	0.54
1:F:25:GLU:O	1:F:29:VAL:HG23	2.07	0.54
1:C:459:ARG:O	1:C:463:GLN:HG3	2.06	0.54
1:A:169:MET:HA	3:A:551:NDP:O1N	2.06	0.54
1:C:133:PRO:HG2	1:C:170:SER:HB3	1.90	0.54
1:D:25:GLU:O	1:D:29:VAL:HG23	2.08	0.54
1:D:333:LYS:HD2	1:D:355:GLU:OE1	2.08	0.54
1:D:229:GLU:O	1:D:230:ALA:HB3	2.08	0.54
1:E:118:VAL:HG22	1:E:456:THR:CG2	2.38	0.54
1:A:245:LYS:HA	1:A:320:ASP:OD1	2.08	0.54
1:A:257:LEU:HD21	4:A:553:GTP:HN21	1.72	0.54
1:E:19:ARG:O	1:E:23:ILE:HG12	2.07	0.54
1:A:62:SER:HB3	1:D:55:CYS:O	2.07	0.53
1:B:25:GLU:O	1:B:29:VAL:HG23	2.08	0.53
1:B:133:PRO:HG2	1:B:170:SER:HB3	1.90	0.53
1:D:411:MET:HA	6:D:587:HOH:O	2.07	0.53
1:F:459:ARG:O	1:F:463:GLN:HG3	2.08	0.53
1:C:431:VAL:HG12	1:D:419:ARG:HH12	1.74	0.53
1:D:478:ARG:HG3	1:D:478:ARG:HH11	1.72	0.53
1:E:303:GLY:H	1:E:309:ILE:HD11	1.73	0.53
1:A:459:ARG:O	1:A:463:GLN:HG3	2.07	0.53
1:E:473:LEU:HD22	1:E:479:THR:HB	1.90	0.53
1:F:19:ARG:O	1:F:23:ILE:HG12	2.08	0.53
1:F:354:PRO:O	1:F:357:ASP:HB2	2.09	0.53
1:A:112:THR:HB	1:A:124:GLY:H	1.74	0.53
1:B:303:GLY:H	1:B:309:ILE:HD11	1.73	0.53
1:A:368:ILE:HG22	1:A:373:LEU:HB2	1.91	0.53
1:B:88:PRO:HB3	1:B:161:GLY:C	2.34	0.53
1:C:497:GLY:HA3	1:D:178:TRP:HD1	1.74	0.53
1:F:187:ILE:HA	5:F:552:H3P:CAK	2.39	0.53
1:C:473:LEU:HD22	1:C:479:THR:HB	1.91	0.53
1:A:55:CYS:O	1:D:62:SER:HB3	2.09	0.53
1:A:303:GLY:H	1:A:309:ILE:HD11	1.73	0.53
1:C:47:GLY:O	1:C:51:ILE:HG13	2.09	0.53
1:C:229:GLU:O	1:C:230:ALA:HB3	2.07	0.53
1:E:133:PRO:HG2	1:E:170:SER:HB3	1.89	0.53
1:E:245:LYS:HA	1:E:320:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PRO:HG2	1:A:170:SER:HB3	1.89	0.53
1:E:110:LEU:O	1:E:114:LYS:HB2	2.08	0.53
1:A:110:LEU:O	1:A:114:LYS:HB2	2.09	0.53
1:B:137:THR:OG1	1:B:140:GLU:HG3	2.08	0.53
1:E:248:ALA:HB1	1:E:272:ALA:HB3	1.91	0.53
1:B:110:LEU:O	1:B:114:LYS:HB2	2.10	0.52
1:B:67:ARG:HD2	1:B:140:GLU:OE2	2.09	0.52
1:C:110:LEU:O	1:C:114:LYS:HB2	2.08	0.52
1:F:316:GLU:O	1:F:340:LYS:HE2	2.09	0.52
1:F:368:ILE:HG22	1:F:373:LEU:HB2	1.91	0.52
1:A:113:TYR:O	1:A:117:VAL:HG23	2.08	0.52
1:C:19:ARG:O	1:C:23:ILE:HG12	2.09	0.52
1:D:118:VAL:HG22	1:D:456:THR:CG2	2.39	0.52
1:D:154:LYS:HD3	1:F:185:SER:O	2.09	0.52
1:C:245:LYS:HA	1:C:320:ASP:OD1	2.09	0.52
1:C:482:TYR:O	1:C:486:ILE:HG13	2.10	0.52
1:B:478:ARG:HG3	1:B:478:ARG:HH11	1.73	0.52
1:C:113:TYR:O	1:C:117:VAL:HG23	2.10	0.52
1:C:303:GLY:H	1:C:309:ILE:HD11	1.75	0.52
1:E:368:ILE:HG22	1:E:373:LEU:HB2	1.91	0.52
1:B:473:LEU:HD22	1:B:479:THR:HB	1.91	0.52
1:C:25:GLU:O	1:C:29:VAL:HG23	2.09	0.52
1:D:410:LEU:O	1:D:413:VAL:HG22	2.10	0.52
1:F:67:ARG:HD2	1:F:140:GLU:OE2	2.10	0.52
1:F:245:LYS:HA	1:F:320:ASP:OD1	2.09	0.52
1:A:92:GLY:H	2:A:550:GLU:N	2.08	0.52
1:C:248:ALA:HB1	1:C:272:ALA:HB3	1.91	0.52
1:C:369:PRO:HB2	1:C:371:LEU:HD23	1.92	0.52
1:D:113:TYR:O	1:D:117:VAL:HG23	2.10	0.52
1:D:245:LYS:HA	1:D:320:ASP:OD1	2.10	0.52
1:E:113:TYR:O	1:E:117:VAL:HG23	2.09	0.52
1:A:209:HIS:CD2	1:A:446:LYS:HG3	2.45	0.52
1:B:315:LEU:HD13	1:B:331:LEU:CD1	2.40	0.52
1:F:88:PRO:HB3	1:F:161:GLY:C	2.35	0.52
1:A:190:TYR:CD1	5:A:552:H3P:CLAE	3.00	0.51
1:A:289:LYS:HA	6:A:581:HOH:O	2.10	0.51
1:C:413:VAL:HG23	1:C:430:ILE:HG13	1.92	0.51
1:D:103:GLU:HG2	1:D:107:LEU:CD2	2.40	0.51
1:F:8:ASN:HD22	1:F:9:PHE:N	2.08	0.51
1:D:473:LEU:HD22	1:D:479:THR:HB	1.93	0.51
1:E:315:LEU:HD13	1:E:331:LEU:CD1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:LYS:NZ	2:F:550:GLU:O	2.43	0.51
1:F:255:VAL:HG11	3:F:551:NDP:O4D	2.10	0.51
1:A:431:VAL:HG12	1:F:419:ARG:HH12	1.76	0.51
1:B:333:LYS:HD2	1:B:355:GLU:OE1	2.09	0.51
1:D:26:ASP:O	1:D:30:GLU:HG3	2.11	0.51
1:D:85:HIS:HD2	1:D:492:VAL:HG21	1.74	0.51
1:F:118:VAL:HG22	1:F:456:THR:CG2	2.40	0.51
1:B:408:HIS:HB3	1:F:436:PHE:HB2	1.92	0.51
1:A:408:HIS:HB3	1:B:436:PHE:HB2	1.92	0.51
1:F:113:TYR:O	1:F:117:VAL:HG23	2.11	0.51
1:C:354:PRO:O	1:C:357:ASP:HB2	2.09	0.51
1:D:112:THR:HB	1:D:124:GLY:H	1.75	0.51
1:D:368:ILE:HG22	1:D:373:LEU:HB2	1.92	0.51
1:F:110:LEU:O	1:F:114:LYS:HB2	2.10	0.51
1:D:19:ARG:O	1:D:23:ILE:HG12	2.11	0.51
1:F:26:ASP:O	1:F:30:GLU:HG3	2.11	0.51
1:F:215:THR:OG1	3:F:551:NDP:H42N	2.11	0.51
1:A:19:ARG:O	1:A:23:ILE:HG12	2.11	0.51
1:A:79:ARG:HD3	1:A:127:ALA:HB2	1.93	0.51
1:A:473:LEU:HB3	1:A:476:ASP:HB3	1.93	0.51
1:C:88:PRO:HB3	1:C:161:GLY:C	2.36	0.51
1:C:368:ILE:HG22	1:C:373:LEU:HB2	1.92	0.51
1:D:354:PRO:O	1:D:357:ASP:HB2	2.11	0.51
1:B:19:ARG:O	1:B:23:ILE:HG12	2.11	0.51
1:C:409:LEU:HD22	1:D:409:LEU:HD21	1.93	0.51
1:D:378:VAL:HA	1:D:381:SER:HB2	1.93	0.51
1:A:419:ARG:HH12	1:B:431:VAL:HG12	1.75	0.51
1:B:126:LYS:NZ	2:B:550:GLU:N	2.59	0.50
1:B:190:TYR:HE2	1:F:162:VAL:HG11	1.75	0.50
1:D:316:GLU:O	1:D:340:LYS:HE2	2.10	0.50
1:D:413:VAL:HG23	1:D:430:ILE:HG13	1.93	0.50
1:A:185:SER:O	1:E:154:LYS:HD3	2.11	0.50
1:B:62:SER:HB3	1:E:55:CYS:O	2.10	0.50
1:B:316:GLU:O	1:B:340:LYS:HE2	2.10	0.50
1:A:410:LEU:O	1:A:413:VAL:HG22	2.12	0.50
1:B:103:GLU:HG2	1:B:107:LEU:CD2	2.42	0.50
1:A:88:PRO:HB3	1:A:161:GLY:C	2.36	0.50
1:A:232:TYR:OH	1:A:469:MET:HE3	2.11	0.50
1:C:26:ASP:O	1:C:30:GLU:HG3	2.11	0.50
1:E:378:VAL:HA	1:E:381:SER:HB2	1.94	0.50
1:E:413:VAL:HG23	1:E:430:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:ASP:OD2	1:F:353:THR:HG21	2.12	0.50
1:C:169:MET:HA	3:C:551:NDP:O1N	2.11	0.50
1:D:67:ARG:HD2	1:D:140:GLU:OE2	2.11	0.50
1:F:378:VAL:HA	1:F:381:SER:HB2	1.94	0.50
1:A:473:LEU:HD22	1:A:479:THR:HB	1.93	0.50
1:D:369:PRO:HB2	1:D:371:LEU:HD23	1.94	0.50
1:B:369:PRO:HB2	1:B:371:LEU:HD23	1.93	0.50
1:D:211:ARG:HH22	3:D:551:NDP:H71N	1.59	0.50
1:E:89:CYS:HB3	1:E:125:ALA:HB2	1.94	0.50
1:E:316:GLU:O	1:E:340:LYS:HE2	2.12	0.50
1:A:316:GLU:O	1:A:340:LYS:HE2	2.11	0.49
1:B:212:ILE:HG13	6:B:564:HOH:O	2.12	0.49
1:C:103:GLU:HG2	1:C:107:LEU:CD2	2.41	0.49
1:E:88:PRO:HB3	1:E:161:GLY:C	2.37	0.49
1:F:378:VAL:HG13	2:F:550:GLU:OE2	2.12	0.49
1:D:183:TYR:CD1	1:D:187:ILE:HD13	2.47	0.49
1:E:354:PRO:O	1:E:357:ASP:HB2	2.12	0.49
1:F:103:GLU:HG2	1:F:107:LEU:CD2	2.42	0.49
1:F:187:ILE:HA	5:F:552:H3P:CAT	2.42	0.49
1:F:303:GLY:H	1:F:309:ILE:HD11	1.76	0.49
1:A:154:LYS:HD3	1:E:185:SER:O	2.13	0.49
1:A:315:LEU:HD13	1:A:331:LEU:CD1	2.43	0.49
1:B:354:PRO:O	1:B:357:ASP:HB2	2.11	0.49
1:C:230:ALA:HA	1:C:233:MET:HB2	1.94	0.49
1:F:369:PRO:HB2	1:F:371:LEU:HD23	1.94	0.49
1:A:413:VAL:HG23	1:A:430:ILE:HG13	1.93	0.49
1:E:26:ASP:O	1:E:30:GLU:HG3	2.12	0.49
1:E:112:THR:HB	1:E:124:GLY:H	1.76	0.49
1:A:26:ASP:O	1:A:30:GLU:HG3	2.13	0.49
1:B:368:ILE:HG22	1:B:373:LEU:HB2	1.94	0.49
1:C:321:ILE:HG12	1:C:343:ILE:HB	1.94	0.49
1:C:410:LEU:O	1:C:413:VAL:HG22	2.13	0.49
1:F:315:LEU:HD13	1:F:331:LEU:CD1	2.43	0.49
1:A:321:ILE:HG12	1:A:343:ILE:HB	1.93	0.49
1:C:497:GLY:HA3	1:D:178:TRP:CD1	2.48	0.49
1:A:7:PRO:HD2	1:A:329:LYS:CD	2.43	0.49
1:A:230:ALA:HA	1:A:233:MET:HB2	1.95	0.49
1:C:417:LEU:CD1	1:D:417:LEU:HD21	2.43	0.49
1:D:88:PRO:HB3	1:D:161:GLY:C	2.37	0.49
1:E:230:ALA:HA	1:E:233:MET:HB2	1.94	0.49
1:E:321:ILE:HG12	1:E:343:ILE:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:LEU:HD13	1:C:331:LEU:CD1	2.41	0.49
1:C:408:HIS:HB3	1:E:436:PHE:HB2	1.94	0.49
1:D:321:ILE:HG12	1:D:343:ILE:HB	1.94	0.49
1:F:183:TYR:CD1	1:F:187:ILE:HD13	2.48	0.49
1:B:410:LEU:O	1:B:413:VAL:HG22	2.13	0.49
1:F:89:CYS:HB3	1:F:125:ALA:HB2	1.94	0.49
1:B:113:TYR:O	1:B:117:VAL:HG23	2.12	0.49
1:C:24:VAL:O	1:C:25:GLU:C	2.56	0.49
1:C:183:TYR:CD1	1:C:187:ILE:HD13	2.48	0.48
2:C:550:GLU:HA	3:C:551:NDP:H41N	1.94	0.48
1:D:465:MET:O	1:D:469:MET:HG2	2.13	0.48
1:F:107:LEU:CB	1:F:126:LYS:HG2	2.42	0.48
1:F:321:ILE:HG12	1:F:343:ILE:HB	1.94	0.48
1:F:473:LEU:HD22	1:F:479:THR:HB	1.95	0.48
1:B:230:ALA:HA	1:B:233:MET:HB2	1.96	0.48
1:C:162:VAL:HG11	1:D:190:TYR:HE2	1.77	0.48
1:D:248:ALA:HB1	1:D:272:ALA:HB3	1.94	0.48
1:B:321:ILE:HG12	1:B:343:ILE:HB	1.95	0.48
1:E:79:ARG:HD3	1:E:127:ALA:HB2	1.96	0.48
1:F:114:LYS:NZ	1:F:349:ASN:HD21	2.11	0.48
1:B:209:HIS:HE1	4:B:553:GTP:O1A	1.97	0.48
1:F:473:LEU:HB3	1:F:476:ASP:HB3	1.95	0.48
1:E:473:LEU:HB3	1:E:476:ASP:HB3	1.94	0.48
1:A:248:ALA:HB1	1:A:272:ALA:HB3	1.95	0.48
1:B:26:ASP:O	1:B:30:GLU:HG3	2.13	0.48
1:C:209:HIS:CD2	1:C:446:LYS:HG3	2.48	0.48
1:D:185:SER:O	1:F:154:LYS:HD3	2.14	0.48
1:E:94:ARG:HB2	1:E:168:ASP:OD2	2.13	0.48
1:F:413:VAL:HG23	1:F:430:ILE:HG13	1.96	0.48
1:A:354:PRO:O	1:A:357:ASP:HB2	2.13	0.48
1:B:24:VAL:O	1:B:25:GLU:C	2.56	0.48
1:C:94:ARG:HB2	1:C:168:ASP:OD2	2.14	0.48
1:B:79:ARG:HD3	1:B:127:ALA:HB2	1.95	0.48
1:D:89:CYS:HB3	1:D:125:ALA:HB2	1.95	0.48
1:D:150:MET:CE	1:F:186:THR:HG22	2.44	0.48
1:B:209:HIS:CD2	1:B:446:LYS:HG3	2.49	0.48
1:A:369:PRO:HB2	1:A:371:LEU:HD23	1.95	0.48
1:E:24:VAL:O	1:E:25:GLU:C	2.56	0.48
1:A:47:GLY:O	1:A:51:ILE:HG13	2.14	0.47
1:B:47:GLY:O	1:B:51:ILE:HG13	2.13	0.47
1:B:413:VAL:HG23	1:B:430:ILE:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:TYR:CD1	1:E:187:ILE:HD13	2.49	0.47
1:F:114:LYS:HZ1	1:F:349:ASN:HD21	1.61	0.47
1:A:23:ILE:HG22	1:A:471:TYR:CD2	2.49	0.47
1:A:150:MET:HE1	6:A:560:HOH:O	2.13	0.47
2:C:550:GLU:O	2:C:550:GLU:HG3	2.14	0.47
1:A:24:VAL:O	1:A:25:GLU:C	2.57	0.47
1:A:67:ARG:HD2	1:A:140:GLU:OE2	2.14	0.47
1:B:221:HIS:HE1	6:B:565:HOH:O	1.96	0.47
1:B:248:ALA:HB1	1:B:272:ALA:HB3	1.97	0.47
1:B:392:VAL:HG13	1:F:382:TYR:OH	2.14	0.47
1:D:47:GLY:O	1:D:51:ILE:HG13	2.15	0.47
1:E:103:GLU:HG2	1:E:107:LEU:CD2	2.44	0.47
1:F:248:ALA:HB1	1:F:272:ALA:HB3	1.96	0.47
1:B:419:ARG:HH12	1:F:431:VAL:CG1	2.28	0.47
1:E:410:LEU:O	1:E:413:VAL:HG22	2.14	0.47
1:F:253:GLY:HA3	3:F:551:NDP:O1A	2.14	0.47
1:F:209:HIS:CE1	4:F:553:GTP:O1A	2.64	0.47
1:D:92:GLY:HA3	2:D:550:GLU:N	2.30	0.47
1:E:369:PRO:HB2	1:E:371:LEU:HD23	1.97	0.47
1:C:132:ASN:C	1:C:132:ASN:HD22	2.22	0.47
1:C:378:VAL:HA	1:C:381:SER:HB2	1.96	0.47
1:D:230:ALA:HA	1:D:233:MET:HB2	1.96	0.47
1:D:315:LEU:HD13	1:D:331:LEU:CD1	2.43	0.47
1:E:107:LEU:CB	1:E:126:LYS:HG2	2.45	0.47
1:E:265:ARG:NH1	4:E:553:GTP:O3G	2.46	0.47
1:E:317:VAL:HG22	1:E:318:ASP:N	2.30	0.47
1:B:89:CYS:HB3	1:B:125:ALA:HB2	1.97	0.47
1:F:250:GLN:NE2	1:F:330:GLN:NE2	2.63	0.47
1:A:260:MET:HE3	1:A:270:CYS:SG	2.55	0.47
1:B:126:LYS:HZ3	2:B:550:GLU:N	2.12	0.47
1:D:24:VAL:O	1:D:25:GLU:C	2.58	0.47
1:E:169:MET:HG2	3:E:551:NDP:O1N	2.15	0.47
1:F:334:SER:O	1:F:337:PRO:HD2	2.15	0.47
5:C:552:H3P:HAI	6:F:572:HOH:O	2.14	0.46
1:E:38:GLU:O	1:E:40:GLN:N	2.47	0.46
1:A:378:VAL:HA	1:A:381:SER:HB2	1.96	0.46
1:E:47:GLY:O	1:E:51:ILE:HG13	2.16	0.46
1:A:382:TYR:OH	1:F:392:VAL:HG13	2.16	0.46
1:B:183:TYR:CD1	1:B:187:ILE:HD13	2.50	0.46
1:A:183:TYR:CD1	1:A:187:ILE:HD13	2.50	0.46
1:C:162:VAL:HG22	1:D:190:TYR:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ARG:HD3	1:D:127:ALA:HB2	1.98	0.46
1:D:83:SER:O	1:D:84:GLN:HG3	2.15	0.46
1:E:346:GLU:OE1	1:E:352:THR:HG23	2.16	0.46
1:F:378:VAL:HG22	6:F:555:HOH:O	2.15	0.46
1:B:378:VAL:HA	1:B:381:SER:HB2	1.96	0.46
1:C:473:LEU:HB3	1:C:476:ASP:HB3	1.97	0.46
1:B:226:PHE:O	1:B:233:MET:HE3	2.15	0.46
1:B:483:VAL:O	1:B:487:GLU:HB2	2.16	0.46
1:C:67:ARG:HD2	1:C:140:GLU:OE2	2.15	0.46
1:E:169:MET:HA	3:E:551:NDP:O1N	2.15	0.46
1:A:107:LEU:CB	1:A:126:LYS:HG2	2.45	0.46
1:A:187:ILE:HG23	5:A:552:H3P:HAKA	1.98	0.46
1:D:169:MET:HG2	3:D:551:NDP:O1N	2.15	0.46
1:F:410:LEU:O	1:F:413:VAL:HG22	2.16	0.46
1:A:258:HIS:CD2	1:A:261:ARG:HD3	2.51	0.46
1:C:346:GLU:OE1	1:C:352:THR:HG23	2.15	0.46
1:E:67:ARG:HD2	1:E:140:GLU:OE2	2.16	0.46
1:B:94:ARG:HB2	1:B:168:ASP:OD2	2.16	0.46
1:B:187:ILE:HG23	5:C:554:H3P:HAKA	1.97	0.46
1:B:346:GLU:OE1	1:B:352:THR:HG23	2.15	0.46
1:D:132:ASN:C	1:D:132:ASN:HD22	2.24	0.46
1:E:232:TYR:OH	1:E:469:MET:HE3	2.16	0.46
1:A:89:CYS:HB3	1:A:125:ALA:HB2	1.97	0.45
1:A:132:ASN:HD22	1:A:132:ASN:C	2.22	0.45
1:C:316:GLU:O	1:C:340:LYS:HE2	2.15	0.45
1:C:409:LEU:HD13	1:D:409:LEU:HD11	1.97	0.45
1:A:335:ASN:N	1:A:335:ASN:ND2	2.64	0.45
1:A:417:LEU:CD1	1:F:417:LEU:HD21	2.46	0.45
1:C:238:MET:HE1	1:C:320:ASP:HB3	1.98	0.45
1:C:465:MET:O	1:C:469:MET:HG2	2.16	0.45
1:D:78:TYR:CE2	1:D:101:VAL:HG22	2.52	0.45
1:C:255:VAL:HG11	3:C:551:NDP:O4D	2.16	0.45
1:E:24:VAL:HG22	1:E:483:VAL:HG22	1.99	0.45
1:E:209:HIS:NE2	1:E:446:LYS:HG3	2.31	0.45
1:A:103:GLU:HG2	1:A:107:LEU:CD2	2.46	0.45
1:B:444:SER:H	1:B:447:ASP:HB2	1.82	0.45
1:B:473:LEU:HB3	1:B:476:ASP:HB3	1.98	0.45
1:C:118:VAL:O	1:C:118:VAL:HG13	2.16	0.45
1:C:287:ASP:HA	1:C:288:PRO:HD3	1.78	0.45
1:E:23:ILE:HG22	1:E:471:TYR:CD2	2.52	0.45
1:F:7:PRO:HD2	1:F:329:LYS:CD	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:ALA:HA	1:F:233:MET:HB2	1.99	0.45
1:F:258:HIS:CD2	1:F:261:ARG:HD3	2.52	0.45
1:A:229:GLU:C	1:A:231:SER:H	2.24	0.45
1:A:483:VAL:O	1:A:487:GLU:HB2	2.17	0.45
1:B:349:ASN:CG	3:B:551:NDP:O2D	2.60	0.45
1:D:346:GLU:OE1	1:D:352:THR:HG23	2.17	0.45
1:F:94:ARG:HB2	1:F:168:ASP:OD2	2.16	0.45
1:A:38:GLU:O	1:A:40:GLN:N	2.49	0.45
1:C:79:ARG:HD3	1:C:127:ALA:HB2	1.99	0.45
1:E:132:ASN:C	1:E:132:ASN:HD22	2.25	0.45
1:F:483:VAL:O	1:F:487:GLU:HB2	2.16	0.45
1:A:364:ASN:HD22	1:A:364:ASN:HA	1.48	0.45
1:D:229:GLU:C	1:D:231:SER:H	2.25	0.45
1:E:260:MET:HE3	1:E:270:CYS:SG	2.57	0.45
1:E:281:TRP:CB	1:E:310:TYR:HB2	2.47	0.45
1:A:331:LEU:HD23	1:A:360:PHE:HE1	1.81	0.45
1:F:90:LYS:NZ	2:F:550:GLU:OE1	2.39	0.45
1:F:107:LEU:HB2	1:F:126:LYS:HG2	1.97	0.45
1:A:369:PRO:HD3	1:A:477:LEU:HB2	1.99	0.45
1:D:232:TYR:OH	1:D:469:MET:HE3	2.16	0.45
1:D:251:GLY:O	1:D:256:GLY:HA3	2.16	0.45
1:E:167:PRO:HG3	1:E:176:MET:CG	2.47	0.45
1:C:258:HIS:CD2	1:C:261:ARG:HD3	2.52	0.44
1:D:107:LEU:CB	1:D:126:LYS:HG2	2.47	0.44
1:D:349:ASN:N	3:D:551:NDP:O2D	2.50	0.44
1:F:24:VAL:O	1:F:25:GLU:C	2.58	0.44
1:C:42:ARG:O	1:C:46:ARG:HG3	2.16	0.44
1:C:126:LYS:NZ	2:C:550:GLU:N	2.65	0.44
1:E:229:GLU:C	1:E:231:SER:H	2.25	0.44
1:B:107:LEU:CB	1:B:126:LYS:HG2	2.47	0.44
1:B:417:LEU:HD21	1:F:417:LEU:CD1	2.47	0.44
1:C:253:GLY:O	1:C:257:LEU:HB3	2.18	0.44
1:D:255:VAL:HG12	3:D:551:NDP:O2N	2.17	0.44
1:E:246:THR:HG22	1:E:269:LYS:HB3	1.98	0.44
1:A:83:SER:O	1:A:84:GLN:HG3	2.18	0.44
1:A:281:TRP:CB	1:A:310:TYR:HB2	2.47	0.44
1:B:258:HIS:CD2	1:B:261:ARG:HD3	2.52	0.44
1:A:478:ARG:HG3	1:A:478:ARG:NH1	2.32	0.44
1:B:364:ASN:HD22	1:B:364:ASN:HA	1.49	0.44
1:D:107:LEU:HB2	1:D:126:LYS:HG2	2.00	0.44
1:D:238:MET:HE1	1:D:320:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:473:LEU:HB3	1:D:476:ASP:HB3	1.98	0.44
1:F:281:TRP:CB	1:F:310:TYR:HB2	2.47	0.44
1:F:346:GLU:OE1	1:F:352:THR:HG23	2.17	0.44
1:C:162:VAL:CG2	1:D:190:TYR:HD2	2.30	0.44
1:D:42:ARG:O	1:D:46:ARG:HG3	2.18	0.44
1:E:331:LEU:HD23	1:E:360:PHE:HE1	1.82	0.44
1:E:358:LYS:O	1:E:362:GLU:HG3	2.17	0.44
1:F:187:ILE:HG23	5:F:552:H3P:HAK	1.98	0.44
1:B:92:GLY:H	2:B:550:GLU:N	2.15	0.44
1:B:281:TRP:CG	1:B:282:ASN:N	2.85	0.44
1:D:186:THR:HG22	1:F:150:MET:HE2	2.00	0.44
1:D:431:VAL:HG12	1:E:419:ARG:HH12	1.83	0.44
1:A:436:PHE:HB2	1:F:408:HIS:HB3	2.00	0.44
1:B:132:ASN:C	1:B:132:ASN:HD22	2.24	0.44
1:C:281:TRP:CG	1:C:282:ASN:N	2.86	0.44
1:D:55:CYS:HA	1:D:82:HIS:HA	2.00	0.44
1:E:12:MET:HG3	1:E:354:PRO:HD3	2.00	0.44
1:C:55:CYS:HA	1:C:82:HIS:HA	2.00	0.44
1:C:167:PRO:HG3	1:C:176:MET:CG	2.48	0.44
1:C:334:SER:O	1:C:337:PRO:HD2	2.17	0.44
1:F:42:ARG:O	1:F:46:ARG:HG3	2.17	0.44
1:F:253:GLY:O	1:F:257:LEU:HB3	2.18	0.44
1:A:99:VAL:O	1:A:130:LYS:HE3	2.17	0.43
1:A:107:LEU:HB2	1:A:126:LYS:HG2	1.99	0.43
1:A:211:ARG:NH2	2:A:550:GLU:OE2	2.51	0.43
1:B:409:LEU:HD21	1:F:409:LEU:HD22	1.99	0.43
1:C:215:THR:O	1:C:219:VAL:HG23	2.18	0.43
1:C:244:ASP:OD2	1:C:245:LYS:NZ	2.50	0.43
1:D:38:GLU:O	1:D:40:GLN:N	2.47	0.43
1:E:55:CYS:HA	1:E:82:HIS:HA	2.00	0.43
1:E:334:SER:O	1:E:337:PRO:HD2	2.17	0.43
1:B:190:TYR:CE2	1:F:162:VAL:HG11	2.52	0.43
1:C:189:HIS:HB3	5:C:554:H3P:CLAF	2.55	0.43
1:F:202:PRO:HA	6:F:574:HOH:O	2.17	0.43
1:A:118:VAL:HG13	1:A:118:VAL:O	2.17	0.43
1:A:253:GLY:O	1:A:257:LEU:HB3	2.18	0.43
1:A:334:SER:O	1:A:337:PRO:HD2	2.19	0.43
1:C:251:GLY:O	1:C:256:GLY:HA3	2.18	0.43
1:D:118:VAL:CG1	1:D:120:VAL:HG23	2.48	0.43
1:D:226:PHE:O	1:D:233:MET:HE3	2.17	0.43
1:E:258:HIS:CD2	1:E:261:ARG:HD3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:478:ARG:HG3	1:F:478:ARG:NH1	2.33	0.43
1:A:116:ALA:O	1:A:488:LYS:HD2	2.19	0.43
1:A:246:THR:HG22	1:A:269:LYS:HB3	2.01	0.43
4:A:553:GTP:N3	4:A:553:GTP:H2'	2.33	0.43
1:D:118:VAL:O	1:D:118:VAL:HG13	2.17	0.43
1:D:319:CYS:O	1:D:341:ALA:HA	2.18	0.43
1:D:332:THR:O	1:D:336:ALA:HB2	2.18	0.43
1:E:99:VAL:O	1:E:130:LYS:HE3	2.17	0.43
1:E:250:GLN:NE2	1:E:330:GLN:NE2	2.64	0.43
1:F:281:TRP:CG	1:F:282:ASN:N	2.87	0.43
1:F:281:TRP:HB3	1:F:310:TYR:HB2	2.00	0.43
1:A:221:HIS:HE1	6:A:557:HOH:O	2.01	0.43
1:C:408:HIS:CE1	1:E:435:GLU:HB3	2.53	0.43
1:F:202:PRO:HB2	1:F:205:GLN:HG2	1.99	0.43
1:A:55:CYS:HA	1:A:82:HIS:HA	1.99	0.43
1:A:401:TYR:CD2	1:B:443:ALA:HB2	2.53	0.43
1:A:491:ARG:CG	1:A:491:ARG:HH11	2.31	0.43
1:B:79:ARG:CD	1:B:127:ALA:HB2	2.49	0.43
1:B:118:VAL:O	1:B:118:VAL:HG13	2.18	0.43
1:B:229:GLU:C	1:B:231:SER:H	2.25	0.43
1:C:38:GLU:O	1:C:40:GLN:N	2.49	0.43
1:C:478:ARG:HG3	1:C:478:ARG:NH1	2.32	0.43
6:C:592:HOH:O	1:D:420:LYS:HB2	2.18	0.43
1:D:410:LEU:HG	1:D:430:ILE:HG22	2.00	0.43
1:D:483:VAL:O	1:D:487:GLU:HB2	2.18	0.43
1:E:281:TRP:HB3	1:E:310:TYR:HB2	2.01	0.43
1:A:42:ARG:O	1:A:46:ARG:HG3	2.19	0.43
1:B:465:MET:O	1:B:469:MET:HG2	2.18	0.43
1:D:334:SER:O	1:D:337:PRO:HD2	2.19	0.43
1:D:335:ASN:N	1:D:335:ASN:ND2	2.65	0.43
1:A:187:ILE:HA	5:A:552:H3P:CAK	2.49	0.43
1:B:78:TYR:CE2	1:B:101:VAL:HG22	2.54	0.43
1:D:253:GLY:HA3	3:D:551:NDP:O1A	2.19	0.43
1:F:250:GLN:HE22	1:F:330:GLN:NE2	2.17	0.43
1:A:118:VAL:CG1	1:A:120:VAL:HG23	2.49	0.43
1:A:202:PRO:HB2	1:A:205:GLN:HG2	2.01	0.43
1:B:58:VAL:O	6:B:570:HOH:O	2.22	0.43
1:B:253:GLY:O	1:B:257:LEU:HB3	2.18	0.43
1:B:410:LEU:HD12	1:B:410:LEU:HA	1.90	0.43
1:D:186:THR:HG22	1:F:150:MET:CE	2.49	0.43
1:E:10:PHE:O	1:E:14:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:ARG:CD	1:E:127:ALA:HB2	2.48	0.43
1:C:89:CYS:HB3	1:C:125:ALA:HB2	2.01	0.43
1:D:94:ARG:HB2	1:D:168:ASP:OD2	2.19	0.43
1:D:150:MET:HE2	1:F:186:THR:HG22	1.99	0.43
1:F:260:MET:HE3	1:F:270:CYS:SG	2.59	0.43
1:A:17:PHE:CE1	1:A:486:ILE:HG12	2.54	0.42
1:A:78:TYR:CE2	1:A:101:VAL:HG22	2.54	0.42
1:B:99:VAL:O	1:B:130:LYS:HE3	2.19	0.42
1:B:378:VAL:HG13	2:B:550:GLU:CD	2.44	0.42
1:D:90:LYS:HD2	1:D:164:VAL:HB	2.01	0.42
1:E:253:GLY:O	1:E:257:LEU:HB3	2.19	0.42
1:F:83:SER:O	1:F:84:GLN:HG3	2.19	0.42
1:F:167:PRO:HG3	1:F:176:MET:CG	2.49	0.42
1:F:336:ALA:CB	1:F:337:PRO:HD3	2.45	0.42
1:B:38:GLU:O	1:B:40:GLN:N	2.50	0.42
1:B:342:LYS:O	1:B:365:ILE:HG23	2.19	0.42
1:B:358:LYS:O	1:B:362:GLU:HG3	2.19	0.42
1:C:392:VAL:HG22	1:E:386:LEU:HG	2.00	0.42
1:E:364:ASN:HD22	1:E:364:ASN:HA	1.47	0.42
1:E:478:ARG:HG3	1:E:478:ARG:NH1	2.33	0.42
1:F:465:MET:O	1:F:469:MET:HG2	2.19	0.42
1:A:346:GLU:OE1	1:A:352:THR:HG23	2.18	0.42
1:D:10:PHE:O	1:D:14:GLU:HG3	2.19	0.42
1:D:445:GLU:O	1:D:449:VAL:HG23	2.20	0.42
1:D:495:GLU:O	1:D:496:ALA:HB3	2.18	0.42
1:A:226:PHE:O	1:A:233:MET:HE3	2.20	0.42
1:A:250:GLN:NE2	1:A:330:GLN:NE2	2.65	0.42
1:B:319:CYS:O	1:B:341:ALA:HA	2.19	0.42
1:D:99:VAL:O	1:D:130:LYS:HE3	2.20	0.42
1:D:167:PRO:HG3	1:D:176:MET:CG	2.49	0.42
1:D:253:GLY:O	1:D:257:LEU:HB3	2.19	0.42
1:E:83:SER:HB2	6:E:559:HOH:O	2.18	0.42
1:F:55:CYS:HA	1:F:82:HIS:HA	2.01	0.42
1:F:287:ASP:HA	1:F:288:PRO:HD3	1.78	0.42
1:A:419:ARG:HH12	1:B:431:VAL:CG1	2.33	0.42
1:B:42:ARG:O	1:B:46:ARG:HG3	2.20	0.42
1:C:226:PHE:O	1:C:233:MET:HE3	2.19	0.42
1:D:281:TRP:CG	1:D:282:ASN:N	2.87	0.42
1:F:38:GLU:O	1:F:40:GLN:N	2.48	0.42
1:F:79:ARG:HD3	1:F:127:ALA:HB2	2.01	0.42
1:F:244:ASP:OD2	1:F:245:LYS:NZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:331:LEU:HD23	1:F:360:PHE:HE1	1.84	0.42
1:A:75:ILE:HD13	1:A:129:VAL:HG13	2.01	0.42
1:D:250:GLN:NE2	1:D:330:GLN:NE2	2.64	0.42
1:E:114:LYS:NZ	2:E:550:GLU:O	2.53	0.42
1:F:126:LYS:NZ	2:F:550:GLU:C	2.78	0.42
1:F:264:HIS:CD2	1:F:288:PRO:HD3	2.55	0.42
1:A:10:PHE:O	1:A:14:GLU:HG3	2.18	0.42
1:A:445:GLU:O	1:A:449:VAL:HG23	2.19	0.42
1:B:55:CYS:HA	1:B:82:HIS:HA	2.01	0.42
1:B:167:PRO:HG3	1:B:176:MET:CG	2.49	0.42
1:B:331:LEU:HD23	1:B:360:PHE:HE1	1.85	0.42
1:E:410:LEU:HG	1:E:430:ILE:HG22	2.02	0.42
1:B:246:THR:HG22	1:B:269:LYS:HB3	2.02	0.42
1:B:260:MET:HE3	1:B:270:CYS:SG	2.60	0.42
1:C:264:HIS:CD2	1:C:288:PRO:HD3	2.55	0.42
1:D:250:GLN:HE22	1:D:330:GLN:HE21	1.63	0.42
1:D:258:HIS:CD2	1:D:261:ARG:HD3	2.54	0.42
3:D:551:NDP:H52N	3:D:551:NDP:H2N	2.02	0.42
1:E:335:ASN:N	1:E:335:ASN:ND2	2.65	0.42
1:B:83:SER:O	1:B:84:GLN:HG3	2.20	0.42
1:B:335:ASN:N	1:B:335:ASN:ND2	2.66	0.42
1:C:107:LEU:CB	1:C:126:LYS:HG2	2.50	0.42
1:C:281:TRP:CB	1:C:310:TYR:HB2	2.50	0.42
1:D:202:PRO:HB2	1:D:205:GLN:HG2	2.02	0.42
1:D:281:TRP:CB	1:D:310:TYR:HB2	2.49	0.42
1:E:118:VAL:O	1:E:118:VAL:HG13	2.20	0.42
1:E:319:CYS:O	1:E:341:ALA:HA	2.19	0.42
1:E:369:PRO:HD3	1:E:477:LEU:HB2	2.02	0.42
1:E:490:PHE:C	1:E:492:VAL:N	2.78	0.42
1:F:132:ASN:HD22	1:F:132:ASN:C	2.27	0.42
1:F:251:GLY:O	1:F:256:GLY:HA3	2.20	0.42
1:A:79:ARG:CD	1:A:127:ALA:HB2	2.50	0.42
1:B:107:LEU:HB2	1:B:126:LYS:HG2	2.01	0.42
1:C:79:ARG:CD	1:C:127:ALA:HB2	2.50	0.42
1:C:229:GLU:C	1:C:231:SER:H	2.27	0.42
1:D:250:GLN:HE22	1:D:330:GLN:NE2	2.17	0.42
1:E:107:LEU:HB2	1:E:126:LYS:HG2	2.01	0.42
1:E:238:MET:HE1	1:E:320:ASP:HB3	2.01	0.42
1:F:47:GLY:O	1:F:51:ILE:HG13	2.19	0.42
1:F:51:ILE:HD13	1:F:498:VAL:HG11	2.01	0.42
1:F:99:VAL:O	1:F:130:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:229:GLU:C	1:F:231:SER:H	2.27	0.42
1:B:190:TYR:HD2	1:F:162:VAL:HG22	1.85	0.41
1:B:287:ASP:OD1	1:B:290:GLU:HG2	2.20	0.41
1:B:370:ASP:C	1:B:372:TYR:H	2.28	0.41
1:B:445:GLU:O	1:B:449:VAL:HG23	2.19	0.41
1:D:364:ASN:HD22	1:D:364:ASN:HA	1.51	0.41
1:E:78:TYR:CE2	1:E:101:VAL:HG22	2.55	0.41
1:A:165:PRO:HD2	1:A:197:CYS:O	2.21	0.41
1:A:215:THR:O	1:A:219:VAL:HG23	2.20	0.41
1:C:90:LYS:HD2	1:C:164:VAL:HB	2.02	0.41
1:C:483:VAL:O	1:C:487:GLU:HB2	2.20	0.41
1:D:83:SER:C	1:D:84:GLN:HG3	2.45	0.41
1:E:118:VAL:CG1	1:E:120:VAL:HG23	2.50	0.41
1:E:465:MET:O	1:E:469:MET:HG2	2.20	0.41
1:A:238:MET:HE1	1:A:320:ASP:HB3	2.01	0.41
1:A:281:TRP:HB3	1:A:310:TYR:HB2	2.02	0.41
1:A:465:MET:O	1:A:469:MET:HG2	2.20	0.41
1:B:75:ILE:HD13	1:B:129:VAL:HG13	2.02	0.41
1:C:369:PRO:HB2	1:C:371:LEU:CD2	2.50	0.41
1:E:202:PRO:HB2	1:E:205:GLN:HG2	2.02	0.41
1:E:281:TRP:CG	1:E:282:ASN:N	2.88	0.41
1:F:362:GLU:C	1:F:364:ASN:H	2.29	0.41
1:B:185:SER:O	1:C:154:LYS:HD3	2.19	0.41
1:B:251:GLY:O	1:B:256:GLY:HA3	2.21	0.41
1:B:409:LEU:HD11	1:F:409:LEU:HD13	2.02	0.41
1:C:362:GLU:C	1:C:364:ASN:H	2.28	0.41
1:D:260:MET:HE3	1:D:270:CYS:SG	2.60	0.41
1:E:441:SER:HB2	6:E:587:HOH:O	2.21	0.41
1:F:27:LYS:HD3	1:F:487:GLU:OE2	2.20	0.41
1:F:92:GLY:O	1:F:126:LYS:HD3	2.20	0.41
1:B:4:GLU:OE1	1:B:4:GLU:HA	2.20	0.41
1:B:281:TRP:CB	1:B:310:TYR:HB2	2.50	0.41
1:B:419:ARG:NH1	1:F:431:VAL:HG12	2.35	0.41
1:C:250:GLN:HE22	1:C:330:GLN:HE21	1.65	0.41
1:C:497:GLY:HA3	1:D:146:ARG:NH2	2.36	0.41
1:D:287:ASP:HA	1:D:288:PRO:HD3	1.76	0.41
1:F:78:TYR:CE2	1:F:101:VAL:HG22	2.56	0.41
1:F:209:HIS:CD2	1:F:446:LYS:HG3	2.55	0.41
1:F:445:GLU:O	1:F:449:VAL:HG23	2.19	0.41
1:A:94:ARG:HB2	1:A:168:ASP:OD2	2.20	0.41
1:A:186:THR:HG22	1:E:150:MET:CE	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLY:HA3	3:A:551:NDP:O1A	2.21	0.41
1:B:490:PHE:O	1:B:491:ARG:C	2.64	0.41
1:C:92:GLY:N	2:C:550:GLU:HB3	2.33	0.41
1:C:248:ALA:CB	1:C:272:ALA:HB3	2.51	0.41
1:E:287:ASP:HA	1:E:288:PRO:HD3	1.79	0.41
1:E:287:ASP:OD1	1:E:290:GLU:HG2	2.21	0.41
1:F:187:ILE:HA	5:F:552:H3P:HAKA	2.02	0.41
1:A:83:SER:C	1:A:84:GLN:HG3	2.46	0.41
1:B:190:TYR:HD2	1:F:162:VAL:CG2	2.33	0.41
1:B:362:GLU:C	1:B:364:ASN:H	2.29	0.41
1:C:7:PRO:O	1:C:329:LYS:NZ	2.51	0.41
1:C:208:ILE:HG13	1:C:445:GLU:CD	2.44	0.41
1:C:255:VAL:HG12	3:C:551:NDP:O2N	2.20	0.41
1:C:319:CYS:O	1:C:341:ALA:HA	2.20	0.41
1:C:410:LEU:HG	1:C:430:ILE:HG22	2.02	0.41
1:C:490:PHE:O	1:C:491:ARG:C	2.64	0.41
1:D:23:ILE:HG22	1:D:471:TYR:CD2	2.56	0.41
1:D:246:THR:HG22	1:D:269:LYS:HB3	2.02	0.41
2:D:550:GLU:CB	3:D:551:NDP:H41N	2.50	0.41
1:F:332:THR:O	1:F:336:ALA:HB2	2.20	0.41
1:A:186:THR:HG22	1:E:150:MET:HE2	2.01	0.41
1:A:358:LYS:O	1:A:362:GLU:HG3	2.21	0.41
1:B:90:LYS:HD2	1:B:164:VAL:HB	2.02	0.41
1:C:162:VAL:HG11	1:D:190:TYR:CE2	2.56	0.41
1:D:209:HIS:CD2	1:D:446:LYS:HG3	2.56	0.41
1:A:251:GLY:O	1:A:256:GLY:HA3	2.21	0.41
1:B:17:PHE:CE2	1:B:53:LYS:HG3	2.56	0.41
1:B:94:ARG:HE	1:B:169:MET:HG3	1.86	0.41
1:B:169:MET:HA	3:B:551:NDP:O1N	2.20	0.41
1:B:264:HIS:CD2	1:B:288:PRO:HD3	2.56	0.41
1:B:497:GLY:O	1:B:498:VAL:C	2.64	0.41
1:C:16:PHE:CG	1:C:478:ARG:HD3	2.55	0.41
1:C:83:SER:O	1:C:84:GLN:HG3	2.21	0.41
1:C:346:GLU:HG2	1:C:351:PRO:HG2	2.02	0.41
1:C:495:GLU:C	1:C:496:ALA:O	2.63	0.41
1:D:92:GLY:O	1:D:126:LYS:HD3	2.21	0.41
1:D:331:LEU:HD23	1:D:360:PHE:HE1	1.84	0.41
1:D:346:GLU:HG2	1:D:351:PRO:CG	2.51	0.41
1:D:433:THR:HG23	1:E:412:SER:HA	2.03	0.41
1:E:83:SER:O	1:E:84:GLN:HG3	2.20	0.41
1:E:226:PHE:O	1:E:233:MET:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:GLY:O	1:E:256:GLY:HA3	2.21	0.41
1:E:253:GLY:HA3	3:E:551:NDP:O1A	2.21	0.41
1:E:332:THR:O	1:E:336:ALA:HB2	2.21	0.41
1:E:445:GLU:O	1:E:449:VAL:HG23	2.21	0.41
1:A:281:TRP:CG	1:A:282:ASN:N	2.89	0.41
1:B:235:ILE:H	1:B:235:ILE:HG13	1.72	0.41
1:B:317:VAL:HG22	1:B:318:ASP:N	2.36	0.41
1:C:20:GLY:O	1:C:24:VAL:HG23	2.21	0.41
1:C:99:VAL:O	1:C:130:LYS:HE3	2.21	0.41
1:E:8:ASN:O	1:E:9:PHE:C	2.64	0.41
1:E:75:ILE:HD13	1:E:129:VAL:HG13	2.03	0.41
1:F:358:LYS:O	1:F:362:GLU:HG3	2.20	0.41
1:A:187:ILE:HG23	5:A:552:H3P:CAK	2.50	0.40
1:A:332:THR:O	1:A:336:ALA:HB2	2.21	0.40
1:B:374:ASN:OD1	1:B:374:ASN:C	2.64	0.40
1:D:378:VAL:HG22	6:D:559:HOH:O	2.21	0.40
1:E:183:TYR:HA	1:E:187:ILE:HD12	2.03	0.40
1:E:483:VAL:O	1:E:487:GLU:HB2	2.20	0.40
1:C:250:GLN:NE2	1:C:330:GLN:NE2	2.66	0.40
1:C:250:GLN:HE22	1:C:330:GLN:NE2	2.19	0.40
1:C:419:ARG:HH12	1:E:431:VAL:HG12	1.86	0.40
1:D:221:HIS:HE1	6:D:562:HOH:O	2.03	0.40
1:E:94:ARG:HG3	1:E:169:MET:HB2	2.03	0.40
1:E:410:LEU:HD12	1:E:410:LEU:HA	1.91	0.40
1:F:319:CYS:O	1:F:341:ALA:HA	2.22	0.40
1:A:53:LYS:O	1:A:82:HIS:HE1	2.04	0.40
1:C:10:PHE:O	1:C:14:GLU:HG3	2.22	0.40
1:D:432:PRO:HB3	1:D:436:PHE:HD2	1.86	0.40
1:E:235:ILE:H	1:E:235:ILE:HG13	1.71	0.40
1:F:8:ASN:OD1	1:F:11:LYS:HE3	2.21	0.40
1:F:118:VAL:CG1	1:F:120:VAL:HG23	2.51	0.40
1:A:167:PRO:HG3	1:A:176:MET:CG	2.52	0.40
1:C:58:VAL:HB	1:F:60:SER:HB2	2.02	0.40
1:D:281:TRP:HB3	1:D:310:TYR:HB2	2.03	0.40
1:D:358:LYS:O	1:D:362:GLU:HG3	2.22	0.40
1:E:9:PHE:O	1:E:12:MET:HB3	2.20	0.40
1:F:215:THR:O	1:F:219:VAL:HG23	2.21	0.40
1:A:162:VAL:HA	6:A:582:HOH:O	2.20	0.40
1:C:281:TRP:HB3	1:C:310:TYR:HB2	2.03	0.40
1:C:287:ASP:OD1	1:C:290:GLU:HG2	2.22	0.40
1:C:348:ALA:HA	3:C:551:NDP:H1D	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:SER:O	1:D:112:THR:HG23	2.21	0.40
1:D:116:ALA:O	1:D:488:LYS:HD2	2.21	0.40
1:D:346:GLU:HG2	1:D:351:PRO:HG2	2.04	0.40
1:F:246:THR:HG22	1:F:269:LYS:HB3	2.04	0.40

