



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:39 am BST

PDB ID : 4ESV  
Title : A New Twist on the Translocation Mechanism of Helicases from the Structure of DnaB with its Substrates  
Authors : Itsathitphaisarn, O.; Wing, R.A.; Eliason, W.K.; Wang, J.; Steitz, T.A.  
Deposited on : 2012-04-23  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

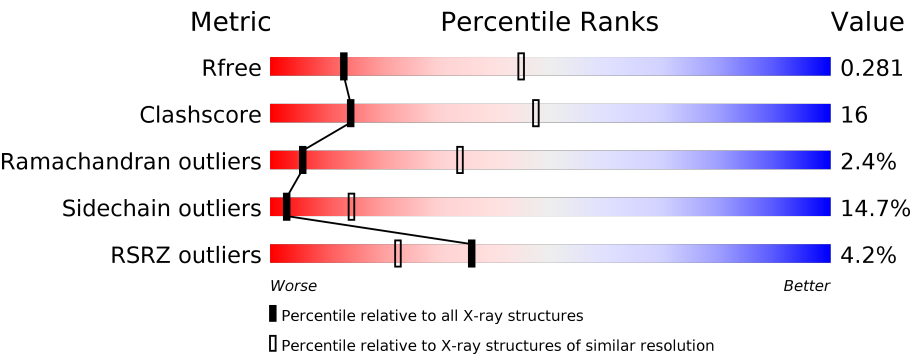
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	V	14	<div><div>7%</div><div>14%</div><div>36%</div><div>50%</div></div>
2	W	13	<div><div>8%</div><div>23%</div><div>69%</div></div>
3	A	454	<div><div>%</div><div>57%</div><div>26%</div><div>8%</div><div>8%</div></div>
3	B	454	<div><div>2%</div><div>55%</div><div>27%</div><div>11%</div><div>5%</div></div>
3	C	454	<div><div>%</div><div>60%</div><div>28%</div><div>7%</div><div>%</div></div>
3	D	454	<div><div>%</div><div>62%</div><div>27%</div><div>6%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
3	E	454	
3	F	454	
3	G	454	
3	H	454	
3	I	454	
3	J	454	
3	K	454	
3	L	454	

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
4	MES	C	505	-	-	-	X
4	MES	W	101	-	-	-	X
5	CA	G	503	-	-	-	X
6	GDP	I	501	-	-	X	-
7	ALF	A	504	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 40296 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 DNA chain called 5'-D(P\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*T P\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	V	14	Total	C	N	O	P	0	0	0
			280	140	28	98	14			

- Molecule 2 is a DNA chain called 5'-D(P\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*T P\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	13	Total	C	N	O	P	0	0	0
			260	130	26	91	13			

- Molecule 3 is a protein called Replicative helicase.

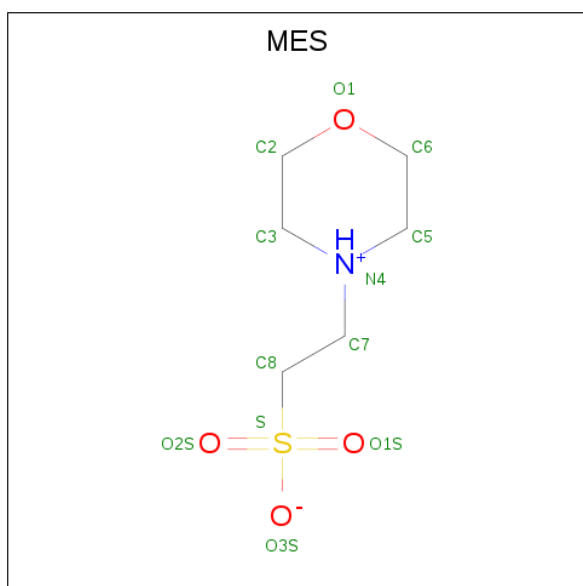
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	418	Total	C	N	O	S	8	1	0
			3255	2036	570	636	13			
3	B	430	Total	C	N	O	S	0	0	0
			3350	2093	591	652	14			
3	C	434	Total	C	N	O	S	0	0	0
			3367	2104	591	658	14			
3	D	431	Total	C	N	O	S	0	0	0
			3333	2084	583	652	14			
3	E	418	Total	C	N	O	S	0	0	0
			3243	2028	565	637	13			
3	F	421	Total	C	N	O	S	0	0	0
			3274	2049	569	643	13			
3	G	421	Total	C	N	O	S	0	0	0
			3259	2037	568	641	13			
3	H	425	Total	C	N	O	S	0	0	0
			3283	2052	572	645	14			
3	I	418	Total	C	N	O	S	0	0	0
			3245	2034	561	637	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	416	Total	C	N	O	S	0	0	0
			3237	2025	563	636	13			
3	K	421	Total	C	N	O	S	0	0	0
			3267	2044	568	642	13			
3	L	419	Total	C	N	O	S	0	0	0
			3246	2031	565	637	13			

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	W	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

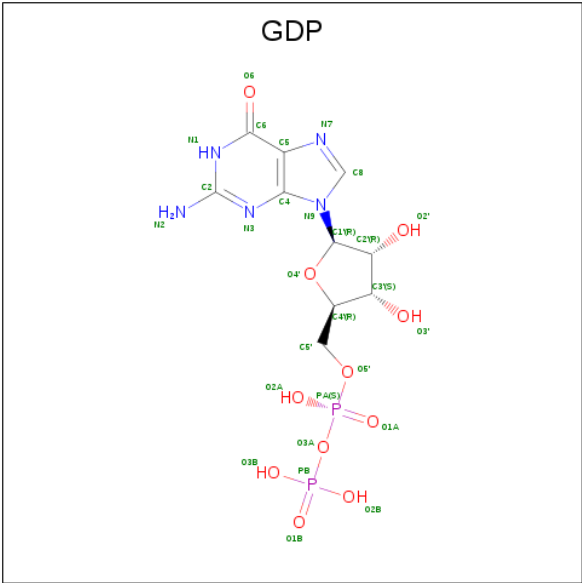
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Ca	0	0
			1	1		
5	D	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	I	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	A	5	Total	Ca	0	0
			5	5		
5	L	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



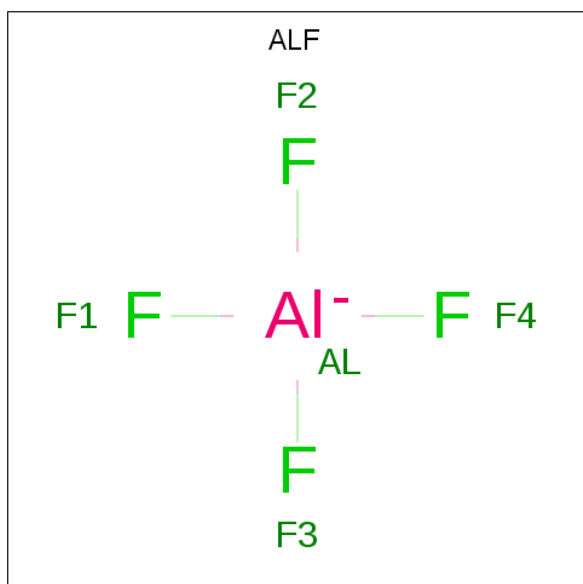
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
6	C	1	Total 28	C 10	N 5	O 11	P 2	0	0
6	D	1	Total 28	C 10	N 5	O 11	P 2	0	0
6	E	1	Total 28	C 10	N 5	O 11	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	G	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	I	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	J	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	K	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	L	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 7 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula:  $\text{AlF}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Al	F	0	0
			5	1	4		
7	C	1	Total	Al	F	0	0
			5	1	4		
7	C	1	Total	Al	F	0	0
			5	1	4		
7	D	1	Total	Al	F	0	0
			5	1	4		
7	E	1	Total	Al	F	0	0
			5	1	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total 5	Al 1	F 4	0	0
7	I	1	Total 5	Al 1	F 4	0	0
7	J	1	Total 5	Al 1	F 4	0	0
7	K	1	Total 5	Al 1	F 4	0	0
7	L	1	Total 5	Al 1	F 4	0	0

- Molecule 8 is water.

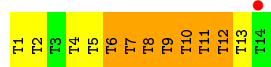
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	O 1	0	0
8	B	1	Total 1	O 1	0	0
8	D	1	Total 1	O 1	0	0
8	E	1	Total 1	O 1	0	0
8	K	1	Total 1	O 1	0	0



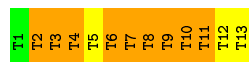
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

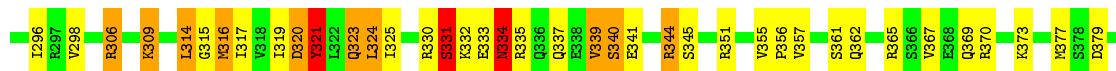
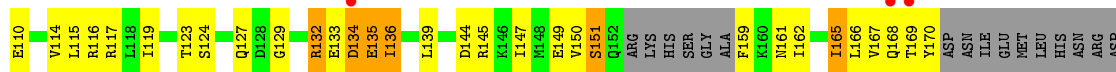
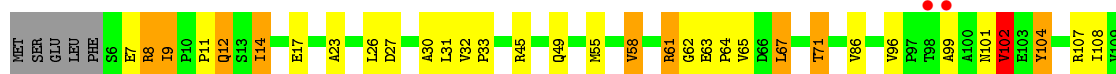
- Molecule 1: 5'-D(P\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*T)-3'



- Molecule 2: 5'-D(P\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*T)-3'

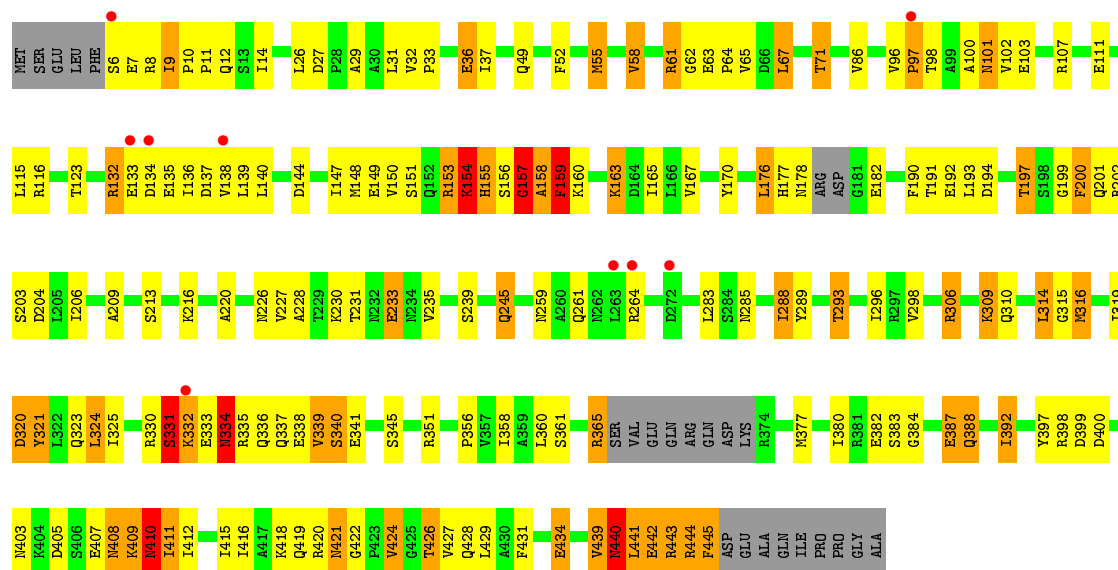


- Molecule 3: Replicative helicase

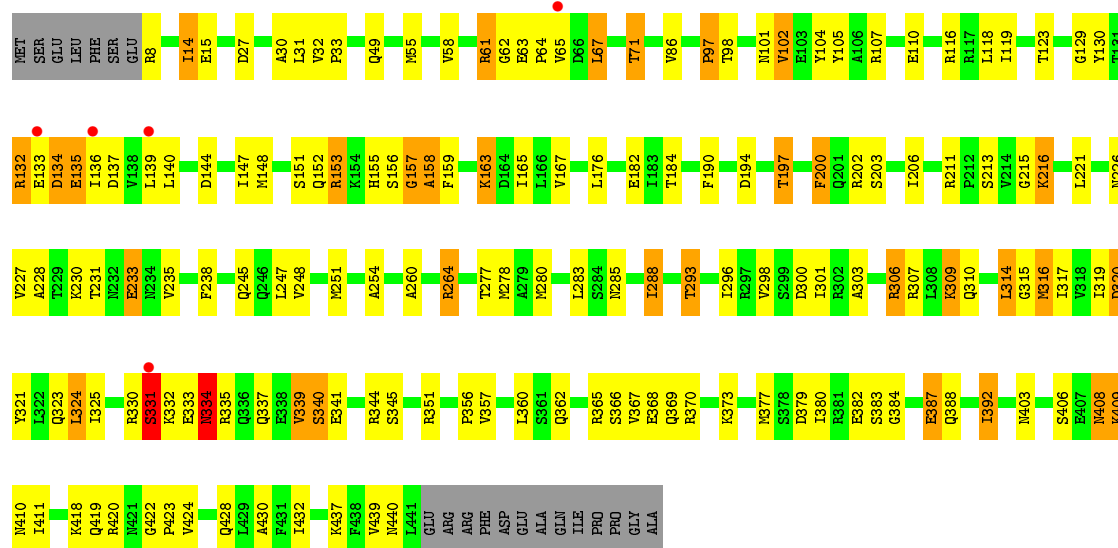


- Molecule 3: Replicative helicase

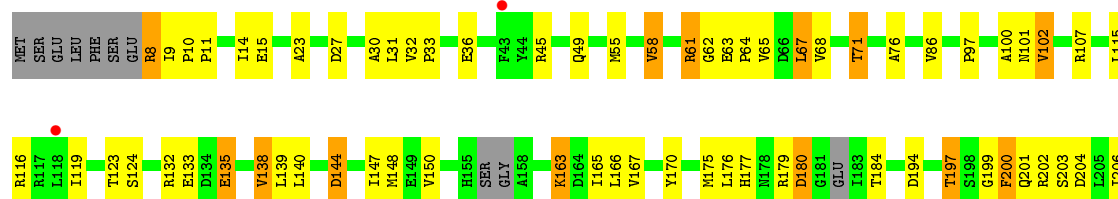


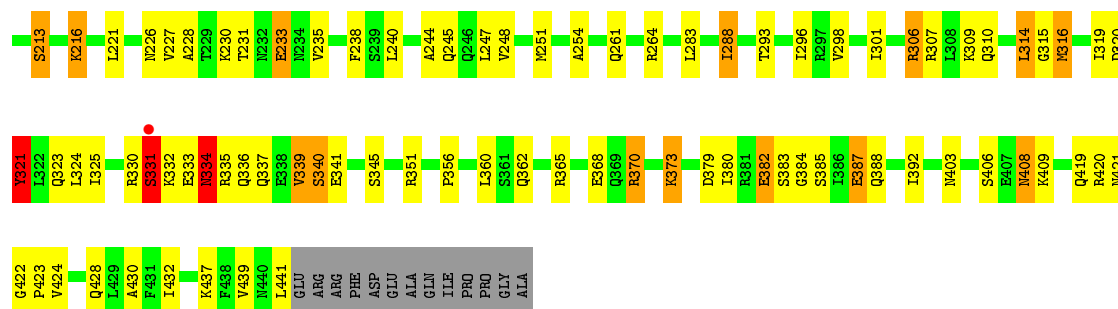


### • Molecule 3: Replicative helicase

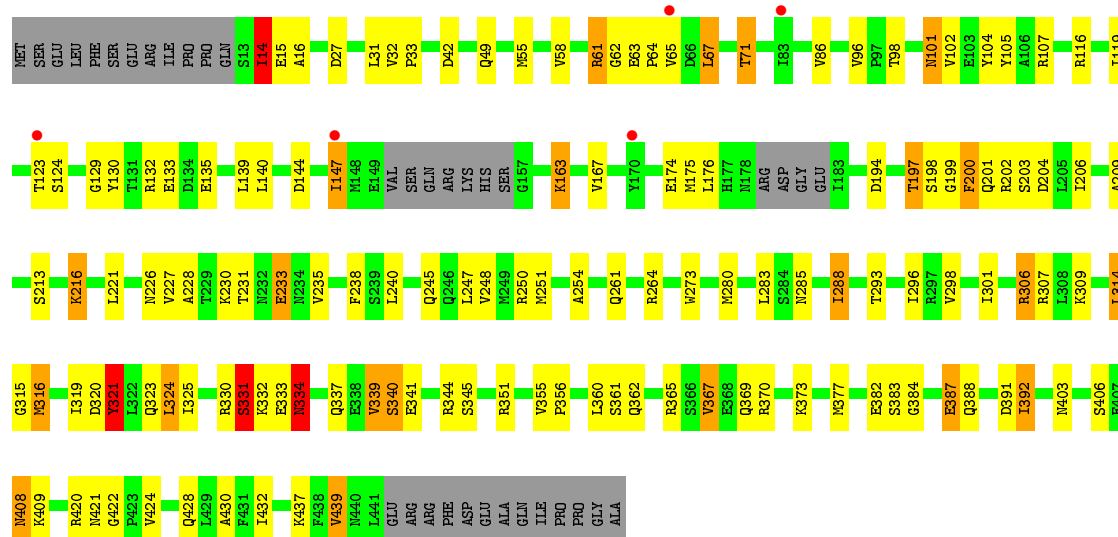


### • Molecule 3: Replicative helicase

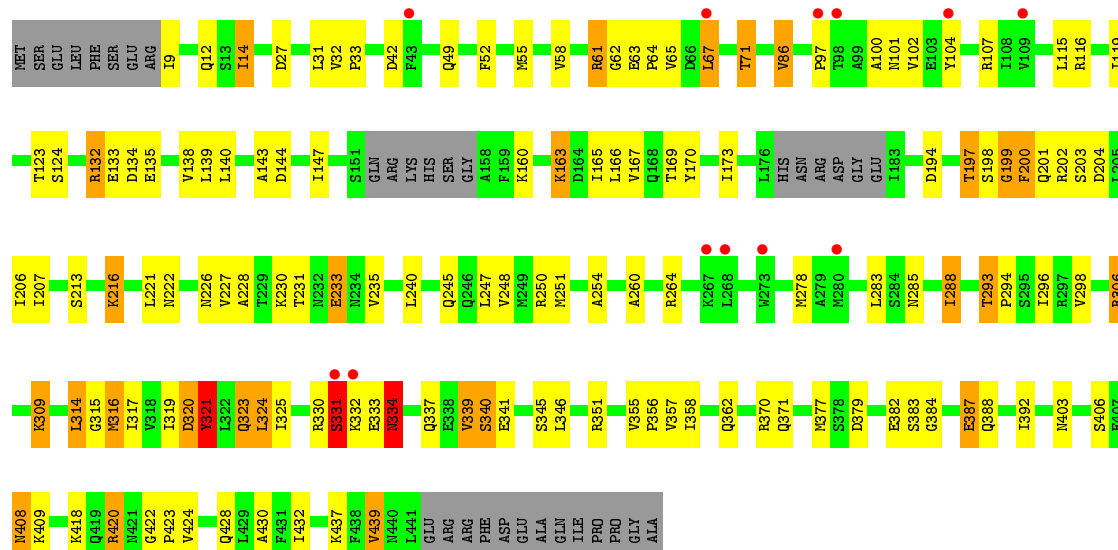




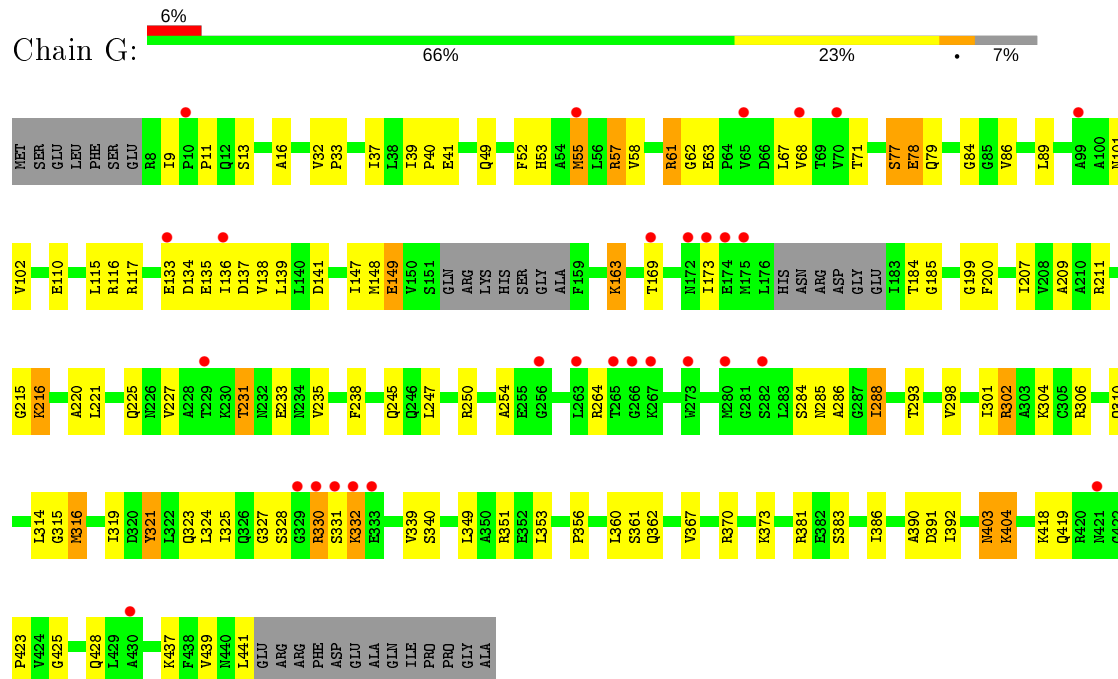
• Molecule 3: Replicative helicase



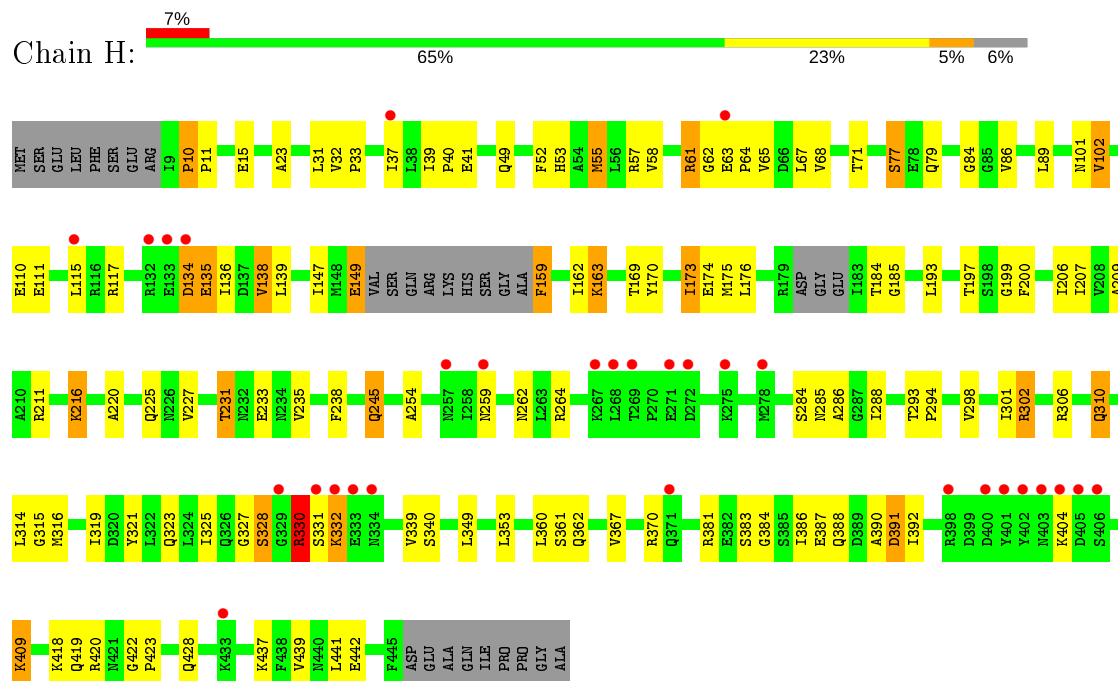
• Molecule 3: Replicative helicase



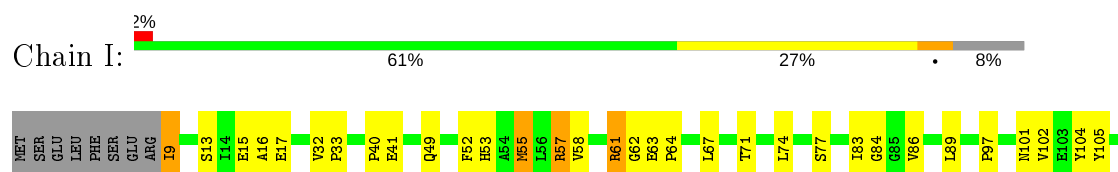
- Molecule 3: Replicative helicase

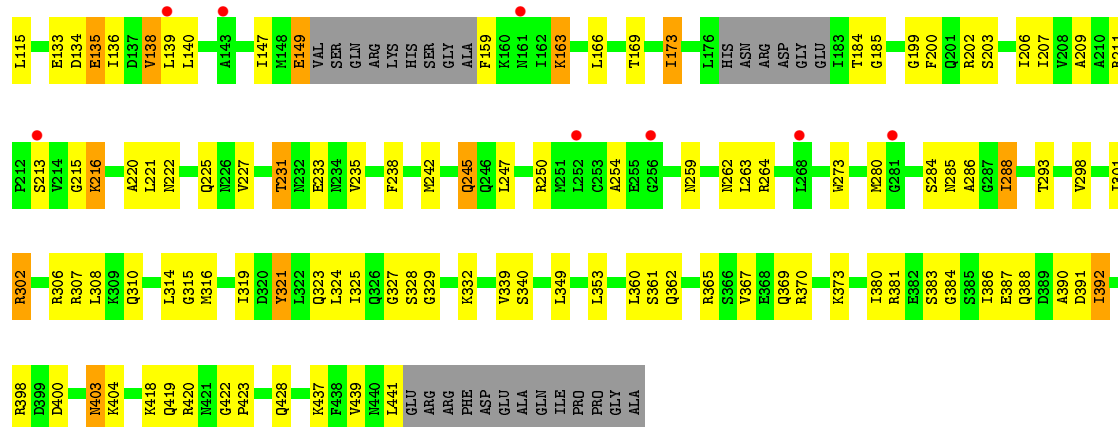


- Molecule 3: Replicative helicase

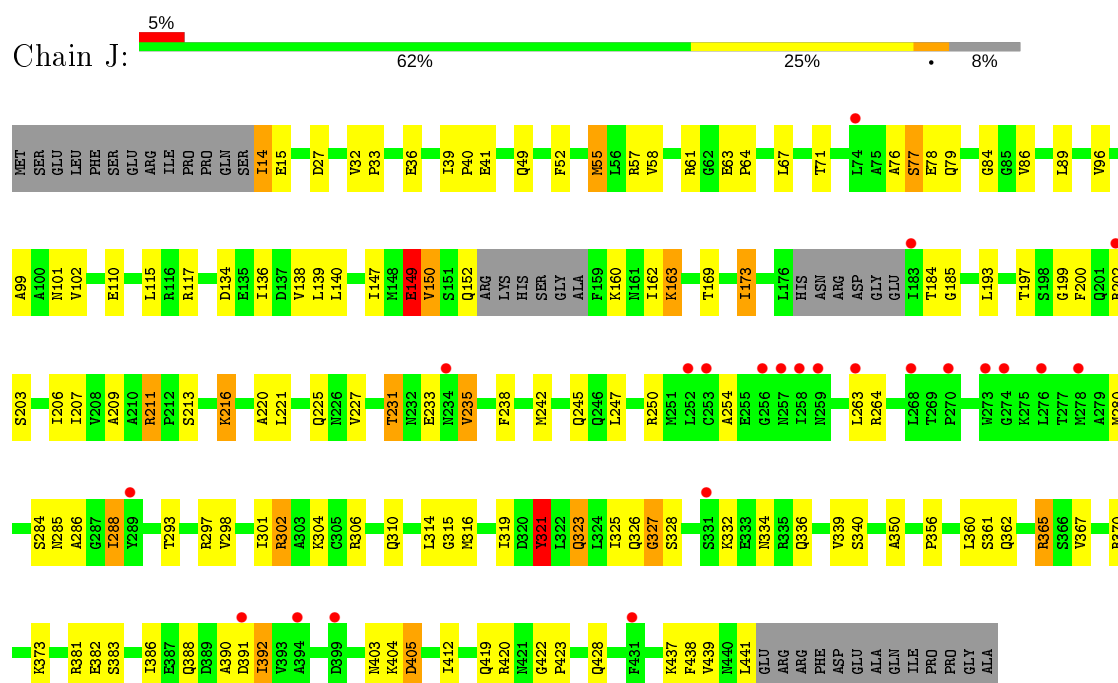


- Molecule 3: Replicative helicase

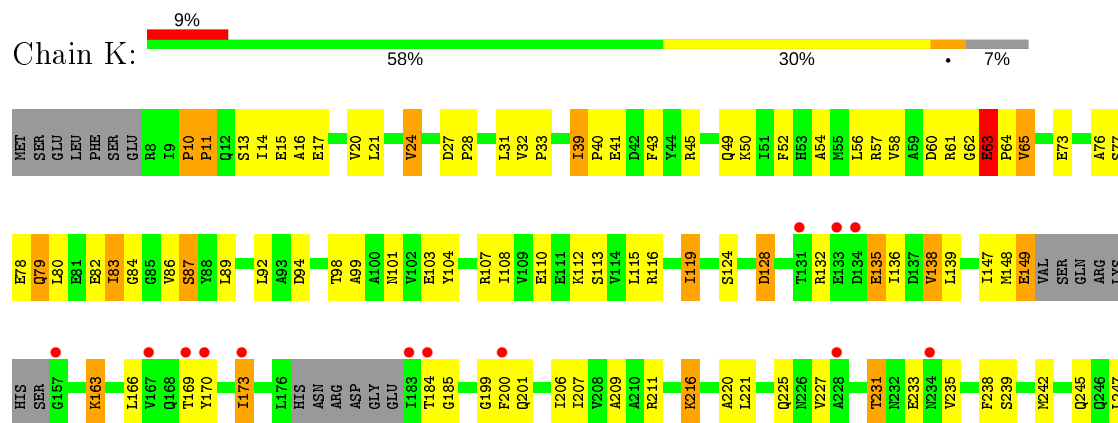


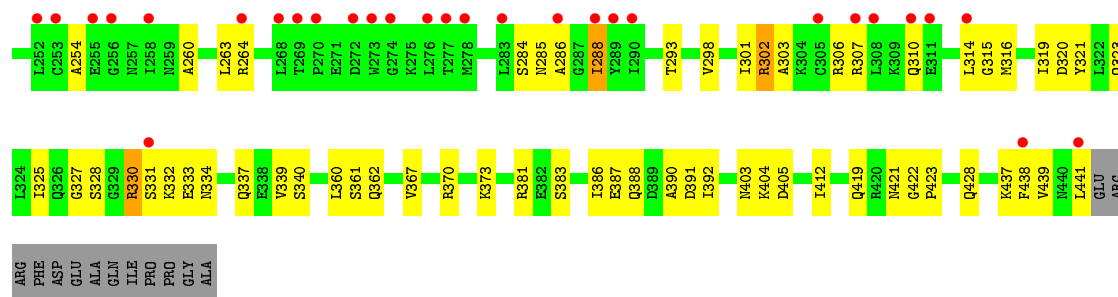


### • Molecule 3: Replicative helicase

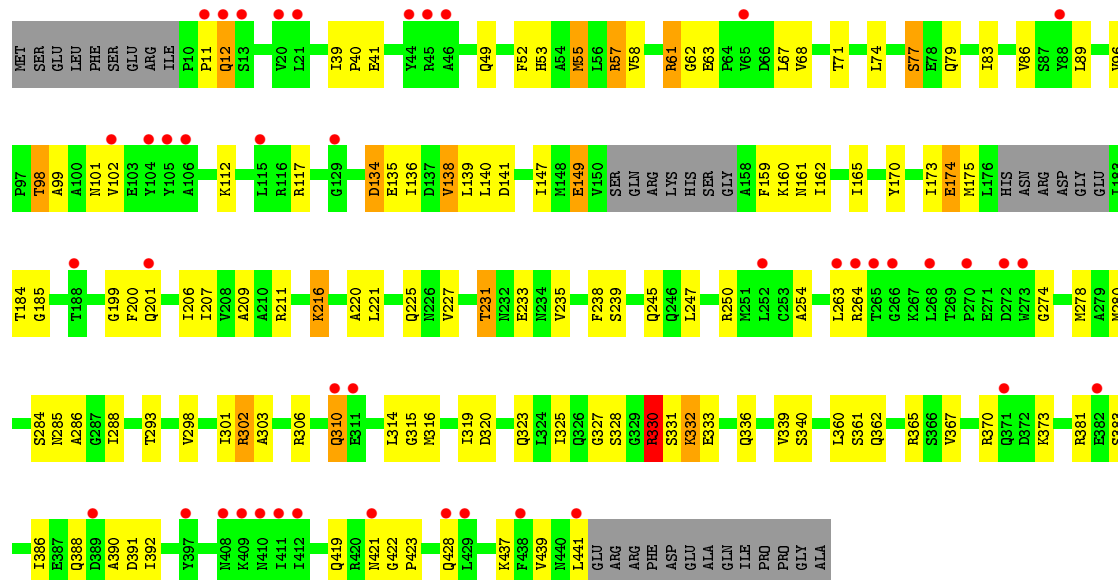


### • Molecule 3: Replicative helicase





• Molecule 3: Replicative helicase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.12Å 180.32Å 279.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.92 – 3.20 47.92 – 3.20	Depositor EDS
% Data completeness (in resolution range)	87.8 (47.92-3.20) 87.8 (47.92-3.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.242 , 0.289 0.239 , 0.281	Depositor DCC
$R_{free}$ test set	5442 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.6	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 83.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	40296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, ALF, CA, MES

