



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 03:38 pm GMT

PDB ID : 5ND3
EMDB ID : EMD-3621
Title : Microtubule-bound MKLP2 motor domain in the with no nucleotide
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 : 6.10 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:

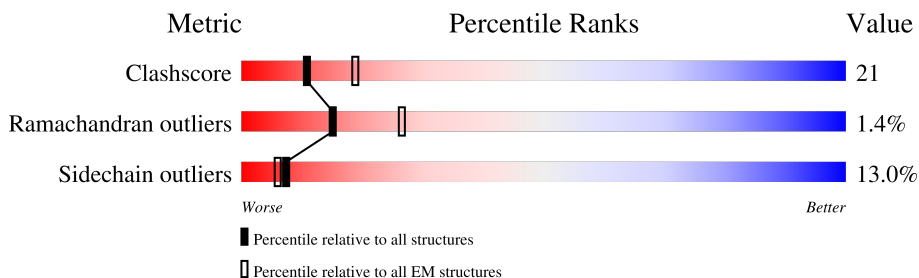
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.10 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
1	5-C	501	
2	1-A	451	
2	2-A	451	
2	3-A	451	

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Mol	Chain	Length	Quality of chain		
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
4	GTP	1-A	500	-	-	X	-
4	GTP	2-A	500	-	-	X	-
4	GTP	3-A	500	-	-	X	-
4	GTP	4-A	500	-	-	X	-
4	GTP	5-A	500	-	-	X	-
6	GDP	1-B	600	-	-	X	-
6	GDP	2-B	600	-	-	X	-
6	GDP	3-B	600	-	-	X	-
6	GDP	4-B	600	-	-	X	-
6	GDP	5-B	600	-	-	X	-

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 45371 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
			Total	C	N	O	S		
1	1-C	296	2375	1508	420	436	11	0	0
1	2-C	296	2375	1508	420	436	11	0	0
1	3-C	295	2366	1502	418	435	11	0	0
1	4-C	296	2375	1508	420	436	11	0	0
1	5-C	296	2375	1508	420	436	11	0	0

- Molecule 2 is a protein called Tubulin alpha chain.

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

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

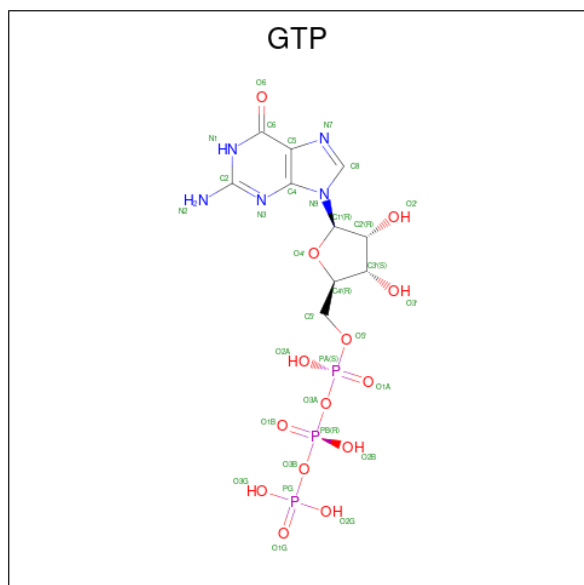
- Molecule 3 is a protein called Tubulin beta-2B chain.

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

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 GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	1-A	1	Total 32	C 10	N 5	O 14	P 3	0
4	2-A	1	Total 32	C 10	N 5	O 14	P 3	0

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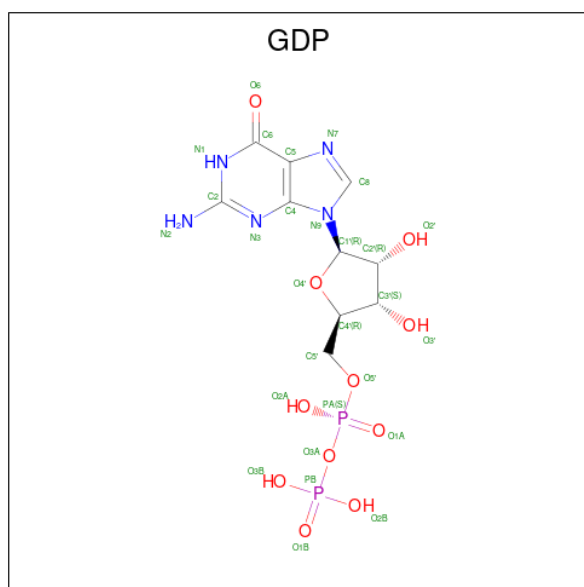
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Mol	Chain	Residues	Atoms				AltConf	
4	3-A	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	4-A	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	5-A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



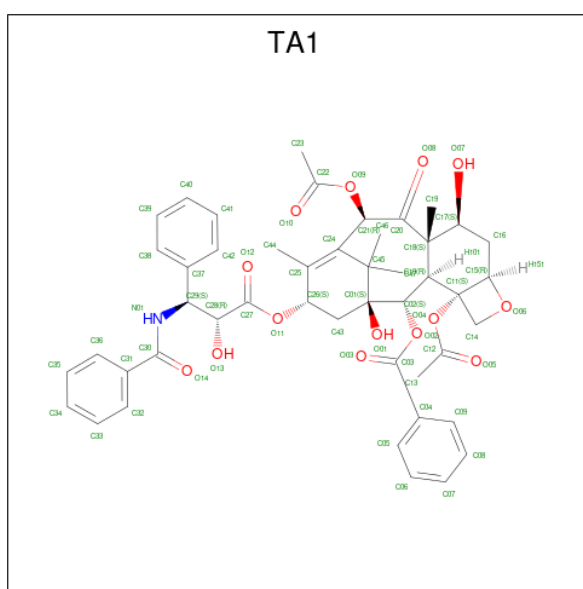
Mol	Chain	Residues	Atoms				AltConf	
6	1-B	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
6	2-B	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	3-B	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	4-B	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	5-B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 7 is TAXOL (three-letter code: TA1) (formula: C₄₇H₅₁NO₁₄).

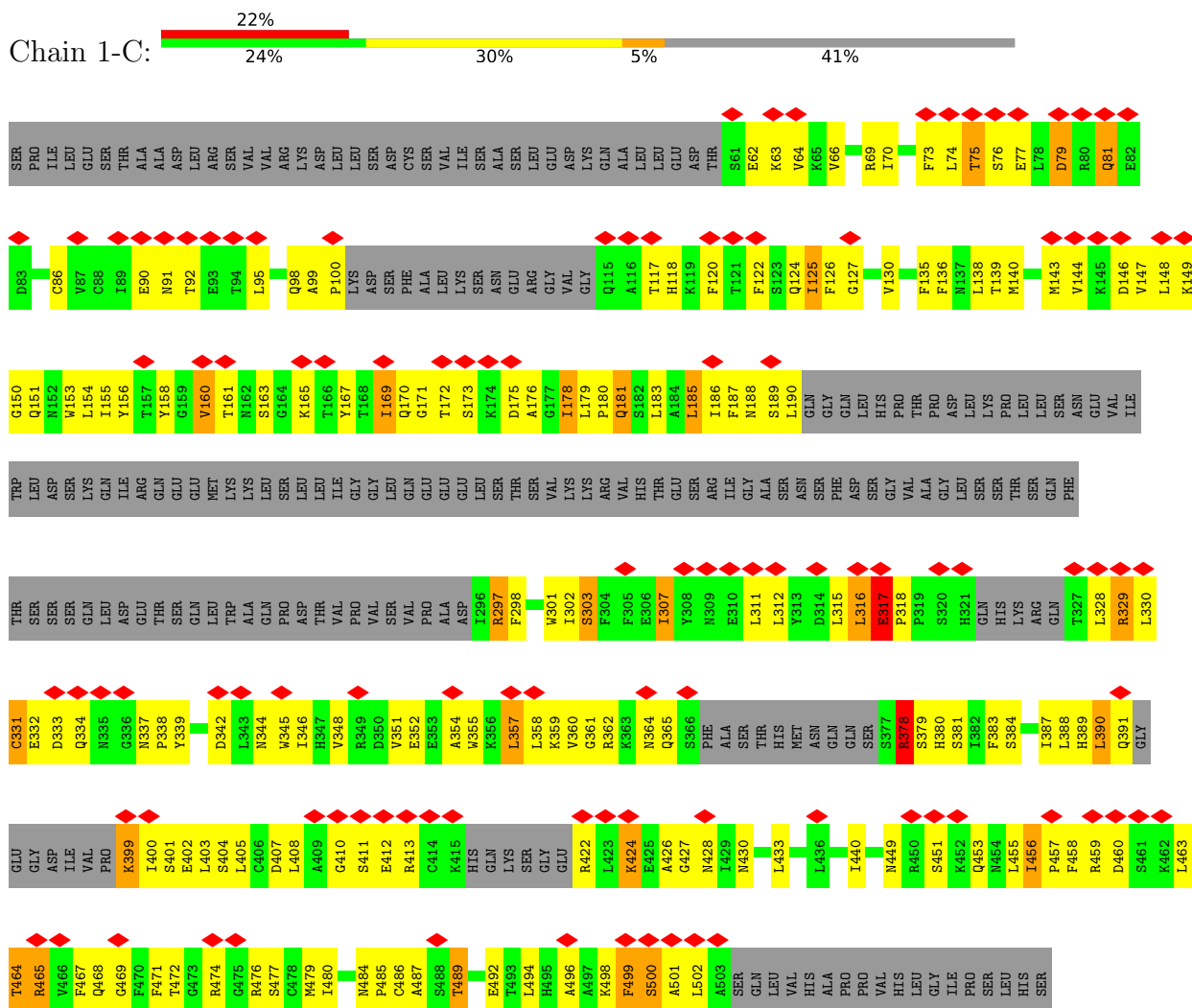


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	1-B	1	Total	C	N	O	0
			62	47	1	14	
7	2-B	1	Total	C	N	O	0
			62	47	1	14	
7	3-B	1	Total	C	N	O	0
			62	47	1	14	
7	4-B	1	Total	C	N	O	0
			62	47	1	14	
7	5-B	1	Total	C	N	O	0
			62	47	1	14	

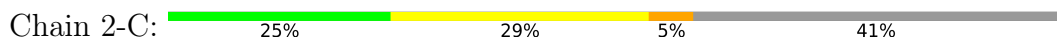
3 Residue-property plots

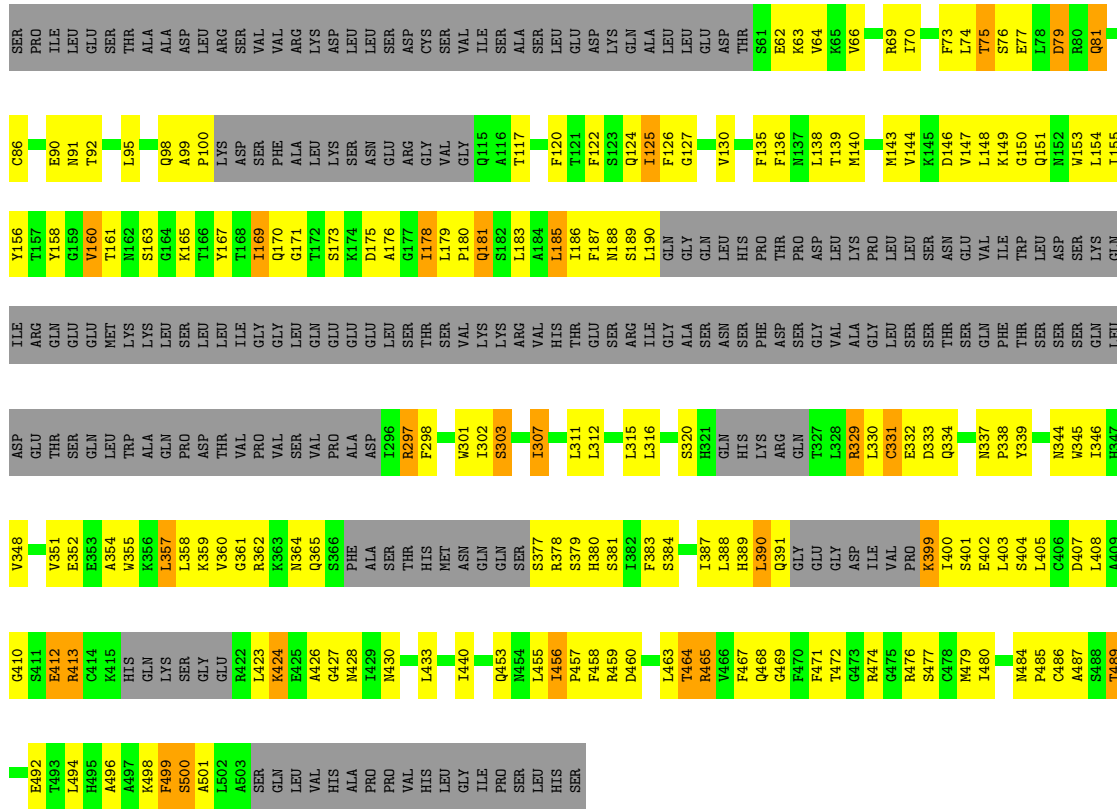
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

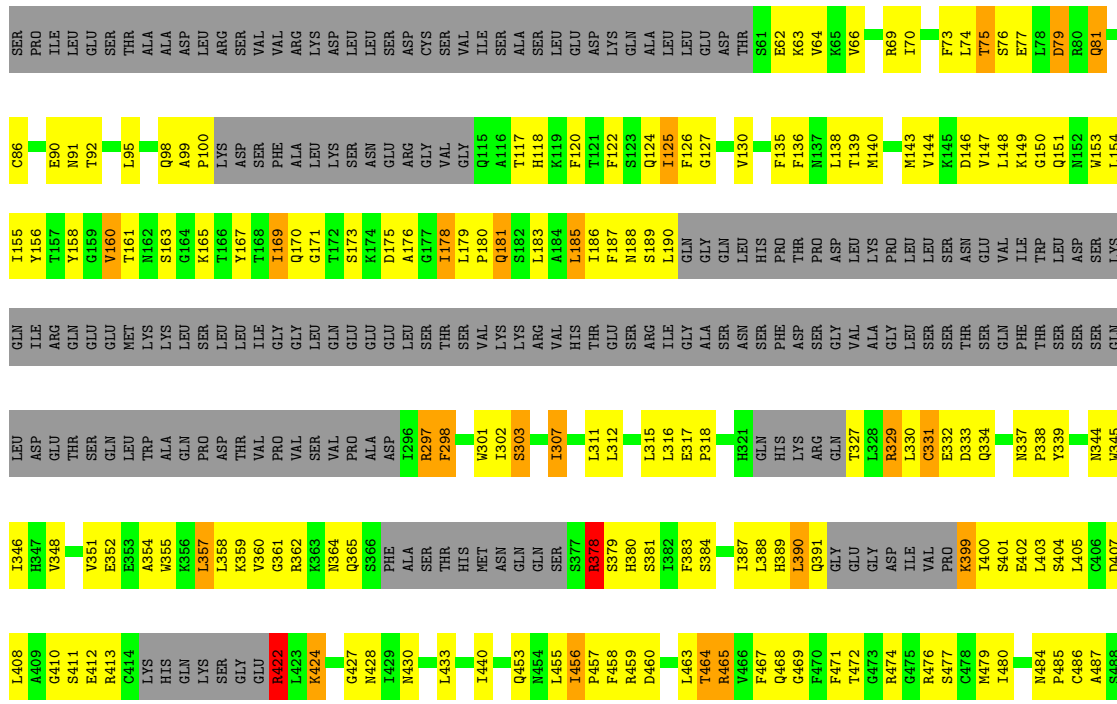
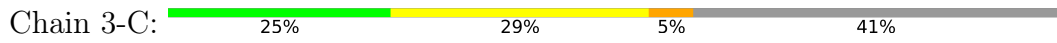


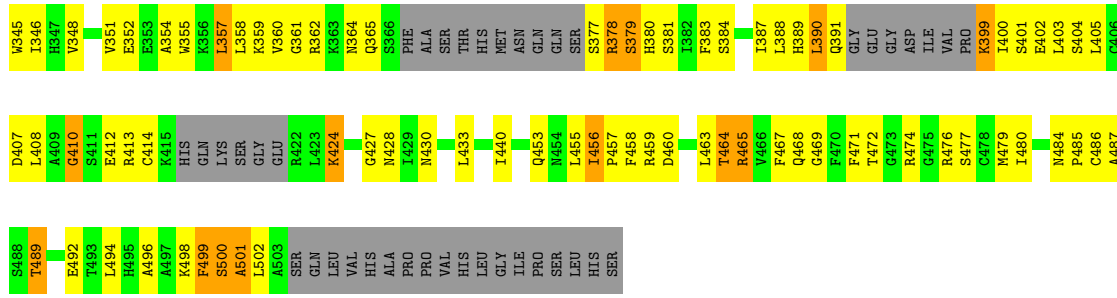
- Molecule 1: Kinesin-like protein KIF20A



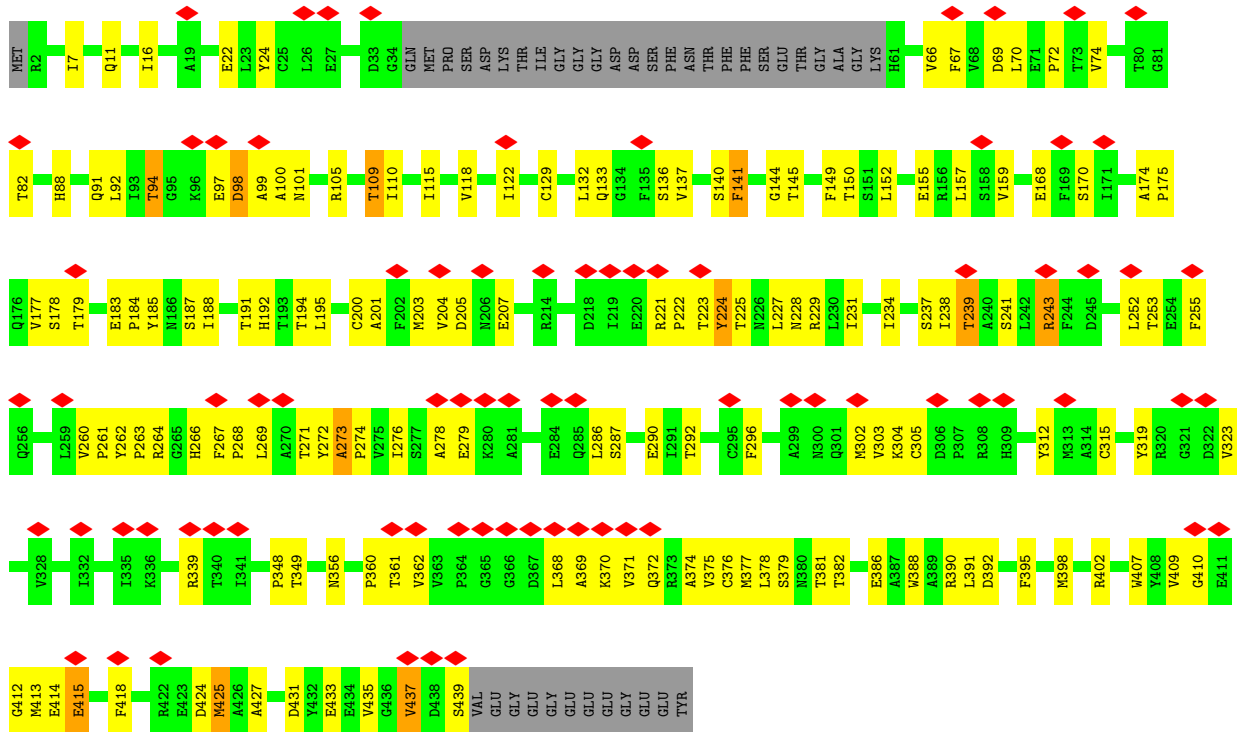


● Molecule 1: Kinesin-like protein KIF20A

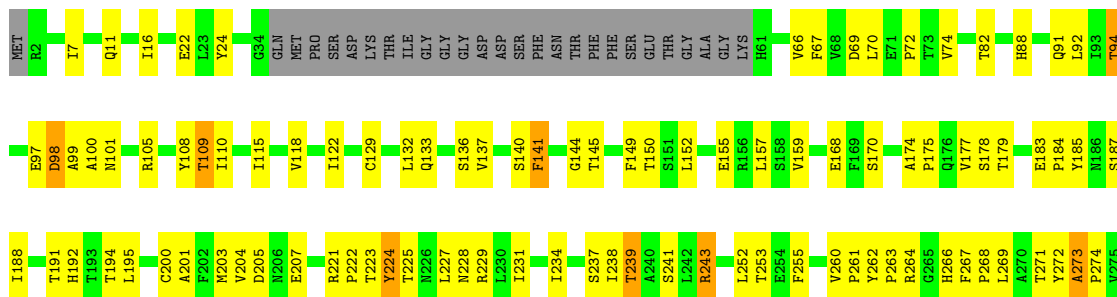


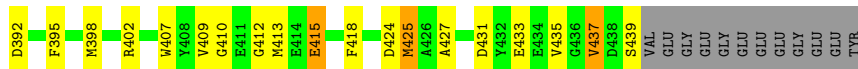


• Molecule 2: Tubulin alpha chain

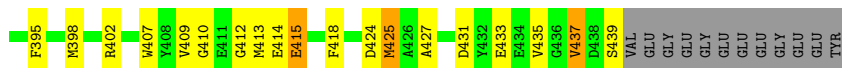
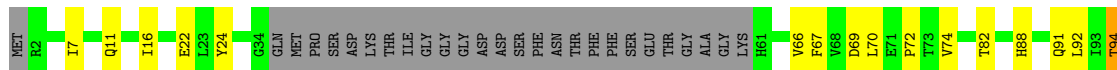


• Molecule 2: Tubulin alpha chain

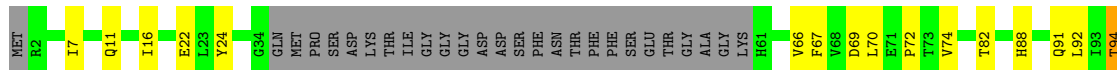




• Molecule 2: Tubulin alpha chain

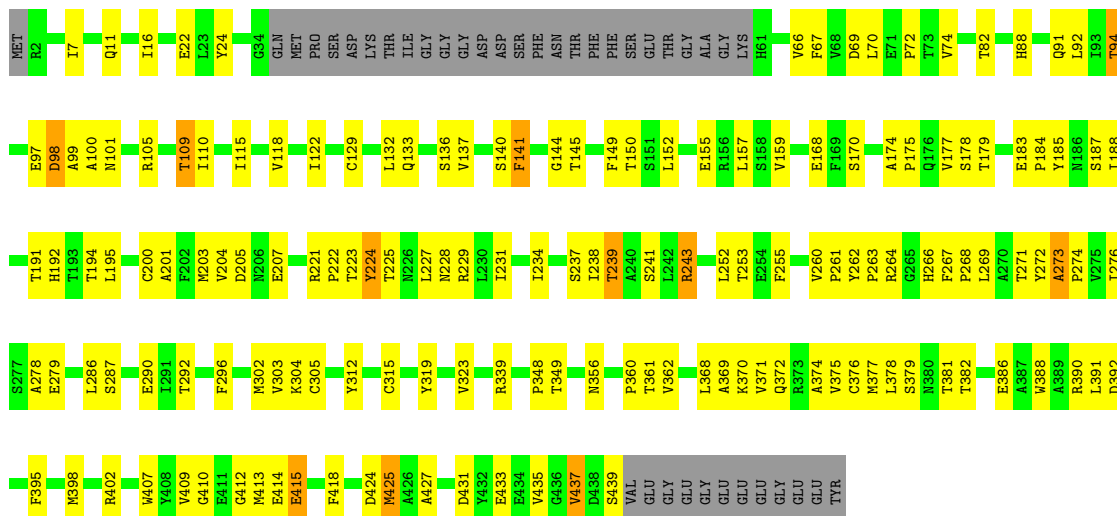


• Molecule 2: Tubulin alpha chain

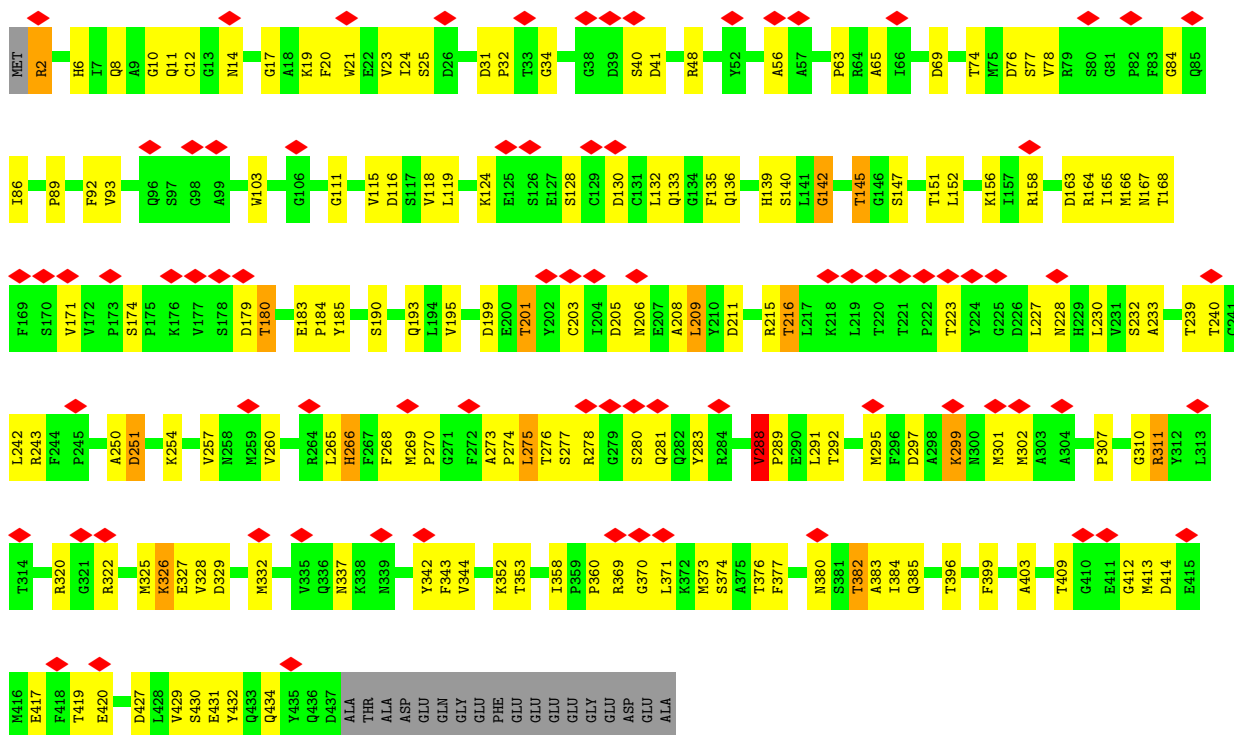


• Molecule 2: Tubulin alpha chain

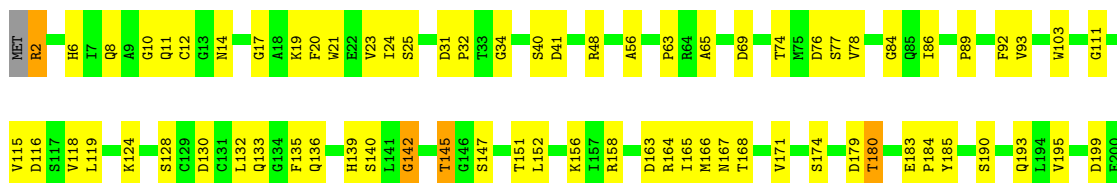


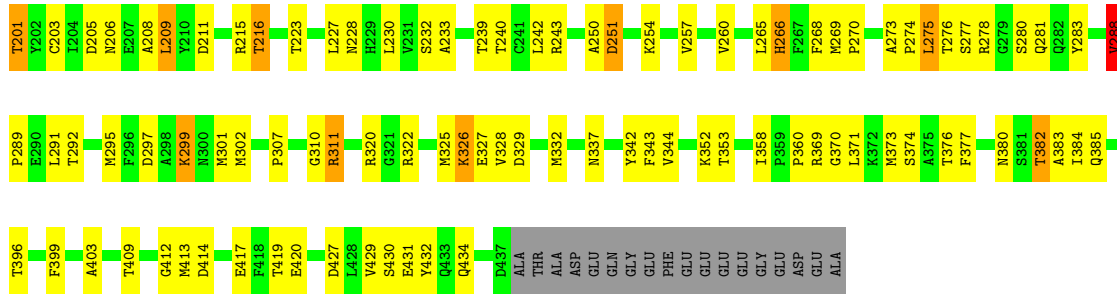


• Molecule 3: Tubulin beta-2B chain

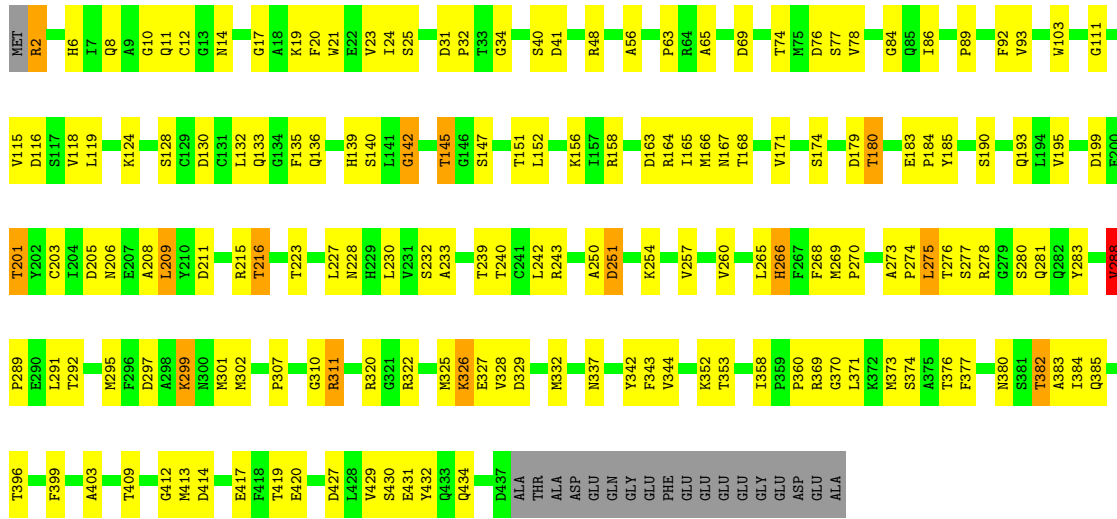


• Molecule 3: Tubulin beta-2B chain

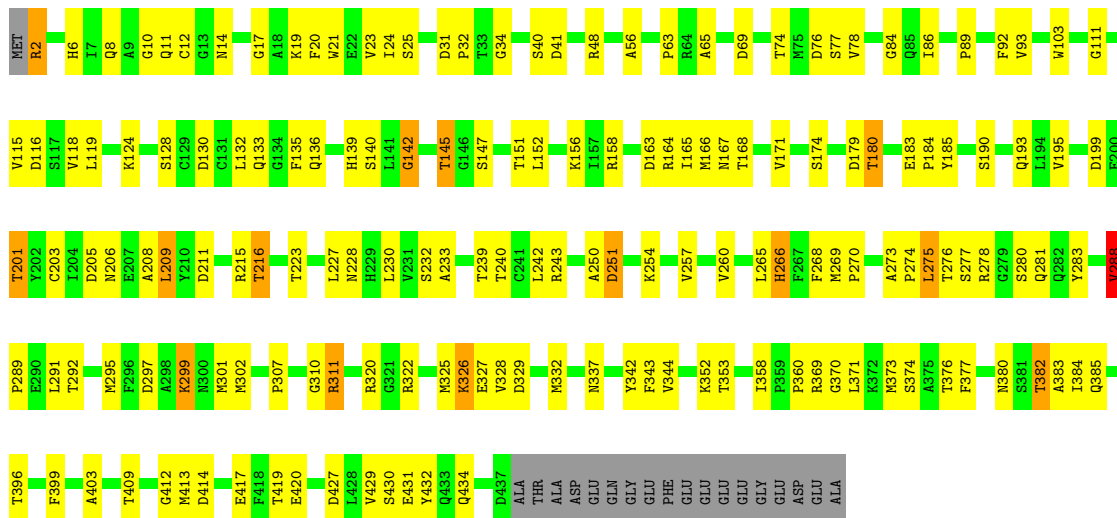




• Molecule 3: Tubulin beta-2B chain

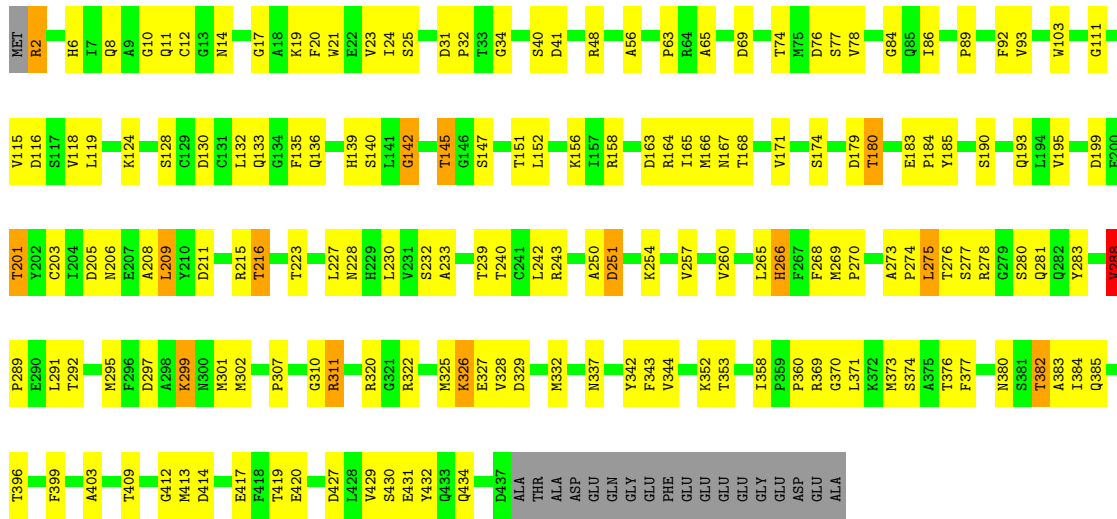


• Molecule 3: Tubulin beta-2B chain



• Molecule 3: Tubulin beta-2B chain

Chain 5-B:  58% 34%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9257	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	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	0.109	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0321	Depositor
Map size (Å)	244.79999, 212.67, 246.33	wwPDB
Map dimensions	160, 139, 161	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.53, 1.53, 1.53	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.59	2/2416 (0.1%)	0.81	7/3254 (0.2%)
1	2-C	0.58	2/2416 (0.1%)	0.80	6/3254 (0.2%)
1	3-C	0.58	2/2407 (0.1%)	0.75	6/3243 (0.2%)
1	4-C	0.58	2/2416 (0.1%)	0.79	6/3254 (0.2%)
1	5-C	0.60	2/2416 (0.1%)	0.80	6/3254 (0.2%)
2	1-A	0.26	0/3300	0.39	0/4482
2	2-A	0.26	0/3300	0.39	0/4482
2	3-A	0.26	0/3300	0.39	0/4482
2	4-A	0.26	0/3300	0.39	0/4482
2	5-A	0.26	0/3300	0.39	0/4482
3	1-B	0.28	0/3426	0.42	0/4642
3	2-B	0.28	0/3426	0.42	0/4642
3	3-B	0.28	0/3426	0.42	0/4642
3	4-B	0.28	0/3426	0.42	0/4642
3	5-B	0.28	0/3426	0.42	0/4642
All	All	0.38	10/45701 (0.0%)	0.53	31/61879 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-C	1	4
1	2-C	1	3
1	3-C	1	2
1	4-C	1	1
1	5-C	1	4
All	All	5	14

