



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:12 PM UTC

PDB ID : 4A6J / pdb_00004a6j
EMDB ID : EMD-1980
Title : Structural model of ParM filament based on CryoEM map
Authors : Gayathri, P.; Fujii, T.; Moller-Jensen, J.; Van Den Ent, F.; Namba, K.; Lowe, J.
Deposited on : 2011-11-04
Resolution : 7.20 Å(reported)
Based on initial model : 4A62

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

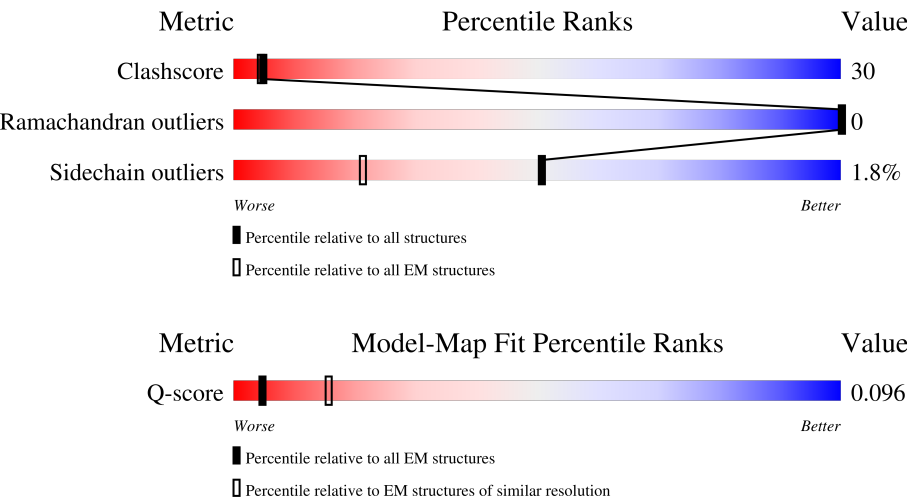
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 7.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	444 (6.70 - 7.70)

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	A	320	100% 81%18%
1	B	320	98% 80%19%
1	C	320	68% 77%23%
1	D	320	42% 77%23%

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Mol	Chain	Length	Quality of chain
1	E	320	41% 77% 23%
1	F	320	41% 77% 23%
1	G	320	42% 77% 23%
1	H	320	43% 77% 23%
1	I	320	49% 81% 18%
1	J	320	80% 82% 18%

2 Entry composition

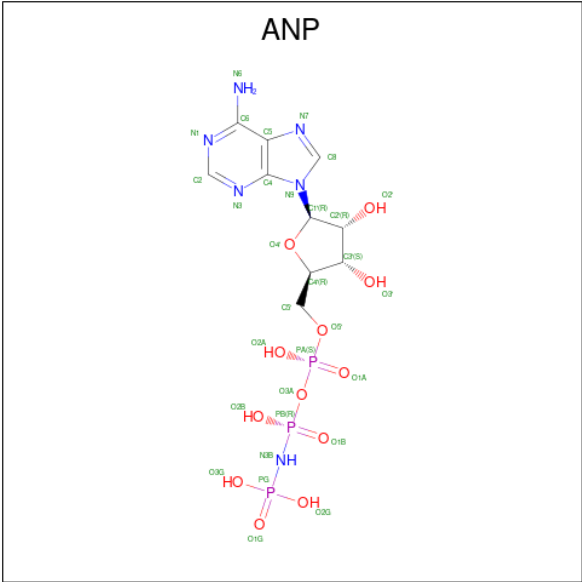
There are 3 unique types of molecules in this entry. The entry contains 25490 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PLASMID SEGREGATION PROTEIN PARM.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	B	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	C	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	D	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	E	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	F	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	G	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	H	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	I	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		
1	J	320	Total	C	N	O	S	1	0
			2517	1585	425	499	8		

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	B	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	C	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	D	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	E	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	F	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	G	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	H	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	I	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	J	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	

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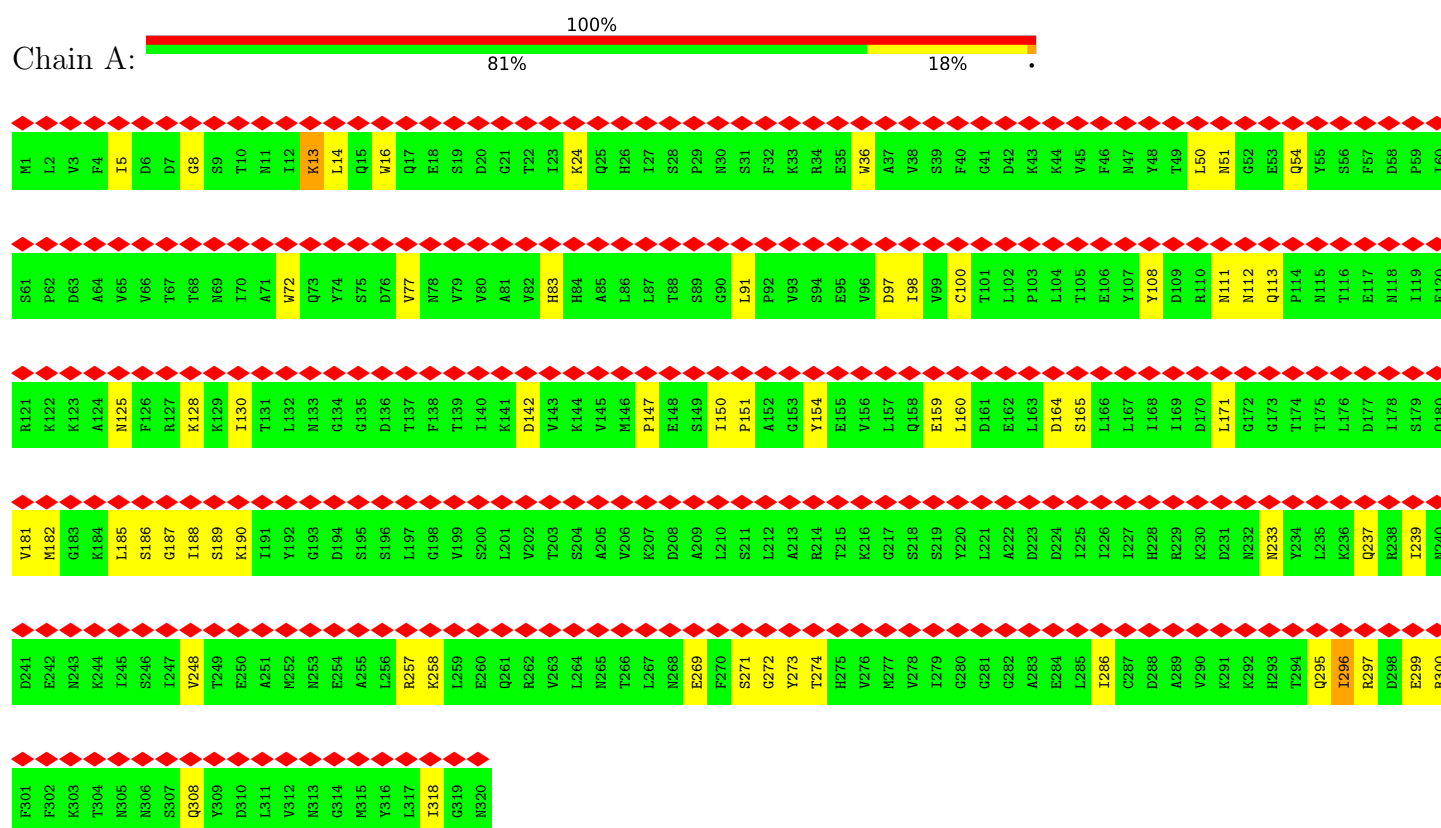
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Mol	Chain	Residues	Atoms		AltConf
3	C	1	Total 1	Mg 1	0
3	D	1	Total 1	Mg 1	0
3	E	1	Total 1	Mg 1	0
3	F	1	Total 1	Mg 1	0
3	G	1	Total 1	Mg 1	0
3	H	1	Total 1	Mg 1	0
3	I	1	Total 1	Mg 1	0
3	J	1	Total 1	Mg 1	0

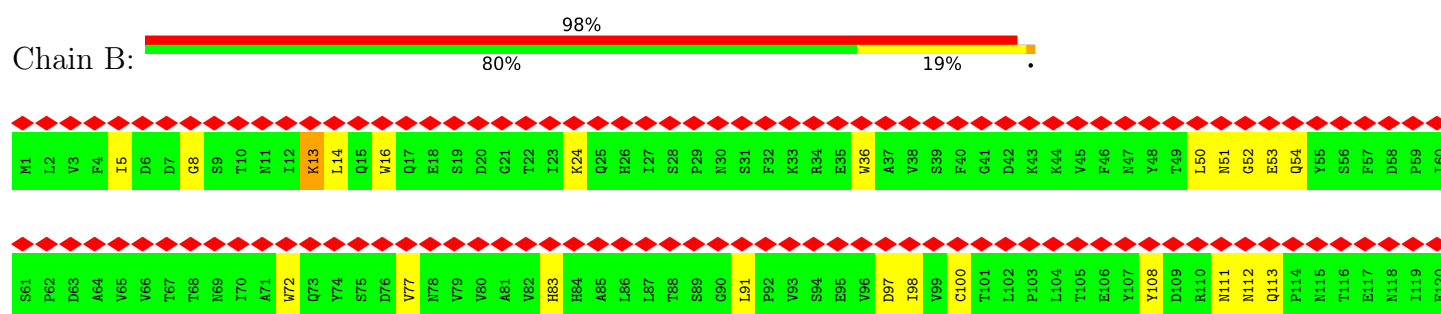
3 Residue-property plots

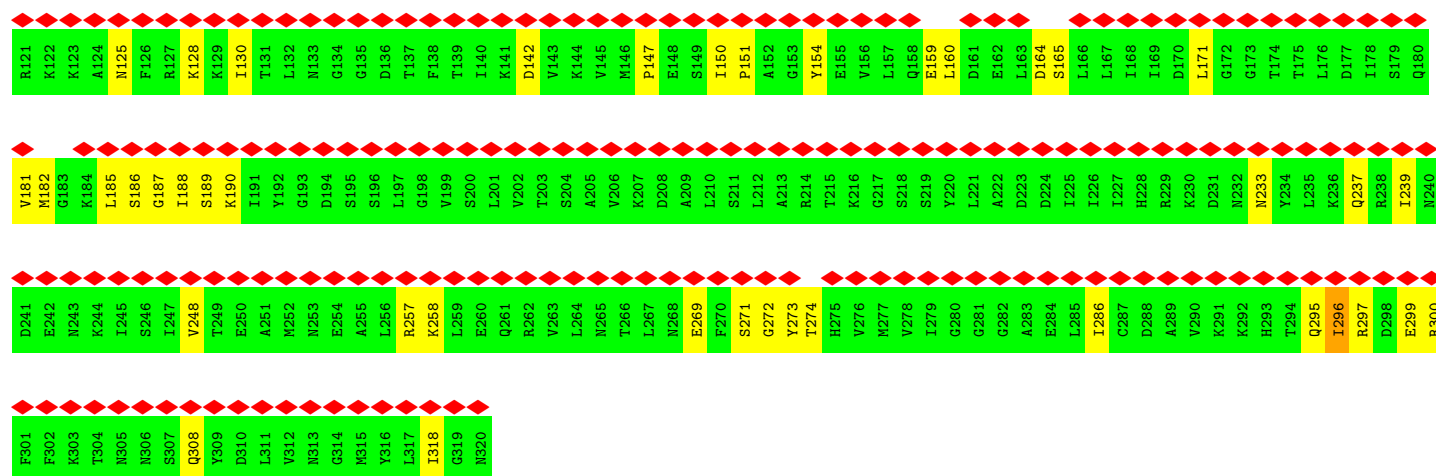
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

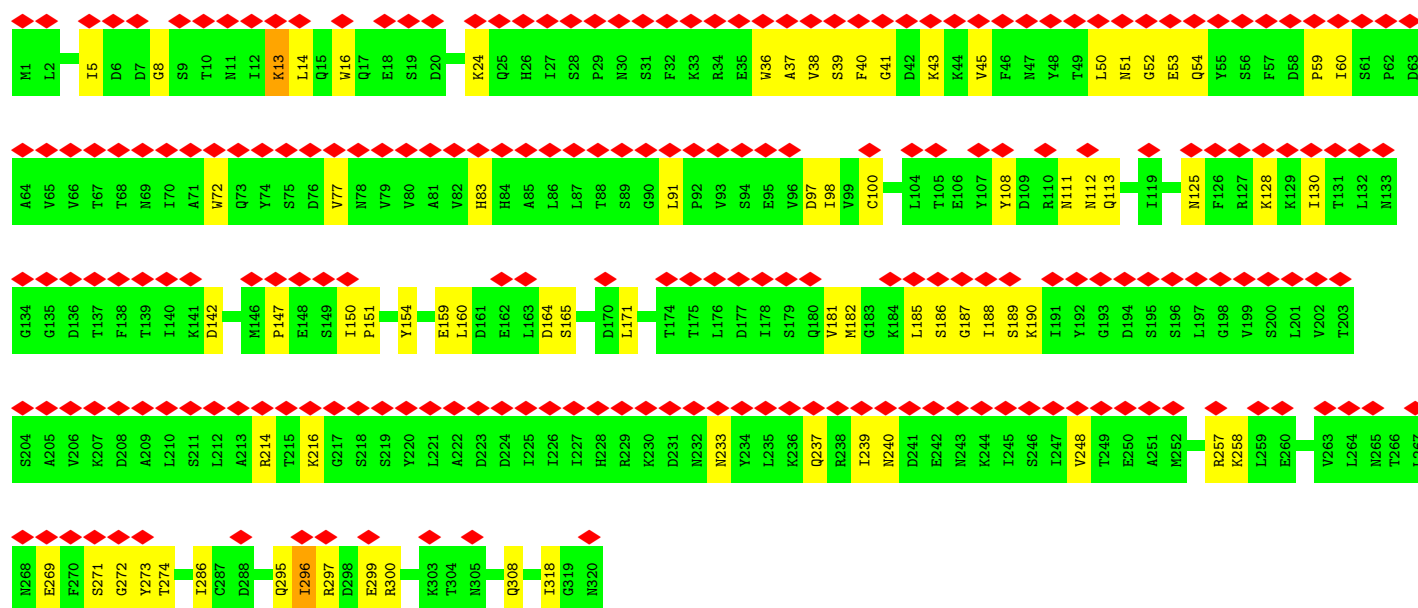
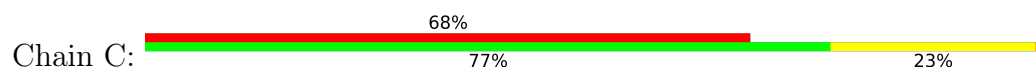


• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

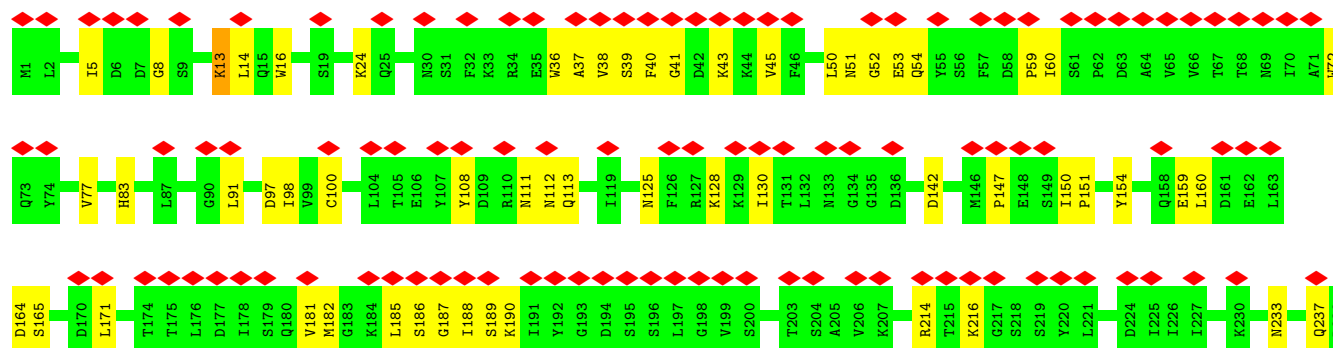
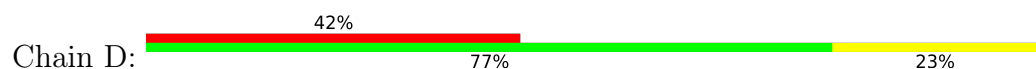




• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

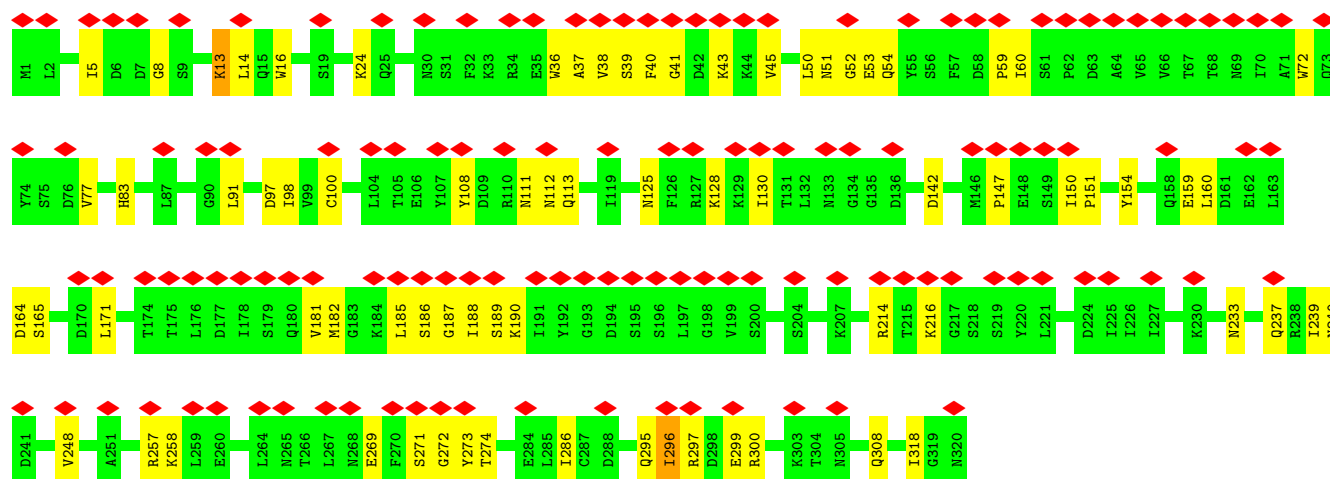
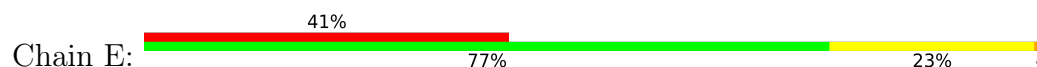


• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

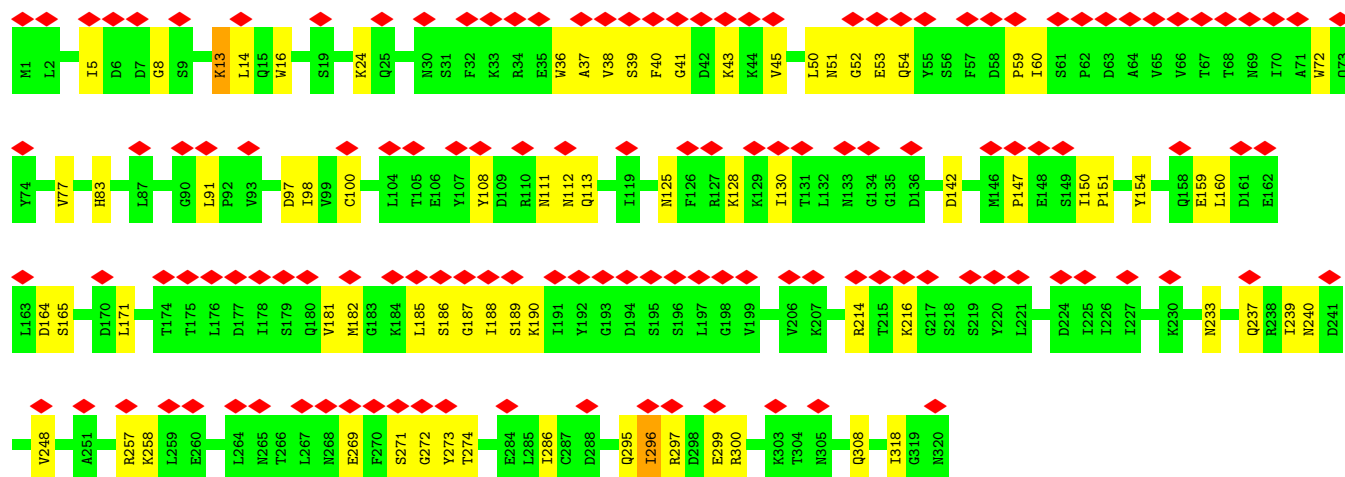
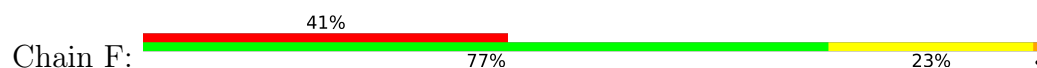




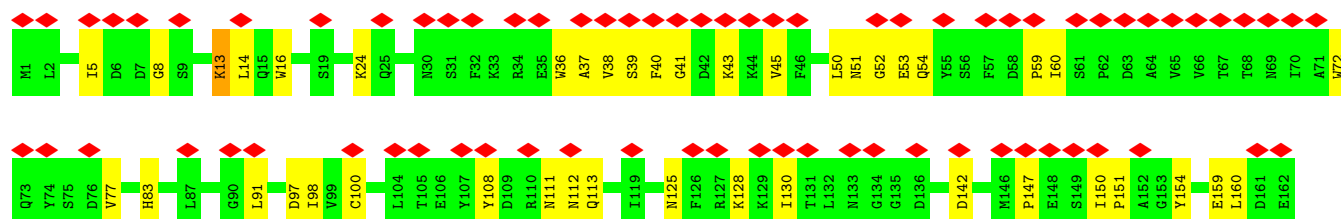
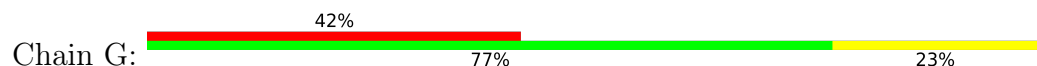
• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

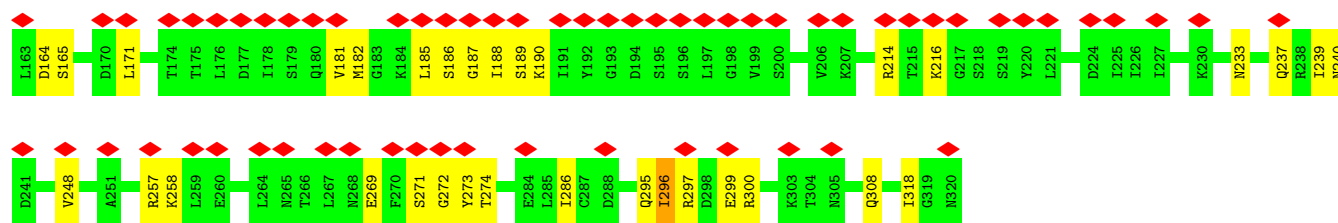


• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

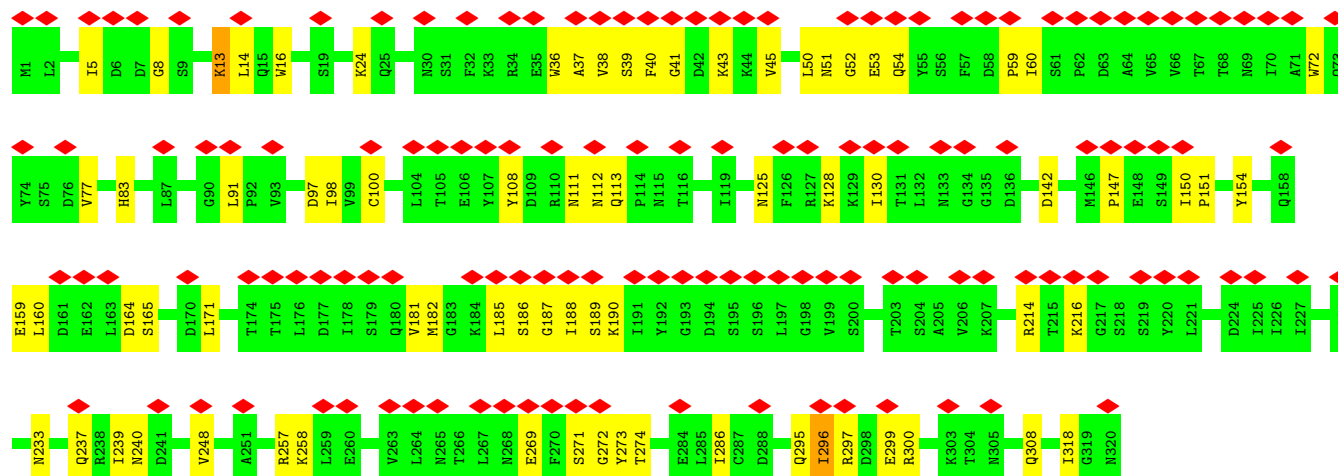
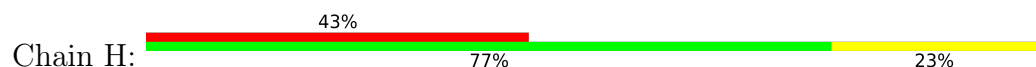


• Molecule 1: PLASMID SEGREGATION PROTEIN PARM

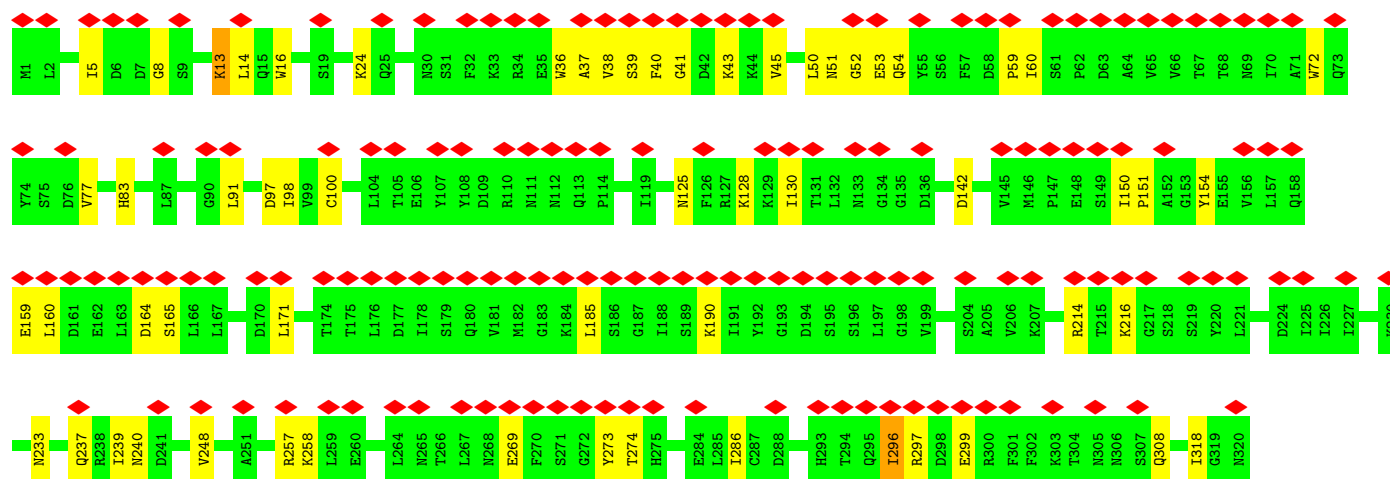
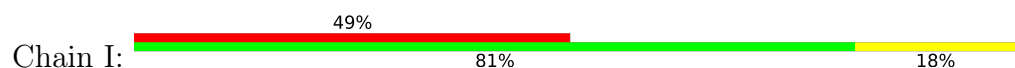




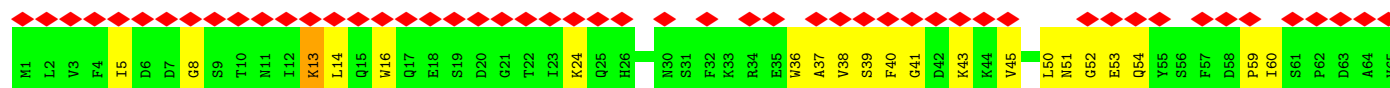
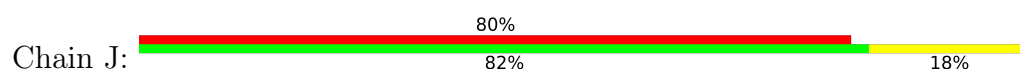
• Molecule 1: PLASMID SEGREGATION PROTEIN PARM



• Molecule 1: PLASMID SEGREGATION PROTEIN PARM



• Molecule 1: PLASMID SEGREGATION PROTEIN PARM



G135	D136	K141	D142	V143	K144	V145	M146	P147	E148	S149	I150	P151	A152	G153	Y154	E155	V156	L157	Q158	E159	L160	D161	E162	L163	D164	S165	L166	L167	I168	I169	D170	L171	G172	G173	T174	T175	L176	D177	I178	S179	Q180	V181	M182	G183	K184	L185	S186	G187	I188	S189	K190	I191	Y192	G193	D194	S195	L196	L197
G198	V199	S200	L201	V202	T203	S204	A205	V206	K207	R214	T215	K216	G217	S218	S219	Y220	L221	D224	I225	I226	I227	H228	R229	K230	N233	Q237	R238	I239	N240	D241	V248	T249	E250	A251	M252	N253	E254	A255	L256	R257	K258	L259	E260	Q261	R262	V263	L264	N265	T266	L267	N268	E269	F270	S271				
G272	Y273	T274	H275	V276	M277	V278	I279	G280	G281	G282	A283	E284	L285	I286	C287	D288	A289	V290	K291	K292	H293	T294	Q295	I296	R297	D298	E299	R300	F301	F302	K303	T304	N305	N306	S307	Q308	Y309	D310	L311	N312	N313	G314	M315	Y316	L317	I318	G319	N320										
V66	T67	N69	I70	A71	W72	Q73	Y74	V77	H83	L87	G90	L91	S94	E95	V96	D97	I98	V99	C100	T101	L102	P103	L104	T105	E106	Y107	Y108	D109	R110	N111	N112	Q113	P114	N115	T116	E117	N118	I119	E120	R121	K122	K123	A124	N125	F126	R127	K128	K129	I130	T131	L132	N133	G134					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	CTFFIND3 EACH PARTICLE	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	91463	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	1.864	Depositor
Minimum map value	-1.246	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.209	Depositor
Recommended contour level	0.631	Depositor
Map size (Å)	164.0, 164.0, 164.0	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.64, 1.64, 1.64	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: ANP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.44	0/2561	0.74	0/3467
1	B	0.44	0/2561	0.74	0/3467
1	C	0.44	0/2561	0.74	0/3467
1	D	0.45	0/2561	0.74	0/3467
1	E	0.44	0/2561	0.74	0/3467
1	F	0.45	0/2561	0.74	0/3467
1	G	0.45	0/2561	0.74	0/3467
1	H	0.45	0/2561	0.74	0/3467
1	I	0.44	0/2561	0.74	0/3467
1	J	0.45	0/2561	0.74	0/3467
All	All	0.45	0/25610	0.74	0/34670

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2517	0	2505	181	0
1	B	2517	0	2505	196	0
1	C	2517	0	2502	335	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2517	0	2502	338	0
1	E	2517	0	2502	333	0
1	F	2517	0	2502	338	0
1	G	2517	0	2502	333	0
1	H	2517	0	2502	337	0
1	I	2517	0	2503	194	0
1	J	2517	0	2503	180	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
2	C	31	0	13	0	0
2	D	31	0	13	0	0
2	E	31	0	13	0	0
2	F	31	0	13	0	0
2	G	31	0	13	0	0
2	H	31	0	13	0	0
2	I	31	0	13	0	0
2	J	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
All	All	25490	0	25158	1503	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 30.

