



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:21 AM UTC

PDB ID : 7PT7 / pdb_00007pt7
EMDB ID : EMD-13620
Title : Structure of MCM2-7 DH complexed with Cdc7-Dbf4 in the presence of ADP:BeF₃, state I
Authors : Saleh, A.; Noguchi, Y.; Aramayo, R.; Ivanova, M.E.; Speck, C.
Deposited on : 2021-09-26
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

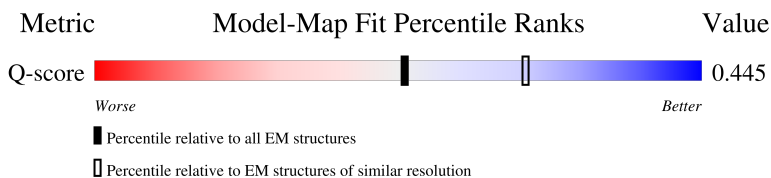
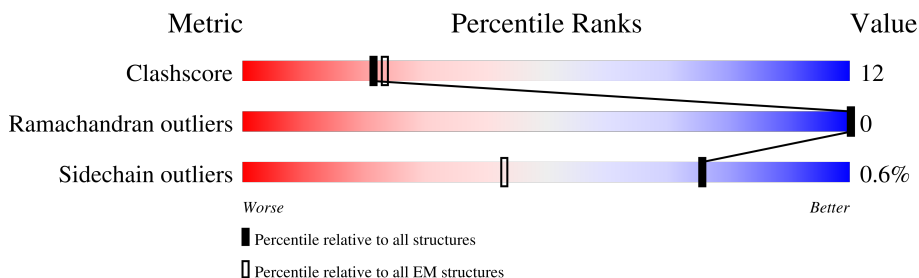
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



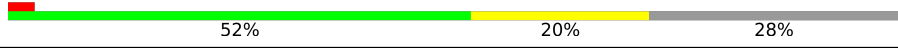
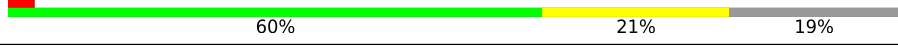
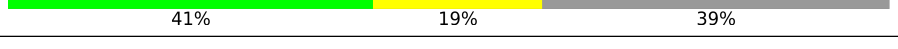
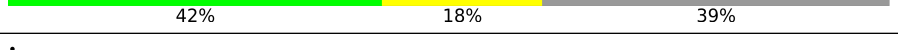
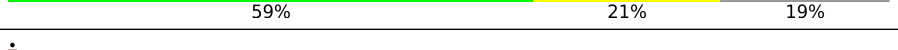
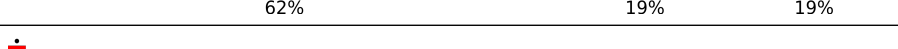
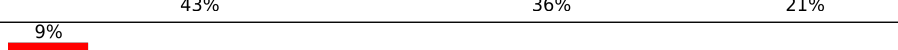
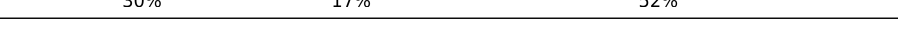
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	1	4	100% 100%
2	2	868	7% 51% 21% 28%
2	B	868	8% 51% 21% 28%
3	3	971	50% 16% 35%

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Mol	Chain	Length	Quality of chain
3	C	971	
4	4	933	
4	D	933	
5	5	775	
5	E	775	
6	6	1017	
6	F	1017	
7	7	845	
7	G	845	
8	8	507	
9	9	704	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 67420 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 Undefined Mcm4 flexible N-terminal tail.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	4	Total	C	N	O	0	0
			20	12	4	4		

- Molecule 2 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	626	Total	C	N	O	S	0	0
			4960	3124	880	937	19		
2	B	626	Total	C	N	O	S	0	0
			4960	3124	880	937	19		

- Molecule 3 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	635	Total	C	N	O	S	0	0
			4986	3152	885	936	13		
3	C	633	Total	C	N	O	S	0	0
			4966	3141	880	932	13		

- Molecule 4 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	668	Total	C	N	O	S	0	0
			5323	3341	920	1033	29		
4	D	668	Total	C	N	O	S	0	0
			5323	3341	920	1033	29		

- Molecule 5 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	628	Total	C	N	O	S	0	0
			4927	3098	844	962	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	628	Total	C	N	O	S	0	0
			4927	3098	844	962	23		

- Molecule 6 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	617	Total	C	N	O	S	0	0
			4889	3083	850	931	25		
6	F	617	Total	C	N	O	S	0	0
			4889	3083	850	931	25		

- Molecule 7 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	683	Total	C	N	O	S	0	0
			5370	3382	924	1034	30		
7	G	683	Total	C	N	O	S	0	0
			5370	3382	924	1034	30		

- Molecule 8 is a protein called Cell division control protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	402	Total	C	N	O	S	0	0
			3292	2126	551	599	16		

- Molecule 9 is a protein called DDK kinase regulatory subunit DBF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	337	Total	C	N	O	S	0	0
			2813	1793	494	514	12		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	5	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	6	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	7	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	8	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	2	1	Total 1	Mg 1	0
11	3	1	Total 1	Mg 1	0
11	4	1	Total 1	Mg 1	0
11	5	1	Total 1	Mg 1	0
11	6	1	Total 1	Mg 1	0
11	7	1	Total 1	Mg 1	0
11	8	2	Total 2	Mg 2	0
11	B	1	Total 1	Mg 1	0
11	C	1	Total 1	Mg 1	0
11	D	1	Total 1	Mg 1	0
11	E	1	Total 1	Mg 1	0
11	F	1	Total 1	Mg 1	0
11	G	1	Total 1	Mg 1	0

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

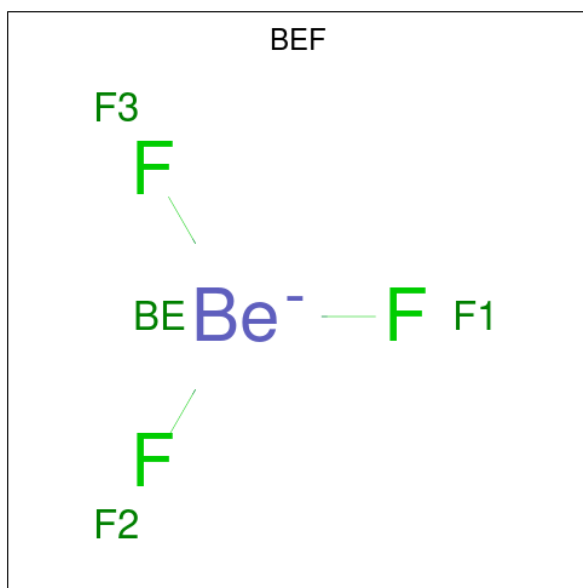
Mol	Chain	Residues	Atoms		AltConf
12	2	1	Total 1	Zn 1	0
12	4	1	Total 1	Zn 1	0
12	5	1	Total 1	Zn 1	0
12	6	1	Total 1	Zn 1	0
12	7	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
12	8	1	Total 1	Zn 1	0
12	9	1	Total 1	Zn 1	0
12	B	1	Total 1	Zn 1	0
12	D	1	Total 1	Zn 1	0
12	E	1	Total 1	Zn 1	0
12	F	1	Total 1	Zn 1	0
12	G	1	Total 1	Zn 1	0

- Molecule 13 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).



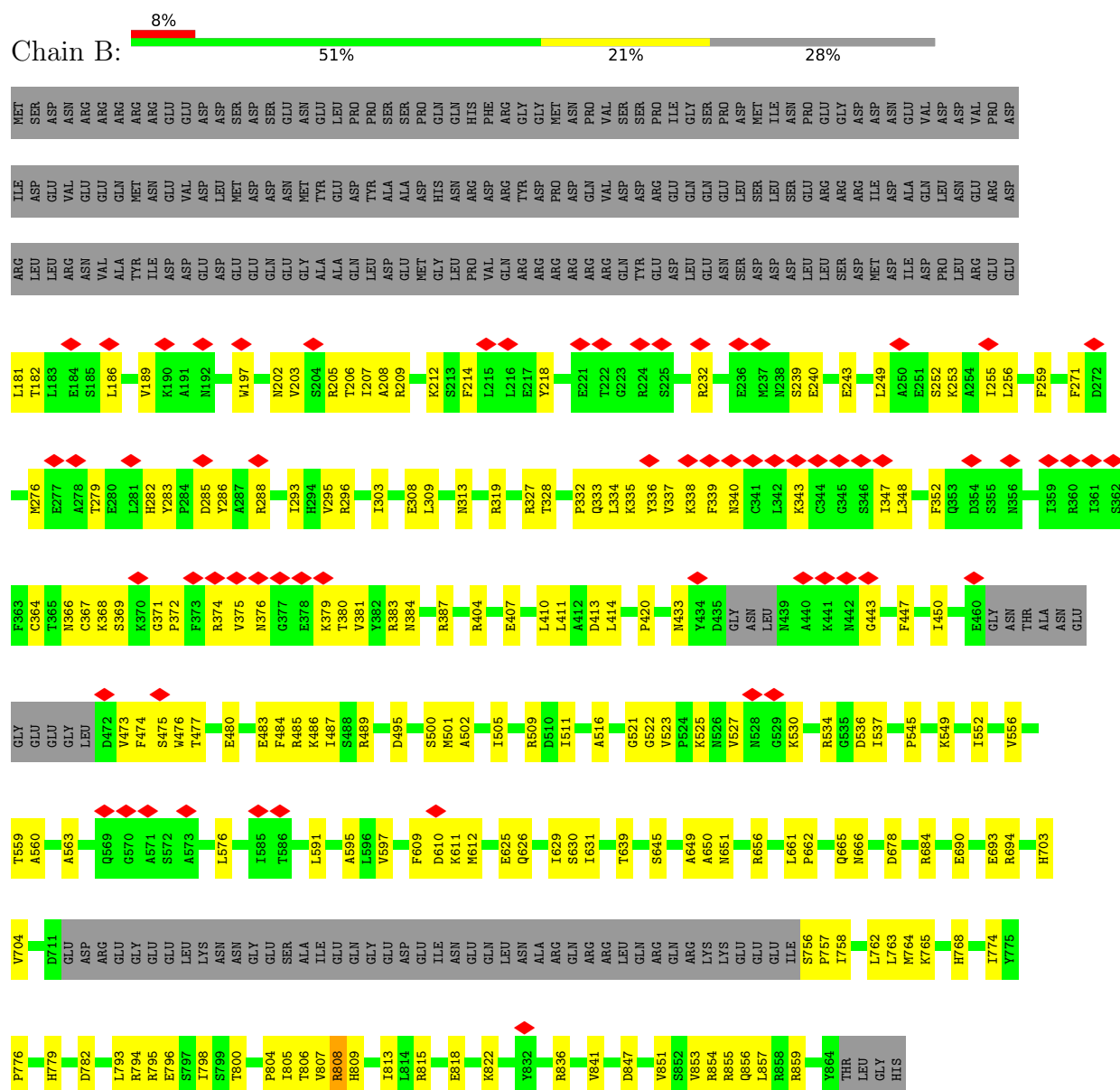
Mol	Chain	Residues	Atoms			AltConf
13	3	1	Total 4	Be 1	F 3	0
13	3	1	Total 4	Be 1	F 3	0
13	4	1	Total 4	Be 1	F 3	0
13	8	1	Total 4	Be 1	F 3	0

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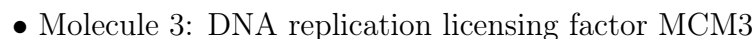
Mol	Chain	Residues	Atoms			AltConf
13	D	1	Total 4	Be 1	F 3	0
13	E	1	Total 4	Be 1	F 3	0
13	G	1	Total 4	Be 1	F 3	0

- Molecule 2: DNA replication licensing factor MCM2



- Molecule 3: DNA replication licensing factor MCM3





M407	M251	I98	MET
V408	G255	S99	GLU
G409	R256	L100	GLY
D410			SER
P411	M261	R104	THR
			GLY
K415	R291	F110	PHE
S416		W111	ASP
Q417			GLY
	V295	L115	ASP
R420	G296		ALA
		F121	THR
I430	L301		THR
G439	G304	P124	PHE
V440	S309	K127	A16
G441	ASN	M136	V25
L442	SER	D137	
T443	ASN	D138	F28
A444	THR	V139	
A445	LEU	P140	Q46
	I315	HIS	
T448	G316	PRO	A54
D449	F317	ASN	
ARG		ALA	N57
GLU	L320	SER	ASP
THR	I321	ALA	ASP
GLY	L322	VAL	GLN
E454			ASP
R455	T325	SER	ASP
		SER	ASP
A465		ARG	ALA
	H330		ASP
D473	A338	H151	GLU
E474	R339		ARG
		L155	ASP
D490	Q340		LEU
V481	M341	F161	LEU
D482			GLY
R483	A368	L166	ASP
V484	P369		ASP
		L171	ASP
A485	I377		GLY
I486	K378	K178	GLY
		L179	ASP
V499	M386	V180	ASP
M490			LEU
E491		K195	GLU
Q492	V389		LYS
Q493	E390	D216	GLU
T494	K391	A217	LYS
V495			LYS
	M395	T220	ALA
S511	G396		ALA
	S397	R224	SER
A516	H398	T255	SER
N517	L399	F226	THR
P518	R400		SER
V519	G401	E234	LEU
	D402		
D524		F244	

LEU	SER	ARG	VAL	ARG	GLU	ILE	MET	ASN	VAL	LEU	LYS	ASP	GLN	ALA	SER	ASP	MET	PHE	ASN	GLU	ILE	LYS	GLN	ASP	VAL	ARG	GLY	VAL	GLY	VAL	ARG
ARG	SER	VAL	ARG	LEU	ASN	LEU	ASN	ARG	VAL																						

• Molecule 4: DNA replication licensing factor MCM4

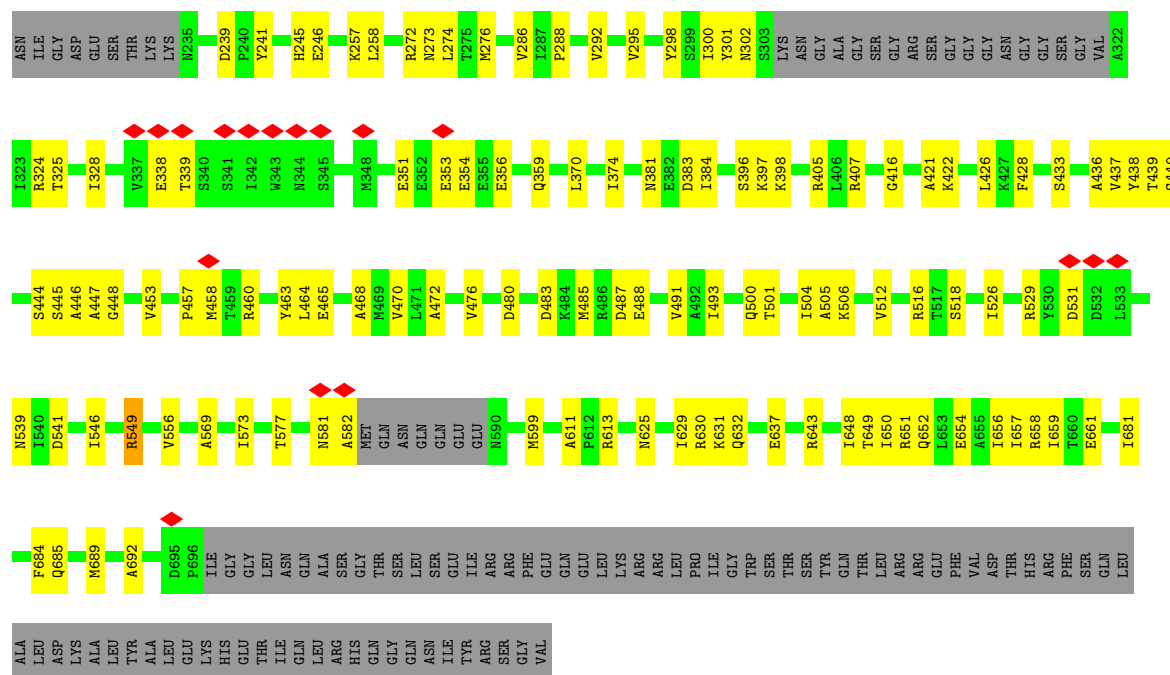
Chain D:  52% 20% 28%

MET	ASN	SER	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	
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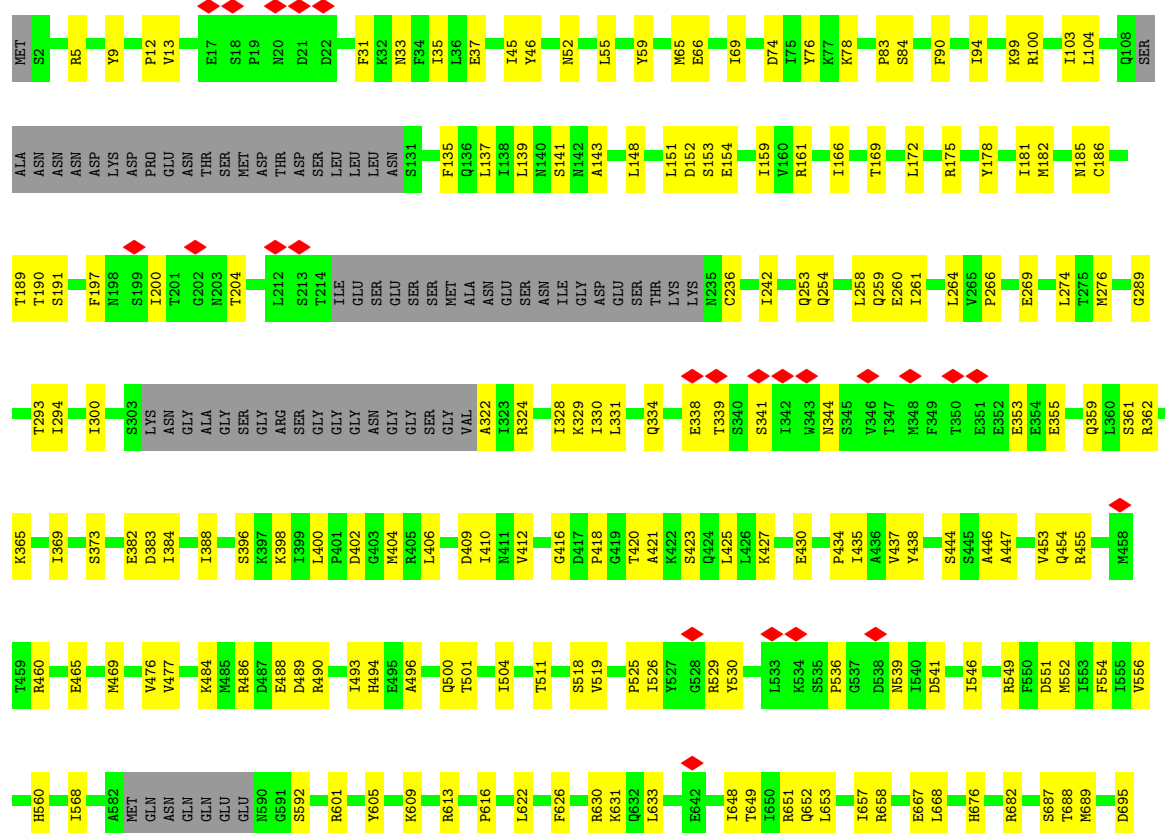
• Molecule 5: Minichromosome maintenance protein 5

Chain 5:  60% 21% 19%

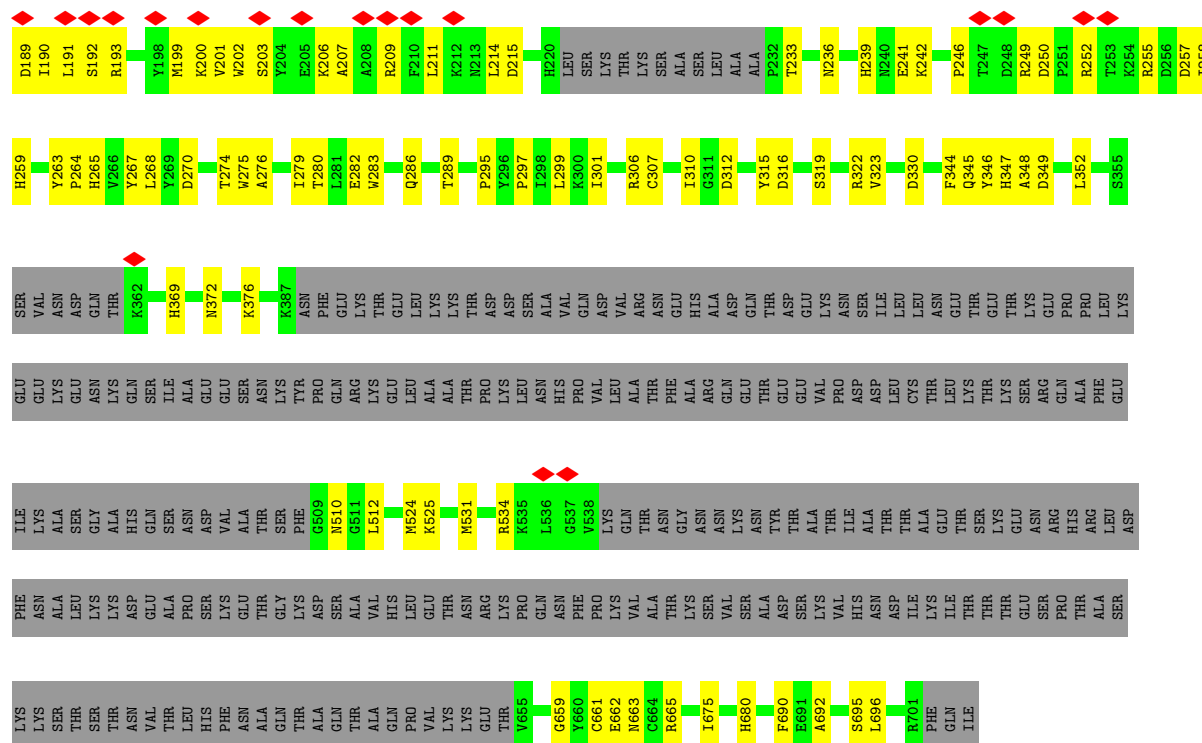
ASP	LYS	ASP	PRO	GLU	ASN	THR	SER	MET	ASP	THR	ASP	SER	LEU	LEU	LEU	LEU	ASN	S131	L137	R149	D150	L151	I159	Y160	R161	T169	Y178	R184	S191	I192	T193	I194	G202	N203	S206	L207	P208	R209	T214	ILE	GLU	SER	GLU	SER	SER	SER	MET	ALA	ASN	ASN	ASN	ASN
MET	S2	R5	Y9	N20	D21	D22	D23	I27	F31	K32	L36	R47	N52	N53	V56	K57	N58	Y59	S60	M65	E66	I69	I75	Y76	L79	S80	D81	E82	P83	I86	I87	P88	L89	F90	I94	R100	Q108	SER	ALA	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN				



• Molecule 5: Minichromosome maintenance protein 5







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30807	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.033	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size ($\text{\AA}$)	385.92, 385.92, 385.92	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, ZN, MG, ADP

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	$\# Z > 5$
2	2	0.18	0/5046	0.38	1/6817 (0.0%)
2	B	0.17	0/5046	0.35	0/6817
3	3	0.21	0/5073	0.33	1/6878 (0.0%)
3	C	0.28	0/5053	0.39	0/6852
4	4	0.25	0/5401	0.43	1/7302 (0.0%)
4	D	0.21	0/5401	0.35	1/7302 (0.0%)
5	5	0.19	0/5000	0.33	0/6766
5	E	0.19	0/5000	0.34	0/6766
6	6	0.31	0/4968	0.55	3/6704 (0.0%)
6	F	0.26	0/4968	0.49	1/6704 (0.0%)
7	7	0.28	0/5451	0.47	1/7368 (0.0%)
7	G	0.21	0/5451	0.29	0/7368
8	8	0.22	0/3373	0.47	1/4549 (0.0%)
9	9	0.20	0/2872	0.40	0/3864
All	All	0.23	0/68103	0.40	10/92057 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	280	ASP	CB-CA-C	-8.12	107.22	116.63
4	D	601	LEU	N-CA-C	-6.91	101.62	110.53
6	6	515	GLU	N-CA-C	-6.73	103.04	111.11
8	8	183	PHE	N-CA-C	-6.73	103.15	112.30
6	F	752	ARG	N-CA-C	-5.83	104.89	112.23
2	2	807	VAL	N-CA-C	-5.71	103.92	111.05
4	4	533	LEU	N-CA-C	-5.13	104.29	110.44
6	6	128	ASP	N-CA-C	-5.11	107.07	113.72
6	6	798	ARG	N-CA-C	-5.09	105.17	111.33
7	7	402	MET	N-CA-C	-5.07	105.84	112.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	20	0	6	0	0
2	2	4960	0	5001	121	0
2	B	4960	0	5002	141	0
3	3	4986	0	5053	111	0
3	C	4966	0	5034	98	0
4	4	5323	0	5387	128	0
4	D	5323	0	5387	130	0
5	5	4927	0	4982	122	0
5	E	4927	0	4982	146	0
6	6	4889	0	4913	134	0
6	F	4889	0	4913	137	0
7	7	5370	0	5426	140	0
7	G	5370	0	5426	101	0
8	8	3292	0	3249	150	0
9	9	2813	0	2821	109	0
10	2	27	0	12	0	0
10	3	27	0	12	3	0
10	4	27	0	12	1	0
10	5	27	0	12	3	0
10	6	27	0	12	2	0
10	7	27	0	12	1	0
10	8	27	0	12	6	0
10	B	27	0	12	3	0
10	C	27	0	12	1	0
10	D	27	0	12	2	0
10	E	27	0	12	2	0
10	F	27	0	12	2	0
10	G	27	0	12	0	0
11	2	1	0	0	0	0
11	3	1	0	0	0	0
11	4	1	0	0	0	0
11	5	1	0	0	0	0
11	6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	7	1	0	0	0	0
11	8	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	F	1	0	0	0	0
11	G	1	0	0	0	0
12	2	1	0	0	0	0
12	4	1	0	0	0	0
12	5	1	0	0	0	0
12	6	1	0	0	0	0
12	7	1	0	0	0	0
12	8	1	0	0	0	0
12	9	1	0	0	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
12	E	1	0	0	0	0
12	F	1	0	0	0	0
12	G	1	0	0	0	0
13	3	8	0	0	1	0
13	4	4	0	0	0	0
13	8	4	0	0	0	0
13	D	4	0	0	1	0
13	E	4	0	0	1	0
13	G	4	0	0	0	0
All	All	67420	0	67738	1583	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 12.