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	V	1.30	2/307 (0.7%)	2.43	29/472 (6.1%)
2	W	1.61	2/285 (0.7%)	2.37	18/438 (4.1%)
3	A	0.61	0/3295	0.77	3/4450 (0.1%)
3	B	0.61	1/3390 (0.0%)	0.82	2/4576 (0.0%)
3	C	0.58	0/3408	0.75	2/4607 (0.0%)
3	D	0.52	0/3372	0.72	0/4557
3	E	0.54	0/3279	0.73	1/4428 (0.0%)
3	F	0.54	0/3312	0.74	2/4475 (0.0%)
3	G	0.40	0/3296	0.61	1/4454 (0.0%)
3	H	0.44	0/3319	0.64	3/4482 (0.1%)
3	I	0.43	0/3283	0.62	1/4437 (0.0%)
3	J	0.43	0/3273	0.65	2/4420 (0.0%)
3	K	0.46	0/3305	0.68	3/4467 (0.1%)
3	L	0.41	0/3284	0.62	0/4437
All	All	0.53	5/40408 (0.0%)	0.76	67/54700 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	4
3	B	0	5
3	C	0	1
3	D	0	2
3	E	0	1
3	F	0	1
3	I	0	1
3	J	0	1
3	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	17

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	421	ASN	CB-CG	5.99	1.64	1.51
2	W	6	DT	C1'-N1	5.61	1.56	1.49
1	V	12	DT	C1'-N1	5.56	1.56	1.49
2	W	11	DT	N1-C2	5.10	1.42	1.38
1	V	8	DT	C3'-O3'	5.03	1.50	1.44

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	8	DT	O4'-C1'-N1	12.56	116.79	108.00
2	W	7	DT	O4'-C1'-N1	10.63	115.44	108.00
2	W	4	DT	C4-C5-C7	10.36	125.22	119.00
2	W	11	DT	O4'-C4'-C3'	-9.32	100.41	106.00
2	W	10	DT	C1'-O4'-C4'	-9.01	101.09	110.10
2	W	10	DT	O4'-C1'-N1	8.91	114.23	108.00
3	B	158	ALA	N-CA-C	-8.32	88.54	111.00
1	V	11	DT	O4'-C1'-N1	-8.23	102.23	108.00
1	V	12	DT	N3-C2-O2	-8.05	117.47	122.30
1	V	12	DT	O4'-C1'-N1	7.88	113.51	108.00
2	W	4	DT	C6-C5-C7	-7.60	118.34	122.90
1	V	7	DT	O4'-C1'-N1	-7.48	102.76	108.00
1	V	9	DT	C5-C4-O4	-7.47	119.67	124.90
1	V	8	DT	C4'-C3'-C2'	-7.30	96.53	103.10
2	W	11	DT	C4'-C3'-C2'	-7.24	96.59	103.10
2	W	2	DT	O4'-C1'-N1	7.17	113.02	108.00
1	V	1	DT	P-O3'-C3'	7.04	128.15	119.70
2	W	4	DT	O4'-C1'-N1	-6.89	103.18	108.00
2	W	13	DT	O4'-C1'-N1	6.71	112.70	108.00
1	V	8	DT	C1'-O4'-C4'	-6.61	103.50	110.10
3	H	10	PRO	N-CA-CB	6.57	111.19	103.30
1	V	2	DT	P-O3'-C3'	6.38	127.36	119.70
1	V	5	DT	O4'-C1'-N1	6.35	112.44	108.00
3	E	321	TYR	CB-CA-C	6.34	123.08	110.40
1	V	11	DT	C4-C5-C7	6.26	122.76	119.00
1	V	12	DT	O4'-C1'-C2'	-6.19	100.95	105.90
3	J	321	TYR	CB-CA-C	6.19	122.78	110.40
1	V	9	DT	N3-C4-O4	6.02	123.51	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	2	DT	C4-C5-C7	5.96	122.58	119.00
1	V	7	DT	C5-C4-O4	-5.93	120.75	124.90
1	V	13	DT	O4'-C1'-N1	5.92	112.15	108.00
2	W	8	DT	N3-C2-O2	-5.87	118.78	122.30
3	F	321	TYR	CB-CA-C	5.86	122.12	110.40
3	B	421	ASN	N-CA-C	-5.83	95.27	111.00
1	V	2	DT	C6-C5-C7	-5.82	119.41	122.90
2	W	9	DT	C4-C5-C7	5.81	122.48	119.00
2	W	8	DT	C4-C5-C7	5.74	122.44	119.00
2	W	3	DT	P-O3'-C3'	5.71	126.55	119.70
1	V	6	DT	O4'-C1'-N1	5.70	111.99	108.00
1	V	11	DT	C4'-C3'-C2'	5.69	108.22	103.10
2	W	8	DT	C6-C5-C7	-5.68	119.49	122.90
1	V	1	DT	C4-C5-C7	5.58	122.35	119.00
3	C	102	VAL	CG1-CB-CG2	5.50	119.70	110.90
3	A	168	GLN	N-CA-C	5.49	125.83	111.00
1	V	10	DT	C4-C5-C7	5.48	122.29	119.00
2	W	9	DT	C6-C5-C7	-5.43	119.64	122.90
3	A	102	VAL	CB-CA-C	-5.40	101.15	111.40
3	H	11	PRO	N-CA-CB	5.36	109.74	103.30
2	W	2	DT	P-O3'-C3'	5.32	126.09	119.70
1	V	7	DT	C3'-C2'-C1'	-5.32	96.12	102.50
1	V	7	DT	O4'-C4'-C3'	-5.31	102.38	104.50
1	V	4	DT	C4-C5-C7	5.27	122.16	119.00
1	V	12	DT	N1-C2-O2	5.26	127.31	123.10
1	V	11	DT	C6-C5-C7	-5.23	119.77	122.90
1	V	2	DT	OP2-P-O3'	5.21	116.67	105.20
3	K	89	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	V	13	DT	C6-N1-C2	-5.19	118.70	121.30
3	C	184	THR	C-N-CA	5.18	133.18	122.30
3	K	63	GLU	C-N-CD	-5.14	109.28	120.60
3	H	84	GLY	N-CA-C	-5.11	100.33	113.10
3	J	84	GLY	N-CA-C	-5.07	100.44	113.10
3	K	84	GLY	N-CA-C	-5.06	100.44	113.10
3	F	199	GLY	N-CA-C	-5.06	100.44	113.10
2	W	9	DT	O4'-C1'-C2'	5.05	109.94	105.90
3	I	84	GLY	N-CA-C	-5.03	100.52	113.10
3	A	200	PHE	CB-CA-C	5.02	120.45	110.40
3	G	84	GLY	N-CA-C	-5.00	100.59	113.10

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	166	LEU	Peptide
3	A	167	VAL	Peptide
3	A	184	THR	Peptide
3	A	320	ASP	Peptide
3	B	151	SER	Peptide
3	B	154	LYS	Peptide
3	B	157	GLY	Peptide
3	B	320	ASP	Peptide
3	B	421	ASN	Peptide
3	C	320	ASP	Peptide
3	D	184	THR	Peptide
3	D	320	ASP	Peptide
3	E	320	ASP	Peptide
3	F	320	ASP	Peptide
3	I	329	GLY	Peptide
3	J	149	GLU	Peptide
3	K	63	GLU	Peptide