All (1503) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PRO:CG	1:C:40:PHE:CE1	1.84	1.60
1:C:147:PRO:CG	1:E:40:PHE:CE1	1.83	1.60
1:E:147:PRO:CG	1:G:40:PHE:CE1	1.82	1.59
1:F:147:PRO:CG	1:H:40:PHE:CE1	1.83	1.58
1:G:147:PRO:CG	1:I:40:PHE:CE1	1.83	1.57
1:B:147:PRO:CG	1:D:40:PHE:CE1	1.82	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:147:PRO:CG	1:J:40:PHE:CE1	1.83	1.57
1:D:147:PRO:CG	1:F:40:PHE:CE1	1.83	1.57
1:A:113:GLN:NE2	1:C:45:VAL:HG21	1.36	1.41
1:E:113:GLN:NE2	1:G:45:VAL:HG21	1.37	1.39
1:G:113:GLN:NE2	1:I:45:VAL:HG21	1.37	1.39
1:H:113:GLN:NE2	1:J:45:VAL:HG21	1.36	1.38
1:F:113:GLN:NE2	1:H:45:VAL:HG21	1.36	1.36
1:C:113:GLN:NE2	1:E:45:VAL:HG21	1.37	1.36
1:D:113:GLN:NE2	1:F:45:VAL:HG21	1.37	1.36
1:B:113:GLN:NE2	1:D:45:VAL:HG21	1.36	1.35
1:F:258:LYS:HG2	1:G:53:GLU:OE2	1.18	1.35
1:C:147:PRO:CD	1:E:40:PHE:HE1	1.42	1.32
1:C:258:LYS:HG2	1:D:53:GLU:OE2	1.18	1.32
1:B:147:PRO:CD	1:D:40:PHE:HE1	1.41	1.32
1:F:147:PRO:CD	1:H:40:PHE:HE1	1.42	1.32
1:G:258:LYS:HG2	1:H:53:GLU:OE2	1.18	1.32
1:B:258:LYS:HG2	1:C:53:GLU:OE2	1.18	1.32
1:I:258:LYS:HG2	1:J:53:GLU:OE2	1.18	1.32
1:G:258:LYS:HG2	1:H:53:GLU:CD	1.56	1.31
1:A:147:PRO:CD	1:C:40:PHE:HE1	1.43	1.31
1:D:258:LYS:HG2	1:E:53:GLU:OE2	1.18	1.31
1:G:147:PRO:CD	1:I:40:PHE:HE1	1.43	1.31
1:H:147:PRO:CD	1:J:40:PHE:HE1	1.43	1.31
1:A:272:GLY:CA	1:C:216:LYS:O	1.79	1.31
1:E:147:PRO:CD	1:G:40:PHE:HE1	1.42	1.31
1:B:258:LYS:HG2	1:C:53:GLU:CD	1.55	1.31
1:E:258:LYS:HG2	1:F:53:GLU:CD	1.56	1.31
1:H:272:GLY:CA	1:J:216:LYS:O	1.79	1.31
1:I:258:LYS:HG2	1:J:53:GLU:CD	1.55	1.31
1:C:272:GLY:CA	1:E:216:LYS:O	1.79	1.30
1:D:258:LYS:HG2	1:E:53:GLU:CD	1.56	1.30
1:E:272:GLY:HA3	1:G:216:LYS:O	1.21	1.30
1:G:147:PRO:HG2	1:I:40:PHE:CE1	1.52	1.30
1:D:147:PRO:HG2	1:F:40:PHE:CE1	1.51	1.30
1:E:272:GLY:CA	1:G:216:LYS:O	1.79	1.30
1:F:258:LYS:HG2	1:G:53:GLU:CD	1.56	1.30
1:F:272:GLY:CA	1:H:216:LYS:O	1.79	1.30
1:G:272:GLY:CA	1:I:216:LYS:O	1.79	1.30
1:H:272:GLY:HA3	1:J:216:LYS:O	1.21	1.30
1:B:147:PRO:HG2	1:D:40:PHE:CE1	1.52	1.30
1:H:111:ASN:O	1:J:37:ALA:C	1.75	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:PRO:CD	1:F:40:PHE:HE1	1.42	1.30
1:A:111:ASN:O	1:C:37:ALA:C	1.75	1.29
1:B:111:ASN:O	1:D:37:ALA:C	1.74	1.29
1:E:258:LYS:HG2	1:F:53:GLU:OE2	1.18	1.29
1:F:111:ASN:O	1:H:37:ALA:C	1.75	1.29
1:F:272:GLY:HA3	1:H:216:LYS:O	1.21	1.29
1:H:258:LYS:HG2	1:I:53:GLU:CD	1.56	1.29
1:H:258:LYS:HG2	1:I:53:GLU:OE2	1.18	1.29
1:A:272:GLY:HA3	1:C:216:LYS:O	1.21	1.29
1:C:111:ASN:O	1:E:37:ALA:C	1.75	1.29
1:C:258:LYS:HG2	1:D:53:GLU:CD	1.56	1.29
1:D:111:ASN:O	1:F:37:ALA:C	1.75	1.29
1:D:272:GLY:CA	1:F:216:LYS:O	1.79	1.29
1:F:147:PRO:HG2	1:H:40:PHE:CE1	1.52	1.29
1:E:111:ASN:O	1:G:37:ALA:C	1.75	1.29
1:G:111:ASN:O	1:I:37:ALA:C	1.75	1.29
1:A:258:LYS:HG2	1:B:53:GLU:CD	1.56	1.28
1:G:272:GLY:HA3	1:I:216:LYS:O	1.21	1.28
1:C:272:GLY:HA3	1:E:216:LYS:O	1.21	1.28
1:E:147:PRO:HG2	1:G:40:PHE:CE1	1.51	1.28
1:H:147:PRO:HG2	1:J:40:PHE:CE1	1.52	1.28
1:G:185:LEU:O	1:I:43:LYS:CG	1.82	1.28
1:D:185:LEU:O	1:F:43:LYS:CG	1.82	1.27
1:B:272:GLY:CA	1:D:216:LYS:O	1.79	1.27
1:C:185:LEU:O	1:E:43:LYS:CG	1.82	1.27
1:D:272:GLY:HA3	1:F:216:LYS:O	1.22	1.27
1:H:185:LEU:O	1:J:43:LYS:CG	1.82	1.27
1:A:185:LEU:O	1:C:43:LYS:CG	1.82	1.27
1:E:185:LEU:O	1:G:43:LYS:CG	1.83	1.27
1:B:272:GLY:HA3	1:D:216:LYS:O	1.21	1.26
1:F:185:LEU:O	1:H:43:LYS:CG	1.82	1.26
1:C:181:VAL:HG13	1:E:43:LYS:NZ	1.49	1.26
1:A:181:VAL:HG13	1:C:43:LYS:NZ	1.50	1.26
1:E:181:VAL:HG13	1:G:43:LYS:NZ	1.50	1.25
1:A:258:LYS:HG2	1:B:53:GLU:OE2	1.18	1.25
1:B:185:LEU:O	1:D:43:LYS:CG	1.84	1.25
1:A:189:SER:OG	1:C:60:ILE:CD1	1.84	1.25
1:C:189:SER:OG	1:E:60:ILE:CD1	1.84	1.25
1:G:181:VAL:HG13	1:I:43:LYS:NZ	1.50	1.25
1:B:189:SER:OG	1:D:60:ILE:CD1	1.84	1.25
1:C:147:PRO:HG2	1:E:40:PHE:CE1	1.52	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:SER:OG	1:G:60:ILE:CD1	1.84	1.25
1:A:147:PRO:HG2	1:C:40:PHE:CE1	1.53	1.24
1:H:112:ASN:O	1:J:38:VAL:CA	1.81	1.24
1:H:189:SER:OG	1:J:60:ILE:CD1	1.84	1.24
1:F:189:SER:OG	1:H:60:ILE:CD1	1.84	1.24
1:G:189:SER:OG	1:I:60:ILE:CD1	1.85	1.24
1:B:181:VAL:HG13	1:D:43:LYS:NZ	1.50	1.24
1:D:189:SER:OG	1:F:60:ILE:CD1	1.84	1.24
1:F:181:VAL:HG13	1:H:43:LYS:NZ	1.50	1.24
1:D:181:VAL:HG13	1:F:43:LYS:NZ	1.49	1.23
1:F:300:ARG:HH22	1:H:237:GLN:C	1.46	1.23
1:H:181:VAL:HG13	1:J:43:LYS:NZ	1.50	1.23
1:H:300:ARG:HH22	1:J:237:GLN:C	1.46	1.23
1:D:111:ASN:O	1:F:37:ALA:O	1.54	1.23
1:D:300:ARG:HH22	1:F:237:GLN:C	1.46	1.23
1:E:111:ASN:O	1:G:37:ALA:O	1.54	1.23
1:F:111:ASN:O	1:H:37:ALA:O	1.55	1.23
1:G:111:ASN:O	1:I:37:ALA:O	1.55	1.23
1:G:300:ARG:HH22	1:I:237:GLN:C	1.46	1.23
1:B:300:ARG:HH22	1:D:237:GLN:C	1.47	1.22
1:G:112:ASN:O	1:I:38:VAL:CA	1.81	1.22
1:B:147:PRO:HG3	1:D:40:PHE:CD1	1.73	1.22
1:E:147:PRO:HG3	1:G:40:PHE:CD1	1.73	1.22
1:A:147:PRO:HG3	1:C:40:PHE:CD1	1.74	1.22
1:C:300:ARG:HH22	1:E:237:GLN:C	1.46	1.22
1:D:147:PRO:HG3	1:F:40:PHE:CD1	1.73	1.22
1:E:300:ARG:HH22	1:G:237:GLN:C	1.47	1.22
1:F:147:PRO:HG3	1:H:40:PHE:CD1	1.74	1.22
1:A:300:ARG:HH22	1:C:237:GLN:C	1.46	1.21
1:D:113:GLN:NE2	1:F:45:VAL:CG2	2.03	1.21
1:C:113:GLN:NE2	1:E:45:VAL:CG2	2.03	1.21
1:F:112:ASN:O	1:H:38:VAL:CA	1.81	1.21
1:G:113:GLN:NE2	1:I:45:VAL:CG2	2.04	1.21
1:B:113:GLN:NE2	1:D:45:VAL:CG2	2.03	1.21
1:C:111:ASN:O	1:E:37:ALA:O	1.55	1.21
1:C:147:PRO:HG3	1:E:40:PHE:CD1	1.73	1.21
1:H:113:GLN:NE2	1:J:45:VAL:CG2	2.04	1.21
1:H:147:PRO:HG3	1:J:40:PHE:CD1	1.74	1.20
1:E:113:GLN:NE2	1:G:45:VAL:CG2	2.03	1.20
1:G:147:PRO:HG3	1:I:40:PHE:CD1	1.74	1.20
1:H:111:ASN:O	1:J:37:ALA:O	1.55	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASN:O	1:D:37:ALA:O	1.54	1.20
1:A:111:ASN:O	1:C:37:ALA:O	1.55	1.20
1:F:113:GLN:NE2	1:H:45:VAL:CG2	2.03	1.20
1:E:112:ASN:O	1:G:38:VAL:CA	1.82	1.19
1:A:113:GLN:NE2	1:C:45:VAL:CG2	2.03	1.19
1:C:113:GLN:HE22	1:E:45:VAL:CG2	1.57	1.18
1:F:113:GLN:HE22	1:H:45:VAL:CG2	1.56	1.18
1:G:185:LEU:O	1:I:43:LYS:HG2	1.42	1.18
1:G:113:GLN:HE22	1:I:45:VAL:CG2	1.57	1.18
1:D:113:GLN:HE22	1:F:45:VAL:CG2	1.56	1.17
1:D:187:GLY:CA	1:F:43:LYS:HD3	1.74	1.17
1:F:187:GLY:CA	1:H:43:LYS:HD3	1.74	1.17
1:H:187:GLY:CA	1:J:43:LYS:HD3	1.75	1.17
1:B:187:GLY:CA	1:D:43:LYS:HD3	1.74	1.17
1:C:112:ASN:O	1:E:38:VAL:CA	1.82	1.17
1:B:113:GLN:HE22	1:D:45:VAL:CG2	1.56	1.17
1:A:112:ASN:O	1:C:38:VAL:CA	1.80	1.16
1:A:187:GLY:CA	1:C:43:LYS:HD3	1.75	1.16
1:A:113:GLN:HE22	1:C:45:VAL:CG2	1.56	1.16
1:D:112:ASN:O	1:F:38:VAL:CA	1.82	1.16
1:F:185:LEU:O	1:H:43:LYS:HG2	1.42	1.16
1:G:187:GLY:CA	1:I:43:LYS:HD3	1.74	1.15
1:C:187:GLY:CA	1:E:43:LYS:HD3	1.74	1.15
1:H:113:GLN:HE22	1:J:45:VAL:CG2	1.57	1.15
1:D:181:VAL:CG1	1:F:43:LYS:NZ	2.10	1.15
1:E:187:GLY:CA	1:G:43:LYS:HD3	1.74	1.15
1:C:181:VAL:CG1	1:E:43:LYS:NZ	2.10	1.14
1:F:181:VAL:CG1	1:H:43:LYS:NZ	2.10	1.14
1:A:181:VAL:CG1	1:C:43:LYS:NZ	2.10	1.14
1:A:185:LEU:O	1:C:43:LYS:HG2	1.42	1.14
1:C:181:VAL:CG1	1:E:43:LYS:HZ1	1.58	1.14
1:E:181:VAL:CG1	1:G:43:LYS:NZ	2.10	1.14
1:E:113:GLN:HE22	1:G:45:VAL:CG2	1.56	1.14
1:G:181:VAL:CG1	1:I:43:LYS:NZ	2.10	1.14
1:D:185:LEU:O	1:F:43:LYS:HG2	1.43	1.13
1:H:181:VAL:CG1	1:J:43:LYS:NZ	2.10	1.13
1:B:185:LEU:O	1:D:43:LYS:HG2	1.44	1.13
1:B:181:VAL:CG1	1:D:43:LYS:NZ	2.11	1.13
1:C:185:LEU:O	1:E:43:LYS:HG2	1.43	1.13
1:D:147:PRO:HG3	1:F:40:PHE:CE1	1.78	1.13
1:E:185:LEU:O	1:G:43:LYS:HG2	1.43	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ASN:O	1:D:38:VAL:CA	1.81	1.13
1:H:300:ARG:NH2	1:J:237:GLN:O	1.84	1.11
1:F:147:PRO:HD2	1:H:40:PHE:HE1	1.15	1.10
1:B:112:ASN:O	1:D:39:SER:N	1.84	1.10
1:G:300:ARG:NH2	1:I:237:GLN:O	1.84	1.10
1:C:300:ARG:NH2	1:E:237:GLN:O	1.85	1.10
1:F:300:ARG:NH2	1:H:237:GLN:O	1.84	1.10
1:D:300:ARG:NH2	1:F:237:GLN:O	1.85	1.10
1:A:112:ASN:O	1:C:39:SER:N	1.85	1.09
1:A:147:PRO:HG3	1:C:40:PHE:CE1	1.79	1.09
1:D:112:ASN:O	1:F:39:SER:N	1.85	1.09
1:B:147:PRO:HG2	1:D:40:PHE:CZ	1.86	1.09
1:B:181:VAL:HG13	1:D:43:LYS:HZ2	0.93	1.09
1:C:112:ASN:O	1:E:39:SER:N	1.85	1.09
1:D:147:PRO:HD2	1:F:40:PHE:HE1	1.15	1.09
1:E:147:PRO:HG2	1:G:40:PHE:CZ	1.87	1.09
1:D:147:PRO:HG2	1:F:40:PHE:CZ	1.87	1.09
1:A:300:ARG:NH2	1:C:237:GLN:O	1.84	1.09
1:C:147:PRO:CD	1:E:40:PHE:CE1	2.26	1.09
1:C:147:PRO:HG2	1:E:40:PHE:CZ	1.87	1.09
1:E:181:VAL:HG13	1:G:43:LYS:HZ2	0.97	1.09
1:E:300:ARG:NH2	1:G:237:GLN:O	1.85	1.09
1:E:181:VAL:CG1	1:G:43:LYS:HZ1	1.63	1.09
1:F:147:PRO:HG3	1:H:40:PHE:CE1	1.79	1.09
1:G:189:SER:OG	1:I:60:ILE:HD11	0.91	1.09
1:H:147:PRO:HG2	1:J:40:PHE:CZ	1.88	1.09
1:D:181:VAL:HG13	1:F:43:LYS:HZ2	0.93	1.08
1:B:300:ARG:NH2	1:D:237:GLN:O	1.86	1.08
1:E:112:ASN:O	1:G:39:SER:N	1.85	1.08
1:H:112:ASN:O	1:J:39:SER:N	1.86	1.08
1:D:147:PRO:CD	1:F:40:PHE:CE1	2.26	1.08
1:F:112:ASN:O	1:H:39:SER:N	1.85	1.08
1:B:147:PRO:CD	1:D:40:PHE:CE1	2.25	1.08
1:B:189:SER:OG	1:D:60:ILE:HD11	0.90	1.08
1:F:147:PRO:HG2	1:H:40:PHE:CZ	1.87	1.08
1:D:189:SER:OG	1:F:60:ILE:HD11	0.91	1.07
1:H:147:PRO:CD	1:J:40:PHE:CE1	2.26	1.07
1:A:147:PRO:HG2	1:C:40:PHE:CZ	1.88	1.07
1:C:147:PRO:HG3	1:E:40:PHE:CE1	1.78	1.07
1:E:189:SER:OG	1:G:60:ILE:HD11	0.91	1.07
1:H:185:LEU:O	1:J:43:LYS:HG2	1.42	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PRO:CD	1:C:40:PHE:CE1	2.26	1.07
1:A:189:SER:OG	1:C:60:ILE:HD11	0.91	1.07
1:D:181:VAL:CG1	1:F:43:LYS:HZ1	1.67	1.07
1:G:112:ASN:O	1:I:39:SER:N	1.86	1.07
1:G:147:PRO:HD2	1:I:40:PHE:HE1	1.15	1.07
1:H:147:PRO:HG3	1:J:40:PHE:CE1	1.79	1.07
1:B:147:PRO:HD2	1:D:40:PHE:HE1	1.15	1.07
1:C:147:PRO:HD2	1:E:40:PHE:HE1	1.15	1.07
1:D:185:LEU:O	1:F:43:LYS:HG3	1.55	1.07
1:H:189:SER:OG	1:J:60:ILE:HD11	0.91	1.07
1:F:147:PRO:CD	1:H:40:PHE:CE1	2.26	1.06
1:H:147:PRO:HD2	1:J:40:PHE:HE1	1.15	1.06
1:G:147:PRO:HG2	1:I:40:PHE:CZ	1.88	1.06
1:C:189:SER:OG	1:E:60:ILE:HD11	0.91	1.06
1:F:189:SER:OG	1:H:60:ILE:HD11	0.91	1.06
1:G:181:VAL:HG13	1:I:43:LYS:HZ2	0.89	1.06
1:H:181:VAL:HG13	1:J:43:LYS:HZ2	0.88	1.05
1:A:147:PRO:HD2	1:C:40:PHE:HE1	1.15	1.05
1:G:185:LEU:O	1:I:43:LYS:HG3	1.54	1.05
1:B:188:ILE:HD11	1:D:40:PHE:CB	1.87	1.05
1:C:181:VAL:HG12	1:E:43:LYS:HZ1	1.17	1.05
1:A:188:ILE:HD11	1:C:40:PHE:CB	1.88	1.04
1:D:188:ILE:HD11	1:F:40:PHE:CB	1.87	1.04
1:F:181:VAL:CG1	1:H:43:LYS:HZ2	1.68	1.04
1:H:188:ILE:HD11	1:J:40:PHE:CB	1.87	1.04
1:B:185:LEU:O	1:D:43:LYS:HG3	1.56	1.04
1:C:185:LEU:O	1:E:43:LYS:HG3	1.55	1.04
1:F:188:ILE:HD11	1:H:40:PHE:CB	1.87	1.04
1:E:147:PRO:HD2	1:G:40:PHE:HE1	1.15	1.04
1:E:188:ILE:HD11	1:G:40:PHE:CB	1.87	1.04
1:F:185:LEU:O	1:H:43:LYS:HG3	1.55	1.04
1:C:188:ILE:HD11	1:E:40:PHE:CB	1.87	1.04
1:G:188:ILE:HD11	1:I:40:PHE:CB	1.87	1.04
1:A:185:LEU:O	1:C:43:LYS:HG3	1.55	1.04
1:E:147:PRO:CD	1:G:40:PHE:CE1	2.26	1.03
1:G:300:ARG:NH2	1:I:237:GLN:HA	1.75	1.02
1:B:181:VAL:CG1	1:D:43:LYS:HZ1	1.69	1.02
1:C:300:ARG:NH2	1:E:237:GLN:HA	1.75	1.02
1:B:300:ARG:NH2	1:D:237:GLN:HA	1.75	1.02
1:D:181:VAL:HG12	1:F:43:LYS:HZ1	1.23	1.02
1:E:185:LEU:O	1:G:43:LYS:HG3	1.55	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:ARG:NH2	1:F:237:GLN:HA	1.74	1.02
1:A:181:VAL:HG13	1:C:43:LYS:HZ2	0.87	1.01
1:F:300:ARG:NH2	1:H:237:GLN:HA	1.75	1.01
1:G:181:VAL:CG1	1:I:43:LYS:HZ1	1.71	1.01
1:G:111:ASN:OD1	1:I:36:TRP:N	1.81	1.01
1:F:258:LYS:CG	1:G:53:GLU:OE2	2.09	1.01
1:G:147:PRO:CD	1:I:40:PHE:CE1	2.26	1.01
1:H:300:ARG:NH2	1:J:237:GLN:HA	1.75	1.01
1:E:300:ARG:NH2	1:G:237:GLN:HA	1.74	1.00
1:E:181:VAL:HG12	1:G:43:LYS:HZ1	1.20	1.00
1:E:258:LYS:CG	1:F:53:GLU:OE2	2.09	1.00
1:B:258:LYS:CG	1:C:53:GLU:OE2	2.09	1.00
1:D:258:LYS:CG	1:E:53:GLU:OE2	2.09	1.00
1:H:185:LEU:O	1:J:43:LYS:HG3	1.54	1.00
1:D:111:ASN:OD1	1:F:36:TRP:N	1.81	1.00
1:G:258:LYS:CG	1:H:53:GLU:OE2	2.09	1.00
1:C:258:LYS:CG	1:D:53:GLU:OE2	2.09	1.00
1:A:300:ARG:NH2	1:C:237:GLN:HA	1.76	0.99
1:B:181:VAL:HG12	1:D:43:LYS:HZ1	1.25	0.99
1:I:258:LYS:CG	1:J:53:GLU:OE2	2.09	0.99
1:A:185:LEU:HD12	1:C:43:LYS:HE3	1.45	0.99
1:C:181:VAL:HG13	1:E:43:LYS:HZ2	1.02	0.99
1:F:147:PRO:CG	1:H:40:PHE:CD1	2.40	0.99
1:A:258:LYS:CG	1:B:53:GLU:OE2	2.09	0.99
1:H:258:LYS:CG	1:I:53:GLU:OE2	2.09	0.99
1:C:185:LEU:HD12	1:E:43:LYS:HE3	1.45	0.98
1:F:181:VAL:HG13	1:H:43:LYS:HZ2	0.81	0.98
1:B:113:GLN:HE21	1:D:45:VAL:HG21	1.19	0.98
1:H:185:LEU:HD12	1:J:43:LYS:HE3	1.45	0.98
1:H:111:ASN:OD1	1:J:36:TRP:N	1.81	0.98
1:C:111:ASN:OD1	1:E:36:TRP:N	1.81	0.98
1:D:300:ARG:HH22	1:F:237:GLN:CA	1.76	0.98
1:D:151:PRO:HD3	1:F:40:PHE:CZ	1.99	0.97
1:G:113:GLN:HE21	1:I:45:VAL:HG21	1.20	0.97
1:H:113:GLN:HE21	1:J:45:VAL:HG21	1.20	0.97
1:B:300:ARG:HH22	1:D:237:GLN:CA	1.76	0.97
1:A:181:VAL:HG12	1:C:43:LYS:HZ1	1.29	0.97
1:E:300:ARG:HH22	1:G:237:GLN:CA	1.76	0.97
1:H:151:PRO:HD3	1:J:40:PHE:CZ	2.00	0.97
1:E:185:LEU:HD12	1:G:43:LYS:HE3	1.45	0.97
1:F:151:PRO:HD3	1:H:40:PHE:CZ	2.00	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLN:HE21	1:C:45:VAL:HG21	1.20	0.97
1:F:185:LEU:HD12	1:H:43:LYS:HE3	1.45	0.97
1:G:300:ARG:HH22	1:I:237:GLN:CA	1.77	0.97
1:E:111:ASN:OD1	1:G:36:TRP:N	1.81	0.97
1:F:300:ARG:HH22	1:H:237:GLN:CA	1.76	0.97
1:G:181:VAL:HG12	1:I:43:LYS:HZ1	1.25	0.97
1:H:181:VAL:HG12	1:J:43:LYS:HZ1	1.27	0.97
1:B:111:ASN:OD1	1:D:36:TRP:N	1.81	0.97
1:D:147:PRO:CG	1:F:40:PHE:CD1	2.40	0.97
1:C:300:ARG:HH22	1:E:237:GLN:CA	1.76	0.96
1:G:185:LEU:HD12	1:I:43:LYS:HE3	1.45	0.96
1:H:300:ARG:HH22	1:J:237:GLN:CA	1.77	0.96
1:B:151:PRO:HD3	1:D:40:PHE:CZ	2.01	0.96
1:B:185:LEU:HD12	1:D:43:LYS:HE3	1.45	0.96
1:E:113:GLN:HE21	1:G:45:VAL:HG21	1.20	0.96
1:C:189:SER:HG	1:E:60:ILE:HD11	1.15	0.96
1:D:185:LEU:HD12	1:F:43:LYS:HE3	1.45	0.96
1:E:147:PRO:CG	1:G:40:PHE:CD1	2.40	0.96
1:G:151:PRO:HD3	1:I:40:PHE:CZ	2.00	0.96
1:D:113:GLN:HE21	1:F:45:VAL:HG21	1.20	0.95
1:A:181:VAL:CG1	1:C:43:LYS:HZ1	1.76	0.95
1:H:181:VAL:CG1	1:J:43:LYS:HZ1	1.73	0.95
1:A:300:ARG:HH22	1:C:237:GLN:CA	1.77	0.95
1:B:258:LYS:CD	1:C:53:GLU:OE1	2.14	0.95
1:D:258:LYS:CD	1:E:53:GLU:OE1	2.14	0.95
1:I:258:LYS:CD	1:J:53:GLU:OE1	2.14	0.95
1:C:151:PRO:HD3	1:E:40:PHE:CZ	2.00	0.95
1:A:258:LYS:CD	1:B:53:GLU:OE1	2.14	0.95
1:F:258:LYS:CD	1:G:53:GLU:OE1	2.14	0.95
1:H:258:LYS:CD	1:I:53:GLU:OE1	2.14	0.95
1:A:147:PRO:CG	1:C:40:PHE:CD1	2.41	0.95
1:A:151:PRO:HD3	1:C:40:PHE:CZ	2.01	0.95
1:E:151:PRO:HD3	1:G:40:PHE:CZ	2.00	0.95
1:E:258:LYS:CD	1:F:53:GLU:OE1	2.14	0.95
1:G:147:PRO:CG	1:I:40:PHE:CD1	2.40	0.95
1:G:258:LYS:CD	1:H:53:GLU:OE1	2.14	0.94
1:A:189:SER:HG	1:C:60:ILE:HD11	1.12	0.94
1:C:258:LYS:CD	1:D:53:GLU:OE1	2.14	0.94
1:D:187:GLY:C	1:F:43:LYS:HD3	1.93	0.94
1:H:181:VAL:CG1	1:J:43:LYS:HZ2	1.77	0.94
1:H:151:PRO:HG3	1:J:40:PHE:HZ	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:PRO:HG3	1:G:40:PHE:CE1	1.78	0.94
1:F:187:GLY:C	1:H:43:LYS:HD3	1.93	0.94
1:E:187:GLY:C	1:G:43:LYS:HD3	1.93	0.93
1:C:113:GLN:HE21	1:E:45:VAL:HG21	1.20	0.93
1:C:151:PRO:HG3	1:E:40:PHE:HZ	1.33	0.93
1:D:151:PRO:HG3	1:F:40:PHE:HZ	1.32	0.93
1:C:187:GLY:C	1:E:43:LYS:HD3	1.93	0.93
1:F:151:PRO:HG3	1:H:40:PHE:HZ	1.32	0.93
1:G:181:VAL:CG1	1:I:43:LYS:HZ2	1.78	0.93
1:B:147:PRO:CG	1:D:40:PHE:CD1	2.40	0.93
1:F:189:SER:HG	1:H:60:ILE:HD11	1.11	0.93
1:A:112:ASN:O	1:C:38:VAL:C	2.12	0.93
1:F:113:GLN:HE21	1:H:45:VAL:HG21	1.20	0.93
1:H:189:SER:HG	1:J:60:ILE:HD11	1.11	0.93
1:B:112:ASN:O	1:D:38:VAL:C	2.12	0.93
1:H:187:GLY:C	1:J:43:LYS:HD3	1.93	0.93
1:A:151:PRO:HG3	1:C:40:PHE:HZ	1.32	0.92
1:E:112:ASN:O	1:G:38:VAL:C	2.13	0.92
1:G:189:SER:HG	1:I:60:ILE:HD11	1.15	0.92
1:B:187:GLY:C	1:D:43:LYS:HD3	1.93	0.92
1:D:113:GLN:HE22	1:F:45:VAL:HG22	1.35	0.92
1:F:112:ASN:O	1:H:38:VAL:C	2.13	0.92
1:G:187:GLY:C	1:I:43:LYS:HD3	1.93	0.92
1:E:189:SER:HG	1:G:60:ILE:HD11	1.14	0.92
1:A:113:GLN:HE22	1:C:45:VAL:HG22	1.35	0.92
1:D:189:SER:HG	1:F:60:ILE:HD11	1.15	0.92
1:H:112:ASN:O	1:J:38:VAL:C	2.13	0.92
1:A:111:ASN:OD1	1:C:36:TRP:N	1.81	0.91
1:E:151:PRO:HG3	1:G:40:PHE:HZ	1.33	0.91
1:G:112:ASN:O	1:I:38:VAL:C	2.13	0.91
1:A:187:GLY:C	1:C:43:LYS:HD3	1.94	0.91
1:F:111:ASN:OD1	1:H:36:TRP:N	1.81	0.91
1:F:181:VAL:HG12	1:H:43:LYS:HZ1	1.35	0.91
1:G:151:PRO:HG3	1:I:40:PHE:HZ	1.32	0.91
1:D:300:ARG:NH2	1:F:237:GLN:C	2.27	0.91
1:H:147:PRO:CG	1:J:40:PHE:CD1	2.40	0.91
1:E:113:GLN:HE22	1:G:45:VAL:HG22	1.35	0.91
1:B:300:ARG:NH2	1:D:237:GLN:C	2.28	0.91
1:F:113:GLN:HE22	1:H:45:VAL:HG22	1.35	0.91
1:B:189:SER:HG	1:D:60:ILE:HD11	1.10	0.91
1:C:112:ASN:O	1:E:38:VAL:C	2.13	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:GLN:HE22	1:J:45:VAL:HG22	1.35	0.91
1:D:112:ASN:O	1:F:38:VAL:C	2.13	0.90
1:G:300:ARG:NH2	1:I:237:GLN:C	2.27	0.90
1:B:113:GLN:HE22	1:D:45:VAL:HG22	1.34	0.90