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	493/501 (98%)	444 (90%)	39 (8%)	10 (2%)	6	28
1	B	493/501 (98%)	442 (90%)	43 (9%)	8 (2%)	7	34
1	C	493/501 (98%)	441 (90%)	44 (9%)	8 (2%)	7	34
1	D	493/501 (98%)	441 (90%)	45 (9%)	7 (1%)	9	36
1	E	493/501 (98%)	435 (88%)	48 (10%)	10 (2%)	6	28
1	F	493/501 (98%)	444 (90%)	42 (8%)	7 (1%)	9	36
All	All	2958/3006 (98%)	2647 (90%)	261 (9%)	50 (2%)	7	32

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	474	GLY
1	A	496	ALA
1	B	39	GLU

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Mol	Chain	Res	Type
1	B	474	GLY
1	C	39	GLU
1	C	474	GLY
1	C	494	ASN
1	D	39	GLU
1	D	474	GLY
1	E	39	GLU
1	E	474	GLY
1	F	39	GLU
1	F	474	GLY
1	A	334	SER
1	A	494	ASN
1	B	5	ASP
1	B	334	SER
1	C	334	SER
1	C	422	GLY
1	D	334	SER
1	D	422	GLY
1	E	334	SER
1	E	495	GLU
1	F	334	SER
1	F	422	GLY
1	A	130	LYS
1	A	422	GLY
1	B	422	GLY
1	E	422	GLY
1	A	9	PHE
1	B	371	LEU
1	D	130	LYS
1	E	8	ASN
1	E	130	LYS
1	F	5	ASP
1	F	130	LYS
1	C	243	GLY
1	F	243	GLY
1	A	243	GLY
1	B	243	GLY
1	C	158	ILE
1	D	243	GLY
1	E	243	GLY
1	A	158	ILE
1	C	440	ILE

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Mol	Chain	Res	Type
1	D	158	ILE
1	E	440	ILE
1	B	158	ILE
1	E	158	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/417 (99%)	384 (93%)	28 (7%)	14	45
1	B	412/417 (99%)	383 (93%)	29 (7%)	14	44
1	C	412/417 (99%)	384 (93%)	28 (7%)	14	45
1	D	412/417 (99%)	383 (93%)	29 (7%)	14	44
1	E	412/417 (99%)	382 (93%)	30 (7%)	13	42
1	F	412/417 (99%)	383 (93%)	29 (7%)	14	44
All	All	2472/2502 (99%)	2299 (93%)	173 (7%)	13	44