## 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	V	280	0	169	11	0
2	W	260	0	157	24	0
3	A	3255	0	3296	128	0
3	B	3350	0	3382	177	0
3	C	3367	0	3384	118	0
3	D	3333	0	3337	119	0
3	E	3243	0	3262	110	0
3	F	3274	0	3305	105	0
3	G	3259	0	3274	87	0
3	H	3283	0	3282	110	0
3	I	3245	0	3268	118	0
3	J	3237	0	3265	108	0
3	K	3267	0	3287	115	0
3	L	3246	0	3263	89	0
4	C	12	0	12	0	0
4	E	12	0	12	0	0
4	I	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	W	12	0	12	4	0
5	A	5	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	L	1	0	0	0	0
6	A	28	0	12	4	0
6	C	28	0	12	4	0
6	D	28	0	12	3	0
6	E	28	0	12	4	0
6	F	28	0	12	4	0
6	G	28	0	12	5	0
6	I	28	0	12	10	0
6	J	28	0	12	6	0
6	K	28	0	12	3	0
6	L	28	0	12	5	0
7	A	5	0	0	2	0
7	C	10	0	0	0	0
7	D	5	0	0	0	0
7	E	5	0	0	0	0
7	G	5	0	0	0	0
7	I	5	0	0	0	0
7	J	5	0	0	0	0
7	K	5	0	0	1	0
7	L	5	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	K	1	0	0	0	0
All	All	40296	0	40099	1249	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (1249) 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)
3:J:403:ASN:HB3	3:J:404:LYS:CA	1.63	1.28
3:A:145:ARG:HD2	3:B:310:GLN:NE2	1.58	1.18
3:E:14:ILE:HD13	3:E:15:GLU:H	1.10	1.16
2:W:6:DT:H2''	2:W:7:DT:H5'	1.29	1.14
3:J:403:ASN:CB	3:J:404:LYS:HA	1.75	1.14
3:K:63:GLU:HB2	3:K:64:PRO:HA	1.13	1.12
3:C:260:ALA:HB1	3:C:264:ARG:HH21	1.03	1.11
3:D:306:ARG:HG3	3:D:306:ARG:HH11	1.16	1.10
3:H:422:GLY:HA2	6:I:501:GDP:C5	1.85	1.10
3:B:154:LYS:N	3:B:155:HIS:HB3	1.69	1.07
3:E:306:ARG:HH11	3:E:306:ARG:HG3	1.16	1.07
3:A:261:GLN:HG2	3:A:264:ARG:NH1	1.70	1.06
3:H:422:GLY:HA2	6:I:501:GDP:N7	1.71	1.04
3:D:370:ARG:HG3	3:D:370:ARG:HH11	1.15	1.04
3:J:365:ARG:HG2	3:J:365:ARG:HH11	0.90	1.04
3:G:148:MET:HG3	3:H:310:GLN:OE1	1.57	1.04
3:D:61:ARG:HH11	3:D:61:ARG:HG2	1.23	1.03
3:B:306:ARG:HH11	3:B:306:ARG:HG3	1.23	1.03
3:E:261:GLN:HG2	3:E:264:ARG:NH2	1.74	1.02
3:F:227:VAL:O	3:F:231:THR:HG22	1.57	1.02
3:A:306:ARG:HH11	3:A:306:ARG:HG3	1.24	1.02
3:B:227:VAL:O	3:B:231:THR:HG22	1.59	1.02
3:K:63:GLU:HB2	3:K:64:PRO:CA	1.86	1.02
3:E:227:VAL:O	3:E:231:THR:HG22	1.59	1.02
3:J:365:ARG:HG2	3:J:365:ARG:NH1	1.62	1.01
3:F:321:TYR:CD2	3:F:324:LEU:HD22	1.95	1.01
3:F:306:ARG:HH11	3:F:306:ARG:HG3	1.22	1.01
3:B:397:TYR:OH	3:B:399:ASP:HB3	1.61	1.00
3:A:61:ARG:HG2	3:A:61:ARG:HH11	1.27	0.99
3:J:365:ARG:HH11	3:J:365:ARG:CG	1.73	0.99
3:B:154:LYS:H	3:B:155:HIS:HB3	1.20	0.99
3:C:227:VAL:O	3:C:231:THR:HG22	1.61	0.99
3:C:306:ARG:HH11	3:C:306:ARG:HG3	1.24	0.99
3:L:141:ASP:OD2	3:L:303:ALA:HB2	1.62	0.98
3:A:104:TYR:HE2	3:A:108:ILE:HD11	1.24	0.97
3:D:421:ASN:HD21	3:E:264:ARG:HD2	1.26	0.97
3:C:61:ARG:HG2	3:C:61:ARG:HH11	1.25	0.97
3:H:409:LYS:H	3:H:409:LYS:HD2	1.24	0.97
3:F:61:ARG:HG2	3:F:61:ARG:HH11	1.29	0.96
1:V:12:DT:H5'	3:B:336:GLN:HG3	1.43	0.95
3:E:61:ARG:HH11	3:E:61:ARG:HG2	1.30	0.95
3:D:227:VAL:O	3:D:231:THR:HG22	1.64	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:68:VAL:HB	3:I:105:TYR:HE2	1.30	0.95
3:E:421:ASN:HD21	3:F:264:ARG:HD3	1.29	0.95
3:B:36:GLU:OE1	3:B:36:GLU:HA	1.63	0.95
3:A:227:VAL:O	3:A:231:THR:HG22	1.67	0.94
3:G:215:GLY:HA2	6:G:501:GDP:O2A	1.67	0.94
3:C:260:ALA:HB1	3:C:264:ARG:NH2	1.83	0.93
6:A:502:GDP:C5	3:F:422:GLY:HA2	2.04	0.93
3:B:444:ARG:HH11	3:B:444:ARG:HG3	1.32	0.92
3:B:61:ARG:HH11	3:B:61:ARG:HG2	1.32	0.92
3:H:32:VAL:HG13	3:I:307:ARG:HD2	1.51	0.92
3:E:261:GLN:HG2	3:E:264:ARG:HH22	1.35	0.91
3:E:14:ILE:HG23	3:E:15:GLU:HG3	1.52	0.91
3:K:173:ILE:HD11	3:L:263:LEU:HD22	1.52	0.91
3:D:421:ASN:HD21	3:E:264:ARG:CD	1.84	0.91
3:F:67:LEU:HD22	3:G:68:VAL:HG21	1.53	0.90
3:E:421:ASN:ND2	3:F:264:ARG:HD3	1.86	0.90
3:C:422:GLY:HA2	6:D:501:GDP:C5	2.07	0.89
3:E:14:ILE:HD13	3:E:15:GLU:N	1.87	0.88
3:B:245:GLN:H	3:B:245:GLN:NE2	1.70	0.88
3:I:422:GLY:HA2	6:J:501:GDP:N7	1.89	0.88
3:B:33:PRO:HA	3:C:307:ARG:HH11	1.38	0.87
3:H:68:VAL:HB	3:I:105:TYR:CE2	2.09	0.87
3:B:245:GLN:N	3:B:245:GLN:HE21	1.73	0.87
3:B:320:ASP:O	3:B:321:TYR:HB3	1.74	0.87
3:F:67:LEU:O	3:F:71:THR:HG23	1.75	0.87
3:I:97:PRO:HG3	3:I:105:TYR:OH	1.75	0.87
3:J:297:ARG:HD2	3:J:327:GLY:O	1.75	0.87
3:B:154:LYS:N	3:B:155:HIS:CB	2.36	0.86
3:G:425:GLY:HA2	3:H:294:PRO:HG2	1.56	0.86
3:I:422:GLY:HA2	6:J:501:GDP:C5	2.10	0.86
3:C:67:LEU:O	3:C:71:THR:HG23	1.75	0.86
3:B:444:ARG:CG	3:B:444:ARG:HH11	1.88	0.86
3:H:68:VAL:CB	3:I:105:TYR:HE2	1.88	0.85
3:J:199:GLY:HA2	3:J:200:PHE:HB2	1.58	0.85
3:L:199:GLY:HA2	3:L:200:PHE:HB2	1.59	0.85
2:W:3:DT:C2'	2:W:4:DT:H5'	2.07	0.85
3:A:145:ARG:HD2	3:B:310:GLN:HE22	1.36	0.85
3:G:199:GLY:HA2	3:G:200:PHE:HB2	1.58	0.85
3:B:33:PRO:HA	3:C:307:ARG:NH1	1.92	0.84
3:I:199:GLY:HA2	3:I:200:PHE:HB2	1.59	0.83
3:B:33:PRO:HG3	3:C:307:ARG:CD	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:199:GLY:HA2	3:K:200:PHE:HB2	1.59	0.83
3:A:145:ARG:HD2	3:B:310:GLN:CD	1.98	0.83
3:C:233:GLU:HG2	3:C:315:GLY:HA3	1.60	0.83
3:D:422:GLY:HA2	6:E:501:GDP:C5	2.13	0.83
3:A:161:ASN:O	3:A:165:ILE:HG13	1.80	0.82
3:A:67:LEU:O	3:A:71:THR:HG23	1.79	0.82
3:D:330:ARG:HH21	3:D:341:GLU:HG3	1.43	0.82
3:L:250:ARG:HH21	6:L:501:GDP:H5'	1.42	0.82
3:B:154:LYS:HG2	3:C:300:ASP:OD2	1.80	0.82
3:E:67:LEU:O	3:E:71:THR:HG23	1.79	0.82
3:D:67:LEU:O	3:D:71:THR:HG23	1.79	0.81
3:I:71:THR:HG22	3:I:89:LEU:HD12	1.63	0.81
3:K:79:GLN:H	3:K:79:GLN:NE2	1.78	0.81
3:H:409:LYS:CD	3:H:409:LYS:H	1.93	0.81
3:B:330:ARG:HH21	3:B:341:GLU:HG3	1.46	0.81
3:K:320:ASP:O	3:K:321:TYR:HB3	1.81	0.81
3:H:199:GLY:HA2	3:H:200:PHE:HB2	1.62	0.81
3:A:104:TYR:CE2	3:A:108:ILE:HD11	2.15	0.80
3:A:330:ARG:HH21	3:A:341:GLU:HG3	1.45	0.80
3:H:162:ILE:HD13	3:I:288:ILE:HD11	1.61	0.80
3:K:79:GLN:H	3:K:79:GLN:HE21	1.23	0.80
3:D:233:GLU:HG2	3:D:315:GLY:HA3	1.64	0.80
3:F:330:ARG:HH21	3:F:341:GLU:HG3	1.46	0.80
3:H:68:VAL:HG11	3:I:105:TYR:CE2	2.17	0.80
3:J:36:GLU:OE2	3:K:307:ARG:CZ	2.29	0.80
3:D:370:ARG:HG3	3:D:370:ARG:NH1	1.92	0.80
3:L:239:SER:HA	3:L:320:ASP:HB2	1.64	0.79
3:L:71:THR:HG22	3:L:89:LEU:HD12	1.64	0.79
3:L:274:GLY:O	3:L:278:MET:HG2	1.83	0.79
3:E:330:ARG:HH21	3:E:341:GLU:HG3	1.45	0.79
3:K:116:ARG:HA	3:K:119:ILE:HD12	1.65	0.79
3:B:36:GLU:CA	3:B:36:GLU:OE1	2.29	0.79
3:E:14:ILE:CD1	3:E:15:GLU:H	1.94	0.79
3:G:351:ARG:HH12	3:H:134:ASP:HA	1.48	0.79
3:H:170:TYR:HD1	3:I:280:MET:SD	2.06	0.79
3:D:306:ARG:NH1	3:D:306:ARG:HG3	1.97	0.78
3:D:36:GLU:OE2	3:E:307:ARG:HD3	1.83	0.78
3:L:12:GLN:HA	3:L:112:LYS:HG2	1.64	0.78
3:B:67:LEU:O	3:B:71:THR:HG23	1.82	0.78
3:I:97:PRO:CG	3:I:105:TYR:OH	2.31	0.78
3:L:12:GLN:CA	3:L:112:LYS:HG2	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:8:DT:H4'	1:V:9:DT:OP1	1.83	0.78
3:K:239:SER:HA	3:K:320:ASP:HB2	1.65	0.77
3:I:215:GLY:HA2	6:I:501:GDP:O2A	1.83	0.77
3:B:233:GLU:HG2	3:B:315:GLY:HA3	1.66	0.77
3:F:233:GLU:HG2	3:F:315:GLY:HA3	1.66	0.77
3:H:68:VAL:CG1	3:I:105:TYR:CE2	2.67	0.77
3:H:68:VAL:CB	3:I:105:TYR:CE2	2.67	0.77
3:A:104:TYR:HE2	3:A:108:ILE:CD1	1.95	0.76
3:B:321:TYR:CE1	3:B:324:LEU:HD13	2.19	0.76
3:B:245:GLN:H	3:B:245:GLN:HE21	0.87	0.76
3:E:422:GLY:HA2	6:F:501:GDP:C5	2.20	0.76
3:C:330:ARG:HH21	3:C:341:GLU:HG3	1.49	0.76
3:A:233:GLU:HG2	3:A:315:GLY:HA3	1.66	0.76
3:D:306:ARG:CG	3:D:306:ARG:HH11	1.97	0.76
3:B:12:GLN:HE21	3:B:14:ILE:CD1	1.99	0.76
3:A:14:ILE:HD12	3:A:45:ARG:HE	1.50	0.75
3:A:61:ARG:CG	3:A:61:ARG:HH11	1.99	0.75
3:E:233:GLU:HG2	3:E:315:GLY:HA3	1.66	0.75
3:D:61:ARG:NH1	3:D:61:ARG:HG2	1.96	0.75
3:H:330:ARG:C	3:H:332:LYS:H	1.90	0.75
3:E:61:ARG:HG2	3:E:61:ARG:NH1	2.02	0.75
1:V:12:DT:H5''	3:B:383:SER:HA	1.67	0.75
3:G:71:THR:HG22	3:G:89:LEU:HD12	1.67	0.75
3:I:207:ILE:HD12	3:I:390:ALA:HB2	1.69	0.75
3:I:202:ARG:O	3:I:203:SER:HB2	1.86	0.75
3:L:319:ILE:HG21	3:L:325:ILE:HD11	1.68	0.74
3:J:71:THR:HG22	3:J:89:LEU:HD12	1.69	0.74
3:H:159:PHE:HE2	3:I:308:LEU:HD22	1.52	0.74
3:D:68:VAL:HB	3:E:105:TYR:HE2	1.53	0.74
3:H:68:VAL:CG1	3:I:105:TYR:HE2	2.01	0.73
3:K:135:GLU:HB2	3:K:138:VAL:HG12	1.70	0.73
2:W:3:DT:H2'	2:W:4:DT:H5'	1.71	0.73
3:C:61:ARG:CG	3:C:61:ARG:HH11	1.99	0.73
2:W:2:DT:H2''	2:W:3:DT:O5'	1.88	0.73
3:B:33:PRO:HG3	3:C:307:ARG:HD3	1.69	0.73
3:D:61:ARG:HH11	3:D:61:ARG:CG	1.98	0.73
3:K:61:ARG:NH2	3:K:73:GLU:OE1	2.21	0.72
3:F:306:ARG:HH11	3:F:306:ARG:CG	2.02	0.72
3:K:319:ILE:HG21	3:K:325:ILE:HD11	1.70	0.72
3:A:23:ALA:CB	3:A:102:VAL:HG13	2.19	0.72
3:K:41:GLU:HA	3:K:49:GLN:HE21	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:79:GLN:N	3:K:79:GLN:HE21	1.86	0.72
3:K:207:ILE:HD12	3:K:390:ALA:HB2	1.71	0.72
3:B:61:ARG:HH11	3:B:61:ARG:CG	2.01	0.72
3:G:184:THR:H	3:G:185:GLY:HA3	1.54	0.71
3:H:71:THR:HG22	3:H:89:LEU:HD12	1.71	0.71
3:K:40:PRO:O	3:K:49:GLN:HG2	1.90	0.71
3:F:61:ARG:CG	3:F:61:ARG:HH11	2.01	0.71
3:L:184:THR:H	3:L:185:GLY:HA3	1.55	0.71
3:E:306:ARG:CG	3:E:306:ARG:HH11	1.98	0.71
3:E:319:ILE:HG21	3:E:325:ILE:HD11	1.72	0.71
3:C:306:ARG:HH11	3:C:306:ARG:CG	2.02	0.71
3:D:166:LEU:HB3	3:E:280:MET:HE3	1.73	0.71
2:W:7:DT:H4'	3:J:382:GLU:O	1.90	0.71
3:H:67:LEU:O	3:H:71:THR:HG23	1.91	0.71
2:W:12:DT:O2	2:W:12:DT:H2'	1.89	0.71
3:A:320:ASP:O	3:A:321:TYR:HB3	1.91	0.71
3:H:117:ARG:HH22	3:H:149:GLU:HB3	1.55	0.70
3:A:23:ALA:HB3	3:A:102:VAL:HG13	1.71	0.70
3:F:61:ARG:HG2	3:F:61:ARG:NH1	2.01	0.70
3:J:297:ARG:CD	3:J:327:GLY:O	2.39	0.70
4:W:101:MES:O3S	3:I:365:ARG:NH1	2.25	0.70
3:A:61:ARG:HG2	3:A:61:ARG:NH1	1.99	0.70
3:C:226:ASN:O	3:C:230:LYS:HB2	1.92	0.70
3:E:61:ARG:CG	3:E:61:ARG:HH11	2.02	0.70
3:K:79:GLN:HB2	3:K:82:GLU:HB3	1.74	0.70
3:D:216:LYS:N	6:D:501:GDP:O2B	2.25	0.70
3:B:7:GLU:HB3	3:B:9:ILE:HG23	1.73	0.70
3:L:207:ILE:HD12	3:L:390:ALA:HB2	1.71	0.70
3:F:67:LEU:CD2	3:G:68:VAL:HG21	2.22	0.70
3:K:227:VAL:O	3:K:231:THR:HG22	1.91	0.70
3:K:166:LEU:HD22	3:L:280:MET:HG2	1.72	0.70
3:B:150:VAL:HG12	3:B:150:VAL:O	1.91	0.70
3:B:388:GLN:CD	3:C:362:GLN:HG2	2.13	0.70
3:J:403:ASN:HB3	3:J:404:LYS:HA	0.79	0.70
3:B:388:GLN:OE1	3:C:362:GLN:HG2	1.91	0.69
3:I:227:VAL:O	3:I:231:THR:HG22	1.92	0.69
3:I:41:GLU:HA	3:I:49:GLN:HE21	1.58	0.69
3:H:422:GLY:CA	6:I:501:GDP:C5	2.72	0.69
3:J:184:THR:H	3:J:185:GLY:HA3	1.58	0.69
3:K:103:GLU:HG3	3:K:107:ARG:HH21	1.57	0.69
3:A:388:GLN:HG3	3:B:138:VAL:HG21	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:170:TYR:CD1	3:I:280:MET:SD	2.86	0.69
3:H:173:ILE:HD11	3:I:263:LEU:HD22	1.74	0.69
3:I:184:THR:H	3:I:185:GLY:HA3	1.58	0.69
3:A:104:TYR:C	3:A:104:TYR:HD2	1.96	0.68
3:G:319:ILE:HG21	3:G:325:ILE:HD11	1.74	0.68
3:A:30:ALA:HB1	3:A:102:VAL:HG21	1.75	0.68
3:B:397:TYR:OH	3:B:399:ASP:CB	2.41	0.68
3:G:207:ILE:HD12	3:G:390:ALA:HB2	1.76	0.68
3:I:319:ILE:HG21	3:I:325:ILE:HD11	1.74	0.68
3:A:127:GLN:OE1	3:B:6:SER:HB2	1.92	0.68
3:A:388:GLN:CG	3:B:138:VAL:HG21	2.24	0.68
3:H:319:ILE:HG21	3:H:325:ILE:HD11	1.75	0.68
3:J:207:ILE:HD12	3:J:390:ALA:HB2	1.76	0.68
3:K:184:THR:H	3:K:185:GLY:HA3	1.57	0.68
3:K:50:LYS:HB2	3:K:83:ILE:HD11	1.76	0.68
3:G:304:LYS:HB3	3:L:159:PHE:HE2	1.58	0.67
3:H:207:ILE:HD12	3:H:390:ALA:HB2	1.76	0.67
3:K:79:GLN:O	3:K:79:GLN:HG2	1.93	0.67
3:A:306:ARG:HH11	3:A:306:ARG:CG	2.03	0.67
3:B:11:PRO:HD2	3:B:116:ARG:HB3	1.77	0.67
3:G:304:LYS:HB3	3:L:159:PHE:CE2	2.30	0.67
3:K:148:MET:SD	3:L:310:GLN:OE1	2.53	0.67
3:K:32:VAL:HB	3:K:33:PRO:HD3	1.75	0.67
3:H:231:THR:HG23	3:H:233:GLU:H	1.59	0.67
3:J:319:ILE:HG21	3:J:325:ILE:HD11	1.76	0.67
3:A:306:ARG:NH1	3:A:306:ARG:HG3	2.03	0.66
3:J:297:ARG:HG2	3:J:326:GLN:O	1.94	0.66
3:L:250:ARG:NH2	6:L:501:GDP:H5'	2.10	0.66
3:A:8:ARG:HD2	3:A:8:ARG:H	1.60	0.66
3:B:231:THR:HG23	3:B:233:GLU:H	1.59	0.66
3:E:216:LYS:N	6:E:501:GDP:O2B	2.29	0.66
3:E:250:ARG:NH2	6:E:501:GDP:O1A	2.24	0.66
3:A:261:GLN:HG2	3:A:264:ARG:HH12	1.56	0.66
3:B:61:ARG:NH1	3:B:61:ARG:HG2	2.04	0.66
3:H:68:VAL:HG11	3:I:105:TYR:CD2	2.31	0.66
2:W:3:DT:H2''	2:W:4:DT:C5'	2.25	0.66
3:D:231:THR:HG23	3:D:233:GLU:H	1.60	0.66
3:L:227:VAL:O	3:L:231:THR:HG22	1.96	0.66
2:W:4:DT:H2'	2:W:5:DT:C6	2.30	0.66
3:D:170:TYR:HD1	3:E:280:MET:SD	2.19	0.66
3:J:216:LYS:HD3	6:J:501:GDP:O2B	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:261:GLN:HG2	3:D:264:ARG:NH2	2.11	0.65
3:D:421:ASN:ND2	3:E:264:ARG:CD	2.56	0.65
3:I:231:THR:HG23	3:I:233:GLU:H	1.61	0.65
3:C:61:ARG:HG2	3:C:61:ARG:NH1	1.98	0.65
3:E:321:TYR:CE2	3:E:324:LEU:HD22	2.30	0.65
3:K:63:GLU:CB	3:K:64:PRO:HA	2.08	0.65
3:E:32:VAL:HB	3:E:33:PRO:HD3	1.79	0.65
3:G:227:VAL:O	3:G:231:THR:HG22	1.97	0.65
3:L:330:ARG:C	3:L:332:LYS:H	2.00	0.65
3:J:231:THR:HG23	3:J:233:GLU:H	1.61	0.65
3:B:200:PHE:N	3:B:200:PHE:HD1	1.95	0.65
3:B:306:ARG:HH11	3:B:306:ARG:CG	2.04	0.65
3:B:36:GLU:HG2	3:C:303:ALA:HB1	1.78	0.65
3:A:104:TYR:CD2	3:A:104:TYR:C	2.69	0.65
3:J:41:GLU:HA	3:J:49:GLN:HE21	1.61	0.65
3:B:397:TYR:O	3:B:412:ILE:HB	1.97	0.65
3:E:422:GLY:HA2	6:F:501:GDP:N7	2.12	0.65
3:J:404:LYS:O	3:J:404:LYS:HG3	1.96	0.65
3:B:32:VAL:HB	3:B:33:PRO:HD3	1.79	0.65
3:H:41:GLU:HA	3:H:49:GLN:HE21	1.62	0.65
3:H:159:PHE:CE2	3:I:308:LEU:HD22	2.31	0.65
3:H:184:THR:H	3:H:185:GLY:HA3	1.61	0.64
3:B:156:SER:O	3:B:157:GLY:C	2.36	0.64
3:A:9:ILE:HG12	3:A:9:ILE:O	1.95	0.64
3:B:158:ALA:O	3:B:159:PHE:C	2.35	0.64
3:G:231:THR:HG23	3:G:233:GLU:H	1.63	0.64
3:A:67:LEU:HD22	3:L:68:VAL:HG21	1.80	0.64
3:H:227:VAL:O	3:H:231:THR:HG22	1.97	0.64
3:C:319:ILE:HG21	3:C:325:ILE:HD11	1.78	0.64
3:D:226:ASN:O	3:D:230:LYS:HB2	1.96	0.64
3:D:68:VAL:HB	3:E:105:TYR:CE2	2.33	0.64
3:D:23:ALA:HB3	3:D:102:VAL:HG13	1.78	0.64
1:V:12:DT:H5'	3:B:336:GLN:CG	2.23	0.64
3:C:231:THR:HG23	3:C:233:GLU:H	1.63	0.64
3:A:319:ILE:HG21	3:A:325:ILE:HD11	1.79	0.64
3:D:388:GLN:CD	3:E:362:GLN:HG2	2.18	0.64
3:H:328:SER:HB3	3:H:330:ARG:HG2	1.78	0.64
3:H:404:LYS:O	3:H:404:LYS:HD2	1.96	0.63
3:A:14:ILE:HD12	3:A:45:ARG:NE	2.13	0.63
3:C:320:ASP:O	3:C:321:TYR:HB3	1.97	0.63
2:W:10:DT:H2''	2:W:11:DT:O4'	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:261:GLN:CG	3:E:264:ARG:HH22	2.11	0.63
3:K:231:THR:HG23	3:K:233:GLU:H	1.63	0.63
3:A:150:VAL:O	3:A:151:SER:HB3	1.98	0.63
3:J:227:VAL:O	3:J:231:THR:HG22	1.99	0.63
3:G:115:LEU:HG	3:H:136:ILE:HD12	1.81	0.63
3:E:200:PHE:HD1	3:E:200:PHE:N	1.97	0.63
3:A:202:ARG:O	3:A:203:SER:HB2	1.99	0.63
3:E:202:ARG:O	3:E:203:SER:HB2	1.99	0.63
3:L:41:GLU:HA	3:L:49:GLN:HE21	1.64	0.63
3:H:207:ILE:HD13	3:H:386:ILE:HG22	1.81	0.62
2:W:3:DT:C2'	2:W:4:DT:C5'	2.77	0.62
3:F:32:VAL:HB	3:F:33:PRO:HD3	1.81	0.62
3:I:163:LYS:HE3	3:I:163:LYS:H	1.64	0.62
3:J:110:GLU:OE1	3:J:152:GLN:CB	2.46	0.62
3:J:36:GLU:OE1	3:K:307:ARG:HB2	1.99	0.62
3:H:117:ARG:NH2	3:H:149:GLU:HB3	2.14	0.62
3:D:32:VAL:HB	3:D:33:PRO:HD3	1.82	0.62
3:E:174:GLU:O	3:E:176:LEU:N	2.31	0.62
3:A:169:THR:CG2	3:A:170:TYR:HA	2.29	0.62
3:D:202:ARG:O	3:D:203:SER:HB2	2.00	0.62
3:L:231:THR:HG23	3:L:233:GLU:H	1.63	0.62
3:B:319:ILE:HG21	3:B:325:ILE:HD11	1.81	0.62
3:B:9:ILE:HG13	3:B:9:ILE:O	2.00	0.62
3:K:57:ARG:NH1	3:K:57:ARG:HB2	2.15	0.62
3:C:202:ARG:O	3:C:203:SER:HB2	2.00	0.61
3:E:254:ALA:O	3:E:437:LYS:HE2	2.00	0.61
3:K:163:LYS:H	3:K:163:LYS:HE3	1.65	0.61
3:F:58:VAL:HG22	3:F:63:GLU:HG3	1.82	0.61
3:A:32:VAL:HB	3:A:33:PRO:HD3	1.81	0.61
3:C:32:VAL:HB	3:C:33:PRO:HD3	1.82	0.61
3:F:14:ILE:HD13	3:F:14:ILE:O	1.99	0.61
3:J:163:LYS:H	3:J:163:LYS:HE3	1.65	0.61
3:B:200:PHE:N	3:B:200:PHE:CD1	2.68	0.61
3:B:331:SER:O	3:B:333:GLU:N	2.33	0.61
3:E:231:THR:HG23	3:E:233:GLU:H	1.64	0.61
3:B:158:ALA:O	3:B:159:PHE:O	2.18	0.61
3:A:280:MET:SD	3:F:170:TYR:HD1	2.23	0.61
3:A:365:ARG:NH2	3:F:387:GLU:OE2	2.30	0.61
3:G:41:GLU:HA	3:G:49:GLN:HE21	1.64	0.61
3:H:163:LYS:HE3	3:H:163:LYS:H	1.65	0.61
3:J:36:GLU:OE1	3:K:307:ARG:HD3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:422:GLY:HA2	6:K:501:GDP:C5	2.36	0.61
3:J:173:ILE:HD11	3:K:263:LEU:HD22	1.82	0.61
3:G:163:LYS:H	3:G:163:LYS:HE3	1.65	0.61
3:F:226:ASN:O	3:F:230:LYS:HB2	2.00	0.61
3:I:13:SER:O	3:I:17:GLU:HG3	2.00	0.60
3:C:384:GLY:HA2	3:C:387:GLU:OE2	2.01	0.60
3:E:101:ASN:HB2	3:E:104:TYR:HD2	1.66	0.60
3:E:226:ASN:O	3:E:230:LYS:HB2	2.01	0.60
3:E:339:VAL:HG22	3:E:383:SER:HB3	1.83	0.60
3:F:306:ARG:NH1	3:F:306:ARG:HG3	2.01	0.60
3:L:12:GLN:O	3:L:112:LYS:HE3	2.01	0.60
3:B:33:PRO:CG	3:C:307:ARG:HD3	2.31	0.60
3:B:170:TYR:HD1	3:C:280:MET:SD	2.24	0.60
3:D:206:ILE:HA	3:D:392:ILE:HG23	1.84	0.60
3:C:331:SER:O	3:C:333:GLU:N	2.35	0.60
3:A:161:ASN:O	3:A:165:ILE:CG1	2.50	0.60
1:V:8:DT:H5"	3:D:336:GLN:HG3	1.83	0.60
3:I:403:ASN:CB	3:I:404:LYS:CA	2.80	0.60
3:F:200:PHE:N	3:F:200:PHE:HD1	1.98	0.60
3:C:370:ARG:NH2	3:C:379:ASP:OD2	2.34	0.60
3:A:231:THR:HG23	3:A:233:GLU:H	1.67	0.59
3:D:179:ARG:CB	3:D:180:ASP:CB	2.80	0.59
3:E:430:ALA:HB3	3:E:439:VAL:HG23	1.83	0.59
3:G:207:ILE:HD13	3:G:386:ILE:HG22	1.83	0.59
3:A:200:PHE:N	3:A:200:PHE:HD1	2.00	0.59
3:C:260:ALA:CB	3:C:264:ARG:HH21	1.96	0.59
3:B:259:ASN:OD1	3:B:434:GLU:HB3	2.02	0.59
3:H:419:GLN:HE21	3:H:423:PRO:HD2	1.68	0.59
3:B:100:ALA:O	3:B:101:ASN:ND2	2.36	0.59
3:B:36:GLU:HG2	3:C:303:ALA:CB	2.32	0.59
3:K:207:ILE:HD13	3:K:386:ILE:HG22	1.84	0.59
3:C:97:PRO:HG2	3:C:105:TYR:OH	2.02	0.59
3:D:206:ILE:HD12	3:D:206:ILE:N	2.18	0.59
3:J:36:GLU:HG2	3:K:303:ALA:HB1	1.85	0.59
3:F:321:TYR:CE2	3:F:324:LEU:HD22	2.37	0.59
3:K:40:PRO:HD3	3:K:52:PHE:HD2	1.68	0.59
3:A:248:VAL:HA	3:A:251:MET:HE2	1.84	0.58
3:B:445:PHE:H	3:B:445:PHE:HD1	1.50	0.58
3:L:330:ARG:HD3	3:L:333:GLU:H	1.68	0.58
3:C:200:PHE:HD1	3:C:200:PHE:N	2.00	0.58
3:D:200:PHE:HD1	3:D:200:PHE:N	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:8:DT:H2"	2:W:9:DT:O5'	2.03	0.58
3:E:58:VAL:HG22	3:E:63:GLU:HG3	1.85	0.58
3:K:112:LYS:O	3:K:116:ARG:HG3	2.02	0.58
3:I:403:ASN:CB	3:I:404:LYS:HA	2.34	0.58
3:B:135:GLU:HB3	3:B:138:VAL:HG12	1.86	0.58
3:G:330:ARG:C	3:G:332:LYS:H	2.07	0.58
3:J:207:ILE:HD13	3:J:386:ILE:HG22	1.85	0.58
3:A:14:ILE:CD1	3:A:45:ARG:HE	2.16	0.58
3:A:226:ASN:O	3:A:230:LYS:HB2	2.03	0.58
3:E:316:MET:HG2	3:E:356:PRO:HG2	1.85	0.58
3:F:206:ILE:HA	3:F:392:ILE:HG23	1.86	0.58
3:F:231:THR:HG23	3:F:233:GLU:H	1.68	0.58
3:A:104:TYR:CE2	3:A:108:ILE:CD1	2.83	0.58
3:L:207:ILE:HD13	3:L:386:ILE:HG22	1.85	0.58
3:E:200:PHE:CD1	3:E:200:PHE:N	2.70	0.58
3:F:319:ILE:HG21	3:F:325:ILE:HD11	1.84	0.58
3:I:115:LEU:HG	3:J:136:ILE:HD12	1.84	0.58
3:K:216:LYS:NZ	3:K:362:GLN:HE22	2.02	0.58
3:B:239:SER:HA	3:B:320:ASP:HB2	1.84	0.58
3:B:33:PRO:HG3	3:C:307:ARG:HD2	1.86	0.58
3:G:288:ILE:HD11	3:L:162:ILE:HD12	1.85	0.58
3:G:133:GLU:HG2	3:H:115:LEU:CD1	2.33	0.58
2:W:3:DT:H2"	2:W:4:DT:H5"	1.84	0.58
3:A:206:ILE:HA	3:A:392:ILE:HG23	1.86	0.57
3:D:316:MET:HG2	3:D:356:PRO:HG2	1.86	0.57
3:E:388:GLN:CD	3:F:362:GLN:HG2	2.24	0.57
3:I:159:PHE:CE2	3:J:304:LYS:HB3	2.39	0.57
3:B:444:ARG:NH1	3:B:444:ARG:HG3	2.07	0.57
3:F:331:SER:O	3:F:333:GLU:N	2.37	0.57
3:J:67:LEU:O	3:J:71:THR:HG23	2.04	0.57
3:K:79:GLN:HB2	3:K:82:GLU:CB	2.33	0.57
3:I:207:ILE:HD13	3:I:386:ILE:HG22	1.85	0.57
3:A:254:ALA:O	3:A:437:LYS:HE2	2.05	0.57
3:E:306:ARG:HG3	3:E:306:ARG:NH1	1.96	0.57
3:F:339:VAL:HG22	3:F:383:SER:HB3	1.86	0.57
3:I:133:GLU:HG2	3:J:115:LEU:HD13	1.86	0.57
3:B:153:ARG:O	3:B:154:LYS:HB2	2.03	0.57
3:B:37:ILE:HG23	3:B:155:HIS:HE1	1.69	0.57
3:C:370:ARG:HH11	3:C:370:ARG:HG3	1.70	0.57
3:B:441:LEU:O	3:B:443:ARG:N	2.37	0.57
3:D:170:TYR:CD1	3:E:280:MET:SD	2.97	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:384:GLY:O	3:I:387:GLU:OE1	2.21	0.57
3:A:403:ASN:HB2	3:A:406:SER:HB2	1.87	0.57
3:C:339:VAL:HG22	3:C:383:SER:HB3	1.87	0.57
3:I:136:ILE:HD12	3:J:115:LEU:HG	1.87	0.57
3:I:67:LEU:O	3:I:71:THR:HG23	2.04	0.57
3:F:403:ASN:HB2	3:F:406:SER:HB2	1.86	0.57
3:B:103:GLU:OE1	3:C:307:ARG:NE	2.38	0.57
3:K:50:LYS:HD2	3:K:79:GLN:HG3	1.87	0.57
3:L:320:ASP:O	3:L:360:LEU:HB2	2.05	0.57
3:A:145:ARG:HG3	3:B:310:GLN:OE1	2.04	0.56
3:F:200:PHE:N	3:F:200:PHE:CD1	2.72	0.56
3:G:321:TYR:CD2	3:G:324:LEU:HD22	2.40	0.56
3:I:302:ARG:HH11	3:I:306:ARG:NH2	2.03	0.56
3:I:216:LYS:NZ	6:I:501:GDP:O3B	2.38	0.56
3:B:226:ASN:O	3:B:230:LYS:HB2	2.04	0.56
3:B:306:ARG:HG3	3:B:306:ARG:NH1	2.03	0.56
3:L:170:TYR:HA	3:L:173:ILE:HD12	1.87	0.56
3:G:67:LEU:O	3:G:71:THR:HG23	2.06	0.56
3:K:339:VAL:HG23	3:K:383:SER:HB2	1.87	0.56
3:K:57:ARG:HH11	3:K:57:ARG:CB	2.17	0.56
3:A:169:THR:HG23	3:A:170:TYR:HA	1.87	0.56
3:B:440:ASN:O	3:B:442:GLU:N	2.38	0.56
3:E:228:ALA:CB	3:E:288:ILE:HG22	2.36	0.56
3:G:321:TYR:HD2	3:G:324:LEU:HD22	1.70	0.56
3:G:117:ARG:HH22	3:G:149:GLU:HB3	1.71	0.56
3:J:321:TYR:CE1	3:J:323:GLN:HG2	2.41	0.56
3:J:419:GLN:HE21	3:J:423:PRO:HD2	1.71	0.56
3:K:387:GLU:OE2	3:L:365:ARG:NH1	2.36	0.56
3:H:174:GLU:OE2	3:I:273:TRP:CH2	2.58	0.56
3:G:288:ILE:HD11	3:L:162:ILE:CD1	2.36	0.56
3:C:384:GLY:HA2	3:D:365:ARG:HH21	1.71	0.56
3:H:254:ALA:O	3:H:437:LYS:HE2	2.06	0.56
3:H:302:ARG:HH11	3:H:306:ARG:NH2	2.04	0.56
3:H:52:PHE:HD1	3:H:55:MET:HE2	1.71	0.56
3:K:422:GLY:HA2	6:L:501:GDP:C8	2.41	0.56
3:A:321:TYR:CE1	3:A:323:GLN:HG2	2.41	0.55
3:D:23:ALA:CB	3:D:102:VAL:HG13	2.36	0.55
3:D:319:ILE:HG22	3:D:321:TYR:H	1.70	0.55
3:D:331:SER:O	3:D:333:GLU:N	2.38	0.55
3:D:165:ILE:HG21	3:E:248:VAL:HG21	1.89	0.55
3:J:302:ARG:HH11	3:J:306:ARG:NH2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:13:SER:HB3	3:I:16:ALA:HB3	1.87	0.55
3:A:228:ALA:CB	3:A:288:ILE:HG22	2.36	0.55
3:C:200:PHE:N	3:C:200:PHE:CD1	2.74	0.55
3:G:215:GLY:CA	6:G:501:GDP:O2A	2.49	0.55
3:J:403:ASN:CB	3:J:404:LYS:CA	2.53	0.55
2:W:9:DT:OP1	3:I:384:GLY:N	2.39	0.55
6:A:502:GDP:N7	3:F:422:GLY:HA2	2.20	0.55
3:F:316:MET:HG2	3:F:356:PRO:HG2	1.87	0.55
3:J:339:VAL:HG23	3:J:383:SER:HB2	1.88	0.55
2:W:6:DT:C2'	2:W:7:DT:H5'	2.18	0.55
3:D:201:GLN:HB2	3:D:204:ASP:OD2	2.06	0.55
3:D:403:ASN:HB2	3:D:406:SER:HB2	1.87	0.55
3:G:250:ARG:NH2	6:G:501:GDP:O1A	2.38	0.55
3:E:331:SER:O	3:E:333:GLU:N	2.40	0.55
3:I:380:ILE:HD12	3:I:387:GLU:HG3	1.88	0.55
3:K:216:LYS:NZ	7:K:502:ALF:F3	2.30	0.55
3:A:23:ALA:HB3	3:A:102:VAL:CG1	2.36	0.55
3:A:321:TYR:HE1	3:A:323:GLN:HG2	1.72	0.55
3:H:207:ILE:HD13	3:H:386:ILE:CG2	2.36	0.55
3:K:302:ARG:HH11	3:K:306:ARG:NH2	2.04	0.55
3:L:52:PHE:HD1	3:L:55:MET:HE1	1.71	0.55
3:D:68:VAL:HG11	3:E:105:TYR:CD2	2.42	0.55
3:I:9:ILE:C	3:I:9:ILE:HD12	2.27	0.55
3:A:261:GLN:CG	3:A:264:ARG:NH1	2.59	0.54
3:D:200:PHE:CD1	3:D:200:PHE:N	2.75	0.54
3:E:55:MET:HG2	3:E:65:VAL:HG11	1.89	0.54
3:K:39:ILE:HG13	3:K:41:GLU:H	1.71	0.54
3:B:321:TYR:CZ	3:B:324:LEU:HD22	2.43	0.54
3:C:306:ARG:HG3	3:C:306:ARG:NH1	2.04	0.54
3:A:437:LYS:HD3	3:A:439:VAL:HG13	1.89	0.54
3:E:421:ASN:HD21	3:F:264:ARG:CD	2.13	0.54
3:L:71:THR:HG22	3:L:89:LEU:CD1	2.37	0.54
1:V:8:DT:C4'	1:V:9:DT:OP1	2.53	0.54
3:A:200:PHE:N	3:A:200:PHE:CD1	2.74	0.54
3:A:261:GLN:HA	3:A:264:ARG:HD3	1.89	0.54
3:B:320:ASP:O	3:B:321:TYR:CB	2.46	0.54
3:G:207:ILE:HD13	3:G:386:ILE:CG2	2.38	0.54
3:K:207:ILE:HD13	3:K:386:ILE:CG2	2.38	0.54
3:L:12:GLN:C	3:L:112:LYS:HG2	2.27	0.54
3:C:30:ALA:HB1	3:C:102:VAL:HG11	1.90	0.54
3:D:319:ILE:HG21	3:D:325:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:321:TYR:HE1	3:J:323:GLN:HG2	1.71	0.54
3:K:16:ALA:O	3:K:20:VAL:HG23	2.08	0.54
3:B:397:TYR:CE1	3:B:398:ARG:C	2.81	0.54
3:A:248:VAL:HA	3:A:251:MET:CE	2.38	0.54
3:C:430:ALA:HB3	3:C:439:VAL:HG23	1.89	0.54
3:E:421:ASN:ND2	3:F:264:ARG:CD	2.66	0.54
3:K:54:ALA:O	3:K:58:VAL:HG23	2.08	0.54
3:B:261:GLN:HE21	3:B:434:GLU:HG2	1.72	0.54
3:B:397:TYR:CD1	3:B:398:ARG:N	2.76	0.54
3:B:58:VAL:HG22	3:B:63:GLU:HG3	1.89	0.54
3:K:254:ALA:O	3:K:437:LYS:HE2	2.08	0.53
3:L:302:ARG:HH11	3:L:306:ARG:NH2	2.05	0.53
3:L:419:GLN:HE21	3:L:423:PRO:HD2	1.73	0.53
3:B:55:MET:HG2	3:B:65:VAL:HG11	1.90	0.53
3:E:403:ASN:HB2	3:E:406:SER:HB2	1.90	0.53
3:I:71:THR:HG22	3:I:89:LEU:CD1	2.36	0.53
3:K:124:SER:O	3:K:128:ASP:HB2	2.07	0.53
3:K:61:ARG:HB2	3:K:62:GLY:HA2	1.89	0.53
3:B:206:ILE:HG13	3:B:392:ILE:CG2	2.38	0.53
3:B:415:ILE:HA	3:B:426:THR:HG23	1.90	0.53
3:L:209:ALA:HB2	3:L:361:SER:HB3	1.90	0.53
3:A:321:TYR:CE2	3:A:324:LEU:HD22	2.44	0.53
3:G:351:ARG:NH1	3:H:134:ASP:HA	2.22	0.53
3:L:207:ILE:HD13	3:L:386:ILE:CG2	2.38	0.53
3:A:12:GLN:NE2	3:A:14:ILE:HG23	2.24	0.53
3:I:216:LYS:HZ3	6:I:501:GDP:PB	2.30	0.53
3:J:321:TYR:HA	3:J:360:LEU:O	2.08	0.53
3:B:154:LYS:CA	3:B:155:HIS:HB3	2.37	0.53
3:F:430:ALA:HB3	3:F:439:VAL:HG23	1.90	0.53
3:J:207:ILE:HD13	3:J:386:ILE:CG2	2.38	0.53
3:B:9:ILE:CG1	3:B:9:ILE:O	2.56	0.53
3:A:339:VAL:HG22	3:A:383:SER:HB3	1.91	0.53
3:I:321:TYR:CD2	3:I:324:LEU:HD22	2.43	0.53
3:I:97:PRO:HG2	3:I:105:TYR:OH	2.08	0.53
3:J:150:VAL:HG23	3:J:152:GLN:C	2.29	0.53
3:C:403:ASN:HB2	3:C:406:SER:HB2	1.91	0.53
3:H:238:PHE:CZ	3:H:301:ILE:HG23	2.43	0.53
3:K:419:GLN:HE21	3:K:423:PRO:HD2	1.73	0.53
3:C:277:THR:HG22	3:C:278:MET:CE	2.39	0.53
3:G:302:ARG:HH11	3:G:306:ARG:NH2	2.07	0.53
3:K:330:ARG:HG2	3:K:333:GLU:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:430:ALA:HB3	3:A:439:VAL:HG23	1.91	0.52
3:B:190:PHE:HA	3:B:440:ASN:ND2	2.24	0.52
3:F:216:LYS:NZ	6:F:501:GDP:O3B	2.42	0.52
3:G:419:GLN:HE21	3:G:423:PRO:HD2	1.73	0.52
3:B:309:LYS:HB2	3:B:314:LEU:HB2	1.91	0.52
3:B:365:ARG:HH21	3:B:365:ARG:CG	2.22	0.52
3:C:388:GLN:CD	3:D:362:GLN:HG2	2.29	0.52
2:W:7:DT:C5'	3:J:336:GLN:HG3	2.39	0.52
3:E:321:TYR:CD2	3:E:324:LEU:HD22	2.45	0.52
3:F:42:ASP:O	3:F:116:ARG:NH2	2.42	0.52
3:G:133:GLU:HG2	3:H:115:LEU:HD13	1.92	0.52
3:A:331:SER:O	3:A:333:GLU:N	2.43	0.52
3:B:298:VAL:HG11	3:B:345:SER:HB3	1.91	0.52
3:B:365:ARG:CZ	3:B:365:ARG:HB3	2.39	0.52
3:C:129:GLY:O	3:D:115:LEU:HD22	2.09	0.52
3:E:206:ILE:HG13	3:E:392:ILE:CG2	2.40	0.52
3:H:135:GLU:CD	3:H:138:VAL:HG11	2.30	0.52
3:I:380:ILE:HB	3:I:387:GLU:OE2	2.09	0.52
3:K:61:ARG:HB2	3:K:62:GLY:CA	2.39	0.52
3:L:67:LEU:O	3:L:71:THR:HG23	2.09	0.52
3:H:37:ILE:O	3:H:110:GLU:HG3	2.10	0.52
3:H:58:VAL:HG13	3:H:63:GLU:HG3	1.92	0.52
3:I:238:PHE:CZ	3:I:301:ILE:HG23	2.45	0.52
3:I:419:GLN:HE21	3:I:423:PRO:HD2	1.74	0.52
3:B:29:ALA:HB1	3:C:310:GLN:CD	2.30	0.52
3:D:384:GLY:HA2	3:D:387:GLU:OE2	2.10	0.52
3:G:362:GLN:HG2	3:L:388:GLN:CD	2.30	0.52
3:B:206:ILE:HA	3:B:392:ILE:HG23	1.91	0.52
3:D:248:VAL:HA	3:D:251:MET:CE	2.40	0.52
3:D:177:HIS:ND1	3:E:273:TRP:HZ2	2.08	0.52
3:E:206:ILE:HA	3:E:392:ILE:HG23	1.91	0.52
3:I:250:ARG:NH2	6:I:501:GDP:O1A	2.43	0.52
3:L:339:VAL:HG23	3:L:383:SER:HB2	1.91	0.52
2:W:4:DT:H2''	2:W:5:DT:O4'	2.10	0.52
3:A:341:GLU:HG2	3:A:344[B]:ARG:NH2	2.25	0.52
3:H:23:ALA:CB	3:H:102:VAL:HG13	2.40	0.52
3:L:367:VAL:HG23	3:L:370:ARG:HH12	1.74	0.52
3:B:439:VAL:HB	3:B:443:ARG:HG3	1.91	0.51
3:F:67:LEU:O	3:F:71:THR:CG2	2.54	0.51
3:I:339:VAL:HG23	3:I:383:SER:HB2	1.91	0.51
3:I:58:VAL:HG13	3:I:63:GLU:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:173:ILE:HD11	3:J:263:LEU:HD22	1.92	0.51
3:K:21:LEU:HB2	3:K:92:LEU:HD13	1.93	0.51
3:L:58:VAL:HG13	3:L:63:GLU:HG3	1.93	0.51
3:A:259:ASN:HD21	3:A:261:GLN:HB2	1.75	0.51
3:B:202:ARG:O	3:B:203:SER:HB2	2.10	0.51
3:C:333:GLU:O	3:C:334:ASN:C	2.48	0.51
3:F:437:LYS:HD3	3:F:439:VAL:HG13	1.91	0.51
3:G:339:VAL:HG23	3:G:383:SER:HB2	1.91	0.51
3:C:116:ARG:HA	3:C:119:ILE:HD12	1.92	0.51
3:D:430:ALA:HB3	3:D:439:VAL:HG23	1.93	0.51
3:G:37:ILE:O	3:G:110:GLU:HG3	2.10	0.51
3:K:24:VAL:HG22	3:K:31:LEU:HB2	1.92	0.51
3:K:103:GLU:HG3	3:K:107:ARG:NH2	2.23	0.51
3:K:31:LEU:HD22	3:K:65:VAL:HG21	1.92	0.51
3:K:40:PRO:HD3	3:K:52:PHE:CD2	2.44	0.51
3:L:238:PHE:CZ	3:L:301:ILE:HG23	2.45	0.51
3:B:339:VAL:HG22	3:B:383:SER:HB3	1.92	0.51
3:I:422:GLY:HA2	6:J:501:GDP:C8	2.44	0.51
3:L:225:GLN:HE22	3:L:254:ALA:HB3	1.75	0.51
3:B:156:SER:O	3:B:158:ALA:N	2.44	0.51
3:C:254:ALA:O	3:C:437:LYS:HE2	2.10	0.51
3:F:228:ALA:CB	3:F:288:ILE:HG22	2.41	0.51
3:K:77:SER:HB2	3:K:79:GLN:HE22	1.74	0.51
3:B:148:MET:C	3:B:150:VAL:H	2.14	0.51
3:B:397:TYR:CZ	3:B:399:ASP:HB3	2.45	0.51
3:C:432:ILE:N	3:C:432:ILE:HD12	2.26	0.51
3:C:151:SER:HA	3:D:140:LEU:HD13	1.93	0.51
3:C:216:LYS:N	6:C:501:GDP:O2B	2.44	0.51
3:H:63:GLU:O	3:I:104:TYR:CG	2.64	0.51
3:J:58:VAL:HG13	3:J:63:GLU:HG3	1.92	0.51
2:W:2:DT:H2''	3:L:336:GLN:HG3	1.93	0.51
3:L:250:ARG:HH21	6:L:501:GDP:C5'	2.20	0.51
3:A:162:ILE:HA	3:A:165:ILE:CD1	2.41	0.51
3:E:309:LYS:HB2	3:E:314:LEU:HB2	1.93	0.51
3:I:40:PRO:O	3:I:49:GLN:HG2	2.11	0.51
3:C:321:TYR:CE1	3:C:324:LEU:HD13	2.46	0.50
3:D:55:MET:HG2	3:D:65:VAL:HG11	1.94	0.50
3:E:319:ILE:HG22	3:E:321:TYR:H	1.76	0.50
3:I:387:GLU:OE2	3:J:365:ARG:NH2	2.43	0.50
3:D:216:LYS:HB3	3:D:360:LEU:HD13	1.94	0.50
3:E:248:VAL:HA	3:E:251:MET:CE	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:163:LYS:H	3:E:163:LYS:HE3	1.76	0.50
3:A:280:MET:HE3	3:F:166:LEU:HB3	1.92	0.50
3:H:174:GLU:OE2	3:I:273:TRP:HH2	1.93	0.50