1:C:147:PRO:CG	1:E:40:PHE:CD1	2.40	0.90
1:F:300:ARG:NH2	1:H:237:GLN:C	2.27	0.90
1:E:258:LYS:HD3	1:F:53:GLU:OE1	1.72	0.90
1:B:151:PRO:HG3	1:D:40:PHE:HZ	1.33	0.90
1:G:258:LYS:HD3	1:H:53:GLU:OE1	1.73	0.89
1:C:113:GLN:HE22	1:E:45:VAL:HG22	1.35	0.89
1:B:147:PRO:HG3	1:D:40:PHE:CE1	1.77	0.89
1:C:258:LYS:HD3	1:D:53:GLU:OE1	1.72	0.89
1:E:300:ARG:NH2	1:G:237:GLN:C	2.28	0.89
1:H:300:ARG:NH2	1:J:237:GLN:C	2.27	0.89
1:A:108:TYR:CD1	1:C:38:VAL:HG13	2.08	0.89
1:D:300:ARG:NH2	1:F:237:GLN:CA	2.35	0.89
1:C:258:LYS:CG	1:D:53:GLU:CD	2.46	0.88
1:I:258:LYS:HD3	1:J:53:GLU:OE1	1.73	0.88
1:G:113:GLN:HE22	1:I:45:VAL:HG22	1.35	0.88
1:A:258:LYS:HD3	1:B:53:GLU:OE1	1.73	0.88
1:C:108:TYR:CD1	1:E:38:VAL:HG13	2.09	0.88
1:G:108:TYR:CD1	1:I:38:VAL:HG13	2.09	0.88
1:C:300:ARG:NH2	1:E:237:GLN:C	2.28	0.88
1:E:108:TYR:CD1	1:G:38:VAL:HG13	2.09	0.88
1:B:108:TYR:CD1	1:D:38:VAL:HG13	2.09	0.88
1:E:258:LYS:CG	1:F:53:GLU:CD	2.46	0.88
1:A:147:PRO:HD2	1:C:40:PHE:CE1	2.02	0.88
1:F:181:VAL:CG1	1:H:43:LYS:HZ1	1.82	0.88
1:G:188:ILE:HD11	1:I:40:PHE:HB2	1.56	0.88
1:B:258:LYS:CG	1:C:53:GLU:CD	2.46	0.88
1:D:108:TYR:CD1	1:F:38:VAL:HG13	2.09	0.87
1:D:258:LYS:CG	1:E:53:GLU:CD	2.47	0.87
1:A:300:ARG:NH2	1:C:237:GLN:C	2.27	0.87
1:G:258:LYS:CG	1:H:53:GLU:CD	2.46	0.87
1:A:300:ARG:NH2	1:C:237:GLN:CA	2.36	0.87
1:F:108:TYR:CD1	1:H:38:VAL:HG13	2.09	0.87
1:G:300:ARG:NH2	1:I:237:GLN:CA	2.35	0.87
1:I:258:LYS:CG	1:J:53:GLU:CD	2.46	0.87
1:F:300:ARG:NH2	1:H:237:GLN:CA	2.36	0.87
1:H:188:ILE:HD11	1:J:40:PHE:HB2	1.56	0.87
1:B:258:LYS:HD3	1:C:53:GLU:OE1	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:108:TYR:CD1	1:J:38:VAL:HG13	2.09	0.87
1:B:187:GLY:H	1:D:43:LYS:HE2	1.41	0.86
1:G:147:PRO:HD2	1:I:40:PHE:CE1	2.03	0.86
1:H:258:LYS:HD3	1:I:53:GLU:OE1	1.73	0.86
1:B:188:ILE:HD11	1:D:40:PHE:HB2	1.55	0.86
1:D:300:ARG:NH1	1:F:237:GLN:O	2.08	0.86
1:D:187:GLY:H	1:F:43:LYS:HE2	1.41	0.86
1:A:188:ILE:HD11	1:C:40:PHE:HB2	1.55	0.86
1:E:187:GLY:H	1:G:43:LYS:HE2	1.41	0.86
1:F:188:ILE:HD11	1:H:40:PHE:HB2	1.55	0.86
1:C:188:ILE:HD11	1:E:40:PHE:HB2	1.55	0.86
1:E:188:ILE:HD11	1:G:40:PHE:HB2	1.55	0.86
1:F:185:LEU:C	1:H:43:LYS:HE2	2.01	0.86
1:F:300:ARG:NH1	1:H:237:GLN:O	2.08	0.86
1:C:187:GLY:H	1:E:43:LYS:HE2	1.41	0.86
1:D:188:ILE:HD11	1:F:40:PHE:HB2	1.56	0.86
1:A:185:LEU:C	1:C:43:LYS:HE2	2.00	0.85
1:E:300:ARG:NH2	1:G:237:GLN:CA	2.36	0.85
1:F:187:GLY:H	1:H:43:LYS:HE2	1.41	0.85
1:F:258:LYS:HD3	1:G:53:GLU:OE1	1.73	0.85
1:G:300:ARG:NH1	1:I:237:GLN:O	2.08	0.85
1:H:187:GLY:H	1:J:43:LYS:HE2	1.41	0.85
1:A:187:GLY:H	1:C:43:LYS:HE2	1.41	0.85
1:A:300:ARG:NH1	1:C:237:GLN:O	2.09	0.85
1:C:300:ARG:NH2	1:E:237:GLN:CA	2.36	0.85
1:H:300:ARG:NH2	1:J:237:GLN:CA	2.36	0.85
1:C:300:ARG:NH1	1:E:237:GLN:O	2.08	0.85
1:D:258:LYS:HD3	1:E:53:GLU:OE1	1.74	0.85
1:H:185:LEU:C	1:J:43:LYS:HE2	2.01	0.85
1:B:300:ARG:NH1	1:D:237:GLN:O	2.08	0.85
1:E:300:ARG:NH1	1:G:237:GLN:O	2.08	0.85
1:G:185:LEU:C	1:I:43:LYS:HE2	2.01	0.85
1:F:147:PRO:HD2	1:H:40:PHE:CE1	2.03	0.85
1:G:187:GLY:H	1:I:43:LYS:HE2	1.41	0.85
1:D:185:LEU:C	1:F:43:LYS:HE2	2.02	0.85
1:H:300:ARG:NH1	1:J:237:GLN:O	2.08	0.85
1:C:185:LEU:C	1:E:43:LYS:HE2	2.02	0.84
1:B:300:ARG:NH2	1:D:237:GLN:CA	2.36	0.84
1:E:185:LEU:C	1:G:43:LYS:HE2	2.02	0.84
1:B:185:LEU:C	1:D:43:LYS:HE2	2.02	0.84
1:F:258:LYS:HG2	1:G:53:GLU:OE1	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:300:ARG:CZ	1:I:237:GLN:O	2.26	0.84
1:C:258:LYS:HG2	1:D:53:GLU:OE1	1.78	0.84
1:A:300:ARG:CZ	1:C:237:GLN:O	2.26	0.84
1:B:147:PRO:HD2	1:D:40:PHE:CE1	2.02	0.84
1:B:258:LYS:HG2	1:C:53:GLU:OE1	1.78	0.84
1:G:151:PRO:CG	1:I:40:PHE:HZ	1.91	0.83
1:C:151:PRO:CG	1:E:40:PHE:HZ	1.92	0.83
1:C:300:ARG:CZ	1:E:237:GLN:O	2.26	0.83
1:D:151:PRO:CG	1:F:40:PHE:HZ	1.91	0.83
1:G:258:LYS:HG2	1:H:53:GLU:OE1	1.78	0.83
1:H:151:PRO:CG	1:J:40:PHE:HZ	1.91	0.83
1:I:258:LYS:HG2	1:J:53:GLU:OE1	1.78	0.83
1:F:185:LEU:C	1:H:43:LYS:CE	2.52	0.83
1:H:300:ARG:CZ	1:J:237:GLN:O	2.26	0.83
1:G:185:LEU:HA	1:I:43:LYS:HE3	1.60	0.83
1:H:185:LEU:C	1:J:43:LYS:CE	2.51	0.83
1:H:185:LEU:HA	1:J:43:LYS:HE3	1.61	0.83
1:B:187:GLY:HA2	1:D:43:LYS:HD3	1.59	0.83
1:G:185:LEU:C	1:I:43:LYS:CE	2.52	0.83
1:C:147:PRO:HD2	1:E:40:PHE:CE1	2.03	0.83
1:E:300:ARG:CZ	1:G:237:GLN:O	2.26	0.83
1:F:185:LEU:HA	1:H:43:LYS:HE3	1.61	0.83
1:A:185:LEU:C	1:C:43:LYS:CE	2.51	0.83
1:A:185:LEU:HA	1:C:43:LYS:HE3	1.61	0.83
1:D:258:LYS:HG2	1:E:53:GLU:OE1	1.78	0.83
1:E:147:PRO:HD2	1:G:40:PHE:CE1	2.03	0.83
1:D:187:GLY:HA2	1:F:43:LYS:HD3	1.60	0.83
1:F:300:ARG:CZ	1:H:237:GLN:O	2.26	0.83
1:G:187:GLY:HA2	1:I:43:LYS:HD3	1.61	0.83
1:A:258:LYS:CG	1:B:53:GLU:CD	2.47	0.83
1:D:185:LEU:HA	1:F:43:LYS:HE3	1.61	0.83
1:F:151:PRO:CG	1:H:40:PHE:HZ	1.92	0.83
1:E:258:LYS:HG2	1:F:53:GLU:OE1	1.78	0.82
1:C:185:LEU:HA	1:E:43:LYS:HE3	1.61	0.82
1:E:185:LEU:C	1:G:43:LYS:CE	2.53	0.82
1:C:185:LEU:C	1:E:43:LYS:CE	2.52	0.82
1:A:151:PRO:CG	1:C:40:PHE:HZ	1.92	0.82
1:A:258:LYS:HG2	1:B:53:GLU:OE1	1.78	0.82
1:D:300:ARG:CZ	1:F:237:GLN:O	2.26	0.82
1:E:151:PRO:CG	1:G:40:PHE:HZ	1.92	0.82
1:F:258:LYS:CG	1:G:53:GLU:CD	2.47	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:258:LYS:CG	1:I:53:GLU:CD	2.47	0.82
1:A:181:VAL:CG1	1:C:43:LYS:HZ2	1.75	0.82
1:D:185:LEU:C	1:F:43:LYS:CE	2.52	0.82
1:B:185:LEU:C	1:D:43:LYS:CE	2.53	0.82
1:H:258:LYS:HG2	1:I:53:GLU:OE1	1.78	0.82
1:E:185:LEU:HA	1:G:43:LYS:HE3	1.62	0.81
1:A:187:GLY:HA2	1:C:43:LYS:HD3	1.60	0.81
1:B:300:ARG:CZ	1:D:237:GLN:O	2.27	0.81
1:E:187:GLY:HA2	1:G:43:LYS:HD3	1.60	0.81
1:H:147:PRO:HD2	1:J:40:PHE:CE1	2.03	0.81
1:H:187:GLY:HA2	1:J:43:LYS:HD3	1.60	0.81
1:C:187:GLY:HA2	1:E:43:LYS:HD3	1.60	0.81
1:B:151:PRO:CG	1:D:40:PHE:HZ	1.92	0.81
1:B:185:LEU:HA	1:D:43:LYS:HE3	1.63	0.81
1:G:147:PRO:HG3	1:I:40:PHE:CE1	1.79	0.81
1:G:151:PRO:CD	1:I:40:PHE:CZ	2.64	0.80
1:F:187:GLY:HA2	1:H:43:LYS:HD3	1.60	0.80
1:C:151:PRO:CD	1:E:40:PHE:CZ	2.64	0.80
1:D:151:PRO:CD	1:F:40:PHE:CZ	2.64	0.80
1:H:151:PRO:CD	1:J:40:PHE:CZ	2.64	0.80
1:A:151:PRO:CD	1:C:40:PHE:CZ	2.65	0.79
1:B:258:LYS:CG	1:C:53:GLU:OE1	2.30	0.79
1:I:258:LYS:CG	1:J:53:GLU:OE1	2.30	0.79
1:E:258:LYS:CG	1:F:53:GLU:OE1	2.31	0.79
1:C:258:LYS:CG	1:D:53:GLU:OE1	2.30	0.79
1:D:147:PRO:HD2	1:F:40:PHE:CE1	2.03	0.79
1:E:151:PRO:CD	1:G:40:PHE:CZ	2.65	0.79
1:D:258:LYS:CG	1:E:53:GLU:OE1	2.31	0.79
1:F:151:PRO:CD	1:H:40:PHE:CZ	2.65	0.79
1:A:258:LYS:CG	1:B:53:GLU:OE1	2.31	0.79
1:H:258:LYS:CG	1:I:53:GLU:OE1	2.31	0.79
1:B:151:PRO:CD	1:D:40:PHE:CZ	2.66	0.79
1:G:258:LYS:CG	1:H:53:GLU:OE1	2.31	0.78
1:F:258:LYS:CG	1:G:53:GLU:OE1	2.31	0.78
1:A:182:MET:HG3	1:C:60:ILE:HD13	1.66	0.78
1:G:182:MET:HG3	1:I:60:ILE:HD13	1.66	0.78
1:B:182:MET:HG3	1:D:60:ILE:HD13	1.66	0.77
1:A:112:ASN:O	1:C:38:VAL:HA	1.14	0.77
1:C:182:MET:HG3	1:E:60:ILE:HD13	1.67	0.77
1:C:272:GLY:HA2	1:E:216:LYS:O	1.84	0.77
1:H:272:GLY:HA2	1:J:216:LYS:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLY:HA2	1:C:216:LYS:O	1.84	0.77
1:E:182:MET:HG3	1:G:60:ILE:HD13	1.67	0.77
1:D:182:MET:HG3	1:F:60:ILE:HD13	1.67	0.77
1:E:272:GLY:HA2	1:G:216:LYS:O	1.85	0.77
1:F:182:MET:HG3	1:H:60:ILE:HD13	1.66	0.77
1:G:258:LYS:HA	1:H:53:GLU:OE2	1.85	0.77
1:F:258:LYS:HA	1:G:53:GLU:OE2	1.85	0.76
1:H:182:MET:HG3	1:J:60:ILE:HD13	1.66	0.76
1:H:258:LYS:HA	1:I:53:GLU:OE2	1.85	0.76
1:A:258:LYS:HA	1:B:53:GLU:OE2	1.85	0.76
1:I:258:LYS:HA	1:J:53:GLU:OE2	1.84	0.76
1:B:257:ARG:NH2	1:C:52:GLY:C	2.44	0.76
1:F:272:GLY:HA2	1:H:216:LYS:O	1.84	0.75
1:G:272:GLY:HA2	1:I:216:LYS:O	1.84	0.75
1:C:258:LYS:HA	1:D:53:GLU:OE2	1.84	0.75
1:D:258:LYS:HA	1:E:53:GLU:OE2	1.85	0.75
1:E:257:ARG:NH2	1:F:52:GLY:C	2.44	0.75
1:E:258:LYS:HA	1:F:53:GLU:OE2	1.85	0.75
1:B:257:ARG:NH2	1:C:52:GLY:O	2.20	0.75
1:C:187:GLY:N	1:E:43:LYS:HD3	2.02	0.75
1:F:187:GLY:N	1:H:43:LYS:HD3	2.02	0.75
1:C:257:ARG:NH2	1:D:52:GLY:C	2.44	0.75
1:C:257:ARG:NH2	1:D:52:GLY:O	2.20	0.75
1:I:257:ARG:NH2	1:J:52:GLY:C	2.44	0.75
1:G:187:GLY:N	1:I:43:LYS:HD3	2.02	0.74
1:A:257:ARG:NH2	1:B:52:GLY:O	2.21	0.74
1:A:257:ARG:NH2	1:B:52:GLY:C	2.45	0.74
1:B:112:ASN:O	1:D:38:VAL:HA	1.15	0.74
1:I:257:ARG:NH2	1:J:52:GLY:O	2.20	0.74
1:A:151:PRO:HG3	1:C:40:PHE:CZ	2.21	0.74
1:F:257:ARG:NH2	1:G:52:GLY:C	2.45	0.74
1:B:258:LYS:HA	1:C:53:GLU:OE2	1.84	0.74
1:G:257:ARG:NH2	1:H:52:GLY:C	2.45	0.74
1:G:257:ARG:NH2	1:H:52:GLY:O	2.20	0.74
1:H:187:GLY:N	1:J:43:LYS:HD3	2.02	0.74
1:H:257:ARG:NH2	1:I:52:GLY:C	2.46	0.74
1:A:187:GLY:N	1:C:43:LYS:HD3	2.02	0.74
1:D:257:ARG:NH2	1:E:52:GLY:O	2.21	0.74
1:E:187:GLY:N	1:G:43:LYS:HE2	2.03	0.74
1:G:185:LEU:CA	1:I:43:LYS:HE3	2.17	0.74
1:B:111:ASN:ND2	1:D:36:TRP:CE3	2.56	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLY:N	1:D:43:LYS:HE2	2.02	0.74
1:C:188:ILE:HD12	1:E:38:VAL:O	1.88	0.74
1:E:151:PRO:HG3	1:G:40:PHE:CZ	2.22	0.74
1:H:257:ARG:NH2	1:I:52:GLY:O	2.21	0.74
1:A:187:GLY:N	1:C:43:LYS:HE2	2.03	0.74
1:D:111:ASN:ND2	1:F:36:TRP:CE3	2.56	0.74
1:A:185:LEU:CA	1:C:43:LYS:HE3	2.17	0.74
1:F:188:ILE:HD12	1:H:38:VAL:O	1.88	0.74
1:H:185:LEU:CA	1:J:43:LYS:HE3	2.18	0.74
1:D:257:ARG:NH2	1:E:52:GLY:C	2.46	0.73
1:E:188:ILE:HD12	1:G:38:VAL:O	1.88	0.73
1:F:187:GLY:N	1:H:43:LYS:HE2	2.03	0.73
1:G:188:ILE:HD12	1:I:38:VAL:O	1.88	0.73
1:F:111:ASN:ND2	1:H:36:TRP:CE3	2.56	0.73
1:F:257:ARG:NH2	1:G:52:GLY:O	2.20	0.73
1:E:257:ARG:NH2	1:F:52:GLY:O	2.20	0.73
1:B:187:GLY:N	1:D:43:LYS:HD3	2.03	0.73
1:H:111:ASN:ND2	1:J:36:TRP:CE3	2.57	0.73
1:D:187:GLY:N	1:F:43:LYS:HD3	2.02	0.73
1:E:187:GLY:N	1:G:43:LYS:HD3	2.02	0.73
1:A:187:GLY:N	1:C:43:LYS:CD	2.51	0.73
1:C:187:GLY:CA	1:E:43:LYS:CD	2.64	0.73
1:H:188:ILE:HD12	1:J:38:VAL:O	1.88	0.73
1:A:188:ILE:HD12	1:C:38:VAL:O	1.88	0.73
1:B:188:ILE:HD12	1:D:38:VAL:O	1.89	0.73
1:C:187:GLY:N	1:E:43:LYS:CD	2.51	0.73
1:D:112:ASN:O	1:F:38:VAL:HA	1.15	0.73
1:E:111:ASN:ND2	1:G:36:TRP:CE3	2.56	0.73
1:G:187:GLY:N	1:I:43:LYS:CD	2.51	0.73
1:H:112:ASN:O	1:J:38:VAL:HA	1.14	0.73
1:B:151:PRO:HG3	1:D:40:PHE:CZ	2.22	0.73
1:D:151:PRO:CD	1:F:40:PHE:HZ	2.02	0.73
1:C:187:GLY:N	1:E:43:LYS:HE2	2.03	0.73
1:E:185:LEU:CA	1:G:43:LYS:HE3	2.19	0.73
1:H:187:GLY:N	1:J:43:LYS:HE2	2.03	0.72
1:H:187:GLY:N	1:J:43:LYS:CD	2.51	0.72
1:C:111:ASN:ND2	1:E:36:TRP:CE3	2.56	0.72
1:D:185:LEU:CA	1:F:43:LYS:HE3	2.18	0.72
1:E:188:ILE:HD11	1:G:40:PHE:N	2.05	0.72
1:B:187:GLY:CA	1:D:43:LYS:CD	2.64	0.72
1:B:187:GLY:N	1:D:43:LYS:CD	2.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:GLY:N	1:F:43:LYS:CD	2.51	0.72
1:D:272:GLY:HA2	1:F:216:LYS:O	1.84	0.72
1:E:187:GLY:N	1:G:43:LYS:CD	2.51	0.72
1:F:187:GLY:N	1:H:43:LYS:CD	2.51	0.72
1:F:185:LEU:CA	1:H:43:LYS:HE3	2.18	0.72
1:G:188:ILE:HD11	1:I:40:PHE:N	2.05	0.72
1:C:185:LEU:CA	1:E:43:LYS:HE3	2.18	0.72
1:F:151:PRO:CD	1:H:40:PHE:HZ	2.03	0.72
1:D:188:ILE:HD12	1:F:38:VAL:O	1.88	0.72
1:H:151:PRO:HG3	1:J:40:PHE:CZ	2.21	0.72
1:F:112:ASN:O	1:H:38:VAL:HA	1.14	0.72
1:G:111:ASN:ND2	1:I:36:TRP:CE3	2.57	0.72
1:G:300:ARG:HH21	1:I:237:GLN:HA	1.52	0.72
1:B:185:LEU:CA	1:D:43:LYS:HE3	2.19	0.72
1:D:187:GLY:N	1:F:43:LYS:HE2	2.03	0.72
1:A:111:ASN:ND2	1:C:36:TRP:CE3	2.57	0.72
1:D:187:GLY:CA	1:F:43:LYS:CD	2.64	0.72
1:D:300:ARG:HH21	1:F:237:GLN:HA	1.52	0.71
1:C:188:ILE:HD11	1:E:40:PHE:N	2.05	0.71
1:G:187:GLY:N	1:I:43:LYS:HE2	2.04	0.71
1:B:151:PRO:CD	1:D:40:PHE:HZ	2.04	0.71
1:G:151:PRO:HG3	1:I:40:PHE:CZ	2.21	0.71
1:A:187:GLY:CA	1:C:43:LYS:CD	2.64	0.71
1:E:300:ARG:HH21	1:G:237:GLN:HA	1.53	0.71
1:H:300:ARG:HH21	1:J:237:GLN:HA	1.53	0.71
1:B:187:GLY:C	1:D:43:LYS:CD	2.64	0.71
1:H:188:ILE:HD11	1:J:40:PHE:N	2.05	0.71
1:D:187:GLY:C	1:F:43:LYS:CD	2.63	0.71
1:E:187:GLY:C	1:G:43:LYS:CD	2.63	0.71
1:A:188:ILE:HD11	1:C:40:PHE:N	2.06	0.71
1:C:187:GLY:C	1:E:43:LYS:CD	2.64	0.71
1:E:271:SER:CB	1:G:216:LYS:CD	2.69	0.71
1:F:188:ILE:CD1	1:H:40:PHE:HB2	2.21	0.71
1:F:300:ARG:HH21	1:H:237:GLN:HA	1.53	0.71
1:B:188:ILE:CD1	1:D:40:PHE:HB2	2.21	0.70
1:C:271:SER:CB	1:E:216:LYS:CD	2.69	0.70
1:D:188:ILE:HD11	1:F:40:PHE:N	2.04	0.70
1:D:188:ILE:CD1	1:F:40:PHE:HB2	2.21	0.70
1:F:187:GLY:CA	1:H:43:LYS:CD	2.64	0.70
1:H:188:ILE:CD1	1:J:40:PHE:HB2	2.21	0.70
1:C:151:PRO:CD	1:E:40:PHE:HZ	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:TYR:O	1:G:240:ASN:ND2	2.24	0.70
1:B:188:ILE:HD11	1:D:40:PHE:N	2.05	0.70
1:G:185:LEU:C	1:I:43:LYS:HG2	2.17	0.70
1:A:271:SER:CB	1:C:216:LYS:CD	2.69	0.70
1:F:188:ILE:HD11	1:H:40:PHE:N	2.05	0.70
1:C:273:TYR:O	1:E:240:ASN:ND2	2.25	0.70
1:D:151:PRO:HG3	1:F:40:PHE:CZ	2.21	0.70
1:F:188:ILE:HD11	1:H:40:PHE:HB3	1.74	0.70
1:G:185:LEU:HD21	1:I:41:GLY:HA3	1.73	0.70
1:C:185:LEU:HD21	1:E:41:GLY:HA3	1.74	0.70
1:F:187:GLY:C	1:H:43:LYS:CD	2.64	0.70
1:B:300:ARG:HH21	1:D:237:GLN:HA	1.54	0.70
1:F:273:TYR:O	1:H:240:ASN:ND2	2.25	0.70
1:G:187:GLY:C	1:I:43:LYS:CD	2.64	0.70
1:H:187:GLY:CA	1:J:43:LYS:CD	2.64	0.70
1:A:273:TYR:O	1:C:240:ASN:ND2	2.25	0.70
1:D:185:LEU:C	1:F:43:LYS:HG2	2.17	0.70
1:E:185:LEU:HD21	1:G:41:GLY:HA3	1.74	0.70
1:H:187:GLY:C	1:J:43:LYS:CD	2.64	0.70
1:H:188:ILE:HD11	1:J:40:PHE:HB3	1.74	0.69
1:F:185:LEU:C	1:H:43:LYS:HG2	2.17	0.69
1:G:271:SER:CB	1:I:216:LYS:CD	2.70	0.69
1:A:188:ILE:CD1	1:C:40:PHE:HB2	2.22	0.69
1:B:108:TYR:CD1	1:D:38:VAL:CG1	2.75	0.69
1:B:108:TYR:OH	1:D:40:PHE:CD1	2.45	0.69
1:C:188:ILE:CD1	1:E:40:PHE:HB2	2.21	0.69
1:C:300:ARG:HH21	1:E:237:GLN:HA	1.53	0.69
1:C:151:PRO:HG3	1:E:40:PHE:CZ	2.22	0.69
1:F:151:PRO:HG3	1:H:40:PHE:CZ	2.21	0.69
1:H:185:LEU:HD21	1:J:41:GLY:HA3	1.74	0.69
1:C:185:LEU:C	1:E:43:LYS:HG2	2.17	0.69
1:D:273:TYR:O	1:F:240:ASN:ND2	2.25	0.69
1:E:188:ILE:CD1	1:G:40:PHE:HB2	2.21	0.69
1:G:188:ILE:CD1	1:I:40:PHE:HB2	2.21	0.69
1:H:273:TYR:O	1:J:240:ASN:ND2	2.25	0.69
1:B:272:GLY:HA2	1:D:216:LYS:O	1.85	0.69
1:G:185:LEU:HG	1:I:43:LYS:HG3	1.75	0.69
1:H:185:LEU:C	1:J:43:LYS:HG2	2.17	0.69
1:A:185:LEU:HD21	1:C:41:GLY:HA3	1.75	0.69
1:B:271:SER:CB	1:D:216:LYS:CD	2.69	0.69
1:B:273:TYR:O	1:D:240:ASN:ND2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LEU:HD21	1:F:41:GLY:HA3	1.73	0.69
1:G:273:TYR:O	1:I:240:ASN:ND2	2.25	0.69
1:H:271:SER:CB	1:J:216:LYS:CD	2.69	0.69
1:F:185:LEU:HD21	1:H:41:GLY:HA3	1.74	0.69
1:D:185:LEU:HG	1:F:43:LYS:HG3	1.75	0.69
1:H:108:TYR:CD1	1:J:38:VAL:CG1	2.76	0.69
1:C:185:LEU:HG	1:E:43:LYS:HG3	1.75	0.68
1:D:108:TYR:CD1	1:F:38:VAL:CG1	2.76	0.68
1:G:108:TYR:CD1	1:I:38:VAL:CG1	2.76	0.68
1:F:108:TYR:CD1	1:H:38:VAL:CG1	2.75	0.68
1:D:271:SER:CB	1:F:216:LYS:CD	2.69	0.68
1:E:185:LEU:HG	1:G:43:LYS:HG3	1.76	0.68
1:G:187:GLY:CA	1:I:43:LYS:CD	2.64	0.68
1:A:185:LEU:C	1:C:43:LYS:HG2	2.18	0.68
1:A:185:LEU:HG	1:C:43:LYS:HG3	1.75	0.68
1:A:108:TYR:OH	1:C:40:PHE:CD1	2.47	0.68
1:A:187:GLY:N	1:C:43:LYS:CE	2.57	0.68
1:F:271:SER:CB	1:H:216:LYS:CD	2.69	0.68
1:H:185:LEU:HA	1:J:43:LYS:CE	2.24	0.68
1:A:108:TYR:CD1	1:C:38:VAL:CG1	2.75	0.68
1:A:300:ARG:HH21	1:C:237:GLN:HA	1.54	0.68
1:A:185:LEU:HA	1:C:43:LYS:CE	2.24	0.68
1:B:188:ILE:HD11	1:D:40:PHE:HB3	1.72	0.68
1:C:108:TYR:CD1	1:E:38:VAL:CG1	2.76	0.68
1:C:108:TYR:OH	1:E:40:PHE:CD1	2.47	0.68
1:C:187:GLY:N	1:E:43:LYS:CE	2.57	0.68
1:F:108:TYR:OH	1:H:40:PHE:CD1	2.47	0.68
1:F:185:LEU:HG	1:H:43:LYS:HG3	1.75	0.68
1:E:187:GLY:N	1:G:43:LYS:CE	2.57	0.67
1:B:185:LEU:HG	1:D:43:LYS:HG3	1.77	0.67
1:E:274:THR:HA	1:G:240:ASN:OD1	1.94	0.67
1:G:151:PRO:CD	1:I:40:PHE:HZ	2.02	0.67
1:H:187:GLY:N	1:J:43:LYS:CE	2.57	0.67
1:B:111:ASN:HA	1:D:36:TRP:O	1.95	0.67
1:F:187:GLY:N	1:H:43:LYS:CE	2.57	0.67
1:E:108:TYR:CD1	1:G:38:VAL:CG1	2.76	0.67
1:E:108:TYR:OH	1:G:40:PHE:CD1	2.46	0.67
1:G:187:GLY:N	1:I:43:LYS:CE	2.57	0.67
1:A:188:ILE:HD11	1:C:40:PHE:HB3	1.74	0.67
1:B:185:LEU:C	1:D:43:LYS:HG2	2.19	0.67
1:C:185:LEU:HA	1:E:43:LYS:CE	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:LEU:C	1:G:43:LYS:HG2	2.18	0.67
1:H:185:LEU:HG	1:J:43:LYS:HG3	1.75	0.67
1:A:151:PRO:CD	1:C:40:PHE:HZ	2.04	0.67
1:B:187:GLY:N	1:D:43:LYS:CE	2.57	0.67
1:G:185:LEU:HA	1:I:43:LYS:CE	2.24	0.67
1:B:185:LEU:HD21	1:D:41:GLY:HA3	1.75	0.67
1:B:274:THR:HA	1:D:240:ASN:OD1	1.94	0.67
1:D:112:ASN:HD22	1:F:38:VAL:H	1.42	0.67
1:D:187:GLY:N	1:F:43:LYS:CE	2.57	0.67
1:D:274:THR:HA	1:F:240:ASN:OD1	1.95	0.67
1:H:108:TYR:OH	1:J:40:PHE:CD1	2.47	0.67
1:A:111:ASN:HA	1:C:36:TRP:O	1.95	0.67
1:D:108:TYR:OH	1:F:40:PHE:CD1	2.47	0.67
1:F:111:ASN:HA	1:H:36:TRP:O	1.95	0.67
1:F:274:THR:HA	1:H:240:ASN:OD1	1.95	0.67
1:H:111:ASN:HA	1:J:36:TRP:O	1.95	0.67
1:H:112:ASN:HD22	1:J:38:VAL:H	1.43	0.67
1:D:111:ASN:ND2	1:F:36:TRP:CD2	2.63	0.67
1:E:111:ASN:HA	1:G:36:TRP:O	1.95	0.67
1:B:112:ASN:HD22	1:D:38:VAL:H	1.43	0.66
