



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:49 AM EDT

PDB ID : 2QAG / pdb\_00002qag  
Title : Crystal structure of human septin trimer 2/6/7  
Authors : Sirajuddin, M.  
Deposited on : 2007-06-15  
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

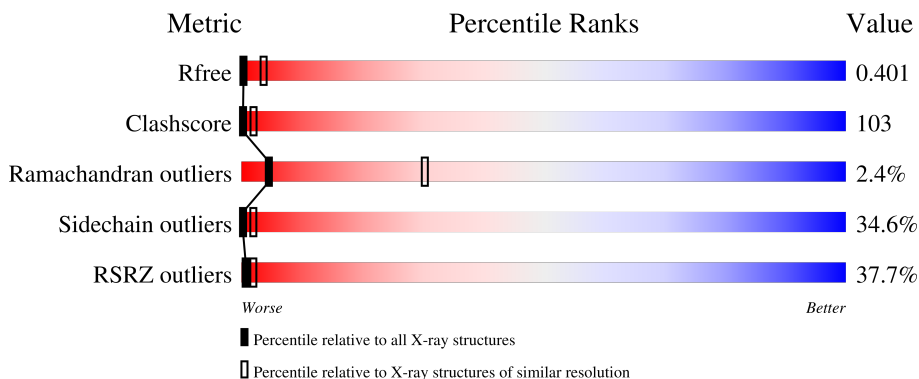
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	361	
2	B	427	
3	C	418	

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	GDP	A	362	-	-	X	-
4	GDP	C	419	-	-	X	-
5	GTP	B	428	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4495 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Septin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	232	1765	1129	302	328	6	0	0	0

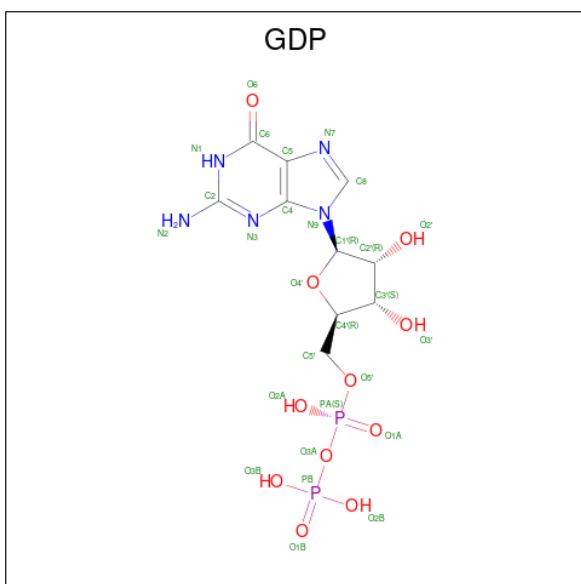
- Molecule 2 is a protein called Septin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	246	1369	837	254	269	9	0	0	0

- Molecule 3 is a protein called Septin-7.

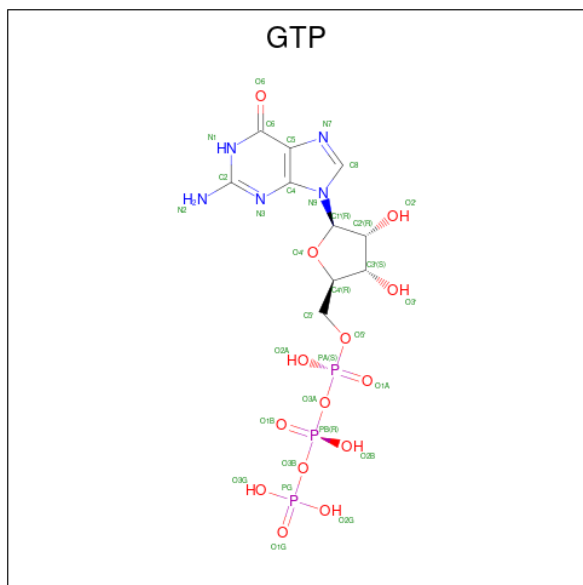
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	224	1273	788	230	247	8	0	0	0

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).

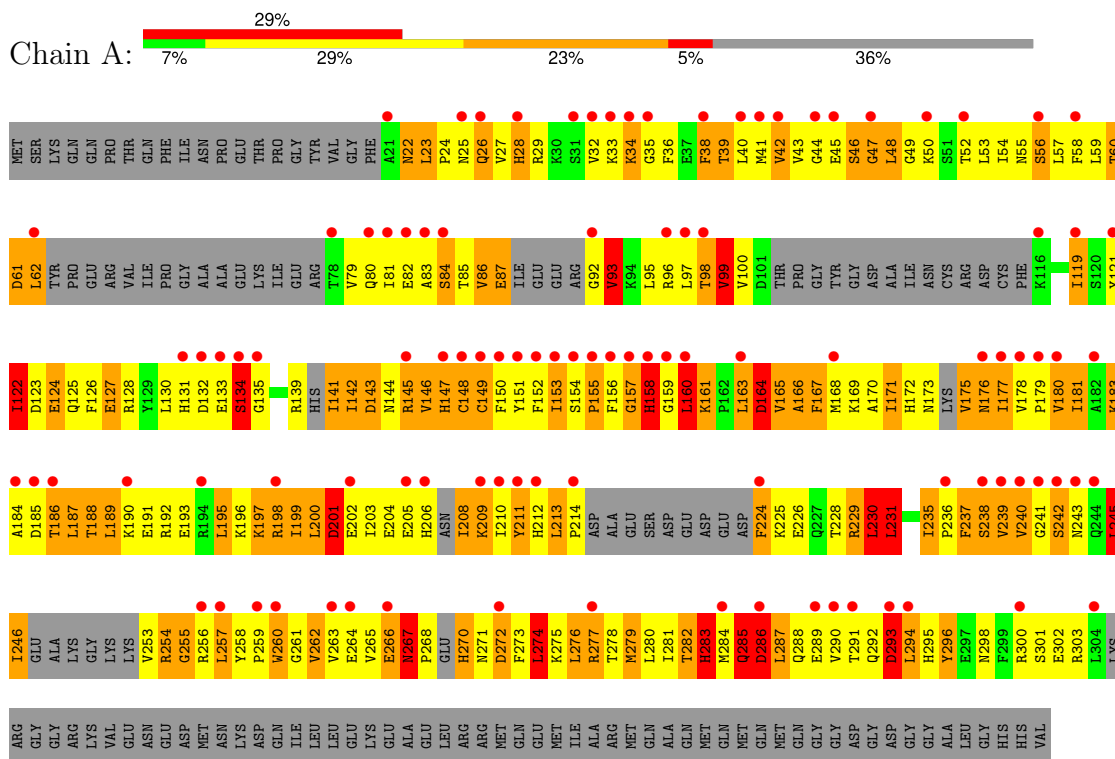


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	32	10	5	14	3	0	0

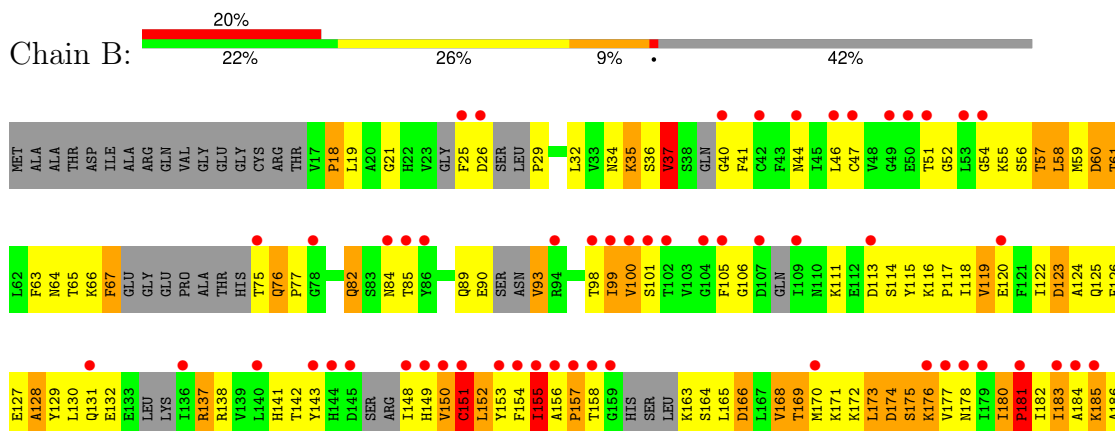
### 3 Residue-property plots i

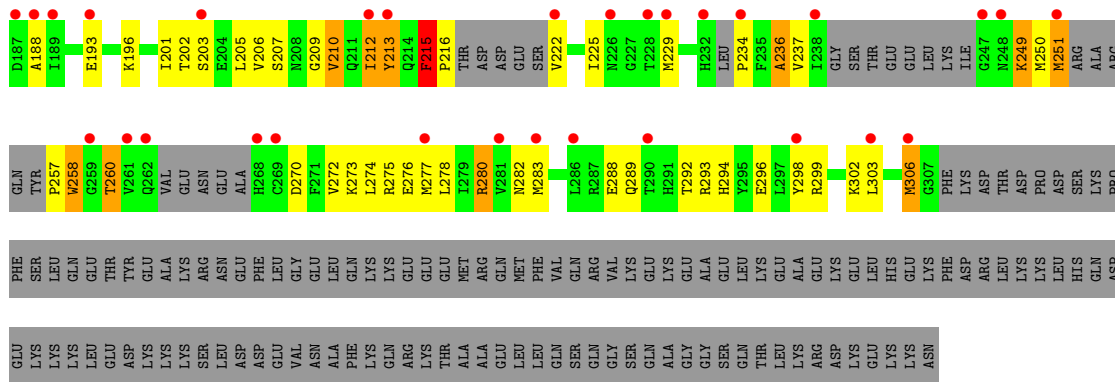
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Septin-2

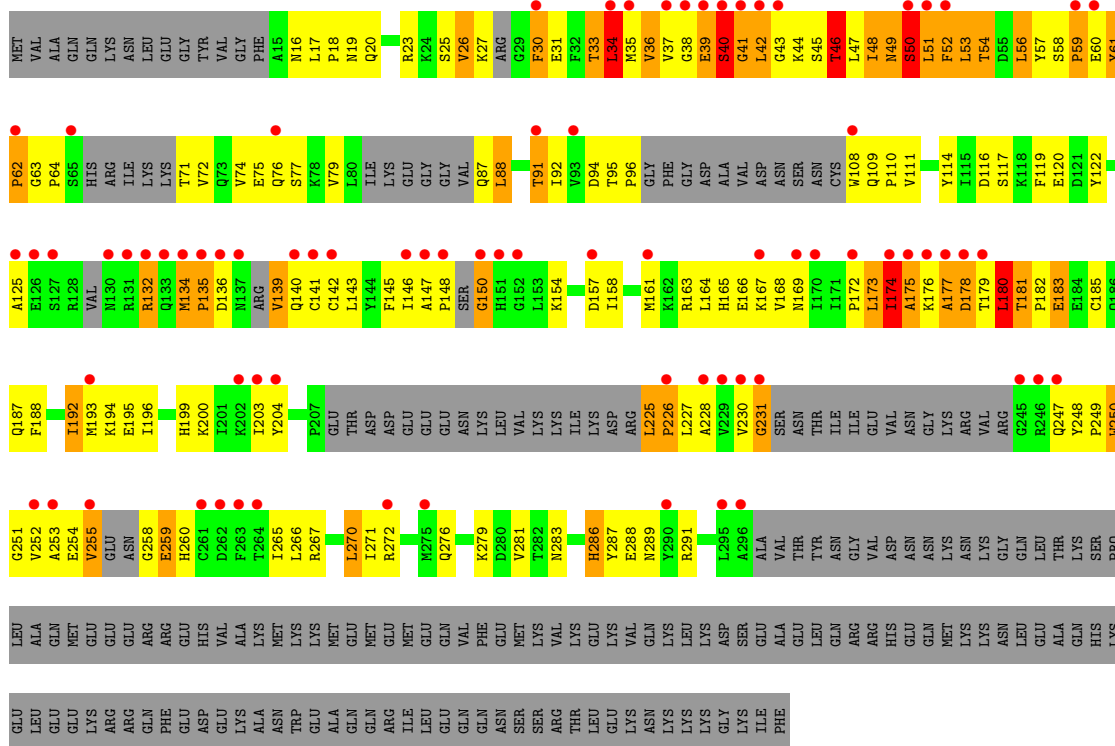


- Molecule 2: Septin-6





• Molecule 3: Septin-7



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	252.51Å 252.51Å 156.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 4.00 49.15 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.15-4.00) 98.2 (49.15-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.23	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.89 (at 4.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.376 , 0.392 0.399 , 0.401	Depositor DCC
$R_{free}$ test set	2125 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	96.4	Xtrriage
Anisotropy	1.176	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 999.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	4495	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.29% 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 i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.65	3/1789 (0.2%)	1.26	33/2421 (1.4%)
2	B	0.53	2/1367 (0.1%)	1.00	8/1865 (0.4%)
3	C	0.83	9/1281 (0.7%)	1.36	29/1762 (1.6%)
All	All	0.68	14/4437 (0.3%)	1.21	70/6048 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	44
2	B	0	49
3	C	0	39
All	All	0	132

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	VAL	CA-CB	-9.00	1.42	1.54
1	A	235	ILE	CA-CB	7.58	1.64	1.54
3	C	173	LEU	CA-C	7.40	1.63	1.53
3	C	230	VAL	CA-CB	-6.82	1.44	1.53
3	C	111	VAL	CA-C	6.72	1.62	1.52
3	C	230	VAL	N-CA	-6.66	1.37	1.47
3	C	172	PRO	CA-C	6.29	1.61	1.52
2	B	141	HIS	CA-C	5.92	1.62	1.53
2	B	201	ILE	CA-CB	-5.76	1.46	1.54
1	A	164	ASP	CA-C	5.53	1.59	1.52
3	C	231	GLY	N-CA	5.28	1.53	1.45
3	C	64	PRO	N-CA	5.16	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	62	PRO	CA-C	5.10	1.59	1.52
3	C	265	ILE	CA-CB	-5.07	1.48	1.54