3:A:58:VAL:HG22	3:A:63:GLU:HG3	1.92	0.50
3:F:260:ALA:HB1	3:F:264:ARG:HH21	1.75	0.50
3:F:86:VAL:HG11	3:G:68:VAL:HG12	1.93	0.50
3:J:388:GLN:CD	3:K:362:GLN:HG2	2.31	0.50
3:J:27:ASP:HB2	3:J:99:ALA:CB	2.41	0.50
3:C:309:LYS:HB2	3:C:314:LEU:HB2	1.93	0.50
3:F:254:ALA:O	3:F:437:LYS:HE2	2.11	0.50
3:B:416:ILE:O	3:B:424:VAL:HG22	2.11	0.50
3:C:148:MET:SD	3:D:144:ASP:OD1	2.69	0.50
3:F:206:ILE:HD12	3:F:206:ILE:N	2.27	0.50
3:K:225:GLN:HE22	3:K:254:ALA:HB3	1.76	0.50
3:B:388:GLN:NE2	3:C:362:GLN:HG2	2.26	0.50
6:G:501:GDP:C5	3:L:422:GLY:HA2	2.47	0.50
3:L:74:LEU:HD13	3:L:83:ILE:HD13	1.94	0.50
3:A:377:MET:HB3	3:A:387:GLU:HG2	1.94	0.49
3:B:384:GLY:HA2	3:B:387:GLU:OE2	2.12	0.49
3:C:377:MET:HB3	3:C:387:GLU:HG2	1.93	0.49
3:I:302:ARG:HH11	3:I:306:ARG:HH22	1.60	0.49
3:I:207:ILE:HD13	3:I:386:ILE:CG2	2.42	0.49
3:I:52:PHE:HD1	3:I:55:MET:HE2	1.77	0.49
3:B:200:PHE:CE2	3:B:358:ILE:HD11	2.47	0.49
3:C:228:ALA:CB	3:C:288:ILE:HG22	2.42	0.49
3:F:337:GLN:HA	3:F:340:SER:HB2	1.93	0.49
3:G:52:PHE:HD1	3:G:55:MET:HE2	1.77	0.49
3:H:53:HIS:HE1	3:H:57:ARG:HH12	1.60	0.49
3:L:254:ALA:O	3:L:437:LYS:HE2	2.12	0.49
3:B:58:VAL:HG13	3:B:63:GLU:HB2	1.94	0.49
3:C:206:ILE:N	3:C:206:ILE:HD12	2.27	0.49
3:D:388:GLN:NE2	3:E:362:GLN:HG2	2.27	0.49
3:B:193:LEU:HA	3:B:427:VAL:HG21	1.94	0.49
3:A:365:ARG:HH21	3:F:384:GLY:HA2	1.76	0.49
2:W:2:DT:C2'	2:W:3:DT:O5'	2.58	0.49
3:D:254:ALA:O	3:D:437:LYS:HE2	2.13	0.49
3:F:206:ILE:HG13	3:F:392:ILE:CG2	2.41	0.49
3:B:154:LYS:N	3:B:155:HIS:HB2	2.23	0.49
1:V:8:DT:H5"	3:D:336:GLN:CG	2.43	0.49
3:F:221:LEU:HD21	3:F:247:LEU:HG	1.95	0.49
3:J:216:LYS:NZ	3:J:362:GLN:HE22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:39:ILE:HD11	3:K:41:GLU:OE1	2.12	0.49
3:B:36:GLU:O	3:B:36:GLU:OE1	2.30	0.49
3:D:58:VAL:HG22	3:D:63:GLU:HG3	1.93	0.49
3:H:209:ALA:HB2	3:H:361:SER:HB3	1.94	0.49
3:A:392:ILE:HA	3:A:418:LYS:O	2.12	0.49
3:B:201:GLN:HB2	3:B:204:ASP:OD2	2.13	0.49
3:E:130:TYR:CZ	3:F:119:ILE:HG21	2.48	0.49
3:F:194:ASP:HA	3:F:197:THR:HG22	1.95	0.49
3:A:298:VAL:HG11	3:A:345:SER:HB3	1.93	0.49
3:B:8:ARG:O	3:B:10:PRO:HD3	2.12	0.49
3:G:225:GLN:HE22	3:G:254:ALA:HB3	1.78	0.49
3:K:57:ARG:HH11	3:K:57:ARG:HB2	1.75	0.49
3:I:53:HIS:HE1	3:I:57:ARG:HH12	1.61	0.49
3:L:173:ILE:O	3:L:175:MET:N	2.45	0.49
3:A:367:VAL:HG23	3:A:370:ARG:NH2	2.28	0.48
3:B:333:GLU:O	3:B:334:ASN:C	2.50	0.48
3:F:432:ILE:N	3:F:432:ILE:HD12	2.28	0.48
3:H:302:ARG:HH11	3:H:306:ARG:HH22	1.60	0.48
3:I:302:ARG:NH1	3:I:306:ARG:NH2	2.60	0.48
3:K:238:PHE:CZ	3:K:301:ILE:HG23	2.47	0.48
3:D:248:VAL:HA	3:D:251:MET:HE2	1.96	0.48
3:D:31:LEU:HD22	3:D:65:VAL:HG21	1.95	0.48
3:D:337:GLN:HA	3:D:340:SER:HB2	1.94	0.48
3:G:58:VAL:HG13	3:G:63:GLU:HG3	1.95	0.48
3:J:302:ARG:HH11	3:J:306:ARG:HH22	1.61	0.48
3:L:199:GLY:CA	3:L:200:PHE:HB2	2.39	0.48
3:C:58:VAL:HG22	3:C:63:GLU:HG3	1.95	0.48
3:J:302:ARG:NH1	3:J:306:ARG:NH2	2.61	0.48
3:A:115:LEU:HG	3:B:136:ILE:HD13	1.95	0.48
3:J:209:ALA:HB2	3:J:361:SER:HB3	1.94	0.48
3:B:190:PHE:HA	3:B:440:ASN:HD21	1.79	0.48
3:F:202:ARG:O	3:F:203:SER:HB2	2.13	0.48
3:H:23:ALA:HB3	3:H:102:VAL:HG13	1.95	0.48
3:B:419:GLN:HG3	3:B:422:GLY:H	1.78	0.48
3:C:315:GLY:O	3:C:356:PRO:HD2	2.14	0.48
3:C:165:ILE:HD13	3:D:244:ALA:HB1	1.95	0.48
3:H:302:ARG:NH1	3:H:306:ARG:NH2	2.61	0.48
3:A:341:GLU:HG2	3:A:344[B]:ARG:CZ	2.44	0.48
3:E:129:GLY:O	3:F:115:LEU:HD22	2.13	0.48
3:J:211:ARG:HH22	3:J:365:ARG:HD2	1.79	0.48
3:A:321:TYR:CD2	3:A:324:LEU:HD22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:14:ILE:O	3:E:16:ALA:N	2.45	0.48
3:G:238:PHE:CZ	3:G:301:ILE:HG23	2.48	0.48
3:K:184:THR:N	3:K:185:GLY:HA3	2.26	0.48
2:W:7:DT:H5"	3:J:336:GLN:CG	2.44	0.48
3:B:316:MET:HG2	3:B:356:PRO:HG2	1.95	0.48
3:E:367:VAL:HG23	3:E:370:ARG:NH2	2.28	0.48
3:F:320:ASP:O	3:F:321:TYR:HB3	2.14	0.48
3:G:117:ARG:NH2	3:G:149:GLU:HB3	2.29	0.48
3:K:221:LEU:HD11	3:K:247:LEU:HG	1.96	0.48
3:K:302:ARG:HH11	3:K:306:ARG:HH22	1.61	0.48
3:K:302:ARG:NH1	3:K:306:ARG:NH2	2.62	0.48
3:L:302:ARG:HH11	3:L:306:ARG:HH22	1.62	0.48
3:L:98:THR:OG1	3:L:99:ALA:N	2.47	0.48
3:B:397:TYR:CZ	3:B:398:ARG:O	2.67	0.48
3:H:199:GLY:CA	3:H:200:PHE:HB2	2.40	0.48
3:H:422:GLY:HA2	6:I:501:GDP:C8	2.47	0.48
3:H:71:THR:HG22	3:H:89:LEU:CD1	2.44	0.48
3:I:32:VAL:HB	3:I:33:PRO:HD3	1.96	0.48
3:J:36:GLU:OE1	3:K:307:ARG:CD	2.62	0.48
3:D:437:LYS:HD3	3:D:439:VAL:HG13	1.96	0.47
3:E:337:GLN:HA	3:E:340:SER:HB2	1.96	0.47
3:F:169:THR:O	3:F:173:ILE:HG13	2.15	0.47
3:D:422:GLY:HA3	3:D:423:PRO:HD3	1.68	0.47
3:J:202:ARG:O	3:J:203:SER:HB2	2.14	0.47
3:B:163:LYS:HE3	3:B:163:LYS:H	1.78	0.47
3:B:228:ALA:CB	3:B:288:ILE:HG22	2.44	0.47
3:B:365:ARG:HH21	3:B:365:ARG:HG3	1.79	0.47
3:B:397:TYR:CG	3:B:398:ARG:N	2.82	0.47
3:G:330:ARG:O	3:G:332:LYS:N	2.37	0.47
3:H:225:GLN:HE22	3:H:254:ALA:HB3	1.79	0.47
3:L:53:HIS:HE1	3:L:57:ARG:HH12	1.62	0.47
3:B:197:THR:HG23	3:B:199:GLY:O	2.14	0.47
3:B:200:PHE:H	3:B:200:PHE:HD1	1.62	0.47
3:D:432:ILE:HD12	3:D:432:ILE:N	2.30	0.47
3:K:260:ALA:HB3	6:K:501:GDP:O6	2.14	0.47
3:B:442:GLU:O	3:B:443:ARG:NE	2.47	0.47
3:H:387:GLU:OE2	3:I:365:ARG:NH2	2.45	0.47
3:E:261:GLN:CG	3:E:264:ARG:NH2	2.62	0.47
3:F:370:ARG:NH2	3:F:379:ASP:OD2	2.47	0.47
3:J:225:GLN:HE22	3:J:254:ALA:HB3	1.80	0.47
3:A:194:ASP:HA	3:A:197:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:156:SER:OG	3:C:293:THR:HG21	2.15	0.47
3:D:135:GLU:HB2	3:D:138:VAL:HG12	1.96	0.47
3:A:365:ARG:NH2	3:F:384:GLY:HA2	2.29	0.47
3:G:53:HIS:HE1	3:G:57:ARG:HH12	1.63	0.47
3:J:254:ALA:O	3:J:437:LYS:HE2	2.14	0.47
3:B:206:ILE:N	3:B:206:ILE:HD12	2.30	0.47
3:C:316:MET:HG2	3:C:356:PRO:HG2	1.97	0.47
3:F:392:ILE:HA	3:F:418:LYS:O	2.15	0.47
3:G:220:ALA:HB2	3:G:360:LEU:HD21	1.97	0.47
3:H:32:VAL:HB	3:H:33:PRO:HD3	1.96	0.47
3:H:420:ARG:HD3	3:I:242:MET:CE	2.44	0.47
2:W:7:DT:H5"	3:J:336:GLN:HG3	1.96	0.47
3:B:428:GLN:O	3:B:429:LEU:HD23	2.15	0.47
3:D:9:ILE:HA	3:D:10:PRO:HD2	1.68	0.47
3:K:387:GLU:OE2	3:L:365:ARG:HD2	2.15	0.47
3:B:134:ASP:HB2	3:B:135:GLU:OE2	2.15	0.47
3:B:154:LYS:CA	3:B:155:HIS:CB	2.93	0.47
3:D:419:GLN:HG3	3:D:422:GLY:H	1.80	0.47
3:G:221:LEU:HD11	3:G:247:LEU:HG	1.97	0.47
3:I:159:PHE:HE2	3:J:304:LYS:HB3	1.78	0.47
4:W:101:MES:H81	3:I:369:GLN:HE22	1.80	0.47
3:B:33:PRO:CB	3:C:307:ARG:HD3	2.45	0.47
3:F:55:MET:HG2	3:F:65:VAL:HG11	1.97	0.47
3:H:339:VAL:HG23	3:H:383:SER:HB2	1.97	0.47
3:A:26:LEU:HB2	3:A:99:ALA:HB2	1.97	0.46
3:B:150:VAL:O	3:B:150:VAL:CG1	2.60	0.46
3:B:408:ASN:O	3:B:411:ILE:HD12	2.15	0.46
3:C:422:GLY:HA2	6:D:501:GDP:N7	2.28	0.46
3:D:315:GLY:O	3:D:356:PRO:HD2	2.15	0.46
3:G:403:ASN:HB3	3:G:404:LYS:CA	2.45	0.46
3:G:184:THR:N	3:G:185:GLY:HA3	2.23	0.46
3:I:133:GLU:HG2	3:J:115:LEU:CD1	2.44	0.46
3:L:302:ARG:NH1	3:L:306:ARG:NH2	2.63	0.46
3:A:145:ARG:CG	3:B:310:GLN:OE1	2.64	0.46
3:C:67:LEU:O	3:C:71:THR:CG2	2.58	0.46
3:D:228:ALA:CB	3:D:288:ILE:HG22	2.46	0.46
3:G:136:ILE:HG21	3:H:111:GLU:HG2	1.98	0.46
3:G:71:THR:HG22	3:G:89:LEU:CD1	2.43	0.46
4:W:101:MES:H51	3:I:369:GLN:NE2	2.30	0.46
3:I:388:GLN:CD	3:J:362:GLN:HG2	2.36	0.46
3:I:58:VAL:HG13	3:I:63:GLU:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:206:ILE:HG13	3:A:392:ILE:CG2	2.45	0.46
3:D:380:ILE:O	3:E:365:ARG:NH2	2.26	0.46
3:E:201:GLN:HB2	3:E:204:ASP:OD2	2.15	0.46
3:F:160:LYS:HB3	3:F:165:ILE:HD11	1.98	0.46
3:H:330:ARG:C	3:H:332:LYS:N	2.58	0.46
3:J:77:SER:HB2	3:J:79:GLN:HG2	1.98	0.46
3:K:199:GLY:CA	3:K:200:PHE:HB2	2.39	0.46
3:A:117:ARG:NH1	3:A:149:GLU:O	2.33	0.46
3:A:333:GLU:O	3:A:334:ASN:C	2.53	0.46
3:A:55:MET:HG2	3:A:65:VAL:HG11	1.96	0.46
3:C:215:GLY:HA2	6:C:501:GDP:O2A	2.15	0.46
3:A:362:GLN:HG2	3:F:388:GLN:CD	2.35	0.46
3:G:367:VAL:HG23	3:G:370:ARG:HH12	1.80	0.46
3:G:209:ALA:HB2	3:G:361:SER:HB3	1.98	0.46
3:G:362:GLN:HG2	3:L:388:GLN:OE1	2.16	0.46
3:J:238:PHE:CZ	3:J:301:ILE:HG23	2.51	0.46
3:B:320:ASP:O	3:B:320:ASP:OD2	2.34	0.46
3:E:377:MET:HB3	3:E:387:GLU:HG2	1.97	0.46
3:H:419:GLN:NE2	3:H:423:PRO:HD2	2.31	0.46
3:I:199:GLY:CA	3:I:200:PHE:HB2	2.39	0.46
3:J:27:ASP:HB2	3:J:99:ALA:HB1	1.98	0.46
3:K:220:ALA:HB2	3:K:360:LEU:HD21	1.98	0.46
3:B:31:LEU:HD22	3:B:65:VAL:HG21	1.98	0.46
3:C:409:LYS:O	3:C:411:ILE:N	2.49	0.46
3:E:206:ILE:HD12	3:E:206:ILE:N	2.31	0.46
3:F:309:LYS:HB2	3:F:314:LEU:HB2	1.97	0.46
3:H:391:ASP:HB3	3:H:420:ARG:NH1	2.31	0.46
3:L:40:PRO:O	3:L:49:GLN:HG2	2.16	0.46
3:B:410:ASN:HD22	3:B:411:ILE:HG13	1.81	0.46
3:B:444:ARG:NH1	3:B:444:ARG:CG	2.58	0.46
3:C:392:ILE:HA	3:C:418:LYS:O	2.15	0.46
3:C:422:GLY:HA3	3:C:423:PRO:HD3	1.72	0.46
3:I:420:ARG:HD3	3:J:242:MET:CE	2.45	0.46
3:I:250:ARG:HH21	6:I:501:GDP:H5'	1.81	0.46
3:J:36:GLU:OE2	3:K:307:ARG:NH2	2.49	0.46
3:A:11:PRO:HD2	3:A:116:ARG:HB3	1.98	0.46
3:B:220:ALA:HB2	3:B:360:LEU:HD21	1.96	0.46
3:C:211:ARG:NE	3:C:368:GLU:OE2	2.49	0.46
3:D:206:ILE:HG13	3:D:392:ILE:CG2	2.46	0.46
3:F:248:VAL:HA	3:F:251:MET:CE	2.46	0.46
3:G:254:ALA:O	3:G:437:LYS:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:425:GLY:CA	3:H:294:PRO:HG2	2.36	0.46
3:J:367:VAL:HG23	3:J:370:ARG:HH12	1.81	0.46
3:K:104:TYR:O	3:K:108:ILE:HD13	2.15	0.46
3:J:36:GLU:CD	3:K:307:ARG:CZ	2.84	0.46
3:K:403:ASN:HB3	3:K:405:ASP:H	1.80	0.46
3:E:58:VAL:HG13	3:E:63:GLU:HB2	1.98	0.45
3:H:77:SER:HB2	3:H:79:GLN:HG2	1.98	0.45
3:J:216:LYS:HB3	3:J:360:LEU:HD13	1.96	0.45
3:A:337:GLN:HA	3:A:340:SER:HB2	1.97	0.45
3:B:337:GLN:HA	3:B:340:SER:HB2	1.98	0.45
3:C:206:ILE:HA	3:C:392:ILE:HG23	1.98	0.45
3:E:333:GLU:O	3:E:334:ASN:C	2.55	0.45
3:K:334:ASN:HD21	3:K:337:GLN:NE2	2.14	0.45
1:V:6:DT:H2"	1:V:7:DT:O5'	2.17	0.45
3:D:163:LYS:H	3:D:163:LYS:HE3	1.80	0.45
3:E:437:LYS:HD3	3:E:439:VAL:HG13	1.97	0.45
3:E:67:LEU:O	3:E:71:THR:CG2	2.56	0.45
3:J:220:ALA:HB2	3:J:360:LEU:HD21	1.98	0.45
3:J:58:VAL:HG13	3:J:63:GLU:CG	2.47	0.45
3:K:422:GLY:HA3	3:K:423:PRO:HD3	1.77	0.45
3:L:221:LEU:HD11	3:L:247:LEU:HG	1.97	0.45
3:C:55:MET:HG2	3:C:65:VAL:HG11	1.99	0.45
3:E:238:PHE:CZ	3:E:301:ILE:HG23	2.50	0.45
3:F:333:GLU:O	3:F:334:ASN:C	2.55	0.45
3:H:349:LEU:HD12	3:H:353:LEU:HD13	1.98	0.45
3:H:419:GLN:HG3	3:H:422:GLY:H	1.81	0.45
3:I:284:SER:C	3:I:286:ALA:H	2.19	0.45
3:J:419:GLN:HG3	3:J:422:GLY:H	1.81	0.45
3:L:422:GLY:HA3	3:L:423:PRO:HD3	1.74	0.45
2:W:11:DT:OP1	3:H:384:GLY:N	2.48	0.45
3:A:206:ILE:N	3:A:206:ILE:HD12	2.32	0.45
3:C:216:LYS:HB2	6:C:501:GDP:O2B	2.15	0.45
3:H:63:GLU:N	3:H:64:PRO:HA	2.32	0.45
3:J:233:GLU:CG	3:J:315:GLY:HA3	2.46	0.45
3:B:321:TYR:HE1	3:B:324:LEU:HD13	1.76	0.45
3:D:240:LEU:N	3:D:240:LEU:HD23	2.31	0.45
3:D:31:LEU:CD2	3:D:65:VAL:HG21	2.47	0.45
1:V:9:DT:OP1	3:D:382:GLU:HA	2.17	0.45
3:D:165:ILE:CG2	3:E:248:VAL:HG21	2.47	0.45
3:E:228:ALA:HB1	3:E:288:ILE:HG22	1.99	0.45
3:F:201:GLN:HB2	3:F:204:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:302:ARG:HH11	3:G:306:ARG:HH22	1.64	0.45
3:G:32:VAL:HB	3:G:33:PRO:HD3	1.98	0.45
3:A:134:ASP:HB2	3:A:135:GLU:HG3	1.98	0.45
3:A:320:ASP:O	3:A:321:TYR:CB	2.62	0.45
3:E:197:THR:HG23	3:E:199:GLY:O	2.16	0.45
3:E:298:VAL:HG11	3:E:345:SER:HB3	1.97	0.45
3:F:250:ARG:NH2	6:F:501:GDP:O1A	2.44	0.45
3:I:222:ASN:HA	3:I:222:ASN:HD22	1.61	0.45
3:A:221:LEU:HD21	3:A:247:LEU:HG	1.99	0.45
3:B:96:VAL:HA	3:B:97:PRO:HD2	1.82	0.45
3:C:298:VAL:HG11	3:C:345:SER:HB3	1.99	0.45
3:D:61:ARG:N	3:D:62:GLY:HA2	2.32	0.45
3:D:68:VAL:CB	3:E:105:TYR:CE2	3.00	0.45
3:F:298:VAL:HG11	3:F:345:SER:HB3	1.99	0.45
3:I:220:ALA:HB2	3:I:360:LEU:HD21	1.99	0.45
3:B:63:GLU:O	3:C:104:TYR:CG	2.70	0.45
3:C:110:GLU:OE1	3:C:153:ARG:CD	2.65	0.45
3:C:321:TYR:CE2	3:C:324:LEU:HD22	2.52	0.45
3:F:116:ARG:HA	3:F:119:ILE:HD12	1.99	0.45
3:F:61:ARG:N	3:F:62:GLY:HA2	2.32	0.45
3:G:137:ASP:O	3:G:141:ASP:HB2	2.17	0.45
3:G:302:ARG:NH1	3:G:306:ARG:NH2	2.65	0.45
3:D:387:GLU:OE2	3:E:365:ARG:NH2	2.43	0.45
3:E:209:ALA:HB2	3:E:361:SER:HB3	1.97	0.45
3:I:419:GLN:HG3	3:I:422:GLY:H	1.82	0.45
3:J:76:ALA:HB1	3:L:134:ASP:HA	1.99	0.45
3:L:233:GLU:CG	3:L:315:GLY:HA3	2.47	0.45
3:B:11:PRO:O	3:B:116:ARG:NH1	2.48	0.44
3:D:339:VAL:HG22	3:D:383:SER:HB3	1.99	0.44
3:F:227:VAL:O	3:F:231:THR:CG2	2.47	0.44
3:K:419:GLN:HG3	3:K:422:GLY:H	1.82	0.44
3:B:315:GLY:O	3:B:356:PRO:HD2	2.17	0.44
3:H:174:GLU:C	3:H:176:LEU:H	2.17	0.44
3:H:233:GLU:CG	3:H:315:GLY:HA3	2.48	0.44
3:J:284:SER:C	3:J:286:ALA:H	2.21	0.44
3:J:206:ILE:HA	3:J:392:ILE:HG23	1.99	0.44
3:J:63:GLU:N	3:J:64:PRO:HA	2.33	0.44
3:K:115:LEU:HG	3:L:136:ILE:HD12	1.98	0.44
3:K:206:ILE:HA	3:K:392:ILE:HG23	1.98	0.44
3:L:117:ARG:NH2	3:L:149:GLU:HB3	2.33	0.44
3:K:148:MET:CE	3:L:310:GLN:OE1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:61:ARG:N	3:B:62:GLY:HA2	2.33	0.44
3:E:384:GLY:HA2	3:E:387:GLU:OE2	2.17	0.44
3:F:31:LEU:HD22	3:F:65:VAL:HG21	1.98	0.44
3:G:199:GLY:CA	3:G:200:PHE:HB2	2.39	0.44
3:J:388:GLN:NE2	3:K:362:GLN:HG2	2.33	0.44
3:C:248:VAL:HA	3:C:251:MET:HE2	1.99	0.44
3:C:130:TYR:CD2	3:D:11:PRO:HD3	2.53	0.44
3:E:194:ASP:HA	3:E:197:THR:HG22	1.98	0.44
3:H:388:GLN:CD	3:I:362:GLN:HG2	2.38	0.44
3:I:215:GLY:CA	6:I:501:GDP:O2A	2.60	0.44
3:J:39:ILE:O	3:J:40:PRO:C	2.56	0.44
3:L:117:ARG:HH22	3:L:149:GLU:HB3	1.83	0.44
3:L:220:ALA:HB2	3:L:360:LEU:HD21	2.00	0.44
3:B:365:ARG:NH2	3:B:365:ARG:HB3	2.33	0.44
3:B:380:ILE:O	3:C:365:ARG:NH2	2.50	0.44
3:C:110:GLU:OE1	3:C:153:ARG:HD2	2.17	0.44
3:C:163:LYS:H	3:C:163:LYS:HE3	1.83	0.44
3:L:216:LYS:NZ	3:L:362:GLN:HE22	2.15	0.44
3:A:127:GLN:OE1	3:B:6:SER:CB	2.64	0.44
3:B:29:ALA:HB1	3:C:310:GLN:OE1	2.17	0.44
3:C:248:VAL:HA	3:C:251:MET:CE	2.47	0.44
3:C:419:GLN:HG3	3:C:422:GLY:H	1.83	0.44
3:D:370:ARG:CG	3:D:370:ARG:NH1	2.70	0.44
3:E:116:ARG:HA	3:E:119:ILE:HD12	1.98	0.44
3:F:86:VAL:CG1	3:G:68:VAL:HG12	2.48	0.44
3:H:206:ILE:HA	3:H:392:ILE:HG23	1.98	0.44
3:B:194:ASP:HA	3:B:197:THR:HG22	2.00	0.44
3:B:445:PHE:N	3:B:445:PHE:HD1	2.16	0.44
3:C:31:LEU:HD22	3:C:65:VAL:HG21	1.99	0.44
3:E:200:PHE:HD1	3:E:200:PHE:H	1.66	0.44
3:C:216:LYS:HB3	3:C:360:LEU:HD13	2.00	0.44
3:H:284:SER:C	3:H:286:ALA:H	2.20	0.44
3:J:221:LEU:HD11	3:J:247:LEU:HG	1.99	0.44
3:J:235:VAL:HG22	3:J:288:ILE:HG22	2.00	0.44
3:D:116:ARG:HA	3:D:119:ILE:HD12	2.00	0.43
3:E:42:ASP:O	3:E:116:ARG:NH2	2.50	0.43
3:E:31:LEU:HD22	3:E:65:VAL:HG21	2.00	0.43
3:F:198:SER:C	3:F:199:GLY:O	2.54	0.43
3:H:149:GLU:OE2	3:H:149:GLU:N	2.51	0.43
3:H:39:ILE:O	3:H:40:PRO:C	2.56	0.43
3:K:14:ILE:HD13	3:K:45:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:228:ALA:HB1	3:A:288:ILE:HG22	2.00	0.43
3:B:135:GLU:CB	3:B:138:VAL:HG12	2.47	0.43
3:D:368:GLU:HA	3:D:373:LYS:NZ	2.34	0.43
3:E:147:ILE:HG12	3:F:143:ALA:HB1	1.99	0.43
3:F:240:LEU:N	3:F:240:LEU:HD23	2.33	0.43
3:H:418:LYS:O	3:H:419:GLN:HB3	2.17	0.43
3:H:61:ARG:N	3:H:62:GLY:HA2	2.33	0.43
3:H:63:GLU:O	3:I:104:TYR:CD2	2.71	0.43
3:I:53:HIS:CE1	3:I:57:ARG:HH12	2.36	0.43
3:I:166:LEU:HD22	3:J:280:MET:HG2	2.00	0.43
3:J:71:THR:HG22	3:J:89:LEU:CD1	2.44	0.43
3:K:10:PRO:HA	3:K:11:PRO:HD3	1.79	0.43
3:K:61:ARG:CB	3:K:62:GLY:CA	2.96	0.43
3:A:291:ASP:OD2	3:A:293:THR:OG1	2.36	0.43
7:A:504:ALF:F3	3:F:420:ARG:NH2	2.19	0.43
3:C:194:ASP:HA	3:C:197:THR:HG22	2.00	0.43
3:C:388:GLN:OE1	3:D:362:GLN:HG2	2.19	0.43
3:D:30:ALA:HB1	3:D:102:VAL:HG21	2.00	0.43
3:D:368:GLU:HA	3:D:368:GLU:OE1	2.17	0.43
3:F:384:GLY:HA2	3:F:387:GLU:OE2	2.18	0.43
3:G:149:GLU:OE2	3:G:149:GLU:N	2.50	0.43
3:I:74:LEU:HD13	3:I:83:ILE:HD13	2.01	0.43
3:A:162:ILE:HA	3:A:165:ILE:HD12	2.00	0.43
3:E:221:LEU:HD21	3:E:247:LEU:HG	2.01	0.43
3:F:163:LYS:O	3:F:167:VAL:HG23	2.18	0.43
3:I:441:LEU:HD12	3:I:441:LEU:HA	1.81	0.43
3:J:404:LYS:O	3:J:405:ASP:HB3	2.18	0.43
3:K:209:ALA:HB2	3:K:361:SER:HB3	2.01	0.43
3:C:132:ARG:C	3:C:134:ASP:H	2.22	0.43
3:E:216:LYS:HB3	3:E:360:LEU:HD13	2.00	0.43
3:I:367:VAL:HG23	3:I:370:ARG:HH12	1.82	0.43
3:J:149:GLU:N	3:J:149:GLU:OE2	2.51	0.43
3:L:160:LYS:HG3	3:L:165:ILE:HD11	2.01	0.43
3:A:324:LEU:HD12	3:A:324:LEU:HA	1.81	0.43
3:A:422:GLY:HA3	3:A:423:PRO:HD3	1.77	0.43
3:A:61:ARG:N	3:A:62:GLY:HA2	2.34	0.43
3:D:194:ASP:HA	3:D:197:THR:HG22	1.99	0.43
3:E:216:LYS:HB2	6:E:501:GDP:O2B	2.18	0.43
3:F:163:LYS:HE3	3:F:163:LYS:H	1.83	0.43
3:G:403:ASN:HB3	3:G:404:LYS:HA	2.00	0.43
3:G:61:ARG:N	3:G:62:GLY:HA2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:254:ALA:O	3:I:437:LYS:HE2	2.19	0.43
3:J:422:GLY:HA3	3:J:423:PRO:HD3	1.75	0.43
3:K:320:ASP:O	3:K:321:TYR:CB	2.60	0.43
3:K:216:LYS:HB3	3:K:360:LEU:HD13	2.00	0.43
3:K:367:VAL:HG23	3:K:370:ARG:HH12	1.84	0.43
3:A:14:ILE:HD12	3:A:45:ARG:HG3	2.01	0.43
3:C:163:LYS:O	3:C:167:VAL:HG23	2.17	0.43
1:V:8:DT:C5'	3:D:336:GLN:HG3	2.48	0.43
3:G:13:SER:HB3	3:G:16:ALA:HB3	2.01	0.43
3:G:39:ILE:O	3:G:40:PRO:C	2.56	0.43
3:H:422:GLY:HA3	3:H:423:PRO:HD3	1.69	0.43
3:A:333:GLU:O	3:A:335:ARG:N	2.52	0.43
3:A:432:ILE:HD12	3:A:432:ILE:N	2.34	0.43
3:C:221:LEU:HD21	3:C:247:LEU:HG	2.01	0.43
3:C:366:SER:O	3:C:369:GLN:HB2	2.18	0.43
3:C:61:ARG:N	3:C:62:GLY:HA2	2.33	0.43
3:H:31:LEU:HD22	3:H:65:VAL:HG21	2.00	0.43
3:K:50:LYS:CB	3:K:83:ILE:HD11	2.47	0.43
3:A:136:ILE:HG21	3:B:111:GLU:HG2	1.99	0.43
3:B:228:ALA:HB1	3:B:288:ILE:HG22	2.01	0.43
3:E:61:ARG:N	3:E:62:GLY:HA2	2.33	0.43
3:J:32:VAL:HB	3:J:33:PRO:HD3	2.01	0.43
3:K:83:ILE:HA	3:K:83:ILE:HD12	1.87	0.43
3:L:206:ILE:HA	3:L:392:ILE:HG23	2.00	0.43
3:A:306:ARG:NH1	3:A:306:ARG:CG	2.71	0.43
3:A:409:LYS:HG2	3:A:409:LYS:H	1.65	0.43
3:A:67:LEU:O	3:A:71:THR:CG2	2.60	0.43
3:C:238:PHE:CZ	3:C:301:ILE:HG23	2.54	0.43
3:H:23:ALA:HB3	3:H:102:VAL:CG1	2.48	0.43
3:J:184:THR:N	3:J:185:GLY:HA3	2.26	0.43
3:K:388:GLN:CD	3:L:362:GLN:HG2	2.38	0.43
3:L:149:GLU:OE2	3:L:149:GLU:N	2.52	0.43
3:A:315:GLY:O	3:A:356:PRO:HD2	2.18	0.42
3:B:163:LYS:O	3:B:167:VAL:HG23	2.19	0.42
3:C:157:GLY:O	3:C:158:ALA:C	2.57	0.42
3:C:437:LYS:HD3	3:C:439:VAL:HG13	1.99	0.42
3:I:225:GLN:HE22	3:I:254:ALA:HB3	1.82	0.42
3:D:306:ARG:CG	3:D:306:ARG:NH1	2.66	0.42
3:F:306:ARG:NH1	3:F:306:ARG:CG	2.71	0.42
3:F:321:TYR:CE1	3:F:323:GLN:HG2	2.54	0.42
3:F:61:ARG:H	3:F:62:GLY:HA2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:259:ASN:O	3:H:262:ASN:HB2	2.20	0.42
3:H:409:LYS:N	3:H:409:LYS:CD	2.72	0.42
3:A:209:ALA:HB2	3:A:361:SER:HB3	2.01	0.42
3:B:12:GLN:HE21	3:B:14:ILE:HD11	1.80	0.42
3:D:58:VAL:HG13	3:D:63:GLU:HB2	2.01	0.42
6:A:502:GDP:C6	3:F:422:GLY:HA2	2.52	0.42
3:F:52:PHE:CD1	3:F:55:MET:HE2	2.54	0.42
3:I:418:LYS:O	3:I:419:GLN:HB3	2.20	0.42
3:J:203:SER:HA	3:J:350:ALA:O	2.19	0.42
3:J:211:ARG:HH22	3:J:365:ARG:CD	2.31	0.42
3:K:17:GLU:HG2	3:K:43:PHE:CD1	2.54	0.42
3:D:309:LYS:HB2	3:D:314:LEU:HB2	2.01	0.42
3:D:298:VAL:HG11	3:D:345:SER:HB3	2.02	0.42
3:E:55:MET:HG2	3:E:65:VAL:CG1	2.48	0.42
3:D:76:ALA:O	3:F:134:ASP:OD1	2.38	0.42
3:H:58:VAL:HG13	3:H:63:GLU:CG	2.50	0.42
3:I:349:LEU:HD12	3:I:353:LEU:HD13	2.01	0.42
3:J:14:ILE:O	3:J:15:GLU:C	2.57	0.42
3:J:199:GLY:CA	3:J:200:PHE:HB2	2.39	0.42
3:L:58:VAL:HG13	3:L:63:GLU:CG	2.48	0.42
3:A:309:LYS:HB2	3:A:314:LEU:HB2	2.01	0.42
3:A:316:MET:HG2	3:A:356:PRO:HG2	2.01	0.42
3:B:293:THR:HG1	3:B:293:THR:H	1.59	0.42
3:B:365:ARG:CB	3:B:365:ARG:NH2	2.83	0.42
3:B:392:ILE:HA	3:B:418:LYS:O	2.20	0.42
3:C:148:MET:SD	3:D:306:ARG:NH2	2.92	0.42
3:D:148:MET:C	3:D:150:VAL:H	2.23	0.42
3:D:199:GLY:HA2	3:D:200:PHE:HB2	2.02	0.42
3:F:248:VAL:HA	3:F:251:MET:HE2	2.01	0.42
3:F:315:GLY:O	3:F:356:PRO:HD2	2.19	0.42
3:I:386:ILE:HG12	3:I:386:ILE:H	1.72	0.42
3:J:441:LEU:HD12	3:J:441:LEU:HA	1.88	0.42
3:L:419:GLN:HG3	3:L:422:GLY:H	1.84	0.42
3:L:216:LYS:N	6:L:501:GDP:O2B	2.50	0.42
3:L:77:SER:HB2	3:L:79:GLN:HG2	2.01	0.42
2:W:4:DT:C2'	2:W:5:DT:C6	3.02	0.42
3:A:14:ILE:HA	3:A:17:GLU:HB2	2.02	0.42
3:A:317:ILE:HB	3:A:357:VAL:HG22	2.02	0.42
3:B:384:GLY:HA2	3:C:365:ARG:HH21	1.83	0.42
3:B:422:GLY:HA2	6:C:501:GDP:C6	2.55	0.42
3:E:163:LYS:O	3:E:167:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:432:ILE:N	3:E:432:ILE:HD12	2.35	0.42
3:F:132:ARG:C	3:F:134:ASP:H	2.23	0.42
3:G:233:GLU:CG	3:G:315:GLY:HA3	2.49	0.42
3:H:33:PRO:O	3:H:37:ILE:HD12	2.19	0.42
3:H:220:ALA:HB2	3:H:360:LEU:HD21	2.01	0.42
3:H:53:HIS:CE1	3:H:57:ARG:NH1	2.87	0.42
3:I:135:GLU:OE1	3:I:138:VAL:HG11	2.19	0.42
3:L:141:ASP:OD2	3:L:303:ALA:CB	2.51	0.42
3:L:184:THR:N	3:L:185:GLY:HA3	2.23	0.42
3:F:197:THR:HG23	3:F:199:GLY:O	2.20	0.42
3:H:367:VAL:HG23	3:H:370:ARG:HH12	1.84	0.42
3:I:149:GLU:OE2	3:I:149:GLU:N	2.53	0.42
3:I:184:THR:N	3:I:185:GLY:HA3	2.27	0.42
3:I:422:GLY:CA	6:J:501:GDP:C5	2.92	0.42
3:K:149:GLU:N	3:K:149:GLU:OE2	2.53	0.42
3:A:320:ASP:O	3:A:320:ASP:CG	2.58	0.42
3:B:52:PHE:CD1	3:B:55:MET:HE2	2.55	0.42
3:F:370:ARG:HH22	3:F:379:ASP:CG	2.23	0.42
3:G:115:LEU:HG	3:H:136:ILE:CD1	2.49	0.42
3:J:420:ARG:HD3	3:K:242:MET:CE	2.49	0.42
3:B:209:ALA:HB2	3:B:361:SER:HB3	2.02	0.42
3:B:239:SER:HA	3:B:320:ASP:CB	2.49	0.42
3:C:233:GLU:CG	3:C:315:GLY:HA3	2.39	0.42
3:D:333:GLU:O	3:D:334:ASN:C	2.57	0.42
3:F:321:TYR:HE1	3:F:323:GLN:HG2	1.83	0.42
3:F:422:GLY:HA3	3:F:423:PRO:HD3	1.70	0.42
3:G:11:PRO:HD2	3:G:116:ARG:HB3	2.01	0.42
3:H:387:GLU:OE2	3:I:365:ARG:NE	2.51	0.42
3:K:233:GLU:CG	3:K:315:GLY:HA3	2.50	0.42
3:L:441:LEU:HA	3:L:441:LEU:HD12	1.87	0.42
3:L:53:HIS:CE1	3:L:57:ARG:HH12	2.38	0.42
6:A:502:GDP:O3B	7:A:504:ALF:F4	2.28	0.42
3:C:337:GLN:HA	3:C:340:SER:HB2	2.02	0.42
3:D:166:LEU:HB3	3:E:280:MET:CE	2.47	0.42
3:F:377:MET:HB3	3:F:387:GLU:HG2	2.01	0.42
3:G:78:GLU:H	3:G:78:GLU:HG2	1.67	0.42
3:H:216:LYS:NZ	3:H:362:GLN:HE22	2.17	0.42
3:I:221:LEU:HD11	3:I:247:LEU:HG	2.01	0.42
3:I:61:ARG:N	3:I:62:GLY:HA2	2.34	0.42
3:K:83:ILE:HG23	3:K:83:ILE:O	2.20	0.42
3:A:61:ARG:H	3:A:62:GLY:HA2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:333:GLU:O	3:B:335:ARG:N	2.53	0.41
3:C:380:ILE:O	3:D:365:ARG:NH2	2.52	0.41
3:C:418:LYS:HG3	3:D:213:SER:HB2	2.00	0.41
6:G:501:GDP:N7	3:L:422:GLY:HA2	2.35	0.41
3:J:117:ARG:HH22	3:J:149:GLU:HB3	1.85	0.41
3:K:104:TYR:O	3:K:108:ILE:CD1	2.68	0.41
3:K:412:ILE:HD13	3:K:438:PHE:HE2	1.85	0.41
3:L:61:ARG:N	3:L:62:GLY:HA2	2.35	0.41
4:W:101:MES:H51	4:W:101:MES:H81	1.75	0.41
3:A:129:GLY:O	3:B:115:LEU:HD22	2.19	0.41
3:A:31:LEU:HD22	3:A:65:VAL:HG21	2.02	0.41
3:B:332:LYS:HD3	3:B:338:GLU:OE2	2.21	0.41
3:D:179:ARG:CA	3:D:180:ASP:CB	2.97	0.41
3:F:200:PHE:CE2	3:F:358:ILE:HD11	2.55	0.41
3:F:233:GLU:CG	3:F:315:GLY:HA3	2.44	0.41
3:G:284:SER:C	3:G:286:ALA:H	2.22	0.41
3:I:245:GLN:HE21	3:I:245:GLN:HB2	1.69	0.41
3:I:259:ASN:O	3:I:262:ASN:HB2	2.20	0.41
3:J:117:ARG:NH2	3:J:149:GLU:HB3	2.35	0.41
3:K:441:LEU:HA	3:K:441:LEU:HD12	1.85	0.41
3:L:330:ARG:C	3:L:332:LYS:N	2.67	0.41
3:B:176:LEU:C	3:B:178:ASN:H	2.23	0.41
3:B:289:TYR:N	3:B:289:TYR:CD1	2.88	0.41
3:B:233:GLU:CG	3:B:315:GLY:HA3	2.44	0.41
3:C:324:LEU:HA	3:C:324:LEU:HD12	1.81	0.41
3:C:370:ARG:HG3	3:C:370:ARG:NH1	2.34	0.41
3:F:200:PHE:HD1	3:F:200:PHE:H	1.68	0.41
3:I:15:GLU:H	3:I:15:GLU:CD	2.24	0.41
3:L:39:ILE:O	3:L:40:PRO:C	2.58	0.41
3:C:14:ILE:O	3:C:15:GLU:C	2.59	0.41
3:C:190:PHE:HA	3:C:440:ASN:HD21	1.85	0.41
3:G:321:TYR:HB3	3:G:324:LEU:HB2	2.01	0.41
3:H:15:GLU:H	3:H:15:GLU:HG2	1.71	0.41
3:J:250:ARG:HH21	6:J:501:GDP:H5'	1.85	0.41
3:K:284:SER:C	3:K:286:ALA:H	2.23	0.41
3:K:27:ASP:HA	3:K:28:PRO:HD3	1.84	0.41
3:K:56:LEU:HD23	3:K:56:LEU:HA	1.64	0.41
3:B:259:ASN:HD21	3:B:261:GLN:HB2	1.85	0.41
3:D:238:PHE:CZ	3:D:301:ILE:HG23	2.55	0.41
3:E:233:GLU:CG	3:E:315:GLY:HA3	2.45	0.41
3:G:349:LEU:HD12	3:G:353:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:418:LYS:O	3:G:419:GLN:HB3	2.21	0.41
3:H:328:SER:HB3	3:H:330:ARG:CG	2.47	0.41
3:H:441:LEU:HA	3:H:441:LEU:HD12	1.76	0.41
3:H:53:HIS:CE1	3:H:57:ARG:HH12	2.38	0.41
3:I:216:LYS:HB3	3:I:360:LEU:HD13	2.02	0.41
3:D:370:ARG:NH2	3:D:379:ASP:OD2	2.54	0.41
3:F:31:LEU:CD2	3:F:65:VAL:HG21	2.51	0.41
3:G:58:VAL:HG13	3:G:63:GLU:CG	2.50	0.41
3:H:193:LEU:O	3:H:197:THR:HG22	2.20	0.41
3:A:201:GLN:HB2	3:A:204:ASP:OD2	2.20	0.41
3:D:221:LEU:HD21	3:D:247:LEU:HG	2.01	0.41
3:G:321:TYR:CG	3:G:324:LEU:HB2	2.55	0.41
3:G:419:GLN:NE2	3:G:423:PRO:HD2	2.36	0.41
3:I:202:ARG:O	3:I:203:SER:CB	2.61	0.41
3:H:388:GLN:OE1	3:I:362:GLN:HG2	2.21	0.41
3:A:116:ARG:HA	3:A:119:ILE:HD12	2.02	0.41
3:B:377:MET:HB3	3:B:387:GLU:HG2	2.03	0.41
3:D:321:TYR:CZ	3:D:362:GLN:NE2	2.89	0.41
3:F:346:LEU:HA	3:F:346:LEU:HD23	1.91	0.41
3:G:441:LEU:HD12	3:G:441:LEU:HA	1.88	0.41
3:I:63:GLU:N	3:I:64:PRO:HA	2.36	0.41
3:J:419:GLN:NE2	3:J:423:PRO:HD2	2.33	0.41
3:J:77:SER:O	3:J:79:GLN:N	2.53	0.41
3:A:110:GLU:O	3:A:114:VAL:HG23	2.20	0.41
3:A:419:GLN:NE2	3:A:423:PRO:HD2	2.36	0.41
3:B:410:ASN:HB2	3:B:431:PHE:H	1.86	0.41
3:E:248:VAL:HA	3:E:251:MET:HE3	2.02	0.41
3:F:58:VAL:HG12	3:F:65:VAL:HG22	2.03	0.41
3:I:209:ALA:HB2	3:I:361:SER:HB3	2.01	0.41
3:I:53:HIS:CE1	3:I:57:ARG:NH1	2.89	0.41
3:K:99:ALA:C	3:K:101:ASN:H	2.24	0.41
3:L:201:GLN:HE22	3:L:421:ASN:HD22	1.69	0.41
3:A:420:ARG:HD3	3:B:137:ASP:OD2	2.21	0.41
3:A:432:ILE:HG21	3:A:435:TYR:CD1	2.56	0.41
3:C:333:GLU:O	3:C:335:ARG:N	2.54	0.41
3:D:14:ILE:HD13	3:D:45:ARG:HG3	2.02	0.41
3:D:8:ARG:HB2	3:D:8:ARG:NH1	2.35	0.41
3:E:61:ARG:H	3:E:62:GLY:HA2	1.86	0.41
3:F:228:ALA:HB1	3:F:288:ILE:HG22	2.02	0.41
3:F:293:THR:HA	3:F:294:PRO:HD3	1.91	0.41
3:G:53:HIS:CE1	3:G:57:ARG:HH12	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:53:HIS:CE1	3:G:57:ARG:NH1	2.89	0.41
3:K:386:ILE:HG12	3:K:386:ILE:H	1.74	0.41
3:L:284:SER:C	3:L:286:ALA:H	2.24	0.41
3:B:398:ARG:HG2	3:B:399:ASP:N	2.35	0.41
3:D:307:ARG:O	3:D:310:GLN:HB3	2.20	0.41
3:D:61:ARG:H	3:D:62:GLY:HA2	1.86	0.41
3:E:198:SER:C	3:E:199:GLY:O	2.57	0.41
3:F:317:ILE:HB	3:F:357:VAL:HG22	2.01	0.41
3:G:403:ASN:CB	3:G:404:LYS:HA	2.50	0.41
3:I:233:GLU:CG	3:I:315:GLY:HA3	2.51	0.41
3:I:398:ARG:C	3:I:400:ASP:N	2.73	0.41
3:J:419:GLN:O	6:K:501:GDP:H3'	2.20	0.41
3:L:135:GLU:OE1	3:L:138:VAL:HG11	2.21	0.41
3:A:407:GLU:HG2	3:A:407:GLU:H	1.75	0.40
3:D:340:SER:HA	3:D:385:SER:OG	2.21	0.40
3:G:330:ARG:C	3:G:332:LYS:N	2.72	0.40
3:J:202:ARG:HA	3:J:356:PRO:HD3	2.03	0.40
3:J:52:PHE:HD1	3:J:55:MET:HE2	1.85	0.40
3:L:216:LYS:HB3	3:L:360:LEU:HD13	2.03	0.40
3:A:132:ARG:C	3:A:134:ASP:H	2.25	0.40
3:B:26:LEU:HD11	3:B:96:VAL:HG13	2.03	0.40
3:D:333:GLU:O	3:D:335:ARG:N	2.54	0.40
3:E:204:ASP:HA	3:E:391:ASP:OD1	2.21	0.40
3:G:216:LYS:NZ	3:G:362:GLN:HE22	2.19	0.40
3:H:245:GLN:HB2	3:H:245:GLN:HE21	1.72	0.40
3:K:403:ASN:HB3	3:K:405:ASP:N	2.36	0.40
1:V:10:DT:H2'	1:V:11:DT:C6	2.56	0.40
3:B:160:LYS:HB2	3:B:165:ILE:HD11	2.04	0.40
3:C:135:GLU:O	3:C:137:ASP:N	2.53	0.40
3:C:317:ILE:HB	3:C:357:VAL:HG22	2.03	0.40
3:D:206:ILE:HG13	3:D:392:ILE:HG21	2.04	0.40
3:D:419:GLN:NE2	3:D:423:PRO:HD2	2.37	0.40
3:E:240:LEU:HD23	3:E:240:LEU:N	2.36	0.40
3:E:261:GLN:HA	3:E:264:ARG:CZ	2.52	0.40
3:G:77:SER:HB2	3:G:79:GLN:HG2	2.04	0.40
3:I:206:ILE:HA	3:I:392:ILE:HG23	2.04	0.40
3:J:412:ILE:HD13	3:J:438:PHE:HE2	1.87	0.40
3:K:216:LYS:HZ2	3:K:362:GLN:HE22	1.66	0.40
3:A:370:ARG:NH2	3:A:379:ASP:OD2	2.51	0.40
3:B:192:GLU:HB2	3:B:427:VAL:HG13	2.03	0.40
3:B:191:THR:H	3:B:440:ASN:ND2	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:61:ARG:H	3:B:62:GLY:HA2	1.85	0.40
3:D:61:ARG:NH1	3:D:61:ARG:CG	2.67	0.40
3:G:40:PRO:O	3:G:49:GLN:HG2	2.22	0.40
2:W:7:DT:H5'	3:J:336:GLN:HG3	2.02	0.40
3:J:162:ILE:CD1	3:K:288:ILE:HD11	2.52	0.40
3:K:201:GLN:HE22	3:K:421:ASN:HD22	1.70	0.40
3:K:61:ARG:CB	3:K:62:GLY:HA2	2.50	0.40
3:A:8:ARG:HD2	3:A:8:ARG:N	2.32	0.40
3:B:132:ARG:C	3:B:134:ASP:H	2.25	0.40
3:C:227:VAL:O	3:C:231:THR:CG2	2.51	0.40
3:C:58:VAL:HG12	3:C:65:VAL:HG22	2.04	0.40
3:C:58:VAL:HG13	3:C:63:GLU:HB2	2.03	0.40
3:D:163:LYS:O	3:D:167:VAL:HG23	2.21	0.40
3:G:316:MET:HG2	3:G:356:PRO:HG2	2.04	0.40
3:H:420:ARG:HD3	3:I:242:MET:HE2	2.03	0.40
3:J:193:LEU:O	3:J:197:THR:HG22	2.22	0.40
3:L:53:HIS:CE1	3:L:57:ARG:NH1	2.89	0.40
2:W:2:DT:C2'	2:W:3:DT:C5'	3.00	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	413/454 (91%)	369 (89%)	31 (8%)	13 (3%)	4	26
3	B	424/454 (93%)	365 (86%)	38 (9%)	21 (5%)	2	16
3	C	432/454 (95%)	385 (89%)	29 (7%)	18 (4%)	3	20
3	D	425/454 (94%)	376 (88%)	37 (9%)	12 (3%)	5	29
3	E	412/454 (91%)	373 (90%)	27 (7%)	12 (3%)	4	28
3	F	415/454 (91%)	377 (91%)	27 (6%)	11 (3%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	415/454 (91%)	374 (90%)	37 (9%)	4 (1%)	15	54
3	H	419/454 (92%)	375 (90%)	39 (9%)	5 (1%)	13	49
3	I	412/454 (91%)	375 (91%)	34 (8%)	3 (1%)	22	61
3	J	410/454 (90%)	369 (90%)	37 (9%)	4 (1%)	15	54
3	K	415/454 (91%)	354 (85%)	51 (12%)	10 (2%)	6	34
3	L	413/454 (91%)	372 (90%)	36 (9%)	5 (1%)	13	49
All	All	5005/5448 (92%)	4464 (89%)	423 (8%)	118 (2%)	6	34