1:E:151:PRO:CD	1:G:40:PHE:HZ	2.03	0.66
1:G:188:ILE:HD11	1:I:40:PHE:HB3	1.74	0.66
1:C:274:THR:HA	1:E:240:ASN:OD1	1.95	0.66
1:F:112:ASN:HD22	1:H:38:VAL:H	1.43	0.66
1:A:111:ASN:ND2	1:C:36:TRP:CD2	2.63	0.66
1:D:185:LEU:HA	1:F:43:LYS:CE	2.24	0.66
1:F:185:LEU:HA	1:H:43:LYS:CE	2.24	0.66
1:H:295:GLN:HB2	1:J:214:ARG:CD	2.23	0.66
1:B:111:ASN:ND2	1:D:36:TRP:CD2	2.62	0.66
1:H:187:GLY:H	1:J:43:LYS:CE	2.09	0.66
1:F:187:GLY:H	1:H:43:LYS:CE	2.09	0.66
1:A:187:GLY:C	1:C:43:LYS:CD	2.65	0.66
1:C:188:ILE:HD11	1:E:40:PHE:HB3	1.74	0.66
1:E:112:ASN:HD22	1:G:38:VAL:H	1.43	0.66
1:C:112:ASN:HD22	1:E:38:VAL:H	1.43	0.66
1:D:111:ASN:HA	1:F:36:TRP:O	1.95	0.66
1:D:187:GLY:H	1:F:43:LYS:CE	2.09	0.66
1:E:188:ILE:HD11	1:G:40:PHE:HB3	1.73	0.66
1:G:112:ASN:HD22	1:I:38:VAL:H	1.43	0.66
1:A:112:ASN:HD22	1:C:38:VAL:H	1.44	0.66
1:H:274:THR:HA	1:J:240:ASN:OD1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLY:H	1:C:43:LYS:CE	2.09	0.66
1:E:187:GLY:CA	1:G:43:LYS:CD	2.64	0.66
1:G:108:TYR:OH	1:I:40:PHE:CD1	2.47	0.66
1:B:187:GLY:H	1:D:43:LYS:CE	2.09	0.65
1:C:187:GLY:H	1:E:43:LYS:CE	2.09	0.65
1:G:274:THR:HA	1:I:240:ASN:OD1	1.96	0.65
1:B:150:ILE:CD1	1:D:40:PHE:CD2	2.80	0.65
1:G:111:ASN:HA	1:I:36:TRP:O	1.96	0.65
1:E:187:GLY:H	1:G:43:LYS:CE	2.09	0.65
1:B:271:SER:CB	1:D:216:LYS:HD3	2.27	0.65
1:C:111:ASN:HA	1:E:36:TRP:O	1.96	0.65
1:H:111:ASN:ND2	1:J:36:TRP:CD2	2.63	0.65
1:C:150:ILE:CD1	1:E:40:PHE:CD2	2.80	0.65
1:B:295:GLN:HB2	1:D:214:ARG:CD	2.24	0.65
1:G:295:GLN:HB2	1:I:214:ARG:CD	2.24	0.65
1:A:274:THR:HA	1:C:240:ASN:OD1	1.95	0.65
1:B:185:LEU:HA	1:D:43:LYS:CE	2.26	0.65
1:C:295:GLN:HB2	1:E:214:ARG:CD	2.24	0.65
1:G:187:GLY:H	1:I:43:LYS:CE	2.09	0.65
1:H:151:PRO:CD	1:J:40:PHE:HZ	2.03	0.65
1:E:185:LEU:HA	1:G:43:LYS:CE	2.25	0.65
1:F:185:LEU:C	1:H:43:LYS:CG	2.69	0.65
1:C:112:ASN:O	1:E:38:VAL:HA	1.15	0.65
1:D:5:ILE:HG12	1:D:14:LEU:CD2	2.27	0.65
1:D:271:SER:CB	1:F:216:LYS:HD3	2.27	0.65
1:E:150:ILE:CD1	1:G:40:PHE:CD2	2.79	0.65
1:F:271:SER:CB	1:H:216:LYS:HD3	2.27	0.65
1:G:150:ILE:CD1	1:I:40:PHE:CD2	2.80	0.64
1:B:5:ILE:HG12	1:B:14:LEU:CD2	2.28	0.64
1:C:151:PRO:HD3	1:E:40:PHE:CE2	2.32	0.64
1:F:5:ILE:HG12	1:F:14:LEU:CD2	2.27	0.64
1:H:271:SER:CB	1:J:216:LYS:HD3	2.28	0.64
1:A:295:GLN:HB2	1:C:214:ARG:CD	2.23	0.64
1:C:185:LEU:C	1:E:43:LYS:CG	2.70	0.64
1:D:188:ILE:HD11	1:F:40:PHE:HB3	1.73	0.64
1:E:151:PRO:HD3	1:G:40:PHE:CE2	2.32	0.64
1:F:150:ILE:CD1	1:H:40:PHE:CD2	2.80	0.64
1:A:151:PRO:HD3	1:C:40:PHE:CE2	2.33	0.64
1:G:151:PRO:HD3	1:I:40:PHE:CE2	2.33	0.64
1:H:150:ILE:CD1	1:J:40:PHE:CD2	2.80	0.64
1:B:151:PRO:HD3	1:D:40:PHE:CE2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:PRO:HD3	1:F:40:PHE:CE2	2.32	0.64
1:I:5:ILE:HG12	1:I:14:LEU:CD2	2.28	0.64
1:A:150:ILE:CD1	1:C:40:PHE:CD2	2.81	0.64
1:G:5:ILE:HG12	1:G:14:LEU:CD2	2.28	0.64
1:H:5:ILE:HG12	1:H:14:LEU:CD2	2.27	0.64
1:E:5:ILE:HG12	1:E:14:LEU:CD2	2.28	0.64
1:G:111:ASN:ND2	1:I:36:TRP:CD2	2.63	0.64
1:G:112:ASN:O	1:I:38:VAL:HA	1.14	0.64
1:B:108:TYR:OH	1:D:40:PHE:HD1	1.80	0.63
1:H:151:PRO:HD3	1:J:40:PHE:CE2	2.32	0.63
1:C:5:ILE:HG12	1:C:14:LEU:CD2	2.28	0.63
1:A:5:ILE:HG12	1:A:14:LEU:CD2	2.28	0.63
1:F:151:PRO:HD3	1:H:40:PHE:CE2	2.32	0.63
1:A:186:SER:N	1:C:43:LYS:HE2	2.14	0.63
1:D:150:ILE:CD1	1:F:40:PHE:CD2	2.79	0.63
1:D:295:GLN:HB2	1:F:214:ARG:CD	2.24	0.63
1:E:111:ASN:ND2	1:G:36:TRP:CD2	2.63	0.63
1:J:5:ILE:HG12	1:J:14:LEU:CD2	2.28	0.63
1:A:271:SER:CB	1:C:216:LYS:HD3	2.27	0.63
1:E:271:SER:CB	1:G:216:LYS:HD3	2.27	0.63
1:F:111:ASN:ND2	1:H:36:TRP:CD2	2.63	0.63
1:H:185:LEU:C	1:J:43:LYS:CG	2.69	0.63
1:D:108:TYR:OH	1:F:40:PHE:HD1	1.81	0.63
1:E:185:LEU:C	1:G:43:LYS:CG	2.70	0.63
1:F:274:THR:HA	1:H:240:ASN:HD21	1.64	0.63
1:B:272:GLY:N	1:D:216:LYS:HB2	2.14	0.62
1:G:271:SER:CB	1:I:216:LYS:HD3	2.28	0.62
1:H:186:SER:N	1:J:43:LYS:HE2	2.14	0.62
1:E:186:SER:C	1:G:43:LYS:HG2	2.24	0.62
1:C:186:SER:C	1:E:43:LYS:HG2	2.25	0.62
1:F:108:TYR:OH	1:H:40:PHE:HD1	1.81	0.62
1:F:186:SER:N	1:H:43:LYS:HE2	2.14	0.62
1:F:272:GLY:N	1:H:216:LYS:HB2	2.14	0.62
1:G:108:TYR:OH	1:I:40:PHE:HD1	1.82	0.62
1:A:108:TYR:OH	1:C:40:PHE:HD1	1.82	0.62
1:A:272:GLY:N	1:C:216:LYS:HB2	2.14	0.62
1:C:111:ASN:ND2	1:E:36:TRP:CD2	2.63	0.62
1:E:108:TYR:OH	1:G:40:PHE:HD1	1.81	0.62
1:G:150:ILE:C	1:I:40:PHE:HE2	2.08	0.62
1:D:274:THR:HA	1:F:240:ASN:HD21	1.65	0.62
1:F:295:GLN:HB2	1:H:214:ARG:CD	2.23	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:SER:C	1:I:43:LYS:HG2	2.25	0.62
1:A:274:THR:HA	1:C:240:ASN:HD21	1.63	0.62
1:D:186:SER:C	1:F:43:LYS:HG2	2.24	0.62
1:D:272:GLY:N	1:F:216:LYS:HB2	2.15	0.62
1:G:272:GLY:N	1:I:216:LYS:HB2	2.15	0.62
1:H:108:TYR:OH	1:J:40:PHE:HD1	1.82	0.62
1:A:186:SER:C	1:C:43:LYS:HG2	2.25	0.62
1:B:186:SER:C	1:D:43:LYS:HG2	2.25	0.62
1:B:274:THR:HA	1:D:240:ASN:HD21	1.64	0.62
1:C:108:TYR:OH	1:E:40:PHE:HD1	1.81	0.62
1:E:272:GLY:N	1:G:216:LYS:HB2	2.15	0.62
1:C:186:SER:N	1:E:43:LYS:HE2	2.15	0.62
1:C:274:THR:HA	1:E:240:ASN:HD21	1.65	0.62
1:E:274:THR:HA	1:G:240:ASN:HD21	1.65	0.62
1:G:185:LEU:C	1:I:43:LYS:CG	2.69	0.61
1:B:185:LEU:C	1:D:43:LYS:CG	2.71	0.61
1:C:271:SER:CB	1:E:216:LYS:HD3	2.28	0.61
1:D:186:SER:N	1:F:43:LYS:HE2	2.15	0.61
1:H:272:GLY:N	1:J:216:LYS:HB2	2.15	0.61
1:C:272:GLY:N	1:E:216:LYS:HB2	2.15	0.61
1:F:186:SER:C	1:H:43:LYS:HG2	2.25	0.61
1:G:186:SER:N	1:I:43:LYS:HE2	2.14	0.61
1:A:185:LEU:CA	1:C:43:LYS:CE	2.78	0.61
1:A:185:LEU:C	1:C:43:LYS:CG	2.70	0.61
1:E:150:ILE:C	1:G:40:PHE:HE2	2.09	0.61
1:E:186:SER:N	1:G:43:LYS:HE2	2.15	0.61
1:G:272:GLY:CA	1:I:216:LYS:C	2.72	0.61
1:H:274:THR:HA	1:J:240:ASN:HD21	1.64	0.61
1:C:150:ILE:C	1:E:40:PHE:HE2	2.09	0.61
1:H:185:LEU:CA	1:J:43:LYS:CE	2.78	0.61
1:H:186:SER:C	1:J:43:LYS:HG2	2.25	0.61
1:B:186:SER:N	1:D:43:LYS:HE2	2.15	0.61
1:D:185:LEU:CA	1:F:43:LYS:CE	2.79	0.61
1:E:150:ILE:HD13	1:G:40:PHE:CD2	2.36	0.61
1:F:185:LEU:CA	1:H:43:LYS:CE	2.79	0.61
1:B:271:SER:HB2	1:D:216:LYS:HD3	1.83	0.60
1:G:274:THR:HA	1:I:240:ASN:HD21	1.64	0.60
1:E:185:LEU:CA	1:G:43:LYS:CE	2.80	0.60
1:D:150:ILE:C	1:F:40:PHE:HE2	2.08	0.60
1:E:112:ASN:O	1:G:38:VAL:HA	1.15	0.60
1:B:150:ILE:HD13	1:D:40:PHE:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:SER:HB2	1:H:216:LYS:HD3	1.84	0.60
1:H:150:ILE:C	1:J:40:PHE:HE2	2.08	0.60
1:C:150:ILE:HD13	1:E:40:PHE:CD2	2.37	0.60
1:D:271:SER:HB2	1:F:216:LYS:HD3	1.84	0.60
1:E:271:SER:HB2	1:G:216:LYS:CD	2.32	0.60
1:H:185:LEU:CD1	1:J:43:LYS:HE3	2.28	0.60
1:D:185:LEU:C	1:F:43:LYS:CG	2.69	0.60
1:F:150:ILE:C	1:H:40:PHE:HE2	2.09	0.60
1:H:271:SER:HB2	1:J:216:LYS:HD3	1.84	0.60
1:A:150:ILE:C	1:C:40:PHE:HE2	2.09	0.60
1:F:185:LEU:CD1	1:H:43:LYS:HE3	2.28	0.59
1:G:150:ILE:HD13	1:I:40:PHE:CD2	2.37	0.59
1:H:150:ILE:HD13	1:J:40:PHE:CD2	2.37	0.59
1:A:271:SER:HB2	1:C:216:LYS:CD	2.32	0.59
1:A:271:SER:HB2	1:C:216:LYS:HD3	1.84	0.59
1:B:185:LEU:CD1	1:D:43:LYS:HE3	2.28	0.59
1:D:185:LEU:CD1	1:F:43:LYS:HE3	2.28	0.59
1:E:295:GLN:HB2	1:G:214:ARG:CD	2.24	0.59
1:F:150:ILE:HD13	1:H:40:PHE:CD2	2.37	0.59
1:H:271:SER:HB2	1:J:216:LYS:CD	2.32	0.59
1:C:271:SER:HB2	1:E:216:LYS:CD	2.32	0.59
1:C:271:SER:HB2	1:E:216:LYS:HD3	1.84	0.59
1:D:150:ILE:HD13	1:F:40:PHE:CD2	2.36	0.59
1:B:150:ILE:C	1:D:40:PHE:HE2	2.10	0.59
1:B:271:SER:HB2	1:D:216:LYS:CD	2.32	0.59
1:B:274:THR:HA	1:D:240:ASN:ND2	2.18	0.59
1:G:271:SER:HB2	1:I:216:LYS:CD	2.32	0.59
1:G:271:SER:HB2	1:I:216:LYS:HD3	1.84	0.59
1:A:274:THR:HA	1:C:240:ASN:ND2	2.18	0.58
1:F:125:ASN:OD1	1:F:128:LYS:NZ	2.32	0.58
1:H:233:ASN:O	1:H:237:GLN:HG2	2.04	0.58
1:F:233:ASN:O	1:F:237:GLN:HG2	2.04	0.58
1:J:233:ASN:O	1:J:237:GLN:HG2	2.03	0.58
1:G:233:ASN:O	1:G:237:GLN:HG2	2.04	0.58
1:D:233:ASN:O	1:D:237:GLN:HG2	2.03	0.58
1:D:271:SER:HB2	1:F:216:LYS:CD	2.32	0.58
1:A:150:ILE:HD13	1:C:40:PHE:CD2	2.38	0.58
1:G:185:LEU:CA	1:I:43:LYS:CE	2.78	0.58
1:C:233:ASN:O	1:C:237:GLN:HG2	2.04	0.58
1:F:274:THR:HA	1:H:240:ASN:ND2	2.19	0.58
1:B:233:ASN:O	1:B:237:GLN:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:SER:HB2	1:G:216:LYS:HD3	1.84	0.57
1:F:271:SER:HB2	1:H:216:LYS:CD	2.32	0.57
1:H:274:THR:HA	1:J:240:ASN:ND2	2.19	0.57
1:A:233:ASN:O	1:A:237:GLN:HG2	2.04	0.57
1:E:233:ASN:O	1:E:237:GLN:HG2	2.04	0.57
1:D:272:GLY:CA	1:F:216:LYS:C	2.72	0.57
1:G:274:THR:HA	1:I:240:ASN:ND2	2.20	0.57
1:I:233:ASN:O	1:I:237:GLN:HG2	2.04	0.57
1:E:274:THR:HA	1:G:240:ASN:ND2	2.20	0.57
1:C:274:THR:HA	1:E:240:ASN:ND2	2.20	0.57
1:D:188:ILE:HD11	1:F:40:PHE:CA	2.35	0.56
1:G:295:GLN:HB2	1:I:214:ARG:HD3	1.87	0.56
1:D:112:ASN:ND2	1:F:38:VAL:H	2.02	0.56
1:E:112:ASN:ND2	1:G:38:VAL:H	2.02	0.56
1:F:188:ILE:HD11	1:H:40:PHE:CA	2.36	0.56
1:H:188:ILE:HD11	1:J:40:PHE:CA	2.36	0.56
1:A:185:LEU:C	1:C:43:LYS:HE3	2.30	0.56
1:D:274:THR:HA	1:F:240:ASN:ND2	2.20	0.56
1:F:295:GLN:HB2	1:H:214:ARG:HD3	1.87	0.56
1:H:185:LEU:C	1:J:43:LYS:HE3	2.31	0.56
1:A:112:ASN:ND2	1:C:38:VAL:H	2.03	0.56
1:C:151:PRO:CG	1:E:40:PHE:CZ	2.82	0.56
1:E:272:GLY:CA	1:G:216:LYS:C	2.72	0.56
1:A:272:GLY:CA	1:C:216:LYS:C	2.72	0.56
1:B:188:ILE:HD11	1:D:40:PHE:CA	2.35	0.56
1:D:295:GLN:HB2	1:F:214:ARG:HD3	1.88	0.55
1:G:112:ASN:ND2	1:I:38:VAL:H	2.02	0.55
1:H:295:GLN:HB2	1:J:214:ARG:HD3	1.87	0.55
1:D:150:ILE:CD1	1:F:40:PHE:CG	2.89	0.55
1:E:188:ILE:HD11	1:G:40:PHE:CA	2.35	0.55
1:B:185:LEU:C	1:D:43:LYS:HE3	2.32	0.55
1:B:295:GLN:HB2	1:D:214:ARG:HD3	1.89	0.55
1:F:108:TYR:CE1	1:H:39:SER:O	2.60	0.55
1:H:182:MET:CG	1:J:60:ILE:HD13	2.36	0.55
1:A:125:ASN:OD1	1:A:128:LYS:NZ	2.32	0.55
1:B:185:LEU:CA	1:D:43:LYS:CE	2.80	0.55
1:B:108:TYR:CE1	1:D:39:SER:O	2.59	0.55
1:B:272:GLY:CA	1:D:216:LYS:C	2.72	0.55
1:F:150:ILE:CD1	1:H:40:PHE:CG	2.90	0.55
1:C:295:GLN:HB2	1:E:214:ARG:HD3	1.88	0.55
1:H:108:TYR:CE1	1:J:39:SER:O	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:GLN:HB2	1:G:214:ARG:HD3	1.89	0.55
1:A:182:MET:CG	1:C:60:ILE:HD13	2.35	0.55
1:B:150:ILE:CD1	1:D:40:PHE:CG	2.90	0.55
1:F:112:ASN:ND2	1:H:38:VAL:H	2.02	0.55
1:G:182:MET:CG	1:I:60:ILE:HD13	2.37	0.55
1:G:185:LEU:HD12	1:I:43:LYS:CE	2.28	0.55
1:A:108:TYR:CG	1:C:38:VAL:CG1	2.90	0.55
1:A:295:GLN:HB2	1:C:214:ARG:HD3	1.87	0.55
1:B:108:TYR:CG	1:D:38:VAL:CG1	2.90	0.55
1:C:108:TYR:CG	1:E:38:VAL:CG1	2.90	0.55
1:E:108:TYR:CE1	1:G:39:SER:O	2.59	0.55
1:E:150:ILE:CD1	1:G:40:PHE:CG	2.90	0.55
1:F:272:GLY:CA	1:H:216:LYS:C	2.72	0.55
1:G:188:ILE:HD11	1:I:40:PHE:CA	2.36	0.55
1:F:185:LEU:C	1:H:43:LYS:HE3	2.31	0.55
1:H:150:ILE:CD1	1:J:40:PHE:CG	2.90	0.55
1:A:258:LYS:CE	1:B:53:GLU:OE1	2.55	0.54
1:C:150:ILE:HD13	1:E:40:PHE:CG	2.43	0.54
1:C:258:LYS:CE	1:D:53:GLU:OE1	2.55	0.54
1:E:108:TYR:CG	1:G:38:VAL:CG1	2.90	0.54
1:H:108:TYR:CG	1:J:38:VAL:CG1	2.90	0.54
1:H:272:GLY:CA	1:J:216:LYS:C	2.72	0.54
1:C:185:LEU:CA	1:E:43:LYS:CE	2.79	0.54
1:C:272:GLY:CA	1:E:216:LYS:C	2.72	0.54
1:D:108:TYR:CE1	1:F:39:SER:O	2.59	0.54
1:D:150:ILE:HD13	1:F:40:PHE:CG	2.42	0.54
1:E:258:LYS:CE	1:F:53:GLU:OE1	2.55	0.54
1:B:150:ILE:HD13	1:D:40:PHE:CG	2.43	0.54
1:C:108:TYR:CE1	1:E:39:SER:O	2.60	0.54
1:E:150:ILE:HD13	1:G:40:PHE:CG	2.42	0.54
1:G:108:TYR:CE1	1:I:39:SER:O	2.60	0.54
1:A:108:TYR:CE1	1:C:39:SER:O	2.60	0.54
1:G:150:ILE:CD1	1:I:40:PHE:CG	2.90	0.54
1:H:112:ASN:ND2	1:J:38:VAL:H	2.02	0.54
1:H:150:ILE:HD13	1:J:40:PHE:CG	2.43	0.54
1:C:185:LEU:O	1:C:185:LEU:HG	2.08	0.54
1:F:108:TYR:CG	1:H:38:VAL:CG1	2.90	0.54
1:G:108:TYR:CG	1:I:38:VAL:CG1	2.90	0.54
1:G:258:LYS:CE	1:H:53:GLU:OE1	2.55	0.54
1:C:188:ILE:HD11	1:E:40:PHE:CA	2.35	0.54
1:E:185:LEU:O	1:E:185:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:ILE:HD13	1:H:40:PHE:CG	2.43	0.54
1:B:182:MET:CG	1:D:60:ILE:HD13	2.36	0.54
1:A:185:LEU:O	1:A:185:LEU:HG	2.08	0.54
1:D:258:LYS:CE	1:E:53:GLU:OE1	2.55	0.54
1:E:150:ILE:HD13	1:G:40:PHE:CB	2.38	0.54
1:G:150:ILE:HD13	1:I:40:PHE:CG	2.43	0.54
1:B:188:ILE:CD1	1:D:40:PHE:CB	2.75	0.54
1:E:182:MET:CG	1:G:60:ILE:HD13	2.37	0.54
1:E:185:LEU:HD12	1:G:43:LYS:CE	2.29	0.54
1:F:258:LYS:CE	1:G:53:GLU:OE1	2.55	0.54
1:G:185:LEU:O	1:G:185:LEU:HG	2.08	0.54
1:G:185:LEU:CD1	1:I:43:LYS:HE3	2.28	0.54
1:B:274:THR:HA	1:D:240:ASN:CG	2.33	0.53
1:C:150:ILE:CD1	1:E:40:PHE:CG	2.90	0.53
1:D:108:TYR:CG	1:F:38:VAL:CG1	2.90	0.53
1:E:185:LEU:CD1	1:G:43:LYS:HE3	2.28	0.53
1:G:150:ILE:HD13	1:I:40:PHE:CB	2.38	0.53
1:H:258:LYS:CE	1:I:53:GLU:OE1	2.55	0.53
1:I:185:LEU:HG	1:I:185:LEU:O	2.08	0.53
1:I:258:LYS:CE	1:J:53:GLU:OE1	2.55	0.53
1:A:150:ILE:CD1	1:C:40:PHE:CG	2.91	0.53
1:B:185:LEU:HD12	1:D:43:LYS:CE	2.29	0.53
1:J:185:LEU:O	1:J:185:LEU:HG	2.08	0.53
1:B:257:ARG:HH22	1:C:52:GLY:C	2.16	0.53
1:C:150:ILE:HD13	1:E:40:PHE:CB	2.38	0.53
1:D:150:ILE:HD13	1:F:40:PHE:CB	2.38	0.53
1:H:150:ILE:HD13	1:J:40:PHE:CB	2.38	0.53
1:B:258:LYS:CE	1:C:53:GLU:OE1	2.55	0.53
1:C:151:PRO:CD	1:E:40:PHE:CE2	2.92	0.53
1:D:125:ASN:OD1	1:D:128:LYS:NZ	2.32	0.53
1:F:151:PRO:CD	1:H:40:PHE:CE2	2.92	0.53
1:F:182:MET:CG	1:H:60:ILE:HD13	2.36	0.53
1:G:151:PRO:CD	1:I:40:PHE:CE2	2.91	0.53
1:A:188:ILE:CD1	1:C:40:PHE:CB	2.76	0.53
1:F:272:GLY:N	1:H:216:LYS:O	2.40	0.53
1:H:185:LEU:O	1:H:185:LEU:HG	2.08	0.53
1:F:185:LEU:O	1:F:185:LEU:HG	2.08	0.53
1:A:150:ILE:HD13	1:C:40:PHE:CG	2.44	0.53
1:C:272:GLY:N	1:E:216:LYS:O	2.40	0.53
1:D:181:VAL:HG12	1:F:43:LYS:NZ	1.97	0.53
1:F:150:ILE:HD13	1:H:40:PHE:CB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:151:PRO:CG	1:I:40:PHE:CZ	2.82	0.53
1:J:125:ASN:OD1	1:J:128:LYS:NZ	2.32	0.53
1:B:272:GLY:HA2	1:D:216:LYS:N	2.24	0.53
1:B:150:ILE:HD13	1:D:40:PHE:CB	2.39	0.53
1:B:185:LEU:O	1:B:185:LEU:HG	2.08	0.53
1:D:185:LEU:O	1:D:185:LEU:HG	2.08	0.53
1:A:188:ILE:HD11	1:C:40:PHE:CA	2.37	0.52
1:E:257:ARG:HH22	1:F:52:GLY:C	2.15	0.52
1:A:274:THR:HA	1:C:240:ASN:CG	2.34	0.52
1:C:125:ASN:OD1	1:C:128:LYS:NZ	2.32	0.52
1:C:188:ILE:CD1	1:E:40:PHE:N	2.72	0.52
1:D:182:MET:CG	1:F:60:ILE:HD13	2.37	0.52
1:D:185:LEU:HD12	1:F:43:LYS:CE	2.28	0.52
1:E:188:ILE:CD1	1:G:40:PHE:N	2.72	0.52
1:G:257:ARG:HH22	1:H:52:GLY:C	2.16	0.52
1:H:274:THR:HA	1:J:240:ASN:CG	2.35	0.52
1:B:5:ILE:O	1:B:100:CYS:HA	2.10	0.52
1:C:185:LEU:CD1	1:E:43:LYS:HE3	2.28	0.52
1:E:272:GLY:HA2	1:G:216:LYS:N	2.25	0.52
1:F:5:ILE:O	1:F:100:CYS:HA	2.10	0.52
1:F:181:VAL:HG12	1:H:43:LYS:NZ	1.98	0.52
1:F:272:GLY:HA2	1:H:216:LYS:N	2.25	0.52
1:G:272:GLY:N	1:I:216:LYS:O	2.40	0.52
1:I:5:ILE:O	1:I:100:CYS:HA	2.10	0.52
1:B:181:VAL:HG12	1:D:43:LYS:NZ	1.99	0.52
1:C:274:THR:HA	1:E:240:ASN:CG	2.35	0.52
1:F:274:THR:HA	1:H:240:ASN:CG	2.35	0.52
1:G:5:ILE:O	1:G:100:CYS:HA	2.10	0.52
1:G:272:GLY:HA2	1:I:216:LYS:N	2.25	0.52
1:A:150:ILE:HD13	1:C:40:PHE:CB	2.39	0.52
1:A:151:PRO:CD	1:C:40:PHE:CE2	2.92	0.52
1:A:272:GLY:HA2	1:C:216:LYS:N	2.24	0.52
1:D:272:GLY:HA2	1:F:216:LYS:N	2.25	0.52
1:G:185:LEU:C	1:I:43:LYS:HE3	2.31	0.52
1:H:5:ILE:O	1:H:100:CYS:HA	2.10	0.52
1:H:151:PRO:CD	1:J:40:PHE:CE2	2.91	0.52
1:I:257:ARG:HH22	1:J:52:GLY:C	2.16	0.52
1:D:5:ILE:O	1:D:100:CYS:HA	2.10	0.52
1:H:272:GLY:HA2	1:J:216:LYS:N	2.25	0.52
1:J:5:ILE:O	1:J:100:CYS:HA	2.10	0.52
1:C:257:ARG:HH22	1:D:52:GLY:C	2.15	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ILE:CD1	1:F:40:PHE:N	2.72	0.52
1:G:188:ILE:CD1	1:I:40:PHE:N	2.73	0.52
1:C:185:LEU:HD12	1:E:43:LYS:CE	2.28	0.52
1:D:274:THR:HA	1:F:240:ASN:CG	2.35	0.52
1:E:5:ILE:O	1:E:100:CYS:HA	2.10	0.52
1:E:271:SER:CB	1:G:216:LYS:HD2	2.40	0.52
1:E:274:THR:HA	1:G:240:ASN:CG	2.34	0.52
1:E:297:ARG:NH1	1:E:299:GLU:OE1	2.43	0.52
1:H:125:ASN:OD1	1:H:128:LYS:NZ	2.32	0.52
1:B:151:PRO:CD	1:D:40:PHE:CE2	2.92	0.51
1:A:297:ARG:NH1	1:A:299:GLU:OE1	2.43	0.51
1:B:188:ILE:CD1	1:D:40:PHE:N	2.73	0.51
1:C:271:SER:CB	1:E:216:LYS:HD2	2.40	0.51
1:H:181:VAL:HG12	1:J:43:LYS:NZ	1.98	0.51
1:F:297:ARG:NH1	1:F:299:GLU:OE1	2.43	0.51
1:H:297:ARG:NH1	1:H:299:GLU:OE1	2.43	0.51
1:F:165:SER:OG	1:F:273:TYR:HA	2.11	0.51
1:A:188:ILE:CD1	1:C:40:PHE:N	2.74	0.51
1:G:274:THR:HA	1:I:240:ASN:CG	2.35	0.51
1:D:151:PRO:CD	1:F:40:PHE:CE2	2.91	0.51
1:C:5:ILE:O	1:C:100:CYS:HA	2.10	0.51
1:C:272:GLY:HA2	1:E:216:LYS:N	2.25	0.51
1:J:297:ARG:NH1	1:J:299:GLU:OE1	2.43	0.51
1:A:5:ILE:O	1:A:100:CYS:HA	2.10	0.51
1:B:272:GLY:N	1:D:216:LYS:O	2.40	0.51
1:D:297:ARG:NH1	1:D:299:GLU:OE1	2.43	0.51
1:F:188:ILE:CD1	1:H:40:PHE:N	2.73	0.51
1:F:271:SER:CB	1:H:216:LYS:HD2	2.40	0.51
1:I:297:ARG:NH1	1:I:299:GLU:OE1	2.43	0.51
1:C:182:MET:CG	1:E:60:ILE:HD13	2.37	0.51
1:D:165:SER:OG	1:D:273:TYR:HA	2.11	0.51
1:H:165:SER:OG	1:H:273:TYR:HA	2.11	0.51
1:J:165:SER:OG	1:J:273:TYR:HA	2.11	0.51
1:B:165:SER:OG	1:B:273:TYR:HA	2.11	0.51
1:D:271:SER:CB	1:F:216:LYS:HD2	2.40	0.51