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	LEU	N-CA-C	13.09	125.08	111.07
2	B	36	SER	N-CA-C	-12.42	99.80	112.97
1	A	86	VAL	CB-CA-C	-10.73	96.26	111.40
3	C	187	GLN	N-CA-C	9.65	121.57	111.14
3	C	50	SER	N-CA-C	9.25	125.36	112.04
3	C	183	GLU	N-CA-C	-9.04	101.43	111.28
3	C	46	THR	N-CA-C	8.64	120.32	111.07
3	C	230	VAL	N-CA-CB	-8.56	103.75	112.06
3	C	200	LYS	N-CA-C	8.35	122.76	111.24
1	A	161	LYS	CA-C-N	8.15	128.61	119.32
1	A	161	LYS	C-N-CA	8.15	128.61	119.32
2	B	213	TYR	N-CA-C	8.03	122.56	109.72
2	B	35	LYS	N-CA-C	7.85	119.47	111.07
3	C	199	HIS	N-CA-C	-7.77	103.79	113.20
1	A	199	ILE	N-CA-C	7.66	118.40	110.36
1	A	272	ASP	N-CA-C	-7.35	104.70	112.93
1	A	262	VAL	N-CA-C	7.25	120.68	108.86
3	C	194	LYS	N-CA-C	-7.24	103.39	111.28
3	C	48	ILE	N-CA-CB	-7.19	102.14	110.55
1	A	199	ILE	CB-CA-C	-7.13	102.76	111.88
3	C	291	ARG	N-CA-C	7.08	121.97	113.12
3	C	63	GLY	CA-C-N	6.76	128.29	119.84
3	C	63	GLY	C-N-CA	6.76	128.29	119.84
3	C	96	PRO	N-CA-CB	6.73	110.41	103.00
1	A	294	LEU	N-CA-C	-6.55	105.82	113.88
1	A	230	LEU	CB-CA-C	-6.47	100.72	110.88
1	A	99	VAL	CB-CA-C	6.33	119.91	110.98
1	A	201	ASP	N-CA-C	-6.33	104.47	111.36
1	A	240	VAL	CB-CA-C	-6.26	101.89	110.77
3	C	177	ALA	N-CA-C	-6.21	106.39	112.97
2	B	203	SER	N-CA-C	-6.20	103.83	111.33
3	C	265	ILE	N-CA-CB	-6.10	102.85	110.47
1	A	293	ASP	N-CA-C	6.10	118.84	111.40
1	A	155	PRO	CB-CA-C	-6.09	102.90	113.20
1	A	127	GLU	N-CA-C	6.08	117.91	111.28
3	C	175	ALA	N-CA-C	6.00	119.72	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	TYR	N-CA-C	-6.00	104.65	111.07
1	A	240	VAL	N-CA-CB	-5.88	104.00	111.64
1	A	42	VAL	N-CA-C	5.87	117.22	108.54
1	A	245	LEU	O-C-N	5.84	129.13	123.29
1	A	245	LEU	N-CA-C	5.83	117.00	108.14
3	C	281	VAL	N-CA-C	5.80	118.34	111.09
3	C	64	PRO	CA-C-N	5.73	132.01	121.70
3	C	64	PRO	C-N-CA	5.73	132.01	121.70
1	A	245	LEU	CA-C-N	5.63	131.84	121.70
1	A	245	LEU	C-N-CA	5.63	131.84	121.70
3	C	39	GLU	N-CA-C	-5.62	100.02	108.96
2	B	77	PRO	CB-CA-C	5.58	119.11	110.25
3	C	48	ILE	N-CA-C	5.54	115.73	110.42
1	A	84	SER	CB-CA-C	5.51	119.51	110.03
1	A	231	LEU	CB-CA-C	-5.49	100.12	110.67
1	A	240	VAL	N-CA-C	5.49	115.76	107.75
3	C	48	ILE	CB-CA-C	-5.48	104.96	111.97
1	A	122	ILE	CB-CA-C	-5.45	104.78	112.14
1	A	93	VAL	CB-CA-C	-5.43	104.25	111.80
1	A	274	LEU	CB-CA-C	-5.42	99.33	110.38
3	C	49	ASN	CB-CA-C	5.42	120.56	109.67
1	A	262	VAL	N-CA-CB	-5.41	101.92	111.93
3	C	39	GLU	CB-CA-C	5.40	119.25	110.22
3	C	36	VAL	CB-CA-C	5.39	118.61	110.63
3	C	62	PRO	N-CA-C	5.38	123.55	112.47
1	A	26	GLN	N-CA-C	-5.37	106.90	113.50
2	B	202	THR	N-CA-C	5.35	116.80	111.07
1	A	155	PRO	N-CA-C	5.34	122.44	113.78
3	C	250	TRP	N-CA-C	-5.28	105.65	112.68
3	C	46	THR	CB-CA-C	-5.23	102.67	110.88
2	B	202	THR	CB-CA-C	-5.19	102.73	110.88
3	C	174	ILE	CB-CA-C	-5.15	103.47	110.42
1	A	25	ASN	N-CA-C	5.12	117.53	111.33
2	B	215	PHE	N-CA-C	5.03	118.43	110.58

There are no chirality outliers.

All (132) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ARG	Peptide
1	A	133	GLU	Peptide
1	A	134	SER	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	A	142	ILE	Peptide
1	A	143	ASP	Peptide
1	A	147	HIS	Peptide
1	A	154	SER	Peptide
1	A	157	GLY	Peptide
1	A	160	LEU	Peptide
1	A	166	ALA	Peptide
1	A	171	ILE	Peptide
1	A	175	VAL	Peptide
1	A	177	ILE	Peptide
1	A	184	ALA	Peptide
1	A	185	ASP	Peptide
1	A	186	THR	Peptide
1	A	198	ARG	Peptide
1	A	209	LYS	Peptide
1	A	22	ASN	Peptide
1	A	238	SER	Peptide
1	A	241	GLY	Peptide
1	A	242	SER	Peptide
1	A	243	ASN	Peptide
1	A	256	ARG	Peptide
1	A	259	PRO	Peptide
1	A	260	TRP	Peptide
1	A	267	ASN	Peptide
1	A	281	ILE	Peptide
1	A	282	THR	Peptide
1	A	283	HIS	Peptide
1	A	285	GLN	Peptide
1	A	286	ASP	Peptide
1	A	287	LEU	Peptide
1	A	300	ARG	Peptide
1	A	301	SER	Peptide
1	A	303	ARG	Peptide
1	A	33	LYS	Peptide
1	A	35	GLY	Peptide
1	A	38	PHE	Peptide
1	A	46	SER	Peptide
1	A	47	GLY	Peptide
1	A	56	SER	Peptide
1	A	60	THR	Peptide
1	A	99	VAL	Peptide
2	B	100	VAL	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
2	B	105	PHE	Peptide
2	B	106	GLY	Peptide
2	B	111	LYS	Peptide
2	B	119	VAL	Peptide
2	B	122	ILE	Peptide
2	B	123	ASP	Peptide
2	B	127	GLU	Peptide
2	B	128	ALA	Peptide
2	B	130	LEU	Peptide
2	B	131	GLN	Peptide
2	B	132	GLU	Peptide
2	B	137	ARG	Peptide
2	B	142	THR	Peptide
2	B	143	TYR	Peptide
2	B	148	ILE	Peptide
2	B	150	VAL	Peptide
2	B	151	CYS	Peptide
2	B	155	ILE	Peptide
2	B	156	ALA	Peptide
2	B	157	PRO	Peptide
2	B	163	LYS	Peptide
2	B	175	SER	Peptide
2	B	176	LYS	Peptide
2	B	18	PRO	Peptide
2	B	180	ILE	Peptide
2	B	181	PRO	Peptide
2	B	183	ILE	Peptide
2	B	207	SER	Peptide
2	B	21	GLY	Peptide
2	B	212	ILE	Peptide
2	B	215	PHE	Peptide
2	B	222	VAL	Peptide
2	B	234	PRO	Peptide
2	B	236	ALA	Peptide
2	B	249	LYS	Peptide
2	B	258	TRP	Peptide
2	B	260	THR	Peptide
2	B	280	ARG	Peptide
2	B	282	ASN	Peptide
2	B	34	ASN	Peptide
2	B	37	VAL	Peptide
2	B	40	GLY	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
2	B	51	THR	Peptide
2	B	76	GLN	Peptide
2	B	82	GLN	Peptide
2	B	89	GLN	Peptide
2	B	93	VAL	Peptide
2	B	99	ILE	Peptide
3	C	117	SER	Peptide
3	C	132	ARG	Peptide
3	C	139	VAL	Peptide
3	C	142	CYS	Peptide
3	C	145	PHE	Peptide
3	C	146	ILE	Peptide
3	C	150	GLY	Peptide
3	C	16	ASN	Peptide
3	C	166	GLU	Peptide
3	C	167	LYS	Peptide
3	C	17	LEU	Peptide
3	C	177	ALA	Peptide
3	C	180	LEU	Peptide
3	C	19	ASN	Peptide
3	C	20	GLN	Peptide
3	C	203	ILE	Peptide
3	C	204	TYR	Peptide
3	C	225	LEU	Peptide
3	C	228	ALA	Peptide
3	C	253	ALA	Peptide
3	C	254	GLU	Peptide
3	C	259	GLU	Peptide
3	C	26	VAL	Peptide
3	C	270	LEU	Peptide
3	C	272	ARG	Peptide
3	C	286	HIS	Peptide
3	C	288	GLU	Peptide
3	C	30	PHE	Peptide
3	C	31	GLU	Peptide
3	C	33	THR	Peptide
3	C	34	LEU	Peptide
3	C	40	SER	Peptide
3	C	41	GLY	Peptide
3	C	42	LEU	Peptide
3	C	74	VAL	Peptide
3	C	75	GLU	Peptide

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Mol	Chain	Res	Type	Group
3	C	76	GLN	Peptide
3	C	88	LEU	Peptide
3	C	91	THR	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1765	0	1694	490	0
2	B	1369	0	854	186	0
3	C	1273	0	822	156	0
4	A	28	0	12	14	0
4	C	28	0	12	16	0
5	B	32	0	12	18	0
All	All	4495	0	3406	812	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 103.

