



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 09:35 AM UTC

PDB ID : 5ND7 / pdb_00005nd7
EMDB ID : EMD-3623
Title : Microtubule-bound MKLP2 motor domain in the presence of AMPPNP
Authors : Atherton, J.; Yu, I.-M.; Cook, A.; Muretta, J.M.; Joseph, A.P.; Major, J.; Sourigues, Y.; Clause, J.; Topf, M.; Rosenfeld, S.S.; Houdusse, A.; Moores, C.A.
Deposited on : 2017-03-07
Resolution : 7.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

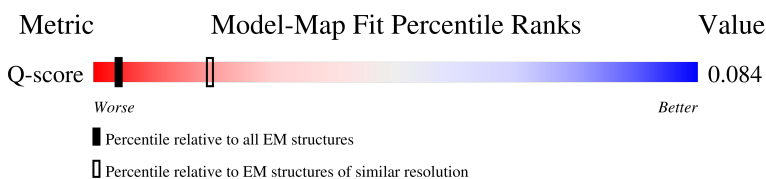
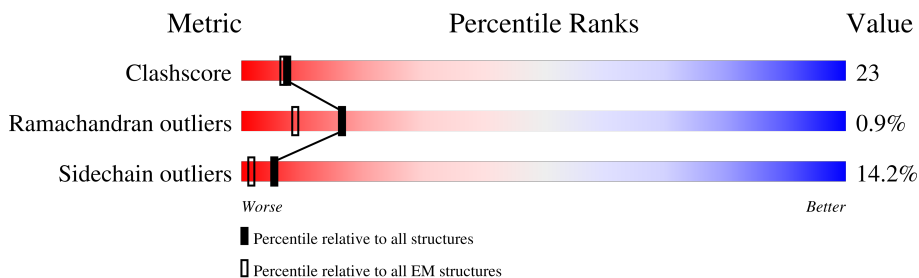
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.90 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.



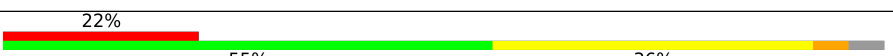
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	366 (7.40 - 8.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-C	501	
1	2-C	501	
1	3-C	501	
1	4-C	501	

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Mol	Chain	Length	Quality of chain
1	5-C	501	
2	1-A	451	
2	2-A	451	
2	3-A	451	
2	4-A	451	
2	5-A	451	
3	1-B	445	
3	2-B	445	
3	3-B	445	
3	4-B	445	
3	5-B	445	

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
6	GTP	1-A	500	-	-	X	-
6	GTP	2-A	500	-	-	X	-
6	GTP	3-A	500	-	-	X	-
6	GTP	4-A	500	-	-	X	-
6	GTP	5-A	500	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 45700 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Kinesin-like protein KIF20A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-C	300	Total	C	N	O	S	0	0
			2407	1531	425	440	11		
1	2-C	300	Total	C	N	O	S	0	0
			2407	1531	425	440	11		
1	3-C	300	Total	C	N	O	S	0	0
			2407	1531	425	440	11		
1	4-C	300	Total	C	N	O	S	0	0
			2407	1531	425	440	11		
1	5-C	300	Total	C	N	O	S	0	0
			2407	1531	425	440	11		

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		
2	2-A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		
2	3-A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		
2	4-A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		
2	5-A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	SER	LEU	conflict	UNP F2Z4C1
A	265	GLY	ILE	conflict	UNP F2Z4C1
A	358	GLU	GLN	conflict	UNP F2Z4C1

- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		
3	2-B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		
3	3-B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		
3	4-B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		
3	5-B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		

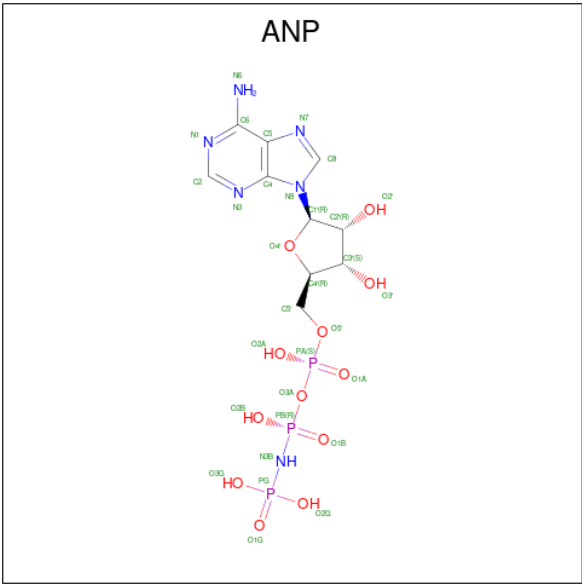
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	57	ALA	THR	conflict	UNP Q6B856
B	172	VAL	MET	conflict	UNP Q6B856
B	298	ALA	SER	conflict	UNP Q6B856
B	318	VAL	ILE	conflict	UNP Q6B856

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	1-C	1	Total	Mg	0
			1	1	
4	2-C	1	Total	Mg	0
			1	1	
4	3-C	1	Total	Mg	0
			1	1	
4	4-C	1	Total	Mg	0
			1	1	
4	5-C	1	Total	Mg	0
			1	1	
4	1-A	1	Total	Mg	0
			1	1	
4	2-A	1	Total	Mg	0
			1	1	
4	3-A	1	Total	Mg	0
			1	1	
4	4-A	1	Total	Mg	0
			1	1	
4	5-A	1	Total	Mg	0
			1	1	

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



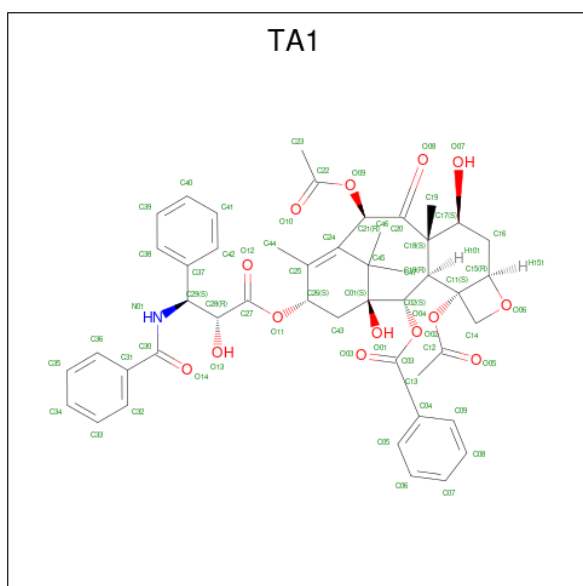
Mol	Chain	Residues	Atoms					AltConf
5	1-C	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	2-C	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	3-C	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	4-C	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	5-C	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
7	1-B	1	Total	C	N	O	P	0
			28	10	5	11	2	
7	2-B	1	Total	C	N	O	P	0
			28	10	5	11	2	
7	3-B	1	Total	C	N	O	P	0
			28	10	5	11	2	
7	4-B	1	Total	C	N	O	P	0
			28	10	5	11	2	
7	5-B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 8 is TAXOL (CCD ID: TA1) (formula: $C_{47}H_{51}NO_{14}$).

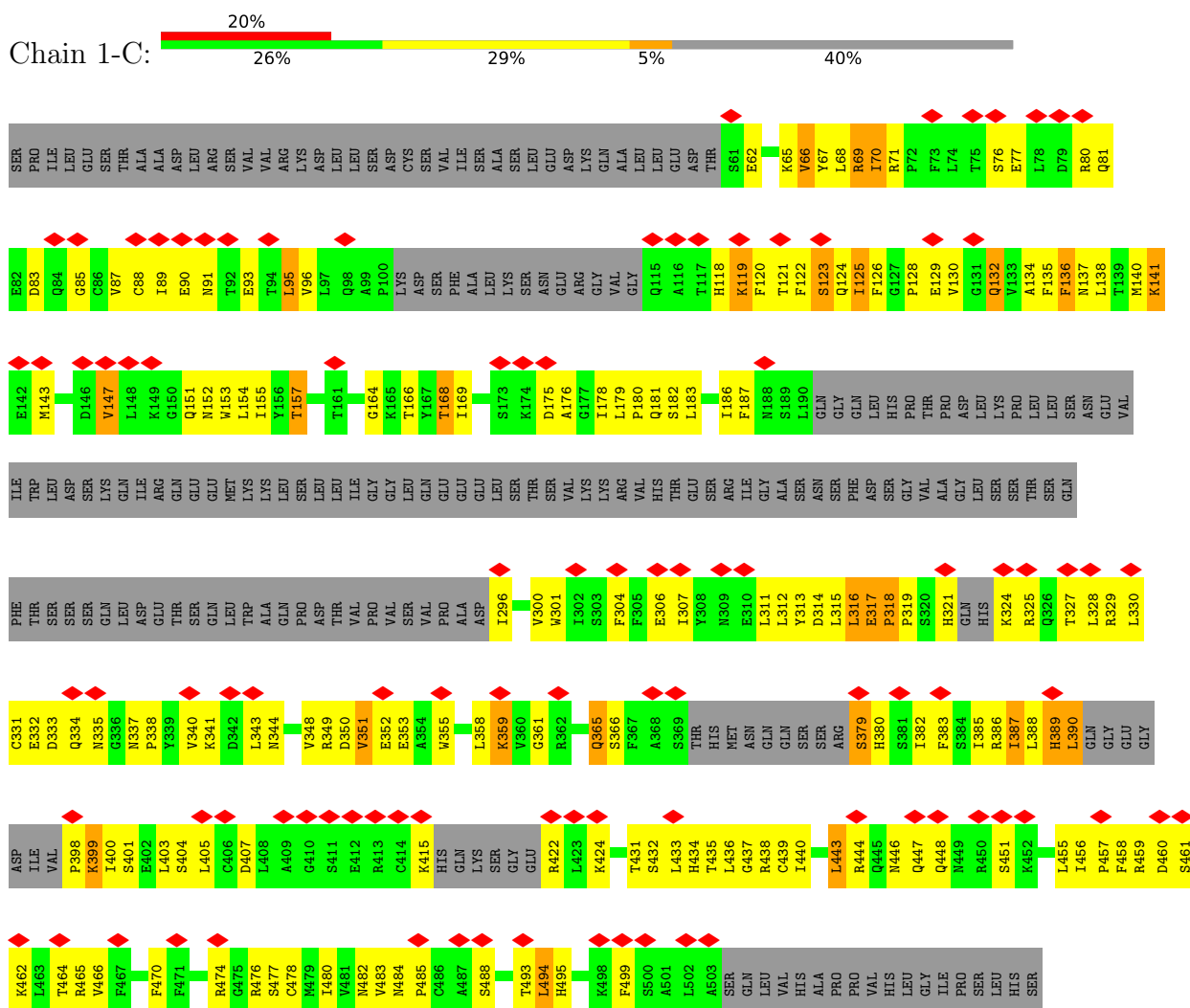


Mol	Chain	Residues	Atoms				AltConf
8	1-B	1	Total	C	N	O	0
			62	47	1	14	
8	2-B	1	Total	C	N	O	0
			62	47	1	14	
8	3-B	1	Total	C	N	O	0
			62	47	1	14	
8	4-B	1	Total	C	N	O	0
			62	47	1	14	
8	5-B	1	Total	C	N	O	0
			62	47	1	14	

3 Residue-property plots

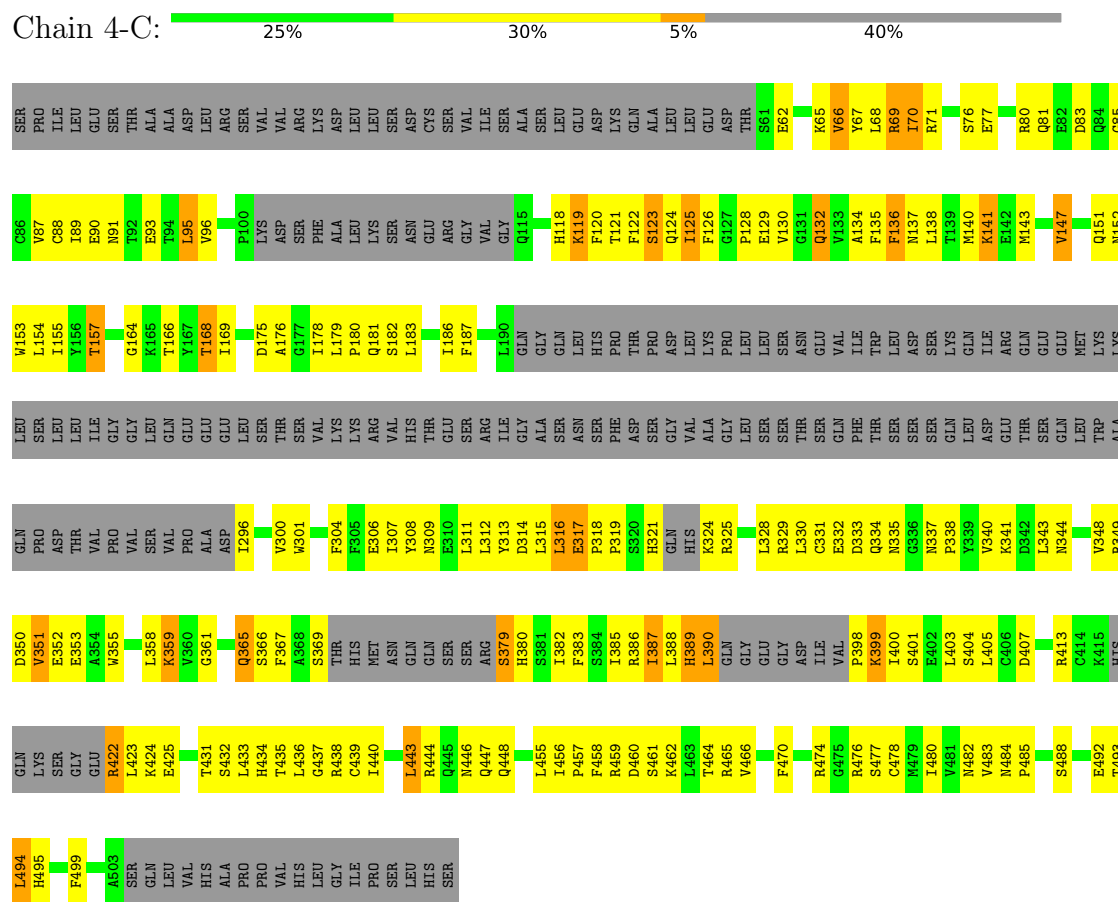
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Kinesin-like protein KIF20A

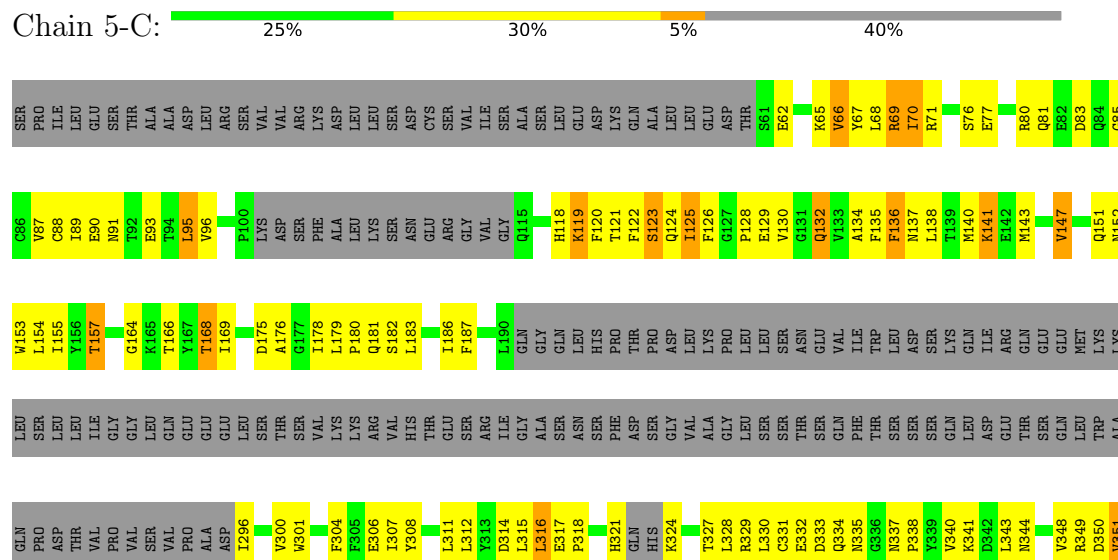


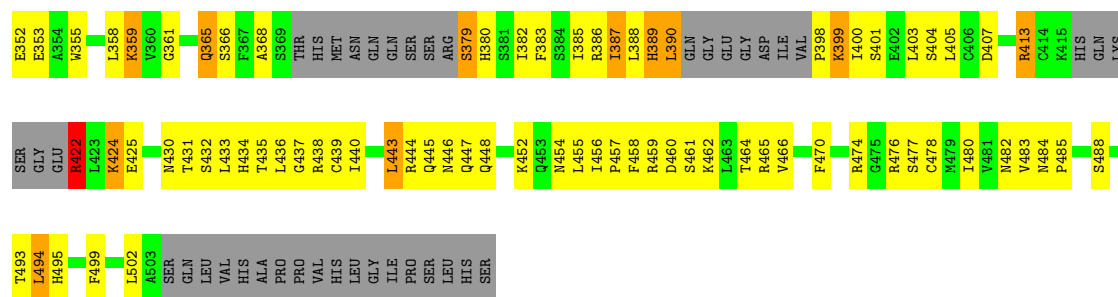


- Molecule 1: Kinesin-like protein KIF20A

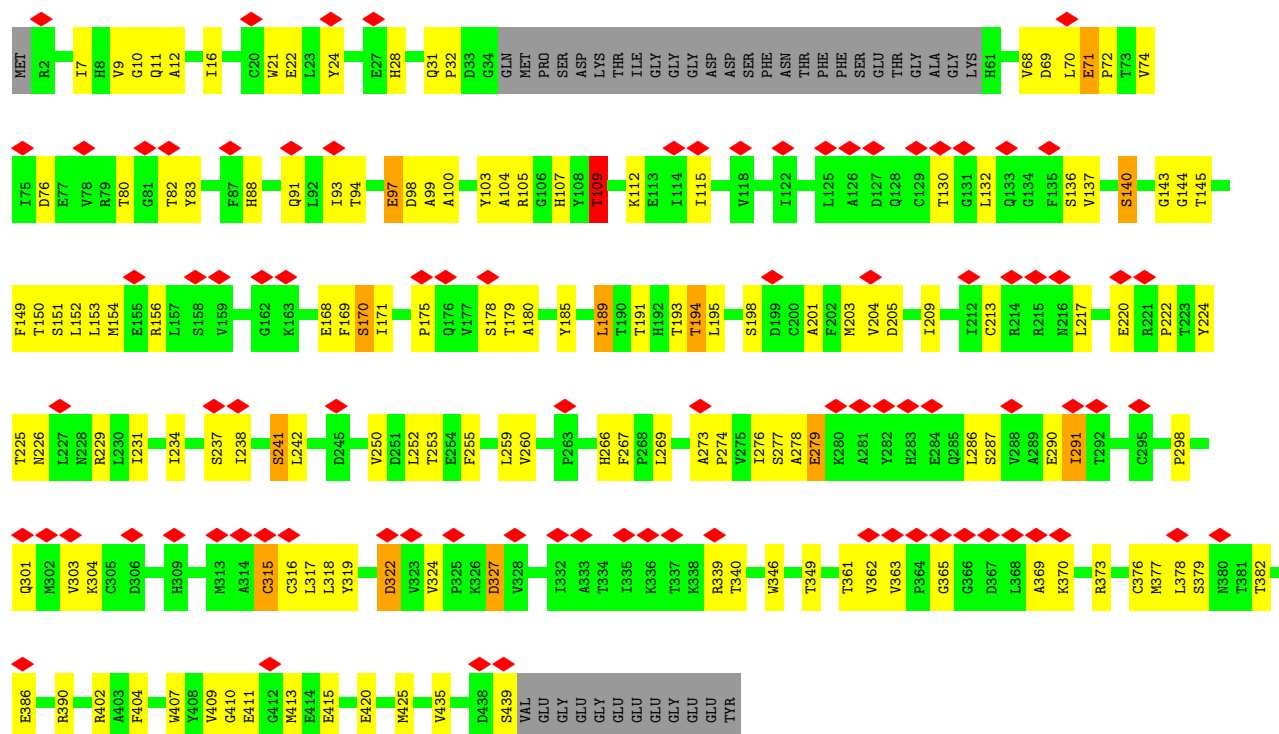


- Molecule 1: Kinesin-like protein KIF20A

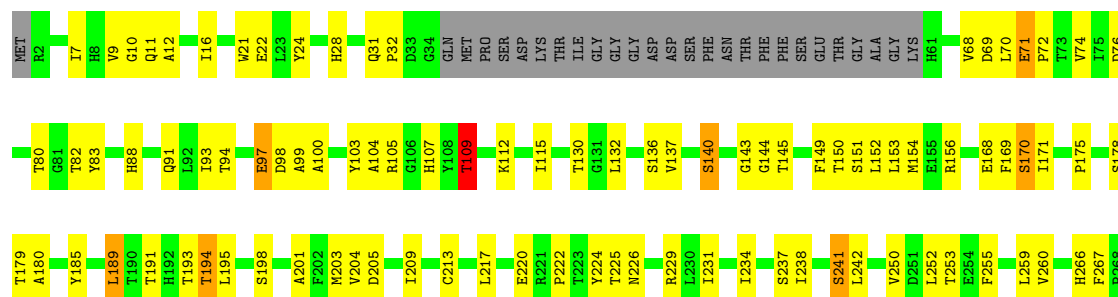


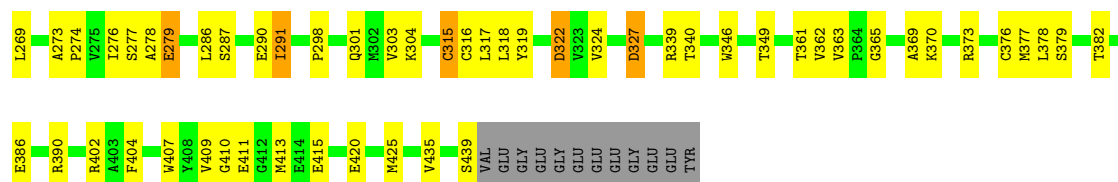


• Molecule 2: Tubulin alpha chain



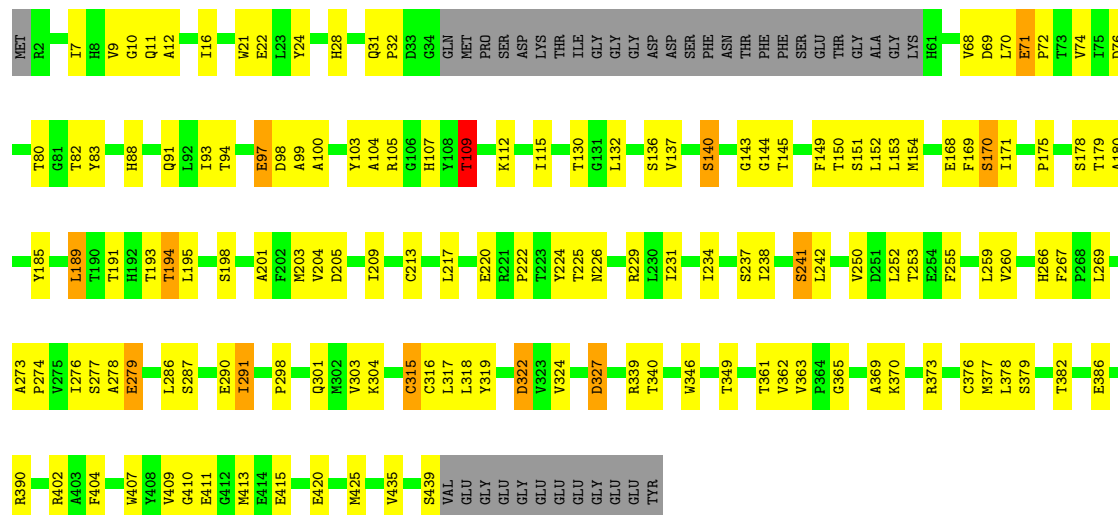
• Molecule 2: Tubulin alpha chain





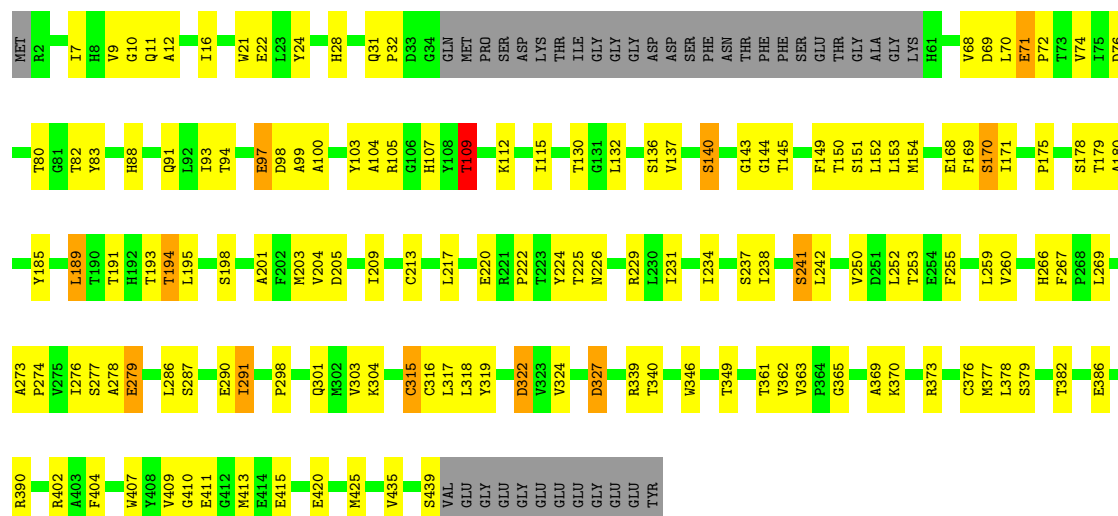
• Molecule 2: Tubulin alpha chain

Chain 3-A: 59% 29% 9%



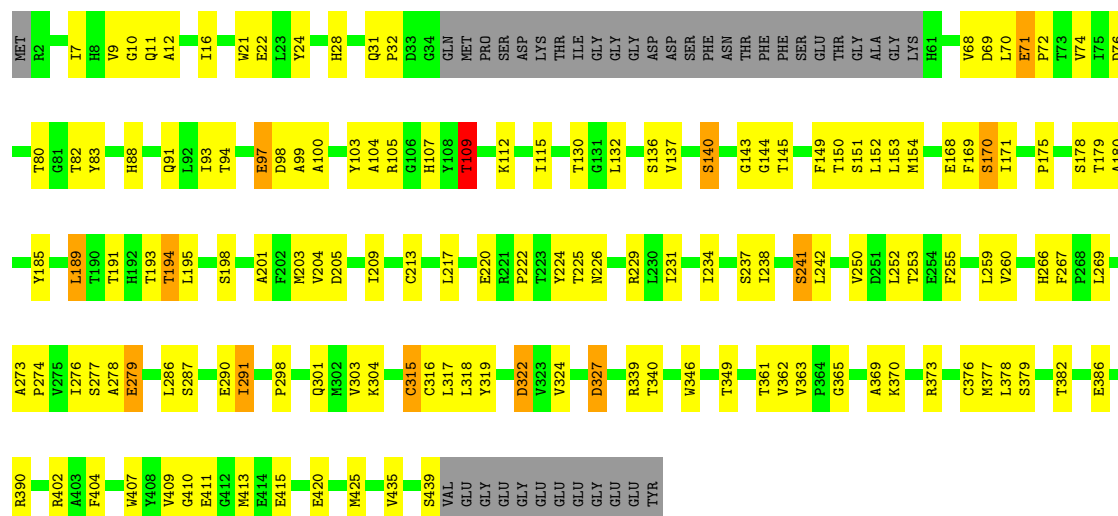
• Molecule 2: Tubulin alpha chain

Chain 4-A: 59% 29% 9%

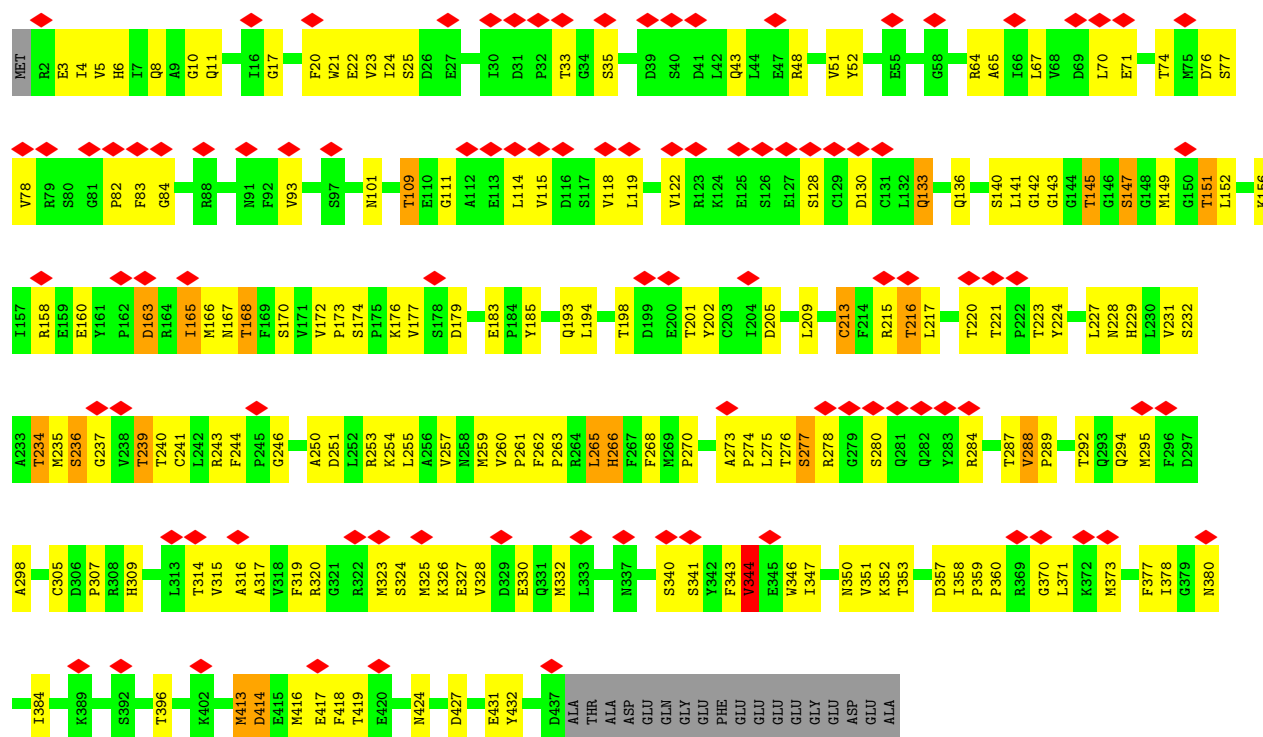


• Molecule 2: Tubulin alpha chain

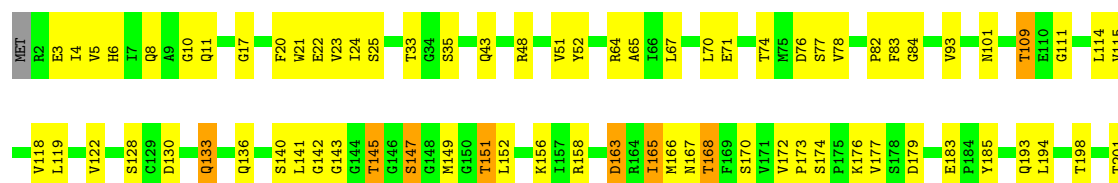
Chain 5-A: 59% 29% 9%

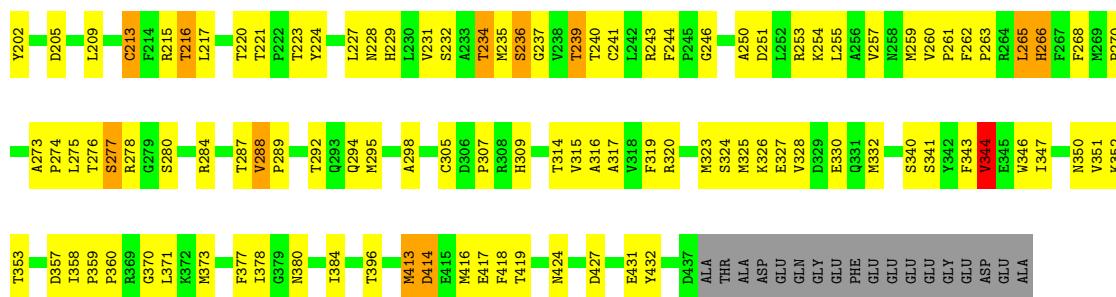


• Molecule 3: Tubulin beta-2B chain



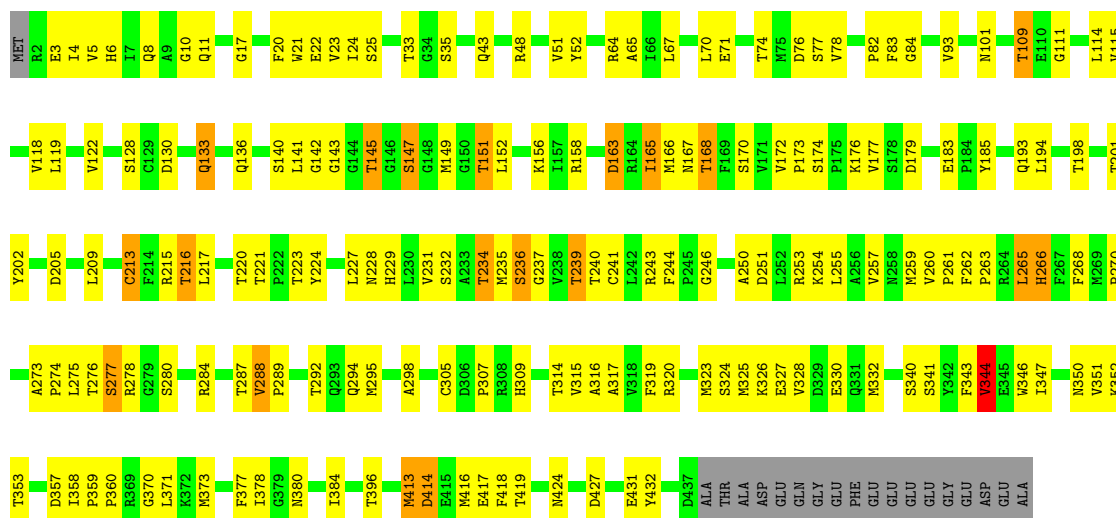
• Molecule 3: Tubulin beta-2B chain





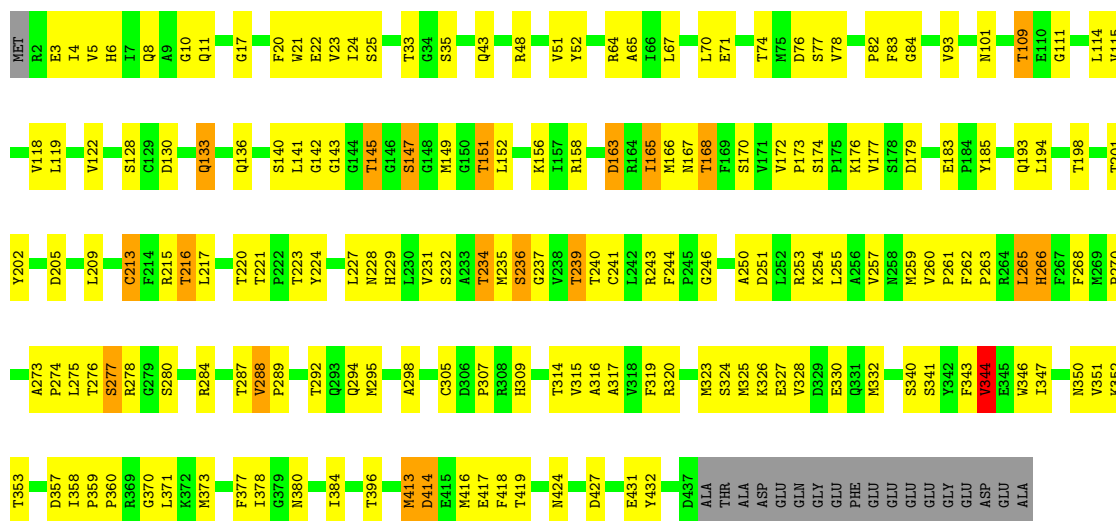
• Molecule 3: Tubulin beta-2B chain

Chain 3-B: 56% 36%



• Molecule 3: Tubulin beta-2B chain

Chain 4-B: 56% 36%



• Molecule 3: Tubulin beta-2B chain

Chain 5-B:

56%

36%

MET	R2	E3	I4	V5	H6	I7	Q8	A9	G10	Q11																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									</
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10858	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0322	Depositor
Map size (Å)	246.4, 214.06, 247.93999	wwPDB
Map dimensions	160, 139, 161	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.54, 1.54, 1.54	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, GTP, TA1, ANP

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	1-C	0.64	0/2450	0.89	1/3299 (0.0%)
1	2-C	0.64	0/2450	0.89	1/3299 (0.0%)
1	3-C	0.64	0/2450	0.89	1/3299 (0.0%)
1	4-C	0.64	0/2450	0.89	1/3299 (0.0%)
1	5-C	0.64	0/2450	0.89	1/3299 (0.0%)
2	1-A	0.37	0/3300	0.77	0/4482
2	2-A	0.37	0/3300	0.77	0/4482
2	3-A	0.37	0/3300	0.77	0/4482
2	4-A	0.37	0/3300	0.77	0/4482
2	5-A	0.37	0/3300	0.77	0/4482
3	1-B	0.39	0/3426	0.78	1/4642 (0.0%)
3	2-B	0.39	0/3426	0.78	1/4642 (0.0%)
3	3-B	0.39	0/3426	0.78	1/4642 (0.0%)
3	4-B	0.39	0/3426	0.78	1/4642 (0.0%)
3	5-B	0.39	0/3426	0.78	1/4642 (0.0%)
All	All	0.47	0/45880	0.81	10/62115 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	5-C	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-C	318	PRO	N-CA-C	5.62	117.56	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-C	318	PRO	N-CA-C	5.62	117.56	110.70
1	3-C	318	PRO	N-CA-C	5.62	117.56	110.70
1	4-C	318	PRO	N-CA-C	5.62	117.56	110.70
1	5-C	318	PRO	N-CA-C	5.62	117.56	110.70
3	1-B	414	ASP	CB-CA-C	-5.06	100.99	109.65
3	2-B	414	ASP	CB-CA-C	-5.06	100.99	109.65
3	3-B	414	ASP	CB-CA-C	-5.06	100.99	109.65
3	4-B	414	ASP	CB-CA-C	-5.06	100.99	109.65
3	5-B	414	ASP	CB-CA-C	-5.06	100.99	109.65

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	5-C	413	ARG	Sidechain
1	5-C	422	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-C	2407	0	2419	185	0
1	2-C	2407	0	2419	195	0
1	3-C	2407	0	2419	191	0
1	4-C	2407	0	2419	196	0
1	5-C	2407	0	2419	186	0
2	1-A	3227	0	3141	125	0
2	2-A	3227	0	3141	128	0
2	3-A	3227	0	3141	124	0
2	4-A	3227	0	3141	123	0
2	5-A	3227	0	3141	123	0
3	1-B	3351	0	3229	153	0
3	2-B	3351	0	3229	150	0
3	3-B	3351	0	3229	149	0
3	4-B	3351	0	3229	150	0
3	5-B	3351	0	3229	150	0
4	1-A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1-C	1	0	0	0	0
4	2-A	1	0	0	0	0
4	2-C	1	0	0	0	0
4	3-A	1	0	0	0	0
4	3-C	1	0	0	0	0
4	4-A	1	0	0	0	0
4	4-C	1	0	0	0	0
4	5-A	1	0	0	0	0
4	5-C	1	0	0	0	0
5	1-C	31	0	13	2	0
5	2-C	31	0	13	2	0
5	3-C	31	0	13	2	0
5	4-C	31	0	13	2	0
5	5-C	31	0	13	2	0
6	1-A	32	0	12	28	0
6	2-A	32	0	12	28	0
6	3-A	32	0	12	28	0
6	4-A	32	0	12	28	0
6	5-A	32	0	12	28	0
7	1-B	28	0	12	8	0
7	2-B	28	0	12	8	0
7	3-B	28	0	12	8	0
7	4-B	28	0	12	8	0
7	5-B	28	0	12	8	0
8	1-B	62	0	51	14	0
8	2-B	62	0	51	14	0
8	3-B	62	0	51	14	0
8	4-B	62	0	51	14	0
8	5-B	62	0	51	14	0
All	All	45700	0	44385	2073	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 23.