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-C	465	ARG	CZ-NH1	6.06	1.41	1.33
1	4-C	465	ARG	CZ-NH1	6.03	1.40	1.33
1	2-C	465	ARG	CZ-NH1	6.01	1.40	1.33
1	3-C	465	ARG	CZ-NH1	6.01	1.40	1.33
1	5-C	465	ARG	CZ-NH1	5.98	1.40	1.33
1	4-C	465	ARG	CZ-NH2	5.56	1.40	1.33
1	3-C	465	ARG	CZ-NH2	5.54	1.40	1.33
1	2-C	465	ARG	CZ-NH2	5.49	1.40	1.33
1	5-C	465	ARG	CZ-NH2	5.48	1.40	1.33
1	1-C	465	ARG	CZ-NH2	5.47	1.40	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-C	378	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	2-C	320	SER	C-N-CA	11.17	149.63	121.70
1	3-C	465	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	5-C	465	ARG	NE-CZ-NH2	-10.39	115.11	120.30
1	4-C	465	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	2-C	465	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	1-C	465	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	4-C	378	ARG	CB-CA-C	-6.74	96.93	110.40
1	3-C	422	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	4-C	451	SER	N-CA-CB	5.87	119.31	110.50
1	5-C	414	CYS	C-N-CA	-5.86	107.06	121.70
1	1-C	318	PRO	N-CA-C	5.85	127.30	112.10
1	2-C	379	SER	C-N-CA	5.74	136.05	121.70
1	4-C	414	CYS	C-N-CA	-5.71	107.43	121.70
1	5-C	317	GLU	O-C-N	5.64	131.82	121.10
1	5-C	410	GLY	C-N-CA	5.63	135.79	121.70
1	4-C	329	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	1-C	379	SER	C-N-CA	5.46	135.35	121.70
1	3-C	378	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	1-C	329	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	1-C	331	CYS	N-CA-CB	5.37	120.26	110.60
1	5-C	331	CYS	N-CA-CB	5.36	120.24	110.60
1	4-C	331	CYS	N-CA-CB	5.35	120.23	110.60
1	2-C	329	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	3-C	329	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	3-C	331	CYS	N-CA-CB	5.34	120.21	110.60
1	5-C	329	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	2-C	331	CYS	N-CA-CB	5.32	120.17	110.60
1	1-C	317	GLU	O-C-N	5.29	131.15	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-C	423	LEU	C-N-CA	5.13	134.52	121.70
1	3-C	411	SER	C-N-CA	-5.11	108.92	121.70

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1-C	297	ARG	CA
1	2-C	297	ARG	CA
1	3-C	297	ARG	CA
1	4-C	297	ARG	CA
1	5-C	297	ARG	CA

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-C	316	LEU	Mainchain
1	1-C	317	GLU	Peptide
1	1-C	378	ARG	Sidechain
1	1-C	459	ARG	Sidechain
1	2-C	410	GLY	Peptide,Mainchain
1	2-C	459	ARG	Sidechain
1	3-C	422	ARG	Sidechain
1	3-C	459	ARG	Sidechain
1	4-C	459	ARG	Sidechain
1	5-C	316	LEU	Mainchain
1	5-C	317	GLU	Peptide
1	5-C	378	ARG	Sidechain
1	5-C	459	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-C	2375	0	2385	147	0
1	2-C	2375	0	2385	144	0
1	3-C	2366	0	2372	144	0
1	4-C	2375	0	2385	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5-C	2375	0	2385	148	0
2	1-A	3227	0	3141	121	0
2	2-A	3227	0	3141	122	0
2	3-A	3227	0	3141	124	0
2	4-A	3227	0	3141	119	0
2	5-A	3227	0	3141	121	0
3	1-B	3351	0	3229	115	0
3	2-B	3351	0	3229	114	0
3	3-B	3351	0	3229	115	0
3	4-B	3351	0	3229	119	0
3	5-B	3351	0	3229	116	0
4	1-A	32	0	12	26	0
4	2-A	32	0	12	26	0
4	3-A	32	0	12	26	0
4	4-A	32	0	12	26	0
4	5-A	32	0	12	26	0
5	1-A	1	0	0	0	0
5	2-A	1	0	0	0	0
5	3-A	1	0	0	0	0
5	4-A	1	0	0	0	0
5	5-A	1	0	0	0	0
6	1-B	28	0	12	11	0
6	2-B	28	0	12	11	0
6	3-B	28	0	12	11	0
6	4-B	28	0	12	11	0
6	5-B	28	0	12	11	0
7	1-B	62	0	51	19	0
7	2-B	62	0	51	19	0
7	3-B	62	0	51	19	0
7	4-B	62	0	51	19	0
7	5-B	62	0	51	19	0
All	All	45371	0	44137	1851	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 21.