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	97	PRO
3	B	154	LYS
3	B	331	SER
3	B	409	LYS
3	B	410	ASN
3	B	411	ILE
3	B	440	ASN
3	B	442	GLU
3	C	136	ILE
3	C	155	HIS
3	C	331	SER
3	C	332	LYS
3	D	321	TYR
3	D	331	SER
3	D	332	LYS
3	E	321	TYR
3	E	331	SER
3	F	321	TYR
3	F	331	SER
3	F	332	LYS
3	G	331	SER
3	H	10	PRO
3	H	330	ARG
3	H	331	SER
3	I	403	ASN
3	J	405	ASP
3	K	11	PRO
3	K	63	GLU
3	K	76	ALA

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Mol	Chain	Res	Type
3	K	87	SER
3	K	331	SER
3	L	330	ARG
3	A	136	ILE
3	A	151	SER
3	A	331	SER
3	A	332	LYS
3	A	408	ASN
3	B	155	HIS
3	B	157	GLY
3	B	159	PHE
3	B	332	LYS
3	B	441	LEU
3	C	97	PRO
3	C	152	GLN
3	C	158	ALA
3	C	408	ASN
3	C	410	ASN
3	D	97	PRO
3	D	180	ASP
3	D	408	ASN
3	E	175	MET
3	E	332	LYS
3	E	408	ASN
3	F	408	ASN
3	G	327	GLY
3	H	327	GLY
3	H	442	GLU
3	I	327	GLY
3	J	327	GLY
3	K	10	PRO
3	K	327	GLY
3	L	174	GLU
3	L	327	GLY
3	L	331	SER
3	A	133	GLU
3	B	133	GLU
3	B	149	GLU
3	C	133	GLU
3	C	156	SER
3	C	157	GLY
3	C	182	GLU

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Mol	Chain	Res	Type
3	C	382	GLU
3	D	100	ALA
3	D	133	GLU
3	D	334	ASN
3	E	133	GLU
3	F	100	ALA
3	F	133	GLU
3	F	382	GLU
3	G	330	ARG
3	J	78	GLU
3	K	110	GLU
3	A	321	TYR
3	A	334	ASN
3	B	177	HIS
3	B	334	ASN
3	B	382	GLU
3	E	334	ASN
3	E	382	GLU
3	K	13	SER
3	K	119	ILE
3	A	382	GLU
3	A	410	ASN
3	C	334	ASN
3	D	382	GLU
3	E	14	ILE
3	F	97	PRO
3	F	334	ASN
3	B	392	ILE
3	D	27	ASP
3	E	27	ASP
3	F	27	ASP
3	C	27	ASP
3	A	392	ILE
3	B	27	ASP
3	C	392	ILE
3	E	392	ILE
3	G	392	ILE
3	I	392	ILE
3	A	27	ASP
3	J	392	ILE
3	L	11	PRO
3	B	64	PRO

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Mol	Chain	Res	Type
3	A	64	PRO
3	C	64	PRO
3	D	64	PRO
3	E	64	PRO
3	F	64	PRO

### 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	
3	A	353/386 (92%)	291 (82%)	62 (18%)	2	9
3	B	362/386 (94%)	293 (81%)	69 (19%)	1	8
3	C	361/386 (94%)	305 (84%)	56 (16%)	2	12
3	D	356/386 (92%)	303 (85%)	53 (15%)	3	14
3	E	348/386 (90%)	293 (84%)	55 (16%)	2	12
3	F	355/386 (92%)	298 (84%)	57 (16%)	2	11
3	G	351/386 (91%)	307 (88%)	44 (12%)	4	21
3	H	350/386 (91%)	308 (88%)	42 (12%)	5	22
3	I	350/386 (91%)	307 (88%)	43 (12%)	4	21
3	J	350/386 (91%)	303 (87%)	47 (13%)	4	18
3	K	352/386 (91%)	300 (85%)	52 (15%)	3	14
3	L	349/386 (90%)	307 (88%)	42 (12%)	5	22
All	All	4237/4632 (92%)	3615 (85%)	622 (15%)	3	14

All (622) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	7	GLU
3	A	8	ARG
3	A	9	ILE
3	A	12	GLN
3	A	14	ILE

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Mol	Chain	Res	Type
3	A	49	GLN
3	A	58	VAL
3	A	61	ARG
3	A	67	LEU
3	A	71	THR
3	A	86	VAL
3	A	96	VAL
3	A	101	ASN
3	A	102	VAL
3	A	104	TYR
3	A	107	ARG
3	A	123	THR
3	A	124	SER
3	A	132	ARG
3	A	134	ASP
3	A	135	GLU
3	A	139	LEU
3	A	144	ASP
3	A	147	ILE
3	A	159	PHE
3	A	165	ILE
3	A	197	THR
3	A	200	PHE
3	A	213	SER
3	A	216	LYS
3	A	233	GLU
3	A	235	VAL
3	A	283	LEU
3	A	285	ASN
3	A	288	ILE
3	A	293	THR
3	A	296	ILE
3	A	306	ARG
3	A	309	LYS
3	A	314	LEU
3	A	316	MET
3	A	321	TYR
3	A	323	GLN
3	A	324	LEU
3	A	331	SER
3	A	334	ASN
3	A	339	VAL

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Mol	Chain	Res	Type
3	A	340	SER
3	A	344[A]	ARG
3	A	344[B]	ARG
3	A	351	ARG
3	A	355	VAL
3	A	369	GLN
3	A	373	LYS
3	A	387	GLU
3	A	408	ASN
3	A	409	LYS
3	A	420	ARG
3	A	424	VAL
3	A	428	GLN
3	A	439	VAL
3	A	441	LEU
3	B	9	ILE
3	B	36	GLU
3	B	49	GLN
3	B	55	MET
3	B	58	VAL
3	B	61	ARG
3	B	67	LEU
3	B	71	THR
3	B	86	VAL
3	B	98	THR
3	B	101	ASN
3	B	102	VAL
3	B	107	ARG
3	B	123	THR
3	B	132	ARG
3	B	139	LEU
3	B	140	LEU
3	B	144	ASP
3	B	147	ILE
3	B	153	ARG
3	B	154	LYS
3	B	159	PHE
3	B	163	LYS
3	B	176	LEU
3	B	182	GLU
3	B	197	THR
3	B	200	PHE

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Mol	Chain	Res	Type
3	B	213	SER
3	B	216	LYS
3	B	233	GLU
3	B	235	VAL
3	B	245	GLN
3	B	264	ARG
3	B	283	LEU
3	B	285	ASN
3	B	288	ILE
3	B	293	THR
3	B	296	ILE
3	B	306	ARG
3	B	309	LYS
3	B	314	LEU
3	B	316	MET
3	B	321	TYR
3	B	323	GLN
3	B	324	LEU
3	B	331	SER
3	B	334	ASN
3	B	339	VAL
3	B	340	SER
3	B	351	ARG
3	B	365	ARG
3	B	387	GLU
3	B	388	GLN
3	B	400	ASP
3	B	403	ASN
3	B	405	ASP
3	B	407	GLU
3	B	408	ASN
3	B	409	LYS
3	B	410	ASN
3	B	420	ARG
3	B	424	VAL
3	B	426	THR
3	B	434	GLU
3	B	439	VAL
3	B	440	ASN
3	B	443	ARG
3	B	444	ARG
3	B	445	PHE

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Mol	Chain	Res	Type
3	C	8	ARG
3	C	14	ILE
3	C	49	GLN
3	C	61	ARG
3	C	67	LEU
3	C	71	THR
3	C	86	VAL
3	C	98	THR
3	C	101	ASN
3	C	107	ARG
3	C	118	LEU
3	C	123	THR
3	C	132	ARG
3	C	134	ASP
3	C	135	GLU
3	C	139	LEU
3	C	140	LEU
3	C	144	ASP
3	C	147	ILE
3	C	153	ARG
3	C	159	PHE
3	C	163	LYS
3	C	176	LEU
3	C	197	THR
3	C	200	PHE
3	C	213	SER
3	C	216	LYS
3	C	233	GLU
3	C	235	VAL
3	C	245	GLN
3	C	264	ARG
3	C	283	LEU
3	C	285	ASN
3	C	288	ILE
3	C	293	THR
3	C	296	ILE
3	C	306	ARG
3	C	309	LYS
3	C	314	LEU
3	C	316	MET
3	C	323	GLN
3	C	324	LEU