All (2073) 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)
2:A:179:THR:CB	6:A:500:GTP:H3'	1.62	1.27
2:A:179:THR:CB	6:A:500:GTP:H3'	1.62	1.27
2:A:179:THR:CB	6:A:500:GTP:H3'	1.62	1.27
2:A:179:THR:CB	6:A:500:GTP:H3'	1.62	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:179:THR:CB	6:A:500:GTP:H3'	1.62	1.27
1:C:369:SER:CB	1:C:413:ARG:HH12	1.46	1.27
1:C:460:ASP:OD2	3:B:263:PRO:HG3	1.33	1.26
1:C:460:ASP:OD2	3:B:263:PRO:HG3	1.36	1.24
1:C:460:ASP:OD2	3:B:263:PRO:HG3	1.37	1.23
1:C:460:ASP:OD2	3:B:263:PRO:HG3	1.38	1.23
1:C:460:ASP:OD2	3:B:263:PRO:HG3	1.37	1.22
2:A:11:GLN:HB3	6:A:500:GTP:O2B	1.53	1.07
2:A:11:GLN:HB3	6:A:500:GTP:O2B	1.53	1.07
2:A:11:GLN:HB3	6:A:500:GTP:O2B	1.53	1.07
2:A:11:GLN:HB3	6:A:500:GTP:O2B	1.53	1.07
2:A:11:GLN:HB3	6:A:500:GTP:O2B	1.53	1.07
1:C:369:SER:OG	1:C:422:ARG:NH1	1.88	1.07
1:C:369:SER:O	1:C:413:ARG:NE	1.88	1.05
1:C:369:SER:CB	1:C:413:ARG:NH1	2.19	1.05
2:A:179:THR:HB	6:A:500:GTP:H3'	1.34	1.02
2:A:179:THR:HB	6:A:500:GTP:H3'	1.34	1.02
2:A:179:THR:HB	6:A:500:GTP:H3'	1.34	1.02
2:A:179:THR:HB	6:A:500:GTP:H3'	1.34	1.02
2:A:179:THR:HB	6:A:500:GTP:H3'	1.34	1.02
1:C:333:ASP:HA	3:B:416:MET:SD	2.02	1.00
2:A:179:THR:CB	6:A:500:GTP:C3'	2.39	0.99
2:A:179:THR:CB	6:A:500:GTP:C3'	2.39	0.99
2:A:179:THR:CB	6:A:500:GTP:C3'	2.39	0.99
2:A:179:THR:CB	6:A:500:GTP:C3'	2.39	0.99
2:A:179:THR:CB	6:A:500:GTP:C3'	2.39	0.99
1:C:333:ASP:HA	3:B:416:MET:SD	2.03	0.99
1:C:333:ASP:HA	3:B:416:MET:SD	2.03	0.98
1:C:333:ASP:HA	3:B:416:MET:SD	2.03	0.98
1:C:333:ASP:HA	3:B:416:MET:SD	2.04	0.97
2:A:179:THR:OG1	6:A:500:GTP:C3'	2.12	0.96
2:A:179:THR:OG1	6:A:500:GTP:C3'	2.12	0.96
2:A:179:THR:OG1	6:A:500:GTP:C3'	2.12	0.96
2:A:179:THR:OG1	6:A:500:GTP:C3'	2.12	0.96
2:A:179:THR:OG1	6:A:500:GTP:C3'	2.12	0.96
1:C:334:GLN:N	3:B:416:MET:SD	2.38	0.96
2:A:179:THR:OG1	6:A:500:GTP:O3'	1.82	0.96
2:A:179:THR:OG1	6:A:500:GTP:O3'	1.82	0.96
2:A:179:THR:OG1	6:A:500:GTP:O3'	1.82	0.96
2:A:179:THR:OG1	6:A:500:GTP:O3'	1.82	0.96
2:A:179:THR:OG1	6:A:500:GTP:O3'	1.82	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:GLN:N	3:B:416:MET:SD	2.40	0.94
2:A:179:THR:CG2	6:A:500:GTP:H3'	1.98	0.93
2:A:179:THR:CG2	6:A:500:GTP:H3'	1.98	0.93
2:A:179:THR:CG2	6:A:500:GTP:H3'	1.98	0.93
2:A:179:THR:CG2	6:A:500:GTP:H3'	1.98	0.93
2:A:179:THR:CG2	6:A:500:GTP:H3'	1.98	0.93
1:C:334:GLN:N	3:B:416:MET:SD	2.41	0.93
1:C:334:GLN:N	3:B:416:MET:SD	2.41	0.93
2:A:11:GLN:CB	6:A:500:GTP:O2B	2.17	0.92
2:A:11:GLN:CB	6:A:500:GTP:O2B	2.17	0.92
2:A:11:GLN:CB	6:A:500:GTP:O2B	2.17	0.92
2:A:11:GLN:CB	6:A:500:GTP:O2B	2.17	0.92
2:A:11:GLN:CB	6:A:500:GTP:O2B	2.17	0.92
2:A:11:GLN:CB	6:A:500:GTP:O2B	2.17	0.92
3:B:10:GLY:HA2	3:B:145:THR:HB	1.54	0.90
3:B:10:GLY:HA2	3:B:145:THR:HB	1.54	0.90
3:B:10:GLY:HA2	3:B:145:THR:HB	1.54	0.90
3:B:10:GLY:HA2	3:B:145:THR:HB	1.54	0.90
3:B:10:GLY:HA2	3:B:145:THR:HB	1.54	0.90
1:C:334:GLN:N	3:B:416:MET:SD	2.44	0.89
1:C:301:TRP:HB2	1:C:386:ARG:HG3	1.51	0.89
1:C:301:TRP:HB2	1:C:386:ARG:HG3	1.51	0.89
1:C:301:TRP:HB2	1:C:386:ARG:HG3	1.51	0.89
1:C:301:TRP:HB2	1:C:386:ARG:HG3	1.51	0.89
1:C:301:TRP:HB2	1:C:386:ARG:HG3	1.51	0.89
1:C:330:LEU:HD11	1:C:466:VAL:HG12	1.53	0.88
1:C:459:ARG:HD3	3:B:427:ASP:OD2	1.71	0.88
1:C:330:LEU:HD11	1:C:466:VAL:HG12	1.54	0.88
1:C:330:LEU:HD11	1:C:466:VAL:HG12	1.53	0.88
1:C:330:LEU:HD11	1:C:466:VAL:HG12	1.53	0.88
1:C:330:LEU:HD11	1:C:466:VAL:HG12	1.53	0.88
1:C:313:TYR:HA	1:C:326:GLN:HE22	1.38	0.88
2:A:278:ALA:HB2	2:A:369:ALA:HA	1.54	0.87
2:A:278:ALA:HB2	2:A:369:ALA:HA	1.54	0.87
2:A:278:ALA:HB2	2:A:369:ALA:HA	1.54	0.87
2:A:278:ALA:HB2	2:A:369:ALA:HA	1.54	0.87
2:A:278:ALA:HB2	2:A:369:ALA:HA	1.54	0.87
1:C:88:CYS:HB2	1:C:96:VAL:HG13	1.57	0.86
1:C:88:CYS:HB2	1:C:96:VAL:HG13	1.57	0.86
1:C:88:CYS:HB2	1:C:96:VAL:HG13	1.57	0.86
1:C:88:CYS:HB2	1:C:96:VAL:HG13	1.57	0.86
1:C:88:CYS:HB2	1:C:96:VAL:HG13	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ARG:HD3	3:B:427:ASP:OD2	1.73	0.86
1:C:459:ARG:HD3	3:B:427:ASP:OD2	1.73	0.86
3:B:173:PRO:HB3	3:B:183:GLU:HG2	1.55	0.86
3:B:173:PRO:HB3	3:B:183:GLU:HG2	1.55	0.86
3:B:173:PRO:HB3	3:B:183:GLU:HG2	1.55	0.86
3:B:173:PRO:HB3	3:B:183:GLU:HG2	1.55	0.86
3:B:173:PRO:HB3	3:B:183:GLU:HG2	1.55	0.86
1:C:415:LYS:HD3	2:A:156:ARG:HH21	1.40	0.85
1:C:460:ASP:CG	3:B:263:PRO:HG3	2.01	0.85
1:C:460:ASP:CG	3:B:263:PRO:HG3	2.02	0.85
1:C:460:ASP:CG	3:B:263:PRO:HG3	2.02	0.85
1:C:369:SER:HB3	1:C:413:ARG:NH1	1.91	0.85
1:C:459:ARG:HD3	3:B:427:ASP:OD2	1.75	0.84
1:C:460:ASP:CG	3:B:263:PRO:HG3	2.02	0.84
3:B:332:MET:HE2	3:B:351:VAL:HG11	1.59	0.84
3:B:332:MET:HE2	3:B:351:VAL:HG11	1.59	0.84
3:B:332:MET:HE2	3:B:351:VAL:HG11	1.59	0.84
3:B:332:MET:HE2	3:B:351:VAL:HG11	1.59	0.84
3:B:332:MET:HE2	3:B:351:VAL:HG11	1.59	0.84
1:C:460:ASP:CG	3:B:263:PRO:HG3	2.03	0.84
2:A:70:LEU:HB2	2:A:99:ALA:HB2	1.58	0.83
2:A:70:LEU:HB2	2:A:99:ALA:HB2	1.58	0.83
2:A:70:LEU:HB2	2:A:99:ALA:HB2	1.58	0.83
2:A:70:LEU:HB2	2:A:99:ALA:HB2	1.58	0.83
2:A:70:LEU:HB2	2:A:99:ALA:HB2	1.58	0.83
1:C:459:ARG:HD3	3:B:427:ASP:OD2	1.77	0.83
3:B:250:ALA:HA	3:B:254:LYS:HD2	1.60	0.83
3:B:250:ALA:HA	3:B:254:LYS:HD2	1.60	0.83
3:B:250:ALA:HA	3:B:254:LYS:HD2	1.60	0.83
3:B:250:ALA:HA	3:B:254:LYS:HD2	1.60	0.83
3:B:250:ALA:HA	3:B:254:LYS:HD2	1.60	0.83
1:C:308:TYR:HE1	1:C:368:ALA:HA	1.42	0.83
1:C:330:LEU:CD1	1:C:466:VAL:HG12	2.08	0.82
1:C:330:LEU:CD1	1:C:466:VAL:HG12	2.08	0.82
1:C:330:LEU:CD1	1:C:466:VAL:HG12	2.08	0.82
1:C:330:LEU:CD1	1:C:466:VAL:HG12	2.08	0.82
1:C:330:LEU:CD1	1:C:466:VAL:HG12	2.08	0.82
1:C:313:TYR:HE1	1:C:324:LYS:HE3	1.43	0.82
1:C:424:LYS:NZ	3:B:163:ASP:OD1	2.13	0.82
1:C:424:LYS:CG	3:B:163:ASP:OD2	2.28	0.82
3:B:246:GLY:HA2	3:B:357:ASP:HB2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:246:GLY:HA2	3:B:357:ASP:HB2	1.62	0.82
3:B:246:GLY:HA2	3:B:357:ASP:HB2	1.62	0.82
3:B:246:GLY:HA2	3:B:357:ASP:HB2	1.62	0.82
1:C:424:LYS:NZ	3:B:163:ASP:OD1	2.13	0.82
3:B:246:GLY:HA2	3:B:357:ASP:HB2	1.62	0.82
1:C:460:ASP:OD2	3:B:263:PRO:CG	2.25	0.81
1:C:424:LYS:NZ	3:B:163:ASP:OD1	2.15	0.80
1:C:424:LYS:NZ	3:B:163:ASP:OD1	2.14	0.80
1:C:424:LYS:CG	3:B:163:ASP:OD2	2.29	0.80
1:C:424:LYS:HG2	3:B:163:ASP:OD2	1.82	0.80
2:A:115:ILE:HD12	2:A:152:LEU:HD13	1.64	0.80
2:A:115:ILE:HD12	2:A:152:LEU:HD13	1.64	0.80
2:A:115:ILE:HD12	2:A:152:LEU:HD13	1.64	0.80
2:A:115:ILE:HD12	2:A:152:LEU:HD13	1.64	0.80
2:A:115:ILE:HD12	2:A:152:LEU:HD13	1.64	0.80
1:C:424:LYS:CG	3:B:163:ASP:OD2	2.30	0.80
1:C:424:LYS:HG2	3:B:163:ASP:OD2	1.82	0.79
1:C:308:TYR:CE1	1:C:368:ALA:HA	2.16	0.79
1:C:424:LYS:CG	3:B:163:ASP:OD2	2.30	0.79
1:C:424:LYS:HG2	3:B:163:ASP:OD2	1.83	0.79
1:C:460:ASP:OD2	3:B:263:PRO:CG	2.27	0.79
1:C:80:ARG:HG3	1:C:81:GLN:HG2	1.65	0.79
1:C:80:ARG:HG3	1:C:81:GLN:HG2	1.65	0.79
1:C:80:ARG:HG3	1:C:81:GLN:HG2	1.65	0.79
3:B:224:TYR:OH	7:B:600:GDP:O2'	2.00	0.79
3:B:224:TYR:OH	7:B:600:GDP:O2'	2.00	0.79
3:B:224:TYR:OH	7:B:600:GDP:O2'	2.00	0.79
3:B:224:TYR:OH	7:B:600:GDP:O2'	2.00	0.79
1:C:460:ASP:OD2	3:B:263:PRO:CG	2.27	0.79
3:B:224:TYR:OH	7:B:600:GDP:O2'	2.00	0.79
1:C:80:ARG:HG3	1:C:81:GLN:HG2	1.65	0.78
1:C:80:ARG:HG3	1:C:81:GLN:HG2	1.65	0.78
1:C:459:ARG:NH1	3:B:424:ASN:HA	1.97	0.78
1:C:330:LEU:CD2	1:C:340:VAL:HG22	2.14	0.78
1:C:424:LYS:NZ	3:B:163:ASP:OD1	2.17	0.78
1:C:330:LEU:CD2	1:C:340:VAL:HG22	2.14	0.78
1:C:330:LEU:CD2	1:C:340:VAL:HG22	2.14	0.78
1:C:330:LEU:CD2	1:C:340:VAL:HG22	2.14	0.78
1:C:424:LYS:CG	3:B:163:ASP:OD2	2.31	0.78
1:C:330:LEU:CD2	1:C:340:VAL:HG22	2.14	0.78
1:C:460:ASP:OD2	3:B:263:PRO:CG	2.28	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ARG:NH1	3:B:424:ASN:HA	1.99	0.78
1:C:313:TYR:CE1	1:C:324:LYS:HE2	2.18	0.77
1:C:460:ASP:OD2	3:B:263:PRO:CG	2.28	0.77
1:C:459:ARG:NH1	3:B:424:ASN:HA	1.99	0.77
1:C:176:ALA:HB3	1:C:181:GLN:HG2	1.67	0.77
1:C:176:ALA:HB3	1:C:181:GLN:HG2	1.67	0.77
1:C:176:ALA:HB3	1:C:181:GLN:HG2	1.67	0.77
1:C:176:ALA:HB3	1:C:181:GLN:HG2	1.67	0.77
1:C:424:LYS:HG2	3:B:163:ASP:OD2	1.84	0.77
1:C:369:SER:HB2	1:C:413:ARG:HH12	1.47	0.77
1:C:459:ARG:NH1	3:B:424:ASN:HA	1.99	0.77
1:C:176:ALA:HB3	1:C:181:GLN:HG2	1.67	0.77
1:C:95:LEU:HB2	1:C:120:PHE:HB2	1.67	0.76
1:C:95:LEU:HB2	1:C:120:PHE:HB2	1.67	0.76
1:C:424:LYS:HG2	3:B:163:ASP:OD2	1.85	0.76
1:C:95:LEU:HB2	1:C:120:PHE:HB2	1.67	0.76
1:C:95:LEU:HB2	1:C:120:PHE:HB2	1.68	0.76
1:C:95:LEU:HB2	1:C:120:PHE:HB2	1.68	0.76
1:C:459:ARG:NH1	3:B:424:ASN:HA	2.00	0.76
1:C:313:TYR:CE1	1:C:324:LYS:HE3	2.20	0.76
2:A:269:LEU:HD22	2:A:303:VAL:HG11	1.67	0.76
2:A:269:LEU:HD22	2:A:303:VAL:HG11	1.67	0.76
2:A:269:LEU:HD22	2:A:303:VAL:HG11	1.67	0.76
2:A:269:LEU:HD22	2:A:303:VAL:HG11	1.67	0.76
2:A:269:LEU:HD22	2:A:303:VAL:HG11	1.67	0.76
1:C:333:ASP:CA	3:B:416:MET:SD	2.74	0.75
1:C:434:HIS:HB2	2:A:409:VAL:HG11	1.67	0.75
2:A:69:ASP:HA	2:A:145:THR:HG21	1.67	0.75
2:A:204:VAL:HG11	2:A:231:ILE:HD12	1.69	0.75
2:A:69:ASP:HA	2:A:145:THR:HG21	1.67	0.75
2:A:204:VAL:HG11	2:A:231:ILE:HD12	1.69	0.75
2:A:69:ASP:HA	2:A:145:THR:HG21	1.67	0.75
2:A:204:VAL:HG11	2:A:231:ILE:HD12	1.69	0.75
2:A:69:ASP:HA	2:A:145:THR:HG21	1.67	0.75
2:A:204:VAL:HG11	2:A:231:ILE:HD12	1.69	0.75
2:A:69:ASP:HA	2:A:145:THR:HG21	1.67	0.75
2:A:204:VAL:HG11	2:A:231:ILE:HD12	1.69	0.75
2:A:69:ASP:HA	2:A:145:THR:HG21	1.67	0.75
2:A:204:VAL:HG11	2:A:231:ILE:HD12	1.69	0.75
3:B:23:VAL:HG13	8:B:601:TA1:C32	2.17	0.75
1:C:147:VAL:HG12	1:C:387:ILE:HG12	1.69	0.75
1:C:434:HIS:HB2	2:A:409:VAL:HG11	1.69	0.75
3:B:23:VAL:HG13	8:B:601:TA1:C32	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:VAL:HG12	1:C:387:ILE:HG12	1.69	0.75
3:B:23:VAL:HG13	8:B:601:TA1:C32	2.17	0.75
3:B:23:VAL:HG13	8:B:601:TA1:C32	2.17	0.75
1:C:333:ASP:CA	3:B:416:MET:SD	2.75	0.75
3:B:23:VAL:HG13	8:B:601:TA1:C32	2.17	0.75
1:C:147:VAL:HG12	1:C:387:ILE:HG12	1.69	0.74
1:C:147:VAL:HG12	1:C:387:ILE:HG12	1.69	0.74
1:C:147:VAL:HG12	1:C:387:ILE:HG12	1.70	0.74
1:C:333:ASP:CA	3:B:416:MET:SD	2.75	0.74
1:C:333:ASP:CA	3:B:416:MET:SD	2.75	0.74
1:C:434:HIS:HB2	2:A:409:VAL:HG11	1.69	0.74
1:C:434:HIS:HB2	2:A:409:VAL:HG11	1.69	0.74
2:A:316:CYS:HB3	2:A:378:LEU:HG	1.70	0.73
2:A:316:CYS:HB3	2:A:378:LEU:HG	1.70	0.73
2:A:316:CYS:HB3	2:A:378:LEU:HG	1.70	0.73
2:A:316:CYS:HB3	2:A:378:LEU:HG	1.70	0.73
2:A:316:CYS:HB3	2:A:378:LEU:HG	1.70	0.73
2:A:179:THR:HG21	6:A:500:GTP:H3'	1.68	0.73
3:B:93:VAL:HG11	3:B:118:VAL:HG22	1.70	0.73
2:A:179:THR:HG21	6:A:500:GTP:H3'	1.68	0.73
3:B:93:VAL:HG11	3:B:118:VAL:HG22	1.70	0.73
2:A:179:THR:HG21	6:A:500:GTP:H3'	1.68	0.73
3:B:93:VAL:HG11	3:B:118:VAL:HG22	1.70	0.73
2:A:179:THR:HG21	6:A:500:GTP:H3'	1.68	0.73
3:B:93:VAL:HG11	3:B:118:VAL:HG22	1.70	0.73
2:A:179:THR:HG21	6:A:500:GTP:H3'	1.68	0.73
3:B:93:VAL:HG11	3:B:118:VAL:HG22	1.70	0.73
1:C:494:LEU:HD11	2:A:420:GLU:CD	2.12	0.73
1:C:333:ASP:CA	3:B:416:MET:SD	2.76	0.73
1:C:434:HIS:HB2	2:A:409:VAL:HG11	1.70	0.73
2:A:242:LEU:HD21	2:A:250:VAL:HB	1.71	0.73
2:A:242:LEU:HD21	2:A:250:VAL:HB	1.71	0.73
2:A:242:LEU:HD21	2:A:250:VAL:HB	1.71	0.73
1:C:314:ASP:HB3	1:C:325:ARG:HH12	1.54	0.73
2:A:242:LEU:HD21	2:A:250:VAL:HB	1.71	0.73
2:A:242:LEU:HD21	2:A:250:VAL:HB	1.71	0.73
3:B:268:PHE:HD1	3:B:380:ASN:HB2	1.54	0.72
3:B:268:PHE:HD1	3:B:380:ASN:HB2	1.54	0.72
3:B:268:PHE:HD1	3:B:380:ASN:HB2	1.54	0.72
3:B:268:PHE:HD1	3:B:380:ASN:HB2	1.54	0.72
3:B:268:PHE:HD1	3:B:380:ASN:HB2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ASP:C	3:B:416:MET:SD	2.73	0.72
1:C:321:HIS:CD2	1:C:366:SER:OG	2.42	0.72
1:C:334:GLN:HG2	3:B:416:MET:HE1	1.71	0.72
1:C:434:HIS:CE1	2:A:409:VAL:HG21	2.25	0.72
1:C:494:LEU:HD11	2:A:420:GLU:CD	2.14	0.72
1:C:334:GLN:HG2	3:B:416:MET:HE1	1.72	0.71
2:A:404:PHE:HB3	2:A:407:TRP:HD1	1.54	0.71
2:A:404:PHE:HB3	2:A:407:TRP:HD1	1.54	0.71
2:A:404:PHE:HB3	2:A:407:TRP:HD1	1.54	0.71
2:A:404:PHE:HB3	2:A:407:TRP:HD1	1.54	0.71
2:A:404:PHE:HB3	2:A:407:TRP:HD1	1.54	0.71
1:C:334:GLN:HG2	3:B:416:MET:HE1	1.72	0.71
1:C:333:ASP:C	3:B:416:MET:SD	2.74	0.71
1:C:313:TYR:HA	1:C:326:GLN:NE2	2.06	0.71
1:C:494:LEU:HD11	2:A:420:GLU:CD	2.14	0.71
1:C:369:SER:HB2	1:C:413:ARG:NH1	2.05	0.71
2:A:260:VAL:HG12	2:A:266:HIS:HB2	1.71	0.71
2:A:260:VAL:HG12	2:A:266:HIS:HB2	1.71	0.71
2:A:260:VAL:HG12	2:A:266:HIS:HB2	1.71	0.71
2:A:260:VAL:HG12	2:A:266:HIS:HB2	1.71	0.71
2:A:260:VAL:HG12	2:A:266:HIS:HB2	1.71	0.71
1:C:494:LEU:HD11	2:A:420:GLU:CD	2.15	0.70
1:C:334:GLN:HG2	3:B:416:MET:HE1	1.73	0.70
3:B:236:SER:HB2	8:B:601:TA1:H401	1.74	0.70
1:C:333:ASP:C	3:B:416:MET:SD	2.75	0.70
3:B:236:SER:HB2	8:B:601:TA1:H401	1.74	0.70
3:B:236:SER:HB2	8:B:601:TA1:H401	1.74	0.70
3:B:236:SER:HB2	8:B:601:TA1:H401	1.74	0.70
3:B:236:SER:HB2	8:B:601:TA1:H401	1.74	0.70
1:C:494:LEU:HD11	2:A:420:GLU:CD	2.16	0.70
1:C:434:HIS:CB	2:A:409:VAL:HG11	2.22	0.70
1:C:333:ASP:C	3:B:416:MET:SD	2.75	0.70
1:C:315:LEU:HB3	1:C:361:GLY:HA2	1.74	0.69
1:C:315:LEU:HB3	1:C:361:GLY:HA2	1.74	0.69
1:C:315:LEU:HB3	1:C:361:GLY:HA2	1.74	0.69
1:C:315:LEU:HB3	1:C:361:GLY:HA2	1.74	0.69
1:C:315:LEU:HB3	1:C:361:GLY:HA2	1.75	0.69
1:C:330:LEU:HD22	1:C:340:VAL:HG22	1.74	0.69
1:C:334:GLN:HG2	3:B:416:MET:HE1	1.74	0.69
1:C:176:ALA:HB1	1:C:180:PRO:HB2	1.75	0.68
1:C:330:LEU:HD22	1:C:340:VAL:HG22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:LEU:HD22	1:C:340:VAL:HG22	1.74	0.68
1:C:330:LEU:HD22	1:C:340:VAL:HG22	1.74	0.68
1:C:176:ALA:HB1	1:C:180:PRO:HB2	1.75	0.68
1:C:176:ALA:HB1	1:C:180:PRO:HB2	1.75	0.68
1:C:333:ASP:C	3:B:416:MET:SD	2.77	0.68
1:C:176:ALA:HB1	1:C:180:PRO:HB2	1.75	0.68
1:C:176:ALA:HB1	1:C:180:PRO:HB2	1.75	0.68
1:C:330:LEU:HD22	1:C:340:VAL:HG22	1.74	0.68
1:C:330:LEU:CD2	1:C:340:VAL:HG13	2.23	0.68
1:C:330:LEU:CD2	1:C:340:VAL:HG13	2.23	0.68
1:C:330:LEU:CD2	1:C:340:VAL:HG13	2.23	0.68
2:A:11:GLN:HA	2:A:74:VAL:HG11	1.76	0.68
3:B:414:ASP:HB2	3:B:417:GLU:CG	2.24	0.68
2:A:11:GLN:HA	2:A:74:VAL:HG11	1.76	0.68
3:B:414:ASP:HB2	3:B:417:GLU:CG	2.24	0.68
2:A:11:GLN:HA	2:A:74:VAL:HG11	1.76	0.68
3:B:414:ASP:HB2	3:B:417:GLU:CG	2.24	0.68
1:C:330:LEU:CD2	1:C:340:VAL:HG13	2.24	0.68
2:A:11:GLN:HA	2:A:74:VAL:HG11	1.76	0.68
3:B:414:ASP:HB2	3:B:417:GLU:CG	2.24	0.68
2:A:11:GLN:HA	2:A:74:VAL:HG11	1.76	0.68
3:B:414:ASP:HB2	3:B:417:GLU:CG	2.24	0.68
1:C:330:LEU:HD11	1:C:466:VAL:CG1	2.24	0.68
1:C:330:LEU:CD2	1:C:340:VAL:HG13	2.24	0.68
1:C:330:LEU:HD11	1:C:466:VAL:CG1	2.24	0.68
1:C:330:LEU:HD11	1:C:466:VAL:CG1	2.24	0.68
1:C:330:LEU:HD11	1:C:466:VAL:CG1	2.24	0.68
1:C:330:LEU:HD11	1:C:466:VAL:CG1	2.24	0.68
2:A:179:THR:HG21	6:A:500:GTP:C2'	2.23	0.67
2:A:179:THR:HG21	6:A:500:GTP:C2'	2.23	0.67
2:A:179:THR:HG21	6:A:500:GTP:C2'	2.23	0.67
2:A:179:THR:HG21	6:A:500:GTP:C2'	2.23	0.67
2:A:179:THR:HG21	6:A:500:GTP:C2'	2.23	0.67
1:C:434:HIS:CB	2:A:409:VAL:HG11	2.24	0.67
1:C:456:ILE:HG13	1:C:457:PRO:HD2	1.76	0.67
1:C:456:ILE:HG13	1:C:457:PRO:HD2	1.76	0.67
1:C:456:ILE:HG13	1:C:457:PRO:HD2	1.76	0.67
1:C:456:ILE:HG13	1:C:457:PRO:HD2	1.76	0.67
1:C:456:ILE:HG13	1:C:457:PRO:HD2	1.76	0.67
2:A:179:THR:HG21	6:A:500:GTP:C3'	2.25	0.67
2:A:179:THR:HG21	6:A:500:GTP:C3'	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:179:THR:HG21	6:A:500:GTP:C3'	2.25	0.67
1:C:434:HIS:CB	2:A:409:VAL:HG11	2.24	0.67
2:A:179:THR:HG21	6:A:500:GTP:C3'	2.25	0.67
2:A:179:THR:HG21	6:A:500:GTP:C3'	2.25	0.67
2:A:10:GLY:HA2	2:A:145:THR:HB	1.77	0.67
2:A:10:GLY:HA2	2:A:145:THR:HB	1.77	0.67
2:A:10:GLY:HA2	2:A:145:THR:HB	1.77	0.67
2:A:10:GLY:HA2	2:A:145:THR:HB	1.77	0.67
2:A:10:GLY:HA2	2:A:145:THR:HB	1.77	0.67
1:C:306:GLU:HA	1:C:380:HIS:O	1.95	0.67
1:C:306:GLU:HA	1:C:380:HIS:O	1.95	0.67
1:C:308:TYR:OH	1:C:368:ALA:HB3	1.94	0.67
1:C:306:GLU:HA	1:C:380:HIS:O	1.95	0.67
1:C:334:GLN:HA	3:B:416:MET:HE1	1.75	0.67
1:C:306:GLU:HA	1:C:380:HIS:O	1.95	0.67
1:C:306:GLU:HA	1:C:380:HIS:O	1.95	0.67
2:A:224:TYR:CD2	6:A:500:GTP:C5	2.83	0.67
3:B:23:VAL:HG13	8:B:601:TA1:H321	1.76	0.67
2:A:224:TYR:CD2	6:A:500:GTP:C5	2.83	0.67
3:B:23:VAL:HG13	8:B:601:TA1:H321	1.76	0.67
2:A:224:TYR:CD2	6:A:500:GTP:C5	2.83	0.67
3:B:23:VAL:HG13	8:B:601:TA1:H321	1.76	0.67
2:A:224:TYR:CD2	6:A:500:GTP:C5	2.83	0.67
3:B:23:VAL:HG13	8:B:601:TA1:H321	1.76	0.67
2:A:224:TYR:CD2	6:A:500:GTP:C5	2.83	0.67
3:B:23:VAL:HG13	8:B:601:TA1:H321	1.76	0.67
1:C:434:HIS:CE1	2:A:409:VAL:HG21	2.30	0.66
1:C:434:HIS:CB	2:A:409:VAL:HG11	2.25	0.66
1:C:434:HIS:CG	2:A:409:VAL:HG11	2.31	0.66
1:C:434:HIS:CE1	2:A:409:VAL:HG21	2.31	0.66
1:C:434:HIS:CE1	2:A:409:VAL:HG21	2.31	0.66
2:A:105:ARG:HA	2:A:109:THR:OG1	1.96	0.66
3:B:5:VAL:HG12	3:B:64:ARG:HD2	1.78	0.66
2:A:105:ARG:HA	2:A:109:THR:OG1	1.96	0.66
3:B:5:VAL:HG12	3:B:64:ARG:HD2	1.78	0.66
2:A:105:ARG:HA	2:A:109:THR:OG1	1.96	0.66
3:B:5:VAL:HG12	3:B:64:ARG:HD2	1.78	0.66
2:A:105:ARG:HA	2:A:109:THR:OG1	1.96	0.66
3:B:5:VAL:HG12	3:B:64:ARG:HD2	1.78	0.66
2:A:105:ARG:HA	2:A:109:THR:OG1	1.96	0.66
3:B:5:VAL:HG12	3:B:64:ARG:HD2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:LYS:HG3	3:B:163:ASP:OD2	1.96	0.66
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.78	0.66
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.78	0.66
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.78	0.66
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.78	0.66
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.78	0.66
3:B:371:LEU:HD13	8:B:601:TA1:H442	1.77	0.66
3:B:371:LEU:HD13	8:B:601:TA1:H442	1.77	0.66
1:C:179:LEU:HB3	1:C:180:PRO:HD3	1.77	0.66
3:B:371:LEU:HD13	8:B:601:TA1:H442	1.77	0.66
1:C:179:LEU:HB3	1:C:180:PRO:HD3	1.77	0.66
3:B:371:LEU:HD13	8:B:601:TA1:H442	1.77	0.66
1:C:179:LEU:HB3	1:C:180:PRO:HD3	1.77	0.66
3:B:371:LEU:HD13	8:B:601:TA1:H442	1.77	0.66
1:C:179:LEU:HB3	1:C:180:PRO:HD3	1.78	0.65
1:C:179:LEU:HB3	1:C:180:PRO:HD3	1.78	0.65
1:C:434:HIS:CB	2:A:409:VAL:HG11	2.26	0.65
3:B:115:VAL:HG21	3:B:152:LEU:HD23	1.79	0.65
3:B:209:LEU:HD23	3:B:227:LEU:HB3	1.77	0.65
3:B:115:VAL:HG21	3:B:152:LEU:HD23	1.79	0.65
3:B:209:LEU:HD23	3:B:227:LEU:HB3	1.77	0.65
3:B:115:VAL:HG21	3:B:152:LEU:HD23	1.79	0.65
3:B:209:LEU:HD23	3:B:227:LEU:HB3	1.77	0.65
3:B:115:VAL:HG21	3:B:152:LEU:HD23	1.79	0.65
3:B:209:LEU:HD23	3:B:227:LEU:HB3	1.77	0.65
3:B:115:VAL:HG21	3:B:152:LEU:HD23	1.79	0.65
3:B:209:LEU:HD23	3:B:227:LEU:HB3	1.77	0.65
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.79	0.65
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.79	0.65
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.79	0.65
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.79	0.65
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.79	0.65
1:C:434:HIS:CE1	2:A:409:VAL:HG21	2.32	0.65
1:C:307:ILE:HB	1:C:380:HIS:HB2	1.78	0.65
1:C:307:ILE:HB	1:C:380:HIS:HB2	1.78	0.64
1:C:307:ILE:HB	1:C:380:HIS:HB2	1.79	0.64
1:C:307:ILE:HB	1:C:380:HIS:HB2	1.79	0.64
1:C:307:ILE:HB	1:C:380:HIS:HB2	1.79	0.64
2:A:100:ALA:HB2	3:B:253:ARG:HB3	1.80	0.64
2:A:100:ALA:HB2	3:B:253:ARG:HB3	1.80	0.64
2:A:100:ALA:HB2	3:B:253:ARG:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:100:ALA:HB2	3:B:253:ARG:HB3	1.80	0.64
2:A:100:ALA:HB2	3:B:253:ARG:HB3	1.80	0.64
8:B:601:TA1:H463	8:B:601:TA1:H261	1.80	0.64
8:B:601:TA1:H463	8:B:601:TA1:H261	1.80	0.64
8:B:601:TA1:H463	8:B:601:TA1:H261	1.80	0.64
8:B:601:TA1:H463	8:B:601:TA1:H261	1.80	0.64
8:B:601:TA1:H463	8:B:601:TA1:H261	1.80	0.64
1:C:334:GLN:HA	3:B:416:MET:HE1	1.78	0.64
1:C:415:LYS:HD3	2:A:156:ARG:NH2	2.13	0.64
1:C:334:GLN:HA	3:B:416:MET:HE1	1.78	0.64
1:C:126:PHE:HB3	1:C:130:VAL:HG21	1.78	0.64
1:C:126:PHE:HB3	1:C:130:VAL:HG21	1.78	0.64
1:C:434:HIS:NE2	2:A:409:VAL:HG21	2.13	0.63
1:C:126:PHE:HB3	1:C:130:VAL:HG21	1.78	0.63
1:C:126:PHE:HB3	1:C:130:VAL:HG21	1.78	0.63
1:C:126:PHE:HB3	1:C:130:VAL:HG21	1.79	0.63
1:C:334:GLN:HA	3:B:416:MET:HE1	1.79	0.63
1:C:413:ARG:HH12	1:C:430:ASN:HD21	1.47	0.63
1:C:328:LEU:HB2	1:C:341:LYS:O	1.99	0.63
1:C:328:LEU:HB2	1:C:341:LYS:O	1.99	0.63
3:B:228:ASN:CG	7:B:600:GDP:HN1	2.07	0.63
3:B:228:ASN:CG	7:B:600:GDP:HN1	2.07	0.63
1:C:328:LEU:HB2	1:C:341:LYS:O	1.99	0.63
3:B:228:ASN:CG	7:B:600:GDP:HN1	2.07	0.63
3:B:228:ASN:CG	7:B:600:GDP:HN1	2.07	0.63
1:C:328:LEU:HB2	1:C:341:LYS:O	1.99	0.63
3:B:228:ASN:CG	7:B:600:GDP:HN1	2.07	0.63
1:C:328:LEU:HB2	1:C:341:LYS:O	1.99	0.63
1:C:455:LEU:HD23	3:B:431:GLU:CD	2.23	0.63
3:B:11:GLN:CB	7:B:600:GDP:O2B	2.47	0.63
3:B:11:GLN:CB	7:B:600:GDP:O2B	2.47	0.63
3:B:11:GLN:CB	7:B:600:GDP:O2B	2.47	0.63
3:B:11:GLN:CB	7:B:600:GDP:O2B	2.47	0.63
3:B:11:GLN:CB	7:B:600:GDP:O2B	2.47	0.63
1:C:334:GLN:CA	3:B:416:MET:HE1	2.29	0.62
1:C:440:ILE:HD12	1:C:499:PHE:HZ	1.63	0.62
1:C:440:ILE:HD12	1:C:499:PHE:HZ	1.63	0.62
1:C:440:ILE:HD12	1:C:499:PHE:HZ	1.63	0.62
1:C:440:ILE:HD12	1:C:499:PHE:HZ	1.63	0.62
3:B:316:ALA:HB3	3:B:378:ILE:HB	1.80	0.62
1:C:415:LYS:HE2	2:A:112:LYS:NZ	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:316:ALA:HB3	3:B:378:ILE:HB	1.80	0.62
3:B:316:ALA:HB3	3:B:378:ILE:HB	1.80	0.62
3:B:316:ALA:HB3	3:B:378:ILE:HB	1.80	0.62
1:C:440:ILE:HD12	1:C:499:PHE:HZ	1.63	0.62
3:B:316:ALA:HB3	3:B:378:ILE:HB	1.80	0.62
2:A:179:THR:HG21	6:A:500:GTP:H2'	1.80	0.62
2:A:179:THR:HG21	6:A:500:GTP:H2'	1.80	0.62
2:A:179:THR:HG21	6:A:500:GTP:H2'	1.80	0.62
2:A:179:THR:HG21	6:A:500:GTP:H2'	1.80	0.62
2:A:179:THR:HG21	6:A:500:GTP:H2'	1.80	0.62
1:C:434:HIS:CD2	2:A:409:VAL:HG21	2.34	0.62
1:C:424:LYS:HG3	3:B:163:ASP:OD2	2.00	0.61
1:C:366:SER:HB2	1:C:379:SER:OG	2.00	0.61
1:C:126:PHE:HZ	1:C:138:LEU:HD22	1.65	0.61
1:C:330:LEU:HD21	1:C:340:VAL:HG22	1.82	0.61
1:C:330:LEU:HD21	1:C:340:VAL:HG22	1.82	0.61
1:C:126:PHE:HZ	1:C:138:LEU:HD22	1.65	0.61
1:C:126:PHE:HZ	1:C:138:LEU:HD22	1.65	0.61
1:C:330:LEU:HD21	1:C:340:VAL:HG22	1.82	0.61
1:C:330:LEU:HD21	1:C:340:VAL:HG22	1.82	0.61
1:C:434:HIS:CG	2:A:409:VAL:HG11	2.35	0.61
1:C:424:LYS:HG3	3:B:163:ASP:OD2	2.00	0.61
1:C:126:PHE:HZ	1:C:138:LEU:HD22	1.65	0.61
1:C:126:PHE:HZ	1:C:138:LEU:HD22	1.65	0.61
1:C:424:LYS:HG3	3:B:163:ASP:OD2	2.00	0.61
1:C:330:LEU:HD23	1:C:340:VAL:HG13	1.82	0.61
1:C:330:LEU:HD21	1:C:340:VAL:HG22	1.82	0.61
1:C:330:LEU:HD23	1:C:340:VAL:HG13	1.82	0.61
2:A:21:TRP:HA	2:A:24:TYR:HB2	1.82	0.61
3:B:10:GLY:CA	3:B:145:THR:HB	2.28	0.61
1:C:434:HIS:CG	2:A:409:VAL:HG11	2.35	0.61
2:A:21:TRP:HA	2:A:24:TYR:HB2	1.82	0.61
3:B:10:GLY:CA	3:B:145:THR:HB	2.28	0.61
2:A:21:TRP:HA	2:A:24:TYR:HB2	1.82	0.61
3:B:10:GLY:CA	3:B:145:THR:HB	2.28	0.61
2:A:21:TRP:HA	2:A:24:TYR:HB2	1.82	0.61
3:B:10:GLY:CA	3:B:145:THR:HB	2.28	0.61
2:A:21:TRP:HA	2:A:24:TYR:HB2	1.82	0.61
3:B:10:GLY:CA	3:B:145:THR:HB	2.28	0.61
1:C:330:LEU:HD23	1:C:340:VAL:HG13	1.82	0.61
1:C:330:LEU:HD23	1:C:340:VAL:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:LEU:HD23	1:C:340:VAL:HG13	1.82	0.61
2:A:9:VAL:HG21	2:A:149:PHE:HB3	1.82	0.60
2:A:9:VAL:HG21	2:A:149:PHE:HB3	1.82	0.60
2:A:9:VAL:HG21	2:A:149:PHE:HB3	1.82	0.60
1:C:321:HIS:HB3	1:C:366:SER:OG	2.01	0.60
2:A:9:VAL:HG21	2:A:149:PHE:HB3	1.82	0.60
2:A:9:VAL:HG21	2:A:149:PHE:HB3	1.82	0.60
1:C:455:LEU:HD23	3:B:431:GLU:CD	2.26	0.60
1:C:434:HIS:CG	2:A:409:VAL:HG11	2.36	0.60
1:C:455:LEU:HD23	3:B:431:GLU:CD	2.26	0.60
1:C:334:GLN:CA	3:B:416:MET:HE1	2.32	0.60
1:C:334:GLN:HA	3:B:416:MET:HE1	1.82	0.60
1:C:334:GLN:CA	3:B:416:MET:HE1	2.32	0.60
1:C:424:LYS:HG3	3:B:163:ASP:OD2	2.01	0.60
1:C:334:GLN:CA	3:B:416:MET:HE1	2.32	0.60
1:C:422:ARG:HH11	1:C:425:GLU:HB2	1.67	0.60
3:B:142:GLY:HA3	3:B:183:GLU:HG3	1.84	0.60
3:B:142:GLY:HA3	3:B:183:GLU:HG3	1.84	0.60
3:B:142:GLY:HA3	3:B:183:GLU:HG3	1.84	0.60
3:B:142:GLY:HA3	3:B:183:GLU:HG3	1.84	0.60
3:B:142:GLY:HA3	3:B:183:GLU:HG3	1.84	0.60
1:C:313:TYR:OH	1:C:319:PRO:HG2	2.01	0.60
1:C:434:HIS:CD2	2:A:409:VAL:HG21	2.36	0.60
1:C:434:HIS:CD2	2:A:409:VAL:HG21	2.36	0.59
1:C:434:HIS:NE2	2:A:409:VAL:HG21	2.17	0.59
1:C:304:PHE:HB3	1:C:316:LEU:HD13	1.84	0.59
1:C:304:PHE:HB3	1:C:316:LEU:HD13	1.84	0.59
1:C:304:PHE:HB3	1:C:316:LEU:HD13	1.84	0.59
1:C:304:PHE:HB3	1:C:316:LEU:HD13	1.84	0.59
1:C:434:HIS:CG	2:A:409:VAL:HG11	2.37	0.59
1:C:70:ILE:HD12	1:C:89:ILE:HD11	1.83	0.59
2:A:179:THR:HB	6:A:500:GTP:C3'	2.17	0.59
2:A:179:THR:HB	6:A:500:GTP:C3'	2.17	0.59
1:C:70:ILE:HD12	1:C:89:ILE:HD11	1.83	0.59
2:A:179:THR:HB	6:A:500:GTP:C3'	2.17	0.59
2:A:179:THR:HB	6:A:500:GTP:C3'	2.17	0.59
1:C:304:PHE:HB3	1:C:316:LEU:HD13	1.84	0.59
2:A:179:THR:HB	6:A:500:GTP:C3'	2.17	0.59
1:C:70:ILE:HD12	1:C:89:ILE:HD11	1.83	0.59
1:C:70:ILE:HD12	1:C:89:ILE:HD11	1.83	0.59
1:C:434:HIS:NE2	2:A:409:VAL:HG21	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ILE:HD12	1:C:89:ILE:HD11	1.83	0.59
1:C:321:HIS:CG	1:C:366:SER:OG	2.56	0.58
1:C:455:LEU:HD23	3:B:431:GLU:CD	2.28	0.58
1:C:455:LEU:HD23	3:B:431:GLU:CD	2.28	0.58
3:B:23:VAL:HA	8:B:601:TA1:C33	2.33	0.58
3:B:23:VAL:HA	8:B:601:TA1:C33	2.33	0.58
3:B:23:VAL:HA	8:B:601:TA1:C33	2.33	0.58
3:B:23:VAL:HA	8:B:601:TA1:C33	2.33	0.58
3:B:23:VAL:HA	8:B:601:TA1:C33	2.33	0.58
1:C:437:GLY:HA2	1:C:499:PHE:CE1	2.39	0.58
1:C:437:GLY:HA2	1:C:499:PHE:CE1	2.39	0.58
1:C:437:GLY:HA2	1:C:499:PHE:CE1	2.39	0.58
1:C:437:GLY:HA2	1:C:499:PHE:CE1	2.39	0.58
1:C:309:ASN:HD21	1:C:422:ARG:HH22	1.52	0.58
1:C:437:GLY:HA2	1:C:499:PHE:CE1	2.39	0.58
1:C:434:HIS:CD2	2:A:409:VAL:HG21	2.38	0.58
1:C:313:TYR:CE1	1:C:324:LYS:HD2	2.39	0.58
1:C:62:GLU:OE2	1:C:65:LYS:HE2	2.04	0.58
1:C:434:HIS:NE2	2:A:409:VAL:HG21	2.19	0.57
1:C:62:GLU:OE2	1:C:65:LYS:HE2	2.04	0.57
1:C:62:GLU:OE2	1:C:65:LYS:HE2	2.04	0.57
1:C:62:GLU:OE2	1:C:65:LYS:HE2	2.04	0.57
1:C:62:GLU:OE2	1:C:65:LYS:HE2	2.04	0.57
1:C:334:GLN:CA	3:B:416:MET:HE1	2.35	0.57
2:A:151:SER:HB3	2:A:193:THR:HG21	1.85	0.57
2:A:151:SER:HB3	2:A:193:THR:HG21	1.85	0.57
1:C:434:HIS:CD2	2:A:409:VAL:HG21	2.38	0.57
2:A:151:SER:HB3	2:A:193:THR:HG21	1.85	0.57
2:A:151:SER:HB3	2:A:193:THR:HG21	1.85	0.57
2:A:151:SER:HB3	2:A:193:THR:HG21	1.85	0.57
1:C:459:ARG:NH1	3:B:424:ASN:HD22	2.03	0.57
2:A:7:ILE:HD11	2:A:137:VAL:HG22	1.86	0.57
2:A:7:ILE:HD11	2:A:137:VAL:HG22	1.86	0.57
2:A:7:ILE:HD11	2:A:137:VAL:HG22	1.86	0.57
2:A:7:ILE:HD11	2:A:137:VAL:HG22	1.86	0.57
2:A:7:ILE:HD11	2:A:137:VAL:HG22	1.86	0.57
1:C:183:LEU:HD21	1:C:383:PHE:HE2	1.69	0.57
3:B:11:GLN:HB3	7:B:600:GDP:O2B	2.05	0.57
3:B:11:GLN:HB3	7:B:600:GDP:O2B	2.05	0.57
3:B:11:GLN:HB3	7:B:600:GDP:O2B	2.05	0.57
3:B:11:GLN:HB3	7:B:600:GDP:O2B	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:11:GLN:HB3	7:B:600:GDP:O2B	2.05	0.57
1:C:183:LEU:HD21	1:C:383:PHE:HE2	1.69	0.57
1:C:183:LEU:HD21	1:C:383:PHE:HE2	1.69	0.57
1:C:183:LEU:HD21	1:C:383:PHE:HE2	1.69	0.57
1:C:434:HIS:NE2	2:A:409:VAL:HG21	2.20	0.57
1:C:183:LEU:HD21	1:C:383:PHE:HE2	1.69	0.57
2:A:237:SER:HA	2:A:241:SER:OG	2.05	0.57
2:A:237:SER:HA	2:A:241:SER:OG	2.05	0.57
2:A:237:SER:HA	2:A:241:SER:OG	2.05	0.57
2:A:237:SER:HA	2:A:241:SER:OG	2.05	0.57
2:A:237:SER:HA	2:A:241:SER:OG	2.05	0.57
1:C:459:ARG:HE	1:C:465:ARG:NH1	2.02	0.57
1:C:330:LEU:CD2	1:C:340:VAL:HA	2.35	0.56
3:B:255:LEU:HB3	3:B:259:MET:HE2	1.87	0.56
3:B:255:LEU:HB3	3:B:259:MET:HE2	1.87	0.56
3:B:255:LEU:HB3	3:B:259:MET:HE2	1.87	0.56
1:C:459:ARG:HE	1:C:465:ARG:NH1	2.02	0.56
3:B:255:LEU:HB3	3:B:259:MET:HE2	1.87	0.56
1:C:459:ARG:HE	1:C:465:ARG:NH1	2.02	0.56
3:B:255:LEU:HB3	3:B:259:MET:HE2	1.87	0.56
1:C:459:ARG:HE	1:C:465:ARG:NH1	2.02	0.56
2:A:104:ALA:HB2	2:A:413:MET:HE2	1.86	0.56
1:C:330:LEU:CD2	1:C:340:VAL:HA	2.35	0.56
2:A:104:ALA:HB2	2:A:413:MET:HE2	1.86	0.56
1:C:330:LEU:CD2	1:C:340:VAL:HA	2.35	0.56
2:A:104:ALA:HB2	2:A:413:MET:HE2	1.86	0.56
1:C:330:LEU:CD2	1:C:340:VAL:HA	2.35	0.56
2:A:104:ALA:HB2	2:A:413:MET:HE2	1.86	0.56
2:A:104:ALA:HB2	2:A:413:MET:HE2	1.86	0.56
1:C:390:LEU:HG	1:C:398:PRO:HB3	1.87	0.56
2:A:100:ALA:O	6:A:500:GTP:O1G	2.23	0.56
2:A:191:THR:HA	2:A:194:THR:HG22	1.87	0.56
2:A:298:PRO:HA	2:A:301:GLN:OE1	2.05	0.56
1:C:390:LEU:HG	1:C:398:PRO:HB3	1.87	0.56
2:A:100:ALA:O	6:A:500:GTP:O1G	2.23	0.56
2:A:191:THR:HA	2:A:194:THR:HG22	1.87	0.56
2:A:298:PRO:HA	2:A:301:GLN:OE1	2.05	0.56
1:C:70:ILE:HD11	1:C:128:PRO:HD3	1.87	0.56
1:C:390:LEU:HG	1:C:398:PRO:HB3	1.87	0.56
1:C:459:ARG:HE	1:C:465:ARG:NH1	2.02	0.56
2:A:100:ALA:O	6:A:500:GTP:O1G	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:191:THR:HA	2:A:194:THR:HG22	1.87	0.56
2:A:298:PRO:HA	2:A:301:GLN:OE1	2.05	0.56
1:C:309:ASN:HD21	1:C:422:ARG:HH22	1.54	0.56
2:A:100:ALA:O	6:A:500:GTP:O1G	2.23	0.56
2:A:191:THR:HA	2:A:194:THR:HG22	1.87	0.56
2:A:298:PRO:HA	2:A:301:GLN:OE1	2.05	0.56
1:C:70:ILE:HD11	1:C:128:PRO:HD3	1.87	0.56
1:C:330:LEU:CD2	1:C:340:VAL:HA	2.35	0.56
1:C:390:LEU:HG	1:C:398:PRO:HB3	1.87	0.56
2:A:100:ALA:O	6:A:500:GTP:O1G	2.23	0.56
2:A:191:THR:HA	2:A:194:THR:HG22	1.87	0.56
2:A:298:PRO:HA	2:A:301:GLN:OE1	2.05	0.56
1:C:424:LYS:HZ2	3:B:163:ASP:CG	2.13	0.56
2:A:234:ILE:O	2:A:238:ILE:HG12	2.06	0.56
2:A:234:ILE:O	2:A:238:ILE:HG12	2.06	0.56
2:A:234:ILE:O	2:A:238:ILE:HG12	2.06	0.56
1:C:390:LEU:HG	1:C:398:PRO:HB3	1.87	0.56
2:A:234:ILE:O	2:A:238:ILE:HG12	2.06	0.56
2:A:234:ILE:O	2:A:238:ILE:HG12	2.06	0.56
1:C:70:ILE:HD11	1:C:128:PRO:HD3	1.88	0.56
1:C:70:ILE:HD11	1:C:128:PRO:HD3	1.88	0.56
1:C:70:ILE:HD11	1:C:128:PRO:HD3	1.88	0.56
3:B:241:CYS:SG	3:B:320:ARG:HB3	2.46	0.56
3:B:241:CYS:SG	3:B:320:ARG:HB3	2.46	0.56
3:B:241:CYS:SG	3:B:320:ARG:HB3	2.46	0.56
3:B:241:CYS:SG	3:B:320:ARG:HB3	2.46	0.56
3:B:241:CYS:SG	3:B:320:ARG:HB3	2.46	0.56
2:A:112:LYS:HD3	2:A:115:ILE:HG21	1.88	0.56
3:B:52:TYR:OH	3:B:136:GLN:HG3	2.05	0.56
3:B:424:ASN:O	3:B:427:ASP:HB3	2.06	0.56
2:A:112:LYS:HD3	2:A:115:ILE:HG21	1.88	0.56
3:B:52:TYR:OH	3:B:136:GLN:HG3	2.05	0.56
3:B:424:ASN:O	3:B:427:ASP:HB3	2.06	0.56
2:A:112:LYS:HD3	2:A:115:ILE:HG21	1.88	0.56
3:B:52:TYR:OH	3:B:136:GLN:HG3	2.05	0.56
3:B:424:ASN:O	3:B:427:ASP:HB3	2.06	0.56
2:A:112:LYS:HD3	2:A:115:ILE:HG21	1.88	0.56
3:B:52:TYR:OH	3:B:136:GLN:HG3	2.05	0.56
3:B:424:ASN:O	3:B:427:ASP:HB3	2.06	0.56
2:A:112:LYS:HD3	2:A:115:ILE:HG21	1.88	0.56
3:B:52:TYR:OH	3:B:136:GLN:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:424:ASN:O	3:B:427:ASP:HB3	2.06	0.56
1:C:340:VAL:HB	1:C:343:LEU:HD11	1.87	0.56
1:C:340:VAL:HB	1:C:343:LEU:HD11	1.87	0.56
1:C:340:VAL:HB	1:C:343:LEU:HD11	1.87	0.56
1:C:459:ARG:HH12	3:B:424:ASN:HA	1.70	0.56
1:C:157:THR:HA	1:C:480:ILE:HB	1.88	0.56
1:C:340:VAL:HB	1:C:343:LEU:HD11	1.87	0.56
1:C:340:VAL:HB	1:C:343:LEU:HD11	1.87	0.56
2:A:175:PRO:HG3	2:A:304:LYS:HG2	1.88	0.55
1:C:157:THR:HA	1:C:480:ILE:HB	1.88	0.55
2:A:175:PRO:HG3	2:A:304:LYS:HG2	1.88	0.55
2:A:175:PRO:HG3	2:A:304:LYS:HG2	1.88	0.55
1:C:157:THR:HA	1:C:480:ILE:HB	1.88	0.55
2:A:175:PRO:HG3	2:A:304:LYS:HG2	1.88	0.55
1:C:157:THR:HA	1:C:480:ILE:HB	1.88	0.55
2:A:175:PRO:HG3	2:A:304:LYS:HG2	1.88	0.55
1:C:157:THR:HA	1:C:480:ILE:HB	1.88	0.55
1:C:457:PRO:O	1:C:460:ASP:HB2	2.07	0.55
1:C:457:PRO:O	1:C:460:ASP:HB2	2.07	0.55
1:C:457:PRO:O	1:C:460:ASP:HB2	2.07	0.55
1:C:457:PRO:O	1:C:460:ASP:HB2	2.07	0.55
2:A:22:GLU:HA	2:A:83:TYR:CE2	2.41	0.55
3:B:373:MET:HE3	3:B:373:MET:HA	1.88	0.55
1:C:457:PRO:O	1:C:460:ASP:HB2	2.07	0.55
2:A:22:GLU:HA	2:A:83:TYR:CE2	2.41	0.55
3:B:373:MET:HE3	3:B:373:MET:HA	1.88	0.55
2:A:22:GLU:HA	2:A:83:TYR:CE2	2.41	0.55
3:B:373:MET:HE3	3:B:373:MET:HA	1.88	0.55
2:A:22:GLU:HA	2:A:83:TYR:CE2	2.41	0.55
3:B:373:MET:HE3	3:B:373:MET:HA	1.88	0.55
2:A:22:GLU:HA	2:A:83:TYR:CE2	2.41	0.55
3:B:373:MET:HE3	3:B:373:MET:HA	1.88	0.55
1:C:136:PHE:HB2	1:C:178:ILE:HA	1.89	0.55
1:C:136:PHE:HB2	1:C:178:ILE:HA	1.89	0.55
1:C:136:PHE:HB2	1:C:178:ILE:HA	1.89	0.55
1:C:389:HIS:HB3	1:C:399:LYS:HG3	1.88	0.55
1:C:179:LEU:HD23	1:C:405:LEU:HG	1.88	0.55
1:C:179:LEU:HD23	1:C:405:LEU:HG	1.88	0.55
1:C:333:ASP:HA	3:B:416:MET:CG	2.36	0.55
1:C:389:HIS:HB3	1:C:399:LYS:HG3	1.88	0.55
1:C:136:PHE:HB2	1:C:178:ILE:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:PHE:HB2	1:C:178:ILE:HA	1.89	0.55
1:C:330:LEU:HD23	1:C:340:VAL:HA	1.89	0.55
1:C:179:LEU:HD23	1:C:405:LEU:HG	1.88	0.55
1:C:330:LEU:HD23	1:C:340:VAL:HA	1.89	0.55
1:C:179:LEU:HD23	1:C:405:LEU:HG	1.88	0.55
1:C:389:HIS:HB3	1:C:399:LYS:HG3	1.88	0.55
1:C:179:LEU:HD23	1:C:405:LEU:HG	1.88	0.55
1:C:389:HIS:HB3	1:C:399:LYS:HG3	1.88	0.55
1:C:389:HIS:HB3	1:C:399:LYS:HG3	1.88	0.55
3:B:3:GLU:HB3	3:B:64:ARG:NH2	2.22	0.55
3:B:3:GLU:HB3	3:B:64:ARG:NH2	2.22	0.55
1:C:330:LEU:HD23	1:C:340:VAL:HA	1.89	0.55
3:B:3:GLU:HB3	3:B:64:ARG:NH2	2.22	0.55
1:C:330:LEU:HD23	1:C:340:VAL:HA	1.89	0.55
3:B:3:GLU:HB3	3:B:64:ARG:NH2	2.22	0.55
3:B:3:GLU:HB3	3:B:64:ARG:NH2	2.22	0.55
3:B:3:GLU:HA	3:B:51:VAL:HA	1.89	0.55
3:B:3:GLU:HA	3:B:51:VAL:HA	1.89	0.55
3:B:3:GLU:HA	3:B:51:VAL:HA	1.89	0.55
3:B:3:GLU:HA	3:B:51:VAL:HA	1.89	0.55
1:C:330:LEU:HD23	1:C:340:VAL:HA	1.89	0.55
3:B:3:GLU:HA	3:B:51:VAL:HA	1.89	0.55
1:C:459:ARG:NH1	3:B:424:ASN:HD22	2.05	0.55
1:C:77:GLU:O	1:C:80:ARG:HG2	2.06	0.54
2:A:137:VAL:HB	2:A:168:GLU:CB	2.37	0.54
1:C:459:ARG:NH1	3:B:424:ASN:HD22	2.05	0.54
2:A:137:VAL:HB	2:A:168:GLU:CB	2.37	0.54
2:A:137:VAL:HB	2:A:168:GLU:CB	2.37	0.54
2:A:137:VAL:HB	2:A:168:GLU:CB	2.37	0.54
2:A:137:VAL:HB	2:A:168:GLU:CB	2.37	0.54
2:A:224:TYR:CE2	6:A:500:GTP:C5	2.95	0.54
2:A:224:TYR:CE2	6:A:500:GTP:C5	2.95	0.54
2:A:224:TYR:CE2	6:A:500:GTP:C5	2.95	0.54
2:A:224:TYR:CE2	6:A:500:GTP:C5	2.95	0.54
2:A:224:TYR:CE2	6:A:500:GTP:C5	2.95	0.54
1:C:77:GLU:O	1:C:80:ARG:HG2	2.06	0.54
1:C:77:GLU:O	1:C:80:ARG:HG2	2.06	0.54
1:C:77:GLU:O	1:C:80:ARG:HG2	2.06	0.54
1:C:296:ILE:HG13	1:C:390:LEU:O	2.06	0.54
1:C:77:GLU:O	1:C:80:ARG:HG2	2.06	0.54
1:C:296:ILE:HG13	1:C:390:LEU:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:PHE:HB2	1:C:351:VAL:HB	1.89	0.54
1:C:296:ILE:HG13	1:C:390:LEU:O	2.06	0.54
2:A:224:TYR:CD2	6:A:500:GTP:C6	2.95	0.54
3:B:360:PRO:HD2	3:B:371:LEU:HB3	1.89	0.54
1:C:187:PHE:HB2	1:C:351:VAL:HB	1.89	0.54
1:C:296:ILE:HG13	1:C:390:LEU:O	2.07	0.54
2:A:224:TYR:CD2	6:A:500:GTP:C6	2.95	0.54
3:B:360:PRO:HD2	3:B:371:LEU:HB3	1.89	0.54
2:A:224:TYR:CD2	6:A:500:GTP:C6	2.95	0.54
3:B:360:PRO:HD2	3:B:371:LEU:HB3	1.89	0.54
1:C:187:PHE:HB2	1:C:351:VAL:HB	1.89	0.54
1:C:296:ILE:HG13	1:C:390:LEU:O	2.07	0.54
2:A:224:TYR:CD2	6:A:500:GTP:C6	2.95	0.54
3:B:360:PRO:HD2	3:B:371:LEU:HB3	1.89	0.54
1:C:187:PHE:HB2	1:C:351:VAL:HB	1.89	0.54
2:A:224:TYR:CD2	6:A:500:GTP:C6	2.95	0.54
3:B:360:PRO:HD2	3:B:371:LEU:HB3	1.89	0.54
1:C:301:TRP:HB2	1:C:386:ARG:CG	2.32	0.54
1:C:424:LYS:NZ	3:B:163:ASP:CG	2.66	0.54
3:B:111:GLY:HA2	3:B:149:MET:HE2	1.89	0.54
3:B:111:GLY:HA2	3:B:149:MET:HE2	1.89	0.54
3:B:111:GLY:HA2	3:B:149:MET:HE2	1.89	0.54
3:B:111:GLY:HA2	3:B:149:MET:HE2	1.89	0.54
3:B:111:GLY:HA2	3:B:149:MET:HE2	1.89	0.54
3:B:228:ASN:OD1	7:B:600:GDP:N1	2.34	0.54
1:C:459:ARG:HH12	3:B:424:ASN:HA	1.72	0.54
3:B:228:ASN:OD1	7:B:600:GDP:N1	2.34	0.54
1:C:187:PHE:HB2	1:C:351:VAL:HB	1.89	0.54
3:B:228:ASN:OD1	7:B:600:GDP:N1	2.34	0.54
3:B:228:ASN:OD1	7:B:600:GDP:N1	2.34	0.54
3:B:228:ASN:OD1	7:B:600:GDP:N1	2.34	0.54
3:B:228:ASN:OD1	7:B:600:GDP:N1	2.34	0.54
3:B:371:LEU:HD13	8:B:601:TA1:C44	2.36	0.54
1:C:301:TRP:HB2	1:C:386:ARG:CG	2.32	0.54
1:C:455:LEU:CD2	3:B:431:GLU:HG3	2.38	0.54
3:B:371:LEU:HD13	8:B:601:TA1:C44	2.36	0.54
1:C:301:TRP:HB2	1:C:386:ARG:CG	2.32	0.54
3:B:371:LEU:HD13	8:B:601:TA1:C44	2.36	0.54
1:C:301:TRP:HB2	1:C:386:ARG:CG	2.32	0.54
3:B:371:LEU:HD13	8:B:601:TA1:C44	2.36	0.54
3:B:371:LEU:HD13	8:B:601:TA1:C44	2.36	0.54
2:A:324:VAL:HB	2:A:327:ASP:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:141:LEU:HD22	3:B:172:VAL:HG12	1.90	0.54
2:A:324:VAL:HB	2:A:327:ASP:HB2	1.89	0.54
3:B:141:LEU:HD22	3:B:172:VAL:HG12	1.90	0.54
2:A:324:VAL:HB	2:A:327:ASP:HB2	1.89	0.54
3:B:141:LEU:HD22	3:B:172:VAL:HG12	1.90	0.54
2:A:324:VAL:HB	2:A:327:ASP:HB2	1.89	0.54
3:B:141:LEU:HD22	3:B:172:VAL:HG12	1.90	0.54
1:C:301:TRP:HB2	1:C:386:ARG:CG	2.32	0.54
2:A:324:VAL:HB	2:A:327:ASP:HB2	1.89	0.54
3:B:141:LEU:HD22	3:B:172:VAL:HG12	1.90	0.54
1:C:319:PRO:HG2	1:C:325:ARG:HH21	1.73	0.54
1:C:455:LEU:CD2	3:B:431:GLU:HG3	2.38	0.54
1:C:455:LEU:CD2	3:B:431:GLU:HG3	2.38	0.53
1:C:459:ARG:HH12	3:B:424:ASN:HA	1.73	0.53
1:C:333:ASP:HA	3:B:416:MET:CG	2.38	0.53
1:C:68:LEU:HD13	1:C:95:LEU:HD13	1.89	0.53
1:C:314:ASP:HB3	1:C:326:GLN:HE22	1.73	0.53
1:C:68:LEU:HD13	1:C:95:LEU:HD13	1.90	0.53
1:C:333:ASP:HA	3:B:416:MET:CG	2.38	0.53
1:C:68:LEU:HD13	1:C:95:LEU:HD13	1.90	0.53
1:C:438:ARG:HD3	2:A:402:ARG:HG3	1.90	0.53
1:C:438:ARG:HD3	2:A:402:ARG:HG3	1.90	0.53
1:C:68:LEU:HD13	1:C:95:LEU:HD13	1.90	0.53
1:C:459:ARG:NH1	3:B:424:ASN:HD22	2.07	0.53
1:C:68:LEU:HD13	1:C:95:LEU:HD13	1.90	0.53
1:C:365:GLN:HG3	1:C:366:SER:O	2.09	0.53
1:C:494:LEU:HD11	2:A:420:GLU:OE1	2.09	0.53
3:B:262:PHE:HB3	3:B:263:PRO:HD2	1.90	0.53
3:B:262:PHE:HB3	3:B:263:PRO:HD2	1.90	0.53
3:B:262:PHE:HB3	3:B:263:PRO:HD2	1.90	0.53
1:C:369:SER:HG	1:C:422:ARG:HH12	1.52	0.53
3:B:262:PHE:HB3	3:B:263:PRO:HD2	1.90	0.53
3:B:262:PHE:HB3	3:B:263:PRO:HD2	1.90	0.53
1:C:333:ASP:HA	3:B:416:MET:CG	2.38	0.53
1:C:369:SER:CB	1:C:422:ARG:NH1	2.70	0.53
1:C:459:ARG:HH12	3:B:424:ASN:HA	1.73	0.53
2:A:286:LEU:HG	2:A:290:GLU:HB2	1.91	0.53
3:B:43:GLN:HA	3:B:244:PHE:CE1	2.44	0.53
3:B:119:LEU:HA	3:B:122:VAL:HG22	1.90	0.53
3:B:326:LYS:O	3:B:330:GLU:HB2	2.09	0.53
2:A:286:LEU:HG	2:A:290:GLU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:43:GLN:HA	3:B:244:PHE:CE1	2.44	0.53
3:B:119:LEU:HA	3:B:122:VAL:HG22	1.90	0.53
3:B:326:LYS:O	3:B:330:GLU:HB2	2.09	0.53
2:A:286:LEU:HG	2:A:290:GLU:HB2	1.91	0.53
3:B:43:GLN:HA	3:B:244:PHE:CE1	2.44	0.53
3:B:119:LEU:HA	3:B:122:VAL:HG22	1.90	0.53
3:B:326:LYS:O	3:B:330:GLU:HB2	2.09	0.53
1:C:438:ARG:HD3	2:A:402:ARG:HG3	1.90	0.53
2:A:286:LEU:HG	2:A:290:GLU:HB2	1.91	0.53
3:B:43:GLN:HA	3:B:244:PHE:CE1	2.44	0.53
3:B:119:LEU:HA	3:B:122:VAL:HG22	1.90	0.53
3:B:326:LYS:O	3:B:330:GLU:HB2	2.09	0.53
2:A:286:LEU:HG	2:A:290:GLU:HB2	1.91	0.53
3:B:43:GLN:HA	3:B:244:PHE:CE1	2.44	0.53
3:B:119:LEU:HA	3:B:122:VAL:HG22	1.90	0.53
3:B:326:LYS:O	3:B:330:GLU:HB2	2.09	0.53
1:C:334:GLN:N	3:B:416:MET:CE	2.71	0.53
1:C:321:HIS:ND1	1:C:366:SER:OG	2.39	0.53
1:C:348:VAL:HG12	1:C:353:GLU:HG2	1.91	0.53
1:C:348:VAL:HG12	1:C:353:GLU:HG2	1.91	0.53
1:C:424:LYS:NZ	3:B:163:ASP:CG	2.67	0.52
1:C:459:ARG:HH12	3:B:424:ASN:HA	1.74	0.52
1:C:348:VAL:HG12	1:C:353:GLU:HG2	1.91	0.52
1:C:455:LEU:CD2	3:B:431:GLU:HG3	2.39	0.52
1:C:348:VAL:HG12	1:C:353:GLU:HG2	1.91	0.52
1:C:313:TYR:HE1	1:C:324:LYS:HD2	1.73	0.52
1:C:348:VAL:HG12	1:C:353:GLU:HG2	1.91	0.52
1:C:438:ARG:HD3	2:A:402:ARG:HG3	1.91	0.52
3:B:215:ARG:HG3	3:B:216:THR:N	2.23	0.52
3:B:215:ARG:HG3	3:B:216:THR:N	2.23	0.52
3:B:215:ARG:HG3	3:B:216:THR:N	2.23	0.52
3:B:215:ARG:HG3	3:B:216:THR:N	2.23	0.52
3:B:215:ARG:HG3	3:B:216:THR:N	2.23	0.52
1:C:321:HIS:NE2	1:C:366:SER:OG	2.43	0.52
1:C:89:ILE:HD12	1:C:125:ILE:HD11	1.92	0.52
1:C:89:ILE:HD12	1:C:125:ILE:HD11	1.92	0.52
1:C:89:ILE:HD12	1:C:125:ILE:HD11	1.92	0.52
1:C:445:GLN:HB2	1:C:450:ARG:NH2	2.25	0.52
1:C:187:PHE:CE1	1:C:300:VAL:HG11	2.45	0.52
3:B:315:VAL:HB	3:B:351:VAL:HG22	1.90	0.52
1:C:494:LEU:HD11	2:A:420:GLU:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:315:VAL:HB	3:B:351:VAL:HG22	1.90	0.52
3:B:315:VAL:HB	3:B:351:VAL:HG22	1.90	0.52
3:B:315:VAL:HB	3:B:351:VAL:HG22	1.90	0.52
3:B:315:VAL:HB	3:B:351:VAL:HG22	1.90	0.52
1:C:382:ILE:HA	1:C:405:LEU:O	2.10	0.52
2:A:22:GLU:HA	2:A:83:TYR:HE2	1.75	0.52
2:A:88:HIS:HB2	2:A:91:GLN:HG3	1.92	0.52
1:C:89:ILE:HD12	1:C:125:ILE:HD11	1.92	0.52
1:C:187:PHE:CE1	1:C:300:VAL:HG11	2.45	0.52
2:A:22:GLU:HA	2:A:83:TYR:HE2	1.75	0.52
2:A:88:HIS:HB2	2:A:91:GLN:HG3	1.92	0.52
1:C:187:PHE:CE1	1:C:300:VAL:HG11	2.45	0.52
1:C:445:GLN:NE2	1:C:452:LYS:HD3	2.25	0.52
2:A:22:GLU:HA	2:A:83:TYR:HE2	1.75	0.52
2:A:88:HIS:HB2	2:A:91:GLN:HG3	1.92	0.52
1:C:187:PHE:CE1	1:C:300:VAL:HG11	2.45	0.52
2:A:22:GLU:HA	2:A:83:TYR:HE2	1.75	0.52
2:A:88:HIS:HB2	2:A:91:GLN:HG3	1.92	0.52
1:C:89:ILE:HD12	1:C:125:ILE:HD11	1.92	0.52
1:C:187:PHE:CE1	1:C:300:VAL:HG11	2.45	0.52
1:C:424:LYS:NZ	3:B:163:ASP:CG	2.68	0.52
2:A:22:GLU:HA	2:A:83:TYR:HE2	1.75	0.52
2:A:88:HIS:HB2	2:A:91:GLN:HG3	1.92	0.52
2:A:269:LEU:O	2:A:378:LEU:HA	2.09	0.52
2:A:269:LEU:O	2:A:378:LEU:HA	2.09	0.52
1:C:459:ARG:NH1	3:B:424:ASN:HD22	2.08	0.52
2:A:269:LEU:O	2:A:378:LEU:HA	2.09	0.52
2:A:269:LEU:O	2:A:378:LEU:HA	2.09	0.52
1:C:382:ILE:HA	1:C:405:LEU:O	2.10	0.52
1:C:455:LEU:CD2	3:B:431:GLU:HG3	2.40	0.52
2:A:269:LEU:O	2:A:378:LEU:HA	2.09	0.52
1:C:334:GLN:N	3:B:416:MET:CE	2.73	0.52
1:C:382:ILE:HA	1:C:405:LEU:O	2.10	0.52
1:C:382:ILE:HA	1:C:405:LEU:O	2.10	0.52
1:C:382:ILE:HA	1:C:405:LEU:O	2.10	0.52
1:C:321:HIS:ND1	1:C:366:SER:OG	2.42	0.52
1:C:494:LEU:HD11	2:A:420:GLU:OE1	2.10	0.52
1:C:423:LEU:HG	1:C:424:LYS:N	2.25	0.51
1:C:494:LEU:HD11	2:A:420:GLU:OE1	2.10	0.51
3:B:176:LYS:HG3	3:B:177:VAL:HG23	1.92	0.51
3:B:176:LYS:HG3	3:B:177:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:176:LYS:HG3	3:B:177:VAL:HG23	1.92	0.51
3:B:176:LYS:HG3	3:B:177:VAL:HG23	1.92	0.51
3:B:176:LYS:HG3	3:B:177:VAL:HG23	1.92	0.51
3:B:251:ASP:H	3:B:254:LYS:HB2	1.76	0.51
1:C:183:LEU:HA	1:C:186:ILE:HG22	1.92	0.51
3:B:251:ASP:H	3:B:254:LYS:HB2	1.76	0.51
1:C:183:LEU:HA	1:C:186:ILE:HG22	1.92	0.51
3:B:251:ASP:H	3:B:254:LYS:HB2	1.76	0.51
3:B:251:ASP:H	3:B:254:LYS:HB2	1.76	0.51
1:C:135:PHE:CE2	1:C:168:THR:HB	2.45	0.51
3:B:251:ASP:H	3:B:254:LYS:HB2	1.76	0.51
1:C:183:LEU:HA	1:C:186:ILE:HG22	1.92	0.51
2:A:362:VAL:HB	2:A:370:LYS:HD3	1.93	0.51
3:B:323:MET:HE2	3:B:328:VAL:HG22	1.92	0.51
2:A:362:VAL:HB	2:A:370:LYS:HD3	1.93	0.51
3:B:323:MET:HE2	3:B:328:VAL:HG22	1.92	0.51
1:C:333:ASP:HA	3:B:416:MET:CG	2.40	0.51
2:A:362:VAL:HB	2:A:370:LYS:HD3	1.93	0.51
3:B:323:MET:HE2	3:B:328:VAL:HG22	1.92	0.51
1:C:183:LEU:HA	1:C:186:ILE:HG22	1.92	0.51
2:A:362:VAL:HB	2:A:370:LYS:HD3	1.93	0.51
3:B:323:MET:HE2	3:B:328:VAL:HG22	1.92	0.51
1:C:183:LEU:HA	1:C:186:ILE:HG22	1.92	0.51
2:A:362:VAL:HB	2:A:370:LYS:HD3	1.93	0.51
3:B:323:MET:HE2	3:B:328:VAL:HG22	1.92	0.51
1:C:330:LEU:CD1	1:C:466:VAL:HA	2.40	0.51
1:C:330:LEU:CD1	1:C:466:VAL:HA	2.40	0.51
1:C:330:LEU:CD1	1:C:466:VAL:HA	2.40	0.51
1:C:314:ASP:HB3	1:C:325:ARG:NH1	2.25	0.51
1:C:334:GLN:N	3:B:416:MET:CE	2.73	0.51
1:C:330:LEU:CD1	1:C:466:VAL:HA	2.40	0.51
2:A:315:CYS:HA	2:A:379:SER:HB3	1.92	0.51
3:B:20:PHE:HA	3:B:232:SER:HB2	1.91	0.51
3:B:70:LEU:HG	3:B:145:THR:HG23	1.93	0.51
2:A:315:CYS:HA	2:A:379:SER:HB3	1.92	0.51
3:B:20:PHE:HA	3:B:232:SER:HB2	1.91	0.51
3:B:70:LEU:HG	3:B:145:THR:HG23	1.93	0.51
2:A:315:CYS:HA	2:A:379:SER:HB3	1.92	0.51
3:B:20:PHE:HA	3:B:232:SER:HB2	1.91	0.51
3:B:70:LEU:HG	3:B:145:THR:HG23	1.93	0.51
1:C:330:LEU:CD1	1:C:466:VAL:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:315:CYS:HA	2:A:379:SER:HB3	1.92	0.51
3:B:20:PHE:HA	3:B:232:SER:HB2	1.91	0.51
3:B:70:LEU:HG	3:B:145:THR:HG23	1.93	0.51
2:A:315:CYS:HA	2:A:379:SER:HB3	1.92	0.51
3:B:20:PHE:HA	3:B:232:SER:HB2	1.91	0.51
3:B:70:LEU:HG	3:B:145:THR:HG23	1.93	0.51
3:B:133:GLN:HG3	3:B:165:ILE:HD11	1.92	0.51
1:C:135:PHE:CE2	1:C:168:THR:HB	2.46	0.51
1:C:329:ARG:NH1	1:C:331:CYS:HB2	2.26	0.51
3:B:133:GLN:HG3	3:B:165:ILE:HD11	1.92	0.51
3:B:133:GLN:HG3	3:B:165:ILE:HD11	1.92	0.51
3:B:133:GLN:HG3	3:B:165:ILE:HD11	1.92	0.51
1:C:329:ARG:NH1	1:C:331:CYS:HB2	2.26	0.51
3:B:133:GLN:HG3	3:B:165:ILE:HD11	1.92	0.51
1:C:329:ARG:NH1	1:C:331:CYS:HB2	2.26	0.51
2:A:191:THR:O	2:A:195:LEU:HB2	2.10	0.51
1:C:424:LYS:NZ	3:B:163:ASP:CG	2.69	0.51
2:A:191:THR:O	2:A:195:LEU:HB2	2.10	0.51
2:A:191:THR:O	2:A:195:LEU:HB2	2.10	0.51
1:C:329:ARG:NH1	1:C:331:CYS:HB2	2.26	0.51
2:A:191:THR:O	2:A:195:LEU:HB2	2.10	0.51
2:A:191:THR:O	2:A:195:LEU:HB2	2.10	0.51
1:C:85:GLY:HA2	1:C:485:PRO:HB3	1.92	0.51
1:C:137:ASN:O	1:C:141:LYS:HB2	2.11	0.51
2:A:224:TYR:CG	6:A:500:GTP:C6	2.98	0.51
1:C:137:ASN:O	1:C:141:LYS:HB2	2.11	0.51
2:A:224:TYR:CG	6:A:500:GTP:C6	2.98	0.51
1:C:85:GLY:HA2	1:C:485:PRO:HB3	1.92	0.51
1:C:329:ARG:NH1	1:C:331:CYS:HB2	2.26	0.51
1:C:443:LEU:HD13	1:C:456:ILE:HD12	1.93	0.51
1:C:494:LEU:HD11	2:A:420:GLU:OE1	2.11	0.51
2:A:224:TYR:CG	6:A:500:GTP:C6	2.98	0.51
2:A:224:TYR:CG	6:A:500:GTP:C6	2.98	0.51
2:A:224:TYR:CG	6:A:500:GTP:C6	2.98	0.51
1:C:70:ILE:HG22	1:C:483:VAL:HG12	1.93	0.50
1:C:443:LEU:HD13	1:C:456:ILE:HD12	1.93	0.50
1:C:70:ILE:HG22	1:C:483:VAL:HG12	1.93	0.50
1:C:443:LEU:HD13	1:C:456:ILE:HD12	1.93	0.50
1:C:70:ILE:HG22	1:C:483:VAL:HG12	1.93	0.50
1:C:137:ASN:O	1:C:141:LYS:HB2	2.11	0.50
1:C:137:ASN:O	1:C:141:LYS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:LEU:HD13	1:C:456:ILE:HD12	1.93	0.50
1:C:70:ILE:HG22	1:C:483:VAL:HG12	1.93	0.50
1:C:137:ASN:O	1:C:141:LYS:HB2	2.11	0.50
1:C:334:GLN:N	3:B:416:MET:CE	2.73	0.50
2:A:7:ILE:HG13	2:A:137:VAL:HA	1.93	0.50
3:B:11:GLN:HB2	7:B:600:GDP:O2B	2.11	0.50
1:C:85:GLY:HA2	1:C:485:PRO:HB3	1.92	0.50
2:A:7:ILE:HG13	2:A:137:VAL:HA	1.93	0.50
3:B:11:GLN:HB2	7:B:600:GDP:O2B	2.11	0.50
1:C:135:PHE:CE2	1:C:168:THR:HB	2.46	0.50
2:A:7:ILE:HG13	2:A:137:VAL:HA	1.93	0.50
3:B:11:GLN:HB2	7:B:600:GDP:O2B	2.11	0.50
1:C:70:ILE:HG22	1:C:483:VAL:HG12	1.94	0.50
1:C:85:GLY:HA2	1:C:485:PRO:HB3	1.92	0.50
2:A:7:ILE:HG13	2:A:137:VAL:HA	1.93	0.50
3:B:11:GLN:HB2	7:B:600:GDP:O2B	2.11	0.50
1:C:85:GLY:HA2	1:C:485:PRO:HB3	1.92	0.50
1:C:443:LEU:HD13	1:C:456:ILE:HD12	1.93	0.50
2:A:7:ILE:HG13	2:A:137:VAL:HA	1.93	0.50
3:B:11:GLN:HB2	7:B:600:GDP:O2B	2.11	0.50
1:C:135:PHE:CE2	1:C:168:THR:HB	2.46	0.50
1:C:438:ARG:HD3	2:A:402:ARG:HG3	1.92	0.50
3:B:277:SER:O	8:B:601:TA1:H191	2.11	0.50
3:B:277:SER:O	8:B:601:TA1:H191	2.11	0.50
3:B:277:SER:O	8:B:601:TA1:H191	2.11	0.50
3:B:277:SER:O	8:B:601:TA1:H191	2.11	0.50
3:B:277:SER:O	8:B:601:TA1:H191	2.11	0.50
2:A:140:SER:HA	2:A:171:ILE:HB	1.92	0.50
2:A:179:THR:OG1	6:A:500:GTP:O2'	2.17	0.50
2:A:286:LEU:HD23	2:A:291:ILE:HG23	1.93	0.50
3:B:3:GLU:HB3	3:B:64:ARG:HH22	1.76	0.50
3:B:237:GLY:HA2	3:B:241:CYS:HB3	1.92	0.50
1:C:365:GLN:HG3	1:C:366:SER:O	2.12	0.50
2:A:140:SER:HA	2:A:171:ILE:HB	1.92	0.50
2:A:179:THR:OG1	6:A:500:GTP:O2'	2.17	0.50
2:A:286:LEU:HD23	2:A:291:ILE:HG23	1.93	0.50
3:B:3:GLU:HB3	3:B:64:ARG:HH22	1.76	0.50
3:B:237:GLY:HA2	3:B:241:CYS:HB3	1.92	0.50
2:A:140:SER:HA	2:A:171:ILE:HB	1.92	0.50