All (1583) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:519:VAL:HG21	3:C:534:ALA:CB	1.72	1.16
3:C:519:VAL:HG21	3:C:534:ALA:HB2	1.34	1.09
4:4:519:TYR:CD1	4:4:811:MET:HE1	1.88	1.07
4:4:519:TYR:HD1	4:4:811:MET:HE1	1.14	1.06
4:4:609:VAL:CG1	7:7:506:MET:HG2	1.88	1.03
2:B:181:LEU:N	2:B:206:THR:HG1	1.56	1.01
3:C:519:VAL:CG2	3:C:534:ALA:HB3	1.95	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3:1001:ADP:H5'2	5:5:651:ARG:HH21	1.31	0.94
4:D:642:ARG:HD3	4:D:698:LEU:HD22	1.50	0.91
2:B:794:ARG:HG2	2:B:805:ILE:HD11	1.52	0.90
3:C:519:VAL:HG21	3:C:534:ALA:HB3	1.53	0.90
3:C:519:VAL:CG2	3:C:534:ALA:CB	2.49	0.90
4:4:519:TYR:HD1	4:4:811:MET:CE	1.86	0.88
4:4:609:VAL:HG11	7:7:506:MET:HG2	1.55	0.86
6:F:362:GLN:HG3	6:F:376:THR:HG22	1.59	0.84
3:C:652:THR:HG22	3:C:654:PRO:HD2	1.61	0.82
4:4:349:CYS:HB3	4:4:352:CYS:SG	2.19	0.82
8:8:398:PHE:HA	8:8:436:TRP:HZ3	1.43	0.82
9:9:120:MET:HA	9:9:123:ASP:HB3	1.61	0.81
7:G:118:CYS:SG	7:G:198:ARG:NH1	2.53	0.81
2:B:327:ARG:HE	2:B:420:PRO:HD3	1.45	0.81
5:5:258:LEU:HB2	5:5:276:MET:HE2	1.62	0.81
2:B:794:ARG:CD	2:B:805:ILE:HD11	2.10	0.80
2:B:794:ARG:CG	2:B:805:ILE:HD11	2.11	0.80
5:5:485:MET:HE1	5:5:493:ILE:HG13	1.64	0.80
9:9:172:ILE:HA	9:9:200:LYS:HE3	1.63	0.79
6:6:312:ASP:HB2	6:6:343:PHE:HB2	1.65	0.79
2:2:195:SER:HG	2:2:263:CYS:HG	1.31	0.77
3:C:216:ASP:OD1	3:C:217:ALA:N	2.16	0.77
6:6:504:PHE:O	6:6:508:LEU:HG	1.81	0.77
7:7:722:VAL:HA	7:7:725:GLU:HG3	1.67	0.77
4:D:474:LEU:HB2	4:D:586:PRO:HD3	1.67	0.76
4:4:609:VAL:HG13	7:7:506:MET:HG2	1.67	0.76
6:6:331:THR:HA	6:6:341:ARG:HD2	1.68	0.76
6:6:505:LEU:HD23	6:6:508:LEU:HD12	1.68	0.76
2:2:693:GLU:HB2	6:6:778:LYS:HD3	1.67	0.75
4:4:422:GLU:HB2	4:4:493:ASN:HA	1.68	0.74
2:2:227:TYR:HA	2:2:230:ARG:HE	1.52	0.74
4:D:351:VAL:HG21	4:D:378:GLU:HG3	1.70	0.74
5:E:185:ASN:ND2	5:E:236:CYS:O	2.21	0.74
3:3:368:ALA:HB3	3:3:378:LYS:HE2	1.70	0.73
7:7:67:LEU:HD11	7:7:121:ILE:HD12	1.71	0.73
4:D:422:GLU:HB2	4:D:493:ASN:HA	1.71	0.73
5:5:630:ARG:NH1	5:5:648:ILE:O	2.21	0.73
6:F:341:ARG:HB3	6:F:344:TRP:HE1	1.54	0.73
2:B:376:ASN:HB3	2:B:379:LYS:HD3	1.69	0.72
8:8:138:LYS:HE3	9:9:348:ALA:N	2.04	0.72
9:9:127:TYR:HD1	9:9:173:VAL:HG22	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:794:ARG:HG2	2:2:805:ILE:HD11	1.72	0.72
8:8:133:ARG:HA	8:8:315:ARG:HG3	1.72	0.72
6:6:513:ILE:O	6:6:517:LYS:HG2	1.89	0.72
8:8:224:PRO:HG2	8:8:226:ILE:HG22	1.72	0.72
7:7:228:ARG:NH2	7:7:327:ILE:O	2.23	0.71
3:C:569:HIS:O	5:E:613:ARG:NH1	2.22	0.71
6:6:614:ARG:HA	6:6:621:TYR:HA	1.71	0.71
6:F:576:ASP:O	6:F:581:LYS:NZ	2.24	0.71
8:8:441:TRP:HB3	8:8:468:PHE:HB2	1.73	0.71
2:B:338:LYS:HD2	2:B:379:LYS:HB3	1.71	0.71
3:3:389:VAL:HG22	3:3:710:THR:HG21	1.73	0.70
3:3:384:MET:HE1	3:3:513:ILE:HB	1.73	0.70
5:E:536:PRO:HB2	5:E:695:ASP:HA	1.74	0.70
8:8:293:CYS:SG	8:8:348:HIS:CE1	2.77	0.70
4:4:639:ASP:OD1	4:4:642:ARG:NH2	2.25	0.70
4:4:471:ASP:HB3	4:4:745:GLU:HG3	1.74	0.69
6:F:600:GLY:HA2	6:F:644:MET:HB2	1.74	0.69
2:2:792:ASP:OD1	2:2:795:ARG:NH1	2.25	0.69
5:5:79:LEU:HA	5:5:86:ILE:HG21	1.75	0.69
6:6:313:MET:HE1	6:F:313:MET:HA	1.74	0.69
5:5:87:ILE:HD11	5:5:137:LEU:HD23	1.74	0.69
3:C:420:ARG:HH22	5:E:501:THR:HG21	1.58	0.69
4:4:609:VAL:CG1	7:7:506:MET:CG	2.69	0.69
5:5:405:ARG:NH2	5:5:500:GLN:OE1	2.25	0.69
8:8:433:GLU:HA	8:8:436:TRP:HD1	1.58	0.69
2:B:800:THR:HG21	2:B:856:GLN:HB2	1.75	0.69
5:E:276:MET:HE1	5:E:294:ILE:HG13	1.75	0.69
2:2:260:LEU:HB2	2:2:267:MET:HE3	1.74	0.69
4:D:335:SER:OG	4:D:395:GLN:NE2	2.26	0.68
6:F:178:LEU:HA	6:F:181:LEU:HD12	1.74	0.68
9:9:203:SER:O	9:9:207:ALA:N	2.24	0.68
8:8:64:HIS:HD2	8:8:105:PRO:HG2	1.59	0.68
6:6:620:ASP:OD1	6:6:621:TYR:N	2.26	0.68
9:9:239:HIS:HA	9:9:242:LYS:HG3	1.74	0.68
7:G:513:LEU:HD13	7:G:540:VAL:HG21	1.76	0.68
6:6:341:ARG:HG3	6:6:344:TRP:HE1	1.58	0.68
9:9:186:LYS:HB3	9:9:192:SER:HB3	1.76	0.68
2:2:485:ARG:NH1	2:2:488:SER:OG	2.27	0.68
7:G:230:ILE:HD12	7:G:239:ILE:HD12	1.74	0.68
2:2:387:ARG:NH2	2:2:407:GLU:OE1	2.27	0.68
8:8:432:GLN:OE1	8:8:436:TRP:NE1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:170:ILE:HD11	6:F:181:LEU:HD11	1.76	0.67
2:2:268:LEU:HD21	2:2:297:ILE:HD11	1.75	0.67
4:4:762:ILE:HA	4:4:817:VAL:HG12	1.76	0.67
3:3:689:ASP:OD1	7:7:606:ARG:NH2	2.27	0.67
2:B:271:PHE:HB3	2:B:295:VAL:HG21	1.76	0.67
9:9:161:GLN:NE2	9:9:162:ILE:O	2.28	0.67
3:3:584:GLU:OE1	5:5:397:LYS:NZ	2.27	0.67
3:C:480:ASP:OD1	3:C:483:ARG:NH2	2.26	0.67
3:3:384:MET:HE3	3:3:405:ILE:HD12	1.77	0.67
7:G:73:ARG:NH2	7:G:130:LYS:O	2.28	0.67
2:2:525:LYS:NZ	5:5:577:THR:OG1	2.28	0.67
2:2:620:ILE:O	2:2:624:MET:HG2	1.95	0.67
4:4:334:ARG:HD3	4:4:617:GLU:HG2	1.76	0.67
2:B:443:GLY:O	6:F:326:LYS:NZ	2.28	0.67
6:6:109:GLU:HB3	6:6:112:ARG:HH21	1.60	0.66
9:9:524:MET:HE1	4:D:271:ILE:HD13	1.76	0.66
6:F:421:LEU:HB3	6:F:444:GLY:HA3	1.76	0.66
4:4:206:ARG:NH1	4:4:247:ASN:OD1	2.29	0.66
8:8:35:LEU:HD11	8:8:48:TYR:HB3	1.76	0.66
8:8:37:ASP:O	8:8:49:LYS:N	2.28	0.66
4:D:429:ALA:O	4:D:587:ARG:NH2	2.28	0.66
3:C:448:THR:HG23	3:C:455:ARG:HH12	1.61	0.66
3:C:430:ILE:HD12	3:C:465:ALA:HB2	1.76	0.66
8:8:80:VAL:O	9:9:663:ASN:ND2	2.29	0.66
3:3:564:HIS:HE2	3:3:627:PRO:HB2	1.61	0.66
8:8:181:VAL:HG21	10:8:1001:ADP:N7	2.11	0.66
6:F:644:MET:O	6:F:649:GLN:NE2	2.28	0.66
9:9:126:ILE:HB	9:9:162:ILE:HA	1.78	0.66
7:7:270:PHE:HB2	5:E:9:TYR:HB2	1.77	0.65
3:C:577:LEU:HB2	3:C:580:GLU:HB2	1.77	0.65
5:E:276:MET:HE2	5:E:330:ILE:HD11	1.78	0.65
2:B:276:MET:HE2	2:B:293:ILE:HG12	1.77	0.65
6:F:173:GLN:OE1	6:F:176:ARG:NH2	2.29	0.65
2:2:181:LEU:N	2:2:209:ARG:HH21	1.95	0.65
2:B:384:ASN:ND2	5:E:152:ASP:OD1	2.27	0.65
2:B:475:SER:O	2:B:765:LYS:NZ	2.30	0.65
4:D:440:ARG:NH1	4:D:462:ASP:OD2	2.30	0.65
4:4:613:GLN:HB2	6:6:617:GLU:HG3	1.77	0.65
4:D:478:THR:HA	4:D:481:ILE:HG22	1.77	0.65
7:G:336:ASN:ND2	7:G:377:GLU:OE2	2.24	0.65
7:G:448:MET:HE2	7:G:450:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:144:ILE:HG13	8:8:309:LEU:HD13	1.79	0.65
2:B:495:ASP:OD1	2:B:836:ARG:NH2	2.30	0.65
8:8:272:ARG:NH2	4:D:294:ASP:OD1	2.27	0.65
8:8:375:ASP:HA	8:8:378:ASN:HB2	1.79	0.65
2:2:543:GLY:HA3	2:2:683:VAL:HG23	1.78	0.64
7:G:396:ASP:OD2	7:G:400:ARG:NH2	2.30	0.64
2:2:364:CYS:HB3	2:2:369:SER:H	1.62	0.64
6:6:504:PHE:CZ	6:6:508:LEU:HD21	2.33	0.64
4:4:559:ARG:HG3	4:4:668:ARG:HG2	1.78	0.64
7:7:417:SER:HB3	7:7:638:MET:HE2	1.80	0.64
5:E:526:ILE:HB	5:E:541:ASP:HB3	1.78	0.64
6:F:190:ARG:HA	6:F:194:PRO:HB3	1.79	0.64
8:8:472:LEU:O	8:8:475:ASN:ND2	2.30	0.64
3:3:689:ASP:O	3:3:693:LYS:NZ	2.31	0.64
7:7:514:VAL:HG21	7:7:557:LEU:HD23	1.80	0.64
2:B:285:ASP:OD2	2:B:288:ARG:NH2	2.30	0.64
5:E:649:THR:H	5:E:652:GLN:HG2	1.63	0.64
5:5:689:MET:HA	5:5:692:ALA:HB3	1.79	0.64
7:7:235:LEU:HD22	7:7:357:PRO:HG3	1.80	0.64
6:F:580:SER:N	10:F:1101:ADP:O2A	2.30	0.64
9:9:236:ASN:HA	9:9:239:HIS:CD2	2.33	0.64
3:C:377:ILE:HD13	3:C:407:MET:HE3	1.79	0.64
6:F:260:GLU:O	6:F:352:ARG:NH1	2.30	0.64
7:G:502:VAL:HG23	7:G:503:THR:HG23	1.80	0.64
6:6:314:CYS:SG	6:6:338:CYS:HB2	2.37	0.64
9:9:171:THR:HA	9:9:199:MET:HE3	1.80	0.64
6:6:528:LYS:HG2	6:6:531:ARG:HH21	1.63	0.63
6:F:186:ARG:NH2	6:F:261:ARG:O	2.29	0.63
2:2:232:ARG:NH1	2:2:283:TYR:OH	2.30	0.63
3:3:481:VAL:HG13	7:7:486:LYS:HD3	1.79	0.63
5:E:409:ASP:O	5:E:658:ARG:NH1	2.31	0.63
6:6:112:ARG:HB2	6:6:180:PHE:HB3	1.81	0.63
2:B:249:LEU:HD11	2:B:256:LEU:HD22	1.80	0.63
5:E:494:HIS:HB3	5:E:549:ARG:HH21	1.62	0.63
2:B:545:PRO:HG3	2:B:651:ASN:HD21	1.63	0.63
3:C:417:GLN:HB3	5:E:404:MET:HE1	1.80	0.63
2:2:816:ILE:HG23	2:2:837:ALA:HB1	1.80	0.63
3:3:211:TYR:HB3	7:7:8:ILE:HD11	1.79	0.63
7:G:89:GLN:OE1	7:G:102:LEU:N	2.32	0.63
6:6:608:LEU:HD23	6:6:652:ILE:HD13	1.79	0.63
4:D:634:PHE:HB3	4:D:675:ALA:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:284:CYS:SG	7:7:286:SER:OG	2.56	0.63
8:8:225:CYS:HA	8:8:227:MET:HE1	1.79	0.63
9:9:307:CYS:HB3	9:9:310:ILE:HG22	1.80	0.63
6:F:777:TYR:OH	6:F:781:ARG:NH1	2.30	0.63
3:3:712:HIS:ND1	3:3:725:ASP:OD1	2.32	0.63
8:8:86:ARG:HH12	9:9:512:LEU:HD21	1.64	0.63
2:2:394:PRO:O	6:6:673:ASN:ND2	2.31	0.63
6:6:605:ALA:N	6:6:648:ASP:OD1	2.31	0.63
8:8:350:LEU:HD21	9:9:268:LEU:HD21	1.81	0.63
7:G:542:GLU:OE2	7:G:687:ARG:NE	2.32	0.62
8:8:432:GLN:HA	8:8:435:ILE:HG12	1.81	0.62
9:9:137:ASN:O	9:9:141:LYS:N	2.30	0.62
4:4:522:LEU:HB3	4:4:541:LEU:HD11	1.81	0.62
7:7:526:PHE:HB3	7:7:567:ALA:HB2	1.81	0.62
3:3:395:ASN:ND2	7:7:421:GLU:OE1	2.31	0.62
9:9:265:HIS:HB3	9:9:282:GLU:HG3	1.81	0.62
2:B:774:ILE:HG22	2:B:776:PRO:HD3	1.81	0.62
5:E:31:PHE:CG	5:E:90:PHE:HD1	2.18	0.62
2:2:327:ARG:NH2	2:2:416:ASP:OD1	2.31	0.62
3:3:443:THR:OG1	3:3:444:ALA:N	2.31	0.62
7:7:16:ASN:ND2	7:7:100:ASP:OD2	2.33	0.62
2:B:813:ILE:HG13	2:B:841:VAL:HG21	1.81	0.62
7:G:526:PHE:HB3	7:G:567:ALA:HB2	1.79	0.62
6:6:409:GLN:HB2	6:6:412:LEU:HD12	1.80	0.62
9:9:306:ARG:NH1	9:9:312:ASP:OD1	2.32	0.62
5:5:649:THR:H	5:5:652:GLN:HG2	1.65	0.62
3:C:368:ALA:HB3	3:C:378:LYS:HE2	1.81	0.62
4:4:529:SER:HA	4:4:735:HIS:CD2	2.35	0.62
6:6:580:SER:N	10:6:1101:ADP:O2A	2.31	0.62
7:7:499:LYS:HB2	7:7:506:MET:SD	2.39	0.62
8:8:219:HIS:HA	8:8:222:PHE:HB2	1.82	0.62
4:4:587:ARG:HH22	6:6:371:GLY:HA3	1.64	0.61
3:C:244:GLU:OE1	7:G:109:ASN:ND2	2.32	0.61
3:C:647:ILE:HD12	3:C:648:PRO:HD2	1.82	0.61
5:E:90:PHE:HE2	5:E:137:LEU:HD13	1.65	0.61
5:E:409:ASP:HB3	5:E:518:SER:HB3	1.80	0.61
6:F:457:CYS:SG	6:F:458:HIS:ND1	2.69	0.61
4:4:727:LEU:O	7:7:442:LYS:NZ	2.33	0.61
5:5:31:PHE:CG	5:5:90:PHE:HD1	2.19	0.61
9:9:510:ASN:HB2	9:9:659:GLY:HA3	1.83	0.61
5:E:359:GLN:OE1	5:E:362:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:508:LYS:HA	4:4:511:GLU:HG2	1.82	0.61
5:5:32:LYS:HZ2	5:5:100:ARG:HH12	1.49	0.61
6:6:608:LEU:HA	6:6:627:ALA:HB3	1.82	0.61
5:5:656:ILE:HD11	5:5:684:PHE:CG	2.36	0.61
2:2:230:ARG:HB3	2:2:242:LEU:HD11	1.81	0.61
2:2:306:LEU:HD23	2:2:406:ARG:HG3	1.83	0.61
5:5:53:ASN:ND2	5:5:60:SER:O	2.27	0.61
9:9:118:LYS:O	9:9:121:LYS:NZ	2.32	0.61
2:2:307:ARG:O	2:2:310:ARG:NH1	2.33	0.61
2:B:243:GLU:HA	2:B:296:ARG:HB2	1.82	0.61
2:B:806:THR:OG1	2:B:808:ARG:HB3	2.01	0.61
2:2:335:LYS:HG3	2:2:383:ARG:HH21	1.65	0.61
6:6:304:LEU:HD23	6:6:323:GLN:HE21	1.66	0.61
6:6:695:LEU:HD23	6:6:792:SER:HB2	1.83	0.61
2:B:335:LYS:HE3	2:B:383:ARG:HD2	1.82	0.61
3:3:409:GLY:HA3	3:3:549:VAL:HG23	1.81	0.61
8:8:398:PHE:HD2	8:8:399:LEU:HD12	1.64	0.61
2:B:796:GLU:HB3	2:B:856:GLN:NE2	2.16	0.61
7:7:426:LEU:HG	7:7:430:LYS:HE3	1.83	0.60
8:8:334:THR:HB	9:9:299:LEU:HD11	1.82	0.60
2:B:855:ARG:HD3	2:B:859:ARG:HH21	1.66	0.60
10:3:1001:ADP:C5'	5:5:651:ARG:HH21	2.10	0.60
5:5:178:TYR:HD1	5:5:193:THR:HG22	1.66	0.60
6:6:828:TYR:OH	6:6:832:ARG:NH1	2.34	0.60
2:B:678:ASP:OD2	2:B:815:ARG:NH2	2.34	0.60
8:8:312:LEU:O	8:8:315:ARG:NH1	2.35	0.60
4:4:609:VAL:HG13	7:7:506:MET:CG	2.31	0.60
5:5:396:SER:O	5:5:398:LYS:NZ	2.33	0.60
2:B:404:ARG:NH2	6:F:387:GLU:OE2	2.35	0.60
9:9:174:ILE:HD12	9:9:202:TRP:HB2	1.84	0.60
8:8:191:ASP:O	8:8:228:ARG:NH2	2.35	0.60
8:8:361:LYS:HB3	8:8:364:GLY:HA3	1.82	0.60
8:8:398:PHE:HA	8:8:436:TRP:CZ3	2.32	0.60
5:5:476:VAL:HG12	5:5:518:SER:HB2	1.84	0.60
6:6:277:ARG:NH2	6:6:363:GLU:OE1	2.34	0.60
2:B:807:VAL:HG21	5:E:568:ILE:HG21	1.83	0.60
6:F:117:GLN:NE2	6:F:121:ASP:OD2	2.34	0.60
6:6:505:LEU:HA	6:6:508:LEU:HD12	1.82	0.60
4:D:600:GLY:HA3	7:G:549:SER:O	2.02	0.60
7:G:437:VAL:O	7:G:646:LYS:NZ	2.27	0.60
4:D:349:CYS:HB3	4:D:354:HIS:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:601:LEU:HB3	4:4:621:LEU:HD23	1.83	0.59
7:7:76:ASN:OD1	7:7:199:ARG:NH2	2.35	0.59
2:B:343:LYS:HD3	2:B:367:CYS:HB3	1.84	0.59
2:B:776:PRO:HG2	2:B:818:GLU:HB2	1.84	0.59
2:2:537:ILE:HG23	2:2:678:ASP:HB2	1.84	0.59
4:4:445:ARG:HH21	4:4:451:ARG:H	1.50	0.59
8:8:293:CYS:SG	8:8:348:HIS:CG	2.87	0.59
2:B:340:ASN:HB3	2:B:347:ILE:HA	1.84	0.59
5:E:388:ILE:HG13	5:E:425:LEU:HD21	1.82	0.59
5:E:536:PRO:HB2	5:E:696:PRO:HD3	1.85	0.59
7:7:258:ILE:HD11	7:7:300:MET:HG2	1.85	0.59
4:D:323:ASP:O	7:G:303:ARG:NH2	2.34	0.59
7:G:209:GLN:HG2	7:G:222:SER:HB2	1.84	0.59
4:4:268:VAL:O	4:4:272:MET:HG3	2.00	0.59
7:7:584:ILE:HG22	7:7:586:LEU:H	1.68	0.59
6:F:570:ASN:CG	6:F:656:MET:HE1	2.28	0.59
5:5:65:MET:SD	5:5:161:ARG:NH1	2.74	0.59
5:5:569:ALA:O	5:5:573:ILE:HG12	2.03	0.59
8:8:265:TYR:O	9:9:259:HIS:N	2.34	0.59
8:8:273:ILE:HD13	9:9:276:ALA:HB3	1.85	0.59
9:9:211:LEU:HD12	9:9:214:LEU:HB2	1.85	0.59
3:C:100:LEU:HD13	3:C:115:LEU:HD11	1.84	0.59
6:6:294:VAL:HG21	6:6:389:ALA:HB1	1.85	0.59
8:8:433:GLU:HA	8:8:436:TRP:CD1	2.36	0.59
8:8:464:LEU:HA	8:8:469:PHE:HD2	1.68	0.59
2:B:794:ARG:CD	2:B:805:ILE:CD1	2.79	0.59
2:2:231:ILE:HD13	2:2:279:THR:HG22	1.83	0.58
3:3:490:MET:HB3	3:3:542:ARG:HD3	1.84	0.58
3:3:537:ASP:OD2	7:7:573:ARG:NH1	2.36	0.58
6:6:139:GLN:HA	6:6:142:PHE:HB3	1.85	0.58
6:6:783:ASP:OD1	6:6:784:ASP:N	2.36	0.58
9:9:534:ARG:HA	4:D:179:ILE:HG12	1.84	0.58
2:B:549:LYS:HD3	2:B:649:ALA:HB1	1.85	0.58
5:E:274:LEU:HD21	5:E:328:ILE:HG13	1.84	0.58
6:6:571:ILE:HG12	6:6:711:LEU:HB2	1.83	0.58
2:2:324:VAL:HG21	2:2:418:SER:HB2	1.85	0.58
6:F:309:PHE:HB3	6:F:344:TRP:HB3	1.86	0.58
5:5:90:PHE:CD2	5:5:137:LEU:HD22	2.39	0.58
7:7:281:LEU:HB2	7:7:298:LEU:HD11	1.86	0.58
7:G:537:ILE:O	7:G:541:MET:HG3	2.04	0.58
5:5:625:ASN:HD22	5:5:681:ILE:HG12	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:400:ARG:HH11	7:G:637:LYS:HE3	1.69	0.58
5:5:464:LEU:HD21	5:5:470:VAL:HG21	1.85	0.58
7:7:413:ARG:HH21	7:7:631:THR:HG23	1.67	0.58
8:8:76:LYS:HB3	8:8:118:ALA:HB3	1.85	0.58
4:D:794:THR:HG22	4:D:796:ARG:H	1.68	0.58
6:F:702:THR:HG22	6:F:705:ILE:HD12	1.86	0.58
6:6:119:LEU:HB3	6:6:136:TYR:CE2	2.37	0.58
4:D:228:LYS:HA	4:D:231:ASN:HD22	1.68	0.58
4:D:578:LEU:HD12	4:D:630:CYS:HB3	1.85	0.58
2:2:319:ARG:HG3	2:2:427:THR:HG22	1.86	0.58
5:5:684:PHE:CD2	5:5:689:MET:HE1	2.39	0.58
6:6:706:MET:HA	6:6:712:PHE:HZ	1.69	0.58
7:7:275:SER:OG	7:7:277:THR:O	2.22	0.58
7:7:452:GLY:H	7:7:694:ARG:HH11	1.51	0.58
3:C:409:GLY:O	3:C:518:PRO:HD3	2.03	0.58
5:E:412:VAL:HG13	5:E:552:MET:HG3	1.86	0.58
3:3:244:GLU:OE1	7:7:109:ASN:ND2	2.37	0.57
7:7:267:TYR:CE2	7:7:288:GLU:HG2	2.39	0.57
9:9:125:ARG:HB3	9:9:170:VAL:HA	1.85	0.57
5:E:434:PRO:HB2	5:E:435:ILE:HD12	1.86	0.57
2:2:338:LYS:HD2	2:2:379:LYS:HB3	1.85	0.57
2:2:445:PRO:HB3	6:6:327:TYR:HE1	1.70	0.57
3:3:701:THR:HG23	3:3:733:LEU:HD21	1.86	0.57
7:7:162:ARG:NH2	7:7:178:ASN:OD1	2.37	0.57
7:7:179:ASP:OD1	7:7:180:ALA:N	2.35	0.57
2:B:477:THR:O	2:B:480:GLU:HG3	2.03	0.57
2:B:609:PHE:HB3	2:B:650:ALA:HB2	1.86	0.57
5:E:626:PHE:CZ	5:E:630:ARG:HD2	2.38	0.57
6:F:310:THR:HB	6:F:345:THR:HB	1.86	0.57
10:3:1001:ADP:H5'2	5:5:651:ARG:NH2	2.11	0.57
4:4:735:HIS:CE1	4:4:737:SER:HB2	2.39	0.57
6:6:306:LYS:HA	6:6:322:GLU:HA	1.84	0.57
4:4:602:THR:OG1	4:4:603:ALA:N	2.38	0.57
9:9:345:GLN:HG2	9:9:346:TYR:CD1	2.39	0.57
2:B:336:TYR:HB2	2:B:381:VAL:HB	1.86	0.57
3:C:440:VAL:HG13	3:C:445:ALA:HB2	1.85	0.57
2:2:343:LYS:HZ3	2:2:372:PRO:HD3	1.68	0.57
9:9:182:ILE:HG22	9:9:184:LEU:H	1.69	0.57
2:B:279:THR:O	2:B:283:TYR:N	2.35	0.57
4:D:519:TYR:CE1	4:D:538:LYS:HE2	2.39	0.57
3:C:442:LEU:HD13	3:C:486:ILE:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:276:MET:HG2	5:5:328:ILE:HB	1.86	0.57
5:E:486:ARG:HG2	5:E:488:GLU:HG2	1.85	0.57
6:F:312:ASP:HB2	6:F:343:PHE:HB3	1.87	0.57
4:4:367:GLU:HG3	6:6:419:SER:HB3	1.85	0.57
6:6:699:LEU:HD13	6:6:701:MET:HE2	1.87	0.57
10:B:901:ADP:O3B	6:F:798:ARG:NH2	2.37	0.57
5:E:90:PHE:CE2	5:E:137:LEU:HD13	2.40	0.57
5:E:369:ILE:HD12	5:E:592:SER:HA	1.85	0.57
3:3:390:GLU:OE1	3:3:467:ARG:NH1	2.33	0.57
7:7:86:LEU:HD22	7:7:207:LEU:HD11	1.86	0.56
9:9:129:ASP:O	9:9:148:ARG:NH1	2.38	0.56
2:2:202:ASN:OD1	2:2:205:ARG:NH1	2.38	0.56
4:4:179:ILE:HG22	4:4:186:SER:HB3	1.87	0.56
4:4:234:ARG:HG3	4:4:280:MET:HE3	1.88	0.56
7:7:479:ARG:NH1	7:7:517:ASP:O	2.38	0.56
2:B:552:ILE:O	2:B:556:VAL:HG23	2.05	0.56
6:F:306:LYS:HG2	6:F:322:GLU:HA	1.86	0.56
2:2:797:SER:HB2	2:2:804:PRO:HA	1.87	0.56
3:3:216:ASP:OD1	3:3:219:THR:OG1	2.23	0.56
4:4:474:LEU:HD23	4:4:748:THR:HG22	1.88	0.56
5:E:455:ARG:NH1	5:E:460:ARG:O	2.36	0.56
6:F:158:LEU:HD11	6:F:166:LEU:HD23	1.86	0.56
2:2:285:ASP:OD2	2:2:288:ARG:NH1	2.37	0.56
8:8:127:GLU:HB2	8:8:130:THR:HG23	1.88	0.56
5:E:353:GLU:HG3	5:E:601:ARG:HH21	1.71	0.56
2:2:289:ILE:O	2:2:290:HIS:ND1	2.39	0.56
2:2:622:GLU:OE1	5:5:445:SER:N	2.38	0.56
5:5:65:MET:HE1	5:5:159:ILE:HG21	1.87	0.56
4:D:195:ARG:HH22	4:D:279:CYS:HA	1.71	0.56
5:E:490:ARG:HD3	5:E:546:ILE:HD11	1.88	0.56
3:3:293:ASN:HB3	3:3:327:TYR:HB2	1.88	0.56
4:4:640:SER:O	6:6:601:LYS:NZ	2.39	0.56
7:7:140:ASP:OD1	7:7:199:ARG:NE	2.37	0.56
2:2:260:LEU:HD21	2:2:297:ILE:HD13	1.88	0.56
5:5:657:ILE:O	5:5:661:GLU:HG2	2.06	0.56
2:B:340:ASN:HA	2:B:348:LEU:HG	1.86	0.56
4:D:239:SER:OG	4:D:299:LYS:NZ	2.39	0.56
3:3:367:LEU:HD12	3:3:421:PHE:HE2	1.72	0.55
7:7:209:GLN:HG3	7:7:222:SER:HB2	1.88	0.55
7:7:396:ASP:O	7:7:399:GLU:HG3	2.06	0.55
8:8:373:VAL:HG23	8:8:399:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:473:ASP:OD1	3:C:474:GLU:N	2.40	0.55
2:2:236:GLU:HG3	2:2:237:MET:SD	2.46	0.55
3:3:364:SER:HA	3:3:367:LEU:HD23	1.87	0.55
8:8:170:LEU:CD1	10:8:1001:ADP:C2	2.89	0.55
8:8:353:GLU:N	9:9:267:TYR:O	2.38	0.55
3:C:526:ASN:OD1	3:C:527:ARG:N	2.39	0.55
4:4:204:LYS:HB3	4:4:221:ASP:HB3	1.87	0.55
3:C:226:PRO:HD3	5:E:242:ILE:HD13	1.88	0.55
7:7:334:HIS:HD2	7:7:375:TYR:CG	2.25	0.55
9:9:113:GLN:O	9:9:117:LYS:N	2.39	0.55
2:B:795:ARG:HA	5:E:560:HIS:CE1	2.42	0.55
4:D:762:ILE:HA	4:D:817:VAL:HB	1.88	0.55
5:5:302:ASN:HA	5:5:324:ARG:HG3	1.87	0.55
6:6:510:SER:HA	6:6:513:ILE:HB	1.87	0.55
3:C:389:VAL:HG22	3:C:710:THR:HG21	1.89	0.55
5:E:90:PHE:CE2	5:E:94:ILE:HD11	2.42	0.55
5:5:151:LEU:HD13	5:5:298:TYR:HE2	1.72	0.55
7:7:193:PRO:HG2	5:E:9:TYR:CD2	2.42	0.55
2:B:384:ASN:HD21	5:E:153:SER:H	1.54	0.55
4:D:470:SER:O	4:D:499:ARG:NH2	2.38	0.55
5:E:169:THR:HB	5:E:254:GLN:HE21	1.71	0.55
6:6:313:MET:HE3	6:F:314:CYS:H	1.70	0.55
8:8:83:SER:N	9:9:662:GLU:OE2	2.39	0.55
8:8:175:LEU:HD13	8:8:177:ARG:HE	1.71	0.55
8:8:398:PHE:HD1	8:8:436:TRP:HE3	1.54	0.55
9:9:149:ASP:OD1	9:9:150:LEU:N	2.40	0.55
2:B:239:SER:O	2:B:286:TYR:OH	2.25	0.55
4:D:684:PRO:HG3	4:D:847:MET:HE3	1.88	0.55
6:F:276:ILE:HD13	6:F:363:GLU:HA	1.87	0.55
2:2:406:ARG:NH2	2:2:449:THR:OG1	2.34	0.55
6:6:303:GLU:HB2	6:6:356:TRP:HB2	1.89	0.55
9:9:179:VAL:HG13	9:9:201:VAL:HG22	1.88	0.55
4:D:778:ARG:HG3	4:D:793:ALA:HB3	1.88	0.55
3:3:386:MET:HE3	3:3:715:VAL:HG22	1.89	0.55
6:F:540:HIS:O	6:F:544:LYS:NZ	2.29	0.55
3:3:97:ILE:HD13	3:3:156:SER:HB2	1.89	0.54
7:7:664:TYR:OH	7:7:668:ARG:NH1	2.40	0.54
6:F:112:ARG:HB2	6:F:180:PHE:HB3	1.89	0.54
6:F:331:THR:HA	6:F:341:ARG:HD3	1.89	0.54
3:3:442:LEU:HD22	3:3:462:MET:HE3	1.89	0.54
5:5:405:ARG:HH21	5:5:516:ARG:HG2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:150:ASN:OD1	7:G:151:GLU:N	2.40	0.54
3:3:233:THR:HG23	3:3:234:GLU:HG2	1.89	0.54
8:8:317:PHE:HB3	8:8:318:PRO:HD3	1.89	0.54
2:B:693:GLU:HB2	6:F:778:LYS:HD3	1.88	0.54
6:F:126:SER:OG	6:F:129:THR:O	2.22	0.54
7:G:621:MET:HE3	7:G:622:HIS:CE1	2.42	0.54
4:4:647:GLU:OE1	4:4:655:SER:N	2.39	0.54
8:8:322:SER:OG	8:8:324:ASP:O	2.26	0.54
4:D:618:SER:HB3	6:F:373:MET:HG2	1.90	0.54
5:E:175:ARG:NH1	5:E:253:GLN:OE1	2.40	0.54
6:F:319:ASP:HB3	6:F:350:ARG:HD3	1.88	0.54
4:4:356:MET:HE1	4:4:372:GLU:H	1.72	0.54
2:2:271:PHE:HD2	2:2:295:VAL:HG21	1.73	0.54
4:4:756:GLU:OE2	4:4:757:HIS:ND1	2.41	0.54
5:5:407:ARG:NH2	5:5:658:ARG:HH22	2.06	0.54
6:6:777:TYR:HB2	6:6:800:LEU:HD13	1.90	0.54
2:2:855:ARG:O	2:2:859:ARG:N	2.40	0.54
6:F:347:ASN:HD21	6:F:350:ARG:HB2	1.73	0.54
2:2:789:VAL:HG11	2:2:838:ILE:HD13	1.89	0.54
3:C:443:THR:OG1	3:C:444:ALA:N	2.41	0.54
3:C:555:GLU:HB2	5:E:631:LYS:HE2	1.90	0.54
4:D:197:PHE:HB2	4:D:254:THR:HG21	1.90	0.54
6:F:115:PHE:HA	6:F:118:PHE:CE1	2.43	0.54
8:8:175:LEU:HB3	8:8:177:ARG:HG2	1.90	0.54
3:C:439:GLY:N	3:C:482:ASP:OD1	2.41	0.54
6:F:362:GLN:HG3	6:F:376:THR:CG2	2.36	0.54
6:F:702:THR:HG23	6:F:704:PRO:HD2	1.90	0.54
7:7:334:HIS:HD2	7:7:375:TYR:CD1	2.26	0.53
7:7:660:VAL:HG11	7:7:693:ILE:HD11	1.91	0.53
8:8:226:ILE:HG12	8:8:231:TYR:HD1	1.72	0.53
5:E:66:GLU:HA	5:E:69:ILE:HD13	1.88	0.53
5:E:172:LEU:HD23	5:E:254:GLN:HB2	1.90	0.53
6:F:737:LYS:HB2	6:F:740:GLU:HB3	1.90	0.53
6:F:790:ARG:O	6:F:837:ARG:NH1	2.41	0.53
4:4:570:PRO:HD3	4:4:680:SER:O	2.07	0.53
5:5:66:GLU:O	5:5:69:ILE:HG12	2.09	0.53
7:7:127:LEU:HD12	7:7:128:PRO:HD2	1.90	0.53
7:7:513:LEU:HD23	7:7:540:VAL:HG21	1.91	0.53
9:9:203:SER:H	9:9:206:LYS:HB2	1.72	0.53
3:C:687:ARG:NH2	7:G:602:ASP:OD1	2.42	0.53
2:2:482:ARG:O	2:2:486:LYS:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:475:PHE:HB3	3:3:516:ALA:HB2	1.89	0.53
6:6:379:VAL:HG22	6:6:454:PHE:HB3	1.90	0.53
3:C:339:ARG:NE	3:C:661:GLN:OE1	2.41	0.53
4:D:656:ILE:HD11	4:D:658:LYS:HD2	1.90	0.53
5:E:530:TYR:HB2	5:E:539:ASN:HB2	1.90	0.53
6:F:589:VAL:HG11	6:F:597:TYR:HB2	1.89	0.53
4:4:725:THR:HB	7:7:657:ASN:HB2	1.91	0.53
8:8:331:GLU:O	8:8:334:THR:OG1	2.22	0.53
8:8:372:PHE:O	8:8:376:LEU:HD23	2.07	0.53
3:C:386:MET:HE3	3:C:715:VAL:HG22	1.90	0.53
5:E:266:PRO:HB2	5:E:269:GLU:HB2	1.89	0.53
5:5:381:ASN:HB3	5:5:384:ILE:HB	1.90	0.53
6:6:137:ARG:HA	6:6:140:ILE:HD12	1.90	0.53
4:D:449:ARG:HD2	4:D:450:GLN:N	2.24	0.53
5:E:551:ASP:OD2	5:E:658:ARG:NH1	2.42	0.53
3:3:507:ASN:ND2	7:7:319:SER:O	2.42	0.53
5:5:374:ILE:HD13	5:5:428:PHE:HE2	1.73	0.53
7:7:149:ARG:HG3	7:7:153:MET:HE3	1.90	0.53
8:8:97:MET:HG3	8:8:157:LYS:HG3	1.91	0.53
8:8:339:LYS:HZ1	8:8:342:ARG:HH22	1.55	0.53
4:D:217:ASN:ND2	4:D:219:THR:OG1	2.42	0.53
4:D:224:LEU:HD13	4:D:227:ILE:HD12	1.91	0.53
4:D:272:MET:HB3	4:D:303:VAL:HG21	1.90	0.53
4:D:354:HIS:CE1	4:D:372:GLU:HB3	2.44	0.53
2:B:309:LEU:O	2:B:313:ASN:ND2	2.41	0.53
2:B:794:ARG:HD3	2:B:805:ILE:HD11	1.89	0.53
4:D:483:GLN:HG3	4:D:484:GLU:HG2	1.89	0.53
4:D:640:SER:O	6:F:601:LYS:NZ	2.42	0.53
7:G:23:ASP:OD2	7:G:88:TYR:OH	2.26	0.53
4:4:321:ASP:HA	4:4:324:LYS:HD3	1.91	0.53
4:4:535:ASP:HA	4:4:538:LYS:HD2	1.90	0.53
9:9:349:ASP:HB3	9:9:352:LEU:HB3	1.91	0.53
2:B:253:LYS:HB3	2:B:256:LEU:HB3	1.91	0.53
6:F:801:GLU:HA	6:F:804:ILE:HD12	1.91	0.53
2:2:599:ALA:O	2:2:644:CYS:HB3	2.09	0.53
6:6:537:VAL:HG11	6:6:584:PHE:CZ	2.44	0.53
8:8:287:PRO:O	8:8:291:MET:HG2	2.09	0.53
2:B:794:ARG:HD3	2:B:805:ILE:CD1	2.38	0.53
3:C:195:LYS:N	3:C:251:ILE:O	2.41	0.53
3:C:402:ASP:HB3	3:C:511:SER:HB3	1.91	0.53
3:C:552:ASP:O	3:C:557:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:720:ASN:HB3	6:F:723:ILE:HG12	1.90	0.53
2:2:477:THR:HG22	2:2:479:GLU:H	1.73	0.53
3:3:480:ASP:O	3:3:484:VAL:HG23	2.09	0.53
5:5:356:GLU:O	5:5:359:GLN:HG3	2.09	0.53
6:6:275:ARG:HD2	6:6:367:GLU:HB2	1.89	0.53
9:9:270:ASP:OD2	9:9:274:THR:N	2.41	0.53
2:B:536:ASP:HB3	2:B:645:SER:HB3	1.89	0.53
3:C:535:LEU:HD22	3:C:539:LEU:HD23	1.91	0.53
4:D:261:LEU:HD22	4:D:272:MET:HE1	1.90	0.53
5:E:65:MET:O	5:E:69:ILE:HD12	2.09	0.53
6:F:310:THR:N	6:F:345:THR:O	2.42	0.53
6:F:379:VAL:HG22	6:F:454:PHE:HB3	1.91	0.53
7:G:451:ARG:NH1	7:G:453:ASP:O	2.42	0.53
2:2:296:ARG:HD2	2:2:454:ASN:O	2.08	0.52
2:2:485:ARG:NH2	2:2:489:ARG:HE	2.06	0.52
4:4:571:SER:OG	7:7:686:PRO:HD2	2.08	0.52
5:5:149:ARG:NH1	5:5:272:ARG:HD3	2.23	0.52
8:8:88:TYR:HE1	9:9:696:LEU:HD13	1.72	0.52
2:B:800:THR:HG23	2:B:856:GLN:HE21	1.74	0.52
2:2:332:PRO:HG2	5:5:300:ILE:HD11	1.91	0.52
6:6:540:HIS:O	6:6:544:LYS:NZ	2.34	0.52
5:E:261:ILE:HD13	5:E:264:LEU:HD12	1.91	0.52
5:E:418:PRO:HA	10:E:802:ADP:O3B	2.09	0.52
2:2:631:ILE:HA	5:5:446:ALA:HB3	1.92	0.52
3:3:579:GLY:O	5:5:611:ALA:N	2.42	0.52
4:4:513:ALA:HA	4:4:518:LEU:HD22	1.92	0.52
4:4:689:THR:HG22	4:4:791:ILE:HG23	1.90	0.52
9:9:136:MET:HG3	9:9:140:ASN:HB3	1.91	0.52
3:C:570:ARG:HA	5:E:613:ARG:HH11	1.75	0.52
6:F:442:SER:OG	6:F:443:LEU:N	2.42	0.52
6:6:526:TYR:HB2	6:6:814:ASN:HD21	1.73	0.52
8:8:281:THR:N	8:8:285:ARG:HH21	2.07	0.52
4:D:187:ILE:HG12	4:D:271:ILE:HD11	1.91	0.52
4:4:347:PHE:HE1	4:4:384:LEU:HD12	1.74	0.52
5:5:422:LYS:HB2	10:5:801:ADP:O2B	2.08	0.52
2:B:332:PRO:HG2	5:E:300:ILE:HD11	1.90	0.52
3:C:566:LEU:O	3:C:570:ARG:HG2	2.10	0.52