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

Mol	Chain	Res	Type
1	A	24	VAL
1	A	33	LYS
1	A	35	ARG
1	A	39	GLU
1	A	75	ILE
1	A	107	LEU
1	A	112	THR
1	A	118	VAL
1	A	130	LYS
1	A	145	THR
1	A	162	VAL
1	A	187	ILE
1	A	254	ASN
1	A	255	VAL

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Mol	Chain	Res	Type
1	A	291	LEU
1	A	331	LEU
1	A	335	ASN
1	A	352	THR
1	A	361	LEU
1	A	364	ASN
1	A	378	VAL
1	A	381	SER
1	A	386	LEU
1	A	392	VAL
1	A	394	TYR
1	A	410	LEU
1	A	491	ARG
1	A	495	GLU
1	B	24	VAL
1	B	33	LYS
1	B	35	ARG
1	B	39	GLU
1	B	75	ILE
1	B	87	THR
1	B	107	LEU
1	B	112	THR
1	B	118	VAL
1	B	130	LYS
1	B	145	THR
1	B	162	VAL
1	B	187	ILE
1	B	254	ASN
1	B	255	VAL
1	B	291	LEU
1	B	331	LEU
1	B	335	ASN
1	B	352	THR
1	B	361	LEU
1	B	364	ASN
1	B	373	LEU
1	B	378	VAL
1	B	381	SER
1	B	386	LEU
1	B	392	VAL
1	B	394	TYR
1	B	406	ASN

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Mol	Chain	Res	Type
1	B	410	LEU
1	C	24	VAL
1	C	33	LYS
1	C	35	ARG
1	C	39	GLU
1	C	75	ILE
1	C	87	THR
1	C	107	LEU
1	C	112	THR
1	C	118	VAL
1	C	130	LYS
1	C	145	THR
1	C	162	VAL
1	C	187	ILE
1	C	254	ASN
1	C	255	VAL
1	C	291	LEU
1	C	331	LEU
1	C	335	ASN
1	C	352	THR
1	C	361	LEU
1	C	364	ASN
1	C	373	LEU
1	C	378	VAL
1	C	381	SER
1	C	386	LEU
1	C	392	VAL
1	C	394	TYR
1	C	410	LEU
1	D	4	GLU
1	D	24	VAL
1	D	33	LYS
1	D	35	ARG
1	D	39	GLU
1	D	75	ILE
1	D	87	THR
1	D	107	LEU
1	D	112	THR
1	D	118	VAL
1	D	130	LYS
1	D	145	THR
1	D	162	VAL

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Mol	Chain	Res	Type
1	D	187	ILE
1	D	254	ASN
1	D	255	VAL
1	D	291	LEU
1	D	331	LEU
1	D	335	ASN
1	D	352	THR
1	D	361	LEU
1	D	364	ASN
1	D	373	LEU
1	D	378	VAL
1	D	381	SER
1	D	386	LEU
1	D	392	VAL
1	D	394	TYR
1	D	410	LEU
1	E	4	GLU
1	E	24	VAL
1	E	33	LYS
1	E	35	ARG
1	E	39	GLU
1	E	75	ILE
1	E	107	LEU
1	E	112	THR
1	E	118	VAL
1	E	130	LYS
1	E	145	THR
1	E	162	VAL
1	E	187	ILE
1	E	254	ASN
1	E	255	VAL
1	E	291	LEU
1	E	331	LEU
1	E	335	ASN
1	E	352	THR
1	E	361	LEU
1	E	364	ASN
1	E	373	LEU
1	E	378	VAL
1	E	381	SER
1	E	386	LEU
1	E	392	VAL

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Mol	Chain	Res	Type
1	E	394	TYR
1	E	410	LEU
1	E	416	SER
1	E	491	ARG
1	F	24	VAL
1	F	33	LYS
1	F	35	ARG
1	F	39	GLU
1	F	75	ILE
1	F	87	THR
1	F	107	LEU
1	F	112	THR
1	F	118	VAL
1	F	130	LYS
1	F	145	THR
1	F	162	VAL
1	F	187	ILE
1	F	254	ASN
1	F	255	VAL
1	F	291	LEU
1	F	331	LEU
1	F	335	ASN
1	F	352	THR
1	F	361	LEU
1	F	364	ASN
1	F	373	LEU
1	F	378	VAL
1	F	381	SER
1	F	386	LEU
1	F	392	VAL
1	F	394	TYR
1	F	410	LEU
1	F	495	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	56	ASN
1	A	82	HIS
1	A	132	ASN
1	A	250	GLN

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Mol	Chain	Res	Type
1	A	254	ASN
1	A	258	HIS
1	A	264	HIS
1	A	298	HIS
1	A	335	ASN
1	A	364	ASN
1	A	388	ASN
1	A	390	ASN
1	A	406	ASN
1	A	408	HIS
1	B	43	ASN
1	B	56	ASN
1	B	82	HIS
1	B	132	ASN
1	B	209	HIS
1	B	250	GLN
1	B	254	ASN
1	B	258	HIS
1	B	264	HIS
1	B	298	HIS
1	B	335	ASN
1	B	364	ASN
1	B	388	ASN
1	B	390	ASN
1	B	406	ASN
1	B	408	HIS
1	B	424	HIS
1	C	43	ASN
1	C	56	ASN
1	C	82	HIS
1	C	132	ASN
1	C	205	GLN
1	C	254	ASN
1	C	258	HIS
1	C	264	HIS
1	C	298	HIS
1	C	330	GLN
1	C	335	ASN
1	C	364	ASN
1	C	390	ASN
1	C	406	ASN
1	C	408	HIS

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Mol	Chain	Res	Type
1	C	424	HIS
1	C	494	ASN
1	D	8	ASN
1	D	43	ASN
1	D	56	ASN
1	D	82	HIS
1	D	132	ASN
1	D	205	GLN
1	D	250	GLN
1	D	254	ASN
1	D	258	HIS
1	D	264	HIS
1	D	298	HIS
1	D	335	ASN
1	D	364	ASN
1	D	388	ASN
1	D	390	ASN
1	D	406	ASN
1	D	408	HIS
1	D	424	HIS
1	E	43	ASN
1	E	56	ASN
1	E	57	HIS
1	E	82	HIS
1	E	132	ASN
1	E	205	GLN
1	E	209	HIS
1	E	250	GLN
1	E	254	ASN
1	E	258	HIS
1	E	264	HIS
1	E	298	HIS
1	E	335	ASN
1	E	364	ASN
1	E	388	ASN
1	E	390	ASN
1	E	406	ASN
1	F	43	ASN
1	F	56	ASN
1	F	82	HIS
1	F	132	ASN
1	F	193	ASN

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Mol	Chain	Res	Type
1	F	209	HIS
1	F	250	GLN
1	F	254	ASN
1	F	258	HIS
1	F	264	HIS
1	F	298	HIS
1	F	335	ASN
1	F	364	ASN
1	F	388	ASN
1	F	390	ASN
1	F	406	ASN
1	F	408	HIS
1	F	424	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GTP	E	553	-	33,34,34	1.92	6 (18%)	50,54,54	3.17	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	H3P	D	552	-	22,22,22	0.69	0	27,33,33	1.21	2 (7%)
3	NDP	E	551	-	51,52,52	1.70	12 (23%)	71,80,80	2.51	23 (32%)
5	H3P	F	552	-	22,22,22	0.57	0	27,33,33	0.81	0
2	GLU	D	550	-	7,8,9	0.91	0	4,9,11	1.07	0
2	GLU	B	550	-	7,8,9	1.02	0	4,9,11	1.11	0
3	NDP	D	551	-	51,52,52	1.86	12 (23%)	71,80,80	2.59	27 (38%)
4	GTP	F	553	-	33,34,34	1.58	6 (18%)	50,54,54	3.16	21 (42%)
2	GLU	C	550	-	7,8,9	0.98	0	4,9,11	0.77	0
3	NDP	F	551	-	51,52,52	1.68	10 (19%)	71,80,80	2.51	26 (36%)
4	GTP	B	553	-	33,34,34	2.21	5 (15%)	50,54,54	3.27	26 (52%)
2	GLU	F	550	-	7,8,9	1.16	0	4,9,11	1.20	0
4	GTP	D	553	-	33,34,34	2.67	6 (18%)	50,54,54	3.79	24 (48%)
3	NDP	A	551	-	51,52,52	2.07	12 (23%)	71,80,80	2.50	24 (33%)
3	NDP	C	551	-	51,52,52	1.76	8 (15%)	71,80,80	2.58	31 (43%)
4	GTP	A	553	-	33,34,34	1.58	5 (15%)	50,54,54	1.73	8 (16%)
3	NDP	B	551	-	51,52,52	1.90	11 (21%)	71,80,80	2.56	27 (38%)
2	GLU	E	550	-	7,8,9	0.99	0	4,9,11	0.90	0
5	H3P	C	552	-	22,22,22	0.38	0	27,33,33	1.31	2 (7%)
5	H3P	A	552	-	22,22,22	0.36	0	27,33,33	0.82	0
5	H3P	B	552	-	22,22,22	0.50	0	27,33,33	1.18	2 (7%)
5	H3P	C	554	-	22,22,22	0.38	0	27,33,33	0.79	0
2	GLU	A	550	-	7,8,9	0.86	0	4,9,11	0.91	0
4	GTP	C	553	-	33,34,34	1.84	8 (24%)	50,54,54	2.00	13 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	E	553	-	-	4/22/38/38	0/3/3/3
5	H3P	D	552	-	-	0/4/4/4	0/2/2/2
3	NDP	E	551	-	-	2/34/77/77	0/5/5/5
5	H3P	F	552	-	-	1/4/4/4	0/2/2/2
2	GLU	D	550	-	-	0/6/7/9	-
2	GLU	B	550	-	-	1/6/7/9	-
3	NDP	D	551	-	-	3/34/77/77	0/5/5/5
4	GTP	F	553	-	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	C	550	-	-	3/6/7/9	-
3	NDP	F	551	-	-	3/34/77/77	0/5/5/5
4	GTP	B	553	-	-	4/22/38/38	0/3/3/3
2	GLU	F	550	-	-	3/6/7/9	-
4	GTP	D	553	-	-	3/22/38/38	0/3/3/3
3	NDP	A	551	-	-	4/34/77/77	0/5/5/5
3	NDP	C	551	-	-	1/34/77/77	0/5/5/5
4	GTP	A	553	-	-	2/22/38/38	0/3/3/3
3	NDP	B	551	-	-	2/34/77/77	0/5/5/5
2	GLU	E	550	-	-	1/6/7/9	-
5	H3P	C	552	-	-	0/4/4/4	0/2/2/2
5	H3P	A	552	-	-	1/4/4/4	0/2/2/2
5	H3P	B	552	-	-	0/4/4/4	0/2/2/2
5	H3P	C	554	-	-	1/4/4/4	0/2/2/2
2	GLU	A	550	-	-	2/6/7/9	-
4	GTP	C	553	-	-	2/22/38/38	0/3/3/3

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	553	GTP	PB-O3A	10.15	1.70	1.59
4	B	553	GTP	PB-O3B	9.97	1.70	1.59
3	A	551	NDP	PN-O3	-8.76	1.50	1.59
3	C	551	NDP	PN-O3	-8.35	1.50	1.59
3	D	551	NDP	PN-O3	-7.99	1.50	1.59
3	B	551	NDP	PN-O3	-7.81	1.51	1.59
4	D	553	GTP	PA-O3A	7.63	1.67	1.59
4	A	553	GTP	PB-O3B	6.32	1.66	1.59
3	E	551	NDP	PN-O3	-6.25	1.52	1.59
4	E	553	GTP	PA-O3A	6.18	1.66	1.59
3	F	551	NDP	PN-O3	-5.43	1.53	1.59
4	C	553	GTP	PB-O3B	4.83	1.64	1.59
4	C	553	GTP	PB-O3A	4.82	1.64	1.59
4	E	553	GTP	PB-O3A	4.75	1.64	1.59
4	F	553	GTP	PA-O3A	4.39	1.64	1.59
3	A	551	NDP	PA-O3	-4.28	1.54	1.59
4	E	553	GTP	PB-O3B	4.28	1.64	1.59
3	F	551	NDP	O4D-C1D	4.25	1.51	1.42
3	D	551	NDP	O4D-C1D	4.06	1.51	1.42
3	B	551	NDP	O4D-C1D	3.82	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	551	NDP	O4D-C1D	3.73	1.50	1.42
3	E	551	NDP	O4D-C1D	3.71	1.50	1.42
3	F	551	NDP	P2B-O2B	3.67	1.66	1.59
4	D	553	GTP	PB-O3B	3.62	1.63	1.59
4	B	553	GTP	C2'-C3'	3.57	1.63	1.53
4	C	553	GTP	C1'-N9	3.43	1.57	1.47
3	B	551	NDP	O4B-C1B	3.40	1.49	1.42
4	D	553	GTP	C3'-C4'	3.37	1.61	1.53
4	F	553	GTP	PB-O3B	3.19	1.62	1.59
3	A	551	NDP	O4B-C1B	3.16	1.49	1.42
3	F	551	NDP	C7N-C3N	-3.15	1.41	1.48
3	A	551	NDP	P2B-O2B	3.07	1.64	1.59
3	A	551	NDP	C5A-C4A	3.01	1.44	1.39
3	C	551	NDP	O4D-C1D	3.01	1.48	1.42
3	B	551	NDP	C5A-N7A	-2.97	1.33	1.39
4	C	553	GTP	C2'-C3'	2.90	1.61	1.53
3	E	551	NDP	C3B-C2B	2.86	1.59	1.53
3	B	551	NDP	PA-O3	-2.85	1.56	1.59
3	A	551	NDP	C5A-N7A	-2.84	1.33	1.39
3	D	551	NDP	P2B-O2B	2.84	1.64	1.59
4	B	553	GTP	C5-N7	-2.82	1.33	1.39
4	B	553	GTP	C3'-C4'	2.77	1.60	1.53
3	D	551	NDP	C7N-C3N	-2.75	1.42	1.48
4	A	553	GTP	C5-N7	-2.72	1.33	1.39
3	B	551	NDP	C5A-C4A	2.69	1.43	1.39
3	E	551	NDP	C5A-C4A	2.68	1.43	1.39
3	B	551	NDP	C1B-N9A	2.66	1.53	1.46
3	A	551	NDP	PA-O5B	2.66	1.69	1.59
4	D	553	GTP	C5-N7	-2.63	1.33	1.39
3	E	551	NDP	P2B-O2B	2.61	1.64	1.59
3	E	551	NDP	O4B-C1B	2.60	1.48	1.42
3	E	551	NDP	P2B-O2X	2.59	1.64	1.54
3	D	551	NDP	O4B-C1B	2.53	1.47	1.42
4	C	553	GTP	C2'-C1'	2.50	1.61	1.53
4	F	553	GTP	C2'-C3'	2.48	1.60	1.53
3	C	551	NDP	P2B-O2X	2.47	1.64	1.54
3	D	551	NDP	C5A-N7A	-2.45	1.34	1.39
3	C	551	NDP	C5A-C4A	2.44	1.43	1.39
3	C	551	NDP	C5A-N7A	-2.43	1.34	1.39
3	A	551	NDP	C5B-C4B	2.42	1.58	1.51
3	A	551	NDP	P2B-O2X	2.41	1.63	1.54
3	B	551	NDP	C5B-C4B	2.41	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	553	GTP	C5-N7	-2.40	1.34	1.39
3	C	551	NDP	C7N-C3N	-2.39	1.43	1.48
3	F	551	NDP	C5A-C4A	2.36	1.43	1.39
3	B	551	NDP	PA-O5B	2.36	1.68	1.59
3	C	551	NDP	PA-O5B	2.34	1.68	1.59
3	D	551	NDP	C1D-N1N	2.33	1.52	1.46
4	C	553	GTP	PA-O3A	2.31	1.62	1.59
3	E	551	NDP	C5A-N7A	-2.28	1.34	1.39
3	F	551	NDP	C1D-N1N	2.27	1.52	1.46
3	F	551	NDP	P2B-O2X	2.25	1.63	1.54
4	A	553	GTP	PG-O3G	2.23	1.63	1.54
4	D	553	GTP	C2'-C3'	2.21	1.59	1.53
3	E	551	NDP	PA-O5B	2.21	1.68	1.59
3	E	551	NDP	P2B-O3X	2.19	1.62	1.54
4	B	553	GTP	PG-O2G	2.18	1.62	1.54
4	C	553	GTP	PG-O3G	2.18	1.62	1.54
3	B	551	NDP	P2B-O2X	2.18	1.62	1.54
4	C	553	GTP	C5-C4	2.18	1.44	1.38
3	B	551	NDP	C7N-C3N	-2.17	1.44	1.48
4	A	553	GTP	O4'-C1'	2.17	1.47	1.42
4	F	553	GTP	C2'-C1'	2.17	1.60	1.53
3	A	551	NDP	C6A-N6A	2.16	1.39	1.34
3	D	551	NDP	PA-O5B	2.16	1.67	1.59
4	E	553	GTP	PA-O2A	2.15	1.65	1.55
3	D	551	NDP	P2B-O3X	2.15	1.62	1.54
4	E	553	GTP	O4'-C1'	2.14	1.46	1.42
3	D	551	NDP	P2B-O2X	2.13	1.62	1.54
4	A	553	GTP	PG-O2G	2.13	1.62	1.54
3	D	551	NDP	C5A-C4A	2.12	1.42	1.39
4	E	553	GTP	C5-N7	-2.12	1.34	1.39
3	E	551	NDP	C1B-N9A	2.12	1.52	1.46
4	F	553	GTP	C3'-C4'	2.11	1.58	1.53
3	C	551	NDP	O4B-C1B	2.10	1.46	1.42
3	D	551	NDP	C5B-C4B	2.08	1.57	1.51
3	E	551	NDP	PN-O2N	2.07	1.64	1.55
3	F	551	NDP	P2B-O3X	2.06	1.62	1.54
3	F	551	NDP	C6A-N6A	2.05	1.39	1.34
3	A	551	NDP	P2B-O3X	2.04	1.62	1.54
3	F	551	NDP	C6N-N1N	2.03	1.42	1.37