2:A:179:THR:OG1	6:A:500:GTP:O2'	2.17	0.50
2:A:286:LEU:HD23	2:A:291:ILE:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3:GLU:HB3	3:B:64:ARG:HH22	1.76	0.50
3:B:237:GLY:HA2	3:B:241:CYS:HB3	1.92	0.50
1:C:135:PHE:CE2	1:C:168:THR:HB	2.46	0.50
2:A:140:SER:HA	2:A:171:ILE:HB	1.92	0.50
2:A:179:THR:OG1	6:A:500:GTP:O2'	2.17	0.50
2:A:286:LEU:HD23	2:A:291:ILE:HG23	1.93	0.50
3:B:3:GLU:HB3	3:B:64:ARG:HH22	1.76	0.50
3:B:237:GLY:HA2	3:B:241:CYS:HB3	1.92	0.50
2:A:140:SER:HA	2:A:171:ILE:HB	1.92	0.50
2:A:179:THR:OG1	6:A:500:GTP:O2'	2.17	0.50
2:A:286:LEU:HD23	2:A:291:ILE:HG23	1.93	0.50
3:B:3:GLU:HB3	3:B:64:ARG:HH22	1.76	0.50
3:B:237:GLY:HA2	3:B:241:CYS:HB3	1.92	0.50
2:A:179:THR:OG1	6:A:500:GTP:C2'	2.59	0.50
3:B:52:TYR:HH	3:B:136:GLN:HG3	1.76	0.50
2:A:179:THR:OG1	6:A:500:GTP:C2'	2.59	0.50
3:B:52:TYR:HH	3:B:136:GLN:HG3	1.76	0.50
2:A:179:THR:OG1	6:A:500:GTP:C2'	2.59	0.50
3:B:52:TYR:HH	3:B:136:GLN:HG3	1.76	0.50
2:A:179:THR:OG1	6:A:500:GTP:C2'	2.59	0.50
3:B:52:TYR:HH	3:B:136:GLN:HG3	1.76	0.50
3:B:232:SER:HA	3:B:235:MET:SD	2.51	0.50
3:B:232:SER:HA	3:B:235:MET:SD	2.51	0.50
3:B:232:SER:HA	3:B:235:MET:SD	2.51	0.50
3:B:232:SER:HA	3:B:235:MET:SD	2.51	0.50
3:B:232:SER:HA	3:B:235:MET:SD	2.51	0.50
2:A:224:TYR:CE2	6:A:500:GTP:C8	2.99	0.50
3:B:21:TRP:HA	3:B:24:ILE:HG22	1.93	0.50
2:A:224:TYR:CE2	6:A:500:GTP:C8	2.99	0.50
3:B:21:TRP:HA	3:B:24:ILE:HG22	1.93	0.50
2:A:224:TYR:CE2	6:A:500:GTP:C8	2.99	0.50
3:B:21:TRP:HA	3:B:24:ILE:HG22	1.93	0.50
2:A:224:TYR:CE2	6:A:500:GTP:C8	2.99	0.50
3:B:21:TRP:HA	3:B:24:ILE:HG22	1.93	0.50
2:A:224:TYR:CE2	6:A:500:GTP:C8	2.99	0.50
3:B:21:TRP:HA	3:B:24:ILE:HG22	1.93	0.50
2:A:137:VAL:HB	2:A:168:GLU:HB3	1.94	0.50
3:B:414:ASP:HB2	3:B:417:GLU:HG3	1.92	0.50
1:C:70:ILE:HD13	1:C:70:ILE:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:137:VAL:HB	2:A:168:GLU:HB3	1.94	0.50
3:B:414:ASP:HB2	3:B:417:GLU:HG3	1.92	0.50
2:A:137:VAL:HB	2:A:168:GLU:HB3	1.94	0.50
3:B:414:ASP:HB2	3:B:417:GLU:HG3	1.92	0.50
2:A:137:VAL:HB	2:A:168:GLU:HB3	1.94	0.50
3:B:414:ASP:HB2	3:B:417:GLU:HG3	1.92	0.50
2:A:137:VAL:HB	2:A:168:GLU:HB3	1.94	0.50
3:B:414:ASP:HB2	3:B:417:GLU:HG3	1.92	0.50
1:C:166:THR:HA	1:C:169:ILE:HG22	1.93	0.49
3:B:101:ASN:ND2	3:B:143:GLY:HA2	2.27	0.49
3:B:198:THR:HG23	3:B:265:LEU:HD13	1.94	0.49
3:B:101:ASN:ND2	3:B:143:GLY:HA2	2.27	0.49
3:B:198:THR:HG23	3:B:265:LEU:HD13	1.94	0.49
1:C:334:GLN:N	3:B:416:MET:CE	2.75	0.49
3:B:101:ASN:ND2	3:B:143:GLY:HA2	2.27	0.49
3:B:198:THR:HG23	3:B:265:LEU:HD13	1.94	0.49
3:B:101:ASN:ND2	3:B:143:GLY:HA2	2.27	0.49
3:B:198:THR:HG23	3:B:265:LEU:HD13	1.94	0.49
3:B:101:ASN:ND2	3:B:143:GLY:HA2	2.27	0.49
3:B:198:THR:HG23	3:B:265:LEU:HD13	1.94	0.49
1:C:70:ILE:HD13	1:C:70:ILE:H	1.77	0.49
1:C:120:PHE:HB3	1:C:122:PHE:CE1	2.46	0.49
1:C:327:THR:HG23	1:C:327:THR:O	2.12	0.49
1:C:166:THR:HA	1:C:169:ILE:HG22	1.93	0.49
1:C:431:THR:O	1:C:435:THR:HG22	2.12	0.49
1:C:120:PHE:HB3	1:C:122:PHE:CE1	2.46	0.49
1:C:166:THR:HA	1:C:169:ILE:HG22	1.93	0.49
1:C:70:ILE:HD13	1:C:70:ILE:H	1.77	0.49
1:C:166:THR:HA	1:C:169:ILE:HG22	1.93	0.49
1:C:334:GLN:HG2	3:B:416:MET:CE	2.41	0.49
1:C:166:THR:HA	1:C:169:ILE:HG22	1.93	0.49
1:C:67:TYR:HA	1:C:124:GLN:O	2.12	0.49
1:C:334:GLN:HG2	3:B:416:MET:CE	2.41	0.49
1:C:431:THR:O	1:C:435:THR:HG22	2.12	0.49
3:B:6:HIS:O	3:B:65:ALA:HA	2.12	0.49
3:B:274:PRO:O	8:B:601:TA1:H151	2.13	0.49
1:C:120:PHE:HB3	1:C:122:PHE:CE1	2.46	0.49
1:C:147:VAL:HG22	1:C:403:LEU:HD21	1.94	0.49
1:C:415:LYS:CD	2:A:156:ARG:HH21	2.19	0.49
3:B:6:HIS:O	3:B:65:ALA:HA	2.12	0.49
3:B:274:PRO:O	8:B:601:TA1:H151	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ILE:HD13	1:C:70:ILE:H	1.77	0.49
3:B:6:HIS:O	3:B:65:ALA:HA	2.12	0.49
3:B:274:PRO:O	8:B:601:TA1:H151	2.13	0.49
1:C:120:PHE:HB3	1:C:122:PHE:CE1	2.46	0.49
1:C:424:LYS:NZ	3:B:163:ASP:CG	2.70	0.49
3:B:6:HIS:O	3:B:65:ALA:HA	2.12	0.49
3:B:274:PRO:O	8:B:601:TA1:H151	2.13	0.49
1:C:67:TYR:HA	1:C:124:GLN:O	2.12	0.49
1:C:70:ILE:HD13	1:C:70:ILE:H	1.77	0.49
1:C:120:PHE:HB3	1:C:122:PHE:CE1	2.46	0.49
1:C:431:THR:O	1:C:435:THR:HG22	2.12	0.49
3:B:6:HIS:O	3:B:65:ALA:HA	2.12	0.49
3:B:274:PRO:O	8:B:601:TA1:H151	2.13	0.49
2:A:224:TYR:CE2	6:A:500:GTP:N7	2.80	0.49
1:C:67:TYR:HA	1:C:124:GLN:O	2.12	0.49
2:A:224:TYR:CE2	6:A:500:GTP:N7	2.80	0.49
1:C:67:TYR:HA	1:C:124:GLN:O	2.12	0.49
1:C:147:VAL:HG22	1:C:403:LEU:HD21	1.94	0.49
1:C:431:THR:O	1:C:435:THR:HG22	2.12	0.49
2:A:224:TYR:CE2	6:A:500:GTP:N7	2.80	0.49
1:C:67:TYR:HA	1:C:124:GLN:O	2.12	0.49
1:C:431:THR:O	1:C:435:THR:HG22	2.12	0.49
2:A:224:TYR:CE2	6:A:500:GTP:N7	2.80	0.49
2:A:224:TYR:CE2	6:A:500:GTP:N7	2.80	0.49
1:C:147:VAL:HG22	1:C:403:LEU:HD21	1.94	0.49
1:C:307:ILE:HA	1:C:311:LEU:O	2.12	0.49
3:B:259:MET:O	3:B:261:PRO:HD3	2.13	0.49
3:B:295:MET:HG2	3:B:377:PHE:HB2	1.94	0.49
3:B:259:MET:O	3:B:261:PRO:HD3	2.13	0.49
3:B:295:MET:HG2	3:B:377:PHE:HB2	1.94	0.49
3:B:259:MET:O	3:B:261:PRO:HD3	2.13	0.49
3:B:295:MET:HG2	3:B:377:PHE:HB2	1.94	0.49
1:C:147:VAL:HG22	1:C:403:LEU:HD21	1.94	0.49
3:B:259:MET:O	3:B:261:PRO:HD3	2.13	0.49
3:B:295:MET:HG2	3:B:377:PHE:HB2	1.94	0.49
3:B:259:MET:O	3:B:261:PRO:HD3	2.13	0.49
3:B:295:MET:HG2	3:B:377:PHE:HB2	1.94	0.49
1:C:455:LEU:HD23	3:B:431:GLU:CG	2.42	0.49
3:B:119:LEU:HD11	3:B:156:LYS:HD3	1.93	0.49
1:C:307:ILE:HA	1:C:311:LEU:O	2.12	0.49
1:C:455:LEU:HD23	3:B:431:GLU:CG	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:119:LEU:HD11	3:B:156:LYS:HD3	1.93	0.49
1:C:140:MET:CE	1:C:178:ILE:HB	2.42	0.49
3:B:119:LEU:HD11	3:B:156:LYS:HD3	1.93	0.49
1:C:140:MET:CE	1:C:178:ILE:HB	2.42	0.49
3:B:119:LEU:HD11	3:B:156:LYS:HD3	1.93	0.49
1:C:307:ILE:HA	1:C:311:LEU:O	2.12	0.49
3:B:119:LEU:HD11	3:B:156:LYS:HD3	1.93	0.49
1:C:140:MET:CE	1:C:178:ILE:HB	2.43	0.49
2:A:205:ASP:O	2:A:209:ILE:HG13	2.12	0.49
1:C:140:MET:CE	1:C:178:ILE:HB	2.42	0.49
1:C:495:HIS:HE1	2:A:415:GLU:HB3	1.76	0.49
2:A:205:ASP:O	2:A:209:ILE:HG13	2.12	0.49
1:C:307:ILE:HA	1:C:311:LEU:O	2.12	0.49
2:A:205:ASP:O	2:A:209:ILE:HG13	2.12	0.49
1:C:307:ILE:HA	1:C:311:LEU:O	2.12	0.49
2:A:205:ASP:O	2:A:209:ILE:HG13	2.12	0.49
1:C:140:MET:CE	1:C:178:ILE:HB	2.43	0.49
1:C:147:VAL:HG22	1:C:403:LEU:HD21	1.95	0.49
1:C:495:HIS:HE1	2:A:415:GLU:HB3	1.76	0.49
2:A:205:ASP:O	2:A:209:ILE:HG13	2.12	0.49
1:C:455:LEU:HD23	3:B:431:GLU:OE2	2.12	0.49
1:C:415:LYS:HE2	2:A:156:ARG:HH21	1.77	0.49
1:C:68:LEU:HD12	1:C:122:PHE:CZ	2.48	0.49
1:C:68:LEU:HD12	1:C:122:PHE:CZ	2.48	0.49
1:C:68:LEU:HD12	1:C:122:PHE:CZ	2.48	0.49
1:C:68:LEU:HD12	1:C:122:PHE:CZ	2.48	0.49
1:C:68:LEU:HD12	1:C:122:PHE:CZ	2.48	0.48
1:C:415:LYS:HE2	2:A:112:LYS:HZ1	1.74	0.48
1:C:155:ILE:HB	1:C:405:LEU:HD13	1.95	0.48
1:C:330:LEU:HD21	1:C:340:VAL:HG13	1.95	0.48
1:C:455:LEU:HD23	3:B:431:GLU:OE2	2.13	0.48
1:C:444:ARG:CZ	1:C:502:LEU:HD21	2.42	0.48
1:C:313:TYR:OH	1:C:318:PRO:HB2	2.13	0.48
3:B:234:THR:HG21	3:B:270:PRO:HB2	1.95	0.48
1:C:334:GLN:HG2	3:B:416:MET:CE	2.42	0.48
3:B:234:THR:HG21	3:B:270:PRO:HB2	1.95	0.48
3:B:234:THR:HG21	3:B:270:PRO:HB2	1.95	0.48
1:C:155:ILE:HB	1:C:405:LEU:HD13	1.95	0.48
1:C:455:LEU:HD23	3:B:431:GLU:CG	2.43	0.48
3:B:234:THR:HG21	3:B:270:PRO:HB2	1.95	0.48
3:B:234:THR:HG21	3:B:270:PRO:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:LEU:HD21	1:C:383:PHE:CE2	2.48	0.48
1:C:155:ILE:HB	1:C:405:LEU:HD13	1.95	0.48
1:C:317:GLU:HG3	1:C:344:ASN:ND2	2.29	0.48
1:C:330:LEU:HD21	1:C:340:VAL:HG13	1.95	0.48
1:C:155:ILE:HB	1:C:405:LEU:HD13	1.95	0.48
1:C:155:ILE:HB	1:C:405:LEU:HD13	1.95	0.48
1:C:330:LEU:HD21	1:C:340:VAL:HG13	1.95	0.48
1:C:495:HIS:HE1	2:A:415:GLU:HB3	1.77	0.48
1:C:330:LEU:HD21	1:C:340:VAL:HG13	1.95	0.48
1:C:455:LEU:HD23	3:B:431:GLU:CG	2.43	0.48
1:C:495:HIS:HE1	2:A:415:GLU:HB3	1.77	0.48
1:C:413:ARG:HH22	1:C:492:GLU:CG	2.26	0.48
1:C:183:LEU:HD21	1:C:383:PHE:CE2	2.48	0.48
1:C:330:LEU:HD21	1:C:340:VAL:HG13	1.95	0.48
1:C:183:LEU:HD21	1:C:383:PHE:CE2	2.48	0.48
1:C:183:LEU:HD21	1:C:383:PHE:CE2	2.48	0.48
1:C:495:HIS:HE1	2:A:415:GLU:HB3	1.77	0.48
1:C:332:GLU:O	3:B:416:MET:HG3	2.13	0.48
1:C:183:LEU:HD21	1:C:383:PHE:CE2	2.48	0.48
1:C:444:ARG:O	1:C:448:GLN:HG3	2.12	0.48
1:C:327:THR:HG23	1:C:327:THR:O	2.14	0.48
1:C:444:ARG:O	1:C:448:GLN:HG3	2.12	0.48
1:C:444:ARG:O	1:C:448:GLN:HG3	2.12	0.48
1:C:444:ARG:O	1:C:448:GLN:HG3	2.12	0.48
1:C:444:ARG:O	1:C:448:GLN:HG3	2.12	0.48
3:B:147:SER:O	3:B:151:THR:HB	2.14	0.48
3:B:147:SER:O	3:B:151:THR:HB	2.14	0.48
3:B:147:SER:O	3:B:151:THR:HB	2.14	0.48
1:C:369:SER:CB	1:C:422:ARG:HH11	2.26	0.48
3:B:147:SER:O	3:B:151:THR:HB	2.14	0.48
3:B:147:SER:O	3:B:151:THR:HB	2.14	0.48
1:C:365:GLN:HG3	1:C:366:SER:N	2.29	0.48
1:C:455:LEU:HD23	3:B:431:GLU:OE2	2.14	0.48
1:C:314:ASP:H	1:C:326:GLN:HE22	1.62	0.48
1:C:317:GLU:CB	1:C:318:PRO:HD2	2.43	0.48
1:C:332:GLU:O	3:B:416:MET:HG3	2.14	0.48
1:C:154:LEU:HD22	1:C:470:PHE:HB3	1.96	0.48
1:C:132:GLN:CD	1:C:168:THR:HA	2.38	0.48
1:C:154:LEU:HD22	1:C:470:PHE:HB3	1.96	0.48
1:C:67:TYR:CE1	1:C:69:ARG:HB2	2.49	0.47
3:B:288:VAL:HB	3:B:289:PRO:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LEU:HD22	1:C:470:PHE:HB3	1.96	0.47
3:B:288:VAL:HB	3:B:289:PRO:CD	2.44	0.47
1:C:154:LEU:HD22	1:C:470:PHE:HB3	1.97	0.47
3:B:288:VAL:HB	3:B:289:PRO:CD	2.44	0.47
3:B:288:VAL:HB	3:B:289:PRO:CD	2.44	0.47
3:B:288:VAL:HB	3:B:289:PRO:CD	2.44	0.47
1:C:365:GLN:HG3	1:C:366:SER:N	2.29	0.47
2:A:180:ALA:HA	3:B:352:LYS:HG2	1.95	0.47
2:A:201:ALA:HB3	2:A:267:PHE:CD1	2.49	0.47
2:A:346:TRP:HZ2	2:A:435:VAL:HG13	1.79	0.47
2:A:407:TRP:CD1	3:B:257:VAL:HA	2.49	0.47
3:B:295:MET:HB3	3:B:377:PHE:CD1	2.50	0.47
1:C:67:TYR:CE1	1:C:69:ARG:HB2	2.49	0.47
1:C:132:GLN:CD	1:C:168:THR:HA	2.38	0.47
2:A:180:ALA:HA	3:B:352:LYS:HG2	1.95	0.47
2:A:201:ALA:HB3	2:A:267:PHE:CD1	2.49	0.47
2:A:346:TRP:HZ2	2:A:435:VAL:HG13	1.79	0.47
2:A:407:TRP:CD1	3:B:257:VAL:HA	2.49	0.47
3:B:295:MET:HB3	3:B:377:PHE:CD1	2.50	0.47
2:A:180:ALA:HA	3:B:352:LYS:HG2	1.95	0.47
2:A:201:ALA:HB3	2:A:267:PHE:CD1	2.49	0.47
2:A:346:TRP:HZ2	2:A:435:VAL:HG13	1.79	0.47
2:A:407:TRP:CD1	3:B:257:VAL:HA	2.49	0.47
3:B:295:MET:HB3	3:B:377:PHE:CD1	2.50	0.47
1:C:67:TYR:CE1	1:C:69:ARG:HB2	2.49	0.47
1:C:154:LEU:HD22	1:C:470:PHE:HB3	1.97	0.47
2:A:180:ALA:HA	3:B:352:LYS:HG2	1.95	0.47
2:A:201:ALA:HB3	2:A:267:PHE:CD1	2.49	0.47
2:A:346:TRP:HZ2	2:A:435:VAL:HG13	1.79	0.47
2:A:407:TRP:CD1	3:B:257:VAL:HA	2.49	0.47
3:B:295:MET:HB3	3:B:377:PHE:CD1	2.50	0.47
2:A:180:ALA:HA	3:B:352:LYS:HG2	1.95	0.47
2:A:201:ALA:HB3	2:A:267:PHE:CD1	2.49	0.47
2:A:346:TRP:HZ2	2:A:435:VAL:HG13	1.79	0.47
2:A:407:TRP:CD1	3:B:257:VAL:HA	2.49	0.47
3:B:295:MET:HB3	3:B:377:PHE:CD1	2.50	0.47
1:C:67:TYR:CE1	1:C:69:ARG:HB2	2.49	0.47
1:C:334:GLN:HG2	3:B:416:MET:CE	2.43	0.47
1:C:132:GLN:CD	1:C:168:THR:HA	2.38	0.47
1:C:91:ASN:HB3	1:C:93:GLU:OE2	2.15	0.47
1:C:67:TYR:CE1	1:C:69:ARG:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ARG:HH22	1:C:77:GLU:HG2	1.79	0.47
1:C:321:HIS:NE2	1:C:324:LYS:HD3	2.30	0.47
1:C:455:LEU:HD23	3:B:431:GLU:CG	2.44	0.47
1:C:71:ARG:HH22	1:C:77:GLU:HG2	1.79	0.47
1:C:91:ASN:HB3	1:C:93:GLU:OE2	2.15	0.47
1:C:335:ASN:HB2	1:C:337:ASN:OD1	2.13	0.47
3:B:194:LEU:O	3:B:198:THR:HG22	2.15	0.47
1:C:71:ARG:HH22	1:C:77:GLU:HG2	1.79	0.47
1:C:91:ASN:HB3	1:C:93:GLU:OE2	2.15	0.47
3:B:194:LEU:O	3:B:198:THR:HG22	2.15	0.47
1:C:132:GLN:CD	1:C:168:THR:HA	2.38	0.47
3:B:194:LEU:O	3:B:198:THR:HG22	2.15	0.47
1:C:71:ARG:HH22	1:C:77:GLU:HG2	1.79	0.47
1:C:335:ASN:HB2	1:C:337:ASN:OD1	2.13	0.47
3:B:194:LEU:O	3:B:198:THR:HG22	2.15	0.47
1:C:91:ASN:HB3	1:C:93:GLU:OE2	2.15	0.47
1:C:132:GLN:NE2	1:C:168:THR:HA	2.29	0.47
1:C:330:LEU:HD11	1:C:466:VAL:CB	2.45	0.47
1:C:335:ASN:HB2	1:C:337:ASN:OD1	2.13	0.47
3:B:194:LEU:O	3:B:198:THR:HG22	2.15	0.47
1:C:318:PRO:HA	1:C:319:PRO:HD3	1.73	0.47
1:C:330:LEU:HD11	1:C:466:VAL:CB	2.45	0.47
1:C:169:ILE:HA	1:C:178:ILE:HG12	1.97	0.47
1:C:330:LEU:HD11	1:C:466:VAL:CB	2.45	0.47
1:C:335:ASN:HB2	1:C:337:ASN:OD1	2.13	0.47
1:C:71:ARG:HH22	1:C:77:GLU:HG2	1.79	0.47
1:C:169:ILE:HA	1:C:178:ILE:HG12	1.97	0.47
1:C:330:LEU:HD11	1:C:466:VAL:CB	2.45	0.47
1:C:335:ASN:HB2	1:C:337:ASN:OD1	2.13	0.47
1:C:91:ASN:HB3	1:C:93:GLU:OE2	2.15	0.47
1:C:169:ILE:HA	1:C:178:ILE:HG12	1.97	0.47
1:C:330:LEU:HD11	1:C:466:VAL:CB	2.45	0.47
1:C:153:TRP:HZ2	1:C:478:CYS:HG	1.63	0.47
1:C:169:ILE:HA	1:C:178:ILE:HG12	1.97	0.47
1:C:153:TRP:HZ2	1:C:478:CYS:HG	1.63	0.47
1:C:169:ILE:HA	1:C:178:ILE:HG12	1.97	0.47
3:B:275:LEU:HD12	3:B:275:LEU:HA	1.80	0.47
3:B:324:SER:O	3:B:328:VAL:HG23	2.14	0.47
1:C:153:TRP:HZ2	1:C:478:CYS:HG	1.63	0.47
1:C:383:PHE:O	1:C:404:SER:HA	2.15	0.47
3:B:275:LEU:HD12	3:B:275:LEU:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:324:SER:O	3:B:328:VAL:HG23	2.14	0.47
3:B:275:LEU:HD12	3:B:275:LEU:HA	1.80	0.47
3:B:324:SER:O	3:B:328:VAL:HG23	2.14	0.47
1:C:153:TRP:HZ2	1:C:478:CYS:HG	1.63	0.47
1:C:440:ILE:HD12	1:C:499:PHE:CZ	2.47	0.47
3:B:275:LEU:HD12	3:B:275:LEU:HA	1.80	0.47
3:B:324:SER:O	3:B:328:VAL:HG23	2.14	0.47
1:C:440:ILE:HD12	1:C:499:PHE:CZ	2.47	0.47
3:B:275:LEU:HD12	3:B:275:LEU:HA	1.80	0.47
3:B:324:SER:O	3:B:328:VAL:HG23	2.14	0.47
1:C:383:PHE:O	1:C:404:SER:HA	2.15	0.47
3:B:229:HIS:NE2	8:B:601:TA1:H361	2.29	0.47
3:B:229:HIS:NE2	8:B:601:TA1:H361	2.29	0.47
3:B:229:HIS:NE2	8:B:601:TA1:H361	2.29	0.47
1:C:383:PHE:O	1:C:404:SER:HA	2.15	0.47
3:B:229:HIS:NE2	8:B:601:TA1:H361	2.29	0.47
3:B:229:HIS:NE2	8:B:601:TA1:H361	2.29	0.47
2:A:70:LEU:HB2	2:A:99:ALA:CB	2.38	0.47
2:A:238:ILE:HD13	2:A:318:LEU:HD12	1.97	0.47
2:A:317:LEU:HB3	2:A:319:TYR:CE1	2.49	0.47
2:A:70:LEU:HB2	2:A:99:ALA:CB	2.38	0.47
2:A:238:ILE:HD13	2:A:318:LEU:HD12	1.97	0.47
2:A:317:LEU:HB3	2:A:319:TYR:CE1	2.49	0.47
1:C:383:PHE:O	1:C:404:SER:HA	2.15	0.47
2:A:70:LEU:HB2	2:A:99:ALA:CB	2.38	0.47
2:A:238:ILE:HD13	2:A:318:LEU:HD12	1.97	0.47
2:A:317:LEU:HB3	2:A:319:TYR:CE1	2.49	0.47
2:A:70:LEU:HB2	2:A:99:ALA:CB	2.38	0.47
2:A:238:ILE:HD13	2:A:318:LEU:HD12	1.97	0.47
2:A:317:LEU:HB3	2:A:319:TYR:CE1	2.49	0.47
1:C:383:PHE:O	1:C:404:SER:HA	2.15	0.47
2:A:70:LEU:HB2	2:A:99:ALA:CB	2.38	0.47
2:A:238:ILE:HD13	2:A:318:LEU:HD12	1.97	0.47
2:A:317:LEU:HB3	2:A:319:TYR:CE1	2.49	0.47
1:C:455:LEU:CD2	3:B:431:GLU:CG	2.93	0.47
3:B:151:THR:HG23	3:B:193:GLN:HG2	1.97	0.47
3:B:413:MET:HG2	3:B:418:PHE:CE2	2.49	0.47
1:C:132:GLN:NE2	1:C:168:THR:HA	2.30	0.47
3:B:151:THR:HG23	3:B:193:GLN:HG2	1.97	0.47
3:B:413:MET:HG2	3:B:418:PHE:CE2	2.49	0.47
1:C:415:LYS:HE2	2:A:112:LYS:HZ1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:151:THR:HG23	3:B:193:GLN:HG2	1.97	0.47
3:B:413:MET:HG2	3:B:418:PHE:CE2	2.49	0.47
1:C:334:GLN:CG	3:B:416:MET:HE1	2.42	0.47
3:B:151:THR:HG23	3:B:193:GLN:HG2	1.97	0.47
3:B:413:MET:HG2	3:B:418:PHE:CE2	2.49	0.47
3:B:151:THR:HG23	3:B:193:GLN:HG2	1.97	0.47
3:B:413:MET:HG2	3:B:418:PHE:CE2	2.49	0.47
1:C:455:LEU:HD22	3:B:431:GLU:HB2	1.97	0.46
3:B:326:LYS:HG3	3:B:327:GLU:N	2.30	0.46
3:B:326:LYS:HG3	3:B:327:GLU:N	2.30	0.46
1:C:332:GLU:O	3:B:416:MET:HG3	2.15	0.46
3:B:326:LYS:HG3	3:B:327:GLU:N	2.30	0.46
3:B:326:LYS:HG3	3:B:327:GLU:N	2.30	0.46
1:C:306:GLU:HB2	1:C:379:SER:CB	2.45	0.46
3:B:326:LYS:HG3	3:B:327:GLU:N	2.30	0.46
1:C:306:GLU:HB2	1:C:379:SER:CB	2.45	0.46
2:A:222:PRO:HD2	3:B:326:LYS:HG2	1.97	0.46
2:A:409:VAL:HA	2:A:413:MET:O	2.14	0.46
2:A:222:PRO:HD2	3:B:326:LYS:HG2	1.97	0.46
2:A:409:VAL:HA	2:A:413:MET:O	2.14	0.46
1:C:306:GLU:HB2	1:C:379:SER:CB	2.45	0.46
2:A:222:PRO:HD2	3:B:326:LYS:HG2	1.97	0.46
2:A:409:VAL:HA	2:A:413:MET:O	2.14	0.46
1:C:306:GLU:HB2	1:C:379:SER:CB	2.45	0.46
2:A:222:PRO:HD2	3:B:326:LYS:HG2	1.97	0.46
2:A:409:VAL:HA	2:A:413:MET:O	2.14	0.46
2:A:222:PRO:HD2	3:B:326:LYS:HG2	1.97	0.46
2:A:409:VAL:HA	2:A:413:MET:O	2.14	0.46
2:A:179:THR:CG2	6:A:500:GTP:C3'	2.75	0.46
2:A:213:CYS:HA	2:A:217:LEU:HB2	1.97	0.46
3:B:114:LEU:O	3:B:118:VAL:HG23	2.16	0.46
3:B:167:ASN:HD21	3:B:202:TYR:HE1	1.62	0.46
1:C:306:GLU:HB2	1:C:379:SER:CB	2.45	0.46
1:C:332:GLU:O	3:B:416:MET:HG3	2.15	0.46
2:A:179:THR:CG2	6:A:500:GTP:C3'	2.75	0.46
2:A:213:CYS:HA	2:A:217:LEU:HB2	1.97	0.46
3:B:114:LEU:O	3:B:118:VAL:HG23	2.16	0.46
3:B:167:ASN:HD21	3:B:202:TYR:HE1	1.62	0.46
1:C:153:TRP:HZ2	1:C:478:CYS:HG	1.64	0.46
2:A:179:THR:CG2	6:A:500:GTP:C3'	2.75	0.46
2:A:213:CYS:HA	2:A:217:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:114:LEU:O	3:B:118:VAL:HG23	2.16	0.46
3:B:167:ASN:HD21	3:B:202:TYR:HE1	1.62	0.46
2:A:179:THR:CG2	6:A:500:GTP:C3'	2.75	0.46
2:A:213:CYS:HA	2:A:217:LEU:HB2	1.97	0.46
3:B:114:LEU:O	3:B:118:VAL:HG23	2.16	0.46
3:B:167:ASN:HD21	3:B:202:TYR:HE1	1.62	0.46
2:A:179:THR:CG2	6:A:500:GTP:C3'	2.75	0.46
2:A:213:CYS:HA	2:A:217:LEU:HB2	1.97	0.46
3:B:114:LEU:O	3:B:118:VAL:HG23	2.16	0.46
3:B:167:ASN:HD21	3:B:202:TYR:HE1	1.62	0.46
1:C:132:GLN:NE2	1:C:168:THR:HA	2.30	0.46
1:C:334:GLN:CG	3:B:416:MET:HE1	2.42	0.46
1:C:132:GLN:NE2	1:C:168:THR:HA	2.30	0.46
2:A:363:VAL:HG12	2:A:365:GLY:H	1.80	0.46
1:C:368:ALA:O	1:C:422:ARG:NH1	2.48	0.46
2:A:363:VAL:HG12	2:A:365:GLY:H	1.80	0.46
1:C:330:LEU:HD12	1:C:466:VAL:HG12	1.96	0.46
2:A:363:VAL:HG12	2:A:365:GLY:H	1.80	0.46
2:A:363:VAL:HG12	2:A:365:GLY:H	1.80	0.46
1:C:330:LEU:HD12	1:C:466:VAL:HG12	1.96	0.46
2:A:363:VAL:HG12	2:A:365:GLY:H	1.80	0.46
1:C:334:GLN:CG	3:B:416:MET:HE1	2.42	0.46
1:C:455:LEU:HD23	3:B:431:GLU:OE2	2.16	0.46
1:C:132:GLN:CD	1:C:168:THR:HA	2.40	0.46
1:C:330:LEU:HD12	1:C:466:VAL:HG12	1.96	0.46
1:C:330:LEU:HD12	1:C:466:VAL:HG12	1.96	0.46
2:A:276:ILE:HG23	2:A:369:ALA:HB3	1.97	0.46
1:C:330:LEU:HD12	1:C:466:VAL:HG12	1.96	0.46
2:A:276:ILE:HG23	2:A:369:ALA:HB3	1.97	0.46
2:A:276:ILE:HG23	2:A:369:ALA:HB3	1.97	0.46
2:A:276:ILE:HG23	2:A:369:ALA:HB3	1.97	0.46
2:A:276:ILE:HG23	2:A:369:ALA:HB3	1.97	0.46
3:B:288:VAL:H	3:B:289:PRO:HD2	1.81	0.46
1:C:369:SER:HB3	1:C:413:ARG:CZ	2.44	0.46
3:B:288:VAL:H	3:B:289:PRO:HD2	1.81	0.46
1:C:153:TRP:O	1:C:403:LEU:HA	2.16	0.46
3:B:288:VAL:H	3:B:289:PRO:HD2	1.81	0.46
1:C:153:TRP:O	1:C:403:LEU:HA	2.16	0.46
1:C:332:GLU:O	3:B:416:MET:HG3	2.16	0.46
3:B:288:VAL:H	3:B:289:PRO:HD2	1.81	0.46
1:C:153:TRP:O	1:C:403:LEU:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:LEU:HD23	3:B:431:GLU:OE2	2.16	0.46
3:B:288:VAL:H	3:B:289:PRO:HD2	1.81	0.46
1:C:153:TRP:O	1:C:403:LEU:HA	2.16	0.46
3:B:265:LEU:HG	3:B:266:HIS:N	2.31	0.46
1:C:153:TRP:O	1:C:403:LEU:HA	2.16	0.46
1:C:455:LEU:CD2	3:B:431:GLU:CG	2.94	0.46
3:B:265:LEU:HG	3:B:266:HIS:N	2.31	0.46
3:B:265:LEU:HG	3:B:266:HIS:N	2.31	0.46
3:B:265:LEU:HG	3:B:266:HIS:N	2.31	0.46
1:C:494:LEU:HD11	2:A:420:GLU:OE2	2.16	0.46
3:B:265:LEU:HG	3:B:266:HIS:N	2.31	0.46
1:C:140:MET:HE2	1:C:178:ILE:HB	1.97	0.45
1:C:334:GLN:HG2	3:B:416:MET:CE	2.45	0.45
1:C:140:MET:HE2	1:C:178:ILE:HB	1.97	0.45
1:C:153:TRP:HA	1:C:476:ARG:O	2.17	0.45
1:C:153:TRP:HA	1:C:476:ARG:O	2.17	0.45
1:C:140:MET:HE2	1:C:178:ILE:HB	1.97	0.45
1:C:455:LEU:CD2	3:B:431:GLU:CG	2.94	0.45
1:C:153:TRP:HA	1:C:476:ARG:O	2.17	0.45
3:B:288:VAL:HB	3:B:289:PRO:HD3	1.97	0.45
1:C:140:MET:HE2	1:C:178:ILE:HB	1.97	0.45
3:B:288:VAL:HB	3:B:289:PRO:HD3	1.97	0.45
3:B:288:VAL:HB	3:B:289:PRO:HD3	1.97	0.45
3:B:288:VAL:HB	3:B:289:PRO:HD3	1.97	0.45
1:C:153:TRP:HA	1:C:476:ARG:O	2.17	0.45
3:B:288:VAL:HB	3:B:289:PRO:HD3	1.97	0.45
2:A:317:LEU:HB3	2:A:319:TYR:HE1	1.82	0.45
2:A:317:LEU:HB3	2:A:319:TYR:HE1	1.82	0.45
2:A:317:LEU:HB3	2:A:319:TYR:HE1	1.82	0.45
1:C:153:TRP:HA	1:C:476:ARG:O	2.17	0.45
2:A:317:LEU:HB3	2:A:319:TYR:HE1	1.82	0.45
1:C:140:MET:HE2	1:C:178:ILE:HB	1.97	0.45
2:A:317:LEU:HB3	2:A:319:TYR:HE1	1.82	0.45
1:C:164:GLY:HA2	5:C:602:ANP:O2A	2.16	0.45
1:C:439:CYS:HB3	1:C:456:ILE:HD11	1.97	0.45
3:B:305:CYS:SG	3:B:384:ILE:HD12	2.57	0.45
1:C:169:ILE:HA	1:C:178:ILE:CG1	2.46	0.45
1:C:439:CYS:HB3	1:C:456:ILE:HD11	1.97	0.45
3:B:305:CYS:SG	3:B:384:ILE:HD12	2.57	0.45
1:C:439:CYS:HB3	1:C:456:ILE:HD11	1.97	0.45
3:B:305:CYS:SG	3:B:384:ILE:HD12	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ILE:HA	1:C:178:ILE:CG1	2.46	0.45
3:B:305:CYS:SG	3:B:384:ILE:HD12	2.57	0.45
3:B:305:CYS:SG	3:B:384:ILE:HD12	2.57	0.45
1:C:483:VAL:HG21	1:C:493:THR:HG23	1.98	0.45
1:C:494:LEU:HD11	2:A:420:GLU:OE2	2.16	0.45
1:C:164:GLY:HA2	5:C:602:ANP:O2A	2.16	0.45
1:C:164:GLY:HA2	5:C:602:ANP:O2A	2.16	0.45
1:C:164:GLY:HA2	5:C:602:ANP:O2A	2.16	0.45
1:C:164:GLY:HA2	5:C:602:ANP:O2A	2.16	0.45
1:C:169:ILE:HA	1:C:178:ILE:CG1	2.46	0.45
1:C:169:ILE:HA	1:C:178:ILE:CG1	2.46	0.45
2:A:252:LEU:O	2:A:255:PHE:HB2	2.16	0.45
1:C:440:ILE:HD12	1:C:499:PHE:CZ	2.47	0.45
1:C:483:VAL:HG21	1:C:493:THR:HG23	1.98	0.45
2:A:252:LEU:O	2:A:255:PHE:HB2	2.16	0.45
1:C:440:ILE:HD12	1:C:499:PHE:CZ	2.47	0.45
1:C:483:VAL:HG21	1:C:493:THR:HG23	1.98	0.45
2:A:252:LEU:O	2:A:255:PHE:HB2	2.16	0.45
1:C:483:VAL:HG21	1:C:493:THR:HG23	1.98	0.45
2:A:252:LEU:O	2:A:255:PHE:HB2	2.16	0.45
1:C:483:VAL:HG21	1:C:493:THR:HG23	1.98	0.45
2:A:252:LEU:O	2:A:255:PHE:HB2	2.16	0.45
1:C:440:ILE:HD12	1:C:499:PHE:CZ	2.47	0.45
3:B:78:VAL:O	3:B:84:GLY:HA3	2.17	0.45
3:B:78:VAL:O	3:B:84:GLY:HA3	2.17	0.45
1:C:169:ILE:HA	1:C:178:ILE:CG1	2.47	0.45
3:B:78:VAL:O	3:B:84:GLY:HA3	2.17	0.45
1:C:132:GLN:NE2	1:C:168:THR:HA	2.32	0.45
1:C:439:CYS:HB3	1:C:456:ILE:HD11	1.97	0.45
3:B:78:VAL:O	3:B:84:GLY:HA3	2.17	0.45
1:C:439:CYS:HB3	1:C:456:ILE:HD11	1.97	0.45
3:B:78:VAL:O	3:B:84:GLY:HA3	2.17	0.45
2:A:205:ASP:CB	2:A:303:VAL:HA	2.47	0.45
3:B:347:ILE:HB	3:B:350:ASN:OD1	2.16	0.45
2:A:205:ASP:CB	2:A:303:VAL:HA	2.47	0.45
3:B:347:ILE:HB	3:B:350:ASN:OD1	2.16	0.45
2:A:205:ASP:CB	2:A:303:VAL:HA	2.47	0.45
3:B:347:ILE:HB	3:B:350:ASN:OD1	2.16	0.45
2:A:205:ASP:CB	2:A:303:VAL:HA	2.47	0.45
3:B:347:ILE:HB	3:B:350:ASN:OD1	2.16	0.45
2:A:205:ASP:CB	2:A:303:VAL:HA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:347:ILE:HB	3:B:350:ASN:OD1	2.16	0.45
1:C:365:GLN:HG3	1:C:366:SER:N	2.32	0.45
1:C:455:LEU:CD2	3:B:431:GLU:CG	2.95	0.45
1:C:435:THR:HG21	1:C:461:SER:HB3	1.99	0.44
1:C:321:HIS:CG	1:C:366:SER:OG	2.71	0.44
1:C:70:ILE:HG22	1:C:483:VAL:CG1	2.47	0.44
3:B:239:THR:O	3:B:243:ARG:HG2	2.16	0.44
3:B:239:THR:O	3:B:243:ARG:HG2	2.16	0.44
1:C:317:GLU:HB3	1:C:318:PRO:CD	2.47	0.44
3:B:239:THR:O	3:B:243:ARG:HG2	2.16	0.44
1:C:70:ILE:HG22	1:C:483:VAL:CG1	2.47	0.44
3:B:239:THR:O	3:B:243:ARG:HG2	2.16	0.44
1:C:70:ILE:HG22	1:C:483:VAL:CG1	2.47	0.44
1:C:435:THR:HG21	1:C:461:SER:HB3	1.99	0.44
3:B:239:THR:O	3:B:243:ARG:HG2	2.16	0.44
1:C:337:ASN:HA	1:C:338:PRO:HD3	1.87	0.44
1:C:435:THR:HG21	1:C:461:SER:HB3	1.99	0.44
1:C:462:LYS:O	1:C:466:VAL:HG13	2.17	0.44
3:B:268:PHE:CD1	3:B:380:ASN:HB2	2.43	0.44
1:C:70:ILE:HG22	1:C:483:VAL:CG1	2.47	0.44
1:C:143:MET:SD	1:C:155:ILE:HD11	2.56	0.44
1:C:462:LYS:O	1:C:466:VAL:HG13	2.17	0.44
3:B:268:PHE:CD1	3:B:380:ASN:HB2	2.43	0.44
1:C:70:ILE:HG22	1:C:483:VAL:CG1	2.47	0.44
1:C:337:ASN:HA	1:C:338:PRO:HD3	1.87	0.44
1:C:435:THR:HG21	1:C:461:SER:HB3	1.99	0.44
1:C:462:LYS:O	1:C:466:VAL:HG13	2.17	0.44
3:B:268:PHE:CD1	3:B:380:ASN:HB2	2.43	0.44
1:C:337:ASN:HA	1:C:338:PRO:HD3	1.87	0.44
1:C:435:THR:HG21	1:C:461:SER:HB3	1.99	0.44
1:C:462:LYS:O	1:C:466:VAL:HG13	2.17	0.44
3:B:268:PHE:CD1	3:B:380:ASN:HB2	2.43	0.44
1:C:143:MET:SD	1:C:155:ILE:HD11	2.56	0.44
3:B:268:PHE:CD1	3:B:380:ASN:HB2	2.43	0.44
1:C:143:MET:SD	1:C:155:ILE:HD11	2.56	0.44
1:C:494:LEU:HD11	2:A:420:GLU:OE2	2.17	0.44
1:C:143:MET:SD	1:C:155:ILE:HD11	2.56	0.44
1:C:334:GLN:CG	3:B:416:MET:HE1	2.45	0.44
1:C:143:MET:SD	1:C:155:ILE:HD11	2.56	0.44
1:C:308:TYR:CZ	1:C:367:PHE:HB2	2.52	0.44
1:C:413:ARG:HH22	1:C:492:GLU:CD	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:GLN:CG	3:B:416:MET:HE1	2.44	0.44
1:C:337:ASN:HA	1:C:338:PRO:HD3	1.87	0.44
1:C:462:LYS:O	1:C:466:VAL:HG13	2.17	0.44
1:C:317:GLU:CB	1:C:318:PRO:HD3	2.48	0.44
1:C:431:THR:OG1	2:A:410:GLY:HA2	2.18	0.44
2:A:259:LEU:HD11	2:A:378:LEU:HD12	1.99	0.44
1:C:337:ASN:HA	1:C:338:PRO:HD3	1.87	0.44
2:A:259:LEU:HD11	2:A:378:LEU:HD12	1.99	0.44
2:A:259:LEU:HD11	2:A:378:LEU:HD12	1.99	0.44
2:A:259:LEU:HD11	2:A:378:LEU:HD12	1.99	0.44
2:A:259:LEU:HD11	2:A:378:LEU:HD12	1.99	0.44
2:A:72:PRO:HA	2:A:94:THR:CG2	2.47	0.44
1:C:136:PHE:HA	1:C:178:ILE:HG22	1.98	0.44
2:A:72:PRO:HA	2:A:94:THR:CG2	2.47	0.44
1:C:317:GLU:HB3	1:C:318:PRO:HD2	1.99	0.44
2:A:72:PRO:HA	2:A:94:THR:CG2	2.47	0.44
1:C:136:PHE:HA	1:C:178:ILE:HG22	1.98	0.44
2:A:72:PRO:HA	2:A:94:THR:CG2	2.47	0.44
1:C:136:PHE:HA	1:C:178:ILE:HG22	1.98	0.44
2:A:72:PRO:HA	2:A:94:THR:CG2	2.47	0.44
1:C:136:PHE:HA	1:C:178:ILE:HG22	1.98	0.44
2:A:317:LEU:HD21	2:A:377:MET:HE2	2.00	0.44
2:A:317:LEU:HD21	2:A:377:MET:HE2	2.00	0.44
2:A:317:LEU:HD21	2:A:377:MET:HE2	2.00	0.44
2:A:317:LEU:HD21	2:A:377:MET:HE2	2.00	0.44
2:A:317:LEU:HD21	2:A:377:MET:HE2	2.00	0.44
2:A:104:ALA:HB1	2:A:411:GLU:HB2	1.99	0.44
2:A:104:ALA:HB1	2:A:411:GLU:HB2	1.99	0.44
1:C:136:PHE:HA	1:C:178:ILE:HG22	1.99	0.44
1:C:455:LEU:HD23	3:B:431:GLU:HG3	1.99	0.44
1:C:494:LEU:HD11	2:A:420:GLU:OE2	2.18	0.44
2:A:104:ALA:HB1	2:A:411:GLU:HB2	1.99	0.44
2:A:104:ALA:HB1	2:A:411:GLU:HB2	1.99	0.44
2:A:104:ALA:HB1	2:A:411:GLU:HB2	1.99	0.44
2:A:31:GLN:HB3	2:A:32:PRO:HD2	1.99	0.44
3:B:23:VAL:HG13	8:B:601:TA1:C31	2.48	0.44
1:C:62:GLU:CD	1:C:476:ARG:HE	2.26	0.44
2:A:31:GLN:HB3	2:A:32:PRO:HD2	1.99	0.44
3:B:23:VAL:HG13	8:B:601:TA1:C31	2.48	0.44
2:A:31:GLN:HB3	2:A:32:PRO:HD2	1.99	0.44
3:B:23:VAL:HG13	8:B:601:TA1:C31	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:GLU:CD	1:C:476:ARG:HE	2.26	0.44
1:C:413:ARG:HH22	1:C:492:GLU:HG3	1.82	0.44
2:A:31:GLN:HB3	2:A:32:PRO:HD2	1.99	0.44
3:B:23:VAL:HG13	8:B:601:TA1:C31	2.48	0.44
1:C:62:GLU:CD	1:C:476:ARG:HE	2.26	0.44
2:A:31:GLN:HB3	2:A:32:PRO:HD2	1.99	0.44
3:B:23:VAL:HG13	8:B:601:TA1:C31	2.48	0.44
1:C:62:GLU:CD	1:C:476:ARG:HE	2.26	0.43
2:A:97:GLU:HB3	2:A:98:ASP:H	1.70	0.43
2:A:97:GLU:HB3	2:A:98:ASP:H	1.70	0.43
1:C:62:GLU:CD	1:C:476:ARG:HE	2.26	0.43
2:A:97:GLU:HB3	2:A:98:ASP:H	1.70	0.43
2:A:97:GLU:HB3	2:A:98:ASP:H	1.70	0.43
1:C:455:LEU:CD2	3:B:431:GLU:CG	2.96	0.43
2:A:97:GLU:HB3	2:A:98:ASP:H	1.70	0.43
1:C:178:ILE:O	1:C:182:SER:HB2	2.18	0.43
3:B:101:ASN:HD21	3:B:143:GLY:HA2	1.83	0.43
3:B:101:ASN:HD21	3:B:143:GLY:HA2	1.83	0.43
1:C:178:ILE:O	1:C:182:SER:HB2	2.18	0.43
3:B:101:ASN:HD21	3:B:143:GLY:HA2	1.83	0.43
1:C:178:ILE:O	1:C:182:SER:HB2	2.18	0.43
1:C:422:ARG:HH12	1:C:425:GLU:CD	2.25	0.43
3:B:101:ASN:HD21	3:B:143:GLY:HA2	1.83	0.43
1:C:178:ILE:O	1:C:182:SER:HB2	2.18	0.43
3:B:101:ASN:HD21	3:B:143:GLY:HA2	1.83	0.43
1:C:325:ARG:HH22	3:B:160:GLU:CD	2.26	0.43
3:B:224:TYR:CE1	7:B:600:GDP:C2	3.06	0.43
1:C:178:ILE:O	1:C:182:SER:HB2	2.18	0.43
3:B:224:TYR:CE1	7:B:600:GDP:C2	3.06	0.43
3:B:224:TYR:CE1	7:B:600:GDP:C2	3.06	0.43
1:C:431:THR:OG1	2:A:410:GLY:HA2	2.18	0.43
3:B:224:TYR:CE1	7:B:600:GDP:C2	3.06	0.43
1:C:187:PHE:CB	1:C:351:VAL:HB	2.48	0.43
1:C:365:GLN:HG3	1:C:366:SER:N	2.33	0.43
3:B:224:TYR:CE1	7:B:600:GDP:C2	3.06	0.43
1:C:333:ASP:HA	3:B:416:MET:HG2	2.00	0.43
2:A:224:TYR:HB3	6:A:500:GTP:O6	2.18	0.43
3:B:213:CYS:HA	3:B:217:LEU:HB2	2.00	0.43
3:B:371:LEU:HD12	3:B:371:LEU:HA	1.82	0.43
1:C:455:LEU:HD23	3:B:431:GLU:HG3	1.99	0.43
2:A:224:TYR:HB3	6:A:500:GTP:O6	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:213:CYS:HA	3:B:217:LEU:HB2	2.00	0.43
3:B:371:LEU:HD12	3:B:371:LEU:HA	1.82	0.43
2:A:224:TYR:HB3	6:A:500:GTP:O6	2.18	0.43
3:B:213:CYS:HA	3:B:217:LEU:HB2	2.00	0.43
3:B:371:LEU:HD12	3:B:371:LEU:HA	1.82	0.43
1:C:187:PHE:CB	1:C:351:VAL:HB	2.48	0.43
2:A:224:TYR:HB3	6:A:500:GTP:O6	2.18	0.43
3:B:213:CYS:HA	3:B:217:LEU:HB2	2.00	0.43
3:B:371:LEU:HD12	3:B:371:LEU:HA	1.82	0.43
2:A:224:TYR:HB3	6:A:500:GTP:O6	2.18	0.43
3:B:213:CYS:HA	3:B:217:LEU:HB2	2.00	0.43
3:B:371:LEU:HD12	3:B:371:LEU:HA	1.82	0.43
1:C:187:PHE:CB	1:C:351:VAL:HB	2.48	0.43
2:A:98:ASP:HB2	3:B:253:ARG:HG3	2.01	0.43
2:A:220:GLU:C	2:A:222:PRO:HD3	2.44	0.43
3:B:8:GLN:HG2	3:B:17:GLY:HA3	2.00	0.43
1:C:187:PHE:CB	1:C:351:VAL:HB	2.48	0.43
1:C:431:THR:OG1	2:A:410:GLY:HA2	2.18	0.43
2:A:98:ASP:HB2	3:B:253:ARG:HG3	2.01	0.43
2:A:220:GLU:C	2:A:222:PRO:HD3	2.44	0.43
3:B:8:GLN:HG2	3:B:17:GLY:HA3	2.00	0.43
1:C:183:LEU:HB3	1:C:351:VAL:HG23	2.01	0.43
2:A:98:ASP:HB2	3:B:253:ARG:HG3	2.01	0.43
2:A:220:GLU:C	2:A:222:PRO:HD3	2.44	0.43
3:B:8:GLN:HG2	3:B:17:GLY:HA3	2.00	0.43
2:A:98:ASP:HB2	3:B:253:ARG:HG3	2.01	0.43
2:A:220:GLU:C	2:A:222:PRO:HD3	2.44	0.43
3:B:8:GLN:HG2	3:B:17:GLY:HA3	2.00	0.43
1:C:502:LEU:N	1:C:502:LEU:HD22	2.34	0.43
2:A:98:ASP:HB2	3:B:253:ARG:HG3	2.01	0.43
2:A:220:GLU:C	2:A:222:PRO:HD3	2.44	0.43
3:B:8:GLN:HG2	3:B:17:GLY:HA3	2.00	0.43
3:B:317:ALA:HB1	3:B:319:PHE:HE1	1.84	0.43
3:B:317:ALA:HB1	3:B:319:PHE:HE1	1.84	0.43
1:C:187:PHE:CB	1:C:351:VAL:HB	2.48	0.43
3:B:317:ALA:HB1	3:B:319:PHE:HE1	1.84	0.43
3:B:317:ALA:HB1	3:B:319:PHE:HE1	1.84	0.43
1:C:183:LEU:HB3	1:C:351:VAL:HG23	2.01	0.43
3:B:317:ALA:HB1	3:B:319:PHE:HE1	1.84	0.43
2:A:11:GLN:HB2	6:A:500:GTP:O2B	2.11	0.43
2:A:339:ARG:HD3	2:A:339:ARG:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:LEU:HB3	1:C:351:VAL:HG23	2.01	0.43
2:A:11:GLN:HB2	6:A:500:GTP:O2B	2.11	0.43
2:A:339:ARG:HD3	2:A:339:ARG:HA	1.85	0.43
1:C:152:ASN:N	1:C:152:ASN:HD22	2.17	0.43
2:A:11:GLN:HB2	6:A:500:GTP:O2B	2.11	0.43
2:A:339:ARG:HD3	2:A:339:ARG:HA	1.85	0.43
1:C:494:LEU:HD11	2:A:420:GLU:OE2	2.19	0.43
2:A:11:GLN:HB2	6:A:500:GTP:O2B	2.11	0.43
2:A:339:ARG:HD3	2:A:339:ARG:HA	1.85	0.43
2:A:11:GLN:HB2	6:A:500:GTP:O2B	2.11	0.43
2:A:339:ARG:HD3	2:A:339:ARG:HA	1.85	0.43
1:C:152:ASN:N	1:C:152:ASN:HD22	2.17	0.43
1:C:183:LEU:HB3	1:C:351:VAL:HG23	2.01	0.43
1:C:306:GLU:HB2	1:C:379:SER:HB3	1.99	0.43
1:C:313:TYR:CG	1:C:321:HIS:NE2	2.82	0.43
8:B:601:TA1:H463	8:B:601:TA1:C26	2.46	0.43
8:B:601:TA1:H463	8:B:601:TA1:C26	2.46	0.43
1:C:306:GLU:HB2	1:C:379:SER:HB3	1.99	0.43
8:B:601:TA1:H463	8:B:601:TA1:C26	2.46	0.43
1:C:152:ASN:N	1:C:152:ASN:HD22	2.17	0.43
1:C:183:LEU:HB3	1:C:351:VAL:HG23	2.01	0.43
8:B:601:TA1:H463	8:B:601:TA1:C26	2.46	0.43
1:C:306:GLU:HB2	1:C:379:SER:HB3	1.99	0.43
8:B:601:TA1:H463	8:B:601:TA1:C26	2.46	0.43
2:A:225:THR:O	2:A:229:ARG:HG2	2.19	0.43
1:C:152:ASN:N	1:C:152:ASN:HD22	2.17	0.43
2:A:225:THR:O	2:A:229:ARG:HG2	2.19	0.43
2:A:225:THR:O	2:A:229:ARG:HG2	2.19	0.43
1:C:306:GLU:HB2	1:C:379:SER:HB3	1.99	0.43
2:A:225:THR:O	2:A:229:ARG:HG2	2.19	0.43
2:A:225:THR:O	2:A:229:ARG:HG2	2.19	0.43
1:C:306:GLU:HB2	1:C:379:SER:HB3	2.00	0.43
1:C:152:ASN:N	1:C:152:ASN:HD22	2.17	0.43
1:C:314:ASP:H	1:C:326:GLN:NE2	2.17	0.42
1:C:183:LEU:HD22	1:C:187:PHE:HE2	1.84	0.42
1:C:183:LEU:HD22	1:C:187:PHE:HE2	1.84	0.42
1:C:183:LEU:HD22	1:C:187:PHE:HE2	1.84	0.42
1:C:183:LEU:HD22	1:C:187:PHE:HE2	1.85	0.42
3:B:23:VAL:HA	8:B:601:TA1:C32	2.49	0.42
3:B:23:VAL:HA	8:B:601:TA1:C32	2.49	0.42
3:B:23:VAL:HA	8:B:601:TA1:C32	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:23:VAL:HA	8:B:601:TA1:C32	2.49	0.42
3:B:23:VAL:HA	8:B:601:TA1:C32	2.49	0.42
1:C:66:VAL:O	1:C:122:PHE:HB3	2.20	0.42
1:C:77:GLU:HA	1:C:80:ARG:HG2	2.01	0.42
1:C:314:ASP:CG	1:C:344:ASN:HD22	2.28	0.42
2:A:12:ALA:O	2:A:16:ILE:HG22	2.19	0.42
2:A:107:HIS:HA	2:A:152:LEU:HD23	2.01	0.42
3:B:260:VAL:HG12	3:B:262:PHE:O	2.18	0.42
1:C:66:VAL:O	1:C:122:PHE:HB3	2.20	0.42
2:A:12:ALA:O	2:A:16:ILE:HG22	2.19	0.42
2:A:107:HIS:HA	2:A:152:LEU:HD23	2.01	0.42
3:B:260:VAL:HG12	3:B:262:PHE:O	2.18	0.42
1:C:66:VAL:O	1:C:122:PHE:HB3	2.20	0.42
1:C:77:GLU:HA	1:C:80:ARG:HG2	2.01	0.42
1:C:314:ASP:CG	1:C:344:ASN:HD22	2.28	0.42
1:C:350:ASP:OD2	1:C:352:GLU:HB3	2.20	0.42
2:A:12:ALA:O	2:A:16:ILE:HG22	2.19	0.42
2:A:107:HIS:HA	2:A:152:LEU:HD23	2.01	0.42
3:B:260:VAL:HG12	3:B:262:PHE:O	2.18	0.42
1:C:317:GLU:HB2	1:C:325:ARG:HH22	1.84	0.42
1:C:455:LEU:HD23	3:B:431:GLU:HG3	2.00	0.42
2:A:12:ALA:O	2:A:16:ILE:HG22	2.19	0.42
2:A:107:HIS:HA	2:A:152:LEU:HD23	2.01	0.42
3:B:260:VAL:HG12	3:B:262:PHE:O	2.18	0.42
1:C:77:GLU:HA	1:C:80:ARG:HG2	2.01	0.42
1:C:183:LEU:HD22	1:C:187:PHE:HE2	1.85	0.42
1:C:422:ARG:NH1	1:C:425:GLU:HB2	2.33	0.42
2:A:12:ALA:O	2:A:16:ILE:HG22	2.19	0.42
2:A:107:HIS:HA	2:A:152:LEU:HD23	2.01	0.42
3:B:260:VAL:HG12	3:B:262:PHE:O	2.18	0.42
1:C:118:HIS:CD2	1:C:119:LYS:H	2.38	0.42
3:B:344:VAL:HG13	3:B:346:TRP:H	1.83	0.42
1:C:118:HIS:CD2	1:C:119:LYS:H	2.38	0.42
1:C:314:ASP:CG	1:C:344:ASN:HD22	2.28	0.42
1:C:350:ASP:OD2	1:C:352:GLU:HB3	2.20	0.42
3:B:344:VAL:HG13	3:B:346:TRP:H	1.83	0.42
3:B:344:VAL:HG13	3:B:346:TRP:H	1.83	0.42
1:C:66:VAL:O	1:C:122:PHE:HB3	2.20	0.42
1:C:118:HIS:CD2	1:C:119:LYS:H	2.38	0.42
1:C:314:ASP:CG	1:C:344:ASN:HD22	2.28	0.42
3:B:344:VAL:HG13	3:B:346:TRP:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:VAL:O	1:C:122:PHE:HB3	2.20	0.42
1:C:118:HIS:CD2	1:C:119:LYS:H	2.38	0.42
1:C:130:VAL:HB	1:C:134:ALA:CB	2.49	0.42
3:B:344:VAL:HG13	3:B:346:TRP:H	1.83	0.42
1:C:90:GLU:HB2	1:C:96:VAL:HG12	2.01	0.42
1:C:130:VAL:HB	1:C:134:ALA:CB	2.50	0.42
2:A:9:VAL:HA	2:A:68:VAL:O	2.19	0.42
3:B:20:PHE:HA	3:B:232:SER:CB	2.50	0.42
1:C:77:GLU:HA	1:C:80:ARG:HG2	2.02	0.42
1:C:130:VAL:HB	1:C:134:ALA:CB	2.50	0.42
1:C:312:LEU:HD13	1:C:328:LEU:HD11	2.01	0.42
1:C:424:LYS:HZ1	3:B:163:ASP:CG	2.26	0.42
2:A:9:VAL:HA	2:A:68:VAL:O	2.19	0.42
3:B:20:PHE:HA	3:B:232:SER:CB	2.50	0.42
1:C:130:VAL:HB	1:C:134:ALA:CB	2.50	0.42
2:A:9:VAL:HA	2:A:68:VAL:O	2.19	0.42
3:B:20:PHE:HA	3:B:232:SER:CB	2.50	0.42
1:C:77:GLU:HA	1:C:80:ARG:HG2	2.02	0.42
1:C:130:VAL:HB	1:C:134:ALA:CB	2.50	0.42
1:C:312:LEU:HD13	1:C:328:LEU:HD11	2.01	0.42
1:C:350:ASP:OD2	1:C:352:GLU:HB3	2.20	0.42
2:A:9:VAL:HA	2:A:68:VAL:O	2.19	0.42
3:B:20:PHE:HA	3:B:232:SER:CB	2.50	0.42
1:C:314:ASP:CG	1:C:344:ASN:HD22	2.28	0.42
1:C:350:ASP:OD2	1:C:352:GLU:HB3	2.20	0.42
2:A:9:VAL:HA	2:A:68:VAL:O	2.19	0.42
3:B:20:PHE:HA	3:B:232:SER:CB	2.50	0.42
1:C:312:LEU:HD13	1:C:328:LEU:HD11	2.01	0.42
1:C:350:ASP:OD2	1:C:352:GLU:HB3	2.20	0.42
2:A:144:GLY:H	6:A:500:GTP:PG	2.43	0.42
1:C:130:VAL:HB	1:C:134:ALA:HB3	2.01	0.42
1:C:143:MET:O	1:C:147:VAL:HG23	2.19	0.42
1:C:455:LEU:HD22	3:B:431:GLU:HB2	2.01	0.42
2:A:144:GLY:H	6:A:500:GTP:PG	2.43	0.42
1:C:90:GLU:HB2	1:C:96:VAL:HG12	2.01	0.42
1:C:118:HIS:CD2	1:C:119:LYS:H	2.38	0.42
1:C:312:LEU:HD13	1:C:328:LEU:HD11	2.01	0.42
2:A:144:GLY:H	6:A:500:GTP:PG	2.43	0.42
1:C:66:VAL:O	1:C:123:SER:HB2	2.19	0.42
2:A:144:GLY:H	6:A:500:GTP:PG	2.43	0.42
1:C:90:GLU:HB2	1:C:96:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:LEU:HD13	1:C:328:LEU:HD11	2.01	0.42
1:C:431:THR:OG1	2:A:410:GLY:HA2	2.19	0.42
1:C:452:LYS:HE3	1:C:454:ASN:HD21	1.85	0.42
1:C:455:LEU:HD23	3:B:431:GLU:HG3	2.01	0.42
2:A:144:GLY:H	6:A:500:GTP:PG	2.43	0.42
1:C:130:VAL:HB	1:C:134:ALA:HB3	2.01	0.42
1:C:143:MET:O	1:C:147:VAL:HG23	2.19	0.42
3:B:43:GLN:HA	3:B:244:PHE:HE1	1.84	0.42
1:C:66:VAL:O	1:C:123:SER:HB2	2.19	0.42
1:C:90:GLU:HB2	1:C:96:VAL:HG12	2.01	0.42
3:B:43:GLN:HA	3:B:244:PHE:HE1	1.84	0.42
1:C:130:VAL:HB	1:C:134:ALA:HB3	2.01	0.42
1:C:143:MET:O	1:C:147:VAL:HG23	2.19	0.42
3:B:43:GLN:HA	3:B:244:PHE:HE1	1.84	0.42
1:C:90:GLU:HB2	1:C:96:VAL:HG12	2.01	0.42
1:C:130:VAL:HB	1:C:134:ALA:HB3	2.01	0.42
1:C:455:LEU:HD22	3:B:431:GLU:HB2	2.01	0.42
3:B:43:GLN:HA	3:B:244:PHE:HE1	1.84	0.42
1:C:66:VAL:O	1:C:123:SER:HB2	2.19	0.42
1:C:130:VAL:HB	1:C:134:ALA:HB3	2.01	0.42
3:B:43:GLN:HA	3:B:244:PHE:HE1	1.84	0.42
1:C:66:VAL:O	1:C:123:SER:HB2	2.19	0.42
3:B:215:ARG:HG3	3:B:216:THR:H	1.85	0.42
3:B:298:ALA:HA	3:B:307:PRO:HD2	2.00	0.42
1:C:316:LEU:HD12	1:C:316:LEU:HA	1.89	0.42
3:B:215:ARG:HG3	3:B:216:THR:H	1.85	0.42
3:B:298:ALA:HA	3:B:307:PRO:HD2	2.00	0.42
1:C:66:VAL:O	1:C:123:SER:HB2	2.19	0.42
1:C:316:LEU:HD12	1:C:316:LEU:HA	1.89	0.42
3:B:215:ARG:HG3	3:B:216:THR:H	1.85	0.42
3:B:298:ALA:HA	3:B:307:PRO:HD2	2.00	0.42
1:C:143:MET:O	1:C:147:VAL:HG23	2.19	0.42
1:C:316:LEU:HD12	1:C:316:LEU:HA	1.89	0.42
1:C:365:GLN:HG3	1:C:366:SER:N	2.35	0.42
1:C:423:LEU:HB3	1:C:424:LYS:H	1.68	0.42
3:B:215:ARG:HG3	3:B:216:THR:H	1.85	0.42
3:B:298:ALA:HA	3:B:307:PRO:HD2	2.00	0.42
1:C:143:MET:O	1:C:147:VAL:HG23	2.20	0.42
1:C:316:LEU:HD12	1:C:316:LEU:HA	1.89	0.42
3:B:215:ARG:HG3	3:B:216:THR:H	1.85	0.42
3:B:298:ALA:HA	3:B:307:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:71:GLU:HB3	2:A:74:VAL:HG23	2.01	0.42
1:C:313:TYR:CE1	1:C:324:LYS:HE3	2.55	0.42
2:A:71:GLU:HB3	2:A:74:VAL:HG23	2.01	0.42
1:C:314:ASP:CB	1:C:326:GLN:HE22	2.33	0.42
2:A:71:GLU:HB3	2:A:74:VAL:HG23	2.01	0.42
2:A:71:GLU:HB3	2:A:74:VAL:HG23	2.01	0.42
2:A:71:GLU:HB3	2:A:74:VAL:HG23	2.01	0.42
2:A:143:GLY:HA3	6:A:500:GTP:O1B	2.20	0.41
2:A:179:THR:CB	6:A:500:GTP:O3'	2.58	0.41
2:A:143:GLY:HA3	6:A:500:GTP:O1B	2.20	0.41
2:A:179:THR:CB	6:A:500:GTP:O3'	2.58	0.41
2:A:143:GLY:HA3	6:A:500:GTP:O1B	2.20	0.41
2:A:179:THR:CB	6:A:500:GTP:O3'	2.58	0.41
2:A:143:GLY:HA3	6:A:500:GTP:O1B	2.20	0.41
2:A:179:THR:CB	6:A:500:GTP:O3'	2.58	0.41
2:A:143:GLY:HA3	6:A:500:GTP:O1B	2.20	0.41
2:A:179:THR:CB	6:A:500:GTP:O3'	2.58	0.41
1:C:424:LYS:NZ	3:B:163:ASP:OD2	2.53	0.41
1:C:439:CYS:SG	1:C:457:PRO:HG2	2.61	0.41
2:A:170:SER:O	2:A:203:MET:HA	2.21	0.41
2:A:386:GLU:O	2:A:390:ARG:HG2	2.20	0.41
2:A:170:SER:O	2:A:203:MET:HA	2.21	0.41
2:A:386:GLU:O	2:A:390:ARG:HG2	2.20	0.41
1:C:439:CYS:SG	1:C:457:PRO:HG2	2.61	0.41
2:A:170:SER:O	2:A:203:MET:HA	2.21	0.41
2:A:386:GLU:O	2:A:390:ARG:HG2	2.20	0.41
2:A:170:SER:O	2:A:203:MET:HA	2.21	0.41
2:A:386:GLU:O	2:A:390:ARG:HG2	2.20	0.41
1:C:439:CYS:SG	1:C:457:PRO:HG2	2.61	0.41
2:A:170:SER:O	2:A:203:MET:HA	2.21	0.41
2:A:386:GLU:O	2:A:390:ARG:HG2	2.20	0.41
1:C:455:LEU:HD23	3:B:431:GLU:HG3	2.01	0.41
2:A:205:ASP:HB3	2:A:303:VAL:HA	2.02	0.41
3:B:370:GLY:O	8:B:601:TA1:H443	2.20	0.41
2:A:205:ASP:HB3	2:A:303:VAL:HA	2.02	0.41
3:B:370:GLY:O	8:B:601:TA1:H443	2.20	0.41
2:A:205:ASP:HB3	2:A:303:VAL:HA	2.02	0.41
3:B:370:GLY:O	8:B:601:TA1:H443	2.20	0.41
1:C:169:ILE:HG21	1:C:407:ASP:HB2	2.02	0.41
1:C:369:SER:HG	1:C:425:GLU:CD	2.28	0.41
1:C:439:CYS:SG	1:C:457:PRO:HG2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:205:ASP:HB3	2:A:303:VAL:HA	2.02	0.41
3:B:370:GLY:O	8:B:601:TA1:H443	2.20	0.41
2:A:205:ASP:HB3	2:A:303:VAL:HA	2.02	0.41
3:B:370:GLY:O	8:B:601:TA1:H443	2.20	0.41
2:A:152:LEU:HD12	2:A:153:LEU:N	2.36	0.41
2:A:154:MET:HE2	2:A:198:SER:OG	2.19	0.41
1:C:169:ILE:HG21	1:C:407:ASP:HB2	2.02	0.41
1:C:439:CYS:SG	1:C:457:PRO:HG2	2.61	0.41
2:A:152:LEU:HD12	2:A:153:LEU:N	2.36	0.41
2:A:154:MET:HE2	2:A:198:SER:OG	2.19	0.41
1:C:169:ILE:HG21	1:C:407:ASP:HB2	2.02	0.41
2:A:152:LEU:HD12	2:A:153:LEU:N	2.36	0.41
2:A:154:MET:HE2	2:A:198:SER:OG	2.19	0.41
2:A:152:LEU:HD12	2:A:153:LEU:N	2.36	0.41
2:A:154:MET:HE2	2:A:198:SER:OG	2.19	0.41
1:C:169:ILE:HG21	1:C:407:ASP:HB2	2.02	0.41
2:A:152:LEU:HD12	2:A:153:LEU:N	2.36	0.41
2:A:154:MET:HE2	2:A:198:SER:OG	2.19	0.41
1:C:169:ILE:HG21	1:C:407:ASP:HB2	2.02	0.41
2:A:103:TYR:CD1	2:A:189:LEU:HD13	2.55	0.41
2:A:322:ASP:O	2:A:373:ARG:HD3	2.20	0.41
3:B:273:ALA:O	3:B:294:GLN:HG2	2.20	0.41
2:A:103:TYR:CD1	2:A:189:LEU:HD13	2.55	0.41
2:A:322:ASP:O	2:A:373:ARG:HD3	2.20	0.41
3:B:273:ALA:O	3:B:294:GLN:HG2	2.20	0.41
2:A:103:TYR:CD1	2:A:189:LEU:HD13	2.55	0.41
2:A:322:ASP:O	2:A:373:ARG:HD3	2.20	0.41
3:B:273:ALA:O	3:B:294:GLN:HG2	2.20	0.41
2:A:103:TYR:CD1	2:A:189:LEU:HD13	2.55	0.41
2:A:322:ASP:O	2:A:373:ARG:HD3	2.20	0.41
3:B:273:ALA:O	3:B:294:GLN:HG2	2.20	0.41
1:C:136:PHE:CG	1:C:181:GLN:HB3	2.56	0.41
1:C:333:ASP:HA	3:B:416:MET:HG2	2.02	0.41
1:C:455:LEU:HD22	3:B:431:GLU:HB2	2.02	0.41
2:A:103:TYR:CD1	2:A:189:LEU:HD13	2.55	0.41
2:A:322:ASP:O	2:A:373:ARG:HD3	2.20	0.41
3:B:273:ALA:O	3:B:294:GLN:HG2	2.20	0.41
1:C:136:PHE:CG	1:C:181:GLN:HB3	2.56	0.41
3:B:4:ILE:HG21	3:B:136:GLN:HG2	2.01	0.41
1:C:136:PHE:CG	1:C:181:GLN:HB3	2.56	0.41
3:B:4:ILE:HG21	3:B:136:GLN:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:VAL:HG23	1:C:122:PHE:O	2.21	0.41
1:C:313:TYR:CZ	1:C:324:LYS:HE2	2.55	0.41
3:B:4:ILE:HG21	3:B:136:GLN:HG2	2.01	0.41
1:C:136:PHE:CG	1:C:181:GLN:HB3	2.56	0.41
3:B:4:ILE:HG21	3:B:136:GLN:HG2	2.01	0.41
1:C:387:ILE:O	1:C:387:ILE:HG13	2.20	0.41
3:B:4:ILE:HG21	3:B:136:GLN:HG2	2.01	0.41
1:C:66:VAL:HG23	1:C:122:PHE:O	2.21	0.41
1:C:387:ILE:O	1:C:387:ILE:HG13	2.20	0.41
1:C:434:HIS:CG	2:A:409:VAL:HG21	2.56	0.41
3:B:22:GLU:HG3	3:B:83:PHE:CD1	2.56	0.41
3:B:228:ASN:ND2	7:B:600:GDP:HN1	2.19	0.41
1:C:313:TYR:CE2	1:C:321:HIS:HB2	2.56	0.41
3:B:22:GLU:HG3	3:B:83:PHE:CD1	2.56	0.41
3:B:228:ASN:ND2	7:B:600:GDP:HN1	2.19	0.41
1:C:136:PHE:CG	1:C:181:GLN:HB3	2.56	0.41
3:B:22:GLU:HG3	3:B:83:PHE:CD1	2.56	0.41
3:B:228:ASN:ND2	7:B:600:GDP:HN1	2.19	0.41
1:C:66:VAL:HG23	1:C:122:PHE:O	2.21	0.41
1:C:333:ASP:HA	3:B:416:MET:HG2	2.02	0.41
3:B:22:GLU:HG3	3:B:83:PHE:CD1	2.56	0.41
3:B:228:ASN:ND2	7:B:600:GDP:HN1	2.19	0.41
1:C:66:VAL:HG23	1:C:122:PHE:O	2.21	0.41
3:B:22:GLU:HG3	3:B:83:PHE:CD1	2.56	0.41
3:B:228:ASN:ND2	7:B:600:GDP:HN1	2.19	0.41
3:B:209:LEU:HD21	3:B:231:VAL:CG2	2.51	0.41
3:B:358:ILE:HA	3:B:359:PRO:HD3	1.81	0.41
1:C:66:VAL:HG23	1:C:122:PHE:O	2.21	0.41
3:B:209:LEU:HD21	3:B:231:VAL:CG2	2.51	0.41
3:B:358:ILE:HA	3:B:359:PRO:HD3	1.81	0.41
1:C:387:ILE:O	1:C:387:ILE:HG13	2.21	0.41
3:B:209:LEU:HD21	3:B:231:VAL:CG2	2.51	0.41
3:B:358:ILE:HA	3:B:359:PRO:HD3	1.81	0.41
1:C:313:TYR:CE2	1:C:321:HIS:HB2	2.56	0.41
1:C:387:ILE:O	1:C:387:ILE:HG13	2.21	0.41
3:B:209:LEU:HD21	3:B:231:VAL:CG2	2.51	0.41
3:B:358:ILE:HA	3:B:359:PRO:HD3	1.81	0.41
3:B:209:LEU:HD21	3:B:231:VAL:CG2	2.51	0.41
3:B:358:ILE:HA	3:B:359:PRO:HD3	1.81	0.41
1:C:143:MET:HG3	1:C:153:TRP:CG	2.55	0.41
1:C:164:GLY:CA	5:C:602:ANP:H8	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:201:ALA:O	2:A:267:PHE:HA	2.21	0.41
2:A:203:MET:HE2	2:A:267:PHE:CB	2.51	0.41
2:A:213:CYS:HA	2:A:217:LEU:CB	2.51	0.41
3:B:320:ARG:HD3	3:B:360:PRO:HG3	2.02	0.41
1:C:143:MET:HG3	1:C:153:TRP:CG	2.55	0.41
1:C:333:ASP:HA	3:B:416:MET:HG2	2.02	0.41
1:C:387:ILE:O	1:C:387:ILE:HG13	2.21	0.41
2:A:201:ALA:O	2:A:267:PHE:HA	2.21	0.41
2:A:203:MET:HE2	2:A:267:PHE:CB	2.51	0.41
2:A:213:CYS:HA	2:A:217:LEU:CB	2.51	0.41
3:B:320:ARG:HD3	3:B:360:PRO:HG3	2.02	0.41
1:C:313:TYR:HE1	1:C:324:LYS:HB3	1.86	0.41
1:C:424:LYS:HZ1	3:B:163:ASP:CG	2.28	0.41
1:C:424:LYS:HZ2	3:B:163:ASP:CG	2.29	0.41
1:C:431:THR:OG1	2:A:410:GLY:HA2	2.21	0.41
2:A:201:ALA:O	2:A:267:PHE:HA	2.21	0.41
2:A:203:MET:HE2	2:A:267:PHE:CB	2.51	0.41
2:A:213:CYS:HA	2:A:217:LEU:CB	2.51	0.41
3:B:320:ARG:HD3	3:B:360:PRO:HG3	2.02	0.41
1:C:143:MET:HG3	1:C:153:TRP:CG	2.55	0.41
1:C:484:ASN:HA	1:C:485:PRO:HD3	1.82	0.41
2:A:201:ALA:O	2:A:267:PHE:HA	2.21	0.41
2:A:203:MET:HE2	2:A:267:PHE:CB	2.51	0.41
2:A:213:CYS:HA	2:A:217:LEU:CB	2.51	0.41
3:B:320:ARG:HD3	3:B:360:PRO:HG3	2.02	0.41
2:A:201:ALA:O	2:A:267:PHE:HA	2.21	0.41
2:A:203:MET:HE2	2:A:267:PHE:CB	2.51	0.41
2:A:213:CYS:HA	2:A:217:LEU:CB	2.51	0.41
3:B:320:ARG:HD3	3:B:360:PRO:HG3	2.02	0.41
1:C:355:TRP:NE1	1:C:359:LYS:HE3	2.36	0.41
1:C:484:ASN:HA	1:C:485:PRO:HD3	1.82	0.41
2:A:407:TRP:HZ2	3:B:260:VAL:HB	1.85	0.41
3:B:11:GLN:HG3	3:B:74:THR:HG21	2.03	0.41
1:C:164:GLY:CA	5:C:602:ANP:H8	2.51	0.41
1:C:355:TRP:NE1	1:C:359:LYS:HE3	2.36	0.41
2:A:407:TRP:HZ2	3:B:260:VAL:HB	1.85	0.41
3:B:11:GLN:HG3	3:B:74:THR:HG21	2.03	0.41
1:C:143:MET:HG3	1:C:153:TRP:CG	2.55	0.41
1:C:355:TRP:NE1	1:C:359:LYS:HE3	2.36	0.41
2:A:407:TRP:HZ2	3:B:260:VAL:HB	1.85	0.41
3:B:11:GLN:HG3	3:B:74:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:LYS:HZ1	3:B:163:ASP:CG	2.28	0.41
2:A:407:TRP:HZ2	3:B:260:VAL:HB	1.85	0.41
3:B:11:GLN:HG3	3:B:74:THR:HG21	2.03	0.41
1:C:143:MET:HG3	1:C:153:TRP:CG	2.55	0.41
1:C:445:GLN:NE2	1:C:452:LYS:HE2	2.36	0.41
1:C:484:ASN:HA	1:C:485:PRO:HD3	1.82	0.41
2:A:407:TRP:HZ2	3:B:260:VAL:HB	1.85	0.41
3:B:11:GLN:HG3	3:B:74:THR:HG21	2.03	0.41
1:C:459:ARG:CZ	3:B:424:ASN:ND2	2.84	0.40
3:B:115:VAL:O	3:B:119:LEU:HG	2.20	0.40
3:B:115:VAL:O	3:B:119:LEU:HG	2.20	0.40
1:C:164:GLY:CA	5:C:602:ANP:H8	2.51	0.40
1:C:484:ASN:HA	1:C:485:PRO:HD3	1.82	0.40
3:B:115:VAL:O	3:B:119:LEU:HG	2.20	0.40
1:C:164:GLY:CA	5:C:602:ANP:H8	2.51	0.40
1:C:355:TRP:NE1	1:C:359:LYS:HE3	2.36	0.40
3:B:115:VAL:O	3:B:119:LEU:HG	2.20	0.40
1:C:164:GLY:CA	5:C:602:ANP:H8	2.51	0.40
1:C:355:TRP:NE1	1:C:359:LYS:HE3	2.36	0.40
1:C:424:LYS:HZ2	3:B:163:ASP:CG	2.29	0.40
3:B:115:VAL:O	3:B:119:LEU:HG	2.20	0.40
1:C:179:LEU:HD23	1:C:405:LEU:CG	2.51	0.40
3:B:168:THR:O	3:B:201:THR:HA	2.21	0.40
3:B:237:GLY:HA2	3:B:241:CYS:CB	2.50	0.40
1:C:484:ASN:HA	1:C:485:PRO:HD3	1.82	0.40
3:B:168:THR:O	3:B:201:THR:HA	2.21	0.40
3:B:237:GLY:HA2	3:B:241:CYS:CB	2.50	0.40
3:B:168:THR:O	3:B:201:THR:HA	2.21	0.40
3:B:237:GLY:HA2	3:B:241:CYS:CB	2.50	0.40
3:B:168:THR:O	3:B:201:THR:HA	2.21	0.40
3:B:237:GLY:HA2	3:B:241:CYS:CB	2.50	0.40
1:C:179:LEU:HD23	1:C:405:LEU:CG	2.51	0.40
3:B:168:THR:O	3:B:201:THR:HA	2.21	0.40
3:B:237:GLY:HA2	3:B:241:CYS:CB	2.50	0.40
2:A:402:ARG:HA	2:A:402:ARG:HD3	1.93	0.40
3:B:156:LYS:HE2	3:B:156:LYS:HA	2.03	0.40
2:A:402:ARG:HA	2:A:402:ARG:HD3	1.93	0.40
3:B:156:LYS:HE2	3:B:156:LYS:HA	2.03	0.40
1:C:179:LEU:HD23	1:C:405:LEU:CG	2.51	0.40
2:A:402:ARG:HA	2:A:402:ARG:HD3	1.93	0.40
3:B:156:LYS:HE2	3:B:156:LYS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:LEU:HD23	1:C:405:LEU:CG	2.51	0.40
2:A:402:ARG:HA	2:A:402:ARG:HD3	1.93	0.40
3:B:156:LYS:HE2	3:B:156:LYS:HA	2.03	0.40
2:A:402:ARG:HA	2:A:402:ARG:HD3	1.93	0.40
3:B:156:LYS:HE2	3:B:156:LYS:HA	2.03	0.40
1:C:179:LEU:HD23	1:C:405:LEU:CG	2.51	0.40
1:C:179:LEU:HD21	1:C:383:PHE:CD2	2.56	0.40
1:C:369:SER:HA	1:C:411:SER:CB	2.51	0.40
1:C:179:LEU:HD21	1:C:383:PHE:CD2	2.56	0.40
1:C:179:LEU:HD21	1:C:383:PHE:CD2	2.56	0.40
1:C:179:LEU:HD21	1:C:383:PHE:CD2	2.57	0.40
2:A:362:VAL:HG21	2:A:370:LYS:HA	2.04	0.40
1:C:70:ILE:HD11	1:C:127:GLY:HA2	2.04	0.40
2:A:362:VAL:HG21	2:A:370:LYS:HA	2.04	0.40
1:C:179:LEU:HD21	1:C:383:PHE:CD2	2.57	0.40
2:A:362:VAL:HG21	2:A:370:LYS:HA	2.04	0.40
2:A:362:VAL:HG21	2:A:370:LYS:HA	2.04	0.40
1:C:355:TRP:HA	1:C:355:TRP:CE3	2.57	0.40
2:A:362:VAL:HG21	2:A:370:LYS:HA	2.04	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 PDB entries followed by that with respect to all EM entries.