All (812) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:VAL:HG12	1:A:266:GLU:CG	1.46	1.43
1:A:183:LYS:HD2	4:A:362:GDP:C5	1.67	1.29
1:A:279:MET:O	1:A:282:THR:HG22	1.34	1.26
1:A:22:ASN:C	1:A:24:PRO:HD2	1.62	1.25
2:B:54:GLY:CA	2:B:57:THR:HG23	1.70	1.22
1:A:183:LYS:HD2	4:A:362:GDP:C4	1.73	1.21
1:A:265:VAL:CG1	1:A:266:GLU:HG2	1.69	1.21
1:A:258:TYR:HB3	1:A:260:TRP:O	1.35	1.19
1:A:282:THR:HG23	1:A:283:HIS:CD2	1.78	1.18
1:A:173:ASN:CA	1:A:294:LEU:HD22	1.73	1.18
2:B:257:PRO:HB2	2:B:258:TRP:CD1	1.79	1.17
3:C:148:PRO:HG2	3:C:150:GLY:CA	1.73	1.17
1:A:245:LEU:C	1:A:246:ILE:HD13	1.67	1.17
1:A:175:VAL:HG12	1:A:176:ASN:HB2	1.17	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:THR:HG23	1:A:283:HIS:H	1.05	1.16
1:A:267:ASN:HB3	1:A:270:HIS:CB	1.77	1.15
2:B:166:ASP:O	2:B:169:THR:HG22	1.47	1.15
3:C:43:GLY:HA2	3:C:46:THR:HG22	1.15	1.15
1:A:208:ILE:HD13	1:A:209:LYS:H	1.10	1.14
2:B:185:LYS:HG3	5:B:428:GTP:C6	1.81	1.14
1:A:173:ASN:HA	1:A:294:LEU:CD2	1.78	1.14
1:A:208:ILE:CD1	1:A:209:LYS:H	1.60	1.13
1:A:224:PHE:C	1:A:224:PHE:CD2	2.27	1.11
2:B:57:THR:HG22	5:B:428:GTP:O1A	1.48	1.11
1:A:139:ARG:H	1:A:141:ILE:HG23	0.96	1.11
2:B:116:LYS:N	2:B:117:PRO:HD2	1.57	1.11
2:B:185:LYS:HE3	5:B:428:GTP:C4	1.85	1.11
3:C:43:GLY:HA2	3:C:46:THR:CG2	1.79	1.10
3:C:45:SER:HA	3:C:48:ILE:HD12	1.21	1.10
1:A:173:ASN:HA	1:A:294:LEU:HD22	1.22	1.10
1:A:179:PRO:HG3	1:A:210:ILE:HD13	1.10	1.09
1:A:275:LYS:O	1:A:279:MET:HB3	1.53	1.08
1:A:23:LEU:N	1:A:24:PRO:HD2	1.67	1.08
1:A:211:TYR:OH	1:A:214:PRO:HD2	1.54	1.08
3:C:42:LEU:HA	4:C:419:GDP:H5''	1.16	1.08
3:C:43:GLY:O	3:C:46:THR:HG23	1.53	1.07
1:A:130:LEU:HB2	1:A:295:HIS:HE1	1.19	1.07
1:A:239:VAL:HG12	1:A:273:PHE:HA	1.24	1.07
3:C:46:THR:O	3:C:50:SER:HB2	1.55	1.06
1:A:122:ILE:HD12	1:A:126:PHE:HE1	1.20	1.06
1:A:179:PRO:CG	1:A:210:ILE:HD13	1.84	1.06
3:C:43:GLY:CA	3:C:46:THR:CG2	2.33	1.06
1:A:143:ASP:OD2	1:A:145:ARG:HD3	1.53	1.05
3:C:148:PRO:HG2	3:C:150:GLY:HA3	1.07	1.05
1:A:283:HIS:HB3	1:A:285:GLN:HE21	1.15	1.05
1:A:282:THR:HG23	1:A:283:HIS:HD2	0.88	1.04
3:C:34:LEU:HD13	3:C:34:LEU:O	1.53	1.04
1:A:79:VAL:HG23	1:A:99:VAL:O	1.57	1.04
1:A:83:ALA:HA	1:A:95:LEU:O	1.57	1.04
2:B:116:LYS:H	2:B:117:PRO:HD2	1.15	1.04
2:B:185:LYS:HA	5:B:428:GTP:O6	1.56	1.03
2:B:54:GLY:CA	2:B:57:THR:CG2	2.36	1.03
1:A:265:VAL:CG1	1:A:266:GLU:CG	2.30	1.03
2:B:46:LEU:O	2:B:151:CYS:HA	1.58	1.03
1:A:282:THR:CG2	1:A:283:HIS:HD2	1.71	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:HB3	1:A:270:HIS:HB3	1.38	1.02
2:B:153:TYR:HB3	2:B:170:MET:HE3	1.40	1.02
1:A:213:LEU:HD23	1:A:213:LEU:O	1.59	1.02
2:B:64:ASN:O	2:B:65:THR:HG23	1.59	1.02
1:A:54:ILE:HG13	1:A:58:PHE:CE2	1.95	1.02
1:A:55:ASN:HA	1:A:60:THR:O	1.61	1.01
1:A:201:ASP:O	1:A:204:GLU:HB2	1.59	1.01
1:A:125:GLN:OE1	1:A:144:ASN:HB2	1.61	1.00
2:B:54:GLY:HA2	2:B:57:THR:CG2	1.92	1.00
2:B:113:ASP:O	2:B:117:PRO:HG3	1.62	1.00
2:B:155:ILE:HD13	2:B:155:ILE:N	1.75	1.00
1:A:156:PHE:HE1	1:A:186:THR:HB	1.26	0.99
1:A:175:VAL:HG12	1:A:176:ASN:CB	1.92	0.99
1:A:239:VAL:CG1	1:A:273:PHE:HA	1.93	0.98
3:C:42:LEU:CA	4:C:419:GDP:H5 <sup>7</sup>	1.93	0.98
3:C:179:THR:HG23	3:C:180:LEU:CD2	1.93	0.98
1:A:175:VAL:CG1	1:A:176:ASN:HB2	1.92	0.98
1:A:258:TYR:HB2	1:A:261:GLY:O	1.63	0.98
1:A:284:MET:O	1:A:287:LEU:HG	1.63	0.98
1:A:179:PRO:HG3	1:A:210:ILE:CD1	1.94	0.98
1:A:267:ASN:OD1	1:A:270:HIS:HB2	1.64	0.97
2:B:249:LYS:CB	2:B:250:MET:HA	1.93	0.97
1:A:156:PHE:CE1	1:A:186:THR:CG2	2.47	0.97
1:A:82:GLU:HG2	1:A:97:LEU:O	1.63	0.97
1:A:57:LEU:HD21	1:A:276:LEU:HD21	1.47	0.97
3:C:148:PRO:CG	3:C:150:GLY:HA3	1.93	0.97
1:A:285:GLN:HA	1:A:287:LEU:HB2	1.46	0.97
1:A:196:LYS:O	1:A:200:LEU:HD12	1.65	0.97
1:A:153:ILE:HG21	1:A:160:LEU:HG	1.45	0.96
1:A:173:ASN:C	1:A:175:VAL:N	2.23	0.96
1:A:282:THR:HG23	1:A:283:HIS:N	1.80	0.96
2:B:249:LYS:CB	2:B:250:MET:SD	2.54	0.96
3:C:42:LEU:HA	4:C:419:GDP:C5 <sup>7</sup>	1.93	0.96
1:A:151:TYR:HD2	1:A:152:PHE:N	1.64	0.95
1:A:139:ARG:N	1:A:141:ILE:HG23	1.82	0.95
3:C:77:SER:HA	3:C:88:LEU:O	1.66	0.95
1:A:173:ASN:C	1:A:294:LEU:HD22	1.91	0.95
1:A:23:LEU:N	1:A:24:PRO:CD	2.30	0.95
1:A:271:ASN:ND2	1:A:273:PHE:HB2	1.82	0.94
2:B:58:LEU:O	2:B:61:THR:HG22	1.67	0.94
3:C:43:GLY:CA	3:C:46:THR:HG22	1.95	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:O	1:A:147:HIS:HB2	1.66	0.94
1:A:177:ILE:HB	1:A:210:ILE:HG22	1.48	0.94
1:A:265:VAL:HG12	1:A:266:GLU:HG3	1.45	0.94
1:A:208:ILE:HD13	1:A:209:LYS:N	1.82	0.93
1:A:29:ARG:O	1:A:32:VAL:HB	1.65	0.93
2:B:54:GLY:HA3	2:B:57:THR:HG23	1.50	0.93
1:A:283:HIS:CD2	1:A:283:HIS:H	1.84	0.93
1:A:268:PRO:HD3	1:A:271:ASN:O	1.69	0.93
2:B:206:VAL:HA	2:B:209:GLY:HA2	1.48	0.93
1:A:237:PHE:H	1:A:237:PHE:HD2	0.99	0.92
1:A:257:LEU:C	1:A:257:LEU:HD23	1.94	0.92
1:A:237:PHE:N	1:A:237:PHE:CD2	2.36	0.92
1:A:265:VAL:HG12	1:A:266:GLU:HG2	0.92	0.92
2:B:114:SER:O	2:B:117:PRO:HG2	1.70	0.91
1:A:130:LEU:HB2	1:A:295:HIS:CE1	2.04	0.91
3:C:182:PRO:HA	3:C:185:CYS:CB	2.00	0.91
1:A:156:PHE:CE1	1:A:186:THR:HG21	2.05	0.91
3:C:286:HIS:HA	3:C:289:ASN:CB	2.00	0.91
1:A:224:PHE:C	1:A:224:PHE:HD2	1.73	0.91
3:C:33:THR:HB	3:C:139:VAL:O	1.70	0.91
1:A:160:LEU:HD12	1:A:199:ILE:HG12	1.52	0.91
2:B:155:ILE:HD13	2:B:155:ILE:H	1.31	0.90
1:A:39:THR:HB	1:A:96:ARG:O	1.71	0.90
3:C:49:ASN:HB3	3:C:54:THR:O	1.69	0.90
1:A:267:ASN:HB3	1:A:270:HIS:HB2	1.49	0.90
3:C:58:SER:N	3:C:59:PRO:HD3	1.87	0.90
3:C:40:SER:HA	3:C:44:LYS:NZ	1.87	0.90
1:A:175:VAL:HG12	1:A:176:ASN:N	1.85	0.90
1:A:39:THR:HA	1:A:96:ARG:O	1.72	0.90
1:A:240:VAL:HG22	4:A:362:GDP:O6	1.71	0.90
1:A:224:PHE:HD2	1:A:224:PHE:O	1.54	0.89
1:A:156:PHE:HE1	1:A:186:THR:CB	1.84	0.89
1:A:57:LEU:CD2	1:A:276:LEU:HD21	2.03	0.89
1:A:81:ILE:HD12	1:A:81:ILE:O	1.72	0.89
1:A:183:LYS:CD	4:A:362:GDP:C5	2.54	0.89
1:A:43:VAL:HG22	1:A:100:VAL:HG21	1.51	0.88
1:A:212:HIS:O	1:A:214:PRO:HD3	1.73	0.88
1:A:285:GLN:HB2	1:A:288:GLN:HG3	1.54	0.88
3:C:36:VAL:HA	3:C:143:LEU:O	1.73	0.88
1:A:36:PHE:O	1:A:93:VAL:HG22	1.75	0.87
2:B:169:THR:O	2:B:173:LEU:HB2	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLN:CB	1:A:288:GLN:HG3	2.04	0.87
1:A:179:PRO:CG	1:A:210:ILE:CD1	2.52	0.86
1:A:199:ILE:O	1:A:203:ILE:HD12	1.75	0.86
1:A:267:ASN:CB	1:A:270:HIS:CB	2.54	0.86
1:A:153:ILE:HD13	1:A:153:ILE:H	1.41	0.86
1:A:82:GLU:CG	1:A:97:LEU:O	2.23	0.85
3:C:49:ASN:OD1	3:C:56:LEU:HG	1.76	0.85
1:A:267:ASN:CB	1:A:270:HIS:HB2	2.06	0.85
2:B:60:ASP:HB3	2:B:65:THR:O	1.75	0.84
2:B:116:LYS:N	2:B:117:PRO:CD	2.39	0.84
3:C:179:THR:HG23	3:C:180:LEU:HD23	1.59	0.84
2:B:153:TYR:CE2	2:B:166:ASP:HB3	2.12	0.84
1:A:122:ILE:HD12	1:A:126:PHE:CE1	2.11	0.84
1:A:177:ILE:HB	1:A:210:ILE:CG2	2.07	0.83
2:B:54:GLY:HA3	2:B:57:THR:CG2	2.05	0.83
3:C:58:SER:N	3:C:59:PRO:CD	2.41	0.83
1:A:282:THR:CG2	1:A:283:HIS:H	1.90	0.83
1:A:199:ILE:O	1:A:203:ILE:CD1	2.27	0.83
1:A:283:HIS:H	1:A:283:HIS:HD2	1.26	0.82
1:A:211:TYR:CZ	1:A:214:PRO:HD2	2.15	0.82
1:A:267:ASN:CG	1:A:270:HIS:HB2	2.05	0.82
3:C:43:GLY:C	3:C:46:THR:HG23	2.03	0.82
2:B:294:HIS:O	2:B:298:TYR:CB	2.27	0.81
3:C:41:GLY:O	4:C:419:GDP:H5''	1.80	0.81
1:A:240:VAL:HG13	4:A:362:GDP:C6	2.14	0.81
1:A:143:ASP:OD2	1:A:145:ARG:HB2	1.81	0.81
3:C:34:LEU:C	3:C:34:LEU:HD22	2.06	0.81
3:C:43:GLY:C	3:C:46:THR:CG2	2.54	0.81
2:B:153:TYR:CB	2:B:170:MET:HE3	2.11	0.80
3:C:179:THR:HG23	3:C:180:LEU:HD22	1.60	0.80
1:A:211:TYR:CD2	1:A:211:TYR:O	2.33	0.80
1:A:283:HIS:HB3	1:A:285:GLN:NE2	1.94	0.80
1:A:285:GLN:HB2	1:A:288:GLN:CG	2.11	0.80
1:A:268:PRO:CD	1:A:271:ASN:O	2.29	0.80
1:A:55:ASN:CA	1:A:60:THR:O	2.29	0.80
3:C:40:SER:HA	3:C:44:LYS:HZ3	1.45	0.80
2:B:166:ASP:HA	2:B:169:THR:CG2	2.12	0.80
2:B:276:GLU:O	2:B:280:ARG:CB	2.30	0.80
1:A:54:ILE:CG1	1:A:58:PHE:CE2	2.64	0.79
1:A:240:VAL:HG13	4:A:362:GDP:O6	1.82	0.79
3:C:188:PHE:O	3:C:192:ILE:CG1	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:O	1:A:32:VAL:CB	2.30	0.79
2:B:44:ASN:O	2:B:149:HIS:HB2	1.83	0.79
3:C:173:LEU:CB	3:C:227:LEU:O	2.31	0.79
1:A:285:GLN:C	1:A:288:GLN:H	1.91	0.79
2:B:115:TYR:O	2:B:118:ILE:CB	2.31	0.79
3:C:258:GLY:C	3:C:260:HIS:CB	2.56	0.79
1:A:151:TYR:CD2	1:A:152:PHE:N	2.50	0.79
3:C:248:TYR:HB2	3:C:251:GLY:O	1.81	0.79
2:B:171:LYS:O	2:B:174:ASP:HB3	1.80	0.79
1:A:175:VAL:HA	1:A:294:LEU:HD13	1.62	0.79
1:A:258:TYR:CB	1:A:261:GLY:O	2.30	0.79
3:C:188:PHE:O	3:C:192:ILE:HG12	1.82	0.79
3:C:179:THR:CG2	3:C:180:LEU:HD23	2.13	0.78
1:A:143:ASP:CG	1:A:145:ARG:HD3	2.08	0.78
1:A:283:HIS:CB	1:A:285:GLN:HE21	1.95	0.78
1:A:122:ILE:CD1	1:A:126:PHE:HE1	1.96	0.77
2:B:182:ILE:HD12	2:B:183:ILE:H	1.47	0.77
1:A:153:ILE:HG22	1:A:164:ASP:OD2	1.84	0.77
2:B:153:TYR:CZ	2:B:169:THR:HG21	2.18	0.77
2:B:64:ASN:O	2:B:65:THR:CG2	2.32	0.77
2:B:250:MET:O	2:B:251:MET:HG3	1.84	0.77
3:C:41:GLY:O	4:C:419:GDP:C5'	2.32	0.77
2:B:168:VAL:O	2:B:172:LYS:HB2	1.85	0.77
1:A:125:GLN:HB3	1:A:144:ASN:O	1.84	0.77
2:B:166:ASP:C	2:B:169:THR:HG22	2.09	0.77
3:C:122:TYR:O	3:C:125:ALA:HB3	1.85	0.77
1:A:279:MET:HG3	1:A:280:LEU:N	1.98	0.77
1:A:151:TYR:HE1	1:A:167:PHE:HB3	1.48	0.76
1:A:258:TYR:CB	1:A:260:TRP:O	2.26	0.76
2:B:185:LYS:HG3	5:B:428:GTP:N1	2.00	0.76
1:A:274:LEU:HD22	1:A:278:THR:OG1	1.86	0.76
3:C:77:SER:CA	3:C:88:LEU:O	2.34	0.76
2:B:54:GLY:HA2	2:B:57:THR:HG23	1.52	0.76
1:A:55:ASN:CG	1:A:61:ASP:HA	2.11	0.76
2:B:153:TYR:CZ	2:B:166:ASP:HB3	2.22	0.75
2:B:153:TYR:OH	2:B:166:ASP:HB3	1.86	0.75
2:B:153:TYR:CE2	2:B:155:ILE:HG23	2.21	0.75
1:A:141:ILE:HD12	1:A:142:ILE:N	2.02	0.75
1:A:177:ILE:CB	1:A:210:ILE:HG22	2.16	0.75
1:A:257:LEU:C	1:A:257:LEU:CD2	2.59	0.75
1:A:36:PHE:O	1:A:93:VAL:CG2	2.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:TYR:O	1:A:211:TYR:HD2	1.70	0.74
1:A:181:ILE:HD11	1:A:236:PRO:HG2	1.69	0.74
1:A:282:THR:CG2	1:A:283:HIS:CD2	2.57	0.74
1:A:172:HIS:HD2	1:A:209:LYS:HB2	1.52	0.74
1:A:211:TYR:CE2	1:A:213:LEU:HA	2.22	0.74
3:C:109:GLN:N	3:C:110:PRO:CD	2.49	0.74
1:A:79:VAL:CG2	1:A:99:VAL:O	2.34	0.74
1:A:153:ILE:HD13	1:A:153:ILE:N	2.02	0.74
1:A:177:ILE:HG22	1:A:179:PRO:N	2.03	0.74
1:A:156:PHE:HE1	1:A:186:THR:CG2	1.94	0.74
1:A:258:TYR:CD2	1:A:260:TRP:CE3	2.76	0.74
3:C:148:PRO:HG2	3:C:150:GLY:N	2.03	0.74
1:A:146:VAL:O	1:A:175:VAL:HG11	1.88	0.74
1:A:224:PHE:CD2	1:A:225:LYS:N	2.55	0.74
1:A:156:PHE:CE1	1:A:186:THR:HB	2.17	0.73
1:A:47:GLY:HA2	2:B:158:THR:HG21	1.70	0.73
1:A:99:VAL:HG12	1:A:100:VAL:O	1.88	0.73
2:B:257:PRO:HB2	2:B:258:TRP:HD1	1.47	0.73
1:A:155:PRO:O	1:A:187:LEU:HD21	1.88	0.73
1:A:183:LYS:CD	4:A:362:GDP:C4	2.65	0.73
1:A:246:ILE:HD13	1:A:246:ILE:N	2.04	0.73
2:B:66:LYS:C	2:B:67:PHE:HD1	1.96	0.73
1:A:211:TYR:CD2	1:A:211:TYR:C	2.67	0.72
1:A:282:THR:CG2	1:A:283:HIS:N	2.48	0.72
1:A:292:GLN:O	1:A:296:TYR:CB	2.38	0.72
3:C:255:VAL:HA	3:C:258:GLY:HA2	1.72	0.72
1:A:49:GLY:CA	1:A:52:THR:HG22	2.19	0.72
1:A:271:ASN:HD21	1:A:273:PHE:HB2	1.52	0.72
3:C:109:GLN:N	3:C:110:PRO:HD2	2.05	0.72
1:A:39:THR:CB	1:A:96:ARG:O	2.38	0.72
1:A:39:THR:CA	1:A:96:ARG:O	2.38	0.71
1:A:173:ASN:CA	1:A:294:LEU:CD2	2.50	0.71
1:A:34:LYS:HD2	1:A:34:LYS:O	1.90	0.71
1:A:132:ASP:O	1:A:135:GLY:N	2.24	0.71
1:A:208:ILE:CD1	1:A:209:LYS:N	2.44	0.71
1:A:121:TYR:O	1:A:125:GLN:HG2	1.89	0.71
2:B:292:THR:O	2:B:296:GLU:CB	2.39	0.71
1:A:156:PHE:CZ	2:B:185:LYS:HB3	2.26	0.70
1:A:61:ASP:C	1:A:62:LEU:HD23	2.16	0.70
1:A:164:ASP:OD1	1:A:164:ASP:N	2.16	0.70
3:C:44:LYS:O	3:C:48:ILE:HG13	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:ILE:N	3:C:174:ILE:HD12	2.05	0.70
3:C:181:THR:O	3:C:185:CYS:N	2.23	0.70
1:A:139:ARG:H	1:A:141:ILE:CG2	1.90	0.70
1:A:172:HIS:CD2	1:A:209:LYS:HB2	2.26	0.70
1:A:288:GLN:O	1:A:291:THR:HG22	1.92	0.70
2:B:153:TYR:CE1	2:B:169:THR:HG21	2.27	0.70
1:A:57:LEU:HD11	1:A:277:ARG:HA	1.74	0.70
1:A:279:MET:O	1:A:282:THR:CG2	2.27	0.70
1:A:239:VAL:HG12	1:A:273:PHE:CA	2.12	0.69
1:A:263:VAL:HG13	2:B:257:PRO:HG3	1.74	0.69
3:C:38:GLY:HA3	3:C:44:LYS:CE	2.23	0.69
2:B:155:ILE:N	2:B:155:ILE:CD1	2.49	0.69
3:C:45:SER:HA	3:C:48:ILE:CD1	2.12	0.69
1:A:198:ARG:O	1:A:202:GLU:HG2	1.92	0.69
2:B:185:LYS:CE	5:B:428:GTP:C4	2.73	0.69
1:A:151:TYR:HE1	1:A:167:PHE:CB	2.05	0.69
1:A:149:CYS:N	1:A:176:ASN:O	2.20	0.69
1:A:237:PHE:HB2	1:A:272:ASP:HB3	1.74	0.69
1:A:201:ASP:O	1:A:204:GLU:CB	2.40	0.69
2:B:119:VAL:O	2:B:123:ASP:N	2.21	0.69
1:A:208:ILE:HD12	1:A:209:LYS:H	1.57	0.68
2:B:57:THR:CG2	5:B:428:GTP:O1A	2.37	0.68
2:B:185:LYS:HD2	5:B:428:GTP:C5	2.29	0.68
2:B:250:MET:C	2:B:251:MET:HG3	2.18	0.68
2:B:251:MET:SD	2:B:251:MET:N	2.65	0.68
1:A:151:TYR:HD2	1:A:152:PHE:H	1.40	0.68
1:A:156:PHE:HZ	2:B:188:ALA:HB2	1.58	0.68
2:B:250:MET:C	2:B:251:MET:CG	2.66	0.68
1:A:264:GLU:H	1:A:270:HIS:CE1	2.12	0.68
1:A:22:ASN:C	1:A:24:PRO:CD	2.54	0.68
2:B:176:LYS:CB	2:B:177:VAL:O	2.42	0.68
1:A:139:ARG:C	1:A:141:ILE:N	2.52	0.68
2:B:171:LYS:HA	2:B:174:ASP:HB3	1.76	0.68
1:A:201:ASP:O	1:A:204:GLU:N	2.26	0.68
1:A:257:LEU:HD23	1:A:258:TYR:N	2.08	0.68
1:A:274:LEU:HD23	1:A:277:ARG:HG2	1.74	0.68
1:A:242:SER:OG	1:A:254:ARG:HB3	1.93	0.68
2:B:174:ASP:HB2	2:B:210:VAL:HG12	1.76	0.68
3:C:47:LEU:O	3:C:51:LEU:CB	2.41	0.68
1:A:81:ILE:HD12	1:A:81:ILE:C	2.19	0.67
3:C:283:ASN:O	3:C:287:TYR:CB	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:O	1:A:187:LEU:CD2	2.42	0.67
2:B:54:GLY:C	2:B:57:THR:HG23	2.19	0.67
1:A:167:PHE:O	1:A:171:ILE:HG22	1.93	0.67
1:A:139:ARG:CB	1:A:141:ILE:N	2.58	0.67
1:A:258:TYR:HD2	1:A:260:TRP:CE3	2.12	0.67
1:A:156:PHE:CE1	2:B:185:LYS:HG2	2.30	0.67
1:A:198:ARG:O	1:A:202:GLU:CG	2.43	0.67
1:A:188:THR:O	1:A:192:ARG:HB2	1.95	0.67
1:A:153:ILE:CG2	1:A:164:ASP:OD2	2.43	0.67
2:B:125:GLN:O	2:B:128:ALA:HB3	1.95	0.66
1:A:43:VAL:HG22	1:A:100:VAL:CG2	2.25	0.66
3:C:45:SER:CA	3:C:48:ILE:HD12	2.11	0.66
2:B:46:LEU:HA	2:B:100:VAL:O	1.95	0.66
2:B:157:PRO:HG3	2:B:184:ALA:O	1.95	0.66
1:A:42:VAL:O	1:A:100:VAL:HG23	1.96	0.66
1:A:149:CYS:SG	1:A:150:PHE:O	2.53	0.66
1:A:271:ASN:ND2	1:A:273:PHE:CB	2.56	0.66
2:B:273:LYS:O	2:B:277:MET:HG2	1.96	0.66
1:A:240:VAL:CG2	4:A:362:GDP:O6	2.43	0.66
3:C:174:ILE:HD11	3:C:226:PRO:HG2	1.78	0.66
3:C:38:GLY:HA3	3:C:44:LYS:HD3	1.76	0.66
3:C:57:TYR:C	3:C:59:PRO:HD3	2.20	0.66
2:B:257:PRO:HB2	2:B:258:TRP:NE1	2.11	0.65
3:C:77:SER:CB	3:C:88:LEU:O	2.45	0.65
2:B:185:LYS:CG	5:B:428:GTP:C6	2.72	0.65
1:A:268:PRO:HG3	1:A:271:ASN:O	1.97	0.65
1:A:197:LYS:HA	1:A:200:LEU:HB2	1.78	0.65
1:A:59:LEU:O	1:A:59:LEU:HG	1.97	0.65
3:C:23:ARG:C	3:C:25:SER:H	2.05	0.65
1:A:245:LEU:HB2	1:A:253:VAL:O	1.96	0.65
1:A:279:MET:SD	1:A:279:MET:C	2.79	0.65
3:C:188:PHE:O	3:C:192:ILE:HG13	1.96	0.65
2:B:302:LYS:O	2:B:306:MET:SD	2.54	0.65
1:A:156:PHE:CE1	1:A:186:THR:CB	2.72	0.65
1:A:283:HIS:CD2	1:A:283:HIS:N	2.61	0.65
2:B:120:GLU:O	2:B:124:ALA:HB2	1.97	0.65
1:A:279:MET:CG	1:A:280:LEU:N	2.58	0.64
1:A:23:LEU:O	1:A:27:VAL:HG23	1.97	0.64
3:C:154:LYS:O	3:C:157:ASP:N	2.30	0.64
1:A:122:ILE:CD1	1:A:126:PHE:CE1	2.77	0.64
3:C:108:TRP:C	3:C:110:PRO:HD2	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:CYS:SG	1:A:149:CYS:O	2.56	0.64
1:A:55:ASN:O	1:A:59:LEU:N	2.30	0.64
1:A:276:LEU:HD23	1:A:277:ARG:N	2.13	0.64
2:B:60:ASP:O	2:B:64:ASN:N	2.30	0.64
1:A:147:HIS:O	1:A:286:ASP:HB2	1.98	0.64
1:A:179:PRO:CD	1:A:210:ILE:CD1	2.76	0.64
1:A:29:ARG:O	1:A:32:VAL:CG2	2.46	0.63
1:A:175:VAL:HG12	1:A:176:ASN:CA	2.28	0.63
3:C:132:ARG:H	3:C:134:MET:HE3	1.63	0.63
2:B:257:PRO:CB	2:B:258:TRP:CD1	2.71	0.63
3:C:79:VAL:HA	3:C:87:GLN:HA	1.80	0.63
3:C:141:CYS:HB2	3:C:169:ASN:O	1.99	0.63
2:B:185:LYS:HA	5:B:428:GTP:C6	2.33	0.63
1:A:177:ILE:HD13	1:A:210:ILE:HG22	1.81	0.63
1:A:285:GLN:O	1:A:288:GLN:HB2	1.98	0.63
1:A:43:VAL:HG11	1:A:167:PHE:CZ	2.33	0.63
1:A:79:VAL:HG22	1:A:80:GLN:N	2.14	0.63
2:B:186:ALA:HB2	2:B:237:VAL:O	1.98	0.63
1:A:165:VAL:HG12	1:A:166:ALA:N	2.13	0.63
2:B:60:ASP:CB	2:B:65:THR:O	2.46	0.63
1:A:285:GLN:CA	1:A:288:GLN:HG3	2.28	0.63
1:A:122:ILE:HD12	1:A:175:VAL:HG23	1.81	0.62
1:A:54:ILE:CG2	1:A:55:ASN:N	2.63	0.62
1:A:179:PRO:HD3	1:A:210:ILE:HG21	1.80	0.62
3:C:40:SER:HA	3:C:44:LYS:HZ1	1.63	0.62
2:B:236:ALA:O	2:B:270:ASP:CB	2.48	0.62
1:A:55:ASN:CB	1:A:60:THR:O	2.47	0.62
1:A:265:VAL:CG1	1:A:266:GLU:HG3	2.11	0.62
1:A:119:ILE:HD11	1:A:170:ALA:O	1.98	0.62
1:A:148:CYS:SG	1:A:149:CYS:N	2.71	0.62
1:A:161:LYS:O	1:A:164:ASP:N	2.33	0.62
1:A:211:TYR:CZ	1:A:214:PRO:CD	2.82	0.62
1:A:177:ILE:H	1:A:177:ILE:HD12	1.64	0.62
2:B:166:ASP:HA	2:B:169:THR:HG22	1.80	0.62
1:A:285:GLN:O	1:A:288:GLN:N	2.30	0.62
3:C:47:LEU:O	3:C:51:LEU:HB3	1.99	0.62
1:A:172:HIS:HD2	1:A:209:LYS:CB	2.13	0.61
1:A:258:TYR:HD2	1:A:260:TRP:HE3	1.47	0.61
2:B:166:ASP:CA	2:B:169:THR:HG22	2.30	0.61
3:C:154:LYS:O	3:C:157:ASP:CB	2.48	0.61
3:C:192:ILE:HA	3:C:195:GLU:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PRO:CD	1:A:210:ILE:HD13	2.31	0.61
1:A:151:TYR:O	1:A:179:PRO:HA	1.99	0.61
1:A:201:ASP:C	1:A:204:GLU:HB2	2.25	0.61
2:B:257:PRO:C	2:B:258:TRP:CD1	2.79	0.61
3:C:192:ILE:O	3:C:195:GLU:CB	2.49	0.61
3:C:30:PHE:O	3:C:88:LEU:HA	2.01	0.61
2:B:185:LYS:HE3	5:B:428:GTP:N9	2.14	0.61
2:B:19:LEU:CB	3:C:77:SER:O	2.48	0.61
3:C:148:PRO:CG	3:C:150:GLY:CA	2.65	0.61
1:A:177:ILE:HG22	1:A:179:PRO:CD	2.31	0.61
1:A:180:VAL:HG22	1:A:181:ILE:N	2.15	0.60
1:A:196:LYS:O	1:A:200:LEU:CD1	2.47	0.60
1:A:84:SER:O	1:A:95:LEU:HB2	2.01	0.60
3:C:173:LEU:C	3:C:174:ILE:HD12	2.27	0.60
1:A:160:LEU:HD23	1:A:164:ASP:HB2	1.82	0.60
1:A:213:LEU:O	1:A:213:LEU:CD2	2.44	0.60
1:A:288:GLN:C	1:A:291:THR:HG22	2.26	0.60
3:C:267:ARG:O	3:C:271:ILE:CB	2.50	0.60
1:A:150:PHE:HB3	1:A:152:PHE:CE1	2.37	0.60
2:B:185:LYS:CD	5:B:428:GTP:C5	2.85	0.60
1:A:208:ILE:HG23	1:A:209:LYS:N	2.16	0.60
1:A:173:ASN:HA	1:A:294:LEU:HD21	1.79	0.60
1:A:265:VAL:HG12	1:A:266:GLU:N	2.15	0.60