1:E:151:PRO:CD	1:G:40:PHE:CE2	2.92	0.51
1:I:125:ASN:OD1	1:I:128:LYS:NZ	2.32	0.51
1:A:271:SER:CB	1:C:216:LYS:HD2	2.40	0.50
1:A:272:GLY:N	1:C:216:LYS:O	2.40	0.50
1:B:125:ASN:OD1	1:B:128:LYS:NZ	2.32	0.50
1:B:297:ARG:NH1	1:B:299:GLU:OE1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:GLY:HA2	1:E:216:LYS:C	2.36	0.50
1:A:185:LEU:HD12	1:C:43:LYS:CE	2.28	0.50
1:H:188:ILE:CD1	1:J:40:PHE:N	2.73	0.50
1:H:257:ARG:HH22	1:I:52:GLY:C	2.17	0.50
1:H:271:SER:CB	1:J:216:LYS:HD2	2.40	0.50
1:A:185:LEU:CD1	1:C:43:LYS:HE3	2.27	0.50
1:B:182:MET:HE3	1:D:59:PRO:HG2	1.94	0.50
1:E:165:SER:OG	1:E:273:TYR:HA	2.11	0.50
1:G:297:ARG:NH1	1:G:299:GLU:OE1	2.43	0.50
1:C:297:ARG:NH1	1:C:299:GLU:OE1	2.43	0.50
1:D:151:PRO:CG	1:F:40:PHE:CZ	2.82	0.50
1:F:185:LEU:HD12	1:H:43:LYS:CE	2.28	0.50
1:G:271:SER:CB	1:I:216:LYS:HD2	2.41	0.50
1:B:271:SER:CB	1:D:216:LYS:HD2	2.40	0.50
1:E:182:MET:HE3	1:G:59:PRO:HG2	1.94	0.50
1:F:182:MET:HE3	1:H:59:PRO:HG2	1.94	0.50
1:F:239:ILE:HD13	1:F:248:VAL:HG21	1.94	0.50
1:G:125:ASN:OD1	1:G:128:LYS:NZ	2.32	0.50
1:G:165:SER:OG	1:G:273:TYR:HA	2.11	0.50
1:H:5:ILE:HD12	1:H:98:ILE:HB	1.94	0.50
1:I:165:SER:OG	1:I:273:TYR:HA	2.11	0.50
1:F:257:ARG:HH22	1:G:52:GLY:C	2.17	0.50
1:H:182:MET:HE3	1:J:59:PRO:HG2	1.94	0.50
1:A:182:MET:HE3	1:C:59:PRO:HG2	1.94	0.50
1:B:272:GLY:HA2	1:D:216:LYS:C	2.36	0.50
1:E:111:ASN:O	1:G:37:ALA:CA	2.58	0.50
1:E:272:GLY:HA2	1:G:216:LYS:C	2.37	0.50
1:F:111:ASN:O	1:H:37:ALA:CA	2.58	0.50
1:A:239:ILE:HD13	1:A:248:VAL:HG21	1.94	0.49
1:B:108:TYR:CG	1:D:38:VAL:HG11	2.47	0.49
1:C:182:MET:HE3	1:E:59:PRO:HG2	1.94	0.49
1:J:5:ILE:HD12	1:J:98:ILE:HB	1.94	0.49
1:C:165:SER:OG	1:C:273:TYR:HA	2.11	0.49
1:H:185:LEU:HD12	1:J:43:LYS:CE	2.28	0.49
1:J:239:ILE:HD13	1:J:248:VAL:HG21	1.94	0.49
1:D:272:GLY:HA2	1:F:216:LYS:C	2.36	0.49
1:F:5:ILE:HD12	1:F:98:ILE:HB	1.94	0.49
1:H:239:ILE:HD13	1:H:248:VAL:HG21	1.94	0.49
1:B:5:ILE:HD12	1:B:98:ILE:HB	1.94	0.49
1:C:188:ILE:CD1	1:E:40:PHE:CB	2.75	0.49
1:D:182:MET:HE3	1:F:59:PRO:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ILE:HB	1:F:38:VAL:O	2.13	0.49
1:E:108:TYR:HE1	1:G:39:SER:O	1.95	0.49
1:E:239:ILE:HD13	1:E:248:VAL:HG21	1.94	0.49
1:G:182:MET:HE3	1:I:59:PRO:HG2	1.94	0.49
1:H:189:SER:HG	1:J:60:ILE:CD1	1.96	0.49
1:H:272:GLY:N	1:J:216:LYS:O	2.40	0.49
1:F:108:TYR:CG	1:H:38:VAL:HG11	2.48	0.49
1:G:272:GLY:HA2	1:I:216:LYS:C	2.36	0.49
1:I:5:ILE:HD12	1:I:98:ILE:HB	1.94	0.49
1:A:257:ARG:HH22	1:B:52:GLY:C	2.17	0.49
1:B:108:TYR:HE1	1:D:39:SER:O	1.95	0.49
1:F:188:ILE:HB	1:H:38:VAL:O	2.13	0.49
1:E:185:LEU:C	1:G:43:LYS:HE3	2.32	0.49
1:G:151:PRO:N	1:I:40:PHE:HE2	2.11	0.49
1:A:165:SER:OG	1:A:273:TYR:HA	2.11	0.49
1:B:151:PRO:CG	1:D:40:PHE:CZ	2.83	0.49
1:F:272:GLY:HA2	1:H:216:LYS:C	2.36	0.49
1:H:188:ILE:HB	1:J:38:VAL:O	2.13	0.49
1:D:108:TYR:HE1	1:F:39:SER:O	1.95	0.49
1:D:239:ILE:HD13	1:D:248:VAL:HG21	1.94	0.49
1:A:5:ILE:HD12	1:A:98:ILE:HB	1.94	0.48
1:H:151:PRO:N	1:J:40:PHE:HE2	2.11	0.48
1:C:239:ILE:HD13	1:C:248:VAL:HG21	1.94	0.48
1:E:125:ASN:OD1	1:E:128:LYS:NZ	2.32	0.48
1:G:239:ILE:HD13	1:G:248:VAL:HG21	1.94	0.48
1:H:108:TYR:CG	1:J:38:VAL:HG11	2.48	0.48
1:D:108:TYR:CG	1:F:38:VAL:HG11	2.48	0.48
1:D:272:GLY:N	1:F:216:LYS:O	2.40	0.48
1:F:151:PRO:N	1:H:40:PHE:HE2	2.11	0.48
1:B:239:ILE:HD13	1:B:248:VAL:HG21	1.94	0.48
1:D:5:ILE:HD12	1:D:98:ILE:HB	1.94	0.48
1:A:111:ASN:O	1:C:37:ALA:CA	2.57	0.48
1:C:112:ASN:ND2	1:E:38:VAL:H	2.02	0.48
1:C:185:LEU:C	1:E:43:LYS:HE3	2.32	0.48
1:C:188:ILE:HB	1:E:38:VAL:O	2.13	0.48
1:G:5:ILE:HD12	1:G:98:ILE:HB	1.94	0.48
1:G:188:ILE:HB	1:I:38:VAL:O	2.13	0.48
1:H:272:GLY:HA2	1:J:216:LYS:C	2.36	0.48
1:E:151:PRO:N	1:G:40:PHE:HE2	2.12	0.48
1:H:108:TYR:HE1	1:J:39:SER:O	1.96	0.48
1:H:257:ARG:HH22	1:I:53:GLU:HG2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ARG:HH22	1:C:53:GLU:HG2	1.79	0.48
1:G:108:TYR:CG	1:I:38:VAL:HG11	2.48	0.48
1:G:108:TYR:HE1	1:I:39:SER:O	1.96	0.48
1:D:151:PRO:N	1:F:40:PHE:HE2	2.11	0.48
1:E:108:TYR:CG	1:G:38:VAL:HG11	2.48	0.48
1:E:272:GLY:N	1:G:216:LYS:O	2.40	0.48
1:F:108:TYR:HE1	1:H:39:SER:O	1.95	0.48
1:A:108:TYR:CG	1:C:38:VAL:HG11	2.47	0.48
1:A:151:PRO:N	1:C:40:PHE:HE2	2.12	0.48
1:B:151:PRO:N	1:D:40:PHE:HE2	2.12	0.48
1:C:108:TYR:CG	1:E:38:VAL:HG11	2.48	0.48
1:C:151:PRO:N	1:E:40:PHE:HE2	2.12	0.48
1:D:188:ILE:CD1	1:F:40:PHE:CB	2.75	0.48
1:E:5:ILE:HD12	1:E:98:ILE:HB	1.94	0.48
1:C:5:ILE:HD12	1:C:98:ILE:HB	1.94	0.47
1:D:257:ARG:HH22	1:E:52:GLY:C	2.17	0.47
1:G:257:ARG:HH22	1:H:53:GLU:HG2	1.79	0.47
1:C:108:TYR:HE1	1:E:39:SER:O	1.96	0.47
1:D:257:ARG:HH22	1:E:53:GLU:HG2	1.79	0.47
1:E:188:ILE:HB	1:G:38:VAL:O	2.13	0.47
1:I:239:ILE:HD13	1:I:248:VAL:HG21	1.94	0.47
1:F:257:ARG:HH22	1:G:53:GLU:HG2	1.79	0.47
1:A:108:TYR:HE1	1:C:39:SER:O	1.96	0.47
1:B:16:TRP:NE1	1:B:91:LEU:HD21	2.30	0.47
1:F:16:TRP:NE1	1:F:91:LEU:HD21	2.30	0.47
1:B:188:ILE:HB	1:D:38:VAL:O	2.14	0.47
1:D:16:TRP:NE1	1:D:91:LEU:HD21	2.30	0.47
1:I:257:ARG:HH22	1:J:53:GLU:HG2	1.79	0.47
1:J:97:ASP:OD1	1:J:142:ASP:HB3	2.15	0.47
1:A:257:ARG:HH22	1:B:53:GLU:HG2	1.79	0.47
1:A:272:GLY:HA2	1:C:216:LYS:C	2.36	0.47
1:C:257:ARG:HH22	1:D:53:GLU:HG2	1.80	0.47
1:D:271:SER:C	1:F:216:LYS:HB2	2.40	0.47
1:F:97:ASP:OD1	1:F:142:ASP:HB3	2.15	0.47
1:H:16:TRP:NE1	1:H:91:LEU:HD21	2.30	0.47
1:I:97:ASP:OD1	1:I:142:ASP:HB3	2.15	0.47
1:C:97:ASP:OD1	1:C:142:ASP:HB3	2.15	0.47
1:D:97:ASP:OD1	1:D:142:ASP:HB3	2.15	0.47
1:F:271:SER:C	1:H:216:LYS:HB2	2.40	0.47
1:G:97:ASP:OD1	1:G:142:ASP:HB3	2.15	0.47
1:E:257:ARG:HH22	1:F:53:GLU:HG2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:LYS:NZ	1:F:269:GLU:O	2.48	0.46
1:H:190:LYS:NZ	1:H:269:GLU:O	2.48	0.46
1:A:16:TRP:NE1	1:A:91:LEU:HD21	2.30	0.46
1:G:16:TRP:NE1	1:G:91:LEU:HD21	2.30	0.46
1:G:190:LYS:NZ	1:G:269:GLU:O	2.49	0.46
1:I:190:LYS:NZ	1:I:269:GLU:O	2.49	0.46
1:E:16:TRP:NE1	1:E:91:LEU:HD21	2.30	0.46
1:E:97:ASP:OD1	1:E:142:ASP:HB3	2.15	0.46
1:F:189:SER:HG	1:H:60:ILE:CD1	1.96	0.46
1:J:16:TRP:NE1	1:J:91:LEU:HD21	2.30	0.46
1:A:181:VAL:HG12	1:C:43:LYS:NZ	1.98	0.46
1:A:188:ILE:HB	1:C:38:VAL:O	2.14	0.46
1:B:97:ASP:OD1	1:B:142:ASP:HB3	2.15	0.46
1:H:271:SER:C	1:J:216:LYS:HB2	2.40	0.46
1:D:190:LYS:NZ	1:D:269:GLU:O	2.48	0.46
1:H:97:ASP:OD1	1:H:142:ASP:HB3	2.15	0.46
1:I:16:TRP:NE1	1:I:91:LEU:HD21	2.30	0.46
1:A:97:ASP:OD1	1:A:142:ASP:HB3	2.15	0.46
1:C:16:TRP:NE1	1:C:91:LEU:HD21	2.30	0.46
1:E:190:LYS:NZ	1:E:269:GLU:O	2.49	0.46
1:E:271:SER:C	1:G:216:LYS:HB2	2.40	0.46
1:G:36:TRP:CD1	1:G:54:GLN:HB3	2.51	0.46
1:H:258:LYS:CA	1:I:53:GLU:OE2	2.61	0.46
1:A:36:TRP:CD1	1:A:54:GLN:HB3	2.51	0.46
1:A:190:LYS:NZ	1:A:269:GLU:O	2.49	0.46
1:B:36:TRP:CD1	1:B:54:GLN:HB3	2.51	0.46
1:H:36:TRP:CD1	1:H:54:GLN:HB3	2.51	0.46
1:B:189:SER:HG	1:D:60:ILE:CD1	1.95	0.46
1:C:190:LYS:NZ	1:C:269:GLU:O	2.49	0.46
1:G:111:ASN:O	1:I:37:ALA:CA	2.58	0.46
1:J:190:LYS:NZ	1:J:269:GLU:O	2.48	0.46
1:F:36:TRP:CD1	1:F:54:GLN:HB3	2.51	0.46
1:J:36:TRP:CD1	1:J:54:GLN:HB3	2.51	0.46
1:B:190:LYS:NZ	1:B:269:GLU:O	2.49	0.45
1:C:271:SER:C	1:E:216:LYS:HB2	2.40	0.45
1:D:111:ASN:O	1:F:37:ALA:CA	2.58	0.45
1:E:258:LYS:CA	1:F:53:GLU:OE2	2.60	0.45
1:I:150:ILE:HB	1:I:151:PRO:HD3	1.98	0.45
1:E:36:TRP:CD1	1:E:54:GLN:HB3	2.51	0.45
1:C:36:TRP:CD1	1:C:54:GLN:HB3	2.51	0.45
1:D:36:TRP:CD1	1:D:54:GLN:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:TRP:CD1	1:I:54:GLN:HB3	2.51	0.45
1:I:50:LEU:HD23	1:I:51:ASN:HB2	1.98	0.45
1:J:150:ILE:HB	1:J:151:PRO:HD3	1.98	0.45
1:B:271:SER:C	1:D:216:LYS:HB2	2.39	0.45
1:J:50:LEU:HD23	1:J:51:ASN:HB2	1.98	0.45
1:B:50:LEU:HD23	1:B:51:ASN:HB2	1.98	0.45
1:F:258:LYS:CA	1:G:53:GLU:OE2	2.60	0.45
1:G:150:ILE:HB	1:G:151:PRO:HD3	1.98	0.45
1:H:150:ILE:HB	1:H:151:PRO:HD3	1.98	0.45
1:D:258:LYS:CA	1:E:53:GLU:OE2	2.61	0.45
1:D:296:ILE:HD12	1:D:296:ILE:HA	1.88	0.45
1:G:50:LEU:HD23	1:G:51:ASN:HB2	1.98	0.45
1:E:150:ILE:HB	1:E:151:PRO:HD3	1.98	0.45
1:F:150:ILE:HB	1:F:151:PRO:HD3	1.98	0.45
1:H:50:LEU:HD23	1:H:51:ASN:HB2	1.98	0.45
1:F:189:SER:OG	1:H:60:ILE:CG1	2.62	0.45
1:B:296:ILE:HD12	1:B:296:ILE:HA	1.88	0.44
1:C:150:ILE:HB	1:C:151:PRO:HD3	1.98	0.44
1:D:150:ILE:HB	1:D:151:PRO:HD3	1.98	0.44
1:B:150:ILE:HB	1:B:151:PRO:HD3	1.98	0.44
1:E:189:SER:OG	1:G:60:ILE:CG1	2.62	0.44
1:G:151:PRO:N	1:I:40:PHE:CE2	2.85	0.44
1:A:150:ILE:HB	1:A:151:PRO:HD3	1.98	0.44
1:A:258:LYS:CA	1:B:53:GLU:OE2	2.61	0.44
1:D:151:PRO:N	1:F:40:PHE:CE2	2.86	0.44
1:E:50:LEU:C	1:E:50:LEU:HD23	2.43	0.44
1:H:111:ASN:O	1:J:37:ALA:CA	2.58	0.44
1:A:50:LEU:HD23	1:A:50:LEU:C	2.43	0.44
1:B:50:LEU:HD23	1:B:50:LEU:C	2.43	0.44
1:B:258:LYS:CA	1:C:53:GLU:OE2	2.60	0.44
1:C:50:LEU:HD23	1:C:51:ASN:HB2	1.98	0.44
1:D:50:LEU:HD23	1:D:51:ASN:HB2	1.98	0.44
1:E:50:LEU:HD23	1:E:51:ASN:HB2	1.98	0.44
1:E:154:TYR:CD1	1:E:318:ILE:HG12	2.53	0.44
1:E:271:SER:HB2	1:G:216:LYS:HD2	2.00	0.44
1:F:50:LEU:HD23	1:F:50:LEU:C	2.43	0.44
1:G:271:SER:C	1:I:216:LYS:HB2	2.40	0.44
1:H:154:TYR:CD1	1:H:318:ILE:HG12	2.53	0.44
1:C:258:LYS:CA	1:D:53:GLU:OE2	2.60	0.44
1:J:50:LEU:HD23	1:J:50:LEU:C	2.43	0.44
1:J:154:TYR:CD1	1:J:318:ILE:HG12	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:TYR:CD1	1:D:318:ILE:HG12	2.53	0.44
1:G:154:TYR:CD1	1:G:318:ILE:HG12	2.53	0.44
1:A:189:SER:HG	1:C:60:ILE:CD1	1.98	0.44
1:C:111:ASN:O	1:E:37:ALA:CA	2.58	0.44
1:E:188:ILE:CD1	1:G:40:PHE:CB	2.75	0.44
1:F:50:LEU:HD23	1:F:51:ASN:HB2	1.98	0.44
1:H:151:PRO:N	1:J:40:PHE:CE2	2.86	0.44
1:I:50:LEU:HD23	1:I:50:LEU:C	2.43	0.44
1:B:108:TYR:OH	1:D:40:PHE:HA	2.18	0.44
1:F:151:PRO:N	1:H:40:PHE:CE2	2.86	0.44
1:A:50:LEU:HD23	1:A:51:ASN:HB2	1.98	0.43
1:C:154:TYR:CD1	1:C:318:ILE:HG12	2.53	0.43
1:F:154:TYR:CD1	1:F:318:ILE:HG12	2.53	0.43
1:B:111:ASN:O	1:D:37:ALA:CA	2.57	0.43
1:D:50:LEU:HD23	1:D:50:LEU:C	2.43	0.43
1:D:108:TYR:OH	1:F:40:PHE:HA	2.19	0.43
1:H:189:SER:OG	1:J:60:ILE:CG1	2.62	0.43
1:A:151:PRO:N	1:C:40:PHE:CE2	2.86	0.43
1:A:296:ILE:HD12	1:C:240:ASN:HB3	2.00	0.43
1:C:189:SER:OG	1:E:60:ILE:CG1	2.62	0.43
1:E:108:TYR:OH	1:G:40:PHE:HA	2.18	0.43
1:F:271:SER:HB2	1:H:216:LYS:HD2	2.00	0.43
1:G:50:LEU:HD23	1:G:50:LEU:C	2.43	0.43
1:G:271:SER:HB2	1:I:216:LYS:HD2	2.00	0.43
1:I:154:TYR:CD1	1:I:318:ILE:HG12	2.53	0.43
1:A:83:HIS:CD2	1:A:130:ILE:HG21	2.54	0.43
1:B:154:TYR:CD1	1:B:318:ILE:HG12	2.53	0.43
1:C:151:PRO:N	1:E:40:PHE:CE2	2.86	0.43
1:E:83:HIS:CD2	1:E:130:ILE:HG21	2.54	0.43
1:F:83:HIS:CD2	1:F:130:ILE:HG21	2.54	0.43
1:H:83:HIS:CD2	1:H:130:ILE:HG21	2.54	0.43
1:J:83:HIS:CD2	1:J:130:ILE:HG21	2.54	0.43
1:A:154:TYR:CD1	1:A:318:ILE:HG12	2.53	0.43
1:A:271:SER:HB2	1:C:216:LYS:HD2	2.00	0.43
1:D:164:ASP:HB3	1:D:274:THR:OG1	2.19	0.43
1:D:271:SER:HB2	1:F:216:LYS:HD2	2.00	0.43
1:F:188:ILE:CD1	1:H:40:PHE:CB	2.75	0.43
1:E:151:PRO:N	1:G:40:PHE:CE2	2.86	0.43
1:A:164:ASP:HB3	1:A:274:THR:OG1	2.19	0.43
1:B:164:ASP:HB3	1:B:274:THR:OG1	2.19	0.43
1:C:50:LEU:HD23	1:C:50:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:HIS:CD2	1:D:130:ILE:HG21	2.54	0.43
1:G:83:HIS:CD2	1:G:130:ILE:HG21	2.54	0.43
1:H:50:LEU:HD23	1:H:50:LEU:C	2.43	0.43
1:H:164:ASP:HB3	1:H:274:THR:OG1	2.19	0.43
1:A:189:SER:OG	1:C:60:ILE:CG1	2.62	0.43
1:B:296:ILE:HD12	1:D:240:ASN:HB3	2.00	0.43
1:J:164:ASP:HB3	1:J:274:THR:OG1	2.19	0.43
1:C:108:TYR:OH	1:E:40:PHE:HA	2.19	0.43
1:C:296:ILE:HD12	1:E:240:ASN:HB3	2.00	0.43
1:D:185:LEU:C	1:F:43:LYS:HE3	2.32	0.43
1:E:112:ASN:ND2	1:G:38:VAL:N	2.62	0.43
1:G:164:ASP:HB3	1:G:274:THR:OG1	2.19	0.43
1:H:296:ILE:HD12	1:J:240:ASN:HB3	2.00	0.43
1:I:83:HIS:CD2	1:I:130:ILE:HG21	2.54	0.42
1:C:181:VAL:HG12	1:E:43:LYS:NZ	1.98	0.42
1:D:296:ILE:HD12	1:F:240:ASN:HB3	2.00	0.42
1:F:108:TYR:OH	1:H:40:PHE:HA	2.19	0.42
1:A:108:TYR:OH	1:C:40:PHE:HA	2.20	0.42
1:A:271:SER:C	1:C:216:LYS:HB2	2.40	0.42
1:E:164:ASP:HB3	1:E:274:THR:OG1	2.19	0.42
1:G:258:LYS:CA	1:H:53:GLU:OE2	2.60	0.42
1:I:164:ASP:HB3	1:I:274:THR:OG1	2.19	0.42
1:B:83:HIS:CD2	1:B:130:ILE:HG21	2.54	0.42
1:C:164:ASP:HB3	1:C:274:THR:OG1	2.19	0.42
1:F:296:ILE:HD12	1:F:296:ILE:HA	1.88	0.42
1:I:258:LYS:CA	1:J:53:GLU:OE2	2.60	0.42
1:E:108:TYR:CG	1:G:38:VAL:HG13	2.54	0.42
1:B:16:TRP:CE2	1:B:24:LYS:HB2	2.55	0.42
1:B:151:PRO:N	1:D:40:PHE:CE2	2.87	0.42
1:C:83:HIS:CD2	1:C:130:ILE:HG21	2.54	0.42
1:D:16:TRP:CE2	1:D:24:LYS:HB2	2.55	0.42
1:G:108:TYR:OH	1:I:40:PHE:HA	2.19	0.42
1:G:296:ILE:HD12	1:I:240:ASN:HB3	2.00	0.42
1:A:8:GLY:O	1:A:72:TRP:CH2	2.73	0.42
1:C:112:ASN:ND2	1:E:38:VAL:N	2.63	0.42
1:E:296:ILE:HD12	1:G:240:ASN:HB3	2.00	0.42
1:G:16:TRP:CE2	1:G:24:LYS:HB2	2.55	0.42
1:G:112:ASN:ND2	1:I:38:VAL:N	2.63	0.42
1:H:271:SER:HB2	1:J:216:LYS:HD2	2.00	0.42
1:B:13:LYS:HD3	1:B:308:GLN:HG2	2.02	0.42
1:B:271:SER:HB2	1:D:216:LYS:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:LYS:HD3	1:F:308:GLN:HG2	2.02	0.42
1:F:164:ASP:HB3	1:F:274:THR:OG1	2.19	0.42
1:F:296:ILE:HD12	1:H:240:ASN:HB3	2.00	0.42
1:G:186:SER:CA	1:I:43:LYS:HG2	2.50	0.42
1:H:296:ILE:HD12	1:H:296:ILE:HA	1.88	0.42
1:I:16:TRP:CE2	1:I:24:LYS:HB2	2.55	0.42
1:D:13:LYS:HD3	1:D:308:GLN:HG2	2.02	0.42
1:E:16:TRP:CE2	1:E:24:LYS:HB2	2.55	0.42
1:F:16:TRP:CE2	1:F:24:LYS:HB2	2.55	0.42
1:I:296:ILE:HD12	1:I:296:ILE:HA	1.88	0.42
1:D:8:GLY:O	1:D:72:TRP:CH2	2.73	0.42
1:H:8:GLY:O	1:H:72:TRP:CH2	2.73	0.42
1:H:186:SER:CA	1:J:43:LYS:HG2	2.50	0.42
1:C:8:GLY:O	1:C:72:TRP:CH2	2.73	0.41
1:H:13:LYS:HD3	1:H:308:GLN:HG2	2.02	0.41
1:J:8:GLY:O	1:J:72:TRP:CH2	2.73	0.41
1:C:16:TRP:CE2	1:C:24:LYS:HB2	2.55	0.41
1:H:108:TYR:OH	1:J:40:PHE:HA	2.19	0.41
1:A:16:TRP:CE2	1:A:24:LYS:HB2	2.55	0.41
1:D:186:SER:CA	1:F:43:LYS:HG2	2.50	0.41
1:F:186:SER:CA	1:H:43:LYS:HG2	2.51	0.41
1:G:189:SER:HG	1:I:60:ILE:CD1	2.02	0.41
1:H:16:TRP:CE2	1:H:24:LYS:HB2	2.55	0.41
1:C:171:LEU:HD22	1:C:286:ILE:HD13	2.03	0.41
1:E:186:SER:CA	1:G:43:LYS:HG2	2.51	0.41
1:F:171:LEU:HD22	1:F:286:ILE:HD13	2.03	0.41
1:I:8:GLY:O	1:I:72:TRP:CH2	2.73	0.41
1:I:13:LYS:HD3	1:I:308:GLN:HG2	2.02	0.41
1:J:13:LYS:HD3	1:J:308:GLN:HG2	2.02	0.41
1:A:5:ILE:HG12	1:A:14:LEU:HD22	2.01	0.41
1:A:171:LEU:HD22	1:A:286:ILE:HD13	2.03	0.41
1:E:8:GLY:O	1:E:72:TRP:CH2	2.73	0.41
1:F:8:GLY:O	1:F:72:TRP:CH2	2.73	0.41
1:J:171:LEU:HD22	1:J:286:ILE:HD13	2.03	0.41
1:B:8:GLY:O	1:B:72:TRP:CH2	2.73	0.41
1:C:186:SER:CA	1:E:43:LYS:HG2	2.51	0.41
1:E:171:LEU:HD22	1:E:286:ILE:HD13	2.03	0.41
1:H:171:LEU:HD22	1:H:286:ILE:HD13	2.03	0.41
1:G:13:LYS:HD3	1:G:308:GLN:HG2	2.02	0.41
1:J:5:ILE:HG12	1:J:14:LEU:HD22	2.01	0.41
1:J:16:TRP:CE2	1:J:24:LYS:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:SER:CA	1:C:43:LYS:HG2	2.51	0.41
1:D:5:ILE:HG12	1:D:14:LEU:HD22	2.01	0.41
1:D:171:LEU:HD22	1:D:286:ILE:HD13	2.03	0.41
1:F:5:ILE:HG12	1:F:14:LEU:HD22	2.01	0.41
1:H:5:ILE:HG12	1:H:14:LEU:HD22	2.01	0.41
1:B:171:LEU:HD22	1:B:286:ILE:HD13	2.03	0.41
1:A:13:LYS:HD3	1:A:308:GLN:HG2	2.02	0.40
1:B:5:ILE:HG12	1:B:14:LEU:HD22	2.01	0.40
1:C:13:LYS:HD3	1:C:308:GLN:HG2	2.02	0.40
1:D:150:ILE:HD12	1:F:40:PHE:CG	2.56	0.40
1:A:112:ASN:ND2	1:C:38:VAL:N	2.64	0.40
1:B:112:ASN:ND2	1:D:38:VAL:N	2.63	0.40
1:B:189:SER:OG	1:D:60:ILE:CG1	2.62	0.40
1:G:171:LEU:HD22	1:G:286:ILE:HD13	2.03	0.40
1:E:13:LYS:HD3	1:E:308:GLN:HG2	2.02	0.40
1:G:8:GLY:O	1:G:72:TRP:CH2	2.73	0.40
1:H:112:ASN:ND2	1:J:38:VAL:N	2.63	0.40
1:B:186:SER:CA	1:D:43:LYS:HG2	2.52	0.40
1:D:112:ASN:ND2	1:F:38:VAL:N	2.62	0.40
1:I:171:LEU:HD22	1:I:286:ILE:HD13	2.03	0.40
1:D:189:SER:HG	1:F:60:ILE:CD1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	B	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	C	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	D	319/320 (100%)	306 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	F	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	G	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	H	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	I	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
1	J	319/320 (100%)	306 (96%)	13 (4%)	0	100	100
All	All	3190/3200 (100%)	3060 (96%)	130 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/284 (100%)	279 (98%)	5 (2%)	51	68
1	B	284/284 (100%)	279 (98%)	5 (2%)	51	68
1	C	284/284 (100%)	279 (98%)	5 (2%)	51	68
1	D	284/284 (100%)	279 (98%)	5 (2%)	51	68
1	E	284/284 (100%)	279 (98%)	5 (2%)	51	68
1	F	284/284 (100%)	279 (98%)	5 (2%)	51	68
1	G	284/284 (100%)	279 (98%)	5 (2%)	51	68
1	H	284/284 (100%)	279 (98%)	5 (2%)	51	68
1	I	284/284 (100%)	279 (98%)	5 (2%)	51	68
1	J	284/284 (100%)	279 (98%)	5 (2%)	51	68
All	All	2840/2840 (100%)	2790 (98%)	50 (2%)	51	68