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	1-C	286/501 (57%)	273 (96%)	11 (4%)	2 (1%)	18	56
1	2-C	286/501 (57%)	272 (95%)	12 (4%)	2 (1%)	18	56
1	3-C	286/501 (57%)	270 (94%)	15 (5%)	1 (0%)	36	72
1	4-C	286/501 (57%)	270 (94%)	15 (5%)	1 (0%)	36	72
1	5-C	286/501 (57%)	271 (95%)	13 (4%)	2 (1%)	18	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1-A	408/451 (90%)	367 (90%)	39 (10%)	2 (0%)	24	63
2	2-A	408/451 (90%)	367 (90%)	39 (10%)	2 (0%)	24	63
2	3-A	408/451 (90%)	367 (90%)	39 (10%)	2 (0%)	24	63
2	4-A	408/451 (90%)	367 (90%)	39 (10%)	2 (0%)	24	63
2	5-A	408/451 (90%)	367 (90%)	39 (10%)	2 (0%)	24	63
3	1-B	424/445 (95%)	384 (91%)	34 (8%)	6 (1%)	9	40
3	2-B	424/445 (95%)	384 (91%)	34 (8%)	6 (1%)	9	40
3	3-B	424/445 (95%)	384 (91%)	34 (8%)	6 (1%)	9	40
3	4-B	424/445 (95%)	384 (91%)	34 (8%)	6 (1%)	9	40
3	5-B	424/445 (95%)	384 (91%)	34 (8%)	6 (1%)	9	40
All	All	5590/6985 (80%)	5111 (91%)	431 (8%)	48 (1%)	16	51