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Mol	Chain	Res	Type
3	C	331	SER
3	C	334	ASN
3	C	339	VAL
3	C	340	SER
3	C	344	ARG
3	C	351	ARG
3	C	367	VAL
3	C	373	LYS
3	C	387	GLU
3	C	408	ASN
3	C	409	LYS
3	C	420	ARG
3	C	424	VAL
3	C	428	GLN
3	D	8	ARG
3	D	15	GLU
3	D	49	GLN
3	D	58	VAL
3	D	61	ARG
3	D	67	LEU
3	D	71	THR
3	D	86	VAL
3	D	101	ASN
3	D	102	VAL
3	D	107	ARG
3	D	123	THR
3	D	124	SER
3	D	132	ARG
3	D	135	GLU
3	D	138	VAL
3	D	139	LEU
3	D	144	ASP
3	D	147	ILE
3	D	163	LYS
3	D	175	MET
3	D	176	LEU
3	D	197	THR
3	D	200	PHE
3	D	213	SER
3	D	216	LYS
3	D	233	GLU
3	D	235	VAL

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Mol	Chain	Res	Type
3	D	245	GLN
3	D	283	LEU
3	D	288	ILE
3	D	293	THR
3	D	296	ILE
3	D	306	ARG
3	D	314	LEU
3	D	316	MET
3	D	321	TYR
3	D	323	GLN
3	D	324	LEU
3	D	331	SER
3	D	334	ASN
3	D	339	VAL
3	D	340	SER
3	D	351	ARG
3	D	370	ARG
3	D	373	LYS
3	D	387	GLU
3	D	408	ASN
3	D	409	LYS
3	D	420	ARG
3	D	424	VAL
3	D	428	GLN
3	D	441	LEU
3	E	14	ILE
3	E	49	GLN
3	E	61	ARG
3	E	67	LEU
3	E	71	THR
3	E	86	VAL
3	E	96	VAL
3	E	98	THR
3	E	101	ASN
3	E	102	VAL
3	E	107	ARG
3	E	123	THR
3	E	124	SER
3	E	132	ARG
3	E	135	GLU
3	E	139	LEU
3	E	140	LEU

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Mol	Chain	Res	Type
3	E	144	ASP
3	E	147	ILE
3	E	163	LYS
3	E	197	THR
3	E	200	PHE
3	E	213	SER
3	E	216	LYS
3	E	233	GLU
3	E	235	VAL
3	E	245	GLN
3	E	283	LEU
3	E	285	ASN
3	E	288	ILE
3	E	293	THR
3	E	296	ILE
3	E	306	ARG
3	E	314	LEU
3	E	316	MET
3	E	321	TYR
3	E	323	GLN
3	E	324	LEU
3	E	331	SER
3	E	334	ASN
3	E	339	VAL
3	E	340	SER
3	E	344	ARG
3	E	351	ARG
3	E	355	VAL
3	E	367	VAL
3	E	369	GLN
3	E	373	LYS
3	E	387	GLU
3	E	408	ASN
3	E	409	LYS
3	E	420	ARG
3	E	424	VAL
3	E	428	GLN
3	E	439	VAL
3	F	9	ILE
3	F	12	GLN
3	F	14	ILE
3	F	49	GLN

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Mol	Chain	Res	Type
3	F	61	ARG
3	F	67	LEU
3	F	71	THR
3	F	86	VAL
3	F	101	ASN
3	F	102	VAL
3	F	104	TYR
3	F	107	ARG
3	F	123	THR
3	F	124	SER
3	F	132	ARG
3	F	135	GLU
3	F	138	VAL
3	F	139	LEU
3	F	140	LEU
3	F	144	ASP
3	F	147	ILE
3	F	163	LYS
3	F	197	THR
3	F	200	PHE
3	F	207	ILE
3	F	213	SER
3	F	216	LYS
3	F	222	ASN
3	F	233	GLU
3	F	235	VAL
3	F	245	GLN
3	F	278	MET
3	F	283	LEU
3	F	285	ASN
3	F	288	ILE
3	F	293	THR
3	F	296	ILE
3	F	306	ARG
3	F	309	LYS
3	F	314	LEU
3	F	316	MET
3	F	323	GLN
3	F	324	LEU
3	F	331	SER
3	F	334	ASN
3	F	339	VAL

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Mol	Chain	Res	Type
3	F	340	SER
3	F	351	ARG
3	F	355	VAL
3	F	371	GLN
3	F	387	GLU
3	F	408	ASN
3	F	409	LYS
3	F	420	ARG
3	F	424	VAL
3	F	428	GLN
3	F	439	VAL
3	G	9	ILE
3	G	55	MET
3	G	57	ARG
3	G	61	ARG
3	G	77	SER
3	G	78	GLU
3	G	86	VAL
3	G	101	ASN
3	G	102	VAL
3	G	134	ASP
3	G	135	GLU
3	G	138	VAL
3	G	139	LEU
3	G	147	ILE
3	G	149	GLU
3	G	163	LYS
3	G	169	THR
3	G	173	ILE
3	G	211	ARG
3	G	216	LYS
3	G	231	THR
3	G	235	VAL
3	G	245	GLN
3	G	264	ARG
3	G	285	ASN
3	G	288	ILE
3	G	293	THR
3	G	298	VAL
3	G	302	ARG
3	G	310	GLN
3	G	314	LEU

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Mol	Chain	Res	Type
3	G	316	MET
3	G	321	TYR
3	G	323	GLN
3	G	328	SER
3	G	332	LYS
3	G	340	SER
3	G	373	LYS
3	G	381	ARG
3	G	391	ASP
3	G	403	ASN
3	G	404	LYS
3	G	428	GLN
3	G	439	VAL
3	H	55	MET
3	H	61	ARG
3	H	77	SER
3	H	86	VAL
3	H	101	ASN
3	H	102	VAL
3	H	134	ASP
3	H	135	GLU
3	H	138	VAL
3	H	139	LEU
3	H	147	ILE
3	H	149	GLU
3	H	159	PHE
3	H	163	LYS
3	H	169	THR
3	H	173	ILE
3	H	175	MET
3	H	211	ARG
3	H	216	LYS
3	H	231	THR
3	H	235	VAL
3	H	245	GLN
3	H	264	ARG
3	H	285	ASN
3	H	288	ILE
3	H	293	THR
3	H	298	VAL
3	H	302	ARG
3	H	310	GLN

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Mol	Chain	Res	Type
3	H	314	LEU
3	H	316	MET
3	H	321	TYR
3	H	323	GLN
3	H	328	SER
3	H	330	ARG
3	H	332	LYS
3	H	340	SER
3	H	381	ARG
3	H	391	ASP
3	H	409	LYS
3	H	428	GLN
3	H	439	VAL
3	I	9	ILE
3	I	55	MET
3	I	57	ARG
3	I	61	ARG
3	I	77	SER
3	I	86	VAL
3	I	101	ASN
3	I	102	VAL
3	I	134	ASP
3	I	135	GLU
3	I	138	VAL
3	I	139	LEU
3	I	140	LEU
3	I	147	ILE
3	I	149	GLU
3	I	163	LYS
3	I	169	THR
3	I	173	ILE
3	I	211	ARG
3	I	213	SER
3	I	216	LYS
3	I	231	THR
3	I	235	VAL
3	I	245	GLN
3	I	264	ARG
3	I	285	ASN
3	I	288	ILE
3	I	293	THR
3	I	298	VAL

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Mol	Chain	Res	Type
3	I	302	ARG
3	I	310	GLN
3	I	314	LEU
3	I	316	MET
3	I	321	TYR
3	I	323	GLN
3	I	328	SER
3	I	332	LYS
3	I	340	SER
3	I	373	LYS
3	I	381	ARG
3	I	391	ASP
3	I	428	GLN
3	I	439	VAL
3	J	14	ILE
3	J	55	MET
3	J	57	ARG
3	J	61	ARG
3	J	77	SER
3	J	86	VAL
3	J	96	VAL
3	J	101	ASN
3	J	102	VAL
3	J	134	ASP
3	J	138	VAL
3	J	139	LEU
3	J	140	LEU
3	J	147	ILE
3	J	149	GLU
3	J	150	VAL
3	J	160	LYS
3	J	163	LYS
3	J	169	THR
3	J	173	ILE
3	J	211	ARG
3	J	213	SER
3	J	216	LYS
3	J	231	THR
3	J	235	VAL
3	J	245	GLN
3	J	264	ARG
3	J	285	ASN

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Mol	Chain	Res	Type
3	J	288	ILE
3	J	293	THR
3	J	298	VAL
3	J	302	ARG
3	J	310	GLN
3	J	314	LEU
3	J	316	MET
3	J	321	TYR
3	J	323	GLN
3	J	328	SER
3	J	332	LYS
3	J	334	ASN
3	J	340	SER
3	J	365	ARG
3	J	373	LYS
3	J	381	ARG
3	J	391	ASP
3	J	428	GLN
3	J	439	VAL
3	K	15	GLU
3	K	24	VAL
3	K	39	ILE
3	K	60	ASP
3	K	63	GLU
3	K	65	VAL
3	K	78	GLU
3	K	79	GLN
3	K	80	LEU
3	K	83	ILE
3	K	86	VAL
3	K	87	SER
3	K	94	ASP
3	K	98	THR
3	K	113	SER
3	K	128	ASP
3	K	132	ARG
3	K	135	GLU
3	K	136	ILE
3	K	138	VAL
3	K	139	LEU
3	K	147	ILE
3	K	149	GLU

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Mol	Chain	Res	Type
3	K	163	LYS
3	K	169	THR
3	K	170	TYR
3	K	173	ILE
3	K	211	ARG
3	K	216	LYS
3	K	231	THR
3	K	235	VAL
3	K	245	GLN
3	K	264	ARG
3	K	285	ASN
3	K	288	ILE
3	K	293	THR
3	K	298	VAL
3	K	302	ARG
3	K	310	GLN
3	K	314	LEU
3	K	316	MET
3	K	323	GLN
3	K	328	SER
3	K	330	ARG
3	K	332	LYS
3	K	340	SER
3	K	373	LYS
3	K	381	ARG
3	K	391	ASP
3	K	404	LYS
3	K	428	GLN
3	K	439	VAL
3	L	12	GLN
3	L	55	MET
3	L	57	ARG
3	L	61	ARG
3	L	77	SER
3	L	86	VAL
3	L	96	VAL
3	L	98	THR
3	L	101	ASN
3	L	102	VAL
3	L	134	ASP
3	L	138	VAL
3	L	139	LEU

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Mol	Chain	Res	Type
3	L	140	LEU
3	L	147	ILE
3	L	149	GLU
3	L	161	ASN
3	L	174	GLU
3	L	211	ARG
3	L	216	LYS
3	L	231	THR
3	L	235	VAL
3	L	245	GLN
3	L	264	ARG
3	L	285	ASN
3	L	288	ILE
3	L	293	THR
3	L	298	VAL
3	L	302	ARG
3	L	310	GLN
3	L	314	LEU
3	L	316	MET
3	L	323	GLN
3	L	328	SER
3	L	330	ARG
3	L	332	LYS
3	L	340	SER
3	L	373	LYS
3	L	381	ARG
3	L	391	ASP
3	L	428	GLN
3	L	439	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	79	GLN
3	A	101	ASN
3	A	225	GLN
3	A	226	ASN
3	A	245	GLN
3	A	259	ASN
3	A	323	GLN
3	A	334	ASN
3	A	369	GLN

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Mol	Chain	Res	Type
3	A	436	ASN
3	B	12	GLN
3	B	79	GLN
3	B	101	ASN
3	B	225	GLN
3	B	226	ASN
3	B	245	GLN
3	B	261	GLN
3	B	323	GLN
3	B	334	ASN
3	B	410	ASN
3	B	440	ASN
3	C	79	GLN
3	C	161	ASN
3	C	172	ASN
3	C	177	HIS
3	C	225	GLN
3	C	226	ASN
3	C	259	ASN
3	C	323	GLN
3	C	334	ASN
3	C	337	GLN
3	C	436	ASN
3	D	12	GLN
3	D	79	GLN
3	D	161	ASN
3	D	225	GLN
3	D	226	ASN
3	D	245	GLN
3	D	259	ASN
3	D	323	GLN
3	D	334	ASN
3	D	371	GLN
3	D	421	ASN
3	E	79	GLN
3	E	225	GLN
3	E	226	ASN
3	E	245	GLN
3	E	259	ASN
3	E	323	GLN
3	E	334	ASN
3	E	421	ASN

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Mol	Chain	Res	Type
3	E	436	ASN
3	F	79	GLN
3	F	225	GLN
3	F	226	ASN
3	F	259	ASN
3	F	323	GLN
3	F	334	ASN
3	F	371	GLN
3	G	49	GLN
3	G	53	HIS
3	G	79	GLN
3	G	161	ASN
3	G	201	GLN
3	G	225	GLN
3	G	226	ASN
3	G	245	GLN
3	G	310	GLN
3	G	323	GLN
3	G	362	GLN
3	G	419	GLN
3	H	49	GLN
3	H	53	HIS
3	H	79	GLN
3	H	161	ASN
3	H	201	GLN
3	H	225	GLN
3	H	226	ASN
3	H	245	GLN
3	H	323	GLN
3	H	362	GLN
3	H	419	GLN
3	I	12	GLN
3	I	49	GLN
3	I	53	HIS
3	I	79	GLN
3	I	201	GLN
3	I	225	GLN
3	I	226	ASN
3	I	245	GLN
3	I	310	GLN
3	I	323	GLN
3	I	362	GLN

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Mol	Chain	Res	Type
3	I	419	GLN
3	J	49	GLN
3	J	53	HIS
3	J	79	GLN
3	J	201	GLN
3	J	225	GLN
3	J	226	ASN
3	J	310	GLN
3	J	323	GLN
3	J	337	GLN
3	J	362	GLN
3	J	419	GLN
3	K	48	HIS
3	K	49	GLN
3	K	79	GLN
3	K	201	GLN
3	K	225	GLN
3	K	226	ASN
3	K	323	GLN
3	K	334	ASN
3	K	362	GLN
3	K	419	GLN
3	L	49	GLN
3	L	53	HIS
3	L	79	GLN
3	L	201	GLN
3	L	225	GLN
3	L	226	ASN
3	L	323	GLN
3	L	362	GLN
3	L	419	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 14 are monoatomic - leaving 24 for Mogul analysis.

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
6	GDP	L	501	5	24,30,30	1.37	2 (8%)	31,47,47	2.42	11 (35%)
7	ALF	E	503	-	0,4,4	0.00	-	-		
7	ALF	A	504	-	0,4,4	0.00	-	-		
6	GDP	C	501	5	24,30,30	1.59	3 (12%)	31,47,47	2.21	13 (41%)
7	ALF	K	502	-	0,4,4	0.00	-	-		
7	ALF	G	502	-	0,4,4	0.00	-	-		
6	GDP	F	501	5	24,30,30	1.44	3 (12%)	31,47,47	2.21	10 (32%)
4	MES	E	504	-	12,12,12	1.94	1 (8%)	14,16,16	7.30	8 (57%)
7	ALF	D	503	-	0,4,4	0.00	-	-		
7	ALF	C	503	-	0,4,4	0.00	-	-		
6	GDP	J	501	-	24,30,30	1.19	3 (12%)	31,47,47	1.85	6 (19%)
6	GDP	E	501	5	24,30,30	1.37	3 (12%)	31,47,47	2.16	10 (32%)
4	MES	I	504	-	12,12,12	1.99	1 (8%)	14,16,16	2.61	7 (50%)
6	GDP	I	501	5	24,30,30	1.21	1 (4%)	31,47,47	2.09	12 (38%)
4	MES	W	101	-	12,12,12	2.17	1 (8%)	14,16,16	2.43	7 (50%)
6	GDP	D	501	5	24,30,30	1.32	3 (12%)	31,47,47	1.90	8 (25%)
7	ALF	L	502	-	0,4,4	0.00	-	-		
4	MES	C	505	-	12,12,12	2.12	1 (8%)	14,16,16	2.66	7 (50%)
7	ALF	I	503	-	0,4,4	0.00	-	-		
7	ALF	J	502	-	0,4,4	0.00	-	-		
6	GDP	G	501	-	24,30,30	1.35	3 (12%)	31,47,47	2.06	7 (22%)
6	GDP	K	501	-	24,30,30	1.31	2 (8%)	31,47,47	2.18	9 (29%)
6	GDP	A	502	5	24,30,30	1.36	3 (12%)	31,47,47	2.07	11 (35%)
7	ALF	C	504	-	0,4,4	0.00	-	-		

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
6	GDP	L	501	5	-	2/12/32/32	0/3/3/3
6	GDP	J	501	-	-	4/12/32/32	0/3/3/3
6	GDP	E	501	5	-	4/12/32/32	0/3/3/3
6	GDP	G	501	-	-	3/12/32/32	0/3/3/3
4	MES	I	504	-	-	3/6/14/14	0/1/1/1
4	MES	C	505	-	-	5/6/14/14	0/1/1/1
6	GDP	C	501	5	-	6/12/32/32	0/3/3/3
6	GDP	I	501	5	-	3/12/32/32	0/3/3/3
6	GDP	K	501	-	-	3/12/32/32	0/3/3/3
6	GDP	A	502	5	-	6/12/32/32	0/3/3/3
4	MES	W	101	-	-	2/6/14/14	0/1/1/1
6	GDP	D	501	5	-	4/12/32/32	0/3/3/3
6	GDP	F	501	5	-	5/12/32/32	0/3/3/3
4	MES	E	504	-	-	3/6/14/14	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	W	101	MES	C8-S	-7.26	1.67	1.77
4	C	505	MES	C8-S	-7.05	1.67	1.77
4	I	504	MES	C8-S	-6.44	1.68	1.77
4	E	504	MES	C8-S	-6.13	1.68	1.77
6	C	501	GDP	C6-C5	4.93	1.49	1.41
6	F	501	GDP	C6-C5	4.82	1.49	1.41
6	E	501	GDP	C6-C5	4.76	1.49	1.41
6	K	501	GDP	C6-C5	4.73	1.49	1.41
6	L	501	GDP	C6-C5	4.67	1.49	1.41
6	G	501	GDP	C6-C5	4.61	1.49	1.41
6	C	501	GDP	O4'-C1'	4.35	1.47	1.41
6	D	501	GDP	C6-C5	4.23	1.48	1.41
6	I	501	GDP	C6-C5	4.16	1.48	1.41
6	J	501	GDP	C6-C5	3.75	1.47	1.41
6	A	502	GDP	O4'-C1'	3.73	1.46	1.41
6	A	502	GDP	C6-C5	3.57	1.47	1.41
6	F	501	GDP	C5-C4	2.94	1.48	1.40
6	C	501	GDP	C5-C4	2.91	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	501	GDP	C5-C4	2.62	1.47	1.40
6	A	502	GDP	C5-C4	2.60	1.47	1.40
6	G	501	GDP	C5-C4	2.57	1.47	1.40
6	K	501	GDP	C5-C4	2.53	1.47	1.40
6	J	501	GDP	C5-C4	2.50	1.47	1.40
6	E	501	GDP	C5-C4	2.48	1.47	1.40
6	D	501	GDP	O4'-C1'	2.46	1.44	1.41
6	F	501	GDP	O4'-C1'	2.32	1.44	1.41
6	L	501	GDP	C5-C4	2.26	1.46	1.40
6	E	501	GDP	O4'-C1'	2.22	1.44	1.41
6	J	501	GDP	O4'-C1'	2.21	1.44	1.41
6	G	501	GDP	O4'-C1'	2.04	1.43	1.41

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	504	MES	O2S-S-C8	-16.10	87.53	106.92
4	E	504	MES	O1S-S-C8	-15.52	88.23	106.92
4	E	504	MES	O3S-S-C8	-12.44	85.64	105.77
6	L	501	GDP	C2-N3-C4	6.63	122.92	115.36
4	I	504	MES	C5-N4-C3	6.32	123.05	108.83
4	E	504	MES	C5-N4-C3	6.25	122.89	108.83
6	F	501	GDP	C6-C5-C4	-6.13	114.94	120.80
6	G	501	GDP	C2-N3-C4	5.56	121.71	115.36
6	K	501	GDP	C2-N3-C4	5.43	121.56	115.36
4	C	505	MES	C5-N4-C3	5.42	121.03	108.83
6	E	501	GDP	C2-N3-C4	5.28	121.39	115.36
6	A	502	GDP	C5-C6-N1	-5.28	116.21	123.43
6	C	501	GDP	C2-N3-C4	5.15	121.24	115.36
6	L	501	GDP	N3-C2-N1	-5.11	120.41	127.22
4	W	101	MES	C5-N4-C3	4.99	120.06	108.83
6	L	501	GDP	C6-C5-C4	-4.97	116.06	120.80
6	K	501	GDP	C6-C5-C4	-4.91	116.11	120.80
6	I	501	GDP	C6-C5-C4	-4.90	116.12	120.80
6	J	501	GDP	C2-N3-C4	4.88	120.93	115.36
6	C	501	GDP	C5-C6-N1	-4.82	116.84	123.43
6	D	501	GDP	C2-N3-C4	4.55	120.55	115.36
6	F	501	GDP	C2-N3-C4	4.45	120.44	115.36
6	A	502	GDP	C2-N3-C4	4.45	120.44	115.36
6	L	501	GDP	C6-N1-C2	4.43	122.96	115.93
4	E	504	MES	O3S-S-O2S	4.31	121.79	111.27
6	E	501	GDP	C6-C5-C4	-4.30	116.69	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	101	MES	C7-N4-C5	4.22	122.03	111.23
6	G	501	GDP	C6-C5-C4	-4.14	116.84	120.80
6	J	501	GDP	C5-C6-N1	-4.14	117.77	123.43
6	K	501	GDP	C6-N1-C2	4.07	122.40	115.93
6	G	501	GDP	C6-N1-C2	4.06	122.38	115.93
6	F	501	GDP	C1'-N9-C4	-3.96	119.67	126.64
6	I	501	GDP	C2-N3-C4	3.95	119.87	115.36
6	G	501	GDP	N3-C2-N1	-3.93	121.97	127.22
6	D	501	GDP	PA-O3A-PB	-3.91	119.42	132.83
6	A	502	GDP	PA-O3A-PB	-3.90	119.44	132.83
6	E	501	GDP	C5-C6-N1	-3.88	118.13	123.43
4	I	504	MES	O1S-S-C8	3.87	111.58	106.92
6	F	501	GDP	C6-N1-C2	3.86	122.06	115.93
6	J	501	GDP	C6-N1-C2	3.77	121.93	115.93
6	K	501	GDP	N3-C2-N1	-3.76	122.21	127.22
6	E	501	GDP	C6-N1-C2	3.72	121.84	115.93
6	I	501	GDP	C1'-N9-C4	-3.71	120.13	126.64
6	C	501	GDP	C6-N1-C2	3.65	121.74	115.93
6	G	501	GDP	C5-C6-N1	-3.63	118.47	123.43
6	D	501	GDP	C5-C6-N1	-3.62	118.48	123.43
6	C	501	GDP	C1'-N9-C4	3.57	132.92	126.64
6	A	502	GDP	C6-N1-C2	3.57	121.60	115.93
6	D	501	GDP	C6-N1-C2	3.52	121.53	115.93
6	K	501	GDP	C5-C6-N1	-3.52	118.62	123.43
6	K	501	GDP	C3'-C2'-C1'	3.51	106.26	100.98
6	L	501	GDP	C4-C5-N7	-3.50	105.75	109.40
4	C	505	MES	C6-C5-N4	-3.45	104.88	110.10
6	E	501	GDP	N3-C2-N1	-3.43	122.64	127.22
4	E	504	MES	C7-N4-C5	3.43	120.00	111.23
4	C	505	MES	C7-N4-C5	3.38	119.88	111.23
4	I	504	MES	C7-N4-C3	3.31	119.70	111.23
6	L	501	GDP	C5-C6-N1	-3.28	118.95	123.43
6	F	501	GDP	N3-C2-N1	-3.26	122.87	127.22
4	C	505	MES	O3S-S-C8	3.26	111.04	105.77
6	C	501	GDP	C3'-C2'-C1'	3.23	105.85	100.98
6	A	502	GDP	O3'-C3'-C4'	-3.19	101.82	111.05
6	F	501	GDP	PA-O3A-PB	-3.18	121.91	132.83
6	K	501	GDP	C4-C5-N7	-3.18	106.09	109.40
4	C	505	MES	C2-C3-N4	-3.15	105.33	110.10
6	D	501	GDP	C6-C5-C4	-3.12	117.81	120.80
6	F	501	GDP	C5-C6-N1	-3.11	119.18	123.43
6	J	501	GDP	N3-C2-N1	-3.08	123.11	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	505	MES	C7-N4-C3	3.07	119.08	111.23
4	W	101	MES	O2S-S-C8	3.06	110.60	106.92
6	E	501	GDP	C3'-C2'-C1'	3.05	105.57	100.98
6	I	501	GDP	PA-O3A-PB	-3.03	122.42	132.83
6	F	501	GDP	O3B-PB-O3A	2.99	114.66	104.64
4	E	504	MES	O3S-S-O1S	2.95	118.48	111.27
6	I	501	GDP	C5-C6-N1	-2.95	119.40	123.43
6	E	501	GDP	PA-O3A-PB	-2.86	123.02	132.83
6	D	501	GDP	O3'-C3'-C4'	-2.82	102.91	111.05
6	I	501	GDP	C6-N1-C2	2.80	120.38	115.93
6	L	501	GDP	PA-O3A-PB	-2.79	123.25	132.83
6	J	501	GDP	PA-O3A-PB	-2.79	123.26	132.83
6	L	501	GDP	C1'-N9-C4	-2.78	121.76	126.64
6	I	501	GDP	O3'-C3'-C2'	-2.76	102.88	111.82
6	G	501	GDP	PA-O3A-PB	-2.73	123.46	132.83
4	C	505	MES	O1S-S-C8	2.70	110.16	106.92
6	C	501	GDP	PA-O3A-PB	-2.69	123.58	132.83
6	K	501	GDP	PA-O3A-PB	-2.67	123.66	132.83
6	G	501	GDP	C4-C5-N7	-2.66	106.63	109.40
6	I	501	GDP	N3-C2-N1	-2.63	123.71	127.22
6	E	501	GDP	C4-C5-N7	-2.63	106.66	109.40
6	A	502	GDP	O5'-C5'-C4'	2.63	118.04	108.99
4	W	101	MES	C7-N4-C3	2.61	117.91	111.23
6	C	501	GDP	O2'-C2'-C1'	2.60	120.45	110.85
6	A	502	GDP	C1'-N9-C4	2.59	131.19	126.64
6	D	501	GDP	C4-C5-N7	-2.56	106.73	109.40
6	C	501	GDP	O5'-C5'-C4'	2.52	117.66	108.99
6	J	501	GDP	C6-C5-C4	-2.50	118.41	120.80
6	L	501	GDP	N2-C2-N1	2.48	121.12	117.25
4	I	504	MES	O1-C2-C3	-2.45	106.40	111.80
6	I	501	GDP	O4'-C4'-C5'	-2.38	101.53	109.37
4	I	504	MES	C7-N4-C5	2.35	117.24	111.23
4	I	504	MES	O2S-S-O1S	-2.34	105.84	113.95
6	A	502	GDP	C3'-C2'-C1'	2.34	104.50	100.98
6	I	501	GDP	O2B-PB-O3A	2.33	112.44	104.64
6	K	501	GDP	C1'-N9-C4	-2.33	122.55	126.64
6	I	501	GDP	C5'-C4'-C3'	2.33	123.90	115.18
6	E	501	GDP	N2-C2-N1	2.30	120.83	117.25
4	E	504	MES	C7-N4-C3	2.30	117.11	111.23
6	I	501	GDP	C4-C5-N7	-2.28	107.02	109.40
6	F	501	GDP	C4-C5-N7	-2.27	107.03	109.40
4	W	101	MES	O3S-S-C8	2.27	109.44	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	501	GDP	O2'-C2'-C3'	-2.26	104.51	111.82
6	C	501	GDP	O4'-C4'-C5'	2.26	116.80	109.37
6	C	501	GDP	C2'-C3'-C4'	2.24	107.00	102.64
6	C	501	GDP	O2B-PB-O3A	2.24	112.13	104.64
6	C	501	GDP	N3-C2-N1	-2.23	124.24	127.22
6	D	501	GDP	N3-C2-N1	-2.23	124.25	127.22
6	C	501	GDP	C4-C5-N7	-2.18	107.13	109.40
6	A	502	GDP	C2'-C3'-C4'	2.17	106.85	102.64
4	W	101	MES	C2-C3-N4	-2.14	106.85	110.10
4	I	504	MES	O3S-S-C8	2.10	109.17	105.77
6	E	501	GDP	C1'-N9-C4	-2.08	122.98	126.64
6	A	502	GDP	O2B-PB-O3A	2.08	111.61	104.64
6	A	502	GDP	O2'-C2'-C1'	-2.07	103.21	110.85
4	W	101	MES	C6-C5-N4	-2.06	106.98	110.10
6	F	501	GDP	N2-C2-N1	2.05	120.43	117.25
6	L	501	GDP	O4'-C1'-C2'	-2.03	103.97	106.93

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	501	GDP	PA-O3A-PB-O2B
6	C	501	GDP	PA-O3A-PB-O3B
6	C	501	GDP	O4'-C4'-C5'-O5'
6	F	501	GDP	C5'-O5'-PA-O1A
6	F	501	GDP	C5'-O5'-PA-O2A
4	E	504	MES	C8-C7-N4-C5
4	E	504	MES	N4-C7-C8-S
6	J	501	GDP	C5'-O5'-PA-O1A
6	J	501	GDP	C5'-O5'-PA-O2A
6	E	501	GDP	C5'-O5'-PA-O3A
6	E	501	GDP	O4'-C4'-C5'-O5'
4	I	504	MES	C8-C7-N4-C3
4	I	504	MES	N4-C7-C8-S
4	W	101	MES	C8-C7-N4-C5
4	W	101	MES	N4-C7-C8-S
6	D	501	GDP	C5'-O5'-PA-O3A
6	D	501	GDP	C5'-O5'-PA-O2A
4	C	505	MES	N4-C7-C8-S
4	C	505	MES	C7-C8-S-O1S
4	C	505	MES	C7-C8-S-O3S
6	K	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
6	A	502	GDP	PA-O3A-PB-O2B
6	A	502	GDP	O4'-C4'-C5'-O5'
6	F	501	GDP	O4'-C4'-C5'-O5'
6	F	501	GDP	C3'-C4'-C5'-O5'
6	I	501	GDP	O4'-C4'-C5'-O5'
6	E	501	GDP	C3'-C4'-C5'-O5'
6	G	501	GDP	O4'-C4'-C5'-O5'
4	I	504	MES	C8-C7-N4-C5
6	J	501	GDP	O4'-C4'-C5'-O5'
6	I	501	GDP	C3'-C4'-C5'-O5'
6	A	502	GDP	PA-O3A-PB-O3B
6	K	501	GDP	C5'-O5'-PA-O3A
6	I	501	GDP	PB-O3A-PA-O2A
6	E	501	GDP	C5'-O5'-PA-O2A
6	K	501	GDP	C5'-O5'-PA-O2A
4	C	505	MES	C7-C8-S-O2S
6	C	501	GDP	C3'-C4'-C5'-O5'
6	C	501	GDP	C4'-C5'-O5'-PA
6	A	502	GDP	C4'-C5'-O5'-PA
6	D	501	GDP	O4'-C4'-C5'-O5'
6	G	501	GDP	PB-O3A-PA-O2A
4	E	504	MES	C8-C7-N4-C3
4	C	505	MES	C8-C7-N4-C3
6	A	502	GDP	PA-O3A-PB-O1B
6	A	502	GDP	C3'-C4'-C5'-O5'
6	L	501	GDP	C5'-O5'-PA-O3A
6	F	501	GDP	C5'-O5'-PA-O3A
6	J	501	GDP	C5'-O5'-PA-O3A
6	L	501	GDP	O4'-C4'-C5'-O5'
6	G	501	GDP	PB-O3A-PA-O1A
6	D	501	GDP	C3'-C4'-C5'-O5'
6	C	501	GDP	PA-O3A-PB-O1B

There are no ring outliers.