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS

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Mol	Chain	Res	Type
1	A	77	VAL
1	A	159	GLU
1	A	160	LEU
1	A	296	ILE
1	B	13	LYS
1	B	77	VAL
1	B	159	GLU
1	B	160	LEU
1	B	296	ILE
1	C	13	LYS
1	C	77	VAL
1	C	159	GLU
1	C	160	LEU
1	C	296	ILE
1	D	13	LYS
1	D	77	VAL
1	D	159	GLU
1	D	160	LEU
1	D	296	ILE
1	E	13	LYS
1	E	77	VAL
1	E	159	GLU
1	E	160	LEU
1	E	296	ILE
1	F	13	LYS
1	F	77	VAL
1	F	159	GLU
1	F	160	LEU
1	F	296	ILE
1	G	13	LYS
1	G	77	VAL
1	G	159	GLU
1	G	160	LEU
1	G	296	ILE
1	H	13	LYS
1	H	77	VAL
1	H	159	GLU
1	H	160	LEU
1	H	296	ILE
1	I	13	LYS
1	I	77	VAL
1	I	159	GLU

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Mol	Chain	Res	Type
1	I	160	LEU
1	I	296	ILE
1	J	13	LYS
1	J	77	VAL
1	J	159	GLU
1	J	160	LEU
1	J	296	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	113	GLN
1	B	78	ASN
1	B	83	HIS
1	B	113	GLN
1	C	78	ASN
1	C	83	HIS
1	C	113	GLN
1	C	233	ASN
1	C	237	GLN
1	D	78	ASN
1	D	83	HIS
1	D	113	GLN
1	E	83	HIS
1	E	113	GLN
1	F	83	HIS
1	F	113	GLN
1	G	78	ASN
1	G	83	HIS
1	G	113	GLN
1	H	78	ASN
1	H	83	HIS
1	H	113	GLN
1	I	83	HIS
1	J	83	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	$\# Z > 2$
2	ANP	I	500	3	33,33,33	2.06	13 (39%)	45,52,52	2.02	14 (31%)
2	ANP	B	500	3	33,33,33	2.06	14 (42%)	45,52,52	2.02	14 (31%)
2	ANP	C	500	3	33,33,33	2.07	13 (39%)	45,52,52	2.01	14 (31%)
2	ANP	D	500	3	33,33,33	2.05	13 (39%)	45,52,52	2.02	14 (31%)
2	ANP	J	500	3	33,33,33	2.04	13 (39%)	45,52,52	2.01	14 (31%)
2	ANP	F	500	3	33,33,33	2.03	12 (36%)	45,52,52	2.02	14 (31%)
2	ANP	H	500	3	33,33,33	2.03	13 (39%)	45,52,52	2.02	14 (31%)
2	ANP	E	500	3	33,33,33	2.06	14 (42%)	45,52,52	2.02	14 (31%)
2	ANP	A	500	3	33,33,33	2.05	13 (39%)	45,52,52	2.01	14 (31%)
2	ANP	G	500	3	33,33,33	2.05	12 (36%)	45,52,52	2.02	14 (31%)

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
2	ANP	I	500	3	-	1/18/38/38	0/3/3/3
2	ANP	B	500	3	-	1/18/38/38	0/3/3/3
2	ANP	C	500	3	-	1/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	D	500	3	-	1/18/38/38	0/3/3/3
2	ANP	J	500	3	-	1/18/38/38	0/3/3/3
2	ANP	F	500	3	-	1/18/38/38	0/3/3/3
2	ANP	H	500	3	-	1/18/38/38	0/3/3/3
2	ANP	E	500	3	-	1/18/38/38	0/3/3/3
2	ANP	A	500	3	-	1/18/38/38	0/3/3/3
2	ANP	G	500	3	-	1/18/38/38	0/3/3/3

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	500	ANP	C5-C4	4.86	1.47	1.39
2	C	500	ANP	PB-N3B	4.85	1.76	1.63
2	D	500	ANP	C5-C4	4.85	1.47	1.39
2	G	500	ANP	C5-C4	4.85	1.47	1.39
2	B	500	ANP	C5-C4	4.83	1.47	1.39
2	C	500	ANP	C5-C4	4.83	1.47	1.39
2	A	500	ANP	C5-C4	4.82	1.47	1.39
2	F	500	ANP	C5-C4	4.82	1.47	1.39
2	E	500	ANP	C5-C4	4.81	1.47	1.39
2	A	500	ANP	PB-N3B	4.79	1.75	1.63
2	I	500	ANP	PB-N3B	4.79	1.75	1.63
2	B	500	ANP	PB-N3B	4.77	1.75	1.63
2	E	500	ANP	PB-N3B	4.77	1.75	1.63
2	C	500	ANP	PG-N3B	4.77	1.75	1.63
2	G	500	ANP	PB-N3B	4.76	1.75	1.63
2	I	500	ANP	PG-N3B	4.76	1.75	1.63
2	G	500	ANP	PG-N3B	4.76	1.75	1.63
2	F	500	ANP	PB-N3B	4.76	1.75	1.63
2	H	500	ANP	C5-C4	4.75	1.47	1.39
2	B	500	ANP	PG-N3B	4.75	1.75	1.63
2	D	500	ANP	PG-N3B	4.75	1.75	1.63
2	A	500	ANP	PG-N3B	4.74	1.75	1.63
2	D	500	ANP	PB-N3B	4.74	1.75	1.63
2	H	500	ANP	PB-N3B	4.74	1.75	1.63
2	E	500	ANP	PG-N3B	4.73	1.75	1.63
2	F	500	ANP	PG-N3B	4.73	1.75	1.63
2	J	500	ANP	PG-N3B	4.73	1.75	1.63
2	J	500	ANP	PB-N3B	4.73	1.75	1.63
2	J	500	ANP	C5-C4	4.72	1.47	1.39
2	H	500	ANP	PG-N3B	4.72	1.75	1.63
2	C	500	ANP	PG-O1G	3.75	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	ANP	PG-O1G	3.74	1.51	1.46
2	I	500	ANP	PG-O1G	3.71	1.51	1.46
2	D	500	ANP	PG-O1G	3.68	1.51	1.46
2	B	500	ANP	PG-O1G	3.68	1.51	1.46
2	G	500	ANP	PG-O1G	3.66	1.51	1.46
2	A	500	ANP	PG-O1G	3.63	1.51	1.46
2	J	500	ANP	PG-O1G	3.62	1.51	1.46
2	H	500	ANP	PG-O1G	3.60	1.51	1.46
2	F	500	ANP	PG-O1G	3.57	1.51	1.46
2	E	500	ANP	C5-C6	2.62	1.48	1.41
2	B	500	ANP	C5-C6	2.61	1.48	1.41
2	D	500	ANP	C5-C6	2.61	1.48	1.41
2	C	500	ANP	C5-C6	2.61	1.48	1.41
2	E	500	ANP	PB-O3A	2.60	1.62	1.59
2	A	500	ANP	C5-C6	2.60	1.48	1.41
2	G	500	ANP	C5-C6	2.60	1.48	1.41
2	J	500	ANP	C5-C6	2.59	1.48	1.41
2	H	500	ANP	C5-C6	2.58	1.48	1.41
2	I	500	ANP	C5-C6	2.58	1.48	1.41
2	C	500	ANP	PB-O3A	2.57	1.62	1.59
2	F	500	ANP	C5-C6	2.53	1.48	1.41
2	G	500	ANP	PB-O3A	2.53	1.62	1.59
2	B	500	ANP	PB-O3A	2.53	1.62	1.59
2	I	500	ANP	PB-O3A	2.51	1.62	1.59
2	J	500	ANP	PB-O3A	2.50	1.62	1.59
2	A	500	ANP	PB-O3A	2.50	1.62	1.59
2	H	500	ANP	PB-O3A	2.46	1.62	1.59
2	D	500	ANP	PB-O3A	2.46	1.62	1.59
2	C	500	ANP	C8-N7	2.42	1.36	1.31
2	F	500	ANP	PB-O3A	2.41	1.62	1.59
2	E	500	ANP	C8-N7	2.39	1.36	1.31
2	A	500	ANP	C8-N7	2.38	1.36	1.31
2	I	500	ANP	C8-N7	2.37	1.36	1.31
2	G	500	ANP	C8-N7	2.36	1.36	1.31
2	J	500	ANP	C8-N7	2.35	1.36	1.31
2	B	500	ANP	C8-N7	2.35	1.36	1.31
2	D	500	ANP	C8-N7	2.34	1.36	1.31
2	H	500	ANP	C8-N7	2.31	1.36	1.31
2	I	500	ANP	C4-N9	-2.29	1.32	1.37
2	A	500	ANP	C4-N9	-2.29	1.32	1.37
2	J	500	ANP	C4-N9	-2.28	1.32	1.37
2	D	500	ANP	C4-N9	-2.28	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	ANP	C8-N7	2.27	1.36	1.31
2	G	500	ANP	C4-N9	-2.27	1.33	1.37
2	F	500	ANP	C4-N9	-2.26	1.33	1.37
2	B	500	ANP	C4-N9	-2.26	1.33	1.37
2	H	500	ANP	C4-N9	-2.26	1.33	1.37
2	E	500	ANP	C4-N9	-2.25	1.33	1.37
2	C	500	ANP	C4-N9	-2.24	1.33	1.37
2	D	500	ANP	PG-O2G	-2.24	1.50	1.56
2	H	500	ANP	PG-O2G	-2.21	1.50	1.56
2	F	500	ANP	PG-O2G	-2.21	1.50	1.56
2	B	500	ANP	PG-O2G	-2.20	1.51	1.56
2	J	500	ANP	PG-O2G	-2.20	1.51	1.56
2	C	500	ANP	PG-O2G	-2.20	1.51	1.56
2	D	500	ANP	PG-O3G	-2.19	1.51	1.56
2	G	500	ANP	PG-O2G	-2.19	1.51	1.56
2	E	500	ANP	PG-O2G	-2.19	1.51	1.56
2	A	500	ANP	PG-O3G	-2.19	1.51	1.56
2	I	500	ANP	PG-O3G	-2.18	1.51	1.56
2	G	500	ANP	PG-O3G	-2.18	1.51	1.56
2	A	500	ANP	PG-O2G	-2.18	1.51	1.56
2	J	500	ANP	PG-O3G	-2.17	1.51	1.56
2	B	500	ANP	PG-O3G	-2.17	1.51	1.56
2	I	500	ANP	PG-O2G	-2.17	1.51	1.56
2	E	500	ANP	PG-O3G	-2.16	1.51	1.56
2	F	500	ANP	PG-O3G	-2.16	1.51	1.56
2	H	500	ANP	PG-O3G	-2.16	1.51	1.56
2	D	500	ANP	C5-N7	-2.13	1.35	1.39
2	C	500	ANP	PG-O3G	-2.12	1.51	1.56
2	A	500	ANP	C5-N7	-2.11	1.35	1.39
2	G	500	ANP	C5-N7	-2.11	1.35	1.39
2	E	500	ANP	PB-O2B	-2.10	1.51	1.56
2	A	500	ANP	PB-O2B	-2.09	1.51	1.56
2	G	500	ANP	PB-O2B	-2.09	1.51	1.56
2	I	500	ANP	PB-O2B	-2.09	1.51	1.56
2	E	500	ANP	PB-O1B	2.08	1.49	1.46
2	E	500	ANP	PA-O3A	2.08	1.61	1.59
2	B	500	ANP	C5-N7	-2.08	1.35	1.39
2	D	500	ANP	PB-O2B	-2.08	1.51	1.56
2	J	500	ANP	C5-N7	-2.07	1.35	1.39
2	H	500	ANP	C5-N7	-2.07	1.35	1.39
2	C	500	ANP	PB-O2B	-2.07	1.51	1.56
2	B	500	ANP	PA-O3A	2.07	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	ANP	PB-O2B	-2.07	1.51	1.56
2	C	500	ANP	C5-N7	-2.07	1.35	1.39
2	H	500	ANP	PB-O2B	-2.07	1.51	1.56
2	H	500	ANP	PB-O1B	2.06	1.49	1.46
2	J	500	ANP	PB-O2B	-2.06	1.51	1.56
2	F	500	ANP	PB-O2B	-2.06	1.51	1.56
2	C	500	ANP	PA-O3A	2.05	1.61	1.59
2	F	500	ANP	C5-N7	-2.05	1.35	1.39
2	J	500	ANP	PB-O1B	2.04	1.49	1.46
2	B	500	ANP	PB-O1B	2.04	1.49	1.46
2	A	500	ANP	PA-O3A	2.04	1.61	1.59
2	I	500	ANP	C5-N7	-2.03	1.35	1.39
2	D	500	ANP	PB-O1B	2.03	1.49	1.46
2	I	500	ANP	PB-O1B	2.02	1.49	1.46
2	E	500	ANP	C5-N7	-2.02	1.35	1.39

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	500	ANP	O1G-PG-N3B	-5.47	103.71	111.77
2	B	500	ANP	O1G-PG-N3B	-5.46	103.72	111.77
2	D	500	ANP	O1G-PG-N3B	-5.45	103.74	111.77
2	G	500	ANP	O1G-PG-N3B	-5.45	103.74	111.77
2	F	500	ANP	O1G-PG-N3B	-5.45	103.75	111.77
2	I	500	ANP	O1G-PG-N3B	-5.44	103.75	111.77
2	C	500	ANP	O1G-PG-N3B	-5.44	103.76	111.77
2	A	500	ANP	O1G-PG-N3B	-5.44	103.76	111.77
2	H	500	ANP	O1G-PG-N3B	-5.43	103.77	111.77
2	E	500	ANP	O1G-PG-N3B	-5.43	103.78	111.77
2	E	500	ANP	C5-C4-N3	-4.81	120.09	126.72
2	I	500	ANP	C5-C4-N3	-4.81	120.10	126.72
2	C	500	ANP	C5-C4-N3	-4.79	120.12	126.72
2	H	500	ANP	C5-C4-N3	-4.78	120.14	126.72
2	F	500	ANP	C5-C4-N3	-4.78	120.14	126.72
2	A	500	ANP	C5-C4-N3	-4.77	120.14	126.72
2	D	500	ANP	C5-C4-N3	-4.77	120.15	126.72
2	J	500	ANP	C5-C4-N3	-4.77	120.15	126.72
2	B	500	ANP	C5-C4-N3	-4.76	120.16	126.72
2	G	500	ANP	C5-C4-N3	-4.75	120.17	126.72
2	I	500	ANP	N3-C4-N9	4.18	134.28	127.17
2	E	500	ANP	N3-C4-N9	4.17	134.27	127.17
2	D	500	ANP	N3-C4-N9	4.17	134.26	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	500	ANP	N3-C4-N9	4.17	134.26	127.17
2	B	500	ANP	N3-C4-N9	4.17	134.25	127.17
2	A	500	ANP	N3-C4-N9	4.16	134.24	127.17
2	H	500	ANP	N3-C4-N9	4.15	134.23	127.17
2	J	500	ANP	N3-C4-N9	4.14	134.20	127.17
2	G	500	ANP	N3-C4-N9	4.14	134.20	127.17
2	C	500	ANP	N3-C4-N9	4.12	134.17	127.17
2	H	500	ANP	N3-C2-N1	-3.87	122.73	128.58
2	F	500	ANP	N3-C2-N1	-3.83	122.78	128.58
2	G	500	ANP	N3-C2-N1	-3.82	122.81	128.58
2	B	500	ANP	N3-C2-N1	-3.81	122.81	128.58
2	J	500	ANP	N3-C2-N1	-3.81	122.81	128.58
2	E	500	ANP	N3-C2-N1	-3.81	122.82	128.58
2	A	500	ANP	N3-C2-N1	-3.79	122.85	128.58
2	C	500	ANP	N3-C2-N1	-3.78	122.87	128.58
2	D	500	ANP	N3-C2-N1	-3.77	122.88	128.58
2	I	500	ANP	N3-C2-N1	-3.75	122.90	128.58
2	I	500	ANP	C4-N9-C8	3.58	109.50	105.74
2	H	500	ANP	C2-N3-C4	3.56	120.53	111.83
2	E	500	ANP	C2-N3-C4	3.55	120.50	111.83
2	J	500	ANP	C2-N3-C4	3.54	120.47	111.83
2	G	500	ANP	C4-N9-C8	3.54	109.45	105.74
2	A	500	ANP	C2-N3-C4	3.54	120.47	111.83
2	B	500	ANP	C2-N3-C4	3.54	120.47	111.83
2	D	500	ANP	C4-N9-C8	3.54	109.45	105.74
2	C	500	ANP	C2-N3-C4	3.53	120.46	111.83
2	I	500	ANP	C2-N3-C4	3.52	120.44	111.83
2	B	500	ANP	C4-N9-C8	3.52	109.44	105.74
2	G	500	ANP	C2-N3-C4	3.52	120.44	111.83
2	A	500	ANP	C4-N9-C8	3.52	109.44	105.74
2	F	500	ANP	C2-N3-C4	3.52	120.43	111.83
2	D	500	ANP	C2-N3-C4	3.52	120.43	111.83
2	F	500	ANP	C4-N9-C8	3.52	109.43	105.74
2	E	500	ANP	C4-N9-C8	3.52	109.43	105.74
2	J	500	ANP	C4-N9-C8	3.51	109.42	105.74
2	H	500	ANP	C4-N9-C8	3.51	109.42	105.74
2	C	500	ANP	C4-N9-C8	3.47	109.38	105.74
2	G	500	ANP	C4-C5-N7	-2.92	107.24	110.58
2	I	500	ANP	C4-C5-N7	-2.92	107.25	110.58
2	F	500	ANP	C4-C5-N7	-2.92	107.25	110.58
2	C	500	ANP	C4-C5-N7	-2.91	107.25	110.58
2	D	500	ANP	C4-C5-N7	-2.89	107.28	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	500	ANP	C4-C5-N7	-2.88	107.29	110.58
2	E	500	ANP	C4-C5-N7	-2.88	107.29	110.58
2	A	500	ANP	C4-C5-N7	-2.86	107.31	110.58
2	B	500	ANP	C4-C5-N7	-2.86	107.31	110.58
2	J	500	ANP	C4-C5-N7	-2.84	107.33	110.58
2	B	500	ANP	C3'-C2'-C1'	2.50	106.20	101.46
2	A	500	ANP	C3'-C2'-C1'	2.49	106.18	101.46
2	C	500	ANP	C3'-C2'-C1'	2.49	106.17	101.46
2	G	500	ANP	C3'-C2'-C1'	2.49	106.17	101.46
2	I	500	ANP	C3'-C2'-C1'	2.48	106.16	101.46
2	D	500	ANP	C3'-C2'-C1'	2.48	106.16	101.46
2	E	500	ANP	C3'-C2'-C1'	2.48	106.16	101.46
2	J	500	ANP	C3'-C2'-C1'	2.48	106.15	101.46
2	G	500	ANP	N9-C8-N7	-2.47	110.43	113.94
2	F	500	ANP	C3'-C2'-C1'	2.47	106.13	101.46
2	H	500	ANP	C3'-C2'-C1'	2.46	106.12	101.46
2	I	500	ANP	N9-C8-N7	-2.44	110.48	113.94
2	H	500	ANP	N9-C8-N7	-2.43	110.48	113.94
2	A	500	ANP	N9-C8-N7	-2.42	110.50	113.94
2	J	500	ANP	N9-C8-N7	-2.42	110.50	113.94
2	G	500	ANP	C5-N7-C8	2.42	107.25	103.45
2	D	500	ANP	N9-C8-N7	-2.41	110.51	113.94
2	C	500	ANP	N9-C8-N7	-2.41	110.52	113.94
2	G	500	ANP	O2B-PB-O1B	2.40	115.02	109.87
2	A	500	ANP	O2B-PB-O1B	2.40	115.02	109.87
2	F	500	ANP	O2B-PB-O1B	2.40	115.01	109.87
2	E	500	ANP	N9-C8-N7	-2.39	110.54	113.94
2	J	500	ANP	O2B-PB-O1B	2.39	115.00	109.87
2	I	500	ANP	O2B-PB-O1B	2.39	114.99	109.87
2	B	500	ANP	N9-C8-N7	-2.39	110.55	113.94
2	E	500	ANP	O2B-PB-O1B	2.38	114.98	109.87
2	D	500	ANP	O2B-PB-O1B	2.38	114.98	109.87
2	H	500	ANP	O2B-PB-O1B	2.38	114.98	109.87
2	C	500	ANP	O2B-PB-O1B	2.38	114.98	109.87
2	F	500	ANP	N9-C8-N7	-2.37	110.57	113.94
2	B	500	ANP	O2B-PB-O1B	2.37	114.96	109.87
2	H	500	ANP	C5-N7-C8	2.37	107.18	103.45
2	D	500	ANP	C5-N7-C8	2.36	107.17	103.45
2	I	500	ANP	C5-N7-C8	2.36	107.16	103.45
2	F	500	ANP	C5-N7-C8	2.36	107.15	103.45
2	C	500	ANP	C5-N7-C8	2.35	107.15	103.45
2	A	500	ANP	C5-N7-C8	2.34	107.13	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	ANP	C5-N7-C8	2.33	107.11	103.45
2	J	500	ANP	C5-N7-C8	2.32	107.10	103.45
2	E	500	ANP	C5-N7-C8	2.32	107.09	103.45
2	F	500	ANP	C2-N1-C6	2.29	122.49	118.73
2	G	500	ANP	C6-C5-N7	2.27	136.47	132.09
2	H	500	ANP	C2-N1-C6	2.27	122.45	118.73
2	D	500	ANP	C2-N1-C6	2.25	122.43	118.73
2	G	500	ANP	C2-N1-C6	2.25	122.43	118.73
2	E	500	ANP	C2-N1-C6	2.25	122.43	118.73
2	D	500	ANP	C6-C5-N7	2.24	136.41	132.09
2	C	500	ANP	C6-C5-N7	2.24	136.41	132.09
2	B	500	ANP	C6-C5-N7	2.24	136.40	132.09
2	B	500	ANP	C2-N1-C6	2.23	122.40	118.73
2	F	500	ANP	C6-C5-N7	2.23	136.39	132.09
2	I	500	ANP	C2-N1-C6	2.22	122.38	118.73
2	A	500	ANP	C2-N1-C6	2.22	122.38	118.73
2	I	500	ANP	C6-C5-N7	2.21	136.36	132.09
2	H	500	ANP	C6-C5-N7	2.21	136.35	132.09
2	A	500	ANP	C6-C5-N7	2.21	136.35	132.09
2	J	500	ANP	C2-N1-C6	2.21	122.36	118.73
2	C	500	ANP	C2-N1-C6	2.21	122.36	118.73
2	J	500	ANP	C6-C5-N7	2.20	136.34	132.09
2	E	500	ANP	C6-C5-N7	2.19	136.31	132.09
2	G	500	ANP	C5'-C4'-C3'	-2.03	107.91	115.21
2	H	500	ANP	C5'-C4'-C3'	-2.03	107.91	115.21
2	D	500	ANP	C5'-C4'-C3'	-2.03	107.92	115.21
2	C	500	ANP	C5'-C4'-C3'	-2.02	107.93	115.21
2	B	500	ANP	C5'-C4'-C3'	-2.02	107.94	115.21
2	I	500	ANP	C5'-C4'-C3'	-2.02	107.95	115.21
2	E	500	ANP	C5'-C4'-C3'	-2.02	107.95	115.21
2	A	500	ANP	C5'-C4'-C3'	-2.02	107.96	115.21
2	F	500	ANP	C5'-C4'-C3'	-2.01	107.96	115.21
2	J	500	ANP	C5'-C4'-C3'	-2.01	107.98	115.21

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	ANP	PB-N3B-PG-O1G
2	B	500	ANP	PB-N3B-PG-O1G
2	C	500	ANP	PB-N3B-PG-O1G
2	D	500	ANP	PB-N3B-PG-O1G

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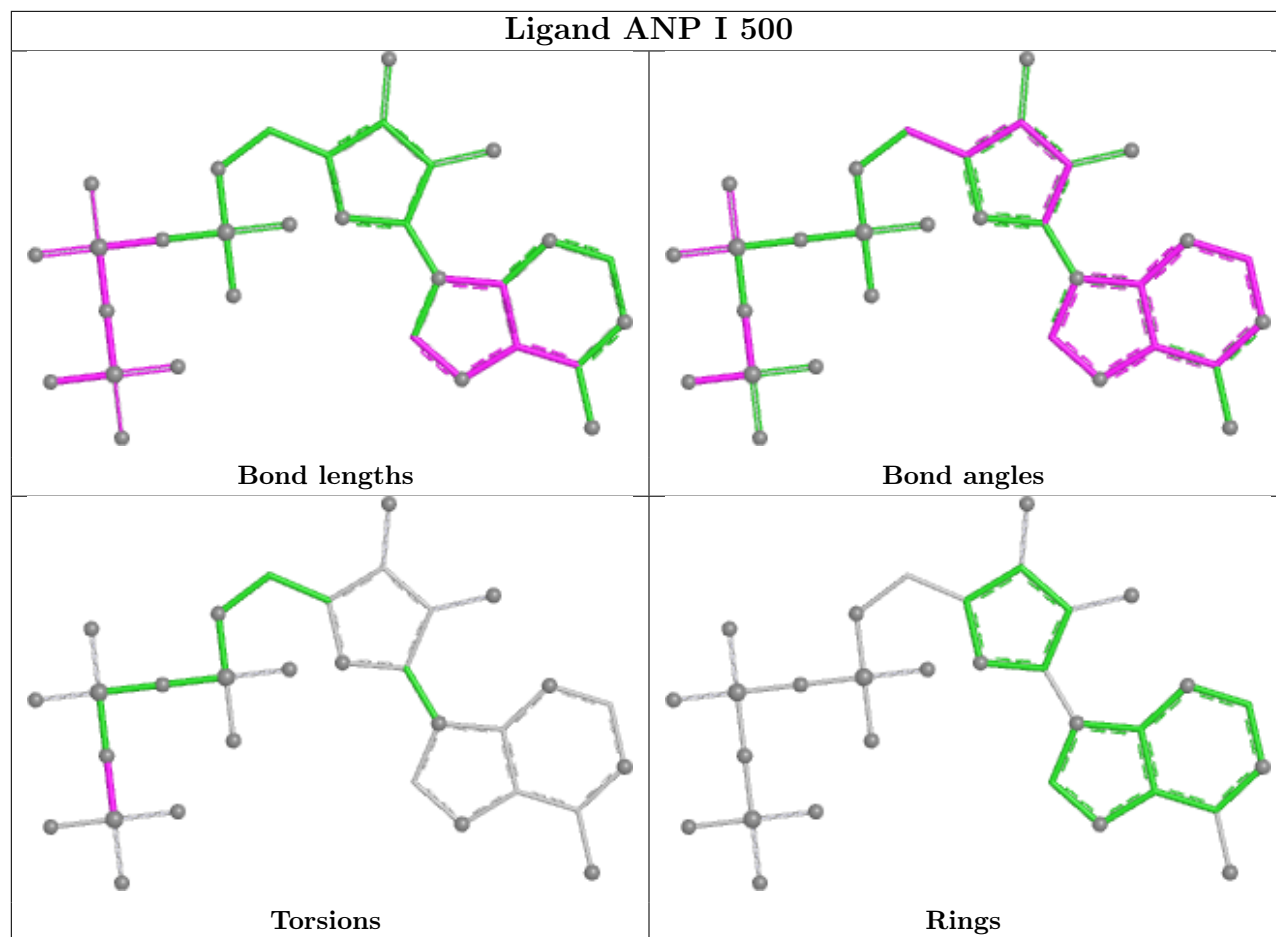
Continued from previous page...