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-C	123	SER
1	1-C	451	SER
1	2-C	123	SER
1	3-C	123	SER
1	4-C	123	SER
1	5-C	123	SER
3	1-B	109	THR
3	1-B	344	VAL
3	2-B	109	THR
3	2-B	344	VAL
3	3-B	109	THR
3	3-B	344	VAL
3	4-B	109	THR
3	4-B	344	VAL
3	5-B	109	THR
3	5-B	344	VAL
2	1-A	109	THR
3	1-B	82	PRO
3	1-B	288	VAL
1	2-C	320	SER
2	2-A	109	THR
3	2-B	82	PRO
3	2-B	288	VAL

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Mol	Chain	Res	Type
2	3-A	109	THR
3	3-B	82	PRO
3	3-B	288	VAL
2	4-A	109	THR
3	4-B	82	PRO
3	4-B	288	VAL
2	5-A	109	THR
3	5-B	82	PRO
3	5-B	288	VAL
2	1-A	279	GLU
2	2-A	279	GLU
2	3-A	279	GLU
2	4-A	279	GLU
2	5-A	279	GLU
3	1-B	266	HIS
3	2-B	266	HIS
3	3-B	266	HIS
3	4-B	266	HIS
1	5-C	424	LYS
3	5-B	266	HIS
3	1-B	278	ARG
3	2-B	278	ARG
3	3-B	278	ARG
3	4-B	278	ARG
3	5-B	278	ARG