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	553	GTP	C4'-O4'-C1'	-10.86	85.49	109.47
4	F	553	GTP	C4'-O4'-C1'	-10.28	86.76	109.47
4	D	553	GTP	C4'-O4'-C1'	-9.50	88.50	109.47
4	D	553	GTP	O2A-PA-O3A	8.55	130.39	107.27
4	E	553	GTP	O2A-PA-O3A	8.49	130.23	107.27
4	D	553	GTP	O3A-PA-O1A	-8.20	86.03	110.70
4	E	553	GTP	C4'-O4'-C1'	-8.10	91.57	109.47
4	E	553	GTP	O3A-PA-O1A	-7.67	87.62	110.70
4	F	553	GTP	O3A-PB-O1B	-7.38	88.50	110.70
4	D	553	GTP	O4'-C1'-N9	7.29	124.89	108.36
4	F	553	GTP	O4'-C1'-N9	7.05	124.34	108.36
3	E	551	NDP	P2B-O2B-C2B	-6.92	104.95	123.43
4	B	553	GTP	O2G-PG-O3B	-6.89	81.53	104.64
4	D	553	GTP	O2B-PB-O3A	-6.89	88.65	107.27
3	D	551	NDP	P2B-O2B-C2B	-6.80	105.27	123.43
4	D	553	GTP	O2A-PA-O1A	-6.61	81.68	112.44
3	A	551	NDP	P2B-O2B-C2B	-6.61	105.79	123.43
4	F	553	GTP	O2B-PB-O3A	-6.48	89.76	107.27
4	E	553	GTP	C5-C4-N3	-6.27	118.41	128.39
3	C	551	NDP	P2B-O2B-C2B	-6.24	106.76	123.43
3	E	551	NDP	O3-PA-O1A	6.22	129.43	110.70
4	D	553	GTP	O5'-PA-O1A	6.12	133.18	108.94
4	D	553	GTP	C5-C4-N3	-6.11	118.66	128.39
4	D	553	GTP	O2A-PA-O5'	-6.09	79.97	107.57
4	B	553	GTP	O4'-C1'-N9	6.07	122.11	108.36
4	C	553	GTP	C5-C4-N3	-6.02	118.81	128.39
3	B	551	NDP	P2B-O2B-C2B	-5.99	107.43	123.43
4	D	553	GTP	O3A-PB-O1B	-5.96	92.78	110.70
3	C	551	NDP	O2N-PN-O5D	-5.90	80.83	107.57
4	B	553	GTP	O3G-PG-O3B	-5.88	84.91	104.64
3	B	551	NDP	C5A-C4A-N3A	-5.88	118.63	126.72
3	D	551	NDP	C5A-C4A-N3A	-5.80	118.73	126.72
4	E	553	GTP	O4'-C1'-N9	5.77	121.44	108.36
3	A	551	NDP	C5A-C4A-N3A	-5.76	118.78	126.72
3	E	551	NDP	O5B-PA-O1A	-5.73	86.23	108.94
3	F	551	NDP	O2N-PN-O5D	-5.70	81.72	107.57
3	E	551	NDP	O2N-PN-O5D	-5.67	81.87	107.57
3	C	551	NDP	C5A-C4A-N3A	-5.63	118.96	126.72
3	D	551	NDP	O5D-PN-O1N	-5.61	86.72	108.94
4	C	553	GTP	C2-N3-C4	5.60	121.95	112.30
3	B	551	NDP	O5B-PA-O1A	-5.58	86.80	108.94
3	C	551	NDP	O3-PA-O1A	5.57	127.46	110.70
4	F	553	GTP	C5-C4-N3	-5.54	119.57	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	553	GTP	N9-C4-N3	5.50	136.96	125.95
3	A	551	NDP	O2N-PN-O5D	-5.50	82.62	107.57
4	E	553	GTP	O5'-PA-O1A	5.49	130.70	108.94
4	A	553	GTP	C5-C4-N3	-5.48	119.67	128.39
3	B	551	NDP	O5D-PN-O1N	-5.43	87.40	108.94
3	C	551	NDP	O5B-PA-O1A	-5.42	87.47	108.94
3	D	551	NDP	O2N-PN-O5D	-5.39	83.13	107.57
4	E	553	GTP	N9-C4-N3	5.35	136.64	125.95
3	F	551	NDP	C5A-C4A-N3A	-5.34	119.36	126.72
3	F	551	NDP	P2B-O2B-C2B	-5.33	109.20	123.43
4	B	553	GTP	C5-C4-N3	-5.32	119.92	128.39
4	E	553	GTP	O2A-PA-O5'	-5.27	83.67	107.57
4	B	553	GTP	O5'-C5'-C4'	-5.25	91.10	108.99
3	E	551	NDP	C5A-C4A-N3A	-5.23	119.51	126.72
3	F	551	NDP	O5D-PN-O1N	-5.20	88.32	108.94
3	F	551	NDP	O5B-PA-O1A	-5.15	88.52	108.94
4	E	553	GTP	C2-N3-C4	5.14	121.14	112.30
3	D	551	NDP	O4B-C1B-C2B	-5.13	97.76	106.59
3	A	551	NDP	C2D-C3D-C4D	5.12	112.50	102.61
4	E	553	GTP	O2A-PA-O1A	-5.08	88.80	112.44
3	B	551	NDP	O2N-PN-O5D	-5.06	84.61	107.57
3	C	551	NDP	O5D-PN-O1N	-5.03	88.99	108.94
3	E	551	NDP	O5D-PN-O1N	-5.03	89.01	108.94
4	B	553	GTP	O3B-PG-O1G	-5.01	84.70	111.04
4	A	553	GTP	C2-N3-C4	4.97	120.87	112.30
3	F	551	NDP	O4D-C1D-N1N	4.96	117.54	108.08
3	A	551	NDP	O5B-PA-O1A	-4.94	89.35	108.94
3	A	551	NDP	O3-PA-O1A	4.94	125.55	110.70
4	F	553	GTP	C2-N3-C4	4.91	120.75	112.30
4	B	553	GTP	C2-N3-C4	4.90	120.73	112.30
4	D	553	GTP	C2-N3-C4	4.89	120.72	112.30
3	A	551	NDP	O4B-C1B-C2B	-4.89	98.18	106.59
3	D	551	NDP	N3A-C4A-N9A	4.84	135.40	127.17
3	B	551	NDP	O4B-C1B-C2B	-4.83	98.28	106.59
3	D	551	NDP	C2D-C3D-C4D	4.80	111.88	102.61
3	A	551	NDP	N3A-C4A-N9A	4.80	135.32	127.17
3	F	551	NDP	O3-PA-O1A	4.78	125.08	110.70
3	B	551	NDP	O4D-C1D-N1N	4.78	117.19	108.08
3	B	551	NDP	C2D-C3D-C4D	4.76	111.81	102.61
4	F	553	GTP	O3B-PB-O1B	4.71	124.89	110.70
3	B	551	NDP	N3A-C4A-N9A	4.71	135.17	127.17
4	D	553	GTP	O2B-PB-O3B	4.65	119.85	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	551	NDP	N3A-C2A-N1A	-4.63	121.58	128.58
4	F	553	GTP	O5'-C5'-C4'	-4.61	93.31	108.99
4	B	553	GTP	N9-C4-N3	4.60	135.16	125.95
4	A	553	GTP	N9-C4-N3	4.54	135.02	125.95
3	C	551	NDP	O4D-C1D-N1N	4.53	116.72	108.08
3	D	551	NDP	O3-PA-O1A	4.53	124.32	110.70
4	F	553	GTP	N9-C4-N3	4.52	134.99	125.95
3	C	551	NDP	N3A-C4A-N9A	4.50	134.81	127.17
3	D	551	NDP	O5B-PA-O1A	-4.48	91.17	108.94
4	D	553	GTP	O3B-PB-O1B	4.46	124.12	110.70
3	A	551	NDP	O5D-PN-O1N	-4.46	91.27	108.94
3	C	551	NDP	O4B-C1B-C2B	-4.44	98.95	106.59
3	B	551	NDP	N3A-C2A-N1A	-4.33	122.03	128.58
3	F	551	NDP	N3A-C2A-N1A	-4.29	122.09	128.58
4	F	553	GTP	O4'-C4'-C5'	4.26	122.98	109.33
3	E	551	NDP	O4B-C1B-C2B	-4.24	99.28	106.59
3	E	551	NDP	N3A-C2A-N1A	-4.23	122.17	128.58
3	A	551	NDP	O4D-C1D-N1N	4.17	116.04	108.08
4	B	553	GTP	C2'-C1'-N9	4.15	124.80	113.25
3	A	551	NDP	N3A-C2A-N1A	-4.14	122.31	128.58
3	B	551	NDP	O3-PA-O1A	4.14	123.16	110.70
3	C	551	NDP	C2D-C3D-C4D	4.13	110.59	102.61
4	B	553	GTP	O4'-C4'-C5'	4.12	122.52	109.33
3	D	551	NDP	O2A-PA-O5B	-4.11	88.95	107.57
4	E	553	GTP	O4'-C4'-C5'	4.08	122.42	109.33
3	E	551	NDP	O2N-PN-O3	4.08	118.29	107.27
3	D	551	NDP	O2A-PA-O3	4.06	118.24	107.27
5	C	552	H3P	CAU-CAK-CAT	-4.04	108.27	117.70
3	F	551	NDP	N3A-C4A-N9A	4.03	134.01	127.17
4	C	553	GTP	N9-C4-N3	4.03	134.00	125.95
3	C	551	NDP	N3A-C2A-N1A	-4.01	122.52	128.58
3	F	551	NDP	O4B-C1B-C2B	-3.99	99.72	106.59
3	F	551	NDP	C2D-C3D-C4D	3.99	110.31	102.61
3	E	551	NDP	C2D-C3D-C4D	3.97	110.29	102.61
3	E	551	NDP	C5A-N7A-C8A	3.92	109.61	103.45
3	D	551	NDP	C5A-N7A-C8A	3.91	109.60	103.45
3	B	551	NDP	C5A-N7A-C8A	3.91	109.60	103.45
3	E	551	NDP	N3A-C4A-N9A	3.91	133.81	127.17
3	A	551	NDP	O2N-PN-O3	3.90	117.81	107.27
3	B	551	NDP	C2A-N3A-C4A	3.83	121.20	111.83
3	F	551	NDP	C5A-N7A-C8A	3.83	109.47	103.45
5	D	552	H3P	CAU-CAK-CAT	-3.83	108.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	551	NDP	C2A-N3A-C4A	3.81	121.14	111.83
3	F	551	NDP	O2A-PA-O5B	-3.80	90.34	107.57
3	C	551	NDP	C5A-N7A-C8A	3.79	109.40	103.45
3	F	551	NDP	C2A-N3A-C4A	3.76	121.02	111.83
3	B	551	NDP	O2A-PA-O5B	-3.72	90.70	107.57
3	A	551	NDP	O2A-PA-O5B	-3.72	90.71	107.57
5	B	552	H3P	CAU-CAK-CAT	-3.67	109.13	117.70
4	B	553	GTP	C3'-C2'-C1'	-3.66	94.53	101.46
3	A	551	NDP	C2A-N3A-C4A	3.66	120.77	111.83
3	B	551	NDP	O3-PN-O1N	3.64	121.66	110.70
3	E	551	NDP	C2A-N3A-C4A	3.63	120.70	111.83
3	F	551	NDP	C4A-C5A-N7A	-3.62	106.44	110.58
3	D	551	NDP	O4B-C1B-N9A	3.61	115.02	108.09
3	A	551	NDP	C5A-N7A-C8A	3.60	109.11	103.45
3	B	551	NDP	O2A-PA-O3	3.54	116.85	107.27
3	E	551	NDP	C4A-C5A-N7A	-3.54	106.53	110.58
3	C	551	NDP	C2A-N3A-C4A	3.53	120.46	111.83
4	C	553	GTP	C4'-O4'-C1'	-3.53	101.68	109.47
3	C	551	NDP	O2N-PN-O3	3.51	116.76	107.27
4	D	553	GTP	O4'-C4'-C5'	3.51	120.57	109.33
3	F	551	NDP	O2N-PN-O3	3.48	116.67	107.27
3	F	551	NDP	O2A-PA-O3	3.44	116.58	107.27
4	F	553	GTP	O2B-PB-O3B	3.40	116.47	107.27
4	E	553	GTP	C8-N7-C5	3.35	110.22	104.26
3	E	551	NDP	O4D-C1D-N1N	3.31	114.40	108.08
4	B	553	GTP	O2G-PG-O1G	3.25	123.49	110.83
3	B	551	NDP	O4B-C1B-N9A	3.21	114.25	108.09
4	B	553	GTP	C2'-C3'-C4'	-3.20	96.43	102.61
4	B	553	GTP	C5'-C4'-C3'	3.20	126.73	115.21
3	D	551	NDP	O4D-C1D-N1N	3.19	114.17	108.08
4	C	553	GTP	O4'-C1'-C2'	-3.18	99.82	106.62
3	B	551	NDP	O2N-PN-O3	3.17	115.84	107.27
4	F	553	GTP	C2'-C3'-C4'	-3.15	96.53	102.61
3	D	551	NDP	C4B-O4B-C1B	-3.13	102.56	109.47
3	C	551	NDP	C4A-C5A-N7A	-3.13	107.01	110.58
3	C	551	NDP	O4B-C1B-N9A	3.13	114.09	108.09
3	C	551	NDP	O2A-PA-O5B	-3.05	93.74	107.57
3	F	551	NDP	C2D-C1D-N1N	-3.05	105.82	113.31
3	D	551	NDP	O2N-PN-O3	3.03	115.45	107.27
3	F	551	NDP	O3-PN-O1N	3.01	119.76	110.70
3	D	551	NDP	C4A-C5A-N7A	-3.00	107.15	110.58
4	C	553	GTP	C8-N7-C5	3.00	109.61	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	551	NDP	C2D-C1D-N1N	-2.97	106.00	113.31
4	D	553	GTP	C8-N7-C5	2.96	109.54	104.26
3	A	551	NDP	O3-PN-O1N	2.96	119.61	110.70
3	A	551	NDP	O2A-PA-O3	2.94	115.23	107.27
3	E	551	NDP	O5D-C5D-C4D	2.93	118.97	108.99
3	B	551	NDP	O4D-C4D-C5D	-2.90	100.06	109.33
3	A	551	NDP	C4A-C5A-N7A	-2.89	107.28	110.58
4	C	553	GTP	C2'-C1'-N9	2.88	121.27	113.25
4	D	553	GTP	C2-N1-C6	-2.86	119.93	125.11
3	F	551	NDP	C4B-O4B-C1B	-2.85	103.17	109.47
4	A	553	GTP	O3G-PG-O3B	2.85	114.19	104.64
3	E	551	NDP	O2A-PA-O5B	-2.83	94.72	107.57
4	F	553	GTP	C8-N7-C5	2.83	109.29	104.26
4	A	553	GTP	C8-N7-C5	2.82	109.28	104.26
4	E	553	GTP	C2-N1-C6	-2.79	120.05	125.11
4	F	553	GTP	C2-N1-C6	-2.78	120.07	125.11
4	F	553	GTP	C2'-C1'-N9	2.78	120.99	113.25
4	C	553	GTP	O5'-C5'-C4'	-2.75	99.63	108.99
4	C	553	GTP	C6-C5-N7	2.75	135.29	130.29
3	C	551	NDP	C3N-C2N-N1N	-2.75	119.17	123.20
3	A	551	NDP	C2D-C1D-N1N	-2.74	106.56	113.31
3	B	551	NDP	C4A-C5A-N7A	-2.74	107.45	110.58
3	D	551	NDP	O3-PN-O1N	2.74	118.94	110.70
3	C	551	NDP	O5D-C5D-C4D	2.74	118.31	108.99
5	C	552	H3P	CAT-CAR-CLAG	-2.68	116.11	120.01
3	C	551	NDP	PN-O5D-C5D	-2.66	106.09	121.35
4	D	553	GTP	C3'-C2'-C1'	-2.66	96.43	101.46
3	E	551	NDP	PN-O5D-C5D	-2.66	106.10	121.35
3	E	551	NDP	O2A-PA-O3	2.65	114.43	107.27
4	B	553	GTP	O2B-PB-O3A	2.64	114.41	107.27
4	D	553	GTP	C1'-N9-C4	2.62	134.23	126.49
4	B	553	GTP	O4'-C1'-C2'	-2.61	101.04	106.62
4	D	553	GTP	C1'-N9-C8	-2.58	119.41	126.73
4	A	553	GTP	O5'-C5'-C4'	-2.56	100.27	108.99
4	A	553	GTP	C2-N1-C6	-2.56	120.46	125.11
4	F	553	GTP	O3A-PA-O1A	2.56	118.41	110.70
4	B	553	GTP	C2-N1-C6	-2.55	120.50	125.11
4	C	553	GTP	C2-N1-C6	-2.54	120.51	125.11
3	C	551	NDP	O2A-PA-O3	2.54	114.13	107.27
3	D	551	NDP	C2B-C1B-N9A	-2.53	109.59	113.75
3	C	551	NDP	C1D-N1N-C6N	-2.53	115.42	120.77
4	C	553	GTP	C4-C5-N7	-2.52	106.67	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	553	GTP	O6-C6-C5	-2.51	119.89	126.53
3	C	551	NDP	C2B-C1B-N9A	-2.51	109.62	113.75
4	D	553	GTP	C2'-C1'-N9	2.51	120.23	113.25
3	B	551	NDP	C4B-O4B-C1B	-2.51	103.93	109.47
3	C	551	NDP	C5D-C4D-C3D	-2.50	106.20	115.21
4	B	553	GTP	O2B-PB-O3B	2.50	114.03	107.27
4	B	553	GTP	C8-N7-C5	2.50	108.71	104.26
3	C	551	NDP	C5B-C4B-C3B	-2.48	106.27	115.21
3	D	551	NDP	PN-O5D-C5D	-2.48	107.13	121.35
3	F	551	NDP	C5D-C4D-C3D	-2.47	106.33	115.21
4	C	553	GTP	O2B-PB-O3A	2.45	113.90	107.27
3	F	551	NDP	PN-O5D-C5D	-2.45	107.31	121.35
3	B	551	NDP	C2D-C1D-N1N	-2.43	107.33	113.31
3	A	551	NDP	PN-O5D-C5D	-2.42	107.46	121.35
3	D	551	NDP	O2B-C2B-C1B	2.42	118.56	110.05
4	E	553	GTP	O5'-C5'-C4'	-2.42	100.77	108.99
3	F	551	NDP	O5D-C5D-C4D	2.41	117.20	108.99
4	F	553	GTP	O4'-C1'-C2'	-2.40	101.48	106.62
3	C	551	NDP	O3-PN-O1N	2.39	117.91	110.70
3	A	551	NDP	O4D-C4D-C5D	-2.34	101.85	109.33
3	E	551	NDP	O3-PN-O1N	2.33	117.72	110.70
5	D	552	H3P	CAL-CAL-CAP	-2.33	118.65	121.77
4	B	553	GTP	O3A-PA-O1A	2.33	117.71	110.70
3	C	551	NDP	C4B-O4B-C1B	-2.33	104.33	109.47
3	B	551	NDP	C1D-N1N-C6N	-2.31	115.88	120.77
3	D	551	NDP	O2N-PN-O1N	2.24	122.85	112.44
4	F	553	GTP	C5'-C4'-C3'	2.23	123.24	115.21
3	D	551	NDP	C5D-C4D-C3D	-2.22	107.21	115.21
4	B	553	GTP	O6-C6-C5	-2.21	120.71	126.53
4	D	553	GTP	C5-C6-N1	2.19	118.83	113.25
4	E	553	GTP	O6-C6-C5	-2.19	120.75	126.53
3	D	551	NDP	O5D-C5D-C4D	2.19	116.45	108.99
3	C	551	NDP	O2N-PN-O1N	2.19	122.62	112.44
3	A	551	NDP	O2B-C2B-C1B	2.17	117.69	110.05
4	B	553	GTP	O3G-PG-O2G	2.17	115.94	107.80
3	F	551	NDP	N9A-C8A-N7A	-2.16	110.88	113.94
3	B	551	NDP	C5B-C4B-C3B	-2.16	107.45	115.21
4	E	553	GTP	C5-C6-N1	2.14	118.71	113.25
3	D	551	NDP	N9A-C8A-N7A	-2.14	110.89	113.94
4	F	553	GTP	O6-C6-C5	-2.13	120.91	126.53
3	E	551	NDP	C1D-N1N-C6N	-2.13	116.27	120.77
3	C	551	NDP	O4D-C1D-C2D	2.12	111.14	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	551	NDP	C3B-C2B-C1B	-2.11	98.76	102.81
4	F	553	GTP	C5-C6-N1	2.10	118.61	113.25
4	E	553	GTP	O2B-PB-O3A	2.10	112.95	107.27
3	E	551	NDP	C5B-C4B-C3B	-2.10	107.65	115.21
3	E	551	NDP	C5D-C4D-C3D	-2.10	107.67	115.21
4	C	553	GTP	C5-C6-N1	2.08	118.55	113.25
4	F	553	GTP	C3'-C2'-C1'	-2.07	97.55	101.46
3	B	551	NDP	C5D-C4D-C3D	-2.07	107.77	115.21
4	A	553	GTP	O2B-PB-O3B	2.06	112.83	107.27
4	E	553	GTP	C4-C5-N7	-2.05	107.42	110.67
4	B	553	GTP	O5'-PA-O1A	2.05	117.07	108.94
5	B	552	H3P	CAP-CAL-CLAC	2.05	121.36	118.81
3	A	551	NDP	C5B-C4B-C3B	-2.04	107.87	115.21
4	B	553	GTP	C1'-N9-C4	2.03	132.49	126.49
4	B	553	GTP	C5-C6-N1	2.03	118.42	113.25
4	D	553	GTP	C2'-C3'-C4'	-2.02	98.70	102.61
3	B	551	NDP	PN-O5D-C5D	-2.02	109.76	121.35
3	A	551	NDP	C5D-C4D-C3D	-2.01	107.98	115.21
3	C	551	NDP	C3N-C7N-N7N	2.01	121.23	117.67
3	F	551	NDP	C6A-C5A-N7A	2.00	135.95	132.09
3	B	551	NDP	C3N-C7N-N7N	2.00	121.22	117.67

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	550	GLU	O-C-CA-CB
2	B	550	GLU	O-C-CA-CB
2	E	550	GLU	O-C-CA-CB
2	F	550	GLU	O-C-CA-CB
2	F	550	GLU	N-CA-CB-CG
2	F	550	GLU	C-CA-CB-CG
3	A	551	NDP	O4D-C1D-N1N-C6N
3	B	551	NDP	O4D-C1D-N1N-C6N
3	D	551	NDP	O4D-C1D-N1N-C6N
3	F	551	NDP	O4D-C1D-N1N-C6N
4	D	553	GTP	C5'-O5'-PA-O1A
4	E	553	GTP	C5'-O5'-PA-O1A
4	B	553	GTP	O4'-C4'-C5'-O5'
3	E	551	NDP	O4D-C1D-N1N-C6N
4	F	553	GTP	O4'-C4'-C5'-O5'
4	C	553	GTP	O4'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
3	C	551	NDP	O4D-C1D-N1N-C6N
4	A	553	GTP	C2'-C1'-N9-C4
4	C	553	GTP	O4'-C1'-N9-C8
4	B	553	GTP	C2'-C1'-N9-C4
2	C	550	GLU	CA-CB-CG-CD
3	A	551	NDP	C5D-O5D-PN-O3
4	B	553	GTP	C5'-O5'-PA-O2A
2	C	550	GLU	OE1-CD-CG-CB
2	C	550	GLU	OE2-CD-CG-CB
4	D	553	GTP	O4'-C4'-C5'-O5'
4	E	553	GTP	O4'-C4'-C5'-O5'
3	B	551	NDP	PN-O3-PA-O1A
3	D	551	NDP	PN-O3-PA-O1A
4	A	553	GTP	C2'-C1'-N9-C8
4	F	553	GTP	C2'-C1'-N9-C8
3	A	551	NDP	PN-O3-PA-O1A
3	A	551	NDP	PA-O3-PN-O2N
3	E	551	NDP	PN-O3-PA-O1A
3	F	551	NDP	PN-O3-PA-O1A
4	E	553	GTP	PB-O3A-PA-O2A
4	F	553	GTP	PG-O3B-PB-O1B
5	A	552	H3P	CAT-CAK-CAU-CAS
5	C	554	H3P	CAT-CAK-CAU-CAS
5	F	552	H3P	CAT-CAK-CAU-CAS
4	B	553	GTP	C2'-C1'-N9-C8
4	E	553	GTP	C2'-C1'-N9-C4
2	A	550	GLU	N-CA-CB-CG
3	D	551	NDP	PA-O3-PN-O2N
3	F	551	NDP	PA-O3-PN-O2N
4	D	553	GTP	PB-O3A-PA-O2A

There are no ring outliers.

21 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	553	GTP	2	0
3	E	551	NDP	5	0
5	F	552	H3P	7	0
2	D	550	GLU	2	0
2	B	550	GLU	4	0
3	D	551	NDP	8	0
4	F	553	GTP	2	0

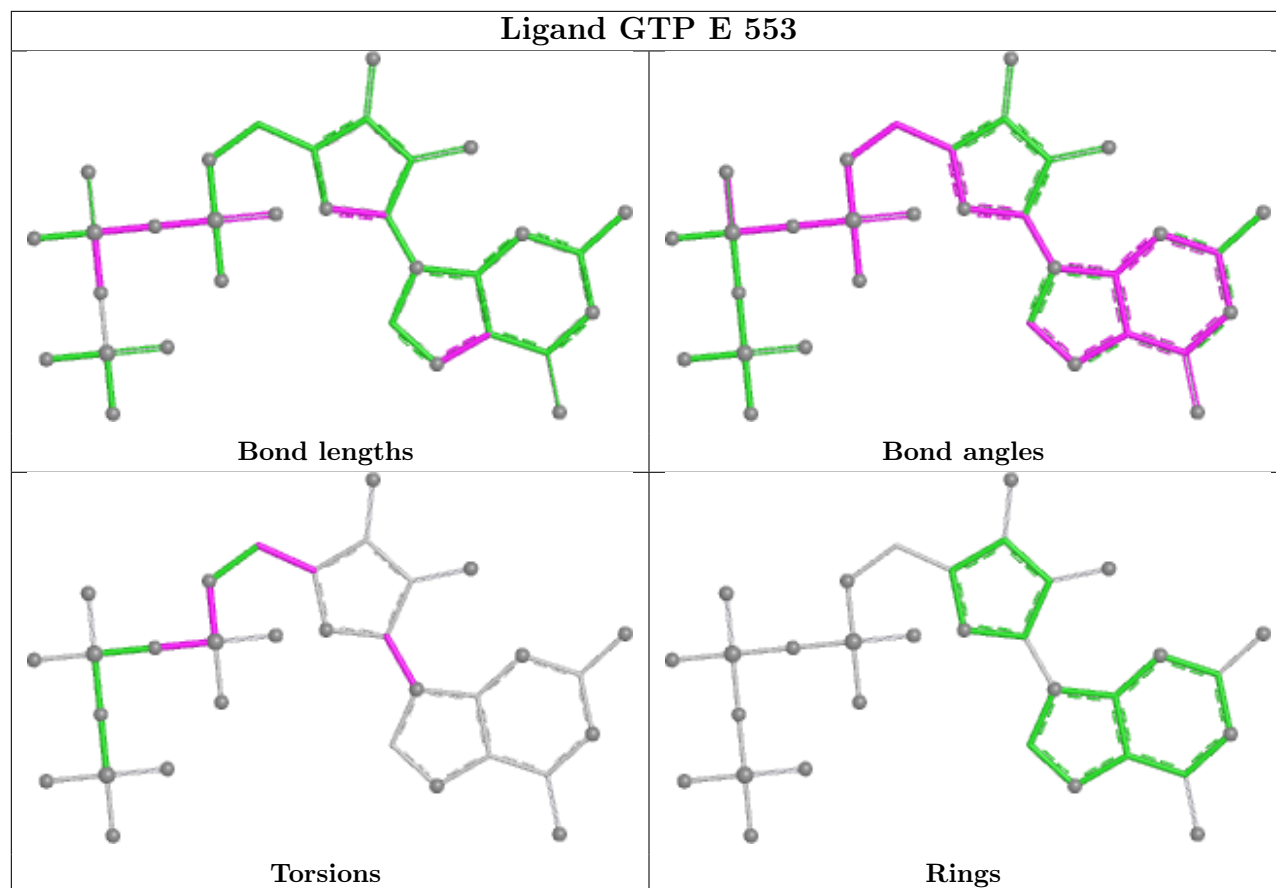
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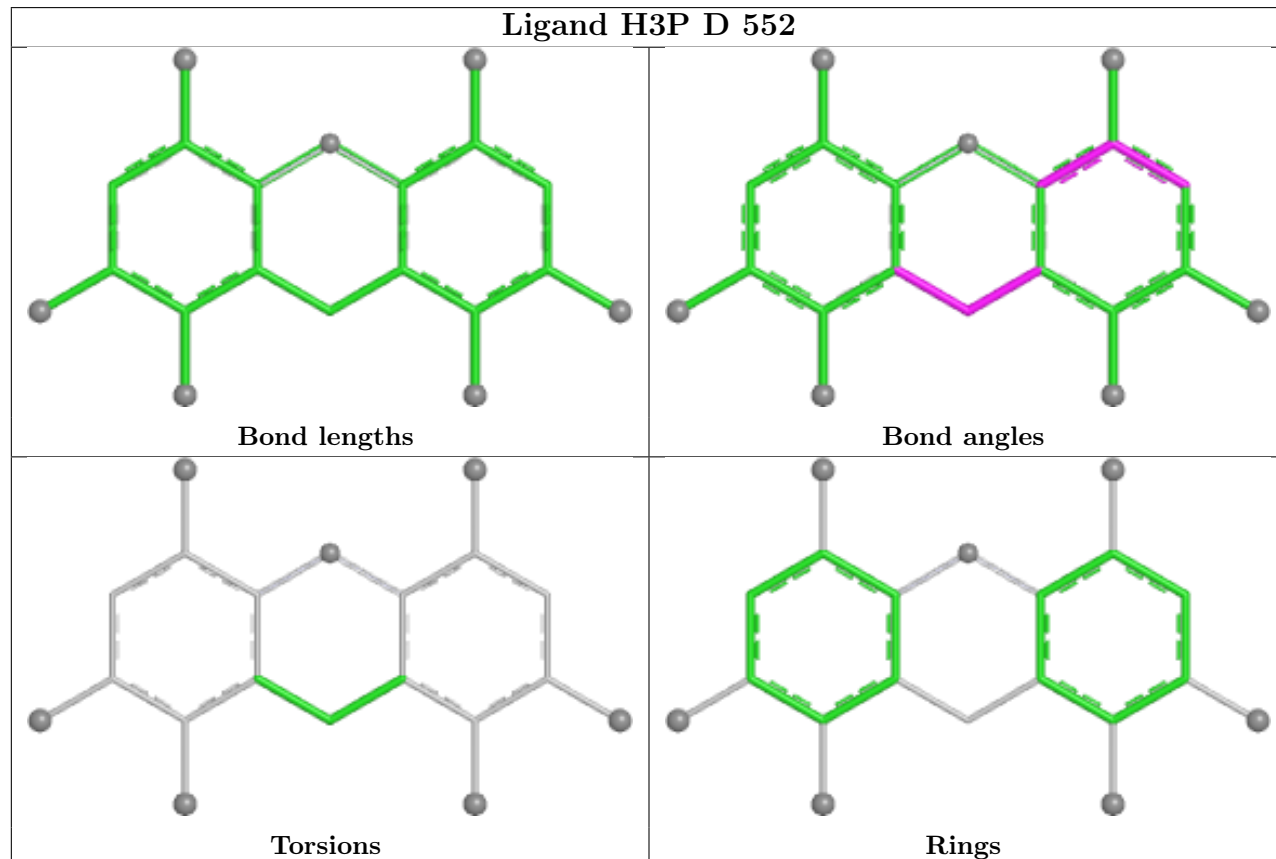
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	550	GLU	5	0
3	F	551	NDP	5	0
4	B	553	GTP	1	0
2	F	550	GLU	4	0
4	D	553	GTP	1	0
3	A	551	NDP	3	0
3	C	551	NDP	7	0
4	A	553	GTP	3	0
3	B	551	NDP	5	0
2	E	550	GLU	1	0
5	C	552	H3P	1	0
5	A	552	H3P	4	0
5	C	554	H3P	3	0
2	A	550	GLU	4	0