2:2:522:GLY:O	2:2:822:LYS:NZ	2.42	0.52
3:3:590:LEU:HG	3:3:592:VAL:HG13	1.92	0.52
6:6:613:VAL:O	6:6:622:THR:N	2.40	0.52
2:B:239:SER:OG	2:B:240:GLU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:HIS:CD2	6:F:565:LEU:HD13	2.45	0.52
7:G:596:ILE:HD11	7:G:695:LEU:HD21	1.91	0.52
3:3:558:ASP:OD2	5:5:630:ARG:HG3	2.10	0.52
3:3:696:PRO:HB3	7:7:573:ARG:HH22	1.75	0.52
4:4:654:ILE:HG23	4:4:665:LEU:HB2	1.91	0.52
8:8:138:LYS:HG2	9:9:344:PHE:CD2	2.45	0.52
4:D:281:VAL:HA	4:D:284:ILE:HD12	1.92	0.52
7:G:143:LEU:HD22	7:G:197:THR:HA	1.92	0.52
3:3:398:HIS:NE2	3:3:493:GLN:OE1	2.32	0.52
6:6:136:TYR:CZ	6:6:140:ILE:HD11	2.45	0.52
4:D:204:LYS:HB3	4:D:221:ASP:HB3	1.91	0.52
3:3:561:ILE:HG21	5:5:650:ILE:HG12	1.92	0.52
4:4:349:CYS:HA	4:4:382:MET:HA	1.92	0.52
4:4:559:ARG:HB2	4:4:652:GLN:HG3	1.90	0.52
4:4:645:LEU:O	4:4:649:MET:HB2	2.09	0.52
6:6:198:ASN:O	6:6:261:ARG:NH1	2.43	0.52
7:7:255:VAL:HG22	7:7:307:PHE:HE1	1.75	0.52
8:8:32:GLU:OE1	8:8:32:GLU:N	2.43	0.52
2:B:447:PHE:CE2	6:F:304:LEU:HD21	2.44	0.52
6:6:614:ARG:NE	6:6:619:GLY:O	2.32	0.52
2:B:181:LEU:N	2:B:206:THR:OG1	2.34	0.52
2:B:856:GLN:HE22	2:B:859:ARG:HD2	1.75	0.52
7:7:423:TYR:HB2	7:7:615:HIS:CD2	2.45	0.51
8:8:138:LYS:HZ1	9:9:347:HIS:HB2	1.74	0.51
2:B:656:ARG:NE	6:F:794:ARG:HG3	2.25	0.51
3:C:489:VAL:HG22	3:C:495:VAL:HG22	1.92	0.51
3:C:683:TYR:OH	3:C:687:ARG:NH1	2.43	0.51
5:5:83:PRO:HG3	5:5:159:ILE:HG13	1.91	0.51
3:C:672:THR:OG1	3:C:721:VAL:O	2.28	0.51
4:D:604:TYR:CE1	4:D:617:GLU:HG2	2.46	0.51
7:G:607:ASP:O	7:G:610:GLU:HG3	2.09	0.51
9:9:246:PRO:O	9:9:249:ARG:NH1	2.43	0.51
4:D:447:ASN:OD1	4:D:450:GLN:NE2	2.28	0.51
5:E:605:TYR:CZ	5:E:609:LYS:HG3	2.46	0.51
6:F:399:GLY:HA3	6:F:456:ALA:HA	1.92	0.51
2:2:525:LYS:HD2	2:2:533:ILE:HD12	1.92	0.51
3:3:700:ARG:HE	10:7:1102:ADP:H5'2	1.76	0.51
6:F:277:ARG:NH2	6:F:372:SER:HB2	2.25	0.51
6:F:290:ILE:HG13	6:F:397:PHE:HB2	1.93	0.51
7:7:607:ASP:OD1	7:7:608:ASP:N	2.42	0.51
4:D:799:GLU:HA	4:D:802:ILE:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:334:ARG:NH1	4:4:617:GLU:OE2	2.43	0.51
6:F:120:GLU:OE2	6:F:137:ARG:NH2	2.28	0.51
3:3:330:HIS:CG	3:3:338:ALA:HB2	2.46	0.51
4:4:373:ARG:HD2	4:4:375:ASP:HB3	1.92	0.51
5:5:581:ASN:OD1	5:5:582:ALA:N	2.43	0.51
8:8:61:PHE:HB3	8:8:64:HIS:HB2	1.93	0.51
8:8:145:TRP:HE1	8:8:472:LEU:HB3	1.76	0.51
9:9:130:ILE:O	9:9:176:ARG:NH2	2.29	0.51
10:C:1001:ADP:O1B	5:E:651:ARG:NH2	2.43	0.51
6:F:122:PHE:HE1	6:F:161:ARG:HB2	1.76	0.51
6:F:629:MET:HE1	6:F:674:ALA:HB2	1.91	0.51
4:4:649:MET:HG2	4:4:701:ARG:HD3	1.92	0.51
7:7:149:ARG:NH2	5:E:13:VAL:O	2.41	0.51
2:B:505:ILE:HD11	10:B:901:ADP:C5	2.46	0.51
2:B:661:LEU:HD22	2:B:665:GLN:HG3	1.93	0.51
3:C:687:ARG:NH1	7:G:609:ASP:OD2	2.44	0.51
3:3:545:LEU:HD11	3:3:708:LEU:HD11	1.93	0.51
5:E:152:ASP:OD1	5:E:153:SER:N	2.44	0.51
5:E:341:SER:H	5:E:344:ASN:HB3	1.76	0.51
4:D:599:VAL:HG12	4:D:604:TYR:HB3	1.92	0.51
5:E:139:LEU:HD12	5:E:331:LEU:HD13	1.93	0.51
2:2:338:LYS:HE2	2:2:350:PRO:HG3	1.92	0.50
8:8:155:HIS:CD2	8:8:298:THR:HB	2.46	0.50
8:8:265:TYR:C	9:9:258:ILE:HG13	2.36	0.50
2:B:296:ARG:NH2	2:B:413:ASP:OD1	2.44	0.50
2:B:796:GLU:HB3	2:B:856:GLN:HE22	1.74	0.50
4:D:534:GLU:OE2	4:D:538:LYS:HD2	2.11	0.50
5:E:182:MET:HE2	5:E:189:THR:HG22	1.93	0.50
2:2:474:PHE:O	2:2:768:HIS:ND1	2.40	0.50
2:2:630:SER:HB3	2:2:639:THR:HG22	1.92	0.50
3:3:214:TYR:CD1	3:3:229:ALA:HB1	2.46	0.50
4:4:308:VAL:HG11	4:4:325:LEU:HD23	1.93	0.50
5:5:453:VAL:HG21	5:5:504:ILE:HG21	1.94	0.50
8:8:170:LEU:HD11	10:8:1001:ADP:C4	2.46	0.50
3:C:255:ARG:NH1	7:G:366:LEU:HA	2.27	0.50
4:D:334:ARG:HD3	4:D:615:VAL:HG11	1.92	0.50
5:E:99:LYS:O	5:E:103:ILE:HG12	2.11	0.50
9:9:187:ASP:O	9:9:193:ARG:NH2	2.44	0.50
4:D:189:GLU:OE2	4:D:193:ASN:ND2	2.45	0.50
5:E:383:ASP:OD1	5:E:682:ARG:NH2	2.27	0.50
6:F:628:LEU:HD11	6:F:652:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:162:ARG:NH2	7:G:178:ASN:OD1	2.44	0.50
7:7:517:ASP:OD1	7:7:560:ARG:N	2.44	0.50
9:9:319:SER:O	9:9:323:VAL:HG23	2.12	0.50
3:C:565:VAL:O	3:C:568:THR:OG1	2.27	0.50
4:D:234:ARG:HB2	4:D:280:MET:HE1	1.93	0.50
4:D:724:LEU:HD12	7:G:689:LEU:HD23	1.93	0.50
5:E:178:TYR:CE1	5:E:191:SER:HB3	2.46	0.50
6:F:821:PRO:HA	6:F:824:ILE:HD12	1.93	0.50
3:3:462:MET:HE1	3:3:486:ILE:HG13	1.94	0.50
7:7:524:ASP:OD2	7:7:525:GLU:N	2.44	0.50
2:B:854:ARG:HH11	2:B:857:LEU:HD22	1.76	0.50
3:C:570:ARG:HH21	5:E:616:PRO:HG3	1.77	0.50
2:2:275:ALA:O	2:2:279:THR:HG23	2.11	0.50
2:2:534:ARG:O	2:2:815:ARG:HD3	2.12	0.50
5:5:69:ILE:HG22	5:5:76:TYR:CG	2.46	0.50
9:9:531:MET:HE3	4:D:178:ARG:HB3	1.93	0.50
4:D:773:ALA:O	4:D:777:MET:HG3	2.11	0.50
4:4:545:PHE:HE1	4:4:751:ILE:HA	1.76	0.50
5:5:444:SER:HB2	5:5:447:ALA:HB3	1.93	0.50
7:7:367:LYS:NZ	7:7:369:GLY:O	2.37	0.50
4:D:352:CYS:SG	4:D:354:HIS:HB2	2.52	0.50
7:7:230:ILE:HD12	7:7:239:ILE:HD12	1.93	0.50
2:2:200:GLN:O	2:2:204:SER:N	2.36	0.50
2:2:390:LEU:HD23	2:2:408:VAL:HB	1.94	0.50
4:4:451:ARG:CZ	6:6:445:VAL:HG13	2.41	0.50
9:9:524:MET:HE1	4:D:271:ILE:HA	1.94	0.50
3:C:402:ASP:OD2	3:C:493:GLN:NE2	2.45	0.50
4:D:778:ARG:HH22	6:F:717:ASP:CG	2.20	0.50
6:F:307:ALA:N	6:F:321:VAL:O	2.45	0.50
7:G:221:SER:OG	7:G:238:LEU:O	2.30	0.50
7:G:481:VAL:HG21	7:G:512:ALA:HB1	1.94	0.50
7:G:692:ILE:HD12	7:G:717:LEU:HD22	1.94	0.50
4:4:548:THR:N	4:4:806:GLU:OE1	2.41	0.49
6:6:357:GLN:NE2	6:6:387:GLU:OE1	2.40	0.49
7:7:529:MET:HE3	7:7:533:ASP:HB2	1.93	0.49
8:8:266:PRO:HA	9:9:258:ILE:HA	1.93	0.49
9:9:241:GLU:OE2	6:F:107:THR:OG1	2.20	0.49
7:G:534:ARG:O	7:G:537:ILE:HG22	2.12	0.49
4:4:647:GLU:HG2	4:4:653:THR:O	2.13	0.49
7:7:621:MET:HE3	7:7:622:HIS:ND1	2.27	0.49
4:D:700:SER:OG	4:D:794:THR:HG21	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:453:VAL:HG23	5:E:504:ILE:HD13	1.92	0.49
6:F:599:SER:OG	6:F:600:GLY:N	2.45	0.49
2:2:296:ARG:HB3	2:2:455:SER:HB2	1.93	0.49
2:2:361:ILE:HB	2:2:373:PHE:HB3	1.93	0.49
2:2:610:ASP:OD1	2:2:610:ASP:N	2.44	0.49
3:3:214:TYR:HD1	3:3:229:ALA:HB1	1.76	0.49
8:8:393:PHE:HB3	9:9:369:HIS:CD2	2.46	0.49
9:9:178:SER:HA	9:9:181:ASN:HB2	1.94	0.49
2:2:402:LEU:HD23	6:6:629:MET:HE1	1.93	0.49
2:2:814:LEU:O	2:2:818:GLU:HG2	2.12	0.49
4:4:371:CYS:HA	4:4:382:MET:HE1	1.95	0.49
8:8:301:ASP:O	8:8:305:VAL:HG23	2.12	0.49
3:C:98:ILE:HG13	3:C:155:LEU:HD11	1.94	0.49
4:D:385:ILE:HG21	4:D:388:ARG:HD3	1.94	0.49
4:D:428:ARG:HH12	4:D:481:ILE:HD11	1.77	0.49
5:E:185:ASN:OD1	5:E:186:CYS:N	2.44	0.49
2:2:309:LEU:HD21	2:2:451:ILE:HD11	1.94	0.49
2:2:524:PRO:HA	2:2:535:GLY:HA3	1.94	0.49
4:4:812:LYS:O	4:4:813:LEU:HB2	2.11	0.49
5:5:32:LYS:HZ2	5:5:100:ARG:HH22	1.61	0.49
4:D:293:LEU:HD23	4:D:293:LEU:H	1.77	0.49
5:E:355:GLU:O	5:E:359:GLN:HG2	2.11	0.49
6:F:115:PHE:HD2	6:F:118:PHE:CE1	2.30	0.49
6:F:579:THR:HB	6:F:715:ILE:HG21	1.94	0.49
2:2:194:TYR:O	2:2:198:ILE:HG12	2.12	0.49
3:3:447:THR:HB	3:3:458:GLU:HG3	1.95	0.49
4:4:721:ALA:HB2	7:7:664:TYR:HD2	1.77	0.49
5:5:90:PHE:HD2	5:5:137:LEU:HD22	1.75	0.49
5:5:656:ILE:HD13	5:5:659:ILE:HD12	1.94	0.49
6:6:696:ARG:NH1	6:6:791:SER:O	2.45	0.49
7:7:117:PHE:O	7:7:121:ILE:HG12	2.11	0.49
7:7:499:LYS:CB	7:7:506:MET:SD	3.01	0.49
9:9:189:ASP:O	9:9:192:SER:OG	2.25	0.49
9:9:534:ARG:HG2	4:D:177:LEU:HD23	1.94	0.49
4:D:199:MET:HE1	4:D:279:CYS:SG	2.53	0.49
7:7:267:TYR:HE2	7:7:288:GLU:HG2	1.78	0.49
4:D:718:ARG:HG2	4:D:722:LYS:HE2	1.94	0.49
7:7:607:ASP:O	7:7:610:GLU:HG3	2.12	0.49
8:8:136:PRO:O	8:8:139:GLY:N	2.44	0.49
9:9:250:ASP:OD1	9:9:250:ASP:N	2.45	0.49
2:B:626:GLN:NE2	5:E:430:GLU:OE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:622:LEU:HD13	5:E:657:ILE:HG12	1.94	0.49
3:3:499:LYS:HD3	7:7:488:SER:HA	1.95	0.49
2:B:364:CYS:HB3	2:B:369:SER:H	1.77	0.49
4:D:512:VAL:HA	4:D:515:ARG:HG3	1.95	0.49
5:E:74:ASP:N	5:E:74:ASP:OD1	2.45	0.49
2:2:589:TRP:HE1	5:5:458:MET:HE1	1.78	0.49
4:4:444:ILE:HD11	6:6:411:GLY:HA2	1.94	0.49
6:6:443:LEU:HD23	7:7:282:SER:HB3	1.93	0.49
8:8:134:ASP:OD1	8:8:134:ASP:N	2.46	0.49
9:9:206:LYS:HA	9:9:209:ARG:HD2	1.95	0.49
3:C:524:ASP:OD2	3:C:527:ARG:NH2	2.45	0.49
7:G:286:SER:O	7:G:290:SER:N	2.44	0.49
4:4:319:PRO:HB3	7:7:253:PRO:HB3	1.95	0.48
6:6:453:SER:OG	6:6:454:PHE:N	2.46	0.48
2:B:534:ARG:HG2	2:B:536:ASP:H	1.78	0.48
3:C:25:VAL:HG21	3:C:127:LYS:HD3	1.94	0.48
4:D:765:ALA:HB1	4:D:819:LEU:HD21	1.95	0.48
5:E:152:ASP:HB3	5:E:154:GLU:HG2	1.95	0.48
2:2:271:PHE:HA	2:2:274:VAL:HG22	1.94	0.48
2:2:325:THR:OG1	2:2:389:THR:O	2.30	0.48
4:4:681:ARG:HH12	7:7:683:GLN:HB3	1.78	0.48
5:5:629:ILE:O	5:5:632:GLN:HG3	2.12	0.48
9:9:144:MET:HE1	9:9:176:ARG:HD2	1.94	0.48
9:9:192:SER:OG	9:9:193:ARG:NH1	2.45	0.48
2:B:335:LYS:HB2	2:B:383:ARG:HD2	1.94	0.48
6:F:309:PHE:HA	6:F:346:LEU:HA	1.95	0.48
2:2:494:ILE:HD11	2:2:824:ARG:HD3	1.95	0.48
6:6:112:ARG:O	6:6:116:GLU:HG3	2.13	0.48
9:9:372:ASN:HA	9:9:376:LYS:HE2	1.94	0.48
3:C:304:GLY:HA3	3:C:317:PHE:CD1	2.48	0.48
4:D:272:MET:O	4:D:276:ILE:HG12	2.13	0.48
6:F:115:PHE:CD1	6:F:181:LEU:HA	2.48	0.48
5:5:90:PHE:HE2	5:5:137:LEU:HD13	1.79	0.48
5:5:654:GLU:O	5:5:658:ARG:NE	2.39	0.48
6:6:280:ARG:HD3	6:6:280:ARG:HA	1.68	0.48
2:B:383:ARG:HH22	2:B:411:LEU:HD13	1.78	0.48
3:3:223:THR:OG1	5:5:246:GLU:OE1	2.31	0.48
4:4:272:MET:O	4:4:276:ILE:HG12	2.14	0.48
5:5:53:ASN:HB3	5:5:58:ASN:O	2.13	0.48
6:6:309:PHE:HB3	6:6:344:TRP:CE3	2.48	0.48
8:8:96:ILE:HG13	8:8:97:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:182:ASP:HB2	10:8:1001:ADP:O2A	2.13	0.48
3:3:233:THR:OG1	5:E:5:ARG:HB2	2.14	0.48
3:3:437:SER:HB3	5:5:505:ALA:HB3	1.96	0.48
7:7:654:GLU:HA	7:7:657:ASN:HD21	1.78	0.48
8:8:162:ARG:HE	8:8:279:ALA:HB3	1.78	0.48
2:B:630:SER:HA	2:B:639:THR:HA	1.95	0.48
7:G:79:ILE:HD13	7:G:203:TYR:HB2	1.95	0.48
2:2:800:THR:HA	2:2:855:ARG:HH21	1.79	0.48
4:4:199:MET:SD	4:4:227:ILE:HD11	2.54	0.48
4:4:340:PRO:HB2	4:4:391:PHE:CD1	2.48	0.48
8:8:426:TYR:CE1	8:8:429:LYS:HE2	2.49	0.48
6:F:110:LYS:O	6:F:113:GLU:HG3	2.13	0.48
3:3:295:VAL:HG12	3:3:325:THR:HB	1.96	0.48
4:4:204:LYS:HB2	4:4:216:ILE:HD11	1.95	0.48
5:5:90:PHE:CE2	5:5:94:ILE:HD11	2.48	0.48
9:9:202:TRP:HE3	9:9:206:LYS:HB3	1.79	0.48
4:D:525:SER:HB3	4:D:747:LEU:HD22	1.96	0.48
6:F:649:GLN:OE1	6:F:701:MET:HE1	2.14	0.48
3:3:687:ARG:NH2	7:7:602:ASP:OD2	2.47	0.48
8:8:274:LYS:HB2	8:8:292:LYS:HE3	1.96	0.48
3:C:28:PHE:HD1	3:C:110:PHE:CE2	2.32	0.48
4:D:268:VAL:HG12	4:D:272:MET:HE3	1.94	0.48
4:D:350:ASN:N	4:D:381:SER:O	2.42	0.48
4:D:431:ASP:OD2	4:D:468:LYS:NZ	2.47	0.48
5:E:178:TYR:HE1	5:E:191:SER:HB3	1.79	0.48
6:F:279:ILE:HG21	6:F:452:ILE:HG21	1.95	0.48
6:F:657:GLU:HG3	6:F:708:ARG:NE	2.29	0.48
7:G:497:VAL:HG13	7:G:497:VAL:O	2.14	0.48
3:3:187:THR:HG21	3:3:259:GLN:OE1	2.14	0.48
3:3:564:HIS:CE1	3:3:628:LEU:HB2	2.49	0.48
3:C:220:THR:HG21	3:C:224:ARG:HG3	1.94	0.48
4:D:727:LEU:O	4:D:733:PRO:HG2	2.14	0.48
4:4:341:ASP:N	4:4:392:ALA:O	2.46	0.47
5:5:457:PRO:HA	5:5:460:ARG:HH11	1.78	0.47
8:8:466:THR:HG23	8:8:469:PHE:H	1.79	0.47
9:9:250:ASP:OD2	9:9:252:ARG:NH2	2.44	0.47
2:B:202:ASN:HA	2:B:205:ARG:HD3	1.96	0.47
5:E:69:ILE:HG13	5:E:76:TYR:CD2	2.49	0.47
5:E:630:ARG:HH12	5:E:649:THR:HA	1.79	0.47
7:G:481:VAL:HG22	7:G:516:ALA:HB2	1.96	0.47
6:6:711:LEU:HD21	6:6:806:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:135:LEU:HD11	8:8:139:GLY:HA3	1.94	0.47
8:8:330:LEU:HD11	9:9:297:PRO:HD2	1.96	0.47
9:9:119:ILE:O	9:9:123:ASP:N	2.47	0.47
5:E:444:SER:HB2	5:E:447:ALA:HB3	1.96	0.47
6:F:803:MET:HG3	6:F:831:LEU:HD12	1.95	0.47
3:3:454:GLU:HG3	3:3:455:ARG:HG3	1.96	0.47
5:5:32:LYS:HZ2	5:5:100:ARG:NH1	2.10	0.47
2:B:809:HIS:O	2:B:813:ILE:HD12	2.13	0.47
5:E:35:ILE:HD11	5:E:90:PHE:CZ	2.49	0.47
6:F:143:MET:SD	6:F:148:LEU:HB2	2.54	0.47
3:3:420:ARG:NH2	5:5:501:THR:OG1	2.47	0.47
5:5:353:GLU:O	5:5:356:GLU:HG2	2.14	0.47
6:6:144:LYS:HG3	6:6:196:LEU:HB3	1.96	0.47
3:C:687:ARG:HG2	7:G:609:ASP:OD2	2.15	0.47
4:D:559:ARG:HB2	4:D:652:GLN:HG3	1.95	0.47
5:E:300:ILE:HG23	5:E:324:ARG:HB3	1.96	0.47
2:2:536:ASP:HB3	2:2:645:SER:HB3	1.95	0.47
2:2:804:PRO:HD3	5:5:529:ARG:NH2	2.30	0.47
3:3:32:LEU:HD13	3:3:132:LEU:HD13	1.96	0.47
6:6:311:CYS:HB2	6:6:344:TRP:CH2	2.49	0.47
6:6:316:ALA:HB3	6:6:334:PRO:HG3	1.96	0.47
6:6:406:ASP:O	6:6:449:THR:OG1	2.21	0.47
6:6:816:VAL:HG21	6:6:823:PHE:HZ	1.79	0.47
7:7:289:CYS:O	7:7:295:LYS:NZ	2.39	0.47
8:8:45:SER:HB2	8:8:78:ILE:HA	1.96	0.47
8:8:138:LYS:HE3	9:9:348:ALA:H	1.79	0.47
2:B:202:ASN:HA	2:B:205:ARG:HH11	1.80	0.47
2:B:433:ASN:HB2	2:B:450:ILE:HG12	1.96	0.47
5:E:200:ILE:HG13	5:E:329:LYS:HZ1	1.80	0.47
5:E:477:VAL:HG13	5:E:519:VAL:HG23	1.96	0.47
3:3:177:ASN:ND2	5:5:245:HIS:O	2.48	0.47
3:3:211:TYR:CD1	7:7:8:ILE:HD11	2.50	0.47
4:4:256:ASP:HB3	7:7:134:TYR:CD2	2.49	0.47
4:4:443:PRO:HB2	4:4:453:LEU:HD13	1.96	0.47
6:6:199:THR:O	6:6:261:ARG:NH2	2.47	0.47
6:6:313:MET:HB3	6:6:338:CYS:SG	2.55	0.47
2:2:814:LEU:HD11	5:5:573:ILE:HG22	1.97	0.47
3:3:223:THR:N	5:5:246:GLU:OE2	2.38	0.47
5:5:169:THR:HG23	5:5:288:PRO:HG3	1.95	0.47
6:6:168:MET:HE2	6:6:168:MET:HA	1.97	0.47
6:6:720:ASN:HB3	6:6:723:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:776:LYS:HD2	6:6:828:TYR:CG	2.50	0.47
6:6:829:ASP:HA	6:6:832:ARG:HG2	1.96	0.47
7:7:499:LYS:HG3	7:7:506:MET:SD	2.55	0.47
7:7:669:GLN:O	7:7:673:ARG:HG3	2.14	0.47
8:8:21:GLN:NE2	8:8:25:ASP:OD2	2.47	0.47
8:8:85:GLN:NE2	8:8:89:ASN:OD1	2.48	0.47
8:8:170:LEU:HD11	10:8:1001:ADP:C2	2.50	0.47
9:9:661:CYS:O	9:9:665:ARG:N	2.47	0.47
2:B:336:TYR:HE2	2:B:352:PHE:HD2	1.62	0.47
3:C:415:LYS:NZ	13:E:801:BEF:F2	2.35	0.47
3:C:544:ASP:OD1	3:C:704:THR:OG1	2.28	0.47
6:F:800:LEU:HA	6:F:803:MET:HE2	1.95	0.47
7:G:367:LYS:HA	7:G:371:LEU:HD12	1.96	0.47
5:5:531:ASP:N	5:5:531:ASP:OD1	2.47	0.47
6:6:144:LYS:HA	6:6:196:LEU:HD13	1.96	0.47
7:7:413:ARG:O	7:7:417:SER:OG	2.26	0.47
7:7:648:LYS:NZ	7:7:704:LEU:HB3	2.30	0.47
8:8:139:GLY:HA2	9:9:344:PHE:CE2	2.50	0.47
2:B:334:LEU:HB3	2:B:337:VAL:HG22	1.97	0.47
3:C:544:ASP:OD1	3:C:707:ARG:NH2	2.36	0.47
4:D:315:ARG:CZ	4:D:413:HIS:HB2	2.45	0.47
4:D:393:ASP:HB3	4:D:424:VAL:HG21	1.97	0.47
2:2:808:ARG:HG3	10:5:801:ADP:H4'	1.97	0.47
3:3:569:HIS:HA	5:5:398:LYS:HD3	1.96	0.47
5:5:20:ASN:N	5:5:23:ASP:OD2	2.48	0.47
5:5:448:GLY:O	5:5:468:ALA:N	2.47	0.47
6:6:611:ALA:HB3	6:6:624:GLU:HB3	1.97	0.47
2:B:189:VAL:HG22	2:B:197:TRP:CG	2.49	0.47
2:B:502:ALA:O	2:B:505:ILE:HG22	2.15	0.47
3:C:519:VAL:HG23	3:C:532:ASN:O	2.15	0.47
5:E:100:ARG:O	5:E:104:LEU:HD23	2.15	0.47
6:F:303:GLU:OE2	6:F:354:LEU:HB2	2.14	0.47
6:F:623:ILE:HD11	6:F:668:ILE:HG21	1.97	0.47
7:G:530:ASP:N	7:G:530:ASP:OD1	2.48	0.47
2:2:553:LEU:HD22	2:2:605:LEU:HD22	1.96	0.47
4:4:356:MET:CE	4:4:372:GLU:H	2.27	0.47
6:6:589:VAL:HG11	6:6:597:TYR:HB2	1.97	0.47
5:E:181:ILE:HG13	5:E:190:THR:HB	1.97	0.47
5:E:338:GLU:HG3	5:E:339:THR:H	1.80	0.47
5:E:486:ARG:HB2	5:E:486:ARG:NH1	2.29	0.47
6:F:500:ASP:HB3	6:F:502:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:529:LEU:HD23	6:F:751:LEU:HD22	1.97	0.47
6:F:580:SER:HB2	6:F:583:GLN:HB2	1.97	0.47
7:G:644:TYR:O	7:G:647:THR:OG1	2.21	0.47
4:4:193:ASN:ND2	4:4:253:GLN:O	2.34	0.46
7:7:472:ALA:O	7:7:476:ILE:HD12	2.15	0.46
8:8:370:LYS:O	8:8:374:TYR:HB2	2.15	0.46
8:8:471:GLU:HG3	9:9:348:ALA:HB1	1.97	0.46
3:C:330:HIS:CG	3:C:338:ALA:HB2	2.50	0.46
3:C:491:GLU:HG2	3:C:700:ARG:HH21	1.80	0.46
4:D:694:LEU:HD13	4:D:698:LEU:HD23	1.96	0.46
7:G:81:ASP:OD1	7:G:205:LYS:HD2	2.15	0.46
2:2:660:THR:HA	2:2:851:VAL:HG22	1.97	0.46
4:4:762:ILE:C	6:6:736:MET:HE1	2.40	0.46
5:5:87:ILE:HG22	5:5:88:PRO:HD3	1.97	0.46
5:5:637:GLU:OE1	5:5:643:ARG:HA	2.15	0.46
7:G:410:VAL:HG21	7:G:641:TYR:CZ	2.50	0.46
7:G:671:SER:HB3	7:G:683:GLN:HA	1.97	0.46
5:5:5:ARG:NH1	3:C:234:GLU:OE2	2.48	0.46
7:7:583:ASN:O	7:7:583:ASN:ND2	2.46	0.46
8:8:379:LYS:NZ	9:9:301:ILE:HB	2.30	0.46
2:B:505:ILE:HD11	10:B:901:ADP:C6	2.50	0.46
2:B:560:ALA:HB3	2:B:563:ALA:HB2	1.97	0.46
5:E:554:PHE:CZ	5:E:687:SER:HB3	2.50	0.46
2:2:760:GLN:O	2:2:764:MET:HG3	2.15	0.46
3:3:384:MET:CE	3:3:513:ILE:HB	2.44	0.46
3:3:415:LYS:HE2	3:3:415:LYS:HB2	1.74	0.46
4:4:528:PRO:HD2	7:7:446:ASP:CG	2.40	0.46
4:4:575:SER:HB2	10:4:1102:ADP:O1A	2.15	0.46
5:5:625:ASN:ND2	5:5:681:ILE:HG12	2.30	0.46
8:8:98:THR:HA	8:8:105:PRO:HB3	1.98	0.46
2:B:591:LEU:O	5:E:259:GLN:NE2	2.41	0.46
5:E:382:GLU:OE1	5:E:382:GLU:N	2.47	0.46
2:2:810:LEU:HA	2:2:813:ILE:HD12	1.97	0.46
4:4:315:ARG:CZ	4:4:413:HIS:HB2	2.45	0.46
4:4:340:PRO:HG3	6:6:452:ILE:HG13	1.97	0.46
2:B:303:ILE:HG13	2:B:319:ARG:HD3	1.96	0.46
3:C:698:THR:CG2	7:G:573:ARG:HH22	2.29	0.46
5:E:484:LYS:HD2	5:E:484:LYS:HA	1.79	0.46
7:G:656:VAL:HG13	7:G:713:VAL:HG21	1.98	0.46
3:3:43:ARG:HA	3:3:43:ARG:HD2	1.73	0.46
5:5:338:GLU:HG3	5:5:339:THR:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:618:TYR:HB3	7:7:626:PRO:HG3	1.97	0.46
2:B:690:GLU:HG3	2:B:694:ARG:NH1	2.30	0.46
3:C:341:MET:SD	3:C:341:MET:N	2.88	0.46
3:3:291:ARG:O	3:3:329:LEU:N	2.34	0.46
4:4:460:TYR:CG	6:6:413:PRO:HB3	2.51	0.46
4:4:761:ILE:HG22	4:4:816:VAL:HG12	1.98	0.46
5:5:439:THR:HG22	5:5:440:SER:O	2.16	0.46
7:7:243:GLY:HA2	7:7:318:LEU:HG	1.97	0.46
7:7:471:LYS:O	7:7:475:LYS:HG2	2.16	0.46
5:5:27:ILE:HG23	5:5:75:ILE:HD11	1.97	0.46
8:8:138:LYS:HZ2	9:9:347:HIS:H	1.63	0.46
8:8:170:LEU:HD11	10:8:1001:ADP:N3	2.31	0.46
8:8:325:ASP:OD1	8:8:326:ALA:N	2.49	0.46
8:8:453:ASP:HB3	8:8:456:LYS:HB3	1.98	0.46
9:9:675:ILE:HA	9:9:680:HIS:CD2	2.51	0.46
2:B:208:ALA:O	2:B:212:LYS:HG3	2.16	0.46
2:B:521:GLY:HA2	2:B:537:ILE:HD12	1.98	0.46
2:B:662:PRO:O	2:B:666:ASN:ND2	2.47	0.46
5:E:552:MET:HB2	5:E:687:SER:HB2	1.98	0.46
2:2:233:THR:HG23	2:2:237:MET:CE	2.45	0.46
2:2:271:PHE:CD2	2:2:295:VAL:HG21	2.50	0.46
2:B:793:LEU:HD12	2:B:805:ILE:HG21	1.98	0.46
2:2:596:LEU:HD11	2:2:620:ILE:HD13	1.98	0.46
3:3:184:GLY:HA2	3:3:261:MET:HG3	1.97	0.46
3:3:363:LEU:HD22	3:3:656:LEU:HD13	1.98	0.46
4:4:437:GLY:HA3	4:4:462:ASP:O	2.15	0.46
6:6:390:LYS:HB2	6:6:393:ASP:HB2	1.98	0.46
4:D:308:VAL:HG13	4:D:308:VAL:O	2.16	0.46
7:G:360:TYR:CZ	7:G:362:GLY:HA3	2.51	0.46
4:4:413:HIS:CG	4:4:414:SER:H	2.33	0.45
5:5:351:GLU:HA	5:5:354:GLU:OE2	2.15	0.45
5:5:681:ILE:O	5:5:685:GLN:HG2	2.16	0.45
6:6:791:SER:OG	6:6:837:ARG:NH2	2.32	0.45
7:7:492:GLY:O	7:7:512:ALA:N	2.41	0.45
3:C:104:ARG:HD3	3:C:111:TRP:CE2	2.51	0.45
3:C:408:VAL:O	3:C:548:VAL:HA	2.16	0.45
4:D:655:SER:HA	4:D:664:THR:HA	1.98	0.45
5:E:369:ILE:O	5:E:373:SER:N	2.49	0.45
2:2:337:VAL:HA	2:2:380:THR:HG23	1.98	0.45
7:7:358:ALA:N	7:7:373:GLU:O	2.45	0.45
8:8:126:GLU:OE2	8:8:173:LEU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:684:ARG:NH2	2:B:847:ASP:OD1	2.48	0.45
4:D:319:PRO:HB3	7:G:253:PRO:HB3	1.99	0.45
3:3:103:LEU:HD21	3:3:114:ILE:HD12	1.99	0.45
4:4:292:ASP:OD1	4:4:292:ASP:N	2.47	0.45
5:5:453:VAL:O	5:5:506:LYS:NZ	2.37	0.45
9:9:175:THR:O	9:9:203:SER:HA	2.17	0.45
3:C:301:LEU:HD12	3:C:320:LEU:HD21	1.97	0.45
4:D:427:CYS:HA	4:D:468:LYS:NZ	2.32	0.45
4:D:570:PRO:HB3	13:D:1103:BEF:F3	2.07	0.45
5:E:148:LEU:HA	5:E:151:LEU:HD23	1.98	0.45
5:5:194:ILE:O	5:5:194:ILE:HG22	2.16	0.45
5:5:257:LYS:HD3	5:5:273:ASN:HD22	1.80	0.45
5:5:487:ASP:OD1	5:5:488:GLU:N	2.50	0.45
6:6:504:PHE:CE2	6:6:508:LEU:HD21	2.50	0.45
7:7:89:GLN:OE1	7:7:102:LEU:N	2.47	0.45
2:B:484:PHE:HZ	2:B:765:LYS:HB3	1.80	0.45
2:B:486:LYS:HA	2:B:486:LYS:HD3	1.79	0.45
5:E:84:SER:HA	5:E:197:PHE:HE2	1.81	0.45
5:E:404:MET:HE3	5:E:404:MET:HB3	1.75	0.45
2:2:549:LYS:HA	2:2:552:ILE:HD12	1.98	0.45
2:2:686:LEU:O	6:6:781:ARG:NH2	2.46	0.45
4:4:432:ARG:HH21	4:4:588:GLY:H	1.64	0.45
5:5:69:ILE:HG22	5:5:76:TYR:CD2	2.52	0.45
5:5:383:ASP:OD1	5:5:383:ASP:N	2.48	0.45
5:5:421:ALA:HB2	10:5:801:ADP:C8	2.51	0.45
7:7:193:PRO:HG2	5:E:9:TYR:CE2	2.52	0.45
9:9:692:ALA:O	9:9:695:SER:OG	2.28	0.45
2:B:853:VAL:HG13	2:B:853:VAL:O	2.16	0.45
3:C:420:ARG:NH1	5:E:501:THR:OG1	2.42	0.45
5:E:83:PRO:HG3	5:E:159:ILE:HG13	1.99	0.45
6:F:326:LYS:HA	6:F:326:LYS:HD3	1.79	0.45
7:G:31:ASP:HB2	7:G:62:LYS:HD3	1.98	0.45
7:G:425:ASN:HB3	7:G:428:VAL:CG2	2.47	0.45
3:3:674:GLU:CD	3:3:723:LYS:HB2	2.42	0.45
6:6:170:ILE:HD12	6:6:181:LEU:HD11	1.98	0.45
8:8:132:TYR:CE2	8:8:133:ARG:HG2	2.51	0.45
8:8:426:TYR:CD1	8:8:429:LYS:HE2	2.52	0.45
9:9:345:GLN:HG2	9:9:346:TYR:HD1	1.81	0.45
2:B:756:SER:HB3	2:B:757:PRO:HD3	1.99	0.45
3:C:662:TYR:CE1	3:C:666:ARG:HG3	2.52	0.45
4:D:696:PRO:N	4:D:697:PRO:HD2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:656:MET:HE2	6:F:656:MET:HB2	1.75	0.45
2:2:576:LEU:HD23	2:2:595:ALA:HB3	1.97	0.45
4:4:474:LEU:HB2	4:4:586:PRO:HD3	1.98	0.45
4:4:712:VAL:HG21	7:7:672:LYS:HB2	1.99	0.45
5:5:208:PRO:HB2	5:5:241:TYR:CE2	2.52	0.45
6:6:568:ASP:N	6:6:568:ASP:OD1	2.50	0.45
4:D:519:TYR:CG	4:D:811:MET:HE1	2.52	0.45
6:F:303:GLU:N	6:F:303:GLU:OE1	2.50	0.45
7:G:158:THR:HA	7:G:185:VAL:HG11	1.97	0.45
2:2:408:VAL:HG22	2:2:451:ILE:HB	1.99	0.45
4:4:799:GLU:OE2	10:6:1101:ADP:O3'	2.31	0.45
5:5:483:ASP:OD1	5:5:483:ASP:N	2.46	0.45
6:6:141:GLU:O	6:6:145:ILE:HG13	2.16	0.45
6:6:177:PHE:O	6:6:181:LEU:HG	2.16	0.45
7:7:434:LEU:HD11	7:7:699:LEU:HG	1.98	0.45
8:8:128:PHE:HA	8:8:131:PHE:CE1	2.52	0.45
2:B:527:VAL:O	2:B:530:LYS:N	2.49	0.45
7:G:310:PHE:HE1	7:G:334:HIS:HD1	1.65	0.45
7:G:535:THR:O	7:G:538:HIS:HB2	2.17	0.45
7:G:627:ASP:OD1	7:G:628:LEU:N	2.50	0.45
4:4:181:TRP:CZ3	7:7:145:GLN:HB3	2.51	0.45
8:8:274:LYS:HE2	9:9:275:TRP:CE3	2.52	0.45
4:D:774:TYR:HD2	6:F:728:ALA:HB2	1.81	0.45
7:G:621:MET:HE3	7:G:622:HIS:ND1	2.32	0.45
4:4:775:VAL:HG21	6:6:725:THR:HG22	1.98	0.45
5:5:286:VAL:HG11	5:5:292:VAL:HG11	1.97	0.45
6:6:193:ALA:N	6:6:194:PRO:HD3	2.32	0.45
7:7:720:VAL:O	7:7:723:SER:OG	2.33	0.45
8:8:356:GLY:HA3	9:9:264:PRO:HB3	1.98	0.45
8:8:425:ALA:HA	8:8:428:LEU:HD12	1.99	0.45
4:D:480:THR:HB	6:F:370:THR:HG21	1.99	0.45
4:D:488:ASN:HB3	4:D:493:ASN:HD21	1.82	0.45
6:F:122:PHE:CE2	6:F:157:HIS:HB3	2.52	0.45
3:3:457:LEU:HA	3:3:457:LEU:HD23	1.84	0.44
3:3:701:THR:HA	3:3:704:THR:HG22	2.00	0.44
4:4:345:ALA:HB3	4:4:365:ILE:HG21	1.97	0.44
6:6:284:ILE:HA	6:6:401:GLU:HB2	1.97	0.44
7:7:533:ASP:O	7:7:537:ILE:HG12	2.17	0.44
2:B:214:PHE:O	2:B:218:TYR:HB2	2.17	0.44
2:B:597:VAL:HG23	2:B:629:ILE:HD12	1.99	0.44
2:B:815:ARG:HA	2:B:818:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:251:TYR:CE2	4:D:253:GLN:HB2	2.51	0.44
7:G:527:ASP:OD1	7:G:527:ASP:N	2.48	0.44
7:G:702:LEU:HD23	7:G:702:LEU:HA	1.84	0.44
2:2:347:ILE:HD13	2:2:379:LYS:HD2	1.98	0.44
4:4:563:ASN:HB2	4:4:649:MET:HE1	1.99	0.44
5:5:549:ARG:HA	5:5:651:ARG:HD3	1.99	0.44
6:6:196:LEU:HD23	6:6:196:LEU:H	1.82	0.44
6:6:275:ARG:HE	6:6:278:ASP:CG	2.26	0.44
2:B:186:LEU:HD22	2:B:207:ILE:HG13	2.00	0.44
2:B:511:ILE:HG21	2:B:552:ILE:HD13	1.99	0.44
3:C:166:LEU:HD12	3:C:171:LEU:HD23	1.98	0.44
4:D:568:GLY:HA3	4:D:708:VAL:O	2.17	0.44
5:E:688:THR:HG22	5:E:689:MET:N	2.33	0.44
2:2:191:ALA:HB3	2:2:197:TRP:HB2	1.98	0.44
2:2:502:ALA:HB1	2:2:505:ILE:HB	1.99	0.44
4:4:610:ASP:HB3	6:6:412:LEU:HD23	1.99	0.44
4:4:696:PRO:N	4:4:697:PRO:HD2	2.31	0.44
5:5:426:LEU:HB3	5:5:438:TYR:HE2	1.82	0.44
6:6:417:PRO:HB2	6:6:448:LEU:HB3	1.99	0.44
6:6:796:THR:O	6:6:799:GLN:HB2	2.17	0.44
7:7:268:GLU:HG3	5:E:13:VAL:HG21	1.99	0.44
8:8:21:GLN:HA	8:8:24:HIS:CD2	2.52	0.44
8:8:219:HIS:CE1	8:8:455:GLN:HB2	2.53	0.44
2:B:522:GLY:O	2:B:822:LYS:NZ	2.50	0.44
5:E:31:PHE:O	5:E:35:ILE:HG12	2.17	0.44
5:E:384:ILE:HD12	5:E:384:ILE:H	1.82	0.44
6:F:339:GLU:O	6:F:341:ARG:NH1	2.49	0.44
6:F:605:ALA:N	6:F:648:ASP:OD1	2.50	0.44
7:G:62:LYS:NZ	7:G:84:ASP:OD2	2.32	0.44
2:2:200:GLN:HB2	2:2:203:VAL:HB	2.00	0.44
2:2:213:SER:HB3	9:9:131:THR:HG21	1.99	0.44
6:6:600:GLY:HA3	6:6:640:GLU:O	2.18	0.44
7:7:541:MET:HG3	7:7:563:ILE:HD12	1.99	0.44
9:9:252:ARG:NE	4:D:373:ARG:HG3	2.33	0.44
2:B:347:ILE:HD13	2:B:379:LYS:HG2	1.98	0.44
2:B:476:TRP:HZ3	2:B:768:HIS:CE1	2.36	0.44
3:3:345:PHE:O	3:3:349:ASN:ND2	2.51	0.44
3:3:446:VAL:HG22	3:3:448:THR:H	1.82	0.44
3:3:472:ILE:O	3:3:514:ALA:HA	2.18	0.44
6:6:770:ARG:O	6:6:774:VAL:HG23	2.17	0.44
7:7:117:PHE:HB3	7:7:202:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:SER:OG	2:B:758:ILE:N	2.43	0.44
3:C:136:MET:HE3	3:C:136:MET:HB2	1.90	0.44
4:D:349:CYS:HB2	4:D:382:MET:HE1	1.99	0.44