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 PDB entries followed by that with respect to all EM entries.

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	1-C	268/447 (60%)	219 (82%)	49 (18%)	2	8
1	2-C	268/447 (60%)	219 (82%)	49 (18%)	2	8
1	3-C	268/447 (60%)	219 (82%)	49 (18%)	2	8
1	4-C	268/447 (60%)	219 (82%)	49 (18%)	2	8
1	5-C	268/447 (60%)	219 (82%)	49 (18%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1-A	347/377 (92%)	311 (90%)	36 (10%)	7	22
2	2-A	347/377 (92%)	311 (90%)	36 (10%)	7	22
2	3-A	347/377 (92%)	311 (90%)	36 (10%)	7	22
2	4-A	347/377 (92%)	311 (90%)	36 (10%)	7	22
2	5-A	347/377 (92%)	311 (90%)	36 (10%)	7	22
3	1-B	367/381 (96%)	313 (85%)	54 (15%)	3	13
3	2-B	367/381 (96%)	313 (85%)	54 (15%)	3	13
3	3-B	367/381 (96%)	313 (85%)	54 (15%)	3	13
3	4-B	367/381 (96%)	313 (85%)	54 (15%)	3	13
3	5-B	367/381 (96%)	313 (85%)	54 (15%)	3	13
All	All	4910/6025 (82%)	4215 (86%)	695 (14%)	5	13

All (695) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-C	66	VAL
1	1-C	69	ARG
1	1-C	70	ILE
1	1-C	76	SER
1	1-C	83	ASP
1	1-C	87	VAL
1	1-C	95	LEU
1	1-C	119	LYS
1	1-C	121	THR
1	1-C	125	ILE
1	1-C	129	GLU
1	1-C	132	GLN
1	1-C	136	PHE
1	1-C	141	LYS
1	1-C	147	VAL
1	1-C	151	GLN
1	1-C	157	THR
1	1-C	168	THR
1	1-C	175	ASP
1	1-C	316	LEU
1	1-C	317	GLU
1	1-C	349	ARG
1	1-C	351	VAL

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Mol	Chain	Res	Type
1	1-C	358	LEU
1	1-C	359	LYS
1	1-C	365	GLN
1	1-C	379	SER
1	1-C	385	ILE
1	1-C	387	ILE
1	1-C	388	LEU
1	1-C	389	HIS
1	1-C	390	LEU
1	1-C	399	LYS
1	1-C	400	ILE
1	1-C	401	SER
1	1-C	422	ARG
1	1-C	432	SER
1	1-C	433	LEU
1	1-C	436	LEU
1	1-C	443	LEU
1	1-C	446	ASN
1	1-C	447	GLN
1	1-C	458	PHE
1	1-C	464	THR
1	1-C	474	ARG
1	1-C	477	SER
1	1-C	482	ASN
1	1-C	488	SER
1	1-C	494	LEU
2	1-A	28	HIS
2	1-A	71	GLU
2	1-A	76	ASP
2	1-A	80	THR
2	1-A	82	THR
2	1-A	93	ILE
2	1-A	97	GLU
2	1-A	109	THR
2	1-A	130	THR
2	1-A	132	LEU
2	1-A	136	SER
2	1-A	140	SER
2	1-A	150	THR
2	1-A	169	PHE
2	1-A	170	SER
2	1-A	178	SER

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Mol	Chain	Res	Type
2	1-A	185	TYR
2	1-A	189	LEU
2	1-A	194	THR
2	1-A	226	ASN
2	1-A	241	SER
2	1-A	253	THR
2	1-A	277	SER
2	1-A	279	GLU
2	1-A	287	SER
2	1-A	291	ILE
2	1-A	315	CYS
2	1-A	322	ASP
2	1-A	327	ASP
2	1-A	340	THR
2	1-A	349	THR
2	1-A	361	THR
2	1-A	376	CYS
2	1-A	382	THR
2	1-A	425	MET
2	1-A	439	SER
3	1-B	25	SER
3	1-B	33	THR
3	1-B	35	SER
3	1-B	48	ARG
3	1-B	67	LEU
3	1-B	71	GLU
3	1-B	76	ASP
3	1-B	77	SER
3	1-B	109	THR
3	1-B	128	SER
3	1-B	130	ASP
3	1-B	133	GLN
3	1-B	140	SER
3	1-B	145	THR
3	1-B	147	SER
3	1-B	151	THR
3	1-B	158	ARG
3	1-B	163	ASP
3	1-B	165	ILE
3	1-B	166	MET
3	1-B	168	THR
3	1-B	170	SER

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Mol	Chain	Res	Type
3	1-B	174	SER
3	1-B	179	ASP
3	1-B	185	TYR
3	1-B	205	ASP
3	1-B	213	CYS
3	1-B	216	THR
3	1-B	220	THR
3	1-B	221	THR
3	1-B	223	THR
3	1-B	234	THR
3	1-B	236	SER
3	1-B	239	THR
3	1-B	240	THR
3	1-B	265	LEU
3	1-B	276	THR
3	1-B	277	SER
3	1-B	280	SER
3	1-B	284	ARG
3	1-B	287	THR
3	1-B	292	THR
3	1-B	309	HIS
3	1-B	314	THR
3	1-B	325	MET
3	1-B	340	SER
3	1-B	341	SER
3	1-B	343	PHE
3	1-B	344	VAL
3	1-B	353	THR
3	1-B	396	THR
3	1-B	413	MET
3	1-B	419	THR
3	1-B	432	TYR
1	2-C	66	VAL
1	2-C	69	ARG
1	2-C	70	ILE
1	2-C	76	SER
1	2-C	83	ASP
1	2-C	87	VAL
1	2-C	95	LEU
1	2-C	119	LYS
1	2-C	121	THR
1	2-C	125	ILE

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Mol	Chain	Res	Type
1	2-C	129	GLU
1	2-C	132	GLN
1	2-C	136	PHE
1	2-C	141	LYS
1	2-C	147	VAL
1	2-C	151	GLN
1	2-C	157	THR
1	2-C	168	THR
1	2-C	175	ASP
1	2-C	316	LEU
1	2-C	317	GLU
1	2-C	349	ARG
1	2-C	351	VAL
1	2-C	358	LEU
1	2-C	359	LYS
1	2-C	365	GLN
1	2-C	379	SER
1	2-C	385	ILE
1	2-C	387	ILE
1	2-C	388	LEU
1	2-C	389	HIS
1	2-C	390	LEU
1	2-C	399	LYS
1	2-C	400	ILE
1	2-C	401	SER
1	2-C	422	ARG
1	2-C	432	SER
1	2-C	433	LEU
1	2-C	436	LEU
1	2-C	443	LEU
1	2-C	446	ASN
1	2-C	447	GLN
1	2-C	458	PHE
1	2-C	464	THR
1	2-C	474	ARG
1	2-C	477	SER
1	2-C	482	ASN
1	2-C	488	SER
1	2-C	494	LEU
2	2-A	28	HIS
2	2-A	71	GLU
2	2-A	76	ASP

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Mol	Chain	Res	Type
2	2-A	80	THR
2	2-A	82	THR
2	2-A	93	ILE
2	2-A	97	GLU
2	2-A	109	THR
2	2-A	130	THR
2	2-A	132	LEU
2	2-A	136	SER
2	2-A	140	SER
2	2-A	150	THR
2	2-A	169	PHE
2	2-A	170	SER
2	2-A	178	SER
2	2-A	185	TYR
2	2-A	189	LEU
2	2-A	194	THR
2	2-A	226	ASN
2	2-A	241	SER
2	2-A	253	THR
2	2-A	277	SER
2	2-A	279	GLU
2	2-A	287	SER
2	2-A	291	ILE
2	2-A	315	CYS
2	2-A	322	ASP
2	2-A	327	ASP
2	2-A	340	THR
2	2-A	349	THR
2	2-A	361	THR
2	2-A	376	CYS
2	2-A	382	THR
2	2-A	425	MET
2	2-A	439	SER
3	2-B	25	SER
3	2-B	33	THR
3	2-B	35	SER
3	2-B	48	ARG
3	2-B	67	LEU
3	2-B	71	GLU
3	2-B	76	ASP
3	2-B	77	SER
3	2-B	109	THR

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Mol	Chain	Res	Type
3	2-B	128	SER
3	2-B	130	ASP
3	2-B	133	GLN
3	2-B	140	SER
3	2-B	145	THR
3	2-B	147	SER
3	2-B	151	THR
3	2-B	158	ARG
3	2-B	163	ASP
3	2-B	165	ILE
3	2-B	166	MET
3	2-B	168	THR
3	2-B	170	SER
3	2-B	174	SER
3	2-B	179	ASP
3	2-B	185	TYR
3	2-B	205	ASP
3	2-B	213	CYS
3	2-B	216	THR
3	2-B	220	THR
3	2-B	221	THR
3	2-B	223	THR
3	2-B	234	THR
3	2-B	236	SER
3	2-B	239	THR
3	2-B	240	THR
3	2-B	265	LEU
3	2-B	276	THR
3	2-B	277	SER
3	2-B	280	SER
3	2-B	284	ARG
3	2-B	287	THR
3	2-B	292	THR
3	2-B	309	HIS
3	2-B	314	THR
3	2-B	325	MET
3	2-B	340	SER
3	2-B	341	SER
3	2-B	343	PHE
3	2-B	344	VAL
3	2-B	353	THR
3	2-B	396	THR

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Mol	Chain	Res	Type
3	2-B	413	MET
3	2-B	419	THR
3	2-B	432	TYR
1	3-C	66	VAL
1	3-C	69	ARG
1	3-C	70	ILE
1	3-C	76	SER
1	3-C	83	ASP
1	3-C	87	VAL
1	3-C	95	LEU
1	3-C	119	LYS
1	3-C	121	THR
1	3-C	125	ILE
1	3-C	129	GLU
1	3-C	132	GLN
1	3-C	136	PHE
1	3-C	141	LYS
1	3-C	147	VAL
1	3-C	151	GLN
1	3-C	157	THR
1	3-C	168	THR
1	3-C	175	ASP
1	3-C	316	LEU
1	3-C	317	GLU
1	3-C	349	ARG
1	3-C	351	VAL
1	3-C	358	LEU
1	3-C	359	LYS
1	3-C	365	GLN
1	3-C	379	SER
1	3-C	385	ILE
1	3-C	387	ILE
1	3-C	388	LEU
1	3-C	389	HIS
1	3-C	390	LEU
1	3-C	399	LYS
1	3-C	400	ILE
1	3-C	401	SER
1	3-C	422	ARG
1	3-C	432	SER
1	3-C	433	LEU
1	3-C	436	LEU

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Mol	Chain	Res	Type
1	3-C	443	LEU
1	3-C	446	ASN
1	3-C	447	GLN
1	3-C	458	PHE
1	3-C	464	THR
1	3-C	474	ARG
1	3-C	477	SER
1	3-C	482	ASN
1	3-C	488	SER
1	3-C	494	LEU
2	3-A	28	HIS
2	3-A	71	GLU
2	3-A	76	ASP
2	3-A	80	THR
2	3-A	82	THR
2	3-A	93	ILE
2	3-A	97	GLU
2	3-A	109	THR
2	3-A	130	THR
2	3-A	132	LEU
2	3-A	136	SER
2	3-A	140	SER
2	3-A	150	THR
2	3-A	169	PHE
2	3-A	170	SER
2	3-A	178	SER
2	3-A	185	TYR
2	3-A	189	LEU
2	3-A	194	THR
2	3-A	226	ASN
2	3-A	241	SER
2	3-A	253	THR
2	3-A	277	SER
2	3-A	279	GLU
2	3-A	287	SER
2	3-A	291	ILE
2	3-A	315	CYS
2	3-A	322	ASP
2	3-A	327	ASP
2	3-A	340	THR
2	3-A	349	THR
2	3-A	361	THR

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Mol	Chain	Res	Type
2	3-A	376	CYS
2	3-A	382	THR
2	3-A	425	MET
2	3-A	439	SER
3	3-B	25	SER
3	3-B	33	THR
3	3-B	35	SER
3	3-B	48	ARG
3	3-B	67	LEU
3	3-B	71	GLU
3	3-B	76	ASP
3	3-B	77	SER
3	3-B	109	THR
3	3-B	128	SER
3	3-B	130	ASP
3	3-B	133	GLN
3	3-B	140	SER
3	3-B	145	THR
3	3-B	147	SER
3	3-B	151	THR
3	3-B	158	ARG
3	3-B	163	ASP
3	3-B	165	ILE
3	3-B	166	MET
3	3-B	168	THR
3	3-B	170	SER
3	3-B	174	SER
3	3-B	179	ASP
3	3-B	185	TYR
3	3-B	205	ASP
3	3-B	213	CYS
3	3-B	216	THR
3	3-B	220	THR
3	3-B	221	THR
3	3-B	223	THR
3	3-B	234	THR
3	3-B	236	SER
3	3-B	239	THR
3	3-B	240	THR
3	3-B	265	LEU
3	3-B	276	THR
3	3-B	277	SER

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Mol	Chain	Res	Type
3	3-B	280	SER
3	3-B	284	ARG
3	3-B	287	THR
3	3-B	292	THR
3	3-B	309	HIS
3	3-B	314	THR
3	3-B	325	MET
3	3-B	340	SER
3	3-B	341	SER
3	3-B	343	PHE
3	3-B	344	VAL
3	3-B	353	THR
3	3-B	396	THR
3	3-B	413	MET
3	3-B	419	THR
3	3-B	432	TYR
1	4-C	66	VAL
1	4-C	69	ARG
1	4-C	70	ILE
1	4-C	76	SER
1	4-C	83	ASP
1	4-C	87	VAL
1	4-C	95	LEU
1	4-C	119	LYS
1	4-C	121	THR
1	4-C	125	ILE
1	4-C	129	GLU
1	4-C	132	GLN
1	4-C	136	PHE
1	4-C	141	LYS
1	4-C	147	VAL
1	4-C	151	GLN
1	4-C	157	THR
1	4-C	168	THR
1	4-C	175	ASP
1	4-C	316	LEU
1	4-C	317	GLU
1	4-C	349	ARG
1	4-C	351	VAL
1	4-C	358	LEU
1	4-C	359	LYS
1	4-C	365	GLN

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Mol	Chain	Res	Type
1	4-C	379	SER
1	4-C	385	ILE
1	4-C	387	ILE
1	4-C	388	LEU
1	4-C	389	HIS
1	4-C	390	LEU
1	4-C	399	LYS
1	4-C	400	ILE
1	4-C	401	SER
1	4-C	422	ARG
1	4-C	432	SER
1	4-C	433	LEU
1	4-C	436	LEU
1	4-C	443	LEU
1	4-C	446	ASN
1	4-C	447	GLN
1	4-C	458	PHE
1	4-C	464	THR
1	4-C	474	ARG
1	4-C	477	SER
1	4-C	482	ASN
1	4-C	488	SER
1	4-C	494	LEU
2	4-A	28	HIS
2	4-A	71	GLU
2	4-A	76	ASP
2	4-A	80	THR
2	4-A	82	THR
2	4-A	93	ILE
2	4-A	97	GLU
2	4-A	109	THR
2	4-A	130	THR
2	4-A	132	LEU
2	4-A	136	SER
2	4-A	140	SER
2	4-A	150	THR
2	4-A	169	PHE
2	4-A	170	SER
2	4-A	178	SER
2	4-A	185	TYR
2	4-A	189	LEU
2	4-A	194	THR

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Mol	Chain	Res	Type
2	4-A	226	ASN
2	4-A	241	SER
2	4-A	253	THR
2	4-A	277	SER
2	4-A	279	GLU
2	4-A	287	SER
2	4-A	291	ILE
2	4-A	315	CYS
2	4-A	322	ASP
2	4-A	327	ASP
2	4-A	340	THR
2	4-A	349	THR
2	4-A	361	THR
2	4-A	376	CYS
2	4-A	382	THR
2	4-A	425	MET
2	4-A	439	SER
3	4-B	25	SER
3	4-B	33	THR
3	4-B	35	SER
3	4-B	48	ARG
3	4-B	67	LEU
3	4-B	71	GLU
3	4-B	76	ASP
3	4-B	77	SER
3	4-B	109	THR
3	4-B	128	SER
3	4-B	130	ASP
3	4-B	133	GLN
3	4-B	140	SER
3	4-B	145	THR
3	4-B	147	SER
3	4-B	151	THR
3	4-B	158	ARG
3	4-B	163	ASP
3	4-B	165	ILE
3	4-B	166	MET
3	4-B	168	THR
3	4-B	170	SER
3	4-B	174	SER
3	4-B	179	ASP
3	4-B	185	TYR

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Mol	Chain	Res	Type
3	4-B	205	ASP
3	4-B	213	CYS
3	4-B	216	THR
3	4-B	220	THR
3	4-B	221	THR
3	4-B	223	THR
3	4-B	234	THR
3	4-B	236	SER
3	4-B	239	THR
3	4-B	240	THR
3	4-B	265	LEU
3	4-B	276	THR
3	4-B	277	SER
3	4-B	280	SER
3	4-B	284	ARG
3	4-B	287	THR
3	4-B	292	THR
3	4-B	309	HIS
3	4-B	314	THR
3	4-B	325	MET
3	4-B	340	SER
3	4-B	341	SER
3	4-B	343	PHE
3	4-B	344	VAL
3	4-B	353	THR
3	4-B	396	THR
3	4-B	413	MET
3	4-B	419	THR
3	4-B	432	TYR
1	5-C	66	VAL
1	5-C	69	ARG
1	5-C	70	ILE
1	5-C	76	SER
1	5-C	83	ASP
1	5-C	87	VAL
1	5-C	95	LEU
1	5-C	119	LYS
1	5-C	121	THR
1	5-C	125	ILE
1	5-C	129	GLU
1	5-C	132	GLN
1	5-C	136	PHE

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Mol	Chain	Res	Type
1	5-C	141	LYS
1	5-C	147	VAL
1	5-C	151	GLN
1	5-C	157	THR
1	5-C	168	THR
1	5-C	175	ASP
1	5-C	316	LEU
1	5-C	317	GLU
1	5-C	349	ARG
1	5-C	351	VAL
1	5-C	358	LEU
1	5-C	359	LYS
1	5-C	365	GLN
1	5-C	379	SER
1	5-C	385	ILE
1	5-C	387	ILE
1	5-C	388	LEU
1	5-C	389	HIS
1	5-C	390	LEU
1	5-C	399	LYS
1	5-C	400	ILE
1	5-C	401	SER
1	5-C	422	ARG
1	5-C	432	SER
1	5-C	433	LEU
1	5-C	436	LEU
1	5-C	443	LEU
1	5-C	446	ASN
1	5-C	447	GLN
1	5-C	458	PHE
1	5-C	464	THR
1	5-C	474	ARG
1	5-C	477	SER
1	5-C	482	ASN
1	5-C	488	SER
1	5-C	494	LEU
2	5-A	28	HIS
2	5-A	71	GLU
2	5-A	76	ASP
2	5-A	80	THR
2	5-A	82	THR
2	5-A	93	ILE

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Mol	Chain	Res	Type
2	5-A	97	GLU
2	5-A	109	THR
2	5-A	130	THR
2	5-A	132	LEU
2	5-A	136	SER
2	5-A	140	SER
2	5-A	150	THR
2	5-A	169	PHE
2	5-A	170	SER
2	5-A	178	SER
2	5-A	185	TYR
2	5-A	189	LEU
2	5-A	194	THR
2	5-A	226	ASN
2	5-A	241	SER
2	5-A	253	THR
2	5-A	277	SER
2	5-A	279	GLU
2	5-A	287	SER
2	5-A	291	ILE
2	5-A	315	CYS
2	5-A	322	ASP
2	5-A	327	ASP
2	5-A	340	THR
2	5-A	349	THR
2	5-A	361	THR
2	5-A	376	CYS
2	5-A	382	THR
2	5-A	425	MET
2	5-A	439	SER
3	5-B	25	SER
3	5-B	33	THR
3	5-B	35	SER
3	5-B	48	ARG
3	5-B	67	LEU
3	5-B	71	GLU
3	5-B	76	ASP
3	5-B	77	SER
3	5-B	109	THR
3	5-B	128	SER
3	5-B	130	ASP
3	5-B	133	GLN

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Mol	Chain	Res	Type
3	5-B	140	SER
3	5-B	145	THR
3	5-B	147	SER
3	5-B	151	THR
3	5-B	158	ARG
3	5-B	163	ASP
3	5-B	165	ILE
3	5-B	166	MET
3	5-B	168	THR
3	5-B	170	SER
3	5-B	174	SER
3	5-B	179	ASP
3	5-B	185	TYR
3	5-B	205	ASP
3	5-B	213	CYS
3	5-B	216	THR
3	5-B	220	THR
3	5-B	221	THR
3	5-B	223	THR
3	5-B	234	THR
3	5-B	236	SER
3	5-B	239	THR
3	5-B	240	THR
3	5-B	265	LEU
3	5-B	276	THR
3	5-B	277	SER
3	5-B	280	SER
3	5-B	284	ARG
3	5-B	287	THR
3	5-B	292	THR
3	5-B	309	HIS
3	5-B	314	THR
3	5-B	325	MET
3	5-B	340	SER
3	5-B	341	SER
3	5-B	343	PHE
3	5-B	344	VAL
3	5-B	353	THR
3	5-B	396	THR
3	5-B	413	MET
3	5-B	419	THR
3	5-B	432	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-C	118	HIS
1	1-C	132	GLN
1	1-C	151	GLN
1	1-C	152	ASN
1	1-C	170	GLN
1	1-C	309	ASN
1	1-C	344	ASN
1	1-C	430	ASN
1	1-C	495	HIS
2	1-A	192	HIS
2	1-A	206	ASN
2	1-A	233	GLN
2	1-A	256	GLN
2	1-A	283	HIS
3	1-B	11	GLN
3	1-B	167	ASN
3	1-B	193	GLN
3	1-B	300	ASN
3	1-B	337	ASN
3	1-B	380	ASN
3	1-B	385	GLN
3	1-B	424	ASN
3	1-B	433	GLN
1	2-C	118	HIS
1	2-C	132	GLN
1	2-C	151	GLN
1	2-C	152	ASN
1	2-C	162	ASN
1	2-C	170	GLN
1	2-C	309	ASN
1	2-C	326	GLN
1	2-C	449	ASN
1	2-C	495	HIS
2	2-A	192	HIS
2	2-A	206	ASN
2	2-A	233	GLN
2	2-A	256	GLN
2	2-A	283	HIS
3	2-B	11	GLN
3	2-B	167	ASN
3	2-B	193	GLN

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Mol	Chain	Res	Type
3	2-B	300	ASN
3	2-B	337	ASN
3	2-B	380	ASN
3	2-B	385	GLN
3	2-B	424	ASN
3	2-B	433	GLN
1	3-C	118	HIS
1	3-C	132	GLN
1	3-C	151	GLN
1	3-C	152	ASN
1	3-C	170	GLN
1	3-C	309	ASN
1	3-C	344	ASN
1	3-C	449	ASN
1	3-C	495	HIS
2	3-A	192	HIS
2	3-A	206	ASN
2	3-A	233	GLN
2	3-A	256	GLN
2	3-A	283	HIS
3	3-B	11	GLN
3	3-B	167	ASN
3	3-B	193	GLN
3	3-B	300	ASN
3	3-B	337	ASN
3	3-B	380	ASN
3	3-B	385	GLN
3	3-B	424	ASN
3	3-B	433	GLN
1	4-C	118	HIS
1	4-C	132	GLN
1	4-C	151	GLN
1	4-C	152	ASN
1	4-C	170	GLN
1	4-C	309	ASN
1	4-C	344	ASN
1	4-C	449	ASN
1	4-C	495	HIS
2	4-A	192	HIS
2	4-A	206	ASN
2	4-A	233	GLN
2	4-A	256	GLN

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Mol	Chain	Res	Type
2	4-A	283	HIS
3	4-B	11	GLN
3	4-B	167	ASN
3	4-B	193	GLN
3	4-B	300	ASN
3	4-B	337	ASN
3	4-B	380	ASN
3	4-B	385	GLN
3	4-B	424	ASN
3	4-B	433	GLN
1	5-C	118	HIS
1	5-C	132	GLN
1	5-C	151	GLN
1	5-C	152	ASN
1	5-C	170	GLN
1	5-C	344	ASN
1	5-C	430	ASN
1	5-C	449	ASN
1	5-C	495	HIS
2	5-A	192	HIS
2	5-A	206	ASN
2	5-A	233	GLN
2	5-A	256	GLN
2	5-A	283	HIS
3	5-B	11	GLN
3	5-B	167	ASN
3	5-B	193	GLN
3	5-B	300	ASN
3	5-B	337	ASN
3	5-B	380	ASN
3	5-B	385	GLN
3	5-B	424	ASN
3	5-B	433	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 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
7	GDP	4-B	600	-	29,30,30	2.85	11 (37%)	45,47,47	3.47	16 (35%)
8	TA1	3-B	601	-	68,68,68	2.20	25 (36%)	105,105,105	1.50	14 (13%)
7	GDP	3-B	600	-	29,30,30	2.85	11 (37%)	45,47,47	3.47	16 (35%)
6	GTP	1-A	500	4	33,34,34	1.91	4 (12%)	50,54,54	0.94	4 (8%)
8	TA1	2-B	601	-	68,68,68	2.20	25 (36%)	105,105,105	1.50	14 (13%)
5	ANP	3-C	602	4	33,33,33	2.18	10 (30%)	45,52,52	2.85	17 (37%)
6	GTP	2-A	500	4	33,34,34	1.91	4 (12%)	50,54,54	0.94	4 (8%)
8	TA1	4-B	601	-	68,68,68	2.20	25 (36%)	105,105,105	1.50	14 (13%)
6	GTP	5-A	500	4	33,34,34	1.91	4 (12%)	50,54,54	0.94	4 (8%)
8	TA1	1-B	601	-	68,68,68	2.20	25 (36%)	105,105,105	1.50	14 (13%)
7	GDP	5-B	600	-	29,30,30	2.85	11 (37%)	45,47,47	3.47	16 (35%)
6	GTP	3-A	500	4	33,34,34	1.91	4 (12%)	50,54,54	0.94	4 (8%)
5	ANP	2-C	602	4	33,33,33	2.17	10 (30%)	45,52,52	2.85	17 (37%)
8	TA1	5-B	601	-	68,68,68	2.20	25 (36%)	105,105,105	1.50	14 (13%)
5	ANP	4-C	602	4	33,33,33	2.17	10 (30%)	45,52,52	2.85	17 (37%)
6	GTP	4-A	500	4	33,34,34	1.91	4 (12%)	50,54,54	0.94	4 (8%)
7	GDP	1-B	600	-	29,30,30	2.85	11 (37%)	45,47,47	3.47	16 (35%)
5	ANP	1-C	602	4	33,33,33	2.17	10 (30%)	45,52,52	2.85	16 (35%)
7	GDP	2-B	600	-	29,30,30	2.85	11 (37%)	45,47,47	3.47	16 (35%)
5	ANP	5-C	602	4	33,33,33	2.18	10 (30%)	45,52,52	2.85	17 (37%)

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
7	GDP	4-B	600	-	-	4/16/32/32	0/3/3/3
8	TA1	3-B	601	-	-	9/41/127/127	0/7/7/7
7	GDP	3-B	600	-	-	4/16/32/32	0/3/3/3
6	GTP	1-A	500	4	-	3/22/38/38	0/3/3/3
8	TA1	2-B	601	-	-	9/41/127/127	0/7/7/7
5	ANP	3-C	602	4	-	9/18/38/38	0/3/3/3
6	GTP	2-A	500	4	-	3/22/38/38	0/3/3/3
8	TA1	4-B	601	-	-	9/41/127/127	0/7/7/7
6	GTP	5-A	500	4	-	3/22/38/38	0/3/3/3
8	TA1	1-B	601	-	-	9/41/127/127	0/7/7/7
7	GDP	5-B	600	-	-	4/16/32/32	0/3/3/3
6	GTP	3-A	500	4	-	3/22/38/38	0/3/3/3
5	ANP	2-C	602	4	-	9/18/38/38	0/3/3/3
8	TA1	5-B	601	-	-	9/41/127/127	0/7/7/7
5	ANP	4-C	602	4	-	9/18/38/38	0/3/3/3
6	GTP	4-A	500	4	-	3/22/38/38	0/3/3/3
7	GDP	1-B	600	-	-	4/16/32/32	0/3/3/3
5	ANP	1-C	602	4	-	9/18/38/38	0/3/3/3
7	GDP	2-B	600	-	-	4/16/32/32	0/3/3/3
5	ANP	5-C	602	4	-	9/18/38/38	0/3/3/3