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

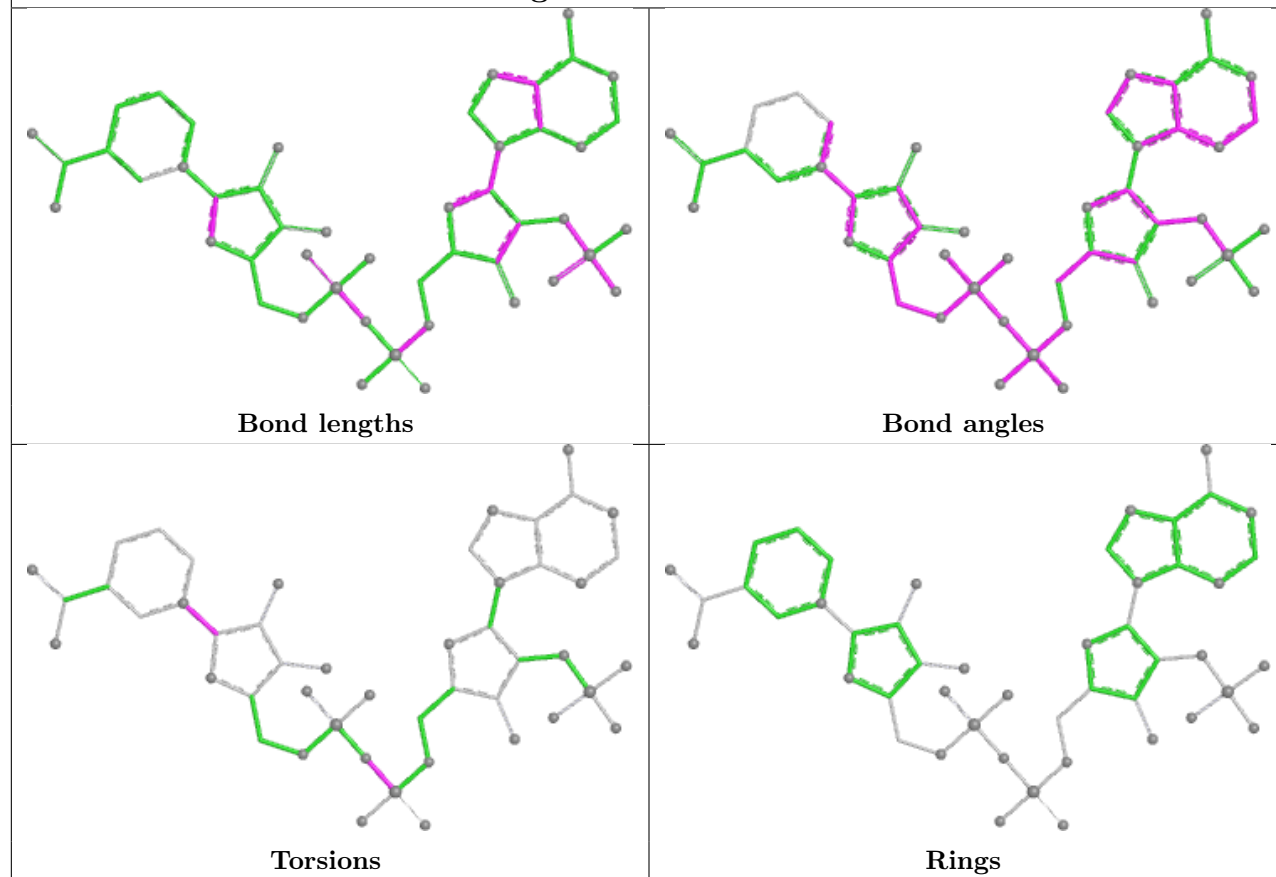
Ligand GTP E 553



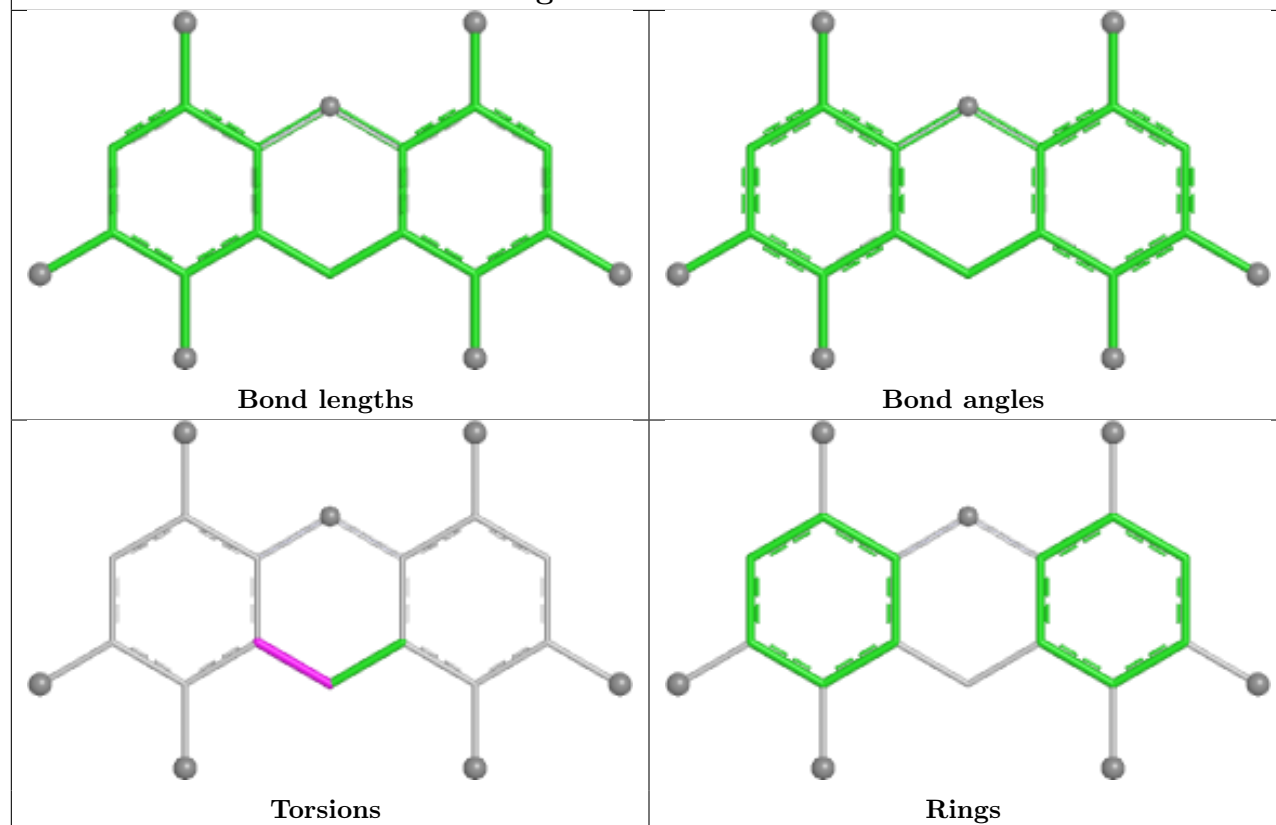
Ligand H3P D 552

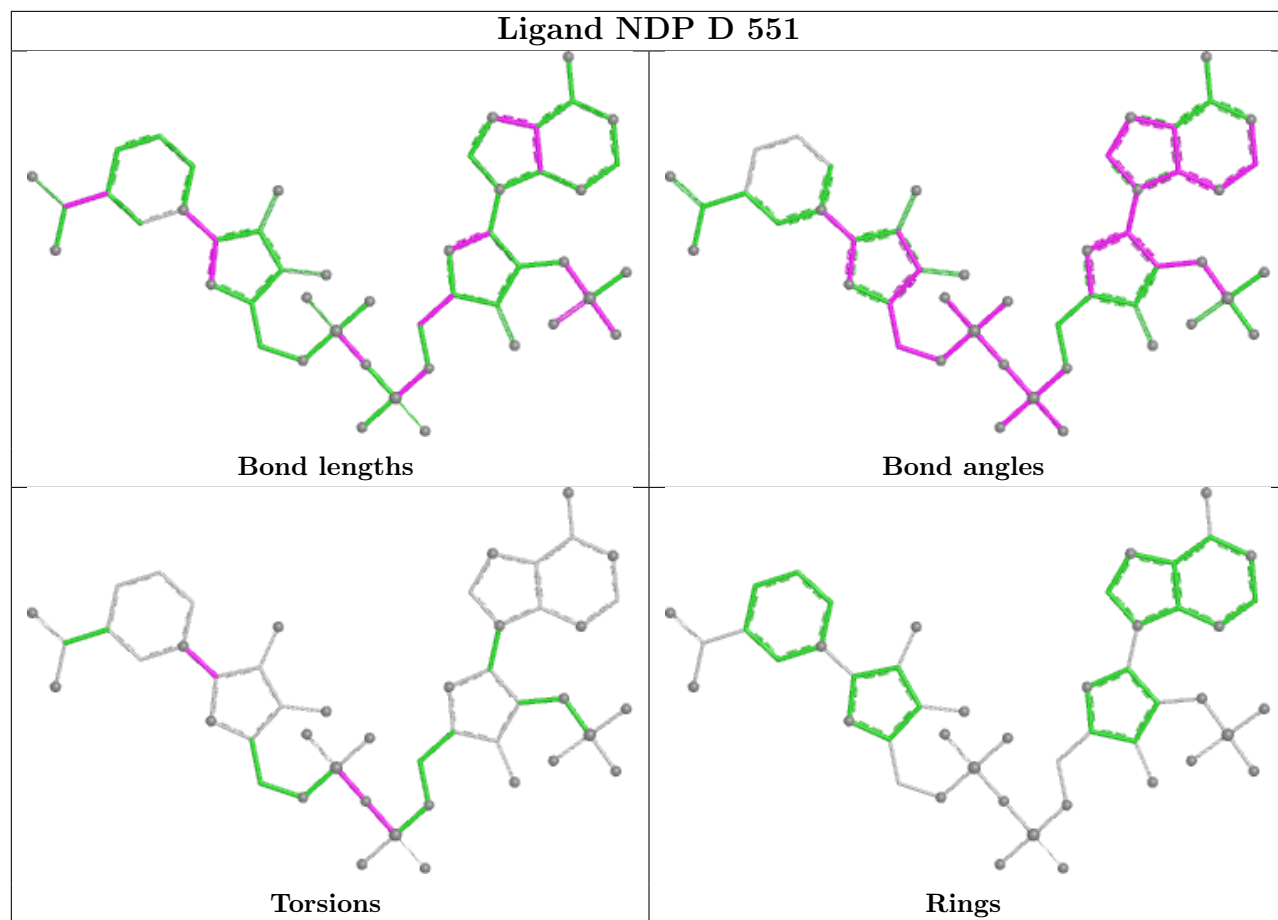


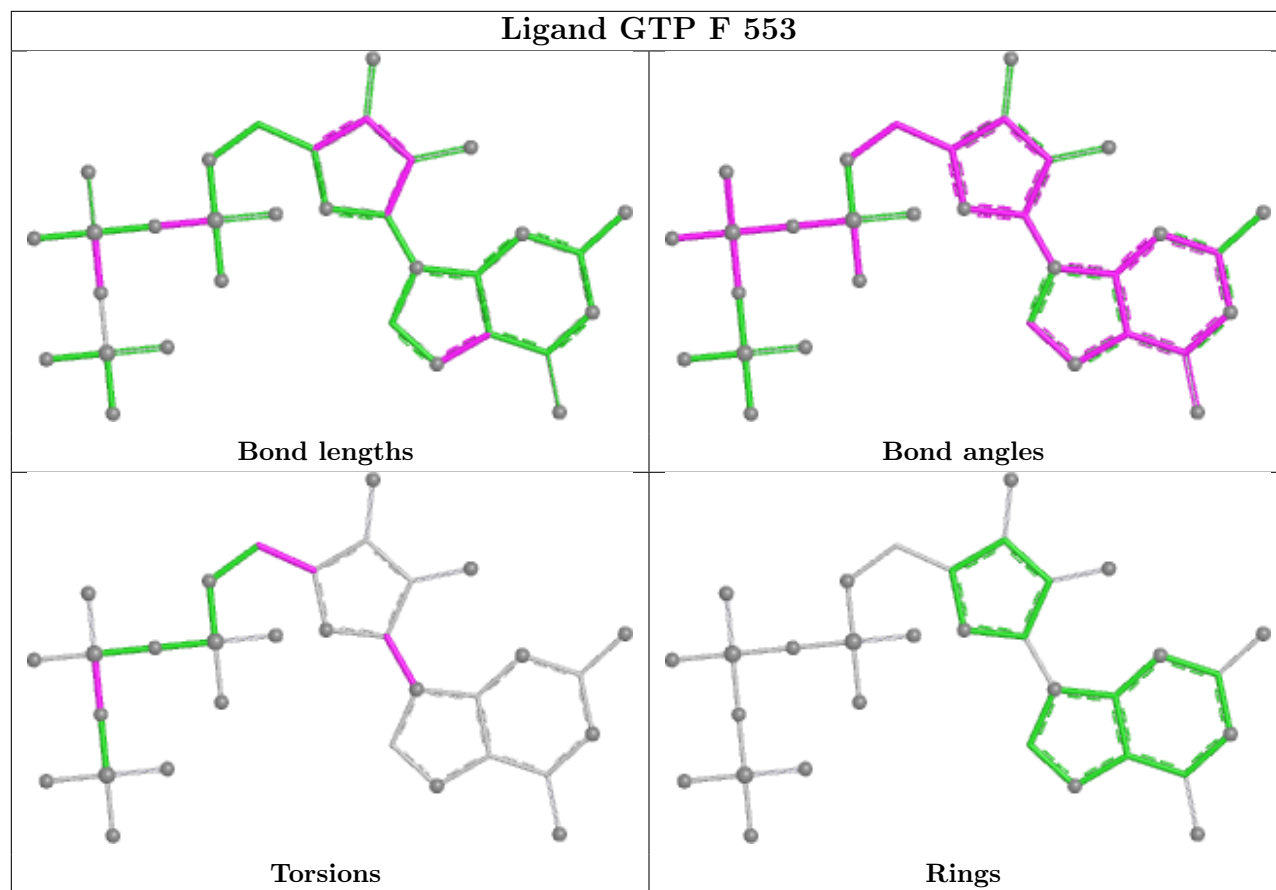
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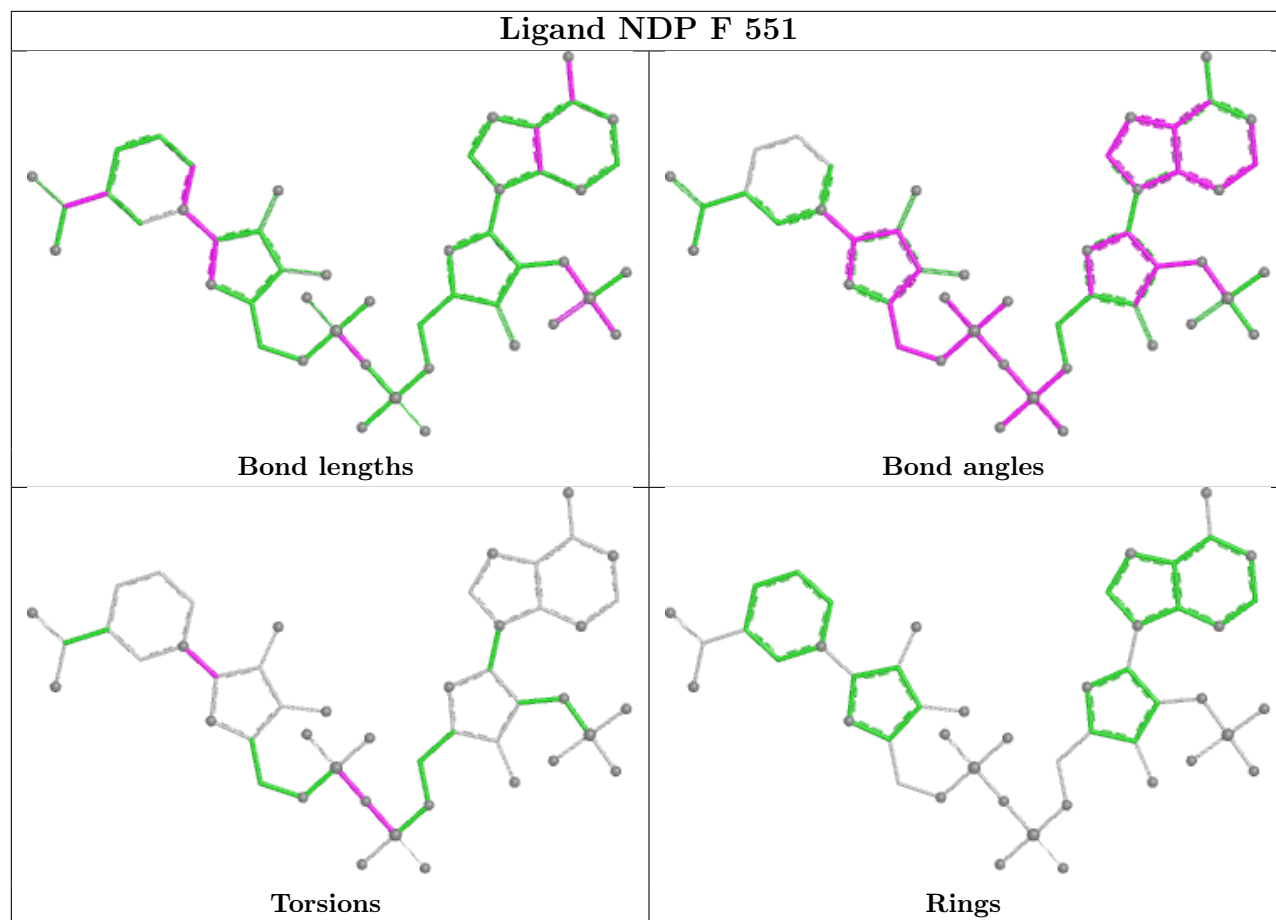