All (1851) 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:OG1	4:A:500:GTP:C3'	1.73	1.34
2:A:179:THR:OG1	4:A:500:GTP:C3'	1.73	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:179:THR:OG1	4:A:500:GTP:C3'	1.73	1.34
2:A:179:THR:OG1	4:A:500:GTP:C3'	1.73	1.34
2:A:179:THR:OG1	4:A:500:GTP:C3'	1.73	1.34
1:C:413:ARG:HD2	1:C:413:ARG:O	1.44	1.16
1:C:388:LEU:HD22	1:C:390:LEU:HD11	1.27	1.13
1:C:388:LEU:HD22	1:C:390:LEU:HD11	1.27	1.13
1:C:388:LEU:HD22	1:C:390:LEU:HD11	1.27	1.13
1:C:388:LEU:HD22	1:C:390:LEU:HD11	1.27	1.13
1:C:388:LEU:HD22	1:C:390:LEU:HD11	1.27	1.13
1:C:413:ARG:HG2	2:A:412:GLY:O	1.49	1.11
1:C:148:LEU:HD23	1:C:387:ILE:HD13	1.18	1.11
1:C:148:LEU:HD23	1:C:387:ILE:HD13	1.19	1.11
1:C:148:LEU:HD23	1:C:387:ILE:HD13	1.19	1.10
1:C:148:LEU:HD23	1:C:387:ILE:HD13	1.19	1.10
1:C:148:LEU:HD23	1:C:387:ILE:HD13	1.19	1.10
1:C:413:ARG:HB2	2:A:414:GLU:OE2	1.51	1.09
2:A:179:THR:OG1	4:A:500:GTP:H3'	0.88	1.04
2:A:179:THR:OG1	4:A:500:GTP:H3'	0.88	1.04
2:A:179:THR:OG1	4:A:500:GTP:H3'	0.88	1.04
2:A:179:THR:OG1	4:A:500:GTP:H3'	0.88	1.04
2:A:179:THR:OG1	4:A:500:GTP:H3'	0.88	1.04
2:A:179:THR:CB	4:A:500:GTP:H3'	1.86	1.04
2:A:179:THR:CB	4:A:500:GTP:H3'	1.86	1.04
2:A:179:THR:CB	4:A:500:GTP:H3'	1.86	1.04
2:A:179:THR:CB	4:A:500:GTP:H3'	1.86	1.04
2:A:179:THR:CB	4:A:500:GTP:H3'	1.86	1.04
2:A:224:TYR:CE1	4:A:500:GTP:C5	2.51	0.98
2:A:224:TYR:CE1	4:A:500:GTP:C5	2.51	0.98
2:A:224:TYR:CE1	4:A:500:GTP:C5	2.51	0.98
2:A:224:TYR:CE1	4:A:500:GTP:C5	2.51	0.98
2:A:224:TYR:CE1	4:A:500:GTP:C5	2.51	0.98
2:A:179:THR:HG1	4:A:500:GTP:C3'	1.72	0.93
2:A:179:THR:HG1	4:A:500:GTP:C3'	1.72	0.93
2:A:179:THR:HG1	4:A:500:GTP:C3'	1.72	0.93
2:A:179:THR:HG1	4:A:500:GTP:C3'	1.72	0.93
2:A:179:THR:HG1	4:A:500:GTP:C3'	1.72	0.93
2:A:179:THR:HG1	4:A:500:GTP:H3'	1.24	0.92
2:A:179:THR:HG1	4:A:500:GTP:H3'	1.24	0.92
2:A:179:THR:HG1	4:A:500:GTP:H3'	1.24	0.92
2:A:179:THR:HG1	4:A:500:GTP:H3'	1.24	0.92
2:A:179:THR:HG1	4:A:500:GTP:H3'	1.24	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:224:TYR:CD1	4:A:500:GTP:C6	2.60	0.89
2:A:224:TYR:CD1	4:A:500:GTP:C6	2.60	0.89
2:A:224:TYR:CD1	4:A:500:GTP:C6	2.60	0.89
2:A:224:TYR:CD1	4:A:500:GTP:C6	2.60	0.89
2:A:224:TYR:CD1	4:A:500:GTP:C6	2.60	0.89
3:B:12:CYS:SG	6:B:600:GDP:C4	2.67	0.88
3:B:12:CYS:SG	6:B:600:GDP:C4	2.67	0.88
3:B:12:CYS:SG	6:B:600:GDP:C4	2.67	0.88
3:B:12:CYS:SG	6:B:600:GDP:C4	2.67	0.88
3:B:12:CYS:SG	6:B:600:GDP:C4	2.67	0.88
3:B:250:ALA:HA	3:B:254:LYS:HD3	1.54	0.87
3:B:250:ALA:HA	3:B:254:LYS:HD3	1.54	0.87
3:B:250:ALA:HA	3:B:254:LYS:HD3	1.54	0.87
3:B:250:ALA:HA	3:B:254:LYS:HD3	1.54	0.87
3:B:250:ALA:HA	3:B:254:LYS:HD3	1.54	0.87
2:A:260:VAL:HG12	2:A:266:HIS:HB2	1.54	0.87
2:A:260:VAL:HG12	2:A:266:HIS:HB2	1.54	0.87
2:A:260:VAL:HG12	2:A:266:HIS:HB2	1.54	0.87
2:A:260:VAL:HG12	2:A:266:HIS:HB2	1.54	0.87
2:A:260:VAL:HG12	2:A:266:HIS:HB2	1.54	0.87
1:C:413:ARG:HG2	2:A:412:GLY:O	1.76	0.86
1:C:148:LEU:CD2	1:C:387:ILE:HD13	2.04	0.85
1:C:148:LEU:CD2	1:C:387:ILE:HD13	2.04	0.85
1:C:148:LEU:CD2	1:C:387:ILE:HD13	2.04	0.85
1:C:148:LEU:CD2	1:C:387:ILE:HD13	2.04	0.85
1:C:148:LEU:CD2	1:C:387:ILE:HD13	2.04	0.85
2:A:175:PRO:HG3	2:A:304:LYS:HG2	1.57	0.85
2:A:175:PRO:HG3	2:A:304:LYS:HG2	1.57	0.85
2:A:175:PRO:HG3	2:A:304:LYS:HG2	1.57	0.85
2:A:175:PRO:HG3	2:A:304:LYS:HG2	1.57	0.85
2:A:175:PRO:HG3	2:A:304:LYS:HG2	1.57	0.85
1:C:456:ILE:HD12	1:C:458:PHE:HE2	1.39	0.84
1:C:456:ILE:HD12	1:C:458:PHE:HE2	1.39	0.84
1:C:388:LEU:HD22	1:C:390:LEU:CD1	2.07	0.84
1:C:456:ILE:HD12	1:C:458:PHE:HE2	1.39	0.84
1:C:388:LEU:HD22	1:C:390:LEU:CD1	2.07	0.84
1:C:388:LEU:HD22	1:C:390:LEU:CD1	2.07	0.84
1:C:456:ILE:HD12	1:C:458:PHE:HE2	1.39	0.84
1:C:388:LEU:HD22	1:C:390:LEU:CD1	2.07	0.84
1:C:388:LEU:HD22	1:C:390:LEU:CD1	2.07	0.84
1:C:456:ILE:HD12	1:C:458:PHE:HE2	1.39	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ILE:HD12	1:C:387:ILE:HD11	1.58	0.84
1:C:186:ILE:HD12	1:C:387:ILE:HD11	1.58	0.84
1:C:186:ILE:HD12	1:C:387:ILE:HD11	1.58	0.84
1:C:186:ILE:HD12	1:C:387:ILE:HD11	1.58	0.84
1:C:413:ARG:HB2	2:A:414:GLU:OE2	1.77	0.84
1:C:484:ASN:HB2	1:C:489:THR:HG21	1.58	0.84
1:C:412:GLU:O	1:C:426:ALA:HB1	1.78	0.84
1:C:484:ASN:HB2	1:C:489:THR:HG21	1.58	0.84
1:C:186:ILE:HD12	1:C:387:ILE:HD11	1.58	0.84
1:C:484:ASN:HB2	1:C:489:THR:HG21	1.58	0.84
1:C:484:ASN:HB2	1:C:489:THR:HG21	1.58	0.84
1:C:484:ASN:HB2	1:C:489:THR:HG21	1.58	0.84
2:A:179:THR:HG21	4:A:500:GTP:C2'	2.08	0.83
2:A:179:THR:HG21	4:A:500:GTP:C2'	2.08	0.83
2:A:179:THR:HG21	4:A:500:GTP:C2'	2.08	0.83
2:A:179:THR:HG21	4:A:500:GTP:C2'	2.08	0.83
2:A:179:THR:HG21	4:A:500:GTP:C2'	2.08	0.83
1:C:453:GLN:HB2	3:B:434:GLN:NE2	1.93	0.83
1:C:453:GLN:HB2	3:B:434:GLN:NE2	1.94	0.82
2:A:224:TYR:CE1	4:A:500:GTP:C4	2.67	0.82
2:A:224:TYR:CE1	4:A:500:GTP:C4	2.67	0.82
1:C:453:GLN:HB2	3:B:434:GLN:NE2	1.95	0.82
2:A:224:TYR:CE1	4:A:500:GTP:C4	2.67	0.82
2:A:224:TYR:CE1	4:A:500:GTP:C4	2.67	0.82
2:A:224:TYR:CE1	4:A:500:GTP:C4	2.67	0.82
3:B:360:PRO:O	7:B:601:TA1:O13	1.97	0.82
3:B:360:PRO:O	7:B:601:TA1:O13	1.97	0.82
3:B:360:PRO:O	7:B:601:TA1:O13	1.97	0.82
3:B:360:PRO:O	7:B:601:TA1:O13	1.97	0.82
3:B:360:PRO:O	7:B:601:TA1:O13	1.97	0.82
1:C:413:ARG:CB	2:A:414:GLU:OE2	2.27	0.81
1:C:453:GLN:HB2	3:B:434:GLN:NE2	1.96	0.81
3:B:12:CYS:HB2	6:B:600:GDP:O1A	1.82	0.80
3:B:12:CYS:HB2	6:B:600:GDP:O1A	1.82	0.80
3:B:12:CYS:HB2	6:B:600:GDP:O1A	1.82	0.80
3:B:12:CYS:HB2	6:B:600:GDP:O1A	1.82	0.80
3:B:12:CYS:HB2	6:B:600:GDP:O1A	1.82	0.80
1:C:453:GLN:HB2	3:B:434:GLN:NE2	1.96	0.80
3:B:254:LYS:HE3	3:B:352:LYS:HE3	1.62	0.80
3:B:254:LYS:HE3	3:B:352:LYS:HE3	1.62	0.80
3:B:254:LYS:HE3	3:B:352:LYS:HE3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:254:LYS:HE3	3:B:352:LYS:HE3	1.62	0.80
3:B:254:LYS:HE3	3:B:352:LYS:HE3	1.62	0.80
1:C:413:ARG:CD	2:A:412:GLY:O	2.30	0.80
3:B:414:ASP:HB3	3:B:417:GLU:HB2	1.64	0.79
3:B:414:ASP:HB3	3:B:417:GLU:HB2	1.64	0.79
3:B:414:ASP:HB3	3:B:417:GLU:HB2	1.64	0.79
3:B:414:ASP:HB3	3:B:417:GLU:HB2	1.64	0.79
3:B:414:ASP:HB3	3:B:417:GLU:HB2	1.64	0.79
3:B:11:GLN:HB3	6:B:600:GDP:O2B	1.83	0.78
3:B:11:GLN:HB3	6:B:600:GDP:O2B	1.83	0.78
3:B:11:GLN:HB3	6:B:600:GDP:O2B	1.83	0.78
3:B:11:GLN:HB3	6:B:600:GDP:O2B	1.83	0.78
3:B:11:GLN:HB3	6:B:600:GDP:O2B	1.83	0.78
1:C:413:ARG:CG	2:A:412:GLY:O	2.31	0.78
1:C:453:GLN:OE1	1:C:455:LEU:HG	1.83	0.78
3:B:360:PRO:HB2	7:B:601:TA1:H281	1.63	0.78
1:C:453:GLN:OE1	1:C:455:LEU:HG	1.83	0.78
3:B:360:PRO:HB2	7:B:601:TA1:H281	1.63	0.78
1:C:453:GLN:OE1	1:C:455:LEU:HG	1.83	0.78
3:B:360:PRO:HB2	7:B:601:TA1:H281	1.63	0.78
3:B:360:PRO:HB2	7:B:601:TA1:H281	1.63	0.78
3:B:360:PRO:HB2	7:B:601:TA1:H281	1.63	0.78
1:C:453:GLN:OE1	1:C:455:LEU:HG	1.83	0.78
1:C:453:GLN:OE1	1:C:455:LEU:HG	1.83	0.78
3:B:230:LEU:CD1	7:B:601:TA1:H081	2.15	0.77
3:B:230:LEU:CD1	7:B:601:TA1:H081	2.15	0.77
3:B:230:LEU:CD1	7:B:601:TA1:H081	2.15	0.77
3:B:230:LEU:CD1	7:B:601:TA1:H081	2.15	0.77
3:B:230:LEU:CD1	7:B:601:TA1:H081	2.15	0.77
1:C:413:ARG:O	1:C:413:ARG:CD	2.32	0.76
1:C:297:ARG:HB3	1:C:390:LEU:HD13	1.67	0.76
1:C:311:LEU:HD12	1:C:327:THR:HB	1.67	0.76
1:C:297:ARG:HB3	1:C:390:LEU:HD13	1.67	0.76
1:C:297:ARG:HB3	1:C:390:LEU:HD13	1.67	0.76
1:C:297:ARG:HB3	1:C:390:LEU:HD13	1.68	0.76
1:C:297:ARG:HB3	1:C:390:LEU:HD13	1.67	0.76
1:C:457:PRO:HB3	1:C:460:ASP:OD2	1.86	0.75
1:C:337:ASN:HB2	1:C:469:GLY:HA2	1.66	0.75
1:C:337:ASN:HB2	1:C:469:GLY:HA2	1.66	0.75
1:C:457:PRO:HB3	1:C:460:ASP:OD2	1.86	0.75
1:C:337:ASN:HB2	1:C:469:GLY:HA2	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:ASN:HB2	1:C:469:GLY:HA2	1.66	0.75
1:C:457:PRO:HB3	1:C:460:ASP:OD2	1.86	0.75
1:C:457:PRO:HB3	1:C:460:ASP:OD2	1.86	0.75
1:C:337:ASN:HB2	1:C:469:GLY:HA2	1.66	0.75
1:C:457:PRO:HB3	1:C:460:ASP:OD2	1.86	0.75
1:C:413:ARG:HD3	2:A:412:GLY:O	1.87	0.74
1:C:311:LEU:HD12	1:C:327:THR:CB	2.17	0.74
1:C:456:ILE:HD12	1:C:458:PHE:CE2	2.22	0.73
1:C:456:ILE:HD12	1:C:458:PHE:CE2	2.22	0.73
1:C:179:LEU:HB3	1:C:180:PRO:HD3	1.70	0.73
1:C:456:ILE:HD12	1:C:458:PHE:CE2	2.22	0.73
1:C:179:LEU:HB3	1:C:180:PRO:HD3	1.70	0.73
1:C:179:LEU:HB3	1:C:180:PRO:HD3	1.70	0.73
1:C:456:ILE:HD12	1:C:458:PHE:CE2	2.22	0.73
2:A:115:ILE:HD12	2:A:152:LEU:HD13	1.69	0.73
1:C:179:LEU:HB3	1:C:180:PRO:HD3	1.70	0.73
2:A:115:ILE:HD12	2:A:152:LEU:HD13	1.69	0.73
1:C:179:LEU:HB3	1:C:180:PRO:HD3	1.70	0.73
2:A:115:ILE:HD12	2:A:152:LEU:HD13	1.69	0.73
2:A:115:ILE:HD12	2:A:152:LEU:HD13	1.69	0.73
1:C:456:ILE:HD12	1:C:458:PHE:CE2	2.22	0.73
2:A:115:ILE:HD12	2:A:152:LEU:HD13	1.69	0.73
3:B:370:GLY:O	7:B:601:TA1:H443	1.87	0.73
3:B:370:GLY:O	7:B:601:TA1:H443	1.87	0.73
3:B:370:GLY:O	7:B:601:TA1:H443	1.87	0.73
3:B:370:GLY:O	7:B:601:TA1:H443	1.87	0.73
3:B:370:GLY:O	7:B:601:TA1:H443	1.87	0.73
2:A:224:TYR:CZ	4:A:500:GTP:C8	2.76	0.72
2:A:224:TYR:CZ	4:A:500:GTP:C8	2.76	0.72
2:A:224:TYR:CZ	4:A:500:GTP:C8	2.76	0.72
2:A:224:TYR:CZ	4:A:500:GTP:C8	2.76	0.72
2:A:224:TYR:CZ	4:A:500:GTP:C8	2.76	0.72
1:C:377:SER:O	1:C:378:ARG:HD3	1.89	0.72
2:A:179:THR:HG21	4:A:500:GTP:H2'	1.72	0.72
2:A:179:THR:HG21	4:A:500:GTP:H2'	1.72	0.72
2:A:179:THR:HG21	4:A:500:GTP:H2'	1.72	0.72
2:A:179:THR:HG21	4:A:500:GTP:H2'	1.72	0.72
2:A:179:THR:HG21	4:A:500:GTP:H2'	1.72	0.72
1:C:458:PHE:HA	1:C:464:THR:HB	1.72	0.72
1:C:458:PHE:HA	1:C:464:THR:HB	1.72	0.72
1:C:458:PHE:HA	1:C:464:THR:HB	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:PHE:HA	1:C:464:THR:HB	1.72	0.71
1:C:458:PHE:HA	1:C:464:THR:HB	1.72	0.71
3:B:273:ALA:HB2	3:B:295:MET:HG3	1.70	0.71
3:B:273:ALA:HB2	3:B:295:MET:HG3	1.70	0.71
3:B:273:ALA:HB2	3:B:295:MET:HG3	1.70	0.71
3:B:273:ALA:HB2	3:B:295:MET:HG3	1.70	0.71
3:B:273:ALA:HB2	3:B:295:MET:HG3	1.70	0.71
3:B:273:ALA:HB2	3:B:295:MET:HG3	1.70	0.71
1:C:170:GLN:HG3	1:C:355:TRP:HH2	1.55	0.71
1:C:170:GLN:HG3	1:C:355:TRP:HH2	1.55	0.71
1:C:170:GLN:HG3	1:C:355:TRP:HH2	1.55	0.71
1:C:170:GLN:HG3	1:C:355:TRP:HH2	1.55	0.71
1:C:170:GLN:HG3	1:C:355:TRP:HH2	1.55	0.71
2:A:278:ALA:HB2	2:A:369:ALA:HA	1.72	0.71
2:A:278:ALA:HB2	2:A:369:ALA:HA	1.72	0.71
2:A:278:ALA:HB2	2:A:369:ALA:HA	1.72	0.71
2:A:278:ALA:HB2	2:A:369:ALA:HA	1.72	0.71
2:A:278:ALA:HB2	2:A:369:ALA:HA	1.72	0.71
3:B:230:LEU:HD13	7:B:601:TA1:H081	1.72	0.71
3:B:230:LEU:HD13	7:B:601:TA1:H081	1.72	0.71
3:B:230:LEU:HD13	7:B:601:TA1:H081	1.72	0.71
3:B:230:LEU:HD13	7:B:601:TA1:H081	1.72	0.71
3:B:230:LEU:HD13	7:B:601:TA1:H081	1.72	0.71
1:C:413:ARG:CG	2:A:412:GLY:O	2.36	0.70
1:C:445:GLN:HB2	1:C:452:LYS:HZ1	1.56	0.70
1:C:183:LEU:HB3	1:C:351:VAL:HG13	1.72	0.70
1:C:183:LEU:HB3	1:C:351:VAL:HG13	1.72	0.70
1:C:183:LEU:HB3	1:C:351:VAL:HG13	1.72	0.70
1:C:183:LEU:HB3	1:C:351:VAL:HG13	1.72	0.70
1:C:183:LEU:HB3	1:C:351:VAL:HG13	1.72	0.70
1:C:144:VAL:HG11	1:C:185:LEU:HB3	1.74	0.69
1:C:144:VAL:HG11	1:C:185:LEU:HB3	1.74	0.69
1:C:144:VAL:HG11	1:C:185:LEU:HB3	1.74	0.69
1:C:144:VAL:HG11	1:C:185:LEU:HB3	1.74	0.69
1:C:144:VAL:HG11	1:C:185:LEU:HB3	1.75	0.69
1:C:355:TRP:NE1	1:C:359:LYS:HE3	2.07	0.69
1:C:355:TRP:NE1	1:C:359:LYS:HE3	2.07	0.69
1:C:355:TRP:NE1	1:C:359:LYS:HE3	2.07	0.69
1:C:355:TRP:NE1	1:C:359:LYS:HE3	2.07	0.69
1:C:355:TRP:NE1	1:C:359:LYS:HE3	2.07	0.69
1:C:424:LYS:NZ	3:B:163:ASP:HA	2.09	0.68
1:C:445:GLN:HB2	1:C:452:LYS:NZ	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:228:ASN:OD1	6:B:600:GDP:N1	2.26	0.67
3:B:228:ASN:OD1	6:B:600:GDP:N1	2.26	0.67
3:B:228:ASN:OD1	6:B:600:GDP:N1	2.26	0.67
3:B:228:ASN:OD1	6:B:600:GDP:N1	2.26	0.67
3:B:228:ASN:OD1	6:B:600:GDP:N1	2.26	0.67
1:C:316:LEU:HD21	1:C:346:ILE:HB	1.77	0.67
1:C:427:GLY:HA3	2:A:410:GLY:O	1.95	0.67
1:C:316:LEU:HD21	1:C:346:ILE:HB	1.77	0.67
1:C:316:LEU:HD21	1:C:346:ILE:HB	1.77	0.67
1:C:357:LEU:O	1:C:360:VAL:HG12	1.94	0.67
1:C:424:LYS:NZ	3:B:163:ASP:HA	2.10	0.67
1:C:316:LEU:HD21	1:C:346:ILE:HB	1.77	0.67
1:C:316:LEU:HD21	1:C:346:ILE:HB	1.77	0.67
1:C:357:LEU:O	1:C:360:VAL:HG12	1.94	0.67
1:C:357:LEU:O	1:C:360:VAL:HG12	1.94	0.67
1:C:357:LEU:O	1:C:360:VAL:HG12	1.94	0.67
1:C:357:LEU:O	1:C:360:VAL:HG12	1.94	0.67
1:C:176:ALA:HB1	1:C:180:PRO:HB2	1.77	0.67
1:C:427:GLY:HA3	2:A:410:GLY:O	1.95	0.67
1:C:176:ALA:HB1	1:C:180:PRO:HB2	1.77	0.67
2:A:238:ILE:HD12	2:A:378:LEU:HD11	1.77	0.67
2:A:238:ILE:HD12	2:A:378:LEU:HD11	1.77	0.67
1:C:176:ALA:HB1	1:C:180:PRO:HB2	1.77	0.67
2:A:238:ILE:HD12	2:A:378:LEU:HD11	1.77	0.67
2:A:238:ILE:HD12	2:A:378:LEU:HD11	1.77	0.67
1:C:176:ALA:HB1	1:C:180:PRO:HB2	1.77	0.67
2:A:238:ILE:HD12	2:A:378:LEU:HD11	1.77	0.67
1:C:176:ALA:HB1	1:C:180:PRO:HB2	1.77	0.67
2:A:67:PHE:HB2	2:A:92:LEU:HD23	1.76	0.66
2:A:67:PHE:HB2	2:A:92:LEU:HD23	1.76	0.66
2:A:67:PHE:HB2	2:A:92:LEU:HD23	1.76	0.66
2:A:67:PHE:HB2	2:A:92:LEU:HD23	1.76	0.66
2:A:67:PHE:HB2	2:A:92:LEU:HD23	1.76	0.66
3:B:23:VAL:HG13	7:B:601:TA1:H321	1.77	0.66
3:B:23:VAL:HG13	7:B:601:TA1:H321	1.77	0.66
3:B:23:VAL:HG13	7:B:601:TA1:H321	1.77	0.66
3:B:23:VAL:HG13	7:B:601:TA1:H321	1.77	0.66
3:B:23:VAL:HG13	7:B:601:TA1:H321	1.77	0.66
3:B:23:VAL:HG13	7:B:601:TA1:C32	2.24	0.66
3:B:23:VAL:HG13	7:B:601:TA1:C32	2.24	0.66
1:C:427:GLY:HA3	2:A:410:GLY:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:23:VAL:HG13	7:B:601:TA1:C32	2.24	0.66
3:B:23:VAL:HG13	7:B:601:TA1:C32	2.24	0.66
3:B:23:VAL:HG13	7:B:601:TA1:C32	2.24	0.66
1:C:423:LEU:HD13	3:B:163:ASP:CB	2.26	0.65
3:B:195:VAL:HA	3:B:265:LEU:HD22	1.78	0.65
3:B:195:VAL:HA	3:B:265:LEU:HD22	1.78	0.65
1:C:424:LYS:NZ	3:B:163:ASP:HA	2.12	0.65
3:B:195:VAL:HA	3:B:265:LEU:HD22	1.78	0.65
3:B:195:VAL:HA	3:B:265:LEU:HD22	1.78	0.65
3:B:195:VAL:HA	3:B:265:LEU:HD22	1.78	0.65
3:B:168:THR:HB	3:B:201:THR:HG23	1.78	0.65
3:B:168:THR:HB	3:B:201:THR:HG23	1.78	0.65
3:B:168:THR:HB	3:B:201:THR:HG23	1.78	0.65
1:C:433:LEU:HG	1:C:499:PHE:HE2	1.60	0.65
3:B:168:THR:HB	3:B:201:THR:HG23	1.78	0.65
3:B:168:THR:HB	3:B:201:THR:HG23	1.78	0.65
1:C:433:LEU:HG	1:C:499:PHE:HE2	1.60	0.65
2:A:7:ILE:HD11	2:A:137:VAL:HG22	1.78	0.65
2:A:7:ILE:HD11	2:A:137:VAL:HG22	1.78	0.65
1:C:433:LEU:HG	1:C:499:PHE:HE2	1.60	0.65
2:A:7:ILE:HD11	2:A:137:VAL:HG22	1.78	0.65
2:A:7:ILE:HD11	2:A:137:VAL:HG22	1.78	0.65
2:A:7:ILE:HD11	2:A:137:VAL:HG22	1.78	0.65
1:C:433:LEU:HG	1:C:499:PHE:HE2	1.60	0.65
1:C:433:LEU:HG	1:C:499:PHE:HE2	1.60	0.65
3:B:69:ASP:HA	3:B:145:THR:HG21	1.78	0.65
3:B:135:PHE:HB2	3:B:166:MET:SD	2.37	0.65
3:B:69:ASP:HA	3:B:145:THR:HG21	1.78	0.65
3:B:135:PHE:HB2	3:B:166:MET:SD	2.37	0.65
3:B:69:ASP:HA	3:B:145:THR:HG21	1.78	0.65
3:B:135:PHE:HB2	3:B:166:MET:SD	2.37	0.65
1:C:424:LYS:NZ	3:B:163:ASP:HA	2.12	0.65
3:B:69:ASP:HA	3:B:145:THR:HG21	1.78	0.65
3:B:135:PHE:HB2	3:B:166:MET:SD	2.37	0.65
3:B:69:ASP:HA	3:B:145:THR:HG21	1.78	0.65
3:B:135:PHE:HB2	3:B:166:MET:SD	2.37	0.65
3:B:242:LEU:HD22	3:B:250:ALA:HB3	1.79	0.65
3:B:242:LEU:HD22	3:B:250:ALA:HB3	1.79	0.65
3:B:242:LEU:HD22	3:B:250:ALA:HB3	1.79	0.65
3:B:242:LEU:HD22	3:B:250:ALA:HB3	1.79	0.65
3:B:242:LEU:HD22	3:B:250:ALA:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:GLY:HA2	1:C:401:SER:HB3	1.79	0.65
1:C:150:GLY:HA2	1:C:401:SER:HB3	1.79	0.65
2:A:129:CYS:SG	2:A:132:LEU:HB3	2.37	0.64
2:A:129:CYS:SG	2:A:132:LEU:HB3	2.37	0.64
1:C:150:GLY:HA2	1:C:401:SER:HB3	1.79	0.64
2:A:129:CYS:SG	2:A:132:LEU:HB3	2.37	0.64
2:A:129:CYS:SG	2:A:132:LEU:HB3	2.37	0.64
2:A:129:CYS:SG	2:A:132:LEU:HB3	2.37	0.64
1:C:150:GLY:HA2	1:C:401:SER:HB3	1.79	0.64
1:C:150:GLY:HA2	1:C:401:SER:HB3	1.80	0.64
1:C:64:VAL:HG11	1:C:440:ILE:HG23	1.79	0.64
1:C:64:VAL:HG11	1:C:440:ILE:HG23	1.79	0.64
1:C:64:VAL:HG11	1:C:440:ILE:HG23	1.79	0.64
1:C:66:VAL:HG21	1:C:500:SER:HB3	1.78	0.64
1:C:413:ARG:HD2	1:C:413:ARG:O	1.96	0.64
1:C:390:LEU:N	1:C:390:LEU:HD12	2.12	0.64
3:B:254:LYS:HE3	3:B:352:LYS:CE	2.27	0.64
1:C:64:VAL:HG11	1:C:440:ILE:HG23	1.79	0.64
3:B:254:LYS:HE3	3:B:352:LYS:CE	2.27	0.64
1:C:66:VAL:HG21	1:C:500:SER:HB3	1.78	0.64
3:B:254:LYS:HE3	3:B:352:LYS:CE	2.27	0.64
1:C:66:VAL:HG21	1:C:500:SER:HB3	1.78	0.64
3:B:254:LYS:HE3	3:B:352:LYS:CE	2.27	0.64
3:B:254:LYS:HE3	3:B:352:LYS:CE	2.27	0.64
1:C:64:VAL:HG11	1:C:440:ILE:HG23	1.79	0.64
3:B:119:LEU:HD21	3:B:156:LYS:HB3	1.79	0.64
1:C:66:VAL:HG21	1:C:500:SER:HB3	1.78	0.64
1:C:424:LYS:NZ	3:B:163:ASP:HA	2.13	0.64
3:B:119:LEU:HD21	3:B:156:LYS:HB3	1.79	0.64
3:B:119:LEU:HD21	3:B:156:LYS:HB3	1.79	0.64
1:C:390:LEU:N	1:C:390:LEU:HD12	2.12	0.64
3:B:119:LEU:HD21	3:B:156:LYS:HB3	1.79	0.64
3:B:119:LEU:HD21	3:B:156:LYS:HB3	1.79	0.64
1:C:66:VAL:HG21	1:C:500:SER:HB3	1.79	0.64
1:C:77:GLU:HB3	1:C:486:CYS:SG	2.38	0.64
1:C:390:LEU:N	1:C:390:LEU:HD12	2.12	0.64
1:C:427:GLY:HA3	2:A:410:GLY:O	1.98	0.64
1:C:390:LEU:N	1:C:390:LEU:HD12	2.12	0.64
1:C:77:GLU:HB3	1:C:486:CYS:SG	2.38	0.64
1:C:390:LEU:N	1:C:390:LEU:HD12	2.12	0.64
1:C:77:GLU:HB3	1:C:486:CYS:SG	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:89:PRO:HA	3:B:92:PHE:HD2	1.62	0.64
3:B:89:PRO:HA	3:B:92:PHE:HD2	1.62	0.64
1:C:77:GLU:HB3	1:C:486:CYS:SG	2.38	0.64
3:B:89:PRO:HA	3:B:92:PHE:HD2	1.62	0.64
1:C:77:GLU:HB3	1:C:486:CYS:SG	2.38	0.64
3:B:89:PRO:HA	3:B:92:PHE:HD2	1.62	0.64
3:B:89:PRO:HA	3:B:92:PHE:HD2	1.62	0.64
1:C:362:ARG:O	1:C:365:GLN:HG3	1.97	0.64
7:B:601:TA1:H463	7:B:601:TA1:H261	1.80	0.64
1:C:362:ARG:O	1:C:365:GLN:HG3	1.97	0.64
7:B:601:TA1:H463	7:B:601:TA1:H261	1.80	0.64
7:B:601:TA1:H463	7:B:601:TA1:H261	1.80	0.64
1:C:362:ARG:O	1:C:365:GLN:HG3	1.97	0.64
7:B:601:TA1:H463	7:B:601:TA1:H261	1.80	0.64
1:C:362:ARG:O	1:C:365:GLN:HG3	1.97	0.64
7:B:601:TA1:H463	7:B:601:TA1:H261	1.80	0.64
1:C:453:GLN:HB2	3:B:434:GLN:HE22	1.63	0.64
2:A:7:ILE:HG13	2:A:137:VAL:HA	1.80	0.64
2:A:7:ILE:HG13	2:A:137:VAL:HA	1.80	0.64
1:C:362:ARG:O	1:C:365:GLN:HG3	1.97	0.64
2:A:7:ILE:HG13	2:A:137:VAL:HA	1.80	0.64
2:A:7:ILE:HG13	2:A:137:VAL:HA	1.80	0.64
2:A:7:ILE:HG13	2:A:137:VAL:HA	1.80	0.64
3:B:206:ASN:ND2	6:B:600:GDP:O2'	2.31	0.63
3:B:206:ASN:ND2	6:B:600:GDP:O2'	2.31	0.63
3:B:206:ASN:ND2	6:B:600:GDP:O2'	2.31	0.63
3:B:206:ASN:ND2	6:B:600:GDP:O2'	2.31	0.63
3:B:206:ASN:ND2	6:B:600:GDP:O2'	2.31	0.63
3:B:140:SER:HA	3:B:171:VAL:HB	1.79	0.63
3:B:140:SER:HA	3:B:171:VAL:HB	1.79	0.63
3:B:140:SER:HA	3:B:171:VAL:HB	1.79	0.63
3:B:140:SER:HA	3:B:171:VAL:HB	1.79	0.63
3:B:140:SER:HA	3:B:171:VAL:HB	1.79	0.63
1:C:453:GLN:HB2	3:B:434:GLN:HE22	1.63	0.63
1:C:427:GLY:HA3	2:A:410:GLY:O	1.99	0.63
1:C:378:ARG:HH11	1:C:378:ARG:HB3	1.64	0.63
1:C:453:GLN:HB2	3:B:434:GLN:HE22	1.64	0.63
1:C:453:GLN:HB2	3:B:434:GLN:HE22	1.63	0.63
1:C:297:ARG:HG2	1:C:298:PHE:H	1.64	0.63
1:C:297:ARG:HG2	1:C:298:PHE:H	1.64	0.63
1:C:126:PHE:HD2	1:C:130:VAL:HG11	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ASN:ND2	1:C:422:ARG:HD3	2.13	0.63
1:C:126:PHE:HD2	1:C:130:VAL:HG11	1.64	0.62
1:C:377:SER:C	1:C:378:ARG:HD2	2.19	0.62
1:C:126:PHE:HD2	1:C:130:VAL:HG11	1.64	0.62
1:C:297:ARG:HG2	1:C:298:PHE:H	1.64	0.62
1:C:126:PHE:HD2	1:C:130:VAL:HG11	1.64	0.62
1:C:297:ARG:HG2	1:C:298:PHE:H	1.64	0.62
1:C:297:ARG:HG2	1:C:298:PHE:H	1.64	0.62
1:C:126:PHE:HD2	1:C:130:VAL:HG11	1.64	0.62
1:C:423:LEU:HD13	3:B:163:ASP:HB2	1.82	0.62
2:A:224:TYR:CZ	4:A:500:GTP:N7	2.68	0.62
2:A:224:TYR:CZ	4:A:500:GTP:C5	2.88	0.62
2:A:224:TYR:CZ	4:A:500:GTP:N7	2.68	0.62
2:A:224:TYR:CZ	4:A:500:GTP:C5	2.88	0.62
2:A:224:TYR:CZ	4:A:500:GTP:N7	2.68	0.62
2:A:224:TYR:CZ	4:A:500:GTP:C5	2.88	0.62
2:A:224:TYR:CZ	4:A:500:GTP:N7	2.68	0.62
2:A:224:TYR:CZ	4:A:500:GTP:C5	2.88	0.62
2:A:224:TYR:CZ	4:A:500:GTP:N7	2.68	0.62
2:A:224:TYR:CZ	4:A:500:GTP:C5	2.88	0.62
1:C:148:LEU:HD13	1:C:189:SER:HB3	1.79	0.62
1:C:148:LEU:HD13	1:C:189:SER:HB3	1.80	0.62
1:C:148:LEU:HD13	1:C:189:SER:HB3	1.80	0.62
1:C:148:LEU:HD13	1:C:189:SER:HB3	1.80	0.62
1:C:148:LEU:HD13	1:C:189:SER:HB3	1.80	0.62
1:C:147:VAL:HG11	1:C:403:LEU:HB2	1.82	0.61
1:C:147:VAL:HG11	1:C:403:LEU:HB2	1.82	0.61
1:C:453:GLN:HB2	3:B:434:GLN:HE22	1.65	0.61
3:B:11:GLN:HA	3:B:74:THR:HG21	1.82	0.61
3:B:11:GLN:HA	3:B:74:THR:HG21	1.82	0.61
1:C:147:VAL:HG11	1:C:403:LEU:HB2	1.82	0.61
3:B:11:GLN:HA	3:B:74:THR:HG21	1.82	0.61
1:C:147:VAL:HG11	1:C:403:LEU:HB2	1.82	0.61
3:B:11:GLN:HA	3:B:74:THR:HG21	1.82	0.61
1:C:147:VAL:HG11	1:C:403:LEU:HB2	1.82	0.61
3:B:11:GLN:HA	3:B:74:THR:HG21	1.82	0.61
3:B:216:THR:HB	3:B:275:LEU:HD12	1.82	0.61
3:B:216:THR:HB	3:B:275:LEU:HD12	1.82	0.61
1:C:64:VAL:HG11	1:C:440:ILE:CG2	2.30	0.61
1:C:413:ARG:NE	2:A:414:GLU:OE2	2.33	0.61
3:B:216:THR:HB	3:B:275:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:VAL:HG11	1:C:440:ILE:CG2	2.30	0.61
3:B:216:THR:HB	3:B:275:LEU:HD12	1.82	0.61
1:C:64:VAL:HG11	1:C:440:ILE:CG2	2.30	0.61
3:B:216:THR:HB	3:B:275:LEU:HD12	1.82	0.61
2:A:271:THR:HB	2:A:377:MET:HB3	1.82	0.61
1:C:64:VAL:HG11	1:C:440:ILE:CG2	2.30	0.61
2:A:271:THR:HB	2:A:377:MET:HB3	1.82	0.61
2:A:271:THR:HB	2:A:377:MET:HB3	1.82	0.61
2:A:271:THR:HB	2:A:377:MET:HB3	1.82	0.61
2:A:271:THR:HB	2:A:377:MET:HB3	1.82	0.61
1:C:64:VAL:HG11	1:C:440:ILE:CG2	2.30	0.61
3:B:209:LEU:HD23	3:B:227:LEU:HB3	1.82	0.61
3:B:209:LEU:HD23	3:B:227:LEU:HB3	1.82	0.61
3:B:209:LEU:HD23	3:B:227:LEU:HB3	1.82	0.61
3:B:209:LEU:HD23	3:B:227:LEU:HB3	1.82	0.61
3:B:209:LEU:HD23	3:B:227:LEU:HB3	1.82	0.61
2:A:224:TYR:OH	4:A:500:GTP:C8	2.53	0.61
2:A:224:TYR:OH	4:A:500:GTP:C8	2.53	0.61
2:A:224:TYR:OH	4:A:500:GTP:C8	2.53	0.61
1:C:328:LEU:HD13	1:C:340:VAL:HG11	1.82	0.61
2:A:224:TYR:OH	4:A:500:GTP:C8	2.53	0.61
2:A:224:TYR:OH	4:A:500:GTP:C8	2.53	0.61
3:B:382:THR:HA	3:B:432:TYR:HD2	1.64	0.60
3:B:382:THR:HA	3:B:432:TYR:HD2	1.64	0.60
3:B:382:THR:HA	3:B:432:TYR:HD2	1.64	0.60
3:B:382:THR:HA	3:B:432:TYR:HD2	1.64	0.60
3:B:382:THR:HA	3:B:432:TYR:HD2	1.64	0.60
3:B:10:GLY:HA2	3:B:145:THR:HB	1.84	0.60
3:B:10:GLY:HA2	3:B:145:THR:HB	1.84	0.60
3:B:10:GLY:HA2	3:B:145:THR:HB	1.84	0.60
1:C:95:LEU:HD21	1:C:125:ILE:HG13	1.83	0.60
3:B:10:GLY:HA2	3:B:145:THR:HB	1.84	0.60
3:B:10:GLY:HA2	3:B:145:THR:HB	1.84	0.60
1:C:95:LEU:HD21	1:C:125:ILE:HG13	1.83	0.60
1:C:95:LEU:HD21	1:C:125:ILE:HG13	1.83	0.60
1:C:95:LEU:HD21	1:C:125:ILE:HG13	1.83	0.60
1:C:95:LEU:HD21	1:C:125:ILE:HG13	1.84	0.60
1:C:380:HIS:HD2	1:C:408:LEU:HG	1.66	0.60
1:C:380:HIS:HD2	1:C:408:LEU:HG	1.66	0.60
1:C:380:HIS:HD2	1:C:408:LEU:HG	1.66	0.60
1:C:424:LYS:HZ1	3:B:163:ASP:HA	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:204:VAL:HG11	2:A:231:ILE:HD12	1.83	0.60
3:B:360:PRO:HB2	7:B:601:TA1:C28	2.31	0.60
2:A:204:VAL:HG11	2:A:231:ILE:HD12	1.83	0.60
3:B:360:PRO:HB2	7:B:601:TA1:C28	2.31	0.60
2:A:204:VAL:HG11	2:A:231:ILE:HD12	1.83	0.60
3:B:360:PRO:HB2	7:B:601:TA1:C28	2.31	0.60
1:C:380:HIS:HD2	1:C:408:LEU:HG	1.66	0.60
2:A:204:VAL:HG11	2:A:231:ILE:HD12	1.83	0.60
3:B:360:PRO:HB2	7:B:601:TA1:C28	2.31	0.60
1:C:380:HIS:HD2	1:C:408:LEU:HG	1.66	0.60
2:A:204:VAL:HG11	2:A:231:ILE:HD12	1.83	0.60
3:B:360:PRO:HB2	7:B:601:TA1:C28	2.31	0.60
1:C:303:SER:HA	1:C:316:LEU:HD12	1.84	0.60
2:A:312:TYR:HA	2:A:381:THR:HG22	1.84	0.60
1:C:303:SER:HA	1:C:316:LEU:HD12	1.84	0.60
2:A:312:TYR:HA	2:A:381:THR:HG22	1.84	0.60
2:A:312:TYR:HA	2:A:381:THR:HG22	1.84	0.60
2:A:312:TYR:HA	2:A:381:THR:HG22	1.84	0.60
2:A:312:TYR:HA	2:A:381:THR:HG22	1.84	0.60
1:C:303:SER:HA	1:C:316:LEU:HD12	1.84	0.60
1:C:303:SER:HA	1:C:316:LEU:HD12	1.84	0.60
1:C:303:SER:HA	1:C:316:LEU:HD12	1.84	0.60
1:C:120:PHE:HB3	1:C:122:PHE:CE2	2.37	0.59
1:C:120:PHE:HB3	1:C:122:PHE:CE2	2.37	0.59
1:C:120:PHE:HB3	1:C:122:PHE:CE2	2.37	0.59
1:C:120:PHE:HB3	1:C:122:PHE:CE2	2.37	0.59
2:A:224:TYR:CD1	4:A:500:GTP:C5	2.87	0.59
2:A:224:TYR:CD1	4:A:500:GTP:C5	2.87	0.59
1:C:120:PHE:HB3	1:C:122:PHE:CE2	2.37	0.59
2:A:224:TYR:CD1	4:A:500:GTP:C5	2.87	0.59
2:A:224:TYR:CD1	4:A:500:GTP:C5	2.87	0.59
2:A:224:TYR:CD1	4:A:500:GTP:C5	2.87	0.59
2:A:224:TYR:CD1	4:A:500:GTP:C5	2.87	0.59
3:B:179:ASP:HB2	6:B:600:GDP:H3'	1.84	0.59
3:B:179:ASP:HB2	6:B:600:GDP:H3'	1.84	0.59
3:B:179:ASP:HB2	6:B:600:GDP:H3'	1.84	0.59
3:B:179:ASP:HB2	6:B:600:GDP:H3'	1.84	0.59
3:B:179:ASP:HB2	6:B:600:GDP:H3'	1.84	0.59
1:C:424:LYS:HD2	1:C:428:ASN:OD1	2.02	0.59
1:C:412:GLU:HG3	1:C:426:ALA:HB1	1.84	0.59
1:C:424:LYS:HD2	1:C:428:ASN:OD1	2.02	0.59
1:C:424:LYS:HD2	1:C:428:ASN:OD1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:LYS:HD2	1:C:428:ASN:OD1	2.02	0.59
1:C:424:LYS:HD2	1:C:428:ASN:OD1	2.02	0.59
2:A:168:GLU:HG3	2:A:201:ALA:HA	1.85	0.59
2:A:168:GLU:HG3	2:A:201:ALA:HA	1.85	0.59
2:A:168:GLU:HG3	2:A:201:ALA:HA	1.85	0.59
2:A:168:GLU:HG3	2:A:201:ALA:HA	1.85	0.59
2:A:168:GLU:HG3	2:A:201:ALA:HA	1.85	0.59
1:C:455:LEU:HD11	3:B:431:GLU:HA	1.83	0.59
3:B:273:ALA:HB3	3:B:274:PRO:HD3	1.85	0.59
3:B:273:ALA:HB3	3:B:274:PRO:HD3	1.85	0.59
3:B:273:ALA:HB3	3:B:274:PRO:HD3	1.85	0.59
3:B:273:ALA:HB3	3:B:274:PRO:HD3	1.85	0.59
3:B:273:ALA:HB3	3:B:274:PRO:HD3	1.85	0.59
3:B:63:PRO:HD3	3:B:86:ILE:HG12	1.84	0.59
3:B:63:PRO:HD3	3:B:86:ILE:HG12	1.84	0.59
3:B:63:PRO:HD3	3:B:86:ILE:HG12	1.84	0.59
3:B:63:PRO:HD3	3:B:86:ILE:HG12	1.84	0.59
1:C:319:PRO:HA	1:C:364:ASN:OD1	2.03	0.59
3:B:63:PRO:HD3	3:B:86:ILE:HG12	1.84	0.59
3:B:297:ASP:OD1	3:B:299:LYS:HG2	2.02	0.58
3:B:297:ASP:OD1	3:B:299:LYS:HG2	2.02	0.58
3:B:297:ASP:OD1	3:B:299:LYS:HG2	2.02	0.58
3:B:297:ASP:OD1	3:B:299:LYS:HG2	2.02	0.58
3:B:297:ASP:OD1	3:B:299:LYS:HG2	2.02	0.58
2:A:224:TYR:OH	4:A:500:GTP:H2'	2.02	0.58
1:C:377:SER:O	1:C:378:ARG:HD2	2.03	0.58
2:A:224:TYR:OH	4:A:500:GTP:H2'	2.02	0.58
2:A:224:TYR:OH	4:A:500:GTP:H2'	2.02	0.58
2:A:224:TYR:OH	4:A:500:GTP:H2'	2.02	0.58
2:A:224:TYR:OH	4:A:500:GTP:H2'	2.02	0.58
2:A:237:SER:HA	2:A:241:SER:OG	2.02	0.58
2:A:237:SER:HA	2:A:241:SER:OG	2.02	0.58
2:A:237:SER:HA	2:A:241:SER:OG	2.02	0.58
2:A:237:SER:HA	2:A:241:SER:OG	2.02	0.58
1:C:455:LEU:HD11	3:B:431:GLU:HA	1.84	0.58
2:A:237:SER:HA	2:A:241:SER:OG	2.02	0.58
1:C:316:LEU:O	1:C:317:GLU:HB2	2.03	0.58
1:C:316:LEU:O	1:C:317:GLU:HB2	2.03	0.58
1:C:301:TRP:HE1	1:C:345:TRP:HA	1.68	0.58
3:B:19:LYS:HG3	3:B:228:ASN:HB2	1.86	0.58
3:B:103:TRP:HZ2	3:B:151:THR:HG21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:TRP:HE1	1:C:345:TRP:HA	1.69	0.58
1:C:378:ARG:HH12	1:C:412:GLU:HG2	1.69	0.58
3:B:19:LYS:HG3	3:B:228:ASN:HB2	1.86	0.58
3:B:103:TRP:HZ2	3:B:151:THR:HG21	1.69	0.58
1:C:301:TRP:HE1	1:C:345:TRP:HA	1.68	0.58
3:B:19:LYS:HG3	3:B:228:ASN:HB2	1.86	0.58
3:B:103:TRP:HZ2	3:B:151:THR:HG21	1.69	0.58
1:C:301:TRP:HE1	1:C:345:TRP:HA	1.68	0.58
3:B:19:LYS:HG3	3:B:228:ASN:HB2	1.86	0.58
3:B:103:TRP:HZ2	3:B:151:THR:HG21	1.69	0.58
3:B:19:LYS:HG3	3:B:228:ASN:HB2	1.86	0.58
3:B:103:TRP:HZ2	3:B:151:THR:HG21	1.69	0.58
1:C:301:TRP:HE1	1:C:345:TRP:HA	1.69	0.58
1:C:186:ILE:CD1	1:C:387:ILE:HD11	2.33	0.58
1:C:186:ILE:CD1	1:C:387:ILE:HD11	2.33	0.57
1:C:302:ILE:HD12	1:C:348:VAL:HG21	1.86	0.57
1:C:186:ILE:CD1	1:C:387:ILE:HD11	2.33	0.57
1:C:186:ILE:CD1	1:C:387:ILE:HD11	2.33	0.57
1:C:302:ILE:HD12	1:C:348:VAL:HG21	1.86	0.57
1:C:186:ILE:CD1	1:C:387:ILE:HD11	2.33	0.57
1:C:302:ILE:HD12	1:C:348:VAL:HG21	1.86	0.57
1:C:302:ILE:HD12	1:C:348:VAL:HG21	1.86	0.57
1:C:302:ILE:HD12	1:C:348:VAL:HG21	1.86	0.57
1:C:307:ILE:HG21	1:C:463:LEU:HD11	1.86	0.57
1:C:307:ILE:HG21	1:C:463:LEU:HD11	1.86	0.57
1:C:307:ILE:HG21	1:C:463:LEU:HD11	1.86	0.57
1:C:307:ILE:HG21	1:C:463:LEU:HD11	1.86	0.57
1:C:315:LEU:CD1	1:C:364:ASN:HB2	2.33	0.57
1:C:455:LEU:HD11	3:B:431:GLU:HA	1.85	0.57
1:C:307:ILE:HG21	1:C:463:LEU:HD11	1.86	0.57
1:C:315:LEU:CD1	1:C:364:ASN:HB2	2.33	0.57
1:C:315:LEU:CD1	1:C:364:ASN:HB2	2.33	0.57
1:C:315:LEU:CD1	1:C:364:ASN:HB2	2.33	0.57
1:C:315:LEU:CD1	1:C:364:ASN:HB2	2.33	0.57
2:A:179:THR:CG2	4:A:500:GTP:C2'	2.83	0.57
2:A:179:THR:CG2	4:A:500:GTP:C2'	2.83	0.57
1:C:424:LYS:HZ1	3:B:163:ASP:HA	1.70	0.57
2:A:179:THR:CG2	4:A:500:GTP:C2'	2.83	0.57
2:A:179:THR:CG2	4:A:500:GTP:C2'	2.83	0.57
2:A:179:THR:CG2	4:A:500:GTP:C2'	2.83	0.57
2:A:360:PRO:HG3	2:A:374:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:230:LEU:HD12	7:B:601:TA1:H081	1.86	0.56
2:A:360:PRO:HG3	2:A:374:ALA:HB2	1.88	0.56
3:B:230:LEU:HD12	7:B:601:TA1:H081	1.86	0.56
2:A:360:PRO:HG3	2:A:374:ALA:HB2	1.88	0.56
3:B:230:LEU:HD12	7:B:601:TA1:H081	1.86	0.56
2:A:360:PRO:HG3	2:A:374:ALA:HB2	1.88	0.56
3:B:230:LEU:HD12	7:B:601:TA1:H081	1.86	0.56
2:A:360:PRO:HG3	2:A:374:ALA:HB2	1.88	0.56
3:B:230:LEU:HD12	7:B:601:TA1:H081	1.86	0.56
3:B:260:VAL:HG12	3:B:266:HIS:HB2	1.87	0.56
3:B:311:ARG:HD2	3:B:342:TYR:HA	1.88	0.56
3:B:260:VAL:HG12	3:B:266:HIS:HB2	1.87	0.56
3:B:311:ARG:HD2	3:B:342:TYR:HA	1.88	0.56
3:B:260:VAL:HG12	3:B:266:HIS:HB2	1.87	0.56
3:B:311:ARG:HD2	3:B:342:TYR:HA	1.88	0.56
3:B:260:VAL:HG12	3:B:266:HIS:HB2	1.87	0.56
3:B:311:ARG:HD2	3:B:342:TYR:HA	1.88	0.56
3:B:260:VAL:HG12	3:B:266:HIS:HB2	1.87	0.56
3:B:311:ARG:HD2	3:B:342:TYR:HA	1.88	0.56
1:C:424:LYS:HZ1	3:B:163:ASP:HA	1.71	0.56
2:A:141:PHE:HE2	2:A:388:TRP:HH2	1.54	0.56
3:B:89:PRO:HA	3:B:92:PHE:CD2	2.38	0.56
1:C:329:ARG:CZ	1:C:331:CYS:HB2	2.35	0.56
2:A:141:PHE:HE2	2:A:388:TRP:HH2	1.54	0.56
3:B:89:PRO:HA	3:B:92:PHE:CD2	2.38	0.56
1:C:329:ARG:CZ	1:C:331:CYS:HB2	2.35	0.56
2:A:141:PHE:HE2	2:A:388:TRP:HH2	1.54	0.56
3:B:89:PRO:HA	3:B:92:PHE:CD2	2.38	0.56
1:C:329:ARG:CZ	1:C:331:CYS:HB2	2.35	0.56
2:A:141:PHE:HE2	2:A:388:TRP:HH2	1.54	0.56
3:B:89:PRO:HA	3:B:92:PHE:CD2	2.38	0.56
1:C:329:ARG:CZ	1:C:331:CYS:HB2	2.35	0.56
2:A:141:PHE:HE2	2:A:388:TRP:HH2	1.54	0.56
3:B:89:PRO:HA	3:B:92:PHE:CD2	2.38	0.56
1:C:329:ARG:CZ	1:C:331:CYS:HB2	2.35	0.56
2:A:141:PHE:HE2	2:A:388:TRP:HH2	1.54	0.56
3:B:89:PRO:HA	3:B:92:PHE:CD2	2.38	0.56
1:C:329:ARG:CZ	1:C:331:CYS:HB2	2.35	0.56
3:B:12:CYS:SG	6:B:600:GDP:C5	2.99	0.56
3:B:12:CYS:SG	6:B:600:GDP:C5	2.99	0.56
3:B:12:CYS:SG	6:B:600:GDP:C5	2.99	0.56
1:C:160:VAL:HG12	1:C:161:THR:H	1.70	0.56
3:B:12:CYS:SG	6:B:600:GDP:C5	2.99	0.56
3:B:12:CYS:SG	6:B:600:GDP:C5	2.99	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:VAL:HG12	1:C:161:THR:H	1.70	0.56
1:C:160:VAL:HG12	1:C:161:THR:H	1.70	0.56
1:C:160:VAL:HG12	1:C:161:THR:H	1.70	0.56
1:C:160:VAL:HG12	1:C:161:THR:H	1.70	0.56
2:A:70:LEU:HB3	2:A:99:ALA:HA	1.86	0.56
2:A:70:LEU:HB3	2:A:99:ALA:HA	1.86	0.56
2:A:70:LEU:HB3	2:A:99:ALA:HA	1.86	0.56
2:A:70:LEU:HB3	2:A:99:ALA:HA	1.86	0.56
2:A:70:LEU:HB3	2:A:99:ALA:HA	1.86	0.56
1:C:455:LEU:HD11	3:B:431:GLU:HA	1.87	0.56
2:A:409:VAL:HA	2:A:413:MET:O	2.06	0.55
1:C:455:LEU:HD11	3:B:431:GLU:HA	1.86	0.55
2:A:409:VAL:HA	2:A:413:MET:O	2.06	0.55
2:A:409:VAL:HA	2:A:413:MET:O	2.06	0.55
2:A:409:VAL:HA	2:A:413:MET:O	2.06	0.55
2:A:409:VAL:HA	2:A:413:MET:O	2.06	0.55
1:C:424:LYS:HZ1	3:B:163:ASP:HA	1.71	0.55
1:C:187:PHE:HA	1:C:190:LEU:HD13	1.87	0.55
1:C:187:PHE:HA	1:C:190:LEU:HD13	1.87	0.55
1:C:187:PHE:HA	1:C:190:LEU:HD13	1.87	0.55
1:C:187:PHE:HA	1:C:190:LEU:HD13	1.87	0.55
1:C:187:PHE:HA	1:C:190:LEU:HD13	1.87	0.55
1:C:360:VAL:HG13	1:C:361:GLY:N	2.21	0.55
3:B:11:GLN:CB	6:B:600:GDP:O2B	2.55	0.55
3:B:20:PHE:HA	3:B:232:SER:HB2	1.89	0.55
3:B:11:GLN:CB	6:B:600:GDP:O2B	2.55	0.55
3:B:20:PHE:HA	3:B:232:SER:HB2	1.89	0.55
1:C:360:VAL:HG13	1:C:361:GLY:N	2.21	0.55
3:B:11:GLN:CB	6:B:600:GDP:O2B	2.55	0.55
3:B:20:PHE:HA	3:B:232:SER:HB2	1.89	0.55
3:B:11:GLN:CB	6:B:600:GDP:O2B	2.55	0.55
3:B:20:PHE:HA	3:B:232:SER:HB2	1.89	0.55
3:B:11:GLN:CB	6:B:600:GDP:O2B	2.55	0.55
3:B:20:PHE:HA	3:B:232:SER:HB2	1.89	0.55
1:C:360:VAL:HG13	1:C:361:GLY:N	2.21	0.55
1:C:360:VAL:HG13	1:C:361:GLY:N	2.21	0.55
1:C:378:ARG:HB3	1:C:378:ARG:NH1	2.22	0.55
1:C:360:VAL:HG13	1:C:361:GLY:N	2.21	0.55
1:C:95:LEU:HD11	1:C:125:ILE:HG13	1.89	0.55
1:C:95:LEU:HD11	1:C:125:ILE:HG13	1.89	0.55
2:A:105:ARG:HA	2:A:109:THR:OG1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:183:GLU:HB3	2:A:184:PRO:HD3	1.88	0.55
2:A:105:ARG:HA	2:A:109:THR:OG1	2.07	0.55
2:A:183:GLU:HB3	2:A:184:PRO:HD3	1.88	0.55
1:C:95:LEU:HD11	1:C:125:ILE:HG13	1.89	0.55
2:A:105:ARG:HA	2:A:109:THR:OG1	2.07	0.55
2:A:183:GLU:HB3	2:A:184:PRO:HD3	1.88	0.55
2:A:105:ARG:HA	2:A:109:THR:OG1	2.07	0.55
2:A:183:GLU:HB3	2:A:184:PRO:HD3	1.88	0.55
2:A:105:ARG:HA	2:A:109:THR:OG1	2.07	0.55
2:A:183:GLU:HB3	2:A:184:PRO:HD3	1.88	0.55
2:A:204:VAL:HG13	2:A:302:MET:HG2	1.89	0.55
1:C:95:LEU:HD11	1:C:125:ILE:HG13	1.89	0.55
2:A:204:VAL:HG13	2:A:302:MET:HG2	1.89	0.55
2:A:204:VAL:HG13	2:A:302:MET:HG2	1.89	0.55
2:A:204:VAL:HG13	2:A:302:MET:HG2	1.89	0.55
1:C:95:LEU:HD11	1:C:125:ILE:HG13	1.89	0.55
2:A:204:VAL:HG13	2:A:302:MET:HG2	1.89	0.55
3:B:179:ASP:CB	6:B:600:GDP:H3'	2.38	0.54
3:B:179:ASP:CB	6:B:600:GDP:H3'	2.38	0.54
3:B:179:ASP:CB	6:B:600:GDP:H3'	2.38	0.54
3:B:179:ASP:CB	6:B:600:GDP:H3'	2.38	0.54
3:B:179:ASP:CB	6:B:600:GDP:H3'	2.38	0.54
1:C:348:VAL:HG11	1:C:354:ALA:HB2	1.90	0.54
3:B:21:TRP:HA	3:B:24:ILE:HG22	1.90	0.54
3:B:21:TRP:HA	3:B:24:ILE:HG22	1.90	0.54
3:B:21:TRP:HA	3:B:24:ILE:HG22	1.90	0.54
1:C:455:LEU:HD11	3:B:434:GLN:HG3	1.88	0.54
3:B:21:TRP:HA	3:B:24:ILE:HG22	1.90	0.54
3:B:21:TRP:HA	3:B:24:ILE:HG22	1.90	0.54
2:A:72:PRO:HA	2:A:94:THR:HG22	1.90	0.54
2:A:234:ILE:O	2:A:238:ILE:HG12	2.07	0.54
3:B:295:MET:HG2	3:B:377:PHE:HB2	1.89	0.54
1:C:348:VAL:HG11	1:C:354:ALA:HB2	1.90	0.54
2:A:72:PRO:HA	2:A:94:THR:HG22	1.90	0.54
2:A:234:ILE:O	2:A:238:ILE:HG12	2.07	0.54
3:B:295:MET:HG2	3:B:377:PHE:HB2	1.89	0.54
2:A:72:PRO:HA	2:A:94:THR:HG22	1.90	0.54
2:A:234:ILE:O	2:A:238:ILE:HG12	2.07	0.54
3:B:295:MET:HG2	3:B:377:PHE:HB2	1.89	0.54
1:C:348:VAL:HG11	1:C:354:ALA:HB2	1.90	0.54
2:A:72:PRO:HA	2:A:94:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:234:ILE:O	2:A:238:ILE:HG12	2.07	0.54
3:B:295:MET:HG2	3:B:377:PHE:HB2	1.89	0.54
1:C:348:VAL:HG11	1:C:354:ALA:HB2	1.90	0.54
2:A:72:PRO:HA	2:A:94:THR:HG22	1.90	0.54
2:A:234:ILE:O	2:A:238:ILE:HG12	2.07	0.54
3:B:295:MET:HG2	3:B:377:PHE:HB2	1.89	0.54
1:C:348:VAL:HG11	1:C:354:ALA:HB2	1.90	0.54
1:C:433:LEU:HG	1:C:499:PHE:CE2	2.42	0.54
2:A:179:THR:HG21	4:A:500:GTP:O2'	2.08	0.54
2:A:179:THR:HG21	4:A:500:GTP:O2'	2.08	0.54
1:C:433:LEU:HG	1:C:499:PHE:CE2	2.42	0.54
2:A:179:THR:HG21	4:A:500:GTP:O2'	2.08	0.54
2:A:179:THR:HG21	4:A:500:GTP:O2'	2.08	0.54
1:C:433:LEU:HG	1:C:499:PHE:CE2	2.42	0.54
2:A:179:THR:HG21	4:A:500:GTP:O2'	2.08	0.54
1:C:315:LEU:HD12	1:C:364:ASN:HB2	1.89	0.54
1:C:433:LEU:HG	1:C:499:PHE:CE2	2.42	0.54
1:C:315:LEU:HD12	1:C:364:ASN:HB2	1.89	0.54
1:C:433:LEU:HG	1:C:499:PHE:CE2	2.42	0.54
1:C:315:LEU:HD12	1:C:364:ASN:HB2	1.89	0.54
1:C:315:LEU:HD12	1:C:364:ASN:HB2	1.89	0.54
1:C:315:LEU:HD12	1:C:364:ASN:HB2	1.89	0.54
3:B:6:HIS:O	3:B:65:ALA:HA	2.08	0.53
3:B:142:GLY:HA3	3:B:183:GLU:HG3	1.89	0.53
3:B:6:HIS:O	3:B:65:ALA:HA	2.08	0.53
3:B:142:GLY:HA3	3:B:183:GLU:HG3	1.89	0.53
3:B:6:HIS:O	3:B:65:ALA:HA	2.08	0.53
3:B:142:GLY:HA3	3:B:183:GLU:HG3	1.89	0.53
3:B:6:HIS:O	3:B:65:ALA:HA	2.08	0.53
3:B:142:GLY:HA3	3:B:183:GLU:HG3	1.89	0.53
3:B:6:HIS:O	3:B:65:ALA:HA	2.08	0.53
3:B:142:GLY:HA3	3:B:183:GLU:HG3	1.89	0.53
3:B:250:ALA:CA	3:B:254:LYS:HD3	2.33	0.53
1:C:413:ARG:NH1	2:A:108:TYR:CE2	2.76	0.53
3:B:250:ALA:CA	3:B:254:LYS:HD3	2.33	0.53
3:B:250:ALA:CA	3:B:254:LYS:HD3	2.33	0.53
3:B:250:ALA:CA	3:B:254:LYS:HD3	2.33	0.53
3:B:250:ALA:CA	3:B:254:LYS:HD3	2.33	0.53
3:B:277:SER:OG	3:B:281:GLN:HB2	2.09	0.53
3:B:291:LEU:HD21	3:B:373:MET:HG2	1.89	0.53
1:C:380:HIS:CD2	1:C:408:LEU:HG	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:277:SER:OG	3:B:281:GLN:HB2	2.09	0.53
3:B:291:LEU:HD21	3:B:373:MET:HG2	1.89	0.53
1:C:380:HIS:CD2	1:C:408:LEU:HG	2.43	0.53
3:B:277:SER:OG	3:B:281:GLN:HB2	2.09	0.53
3:B:291:LEU:HD21	3:B:373:MET:HG2	1.89	0.53
1:C:380:HIS:CD2	1:C:408:LEU:HG	2.43	0.53
3:B:277:SER:OG	3:B:281:GLN:HB2	2.09	0.53
3:B:291:LEU:HD21	3:B:373:MET:HG2	1.89	0.53
3:B:277:SER:OG	3:B:281:GLN:HB2	2.09	0.53
3:B:291:LEU:HD21	3:B:373:MET:HG2	1.89	0.53
1:C:380:HIS:CD2	1:C:408:LEU:HG	2.43	0.53
1:C:380:HIS:CD2	1:C:408:LEU:HG	2.44	0.53
2:A:177:VAL:HG13	3:B:329:ASP:HB3	1.90	0.53
2:A:269:LEU:HD13	2:A:303:VAL:HG11	1.90	0.53
2:A:319:TYR:HB3	2:A:323:VAL:HG21	1.91	0.53
2:A:177:VAL:HG13	3:B:329:ASP:HB3	1.90	0.53
2:A:269:LEU:HD13	2:A:303:VAL:HG11	1.90	0.53
2:A:319:TYR:HB3	2:A:323:VAL:HG21	1.91	0.53
2:A:177:VAL:HG13	3:B:329:ASP:HB3	1.90	0.53
2:A:269:LEU:HD13	2:A:303:VAL:HG11	1.90	0.53
2:A:319:TYR:HB3	2:A:323:VAL:HG21	1.91	0.53
2:A:177:VAL:HG13	3:B:329:ASP:HB3	1.90	0.53
2:A:269:LEU:HD13	2:A:303:VAL:HG11	1.90	0.53
2:A:319:TYR:HB3	2:A:323:VAL:HG21	1.91	0.53
2:A:177:VAL:HG13	3:B:329:ASP:HB3	1.90	0.53
2:A:269:LEU:HD13	2:A:303:VAL:HG11	1.90	0.53
2:A:319:TYR:HB3	2:A:323:VAL:HG21	1.91	0.53
2:A:179:THR:CG2	4:A:500:GTP:O2'	2.57	0.53
2:A:179:THR:CG2	4:A:500:GTP:O2'	2.57	0.53
2:A:179:THR:CG2	4:A:500:GTP:O2'	2.57	0.53
2:A:179:THR:CG2	4:A:500:GTP:O2'	2.57	0.53
1:C:155:ILE:HG23	1:C:405:LEU:HA	1.91	0.53
2:A:179:THR:CG2	4:A:500:GTP:O2'	2.57	0.53
1:C:155:ILE:HG23	1:C:405:LEU:HA	1.91	0.53
1:C:155:ILE:HG23	1:C:405:LEU:HA	1.91	0.53
1:C:155:ILE:HG23	1:C:405:LEU:HA	1.92	0.52
1:C:155:ILE:HG23	1:C:405:LEU:HA	1.91	0.52
3:B:382:THR:HA	3:B:432:TYR:CD2	2.43	0.52
3:B:382:THR:HA	3:B:432:TYR:CD2	2.43	0.52
3:B:382:THR:HA	3:B:432:TYR:CD2	2.43	0.52
1:C:90:GLU:O	1:C:91:ASN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:382:THR:HA	3:B:432:TYR:CD2	2.43	0.52
1:C:90:GLU:O	1:C:91:ASN:HB2	2.09	0.52
3:B:382:THR:HA	3:B:432:TYR:CD2	2.43	0.52
1:C:90:GLU:O	1:C:91:ASN:HB2	2.09	0.52
1:C:90:GLU:O	1:C:91:ASN:HB2	2.09	0.52
1:C:328:LEU:HD13	1:C:340:VAL:CG1	2.39	0.52
1:C:90:GLU:O	1:C:91:ASN:HB2	2.09	0.52
1:C:120:PHE:HB3	1:C:122:PHE:HE2	1.75	0.52
3:B:310:GLY:HA3	3:B:383:ALA:HB2	1.91	0.52
1:C:120:PHE:HB3	1:C:122:PHE:HE2	1.75	0.52
3:B:310:GLY:HA3	3:B:383:ALA:HB2	1.91	0.52
3:B:310:GLY:HA3	3:B:383:ALA:HB2	1.91	0.52
1:C:120:PHE:HB3	1:C:122:PHE:HE2	1.75	0.52
3:B:310:GLY:HA3	3:B:383:ALA:HB2	1.91	0.52
1:C:120:PHE:HB3	1:C:122:PHE:HE2	1.75	0.52
3:B:310:GLY:HA3	3:B:383:ALA:HB2	1.91	0.52
1:C:120:PHE:HB3	1:C:122:PHE:HE2	1.75	0.52
2:A:174:ALA:HB1	2:A:207:GLU:HB2	1.90	0.52
2:A:174:ALA:HB1	2:A:207:GLU:HB2	1.90	0.52
2:A:174:ALA:HB1	2:A:207:GLU:HB2	1.90	0.52
2:A:174:ALA:HB1	2:A:207:GLU:HB2	1.90	0.52
2:A:174:ALA:HB1	2:A:207:GLU:HB2	1.90	0.52
1:C:143:MET:HG3	1:C:153:TRP:CD2	2.44	0.52
3:B:2:ARG:HD2	3:B:133:GLN:OE1	2.10	0.52
3:B:31:ASP:HB3	3:B:34:GLY:HA3	1.90	0.52
3:B:2:ARG:HD2	3:B:133:GLN:OE1	2.10	0.52
3:B:31:ASP:HB3	3:B:34:GLY:HA3	1.90	0.52
1:C:332:GLU:HB2	3:B:420:GLU:OE1	2.10	0.52
3:B:2:ARG:HD2	3:B:133:GLN:OE1	2.10	0.52
3:B:31:ASP:HB3	3:B:34:GLY:HA3	1.90	0.52
3:B:2:ARG:HD2	3:B:133:GLN:OE1	2.10	0.52
3:B:31:ASP:HB3	3:B:34:GLY:HA3	1.90	0.52
1:C:316:LEU:HD22	1:C:344:ASN:HB3	1.92	0.52
3:B:2:ARG:HD2	3:B:133:GLN:OE1	2.10	0.52
3:B:31:ASP:HB3	3:B:34:GLY:HA3	1.90	0.52
1:C:143:MET:HG3	1:C:153:TRP:CD2	2.44	0.52
1:C:143:MET:HG3	1:C:153:TRP:CD2	2.44	0.52
1:C:143:MET:HG3	1:C:153:TRP:CD2	2.44	0.52
1:C:316:LEU:HD22	1:C:344:ASN:HB3	1.92	0.52
1:C:422:ARG:HA	1:C:422:ARG:NE	2.25	0.52
1:C:143:MET:HG3	1:C:153:TRP:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:LEU:HD11	3:B:434:GLN:HG3	1.91	0.52
1:C:316:LEU:HD22	1:C:344:ASN:HB3	1.92	0.52
1:C:316:LEU:HD22	1:C:344:ASN:HB3	1.92	0.52
1:C:316:LEU:HD22	1:C:344:ASN:HB3	1.92	0.52
2:A:203:MET:HG3	2:A:267:PHE:HB3	1.91	0.51
2:A:203:MET:HG3	2:A:267:PHE:HB3	1.91	0.51
2:A:203:MET:HG3	2:A:267:PHE:HB3	1.91	0.51
2:A:203:MET:HG3	2:A:267:PHE:HB3	1.91	0.51
2:A:203:MET:HG3	2:A:267:PHE:HB3	1.91	0.51
1:C:330:LEU:HD13	1:C:465:ARG:HB3	1.91	0.51
1:C:330:LEU:HD13	1:C:465:ARG:HB3	1.91	0.51
1:C:330:LEU:HD13	1:C:465:ARG:HB3	1.91	0.51
1:C:86:CYS:SG	1:C:487:ALA:HA	2.50	0.51
1:C:86:CYS:SG	1:C:487:ALA:HA	2.50	0.51
1:C:330:LEU:HD13	1:C:465:ARG:HB3	1.91	0.51
1:C:330:LEU:HD13	1:C:465:ARG:HB3	1.91	0.51
2:A:179:THR:CG2	4:A:500:GTP:H3'	2.39	0.51
2:A:303:VAL:HG13	2:A:305:CYS:H	1.75	0.51
2:A:179:THR:CG2	4:A:500:GTP:H3'	2.39	0.51
2:A:303:VAL:HG13	2:A:305:CYS:H	1.75	0.51
1:C:86:CYS:SG	1:C:487:ALA:HA	2.50	0.51
2:A:179:THR:CG2	4:A:500:GTP:H3'	2.39	0.51
2:A:303:VAL:HG13	2:A:305:CYS:H	1.75	0.51
2:A:179:THR:CG2	4:A:500:GTP:H3'	2.39	0.51
2:A:303:VAL:HG13	2:A:305:CYS:H	1.75	0.51
2:A:179:THR:CG2	4:A:500:GTP:H3'	2.39	0.51
2:A:303:VAL:HG13	2:A:305:CYS:H	1.75	0.51
1:C:86:CYS:SG	1:C:487:ALA:HA	2.50	0.51
1:C:135:PHE:HZ	1:C:480:ILE:HG12	1.76	0.51
1:C:413:ARG:HD3	2:A:414:GLU:OE1	2.10	0.51
2:A:273:ALA:HB2	2:A:375:VAL:HB	1.93	0.51
2:A:273:ALA:HB2	2:A:375:VAL:HB	1.93	0.51
1:C:135:PHE:HZ	1:C:480:ILE:HG12	1.76	0.51
2:A:273:ALA:HB2	2:A:375:VAL:HB	1.93	0.51
1:C:135:PHE:HZ	1:C:480:ILE:HG12	1.76	0.51
1:C:424:LYS:HZ1	3:B:163:ASP:HA	1.76	0.51
2:A:273:ALA:HB2	2:A:375:VAL:HB	1.93	0.51
1:C:86:CYS:SG	1:C:487:ALA:HA	2.50	0.51
1:C:158:TYR:CE1	1:C:410:GLY:HA2	2.46	0.51
2:A:273:ALA:HB2	2:A:375:VAL:HB	1.93	0.51
1:C:135:PHE:HZ	1:C:480:ILE:HG12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:PHE:HZ	1:C:480:ILE:HG12	1.76	0.51
2:A:137:VAL:HB	2:A:168:GLU:HB3	1.93	0.51
2:A:137:VAL:HB	2:A:168:GLU:HB3	1.93	0.51
1:C:455:LEU:HD11	3:B:434:GLN:HG3	1.92	0.51
2:A:137:VAL:HB	2:A:168:GLU:HB3	1.93	0.51
2:A:137:VAL:HB	2:A:168:GLU:HB3	1.93	0.51
2:A:137:VAL:HB	2:A:168:GLU:HB3	1.93	0.51
1:C:136:PHE:CE1	1:C:181:GLN:HG2	2.46	0.51
1:C:411:SER:HB3	1:C:433:LEU:HD23	1.93	0.51
2:A:122:ILE:HD12	2:A:157:LEU:HD21	1.91	0.51
1:C:136:PHE:CE1	1:C:181:GLN:HG2	2.46	0.51
2:A:122:ILE:HD12	2:A:157:LEU:HD21	1.91	0.51
1:C:136:PHE:CE1	1:C:181:GLN:HG2	2.46	0.51
2:A:122:ILE:HD12	2:A:157:LEU:HD21	1.91	0.51
1:C:136:PHE:CE1	1:C:181:GLN:HG2	2.46	0.51