3:C:43:GLY:O	3:C:46:THR:CG2	2.39	0.60
1:A:61:ASP:O	1:A:62:LEU:HD23	2.01	0.60
1:A:268:PRO:CG	1:A:271:ASN:O	2.50	0.60
2:B:185:LYS:HG3	5:B:428:GTP:C5	2.37	0.60
3:C:34:LEU:HB3	3:C:91:THR:O	2.01	0.60
1:A:204:GLU:C	1:A:206:HIS:H	2.10	0.59
1:A:189:LEU:HA	1:A:192:ARG:HB2	1.83	0.59
2:B:274:LEU:O	2:B:278:LEU:CB	2.50	0.59
2:B:166:ASP:N	2:B:166:ASP:OD1	2.34	0.59
1:A:240:VAL:CG1	4:A:362:GDP:O6	2.50	0.59
1:A:279:MET:SD	1:A:280:LEU:HA	2.42	0.59
2:B:19:LEU:CB	3:C:77:SER:N	2.65	0.59
2:B:206:VAL:HA	2:B:209:GLY:CA	2.27	0.59
3:C:140:GLN:O	3:C:168:VAL:CB	2.51	0.59
3:C:259:GLU:N	3:C:260:HIS:CB	2.66	0.59
1:A:180:VAL:CG2	1:A:181:ILE:N	2.64	0.59
1:A:200:LEU:O	1:A:203:ILE:HB	2.03	0.59
2:B:154:PHE:HA	2:B:182:ILE:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ASN:O	1:A:24:PRO:HD2	2.00	0.58
2:B:175:SER:N	2:B:176:LYS:HA	2.17	0.58
1:A:173:ASN:C	1:A:175:VAL:CA	2.76	0.58
2:B:67:PHE:HD1	2:B:67:PHE:N	2.01	0.58
3:C:47:LEU:O	3:C:51:LEU:HB2	2.02	0.58
2:B:171:LYS:C	2:B:174:ASP:HB3	2.28	0.58
1:A:45:GLU:O	1:A:47:GLY:HA3	2.03	0.58
1:A:49:GLY:HA2	4:A:362:GDP:O1A	2.04	0.58
2:B:85:THR:CB	2:B:98:THR:HA	2.34	0.58
3:C:42:LEU:CA	4:C:419:GDP:C5'	2.69	0.58
3:C:41:GLY:C	4:C:419:GDP:H5''	2.28	0.58
1:A:38:PHE:CE1	1:A:147:HIS:HB3	2.38	0.58
1:A:87:GLU:C	1:A:92:GLY:HA2	2.28	0.58
1:A:263:VAL:HG13	2:B:257:PRO:CG	2.33	0.58
3:C:110:PRO:O	3:C:114:TYR:N	2.35	0.58
1:A:29:ARG:HA	1:A:32:VAL:HG23	1.85	0.58
2:B:165:LEU:O	2:B:169:THR:HB	2.03	0.58
1:A:156:PHE:CZ	1:A:186:THR:CG2	2.86	0.57
2:B:185:LYS:HE3	5:B:428:GTP:N3	2.19	0.57
1:A:199:ILE:O	1:A:203:ILE:HD13	2.04	0.57
2:B:225:ILE:O	2:B:229:MET:HG2	2.04	0.57
3:C:38:GLY:HA3	3:C:44:LYS:CD	2.34	0.57
3:C:48:ILE:O	3:C:52:PHE:HB2	2.04	0.57
1:A:229:ARG:NH2	1:A:230:LEU:CD1	2.67	0.57
2:B:171:LYS:O	2:B:174:ASP:CB	2.52	0.57
2:B:277:MET:HG3	2:B:278:LEU:N	2.18	0.57
3:C:34:LEU:O	3:C:34:LEU:CD1	2.42	0.57
3:C:174:ILE:N	3:C:174:ILE:CD1	2.67	0.57
1:A:151:TYR:CE1	1:A:167:PHE:HB3	2.36	0.57
2:B:171:LYS:CA	2:B:174:ASP:HB3	2.35	0.57
1:A:41:MET:HA	1:A:98:THR:O	2.05	0.57
1:A:80:GLN:HA	1:A:80:GLN:OE1	2.04	0.57
1:A:265:VAL:CB	1:A:266:GLU:HG3	2.34	0.57
1:A:28:HIS:C	1:A:28:HIS:CD2	2.83	0.56
1:A:47:GLY:HA2	2:B:158:THR:CG2	2.35	0.56
1:A:143:ASP:OD2	1:A:145:ARG:CD	2.42	0.56
1:A:151:TYR:CD2	1:A:151:TYR:C	2.82	0.56
3:C:43:GLY:HA2	4:C:419:GDP:O1A	2.04	0.56
1:A:265:VAL:C	1:A:266:GLU:HG3	2.29	0.56
3:C:157:ASP:O	3:C:161:MET:HG3	2.05	0.56
3:C:43:GLY:CA	3:C:46:THR:HG21	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:MET:O	3:C:143:LEU:N	2.38	0.56
1:A:55:ASN:O	1:A:60:THR:N	2.38	0.56
1:A:143:ASP:CB	1:A:145:ARG:HD3	2.36	0.56
1:A:200:LEU:HA	1:A:203:ILE:HD13	1.88	0.56
2:B:120:GLU:O	2:B:124:ALA:CB	2.54	0.56
3:C:51:LEU:HD12	3:C:51:LEU:O	2.06	0.56
1:A:211:TYR:HH	1:A:214:PRO:HD2	1.67	0.56
2:B:67:PHE:N	2:B:67:PHE:CD1	2.72	0.56
1:A:151:TYR:HD2	1:A:151:TYR:C	2.14	0.56
1:A:172:HIS:HD2	1:A:209:LYS:HG3	1.71	0.56
1:A:263:VAL:HG22	2:B:257:PRO:HG3	1.86	0.56
2:B:182:ILE:CD1	2:B:183:ILE:H	2.16	0.56
2:B:54:GLY:HA3	2:B:57:THR:HG21	1.87	0.55
1:A:276:LEU:HD23	1:A:276:LEU:C	2.31	0.55
2:B:90:GLU:N	2:B:93:VAL:O	2.32	0.55
1:A:122:ILE:HG13	1:A:126:PHE:CD1	2.42	0.55
3:C:71:THR:CB	3:C:95:THR:CB	2.84	0.55
1:A:177:ILE:HG22	1:A:178:VAL:C	2.32	0.55
1:A:179:PRO:CD	1:A:210:ILE:HD12	2.37	0.55
3:C:34:LEU:O	3:C:92:ILE:HA	2.07	0.55
3:C:141:CYS:HA	3:C:168:VAL:CB	2.37	0.55
1:A:43:VAL:HG11	1:A:167:PHE:CE1	2.42	0.55
2:B:60:ASP:O	2:B:64:ASN:CA	2.55	0.55
1:A:38:PHE:CE2	1:A:40:LEU:HB3	2.41	0.55
1:A:206:HIS:CD2	1:A:208:ILE:HG13	2.42	0.55
2:B:153:TYR:HE2	2:B:155:ILE:HG23	1.69	0.55
1:A:173:ASN:C	1:A:175:VAL:HA	2.32	0.54
1:A:177:ILE:HG22	1:A:179:PRO:HD3	1.89	0.54
2:B:60:ASP:O	2:B:64:ASN:HA	2.07	0.54
1:A:224:PHE:O	1:A:228:THR:HG22	2.07	0.54
1:A:203:ILE:HD12	1:A:203:ILE:H	1.73	0.54
1:A:285:GLN:HB2	1:A:288:GLN:CD	2.32	0.54
3:C:192:ILE:HD11	3:C:226:PRO:CD	2.38	0.54
2:B:19:LEU:CB	3:C:77:SER:H	2.20	0.54
2:B:249:LYS:CB	2:B:250:MET:CA	2.75	0.54
2:B:114:SER:C	2:B:117:PRO:HG2	2.33	0.54
1:A:290:VAL:HA	1:A:294:LEU:HD12	1.89	0.53
1:A:148:CYS:SG	1:A:149:CYS:C	2.91	0.53
1:A:274:LEU:CD2	1:A:277:ARG:HG2	2.37	0.53
1:A:29:ARG:O	1:A:32:VAL:HG23	2.08	0.53
1:A:298:ASN:O	1:A:302:GLU:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:TYR:HE2	2:B:166:ASP:HB3	1.68	0.53
3:C:46:THR:O	3:C:50:SER:CB	2.45	0.53
1:A:263:VAL:HG22	2:B:257:PRO:CG	2.38	0.53
3:C:43:GLY:N	4:C:419:GDP:H5'	2.24	0.53
1:A:156:PHE:CZ	1:A:186:THR:HG22	2.43	0.53
2:B:205:LEU:O	2:B:209:GLY:HA2	2.09	0.53
2:B:205:LEU:O	2:B:210:VAL:HG23	2.09	0.53
3:C:176:LYS:O	3:C:179:THR:N	2.38	0.53
1:A:212:HIS:O	1:A:214:PRO:CD	2.54	0.53
2:B:166:ASP:HA	2:B:169:THR:HG21	1.88	0.53
1:A:44:GLY:O	1:A:50:LYS:HE2	2.09	0.53
2:B:35:LYS:C	2:B:37:VAL:H	2.17	0.53
3:C:39:GLU:O	3:C:44:LYS:NZ	2.41	0.53
1:A:285:GLN:O	1:A:288:GLN:CB	2.57	0.53
3:C:72:VAL:O	3:C:94:ASP:O	2.26	0.53
1:A:39:THR:CG2	1:A:145:ARG:O	2.57	0.52
1:A:97:LEU:C	1:A:97:LEU:HD23	2.34	0.52
1:A:178:VAL:HG12	1:A:179:PRO:O	2.10	0.52
1:A:189:LEU:HD12	1:A:190:LYS:N	2.24	0.52
1:A:242:SER:CB	1:A:255:GLY:O	2.56	0.52
1:A:242:SER:HB3	1:A:255:GLY:O	2.09	0.52
2:B:119:VAL:O	2:B:123:ASP:CB	2.57	0.52
3:C:116:ASP:O	3:C:120:GLU:N	2.37	0.52
1:A:45:GLU:O	1:A:48:LEU:HG	2.09	0.52
1:A:196:LYS:HB2	1:A:197:LYS:HE3	1.91	0.52
1:A:288:GLN:O	1:A:291:THR:CG2	2.58	0.52
1:A:122:ILE:CG1	1:A:123:ASP:N	2.68	0.52
1:A:201:ASP:HA	1:A:204:GLU:HB2	1.91	0.52
2:B:257:PRO:C	2:B:258:TRP:CG	2.88	0.52
3:C:60:GLU:HG2	4:C:419:GDP:O3B	2.10	0.52
2:B:153:TYR:HB3	2:B:170:MET:CE	2.28	0.52
2:B:299:ARG:O	2:B:303:LEU:N	2.30	0.52
2:B:56:SER:O	2:B:60:ASP:OD2	2.27	0.52
1:A:289:GLU:O	1:A:293:ASP:N	2.32	0.52
1:A:125:GLN:CB	1:A:144:ASN:O	2.58	0.52
1:A:175:VAL:CG1	1:A:176:ASN:N	2.56	0.52
1:A:131:HIS:HD2	1:A:132:ASP:OD1	1.93	0.51
1:A:285:GLN:HB3	1:A:288:GLN:NE2	2.25	0.51
3:C:34:LEU:HD22	3:C:35:MET:N	2.25	0.51
3:C:42:LEU:N	4:C:419:GDP:H5''	2.25	0.51
2:B:185:LYS:HD2	5:B:428:GTP:N7	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:TYR:CD1	3:C:61:TYR:C	2.86	0.51
1:A:265:VAL:CG1	1:A:266:GLU:N	2.73	0.51
1:A:61:ASP:OD2	1:A:62:LEU:N	2.44	0.51
1:A:189:LEU:HD12	1:A:190:LYS:H	1.75	0.51
1:A:28:HIS:CG	1:A:29:ARG:N	2.78	0.51
1:A:122:ILE:HB	1:A:146:VAL:HG21	1.93	0.51
2:B:113:ASP:O	2:B:117:PRO:CG	2.46	0.51
1:A:151:TYR:HE1	1:A:167:PHE:CG	2.29	0.51
1:A:54:ILE:HG13	1:A:58:PHE:CZ	2.45	0.50
1:A:186:THR:O	5:B:428:GTP:N2	2.44	0.50
1:A:29:ARG:C	1:A:32:VAL:HG23	2.36	0.50
1:A:153:ILE:HG21	1:A:160:LEU:CG	2.29	0.50
1:A:173:ASN:O	1:A:175:VAL:N	2.44	0.50
3:C:38:GLY:HA3	3:C:44:LYS:HE2	1.92	0.50
1:A:163:LEU:C	1:A:163:LEU:HD13	2.36	0.50
1:A:278:THR:O	1:A:282:THR:HB	2.12	0.50
1:A:285:GLN:HB3	1:A:288:GLN:HE21	1.77	0.50
2:B:166:ASP:O	2:B:170:MET:N	2.42	0.50
1:A:146:VAL:HB	1:A:175:VAL:HG21	1.93	0.50
1:A:156:PHE:CZ	2:B:185:LYS:CB	2.95	0.50
1:A:268:PRO:O	1:A:270:HIS:N	2.45	0.50
2:B:174:ASP:HB2	2:B:210:VAL:CG1	2.41	0.50
3:C:135:PRO:CB	3:C:136:ASP:HA	2.41	0.50
1:A:82:GLU:CB	1:A:97:LEU:O	2.59	0.50
1:A:151:TYR:OH	1:A:164:ASP:HA	2.11	0.50
1:A:229:ARG:HH21	1:A:230:LEU:HD13	1.76	0.50
2:B:153:TYR:HE2	2:B:155:ILE:CG2	2.25	0.50
3:C:147:ALA:HB2	3:C:175:ALA:H	1.77	0.50
1:A:284:MET:O	1:A:287:LEU:CG	2.48	0.50
1:A:57:LEU:CD2	1:A:276:LEU:CD2	2.83	0.50
1:A:122:ILE:HG13	1:A:126:PHE:HD1	1.76	0.50
1:A:271:ASN:CG	1:A:273:PHE:HB2	2.37	0.50
1:A:188:THR:O	1:A:192:ARG:N	2.45	0.49
1:A:258:TYR:CD2	1:A:260:TRP:CZ3	3.01	0.49
1:A:172:HIS:HD2	1:A:209:LYS:CG	2.25	0.49
1:A:181:ILE:HB	1:A:238:SER:OG	2.13	0.49
1:A:206:HIS:CD2	1:A:208:ILE:CG1	2.95	0.49
1:A:177:ILE:CG1	1:A:210:ILE:HG22	2.42	0.49
3:C:40:SER:HB3	4:C:419:GDP:O3B	2.13	0.49
3:C:116:ASP:C	3:C:119:PHE:H	2.20	0.49
1:A:54:ILE:HG13	1:A:58:PHE:CD2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:PHE:CE2	2:B:185:LYS:CB	2.96	0.49
1:A:57:LEU:HD22	1:A:276:LEU:HD21	1.88	0.49
1:A:139:ARG:CA	1:A:141:ILE:N	2.76	0.49
1:A:258:TYR:CE2	1:A:260:TRP:CZ3	3.00	0.49
2:B:116:LYS:H	2:B:117:PRO:CD	2.04	0.49
3:C:23:ARG:C	3:C:25:SER:N	2.68	0.49
1:A:156:PHE:CE2	2:B:185:LYS:HB3	2.48	0.48
1:A:263:VAL:HG13	2:B:257:PRO:HD3	1.94	0.48
3:C:49:ASN:CB	3:C:54:THR:O	2.53	0.48
1:A:34:LYS:HD2	1:A:34:LYS:C	2.35	0.48
1:A:153:ILE:H	1:A:153:ILE:CD1	2.05	0.48
1:A:183:LYS:HG3	4:A:362:GDP:C6	2.47	0.48
1:A:197:LYS:O	1:A:200:LEU:HB2	2.13	0.48
1:A:229:ARG:HE	1:A:229:ARG:HB3	1.36	0.48
2:B:250:MET:C	2:B:251:MET:SD	2.96	0.48
3:C:154:LYS:O	3:C:157:ASP:CA	2.61	0.48
1:A:199:ILE:HG22	1:A:203:ILE:CD1	2.44	0.48
3:C:41:GLY:O	4:C:419:GDP:O5'	2.31	0.48
1:A:49:GLY:HA2	1:A:52:THR:HG22	1.95	0.48
1:A:130:LEU:CD1	1:A:295:HIS:CE1	2.96	0.48
1:A:141:ILE:HD12	1:A:142:ILE:H	1.74	0.48
2:B:151:CYS:SG	2:B:152:LEU:C	2.96	0.48
2:B:155:ILE:HD13	2:B:182:ILE:O	2.14	0.48
3:C:147:ALA:CB	3:C:175:ALA:H	2.27	0.48
1:A:228:THR:HG23	1:A:229:ARG:N	2.29	0.48
2:B:272:VAL:O	2:B:275:ARG:N	2.46	0.48
2:B:64:ASN:C	2:B:65:THR:HG23	2.35	0.48
3:C:266:LEU:O	3:C:270:LEU:CB	2.62	0.48
1:A:79:VAL:HG22	1:A:80:GLN:H	1.78	0.48
1:A:130:LEU:HD12	1:A:295:HIS:CE1	2.49	0.47
1:A:179:PRO:HD2	1:A:210:ILE:HD12	1.95	0.47
3:C:154:LYS:O	3:C:158:ILE:N	2.45	0.47
1:A:163:LEU:HD13	1:A:163:LEU:O	2.13	0.47
1:A:195:LEU:O	1:A:199:ILE:HG13	2.13	0.47
1:A:23:LEU:O	1:A:27:VAL:N	2.29	0.47
1:A:195:LEU:O	1:A:199:ILE:CG1	2.62	0.47
1:A:258:TYR:CE2	1:A:260:TRP:HZ3	2.33	0.47
1:A:83:ALA:CA	1:A:95:LEU:O	2.46	0.47
1:A:49:GLY:O	1:A:53:LEU:HB3	2.15	0.47
1:A:122:ILE:O	1:A:126:PHE:CD1	2.68	0.47
1:A:177:ILE:CD1	1:A:210:ILE:HG22	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:THR:O	2:B:76:GLN:CB	2.61	0.47
2:B:153:TYR:OH	2:B:166:ASP:CB	2.59	0.47
1:A:39:THR:O	1:A:147:HIS:CB	2.53	0.47
1:A:49:GLY:HA3	1:A:52:THR:HG22	1.94	0.47
1:A:121:TYR:HA	1:A:124:GLU:HB3	1.97	0.47
1:A:204:GLU:C	1:A:206:HIS:N	2.73	0.47
1:A:245:LEU:CA	1:A:246:ILE:HD13	2.39	0.47
2:B:169:THR:O	2:B:173:LEU:CB	2.56	0.47
2:B:170:MET:O	2:B:174:ASP:N	2.48	0.47
3:C:26:VAL:O	3:C:27:LYS:O	2.31	0.47
1:A:50:LYS:NZ	4:A:362:GDP:O2B	2.42	0.47
3:C:248:TYR:HB3	3:C:249:PRO:HD2	1.96	0.47
3:C:33:THR:O	3:C:139:VAL:O	2.31	0.46
3:C:33:THR:HG23	3:C:91:THR:CB	2.45	0.46
1:A:197:LYS:O	1:A:201:ASP:N	2.44	0.46
1:A:258:TYR:CD2	1:A:260:TRP:HE3	2.26	0.46
3:C:50:SER:O	3:C:53:LEU:HD23	2.15	0.46
1:A:40:LEU:HA	1:A:148:CYS:O	2.14	0.46
1:A:268:PRO:HA	1:A:270:HIS:N	2.30	0.46
2:B:25:PHE:O	2:B:26:ASP:C	2.58	0.46
1:A:54:ILE:HG23	1:A:55:ASN:N	2.31	0.46
1:A:52:THR:HG23	1:A:53:LEU:N	2.31	0.46
1:A:240:VAL:CG1	4:A:362:GDP:C6	2.93	0.46
1:A:176:ASN:HD22	1:A:176:ASN:HA	1.58	0.46
1:A:201:ASP:CA	1:A:204:GLU:HB2	2.46	0.46
3:C:163:ARG:C	3:C:165:HIS:H	2.24	0.46
3:C:176:LYS:O	3:C:179:THR:HB	2.16	0.46
3:C:161:MET:HE3	3:C:161:MET:HB3	1.77	0.46
1:A:79:VAL:CG2	1:A:80:GLN:N	2.79	0.46
2:B:155:ILE:O	2:B:183:ILE:HA	2.16	0.46
3:C:276:GLN:O	3:C:279:LYS:HG2	2.16	0.46
1:A:81:ILE:C	1:A:81:ILE:CD1	2.88	0.45
1:A:156:PHE:CZ	1:A:186:THR:HG21	2.50	0.45
1:A:289:GLU:C	1:A:291:THR:N	2.73	0.45
1:A:167:PHE:O	1:A:171:ILE:CG2	2.61	0.45
1:A:245:LEU:O	1:A:246:ILE:HD13	2.12	0.45
1:A:46:SER:HB3	1:A:50:LYS:NZ	2.31	0.45
1:A:286:ASP:OD1	1:A:286:ASP:N	2.31	0.45
2:B:84:ASN:O	2:B:99:ILE:O	2.34	0.45
2:B:170:MET:O	2:B:173:LEU:C	2.59	0.45
1:A:54:ILE:O	1:A:58:PHE:CG	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:ARG:CB	2:B:138:ARG:CB	2.93	0.45
1:A:55:ASN:OD1	1:A:61:ASP:HA	2.16	0.45
1:A:172:HIS:CD2	1:A:209:LYS:HG3	2.50	0.45
1:A:271:ASN:C	1:A:273:PHE:H	2.24	0.45
1:A:231:LEU:HD12	1:A:231:LEU:HA	1.67	0.45
1:A:82:GLU:O	1:A:97:LEU:N	2.49	0.45
1:A:164:ASP:O	1:A:168:MET:HG3	2.16	0.45
2:B:169:THR:CG2	2:B:170:MET:N	2.79	0.45
1:A:143:ASP:HB2	1:A:145:ARG:HD3	1.97	0.45
3:C:79:VAL:CB	3:C:87:GLN:CB	2.95	0.45
3:C:148:PRO:CB	3:C:150:GLY:HA3	2.47	0.45
1:A:39:THR:HG21	1:A:145:ARG:O	2.17	0.45
1:A:155:PRO:O	1:A:187:LEU:HD22	2.17	0.45
1:A:158:HIS:HB3	1:A:159:GLY:H	1.55	0.45
1:A:160:LEU:CD1	1:A:199:ILE:HG12	2.35	0.45
1:A:213:LEU:O	1:A:214:PRO:C	2.60	0.45
2:B:25:PHE:O	2:B:26:ASP:O	2.35	0.45
2:B:60:ASP:HA	2:B:65:THR:O	2.17	0.45
3:C:46:THR:O	3:C:50:SER:N	2.44	0.45
2:B:180:ILE:HA	2:B:181:PRO:HD3	1.37	0.44
3:C:178:ASP:OD2	3:C:248:TYR:OH	2.29	0.44
3:C:248:TYR:HB3	3:C:249:PRO:CD	2.47	0.44
3:C:258:GLY:HA3	3:C:259:GLU:HA	1.64	0.44
1:A:57:LEU:HD21	1:A:276:LEU:CD2	2.33	0.44
1:A:149:CYS:SG	1:A:150:PHE:N	2.90	0.44
1:A:153:ILE:CG2	1:A:160:LEU:HG	2.31	0.44
2:B:288:GLU:O	2:B:292:THR:CB	2.65	0.44
2:B:29:PRO:O	2:B:32:LEU:N	2.51	0.44
2:B:126:PHE:C	2:B:129:TYR:H	2.26	0.44
3:C:51:LEU:HD12	3:C:51:LEU:C	2.42	0.44
1:A:122:ILE:HG13	1:A:123:ASP:N	2.22	0.44
1:A:183:LYS:HD2	4:A:362:GDP:C8	2.52	0.44
3:C:178:ASP:CG	4:C:419:GDP:HN1	2.25	0.44
1:A:271:ASN:CG	1:A:273:PHE:CB	2.91	0.44
2:B:58:LEU:C	2:B:61:THR:HG22	2.40	0.44
3:C:179:THR:CG2	3:C:180:LEU:N	2.80	0.44
3:C:181:THR:HA	3:C:182:PRO:HD3	1.74	0.44
3:C:192:ILE:O	3:C:195:GLU:N	2.50	0.44
3:C:231:GLY:HA3	4:C:419:GDP:N7	2.32	0.44
1:A:150:PHE:N	1:A:150:PHE:CD1	2.86	0.44
1:A:161:LYS:HB2	1:A:164:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:CA	1:A:32:VAL:HG23	2.47	0.43
1:A:188:THR:OG1	1:A:191:GLU:HG3	2.18	0.43
2:B:193:GLU:C	2:B:196:LYS:H	2.27	0.43
2:B:155:ILE:CD1	2:B:182:ILE:O	2.67	0.43
3:C:247:GLN:CB	3:C:252:VAL:CB	2.97	0.43
3:C:249:PRO:HB2	3:C:250:TRP:CE3	2.53	0.43
1:A:156:PHE:O	1:A:157:GLY:C	2.60	0.43
1:A:54:ILE:HG22	1:A:55:ASN:N	2.34	0.43
1:A:163:LEU:HA	1:A:163:LEU:HD22	1.64	0.43
1:A:288:GLN:CA	1:A:291:THR:HG22	2.49	0.43
2:B:277:MET:HG3	2:B:278:LEU:H	1.83	0.43
2:B:57:THR:O	2:B:61:THR:HB	2.19	0.43
3:C:39:GLU:O	3:C:44:LYS:CE	2.67	0.43
3:C:43:GLY:H	4:C:419:GDP:PA	2.41	0.43
1:A:176:ASN:OD1	1:A:290:VAL:HG22	2.18	0.43
1:A:172:HIS:HB2	1:A:209:LYS:O	2.19	0.43
1:A:199:ILE:O	1:A:202:GLU:HB2	2.19	0.43
1:A:202:GLU:C	1:A:204:GLU:H	2.24	0.43
2:B:82:GLN:O	2:B:101:SER:O	2.37	0.43
2:B:186:ALA:CB	2:B:237:VAL:O	2.65	0.43
1:A:82:GLU:HB2	1:A:97:LEU:HB3	2.01	0.42
3:C:182:PRO:HA	3:C:185:CYS:H	1.84	0.42
1:A:189:LEU:O	1:A:193:GLU:HG2	2.19	0.42
2:B:63:PHE:O	2:B:64:ASN:C	2.60	0.42
1:A:119:ILE:O	1:A:119:ILE:CG2	2.64	0.42
1:A:150:PHE:CB	1:A:152:PHE:CE1	3.02	0.42
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.75	0.42
1:A:206:HIS:HB3	1:A:208:ILE:HB	2.00	0.42
1:A:263:VAL:HG13	2:B:257:PRO:CD	2.49	0.42
2:B:19:LEU:CB	3:C:77:SER:C	2.92	0.42
2:B:149:HIS:O	2:B:178:ASN:CB	2.67	0.42
3:C:164:LEU:O	3:C:165:HIS:C	2.62	0.42
3:C:179:THR:HG23	3:C:180:LEU:N	2.34	0.42
1:A:29:ARG:HA	1:A:32:VAL:CG2	2.49	0.42
2:B:57:THR:HG21	5:B:428:GTP:H5'	2.01	0.42
2:B:182:ILE:HD12	2:B:183:ILE:N	2.24	0.42
1:A:156:PHE:CD1	2:B:185:LYS:HE2	2.55	0.42
1:A:164:ASP:O	1:A:168:MET:N	2.46	0.42
2:B:55:LYS:O	2:B:59:MET:HG2	2.19	0.42
2:B:185:LYS:CG	5:B:428:GTP:C5	3.01	0.42
2:B:289:GLN:O	2:B:293:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLU:O	1:A:230:LEU:HB2	2.19	0.42
2:B:151:CYS:SG	2:B:153:TYR:N	2.92	0.42
3:C:192:ILE:O	3:C:196:ILE:N	2.53	0.42
3:C:192:ILE:C	3:C:195:GLU:H	2.28	0.42
1:A:43:VAL:O	1:A:152:PHE:CD1	2.73	0.42
1:A:43:VAL:HG12	1:A:44:GLY:N	2.34	0.42
1:A:242:SER:HB2	1:A:255:GLY:O	2.19	0.42
1:A:288:GLN:HA	1:A:291:THR:HG22	2.01	0.42
2:B:186:ALA:HB2	2:B:237:VAL:C	2.44	0.42
3:C:116:ASP:O	3:C:119:PHE:N	2.52	0.42
3:C:193:MET:CE	3:C:225:LEU:O	2.67	0.42
1:A:38:PHE:O	1:A:95:LEU:HD23	2.20	0.42
1:A:149:CYS:O	1:A:177:ILE:HA	2.20	0.42
2:B:215:PHE:CB	2:B:216:PRO:CD	2.97	0.42
1:A:177:ILE:CG2	1:A:179:PRO:HD3	2.48	0.42
1:A:289:GLU:C	1:A:291:THR:H	2.26	0.42
1:A:151:TYR:CE1	1:A:167:PHE:CG	3.09	0.41
1:A:56:SER:OG	1:A:254:ARG:NH2	2.41	0.41
1:A:134:SER:HA	1:A:135:GLY:HA3	1.79	0.41
1:A:193:GLU:HA	1:A:196:LYS:HE3	2.02	0.41
1:A:229:ARG:NH2	1:A:230:LEU:HD13	2.32	0.41
1:A:198:ARG:O	1:A:202:GLU:HG3	2.18	0.41
3:C:132:ARG:N	3:C:134:MET:HE3	2.32	0.41
3:C:226:PRO:HB2	3:C:227:LEU:H	1.61	0.41
1:A:237:PHE:CB	1:A:272:ASP:HB3	2.47	0.41
2:B:182:ILE:HD11	2:B:237:VAL:CB	2.51	0.41
1:A:148:CYS:HA	1:A:176:ASN:HB3	2.03	0.41
2:B:85:THR:HA	2:B:98:THR:HA	2.02	0.41
1:A:36:PHE:O	1:A:93:VAL:HG23	2.17	0.41
1:A:165:VAL:CG1	1:A:166:ALA:N	2.73	0.41
1:A:197:LYS:HA	1:A:200:LEU:HD13	2.03	0.41
1:A:197:LYS:HB3	1:A:197:LYS:HE2	1.80	0.41
1:A:165:VAL:HG22	1:A:206:HIS:CE1	2.56	0.41
1:A:181:ILE:HD13	1:A:238:SER:OG	2.21	0.41
1:A:197:LYS:CA	1:A:200:LEU:HB2	2.48	0.41
2:B:206:VAL:CA	2:B:209:GLY:HA2	2.33	0.41
1:A:119:ILE:O	1:A:119:ILE:HG23	2.21	0.41
1:A:150:PHE:CB	1:A:152:PHE:HE1	2.34	0.41
1:A:193:GLU:O	1:A:197:LYS:HD2	2.20	0.41
2:B:47:CYS:HA	2:B:152:LEU:O	2.20	0.41
1:A:26:GLN:NE2	1:A:26:GLN:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:PHE:H	1:A:93:VAL:HG23	1.86	0.41
1:A:168:MET:HE1	1:A:179:PRO:HB3	2.03	0.41
1:A:254:ARG:O	1:A:265:VAL:HG23	2.21	0.41
1:A:268:PRO:HA	1:A:270:HIS:C	2.46	0.41
1:A:43:VAL:HG21	1:A:167:PHE:CE2	2.57	0.40
1:A:173:ASN:HD22	1:A:294:LEU:CD2	2.34	0.40
3:C:34:LEU:HD13	3:C:34:LEU:C	2.37	0.40
1:A:126:PHE:CZ	1:A:175:VAL:HG22	2.56	0.40
1:A:279:MET:HE3	1:A:280:LEU:HD12	2.02	0.40
2:B:54:GLY:CA	2:B:57:THR:HG21	2.39	0.40
1:A:156:PHE:CZ	2:B:185:LYS:HG2	2.56	0.40
1:A:165:VAL:O	1:A:169:LYS:N	2.53	0.40
1:A:224:PHE:CD2	1:A:224:PHE:O	2.42	0.40
1:A:258:TYR:O	1:A:261:GLY:O	2.40	0.40
1:A:150:PHE:N	1:A:150:PHE:HD1	2.20	0.40
1:A:165:VAL:HG22	1:A:206:HIS:HE1	1.87	0.40
1:A:285:GLN:CB	1:A:288:GLN:NE2	2.84	0.40
2:B:212:ILE:HD12	2:B:213:TYR:C	2.46	0.40
3:C:182:PRO:HD2	3:C:183:GLU:H	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	212/361 (59%)	189 (89%)	18 (8%)	5 (2%)	<b>4</b> 30
2	B	216/427 (51%)	190 (88%)	21 (10%)	5 (2%)	<b>5</b> 31
3	C	202/418 (48%)	172 (85%)	25 (12%)	5 (2%)	<b>4</b> 29
All	All	630/1206 (52%)	551 (88%)	64 (10%)	15 (2%)	<b>4</b> 30