All (250) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-B	600	GDP	PA-O3A	7.57	1.67	1.59
7	2-B	600	GDP	PA-O3A	7.57	1.67	1.59
7	3-B	600	GDP	PA-O3A	7.57	1.67	1.59
7	4-B	600	GDP	PA-O3A	7.57	1.67	1.59
7	5-B	600	GDP	PA-O3A	7.57	1.67	1.59
8	1-B	601	TA1	C06-C05	6.50	1.50	1.38
8	2-B	601	TA1	C06-C05	6.50	1.50	1.38
8	3-B	601	TA1	C06-C05	6.50	1.50	1.38
8	4-B	601	TA1	C06-C05	6.50	1.50	1.38
8	5-B	601	TA1	C06-C05	6.50	1.50	1.38
5	4-C	602	ANP	PB-O2B	-6.34	1.40	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2-C	602	ANP	PB-O2B	-6.32	1.40	1.56
5	5-C	602	ANP	PB-O2B	-6.31	1.40	1.56
5	1-C	602	ANP	PB-O2B	-6.30	1.40	1.56
5	3-C	602	ANP	PB-O2B	-6.25	1.40	1.56
6	1-A	500	GTP	PA-O3A	-6.07	1.52	1.59
6	2-A	500	GTP	PA-O3A	-6.07	1.52	1.59
6	3-A	500	GTP	PA-O3A	-6.07	1.52	1.59
6	4-A	500	GTP	PA-O3A	-6.07	1.52	1.59
6	5-A	500	GTP	PA-O3A	-6.07	1.52	1.59
7	1-B	600	GDP	O6-C6	5.93	1.34	1.23
7	2-B	600	GDP	O6-C6	5.93	1.34	1.23
7	3-B	600	GDP	O6-C6	5.93	1.34	1.23
7	4-B	600	GDP	O6-C6	5.93	1.34	1.23
7	5-B	600	GDP	O6-C6	5.93	1.34	1.23
7	1-B	600	GDP	C8-N9	5.87	1.50	1.37
7	2-B	600	GDP	C8-N9	5.87	1.50	1.37
7	3-B	600	GDP	C8-N9	5.87	1.50	1.37
7	4-B	600	GDP	C8-N9	5.87	1.50	1.37
7	5-B	600	GDP	C8-N9	5.87	1.50	1.37
8	1-B	601	TA1	C08-C07	-5.70	1.25	1.38
8	2-B	601	TA1	C08-C07	-5.70	1.25	1.38
8	3-B	601	TA1	C08-C07	-5.70	1.25	1.38
8	4-B	601	TA1	C08-C07	-5.70	1.25	1.38
8	5-B	601	TA1	C08-C07	-5.70	1.25	1.38
6	1-A	500	GTP	PB-O3A	-5.65	1.53	1.59
6	2-A	500	GTP	PB-O3A	-5.65	1.53	1.59
6	3-A	500	GTP	PB-O3A	-5.65	1.53	1.59
6	4-A	500	GTP	PB-O3A	-5.65	1.53	1.59
6	5-A	500	GTP	PB-O3A	-5.65	1.53	1.59
6	1-A	500	GTP	PB-O3B	5.39	1.65	1.59
6	2-A	500	GTP	PB-O3B	5.39	1.65	1.59
6	3-A	500	GTP	PB-O3B	5.39	1.65	1.59
6	4-A	500	GTP	PB-O3B	5.39	1.65	1.59
6	5-A	500	GTP	PB-O3B	5.39	1.65	1.59
8	1-B	601	TA1	C18-C10	5.36	1.69	1.57
8	2-B	601	TA1	C18-C10	5.36	1.69	1.57
8	3-B	601	TA1	C18-C10	5.36	1.69	1.57
8	4-B	601	TA1	C18-C10	5.36	1.69	1.57
8	5-B	601	TA1	C18-C10	5.36	1.69	1.57
5	1-C	602	ANP	PB-O3A	5.07	1.65	1.59
5	4-C	602	ANP	PB-O3A	5.02	1.65	1.59
5	5-C	602	ANP	PB-O3A	4.99	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2-C	602	ANP	PB-O3A	4.97	1.65	1.59
5	3-C	602	ANP	PB-O3A	4.94	1.65	1.59
8	1-B	601	TA1	C05-C04	4.82	1.46	1.39
8	2-B	601	TA1	C05-C04	4.82	1.46	1.39
8	3-B	601	TA1	C05-C04	4.82	1.46	1.39
8	4-B	601	TA1	C05-C04	4.82	1.46	1.39
8	5-B	601	TA1	C05-C04	4.82	1.46	1.39
7	1-B	600	GDP	C2-N1	4.74	1.49	1.37
7	2-B	600	GDP	C2-N1	4.74	1.49	1.37
7	3-B	600	GDP	C2-N1	4.74	1.49	1.37
7	4-B	600	GDP	C2-N1	4.74	1.49	1.37
7	5-B	600	GDP	C2-N1	4.74	1.49	1.37
8	1-B	601	TA1	C45-C24	4.27	1.61	1.54
8	2-B	601	TA1	C45-C24	4.27	1.61	1.54
8	3-B	601	TA1	C45-C24	4.27	1.61	1.54
8	4-B	601	TA1	C45-C24	4.27	1.61	1.54
8	5-B	601	TA1	C45-C24	4.27	1.61	1.54
5	3-C	602	ANP	PA-O3A	3.91	1.63	1.59
7	1-B	600	GDP	PB-O2B	-3.89	1.40	1.54
7	2-B	600	GDP	PB-O2B	-3.89	1.40	1.54
7	3-B	600	GDP	PB-O2B	-3.89	1.40	1.54
7	4-B	600	GDP	PB-O2B	-3.89	1.40	1.54
7	5-B	600	GDP	PB-O2B	-3.89	1.40	1.54
5	5-C	602	ANP	PG-O2G	-3.84	1.46	1.56
5	1-C	602	ANP	PG-O2G	-3.83	1.46	1.56
5	2-C	602	ANP	PG-O2G	-3.81	1.46	1.56
5	4-C	602	ANP	PG-O2G	-3.81	1.46	1.56
5	5-C	602	ANP	PA-O3A	3.81	1.63	1.59
5	3-C	602	ANP	PG-O2G	-3.81	1.46	1.56
8	1-B	601	TA1	C36-C31	3.78	1.45	1.39
8	2-B	601	TA1	C36-C31	3.78	1.45	1.39
8	3-B	601	TA1	C36-C31	3.78	1.45	1.39
8	4-B	601	TA1	C36-C31	3.78	1.45	1.39
8	5-B	601	TA1	C36-C31	3.78	1.45	1.39
5	1-C	602	ANP	PA-O3A	3.76	1.63	1.59
5	4-C	602	ANP	PA-O3A	3.75	1.63	1.59
5	2-C	602	ANP	PA-O3A	3.72	1.63	1.59
8	1-B	601	TA1	O02-C03	3.53	1.41	1.34
8	2-B	601	TA1	O02-C03	3.53	1.41	1.34
8	3-B	601	TA1	O02-C03	3.53	1.41	1.34
8	4-B	601	TA1	O02-C03	3.53	1.41	1.34
8	5-B	601	TA1	O02-C03	3.53	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-B	600	GDP	O4'-C1'	3.34	1.49	1.42
7	2-B	600	GDP	O4'-C1'	3.34	1.49	1.42
7	3-B	600	GDP	O4'-C1'	3.34	1.49	1.42
7	4-B	600	GDP	O4'-C1'	3.34	1.49	1.42
7	5-B	600	GDP	O4'-C1'	3.34	1.49	1.42
8	1-B	601	TA1	C25-C24	3.33	1.39	1.34
8	2-B	601	TA1	C25-C24	3.33	1.39	1.34
8	3-B	601	TA1	C25-C24	3.33	1.39	1.34
8	4-B	601	TA1	C25-C24	3.33	1.39	1.34
8	5-B	601	TA1	C25-C24	3.33	1.39	1.34
8	1-B	601	TA1	C43-C01	3.25	1.61	1.54
8	2-B	601	TA1	C43-C01	3.25	1.61	1.54
8	3-B	601	TA1	C43-C01	3.25	1.61	1.54
8	4-B	601	TA1	C43-C01	3.25	1.61	1.54
8	5-B	601	TA1	C43-C01	3.25	1.61	1.54
8	1-B	601	TA1	C46-C45	3.22	1.60	1.53
8	2-B	601	TA1	C46-C45	3.22	1.60	1.53
8	3-B	601	TA1	C46-C45	3.22	1.60	1.53
8	4-B	601	TA1	C46-C45	3.22	1.60	1.53
8	5-B	601	TA1	C46-C45	3.22	1.60	1.53
8	1-B	601	TA1	C11-C10	3.06	1.61	1.54
8	2-B	601	TA1	C11-C10	3.06	1.61	1.54
8	3-B	601	TA1	C11-C10	3.06	1.61	1.54
8	4-B	601	TA1	C11-C10	3.06	1.61	1.54
8	5-B	601	TA1	C11-C10	3.06	1.61	1.54
5	3-C	602	ANP	C6-N6	-3.05	1.26	1.34
5	2-C	602	ANP	C6-N6	-3.01	1.26	1.34
5	5-C	602	ANP	C6-N6	-3.01	1.26	1.34
7	1-B	600	GDP	C8-N7	3.01	1.41	1.32
7	2-B	600	GDP	C8-N7	3.01	1.41	1.32
7	3-B	600	GDP	C8-N7	3.01	1.41	1.32
7	4-B	600	GDP	C8-N7	3.01	1.41	1.32
7	5-B	600	GDP	C8-N7	3.01	1.41	1.32
5	4-C	602	ANP	C6-N6	-3.01	1.26	1.34
5	1-C	602	ANP	C6-N6	-3.00	1.26	1.34
5	3-C	602	ANP	C2-N1	2.90	1.39	1.33
5	3-C	602	ANP	PG-O1G	2.87	1.50	1.46
5	5-C	602	ANP	PG-O1G	2.87	1.50	1.46
5	5-C	602	ANP	C2-N1	2.86	1.39	1.33
5	1-C	602	ANP	C2-N1	2.85	1.39	1.33
7	1-B	600	GDP	C5-N7	-2.85	1.33	1.39
7	2-B	600	GDP	C5-N7	-2.85	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3-B	600	GDP	C5-N7	-2.85	1.33	1.39
7	4-B	600	GDP	C5-N7	-2.85	1.33	1.39
7	5-B	600	GDP	C5-N7	-2.85	1.33	1.39
5	4-C	602	ANP	PG-O1G	2.85	1.50	1.46
5	2-C	602	ANP	PG-O1G	2.84	1.50	1.46
5	4-C	602	ANP	C2-N1	2.83	1.39	1.33
5	2-C	602	ANP	C2-N1	2.81	1.38	1.33
5	1-C	602	ANP	PG-O1G	2.81	1.50	1.46
8	1-B	601	TA1	C43-C26	2.75	1.58	1.52
8	2-B	601	TA1	C43-C26	2.75	1.58	1.52
8	3-B	601	TA1	C43-C26	2.75	1.58	1.52
8	4-B	601	TA1	C43-C26	2.75	1.58	1.52
8	5-B	601	TA1	C43-C26	2.75	1.58	1.52
7	1-B	600	GDP	C5-C4	2.64	1.46	1.38
7	2-B	600	GDP	C5-C4	2.64	1.46	1.38
7	3-B	600	GDP	C5-C4	2.64	1.46	1.38
7	4-B	600	GDP	C5-C4	2.64	1.46	1.38
7	5-B	600	GDP	C5-C4	2.64	1.46	1.38
8	1-B	601	TA1	C26-C25	2.56	1.56	1.51
8	2-B	601	TA1	C26-C25	2.56	1.56	1.51
8	3-B	601	TA1	C26-C25	2.56	1.56	1.51
8	4-B	601	TA1	C26-C25	2.56	1.56	1.51
8	5-B	601	TA1	C26-C25	2.56	1.56	1.51
8	1-B	601	TA1	C01-C45	2.50	1.66	1.56
8	2-B	601	TA1	C01-C45	2.50	1.66	1.56
8	3-B	601	TA1	C01-C45	2.50	1.66	1.56
8	4-B	601	TA1	C01-C45	2.50	1.66	1.56
8	5-B	601	TA1	C01-C45	2.50	1.66	1.56
8	1-B	601	TA1	C18-C20	2.50	1.62	1.55
8	2-B	601	TA1	C18-C20	2.50	1.62	1.55
8	3-B	601	TA1	C18-C20	2.50	1.62	1.55
8	4-B	601	TA1	C18-C20	2.50	1.62	1.55
8	5-B	601	TA1	C18-C20	2.50	1.62	1.55
5	1-C	602	ANP	PG-O3G	-2.48	1.50	1.56
5	4-C	602	ANP	C5-N7	-2.48	1.34	1.39
7	1-B	600	GDP	PB-O3B	2.48	1.64	1.54
7	2-B	600	GDP	PB-O3B	2.48	1.64	1.54
7	3-B	600	GDP	PB-O3B	2.48	1.64	1.54
7	4-B	600	GDP	PB-O3B	2.48	1.64	1.54
7	5-B	600	GDP	PB-O3B	2.48	1.64	1.54
5	5-C	602	ANP	C5-N7	-2.47	1.34	1.39
8	1-B	601	TA1	C04-C03	-2.47	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2-B	601	TA1	C04-C03	-2.47	1.44	1.50
8	3-B	601	TA1	C04-C03	-2.47	1.44	1.50
8	4-B	601	TA1	C04-C03	-2.47	1.44	1.50
8	5-B	601	TA1	C04-C03	-2.47	1.44	1.50
5	3-C	602	ANP	PG-O3G	-2.47	1.50	1.56
5	2-C	602	ANP	PG-O3G	-2.46	1.50	1.56
7	1-B	600	GDP	C2-N3	-2.46	1.27	1.33
7	2-B	600	GDP	C2-N3	-2.46	1.27	1.33
7	3-B	600	GDP	C2-N3	-2.46	1.27	1.33
7	4-B	600	GDP	C2-N3	-2.46	1.27	1.33
7	5-B	600	GDP	C2-N3	-2.46	1.27	1.33
5	5-C	602	ANP	PG-O3G	-2.45	1.50	1.56
5	4-C	602	ANP	PG-O3G	-2.45	1.50	1.56
5	2-C	602	ANP	C5-N7	-2.44	1.34	1.39
5	3-C	602	ANP	C5-N7	-2.44	1.34	1.39
5	1-C	602	ANP	C5'-C4'	2.43	1.58	1.51
5	1-C	602	ANP	C5-N7	-2.43	1.34	1.39
5	3-C	602	ANP	C5'-C4'	2.40	1.58	1.51
5	4-C	602	ANP	C5'-C4'	2.39	1.58	1.51
5	5-C	602	ANP	C5'-C4'	2.37	1.58	1.51
5	2-C	602	ANP	C5'-C4'	2.37	1.58	1.51
8	1-B	601	TA1	C41-C42	2.36	1.42	1.38
8	2-B	601	TA1	C41-C42	2.36	1.42	1.38
8	3-B	601	TA1	C41-C42	2.36	1.42	1.38
8	4-B	601	TA1	C41-C42	2.36	1.42	1.38
8	5-B	601	TA1	C41-C42	2.36	1.42	1.38
8	1-B	601	TA1	C16-C15	2.32	1.56	1.52
8	2-B	601	TA1	C16-C15	2.32	1.56	1.52
8	3-B	601	TA1	C16-C15	2.32	1.56	1.52
8	4-B	601	TA1	C16-C15	2.32	1.56	1.52
8	5-B	601	TA1	C16-C15	2.32	1.56	1.52
8	1-B	601	TA1	C33-C32	2.17	1.42	1.38
8	2-B	601	TA1	C33-C32	2.17	1.42	1.38
8	3-B	601	TA1	C33-C32	2.17	1.42	1.38
8	4-B	601	TA1	C33-C32	2.17	1.42	1.38
8	5-B	601	TA1	C33-C32	2.17	1.42	1.38
8	1-B	601	TA1	O09-C21	2.16	1.49	1.44
8	2-B	601	TA1	O09-C21	2.16	1.49	1.44
8	3-B	601	TA1	O09-C21	2.16	1.49	1.44
8	4-B	601	TA1	O09-C21	2.16	1.49	1.44
8	5-B	601	TA1	O09-C21	2.16	1.49	1.44
8	1-B	601	TA1	C08-C09	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2-B	601	TA1	C08-C09	2.16	1.42	1.38
8	3-B	601	TA1	C08-C09	2.16	1.42	1.38
8	4-B	601	TA1	C08-C09	2.16	1.42	1.38
8	5-B	601	TA1	C08-C09	2.16	1.42	1.38
8	1-B	601	TA1	C37-C29	2.14	1.54	1.52
8	2-B	601	TA1	C37-C29	2.14	1.54	1.52
8	3-B	601	TA1	C37-C29	2.14	1.54	1.52
8	4-B	601	TA1	C37-C29	2.14	1.54	1.52
8	5-B	601	TA1	C37-C29	2.14	1.54	1.52
8	1-B	601	TA1	C10-C02	2.14	1.62	1.57
8	2-B	601	TA1	C10-C02	2.14	1.62	1.57
8	3-B	601	TA1	C10-C02	2.14	1.62	1.57
8	4-B	601	TA1	C10-C02	2.14	1.62	1.57
8	5-B	601	TA1	C10-C02	2.14	1.62	1.57
8	1-B	601	TA1	C07-C06	2.06	1.42	1.38
8	2-B	601	TA1	C07-C06	2.06	1.42	1.38
8	3-B	601	TA1	C07-C06	2.06	1.42	1.38
8	4-B	601	TA1	C07-C06	2.06	1.42	1.38
8	5-B	601	TA1	C07-C06	2.06	1.42	1.38
8	1-B	601	TA1	C34-C33	2.02	1.42	1.38
8	2-B	601	TA1	C34-C33	2.02	1.42	1.38
8	3-B	601	TA1	C34-C33	2.02	1.42	1.38
8	4-B	601	TA1	C34-C33	2.02	1.42	1.38
8	5-B	601	TA1	C34-C33	2.02	1.42	1.38
6	1-A	500	GTP	PB-O2B	-2.02	1.46	1.55
6	2-A	500	GTP	PB-O2B	-2.02	1.46	1.55
6	3-A	500	GTP	PB-O2B	-2.02	1.46	1.55
6	4-A	500	GTP	PB-O2B	-2.02	1.46	1.55
6	5-A	500	GTP	PB-O2B	-2.02	1.46	1.55

All (254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	1-B	600	GDP	N9-C8-N7	-10.73	93.51	113.40
7	2-B	600	GDP	N9-C8-N7	-10.73	93.51	113.40
7	3-B	600	GDP	N9-C8-N7	-10.73	93.51	113.40
7	4-B	600	GDP	N9-C8-N7	-10.73	93.51	113.40
7	5-B	600	GDP	N9-C8-N7	-10.73	93.51	113.40
7	1-B	600	GDP	C8-N7-C5	9.19	120.62	104.26
7	2-B	600	GDP	C8-N7-C5	9.19	120.62	104.26
7	3-B	600	GDP	C8-N7-C5	9.19	120.62	104.26
7	4-B	600	GDP	C8-N7-C5	9.19	120.62	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	5-B	600	GDP	C8-N7-C5	9.19	120.62	104.26
5	3-C	602	ANP	O2B-PB-O1B	8.63	128.39	109.87
5	1-C	602	ANP	O2B-PB-O1B	8.61	128.33	109.87
5	5-C	602	ANP	O2B-PB-O1B	8.60	128.33	109.87
5	4-C	602	ANP	O2B-PB-O1B	8.60	128.32	109.87
5	2-C	602	ANP	O2B-PB-O1B	8.58	128.26	109.87
7	1-B	600	GDP	C6-C5-N7	8.56	145.88	130.29
7	2-B	600	GDP	C6-C5-N7	8.56	145.88	130.29
7	3-B	600	GDP	C6-C5-N7	8.56	145.88	130.29
7	4-B	600	GDP	C6-C5-N7	8.56	145.88	130.29
7	5-B	600	GDP	C6-C5-N7	8.56	145.88	130.29
5	5-C	602	ANP	O5'-PA-O1A	-7.90	77.61	108.94
5	1-C	602	ANP	O5'-PA-O1A	-7.90	77.62	108.94
5	4-C	602	ANP	O5'-PA-O1A	-7.90	77.62	108.94
5	2-C	602	ANP	O5'-PA-O1A	-7.90	77.64	108.94
5	3-C	602	ANP	O5'-PA-O1A	-7.89	77.68	108.94
7	1-B	600	GDP	N2-C2-N3	6.30	131.96	119.67
7	2-B	600	GDP	N2-C2-N3	6.30	131.96	119.67
7	3-B	600	GDP	N2-C2-N3	6.30	131.96	119.67
7	4-B	600	GDP	N2-C2-N3	6.30	131.96	119.67
7	5-B	600	GDP	N2-C2-N3	6.30	131.96	119.67
5	2-C	602	ANP	O2B-PB-O3A	-6.25	83.79	104.64
5	1-C	602	ANP	O2B-PB-O3A	-6.24	83.81	104.64
5	3-C	602	ANP	O2B-PB-O3A	-6.23	83.84	104.64
5	5-C	602	ANP	O2B-PB-O3A	-6.23	83.85	104.64
5	4-C	602	ANP	O2B-PB-O3A	-6.22	83.88	104.64
7	1-B	600	GDP	C6-C5-C4	-6.19	109.52	118.83
7	2-B	600	GDP	C6-C5-C4	-6.19	109.52	118.83
7	3-B	600	GDP	C6-C5-C4	-6.19	109.52	118.83
7	4-B	600	GDP	C6-C5-C4	-6.19	109.52	118.83
7	5-B	600	GDP	C6-C5-C4	-6.19	109.52	118.83
5	2-C	602	ANP	O2A-PA-O5'	-6.19	79.53	107.57
5	4-C	602	ANP	O2A-PA-O5'	-6.18	79.54	107.57
5	1-C	602	ANP	O2A-PA-O5'	-6.18	79.55	107.57
5	5-C	602	ANP	O2A-PA-O5'	-6.18	79.57	107.57
5	3-C	602	ANP	O2A-PA-O5'	-6.17	79.59	107.57
5	5-C	602	ANP	O3A-PB-N3B	-6.10	89.66	106.59
5	1-C	602	ANP	O3A-PB-N3B	-6.10	89.67	106.59
5	3-C	602	ANP	O3A-PB-N3B	-6.09	89.68	106.59
5	2-C	602	ANP	O3A-PB-N3B	-6.09	89.70	106.59
5	4-C	602	ANP	O3A-PB-N3B	-6.08	89.73	106.59
7	1-B	600	GDP	C8-N9-C4	5.85	117.00	106.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	2-B	600	GDP	C8-N9-C4	5.85	117.00	106.03
7	3-B	600	GDP	C8-N9-C4	5.85	117.00	106.03
7	4-B	600	GDP	C8-N9-C4	5.85	117.00	106.03
7	5-B	600	GDP	C8-N9-C4	5.85	117.00	106.03
8	1-B	601	TA1	C06-C05-C04	-5.84	114.62	120.36
8	2-B	601	TA1	C06-C05-C04	-5.84	114.62	120.36
8	3-B	601	TA1	C06-C05-C04	-5.84	114.62	120.36
8	4-B	601	TA1	C06-C05-C04	-5.84	114.62	120.36
8	5-B	601	TA1	C06-C05-C04	-5.84	114.62	120.36
8	1-B	601	TA1	C07-C08-C09	5.79	127.38	120.24
8	2-B	601	TA1	C07-C08-C09	5.79	127.38	120.24
8	3-B	601	TA1	C07-C08-C09	5.79	127.38	120.24
8	4-B	601	TA1	C07-C08-C09	5.79	127.38	120.24
8	5-B	601	TA1	C07-C08-C09	5.79	127.38	120.24
7	1-B	600	GDP	C5-C6-N1	4.48	124.66	113.25
7	2-B	600	GDP	C5-C6-N1	4.48	124.66	113.25
7	3-B	600	GDP	C5-C6-N1	4.48	124.66	113.25
7	4-B	600	GDP	C5-C6-N1	4.48	124.66	113.25
7	5-B	600	GDP	C5-C6-N1	4.48	124.66	113.25
7	1-B	600	GDP	N2-C2-N1	-4.25	107.80	116.76
7	2-B	600	GDP	N2-C2-N1	-4.25	107.80	116.76
7	3-B	600	GDP	N2-C2-N1	-4.25	107.80	116.76
7	4-B	600	GDP	N2-C2-N1	-4.25	107.80	116.76
7	5-B	600	GDP	N2-C2-N1	-4.25	107.80	116.76
7	1-B	600	GDP	C2-N3-C4	4.12	119.40	112.30
7	2-B	600	GDP	C2-N3-C4	4.12	119.40	112.30
7	3-B	600	GDP	C2-N3-C4	4.12	119.40	112.30
7	4-B	600	GDP	C2-N3-C4	4.12	119.40	112.30
7	5-B	600	GDP	C2-N3-C4	4.12	119.40	112.30
8	1-B	601	TA1	C05-C04-C03	-4.02	111.53	120.40
8	2-B	601	TA1	C05-C04-C03	-4.02	111.53	120.40
8	3-B	601	TA1	C05-C04-C03	-4.02	111.53	120.40
8	4-B	601	TA1	C05-C04-C03	-4.02	111.53	120.40
8	5-B	601	TA1	C05-C04-C03	-4.02	111.53	120.40
7	1-B	600	GDP	O6-C6-C5	-3.96	116.09	126.53
7	2-B	600	GDP	O6-C6-C5	-3.96	116.09	126.53
7	3-B	600	GDP	O6-C6-C5	-3.96	116.09	126.53
7	4-B	600	GDP	O6-C6-C5	-3.96	116.09	126.53
7	5-B	600	GDP	O6-C6-C5	-3.96	116.09	126.53
7	1-B	600	GDP	C4-C5-N7	-3.83	104.61	110.67
7	2-B	600	GDP	C4-C5-N7	-3.83	104.61	110.67
7	3-B	600	GDP	C4-C5-N7	-3.83	104.61	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	4-B	600	GDP	C4-C5-N7	-3.83	104.61	110.67
7	5-B	600	GDP	C4-C5-N7	-3.83	104.61	110.67
7	1-B	600	GDP	C2-N1-C6	-3.78	118.26	125.11
7	2-B	600	GDP	C2-N1-C6	-3.78	118.26	125.11
7	3-B	600	GDP	C2-N1-C6	-3.78	118.26	125.11
7	4-B	600	GDP	C2-N1-C6	-3.78	118.26	125.11
7	5-B	600	GDP	C2-N1-C6	-3.78	118.26	125.11
5	4-C	602	ANP	N3-C2-N1	-3.64	123.08	128.58
5	2-C	602	ANP	N3-C2-N1	-3.61	123.12	128.58
5	5-C	602	ANP	N3-C2-N1	-3.60	123.14	128.58
8	1-B	601	TA1	C09-C04-C03	3.60	128.33	120.40
8	2-B	601	TA1	C09-C04-C03	3.60	128.33	120.40
8	3-B	601	TA1	C09-C04-C03	3.60	128.33	120.40
8	4-B	601	TA1	C09-C04-C03	3.60	128.33	120.40
8	5-B	601	TA1	C09-C04-C03	3.60	128.33	120.40
5	1-C	602	ANP	N3-C2-N1	-3.59	123.15	128.58
5	3-C	602	ANP	N3-C2-N1	-3.57	123.17	128.58
5	4-C	602	ANP	O2A-PA-O3A	3.53	116.82	107.27
5	3-C	602	ANP	O2A-PA-O3A	3.53	116.81	107.27
5	1-C	602	ANP	O2A-PA-O3A	3.52	116.80	107.27
5	2-C	602	ANP	O2A-PA-O3A	3.52	116.80	107.27
5	5-C	602	ANP	O2A-PA-O3A	3.51	116.77	107.27
7	1-B	600	GDP	C2'-C3'-C4'	3.42	109.22	102.61
7	2-B	600	GDP	C2'-C3'-C4'	3.42	109.22	102.61
7	3-B	600	GDP	C2'-C3'-C4'	3.42	109.22	102.61
7	4-B	600	GDP	C2'-C3'-C4'	3.42	109.22	102.61
7	5-B	600	GDP	C2'-C3'-C4'	3.42	109.22	102.61
5	2-C	602	ANP	C2-N1-C6	3.37	124.26	118.73
5	4-C	602	ANP	C2-N1-C6	3.37	124.26	118.73
5	1-C	602	ANP	C2-N1-C6	3.34	124.22	118.73
5	5-C	602	ANP	C2-N1-C6	3.34	124.21	118.73
5	3-C	602	ANP	C2-N1-C6	3.33	124.21	118.73
8	1-B	601	TA1	C17-C18-C20	3.23	109.82	102.58
8	2-B	601	TA1	C17-C18-C20	3.23	109.82	102.58
8	3-B	601	TA1	C17-C18-C20	3.23	109.82	102.58
8	4-B	601	TA1	C17-C18-C20	3.23	109.82	102.58
8	5-B	601	TA1	C17-C18-C20	3.23	109.82	102.58
8	1-B	601	TA1	O04-C11-C14	-3.04	101.69	108.13
8	2-B	601	TA1	O04-C11-C14	-3.04	101.69	108.13
8	3-B	601	TA1	O04-C11-C14	-3.04	101.69	108.13
8	4-B	601	TA1	O04-C11-C14	-3.04	101.69	108.13
8	5-B	601	TA1	O04-C11-C14	-3.04	101.69	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1-B	601	TA1	C45-C01-C02	3.02	115.25	111.93
8	2-B	601	TA1	C45-C01-C02	3.02	115.25	111.93
8	3-B	601	TA1	C45-C01-C02	3.02	115.25	111.93
8	4-B	601	TA1	C45-C01-C02	3.02	115.25	111.93
8	5-B	601	TA1	C45-C01-C02	3.02	115.25	111.93
5	2-C	602	ANP	O4'-C4'-C3'	-2.99	99.21	105.15
5	5-C	602	ANP	O4'-C4'-C3'	-2.99	99.22	105.15
5	1-C	602	ANP	O4'-C4'-C3'	-2.99	99.22	105.15
5	3-C	602	ANP	O4'-C4'-C3'	-2.97	99.25	105.15
5	4-C	602	ANP	O4'-C4'-C3'	-2.96	99.27	105.15
7	1-B	600	GDP	C1'-N9-C8	-2.67	119.14	126.73
7	2-B	600	GDP	C1'-N9-C8	-2.67	119.14	126.73
7	3-B	600	GDP	C1'-N9-C8	-2.67	119.14	126.73
7	4-B	600	GDP	C1'-N9-C8	-2.67	119.14	126.73
7	5-B	600	GDP	C1'-N9-C8	-2.67	119.14	126.73
8	1-B	601	TA1	O01-C01-C43	2.47	113.34	107.04
8	2-B	601	TA1	O01-C01-C43	2.47	113.34	107.04
8	3-B	601	TA1	O01-C01-C43	2.47	113.34	107.04
8	4-B	601	TA1	O01-C01-C43	2.47	113.34	107.04
8	5-B	601	TA1	O01-C01-C43	2.47	113.34	107.04
6	1-A	500	GTP	O3A-PB-O1B	-2.46	103.29	110.70
6	2-A	500	GTP	O3A-PB-O1B	-2.46	103.29	110.70
6	3-A	500	GTP	O3A-PB-O1B	-2.46	103.29	110.70
6	4-A	500	GTP	O3A-PB-O1B	-2.46	103.29	110.70
6	5-A	500	GTP	O3A-PB-O1B	-2.46	103.29	110.70
5	3-C	602	ANP	O2A-PA-O1A	2.46	123.91	112.44
5	5-C	602	ANP	O2A-PA-O1A	2.45	123.86	112.44
5	1-C	602	ANP	O2A-PA-O1A	2.45	123.83	112.44
5	2-C	602	ANP	O2A-PA-O1A	2.44	123.81	112.44
5	4-C	602	ANP	O2A-PA-O1A	2.44	123.80	112.44
5	2-C	602	ANP	O1B-PB-N3B	2.39	115.29	111.77
5	4-C	602	ANP	O5'-C5'-C4'	-2.39	100.86	108.99
5	3-C	602	ANP	O1B-PB-N3B	2.39	115.29	111.77
5	2-C	602	ANP	O5'-C5'-C4'	-2.38	100.89	108.99
5	5-C	602	ANP	O1B-PB-N3B	2.38	115.27	111.77
8	1-B	601	TA1	C08-C09-C04	-2.38	118.03	120.36
8	2-B	601	TA1	C08-C09-C04	-2.38	118.03	120.36
8	3-B	601	TA1	C08-C09-C04	-2.38	118.03	120.36
8	4-B	601	TA1	C08-C09-C04	-2.38	118.03	120.36
8	5-B	601	TA1	C08-C09-C04	-2.38	118.03	120.36
5	5-C	602	ANP	O5'-C5'-C4'	-2.38	100.90	108.99
5	1-C	602	ANP	O5'-C5'-C4'	-2.37	100.91	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	3-C	602	ANP	O5'-C5'-C4'	-2.37	100.92	108.99
5	1-C	602	ANP	O1B-PB-N3B	2.36	115.25	111.77
5	4-C	602	ANP	O1B-PB-N3B	2.35	115.23	111.77
7	1-B	600	GDP	O2'-C2'-C3'	2.30	119.18	111.82
7	2-B	600	GDP	O2'-C2'-C3'	2.30	119.18	111.82
7	3-B	600	GDP	O2'-C2'-C3'	2.30	119.18	111.82
7	4-B	600	GDP	O2'-C2'-C3'	2.30	119.18	111.82
7	5-B	600	GDP	O2'-C2'-C3'	2.30	119.18	111.82
8	1-B	601	TA1	C14-C11-C15	-2.27	83.04	85.38
8	2-B	601	TA1	C14-C11-C15	-2.27	83.04	85.38
8	3-B	601	TA1	C14-C11-C15	-2.27	83.04	85.38
8	4-B	601	TA1	C14-C11-C15	-2.27	83.04	85.38
8	5-B	601	TA1	C14-C11-C15	-2.27	83.04	85.38
8	1-B	601	TA1	C10-C18-C17	-2.22	102.33	106.55
8	2-B	601	TA1	C10-C18-C17	-2.22	102.33	106.55
8	3-B	601	TA1	C10-C18-C17	-2.22	102.33	106.55
8	4-B	601	TA1	C10-C18-C17	-2.22	102.33	106.55
8	5-B	601	TA1	C10-C18-C17	-2.22	102.33	106.55
8	1-B	601	TA1	O06-C15-C11	2.22	93.01	90.58
8	2-B	601	TA1	O06-C15-C11	2.22	93.01	90.58
8	3-B	601	TA1	O06-C15-C11	2.22	93.01	90.58
8	4-B	601	TA1	O06-C15-C11	2.22	93.01	90.58
8	5-B	601	TA1	O06-C15-C11	2.22	93.01	90.58
5	4-C	602	ANP	O3G-PG-O1G	-2.21	107.92	113.45
6	1-A	500	GTP	O2B-PB-O3A	2.20	113.21	107.27
6	2-A	500	GTP	O2B-PB-O3A	2.20	113.21	107.27
6	3-A	500	GTP	O2B-PB-O3A	2.20	113.21	107.27
6	4-A	500	GTP	O2B-PB-O3A	2.20	113.21	107.27
6	5-A	500	GTP	O2B-PB-O3A	2.20	113.21	107.27
5	3-C	602	ANP	O2G-PG-O1G	-2.18	107.97	113.45
5	3-C	602	ANP	O3G-PG-O1G	-2.18	107.98	113.45
5	1-C	602	ANP	O3G-PG-O1G	-2.18	107.98	113.45
5	2-C	602	ANP	O3G-PG-O1G	-2.18	107.99	113.45
5	5-C	602	ANP	O3G-PG-O1G	-2.18	107.99	113.45
5	2-C	602	ANP	O2G-PG-O1G	-2.17	108.01	113.45
5	5-C	602	ANP	O2G-PG-O1G	-2.17	108.01	113.45
5	4-C	602	ANP	O2G-PG-O1G	-2.17	108.02	113.45
5	1-C	602	ANP	O2G-PG-O1G	-2.16	108.03	113.45
6	1-A	500	GTP	O5'-C5'-C4'	2.13	116.24	108.99
6	2-A	500	GTP	O5'-C5'-C4'	2.13	116.24	108.99
6	3-A	500	GTP	O5'-C5'-C4'	2.13	116.24	108.99
6	4-A	500	GTP	O5'-C5'-C4'	2.13	116.24	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5-A	500	GTP	O5'-C5'-C4'	2.13	116.24	108.99
7	1-B	600	GDP	C4'-O4'-C1'	2.06	114.02	109.47
7	2-B	600	GDP	C4'-O4'-C1'	2.06	114.02	109.47
7	3-B	600	GDP	C4'-O4'-C1'	2.06	114.02	109.47
7	4-B	600	GDP	C4'-O4'-C1'	2.06	114.02	109.47
7	5-B	600	GDP	C4'-O4'-C1'	2.06	114.02	109.47
5	2-C	602	ANP	C6-C5-C4	2.05	119.98	117.18
5	1-C	602	ANP	C5-N7-C8	2.05	106.67	103.45
5	2-C	602	ANP	C5-N7-C8	2.04	106.66	103.45
5	2-C	602	ANP	C5-C6-N1	-2.04	112.34	117.51
5	4-C	602	ANP	C5-N7-C8	2.03	106.65	103.45
5	3-C	602	ANP	C5-N7-C8	2.03	106.64	103.45
6	1-A	500	GTP	O3G-PG-O3B	2.03	111.43	104.64
6	2-A	500	GTP	O3G-PG-O3B	2.03	111.43	104.64
6	3-A	500	GTP	O3G-PG-O3B	2.03	111.43	104.64
6	4-A	500	GTP	O3G-PG-O3B	2.03	111.43	104.64
6	5-A	500	GTP	O3G-PG-O3B	2.03	111.43	104.64
5	5-C	602	ANP	C6-C5-C4	2.02	119.94	117.18
5	5-C	602	ANP	C5-C6-N1	-2.02	112.38	117.51
5	3-C	602	ANP	C6-C5-C4	2.02	119.93	117.18
5	3-C	602	ANP	C5-C6-N1	-2.02	112.39	117.51
8	1-B	601	TA1	C21-O09-C22	2.02	120.11	115.95
8	2-B	601	TA1	C21-O09-C22	2.02	120.11	115.95
8	3-B	601	TA1	C21-O09-C22	2.02	120.11	115.95
8	4-B	601	TA1	C21-O09-C22	2.02	120.11	115.95
8	5-B	601	TA1	C21-O09-C22	2.02	120.11	115.95
5	5-C	602	ANP	C5-N7-C8	2.01	106.61	103.45
5	4-C	602	ANP	C5-C6-N1	-2.01	112.41	117.51
5	1-C	602	ANP	C6-C5-C4	2.01	119.92	117.18
5	4-C	602	ANP	C6-C5-C4	2.00	119.91	117.18
8	1-B	601	TA1	O11-C27-O12	2.00	127.56	123.95
8	2-B	601	TA1	O11-C27-O12	2.00	127.56	123.95
8	3-B	601	TA1	O11-C27-O12	2.00	127.56	123.95
8	4-B	601	TA1	O11-C27-O12	2.00	127.56	123.95
8	5-B	601	TA1	O11-C27-O12	2.00	127.56	123.95

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1-C	602	ANP	PG-N3B-PB-O1B
5	1-C	602	ANP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
5	1-C	602	ANP	C5'-O5'-PA-O1A
5	1-C	602	ANP	C5'-O5'-PA-O2A
5	1-C	602	ANP	C5'-O5'-PA-O3A
5	2-C	602	ANP	PG-N3B-PB-O1B
5	2-C	602	ANP	PA-O3A-PB-O2B
5	2-C	602	ANP	C5'-O5'-PA-O1A
5	2-C	602	ANP	C5'-O5'-PA-O2A
5	2-C	602	ANP	C5'-O5'-PA-O3A
5	3-C	602	ANP	PG-N3B-PB-O1B
5	3-C	602	ANP	PA-O3A-PB-O2B
5	3-C	602	ANP	C5'-O5'-PA-O1A
5	3-C	602	ANP	C5'-O5'-PA-O2A
5	3-C	602	ANP	C5'-O5'-PA-O3A
5	4-C	602	ANP	PG-N3B-PB-O1B
5	4-C	602	ANP	PA-O3A-PB-O2B
5	4-C	602	ANP	C5'-O5'-PA-O1A
5	4-C	602	ANP	C5'-O5'-PA-O2A
5	4-C	602	ANP	C5'-O5'-PA-O3A
5	5-C	602	ANP	PG-N3B-PB-O1B
5	5-C	602	ANP	PA-O3A-PB-O2B
5	5-C	602	ANP	C5'-O5'-PA-O1A
5	5-C	602	ANP	C5'-O5'-PA-O2A
5	5-C	602	ANP	C5'-O5'-PA-O3A
7	1-B	600	GDP	PA-O3A-PB-O2B
7	1-B	600	GDP	C5'-O5'-PA-O3A
7	1-B	600	GDP	C5'-O5'-PA-O1A
7	2-B	600	GDP	PA-O3A-PB-O2B
7	2-B	600	GDP	C5'-O5'-PA-O3A
7	2-B	600	GDP	C5'-O5'-PA-O1A
7	3-B	600	GDP	PA-O3A-PB-O2B
7	3-B	600	GDP	C5'-O5'-PA-O3A
7	3-B	600	GDP	C5'-O5'-PA-O1A
7	4-B	600	GDP	PA-O3A-PB-O2B
7	4-B	600	GDP	C5'-O5'-PA-O3A
7	4-B	600	GDP	C5'-O5'-PA-O1A
7	5-B	600	GDP	PA-O3A-PB-O2B
7	5-B	600	GDP	C5'-O5'-PA-O3A
7	5-B	600	GDP	C5'-O5'-PA-O1A
8	1-B	601	TA1	O02-C03-C04-C05
8	2-B	601	TA1	O02-C03-C04-C05
8	3-B	601	TA1	O02-C03-C04-C05
8	4-B	601	TA1	O02-C03-C04-C05