10:D:1102:ADP:O2'	7:G:448:MET:HE3	2.17	0.44
6:F:143:MET:HE1	6:F:150:THR:O	2.18	0.44
6:F:776:LYS:HD2	6:F:828:TYR:CD2	2.52	0.44
7:G:269:VAL:HG21	7:G:285:THR:HB	2.00	0.44
5:5:161:ARG:HG2	5:5:295:VAL:HG22	1.99	0.44
7:7:255:VAL:HG22	7:7:307:PHE:CE1	2.53	0.44
7:7:570:LEU:HD23	7:7:571:TYR:CG	2.53	0.44
8:8:159:ILE:HA	8:8:189:GLN:H	1.83	0.44
7:G:73:ARG:NE	7:G:136:ASP:OD2	2.51	0.44
7:G:183:GLU:O	7:G:186:GLU:HG3	2.18	0.44
7:G:425:ASN:HB3	7:G:428:VAL:HG22	1.99	0.44
2:2:233:THR:HG23	2:2:237:MET:HE1	2.00	0.44
2:2:547:THR:HG22	2:2:547:THR:O	2.18	0.44
3:3:517:ASN:ND2	13:3:1002:BEF:F2	2.41	0.44
8:8:260:ASP:HB3	8:8:262:THR:HG23	2.00	0.44
8:8:352:PHE:HD1	9:9:268:LEU:HB2	1.82	0.44
3:C:291:ARG:HH22	5:E:511:THR:HB	1.83	0.44
4:D:437:GLY:HA3	4:D:462:ASP:O	2.18	0.44
4:D:518:LEU:HD23	4:D:812:LYS:HD3	2.00	0.44
5:E:166:ILE:O	5:E:289:GLY:N	2.30	0.44
5:E:453:VAL:HG21	5:E:504:ILE:HG21	2.00	0.44
6:F:125:GLN:HA	6:F:132:VAL:HG23	1.98	0.44
6:F:552:LEU:HD13	6:F:813:ALA:HB2	1.98	0.44
6:F:609:THR:O	6:F:626:GLY:HA3	2.17	0.44
7:G:364:LYS:HD3	7:G:364:LYS:HA	1.79	0.44
7:G:423:TYR:HB2	7:G:615:HIS:CG	2.53	0.44
3:3:662:TYR:CE1	3:3:666:ARG:HG3	2.53	0.44
7:7:481:VAL:HG22	7:7:516:ALA:HB2	1.99	0.44
9:9:233:THR:HB	9:9:236:ASN:HB3	1.98	0.44
3:C:369:PRO:HD2	5:E:402:ASP:OD2	2.17	0.44
3:C:741:ASP:N	3:C:741:ASP:OD1	2.51	0.44
6:F:644:MET:HE2	6:F:649:GLN:HG3	1.99	0.44
7:G:252:LYS:HA	7:G:252:LYS:HD3	1.73	0.44
4:4:512:VAL:HG21	4:4:746:PHE:CE2	2.53	0.44
4:4:728:TYR:HA	7:7:442:LYS:NZ	2.33	0.44
2:B:181:LEU:HB3	2:B:182:THR:H	1.61	0.44
2:B:202:ASN:OD1	2:B:203:VAL:N	2.51	0.44
5:E:410:ILE:O	5:E:518:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:330:PRO:HD2	6:F:344:TRP:CE2	2.53	0.44
6:F:764:ILE:N	6:F:817:ASP:O	2.43	0.44
2:2:774:ILE:HG22	2:2:776:PRO:HD3	1.99	0.43
3:3:115:LEU:HD23	3:3:115:LEU:HA	1.76	0.43
4:4:752:SER:O	4:4:756:GLU:HG3	2.19	0.43
5:5:52:ASN:O	5:5:56:VAL:HG23	2.18	0.43
7:7:690:LEU:HD23	7:7:690:LEU:HA	1.81	0.43
8:8:137:ILE:HA	8:8:140:ILE:HD13	1.99	0.43
8:8:287:PRO:HD3	8:8:303:TRP:CE2	2.53	0.43
2:B:473:VAL:HG23	2:B:474:PHE:CD1	2.53	0.43
2:B:851:VAL:O	2:B:854:ARG:HG2	2.18	0.43
3:C:552:ASP:HB2	3:C:557:ARG:HH22	1.83	0.43
4:D:533:LEU:HD12	4:D:536:VAL:HG21	2.00	0.43
6:F:629:MET:N	6:F:629:MET:HE2	2.32	0.43
4:4:701:ARG:HA	4:4:796:ARG:HD2	1.99	0.43
5:5:36:LEU:HB3	5:5:47:ARG:HH21	1.83	0.43
5:5:301:TYR:O	5:5:325:THR:N	2.41	0.43
6:6:644:MET:SD	6:6:648:ASP:HB2	2.58	0.43
7:7:583:ASN:C	7:7:583:ASN:HD22	2.25	0.43
9:9:315:TYR:HB3	9:9:322:ARG:NH1	2.34	0.43
2:B:255:ILE:HG13	2:B:259:PHE:CZ	2.53	0.43
2:B:483:GLU:O	2:B:487:ILE:HD12	2.17	0.43
5:E:396:SER:OG	5:E:398:LYS:NZ	2.42	0.43
6:F:284:ILE:HA	6:F:401:GLU:HG3	1.99	0.43
6:F:608:LEU:HD13	6:F:652:ILE:CG1	2.48	0.43
6:6:585:LEU:HB3	6:6:637:CYS:HB3	2.00	0.43
6:6:623:ILE:HG21	6:6:672:LEU:HD21	1.98	0.43
8:8:265:TYR:CD1	9:9:280:THR:HG21	2.53	0.43
2:B:485:ARG:O	2:B:489:ARG:HG3	2.19	0.43
4:D:715:LYS:HB3	4:D:715:LYS:HE2	1.70	0.43
7:G:398:GLU:O	7:G:402:MET:HG2	2.18	0.43
7:G:401:VAL:O	7:G:405:ILE:HG12	2.18	0.43
2:2:306:LEU:HD13	2:2:392:GLU:HG2	2.00	0.43
2:2:485:ARG:HD2	2:2:485:ARG:HA	1.90	0.43
4:4:684:PRO:HG3	4:4:847:MET:HE3	2.00	0.43
5:5:209:ARG:HD2	5:5:209:ARG:N	2.34	0.43
7:7:702:LEU:HD23	7:7:702:LEU:HA	1.70	0.43
8:8:38:LYS:HB2	8:8:48:TYR:CE1	2.53	0.43
8:8:107:CYS:HB2	8:8:119:VAL:HG12	2.00	0.43
8:8:140:ILE:H	8:8:140:ILE:HD12	1.84	0.43
8:8:299:LYS:HA	8:8:302:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:PHE:CE1	2:B:375:VAL:HG22	2.53	0.43
4:D:209:LEU:HG	4:D:250:ALA:HA	2.00	0.43
4:D:839:ASP:HB3	4:D:842:THR:O	2.19	0.43
6:F:313:MET:HE1	6:F:338:CYS:HA	1.99	0.43
7:G:313:CYS:HB2	7:G:333:ILE:HB	2.01	0.43
4:4:234:ARG:HH21	4:4:235:GLU:HG2	1.84	0.43
4:4:461:VAL:HG12	4:4:462:ASP:O	2.18	0.43
4:4:512:VAL:HG21	4:4:746:PHE:HE2	1.83	0.43
5:5:383:ASP:OD1	5:5:384:ILE:HD12	2.18	0.43
7:7:546:ILE:O	7:7:557:LEU:N	2.52	0.43
8:8:29:ILE:HD11	8:8:110:LYS:HD3	2.00	0.43
8:8:261:LEU:HD23	9:9:258:ILE:HD12	2.01	0.43
8:8:297:SER:O	8:8:300:ILE:HG12	2.17	0.43
8:8:330:LEU:O	8:8:334:THR:HG23	2.18	0.43
8:8:458:SER:HB2	8:8:462:ASP:HB2	2.00	0.43
2:B:252:SER:OG	2:B:253:LYS:N	2.51	0.43
3:C:121:PHE:C	3:C:124:PRO:HD2	2.44	0.43
4:D:613:GLN:HA	6:F:617:GLU:HG2	1.99	0.43
5:E:365:LYS:O	5:E:369:ILE:HG12	2.18	0.43
6:F:145:ILE:HG22	6:F:146:TYR:CD1	2.53	0.43
6:F:820:THR:OG1	6:F:822:SER:OG	2.33	0.43
7:G:138:VAL:HG21	7:G:303:ARG:NH1	2.34	0.43
7:G:675:MET:SD	7:G:676:ASP:HB2	2.58	0.43
3:3:112:SER:O	3:3:116:VAL:HG12	2.18	0.43
3:3:301:LEU:HD12	3:3:320:LEU:HD21	1.99	0.43
4:4:315:ARG:NH1	4:4:413:HIS:HB2	2.33	0.43
4:4:721:ALA:HB2	7:7:664:TYR:CD2	2.53	0.43
6:6:632:ASP:OD1	6:6:675:ARG:N	2.52	0.43
8:8:45:SER:OG	8:8:46:SER:N	2.52	0.43
9:9:263:TYR:HB3	9:9:264:PRO:HD2	1.99	0.43
9:9:534:ARG:HD3	4:D:177:LEU:HA	2.01	0.43
2:B:333:GLN:O	2:B:383:ARG:HG2	2.18	0.43
3:C:570:ARG:NH2	5:E:616:PRO:HG3	2.33	0.43
5:E:74:ASP:HB2	5:E:78:LYS:NZ	2.33	0.43
6:F:306:LYS:HA	6:F:323:GLN:H	1.84	0.43
7:G:179:ASP:O	7:G:182:ARG:NH2	2.52	0.43
4:4:252:LYS:HA	4:4:255:GLU:HG3	1.99	0.43
4:4:631:ILE:O	4:4:673:ALA:HA	2.19	0.43
5:5:184:ARG:NH1	5:5:239:ASP:O	2.52	0.43
7:7:143:LEU:HD22	7:7:197:THR:HA	2.01	0.43
8:8:47:VAL:HG22	8:8:76:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:81:THR:OG1	9:9:661:CYS:HA	2.19	0.43
8:8:185:LEU:HG	8:8:279:ALA:HB1	2.00	0.43
3:C:104:ARG:HB2	3:C:111:TRP:CD1	2.53	0.43
3:C:484:VAL:HG22	7:G:528:LYS:HD3	2.00	0.43
4:D:178:ARG:HA	4:D:178:ARG:HD2	1.89	0.43
5:E:259:GLN:HG2	5:E:260:GLU:O	2.19	0.43
5:E:489:ASP:O	5:E:493:ILE:HG12	2.19	0.43
6:F:118:PHE:O	6:F:122:PHE:HB2	2.19	0.43
2:2:252:SER:OG	2:2:253:LYS:N	2.49	0.43
3:3:696:PRO:HB3	7:7:573:ARG:NH2	2.33	0.43
6:6:318:VAL:HG21	6:6:334:PRO:HD3	2.01	0.43
6:6:338:CYS:SG	6:6:340:ASN:HB2	2.59	0.43
8:8:352:PHE:HA	9:9:268:LEU:HA	2.01	0.43
2:B:523:VAL:H	2:B:818:GLU:HG3	1.84	0.43
4:D:524:ARG:HD2	4:D:739:ASP:OD2	2.19	0.43
4:D:777:MET:HG2	4:D:830:ARG:NH2	2.34	0.43
5:E:190:THR:HG22	5:E:191:SER:N	2.33	0.43
6:F:608:LEU:HA	6:F:627:ALA:HB3	2.00	0.43
2:2:790:TYR:HB2	2:2:810:LEU:HD13	2.01	0.43
4:4:375:ASP:OD1	4:4:376:CYS:N	2.52	0.43
4:4:451:ARG:NH1	6:6:445:VAL:HG13	2.33	0.43
6:6:308:SER:O	6:6:346:LEU:HA	2.19	0.43
9:9:268:LEU:HB3	9:9:279:ILE:HG22	2.01	0.43
9:9:316:ASP:O	9:9:322:ARG:HD3	2.18	0.43
3:C:395:ASN:OD1	3:C:396:GLY:N	2.52	0.43
3:C:491:GLU:HB2	3:C:542:ARG:HD2	2.00	0.43
5:E:59:TYR:HA	5:E:135:PHE:CZ	2.54	0.43
5:E:65:MET:HE2	5:E:141:SER:HB2	2.00	0.43
6:F:195:GLU:H	6:F:195:GLU:CD	2.26	0.43
2:2:227:TYR:HB3	9:9:165:PHE:HE2	1.82	0.43
2:2:580:VAL:HG23	2:2:631:ILE:HD11	2.01	0.43
3:3:413:THR:O	3:3:413:THR:HG22	2.19	0.43
5:5:178:TYR:CE1	5:5:191:SER:HB3	2.53	0.43
5:5:206:SER:HB2	5:5:209:ARG:NH2	2.34	0.43
6:6:122:PHE:HE1	6:6:160:MET:HE1	1.84	0.43
7:7:29:LYS:HB3	7:7:61:PRO:HA	2.01	0.43
7:7:654:GLU:HA	7:7:657:ASN:ND2	2.33	0.43
8:8:285:ARG:HG2	8:8:289:VAL:HG13	2.00	0.43
4:D:477:ASP:OD1	4:D:479:SER:OG	2.35	0.43
4:D:704:LEU:HD11	4:D:804:LEU:HD21	2.00	0.43
4:D:711:LYS:HE2	4:D:847:MET:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:622:LEU:HD23	5:E:622:LEU:HA	1.90	0.43
2:2:609:PHE:HB3	2:2:650:ALA:HB2	2.00	0.42
3:3:214:TYR:OH	3:3:232:PRO:HD3	2.19	0.42
3:3:474:GLU:HB3	3:3:477:LYS:HD3	2.01	0.42
7:7:312:GLU:HB3	7:7:502:VAL:HG21	2.01	0.42
8:8:369:LEU:O	8:8:373:VAL:HG22	2.19	0.42
9:9:190:ILE:HG13	9:9:191:LEU:N	2.34	0.42
9:9:283:TRP:CD1	9:9:295:PRO:HG2	2.54	0.42
9:9:316:ASP:OD2	9:9:319:SER:N	2.52	0.42
3:C:698:THR:H	3:C:701:THR:HG23	1.83	0.42
4:D:739:ASP:OD1	4:D:739:ASP:N	2.51	0.42
6:F:706:MET:HA	6:F:712:PHE:HZ	1.84	0.42
2:2:182:THR:O	2:2:185:SER:OG	2.34	0.42
3:3:474:GLU:OE1	3:3:477:LYS:NZ	2.46	0.42
3:3:741:ASP:OD1	3:3:741:ASP:N	2.51	0.42
6:6:341:ARG:HG3	6:6:344:TRP:NE1	2.30	0.42
7:7:267:TYR:CE1	5:E:12:PRO:HB3	2.53	0.42
7:7:272:GLU:OE2	5:E:9:TYR:OH	2.37	0.42
8:8:90:GLU:OE1	8:8:184:GLY:HA2	2.18	0.42
8:8:102:ARG:NH1	8:8:149:ARG:HG2	2.34	0.42
8:8:429:LYS:HA	8:8:432:GLN:HG3	2.01	0.42
2:B:186:LEU:HD11	2:B:206:THR:HG22	2.01	0.42
2:B:206:THR:O	2:B:209:ARG:HG2	2.19	0.42
2:B:271:PHE:CB	2:B:295:VAL:HG21	2.46	0.42
2:B:371:GLY:N	2:B:372:PRO:HD3	2.34	0.42
2:B:501:MET:HG3	2:B:516:ALA:HB2	2.00	0.42
3:C:483:ARG:O	3:C:486:ILE:HG22	2.19	0.42
4:D:336:THR:HG22	4:D:396:VAL:H	1.85	0.42
5:E:31:PHE:CE2	5:E:90:PHE:HB2	2.54	0.42
5:E:200:ILE:HD13	5:E:204:THR:HG21	2.01	0.42
2:2:537:ILE:HD11	2:2:815:ARG:HB3	2.01	0.42
3:3:342:LEU:HD21	3:3:662:TYR:HB2	2.01	0.42
3:3:473:ASP:OD1	3:3:474:GLU:N	2.52	0.42
5:5:437:VAL:HG23	5:5:472:ALA:HB2	2.00	0.42
7:7:260:TYR:HB2	7:7:269:VAL:HG23	2.01	0.42
7:7:425:ASN:HB3	7:7:428:VAL:CG2	2.49	0.42
8:8:144:ILE:O	8:8:148:LEU:HD23	2.19	0.42
8:8:297:SER:OG	8:8:298:THR:N	2.51	0.42
3:C:390:GLU:OE2	3:C:398:HIS:HE1	2.02	0.42
6:F:150:THR:HG23	6:F:264:GLN:HB3	2.00	0.42
6:F:347:ASN:ND2	6:F:350:ARG:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:772:TYR:HD2	6:F:824:ILE:HB	1.84	0.42
6:F:777:TYR:HB2	6:F:800:LEU:HD13	2.01	0.42
7:G:722:VAL:HA	7:G:725:GLU:HB2	2.01	0.42
4:4:360:ILE:HD11	4:4:363:GLY:HA2	2.02	0.42
4:4:544:LEU:HD23	4:4:544:LEU:HA	1.81	0.42
5:5:463:TYR:OH	5:5:465:GLU:HG2	2.20	0.42
6:6:581:LYS:HB2	6:6:581:LYS:HE2	1.80	0.42
7:7:493:LEU:HG	7:7:513:LEU:HD13	2.00	0.42
2:B:328:THR:HG1	2:B:387:ARG:H	1.66	0.42
2:B:704:VAL:HG11	6:F:770:ARG:HH21	1.84	0.42
2:B:779:HIS:HB3	2:B:782:ASP:OD1	2.18	0.42
2:B:800:THR:CG2	2:B:856:GLN:HE21	2.32	0.42
3:C:400:ARG:HH21	3:C:707:ARG:HH22	1.68	0.42
4:D:568:GLY:HA3	4:D:708:VAL:HG23	2.01	0.42
5:E:52:ASN:HA	5:E:55:LEU:HD12	2.01	0.42
5:E:525:PRO:HG2	5:E:530:TYR:HD1	1.83	0.42
6:F:723:ILE:O	6:F:726:GLU:HG2	2.20	0.42
3:3:407:MET:HE3	3:3:407:MET:HB2	1.87	0.42
6:6:566:ARG:NH2	6:6:710:ASP:OD1	2.52	0.42
6:6:600:GLY:N	6:6:639:ASP:O	2.52	0.42
2:B:804:PRO:HD3	5:E:529:ARG:NH2	2.33	0.42
3:C:296:GLY:HA3	3:C:322:LEU:O	2.20	0.42
5:E:409:ASP:HB2	5:E:500:GLN:HE22	1.84	0.42
6:F:800:LEU:HA	6:F:803:MET:CE	2.50	0.42
7:G:265:CYS:SG	7:G:267:TYR:HB2	2.59	0.42
7:G:334:HIS:HD2	7:G:375:TYR:CG	2.37	0.42
7:G:552:GLY:O	7:G:553:ILE:HD13	2.19	0.42
7:G:653:SER:HB2	7:G:707:MET:HE3	2.01	0.42
2:2:476:TRP:HA	2:2:765:LYS:HD2	2.01	0.42
2:2:658:ASN:ND2	2:2:661:LEU:HG	2.34	0.42
3:3:362:ILE:HD13	3:3:362:ILE:HA	1.94	0.42
3:3:448:THR:HG22	3:3:455:ARG:NH2	2.34	0.42
5:5:440:SER:HA	5:5:480:ASP:OD1	2.20	0.42
6:6:136:TYR:O	6:6:139:GLN:HG2	2.20	0.42
6:6:701:MET:HB2	6:6:706:MET:HE1	2.01	0.42
7:7:115:GLU:HA	7:7:118:CYS:SG	2.60	0.42
7:7:586:LEU:HD22	7:7:590:LEU:HD23	2.01	0.42
8:8:15:ILE:O	8:8:19:MET:HG3	2.19	0.42
8:8:55:GLY:O	8:8:58:THR:OG1	2.24	0.42
8:8:138:LYS:HD3	9:9:344:PHE:C	2.45	0.42
8:8:228:ARG:HA	8:8:228:ARG:HD3	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:396:GLY:O	7:G:475:LYS:HE3	2.20	0.42
6:F:401:GLU:OE2	6:F:452:ILE:HG23	2.20	0.42
2:2:756:SER:HB2	2:2:757:PRO:HD3	2.02	0.42
2:2:786:VAL:HG12	2:2:834:LEU:HD21	2.01	0.42
3:3:211:TYR:CE1	7:7:6:PRO:HB2	2.55	0.42
3:3:423:LEU:HD13	3:3:431:ALA:HB2	2.02	0.42
3:3:716:ARG:NH2	3:3:725:ASP:OD2	2.39	0.42
6:6:364:ASN:O	6:6:368:ILE:HG13	2.20	0.42
7:7:196:LEU:HD21	7:7:257:VAL:HG21	2.02	0.42
8:8:14:GLU:HA	8:8:17:GLU:OE1	2.19	0.42
8:8:41:GLU:OE2	8:8:79:TYR:OH	2.36	0.42
8:8:102:ARG:HA	8:8:179:VAL:HG12	2.02	0.42
9:9:255:ARG:C	9:9:257:ASP:H	2.27	0.42
2:B:576:LEU:HD23	2:B:595:ALA:HB3	2.01	0.42
4:D:585:THR:HG21	4:D:628:VAL:HB	2.02	0.42
4:D:587:ARG:O	4:D:627:GLY:HA3	2.19	0.42
4:D:613:GLN:O	4:D:615:VAL:HG23	2.20	0.42
5:E:476:VAL:HG12	5:E:518:SER:OG	2.19	0.42
5:E:667:GLU:CD	5:E:676:HIS:HE2	2.27	0.42
7:G:16:ASN:ND2	7:G:100:ASP:OD2	2.53	0.42
8:8:389:TYR:OH	9:9:330:ASP:OD1	2.27	0.42
8:8:464:LEU:HA	8:8:469:PHE:CD2	2.53	0.42
2:B:366:ASN:O	2:B:368:LYS:NZ	2.53	0.42
4:D:711:LYS:NZ	4:D:847:MET:SD	2.72	0.42
6:F:764:ILE:O	6:F:818:GLU:HA	2.19	0.42
2:2:211:LEU:HD22	2:2:271:PHE:CD1	2.54	0.42
3:3:406:LEU:HD23	3:3:546:LEU:HD13	2.02	0.42
4:4:251:TYR:HB3	4:4:254:THR:HG22	2.01	0.42
4:4:678:ILE:HD13	4:4:693:ASP:OD2	2.19	0.42
5:5:460:ARG:HA	5:5:460:ARG:HD2	1.81	0.42
6:6:656:MET:HE2	6:6:656:MET:HB2	1.84	0.42
7:7:417:SER:CB	7:7:638:MET:HE2	2.49	0.42
8:8:22:LEU:HD12	8:8:26:LEU:HD23	2.01	0.42
2:B:485:ARG:HD3	2:B:485:ARG:HA	1.87	0.42
3:C:400:ARG:HG3	3:C:493:GLN:NE2	2.35	0.42
4:D:451:ARG:HD2	6:F:445:VAL:HG21	2.01	0.42
4:D:452:VAL:HG12	7:G:277:THR:HG22	2.01	0.42
4:D:642:ARG:HD3	4:D:698:LEU:CD2	2.36	0.42
5:E:400:LEU:HD23	5:E:406:LEU:HD23	2.00	0.42
6:F:416:LYS:HD3	6:F:416:LYS:HA	1.85	0.42
7:G:589:ALA:O	7:G:593:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:574:VAL:HB	2:2:595:ALA:HB2	2.02	0.42
4:4:522:LEU:HB3	4:4:541:LEU:CD1	2.50	0.42
4:4:590:TYR:OH	4:4:632:ASP:OD2	2.34	0.42
4:4:712:VAL:HB	7:7:672:LYS:HD3	2.01	0.42
6:6:120:GLU:OE2	6:6:188:VAL:HG13	2.19	0.42
6:6:655:ALA:O	6:6:659:GLN:N	2.50	0.42
7:7:138:VAL:O	7:7:141:VAL:HG22	2.20	0.42
8:8:29:ILE:HG23	8:8:33:TYR:HD2	1.85	0.42
2:B:407:GLU:HB3	2:B:450:ILE:HG22	2.01	0.42
4:D:575:SER:HB2	10:D:1102:ADP:O1A	2.20	0.42
4:D:769:GLU:OE1	4:D:819:LEU:HB3	2.20	0.42
5:E:633:LEU:HD22	5:E:648:ILE:HG12	2.01	0.42
6:F:158:LEU:HG	6:F:167:ALA:HB2	2.01	0.42
6:F:330:PRO:HD2	6:F:344:TRP:NE1	2.34	0.42
7:G:457:CYS:HB2	7:G:594:PHE:CD1	2.55	0.42
7:G:685:THR:O	7:G:688:THR:OG1	2.27	0.42
2:2:281:LEU:HB3	9:9:164:GLN:HG2	2.01	0.41
3:3:555:GLU:HG3	5:5:631:LYS:HD3	2.01	0.41
4:4:397:ILE:O	4:4:417:LEU:N	2.46	0.41
7:7:396:ASP:OD1	7:7:397:VAL:N	2.52	0.41
8:8:299:LYS:HD3	8:8:457:ARG:HB3	2.03	0.41
2:B:333:GLN:HE22	5:E:322:ALA:HB1	1.84	0.41
3:C:486:ILE:HG13	3:C:490:MET:HG3	2.02	0.41
5:E:258:LEU:HB2	5:E:276:MET:SD	2.59	0.41
6:F:505:LEU:HD23	6:F:505:LEU:HA	1.82	0.41
7:G:428:VAL:O	7:G:432:LEU:HG	2.20	0.41
5:5:32:LYS:HZ2	5:5:100:ARG:NH2	2.18	0.41
6:6:653:HIS:CG	6:6:705:ILE:HD12	2.55	0.41
8:8:271:ARG:HE	9:9:275:TRP:C	2.27	0.41
3:C:161:PHE:CZ	3:C:295:VAL:HG21	2.55	0.41
3:C:391:LYS:HB2	3:C:399:LEU:HD12	2.01	0.41
2:2:511:ILE:HD13	2:2:681:CYS:HB3	2.02	0.41
2:2:534:ARG:HG2	2:2:536:ASP:H	1.85	0.41
3:3:576:TYR:CE2	3:3:582:VAL:HA	2.55	0.41
4:4:755:LYS:HA	4:4:810:LYS:HD3	2.02	0.41
5:5:370:LEU:HD22	5:5:599:MET:HE3	2.02	0.41
5:5:416:GLY:HA2	5:5:556:VAL:O	2.20	0.41
7:7:442:LYS:HD2	7:7:442:LYS:HA	1.85	0.41
7:7:633:VAL:O	7:7:638:MET:HE3	2.20	0.41
8:8:374:TYR:HB2	8:8:399:LEU:HD23	2.02	0.41
2:B:410:LEU:HD23	2:B:414:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:GLN:HE22	3:C:137:ASP:HB2	1.85	0.41
3:C:98:ILE:CG1	3:C:155:LEU:HD11	2.50	0.41
4:D:217:ASN:OD1	4:D:218:ASN:N	2.54	0.41
4:D:231:ASN:HA	4:D:234:ARG:NH1	2.35	0.41
6:F:633:ASN:N	6:F:675:ARG:O	2.46	0.41
7:G:435:LEU:HD21	7:G:564:LEU:HB2	2.02	0.41
3:3:472:ILE:HG21	3:3:475:PHE:HD1	1.85	0.41
4:4:203:TYR:CZ	4:4:206:ARG:HD3	2.55	0.41
6:6:137:ARG:HD2	6:6:192:TYR:CD2	2.55	0.41
6:6:141:GLU:HA	6:6:144:LYS:HB3	2.01	0.41
7:7:681:PHE:HZ	7:7:727:LEU:HD21	1.85	0.41
8:8:269:GLU:H	9:9:525:LYS:HZ1	1.66	0.41
8:8:306:GLY:HA3	8:8:449:CYS:SG	2.61	0.41
9:9:125:ARG:C	9:9:170:VAL:HG13	2.45	0.41
5:E:33:ASN:O	5:E:37:GLU:HB2	2.19	0.41
5:E:143:ALA:HB3	5:E:161:ARG:HE	1.86	0.41
7:G:677:SER:OG	7:G:678:LYS:N	2.53	0.41
2:2:522:GLY:C	2:2:822:LYS:HZ2	2.29	0.41
3:3:41:SER:O	3:3:45:ILE:HG12	2.20	0.41
3:3:276:VAL:HG22	3:3:321:ILE:HB	2.02	0.41
5:5:9:TYR:HB2	7:G:270:PHE:HB2	2.03	0.41
6:6:312:ASP:HB3	6:6:342:ALA:HB3	2.01	0.41
6:6:321:VAL:HG11	6:6:330:PRO:HD3	2.02	0.41
7:7:631:THR:HG23	7:7:631:THR:O	2.20	0.41
2:B:625:GLU:OE2	5:E:438:TYR:OH	2.36	0.41
2:B:758:ILE:HG23	2:B:762:LEU:HD23	2.02	0.41
5:E:688:THR:HG22	5:E:689:MET:H	1.85	0.41
3:3:100:LEU:HD23	3:3:100:LEU:HA	1.88	0.41
3:3:346:ASP:OD2	3:3:658:LYS:NZ	2.39	0.41
4:4:394:LYS:HB3	4:4:394:LYS:HE2	1.77	0.41
4:4:830:ARG:NH1	4:4:835:ASP:OD2	2.47	0.41
6:6:134:LYS:HG3	6:6:137:ARG:HH12	1.86	0.41
6:6:658:GLN:HG3	6:6:660:THR:H	1.85	0.41
7:7:490:GLY:O	7:7:494:THR:HG23	2.20	0.41
9:9:137:ASN:H	9:9:140:ASN:HB3	1.86	0.41
9:9:286:GLN:O	9:9:289:THR:OG1	2.31	0.41
2:B:308:GLU:N	2:B:308:GLU:OE1	2.54	0.41
2:B:500:SER:HB3	2:B:763:LEU:HD22	2.03	0.41
3:C:178:LYS:O	3:C:180:VAL:HG13	2.21	0.41
3:C:295:VAL:CG1	3:C:325:THR:HB	2.51	0.41
4:D:321:ASP:HA	4:D:324:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:371:CYS:HA	4:D:382:MET:CE	2.50	0.41
4:D:594:LYS:HD2	4:D:594:LYS:HA	1.63	0.41
5:E:536:PRO:HA	5:E:539:ASN:ND2	2.35	0.41
5:E:626:PHE:CG	5:E:653:LEU:HD12	2.56	0.41
6:F:305:TYR:HB2	6:F:354:LEU:HG	2.02	0.41
6:F:763:PRO:HB2	6:F:819:ILE:HD11	2.02	0.41
7:G:458:LEU:HD22	7:G:600:MET:HE2	2.02	0.41
2:2:629:ILE:O	2:2:640:LEU:N	2.50	0.41
3:3:528:ASP:OD1	3:3:528:ASP:N	2.51	0.41
4:4:256:ASP:HB3	7:7:134:TYR:HD2	1.84	0.41
4:4:457:TYR:HB2	7:7:253:PRO:HG2	2.03	0.41
5:5:526:ILE:HG22	5:5:539:ASN:O	2.20	0.41
7:7:482:TYR:OH	7:7:524:ASP:OD1	2.26	0.41
9:9:125:ARG:HB3	9:9:170:VAL:HG13	2.02	0.41
2:B:559:THR:HA	2:B:764:MET:HE2	2.02	0.41
4:D:180:ILE:HB	4:D:183:THR:OG1	2.21	0.41
4:D:798:LEU:HA	4:D:801:MET:HE3	2.02	0.41
4:D:798:LEU:HA	4:D:801:MET:CE	2.50	0.41
5:E:69:ILE:HG13	5:E:76:TYR:CG	2.56	0.41
5:E:293:THR:HB	5:E:334:GLN:HB3	2.02	0.41
6:F:115:PHE:CE2	6:F:119:LEU:HD21	2.56	0.41
6:F:122:PHE:CE1	6:F:161:ARG:HB2	2.55	0.41
6:F:419:SER:OG	6:F:446:ARG:NH1	2.54	0.41
7:G:255:VAL:HA	7:G:307:PHE:HD1	1.86	0.41
2:2:674:LEU:HD12	2:2:674:LEU:HA	1.92	0.41
3:3:483:ARG:O	3:3:486:ILE:HG22	2.21	0.41
3:3:703:GLU:HB3	3:3:707:ARG:HH12	1.86	0.41
4:4:545:PHE:CE1	4:4:751:ILE:HA	2.54	0.41
4:4:663:THR:HG21	6:6:374:PRO:HG3	2.03	0.41
5:5:75:ILE:HD12	5:5:75:ILE:HA	1.94	0.41
6:6:110:LYS:O	6:6:113:GLU:HG3	2.20	0.41
6:6:149:ASN:O	6:6:264:GLN:N	2.34	0.41
6:6:277:ARG:HE	6:6:277:ARG:HB2	1.75	0.41
6:6:306:LYS:HB3	6:6:352:ARG:HB2	2.03	0.41
6:6:555:VAL:HG12	6:6:557:LYS:HG3	2.03	0.41
7:7:420:PRO:HB2	7:7:625:GLN:HB3	2.03	0.41
8:8:272:ARG:NE	4:D:297:GLU:OE2	2.53	0.41
2:B:232:ARG:HD3	2:B:282:HIS:CE1	2.56	0.41
2:B:609:PHE:O	2:B:612:MET:HG3	2.20	0.41
5:E:361:SER:HB2	5:E:668:LEU:HD13	2.03	0.41
5:E:423:SER:O	5:E:427:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:469:MET:HE2	5:E:496:ALA:HB1	2.03	0.41
6:F:170:ILE:HD12	6:F:170:ILE:HA	1.91	0.41
6:F:177:PHE:O	6:F:181:LEU:HG	2.20	0.41
6:F:831:LEU:O	6:F:835:ILE:HG22	2.20	0.41
7:G:517:ASP:OD1	7:G:560:ARG:HG2	2.20	0.41
7:G:670:ASP:O	7:G:674:GLU:HG2	2.21	0.41
2:2:279:THR:O	2:2:283:TYR:N	2.39	0.41
2:2:414:LEU:HD11	2:2:454:ASN:O	2.21	0.41
2:2:673:ILE:HA	2:2:676:ARG:HG2	2.03	0.41
3:3:330:HIS:N	3:3:589:SER:O	2.51	0.41
3:3:570:ARG:HB3	5:5:613:ARG:HH21	1.85	0.41
4:4:265:PRO:O	4:4:269:ILE:HB	2.21	0.41
4:4:524:ARG:HD2	4:4:739:ASP:OD2	2.21	0.41
5:5:274:LEU:HD12	5:5:274:LEU:HA	1.89	0.41
5:5:458:MET:N	5:5:458:MET:HE2	2.36	0.41
5:5:526:ILE:HB	5:5:541:ASP:HB2	2.03	0.41
7:7:160:GLU:O	7:7:164:GLU:HG2	2.20	0.41
7:7:298:LEU:H	7:7:298:LEU:HD23	1.86	0.41
8:8:66:TRP:HZ2	8:8:179:VAL:HG13	1.86	0.41
8:8:114:ASP:HA	9:9:690:PHE:CE2	2.56	0.41
8:8:427:GLU:HA	8:8:430:LYS:HD3	2.02	0.41
8:8:449:CYS:SG	8:8:450:PHE:N	2.93	0.41
2:B:337:VAL:HA	2:B:380:THR:HG23	2.03	0.41
2:B:340:ASN:OD1	2:B:374:ARG:HB3	2.21	0.41
2:B:525:LYS:HD2	2:B:525:LYS:HA	1.96	0.41
4:D:183:THR:HG22	4:D:264:TYR:CD1	2.56	0.41
4:D:218:ASN:OD1	4:D:219:THR:HG23	2.21	0.41
4:D:535:ASP:O	4:D:706:TYR:OH	2.29	0.41
5:E:45:ILE:HG13	5:E:46:TYR:N	2.36	0.41
5:E:416:GLY:HA3	5:E:556:VAL:HG23	2.03	0.41
5:E:420:THR:HG22	5:E:420:THR:O	2.21	0.41
5:E:437:VAL:HG23	5:E:477:VAL:HG23	2.02	0.41
6:F:707:SER:HB3	6:F:798:ARG:NH1	2.36	0.41
7:G:138:VAL:HA	7:G:141:VAL:HG12	2.03	0.41
7:G:491:VAL:HB	7:G:493:LEU:O	2.20	0.41
7:G:500:ASP:HB3	7:G:503:THR:O	2.21	0.41
2:2:217:GLU:OE1	9:9:190:ILE:HD13	2.20	0.41
3:3:350:ILE:HG23	3:3:659:TYR:CD2	2.56	0.41
6:6:628:LEU:HD11	6:6:652:ILE:HD12	2.02	0.41
7:7:548:ILE:HD12	7:7:557:LEU:HD13	2.03	0.41
7:7:668:ARG:HA	7:7:668:ARG:HD2	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:148:LEU:HD21	8:8:305:VAL:HG11	2.02	0.41
8:8:227:MET:HE2	8:8:295:ALA:HB2	2.02	0.41
2:B:610:ASP:OD1	2:B:611:LYS:N	2.54	0.41
2:B:631:ILE:HD12	5:E:446:ALA:HB3	2.03	0.41
2:B:798:ILE:HD12	2:B:798:ILE:HA	1.92	0.41
5:E:454:GLN:HB2	5:E:465:GLU:HG3	2.03	0.41
2:2:220:ASP:CG	2:2:226:VAL:HG22	2.46	0.40
3:3:176:LEU:HD22	3:3:300:SER:HB3	2.03	0.40
3:3:477:LYS:HG2	5:5:491:VAL:HG12	2.03	0.40
4:4:186:SER:OG	4:4:189:GLU:HB2	2.20	0.40
7:7:138:VAL:HG11	7:7:303:ARG:NH1	2.36	0.40
8:8:160:ILE:N	8:8:187:GLU:O	2.42	0.40
4:D:370:ARG:HA	4:D:379:PRO:HA	2.04	0.40
5:E:605:TYR:CE1	5:E:609:LYS:HG3	2.56	0.40
6:F:578:SER:O	10:F:1101:ADP:H8	2.05	0.40
7:G:360:TYR:HB2	7:G:371:LEU:O	2.21	0.40
2:2:343:LYS:NZ	2:2:372:PRO:HD3	2.34	0.40
4:4:239:SER:OG	4:4:299:LYS:HD3	2.21	0.40
4:4:651:GLN:HG2	4:4:653:THR:HG22	2.03	0.40
7:7:67:LEU:HB3	7:7:126:PRO:CD	2.51	0.40
8:8:357:LEU:HD12	8:8:357:LEU:H	1.85	0.40
9:9:211:LEU:O	9:9:215:ASP:N	2.25	0.40
2:B:384:ASN:ND2	5:E:153:SER:H	2.19	0.40
6:F:143:MET:HG3	6:F:196:LEU:HD23	2.03	0.40
3:3:572:LEU:HD23	3:3:573:PRO:O	2.22	0.40
3:C:408:VAL:HA	3:C:516:ALA:O	2.22	0.40
4:D:333:LEU:HD11	4:D:400:GLN:HB2	2.03	0.40
6:F:122:PHE:HD1	6:F:161:ARG:HH11	1.69	0.40
6:F:124:VAL:HB	6:F:135:VAL:HG11	2.04	0.40
7:G:652:MET:HA	7:G:708:VAL:HB	2.03	0.40
2:2:796:GLU:OE2	2:2:859:ARG:HB3	2.21	0.40
3:3:333:SER:OG	5:5:512:VAL:HG23	2.21	0.40
3:3:483:ARG:HB3	3:3:539:LEU:HD11	2.03	0.40
3:3:733:LEU:HD12	3:3:733:LEU:HA	1.82	0.40
4:4:319:PRO:O	4:4:322:ILE:HG12	2.21	0.40
4:4:529:SER:HA	4:4:735:HIS:NE2	2.35	0.40
6:6:259:THR:HG22	6:6:260:GLU:HG3	2.03	0.40
6:6:699:LEU:HD23	6:6:699:LEU:HA	1.92	0.40
8:8:138:LYS:HG2	9:9:344:PHE:HD2	1.85	0.40
2:B:509:ARG:NH1	2:B:509:ARG:HB3	2.37	0.40
3:C:410:ASP:HB3	3:C:411:PRO:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:336:THR:CG2	4:D:396:VAL:H	2.34	0.40
6:F:333:CYS:SG	6:F:338:CYS:HB3	2.61	0.40
7:G:493:LEU:HD21	7:G:548:ILE:HD11	2.03	0.40
3:3:622:PHE:CE2	3:3:649:LYS:HD3	2.57	0.40
5:5:433:SER:OG	5:5:436:ALA:HB2	2.21	0.40
7:7:331:LEU:HD21	7:7:376:LEU:HB2	2.02	0.40
8:8:399:LEU:O	8:8:403:LEU:HB2	2.22	0.40
9:9:239:HIS:HB2	9:9:242:LYS:NZ	2.36	0.40
2:B:855:ARG:HD3	2:B:859:ARG:NH2	2.34	0.40
3:C:226:PRO:HG2	5:E:242:ILE:HG21	2.03	0.40
3:C:261:MET:HE1	3:C:588:LEU:HD11	2.03	0.40
3:C:675:ALA:O	3:C:676:ILE:C	2.64	0.40
4:D:349:CYS:HB3	4:D:354:HIS:N	2.33	0.40
4:D:574:LYS:O	4:D:578:LEU:HD23	2.22	0.40
4:D:730:GLU:O	7:G:442:LYS:NZ	2.30	0.40
5:E:421:ALA:HA	10:E:802:ADP:H5'2	2.04	0.40
5:E:631:LYS:HD3	5:E:631:LYS:HA	1.75	0.40
7:G:592:SER:OG	7:G:687:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	618/868 (71%)	596 (96%)	22 (4%)	0	100	100
2	B	618/868 (71%)	594 (96%)	24 (4%)	0	100	100
3	3	621/971 (64%)	601 (97%)	20 (3%)	0	100	100
3	C	619/971 (64%)	595 (96%)	24 (4%)	0	100	100
4	4	664/933 (71%)	639 (96%)	25 (4%)	0	100	100
4	D	664/933 (71%)	645 (97%)	19 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	5	618/775 (80%)	604 (98%)	14 (2%)	0	100	100
5	E	618/775 (80%)	598 (97%)	20 (3%)	0	100	100
6	6	607/1017 (60%)	589 (97%)	18 (3%)	0	100	100
6	F	607/1017 (60%)	588 (97%)	19 (3%)	0	100	100
7	7	675/845 (80%)	655 (97%)	20 (3%)	0	100	100
7	G	675/845 (80%)	652 (97%)	23 (3%)	0	100	100
8	8	394/507 (78%)	381 (97%)	13 (3%)	0	100	100
9	9	327/704 (46%)	312 (95%)	15 (5%)	0	100	100
All	All	8325/12029 (69%)	8049 (97%)	276 (3%)	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	
2	2	551/770 (72%)	550 (100%)	1 (0%)	87	87
2	B	551/770 (72%)	550 (100%)	1 (0%)	87	87
3	3	550/835 (66%)	548 (100%)	2 (0%)	84	83
3	C	548/835 (66%)	548 (100%)	0	100	100
4	4	607/848 (72%)	602 (99%)	5 (1%)	73	76
4	D	607/848 (72%)	607 (100%)	0	100	100
5	5	564/688 (82%)	562 (100%)	2 (0%)	84	83
5	E	564/688 (82%)	564 (100%)	0	100	100
6	6	541/886 (61%)	528 (98%)	13 (2%)	43	62
6	F	541/886 (61%)	532 (98%)	9 (2%)	53	67
7	7	603/753 (80%)	595 (99%)	8 (1%)	61	71
7	G	603/753 (80%)	603 (100%)	0	100	100
8	8	356/454 (78%)	353 (99%)	3 (1%)	73	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	9	313/639 (49%)	309 (99%)	4 (1%)	61	71
All	All	7499/10653 (70%)	7451 (99%)	48 (1%)	76	79