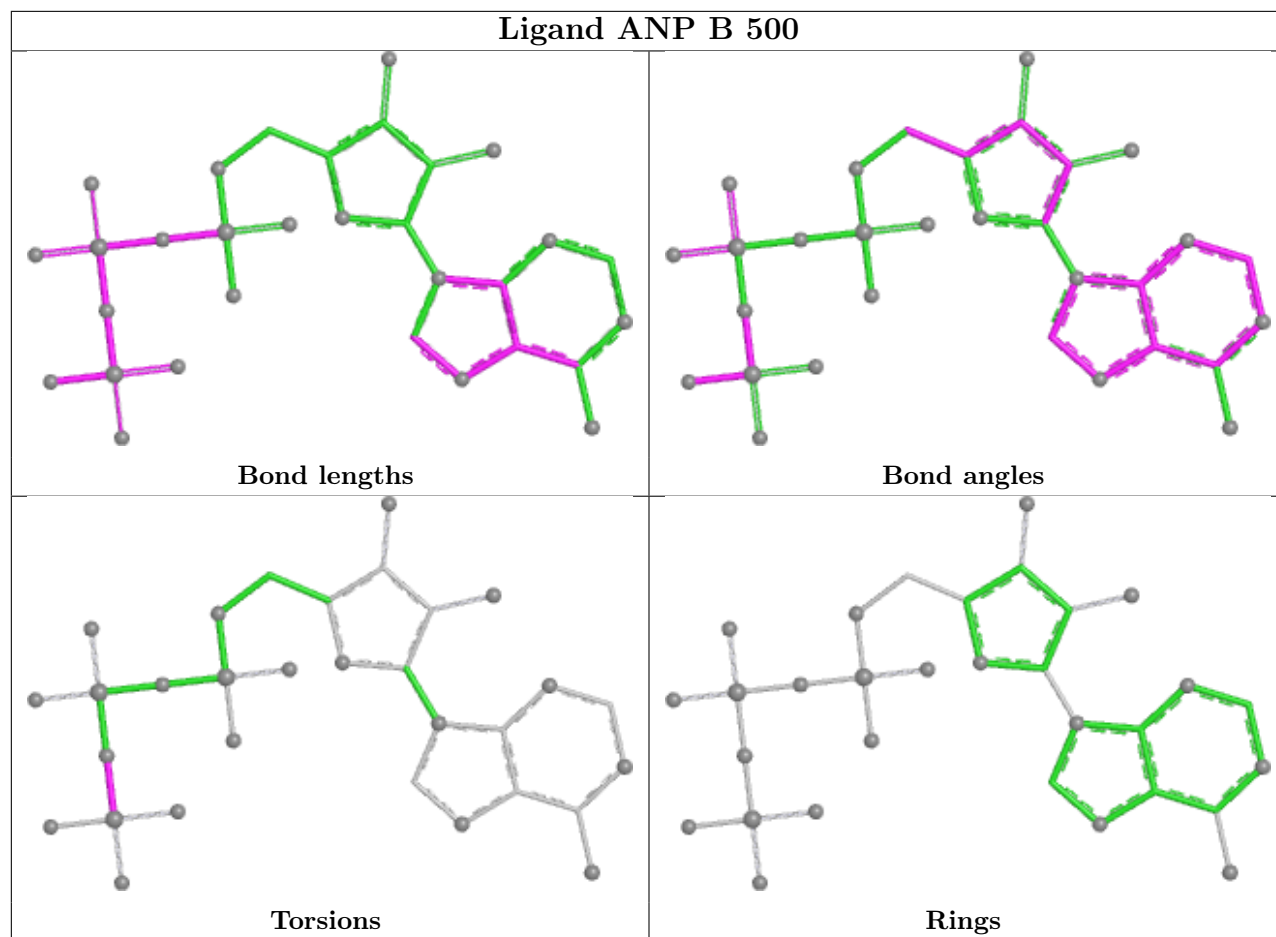
Mol	Chain	Res	Type	Atoms
2	E	500	ANP	PB-N3B-PG-O1G
2	F	500	ANP	PB-N3B-PG-O1G
2	G	500	ANP	PB-N3B-PG-O1G
2	H	500	ANP	PB-N3B-PG-O1G
2	I	500	ANP	PB-N3B-PG-O1G
2	J	500	ANP	PB-N3B-PG-O1G

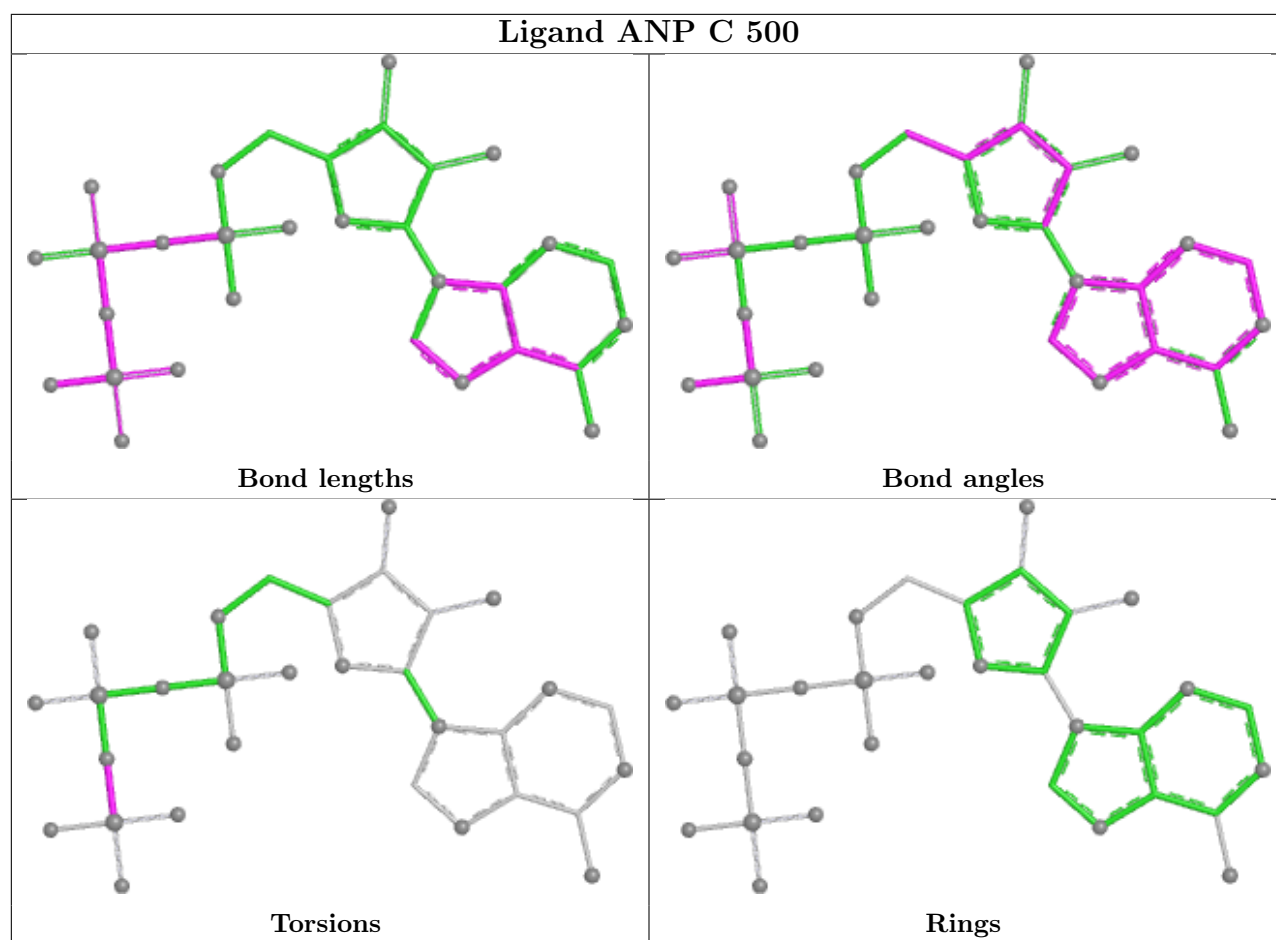
There are no ring outliers.

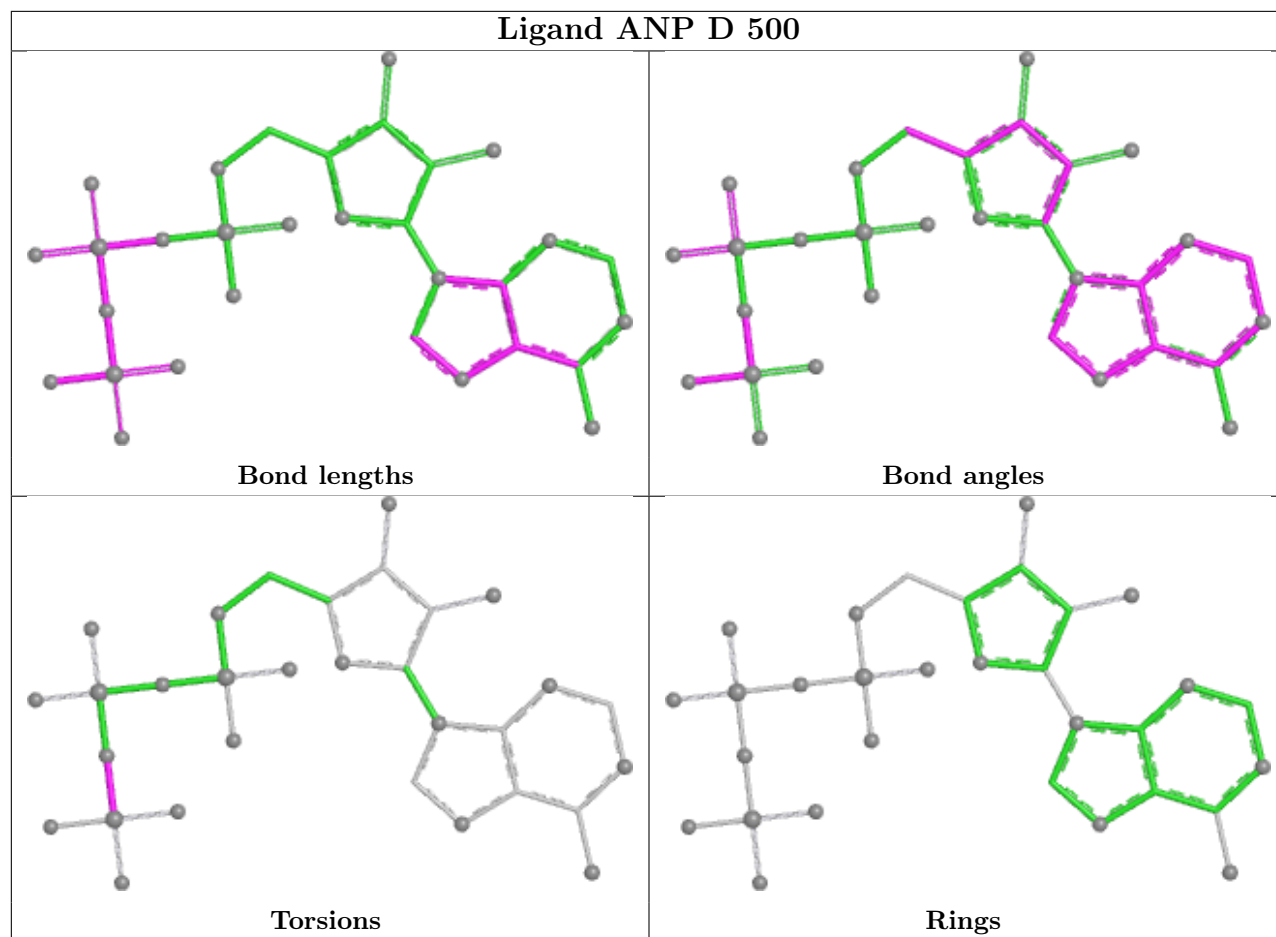
No monomer is involved in short contacts.

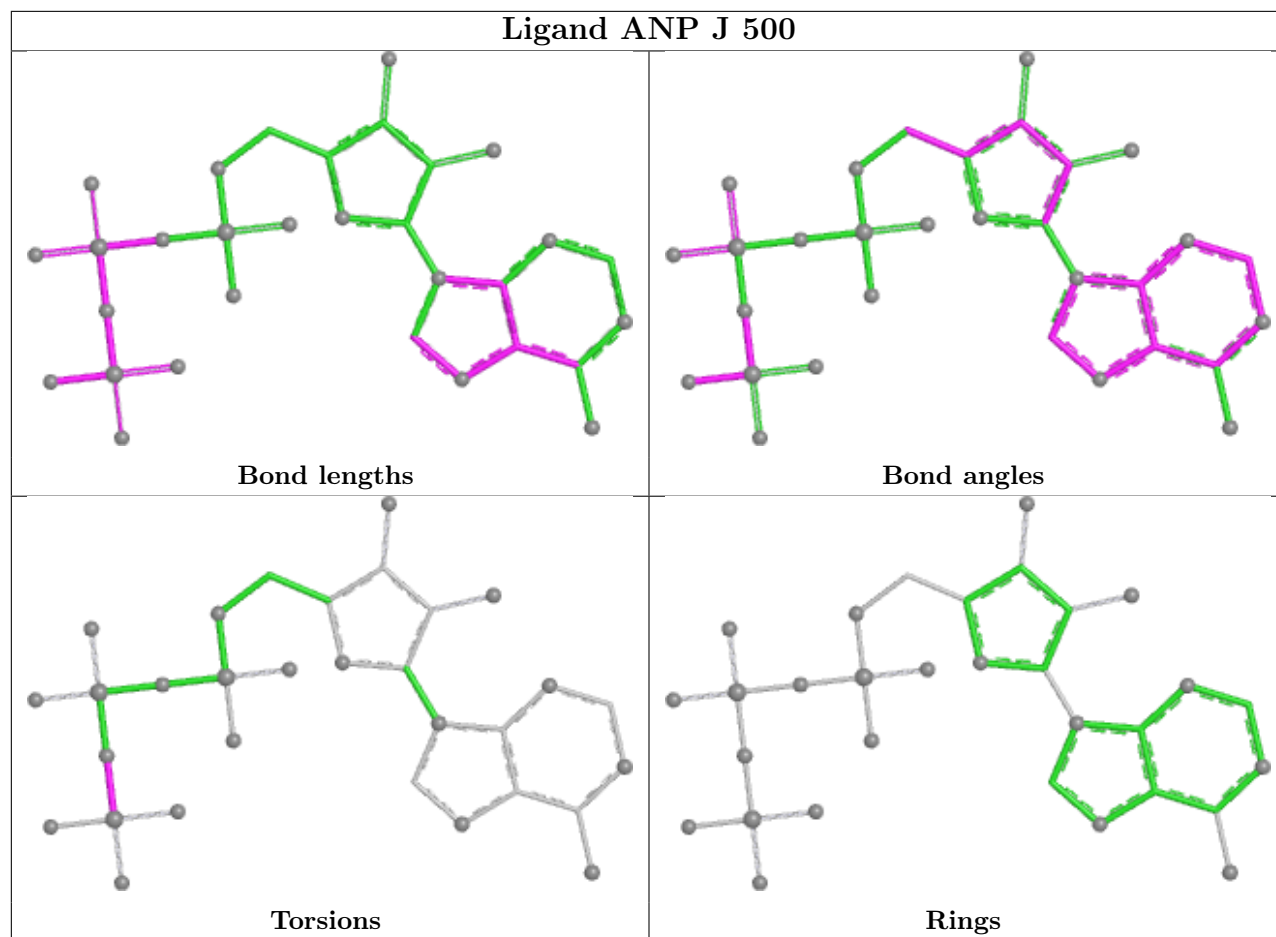
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