Ligand H3P F 552

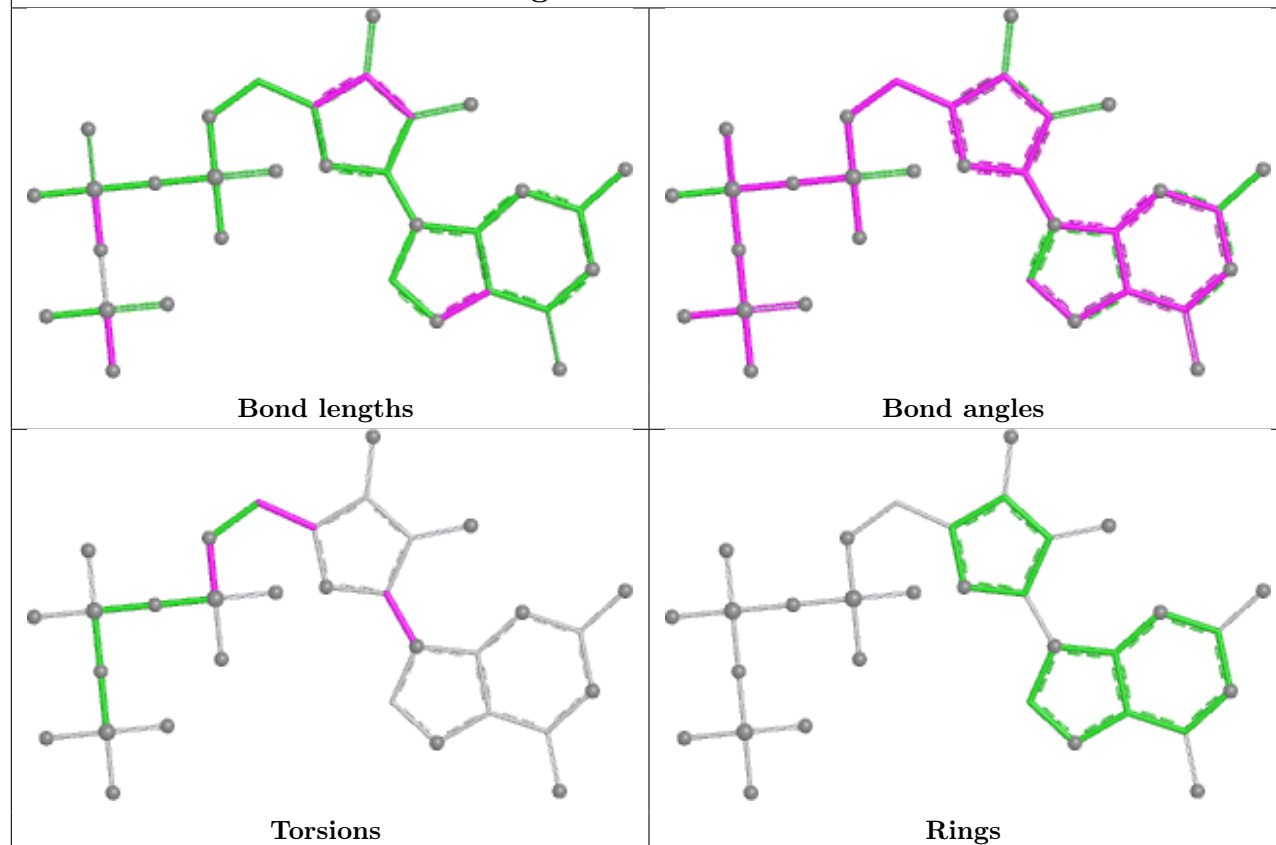




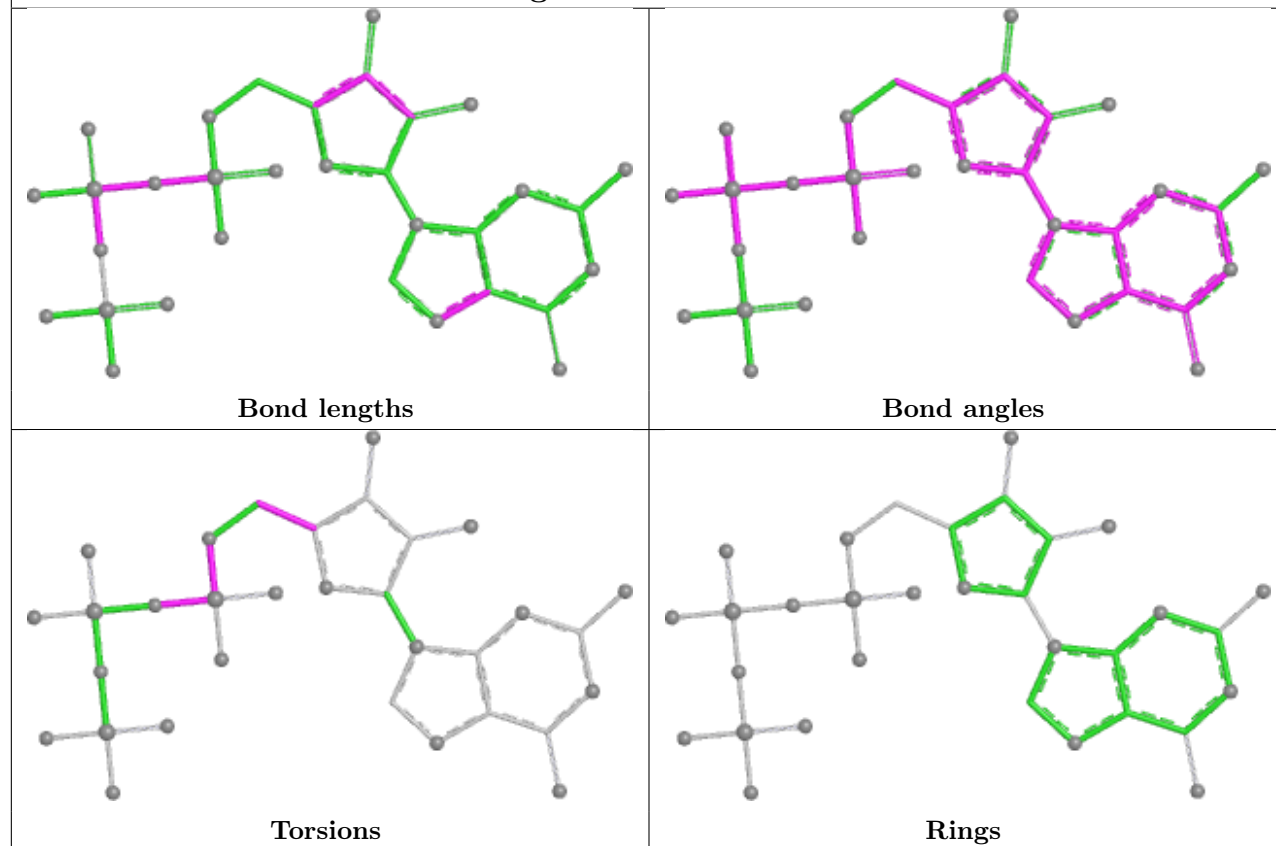


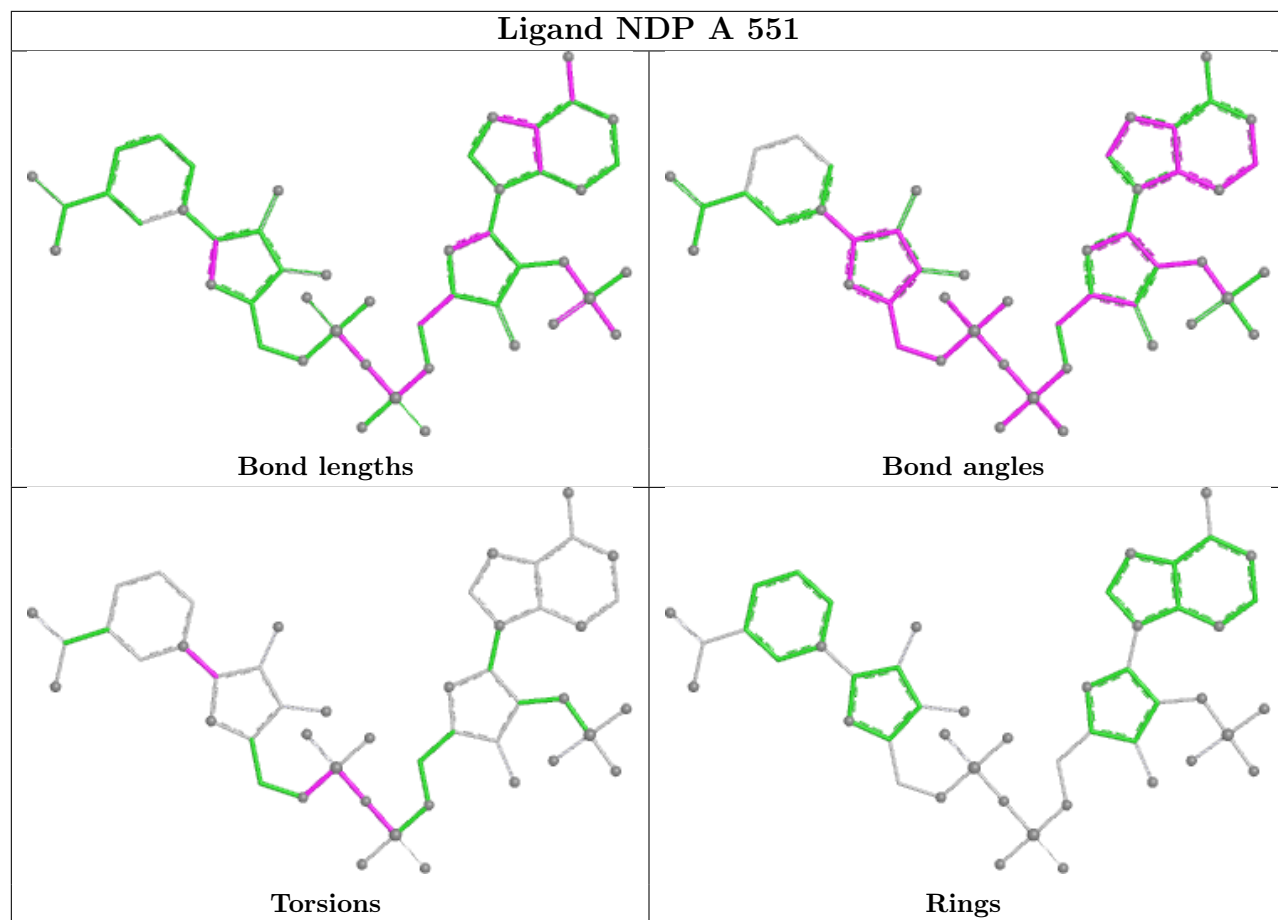


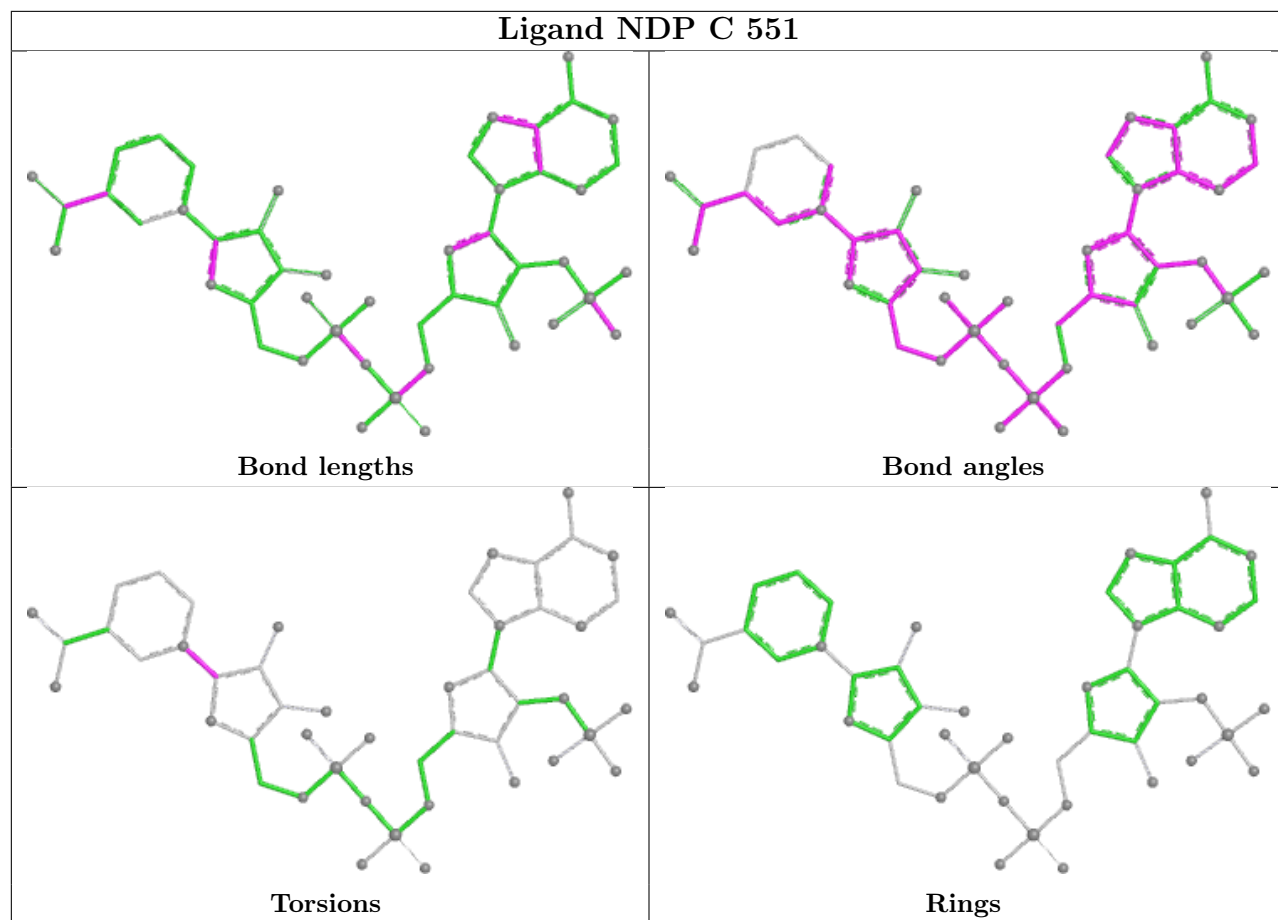
Ligand GTP B 553

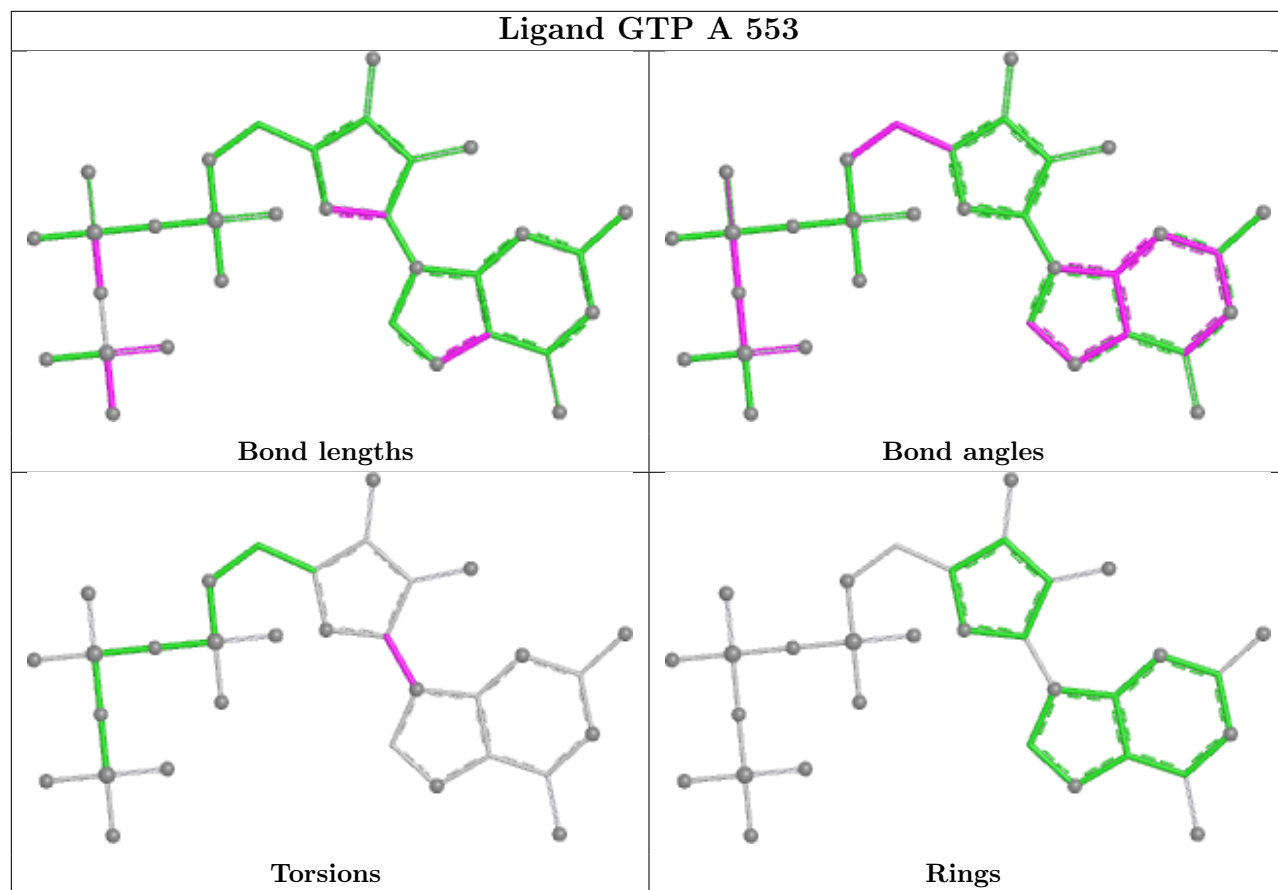


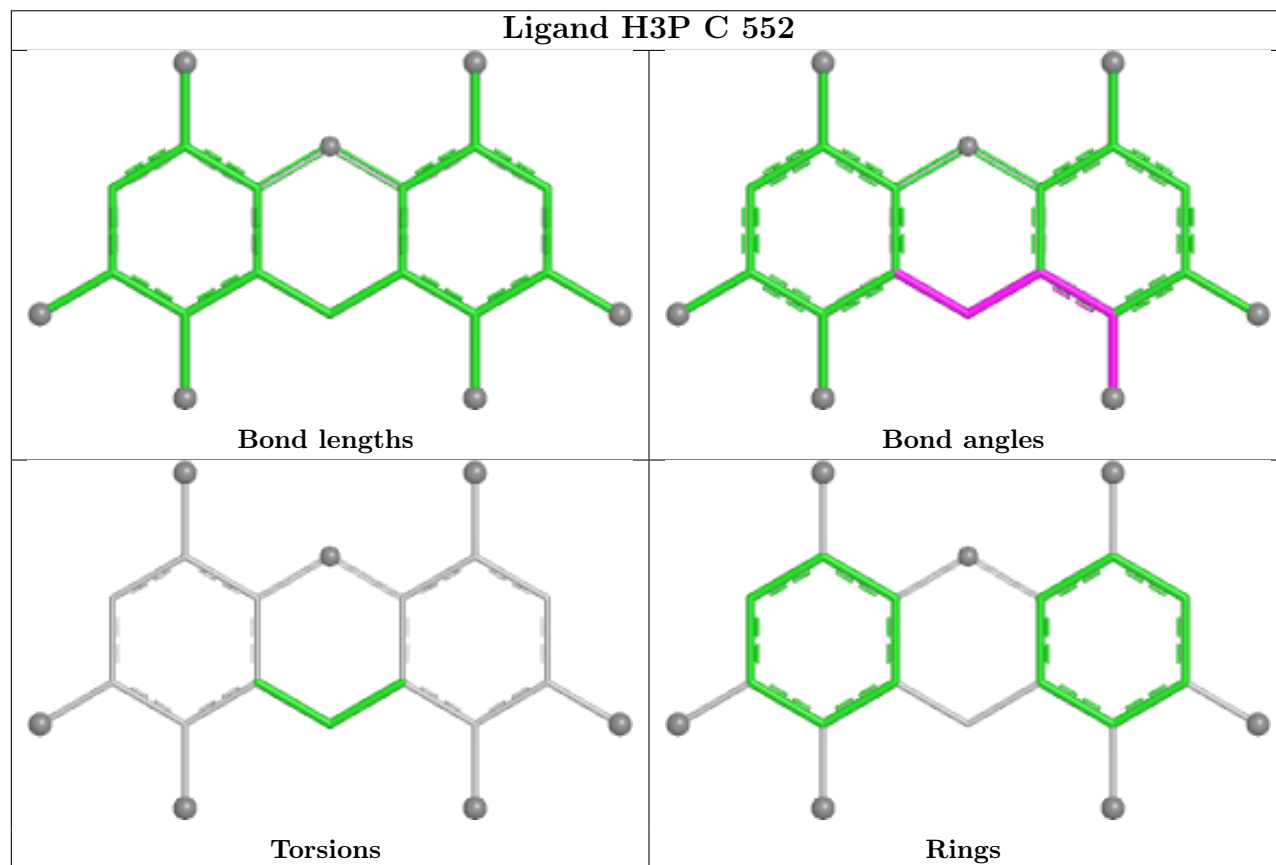
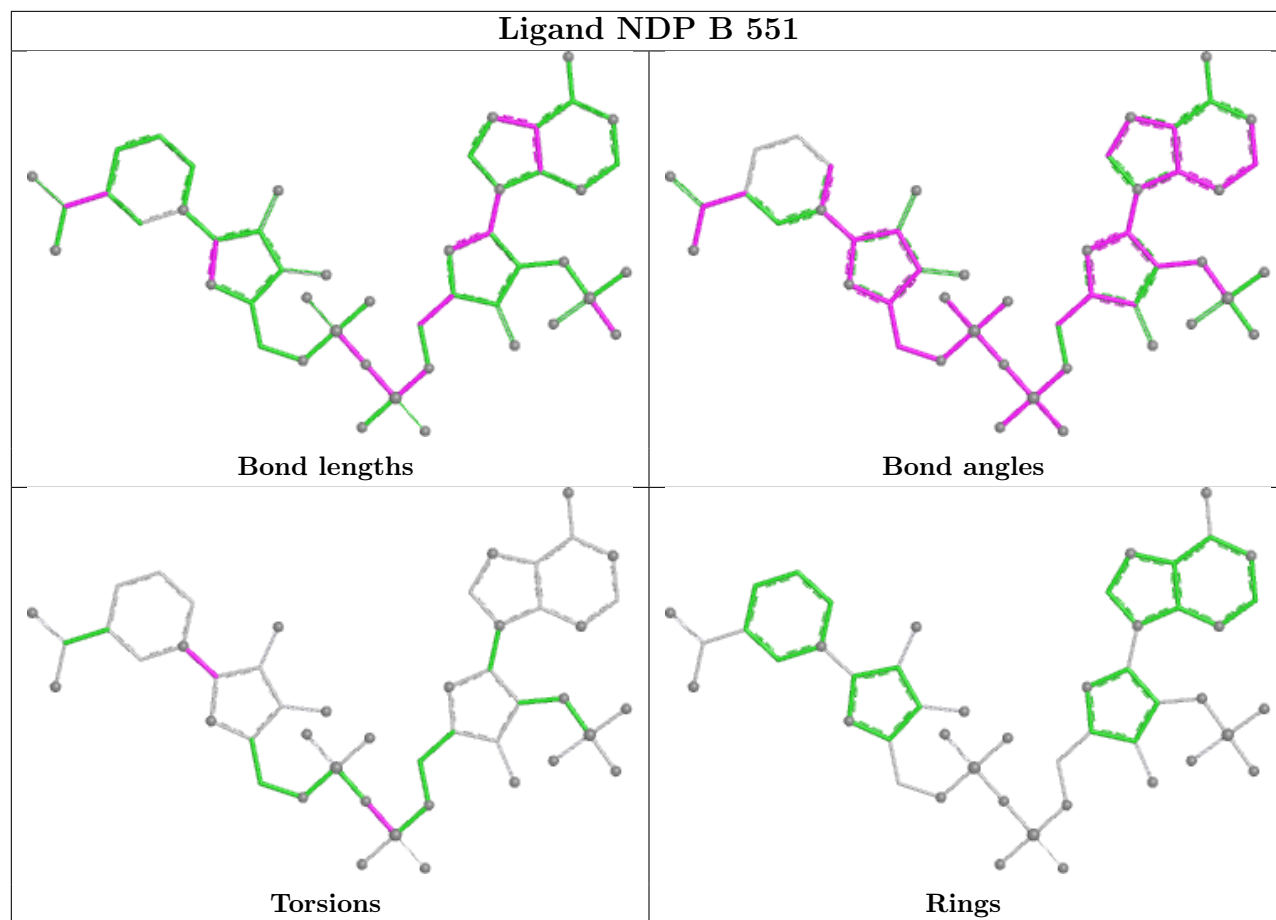
Ligand GTP D 553



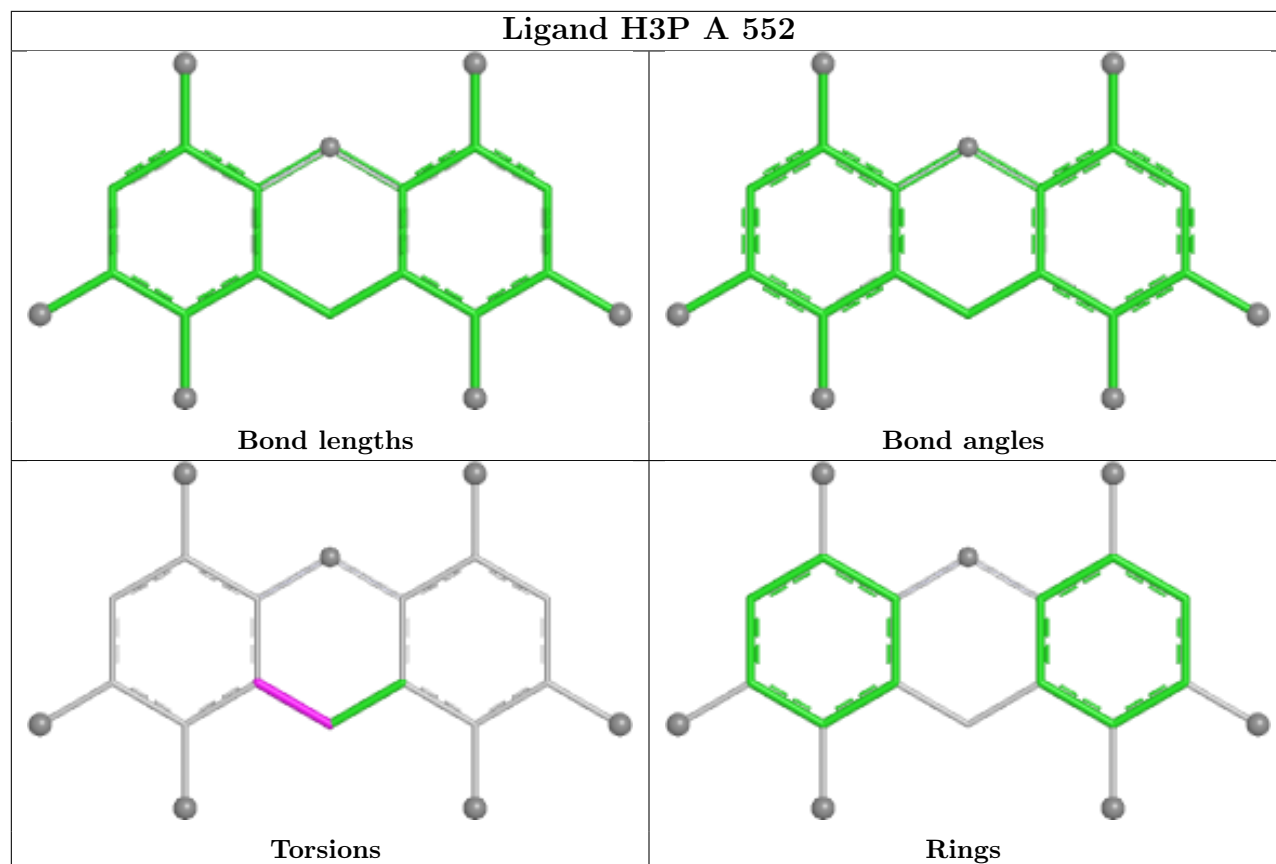




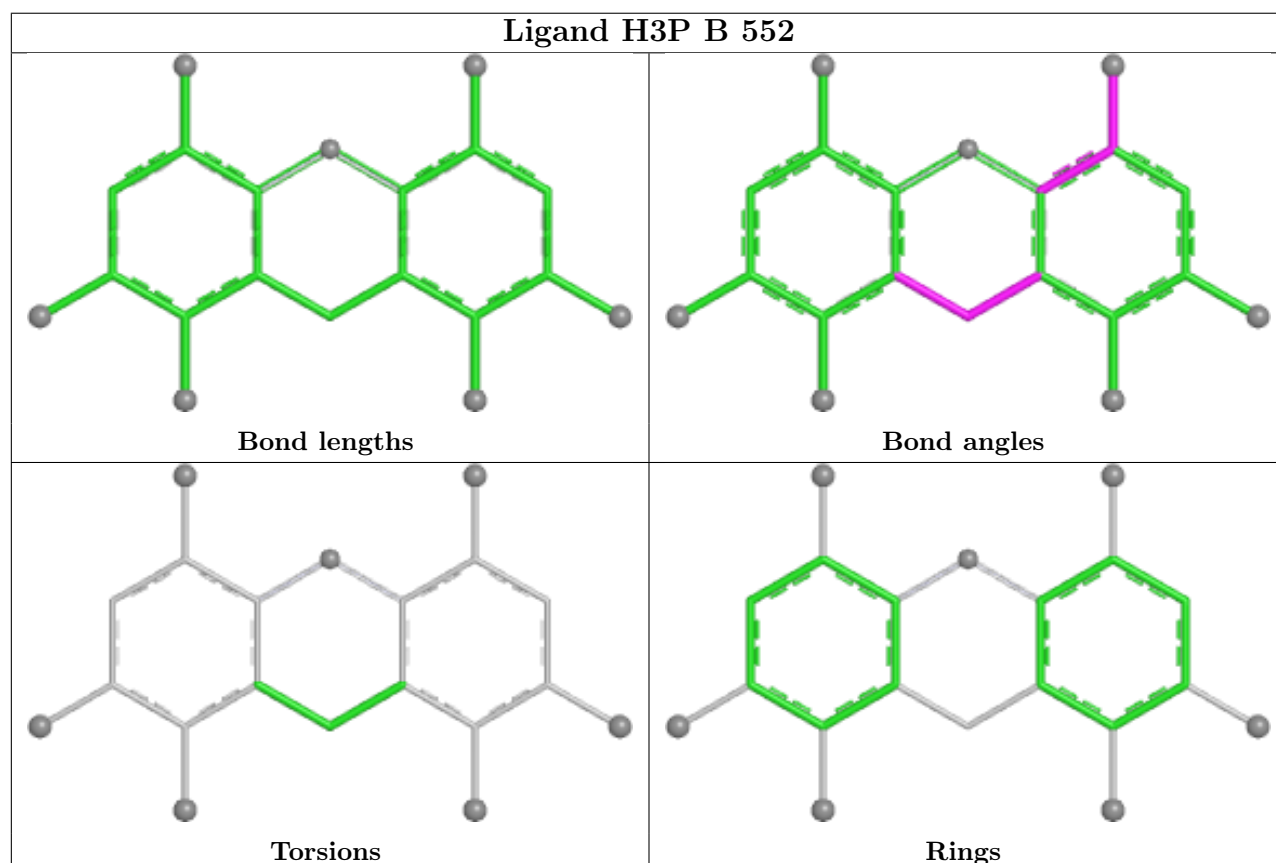




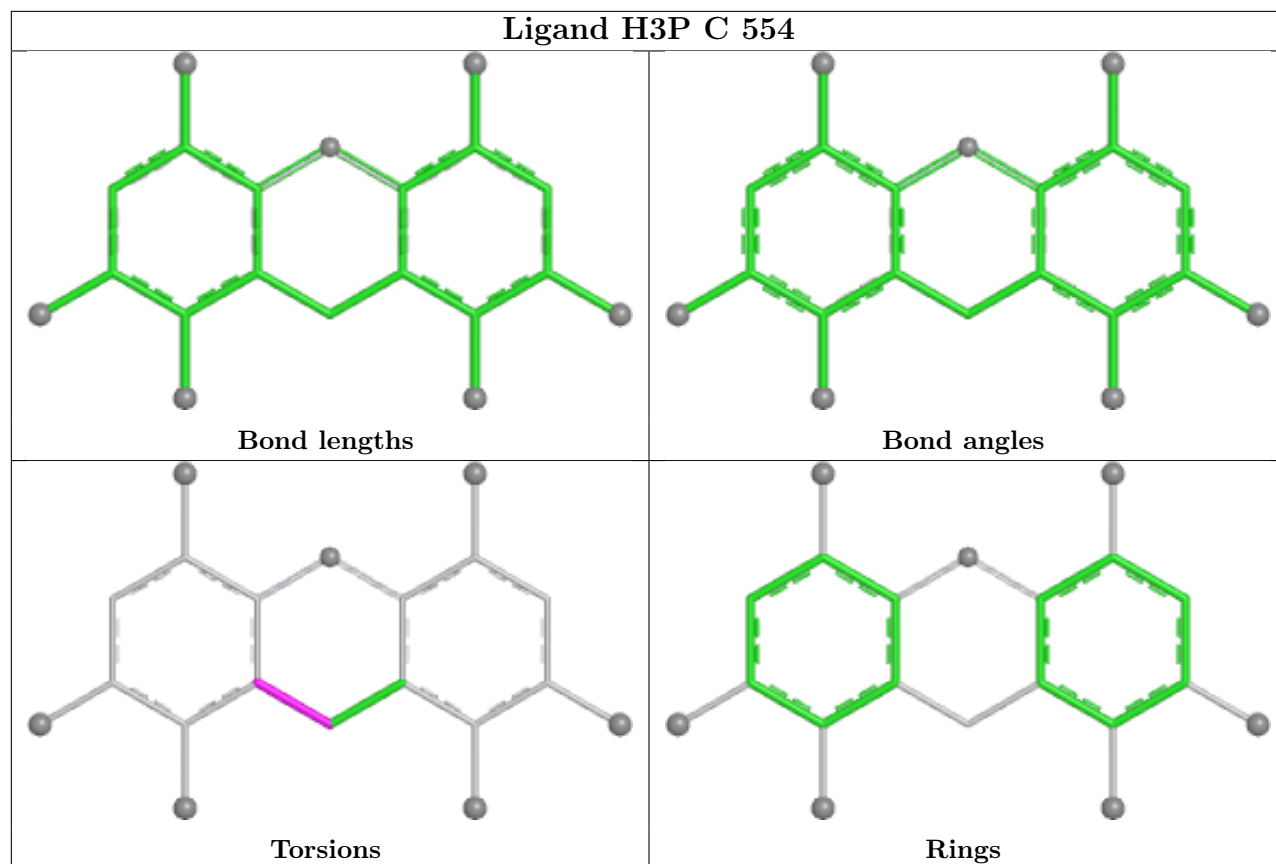
Ligand H3P A 552



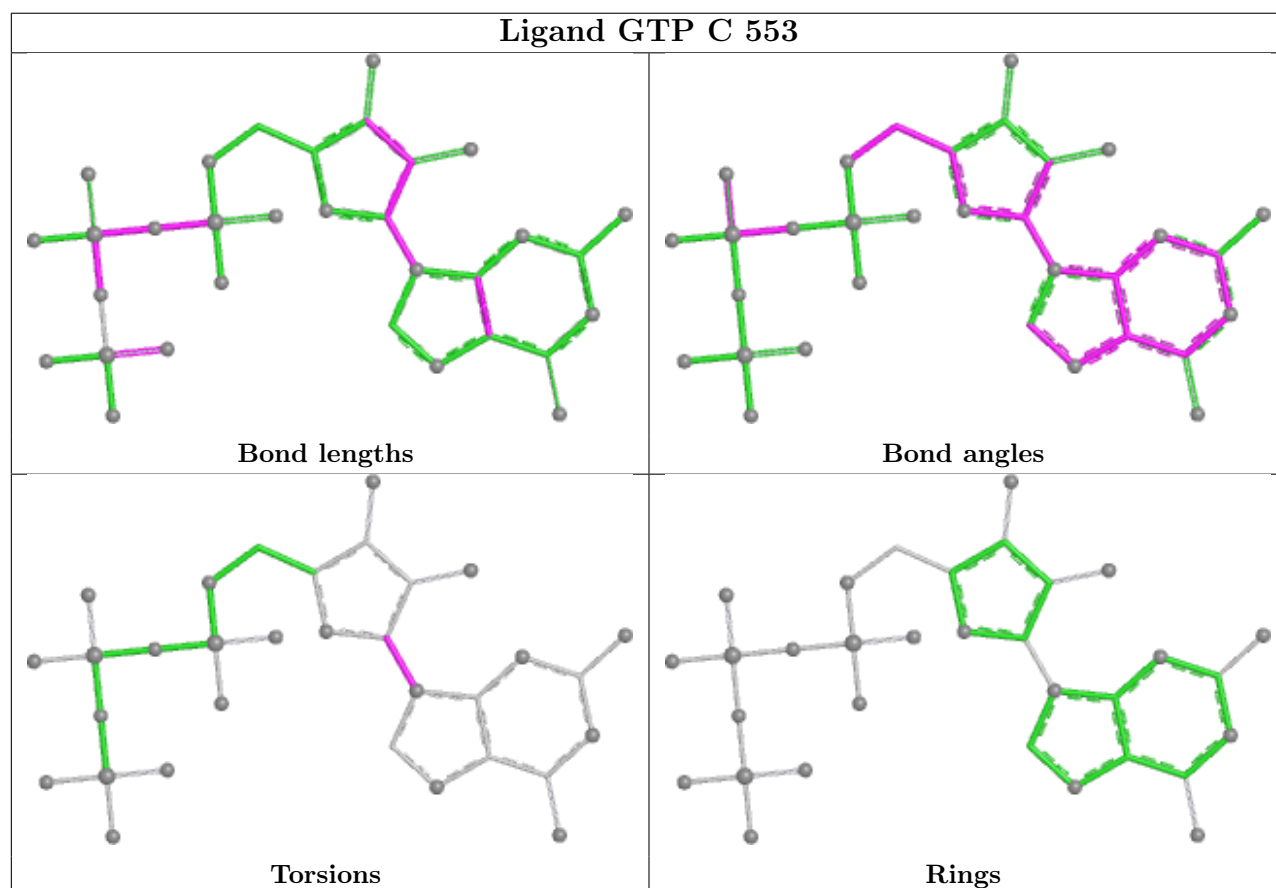
Ligand H3P B 552



Ligand H3P C 554



Ligand GTP C 553



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	495/501 (98%)	1.24	95 (19%) 3 2	67, 92, 109, 124	0
1	B	495/501 (98%)	1.01	54 (10%) 10 6	65, 90, 108, 123	0
1	C	495/501 (98%)	1.06	63 (12%) 8 5	64, 91, 108, 124	0
1	D	495/501 (98%)	1.16	81 (16%) 4 3	67, 92, 109, 123	0
1	E	495/501 (98%)	1.02	69 (13%) 6 4	66, 91, 110, 125	0
1	F	495/501 (98%)	1.08	61 (12%) 8 5	65, 92, 109, 124	0
All	All	2970/3006 (98%)	1.10	423 (14%) 6 4	64, 91, 109, 125	0