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	808	ARG
3	3	277	ILE
3	3	281	ASP
4	4	536	VAL
4	4	573	SER
4	4	668	ARG
4	4	814	LYS
4	4	815	ASN
5	5	546	ILE
5	5	549	ARG
6	6	131	GLU
6	6	306	LYS
6	6	308	SER
6	6	310	THR
6	6	511	ASP
6	6	515	GLU
6	6	520	VAL
6	6	521	LYS
6	6	656	MET
6	6	759	ARG
6	6	798	ARG
6	6	801	GLU
6	6	815	CYS
7	7	401	VAL
7	7	507	ILE
7	7	508	LEU
7	7	648	LYS
7	7	685	THR
7	7	686	PRO
7	7	689	LEU
7	7	704	LEU
8	8	70	SER
8	8	174	GLU
8	8	185	LEU
9	9	122	ARG
9	9	123	ASP

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Mol	Chain	Res	Type
9	9	125	ARG
9	9	126	ILE
2	B	808	ARG
6	F	501	GLN
6	F	502	GLU
6	F	515	GLU
6	F	652	ILE
6	F	653	HIS
6	F	656	MET
6	F	759	ARG
6	F	762	LYS
6	F	815	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	238	ASN
2	2	333	GLN
2	2	626	GLN
2	2	760	GLN
2	2	780	GLN
3	3	55	ASN
3	3	374	HIS
3	3	392	ASN
3	3	517	ASN
3	3	673	GLN
3	3	677	ASN
4	4	231	ASN
4	4	263	ASN
4	4	377	ASN
4	4	543	GLN
4	4	676	ASN
4	4	723	HIS
4	4	808	HIS
5	5	334	GLN
5	5	424	GLN
5	5	625	ASN
6	6	182	GLN
6	6	364	ASN
6	6	514	ASN
6	6	540	HIS
6	6	683	ASN