13 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	501	GDP	5	0
7	A	504	ALF	2	0
6	C	501	GDP	4	0
7	K	502	ALF	1	0
6	F	501	GDP	4	0

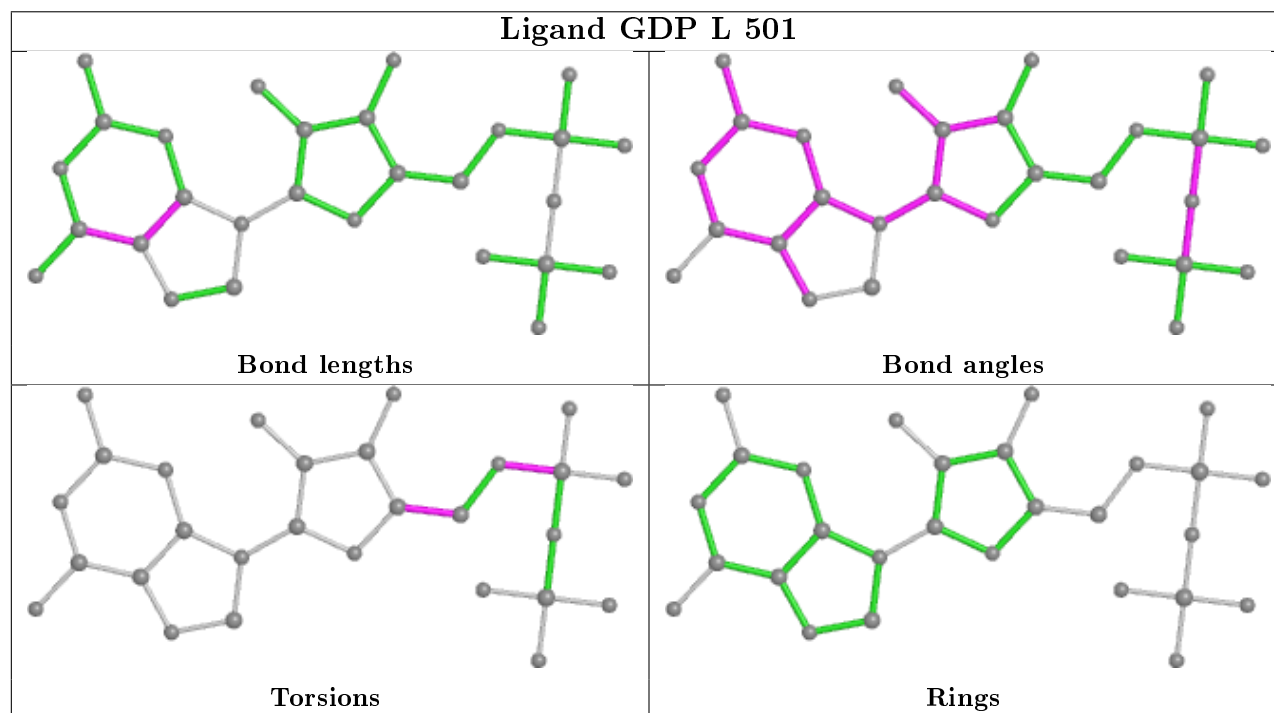
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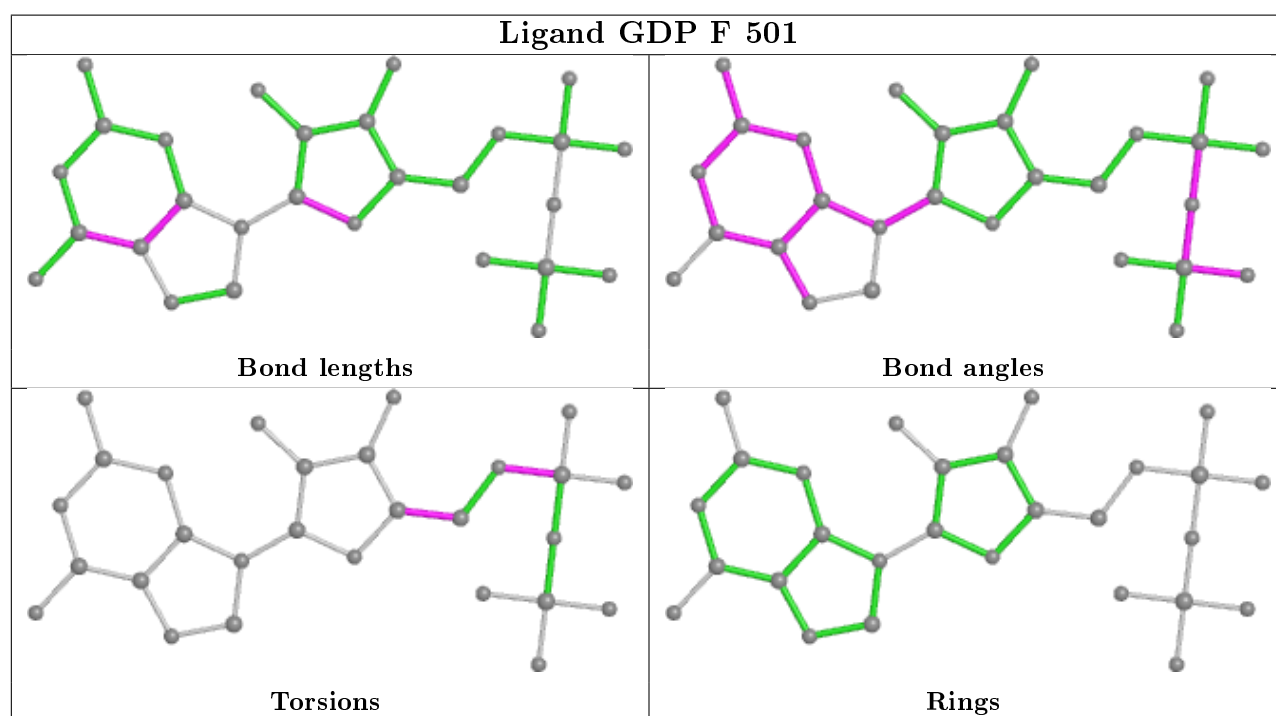
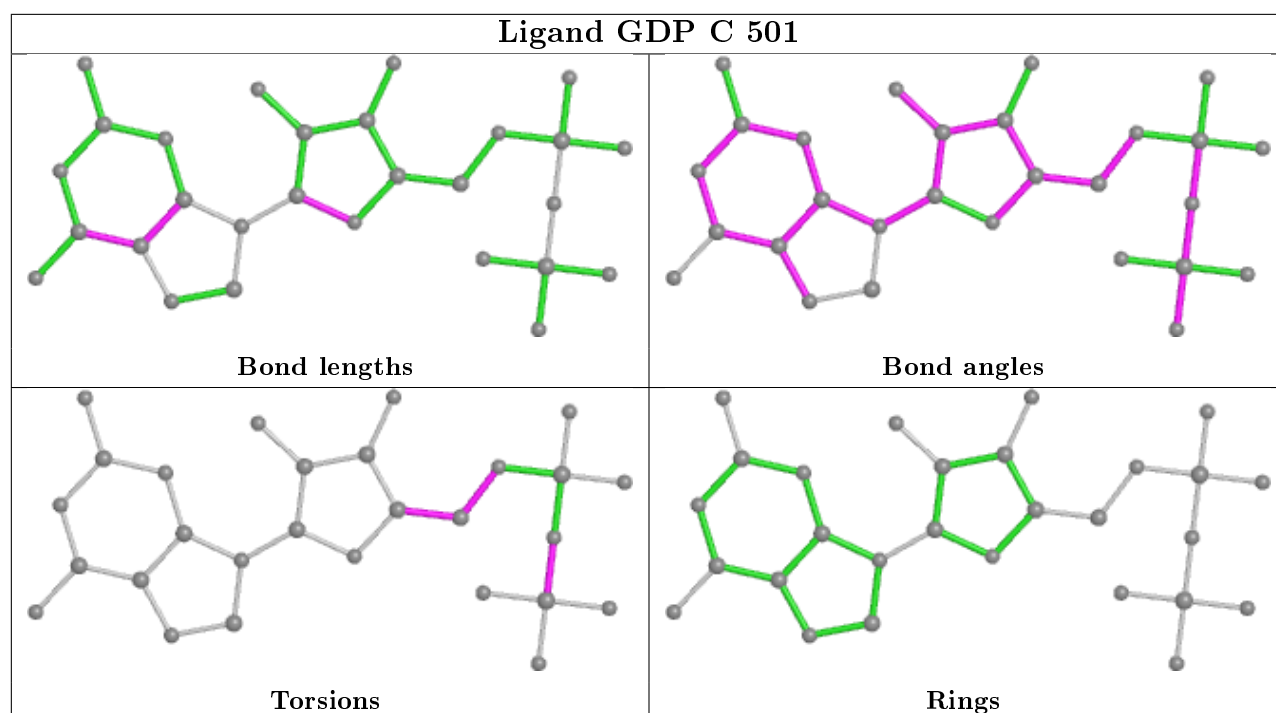


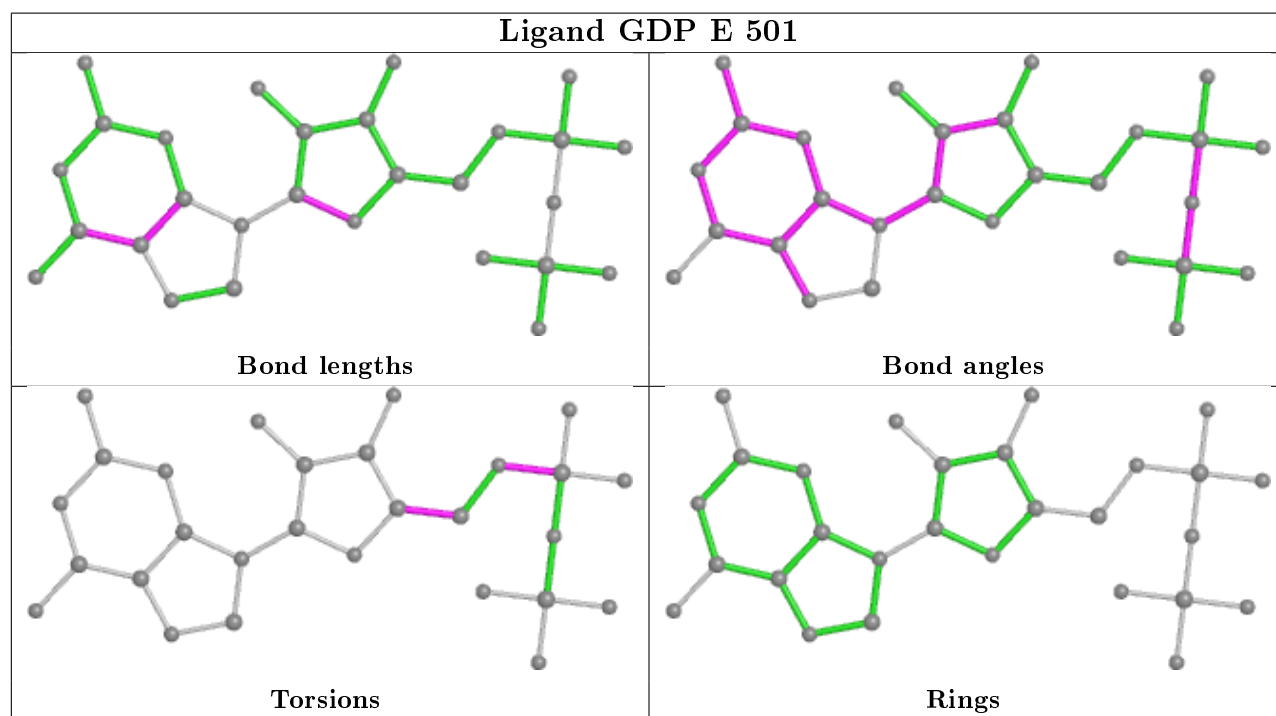
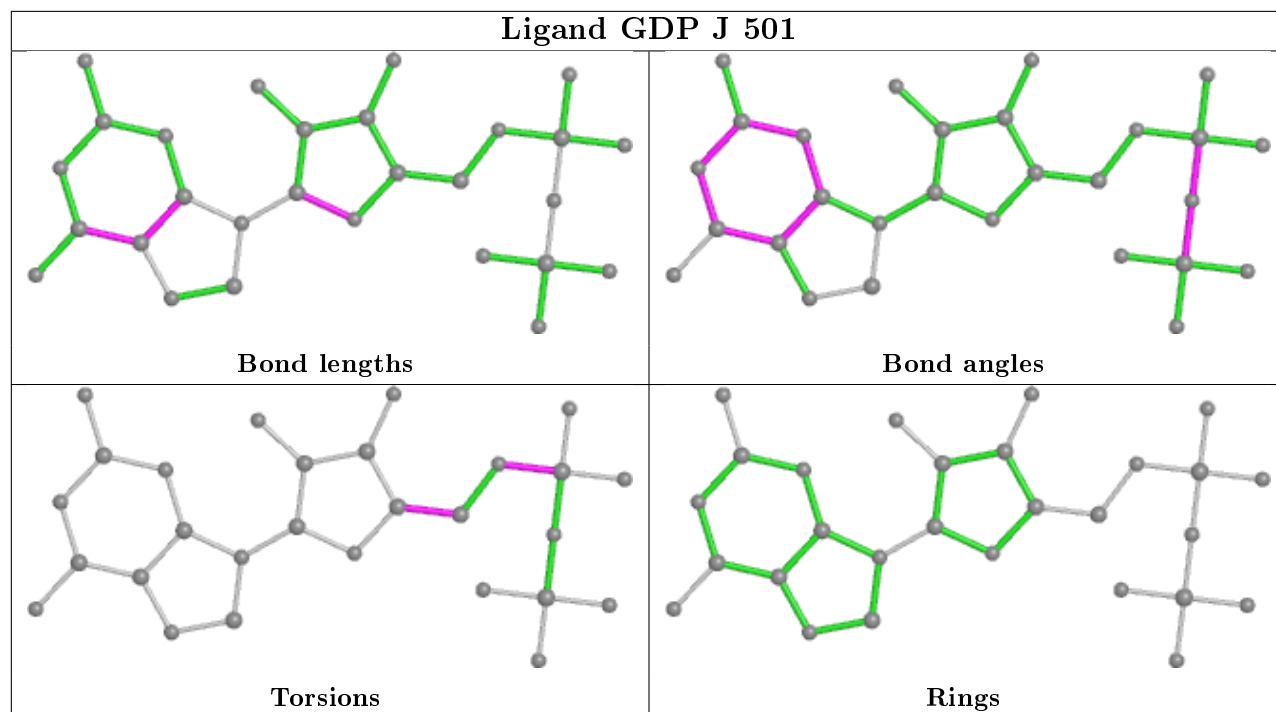
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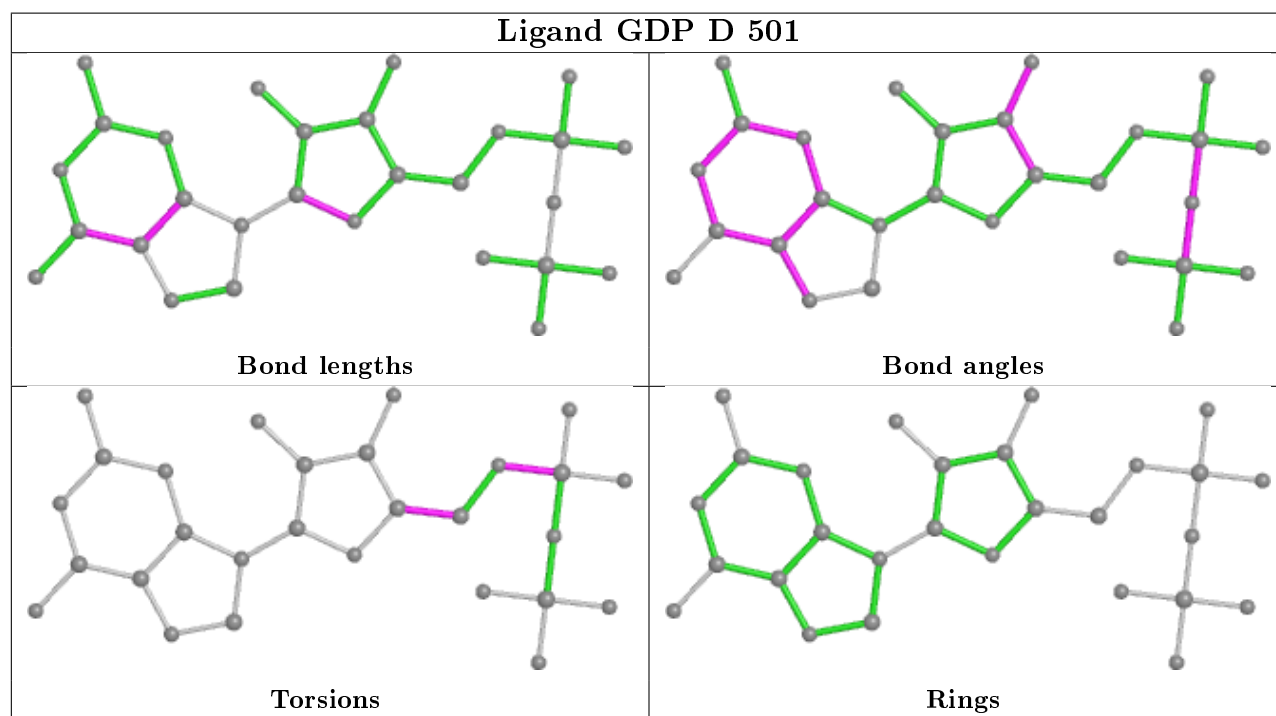
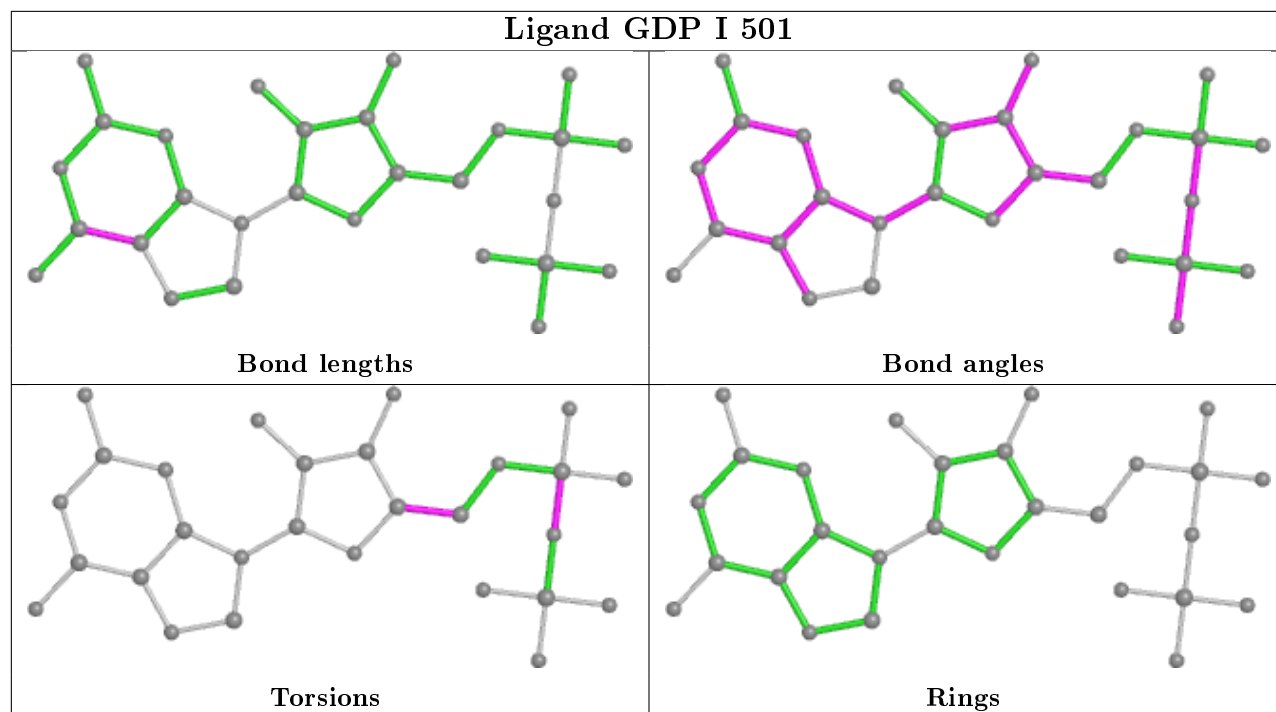
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	501	GDP	6	0
6	E	501	GDP	4	0
6	I	501	GDP	10	0
4	W	101	MES	4	0
6	D	501	GDP	3	0
6	G	501	GDP	5	0
6	K	501	GDP	3	0
6	A	502	GDP	4	0

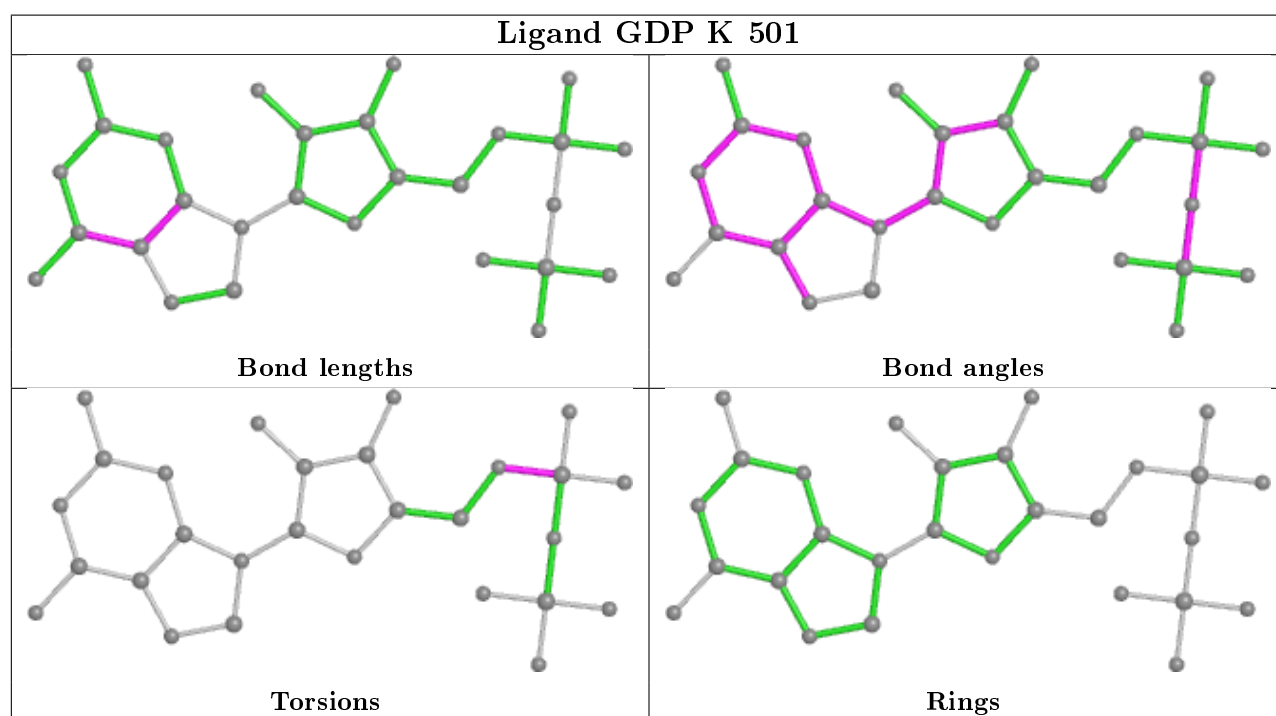
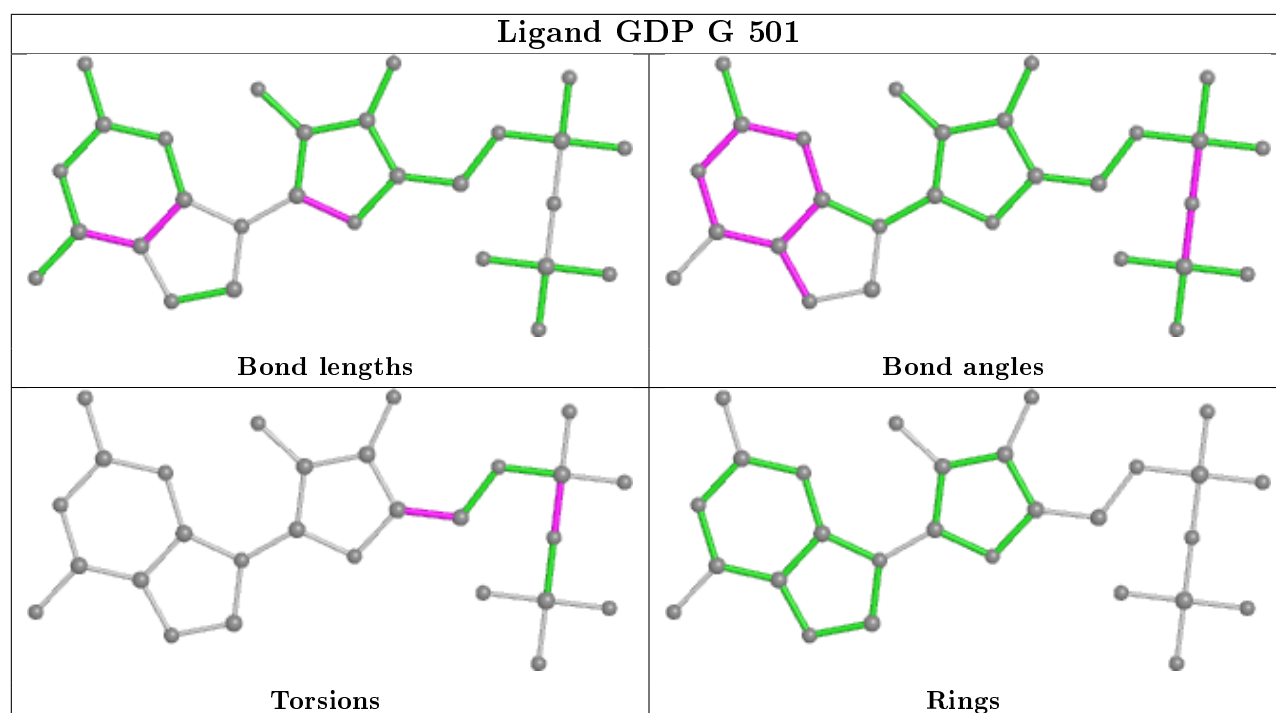
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

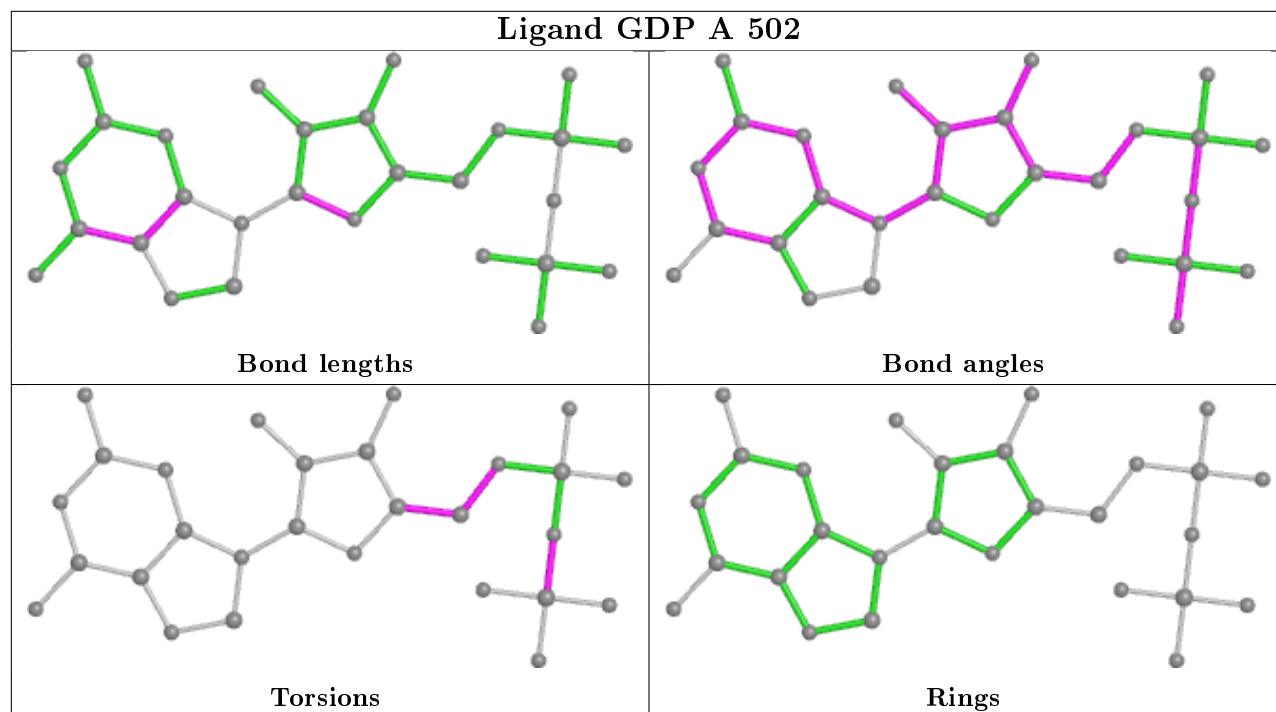












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	V	14/14 (100%)	-0.19	1 (7%) 16 9	82, 91, 181, 202	0
2	W	13/13 (100%)	-0.55	0 100 100	92, 107, 167, 208	0
3	A	418/454 (92%)	-0.18	6 (1%) 75 63	69, 100, 162, 214	3 (0%)
3	B	430/454 (94%)	-0.06	9 (2%) 63 49	66, 111, 181, 236	0
3	C	434/454 (95%)	-0.16	5 (1%) 79 67	66, 102, 157, 213	0
3	D	431/454 (94%)	-0.12	3 (0%) 87 81	67, 109, 171, 229	0
3	E	418/454 (92%)	-0.08	5 (1%) 79 67	68, 108, 164, 221	0
3	F	421/454 (92%)	-0.01	12 (2%) 51 36	66, 108, 167, 212	0
3	G	421/454 (92%)	0.42	29 (6%) 16 9	100, 165, 252, 322	0
3	H	425/454 (93%)	0.39	30 (7%) 16 9	95, 149, 253, 284	0
3	I	418/454 (92%)	0.20	8 (1%) 66 53	92, 158, 248, 326	0
3	J	416/454 (91%)	0.38	23 (5%) 25 14	89, 177, 285, 314	1 (0%)
3	K	421/454 (92%)	0.42	42 (9%) 7 4	77, 169, 283, 310	0
3	L	419/454 (92%)	0.56	43 (10%) 6 4	112, 174, 247, 301	0
All	All	5099/5475 (93%)	0.14	216 (4%) 36 23	66, 134, 228, 326	4 (0%)