All (423) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	315	LEU	6.2
1	E	347	GLY	5.9
1	D	497	GLY	5.4
1	A	498	VAL	5.3
1	A	490	PHE	5.0
1	B	497	GLY	4.8
1	C	397	LEU	4.6
1	E	153	ALA	4.5
1	B	270	CYS	4.1
1	B	204	SER	4.1
1	A	493	TYR	4.0
1	C	375	ALA	4.0
1	D	406	ASN	4.0
1	C	349	ASN	3.9
1	E	273	VAL	3.8
1	A	322	LEU	3.8
1	D	461	ALA	3.8
1	E	181	ASP	3.8
1	D	58	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	161	GLY	3.8
1	D	421	PHE	3.7
1	C	498	VAL	3.7
1	D	464	ILE	3.7
1	C	398	THR	3.7
1	D	161	GLY	3.6
1	D	212	ILE	3.6
1	C	145	THR	3.6
1	D	302	LEU	3.6
1	B	84	GLN	3.5
1	E	421	PHE	3.5
1	A	347	GLY	3.5
1	A	197	CYS	3.5
1	F	431	VAL	3.5
1	B	286	ILE	3.5
1	A	421	PHE	3.4
1	D	373	LEU	3.4
1	F	485	ALA	3.4
1	E	376	GLY	3.4
1	C	9	PHE	3.4
1	E	13	VAL	3.4
1	F	158	ILE	3.4
1	F	421	PHE	3.4
1	A	489	VAL	3.4
1	E	160	PRO	3.3
1	A	464	ILE	3.3
1	C	448	ILE	3.3
1	E	57	HIS	3.3
1	E	150	MET	3.3
1	A	467	THR	3.2
1	F	64	PRO	3.2
1	D	160	PRO	3.2
1	C	451	SER	3.2
1	F	456	THR	3.2
1	A	453	LEU	3.2
1	E	324	PRO	3.2
1	F	83	SER	3.2
1	C	443	ALA	3.2
1	B	195	HIS	3.1
1	D	321	ILE	3.1
1	A	424	HIS	3.1
1	D	107	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	198	VAL	3.1
1	A	232	TYR	3.1
1	A	241	GLY	3.1
1	B	156	GLY	3.1
1	F	95	TYR	3.1
1	E	498	VAL	3.1
1	D	52	ILE	3.1
1	B	196	ALA	3.0
1	F	430	ILE	3.0
1	D	371	LEU	3.0
1	E	303	GLY	3.0
1	A	482	TYR	3.0
1	A	330	GLN	3.0
1	B	474	GLY	3.0
1	F	118	VAL	3.0
1	C	379	THR	3.0
1	A	223	ILE	3.0
1	A	324	PRO	3.0
1	D	167	PRO	3.0
1	D	273	VAL	3.0
1	A	175	GLU	2.9
1	D	498	VAL	2.9
1	E	20	GLY	2.9
1	A	148	PHE	2.9
1	C	160	PRO	2.9
1	A	474	GLY	2.9
1	D	397	LEU	2.9
1	E	379	THR	2.9
1	F	406	ASN	2.9
1	D	354	PRO	2.9
1	F	272	ALA	2.9
1	D	92	GLY	2.9
1	B	339	VAL	2.9
1	E	17	PHE	2.9
1	A	75	ILE	2.9
1	F	486	ILE	2.9
1	F	120	VAL	2.9
1	D	425	GLY	2.9
1	E	16	PHE	2.9
1	A	280	ILE	2.9
1	C	440	ILE	2.9
1	B	206	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	113	TYR	2.8
1	C	52	ILE	2.8
1	F	453	LEU	2.8
1	B	83	SER	2.8
1	C	214	ALA	2.8
1	D	148	PHE	2.8
1	E	148	PHE	2.8
1	A	248	ALA	2.8
1	C	255	VAL	2.8
1	D	379	THR	2.8
1	A	409	LEU	2.8
1	C	385	TRP	2.8
1	A	195	HIS	2.8
1	F	481	ALA	2.8
1	A	331	LEU	2.8
1	F	371	LEU	2.8
1	E	9	PHE	2.8
1	F	489	VAL	2.8
1	A	144	ILE	2.8
1	A	227	ILE	2.8
1	A	449	VAL	2.7
1	A	397	LEU	2.7
1	B	347	GLY	2.7
1	E	81	GLN	2.7
1	A	89	CYS	2.7
1	F	331	LEU	2.7
1	A	65	ILE	2.7
1	A	314	ILE	2.7
1	F	457	MET	2.7
1	B	425	GLY	2.7
1	D	195	HIS	2.7
1	F	498	VAL	2.7
1	A	359	ILE	2.7
1	A	366	MET	2.7
1	A	485	ALA	2.7
1	E	45	VAL	2.7
1	A	57	HIS	2.7
1	F	154	LYS	2.6
1	E	377	GLY	2.6
1	E	236	LEU	2.6
1	F	473	LEU	2.6
1	E	314	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	406	ASN	2.6
1	D	62	SER	2.6
1	F	195	HIS	2.6
1	F	493	TYR	2.6
1	C	167	PRO	2.6
1	D	191	ASP	2.6
1	A	486	ILE	2.6
1	A	349	ASN	2.6
1	C	315	LEU	2.6
1	A	476	ASP	2.6
1	D	291	LEU	2.6
1	E	129	VAL	2.6
1	E	154	LYS	2.6
1	E	131	ILE	2.5
1	E	309	ILE	2.5
1	B	259	SER	2.5
1	E	259	SER	2.5
1	C	251	GLY	2.5
1	F	417	LEU	2.5
1	F	477	LEU	2.5
1	B	498	VAL	2.5
1	A	52	ILE	2.5
1	A	309	ILE	2.5
1	C	428	ILE	2.5
1	C	195	HIS	2.5
1	B	405	SER	2.5
1	C	409	LEU	2.5
1	B	13	VAL	2.5
1	C	378	VAL	2.5
1	A	163	ASP	2.5
1	A	328	GLU	2.5
1	D	359	ILE	2.5
1	E	474	GLY	2.5
1	C	392	VAL	2.5
1	D	349	ASN	2.5
1	C	421	PHE	2.5
1	C	85	HIS	2.5
1	D	493	TYR	2.5
1	C	83	SER	2.5
1	B	10	PHE	2.5
1	E	493	TYR	2.5
1	E	104	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	325	ALA	2.4
1	D	184	ALA	2.4
1	E	272	ALA	2.4
1	C	405	SER	2.4
1	D	309	ILE	2.4
1	E	368	ILE	2.4
1	F	57	HIS	2.4
1	F	78	TYR	2.4
1	A	222	GLY	2.4
1	A	367	VAL	2.4
1	C	218	GLY	2.4
1	E	380	VAL	2.4
1	F	492	VAL	2.4
1	A	345	ALA	2.4
1	D	356	ALA	2.4
1	E	93	ILE	2.4
1	D	76	GLU	2.4
1	E	109	SER	2.4
1	F	9	PHE	2.4
1	D	257	LEU	2.4
1	A	200	GLY	2.4
1	D	241	GLY	2.4
1	D	48	ILE	2.4
1	D	260	MET	2.4
1	B	371	LEU	2.4
1	A	494	ASN	2.4
1	E	149	THR	2.4
1	D	95	TYR	2.4
1	D	123	GLY	2.4
1	D	481	ALA	2.4
1	F	360	PHE	2.4
1	A	479	THR	2.4
1	F	117	VAL	2.4
1	F	121	PRO	2.4
1	B	254	ASN	2.4
1	A	85	HIS	2.4
1	A	125	ALA	2.4
1	A	343	ILE	2.4
1	B	51	ILE	2.4
1	B	116	ALA	2.4
1	F	365	ILE	2.4
1	D	220	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	107	LEU	2.4
1	C	133	PRO	2.4
1	E	24	VAL	2.4
1	D	87	THR	2.3
1	A	179	ILE	2.3
1	A	325	ALA	2.3
1	C	480	ALA	2.3
1	D	221	HIS	2.3
1	F	455	TYR	2.3
1	B	473	LEU	2.3
1	D	409	LEU	2.3
1	E	61	LEU	2.3
1	E	84	GLN	2.3
1	F	397	LEU	2.3
1	F	175	GLU	2.3
1	F	413	VAL	2.3
1	B	208	ILE	2.3
1	B	314	ILE	2.3
1	F	135	ASN	2.3
1	F	233	MET	2.3
1	A	323	ILE	2.3
1	E	178	TRP	2.3
1	B	496	ALA	2.3
1	D	194	ALA	2.3
1	D	394	TYR	2.3
1	E	247	PHE	2.3
1	B	162	VAL	2.3
1	F	380	VAL	2.3
1	A	192	ILE	2.3
1	C	377	GLY	2.3
1	E	80	ALA	2.3
1	A	457	MET	2.3
1	A	405	SER	2.3
1	F	352	THR	2.3
1	B	453	LEU	2.3
1	B	455	TYR	2.3
1	D	372	TYR	2.3
1	A	104	VAL	2.3
1	A	487	GLU	2.3
1	A	344	ILE	2.3
1	B	93	ILE	2.3
1	C	196	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	479	THR	2.3
1	C	394	TYR	2.3
1	C	493	TYR	2.3
1	B	81	GLN	2.3
1	D	489	VAL	2.3
1	C	38	GLU	2.2
1	C	151	GLU	2.2
1	A	187	ILE	2.2
1	A	286	ILE	2.2
1	B	368	ILE	2.2
1	D	314	ILE	2.2
1	A	315	LEU	2.2
1	C	322	LEU	2.2
1	F	59	LEU	2.2
1	F	405	SER	2.2
1	A	219	VAL	2.2
1	C	99	VAL	2.2
1	E	254	ASN	2.2
1	F	435	GLU	2.2
1	C	184	ALA	2.2
1	D	218	GLY	2.2
1	F	410	LEU	2.2
1	D	9	PHE	2.2
1	D	155	LYS	2.2
1	F	226	PHE	2.2
1	C	113	TYR	2.2
1	E	120	VAL	2.2
1	A	484	ASN	2.2
1	A	131	ILE	2.2
1	C	319	CYS	2.2
1	D	223	ILE	2.2
1	A	244	ASP	2.2
1	A	350	GLY	2.2
1	C	324	PRO	2.2
1	D	61	LEU	2.2
1	E	481	ALA	2.2
1	F	496	ALA	2.2
1	C	63	PHE	2.2
1	D	466	ARG	2.2
1	E	195	HIS	2.2
1	D	170	SER	2.2
1	B	205	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	51	ILE	2.2
1	E	286	ILE	2.2
1	F	48	ILE	2.2
1	D	390	ASN	2.2
1	C	28	LEU	2.2
1	F	315	LEU	2.2
1	B	108	ALA	2.2
1	C	270	CYS	2.2
1	E	128	GLY	2.2
1	B	421	PHE	2.2
1	E	436	PHE	2.2
1	C	479	THR	2.2
1	D	382	TYR	2.2
1	E	249	VAL	2.2
1	A	313	SER	2.2
1	D	84	GLN	2.2
1	F	204	SER	2.2
1	F	314	ILE	2.2
1	A	160	PRO	2.2
1	A	329	LYS	2.2
1	A	337	PRO	2.2
1	D	64	PRO	2.2
1	D	419	ARG	2.2
1	A	117	VAL	2.1
1	C	45	VAL	2.1
1	E	95	TYR	2.1
1	C	48	ILE	2.1
1	C	51	ILE	2.1
1	E	397	LEU	2.1
1	F	28	LEU	2.1
1	E	100	SER	2.1
1	E	63	PHE	2.1
1	E	383	PHE	2.1
1	A	380	VAL	2.1
1	C	87	THR	2.1
1	C	208	ILE	2.1
1	F	321	ILE	2.1
1	F	386	LEU	2.1
1	B	341	ALA	2.1
1	A	460	SER	2.1
1	C	64	PRO	2.1
1	E	133	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	254	ASN	2.1
1	B	349	ASN	2.1
1	F	228	ASN	2.1
1	A	162	VAL	2.1
1	E	270	CYS	2.1
1	A	450	HIS	2.1
1	D	424	HIS	2.1
1	A	87	THR	2.1
1	B	48	ILE	2.1
1	B	448	ILE	2.1
1	C	291	LEU	2.1
1	D	59	LEU	2.1
1	D	315	LEU	2.1
1	E	366	MET	2.1
1	B	160	PRO	2.1
1	B	383	PHE	2.1
1	B	451	SER	2.1
1	B	164	VAL	2.1
1	D	317	VAL	2.1
1	F	339	VAL	2.1
1	A	368	ILE	2.1
1	A	371	LEU	2.1
1	D	301	ILE	2.1
1	E	424	HIS	2.1
1	F	5	ASP	2.1
1	B	485	ALA	2.1
1	C	348	ALA	2.1
1	B	452	GLY	2.1
1	D	474	GLY	2.1
1	D	294	PHE	2.1
1	D	383	PHE	2.1
1	A	22	SER	2.1
1	D	109	SER	2.1
1	C	439	ARG	2.1
1	D	410	LEU	2.1
1	E	440	ILE	2.1
1	E	293	ASP	2.1
1	A	270	CYS	2.1
1	C	194	ALA	2.1
1	D	480	ALA	2.1
1	C	123	GLY	2.1
1	C	483	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	162	VAL	2.0
1	A	23	ILE	2.0
1	B	28	LEU	2.0
1	E	323	ILE	2.0
1	A	465	MET	2.0
1	B	450	HIS	2.0
1	D	85	HIS	2.0
1	D	366	MET	2.0
1	B	352	THR	2.0
1	A	369	PRO	2.0
1	A	436	PHE	2.0
1	B	426	GLY	2.0
1	E	151	GLU	2.0
1	A	74	VAL	2.0
1	A	417	LEU	2.0
1	C	177	SER	2.0
1	E	52	ILE	2.0
1	D	348	ALA	2.0
1	A	191	ASP	2.0
1	E	360	PHE	2.0
1	F	20	GLY	2.0
1	E	64	PRO	2.0
1	D	396	ARG	2.0
1	B	110	LEU	2.0
1	C	309	ILE	2.0
1	E	223	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

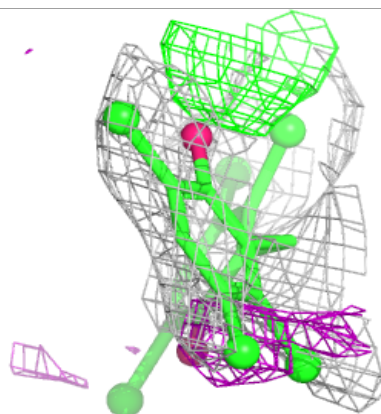
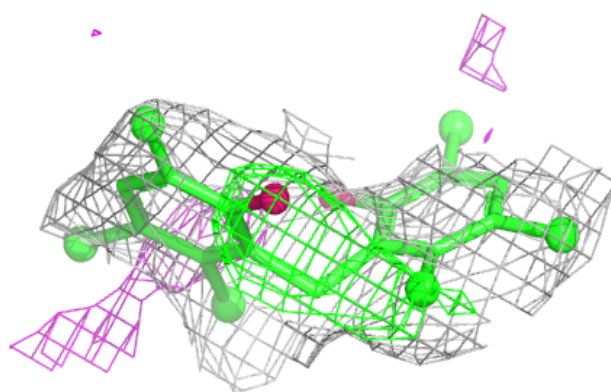
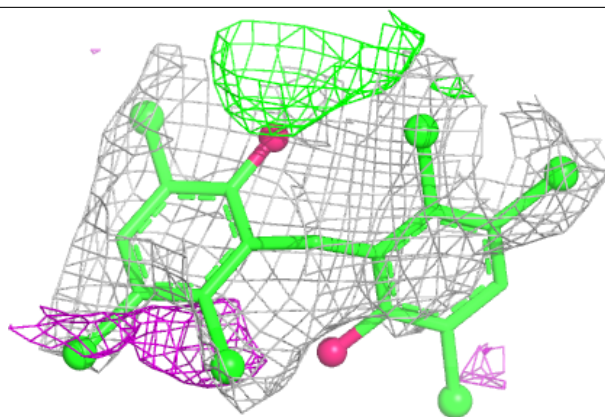
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	H3P	C	554	21/21	0.46	0.18	122,128,130,135	0
2	GLU	F	550	9/10	0.58	0.25	97,100,101,102	0
5	H3P	B	552	21/21	0.62	0.17	119,131,139,143	0
5	H3P	A	552	21/21	0.65	0.16	124,129,131,137	0
2	GLU	D	550	9/10	0.67	0.19	100,102,102,102	0
5	H3P	C	552	21/21	0.68	0.16	117,131,136,139	0
3	NDP	D	551	48/48	0.69	0.17	89,97,102,106	0
4	GTP	A	553	32/32	0.69	0.15	123,134,150,151	0
4	GTP	D	553	32/32	0.70	0.13	116,121,123,124	0
4	GTP	F	553	32/32	0.70	0.13	126,132,135,136	0
4	GTP	E	553	32/32	0.71	0.12	124,130,133,133	0
5	H3P	F	552	21/21	0.71	0.15	122,128,131,134	0
2	GLU	A	550	9/10	0.72	0.21	97,97,98,98	0
5	H3P	D	552	21/21	0.74	0.14	118,132,138,143	0
2	GLU	B	550	9/10	0.74	0.19	76,80,83,84	0
3	NDP	F	551	48/48	0.75	0.16	103,111,114,115	0
4	GTP	B	553	32/32	0.76	0.12	109,117,122,125	0
3	NDP	E	551	48/48	0.77	0.15	104,115,126,128	0
3	NDP	A	551	48/48	0.78	0.16	87,100,105,108	0
4	GTP	C	553	32/32	0.79	0.12	112,130,133,133	0
2	GLU	C	550	9/10	0.81	0.17	85,88,88,89	0
3	NDP	B	551	48/48	0.82	0.15	88,95,103,106	0
3	NDP	C	551	48/48	0.85	0.12	84,91,94,95	0
2	GLU	E	550	9/10	0.85	0.15	86,89,89,90	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.

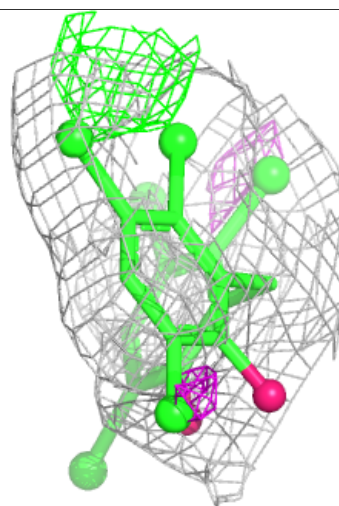
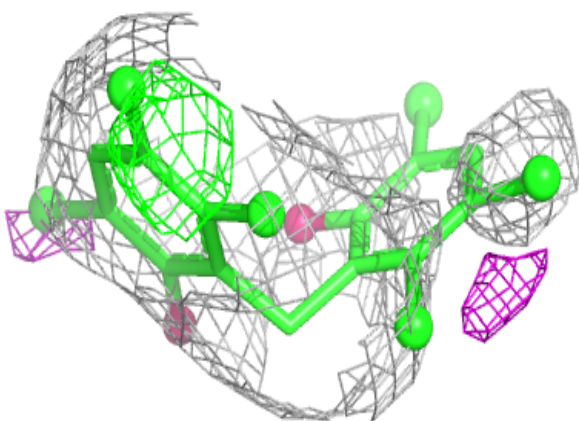
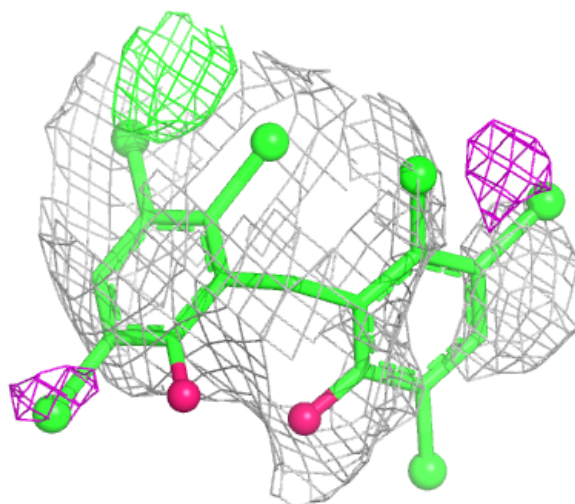
Electron density around H3P C 554:

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



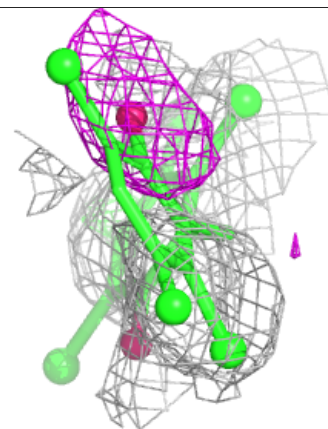
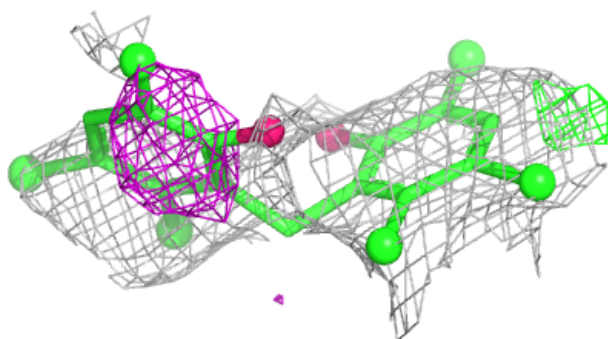
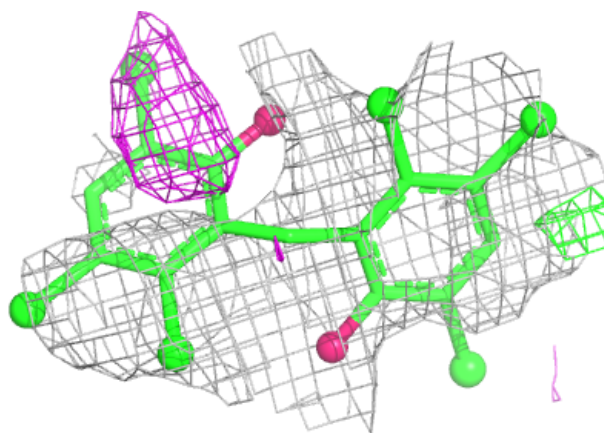
Electron density around H3P B 552:

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



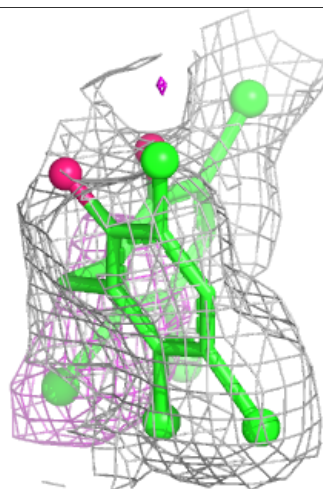
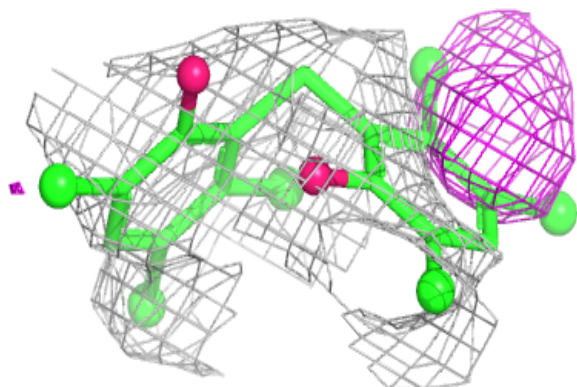
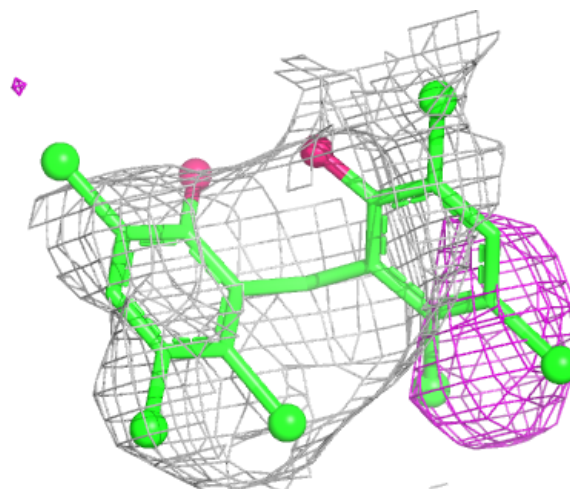
Electron density around H3P A 552:

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



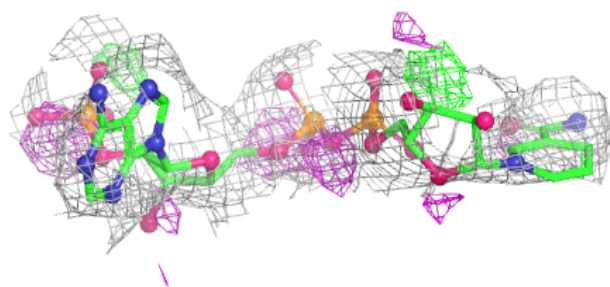
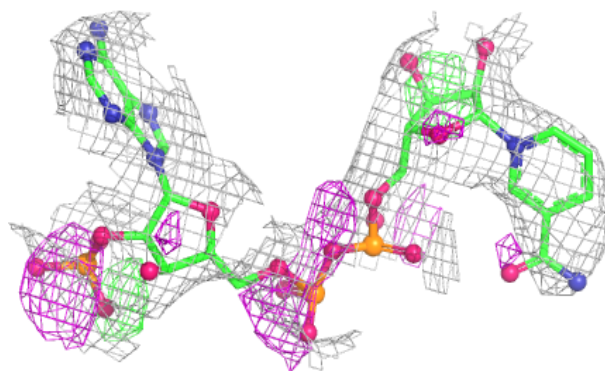
Electron density around H3P C 552:

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

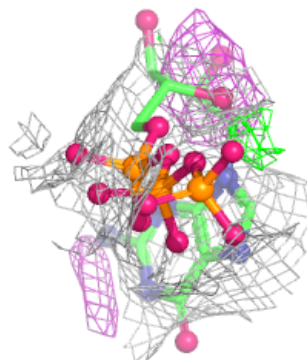
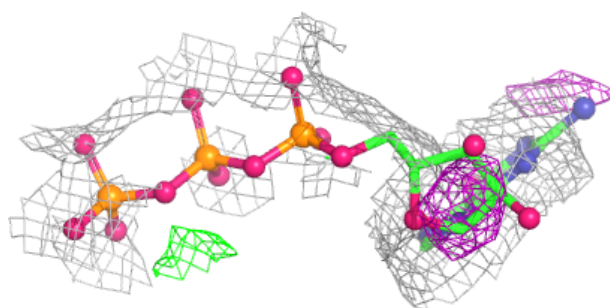
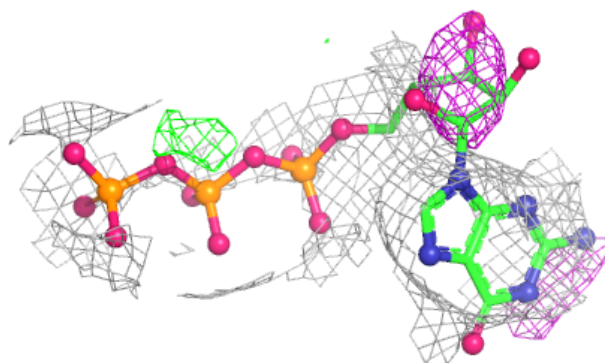


Electron density around NDP D 551:

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

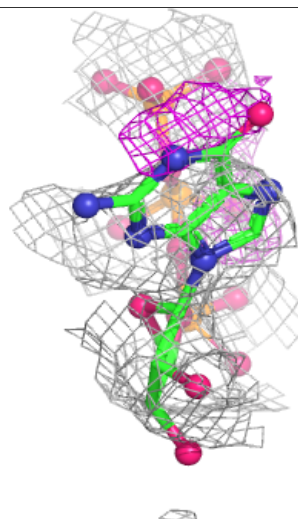
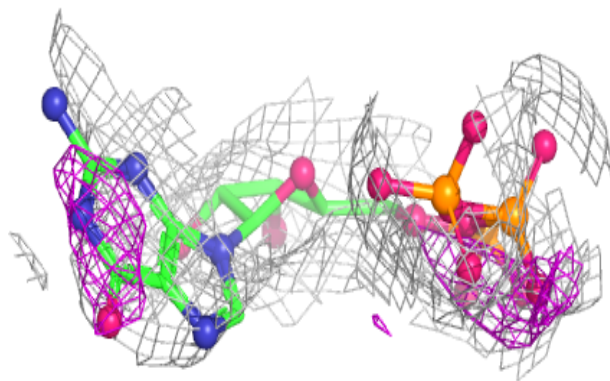
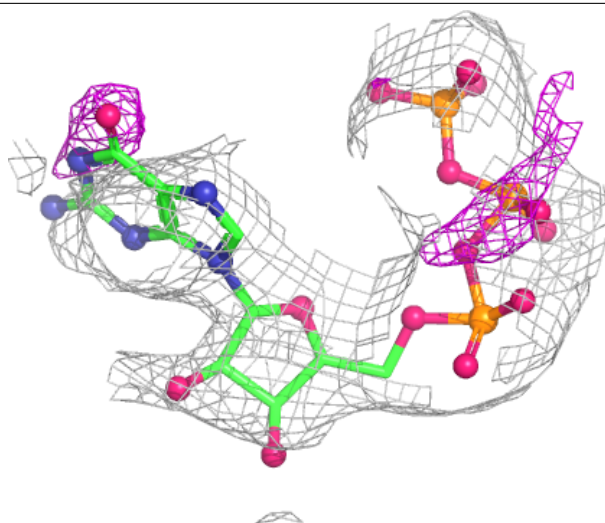
**Electron density around GTP A 553:**

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



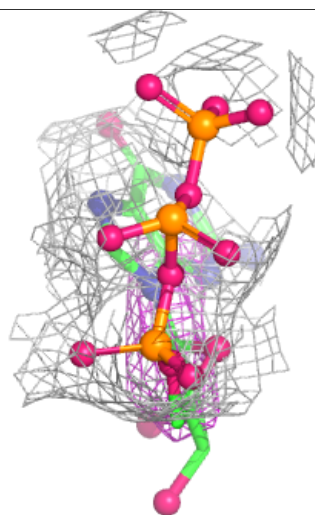
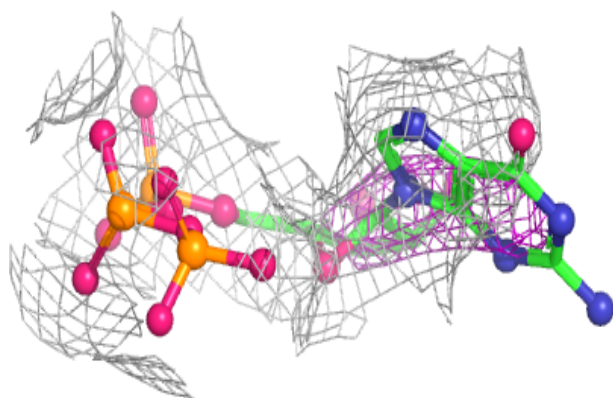
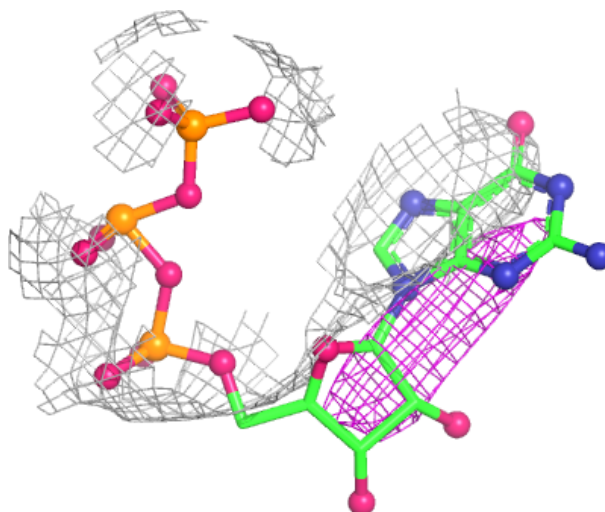
Electron density around GTP D 553:

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



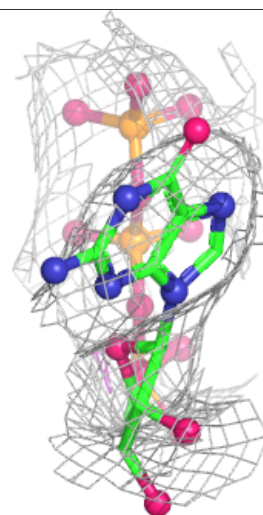
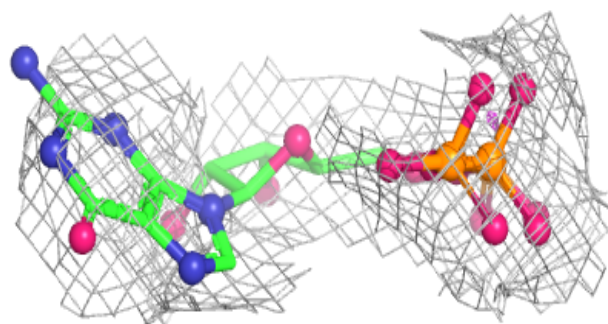
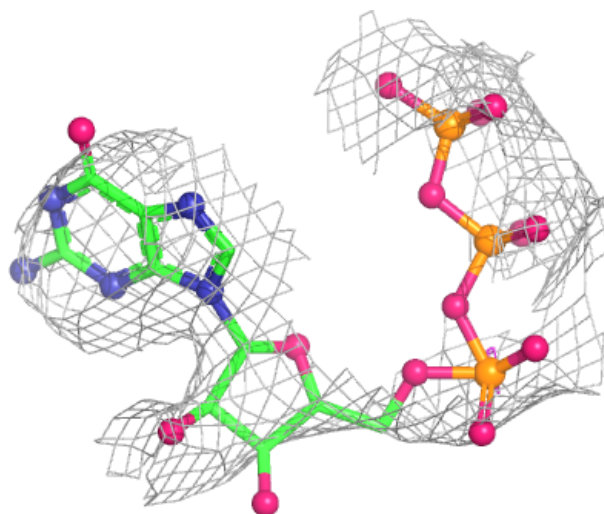
Electron density around GTP F 553:

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



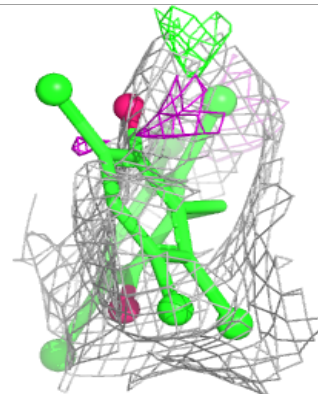
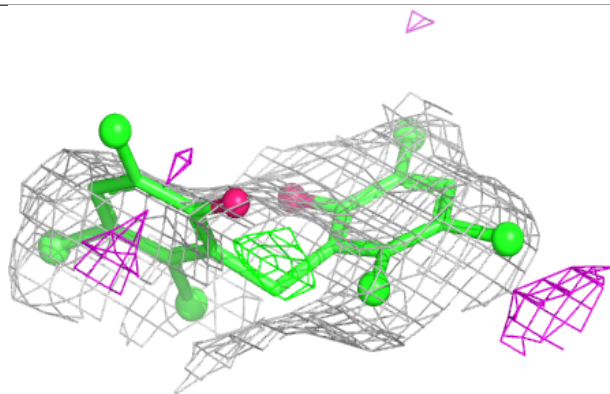
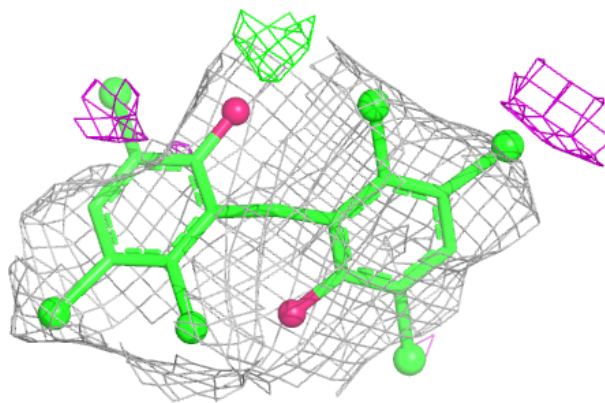
Electron density around GTP E 553:

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



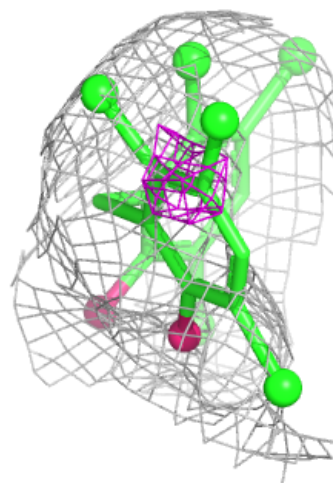
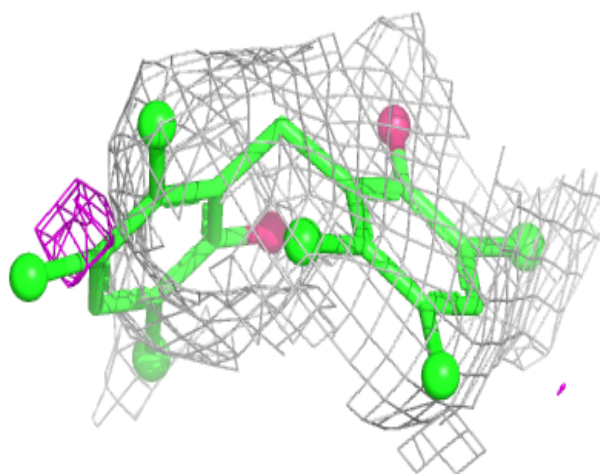
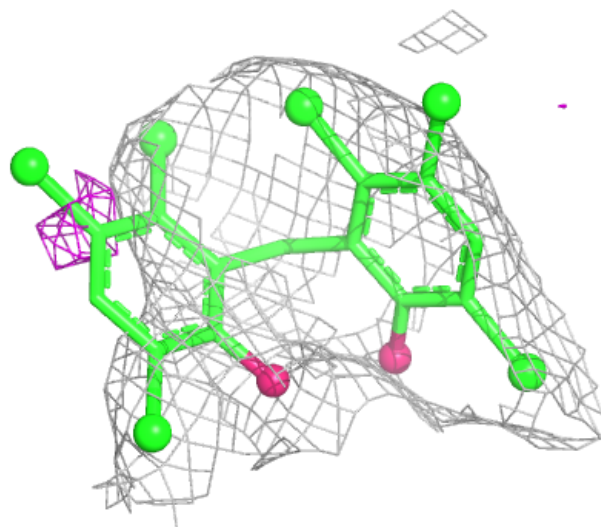
Electron density around H3P F 552:

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



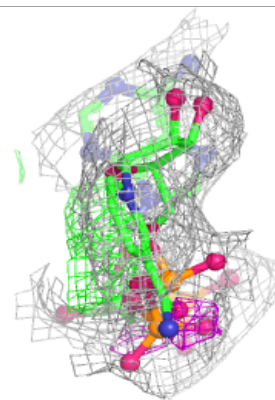
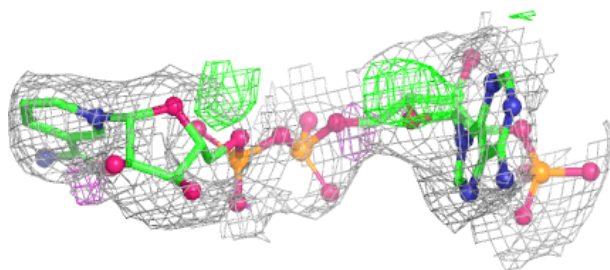
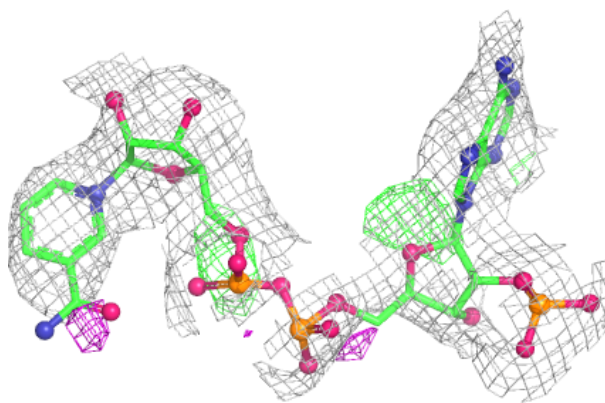
Electron density around H3P D 552:

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



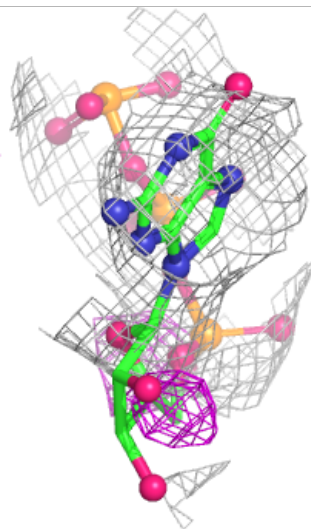
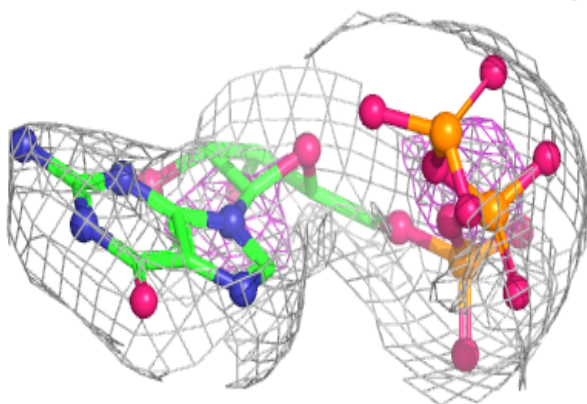
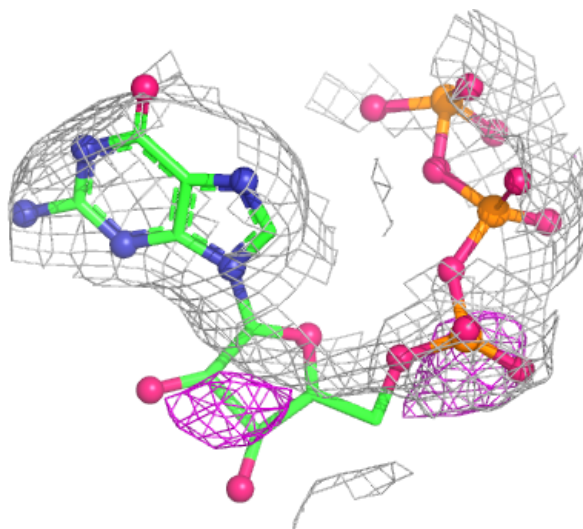
Electron density around NDP F 551:

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



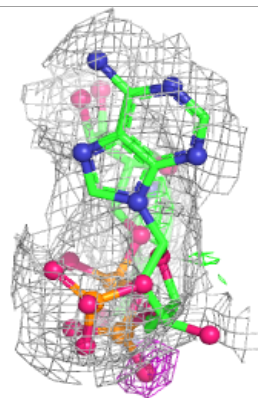
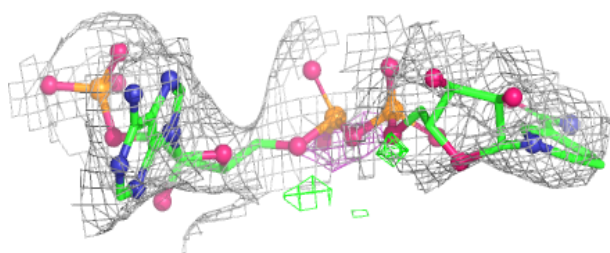
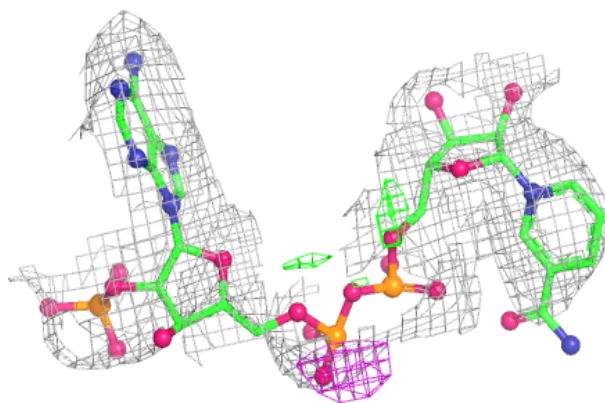
Electron density around GTP B 553:

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

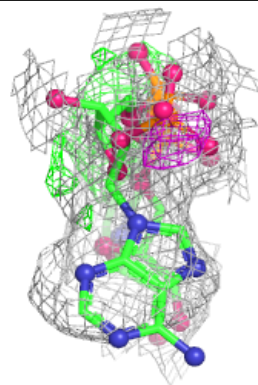
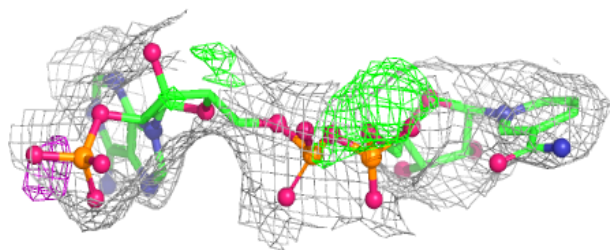
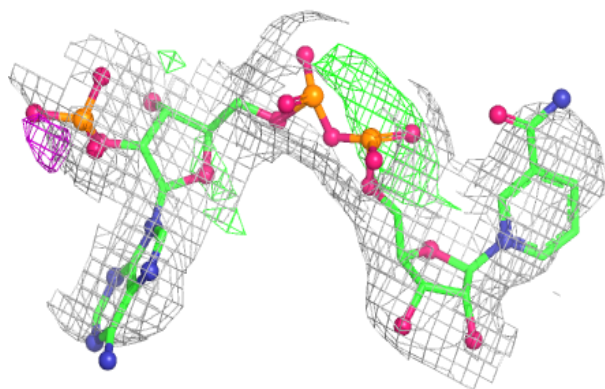


Electron density around NDP E 551:

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

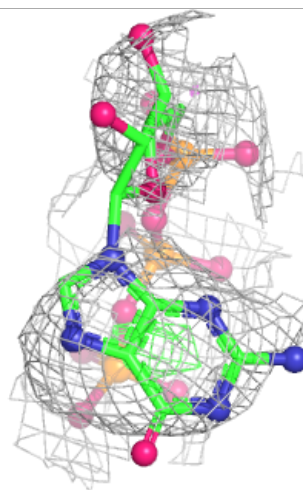
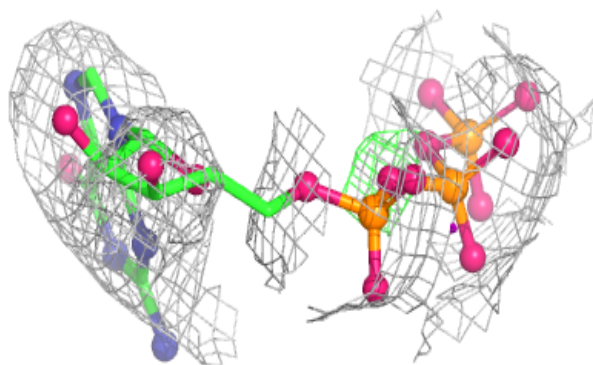
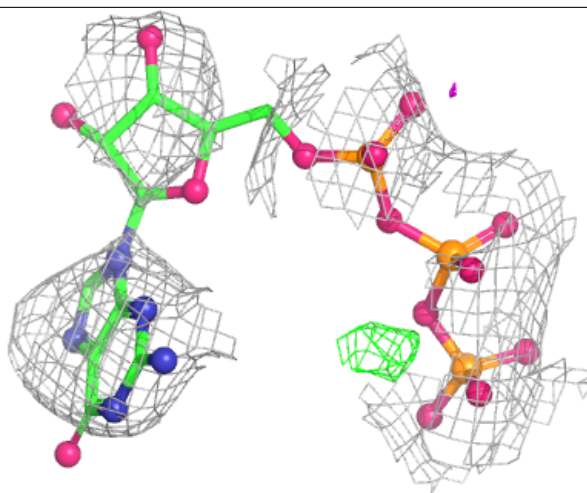
**Electron density around NDP A 551:**

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



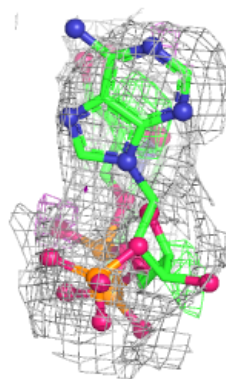
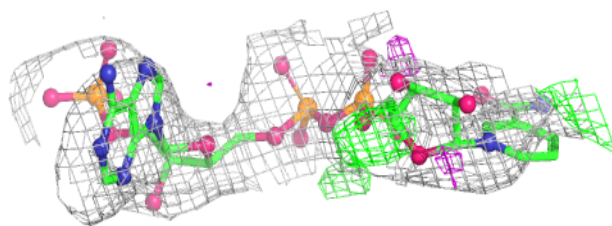
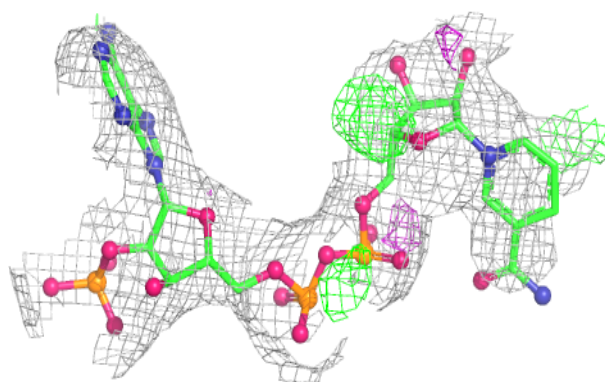
Electron density around GTP C 553:

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

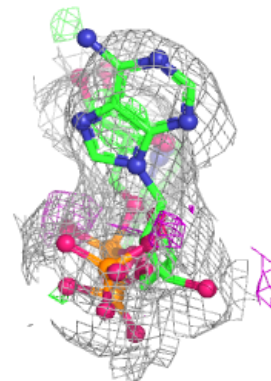
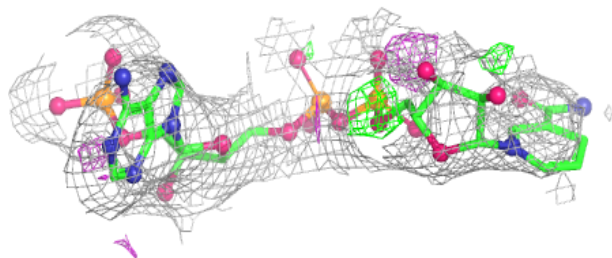
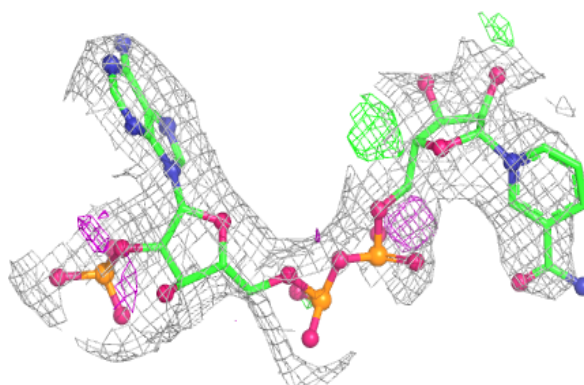


Electron density around NDP B 551:

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

**Electron density around NDP 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.