2:A:122:ILE:HD12	2:A:157:LEU:HD21	1.91	0.51
1:C:136:PHE:CE1	1:C:181:GLN:HG2	2.46	0.51
2:A:122:ILE:HD12	2:A:157:LEU:HD21	1.91	0.51
2:A:144:GLY:H	4:A:500:GTP:PG	2.34	0.50
3:B:179:ASP:OD2	6:B:600:GDP:C3'	2.59	0.50
2:A:144:GLY:H	4:A:500:GTP:PG	2.34	0.50
3:B:179:ASP:OD2	6:B:600:GDP:C3'	2.59	0.50
2:A:144:GLY:H	4:A:500:GTP:PG	2.34	0.50
3:B:179:ASP:OD2	6:B:600:GDP:C3'	2.59	0.50
2:A:144:GLY:H	4:A:500:GTP:PG	2.34	0.50
3:B:179:ASP:OD2	6:B:600:GDP:C3'	2.59	0.50
2:A:144:GLY:H	4:A:500:GTP:PG	2.34	0.50
3:B:179:ASP:OD2	6:B:600:GDP:C3'	2.59	0.50
2:A:144:GLY:H	4:A:500:GTP:PG	2.34	0.50
3:B:179:ASP:OD2	6:B:600:GDP:C3'	2.59	0.50
1:C:332:GLU:HB2	3:B:420:GLU:OE1	2.11	0.50
2:A:388:TRP:CE3	2:A:388:TRP:HA	2.46	0.50
2:A:388:TRP:CE3	2:A:388:TRP:HA	2.46	0.50
1:C:118:HIS:NE2	1:C:502:LEU:HD11	2.25	0.50
2:A:388:TRP:CE3	2:A:388:TRP:HA	2.46	0.50
1:C:402:GLU:O	1:C:402:GLU:HG3	2.10	0.50
2:A:388:TRP:CE3	2:A:388:TRP:HA	2.46	0.50
1:C:402:GLU:O	1:C:402:GLU:HG3	2.10	0.50
2:A:388:TRP:CE3	2:A:388:TRP:HA	2.46	0.50
1:C:402:GLU:O	1:C:402:GLU:HG3	2.10	0.50
1:C:402:GLU:O	1:C:402:GLU:HG3	2.10	0.50
1:C:402:GLU:O	1:C:402:GLU:HG3	2.10	0.50
1:C:455:LEU:HD11	3:B:434:GLN:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:288:VAL:HG21	3:B:327:GLU:HG3	1.92	0.50
1:C:332:GLU:HB2	3:B:420:GLU:OE1	2.12	0.50
3:B:288:VAL:HG21	3:B:327:GLU:HG3	1.92	0.50
3:B:288:VAL:HG21	3:B:327:GLU:HG3	1.92	0.50
3:B:288:VAL:HG21	3:B:327:GLU:HG3	1.92	0.50
3:B:288:VAL:HG21	3:B:327:GLU:HG3	1.92	0.50
3:B:276:THR:O	7:B:601:TA1:O06	2.29	0.50
1:C:413:ARG:HD2	1:C:413:ARG:C	2.28	0.50
3:B:276:THR:O	7:B:601:TA1:O06	2.29	0.50
3:B:276:THR:O	7:B:601:TA1:O06	2.29	0.50
3:B:276:THR:O	7:B:601:TA1:O06	2.29	0.50
3:B:276:THR:O	7:B:601:TA1:O06	2.29	0.50
1:C:422:ARG:HA	1:C:422:ARG:NE	2.27	0.50
2:A:174:ALA:HB3	2:A:177:VAL:O	2.12	0.50
2:A:269:LEU:O	2:A:378:LEU:HA	2.11	0.50
2:A:174:ALA:HB3	2:A:177:VAL:O	2.12	0.50
2:A:269:LEU:O	2:A:378:LEU:HA	2.11	0.50
2:A:174:ALA:HB3	2:A:177:VAL:O	2.12	0.50
2:A:269:LEU:O	2:A:378:LEU:HA	2.11	0.50
2:A:174:ALA:HB3	2:A:177:VAL:O	2.12	0.50
2:A:269:LEU:O	2:A:378:LEU:HA	2.11	0.50
1:C:332:GLU:HB2	3:B:420:GLU:OE1	2.12	0.50
2:A:174:ALA:HB3	2:A:177:VAL:O	2.12	0.50
2:A:269:LEU:O	2:A:378:LEU:HA	2.11	0.50
2:A:188:ILE:HG23	2:A:425:MET:HG3	1.93	0.49
3:B:233:ALA:O	7:B:601:TA1:C39	2.61	0.49
2:A:188:ILE:HG23	2:A:425:MET:HG3	1.93	0.49
3:B:233:ALA:O	7:B:601:TA1:C39	2.61	0.49
2:A:188:ILE:HG23	2:A:425:MET:HG3	1.93	0.49
3:B:233:ALA:O	7:B:601:TA1:C39	2.61	0.49
2:A:188:ILE:HG23	2:A:425:MET:HG3	1.93	0.49
3:B:233:ALA:O	7:B:601:TA1:C39	2.61	0.49
2:A:188:ILE:HG23	2:A:425:MET:HG3	1.93	0.49
3:B:233:ALA:O	7:B:601:TA1:C39	2.61	0.49
1:C:118:HIS:NE2	1:C:502:LEU:HD11	2.27	0.49
1:C:307:ILE:HB	1:C:312:LEU:HD23	1.93	0.49
1:C:307:ILE:HB	1:C:312:LEU:HD23	1.93	0.49
2:A:174:ALA:CB	2:A:207:GLU:HB2	2.42	0.49
2:A:174:ALA:CB	2:A:207:GLU:HB2	2.42	0.49
2:A:174:ALA:CB	2:A:207:GLU:HB2	2.42	0.49
1:C:307:ILE:HB	1:C:312:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:174:ALA:CB	2:A:207:GLU:HB2	2.42	0.49
1:C:307:ILE:HB	1:C:312:LEU:HD23	1.93	0.49
2:A:174:ALA:CB	2:A:207:GLU:HB2	2.42	0.49
1:C:307:ILE:HB	1:C:312:LEU:HD23	1.93	0.49
2:A:100:ALA:O	4:A:500:GTP:O1G	2.29	0.49
2:A:100:ALA:O	4:A:500:GTP:O1G	2.29	0.49
2:A:100:ALA:O	4:A:500:GTP:O1G	2.29	0.49
2:A:100:ALA:O	4:A:500:GTP:O1G	2.29	0.49
2:A:100:ALA:O	4:A:500:GTP:O1G	2.29	0.49
3:B:115:VAL:HG21	3:B:152:LEU:HD23	1.95	0.49
3:B:268:PHE:HD1	3:B:380:ASN:HB2	1.77	0.49
1:C:400:ILE:HG23	1:C:400:ILE:O	2.12	0.49
3:B:115:VAL:HG21	3:B:152:LEU:HD23	1.95	0.49
3:B:268:PHE:HD1	3:B:380:ASN:HB2	1.77	0.49
1:C:400:ILE:HG23	1:C:400:ILE:O	2.12	0.49
3:B:115:VAL:HG21	3:B:152:LEU:HD23	1.95	0.49
3:B:268:PHE:HD1	3:B:380:ASN:HB2	1.77	0.49
3:B:115:VAL:HG21	3:B:152:LEU:HD23	1.95	0.49
3:B:268:PHE:HD1	3:B:380:ASN:HB2	1.77	0.49
1:C:400:ILE:HG23	1:C:400:ILE:O	2.12	0.49
3:B:115:VAL:HG21	3:B:152:LEU:HD23	1.95	0.49
3:B:268:PHE:HD1	3:B:380:ASN:HB2	1.77	0.49
1:C:400:ILE:HG23	1:C:400:ILE:O	2.12	0.49
1:C:455:LEU:HD11	3:B:434:GLN:HG3	1.94	0.49
2:A:224:TYR:CE1	4:A:500:GTP:C6	2.91	0.49
2:A:224:TYR:CE1	4:A:500:GTP:C6	2.91	0.49
2:A:224:TYR:CE1	4:A:500:GTP:C6	2.91	0.49
1:C:400:ILE:HG23	1:C:400:ILE:O	2.12	0.49
2:A:224:TYR:CE1	4:A:500:GTP:C6	2.91	0.49
2:A:224:TYR:CE1	4:A:500:GTP:C6	2.91	0.49
1:C:64:VAL:O	1:C:64:VAL:HG13	2.12	0.49
1:C:143:MET:HG3	1:C:153:TRP:CG	2.48	0.49
2:A:184:PRO:HG2	2:A:398:MET:CE	2.43	0.49
1:C:64:VAL:O	1:C:64:VAL:HG13	2.12	0.49
1:C:143:MET:HG3	1:C:153:TRP:CG	2.48	0.49
2:A:184:PRO:HG2	2:A:398:MET:CE	2.43	0.49
1:C:64:VAL:O	1:C:64:VAL:HG13	2.12	0.49
2:A:184:PRO:HG2	2:A:398:MET:CE	2.43	0.49
2:A:184:PRO:HG2	2:A:398:MET:CE	2.43	0.49
1:C:64:VAL:O	1:C:64:VAL:HG13	2.12	0.49
2:A:184:PRO:HG2	2:A:398:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:MET:HG3	1:C:153:TRP:CG	2.48	0.49
1:C:64:VAL:O	1:C:64:VAL:HG13	2.12	0.49
1:C:143:MET:HG3	1:C:153:TRP:CG	2.48	0.49
1:C:143:MET:HG3	1:C:153:TRP:CG	2.48	0.49
1:C:70:ILE:HG12	1:C:125:ILE:HD11	1.95	0.48
1:C:449:ASN:ND2	1:C:451:SER:H	2.10	0.48
2:A:262:TYR:HB3	2:A:263:PRO:HD2	1.95	0.48
3:B:370:GLY:O	7:B:601:TA1:C44	2.58	0.48
1:C:70:ILE:HG12	1:C:125:ILE:HD11	1.95	0.48
2:A:262:TYR:HB3	2:A:263:PRO:HD2	1.95	0.48
3:B:370:GLY:O	7:B:601:TA1:C44	2.58	0.48
1:C:301:TRP:NE1	1:C:345:TRP:HA	2.28	0.48
2:A:262:TYR:HB3	2:A:263:PRO:HD2	1.95	0.48
3:B:370:GLY:O	7:B:601:TA1:C44	2.58	0.48
1:C:70:ILE:HG12	1:C:125:ILE:HD11	1.95	0.48
1:C:332:GLU:HB2	3:B:420:GLU:OE1	2.13	0.48
2:A:262:TYR:HB3	2:A:263:PRO:HD2	1.95	0.48
3:B:370:GLY:O	7:B:601:TA1:C44	2.58	0.48
1:C:70:ILE:HG12	1:C:125:ILE:HD11	1.95	0.48
2:A:262:TYR:HB3	2:A:263:PRO:HD2	1.95	0.48
3:B:370:GLY:O	7:B:601:TA1:C44	2.58	0.48
1:C:301:TRP:NE1	1:C:345:TRP:HA	2.28	0.48
1:C:301:TRP:NE1	1:C:345:TRP:HA	2.28	0.48
1:C:70:ILE:HG12	1:C:125:ILE:HD11	1.95	0.48
1:C:301:TRP:NE1	1:C:345:TRP:HA	2.28	0.48
1:C:301:TRP:NE1	1:C:345:TRP:HA	2.28	0.48
2:A:276:ILE:HG23	2:A:369:ALA:HB3	1.95	0.48
2:A:286:LEU:HG	2:A:290:GLU:HB3	1.96	0.48
2:A:276:ILE:HG23	2:A:369:ALA:HB3	1.95	0.48
2:A:286:LEU:HG	2:A:290:GLU:HB3	1.96	0.48
2:A:276:ILE:HG23	2:A:369:ALA:HB3	1.95	0.48
2:A:286:LEU:HG	2:A:290:GLU:HB3	1.96	0.48
2:A:276:ILE:HG23	2:A:369:ALA:HB3	1.95	0.48
2:A:286:LEU:HG	2:A:290:GLU:HB3	1.96	0.48
2:A:276:ILE:HG23	2:A:369:ALA:HB3	1.95	0.48
2:A:286:LEU:HG	2:A:290:GLU:HB3	1.96	0.48
3:B:320:ARG:HB2	3:B:358:ILE:O	2.12	0.48
3:B:320:ARG:HB2	3:B:358:ILE:O	2.12	0.48
3:B:320:ARG:HB2	3:B:358:ILE:O	2.12	0.48
3:B:320:ARG:HB2	3:B:358:ILE:O	2.12	0.48
3:B:320:ARG:HB2	3:B:358:ILE:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:328:VAL:O	3:B:332:MET:HG2	2.14	0.48
3:B:328:VAL:O	3:B:332:MET:HG2	2.14	0.48
3:B:328:VAL:O	3:B:332:MET:HG2	2.14	0.48
3:B:328:VAL:O	3:B:332:MET:HG2	2.14	0.48
3:B:328:VAL:O	3:B:332:MET:HG2	2.14	0.48
1:C:411:SER:HB3	1:C:433:LEU:CD2	2.43	0.48
1:C:362:ARG:HA	1:C:365:GLN:HG3	1.94	0.48
1:C:118:HIS:NE2	1:C:502:LEU:HD11	2.28	0.48
1:C:362:ARG:HA	1:C:365:GLN:HG3	1.94	0.48
2:A:377:MET:HE3	2:A:379:SER:HB3	1.96	0.48
2:A:377:MET:HE3	2:A:379:SER:HB3	1.96	0.48
2:A:377:MET:HE3	2:A:379:SER:HB3	1.96	0.48
2:A:377:MET:HE3	2:A:379:SER:HB3	1.96	0.48
1:C:455:LEU:CD1	3:B:431:GLU:HA	2.44	0.48
2:A:377:MET:HE3	2:A:379:SER:HB3	1.96	0.48
1:C:127:GLY:H	1:C:130:VAL:HB	1.79	0.48
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.94	0.48
1:C:127:GLY:H	1:C:130:VAL:HB	1.79	0.48
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.94	0.48
1:C:127:GLY:H	1:C:130:VAL:HB	1.79	0.48
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.94	0.48
1:C:127:GLY:H	1:C:130:VAL:HB	1.79	0.48
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.94	0.48
1:C:127:GLY:H	1:C:130:VAL:HB	1.79	0.48
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.94	0.48
1:C:127:GLY:H	1:C:130:VAL:HB	1.79	0.48
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.94	0.48
1:C:362:ARG:HA	1:C:365:GLN:HG3	1.94	0.48
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.94	0.48
1:C:362:ARG:HA	1:C:365:GLN:HG3	1.94	0.47
1:C:362:ARG:HA	1:C:365:GLN:HG3	1.94	0.47
1:C:333:ASP:HB2	1:C:339:TYR:HE2	1.79	0.47
1:C:333:ASP:HB2	1:C:339:TYR:HE2	1.79	0.47
1:C:455:LEU:CD1	3:B:431:GLU:HA	2.45	0.47
1:C:333:ASP:HB2	1:C:339:TYR:HE2	1.79	0.47
1:C:333:ASP:HB2	1:C:339:TYR:HE2	1.79	0.47
1:C:333:ASP:HB2	1:C:339:TYR:HE2	1.79	0.47
2:A:286:LEU:HG	2:A:290:GLU:CB	2.44	0.47
3:B:12:CYS:SG	6:B:600:GDP:N9	2.87	0.47
1:C:333:ASP:HB2	1:C:339:TYR:CE2	2.49	0.47
2:A:286:LEU:HG	2:A:290:GLU:CB	2.44	0.47
3:B:12:CYS:SG	6:B:600:GDP:N9	2.87	0.47
2:A:286:LEU:HG	2:A:290:GLU:CB	2.44	0.47
3:B:12:CYS:SG	6:B:600:GDP:N9	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:VAL:HG21	1:C:403:LEU:HD12	1.95	0.47
2:A:286:LEU:HG	2:A:290:GLU:CB	2.44	0.47
3:B:12:CYS:SG	6:B:600:GDP:N9	2.87	0.47
1:C:333:ASP:HB2	1:C:339:TYR:CE2	2.49	0.47
2:A:286:LEU:HG	2:A:290:GLU:CB	2.44	0.47
3:B:12:CYS:SG	6:B:600:GDP:N9	2.87	0.47
1:C:147:VAL:HG21	1:C:403:LEU:HD12	1.95	0.47
1:C:333:ASP:HB2	1:C:339:TYR:CE2	2.49	0.47
2:A:201:ALA:HB3	2:A:267:PHE:CD2	2.50	0.47
1:C:147:VAL:HG21	1:C:403:LEU:HD12	1.95	0.47
2:A:201:ALA:HB3	2:A:267:PHE:CD2	2.50	0.47
1:C:147:VAL:HG21	1:C:403:LEU:HD12	1.95	0.47
1:C:333:ASP:HB2	1:C:339:TYR:CE2	2.50	0.47
2:A:201:ALA:HB3	2:A:267:PHE:CD2	2.50	0.47
1:C:333:ASP:HB2	1:C:339:TYR:CE2	2.49	0.47
2:A:201:ALA:HB3	2:A:267:PHE:CD2	2.50	0.47
1:C:147:VAL:HG21	1:C:403:LEU:HD12	1.95	0.47
2:A:201:ALA:HB3	2:A:267:PHE:CD2	2.50	0.47
2:A:362:VAL:HG11	2:A:368:LEU:HB2	1.97	0.47
2:A:362:VAL:HG11	2:A:368:LEU:HB2	1.97	0.47
2:A:362:VAL:HG11	2:A:368:LEU:HB2	1.97	0.47
2:A:362:VAL:HG11	2:A:368:LEU:HB2	1.97	0.47
2:A:362:VAL:HG11	2:A:368:LEU:HB2	1.97	0.47
1:C:449:ASN:HD22	1:C:451:SER:H	1.63	0.47
3:B:180:THR:O	3:B:183:GLU:HB2	2.14	0.47
3:B:326:LYS:HG3	3:B:327:GLU:N	2.29	0.47
3:B:180:THR:O	3:B:183:GLU:HB2	2.14	0.47
3:B:326:LYS:HG3	3:B:327:GLU:N	2.29	0.47
3:B:180:THR:O	3:B:183:GLU:HB2	2.14	0.47
3:B:326:LYS:HG3	3:B:327:GLU:N	2.29	0.47
1:C:327:THR:HG23	1:C:328:LEU:N	2.30	0.47
3:B:180:THR:O	3:B:183:GLU:HB2	2.14	0.47
3:B:326:LYS:HG3	3:B:327:GLU:N	2.29	0.47
1:C:413:ARG:HD2	1:C:413:ARG:C	2.34	0.47
3:B:180:THR:O	3:B:183:GLU:HB2	2.14	0.47
3:B:326:LYS:HG3	3:B:327:GLU:N	2.29	0.47
2:A:415:GLU:HA	2:A:418:PHE:HD2	1.79	0.47
3:B:243:ARG:NH1	3:B:251:ASP:HB2	2.30	0.47
2:A:415:GLU:HA	2:A:418:PHE:HD2	1.79	0.47
3:B:243:ARG:NH1	3:B:251:ASP:HB2	2.30	0.47
2:A:415:GLU:HA	2:A:418:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:243:ARG:NH1	3:B:251:ASP:HB2	2.30	0.47
2:A:415:GLU:HA	2:A:418:PHE:HD2	1.79	0.47
3:B:243:ARG:NH1	3:B:251:ASP:HB2	2.30	0.47
2:A:415:GLU:HA	2:A:418:PHE:HD2	1.79	0.47
3:B:243:ARG:NH1	3:B:251:ASP:HB2	2.30	0.47
3:B:360:PRO:HD2	3:B:371:LEU:HB3	1.95	0.47
3:B:360:PRO:HD2	3:B:371:LEU:HB3	1.95	0.47
3:B:360:PRO:HD2	3:B:371:LEU:HB3	1.95	0.47
1:C:311:LEU:HD12	1:C:327:THR:CG2	2.44	0.47
3:B:360:PRO:HD2	3:B:371:LEU:HB3	1.95	0.47
3:B:360:PRO:HD2	3:B:371:LEU:HB3	1.95	0.47
3:B:278:ARG:HG3	7:B:601:TA1:O08	2.15	0.47
3:B:278:ARG:HG3	7:B:601:TA1:O08	2.15	0.47
1:C:455:LEU:CD1	3:B:431:GLU:HA	2.46	0.47
3:B:278:ARG:HG3	7:B:601:TA1:O08	2.15	0.47
3:B:278:ARG:HG3	7:B:601:TA1:O08	2.15	0.47
3:B:278:ARG:HG3	7:B:601:TA1:O08	2.15	0.47
2:A:118:VAL:HG21	2:A:149:PHE:HZ	1.80	0.46
2:A:137:VAL:HB	2:A:168:GLU:CB	2.45	0.46
2:A:118:VAL:HG21	2:A:149:PHE:HZ	1.80	0.46
2:A:137:VAL:HB	2:A:168:GLU:CB	2.45	0.46
2:A:118:VAL:HG21	2:A:149:PHE:HZ	1.80	0.46
2:A:137:VAL:HB	2:A:168:GLU:CB	2.45	0.46
2:A:118:VAL:HG21	2:A:149:PHE:HZ	1.80	0.46
2:A:137:VAL:HB	2:A:168:GLU:CB	2.45	0.46
2:A:118:VAL:HG21	2:A:149:PHE:HZ	1.80	0.46
2:A:137:VAL:HB	2:A:168:GLU:CB	2.45	0.46
1:C:74:LEU:HB3	1:C:77:GLU:HG3	1.97	0.46
2:A:237:SER:HA	2:A:241:SER:HG	1.80	0.46
3:B:111:GLY:O	3:B:115:VAL:HG23	2.16	0.46
3:B:168:THR:O	3:B:201:THR:HA	2.16	0.46
2:A:237:SER:HA	2:A:241:SER:HG	1.80	0.46
3:B:111:GLY:O	3:B:115:VAL:HG23	2.16	0.46
3:B:168:THR:O	3:B:201:THR:HA	2.16	0.46
2:A:237:SER:HA	2:A:241:SER:HG	1.80	0.46
3:B:111:GLY:O	3:B:115:VAL:HG23	2.16	0.46
3:B:168:THR:O	3:B:201:THR:HA	2.16	0.46
1:C:74:LEU:HB3	1:C:77:GLU:HG3	1.97	0.46
2:A:237:SER:HA	2:A:241:SER:HG	1.80	0.46
3:B:111:GLY:O	3:B:115:VAL:HG23	2.16	0.46
3:B:168:THR:O	3:B:201:THR:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:ASN:HD22	2:A:412:GLY:HA2	1.81	0.46
2:A:237:SER:HA	2:A:241:SER:HG	1.80	0.46
3:B:111:GLY:O	3:B:115:VAL:HG23	2.16	0.46
3:B:168:THR:O	3:B:201:THR:HA	2.16	0.46
2:A:11:GLN:HB3	4:A:500:GTP:O2B	2.14	0.46
3:B:132:LEU:O	3:B:164:ARG:HD2	2.15	0.46
3:B:151:THR:HG23	3:B:193:GLN:HG2	1.97	0.46
3:B:183:GLU:N	3:B:184:PRO:HD2	2.31	0.46
1:C:74:LEU:HB3	1:C:77:GLU:HG3	1.98	0.46
2:A:11:GLN:HB3	4:A:500:GTP:O2B	2.14	0.46
3:B:132:LEU:O	3:B:164:ARG:HD2	2.15	0.46
3:B:151:THR:HG23	3:B:193:GLN:HG2	1.97	0.46
3:B:183:GLU:N	3:B:184:PRO:HD2	2.31	0.46
2:A:11:GLN:HB3	4:A:500:GTP:O2B	2.14	0.46
3:B:132:LEU:O	3:B:164:ARG:HD2	2.15	0.46
3:B:151:THR:HG23	3:B:193:GLN:HG2	1.97	0.46
3:B:183:GLU:N	3:B:184:PRO:HD2	2.31	0.46
1:C:86:CYS:HB3	1:C:485:PRO:O	2.15	0.46
1:C:413:ARG:HD2	1:C:413:ARG:C	2.35	0.46
2:A:11:GLN:HB3	4:A:500:GTP:O2B	2.14	0.46
3:B:132:LEU:O	3:B:164:ARG:HD2	2.15	0.46
3:B:151:THR:HG23	3:B:193:GLN:HG2	1.97	0.46
3:B:183:GLU:N	3:B:184:PRO:HD2	2.31	0.46
1:C:74:LEU:HB3	1:C:77:GLU:HG3	1.98	0.46
2:A:11:GLN:HB3	4:A:500:GTP:O2B	2.14	0.46
3:B:132:LEU:O	3:B:164:ARG:HD2	2.15	0.46
3:B:151:THR:HG23	3:B:193:GLN:HG2	1.97	0.46
3:B:183:GLU:N	3:B:184:PRO:HD2	2.31	0.46
2:A:179:THR:CG2	4:A:500:GTP:C3'	2.93	0.46
1:C:86:CYS:HB3	1:C:485:PRO:O	2.15	0.46
2:A:179:THR:CG2	4:A:500:GTP:C3'	2.93	0.46
1:C:74:LEU:HB3	1:C:77:GLU:HG3	1.98	0.46
1:C:86:CYS:HB3	1:C:485:PRO:O	2.16	0.46
2:A:179:THR:CG2	4:A:500:GTP:C3'	2.93	0.46
2:A:179:THR:CG2	4:A:500:GTP:C3'	2.93	0.46
2:A:179:THR:CG2	4:A:500:GTP:C3'	2.93	0.46
1:C:86:CYS:HB3	1:C:485:PRO:O	2.16	0.46
1:C:154:LEU:CD2	1:C:404:SER:HB2	2.46	0.46
1:C:430:ASN:HD22	2:A:412:GLY:HA2	1.81	0.46
1:C:86:CYS:HB3	1:C:485:PRO:O	2.16	0.46
1:C:154:LEU:CD2	1:C:404:SER:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:ARG:O	1:C:379:SER:HB2	2.14	0.46
1:C:92:THR:HA	1:C:125:ILE:HG22	1.96	0.46
1:C:154:LEU:CD2	1:C:404:SER:HB2	2.46	0.46
2:A:243:ARG:HE	2:A:243:ARG:HA	1.81	0.46
2:A:243:ARG:HE	2:A:243:ARG:HA	1.81	0.46
1:C:92:THR:HA	1:C:125:ILE:HG22	1.96	0.46
1:C:154:LEU:CD2	1:C:404:SER:HB2	2.46	0.46
2:A:243:ARG:HE	2:A:243:ARG:HA	1.81	0.46
1:C:154:LEU:CD2	1:C:404:SER:HB2	2.46	0.46
2:A:243:ARG:HE	2:A:243:ARG:HA	1.81	0.46
1:C:92:THR:HA	1:C:125:ILE:HG22	1.96	0.46
2:A:243:ARG:HE	2:A:243:ARG:HA	1.81	0.46
1:C:312:LEU:HB2	1:C:328:LEU:HD23	1.97	0.46
3:B:203:CYS:SG	3:B:384:ILE:HD11	2.55	0.46
1:C:92:THR:HA	1:C:125:ILE:HG22	1.96	0.46
3:B:203:CYS:SG	3:B:384:ILE:HD11	2.55	0.46
3:B:203:CYS:SG	3:B:384:ILE:HD11	2.55	0.46
1:C:92:THR:HA	1:C:125:ILE:HG22	1.96	0.46
3:B:203:CYS:SG	3:B:384:ILE:HD11	2.55	0.46
3:B:203:CYS:SG	3:B:384:ILE:HD11	2.55	0.46
2:A:97:GLU:HB2	2:A:110:ILE:HD11	1.97	0.46
2:A:184:PRO:HA	2:A:187:SER:OG	2.15	0.46
3:B:78:VAL:O	3:B:84:GLY:HA3	2.16	0.46
2:A:97:GLU:HB2	2:A:110:ILE:HD11	1.97	0.46
2:A:184:PRO:HA	2:A:187:SER:OG	2.15	0.46
3:B:78:VAL:O	3:B:84:GLY:HA3	2.16	0.46
1:C:317:GLU:N	1:C:318:PRO:HD3	2.30	0.46
2:A:97:GLU:HB2	2:A:110:ILE:HD11	1.97	0.46
2:A:184:PRO:HA	2:A:187:SER:OG	2.15	0.46
3:B:78:VAL:O	3:B:84:GLY:HA3	2.16	0.46
2:A:97:GLU:HB2	2:A:110:ILE:HD11	1.97	0.46
2:A:184:PRO:HA	2:A:187:SER:OG	2.15	0.46
3:B:78:VAL:O	3:B:84:GLY:HA3	2.16	0.46
2:A:97:GLU:HB2	2:A:110:ILE:HD11	1.97	0.46
2:A:184:PRO:HA	2:A:187:SER:OG	2.15	0.46
3:B:78:VAL:O	3:B:84:GLY:HA3	2.16	0.46
2:A:431:ASP:O	2:A:435:VAL:HG23	2.16	0.46
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.98	0.46
2:A:431:ASP:O	2:A:435:VAL:HG23	2.16	0.46
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.98	0.46
2:A:431:ASP:O	2:A:435:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.98	0.46
2:A:431:ASP:O	2:A:435:VAL:HG23	2.16	0.46
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.98	0.46
2:A:431:ASP:O	2:A:435:VAL:HG23	2.16	0.46
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.98	0.46
1:C:86:CYS:HA	1:C:98:GLN:O	2.16	0.45
2:A:184:PRO:HG2	2:A:398:MET:HE2	1.98	0.45
3:B:103:TRP:CZ2	3:B:151:THR:HG21	2.50	0.45
1:C:424:LYS:O	1:C:428:ASN:HB2	2.16	0.45
2:A:184:PRO:HG2	2:A:398:MET:HE2	1.98	0.45
3:B:103:TRP:CZ2	3:B:151:THR:HG21	2.50	0.45
1:C:86:CYS:HA	1:C:98:GLN:O	2.16	0.45
2:A:184:PRO:HG2	2:A:398:MET:HE2	1.98	0.45
3:B:103:TRP:CZ2	3:B:151:THR:HG21	2.50	0.45
1:C:86:CYS:HA	1:C:98:GLN:O	2.16	0.45
1:C:424:LYS:O	1:C:428:ASN:HB2	2.16	0.45
1:C:455:LEU:CD1	3:B:431:GLU:HA	2.47	0.45
2:A:184:PRO:HG2	2:A:398:MET:HE2	1.98	0.45
3:B:103:TRP:CZ2	3:B:151:THR:HG21	2.50	0.45
2:A:184:PRO:HG2	2:A:398:MET:HE2	1.98	0.45
3:B:103:TRP:CZ2	3:B:151:THR:HG21	2.50	0.45
1:C:424:LYS:O	1:C:428:ASN:HB2	2.16	0.45
2:A:118:VAL:HG21	2:A:149:PHE:CZ	2.51	0.45
2:A:118:VAL:HG21	2:A:149:PHE:CZ	2.51	0.45
1:C:424:LYS:O	1:C:428:ASN:HB2	2.16	0.45
2:A:118:VAL:HG21	2:A:149:PHE:CZ	2.51	0.45
2:A:118:VAL:HG21	2:A:149:PHE:CZ	2.51	0.45
1:C:86:CYS:HA	1:C:98:GLN:O	2.16	0.45
2:A:118:VAL:HG21	2:A:149:PHE:CZ	2.51	0.45
1:C:302:ILE:HA	1:C:384:SER:O	2.17	0.45
1:C:86:CYS:HA	1:C:98:GLN:O	2.16	0.45
1:C:302:ILE:HA	1:C:384:SER:O	2.17	0.45
1:C:302:ILE:HA	1:C:384:SER:O	2.17	0.45
1:C:413:ARG:HD2	1:C:413:ARG:O	2.16	0.45
1:C:430:ASN:HD22	2:A:412:GLY:HA2	1.82	0.45
1:C:302:ILE:HA	1:C:384:SER:O	2.17	0.45
1:C:424:LYS:O	1:C:428:ASN:HB2	2.17	0.45
1:C:389:HIS:NE2	1:C:399:LYS:HG2	2.31	0.45
1:C:391:GLN:CD	1:C:391:GLN:H	2.20	0.45
1:C:389:HIS:NE2	1:C:399:LYS:HG2	2.31	0.45
1:C:391:GLN:CD	1:C:391:GLN:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:HIS:NE2	1:C:399:LYS:HG2	2.31	0.45
1:C:302:ILE:HA	1:C:384:SER:O	2.17	0.45
1:C:389:HIS:NE2	1:C:399:LYS:HG2	2.31	0.45
1:C:391:GLN:CD	1:C:391:GLN:H	2.20	0.45
1:C:389:HIS:NE2	1:C:399:LYS:HG2	2.31	0.45
1:C:391:GLN:CD	1:C:391:GLN:H	2.20	0.45
1:C:453:GLN:HB2	3:B:434:GLN:CD	2.36	0.45
2:A:70:LEU:HB3	2:A:98:ASP:O	2.16	0.45
2:A:70:LEU:HB3	2:A:98:ASP:O	2.16	0.45
1:C:158:TYR:CE1	1:C:410:GLY:HA2	2.52	0.45
1:C:391:GLN:CD	1:C:391:GLN:H	2.20	0.45
2:A:70:LEU:HB3	2:A:98:ASP:O	2.16	0.45
2:A:70:LEU:HB3	2:A:98:ASP:O	2.16	0.45
2:A:70:LEU:HB3	2:A:98:ASP:O	2.16	0.45
2:A:155:GLU:O	2:A:159:VAL:HG23	2.17	0.45
2:A:188:ILE:HG13	2:A:395:PHE:CG	2.51	0.45
2:A:155:GLU:O	2:A:159:VAL:HG23	2.17	0.45
2:A:188:ILE:HG13	2:A:395:PHE:CG	2.51	0.45
2:A:155:GLU:O	2:A:159:VAL:HG23	2.17	0.45
2:A:188:ILE:HG13	2:A:395:PHE:CG	2.51	0.45
2:A:155:GLU:O	2:A:159:VAL:HG23	2.17	0.45
2:A:188:ILE:HG13	2:A:395:PHE:CG	2.51	0.45
2:A:155:GLU:O	2:A:159:VAL:HG23	2.17	0.45
2:A:188:ILE:HG13	2:A:395:PHE:CG	2.51	0.45
2:A:155:GLU:O	2:A:159:VAL:HG23	2.17	0.45
2:A:188:ILE:HG13	2:A:395:PHE:CG	2.51	0.45
1:C:424:LYS:O	1:C:424:LYS:HG3	2.17	0.45
1:C:163:SER:HA	1:C:484:ASN:OD1	2.17	0.45
1:C:424:LYS:O	1:C:424:LYS:HG3	2.17	0.45
3:B:360:PRO:O	7:B:601:TA1:C28	2.65	0.45
1:C:455:LEU:CD1	3:B:431:GLU:HA	2.47	0.45
3:B:360:PRO:O	7:B:601:TA1:C28	2.65	0.45
3:B:360:PRO:O	7:B:601:TA1:C28	2.65	0.45
1:C:424:LYS:O	1:C:424:LYS:HG3	2.17	0.45
3:B:360:PRO:O	7:B:601:TA1:C28	2.65	0.45
1:C:424:LYS:O	1:C:424:LYS:HG3	2.17	0.45
3:B:360:PRO:O	7:B:601:TA1:C28	2.65	0.45
1:C:163:SER:HA	1:C:484:ASN:OD1	2.17	0.45
2:A:191:THR:O	2:A:195:LEU:HB2	2.16	0.45
3:B:201:THR:OG1	3:B:265:LEU:HD11	2.17	0.45
1:C:163:SER:HA	1:C:484:ASN:OD1	2.17	0.45
1:C:424:LYS:O	1:C:424:LYS:HG3	2.17	0.45
2:A:191:THR:O	2:A:195:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:201:THR:OG1	3:B:265:LEU:HD11	2.17	0.45
1:C:163:SER:HA	1:C:484:ASN:OD1	2.17	0.45
2:A:191:THR:O	2:A:195:LEU:HB2	2.16	0.45
3:B:201:THR:OG1	3:B:265:LEU:HD11	2.17	0.45
1:C:328:LEU:HB3	1:C:340:VAL:HG12	1.98	0.45
2:A:191:THR:O	2:A:195:LEU:HB2	2.16	0.45
3:B:201:THR:OG1	3:B:265:LEU:HD11	2.17	0.45
2:A:191:THR:O	2:A:195:LEU:HB2	2.16	0.45
3:B:201:THR:OG1	3:B:265:LEU:HD11	2.17	0.45
2:A:16:ILE:HA	2:A:228:ASN:HB3	1.99	0.45
1:C:430:ASN:HD22	2:A:412:GLY:HA2	1.82	0.45
2:A:16:ILE:HA	2:A:228:ASN:HB3	1.99	0.45
2:A:16:ILE:HA	2:A:228:ASN:HB3	1.99	0.45
1:C:163:SER:HA	1:C:484:ASN:OD1	2.17	0.45
2:A:16:ILE:HA	2:A:228:ASN:HB3	1.99	0.45
1:C:453:GLN:HB2	3:B:434:GLN:CD	2.36	0.45
2:A:16:ILE:HA	2:A:228:ASN:HB3	1.99	0.45
1:C:316:LEU:HB3	1:C:344:ASN:HB2	1.99	0.44
1:C:316:LEU:HB3	1:C:344:ASN:HB2	1.99	0.44
1:C:423:LEU:HD13	3:B:163:ASP:HB3	1.97	0.44
1:C:167:TYR:O	1:C:171:GLY:HA2	2.18	0.44
1:C:316:LEU:HD11	1:C:346:ILE:HG22	1.99	0.44
1:C:316:LEU:HB3	1:C:344:ASN:HB2	1.99	0.44
1:C:316:LEU:HB3	1:C:344:ASN:HB2	1.99	0.44
1:C:430:ASN:HD22	2:A:412:GLY:HA2	1.83	0.44
1:C:167:TYR:O	1:C:171:GLY:HA2	2.18	0.44
1:C:316:LEU:HD11	1:C:346:ILE:HG22	1.99	0.44
1:C:167:TYR:O	1:C:171:GLY:HA2	2.18	0.44
1:C:316:LEU:HD11	1:C:346:ILE:HG22	1.99	0.44
1:C:167:TYR:O	1:C:171:GLY:HA2	2.18	0.44
1:C:316:LEU:HD11	1:C:346:ILE:HG22	1.99	0.44
1:C:316:LEU:HB3	1:C:344:ASN:HB2	1.99	0.44
1:C:500:SER:O	1:C:501:ALA:HB3	2.18	0.44
1:C:167:TYR:O	1:C:171:GLY:HA2	2.18	0.44
1:C:318:PRO:HG2	1:C:364:ASN:ND2	2.32	0.44
1:C:383:PHE:O	1:C:404:SER:HA	2.18	0.44
1:C:316:LEU:HD11	1:C:346:ILE:HG22	2.00	0.44
1:C:383:PHE:O	1:C:404:SER:HA	2.18	0.44
1:C:135:PHE:CZ	1:C:480:ILE:HG12	2.52	0.44
1:C:383:PHE:O	1:C:404:SER:HA	2.18	0.44
1:C:135:PHE:CZ	1:C:480:ILE:HG12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:PHE:O	1:C:404:SER:HA	2.18	0.44
1:C:135:PHE:CZ	1:C:480:ILE:HG12	2.52	0.44
1:C:383:PHE:O	1:C:404:SER:HA	2.18	0.44
1:C:360:VAL:CG1	1:C:361:GLY:N	2.81	0.44
1:C:360:VAL:CG1	1:C:361:GLY:N	2.81	0.44
2:A:225:THR:O	2:A:229:ARG:HG3	2.17	0.44
3:B:8:GLN:OE1	3:B:14:ASN:HA	2.17	0.44
2:A:225:THR:O	2:A:229:ARG:HG3	2.17	0.44
3:B:8:GLN:OE1	3:B:14:ASN:HA	2.17	0.44
1:C:360:VAL:CG1	1:C:361:GLY:N	2.81	0.44
1:C:453:GLN:HB2	3:B:434:GLN:CD	2.37	0.44
2:A:225:THR:O	2:A:229:ARG:HG3	2.17	0.44
3:B:8:GLN:OE1	3:B:14:ASN:HA	2.17	0.44
1:C:135:PHE:CZ	1:C:480:ILE:HG12	2.52	0.44
2:A:225:THR:O	2:A:229:ARG:HG3	2.17	0.44
3:B:8:GLN:OE1	3:B:14:ASN:HA	2.17	0.44
1:C:135:PHE:CZ	1:C:480:ILE:HG12	2.52	0.44
1:C:360:VAL:CG1	1:C:361:GLY:N	2.81	0.44
2:A:225:THR:O	2:A:229:ARG:HG3	2.17	0.44
3:B:8:GLN:OE1	3:B:14:ASN:HA	2.17	0.44
1:C:328:LEU:HD12	1:C:342:ASP:HB3	2.00	0.44
1:C:158:TYR:HE2	1:C:496:ALA:HA	1.83	0.44
1:C:360:VAL:CG1	1:C:361:GLY:N	2.81	0.44
1:C:158:TYR:HE2	1:C:496:ALA:HA	1.83	0.44
1:C:158:TYR:HE2	1:C:496:ALA:HA	1.83	0.44
1:C:158:TYR:HE2	1:C:496:ALA:HA	1.83	0.44
1:C:424:LYS:HZ3	3:B:163:ASP:HA	1.80	0.44
1:C:158:TYR:HE2	1:C:496:ALA:HA	1.83	0.44
2:A:69:ASP:HA	2:A:145:THR:HG21	2.00	0.44
3:B:301:MET:HG3	3:B:307:PRO:HD3	1.99	0.44
2:A:69:ASP:HA	2:A:145:THR:HG21	2.00	0.44
3:B:301:MET:HG3	3:B:307:PRO:HD3	1.99	0.44
2:A:69:ASP:HA	2:A:145:THR:HG21	2.00	0.44
3:B:301:MET:HG3	3:B:307:PRO:HD3	1.99	0.44
2:A:69:ASP:HA	2:A:145:THR:HG21	2.00	0.44
3:B:301:MET:HG3	3:B:307:PRO:HD3	1.99	0.44
2:A:69:ASP:HA	2:A:145:THR:HG21	2.00	0.44
3:B:301:MET:HG3	3:B:307:PRO:HD3	1.99	0.44
2:A:69:ASP:HA	2:A:145:THR:HG21	2.00	0.44
3:B:301:MET:HG3	3:B:307:PRO:HD3	1.99	0.44
1:C:331:CYS:SG	1:C:332:GLU:N	2.91	0.43
1:C:308:TYR:OH	1:C:422:ARG:HG3	2.18	0.43
1:C:331:CYS:SG	1:C:332:GLU:N	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:CYS:SG	1:C:332:GLU:N	2.91	0.43
1:C:331:CYS:SG	1:C:332:GLU:N	2.92	0.43
2:A:204:VAL:HG11	2:A:231:ILE:CD1	2.48	0.43
1:C:331:CYS:SG	1:C:332:GLU:N	2.92	0.43
2:A:204:VAL:HG11	2:A:231:ILE:CD1	2.48	0.43
2:A:204:VAL:HG11	2:A:231:ILE:CD1	2.48	0.43
2:A:204:VAL:HG11	2:A:231:ILE:CD1	2.48	0.43
1:C:155:ILE:CG2	1:C:405:LEU:HA	2.48	0.43
2:A:204:VAL:HG11	2:A:231:ILE:CD1	2.48	0.43
2:A:201:ALA:O	2:A:268:PRO:HD2	2.18	0.43
2:A:224:TYR:HD1	2:A:227:LEU:HD12	1.83	0.43
1:C:155:ILE:CG2	1:C:405:LEU:HA	2.48	0.43
2:A:201:ALA:O	2:A:268:PRO:HD2	2.18	0.43
2:A:224:TYR:HD1	2:A:227:LEU:HD12	1.83	0.43
1:C:155:ILE:CG2	1:C:405:LEU:HA	2.48	0.43
2:A:201:ALA:O	2:A:268:PRO:HD2	2.18	0.43
2:A:224:TYR:HD1	2:A:227:LEU:HD12	1.83	0.43
1:C:155:ILE:CG2	1:C:405:LEU:HA	2.48	0.43
2:A:201:ALA:O	2:A:268:PRO:HD2	2.18	0.43
2:A:224:TYR:HD1	2:A:227:LEU:HD12	1.83	0.43
1:C:154:LEU:HD22	1:C:404:SER:O	2.18	0.43
2:A:201:ALA:O	2:A:268:PRO:HD2	2.18	0.43
2:A:224:TYR:HD1	2:A:227:LEU:HD12	1.83	0.43
1:C:154:LEU:HD22	1:C:404:SER:O	2.18	0.43
1:C:155:ILE:CG2	1:C:405:LEU:HA	2.48	0.43
1:C:380:HIS:HA	1:C:407:ASP:O	2.19	0.43
2:A:11:GLN:HA	2:A:74:VAL:HG11	2.01	0.43
2:A:88:HIS:O	2:A:91:GLN:HG3	2.18	0.43
2:A:386:GLU:O	2:A:390:ARG:HG2	2.18	0.43
3:B:8:GLN:CD	3:B:17:GLY:HA3	2.39	0.43
3:B:211:ASP:O	3:B:215:ARG:HG2	2.18	0.43
3:B:269:MET:HG3	3:B:384:ILE:HD12	1.99	0.43
3:B:270:PRO:HD2	3:B:302:MET:HB3	2.00	0.43
3:B:276:THR:HB	3:B:281:GLN:HB3	2.00	0.43
1:C:154:LEU:HD22	1:C:404:SER:O	2.18	0.43
1:C:380:HIS:HA	1:C:407:ASP:O	2.19	0.43
2:A:11:GLN:HA	2:A:74:VAL:HG11	2.01	0.43
2:A:88:HIS:O	2:A:91:GLN:HG3	2.18	0.43
2:A:386:GLU:O	2:A:390:ARG:HG2	2.18	0.43
3:B:8:GLN:CD	3:B:17:GLY:HA3	2.39	0.43
3:B:211:ASP:O	3:B:215:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:269:MET:HG3	3:B:384:ILE:HD12	1.99	0.43
3:B:270:PRO:HD2	3:B:302:MET:HB3	2.00	0.43
3:B:276:THR:HB	3:B:281:GLN:HB3	2.00	0.43
1:C:154:LEU:HD22	1:C:404:SER:O	2.18	0.43
2:A:11:GLN:HA	2:A:74:VAL:HG11	2.01	0.43
2:A:88:HIS:O	2:A:91:GLN:HG3	2.18	0.43
2:A:386:GLU:O	2:A:390:ARG:HG2	2.18	0.43
3:B:8:GLN:CD	3:B:17:GLY:HA3	2.39	0.43
3:B:211:ASP:O	3:B:215:ARG:HG2	2.18	0.43
3:B:269:MET:HG3	3:B:384:ILE:HD12	1.99	0.43
3:B:270:PRO:HD2	3:B:302:MET:HB3	2.00	0.43
3:B:276:THR:HB	3:B:281:GLN:HB3	2.00	0.43
1:C:154:LEU:HD22	1:C:404:SER:O	2.18	0.43
1:C:380:HIS:HA	1:C:407:ASP:O	2.19	0.43
2:A:11:GLN:HA	2:A:74:VAL:HG11	2.01	0.43
2:A:88:HIS:O	2:A:91:GLN:HG3	2.18	0.43
2:A:386:GLU:O	2:A:390:ARG:HG2	2.18	0.43
3:B:8:GLN:CD	3:B:17:GLY:HA3	2.39	0.43
3:B:211:ASP:O	3:B:215:ARG:HG2	2.18	0.43
3:B:269:MET:HG3	3:B:384:ILE:HD12	1.99	0.43
3:B:270:PRO:HD2	3:B:302:MET:HB3	2.00	0.43
3:B:276:THR:HB	3:B:281:GLN:HB3	2.00	0.43
2:A:11:GLN:HA	2:A:74:VAL:HG11	2.01	0.43
2:A:88:HIS:O	2:A:91:GLN:HG3	2.18	0.43
2:A:386:GLU:O	2:A:390:ARG:HG2	2.18	0.43
3:B:8:GLN:CD	3:B:17:GLY:HA3	2.39	0.43
3:B:211:ASP:O	3:B:215:ARG:HG2	2.18	0.43
3:B:269:MET:HG3	3:B:384:ILE:HD12	1.99	0.43
3:B:270:PRO:HD2	3:B:302:MET:HB3	2.00	0.43
3:B:276:THR:HB	3:B:281:GLN:HB3	2.00	0.43
2:A:133:GLN:HG2	2:A:252:LEU:HB2	1.99	0.43
2:A:371:VAL:HG12	2:A:372:GLN:N	2.34	0.43
7:B:601:TA1:H463	7:B:601:TA1:C26	2.46	0.43
1:C:140:MET:O	1:C:144:VAL:HG23	2.18	0.43
2:A:133:GLN:HG2	2:A:252:LEU:HB2	1.99	0.43
2:A:371:VAL:HG12	2:A:372:GLN:N	2.34	0.43
7:B:601:TA1:H463	7:B:601:TA1:C26	2.46	0.43
1:C:140:MET:O	1:C:144:VAL:HG23	2.18	0.43
1:C:380:HIS:HA	1:C:407:ASP:O	2.19	0.43
2:A:133:GLN:HG2	2:A:252:LEU:HB2	1.99	0.43
2:A:371:VAL:HG12	2:A:372:GLN:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:601:TA1:H463	7:B:601:TA1:C26	2.46	0.43
2:A:133:GLN:HG2	2:A:252:LEU:HB2	1.99	0.43
2:A:371:VAL:HG12	2:A:372:GLN:N	2.34	0.43
7:B:601:TA1:H463	7:B:601:TA1:C26	2.46	0.43
2:A:133:GLN:HG2	2:A:252:LEU:HB2	1.99	0.43
2:A:371:VAL:HG12	2:A:372:GLN:N	2.34	0.43
7:B:601:TA1:H463	7:B:601:TA1:C26	2.46	0.43
1:C:140:MET:O	1:C:144:VAL:HG23	2.18	0.43
1:C:140:MET:O	1:C:144:VAL:HG23	2.18	0.43
1:C:140:MET:O	1:C:144:VAL:HG23	2.18	0.43
1:C:380:HIS:HA	1:C:407:ASP:O	2.19	0.43
1:C:424:LYS:HZ3	3:B:163:ASP:HA	1.82	0.43
1:C:312:LEU:HB2	1:C:328:LEU:CD2	2.49	0.43
1:C:332:GLU:HA	1:C:338:PRO:HA	2.01	0.43
3:B:288:VAL:N	3:B:289:PRO:HD2	2.33	0.43
1:C:332:GLU:HA	1:C:338:PRO:HA	2.01	0.43
3:B:288:VAL:N	3:B:289:PRO:HD2	2.33	0.43
1:C:332:GLU:HA	1:C:338:PRO:HA	2.01	0.43
3:B:288:VAL:N	3:B:289:PRO:HD2	2.33	0.43
3:B:288:VAL:N	3:B:289:PRO:HD2	2.33	0.43
1:C:332:GLU:HA	1:C:338:PRO:HA	2.01	0.43
3:B:288:VAL:N	3:B:289:PRO:HD2	2.33	0.43
3:B:385:GLN:HB2	3:B:429:VAL:HG13	2.01	0.42
1:C:100:PRO:O	1:C:487:ALA:HB1	2.19	0.42
3:B:385:GLN:HB2	3:B:429:VAL:HG13	2.01	0.42
3:B:385:GLN:HB2	3:B:429:VAL:HG13	2.01	0.42
1:C:100:PRO:O	1:C:487:ALA:HB1	2.19	0.42
1:C:158:TYR:CE1	1:C:410:GLY:HA2	2.54	0.42
1:C:332:GLU:HA	1:C:338:PRO:HA	2.01	0.42
3:B:385:GLN:HB2	3:B:429:VAL:HG13	2.01	0.42
1:C:100:PRO:O	1:C:487:ALA:HB1	2.19	0.42
1:C:456:ILE:HA	1:C:457:PRO:HD3	1.74	0.42
3:B:385:GLN:HB2	3:B:429:VAL:HG13	2.01	0.42
1:C:100:PRO:O	1:C:487:ALA:HB1	2.19	0.42
1:C:358:LEU:HD23	1:C:362:ARG:NH1	2.35	0.42
1:C:456:ILE:HA	1:C:457:PRO:HD3	1.74	0.42
2:A:66:VAL:HG12	2:A:91:GLN:HB3	2.01	0.42
2:A:273:ALA:H	2:A:274:PRO:HD2	1.83	0.42
1:C:500:SER:O	1:C:501:ALA:HB3	2.19	0.42
2:A:66:VAL:HG12	2:A:91:GLN:HB3	2.01	0.42
2:A:273:ALA:H	2:A:274:PRO:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:PRO:O	1:C:487:ALA:HB1	2.19	0.42
2:A:66:VAL:HG12	2:A:91:GLN:HB3	2.01	0.42
2:A:273:ALA:H	2:A:274:PRO:HD2	1.83	0.42
1:C:311:LEU:CD1	1:C:327:THR:HG21	2.49	0.42
1:C:456:ILE:HA	1:C:457:PRO:HD3	1.74	0.42
2:A:66:VAL:HG12	2:A:91:GLN:HB3	2.01	0.42
2:A:273:ALA:H	2:A:274:PRO:HD2	1.83	0.42
2:A:66:VAL:HG12	2:A:91:GLN:HB3	2.01	0.42
2:A:273:ALA:H	2:A:274:PRO:HD2	1.83	0.42
1:C:66:VAL:HA	1:C:479:MET:HB3	2.02	0.42
1:C:66:VAL:HA	1:C:479:MET:HB3	2.02	0.42
1:C:358:LEU:HD23	1:C:362:ARG:NH1	2.35	0.42
1:C:165:LYS:O	1:C:169:ILE:HG22	2.20	0.42
1:C:358:LEU:HD23	1:C:362:ARG:NH1	2.35	0.42
1:C:453:GLN:HB2	3:B:434:GLN:CD	2.39	0.42
1:C:456:ILE:HA	1:C:457:PRO:HD3	1.74	0.42
1:C:165:LYS:O	1:C:169:ILE:HG22	2.20	0.42
1:C:358:LEU:HD23	1:C:362:ARG:NH1	2.35	0.42
1:C:456:ILE:HA	1:C:457:PRO:HD3	1.74	0.42
1:C:66:VAL:HA	1:C:479:MET:HB3	2.02	0.42
1:C:165:LYS:O	1:C:169:ILE:HG22	2.20	0.42
1:C:358:LEU:HD23	1:C:362:ARG:NH1	2.35	0.42
1:C:456:ILE:HA	1:C:457:PRO:HD3	1.74	0.42
1:C:66:VAL:HA	1:C:479:MET:HB3	2.02	0.42
1:C:66:VAL:HA	1:C:479:MET:HB3	2.02	0.42
1:C:165:LYS:O	1:C:169:ILE:HG22	2.20	0.42
1:C:378:ARG:HH12	1:C:412:GLU:CG	2.32	0.42
1:C:500:SER:O	1:C:501:ALA:HB3	2.20	0.42
1:C:165:LYS:O	1:C:169:ILE:HG22	2.20	0.42
2:A:227:LEU:O	2:A:231:ILE:HG12	2.20	0.42
2:A:227:LEU:O	2:A:231:ILE:HG12	2.20	0.42
1:C:156:TYR:HB3	1:C:479:MET:HA	2.01	0.42
2:A:227:LEU:O	2:A:231:ILE:HG12	2.20	0.42
2:A:227:LEU:O	2:A:231:ILE:HG12	2.20	0.42
2:A:227:LEU:O	2:A:231:ILE:HG12	2.20	0.42
1:C:156:TYR:HB3	1:C:479:MET:HA	2.01	0.42
3:B:268:PHE:CD1	3:B:380:ASN:HB2	2.54	0.42
1:C:156:TYR:HB3	1:C:479:MET:HA	2.01	0.42
3:B:268:PHE:CD1	3:B:380:ASN:HB2	2.54	0.42
3:B:268:PHE:CD1	3:B:380:ASN:HB2	2.54	0.42
1:C:156:TYR:HB3	1:C:479:MET:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:268:PHE:CD1	3:B:380:ASN:HB2	2.54	0.42
1:C:156:TYR:HB3	1:C:479:MET:HA	2.01	0.42
3:B:268:PHE:CD1	3:B:380:ASN:HB2	2.54	0.42
2:A:407:TRP:CG	3:B:257:VAL:HG13	2.54	0.42
3:B:93:VAL:HG11	3:B:118:VAL:HG22	2.01	0.42
3:B:230:LEU:HD13	7:B:601:TA1:C08	2.47	0.42
2:A:407:TRP:CG	3:B:257:VAL:HG13	2.54	0.42
3:B:93:VAL:HG11	3:B:118:VAL:HG22	2.01	0.42
3:B:230:LEU:HD13	7:B:601:TA1:C08	2.47	0.42
2:A:407:TRP:CG	3:B:257:VAL:HG13	2.54	0.42
3:B:93:VAL:HG11	3:B:118:VAL:HG22	2.01	0.42
3:B:230:LEU:HD13	7:B:601:TA1:C08	2.47	0.42
2:A:407:TRP:CG	3:B:257:VAL:HG13	2.54	0.42
3:B:93:VAL:HG11	3:B:118:VAL:HG22	2.01	0.42
3:B:230:LEU:HD13	7:B:601:TA1:C08	2.47	0.42
2:A:407:TRP:CG	3:B:257:VAL:HG13	2.54	0.42
3:B:93:VAL:HG11	3:B:118:VAL:HG22	2.01	0.42
3:B:230:LEU:HD13	7:B:601:TA1:C08	2.47	0.42
1:C:330:LEU:HD13	1:C:465:ARG:CB	2.50	0.42
2:A:398:MET:HE3	2:A:398:MET:HB2	1.89	0.42
3:B:195:VAL:HG23	3:B:265:LEU:HB3	2.01	0.42
1:C:330:LEU:HD13	1:C:465:ARG:CB	2.50	0.42
2:A:398:MET:HE3	2:A:398:MET:HB2	1.89	0.42
3:B:195:VAL:HG23	3:B:265:LEU:HB3	2.01	0.42
1:C:330:LEU:HD13	1:C:465:ARG:CB	2.50	0.42
2:A:398:MET:HE3	2:A:398:MET:HB2	1.89	0.42
3:B:195:VAL:HG23	3:B:265:LEU:HB3	2.01	0.42
1:C:330:LEU:HD13	1:C:465:ARG:CB	2.50	0.42
2:A:398:MET:HE3	2:A:398:MET:HB2	1.89	0.42
3:B:195:VAL:HG23	3:B:265:LEU:HB3	2.01	0.42
1:C:500:SER:O	1:C:501:ALA:HB3	2.20	0.42
2:A:398:MET:HE3	2:A:398:MET:HB2	1.89	0.42
3:B:195:VAL:HG23	3:B:265:LEU:HB3	2.01	0.42
2:A:427:ALA:O	2:A:431:ASP:HB2	2.20	0.42
2:A:427:ALA:O	2:A:431:ASP:HB2	2.20	0.42
2:A:427:ALA:O	2:A:431:ASP:HB2	2.20	0.42
2:A:427:ALA:O	2:A:431:ASP:HB2	2.20	0.42
1:C:330:LEU:HD13	1:C:465:ARG:CB	2.50	0.42
2:A:427:ALA:O	2:A:431:ASP:HB2	2.20	0.42
1:C:456:ILE:H	1:C:456:ILE:HG12	1.53	0.41
1:C:494:LEU:HG	1:C:498:LYS:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:230:LEU:HB2	7:B:601:TA1:HC71	2.01	0.41
1:C:330:LEU:CD1	1:C:465:ARG:HB2	2.50	0.41
3:B:230:LEU:HB2	7:B:601:TA1:HC71	2.01	0.41
1:C:311:LEU:HD13	1:C:311:LEU:HA	1.90	0.41
3:B:230:LEU:HB2	7:B:601:TA1:HC71	2.01	0.41
3:B:230:LEU:HB2	7:B:601:TA1:HC71	2.01	0.41
3:B:230:LEU:HB2	7:B:601:TA1:HC71	2.01	0.41
1:C:311:LEU:HD13	1:C:311:LEU:HA	1.90	0.41
1:C:330:LEU:CD1	1:C:465:ARG:HB2	2.50	0.41
2:A:183:GLU:HB3	2:A:184:PRO:CD	2.50	0.41
3:B:156:LYS:HA	3:B:156:LYS:HD3	1.89	0.41
3:B:396:THR:HA	3:B:399:PHE:HB3	2.01	0.41
1:C:75:THR:O	1:C:79:ASP:HB2	2.20	0.41
1:C:311:LEU:HD13	1:C:311:LEU:HA	1.90	0.41
2:A:183:GLU:HB3	2:A:184:PRO:CD	2.50	0.41
3:B:156:LYS:HA	3:B:156:LYS:HD3	1.89	0.41
3:B:396:THR:HA	3:B:399:PHE:HB3	2.01	0.41
1:C:95:LEU:HD11	1:C:125:ILE:HB	2.01	0.41
2:A:183:GLU:HB3	2:A:184:PRO:CD	2.50	0.41
3:B:156:LYS:HA	3:B:156:LYS:HD3	1.89	0.41
3:B:396:THR:HA	3:B:399:PHE:HB3	2.01	0.41
1:C:330:LEU:CD1	1:C:465:ARG:HB2	2.50	0.41
1:C:423:LEU:CD1	3:B:163:ASP:HB2	2.48	0.41
1:C:453:GLN:HB2	3:B:434:GLN:CD	2.39	0.41
1:C:494:LEU:HG	1:C:498:LYS:HE3	2.01	0.41
2:A:183:GLU:HB3	2:A:184:PRO:CD	2.50	0.41
3:B:156:LYS:HA	3:B:156:LYS:HD3	1.89	0.41
3:B:396:THR:HA	3:B:399:PHE:HB3	2.01	0.41
1:C:95:LEU:HD11	1:C:125:ILE:HB	2.01	0.41
1:C:149:LYS:HB3	1:C:149:LYS:HE2	1.89	0.41
1:C:311:LEU:HD13	1:C:311:LEU:HA	1.90	0.41
1:C:330:LEU:CD1	1:C:465:ARG:HB2	2.50	0.41
1:C:456:ILE:H	1:C:456:ILE:HG12	1.53	0.41
1:C:494:LEU:HG	1:C:498:LYS:HE3	2.01	0.41
2:A:183:GLU:HB3	2:A:184:PRO:CD	2.50	0.41
3:B:156:LYS:HA	3:B:156:LYS:HD3	1.89	0.41
3:B:396:THR:HA	3:B:399:PHE:HB3	2.01	0.41
1:C:75:THR:O	1:C:79:ASP:HB2	2.21	0.41
1:C:149:LYS:HB3	1:C:149:LYS:HE2	1.89	0.41
1:C:154:LEU:HG	1:C:467:PHE:HE1	1.85	0.41
2:A:224:TYR:HE1	4:A:500:GTP:C4	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:LEU:HD11	1:C:125:ILE:HB	2.01	0.41
1:C:456:ILE:H	1:C:456:ILE:HG12	1.53	0.41
1:C:494:LEU:HG	1:C:498:LYS:HE3	2.01	0.41
2:A:224:TYR:HE1	4:A:500:GTP:C4	2.34	0.41
1:C:75:THR:O	1:C:79:ASP:HB2	2.21	0.41
1:C:330:LEU:CD1	1:C:465:ARG:HB2	2.50	0.41
1:C:494:LEU:HG	1:C:498:LYS:HE3	2.01	0.41
2:A:224:TYR:HE1	4:A:500:GTP:C4	2.34	0.41
1:C:75:THR:O	1:C:79:ASP:HB2	2.21	0.41
1:C:95:LEU:HD11	1:C:125:ILE:HB	2.01	0.41
1:C:311:LEU:HD13	1:C:311:LEU:HA	1.90	0.41
2:A:224:TYR:HE1	4:A:500:GTP:C4	2.34	0.41
2:A:224:TYR:HE1	4:A:500:GTP:C4	2.34	0.41
1:C:95:LEU:HD11	1:C:125:ILE:HB	2.01	0.41
1:C:100:PRO:HD2	1:C:487:ALA:CB	2.51	0.41
1:C:455:LEU:HD13	3:B:431:GLU:HG2	2.02	0.41
1:C:149:LYS:HB3	1:C:149:LYS:HE2	1.89	0.41
1:C:149:LYS:HB3	1:C:149:LYS:HE2	1.89	0.41
1:C:456:ILE:H	1:C:456:ILE:HG12	1.53	0.41
1:C:413:ARG:O	1:C:413:ARG:NH1	2.41	0.41
1:C:75:THR:O	1:C:79:ASP:HB2	2.21	0.41
1:C:154:LEU:HG	1:C:467:PHE:HE1	1.85	0.41
1:C:100:PRO:HD2	1:C:487:ALA:CB	2.51	0.41
1:C:154:LEU:HG	1:C:467:PHE:HE1	1.85	0.41
1:C:100:PRO:HD2	1:C:487:ALA:CB	2.51	0.41
1:C:154:LEU:HG	1:C:467:PHE:HE1	1.85	0.41
1:C:100:PRO:HD2	1:C:487:ALA:CB	2.51	0.41
1:C:149:LYS:HB3	1:C:149:LYS:HE2	1.89	0.41
1:C:154:LEU:HG	1:C:467:PHE:HE1	1.85	0.41
1:C:456:ILE:H	1:C:456:ILE:HG12	1.53	0.41
1:C:100:PRO:HD2	1:C:487:ALA:CB	2.51	0.41
1:C:158:TYR:CE1	1:C:410:GLY:HA2	2.55	0.41
2:A:371:VAL:HG12	2:A:372:GLN:H	1.85	0.41
2:A:371:VAL:HG12	2:A:372:GLN:H	1.85	0.41
2:A:371:VAL:HG12	2:A:372:GLN:H	1.85	0.41
1:C:81:GLN:HE21	1:C:81:GLN:HB2	1.74	0.41
1:C:465:ARG:O	1:C:468:GLN:HB3	2.21	0.41
2:A:371:VAL:HG12	2:A:372:GLN:H	1.85	0.41
1:C:81:GLN:HE21	1:C:81:GLN:HB2	1.74	0.41
1:C:465:ARG:O	1:C:468:GLN:HB3	2.21	0.41
2:A:371:VAL:HG12	2:A:372:GLN:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLN:HE21	1:C:81:GLN:HB2	1.74	0.41
1:C:465:ARG:O	1:C:468:GLN:HB3	2.21	0.41
2:A:188:ILE:HD11	2:A:392:ASP:HA	2.02	0.41
1:C:81:GLN:HE21	1:C:81:GLN:HB2	1.74	0.41
1:C:465:ARG:O	1:C:468:GLN:HB3	2.21	0.41
2:A:188:ILE:HD11	2:A:392:ASP:HA	2.02	0.41
1:C:81:GLN:HE21	1:C:81:GLN:HB2	1.74	0.41
2:A:188:ILE:HD11	2:A:392:ASP:HA	2.02	0.41
1:C:311:LEU:HD12	1:C:327:THR:HG21	2.02	0.41
2:A:188:ILE:HD11	2:A:392:ASP:HA	2.02	0.41
2:A:188:ILE:HD11	2:A:392:ASP:HA	2.02	0.41
1:C:99:ALA:HA	1:C:100:PRO:HD3	1.75	0.41
2:A:205:ASP:CB	2:A:303:VAL:HA	2.51	0.41
3:B:205:ASP:HB3	3:B:208:ALA:HB3	2.02	0.41
3:B:243:ARG:HA	3:B:243:ARG:HD3	1.86	0.41
1:C:99:ALA:HA	1:C:100:PRO:HD3	1.75	0.41
2:A:205:ASP:CB	2:A:303:VAL:HA	2.51	0.41
3:B:205:ASP:HB3	3:B:208:ALA:HB3	2.02	0.41
3:B:243:ARG:HA	3:B:243:ARG:HD3	1.86	0.41
1:C:99:ALA:HA	1:C:100:PRO:HD3	1.75	0.41
1:C:465:ARG:O	1:C:468:GLN:HB3	2.21	0.41
2:A:205:ASP:CB	2:A:303:VAL:HA	2.51	0.41
3:B:205:ASP:HB3	3:B:208:ALA:HB3	2.02	0.41
3:B:243:ARG:HA	3:B:243:ARG:HD3	1.86	0.41
1:C:99:ALA:HA	1:C:100:PRO:HD3	1.75	0.41
2:A:205:ASP:CB	2:A:303:VAL:HA	2.51	0.41
3:B:205:ASP:HB3	3:B:208:ALA:HB3	2.02	0.41
3:B:243:ARG:HA	3:B:243:ARG:HD3	1.86	0.41
1:C:99:ALA:HA	1:C:100:PRO:HD3	1.75	0.41
1:C:312:LEU:O	1:C:328:LEU:HD13	2.20	0.41
1:C:378:ARG:NH1	1:C:412:GLU:OE1	2.44	0.41
2:A:205:ASP:CB	2:A:303:VAL:HA	2.51	0.41
3:B:205:ASP:HB3	3:B:208:ALA:HB3	2.02	0.41
3:B:243:ARG:HA	3:B:243:ARG:HD3	1.86	0.41
1:C:62:GLU:CD	1:C:474:ARG:HH22	2.24	0.41
1:C:154:LEU:HG	1:C:467:PHE:CE1	2.56	0.41
1:C:337:ASN:HA	1:C:338:PRO:HD3	1.85	0.41
2:A:24:TYR:OH	2:A:239:THR:HB	2.21	0.41
2:A:339:ARG:HA	2:A:339:ARG:HD3	1.84	0.41
2:A:369:ALA:O	2:A:370:LYS:HB3	2.21	0.41
1:C:154:LEU:HG	1:C:467:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:ASN:HA	1:C:338:PRO:HD3	1.85	0.41
2:A:24:TYR:OH	2:A:239:THR:HB	2.21	0.41
2:A:339:ARG:HA	2:A:339:ARG:HD3	1.84	0.41
2:A:369:ALA:O	2:A:370:LYS:HB3	2.21	0.41
1:C:154:LEU:HG	1:C:467:PHE:CE1	2.56	0.41
2:A:24:TYR:OH	2:A:239:THR:HB	2.21	0.41
2:A:339:ARG:HA	2:A:339:ARG:HD3	1.84	0.41
2:A:369:ALA:O	2:A:370:LYS:HB3	2.21	0.41
1:C:154:LEU:HG	1:C:467:PHE:CE1	2.56	0.41
2:A:24:TYR:OH	2:A:239:THR:HB	2.21	0.41
2:A:339:ARG:HA	2:A:339:ARG:HD3	1.84	0.41
2:A:369:ALA:O	2:A:370:LYS:HB3	2.21	0.41
1:C:154:LEU:HG	1:C:467:PHE:CE1	2.56	0.41
1:C:337:ASN:HA	1:C:338:PRO:HD3	1.85	0.41
1:C:455:LEU:HD13	3:B:431:GLU:HG2	2.03	0.41
2:A:24:TYR:OH	2:A:239:THR:HB	2.21	0.41
2:A:339:ARG:HA	2:A:339:ARG:HD3	1.84	0.41
2:A:369:ALA:O	2:A:370:LYS:HB3	2.21	0.41
1:C:92:THR:HB	1:C:124:GLN:OE1	2.21	0.41
2:A:221:ARG:N	2:A:222:PRO:HD3	2.36	0.41
2:A:260:VAL:HA	2:A:261:PRO:HD3	1.89	0.41
2:A:362:VAL:CG1	2:A:368:LEU:HB2	2.52	0.41
2:A:433:GLU:HG3	2:A:437:VAL:HG21	2.03	0.41
1:C:62:GLU:CD	1:C:474:ARG:HH22	2.25	0.41
1:C:92:THR:HB	1:C:124:GLN:OE1	2.21	0.41
2:A:221:ARG:N	2:A:222:PRO:HD3	2.36	0.41
2:A:260:VAL:HA	2:A:261:PRO:HD3	1.89	0.41
2:A:362:VAL:CG1	2:A:368:LEU:HB2	2.52	0.41
2:A:433:GLU:HG3	2:A:437:VAL:HG21	2.03	0.41
1:C:62:GLU:CD	1:C:474:ARG:HH22	2.25	0.41
1:C:337:ASN:HA	1:C:338:PRO:HD3	1.85	0.41
2:A:221:ARG:N	2:A:222:PRO:HD3	2.36	0.41
2:A:260:VAL:HA	2:A:261:PRO:HD3	1.89	0.41
2:A:362:VAL:CG1	2:A:368:LEU:HB2	2.52	0.41
2:A:433:GLU:HG3	2:A:437:VAL:HG21	2.03	0.41
1:C:62:GLU:CD	1:C:474:ARG:HH22	2.25	0.41
1:C:337:ASN:HA	1:C:338:PRO:HD3	1.85	0.41
2:A:221:ARG:N	2:A:222:PRO:HD3	2.36	0.41
2:A:260:VAL:HA	2:A:261:PRO:HD3	1.89	0.41
2:A:362:VAL:CG1	2:A:368:LEU:HB2	2.52	0.41
2:A:433:GLU:HG3	2:A:437:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:GLU:CD	1:C:474:ARG:HH22	2.25	0.41
1:C:92:THR:HB	1:C:124:GLN:OE1	2.21	0.41
2:A:221:ARG:N	2:A:222:PRO:HD3	2.36	0.41
2:A:260:VAL:HA	2:A:261:PRO:HD3	1.89	0.41
2:A:362:VAL:CG1	2:A:368:LEU:HB2	2.52	0.41
2:A:433:GLU:HG3	2:A:437:VAL:HG21	2.03	0.41
1:C:92:THR:HB	1:C:124:GLN:OE1	2.21	0.40
1:C:455:LEU:HD13	3:B:431:GLU:HG2	2.03	0.40
1:C:92:THR:HB	1:C:124:GLN:OE1	2.21	0.40
2:A:391:LEU:HD12	2:A:391:LEU:HA	1.98	0.40
2:A:391:LEU:HD12	2:A:391:LEU:HA	1.98	0.40
2:A:391:LEU:HD12	2:A:391:LEU:HA	1.98	0.40
2:A:391:LEU:HD12	2:A:391:LEU:HA	1.98	0.40
2:A:391:LEU:HD12	2:A:391:LEU:HA	1.98	0.40
3:B:31:ASP:CG	3:B:32:PRO:HD2	2.41	0.40
3:B:136:GLN:HA	3:B:167:ASN:O	2.21	0.40
3:B:360:PRO:HB3	7:B:601:TA1:C37	2.51	0.40
3:B:31:ASP:CG	3:B:32:PRO:HD2	2.41	0.40
3:B:136:GLN:HA	3:B:167:ASN:O	2.21	0.40
3:B:360:PRO:HB3	7:B:601:TA1:C37	2.51	0.40
3:B:31:ASP:CG	3:B:32:PRO:HD2	2.41	0.40
3:B:136:GLN:HA	3:B:167:ASN:O	2.21	0.40
3:B:360:PRO:HB3	7:B:601:TA1:C37	2.51	0.40
1:C:169:ILE:HA	1:C:178:ILE:HG22	2.03	0.40
3:B:31:ASP:CG	3:B:32:PRO:HD2	2.41	0.40
3:B:136:GLN:HA	3:B:167:ASN:O	2.21	0.40
3:B:360:PRO:HB3	7:B:601:TA1:C37	2.51	0.40
1:C:169:ILE:HA	1:C:178:ILE:HG22	2.03	0.40
3:B:31:ASP:CG	3:B:32:PRO:HD2	2.41	0.40
3:B:136:GLN:HA	3:B:167:ASN:O	2.21	0.40
3:B:360:PRO:HB3	7:B:601:TA1:C37	2.51	0.40
2:A:201:ALA:O	2:A:267:PHE:HA	2.21	0.40
2:A:292:THR:HG22	2:A:296:PHE:HE2	1.87	0.40
1:C:169:ILE:HA	1:C:178:ILE:HG22	2.03	0.40
2:A:201:ALA:O	2:A:267:PHE:HA	2.21	0.40
2:A:292:THR:HG22	2:A:296:PHE:HE2	1.87	0.40
2:A:201:ALA:O	2:A:267:PHE:HA	2.21	0.40
2:A:292:THR:HG22	2:A:296:PHE:HE2	1.87	0.40
2:A:201:ALA:O	2:A:267:PHE:HA	2.21	0.40
2:A:292:THR:HG22	2:A:296:PHE:HE2	1.87	0.40
1:C:378:ARG:HD3	1:C:378:ARG:HA	1.82	0.40