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	405	ASP	11.8
3	H	400	ASP	7.5
3	L	270	PRO	7.2
3	H	404	LYS	6.7
3	K	256	GLY	6.6
3	F	331	SER	6.5
3	G	266	GLY	6.5
3	K	276	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
3	K	133	GLU	6.2
3	K	289	TYR	6.0
3	H	403	ASN	6.0
3	L	265	THR	5.7
3	G	173	ILE	5.7
3	G	267	LYS	5.7
3	A	99	ALA	5.6
3	J	257	ASN	5.4
3	G	265	THR	5.4
3	J	258	ILE	5.1
3	G	172	ASN	5.0
3	G	331	SER	4.9
3	G	133	GLU	4.8
3	L	410	ASN	4.7
3	H	402	TYR	4.7
3	H	401	TYR	4.5
3	C	133	GLU	4.5
3	H	267	LYS	4.4
3	K	277	THR	4.4
3	K	258	ILE	4.4
3	H	331	SER	4.3
3	H	333	GLU	4.3
3	L	408	ASN	4.3
3	L	411	ILE	4.2
3	K	288	ILE	4.2
3	L	438	PHE	4.0
3	B	264	ARG	4.0
3	C	331	SER	4.0
3	K	170	TYR	4.0
3	H	269	THR	3.9
3	K	308	LEU	3.9
3	K	270	PRO	3.9
3	J	183	ILE	3.9
3	K	134	ASP	3.9
3	K	268	LEU	3.9
3	I	161	ASN	3.8
3	K	331	SER	3.7
3	L	13	SER	3.7
3	K	314	LEU	3.7
3	L	266	GLY	3.7
3	J	252	LEU	3.6
3	H	268	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
3	J	276	LEU	3.6
3	K	278	MET	3.5
3	K	252	LEU	3.5
3	K	286	ALA	3.5
3	B	134	ASP	3.4
3	L	371	GLN	3.4
3	A	169	THR	3.4
3	L	428	GLN	3.4
3	J	270	PRO	3.4
3	K	438	PHE	3.4
3	E	65	VAL	3.3
3	H	259	ASN	3.3
3	F	332	LYS	3.3
3	H	275	LYS	3.3
3	H	332	LYS	3.2
3	H	406	SER	3.2
3	K	283	LEU	3.2
3	A	421	ASN	3.2
3	L	104	TYR	3.2
3	G	263	LEU	3.1
3	K	310	GLN	3.1
3	C	136	ILE	3.1
3	L	429	LEU	3.1
3	G	282	SER	3.0
3	K	255	GLU	3.0
3	C	65	VAL	3.0
3	B	133	GLU	3.0
3	G	329	GLY	3.0
3	G	99	ALA	3.0
3	K	264	ARG	3.0
3	K	173	ILE	3.0
3	A	168	GLN	3.0
3	I	256	GLY	3.0
3	G	229	THR	2.9
3	J	331	SER	2.9
3	L	263	LEU	2.9
3	G	256	GLY	2.9
3	L	11	PRO	2.9
3	G	136	ILE	2.9
3	L	264	ARG	2.9
3	L	44	TYR	2.9
3	L	441	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	G	174	GLU	2.8
3	K	131	THR	2.8
3	E	170	TYR	2.8
3	L	273	TRP	2.8
3	A	134	ASP	2.8
3	F	97	PRO	2.8
3	J	263	LEU	2.8
3	J	273	TRP	2.8
3	L	21	LEU	2.8
3	J	253	CYS	2.7
3	B	272	ASP	2.7
3	F	273	TRP	2.7
3	I	281	GLY	2.7
3	B	97	PRO	2.7
3	H	329	GLY	2.7
3	B	6	SER	2.7
3	D	331	SER	2.7
3	K	441	LEU	2.7
3	H	134	ASP	2.7
3	C	139	LEU	2.6
3	G	273	TRP	2.6
1	V	14	DT	2.6
3	H	278	MET	2.6
3	G	332	LYS	2.6
3	G	175	MET	2.6
3	F	98	THR	2.6
3	L	88	TYR	2.6
3	L	65	VAL	2.6
3	K	274	GLY	2.6
3	J	391	ASP	2.6
3	K	253	CYS	2.5
3	H	115	LEU	2.5
3	K	234	ASN	2.5
3	K	305	CYS	2.5
3	D	118	LEU	2.5
3	L	252	LEU	2.5
3	F	43	PHE	2.5
3	L	102	VAL	2.5
3	F	280	MET	2.5
3	G	68	VAL	2.5
3	H	398	ARG	2.5
3	G	421	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	67	LEU	2.5
3	H	272	ASP	2.5
3	K	200	PHE	2.5
3	J	234	ASN	2.5
3	G	169	THR	2.5
3	F	104	TYR	2.5
3	L	389	ASP	2.5
3	G	280	MET	2.4
3	H	371	GLN	2.4
3	I	252	LEU	2.4
3	K	167	VAL	2.4
3	J	259	ASN	2.4
3	K	169	THR	2.4
3	K	311	GLU	2.4
3	K	290	ILE	2.4
3	G	330	ARG	2.4
3	K	307	ARG	2.4
3	L	382	GLU	2.4
3	J	268	LEU	2.4
3	J	274	GLY	2.4
3	F	268	LEU	2.4
3	H	433	LYS	2.3
3	J	289	TYR	2.3
3	L	412	ILE	2.3
3	J	256	GLY	2.3
3	K	157	GLY	2.3
3	L	268	LEU	2.3
3	L	397	TYR	2.3
3	G	70	VAL	2.3
3	L	129	GLY	2.3
3	G	333	GLU	2.3
3	B	263	LEU	2.3
3	L	409	LYS	2.2
3	L	310	GLN	2.2
3	K	272	ASP	2.2
3	L	272	ASP	2.2
3	H	257	ASN	2.2
3	K	273	TRP	2.2
3	G	65	VAL	2.2
3	F	267	LYS	2.2
3	B	332	LYS	2.2
3	L	201	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
3	I	139	LEU	2.2
3	D	43	PHE	2.2
3	J	278	MET	2.2
3	K	228	ALA	2.2
3	J	399	ASP	2.2
3	H	334	ASN	2.2
3	K	184	THR	2.2
3	L	45	ARG	2.2
3	J	74	LEU	2.2
3	J	431	PHE	2.2
3	L	421	ASN	2.2
3	F	109	VAL	2.2
3	J	202	ARG	2.2
3	E	147	ILE	2.2
3	H	37	ILE	2.2
3	G	430	ALA	2.1
3	L	20	VAL	2.1
3	I	268	LEU	2.1
3	I	143	ALA	2.1
3	L	46	ALA	2.1
3	L	12	GLN	2.1
3	L	105	TYR	2.1
3	E	83	ILE	2.1
3	G	10	PRO	2.1
3	I	213	SER	2.1
3	H	132	ARG	2.1
3	G	55	MET	2.1
3	E	123	THR	2.1
3	K	183	ILE	2.1
3	L	115	LEU	2.1
3	B	138	VAL	2.0
3	K	269	THR	2.0
3	L	106	ALA	2.0
3	H	133	GLU	2.0
3	H	271	GLU	2.0
3	J	394	ALA	2.0
3	A	98	THR	2.0
3	L	311	GLU	2.0
3	H	63	GLU	2.0
3	L	188	THR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

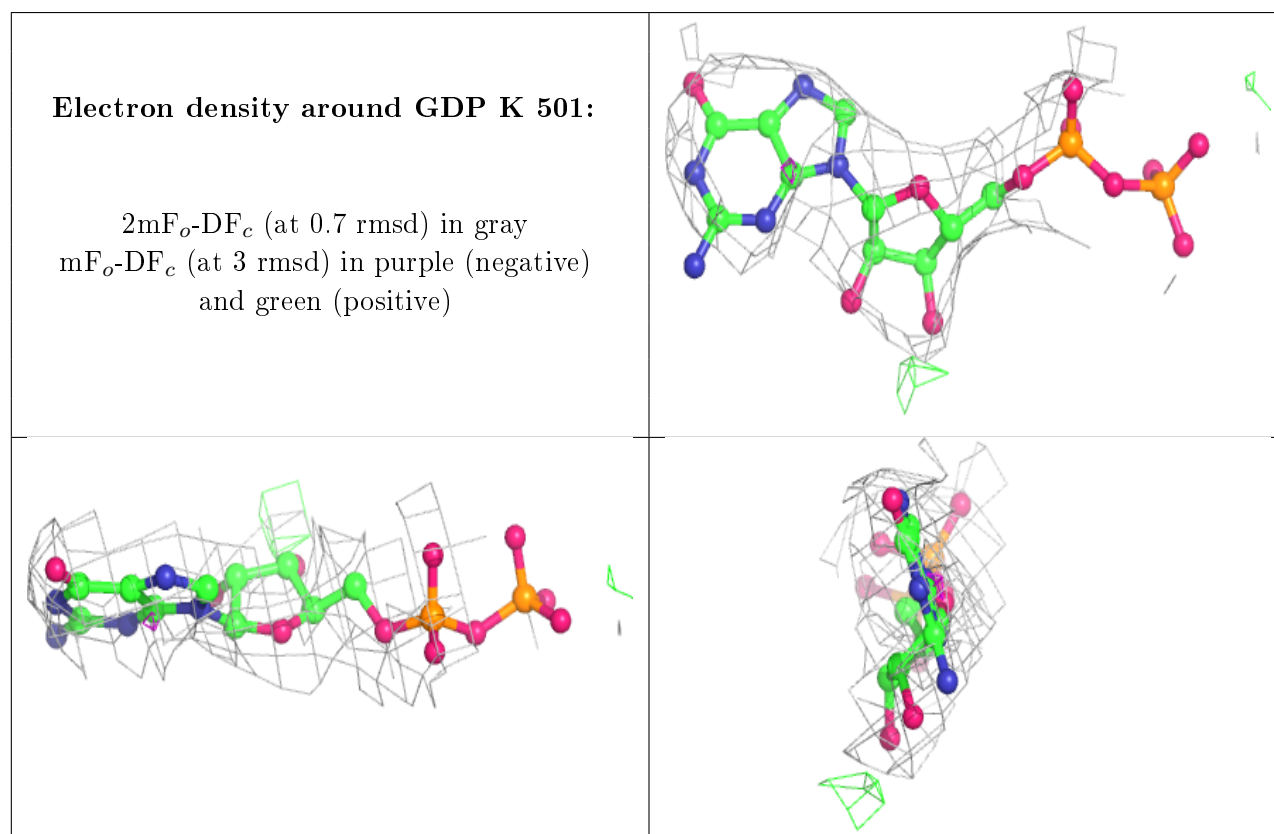
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MES	C	505	12/12	0.64	0.85	232,233,234,235	0
4	MES	W	101	12/12	0.68	0.66	247,250,253,253	0
5	CA	G	503	1/1	0.80	0.48	141,141,141,141	0
5	CA	B	501	1/1	0.81	0.58	147,147,147,147	0
6	GDP	K	501	28/28	0.82	0.24	165,178,204,208	0
5	CA	A	507	1/1	0.84	0.27	134,134,134,134	0
5	CA	A	505	1/1	0.85	0.26	117,117,117,117	0
6	GDP	L	501	28/28	0.86	0.23	129,162,173,177	0
4	MES	I	504	12/12	0.87	0.16	111,121,151,151	0
6	GDP	J	501	28/28	0.89	0.22	140,157,182,186	0
6	GDP	E	501	28/28	0.90	0.23	67,89,110,118	0
5	CA	A	506	1/1	0.90	0.36	140,140,140,140	0
4	MES	E	504	12/12	0.91	0.16	122,127,144,148	0
5	CA	A	501	1/1	0.92	0.22	109,109,109,109	0
6	GDP	G	501	28/28	0.92	0.23	118,157,181,186	0
5	CA	D	504	1/1	0.92	0.16	131,131,131,131	0
7	ALF	G	502	5/5	0.92	0.40	120,127,139,141	0
6	GDP	F	501	28/28	0.92	0.24	71,90,105,111	0
7	ALF	J	502	5/5	0.93	0.39	119,120,129,130	0
6	GDP	I	501	28/28	0.93	0.23	71,84,103,109	0
6	GDP	C	501	28/28	0.95	0.24	66,69,83,87	0
6	GDP	D	501	28/28	0.95	0.18	65,81,90,97	0
6	GDP	A	502	28/28	0.95	0.20	67,75,87,90	0
7	ALF	K	502	5/5	0.96	0.31	121,126,137,144	0
7	ALF	A	504	5/5	0.96	0.21	84,89,97,97	0
5	CA	F	502	1/1	0.97	0.37	92,92,92,92	0
7	ALF	E	503	5/5	0.97	0.36	88,88,100,101	0

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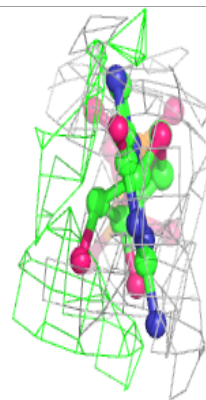
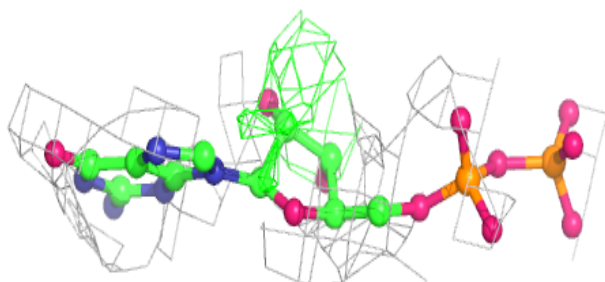
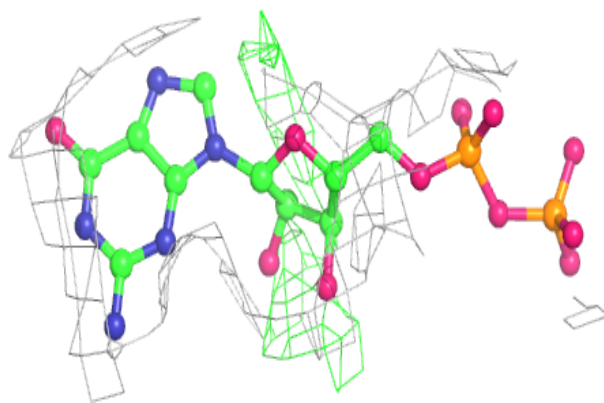
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	ALF	D	503	5/5	0.98	0.37	80,88,97,109	0
5	CA	D	502	1/1	0.98	0.26	90,90,90,90	0
7	ALF	I	503	5/5	0.98	0.28	89,90,95,97	0
7	ALF	L	502	5/5	0.98	0.21	118,121,124,126	0
5	CA	C	502	1/1	0.98	0.41	101,101,101,101	0
5	CA	I	502	1/1	0.99	0.32	117,117,117,117	0
5	CA	E	502	1/1	0.99	0.34	110,110,110,110	0
7	ALF	C	503	5/5	0.99	0.31	66,70,86,88	0
5	CA	L	503	1/1	0.99	0.30	155,155,155,155	0
5	CA	A	503	1/1	0.99	0.28	103,103,103,103	0
7	ALF	C	504	5/5	0.99	0.32	67,74,92,94	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.

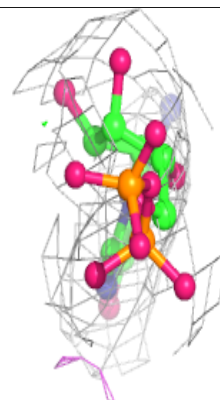
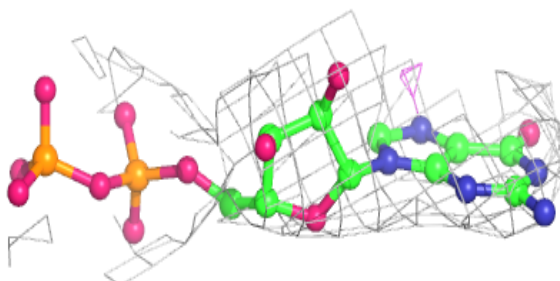
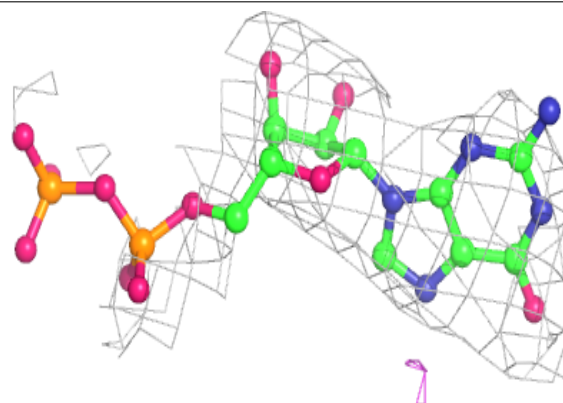


**Electron density around GDP L 501:**

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

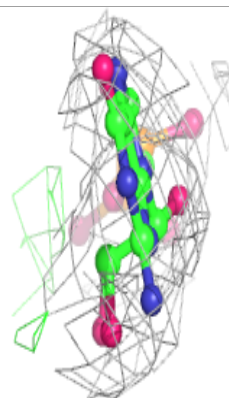
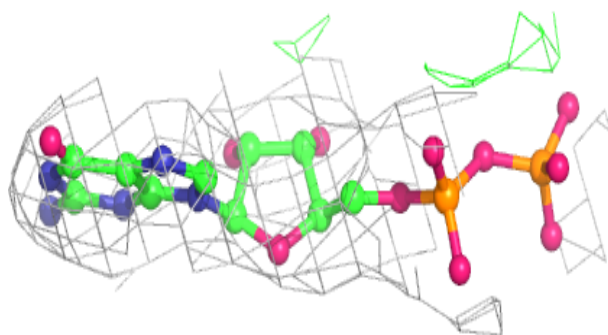
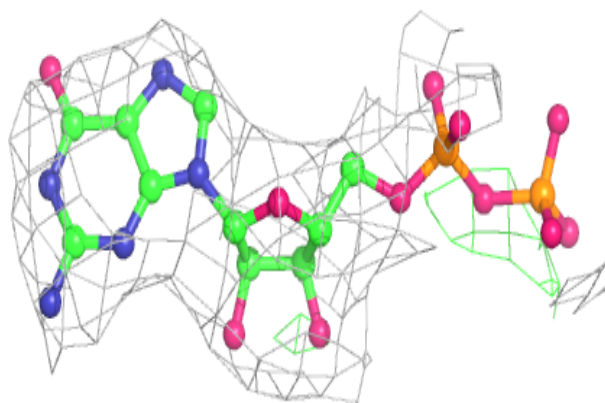
**Electron density around GDP J 501:**

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

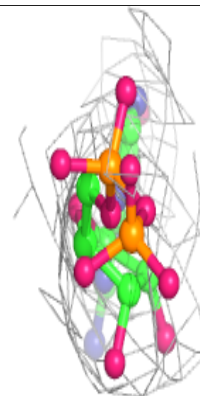
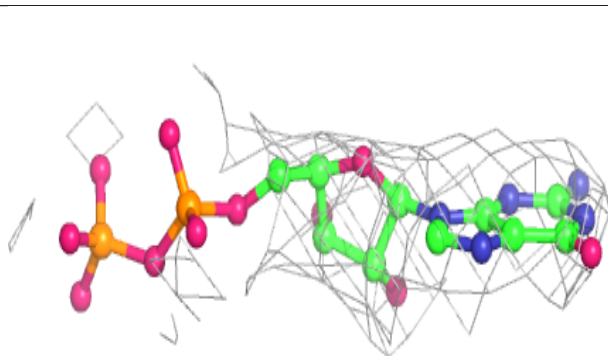
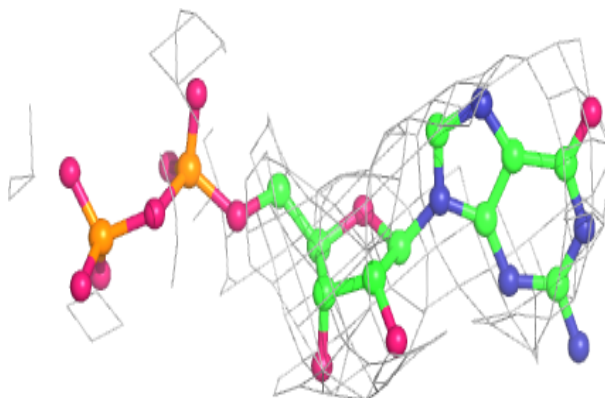


**Electron density around GDP E 501:**

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

**Electron density around GDP G 501:**

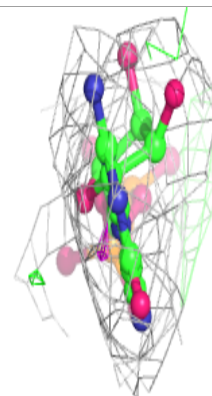
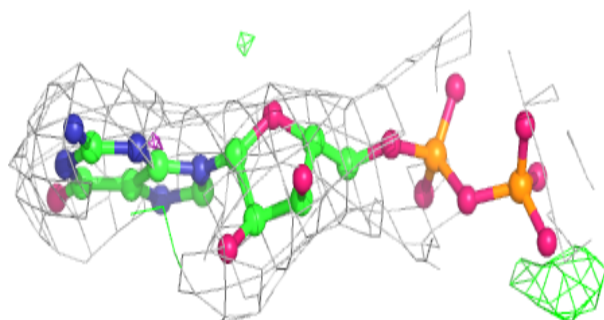
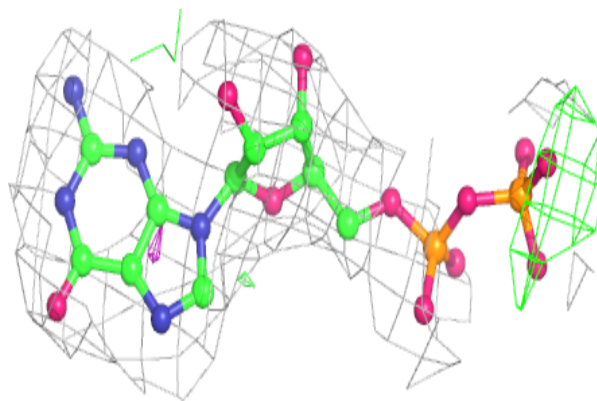
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



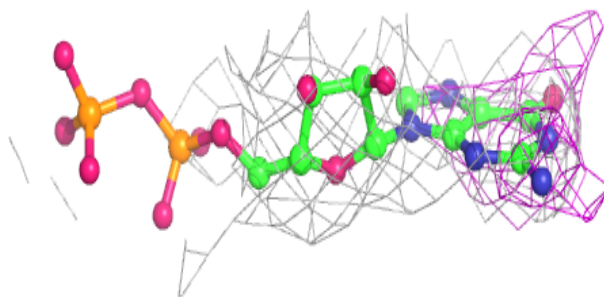
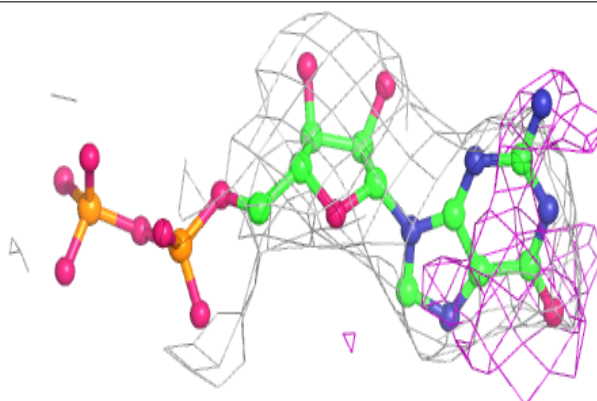


**Electron density around GDP F 501:**

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

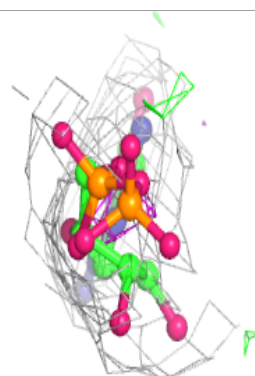
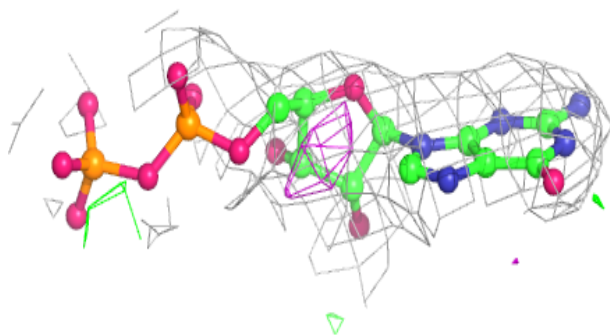
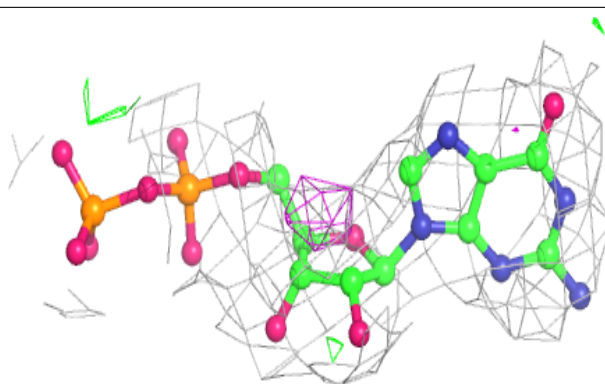
**Electron density around GDP I 501:**

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

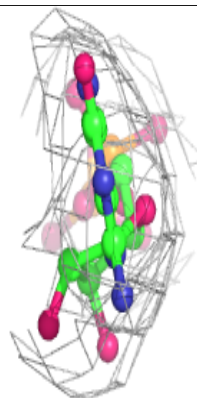
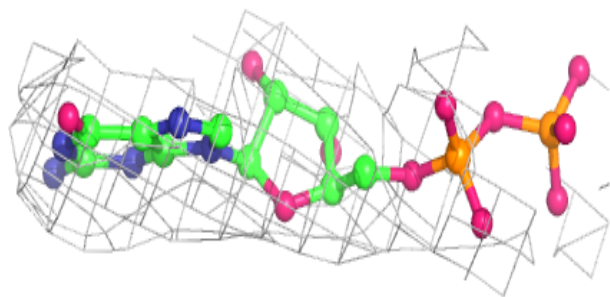
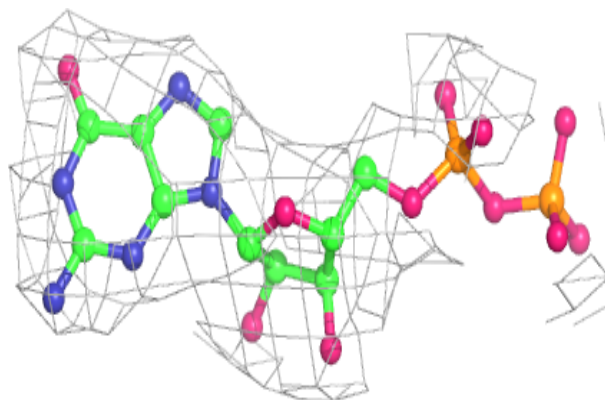


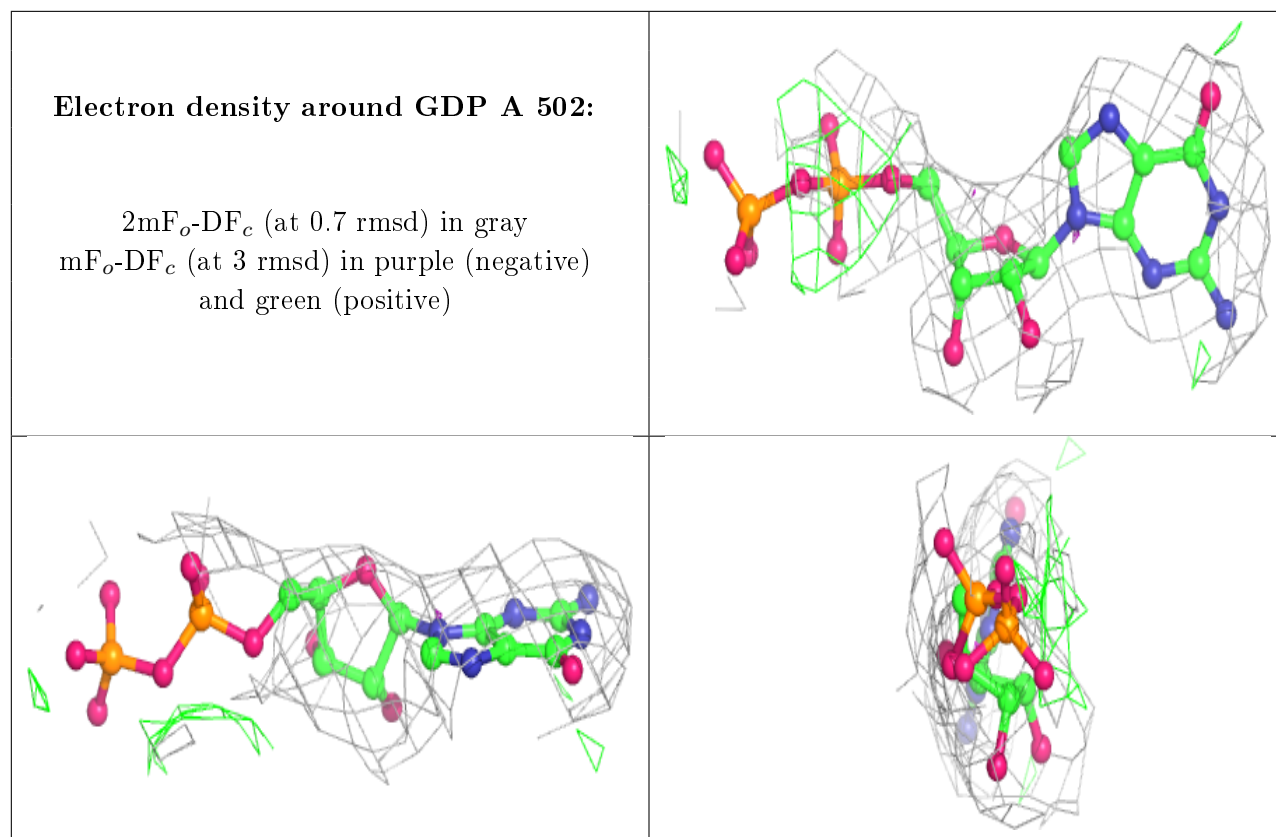
**Electron density around GDP C 501:**

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

**Electron density around GDP D 501:**

$2mF_o-DF_c$  (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.