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	18	PRO
2	B	181	PRO
1	A	158	HIS
2	B	41	PHE
3	C	59	PRO
3	C	226	PRO
1	A	255	GLY
1	A	205	GLU
3	C	62	PRO
1	A	213	LEU
3	C	135	PRO
2	B	52	GLY
2	B	37	VAL
3	C	18	PRO
1	A	267	ASN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/320 (58%)	122 (66%)	64 (34%)	0	2
2	B	54/381 (14%)	33 (61%)	21 (39%)	0	1
3	C	58/380 (15%)	40 (69%)	18 (31%)	0	2
All	All	298/1081 (28%)	195 (65%)	103 (35%)	0	2

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	28	HIS
1	A	34	LYS
1	A	39	THR
1	A	48	LEU
1	A	61	ASP
1	A	62	LEU
1	A	85	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	86	VAL
1	A	87	GLU
1	A	93	VAL
1	A	98	THR
1	A	119	ILE
1	A	122	ILE
1	A	124	GLU
1	A	127	GLU
1	A	134	SER
1	A	141	ILE
1	A	145	ARG
1	A	146	VAL
1	A	148	CYS
1	A	149	CYS
1	A	153	ILE
1	A	158	HIS
1	A	160	LEU
1	A	163	LEU
1	A	164	ASP
1	A	165	VAL
1	A	167	PHE
1	A	176	ASN
1	A	180	VAL
1	A	181	ILE
1	A	183	LYS
1	A	187	LEU
1	A	188	THR
1	A	189	LEU
1	A	195	LEU
1	A	197	LYS
1	A	200	LEU
1	A	201	ASP
1	A	208	ILE
1	A	211	TYR
1	A	224	PHE
1	A	229	ARG
1	A	230	LEU
1	A	231	LEU
1	A	235	ILE
1	A	237	PHE
1	A	239	VAL
1	A	245	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	246	ILE
1	A	254	ARG
1	A	257	LEU
1	A	262	VAL
1	A	266	GLU
1	A	270	HIS
1	A	274	LEU
1	A	276	LEU
1	A	277	ARG
1	A	279	MET
1	A	283	HIS
1	A	285	GLN
1	A	286	ASP
1	A	293	ASP
2	B	57	THR
2	B	58	LEU
2	B	60	ASP
2	B	61	THR
2	B	67	PHE
2	B	150	VAL
2	B	151	CYS
2	B	152	LEU
2	B	155	ILE
2	B	164	SER
2	B	166	ASP
2	B	168	VAL
2	B	169	THR
2	B	173	LEU
2	B	174	ASP
2	B	185	LYS
2	B	210	VAL
2	B	251	MET
2	B	260	THR
2	B	283	MET
2	B	306	MET
3	C	34	LEU
3	C	37	VAL
3	C	40	SER
3	C	46	THR
3	C	50	SER
3	C	51	LEU
3	C	52	PHE