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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	0.40
2:A:292:THR:HG22	2:A:296:PHE:HE2	1.87	0.40
1:C:169:ILE:HA	1:C:178:ILE:HG22	2.04	0.40
1:C:169:ILE:HA	1:C:178:ILE:HG22	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	282/501 (56%)	267 (95%)	10 (4%)	5 (2%)	8	40
1	2-C	282/501 (56%)	265 (94%)	14 (5%)	3 (1%)	14	52
1	3-C	281/501 (56%)	266 (95%)	10 (4%)	5 (2%)	8	40
1	4-C	282/501 (56%)	266 (94%)	12 (4%)	4 (1%)	11	46
1	5-C	282/501 (56%)	265 (94%)	11 (4%)	6 (2%)	7	36
2	1-A	408/451 (90%)	366 (90%)	38 (9%)	4 (1%)	15	54
2	2-A	408/451 (90%)	366 (90%)	38 (9%)	4 (1%)	15	54
2	3-A	408/451 (90%)	366 (90%)	38 (9%)	4 (1%)	15	54
2	4-A	408/451 (90%)	366 (90%)	38 (9%)	4 (1%)	15	54
2	5-A	408/451 (90%)	366 (90%)	38 (9%)	4 (1%)	15	54
3	1-B	424/445 (95%)	379 (89%)	38 (9%)	7 (2%)	9	42
3	2-B	424/445 (95%)	379 (89%)	38 (9%)	7 (2%)	9	42
3	3-B	424/445 (95%)	379 (89%)	38 (9%)	7 (2%)	9	42
3	4-B	424/445 (95%)	379 (89%)	38 (9%)	7 (2%)	9	42
3	5-B	424/445 (95%)	379 (89%)	38 (9%)	7 (2%)	9	42
All	All	5569/6985 (80%)	5054 (91%)	437 (8%)	78 (1%)	15	46