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Mol	Chain	Res	Type
6	6	814	ASN
7	7	112	HIS
7	7	311	GLN
7	7	334	HIS
7	7	568	ASN
8	8	64	HIS
8	8	85	GLN
8	8	89	ASN
8	8	363	ASN
8	8	448	GLN
8	8	475	ASN
9	9	369	HIS
2	B	391	GLN
2	B	526	ASN
2	B	613	ASN
2	B	653	ASN
2	B	856	GLN
3	C	293	ASN
3	C	324	ASN
3	C	365	GLN
3	C	392	ASN
3	C	661	GLN
4	D	188	GLN
4	D	240	ASN
4	D	242	ASN
4	D	410	GLN
4	D	488	ASN
4	D	500	GLN
4	D	685	ASN
5	E	344	ASN
5	E	424	GLN
5	E	499	GLN
5	E	539	ASN
5	E	561	ASN
5	E	590	ASN
5	E	632	GLN
6	F	347	ASN
6	F	366	ASN
6	F	658	GLN
6	F	700	ASN
7	G	68	GLN
7	G	326	HIS

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Mol	Chain	Res	Type
7	G	332	ASN
7	G	518	ASN
7	G	622	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 26 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	BEF	E	801	10	0,3,3	-	-	-		
13	BEF	G	1103	10	0,3,3	-	-	-		
13	BEF	3	1002	10	0,3,3	-	-	-		
10	ADP	4	1102	11,13	28,29,29	0.49	0	43,45,45	0.50	0
10	ADP	3	1001	11,13	28,29,29	0.53	0	43,45,45	0.47	0
10	ADP	F	1101	11	28,29,29	3.22	16 (57%)	43,45,45	2.24	11 (25%)
13	BEF	4	1103	10	0,3,3	-	-	-		
13	BEF	3	1004	10	0,3,3	-	-	-		
13	BEF	D	1103	10	0,3,3	-	-	-		
10	ADP	5	801	11	28,29,29	0.53	0	43,45,45	0.42	0
10	ADP	D	1102	11,13	28,29,29	0.49	0	43,45,45	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	ADP	7	1102	11,13	28,29,29	0.49	0	43,45,45	0.48	0
10	ADP	C	1001	11,13	28,29,29	0.54	0	43,45,45	0.47	0
13	BEF	8	1003	10	0,3,3	-	-	-		
10	ADP	8	1001	11,13	28,29,29	0.49	0	43,45,45	0.48	0
10	ADP	6	1101	11	28,29,29	3.22	16 (57%)	43,45,45	2.25	11 (25%)
10	ADP	2	901	11	28,29,29	0.49	0	43,45,45	0.51	0
10	ADP	G	1102	11,13	28,29,29	0.50	0	43,45,45	0.48	0
10	ADP	E	802	11	28,29,29	0.49	0	43,45,45	0.53	0
10	ADP	B	901	11	28,29,29	0.52	0	43,45,45	0.46	0