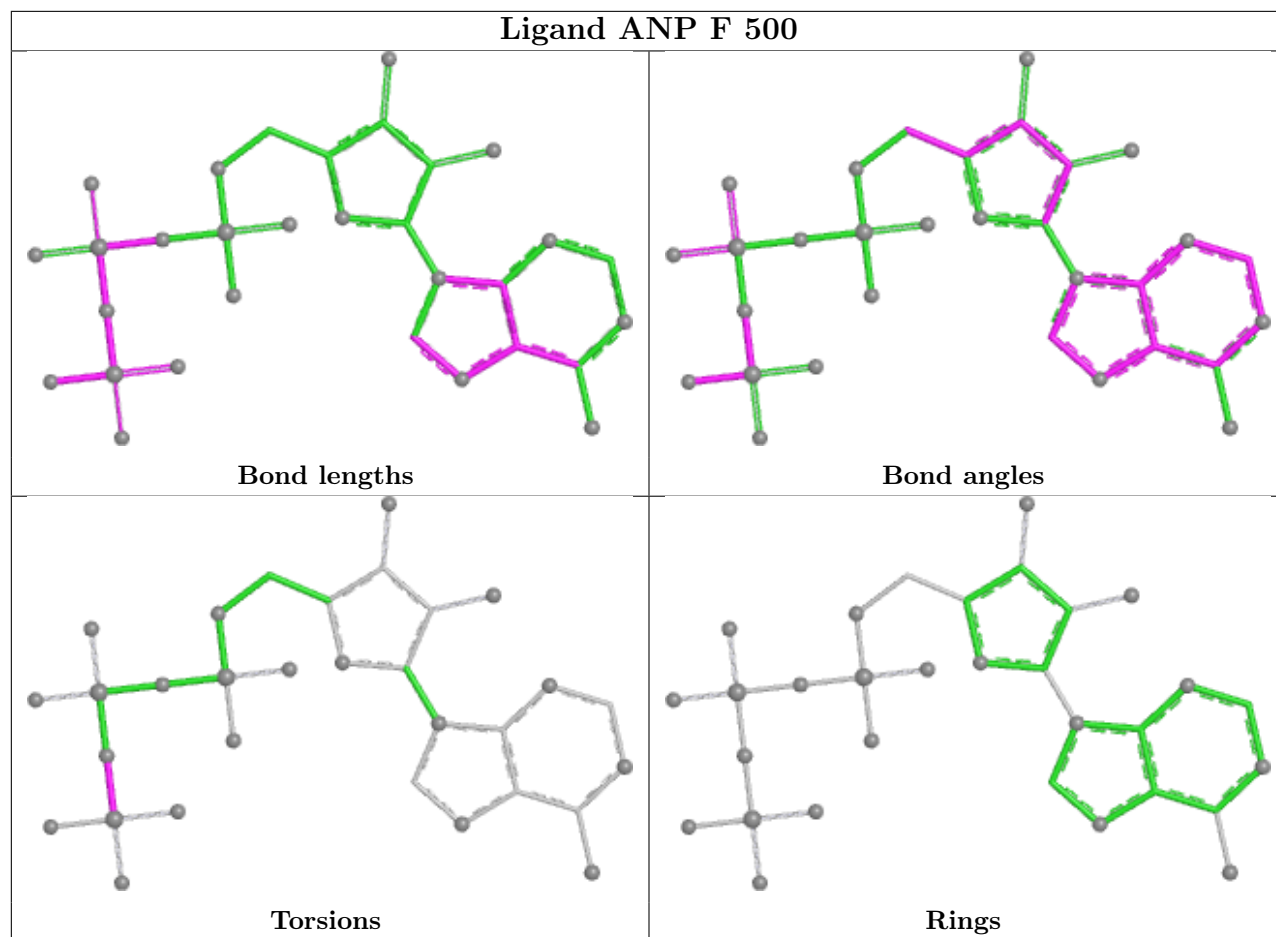


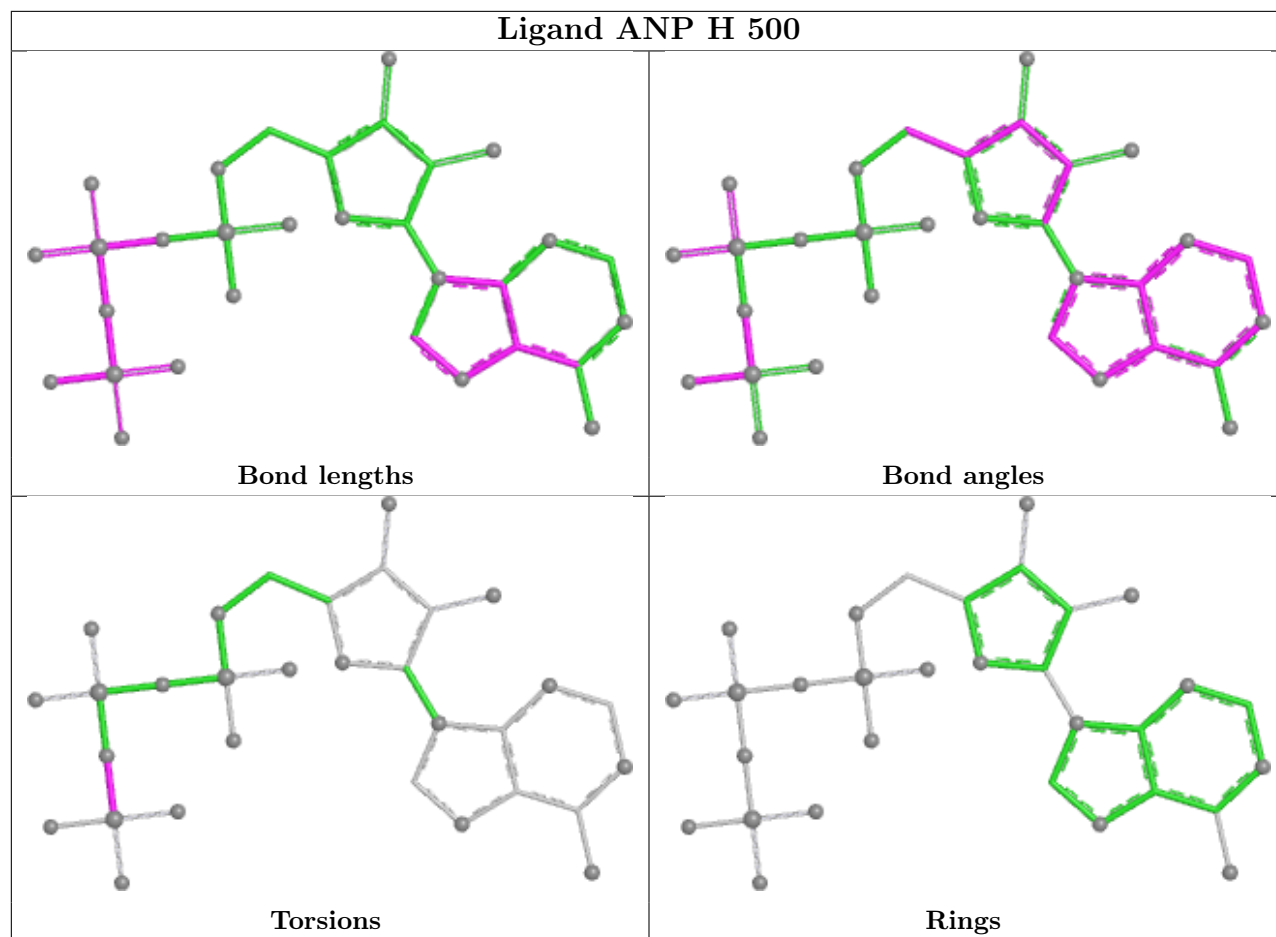


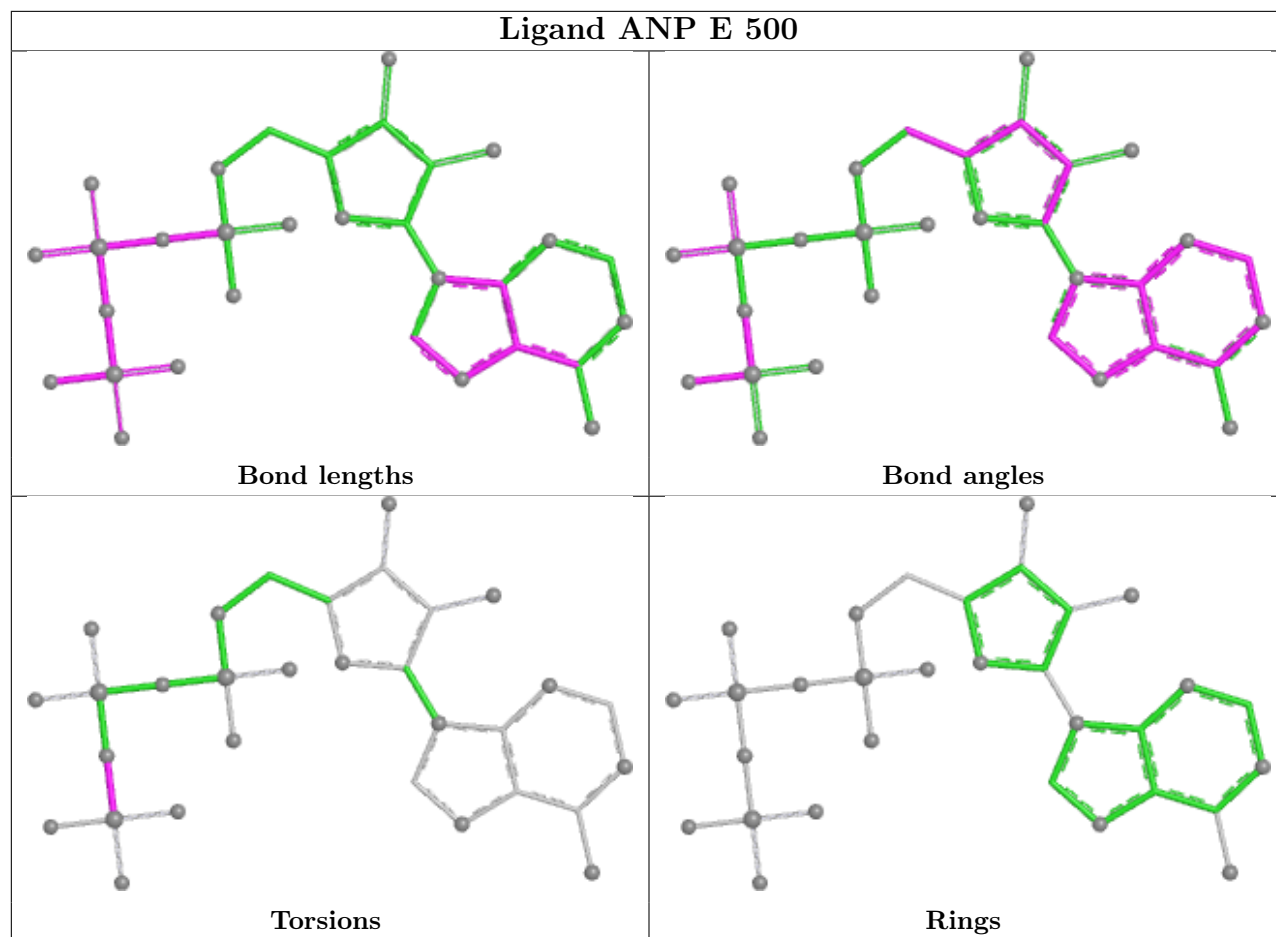


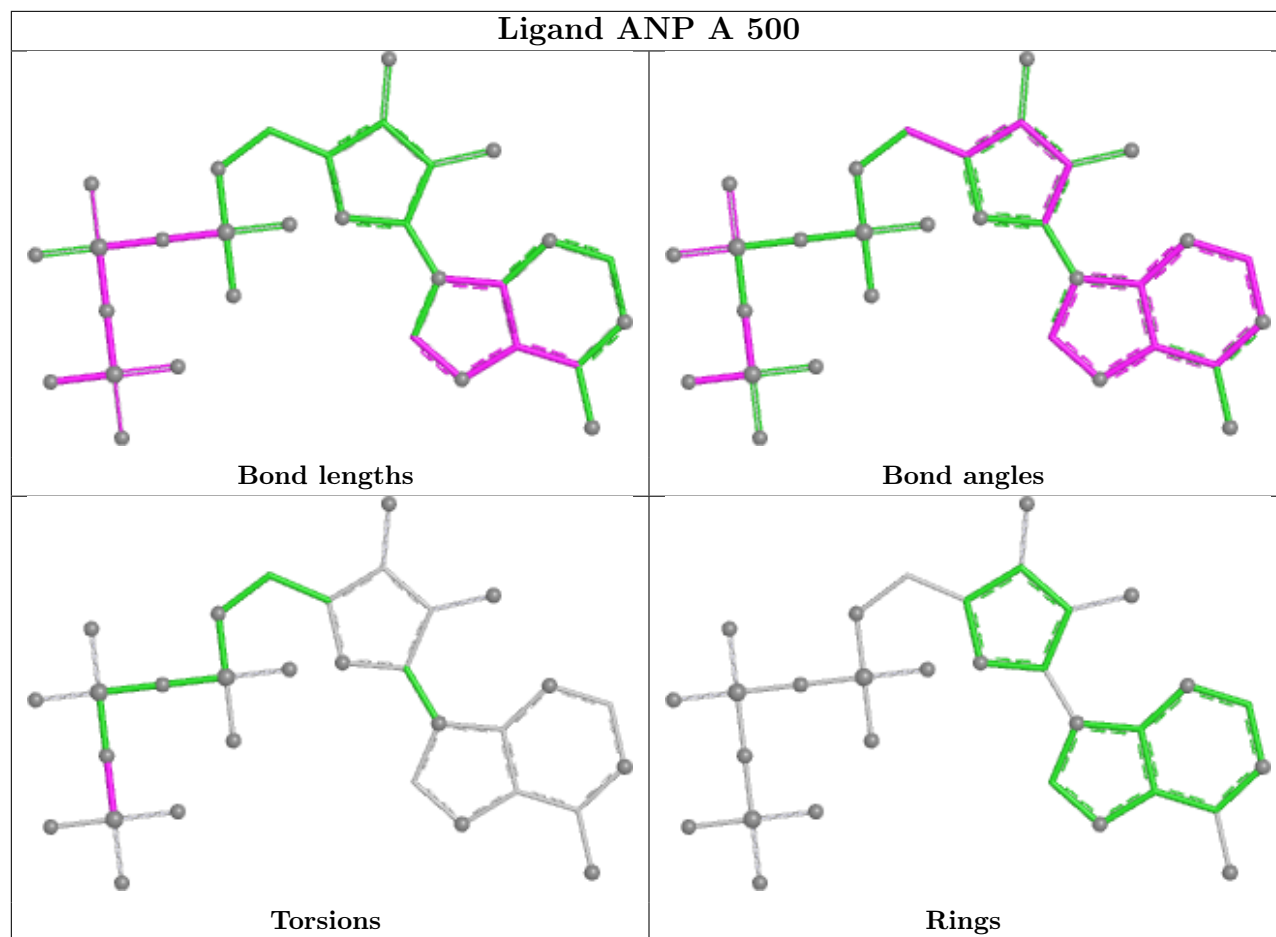


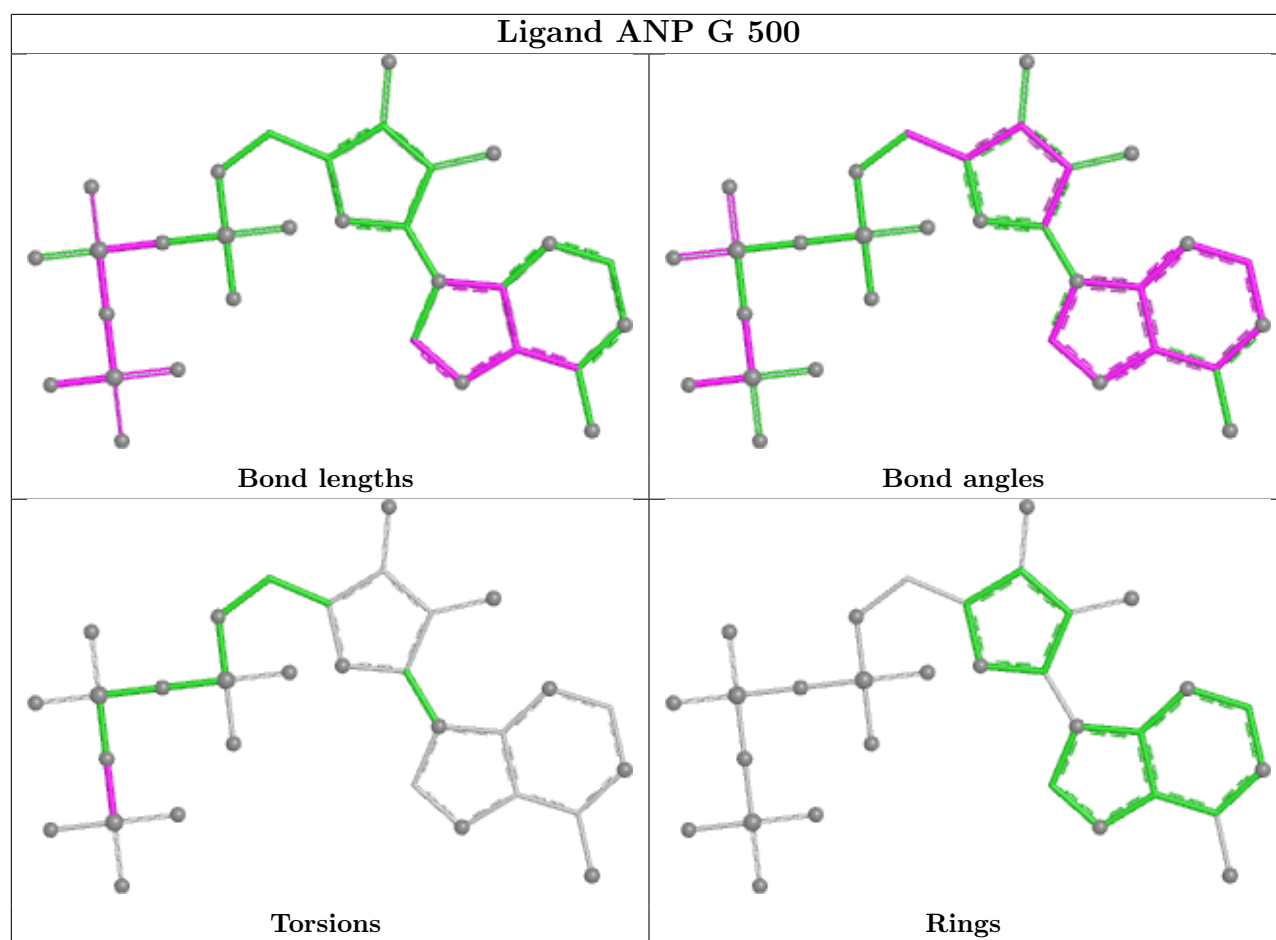












5.7 Other polymers [i](#)

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-1980. These allow visual inspection of the internal detail of the map and identification of artifacts.

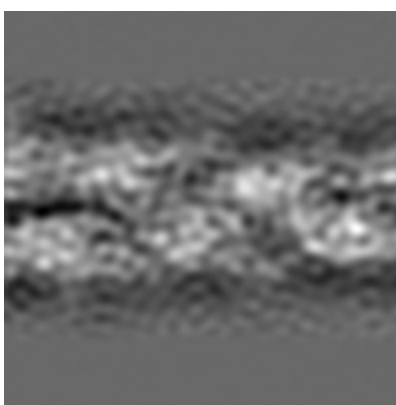
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

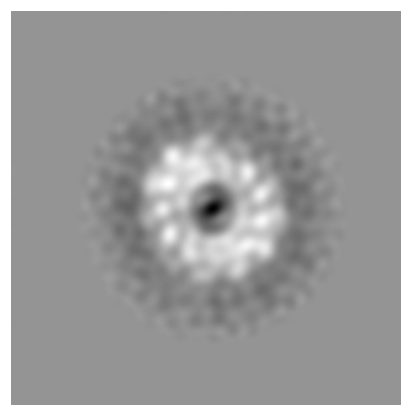
6.1.1 Primary map



X



Y



Z

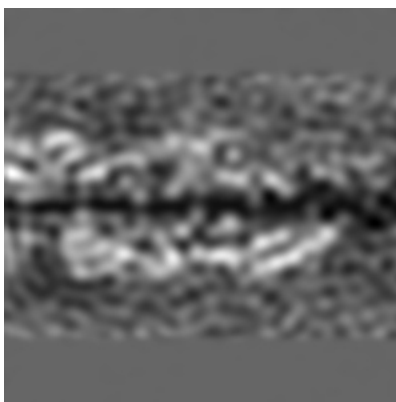
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

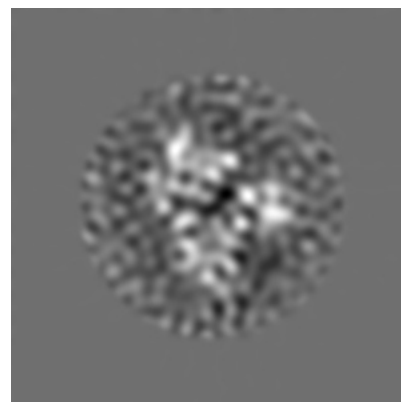
6.2.1 Primary map



X Index: 50



Y Index: 50



Z Index: 50

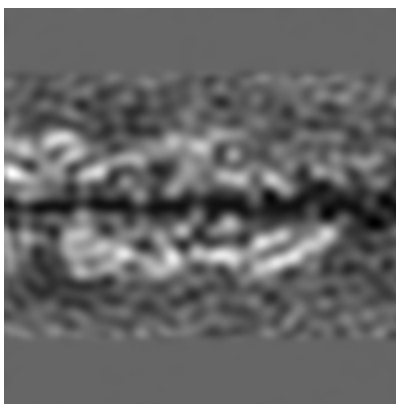
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

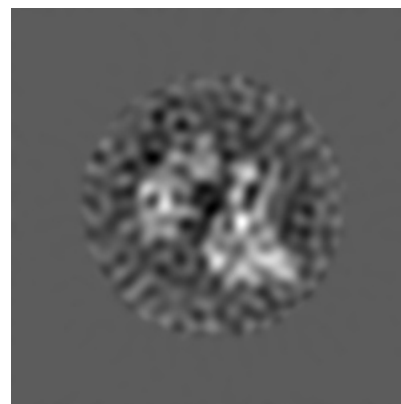
6.3.1 Primary map



X Index: 50



Y Index: 50

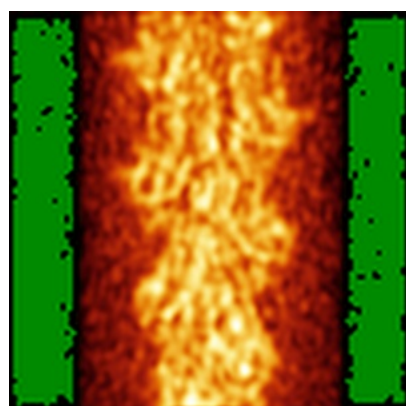


Z Index: 30

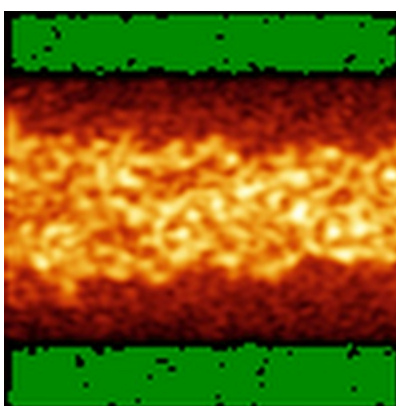
The images above show the largest variance slices of the map in three orthogonal directions.

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

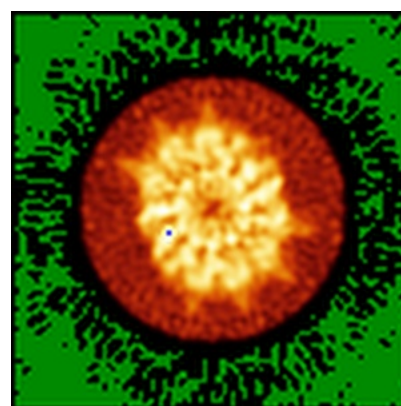
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

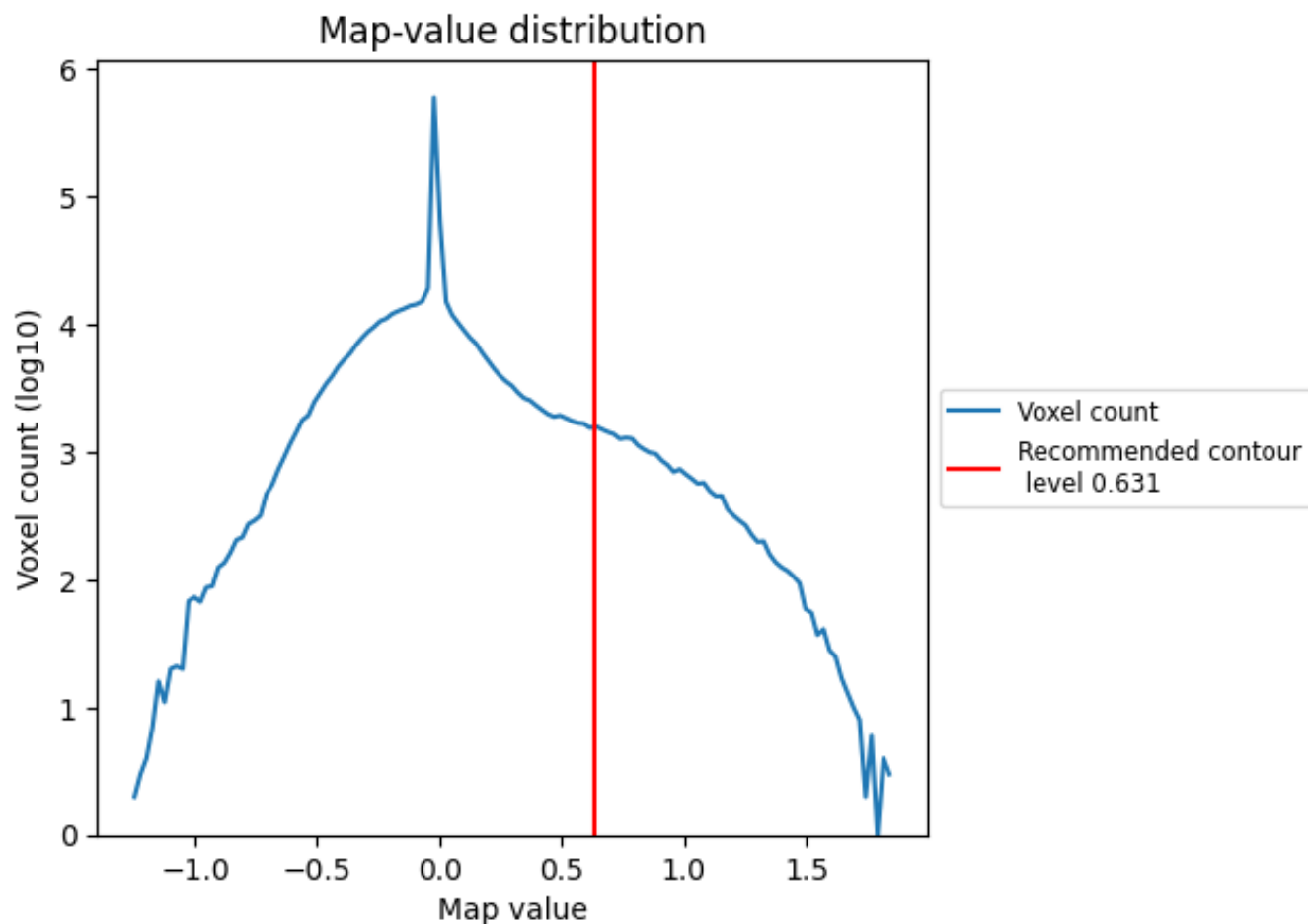
6.6 Mask visualisation

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

7 Map analysis [i](#)

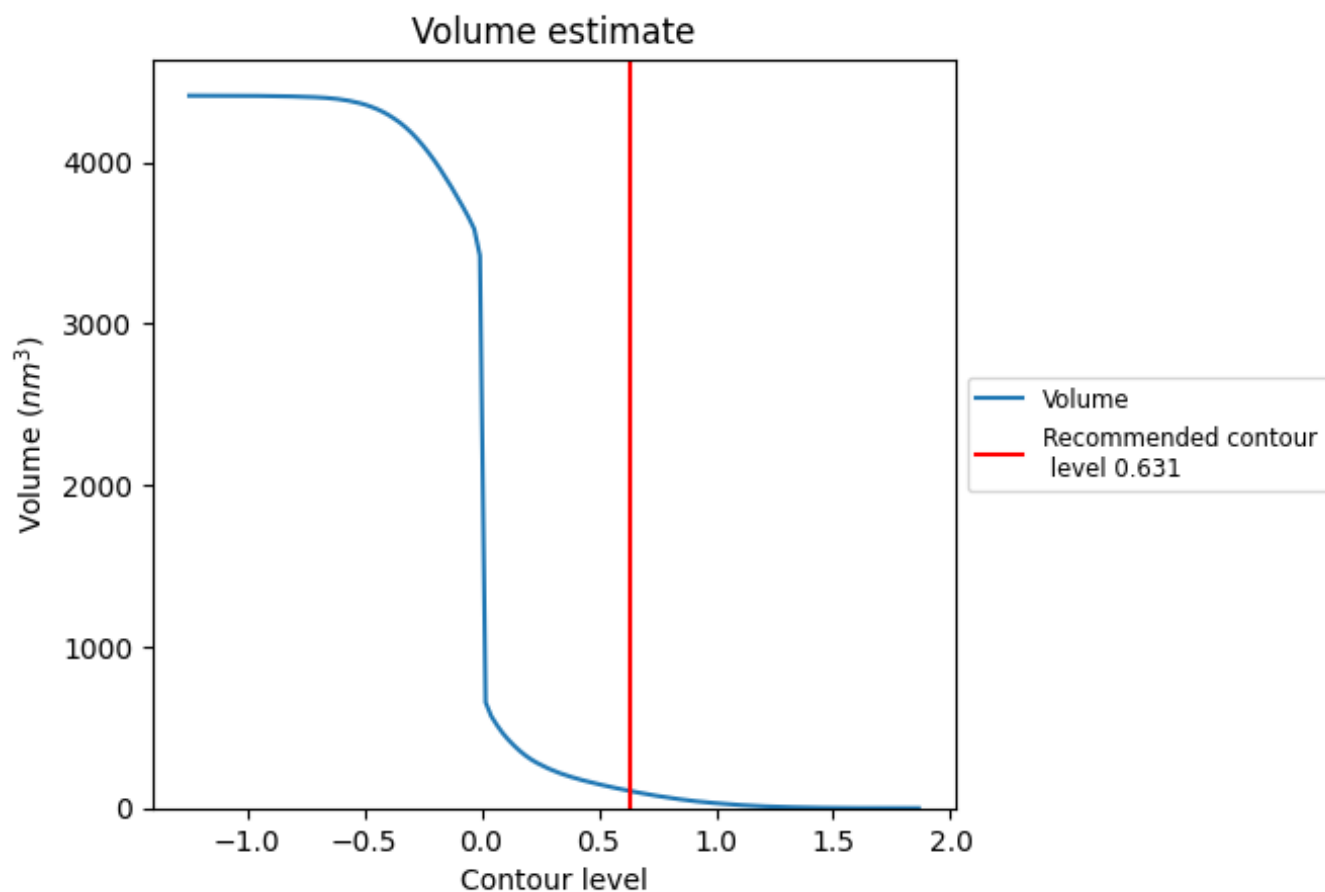
This section contains the results of statistical analysis of the map.

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.

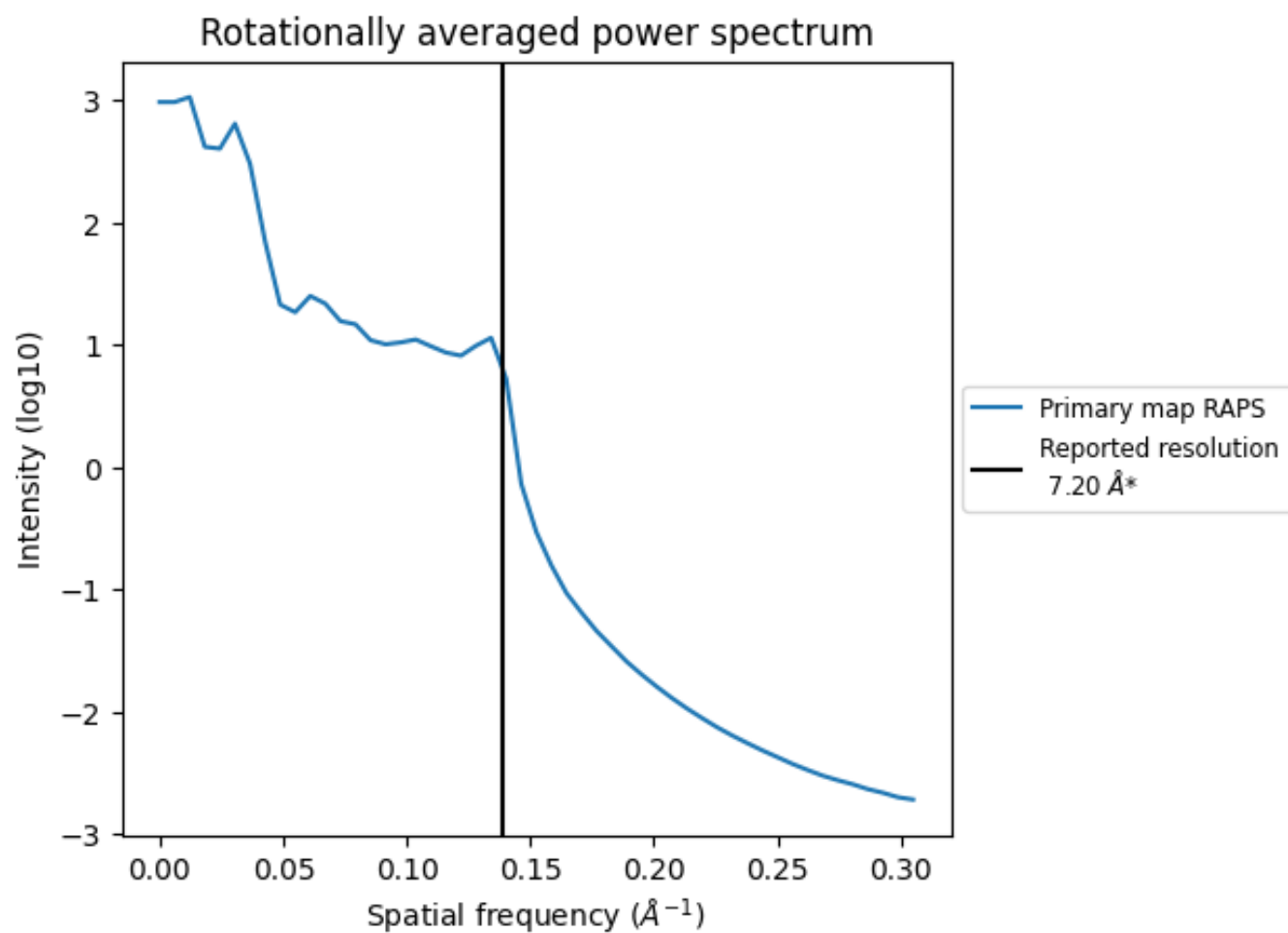
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm³; this corresponds to an approximate mass of 97 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.139 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

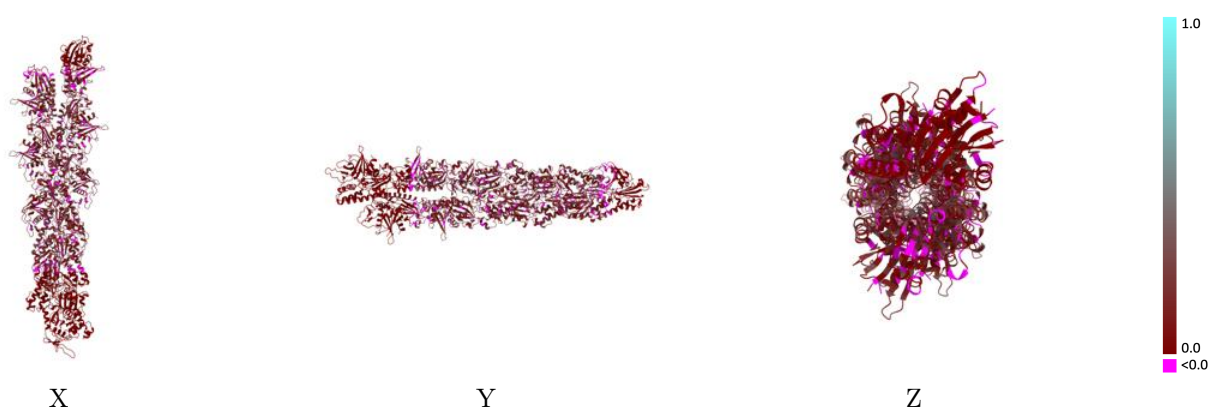
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1980 and PDB model 4A6J. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

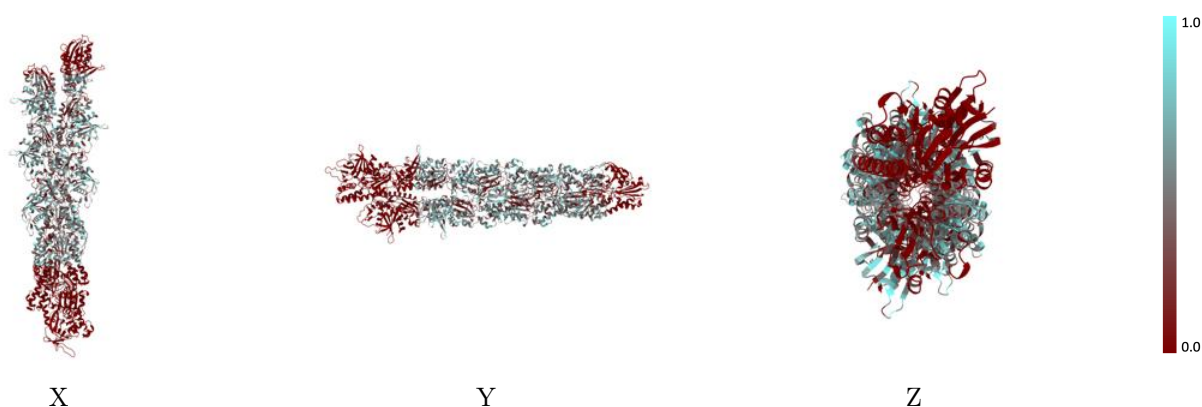
This section was not generated.

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



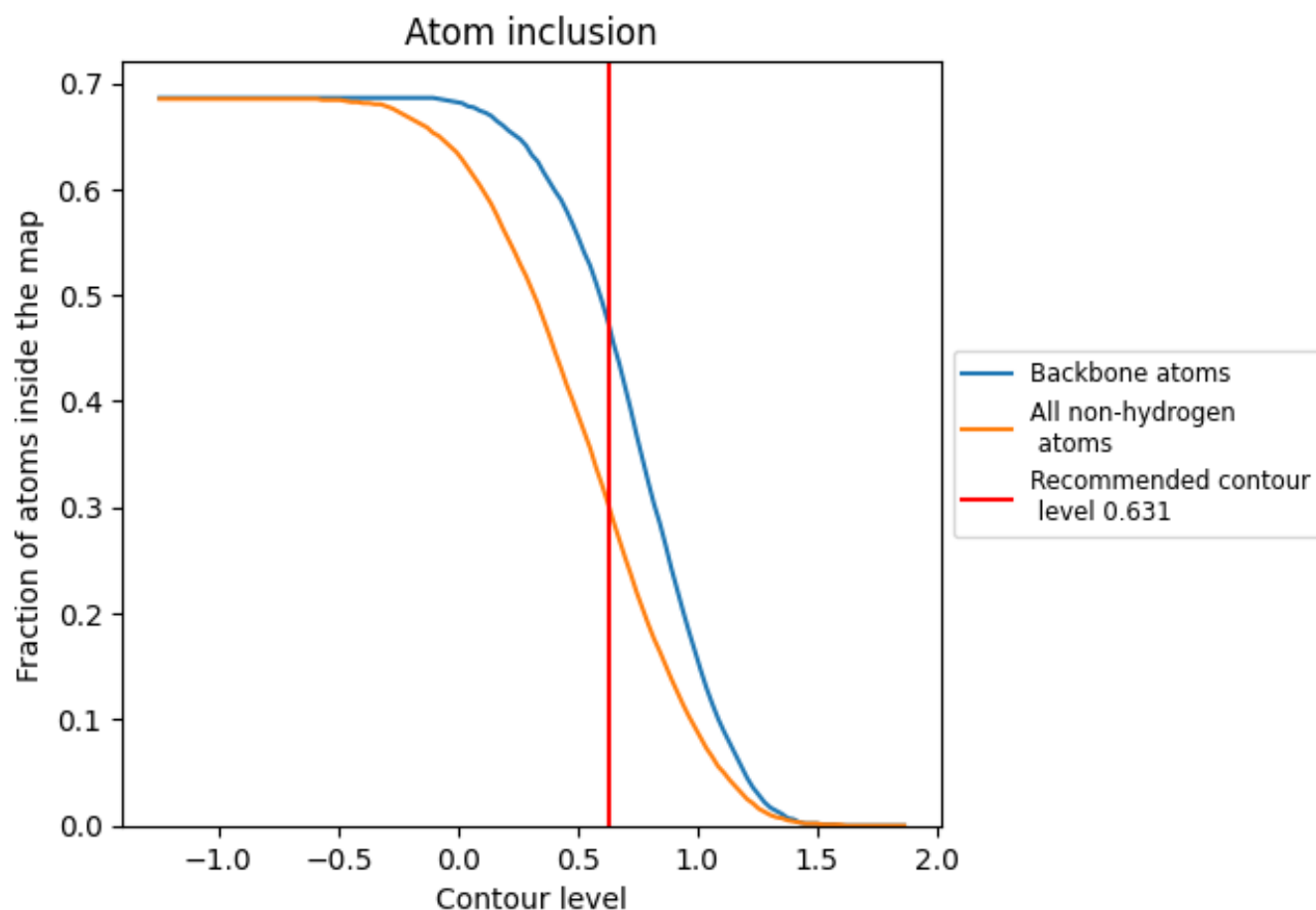
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.631).

9.4 Atom inclusion [i](#)



At the recommended contour level, 47% of all backbone atoms, 30% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.631) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3010	0.0960
A	0.0000	0.0000
B	0.0240	0.0080
C	0.2410	0.0730
D	0.4370	0.1380
E	0.4450	0.1420
F	0.4410	0.1430
G	0.4390	0.1420
H	0.4340	0.1420
I	0.3910	0.1230
J	0.1540	0.0450

1.0
0.0
<0.0