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-C	317	GLU
3	1-B	288	VAL
3	2-B	288	VAL
1	3-C	379	SER
3	3-B	288	VAL
3	4-B	288	VAL
1	5-C	317	GLU
3	5-B	288	VAL
1	1-C	297	ARG
1	1-C	501	ALA
2	1-A	279	GLU
1	2-C	297	ARG
2	2-A	279	GLU
1	3-C	297	ARG
2	3-A	279	GLU
1	4-C	297	ARG
1	4-C	501	ALA
2	4-A	279	GLU
1	5-C	297	ARG
1	5-C	501	ALA
2	5-A	279	GLU
1	1-C	73	PHE
3	1-B	56	ALA
1	2-C	73	PHE
3	2-B	56	ALA
1	3-C	73	PHE
1	3-C	501	ALA
3	3-B	56	ALA
1	4-C	73	PHE
3	4-B	56	ALA
1	5-C	73	PHE
3	5-B	56	ALA
3	1-B	344	VAL
3	1-B	403	ALA
3	2-B	344	VAL
3	2-B	403	ALA
3	3-B	344	VAL
3	3-B	403	ALA
3	4-B	344	VAL
3	4-B	403	ALA
1	5-C	379	SER
3	5-B	344	VAL

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Mol	Chain	Res	Type
3	5-B	403	ALA
2	1-A	273	ALA
2	1-A	348	PRO
3	1-B	266	HIS
2	2-A	273	ALA
2	2-A	348	PRO
3	2-B	266	HIS
2	3-A	273	ALA
2	3-A	348	PRO
3	3-B	266	HIS
2	4-A	273	ALA
2	4-A	348	PRO
3	4-B	266	HIS
2	5-A	273	ALA
2	5-A	348	PRO
3	5-B	266	HIS
1	1-C	160	VAL
1	2-C	160	VAL
1	3-C	160	VAL
1	4-C	160	VAL
1	5-C	160	VAL
2	1-A	437	VAL
3	1-B	142	GLY
3	1-B	412	GLY
2	2-A	437	VAL
3	2-B	142	GLY
3	2-B	412	GLY
2	3-A	437	VAL
3	3-B	142	GLY
3	3-B	412	GLY
2	4-A	437	VAL
3	4-B	142	GLY
3	4-B	412	GLY
2	5-A	437	VAL
3	5-B	142	GLY
3	5-B	412	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	265/447 (59%)	224 (84%)	41 (16%)	2	14
1	2-C	265/447 (59%)	225 (85%)	40 (15%)	3	15
1	3-C	264/447 (59%)	221 (84%)	43 (16%)	2	13
1	4-C	265/447 (59%)	225 (85%)	40 (15%)	3	15
1	5-C	265/447 (59%)	225 (85%)	40 (15%)	3	15
2	1-A	347/377 (92%)	311 (90%)	36 (10%)	7	25
2	2-A	347/377 (92%)	311 (90%)	36 (10%)	7	25
2	3-A	347/377 (92%)	311 (90%)	36 (10%)	7	25
2	4-A	347/377 (92%)	311 (90%)	36 (10%)	7	25
2	5-A	347/377 (92%)	311 (90%)	36 (10%)	7	25
3	1-B	367/381 (96%)	317 (86%)	50 (14%)	3	17
3	2-B	367/381 (96%)	317 (86%)	50 (14%)	3	17
3	3-B	367/381 (96%)	317 (86%)	50 (14%)	3	17
3	4-B	367/381 (96%)	317 (86%)	50 (14%)	3	17
3	5-B	367/381 (96%)	317 (86%)	50 (14%)	3	17
All	All	4894/6025 (81%)	4260 (87%)	634 (13%)	7	18

All (634) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-C	63	LYS
1	1-C	69	ARG
1	1-C	75	THR
1	1-C	76	SER
1	1-C	79	ASP
1	1-C	81	GLN
1	1-C	117	THR
1	1-C	125	ILE
1	1-C	138	LEU
1	1-C	139	THR
1	1-C	146	ASP
1	1-C	151	GLN
1	1-C	169	ILE
1	1-C	172	THR
1	1-C	173	SER

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Mol	Chain	Res	Type
1	1-C	175	ASP
1	1-C	178	ILE
1	1-C	181	GLN
1	1-C	185	LEU
1	1-C	188	ASN
1	1-C	303	SER
1	1-C	307	ILE
1	1-C	317	GLU
1	1-C	334	GLN
1	1-C	352	GLU
1	1-C	357	LEU
1	1-C	378	ARG
1	1-C	381	SER
1	1-C	390	LEU
1	1-C	399	LYS
1	1-C	424	LYS
1	1-C	456	ILE
1	1-C	464	THR
1	1-C	471	PHE
1	1-C	472	THR
1	1-C	476	ARG
1	1-C	477	SER
1	1-C	489	THR
1	1-C	492	GLU
1	1-C	499	PHE
1	1-C	500	SER
2	1-A	22	GLU
2	1-A	82	THR
2	1-A	94	THR
2	1-A	98	ASP
2	1-A	101	ASN
2	1-A	109	THR
2	1-A	136	SER
2	1-A	140	SER
2	1-A	141	PHE
2	1-A	150	THR
2	1-A	170	SER
2	1-A	178	SER
2	1-A	185	TYR
2	1-A	192	HIS
2	1-A	194	THR
2	1-A	200	CYS

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Mol	Chain	Res	Type
2	1-A	223	THR
2	1-A	224	TYR
2	1-A	239	THR
2	1-A	243	ARG
2	1-A	253	THR
2	1-A	255	PHE
2	1-A	264	ARG
2	1-A	272	TYR
2	1-A	287	SER
2	1-A	315	CYS
2	1-A	349	THR
2	1-A	356	ASN
2	1-A	361	THR
2	1-A	376	CYS
2	1-A	382	THR
2	1-A	402	ARG
2	1-A	415	GLU
2	1-A	424	ASP
2	1-A	425	MET
2	1-A	439	SER
3	1-B	2	ARG
3	1-B	25	SER
3	1-B	40	SER
3	1-B	41	ASP
3	1-B	48	ARG
3	1-B	76	ASP
3	1-B	77	SER
3	1-B	116	ASP
3	1-B	124	LYS
3	1-B	128	SER
3	1-B	130	ASP
3	1-B	139	HIS
3	1-B	145	THR
3	1-B	147	SER
3	1-B	158	ARG
3	1-B	165	ILE
3	1-B	174	SER
3	1-B	180	THR
3	1-B	185	TYR
3	1-B	190	SER
3	1-B	199	ASP
3	1-B	201	THR

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Mol	Chain	Res	Type
3	1-B	209	LEU
3	1-B	216	THR
3	1-B	223	THR
3	1-B	239	THR
3	1-B	240	THR
3	1-B	251	ASP
3	1-B	275	LEU
3	1-B	280	SER
3	1-B	283	TYR
3	1-B	288	VAL
3	1-B	292	THR
3	1-B	299	LYS
3	1-B	311	ARG
3	1-B	322	ARG
3	1-B	325	MET
3	1-B	326	LYS
3	1-B	337	ASN
3	1-B	343	PHE
3	1-B	353	THR
3	1-B	369	ARG
3	1-B	374	SER
3	1-B	376	THR
3	1-B	382	THR
3	1-B	409	THR
3	1-B	413	MET
3	1-B	419	THR
3	1-B	427	ASP
3	1-B	430	SER
1	2-C	63	LYS
1	2-C	69	ARG
1	2-C	75	THR
1	2-C	76	SER
1	2-C	79	ASP
1	2-C	81	GLN
1	2-C	117	THR
1	2-C	125	ILE
1	2-C	138	LEU
1	2-C	139	THR
1	2-C	146	ASP
1	2-C	151	GLN
1	2-C	169	ILE
1	2-C	173	SER

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Mol	Chain	Res	Type
1	2-C	175	ASP
1	2-C	178	ILE
1	2-C	181	GLN
1	2-C	185	LEU
1	2-C	188	ASN
1	2-C	303	SER
1	2-C	307	ILE
1	2-C	334	GLN
1	2-C	352	GLU
1	2-C	357	LEU
1	2-C	381	SER
1	2-C	390	LEU
1	2-C	399	LYS
1	2-C	412	GLU
1	2-C	413	ARG
1	2-C	424	LYS
1	2-C	456	ILE
1	2-C	464	THR
1	2-C	471	PHE
1	2-C	472	THR
1	2-C	476	ARG
1	2-C	477	SER
1	2-C	489	THR
1	2-C	492	GLU
1	2-C	499	PHE
1	2-C	500	SER
2	2-A	22	GLU
2	2-A	82	THR
2	2-A	94	THR
2	2-A	98	ASP
2	2-A	101	ASN
2	2-A	109	THR
2	2-A	136	SER
2	2-A	140	SER
2	2-A	141	PHE
2	2-A	150	THR
2	2-A	170	SER
2	2-A	178	SER
2	2-A	185	TYR
2	2-A	192	HIS
2	2-A	194	THR
2	2-A	200	CYS

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Mol	Chain	Res	Type
2	2-A	223	THR
2	2-A	224	TYR
2	2-A	239	THR
2	2-A	243	ARG
2	2-A	253	THR
2	2-A	255	PHE
2	2-A	264	ARG
2	2-A	272	TYR
2	2-A	287	SER
2	2-A	315	CYS
2	2-A	349	THR
2	2-A	356	ASN
2	2-A	361	THR
2	2-A	376	CYS
2	2-A	382	THR
2	2-A	402	ARG
2	2-A	415	GLU
2	2-A	424	ASP
2	2-A	425	MET
2	2-A	439	SER
3	2-B	2	ARG
3	2-B	25	SER
3	2-B	40	SER
3	2-B	41	ASP
3	2-B	48	ARG
3	2-B	76	ASP
3	2-B	77	SER
3	2-B	116	ASP
3	2-B	124	LYS
3	2-B	128	SER
3	2-B	130	ASP
3	2-B	139	HIS
3	2-B	145	THR
3	2-B	147	SER
3	2-B	158	ARG
3	2-B	165	ILE
3	2-B	174	SER
3	2-B	180	THR
3	2-B	185	TYR
3	2-B	190	SER
3	2-B	199	ASP
3	2-B	201	THR