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
10	ADP	7	1102	11,13	-	8/16/32/32	0/3/3/3
10	ADP	C	1001	11,13	-	4/16/32/32	0/3/3/3
10	ADP	G	1102	11,13	-	8/16/32/32	0/3/3/3
10	ADP	8	1001	11,13	-	1/16/32/32	0/3/3/3
10	ADP	4	1102	11,13	-	2/16/32/32	0/3/3/3
10	ADP	3	1001	11,13	-	4/16/32/32	0/3/3/3
10	ADP	E	802	11	-	3/16/32/32	0/3/3/3
10	ADP	5	801	11	-	4/16/32/32	0/3/3/3
10	ADP	6	1101	11	-	4/16/32/32	0/3/3/3
10	ADP	B	901	11	-	6/16/32/32	0/3/3/3
10	ADP	F	1101	11	-	4/16/32/32	0/3/3/3
10	ADP	2	901	11	-	4/16/32/32	0/3/3/3
10	ADP	D	1102	11,13	-	2/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	6	1101	ADP	C2'-C3'	-10.04	1.26	1.53
10	F	1101	ADP	C2'-C3'	-10.02	1.26	1.53
10	F	1101	ADP	C6-N6	6.37	1.50	1.34
10	6	1101	ADP	C6-N6	6.36	1.50	1.34
10	F	1101	ADP	C5'-C4'	-4.67	1.37	1.51
10	6	1101	ADP	C5'-C4'	-4.64	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	1101	ADP	C2'-C1'	4.15	1.66	1.53
10	6	1101	ADP	C2'-C1'	4.14	1.66	1.53
10	6	1101	ADP	O4'-C1'	-3.72	1.33	1.42
10	F	1101	ADP	O4'-C1'	-3.71	1.33	1.42
10	F	1101	ADP	PA-O3A	3.44	1.63	1.59
10	6	1101	ADP	PA-O3A	3.43	1.63	1.59
10	6	1101	ADP	C3'-C4'	3.26	1.61	1.53
10	F	1101	ADP	C3'-C4'	3.25	1.61	1.53
10	6	1101	ADP	O4'-C4'	3.00	1.51	1.45
10	F	1101	ADP	O4'-C4'	2.97	1.51	1.45
10	6	1101	ADP	C5-C6	-2.81	1.33	1.41
10	F	1101	ADP	C5-C6	-2.79	1.33	1.41
10	F	1101	ADP	C5-N7	-2.76	1.34	1.39
10	6	1101	ADP	C5-N7	-2.74	1.34	1.39
10	F	1101	ADP	C5-C4	-2.51	1.34	1.39
10	6	1101	ADP	C5-C4	-2.50	1.34	1.39
10	6	1101	ADP	PA-O5'	2.43	1.68	1.59
10	F	1101	ADP	PA-O5'	2.41	1.68	1.59
10	6	1101	ADP	PA-O1A	2.39	1.59	1.50
10	F	1101	ADP	PA-O1A	2.37	1.59	1.50
10	F	1101	ADP	O2'-C2'	2.29	1.48	1.43
10	6	1101	ADP	O2'-C2'	2.29	1.48	1.43
10	F	1101	ADP	C8-N9	-2.20	1.33	1.37
10	6	1101	ADP	C8-N9	-2.20	1.33	1.37
10	6	1101	ADP	O5'-C5'	-2.11	1.36	1.44
10	F	1101	ADP	O5'-C5'	-2.11	1.36	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	6	1101	ADP	N3-C2-N1	-5.66	120.02	128.58
10	F	1101	ADP	N3-C2-N1	-5.64	120.05	128.58
10	6	1101	ADP	N9-C8-N7	-5.25	106.48	113.94
10	F	1101	ADP	N9-C8-N7	-5.24	106.50	113.94
10	F	1101	ADP	N6-C6-N1	-5.21	106.78	118.38
10	6	1101	ADP	N6-C6-N1	-5.20	106.79	118.38
10	6	1101	ADP	C5-C4-N3	-4.82	120.08	126.72
10	F	1101	ADP	C5-C4-N3	-4.78	120.13	126.72
10	6	1101	ADP	C4-N9-C8	4.04	109.98	105.74
10	F	1101	ADP	C4-N9-C8	4.03	109.97	105.74
10	6	1101	ADP	C5-C6-N6	3.92	132.99	123.29
10	F	1101	ADP	C5-C6-N6	3.91	132.97	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	6	1101	ADP	N3-C4-N9	3.55	133.21	127.17
10	F	1101	ADP	N3-C4-N9	3.55	133.20	127.17
10	6	1101	ADP	C2-N3-C4	3.33	119.96	111.83
10	F	1101	ADP	C2-N3-C4	3.32	119.94	111.83
10	6	1101	ADP	C5-N7-C8	3.19	108.46	103.45
10	F	1101	ADP	C5-N7-C8	3.18	108.45	103.45
10	F	1101	ADP	C4-N9-C1'	-3.03	119.54	126.63
10	6	1101	ADP	C4-N9-C1'	-3.03	119.55	126.63
10	F	1101	ADP	C3'-C2'-C1'	2.59	106.35	101.46
10	6	1101	ADP	C3'-C2'-C1'	2.58	106.35	101.46

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	2	901	ADP	PA-O3A-PB-O2B
10	2	901	ADP	PA-O3A-PB-O3B
10	2	901	ADP	C5'-O5'-PA-O2A
10	2	901	ADP	C5'-O5'-PA-O3A
10	3	1001	ADP	PA-O3A-PB-O2B
10	4	1102	ADP	O4'-C4'-C5'-O5'
10	5	801	ADP	PA-O3A-PB-O2B
10	6	1101	ADP	C5'-O5'-PA-O1A
10	6	1101	ADP	C5'-O5'-PA-O2A
10	6	1101	ADP	C5'-O5'-PA-O3A
10	7	1102	ADP	O4'-C4'-C5'-O5'
10	B	901	ADP	C5'-O5'-PA-O1A
10	C	1001	ADP	PA-O3A-PB-O2B
10	D	1102	ADP	O4'-C4'-C5'-O5'
10	E	802	ADP	C5'-O5'-PA-O3A
10	F	1101	ADP	C5'-O5'-PA-O1A
10	F	1101	ADP	C5'-O5'-PA-O2A
10	F	1101	ADP	C5'-O5'-PA-O3A
10	G	1102	ADP	O4'-C4'-C5'-O5'
10	4	1102	ADP	C3'-C4'-C5'-O5'
10	D	1102	ADP	C3'-C4'-C5'-O5'
10	7	1102	ADP	C3'-C4'-C5'-O5'
10	B	901	ADP	O4'-C4'-C5'-O5'
10	B	901	ADP	C3'-C4'-C5'-O5'
10	G	1102	ADP	C3'-C4'-C5'-O5'
10	5	801	ADP	C3'-C4'-C5'-O5'
10	5	801	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
10	7	1102	ADP	PA-O3A-PB-O1B
10	G	1102	ADP	PA-O3A-PB-O1B
10	3	1001	ADP	O4'-C4'-C5'-O5'
10	C	1001	ADP	O4'-C4'-C5'-O5'
10	7	1102	ADP	C5'-O5'-PA-O1A
10	7	1102	ADP	C5'-O5'-PA-O2A
10	7	1102	ADP	C5'-O5'-PA-O3A
10	B	901	ADP	C5'-O5'-PA-O2A
10	B	901	ADP	C5'-O5'-PA-O3A
10	E	802	ADP	C5'-O5'-PA-O1A
10	G	1102	ADP	C5'-O5'-PA-O1A
10	G	1102	ADP	C5'-O5'-PA-O2A
10	G	1102	ADP	C5'-O5'-PA-O3A
10	B	901	ADP	C4'-C5'-O5'-PA
10	5	801	ADP	C4'-C5'-O5'-PA
10	6	1101	ADP	O4'-C4'-C5'-O5'
10	F	1101	ADP	O4'-C4'-C5'-O5'
10	3	1001	ADP	C3'-C4'-C5'-O5'
10	C	1001	ADP	C3'-C4'-C5'-O5'
10	3	1001	ADP	PA-O3A-PB-O1B
10	C	1001	ADP	PA-O3A-PB-O1B
10	7	1102	ADP	PA-O3A-PB-O2B
10	7	1102	ADP	PA-O3A-PB-O3B
10	G	1102	ADP	PA-O3A-PB-O2B
10	G	1102	ADP	PA-O3A-PB-O3B
10	8	1001	ADP	PB-O3A-PA-O1A
10	E	802	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

14 monomers are involved in 29 short contacts:

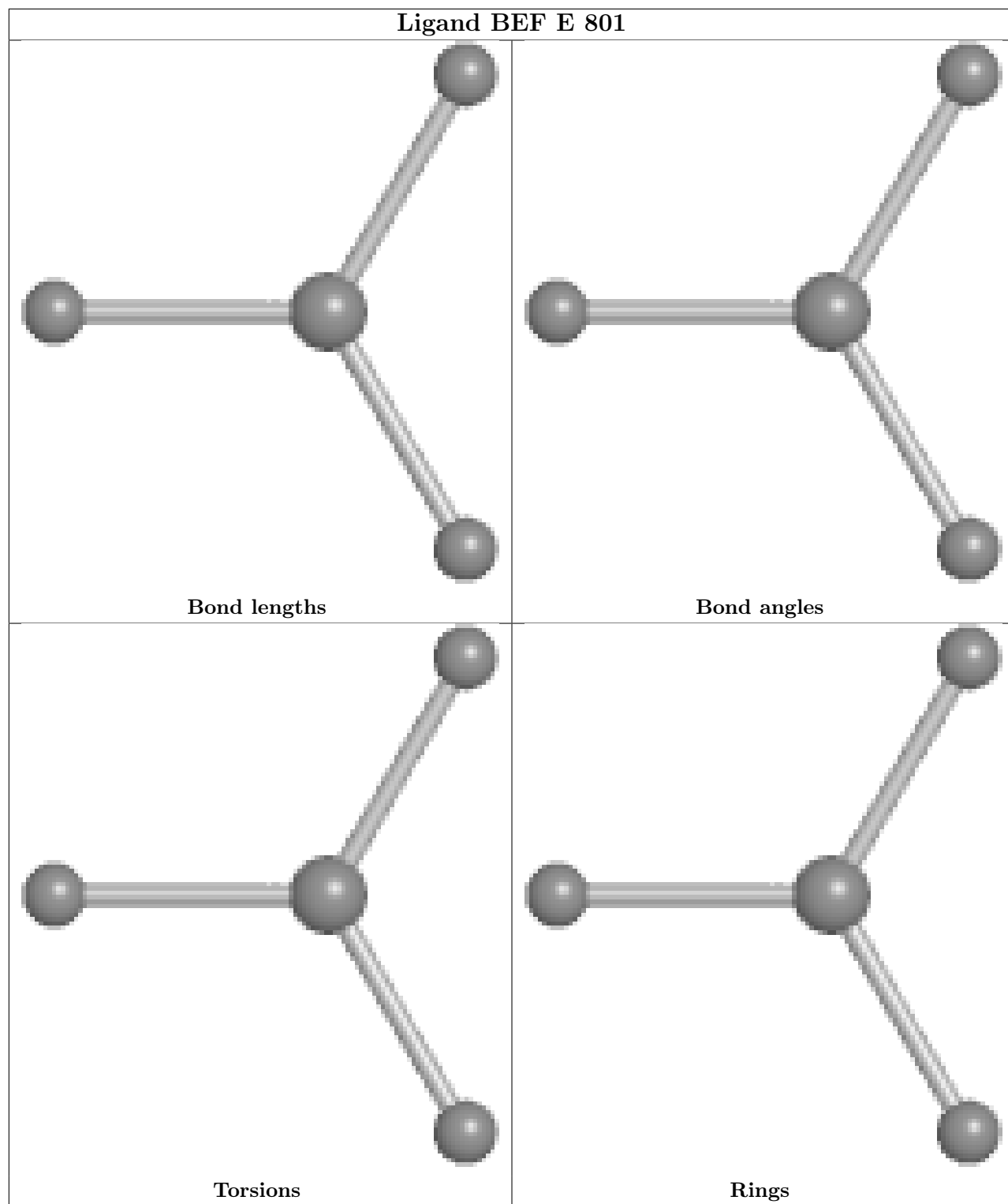
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	801	BEF	1	0
13	3	1002	BEF	1	0
10	4	1102	ADP	1	0
10	3	1001	ADP	3	0
10	F	1101	ADP	2	0
13	D	1103	BEF	1	0
10	5	801	ADP	3	0
10	D	1102	ADP	2	0
10	7	1102	ADP	1	0
10	C	1001	ADP	1	0