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Mol	Chain	Res	Type	Atoms
8	5-B	601	TA1	O02-C03-C04-C05
8	1-B	601	TA1	O02-C03-C04-C09
8	2-B	601	TA1	O02-C03-C04-C09
8	3-B	601	TA1	O02-C03-C04-C09
8	4-B	601	TA1	O02-C03-C04-C09
8	5-B	601	TA1	O02-C03-C04-C09
5	1-C	602	ANP	C3'-C4'-C5'-O5'
5	2-C	602	ANP	C3'-C4'-C5'-O5'
5	3-C	602	ANP	C3'-C4'-C5'-O5'
5	4-C	602	ANP	C3'-C4'-C5'-O5'
5	5-C	602	ANP	C3'-C4'-C5'-O5'
8	1-B	601	TA1	O03-C03-C04-C09
8	2-B	601	TA1	O03-C03-C04-C09
8	3-B	601	TA1	O03-C03-C04-C09
8	4-B	601	TA1	O03-C03-C04-C09
8	5-B	601	TA1	O03-C03-C04-C09
8	1-B	601	TA1	O03-C03-C04-C05
8	2-B	601	TA1	O03-C03-C04-C05
8	3-B	601	TA1	O03-C03-C04-C05
8	4-B	601	TA1	O03-C03-C04-C05
8	5-B	601	TA1	O03-C03-C04-C05
8	1-B	601	TA1	N01-C30-C31-C36
8	2-B	601	TA1	N01-C30-C31-C36
8	3-B	601	TA1	N01-C30-C31-C36
8	4-B	601	TA1	N01-C30-C31-C36
8	5-B	601	TA1	N01-C30-C31-C36
5	1-C	602	ANP	O4'-C4'-C5'-O5'
5	2-C	602	ANP	O4'-C4'-C5'-O5'
5	3-C	602	ANP	O4'-C4'-C5'-O5'
5	4-C	602	ANP	O4'-C4'-C5'-O5'
5	5-C	602	ANP	O4'-C4'-C5'-O5'
8	1-B	601	TA1	O14-C30-C31-C36
8	2-B	601	TA1	O14-C30-C31-C36
8	3-B	601	TA1	O14-C30-C31-C36
8	4-B	601	TA1	O14-C30-C31-C36
8	5-B	601	TA1	O14-C30-C31-C36
8	1-B	601	TA1	N01-C30-C31-C32
8	2-B	601	TA1	N01-C30-C31-C32
8	3-B	601	TA1	N01-C30-C31-C32
8	4-B	601	TA1	N01-C30-C31-C32
8	5-B	601	TA1	N01-C30-C31-C32
8	1-B	601	TA1	O14-C30-C31-C32

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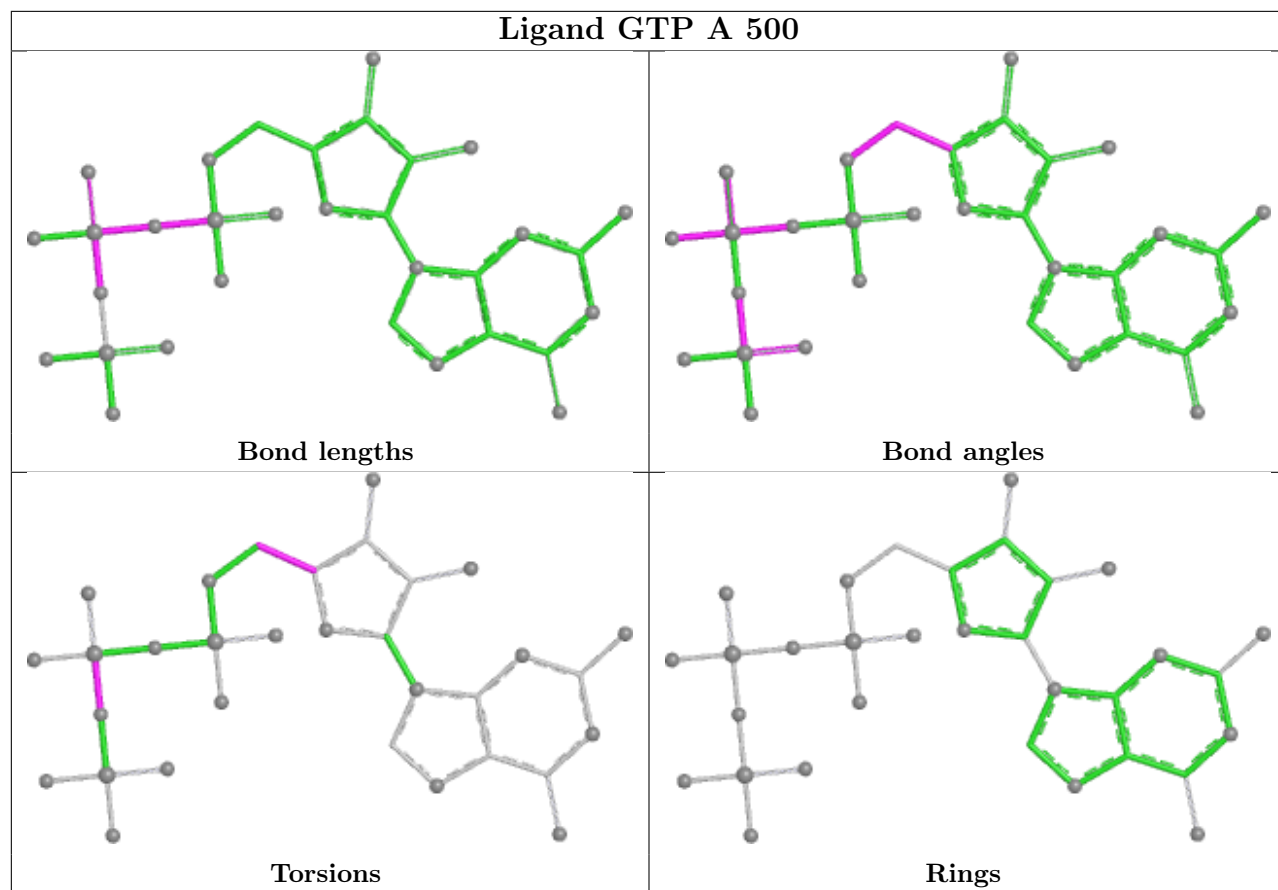
Mol	Chain	Res	Type	Atoms
8	2-B	601	TA1	O14-C30-C31-C32
8	3-B	601	TA1	O14-C30-C31-C32
8	4-B	601	TA1	O14-C30-C31-C32
8	5-B	601	TA1	O14-C30-C31-C32
6	1-A	500	GTP	C3'-C4'-C5'-O5'
6	2-A	500	GTP	C3'-C4'-C5'-O5'
6	3-A	500	GTP	C3'-C4'-C5'-O5'
6	4-A	500	GTP	C3'-C4'-C5'-O5'
6	5-A	500	GTP	C3'-C4'-C5'-O5'
6	1-A	500	GTP	O4'-C4'-C5'-O5'
6	2-A	500	GTP	O4'-C4'-C5'-O5'
6	3-A	500	GTP	O4'-C4'-C5'-O5'
6	4-A	500	GTP	O4'-C4'-C5'-O5'
6	5-A	500	GTP	O4'-C4'-C5'-O5'
7	1-B	600	GDP	PA-O3A-PB-O3B
7	2-B	600	GDP	PA-O3A-PB-O3B
7	3-B	600	GDP	PA-O3A-PB-O3B
7	4-B	600	GDP	PA-O3A-PB-O3B
7	5-B	600	GDP	PA-O3A-PB-O3B
5	1-C	602	ANP	PB-O3A-PA-O1A
5	2-C	602	ANP	PB-O3A-PA-O1A
5	3-C	602	ANP	PB-O3A-PA-O1A
5	4-C	602	ANP	PB-O3A-PA-O1A
5	5-C	602	ANP	PB-O3A-PA-O1A
6	1-A	500	GTP	PG-O3B-PB-O1B
6	2-A	500	GTP	PG-O3B-PB-O1B
6	3-A	500	GTP	PG-O3B-PB-O1B
6	4-A	500	GTP	PG-O3B-PB-O1B
6	5-A	500	GTP	PG-O3B-PB-O1B
8	1-B	601	TA1	C15-C11-O04-C12
8	2-B	601	TA1	C15-C11-O04-C12
8	3-B	601	TA1	C15-C11-O04-C12
8	4-B	601	TA1	C15-C11-O04-C12
8	5-B	601	TA1	C15-C11-O04-C12
5	1-C	602	ANP	PA-O3A-PB-O1B
5	2-C	602	ANP	PA-O3A-PB-O1B
5	3-C	602	ANP	PA-O3A-PB-O1B
5	4-C	602	ANP	PA-O3A-PB-O1B
5	5-C	602	ANP	PA-O3A-PB-O1B

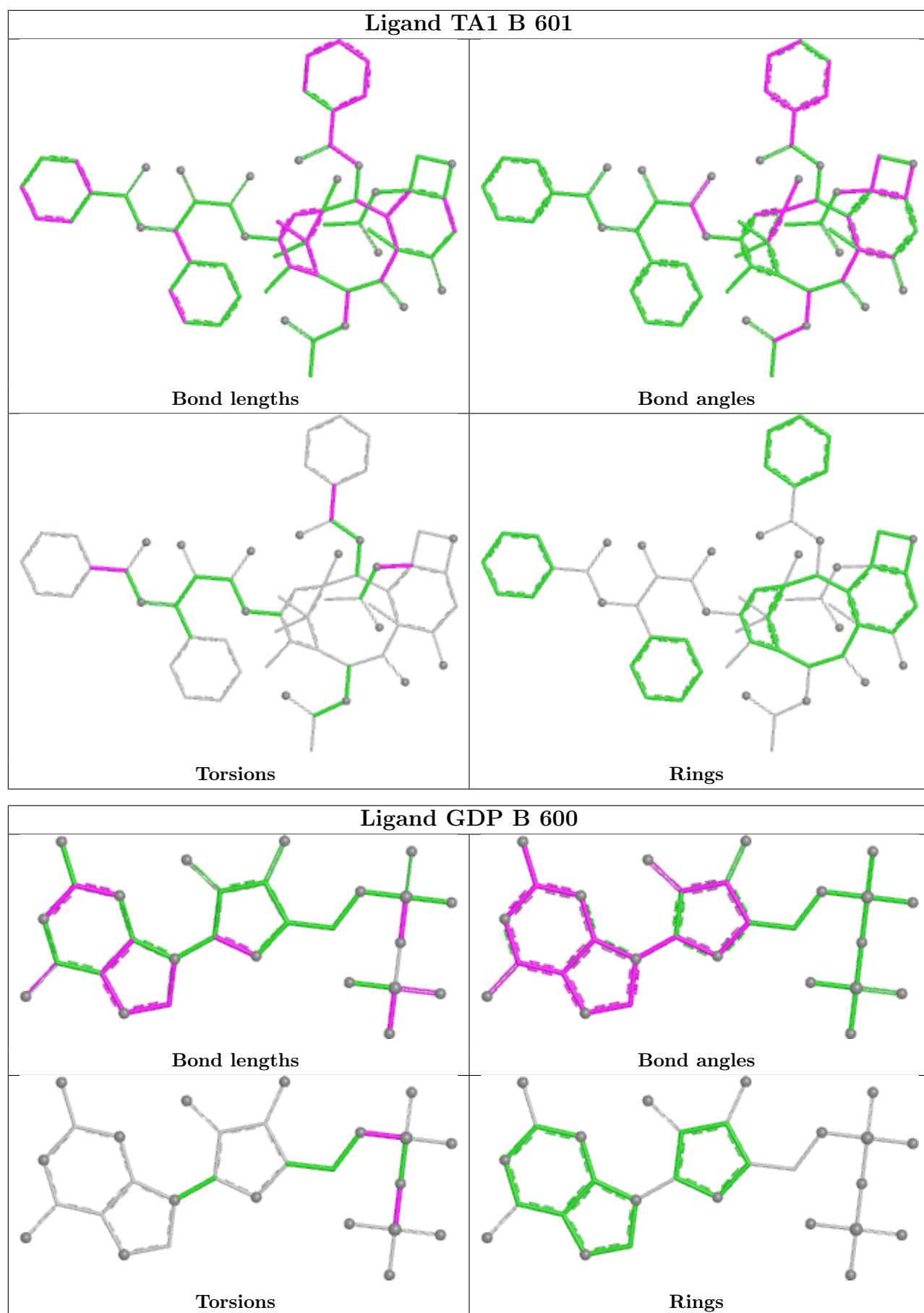
There are no ring outliers.

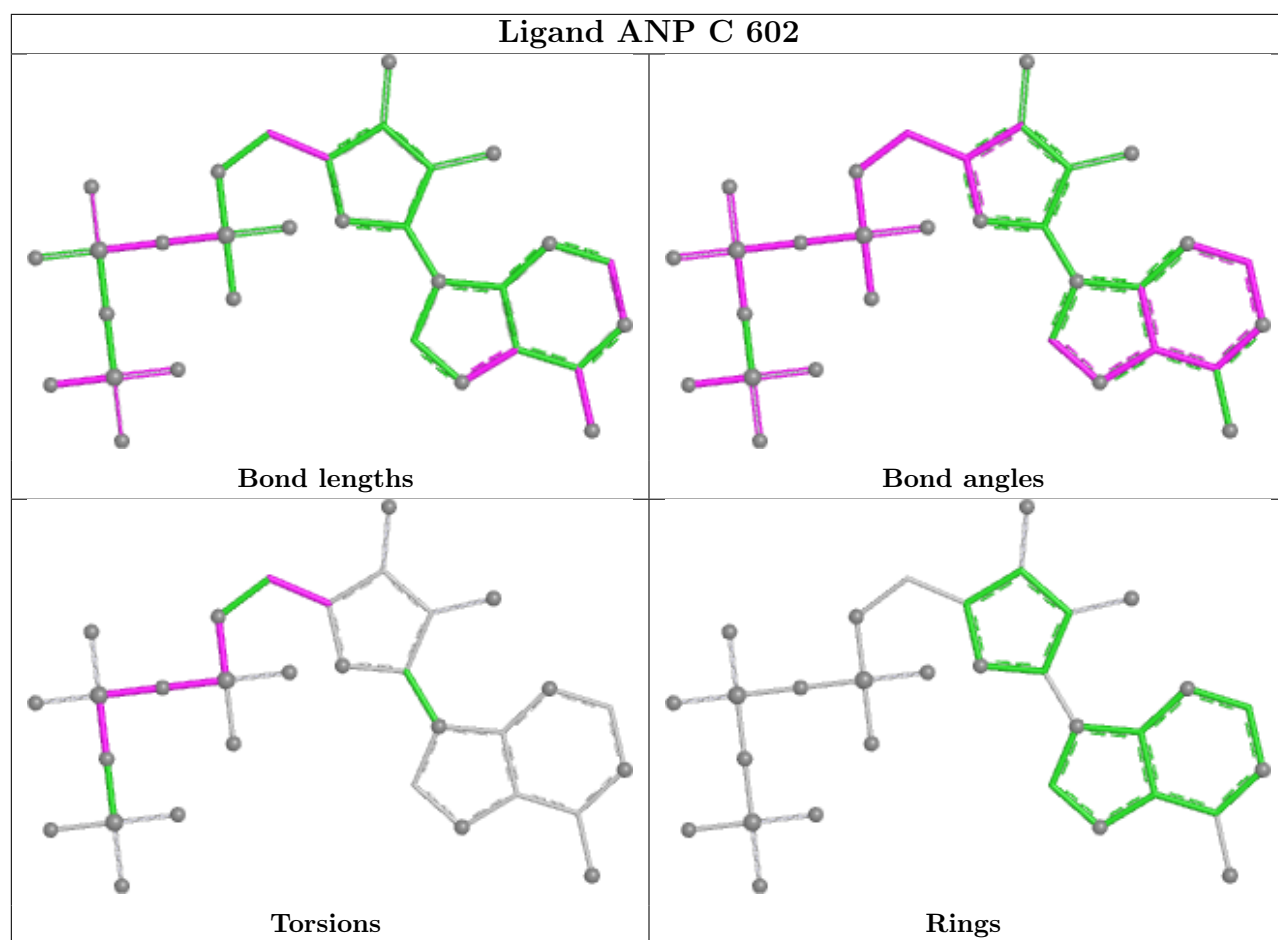
20 monomers are involved in 260 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	4-B	600	GDP	8	0
8	3-B	601	TA1	14	0
7	3-B	600	GDP	8	0
6	1-A	500	GTP	28	0
8	2-B	601	TA1	14	0
5	3-C	602	ANP	2	0
6	2-A	500	GTP	28	0
8	4-B	601	TA1	14	0
6	5-A	500	GTP	28	0
8	1-B	601	TA1	14	0
7	5-B	600	GDP	8	0
6	3-A	500	GTP	28	0
5	2-C	602	ANP	2	0
8	5-B	601	TA1	14	0
5	4-C	602	ANP	2	0
6	4-A	500	GTP	28	0
7	1-B	600	GDP	8	0
5	1-C	602	ANP	2	0
7	2-B	600	GDP	8	0
5	5-C	602	ANP	2	0

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







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.

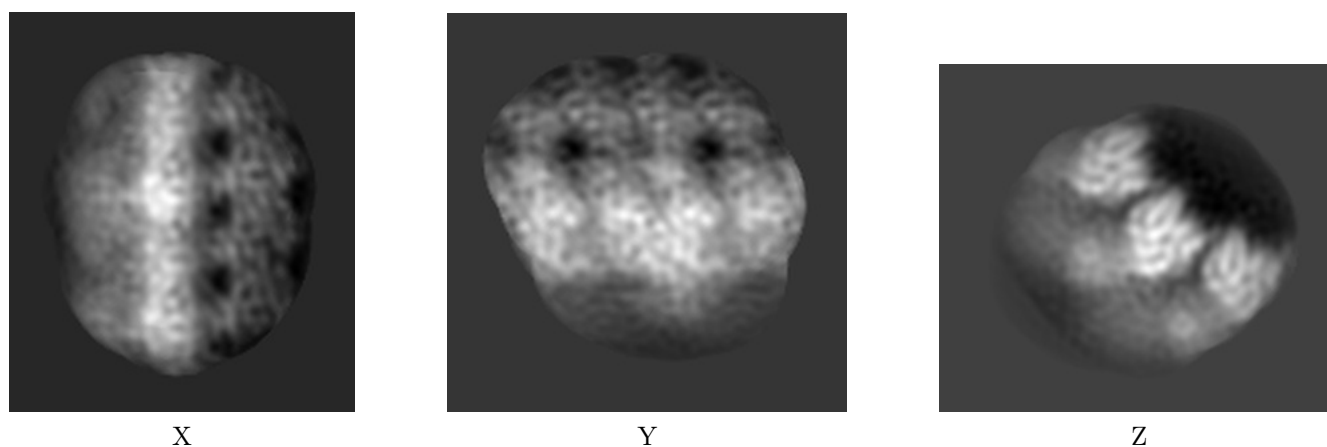
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3623. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

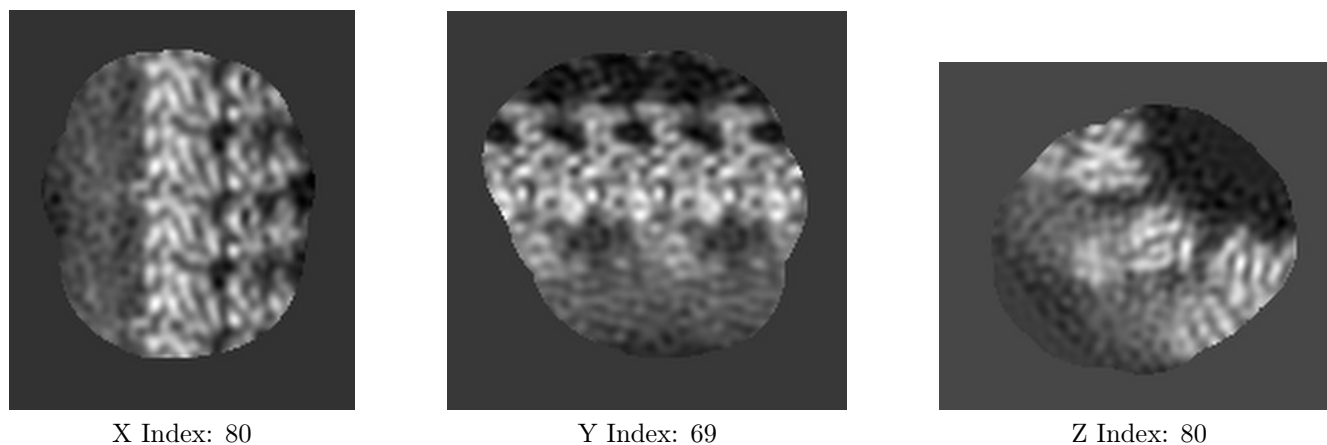
6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

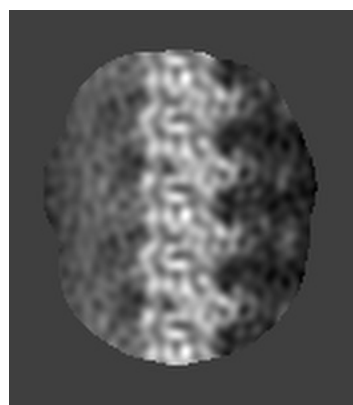
6.2.1 Primary map



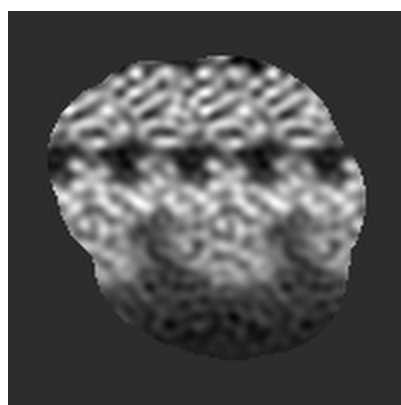
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

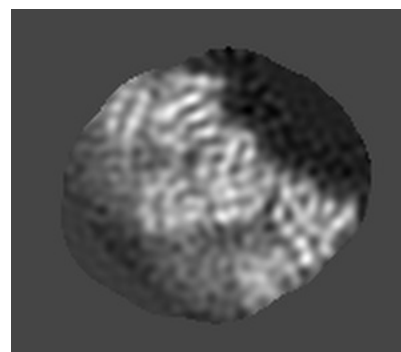
6.3.1 Primary map



X Index: 85



Y Index: 57

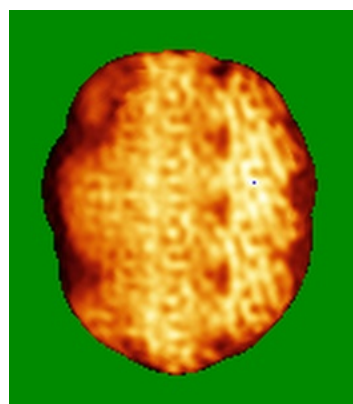


Z Index: 92

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

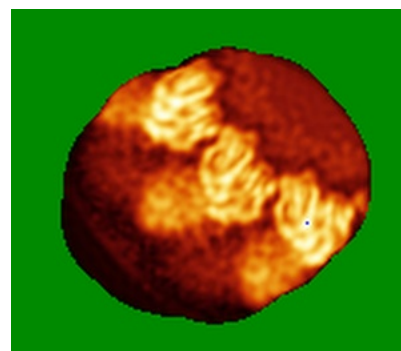
6.4.1 Primary map



X



Y

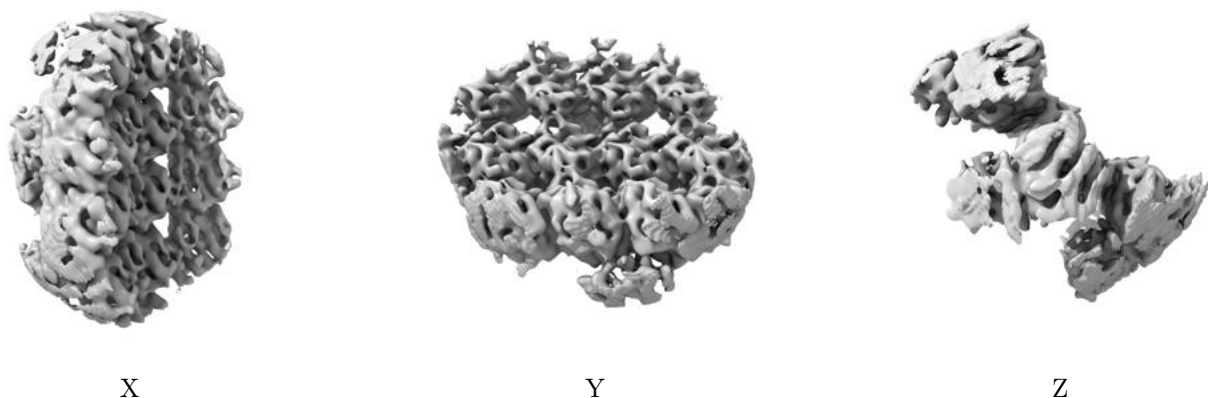


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0322. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

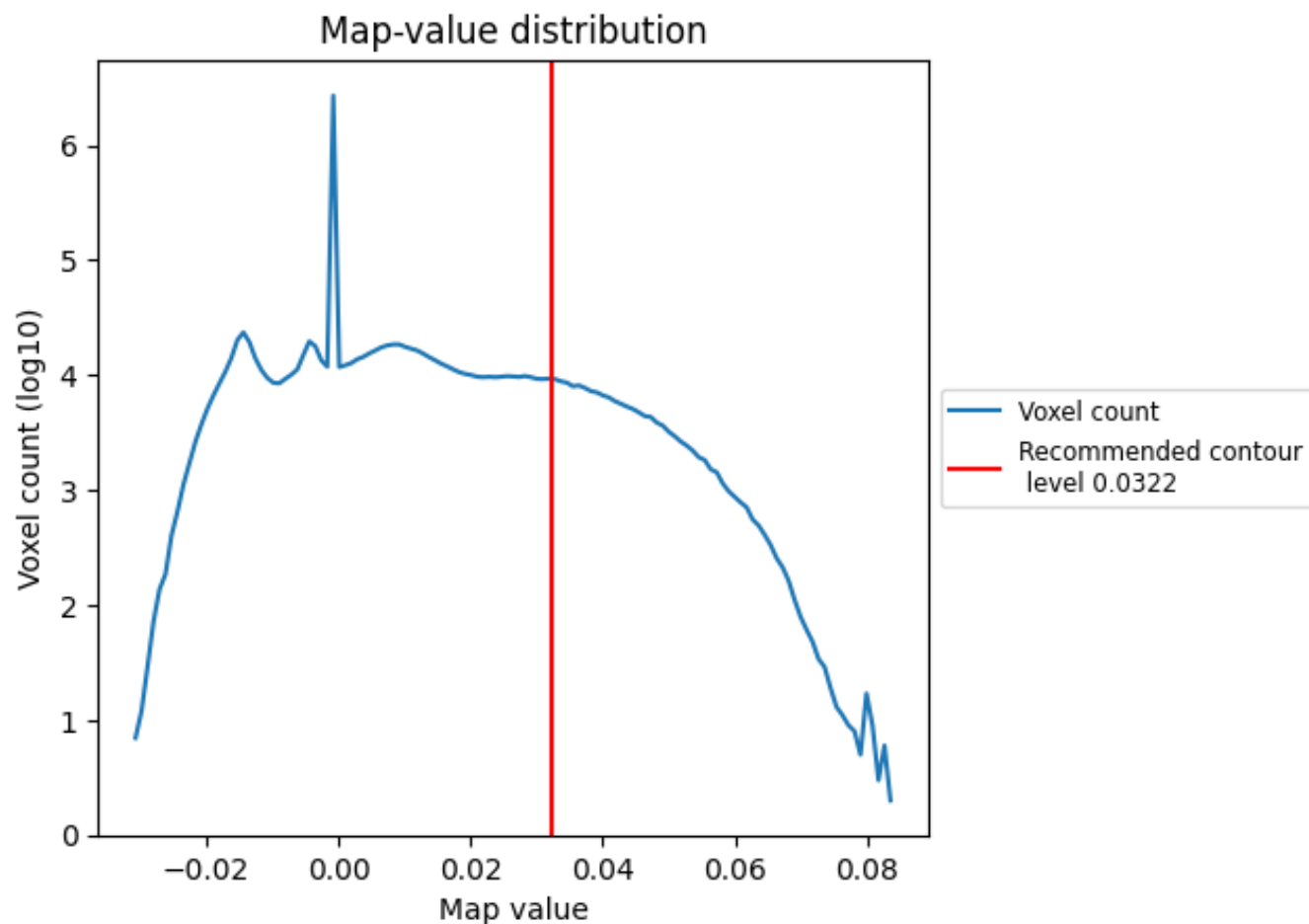
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

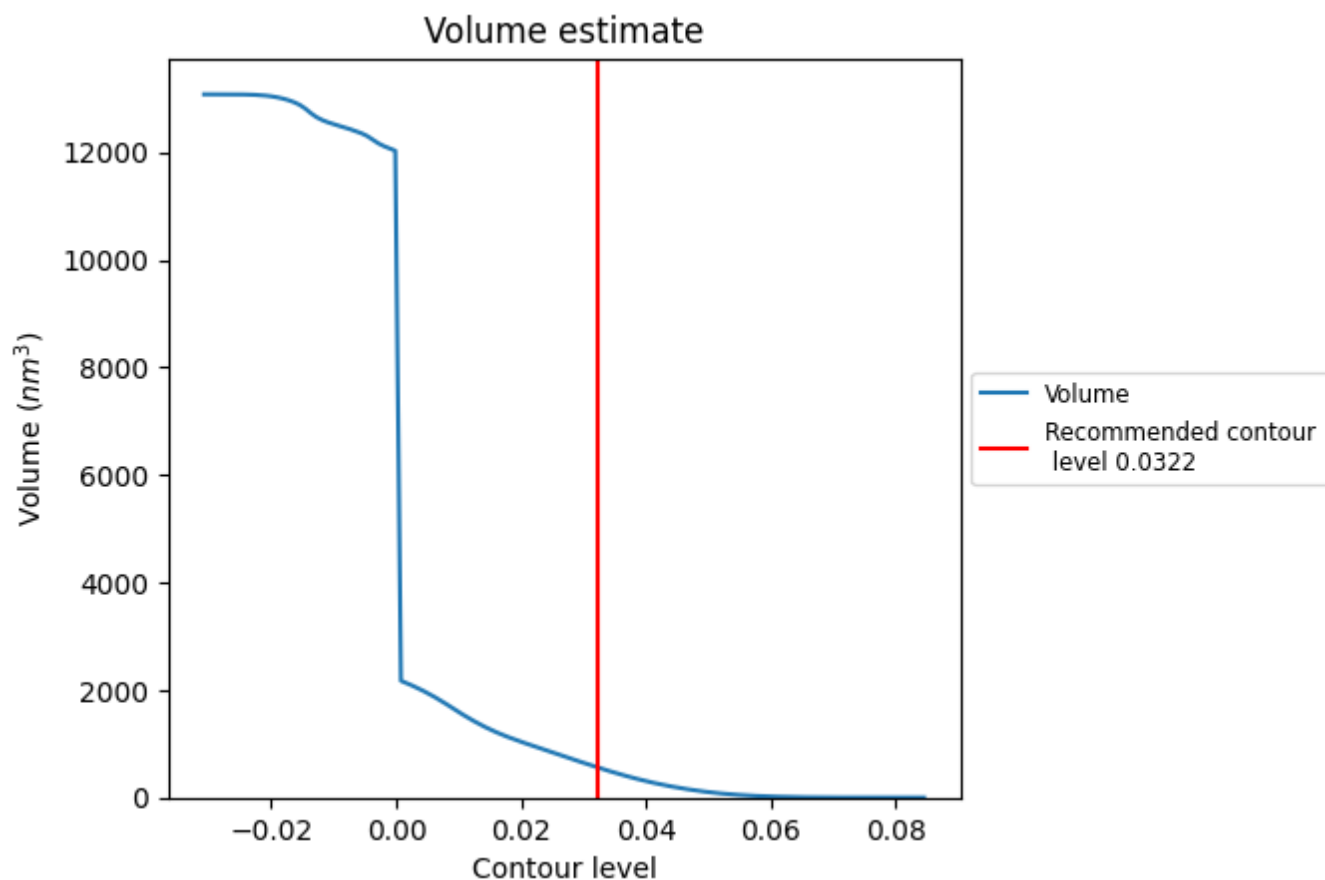
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 563 nm³; this corresponds to an approximate mass of 509 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

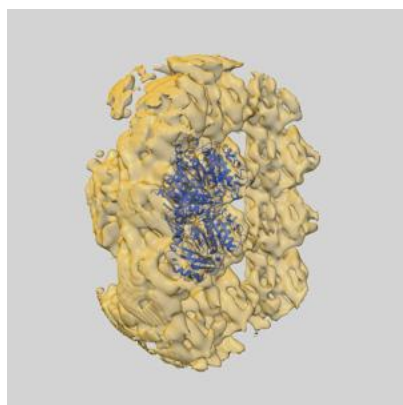
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

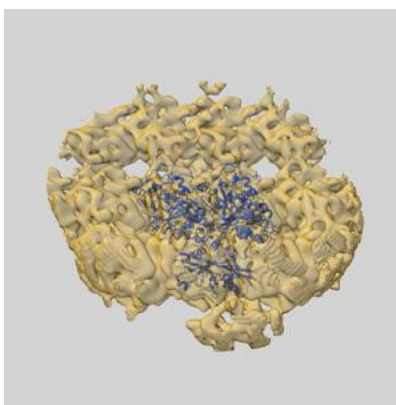
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3623 and PDB model 5ND7. Per-residue inclusion information can be found in section [3](#) on page [9](#).

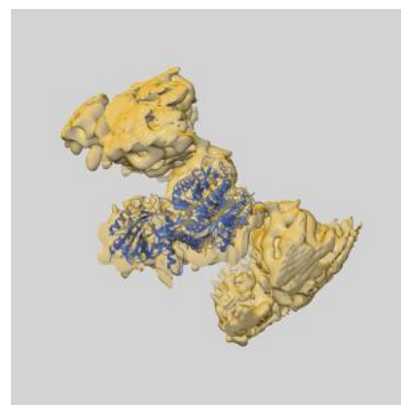
9.1 Map-model overlay [i](#)



X



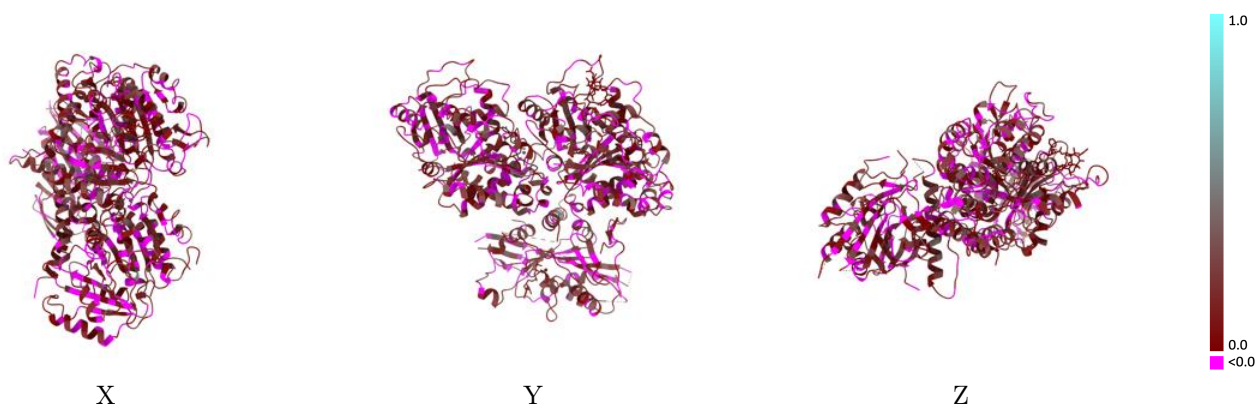
Y



Z

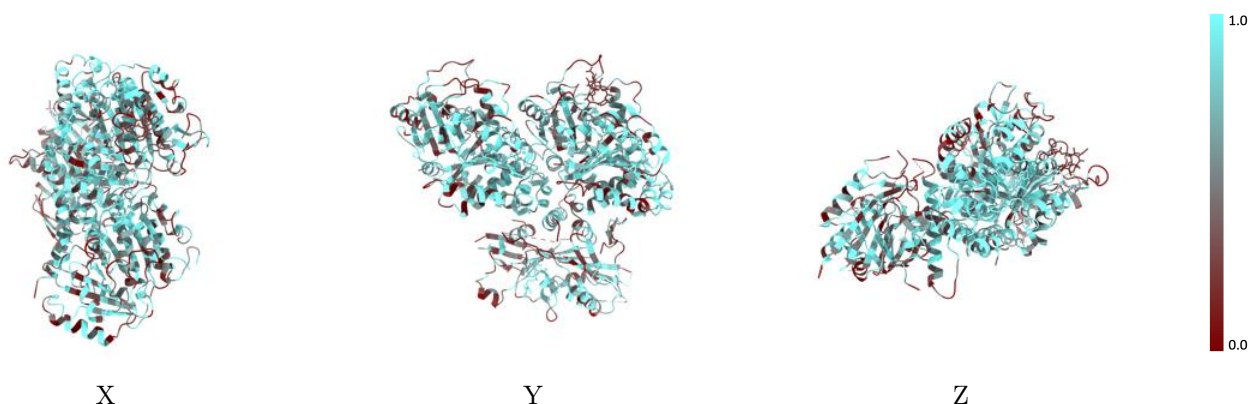
The images above show the 3D surface view of the map at the recommended contour level 0.0322 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



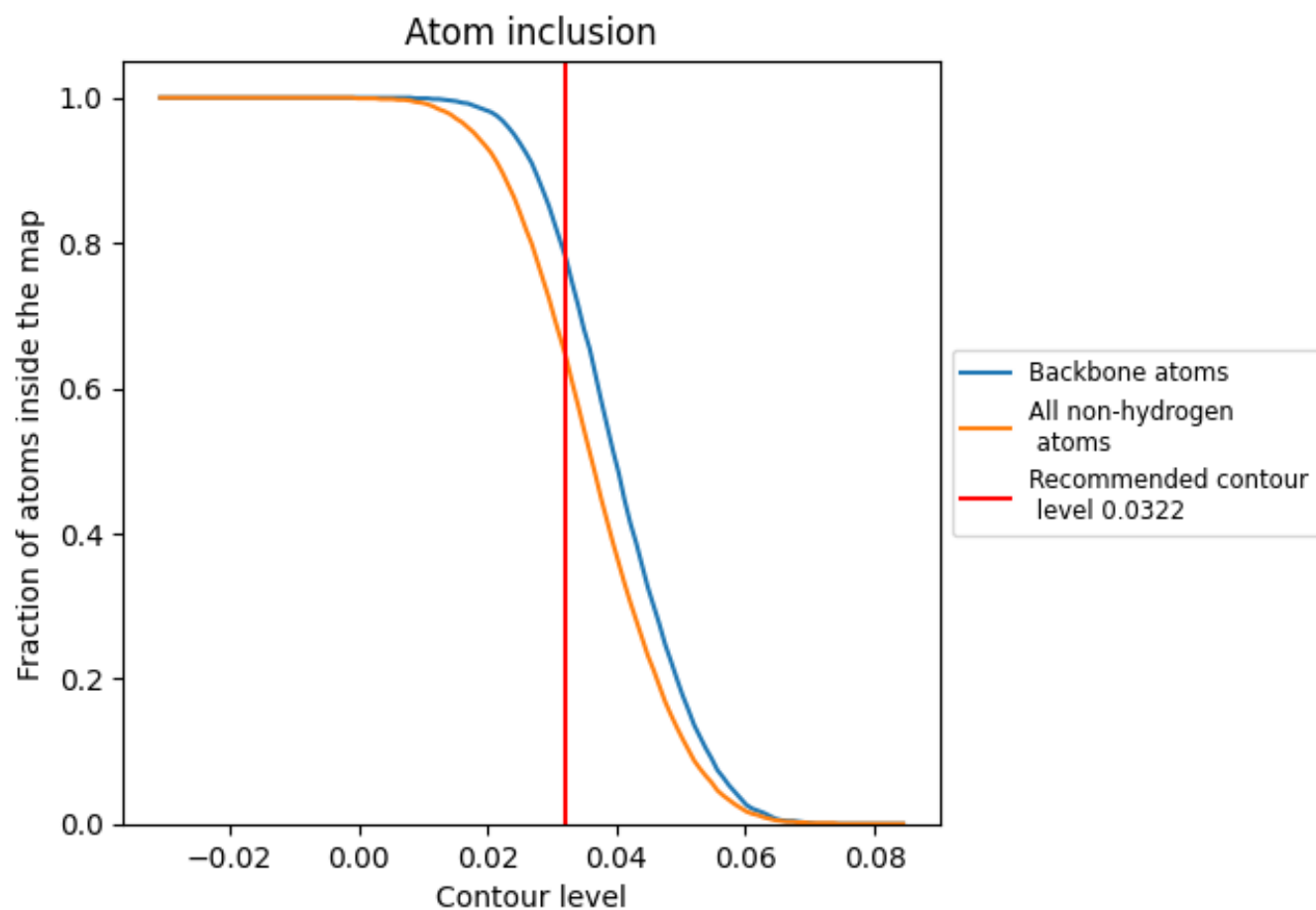
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0322).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0322) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6430	0.0840
A	0.6750	0.0860
B	0.6690	0.0800
C	0.5620	0.0880