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Mol	Chain	Res	Type
3	2-B	209	LEU
3	2-B	216	THR
3	2-B	223	THR
3	2-B	239	THR
3	2-B	240	THR
3	2-B	251	ASP
3	2-B	275	LEU
3	2-B	280	SER
3	2-B	283	TYR
3	2-B	288	VAL
3	2-B	292	THR
3	2-B	299	LYS
3	2-B	311	ARG
3	2-B	322	ARG
3	2-B	325	MET
3	2-B	326	LYS
3	2-B	337	ASN
3	2-B	343	PHE
3	2-B	353	THR
3	2-B	369	ARG
3	2-B	374	SER
3	2-B	376	THR
3	2-B	382	THR
3	2-B	409	THR
3	2-B	413	MET
3	2-B	419	THR
3	2-B	427	ASP
3	2-B	430	SER
1	3-C	63	LYS
1	3-C	69	ARG
1	3-C	75	THR
1	3-C	76	SER
1	3-C	79	ASP
1	3-C	81	GLN
1	3-C	117	THR
1	3-C	125	ILE
1	3-C	138	LEU
1	3-C	139	THR
1	3-C	146	ASP
1	3-C	151	GLN
1	3-C	169	ILE
1	3-C	173	SER

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Mol	Chain	Res	Type
1	3-C	175	ASP
1	3-C	178	ILE
1	3-C	181	GLN
1	3-C	185	LEU
1	3-C	188	ASN
1	3-C	298	PHE
1	3-C	303	SER
1	3-C	307	ILE
1	3-C	327	THR
1	3-C	334	GLN
1	3-C	352	GLU
1	3-C	357	LEU
1	3-C	378	ARG
1	3-C	381	SER
1	3-C	390	LEU
1	3-C	399	LYS
1	3-C	412	GLU
1	3-C	422	ARG
1	3-C	424	LYS
1	3-C	456	ILE
1	3-C	464	THR
1	3-C	471	PHE
1	3-C	472	THR
1	3-C	476	ARG
1	3-C	477	SER
1	3-C	489	THR
1	3-C	492	GLU
1	3-C	499	PHE
1	3-C	500	SER
2	3-A	22	GLU
2	3-A	82	THR
2	3-A	94	THR
2	3-A	98	ASP
2	3-A	101	ASN
2	3-A	109	THR
2	3-A	136	SER
2	3-A	140	SER
2	3-A	141	PHE
2	3-A	150	THR
2	3-A	170	SER
2	3-A	178	SER
2	3-A	185	TYR

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Mol	Chain	Res	Type
2	3-A	192	HIS
2	3-A	194	THR
2	3-A	200	CYS
2	3-A	223	THR
2	3-A	224	TYR
2	3-A	239	THR
2	3-A	243	ARG
2	3-A	253	THR
2	3-A	255	PHE
2	3-A	264	ARG
2	3-A	272	TYR
2	3-A	287	SER
2	3-A	315	CYS
2	3-A	349	THR
2	3-A	356	ASN
2	3-A	361	THR
2	3-A	376	CYS
2	3-A	382	THR
2	3-A	402	ARG
2	3-A	415	GLU
2	3-A	424	ASP
2	3-A	425	MET
2	3-A	439	SER
3	3-B	2	ARG
3	3-B	25	SER
3	3-B	40	SER
3	3-B	41	ASP
3	3-B	48	ARG
3	3-B	76	ASP
3	3-B	77	SER
3	3-B	116	ASP
3	3-B	124	LYS
3	3-B	128	SER
3	3-B	130	ASP
3	3-B	139	HIS
3	3-B	145	THR
3	3-B	147	SER
3	3-B	158	ARG
3	3-B	165	ILE
3	3-B	174	SER
3	3-B	180	THR
3	3-B	185	TYR

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Mol	Chain	Res	Type
3	3-B	190	SER
3	3-B	199	ASP
3	3-B	201	THR
3	3-B	209	LEU
3	3-B	216	THR
3	3-B	223	THR
3	3-B	239	THR
3	3-B	240	THR
3	3-B	251	ASP
3	3-B	275	LEU
3	3-B	280	SER
3	3-B	283	TYR
3	3-B	288	VAL
3	3-B	292	THR
3	3-B	299	LYS
3	3-B	311	ARG
3	3-B	322	ARG
3	3-B	325	MET
3	3-B	326	LYS
3	3-B	337	ASN
3	3-B	343	PHE
3	3-B	353	THR
3	3-B	369	ARG
3	3-B	374	SER
3	3-B	376	THR
3	3-B	382	THR
3	3-B	409	THR
3	3-B	413	MET
3	3-B	419	THR
3	3-B	427	ASP
3	3-B	430	SER
1	4-C	63	LYS
1	4-C	69	ARG
1	4-C	75	THR
1	4-C	76	SER
1	4-C	79	ASP
1	4-C	81	GLN
1	4-C	117	THR
1	4-C	125	ILE
1	4-C	138	LEU
1	4-C	139	THR
1	4-C	146	ASP

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Mol	Chain	Res	Type
1	4-C	151	GLN
1	4-C	169	ILE
1	4-C	173	SER
1	4-C	175	ASP
1	4-C	178	ILE
1	4-C	181	GLN
1	4-C	185	LEU
1	4-C	188	ASN
1	4-C	298	PHE
1	4-C	303	SER
1	4-C	307	ILE
1	4-C	334	GLN
1	4-C	352	GLU
1	4-C	357	LEU
1	4-C	381	SER
1	4-C	390	LEU
1	4-C	399	LYS
1	4-C	412	GLU
1	4-C	424	LYS
1	4-C	456	ILE
1	4-C	464	THR
1	4-C	471	PHE
1	4-C	472	THR
1	4-C	476	ARG
1	4-C	477	SER
1	4-C	489	THR
1	4-C	492	GLU
1	4-C	499	PHE
1	4-C	500	SER
2	4-A	22	GLU
2	4-A	82	THR
2	4-A	94	THR
2	4-A	98	ASP
2	4-A	101	ASN
2	4-A	109	THR
2	4-A	136	SER
2	4-A	140	SER
2	4-A	141	PHE
2	4-A	150	THR
2	4-A	170	SER
2	4-A	178	SER
2	4-A	185	TYR

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Mol	Chain	Res	Type
2	4-A	192	HIS
2	4-A	194	THR
2	4-A	200	CYS
2	4-A	223	THR
2	4-A	224	TYR
2	4-A	239	THR
2	4-A	243	ARG
2	4-A	253	THR
2	4-A	255	PHE
2	4-A	264	ARG
2	4-A	272	TYR
2	4-A	287	SER
2	4-A	315	CYS
2	4-A	349	THR
2	4-A	356	ASN
2	4-A	361	THR
2	4-A	376	CYS
2	4-A	382	THR
2	4-A	402	ARG
2	4-A	415	GLU
2	4-A	424	ASP
2	4-A	425	MET
2	4-A	439	SER
3	4-B	2	ARG
3	4-B	25	SER
3	4-B	40	SER
3	4-B	41	ASP
3	4-B	48	ARG
3	4-B	76	ASP
3	4-B	77	SER
3	4-B	116	ASP
3	4-B	124	LYS
3	4-B	128	SER
3	4-B	130	ASP
3	4-B	139	HIS
3	4-B	145	THR
3	4-B	147	SER
3	4-B	158	ARG
3	4-B	165	ILE
3	4-B	174	SER
3	4-B	180	THR
3	4-B	185	TYR

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Mol	Chain	Res	Type
3	4-B	190	SER
3	4-B	199	ASP
3	4-B	201	THR
3	4-B	209	LEU
3	4-B	216	THR
3	4-B	223	THR
3	4-B	239	THR
3	4-B	240	THR
3	4-B	251	ASP
3	4-B	275	LEU
3	4-B	280	SER
3	4-B	283	TYR
3	4-B	288	VAL
3	4-B	292	THR
3	4-B	299	LYS
3	4-B	311	ARG
3	4-B	322	ARG
3	4-B	325	MET
3	4-B	326	LYS
3	4-B	337	ASN
3	4-B	343	PHE
3	4-B	353	THR
3	4-B	369	ARG
3	4-B	374	SER
3	4-B	376	THR
3	4-B	382	THR
3	4-B	409	THR
3	4-B	413	MET
3	4-B	419	THR
3	4-B	427	ASP
3	4-B	430	SER
1	5-C	63	LYS
1	5-C	69	ARG
1	5-C	75	THR
1	5-C	76	SER
1	5-C	79	ASP
1	5-C	81	GLN
1	5-C	117	THR
1	5-C	125	ILE
1	5-C	138	LEU
1	5-C	139	THR
1	5-C	146	ASP

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Mol	Chain	Res	Type
1	5-C	151	GLN
1	5-C	169	ILE
1	5-C	172	THR
1	5-C	173	SER
1	5-C	175	ASP
1	5-C	178	ILE
1	5-C	181	GLN
1	5-C	185	LEU
1	5-C	188	ASN
1	5-C	303	SER
1	5-C	307	ILE
1	5-C	317	GLU
1	5-C	334	GLN
1	5-C	352	GLU
1	5-C	357	LEU
1	5-C	381	SER
1	5-C	390	LEU
1	5-C	399	LYS
1	5-C	424	LYS
1	5-C	456	ILE
1	5-C	464	THR
1	5-C	471	PHE
1	5-C	472	THR
1	5-C	476	ARG
1	5-C	477	SER
1	5-C	489	THR
1	5-C	492	GLU
1	5-C	499	PHE
1	5-C	500	SER
2	5-A	22	GLU
2	5-A	82	THR
2	5-A	94	THR
2	5-A	98	ASP
2	5-A	101	ASN
2	5-A	109	THR
2	5-A	136	SER
2	5-A	140	SER
2	5-A	141	PHE
2	5-A	150	THR
2	5-A	170	SER
2	5-A	178	SER
2	5-A	185	TYR

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Mol	Chain	Res	Type
2	5-A	192	HIS
2	5-A	194	THR
2	5-A	200	CYS
2	5-A	223	THR
2	5-A	224	TYR
2	5-A	239	THR
2	5-A	243	ARG
2	5-A	253	THR
2	5-A	255	PHE
2	5-A	264	ARG
2	5-A	272	TYR
2	5-A	287	SER
2	5-A	315	CYS
2	5-A	349	THR
2	5-A	356	ASN
2	5-A	361	THR
2	5-A	376	CYS
2	5-A	382	THR
2	5-A	402	ARG
2	5-A	415	GLU
2	5-A	424	ASP
2	5-A	425	MET
2	5-A	439	SER
3	5-B	2	ARG
3	5-B	25	SER
3	5-B	40	SER
3	5-B	41	ASP
3	5-B	48	ARG
3	5-B	76	ASP
3	5-B	77	SER
3	5-B	116	ASP
3	5-B	124	LYS
3	5-B	128	SER
3	5-B	130	ASP
3	5-B	139	HIS
3	5-B	145	THR
3	5-B	147	SER
3	5-B	158	ARG
3	5-B	165	ILE
3	5-B	174	SER
3	5-B	180	THR
3	5-B	185	TYR

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Mol	Chain	Res	Type
3	5-B	190	SER
3	5-B	199	ASP
3	5-B	201	THR
3	5-B	209	LEU
3	5-B	216	THR
3	5-B	223	THR
3	5-B	239	THR
3	5-B	240	THR
3	5-B	251	ASP
3	5-B	275	LEU
3	5-B	280	SER
3	5-B	283	TYR
3	5-B	288	VAL
3	5-B	292	THR
3	5-B	299	LYS
3	5-B	311	ARG
3	5-B	322	ARG
3	5-B	325	MET
3	5-B	326	LYS
3	5-B	337	ASN
3	5-B	343	PHE
3	5-B	353	THR
3	5-B	369	ARG
3	5-B	374	SER
3	5-B	376	THR
3	5-B	382	THR
3	5-B	409	THR
3	5-B	413	MET
3	5-B	419	THR
3	5-B	427	ASP
3	5-B	430	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-C	84	GLN
1	1-C	181	GLN
1	1-C	365	GLN
1	1-C	449	ASN
2	1-A	197	HIS
3	1-B	206	ASN
3	1-B	337	ASN

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Mol	Chain	Res	Type
3	1-B	434	GLN
1	2-C	84	GLN
1	2-C	181	GLN
1	2-C	365	GLN
1	2-C	445	GLN
2	2-A	197	HIS
3	2-B	206	ASN
3	2-B	337	ASN
3	2-B	434	GLN
1	3-C	84	GLN
1	3-C	181	GLN
1	3-C	365	GLN
1	3-C	445	GLN
2	3-A	197	HIS
3	3-B	206	ASN
3	3-B	337	ASN
3	3-B	434	GLN
1	4-C	84	GLN
1	4-C	118	HIS
1	4-C	181	GLN
1	4-C	309	ASN
1	4-C	365	GLN
1	4-C	445	GLN
1	4-C	449	ASN
2	4-A	197	HIS
3	4-B	206	ASN
3	4-B	337	ASN
3	4-B	434	GLN
1	5-C	84	GLN
1	5-C	181	GLN
1	5-C	365	GLN
1	5-C	445	GLN
2	5-A	197	HIS
3	5-B	206	ASN
3	5-B	337	ASN
3	5-B	434	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 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	TA1	1-B	601	-	68,68,68	2.00	19 (27%)	105,105,105	1.39	11 (10%)
6	GDP	2-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
6	GDP	1-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
7	TA1	4-B	601	-	68,68,68	2.00	19 (27%)	105,105,105	1.39	11 (10%)
4	GTP	2-A	500	2,5	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)
4	GTP	1-A	500	2,5	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)
7	TA1	5-B	601	-	68,68,68	2.00	19 (27%)	105,105,105	1.39	11 (10%)
4	GTP	5-A	500	2,5	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)
6	GDP	3-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
6	GDP	4-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
6	GDP	5-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
7	TA1	3-B	601	-	68,68,68	2.00	19 (27%)	105,105,105	1.39	11 (10%)
4	GTP	4-A	500	2,5	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)
4	GTP	3-A	500	2,5	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)
7	TA1	2-B	601	-	68,68,68	2.00	19 (27%)	105,105,105	1.39	11 (10%)

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	TA1	1-B	601	-	-	9/41/127/127	0/7/7/7
6	GDP	2-B	600	-	-	4/12/32/32	0/3/3/3
6	GDP	1-B	600	-	-	4/12/32/32	0/3/3/3
7	TA1	4-B	601	-	-	9/41/127/127	0/7/7/7
4	GTP	2-A	500	2,5	-	3/18/38/38	0/3/3/3
4	GTP	1-A	500	2,5	-	3/18/38/38	0/3/3/3
7	TA1	5-B	601	-	-	9/41/127/127	0/7/7/7
4	GTP	5-A	500	2,5	-	3/18/38/38	0/3/3/3
6	GDP	3-B	600	-	-	4/12/32/32	0/3/3/3
6	GDP	4-B	600	-	-	4/12/32/32	0/3/3/3
6	GDP	5-B	600	-	-	4/12/32/32	0/3/3/3
7	TA1	3-B	601	-	-	9/41/127/127	0/7/7/7
4	GTP	4-A	500	2,5	-	3/18/38/38	0/3/3/3
4	GTP	3-A	500	2,5	-	3/18/38/38	0/3/3/3
7	TA1	2-B	601	-	-	9/41/127/127	0/7/7/7

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1-B	600	GDP	O4'-C1'	6.36	1.50	1.41
6	2-B	600	GDP	O4'-C1'	6.36	1.50	1.41
6	3-B	600	GDP	O4'-C1'	6.36	1.50	1.41
6	4-B	600	GDP	O4'-C1'	6.36	1.50	1.41
6	5-B	600	GDP	O4'-C1'	6.36	1.50	1.41
6	1-B	600	GDP	O6-C6	5.65	1.34	1.23
6	2-B	600	GDP	O6-C6	5.65	1.34	1.23
6	3-B	600	GDP	O6-C6	5.65	1.34	1.23
6	4-B	600	GDP	O6-C6	5.65	1.34	1.23
6	5-B	600	GDP	O6-C6	5.65	1.34	1.23
7	1-B	601	TA1	C06-C05	5.30	1.50	1.38
7	2-B	601	TA1	C06-C05	5.30	1.50	1.38
7	3-B	601	TA1	C06-C05	5.30	1.50	1.38
7	4-B	601	TA1	C06-C05	5.30	1.50	1.38
7	5-B	601	TA1	C06-C05	5.30	1.50	1.38
7	1-B	601	TA1	C18-C10	5.09	1.69	1.57
7	2-B	601	TA1	C18-C10	5.09	1.69	1.57
7	3-B	601	TA1	C18-C10	5.09	1.69	1.57
7	4-B	601	TA1	C18-C10	5.09	1.69	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	5-B	601	TA1	C18-C10	5.09	1.69	1.57
6	1-B	600	GDP	C2-N1	4.70	1.49	1.37
6	2-B	600	GDP	C2-N1	4.70	1.49	1.37
6	3-B	600	GDP	C2-N1	4.70	1.49	1.37
6	4-B	600	GDP	C2-N1	4.70	1.49	1.37
6	5-B	600	GDP	C2-N1	4.70	1.49	1.37
7	1-B	601	TA1	C08-C07	-4.55	1.25	1.38
7	2-B	601	TA1	C08-C07	-4.55	1.25	1.38
7	3-B	601	TA1	C08-C07	-4.55	1.25	1.38
7	4-B	601	TA1	C08-C07	-4.55	1.25	1.38
7	5-B	601	TA1	C08-C07	-4.55	1.25	1.38
7	1-B	601	TA1	C05-C04	4.35	1.46	1.39
7	2-B	601	TA1	C05-C04	4.35	1.46	1.39
7	3-B	601	TA1	C05-C04	4.35	1.46	1.39
7	4-B	601	TA1	C05-C04	4.35	1.46	1.39
7	5-B	601	TA1	C05-C04	4.35	1.46	1.39
7	1-B	601	TA1	C45-C24	3.97	1.61	1.54
7	2-B	601	TA1	C45-C24	3.97	1.61	1.54
7	3-B	601	TA1	C45-C24	3.97	1.61	1.54
7	4-B	601	TA1	C45-C24	3.97	1.61	1.54
7	5-B	601	TA1	C45-C24	3.97	1.61	1.54
6	1-B	600	GDP	PB-O2B	-3.81	1.40	1.54
6	2-B	600	GDP	PB-O2B	-3.81	1.40	1.54
6	3-B	600	GDP	PB-O2B	-3.81	1.40	1.54
6	4-B	600	GDP	PB-O2B	-3.81	1.40	1.54
6	5-B	600	GDP	PB-O2B	-3.81	1.40	1.54
4	1-A	500	GTP	C5-C6	-3.74	1.39	1.47
4	2-A	500	GTP	C5-C6	-3.74	1.39	1.47
4	3-A	500	GTP	C5-C6	-3.74	1.39	1.47
4	4-A	500	GTP	C5-C6	-3.74	1.39	1.47
4	5-A	500	GTP	C5-C6	-3.74	1.39	1.47
7	1-B	601	TA1	O02-C03	3.61	1.42	1.34
7	2-B	601	TA1	O02-C03	3.61	1.42	1.34
7	3-B	601	TA1	O02-C03	3.61	1.42	1.34
7	4-B	601	TA1	O02-C03	3.61	1.42	1.34
7	5-B	601	TA1	O02-C03	3.61	1.42	1.34
6	1-B	600	GDP	C8-N7	3.45	1.40	1.35
6	2-B	600	GDP	C8-N7	3.45	1.40	1.35
6	3-B	600	GDP	C8-N7	3.45	1.40	1.35
6	4-B	600	GDP	C8-N7	3.45	1.40	1.35
6	5-B	600	GDP	C8-N7	3.45	1.40	1.35
7	1-B	601	TA1	C36-C31	3.33	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-B	601	TA1	C36-C31	3.33	1.45	1.39
7	3-B	601	TA1	C36-C31	3.33	1.45	1.39
7	4-B	601	TA1	C36-C31	3.33	1.45	1.39
7	5-B	601	TA1	C36-C31	3.33	1.45	1.39
7	1-B	601	TA1	C25-C24	3.25	1.39	1.34
7	2-B	601	TA1	C25-C24	3.25	1.39	1.34
7	3-B	601	TA1	C25-C24	3.25	1.39	1.34
7	4-B	601	TA1	C25-C24	3.25	1.39	1.34
7	5-B	601	TA1	C25-C24	3.25	1.39	1.34
7	1-B	601	TA1	C46-C45	3.16	1.60	1.53
7	2-B	601	TA1	C46-C45	3.16	1.60	1.53
7	3-B	601	TA1	C46-C45	3.16	1.60	1.53
7	4-B	601	TA1	C46-C45	3.16	1.60	1.53
7	5-B	601	TA1	C46-C45	3.16	1.60	1.53
7	1-B	601	TA1	C43-C01	3.07	1.60	1.54
7	2-B	601	TA1	C43-C01	3.07	1.60	1.54
7	3-B	601	TA1	C43-C01	3.07	1.60	1.54
7	4-B	601	TA1	C43-C01	3.07	1.60	1.54
7	5-B	601	TA1	C43-C01	3.07	1.60	1.54
7	1-B	601	TA1	C11-C10	3.06	1.61	1.54
7	2-B	601	TA1	C11-C10	3.06	1.61	1.54
7	3-B	601	TA1	C11-C10	3.06	1.61	1.54
7	4-B	601	TA1	C11-C10	3.06	1.61	1.54
7	5-B	601	TA1	C11-C10	3.06	1.61	1.54
6	1-B	600	GDP	C5-C6	-2.89	1.41	1.47
6	2-B	600	GDP	C5-C6	-2.89	1.41	1.47
6	3-B	600	GDP	C5-C6	-2.89	1.41	1.47
6	4-B	600	GDP	C5-C6	-2.89	1.41	1.47
6	5-B	600	GDP	C5-C6	-2.89	1.41	1.47
7	1-B	601	TA1	C43-C26	2.78	1.58	1.52
7	2-B	601	TA1	C43-C26	2.78	1.58	1.52
7	3-B	601	TA1	C43-C26	2.78	1.58	1.52
7	4-B	601	TA1	C43-C26	2.78	1.58	1.52
7	5-B	601	TA1	C43-C26	2.78	1.58	1.52
4	1-A	500	GTP	C6-N1	2.54	1.41	1.37
4	2-A	500	GTP	C6-N1	2.54	1.41	1.37
4	3-A	500	GTP	C6-N1	2.54	1.41	1.37
4	4-A	500	GTP	C6-N1	2.54	1.41	1.37
4	5-A	500	GTP	C6-N1	2.54	1.41	1.37
7	1-B	601	TA1	C26-C25	2.48	1.56	1.51
7	2-B	601	TA1	C26-C25	2.48	1.56	1.51
7	3-B	601	TA1	C26-C25	2.48	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	4-B	601	TA1	C26-C25	2.48	1.56	1.51
7	5-B	601	TA1	C26-C25	2.48	1.56	1.51
6	1-B	600	GDP	C2-N3	-2.43	1.27	1.33
6	2-B	600	GDP	C2-N3	-2.43	1.27	1.33
6	3-B	600	GDP	C2-N3	-2.43	1.27	1.33
6	4-B	600	GDP	C2-N3	-2.43	1.27	1.33
6	5-B	600	GDP	C2-N3	-2.43	1.27	1.33
7	1-B	601	TA1	C18-C20	2.41	1.62	1.55
7	2-B	601	TA1	C18-C20	2.41	1.62	1.55
7	3-B	601	TA1	C18-C20	2.41	1.62	1.55
7	4-B	601	TA1	C18-C20	2.41	1.62	1.55
7	5-B	601	TA1	C18-C20	2.41	1.62	1.55
4	1-A	500	GTP	C8-N7	-2.40	1.30	1.35
4	2-A	500	GTP	C8-N7	-2.40	1.30	1.35
4	3-A	500	GTP	C8-N7	-2.40	1.30	1.35
4	4-A	500	GTP	C8-N7	-2.40	1.30	1.35
4	5-A	500	GTP	C8-N7	-2.40	1.30	1.35
6	1-B	600	GDP	PB-O3B	2.36	1.64	1.54
6	2-B	600	GDP	PB-O3B	2.36	1.64	1.54
6	3-B	600	GDP	PB-O3B	2.36	1.64	1.54
6	4-B	600	GDP	PB-O3B	2.36	1.64	1.54
6	5-B	600	GDP	PB-O3B	2.36	1.64	1.54
7	1-B	601	TA1	C04-C03	-2.35	1.44	1.50
7	2-B	601	TA1	C04-C03	-2.35	1.44	1.50
7	3-B	601	TA1	C04-C03	-2.35	1.44	1.50
7	4-B	601	TA1	C04-C03	-2.35	1.44	1.50
7	5-B	601	TA1	C04-C03	-2.35	1.44	1.50
7	1-B	601	TA1	C01-C45	2.35	1.66	1.56
7	2-B	601	TA1	C01-C45	2.35	1.66	1.56
7	3-B	601	TA1	C01-C45	2.35	1.66	1.56
7	4-B	601	TA1	C01-C45	2.35	1.66	1.56
7	5-B	601	TA1	C01-C45	2.35	1.66	1.56
7	1-B	601	TA1	C16-C15	2.26	1.57	1.52
7	2-B	601	TA1	C16-C15	2.26	1.57	1.52
7	3-B	601	TA1	C16-C15	2.26	1.57	1.52
7	4-B	601	TA1	C16-C15	2.26	1.57	1.52
7	5-B	601	TA1	C16-C15	2.26	1.57	1.52
4	1-A	500	GTP	O4'-C1'	2.19	1.44	1.41
4	2-A	500	GTP	O4'-C1'	2.19	1.44	1.41
4	3-A	500	GTP	O4'-C1'	2.19	1.44	1.41
4	4-A	500	GTP	O4'-C1'	2.19	1.44	1.41
4	5-A	500	GTP	O4'-C1'	2.19	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-B	601	TA1	C10-C02	2.12	1.62	1.57
7	2-B	601	TA1	C10-C02	2.12	1.62	1.57
7	3-B	601	TA1	C10-C02	2.12	1.62	1.57
7	4-B	601	TA1	C10-C02	2.12	1.62	1.57
7	5-B	601	TA1	C10-C02	2.12	1.62	1.57
7	1-B	601	TA1	C37-C29	2.07	1.54	1.52
7	2-B	601	TA1	C37-C29	2.07	1.54	1.52
7	3-B	601	TA1	C37-C29	2.07	1.54	1.52
7	4-B	601	TA1	C37-C29	2.07	1.54	1.52
7	5-B	601	TA1	C37-C29	2.07	1.54	1.52
6	1-B	600	GDP	O3'-C3'	2.02	1.47	1.43
6	2-B	600	GDP	O3'-C3'	2.02	1.47	1.43
6	3-B	600	GDP	O3'-C3'	2.02	1.47	1.43
6	4-B	600	GDP	O3'-C3'	2.02	1.47	1.43
6	5-B	600	GDP	O3'-C3'	2.02	1.47	1.43

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1-B	600	GDP	C8-N7-C5	9.30	120.71	102.99
6	2-B	600	GDP	C8-N7-C5	9.30	120.71	102.99
6	3-B	600	GDP	C8-N7-C5	9.30	120.71	102.99
6	4-B	600	GDP	C8-N7-C5	9.30	120.71	102.99
6	5-B	600	GDP	C8-N7-C5	9.30	120.71	102.99
6	1-B	600	GDP	N2-C2-N3	6.29	131.99	119.74
6	2-B	600	GDP	N2-C2-N3	6.29	131.99	119.74
6	3-B	600	GDP	N2-C2-N3	6.29	131.99	119.74
6	4-B	600	GDP	N2-C2-N3	6.29	131.99	119.74
6	5-B	600	GDP	N2-C2-N3	6.29	131.99	119.74
6	1-B	600	GDP	C5-C6-N1	6.07	124.66	113.95
6	2-B	600	GDP	C5-C6-N1	6.07	124.66	113.95
6	3-B	600	GDP	C5-C6-N1	6.07	124.66	113.95
6	4-B	600	GDP	C5-C6-N1	6.07	124.66	113.95
6	5-B	600	GDP	C5-C6-N1	6.07	124.66	113.95
7	1-B	601	TA1	C06-C05-C04	-4.87	114.58	120.34
7	2-B	601	TA1	C06-C05-C04	-4.87	114.58	120.34
7	3-B	601	TA1	C06-C05-C04	-4.87	114.58	120.34
7	4-B	601	TA1	C06-C05-C04	-4.87	114.58	120.34
7	5-B	601	TA1	C06-C05-C04	-4.87	114.58	120.34
7	1-B	601	TA1	C07-C08-C09	4.72	127.38	120.19
7	2-B	601	TA1	C07-C08-C09	4.72	127.38	120.19
7	3-B	601	TA1	C07-C08-C09	4.72	127.38	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	4-B	601	TA1	C07-C08-C09	4.72	127.38	120.19
7	5-B	601	TA1	C07-C08-C09	4.72	127.38	120.19
6	1-B	600	GDP	O6-C6-C5	-4.23	116.11	124.37
6	2-B	600	GDP	O6-C6-C5	-4.23	116.11	124.37
6	3-B	600	GDP	O6-C6-C5	-4.23	116.11	124.37
6	4-B	600	GDP	O6-C6-C5	-4.23	116.11	124.37
6	5-B	600	GDP	O6-C6-C5	-4.23	116.11	124.37
6	1-B	600	GDP	N2-C2-N1	-4.21	107.75	116.71
6	2-B	600	GDP	N2-C2-N1	-4.21	107.75	116.71
6	3-B	600	GDP	N2-C2-N1	-4.21	107.75	116.71
6	4-B	600	GDP	N2-C2-N1	-4.21	107.75	116.71
6	5-B	600	GDP	N2-C2-N1	-4.21	107.75	116.71
7	1-B	601	TA1	C05-C04-C03	-3.97	111.44	120.40
7	2-B	601	TA1	C05-C04-C03	-3.97	111.44	120.40
7	3-B	601	TA1	C05-C04-C03	-3.97	111.44	120.40
7	4-B	601	TA1	C05-C04-C03	-3.97	111.44	120.40
7	5-B	601	TA1	C05-C04-C03	-3.97	111.44	120.40
6	1-B	600	GDP	C2-N1-C6	-3.73	118.23	125.10
6	2-B	600	GDP	C2-N1-C6	-3.73	118.23	125.10
6	3-B	600	GDP	C2-N1-C6	-3.73	118.23	125.10
6	4-B	600	GDP	C2-N1-C6	-3.73	118.23	125.10
6	5-B	600	GDP	C2-N1-C6	-3.73	118.23	125.10
7	1-B	601	TA1	C09-C04-C03	3.55	128.42	120.40
7	2-B	601	TA1	C09-C04-C03	3.55	128.42	120.40
7	3-B	601	TA1	C09-C04-C03	3.55	128.42	120.40
7	4-B	601	TA1	C09-C04-C03	3.55	128.42	120.40
7	5-B	601	TA1	C09-C04-C03	3.55	128.42	120.40
6	1-B	600	GDP	C2'-C3'-C4'	3.38	109.22	102.64
6	2-B	600	GDP	C2'-C3'-C4'	3.38	109.22	102.64
6	3-B	600	GDP	C2'-C3'-C4'	3.38	109.22	102.64
6	4-B	600	GDP	C2'-C3'-C4'	3.38	109.22	102.64
6	5-B	600	GDP	C2'-C3'-C4'	3.38	109.22	102.64
7	1-B	601	TA1	C17-C18-C20	3.15	109.88	102.59
7	2-B	601	TA1	C17-C18-C20	3.15	109.88	102.59
7	3-B	601	TA1	C17-C18-C20	3.15	109.88	102.59
7	4-B	601	TA1	C17-C18-C20	3.15	109.88	102.59
7	5-B	601	TA1	C17-C18-C20	3.15	109.88	102.59
7	1-B	601	TA1	C45-C01-C02	2.99	115.18	111.91
7	2-B	601	TA1	C45-C01-C02	2.99	115.18	111.91
7	3-B	601	TA1	C45-C01-C02	2.99	115.18	111.91
7	4-B	601	TA1	C45-C01-C02	2.99	115.18	111.91
7	5-B	601	TA1	C45-C01-C02	2.99	115.18	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	1-B	601	TA1	O04-C11-C14	-2.90	101.75	108.09
7	2-B	601	TA1	O04-C11-C14	-2.90	101.75	108.09
7	3-B	601	TA1	O04-C11-C14	-2.90	101.75	108.09
7	4-B	601	TA1	O04-C11-C14	-2.90	101.75	108.09
7	5-B	601	TA1	O04-C11-C14	-2.90	101.75	108.09
7	1-B	601	TA1	O01-C01-C43	2.54	113.38	107.03
7	2-B	601	TA1	O01-C01-C43	2.54	113.38	107.03
7	3-B	601	TA1	O01-C01-C43	2.54	113.38	107.03
7	4-B	601	TA1	O01-C01-C43	2.54	113.38	107.03
7	5-B	601	TA1	O01-C01-C43	2.54	113.38	107.03
6	1-B	600	GDP	O2'-C2'-C3'	2.26	119.13	111.82
6	2-B	600	GDP	O2'-C2'-C3'	2.26	119.13	111.82
6	3-B	600	GDP	O2'-C2'-C3'	2.26	119.13	111.82
6	4-B	600	GDP	O2'-C2'-C3'	2.26	119.13	111.82
6	5-B	600	GDP	O2'-C2'-C3'	2.26	119.13	111.82
7	1-B	601	TA1	C14-C11-C15	-2.16	83.10	85.40
7	2-B	601	TA1	C14-C11-C15	-2.16	83.10	85.40
7	3-B	601	TA1	C14-C11-C15	-2.16	83.10	85.40
7	4-B	601	TA1	C14-C11-C15	-2.16	83.10	85.40
7	5-B	601	TA1	C14-C11-C15	-2.16	83.10	85.40
7	1-B	601	TA1	C10-C18-C17	-2.16	102.33	106.54
7	2-B	601	TA1	C10-C18-C17	-2.16	102.33	106.54
7	3-B	601	TA1	C10-C18-C17	-2.16	102.33	106.54
7	4-B	601	TA1	C10-C18-C17	-2.16	102.33	106.54
7	5-B	601	TA1	C10-C18-C17	-2.16	102.33	106.54
7	1-B	601	TA1	O06-C15-C11	2.13	92.98	90.58
7	2-B	601	TA1	O06-C15-C11	2.13	92.98	90.58
7	3-B	601	TA1	O06-C15-C11	2.13	92.98	90.58
7	4-B	601	TA1	O06-C15-C11	2.13	92.98	90.58
7	5-B	601	TA1	O06-C15-C11	2.13	92.98	90.58
4	1-A	500	GTP	O5'-C5'-C4'	2.07	116.13	108.99
4	2-A	500	GTP	O5'-C5'-C4'	2.07	116.13	108.99
4	3-A	500	GTP	O5'-C5'-C4'	2.07	116.13	108.99
4	4-A	500	GTP	O5'-C5'-C4'	2.07	116.13	108.99
4	5-A	500	GTP	O5'-C5'-C4'	2.07	116.13	108.99
4	1-A	500	GTP	O3G-PG-O3B	2.02	111.40	104.64
4	2-A	500	GTP	O3G-PG-O3B	2.02	111.40	104.64
4	3-A	500	GTP	O3G-PG-O3B	2.02	111.40	104.64
4	4-A	500	GTP	O3G-PG-O3B	2.02	111.40	104.64
4	5-A	500	GTP	O3G-PG-O3B	2.02	111.40	104.64