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Mol	Chain	Res	Type
3	C	53	LEU
3	C	54	THR
3	C	56	LEU
3	C	61	TYR
3	C	134	MET
3	C	174	ILE
3	C	178	ASP
3	C	180	LEU
3	C	181	THR
3	C	192	ILE
3	C	255	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	172	HIS
1	A	173	ASN
1	A	206	HIS
1	A	212	HIS
1	A	270	HIS
1	A	283	HIS
1	A	285	GLN
1	A	295	HIS
2	B	262	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GTP	B	428	-	33,34,34	0.94	1 (3%)	50,54,54	1.62	9 (18%)
4	GDP	C	419	-	29,30,30	1.16	3 (10%)	45,47,47	1.80	7 (15%)
4	GDP	A	362	-	29,30,30	1.17	3 (10%)	45,47,47	1.80	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	B	428	-	-	4/22/38/38	0/3/3/3
4	GDP	C	419	-	-	5/16/32/32	0/3/3/3
4	GDP	A	362	-	-	2/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	362	GDP	C5-C4	3.22	1.47	1.38
4	C	419	GDP	C5-C4	3.18	1.47	1.38
4	A	362	GDP	C6-N1	-2.44	1.34	1.38
4	C	419	GDP	C6-N1	-2.39	1.34	1.38
5	B	428	GTP	C2-N3	2.22	1.38	1.33
4	C	419	GDP	C5-N7	-2.03	1.35	1.39
4	A	362	GDP	C5-N7	-2.02	1.35	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	419	GDP	C5-C4-N3	-6.16	118.58	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	362	GDP	C5-C4-N3	-6.15	118.60	128.39
5	B	428	GTP	C5-C4-N3	-5.08	120.30	128.39
4	A	362	GDP	C2-N3-C4	5.04	120.98	112.30
4	C	419	GDP	C2-N3-C4	5.04	120.98	112.30
5	B	428	GTP	C2-N3-C4	4.63	120.27	112.30
4	A	362	GDP	N9-C4-N3	4.58	135.10	125.95
4	C	419	GDP	N9-C4-N3	4.56	135.07	125.95
5	B	428	GTP	N9-C4-N3	3.27	132.50	125.95
4	A	362	GDP	C6-C5-N7	3.25	136.20	130.29
4	C	419	GDP	C6-C5-N7	3.24	136.19	130.29
5	B	428	GTP	C2-N1-C6	-2.90	119.86	125.11
5	B	428	GTP	N9-C8-N7	-2.60	108.58	113.40
4	C	419	GDP	C4-C5-N7	-2.59	106.57	110.67
4	A	362	GDP	C4-C5-N7	-2.57	106.59	110.67
4	C	419	GDP	C3'-C2'-C1'	2.54	106.27	101.46
4	A	362	GDP	C3'-C2'-C1'	2.53	106.24	101.46
5	B	428	GTP	C5-C6-N1	2.49	119.59	113.25
5	B	428	GTP	C8-N7-C5	2.48	108.68	104.26
5	B	428	GTP	O6-C6-C5	-2.40	120.20	126.53
5	B	428	GTP	C3'-C2'-C1'	2.32	105.86	101.46
4	A	362	GDP	O6-C6-C5	-2.12	120.94	126.53
4	C	419	GDP	O6-C6-C5	-2.09	121.01	126.53