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	1-B	600	GDP	PA-O3A-PB-O2B
6	1-B	600	GDP	C5'-O5'-PA-O3A
6	1-B	600	GDP	C5'-O5'-PA-O1A
6	2-B	600	GDP	PA-O3A-PB-O2B
6	2-B	600	GDP	C5'-O5'-PA-O3A
6	2-B	600	GDP	C5'-O5'-PA-O1A
6	3-B	600	GDP	PA-O3A-PB-O2B
6	3-B	600	GDP	C5'-O5'-PA-O3A
6	3-B	600	GDP	C5'-O5'-PA-O1A
6	4-B	600	GDP	PA-O3A-PB-O2B
6	4-B	600	GDP	C5'-O5'-PA-O3A
6	4-B	600	GDP	C5'-O5'-PA-O1A
6	5-B	600	GDP	PA-O3A-PB-O2B
6	5-B	600	GDP	C5'-O5'-PA-O3A
6	5-B	600	GDP	C5'-O5'-PA-O1A
7	1-B	601	TA1	O02-C03-C04-C05
7	2-B	601	TA1	O02-C03-C04-C05
7	3-B	601	TA1	O02-C03-C04-C05
7	4-B	601	TA1	O02-C03-C04-C05
7	5-B	601	TA1	O02-C03-C04-C05
7	1-B	601	TA1	O02-C03-C04-C09
7	2-B	601	TA1	O02-C03-C04-C09
7	3-B	601	TA1	O02-C03-C04-C09
7	4-B	601	TA1	O02-C03-C04-C09
7	5-B	601	TA1	O02-C03-C04-C09
7	1-B	601	TA1	O03-C03-C04-C09
7	2-B	601	TA1	O03-C03-C04-C09
7	3-B	601	TA1	O03-C03-C04-C09
7	4-B	601	TA1	O03-C03-C04-C09
7	5-B	601	TA1	O03-C03-C04-C09
7	1-B	601	TA1	O03-C03-C04-C05
7	2-B	601	TA1	O03-C03-C04-C05
7	3-B	601	TA1	O03-C03-C04-C05
7	4-B	601	TA1	O03-C03-C04-C05
7	5-B	601	TA1	O03-C03-C04-C05
7	1-B	601	TA1	N01-C30-C31-C36
7	2-B	601	TA1	N01-C30-C31-C36
7	3-B	601	TA1	N01-C30-C31-C36
7	4-B	601	TA1	N01-C30-C31-C36
7	5-B	601	TA1	N01-C30-C31-C36
7	1-B	601	TA1	O14-C30-C31-C36
7	2-B	601	TA1	O14-C30-C31-C36

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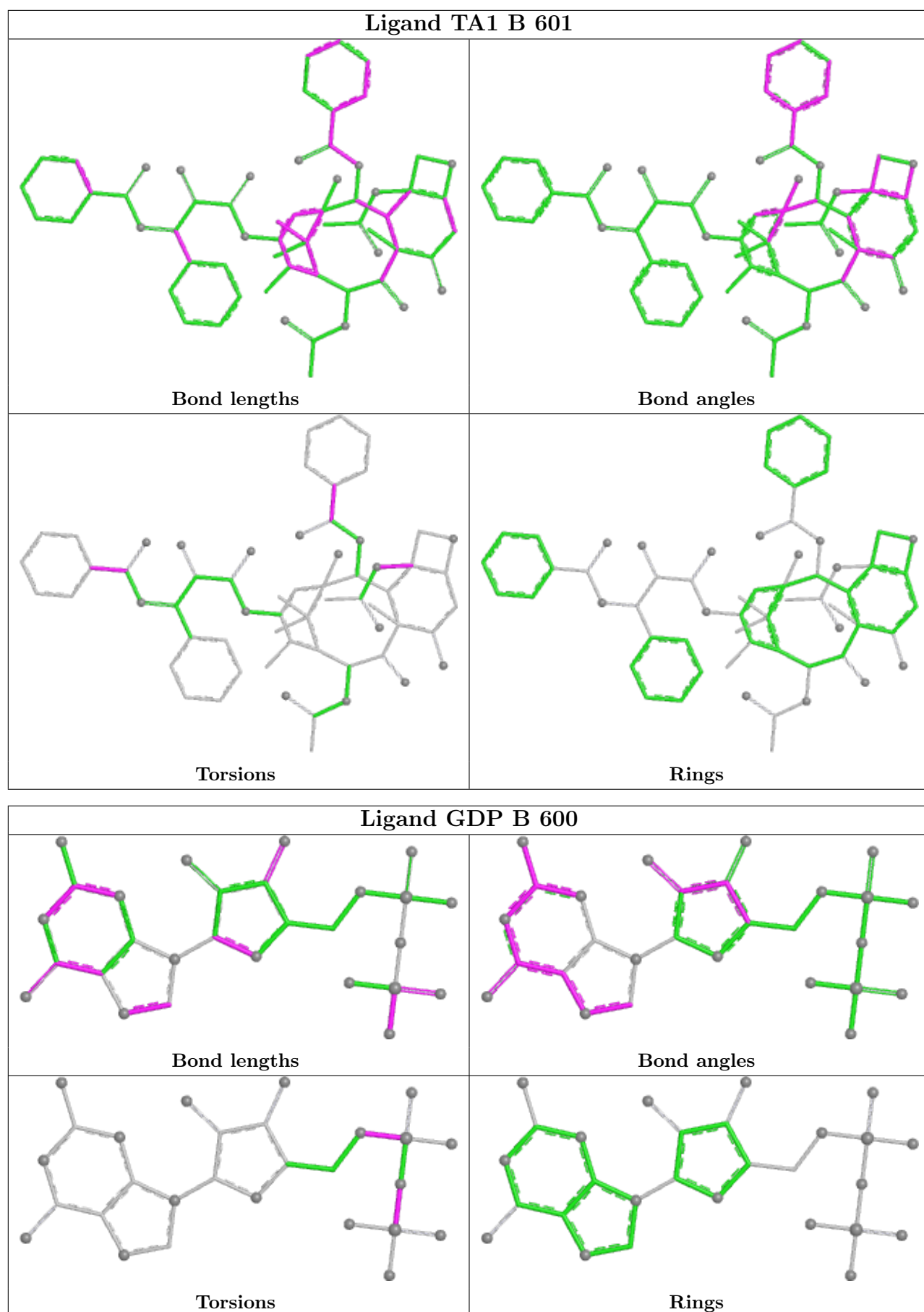
Mol	Chain	Res	Type	Atoms
7	3-B	601	TA1	O14-C30-C31-C36
7	4-B	601	TA1	O14-C30-C31-C36
7	5-B	601	TA1	O14-C30-C31-C36
7	1-B	601	TA1	N01-C30-C31-C32
7	2-B	601	TA1	N01-C30-C31-C32
7	3-B	601	TA1	N01-C30-C31-C32
7	4-B	601	TA1	N01-C30-C31-C32
7	5-B	601	TA1	N01-C30-C31-C32
7	1-B	601	TA1	O14-C30-C31-C32
7	2-B	601	TA1	O14-C30-C31-C32
7	3-B	601	TA1	O14-C30-C31-C32
7	4-B	601	TA1	O14-C30-C31-C32
7	5-B	601	TA1	O14-C30-C31-C32
4	1-A	500	GTP	C3'-C4'-C5'-O5'
4	2-A	500	GTP	C3'-C4'-C5'-O5'
4	3-A	500	GTP	C3'-C4'-C5'-O5'
4	4-A	500	GTP	C3'-C4'-C5'-O5'
4	5-A	500	GTP	C3'-C4'-C5'-O5'
4	1-A	500	GTP	O4'-C4'-C5'-O5'
4	2-A	500	GTP	O4'-C4'-C5'-O5'
4	3-A	500	GTP	O4'-C4'-C5'-O5'
4	4-A	500	GTP	O4'-C4'-C5'-O5'
4	5-A	500	GTP	O4'-C4'-C5'-O5'
6	1-B	600	GDP	PA-O3A-PB-O3B
6	2-B	600	GDP	PA-O3A-PB-O3B
6	3-B	600	GDP	PA-O3A-PB-O3B
6	4-B	600	GDP	PA-O3A-PB-O3B
6	5-B	600	GDP	PA-O3A-PB-O3B
4	1-A	500	GTP	PG-O3B-PB-O1B
4	2-A	500	GTP	PG-O3B-PB-O1B
4	3-A	500	GTP	PG-O3B-PB-O1B
4	4-A	500	GTP	PG-O3B-PB-O1B
4	5-A	500	GTP	PG-O3B-PB-O1B
7	1-B	601	TA1	C15-C11-O04-C12
7	2-B	601	TA1	C15-C11-O04-C12
7	3-B	601	TA1	C15-C11-O04-C12
7	4-B	601	TA1	C15-C11-O04-C12
7	5-B	601	TA1	C15-C11-O04-C12

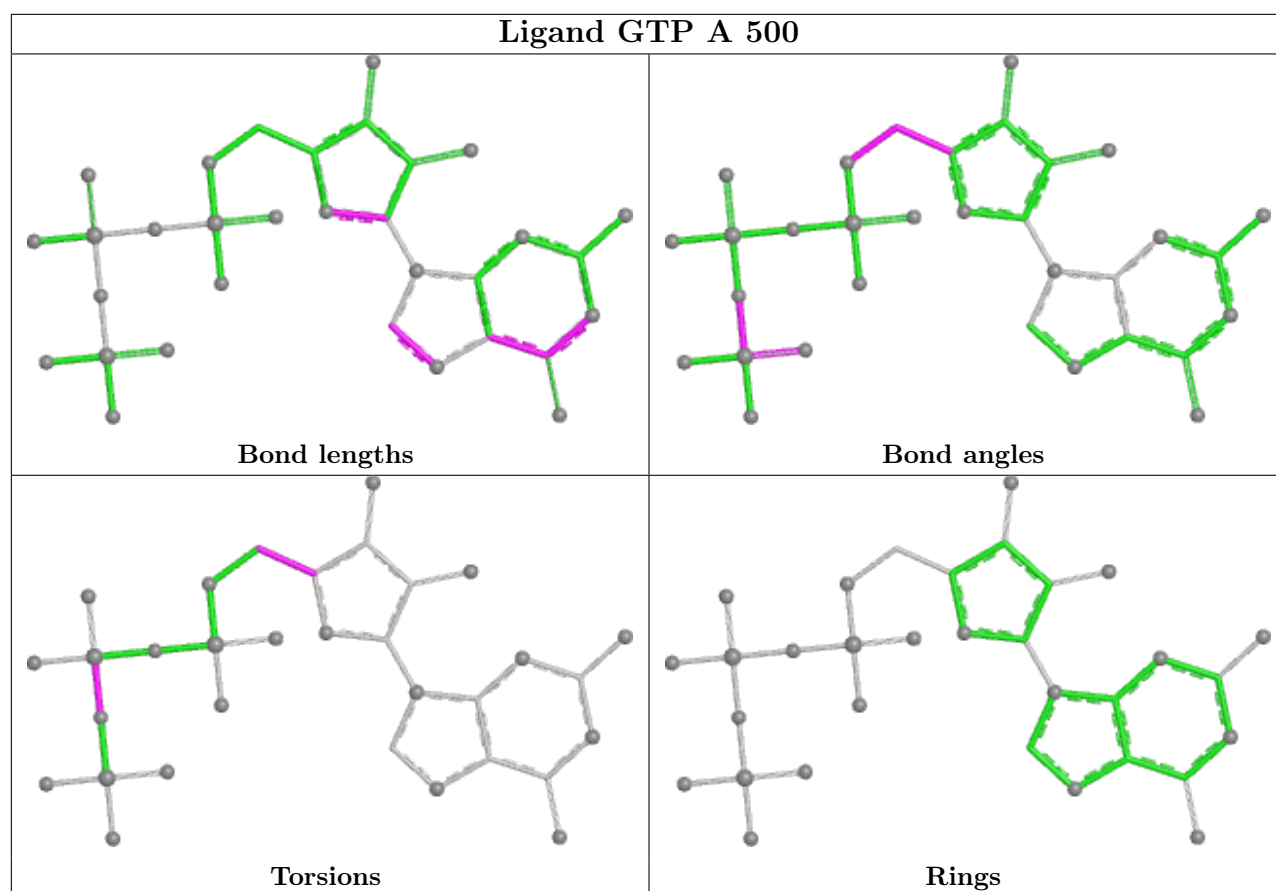
There are no ring outliers.

15 monomers are involved in 280 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	1-B	601	TA1	19	0
6	2-B	600	GDP	11	0
6	1-B	600	GDP	11	0
7	4-B	601	TA1	19	0
4	2-A	500	GTP	26	0
4	1-A	500	GTP	26	0
7	5-B	601	TA1	19	0
4	5-A	500	GTP	26	0
6	3-B	600	GDP	11	0
6	4-B	600	GDP	11	0
6	5-B	600	GDP	11	0
7	3-B	601	TA1	19	0
4	4-A	500	GTP	26	0
4	3-A	500	GTP	26	0
7	2-B	601	TA1	19	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.

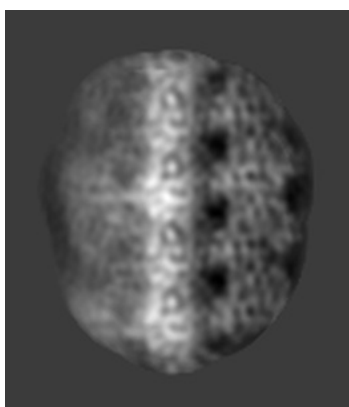
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3621. These allow visual inspection of the internal detail of the map and identification of artifacts.

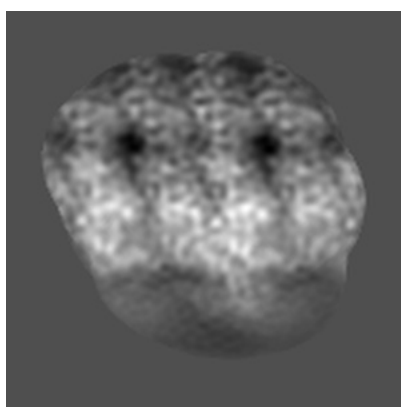
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

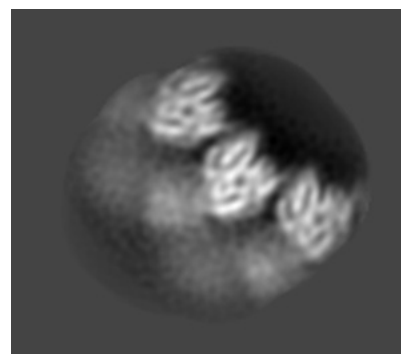
6.1.1 Primary map



X



Y

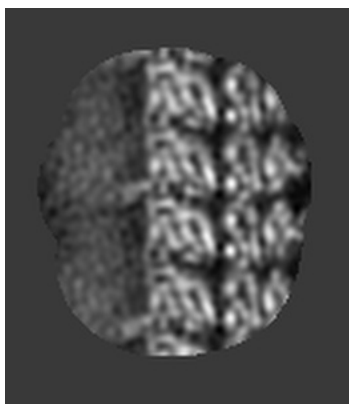


Z

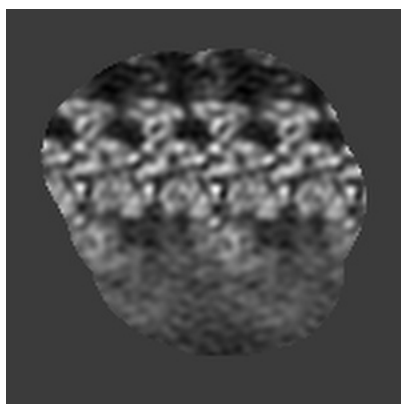
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

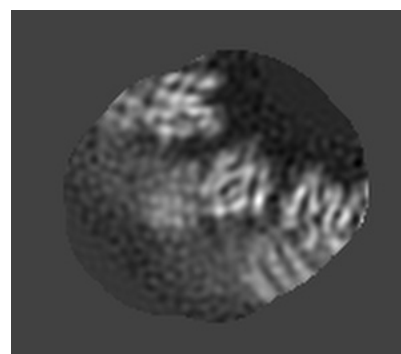
6.2.1 Primary map



X Index: 80



Y Index: 69

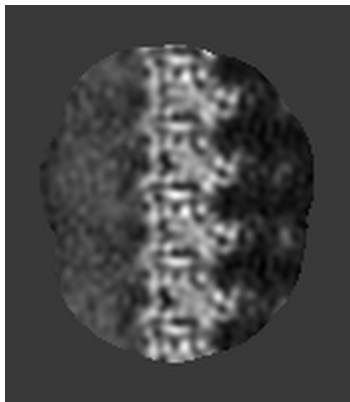


Z Index: 80

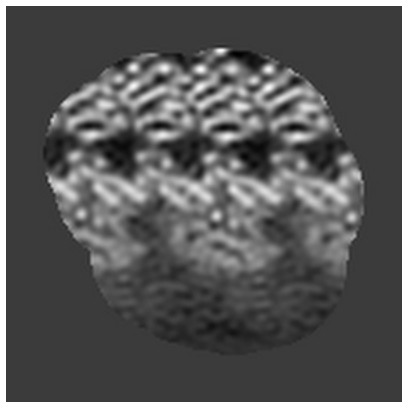
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

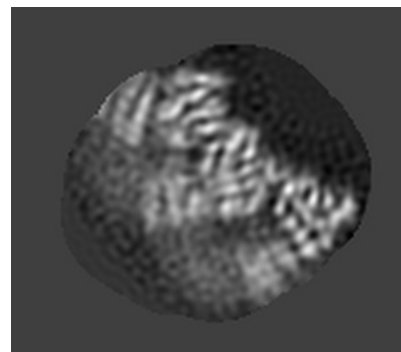
6.3.1 Primary map



X Index: 87



Y Index: 59



Z Index: 91

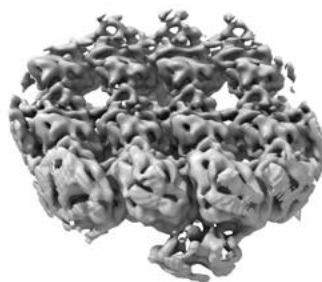
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

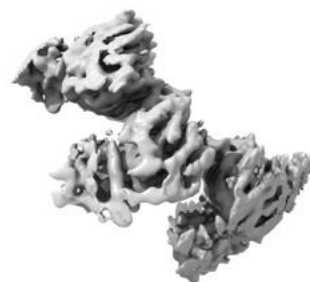
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0321. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

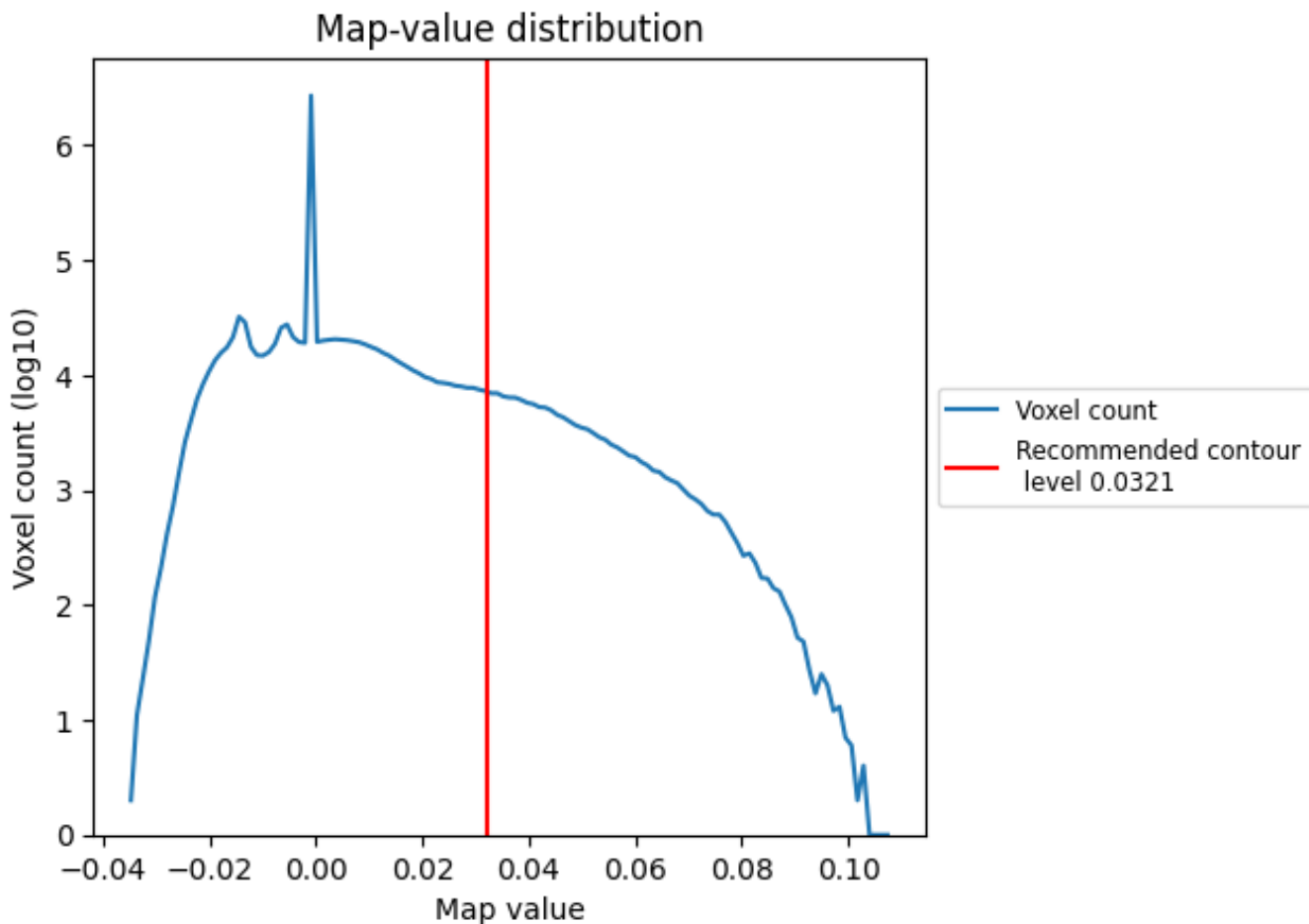
6.5 Mask visualisation

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

7 Map analysis [i](#)

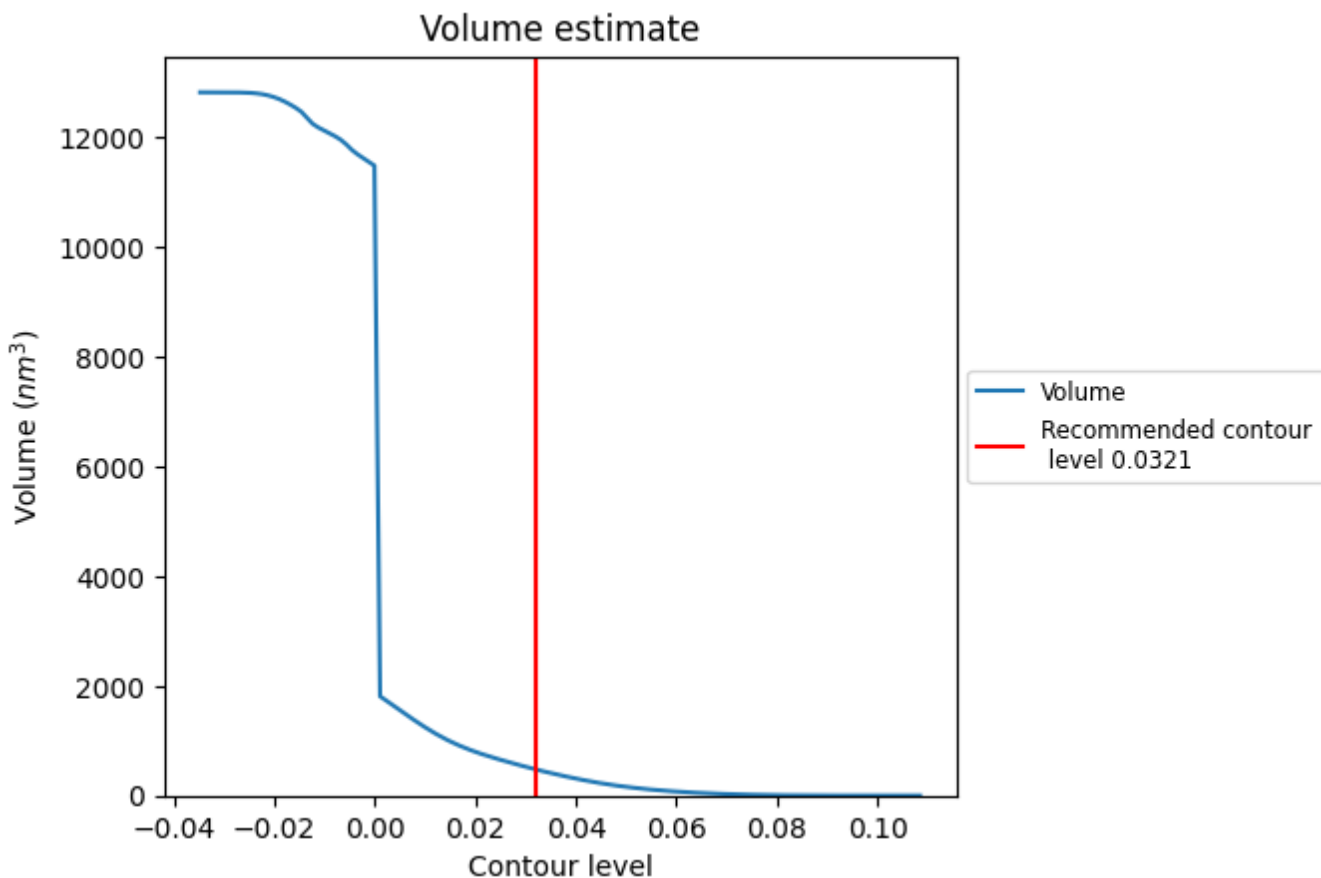
This section contains the results of statistical analysis of the map.

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 476 nm³; this corresponds to an approximate mass of 430 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.

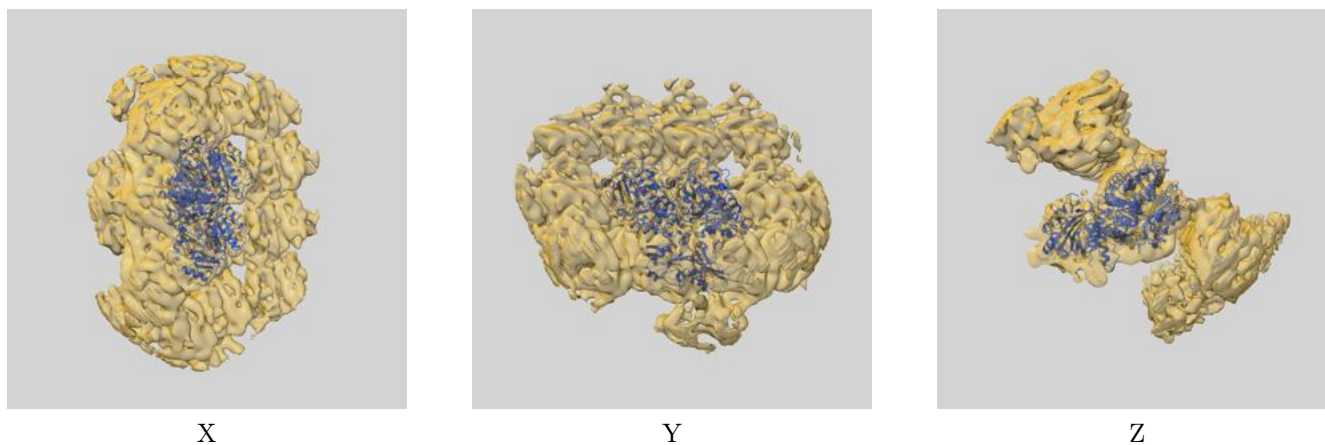
8 Fourier-Shell correlation

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-3621 and PDB model 5ND3. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

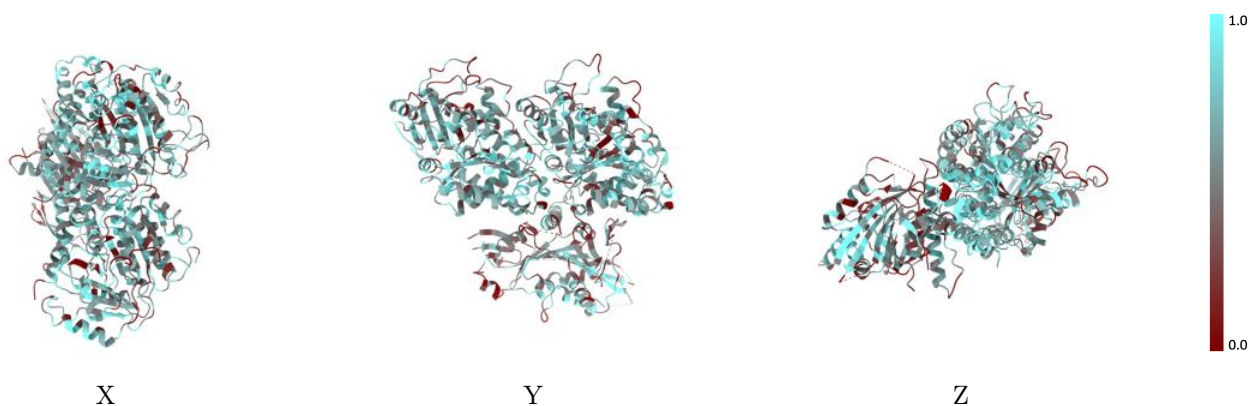


The images above show the 3D surface view of the map at the recommended contour level 0.0321 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

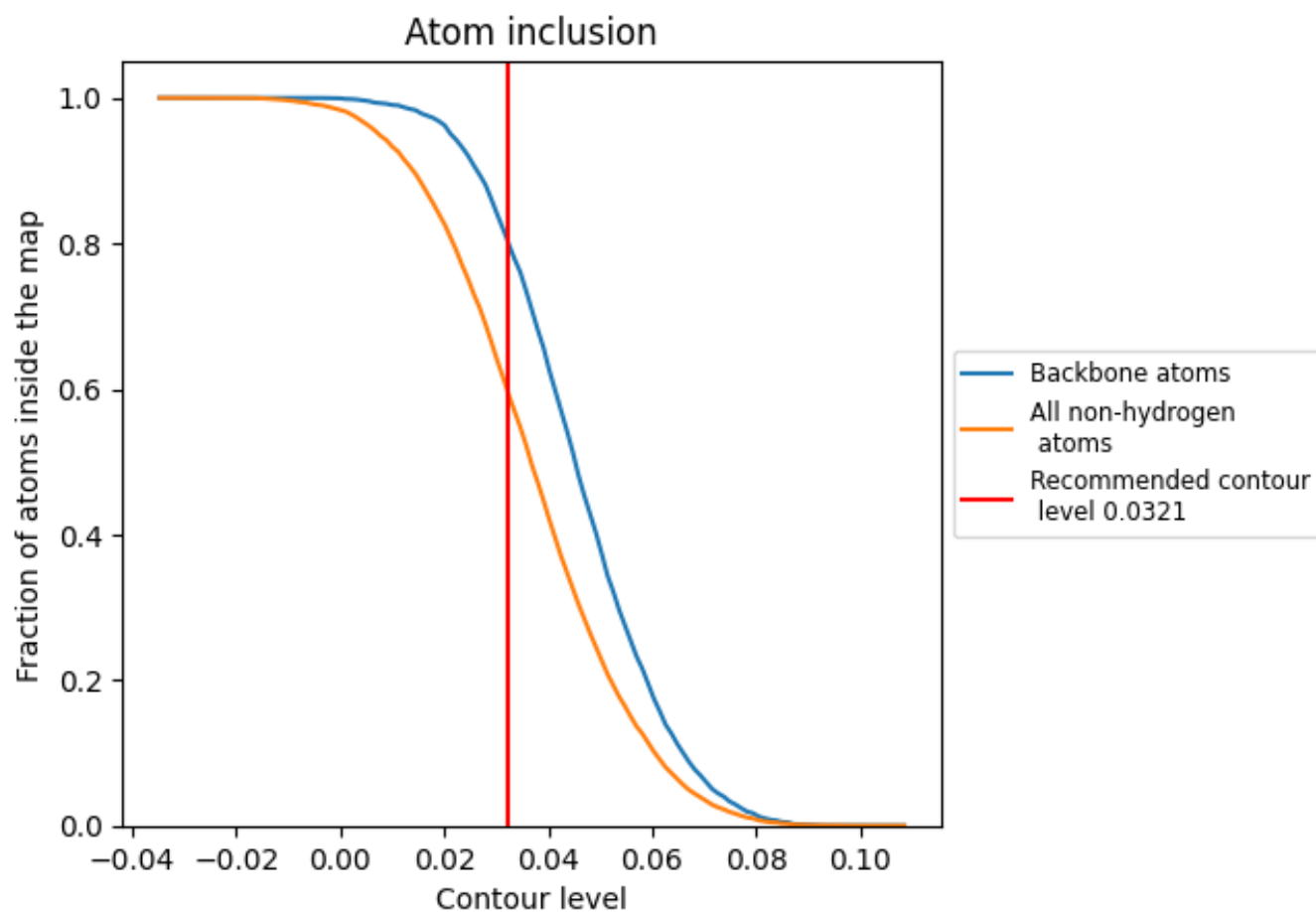
This section was not generated.

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 (0.0321).





9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0321) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.5997
A	 0.6389
B	 0.6322
C	 0.4985