There are no chirality outliers.

All (11) torsion outliers are listed below:

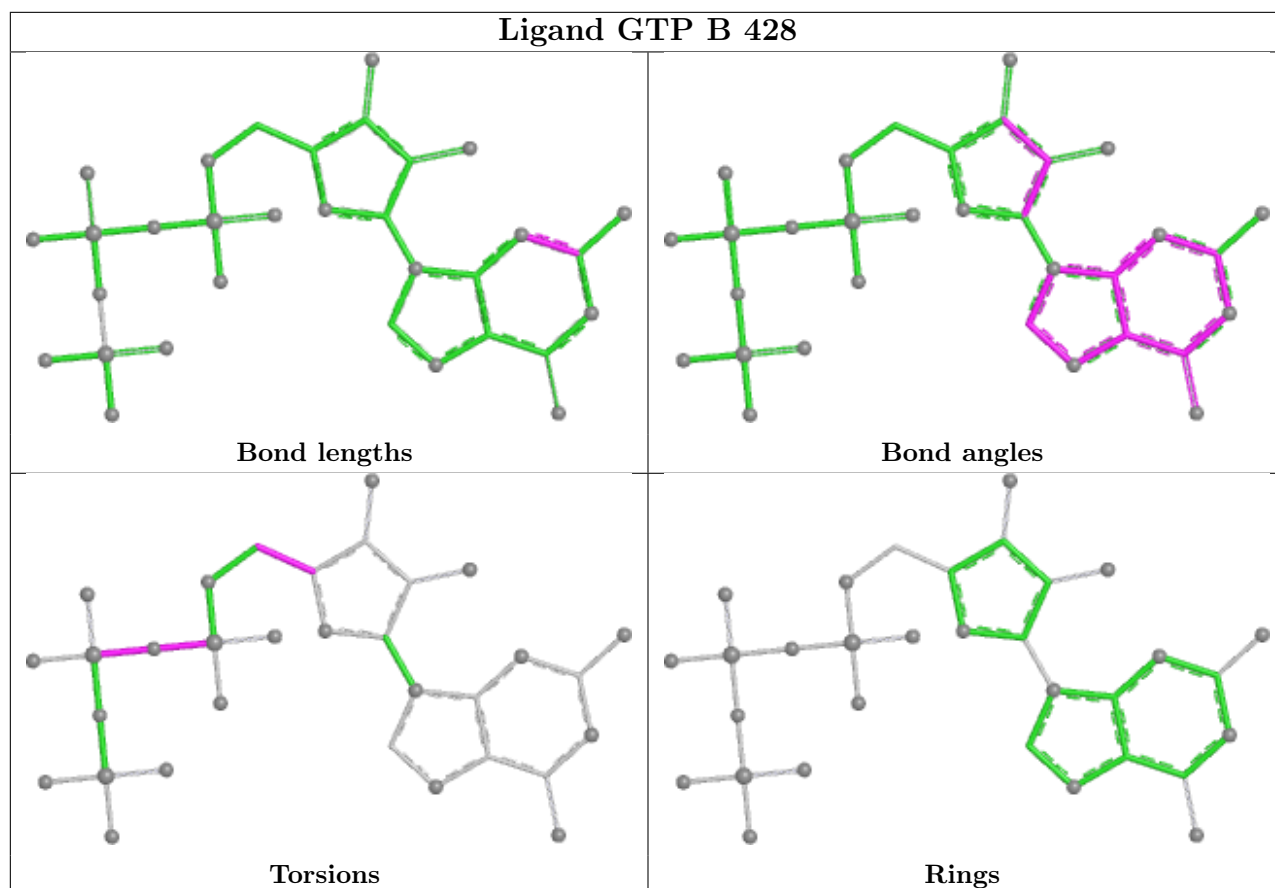
Mol	Chain	Res	Type	Atoms
4	C	419	GDP	C5'-O5'-PA-O3A
4	C	419	GDP	C5'-O5'-PA-O1A
4	A	362	GDP	O4'-C4'-C5'-O5'
4	A	362	GDP	C3'-C4'-C5'-O5'
5	B	428	GTP	O4'-C4'-C5'-O5'
5	B	428	GTP	PA-O3A-PB-O1B
4	C	419	GDP	C5'-O5'-PA-O2A
4	C	419	GDP	PB-O3A-PA-O1A
4	C	419	GDP	C4'-C5'-O5'-PA
5	B	428	GTP	C3'-C4'-C5'-O5'
5	B	428	GTP	PB-O3A-PA-O2A

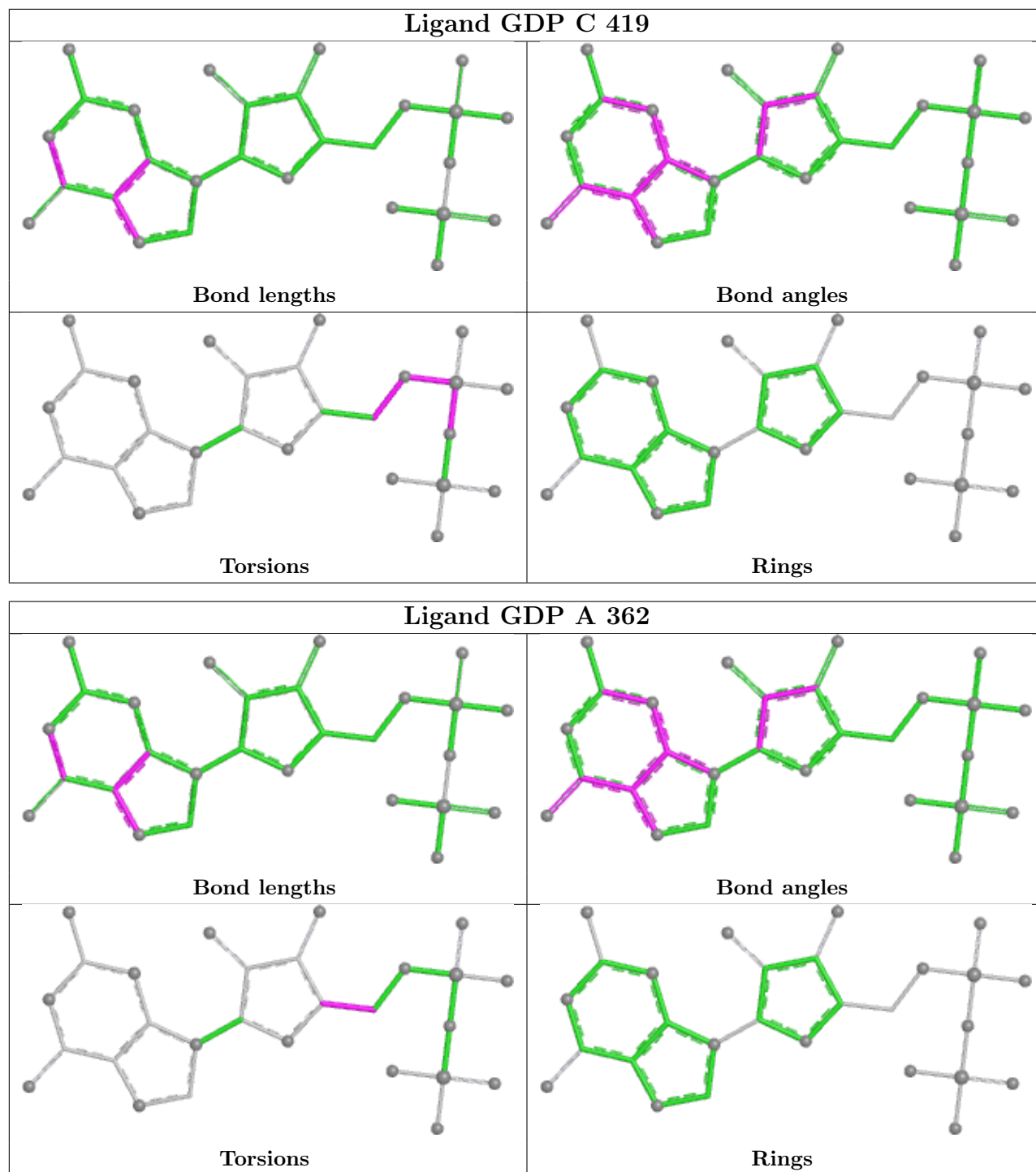
There are no ring outliers.

3 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	428	GTP	18	0
4	C	419	GDP	16	0
4	A	362	GDP	14	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	A	232/361 (64%)	2.10	103 (44%) <b>0</b> <b>1</b>	2, 81, 122, 148	0
2	B	246/427 (57%)	1.71	85 (34%) <b>1</b> <b>2</b>	3, 60, 134, 139	0
3	C	224/418 (53%)	1.70	77 (34%) <b>1</b> <b>2</b>	26, 80, 134, 156	0
All	All	702/1206 (58%)	1.84	265 (37%) <b>1</b> <b>2</b>	2, 73, 130, 156	0

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	SER	9.2
2	B	26	ASP	7.0
1	A	156	PHE	6.9
3	C	137	ASN	6.8
3	C	41	GLY	6.7
2	B	247	GLY	6.6
2	B	145	ASP	6.3
1	A	289	GLU	6.3
3	C	133	GLN	6.2
3	C	245	GLY	6.0
1	A	241	GLY	5.9
2	B	178	ASN	5.8
3	C	134	MET	5.8
2	B	179	ILE	5.6
2	B	144	HIS	5.5
2	B	131	GLN	5.4
2	B	184	ALA	5.4
1	A	41	MET	5.4
3	C	179	THR	5.3
1	A	81	ILE	5.1
1	A	186	THR	4.9
1	A	98	THR	4.9
1	A	210	ILE	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	149	CYS	4.8
2	B	75	THR	4.8
1	A	293	ASP	4.7
1	A	34	LYS	4.7
1	A	116	LYS	4.6
3	C	169	ASN	4.6
1	A	45	GLU	4.5
3	C	39	GLU	4.5
3	C	37	VAL	4.5
2	B	159	GLY	4.5
1	A	82	GLU	4.4
1	A	121	TYR	4.4
1	A	185	ASP	4.4
2	B	136	ILE	4.4
2	B	262	GLN	4.4
2	B	193	GLU	4.3
3	C	151	HIS	4.3
3	C	176	LYS	4.2
2	B	85	THR	4.2
2	B	234	PRO	4.2
1	A	158	HIS	4.1
3	C	263	PHE	4.1
3	C	175	ALA	4.1
3	C	295	LEU	4.1
3	C	231	GLY	4.1
1	A	259	PRO	4.0
1	A	177	ILE	4.0
2	B	261	VAL	4.0
1	A	35	GLY	3.9
2	B	183	ILE	3.9
3	C	135	PRO	3.9
2	B	107	ASP	3.9
1	A	206	HIS	3.9
2	B	51	THR	3.8
3	C	262	ASP	3.8
1	A	28	HIS	3.8
1	A	209	LYS	3.8
3	C	147	ALA	3.8
2	B	259	GLY	3.8
2	B	100	VAL	3.8
2	B	248	ASN	3.8
1	A	176	ASN	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	31	SER	3.8
2	B	268	HIS	3.8
1	A	243	ASN	3.7
1	A	56	SER	3.7
2	B	86	TYR	3.7
1	A	148	CYS	3.7
3	C	170	ILE	3.7
3	C	290	TYR	3.7
3	C	141	CYS	3.7
3	C	174	ILE	3.6
3	C	161	MET	3.6
1	A	40	LEU	3.6
3	C	261	CYS	3.6
2	B	154	PHE	3.6
2	B	213	TYR	3.6
3	C	38	GLY	3.6
3	C	177	ALA	3.5
1	A	133	GLU	3.5
2	B	113	ASP	3.5
1	A	155	PRO	3.5
3	C	255	VAL	3.4
1	A	42	VAL	3.4
1	A	178	VAL	3.4
3	C	146	ILE	3.4
2	B	269	CYS	3.4
3	C	91	THR	3.4
2	B	153	TYR	3.4
3	C	252	VAL	3.4
2	B	84	ASN	3.4
3	C	142	CYS	3.3
1	A	240	VAL	3.3
1	A	97	LEU	3.3
2	B	283	MET	3.3
2	B	176	LYS	3.3
2	B	185	LYS	3.3
2	B	156	ALA	3.3
3	C	35	MET	3.2
1	A	211	TYR	3.2
1	A	202	GLU	3.2
2	B	157	PRO	3.2
1	A	242	SER	3.2
2	B	98	THR	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	80	GLN	3.2
3	C	140	GLN	3.2
3	C	275	MET	3.2
2	B	50	GLU	3.2
1	A	179	PRO	3.2
1	A	96	ARG	3.2
2	B	42	CYS	3.1
3	C	62	PRO	3.1
3	C	148	PRO	3.1
1	A	160	LEU	3.1
2	B	47	CYS	3.1
3	C	60	GLU	3.1
1	A	238	SER	3.1
3	C	40	SER	3.1
3	C	59	PRO	3.0
1	A	153	ILE	3.0
2	B	188	ALA	3.0
3	C	127	SER	3.0
3	C	247	GLN	3.0
1	A	198	ARG	3.0
3	C	132	ARG	3.0
3	C	30	PHE	3.0
1	A	180	VAL	3.0
3	C	253	ALA	2.9
2	B	229	MET	2.9
2	B	49	GLY	2.9
1	A	38	PHE	2.9
2	B	155	ILE	2.9
1	A	92	GLY	2.9
2	B	53	LEU	2.9
2	B	78	GLY	2.9
2	B	148	ILE	2.9
2	B	102	THR	2.9
3	C	136	ASP	2.9
2	B	46	LEU	2.9
3	C	93	VAL	2.8
1	A	266	GLU	2.8
3	C	108	TRP	2.8
2	B	25	PHE	2.8
2	B	140	LEU	2.8
2	B	203	SER	2.8
1	A	135	GLY	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	152	GLY	2.8
1	A	257	LEU	2.8
1	A	154	SER	2.8
1	A	184	ALA	2.8
3	C	52	PHE	2.8
2	B	177	VAL	2.8
1	A	33	LYS	2.8
1	A	244	GLN	2.8
1	A	290	VAL	2.8
2	B	286	LEU	2.8
3	C	178	ASP	2.8
2	B	143	TYR	2.7
1	A	52	THR	2.7
1	A	286	ASP	2.7
3	C	264	THR	2.7
2	B	149	HIS	2.7
1	A	260	TRP	2.7
3	C	131	ARG	2.7
3	C	296	ALA	2.7
3	C	246	ARG	2.7
3	C	42	LEU	2.7
1	A	182	ALA	2.6
1	A	26	GLN	2.6
1	A	84	SER	2.6
1	A	272	ASP	2.6
2	B	170	MET	2.6
2	B	303	LEU	2.6
1	A	151	TYR	2.6
3	C	272	ARG	2.6
1	A	83	ALA	2.6
1	A	131	HIS	2.5
1	A	147	HIS	2.5
3	C	202	LYS	2.5
3	C	228	ALA	2.5
1	A	214	PRO	2.5
1	A	212	HIS	2.5
2	B	44	ASN	2.5
1	A	21	ALA	2.5
2	B	298	TYR	2.5
2	B	109	ILE	2.5
2	B	181	PRO	2.5
2	B	212	ILE	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	290	THR	2.5
1	A	150	PHE	2.5
2	B	277	MET	2.4
1	A	78	THR	2.4
3	C	230	VAL	2.4
1	A	47	GLY	2.4
3	C	167	LYS	2.4
1	A	62	LEU	2.4
1	A	25	ASN	2.4
3	C	130	ASN	2.4
2	B	54	GLY	2.4
3	C	34	LEU	2.4
1	A	132	ASP	2.4
3	C	203	ILE	2.4
1	A	264	GLU	2.4
2	B	101	SER	2.4
2	B	187	ASP	2.4
1	A	168	MET	2.4
1	A	194	ARG	2.4
2	B	189	ILE	2.4
1	A	256	ARG	2.4
3	C	150	GLY	2.3
2	B	150	VAL	2.3
1	A	263	VAL	2.3
1	A	284	MET	2.3
1	A	277	ARG	2.3
2	B	251	MET	2.3
2	B	306	MET	2.3
2	B	120	GLU	2.3
3	C	65	SER	2.3
2	B	238	ILE	2.3
1	A	44	GLY	2.3
2	B	281	VAL	2.3
1	A	300	ARG	2.3
2	B	151	CYS	2.3
3	C	226	PRO	2.3
2	B	99	ILE	2.2
3	C	43	GLY	2.2
2	B	222	VAL	2.2
1	A	205	GLU	2.2
1	A	224	PHE	2.2
1	A	304	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	104	GLY	2.2
1	A	291	THR	2.2
1	A	119	ILE	2.2
2	B	105	PHE	2.2
1	A	50	LYS	2.2
1	A	294	LEU	2.2
3	C	76	GLN	2.2
1	A	157	GLY	2.2
2	B	40	GLY	2.2
1	A	58	PHE	2.2
2	B	228	THR	2.2
3	C	204	TYR	2.1
3	C	229	VAL	2.1
3	C	126	GLU	2.1
1	A	159	GLY	2.1
1	A	163	LEU	2.1
1	A	190	LYS	2.1
1	A	236	PRO	2.1
3	C	172	PRO	2.1
2	B	226	ASN	2.1
1	A	152	PHE	2.1
2	B	94	ARG	2.1
1	A	32	VAL	2.1
1	A	239	VAL	2.1
2	B	232	HIS	2.1
3	C	50	SER	2.1
3	C	125	ALA	2.0
3	C	193	MET	2.0
2	B	158	THR	2.0
3	C	51	LEU	2.0
3	C	157	ASP	2.0
1	A	145	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

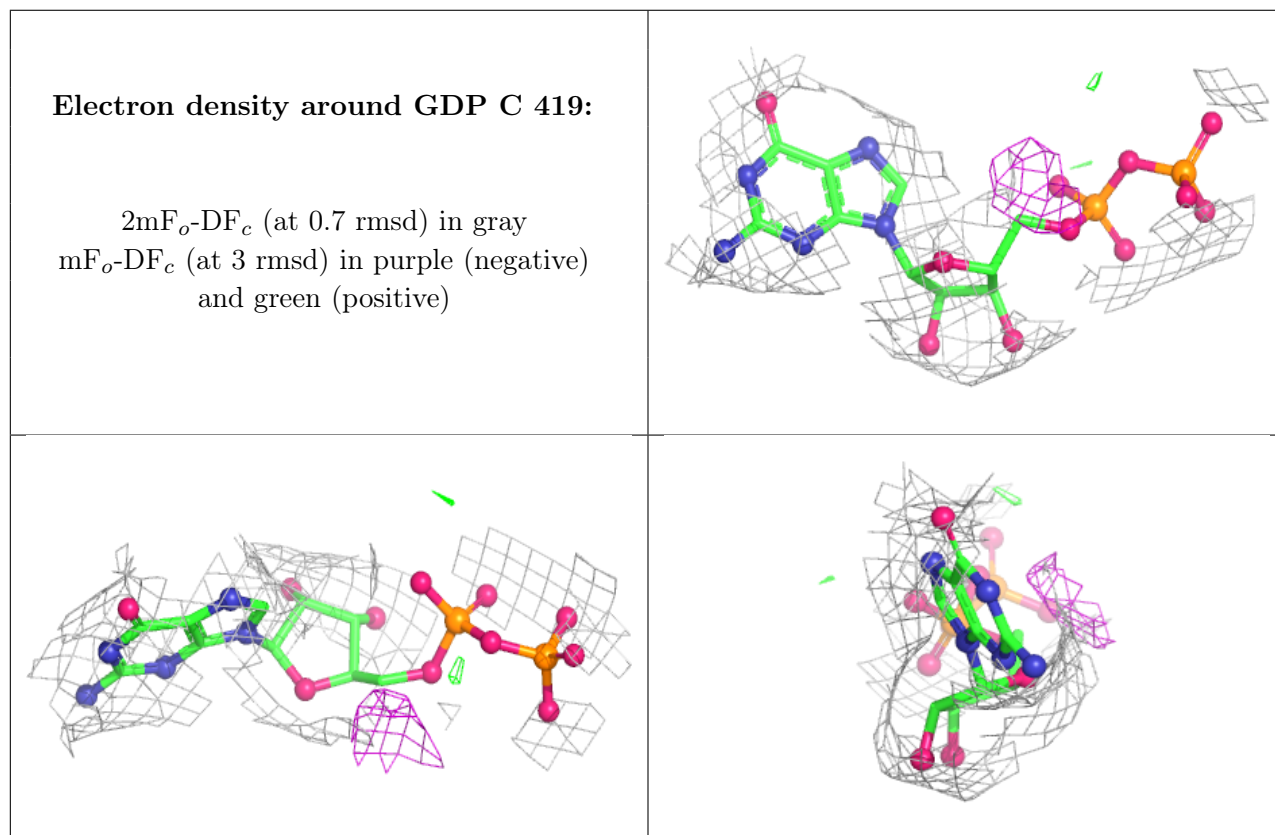
There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

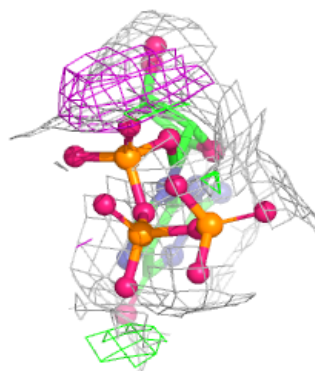
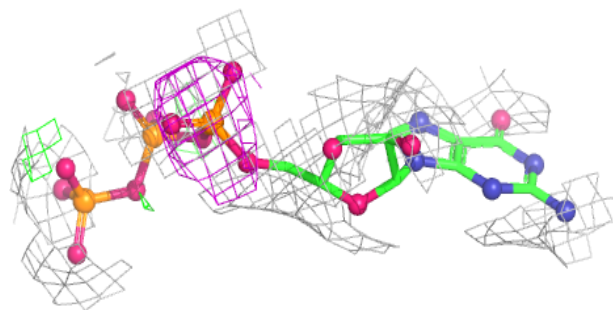
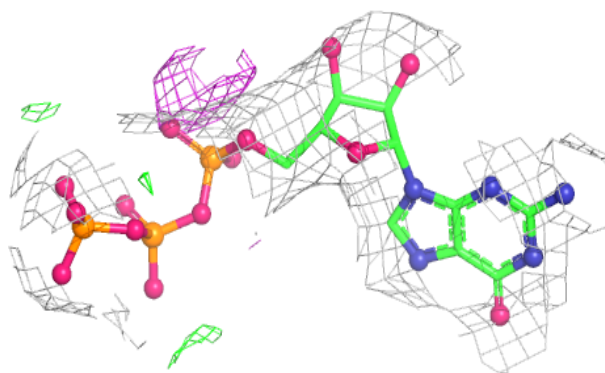
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GDP	C	419	28/28	0.85	0.15	83,89,97,100	0
5	GTP	B	428	32/32	0.86	0.17	35,56,65,67	0
4	GDP	A	362	28/28	0.87	0.19	53,75,81,81	0

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

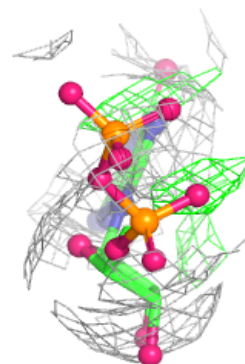
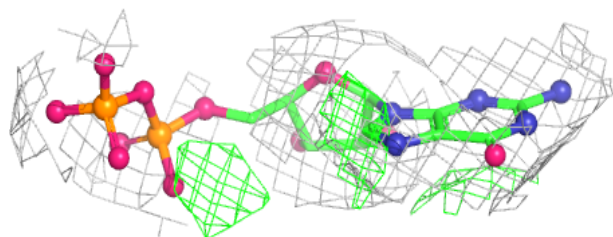
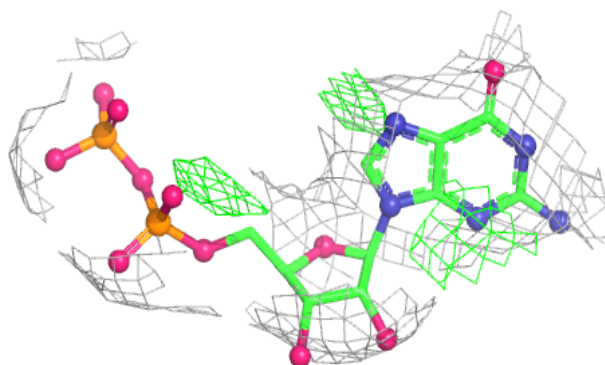


**Electron density around GTP B 428:**

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

**Electron density around GDP A 362:**

$2mF_o-DF_c$  (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.