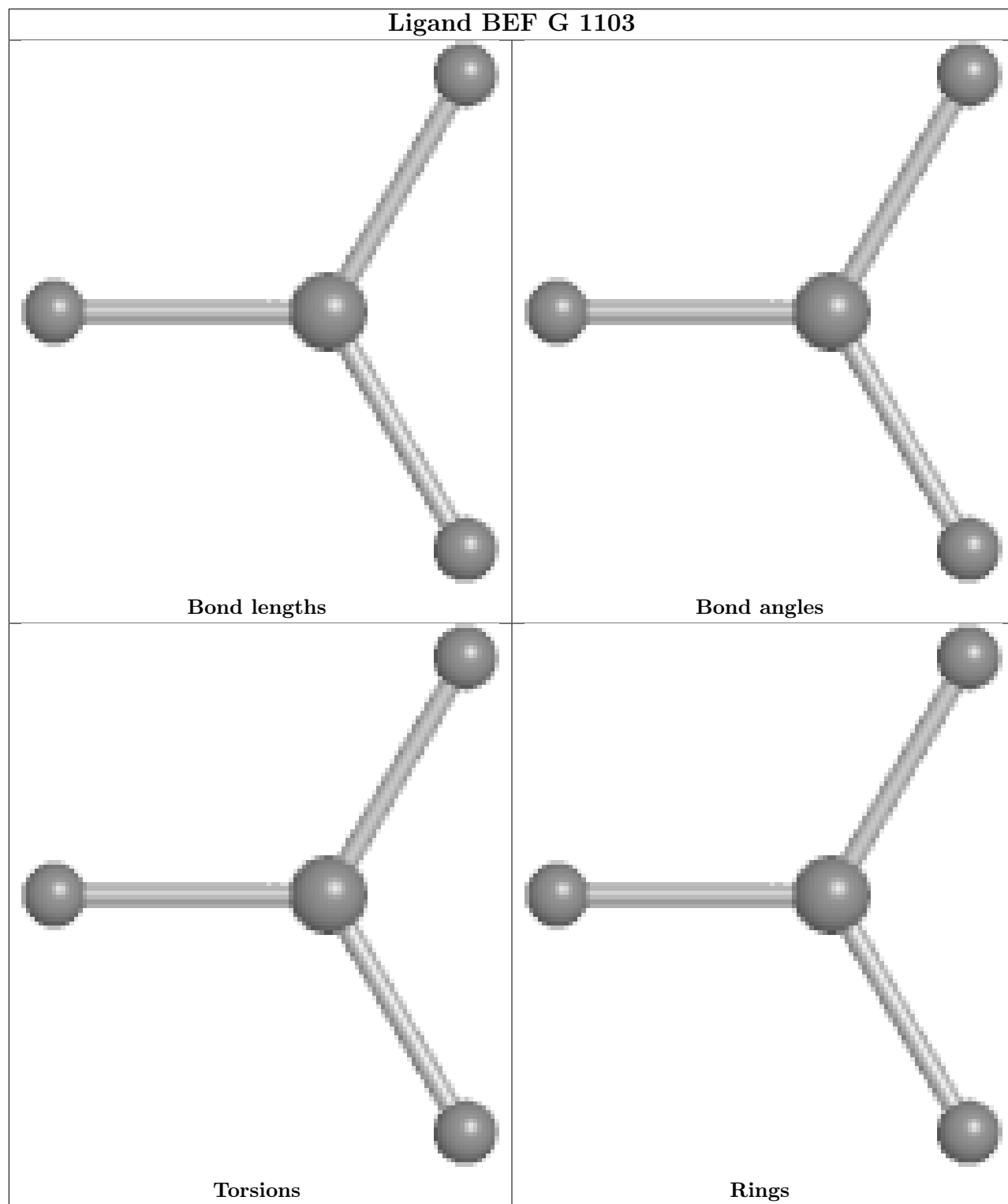
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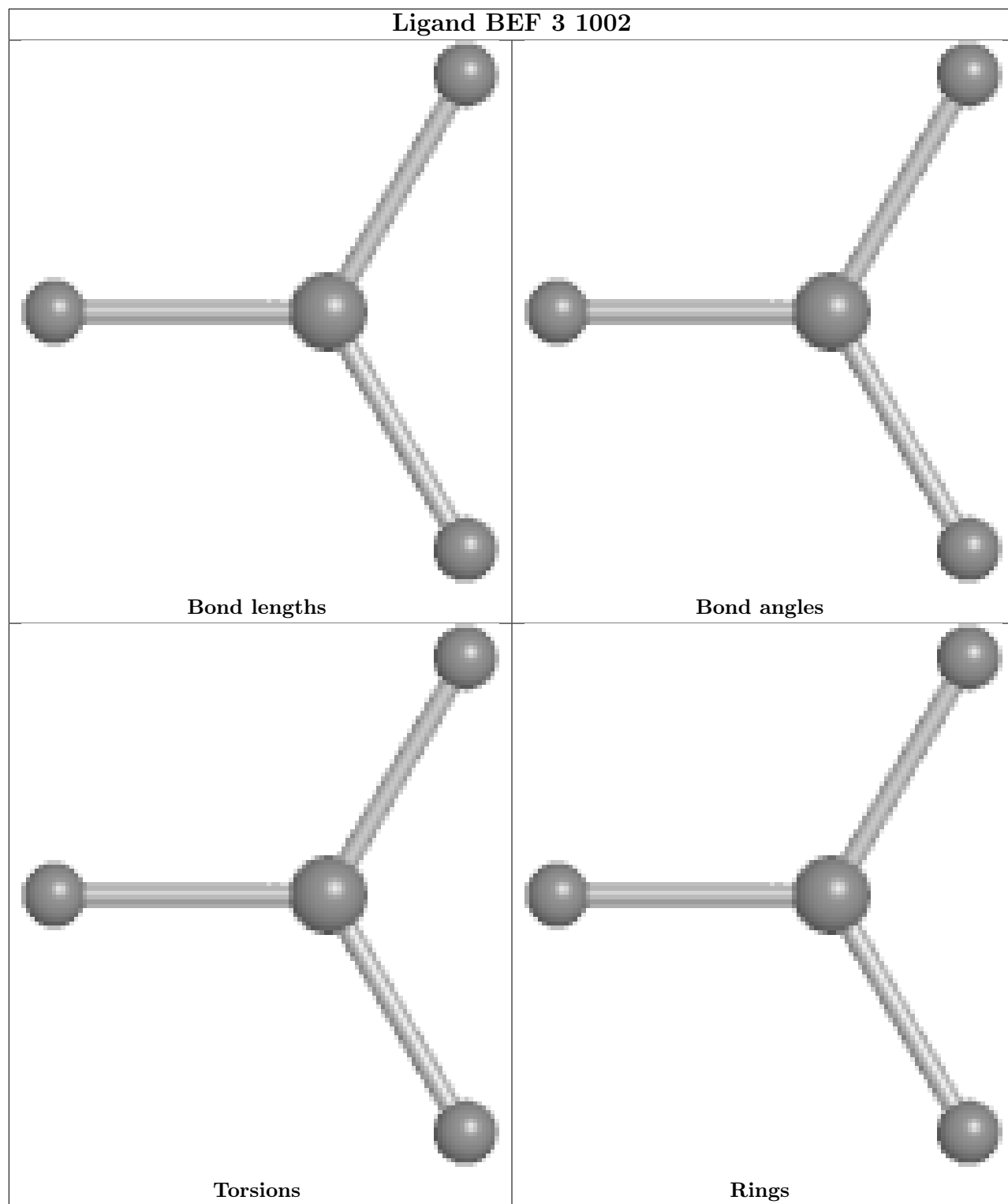
Continued from previous page...

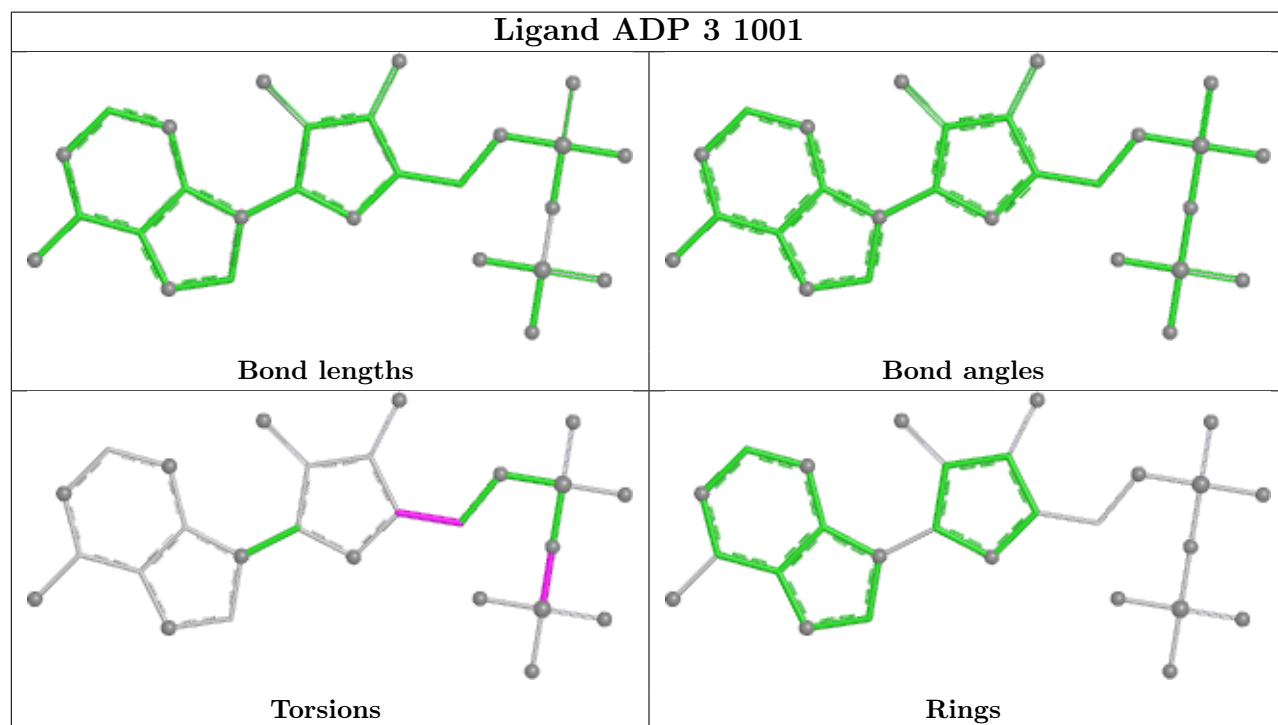
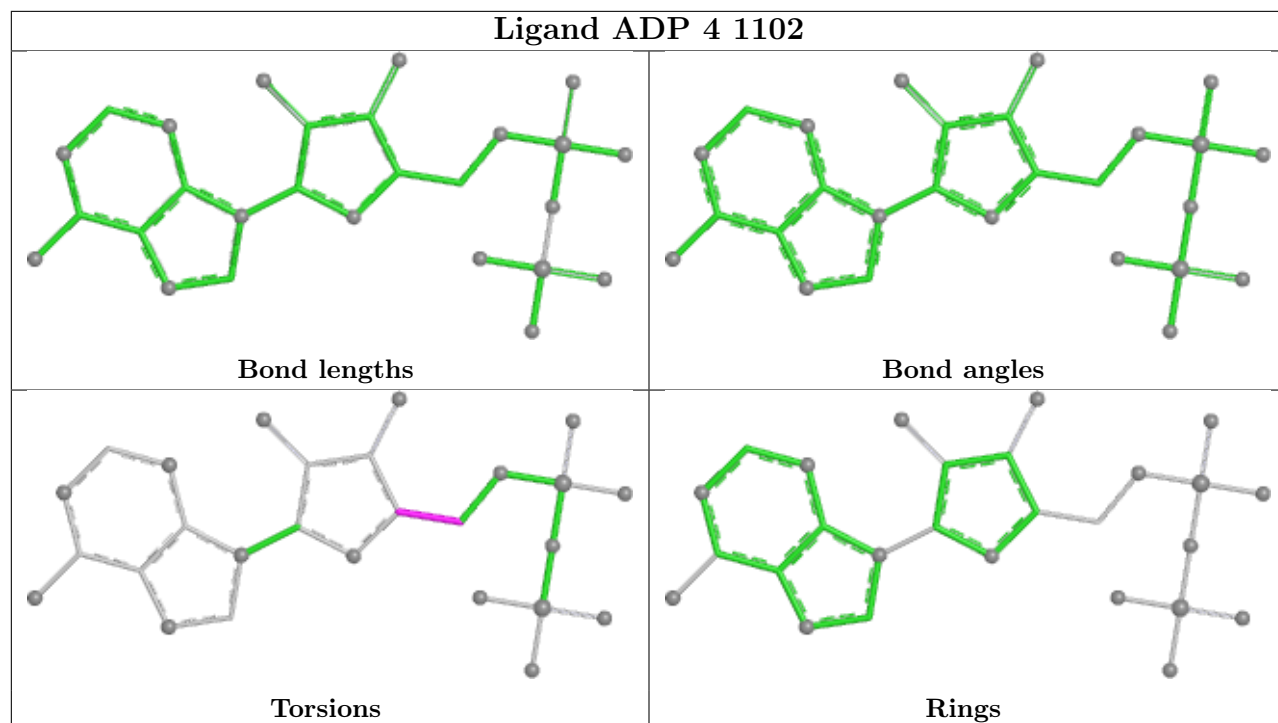
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	8	1001	ADP	6	0
10	6	1101	ADP	2	0
10	E	802	ADP	2	0
10	B	901	ADP	3	0

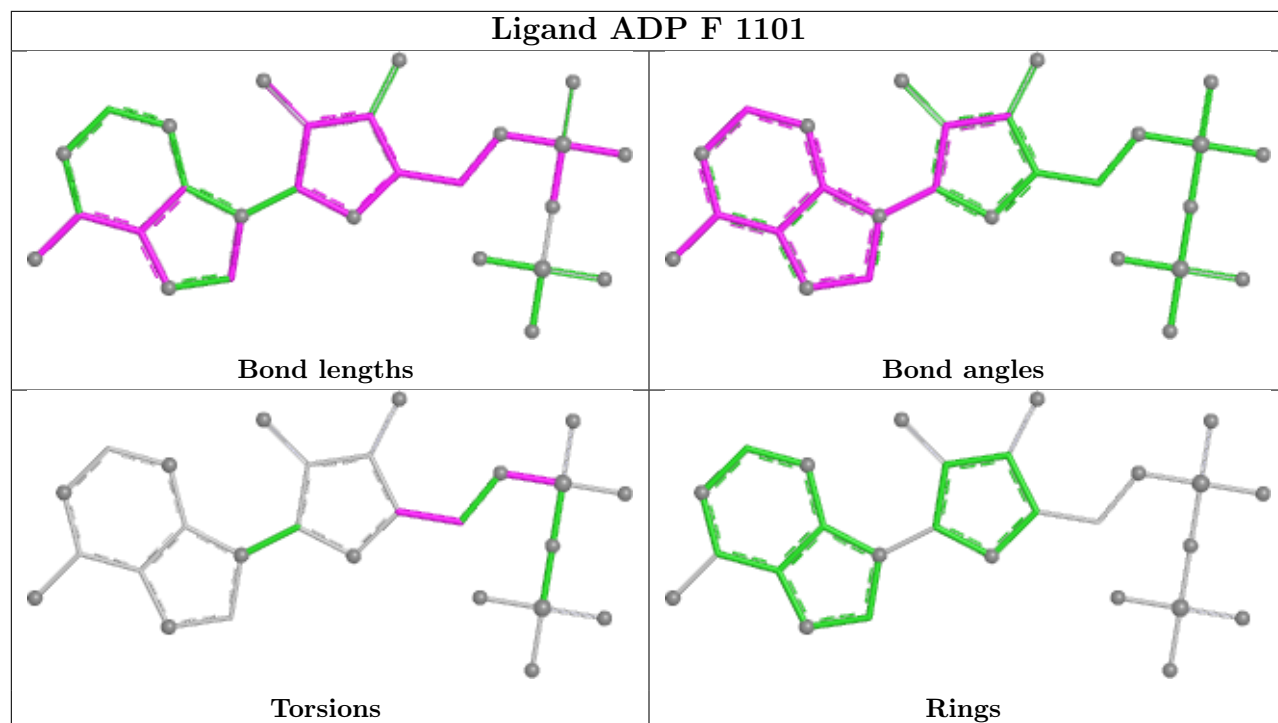
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

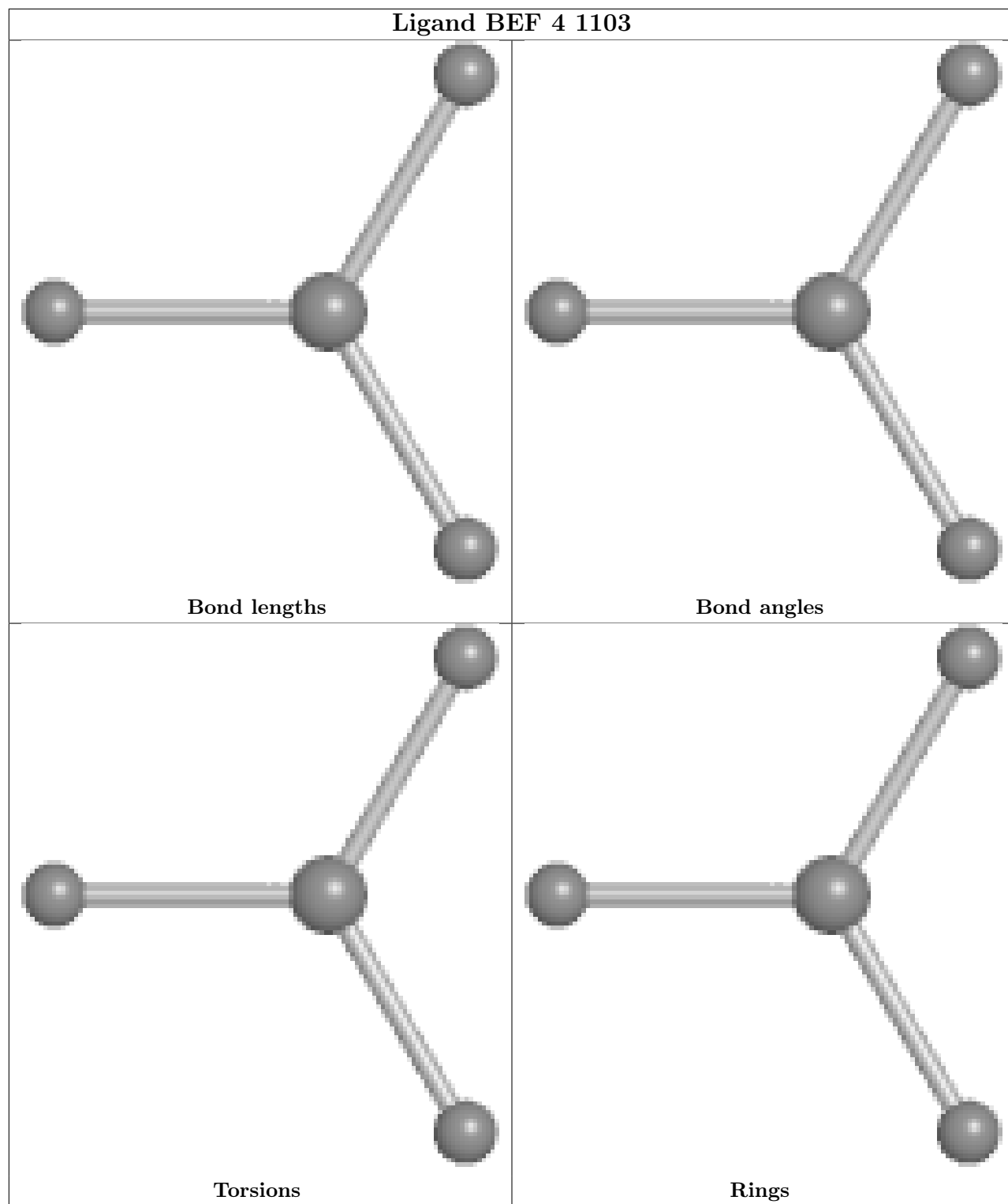


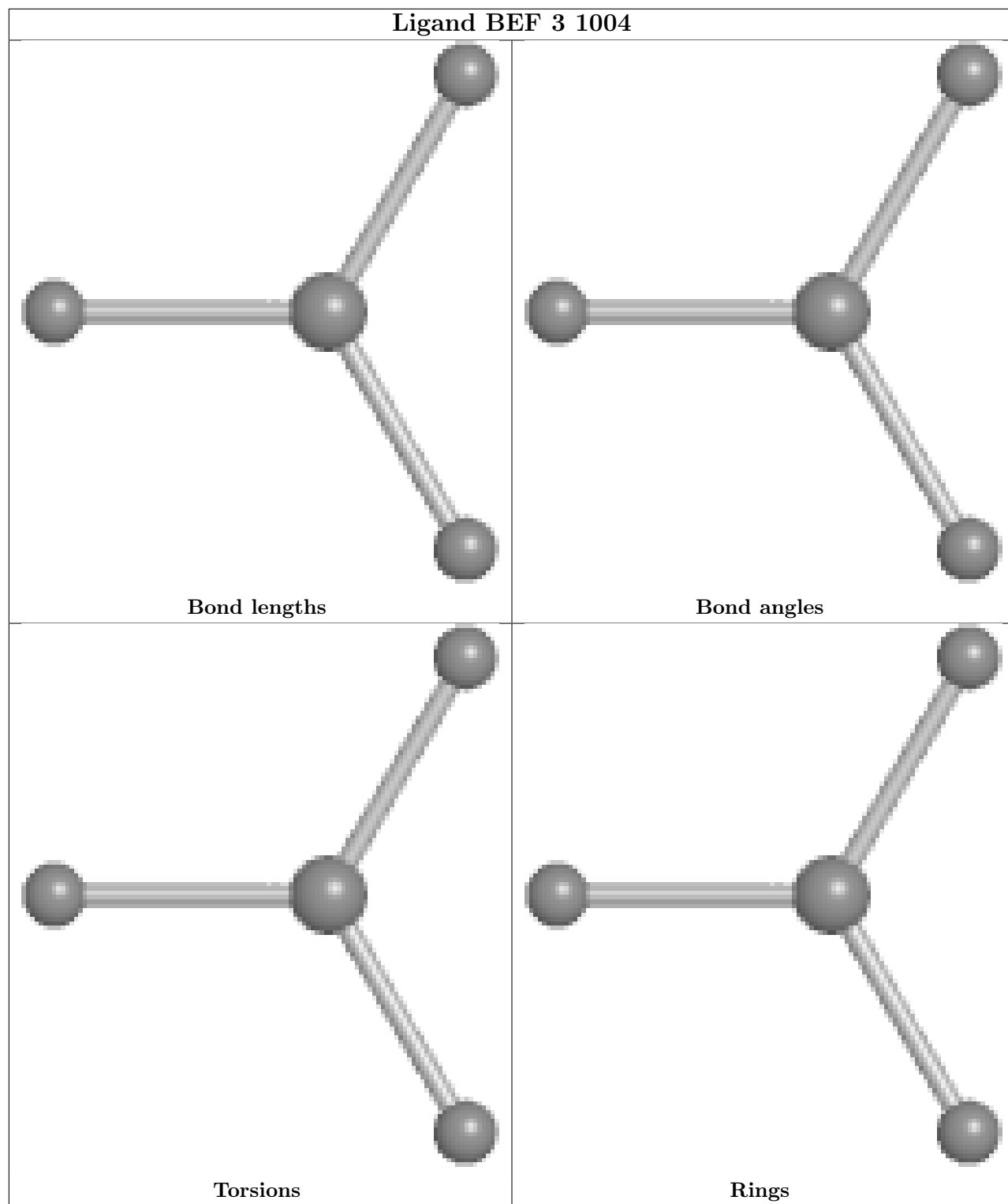


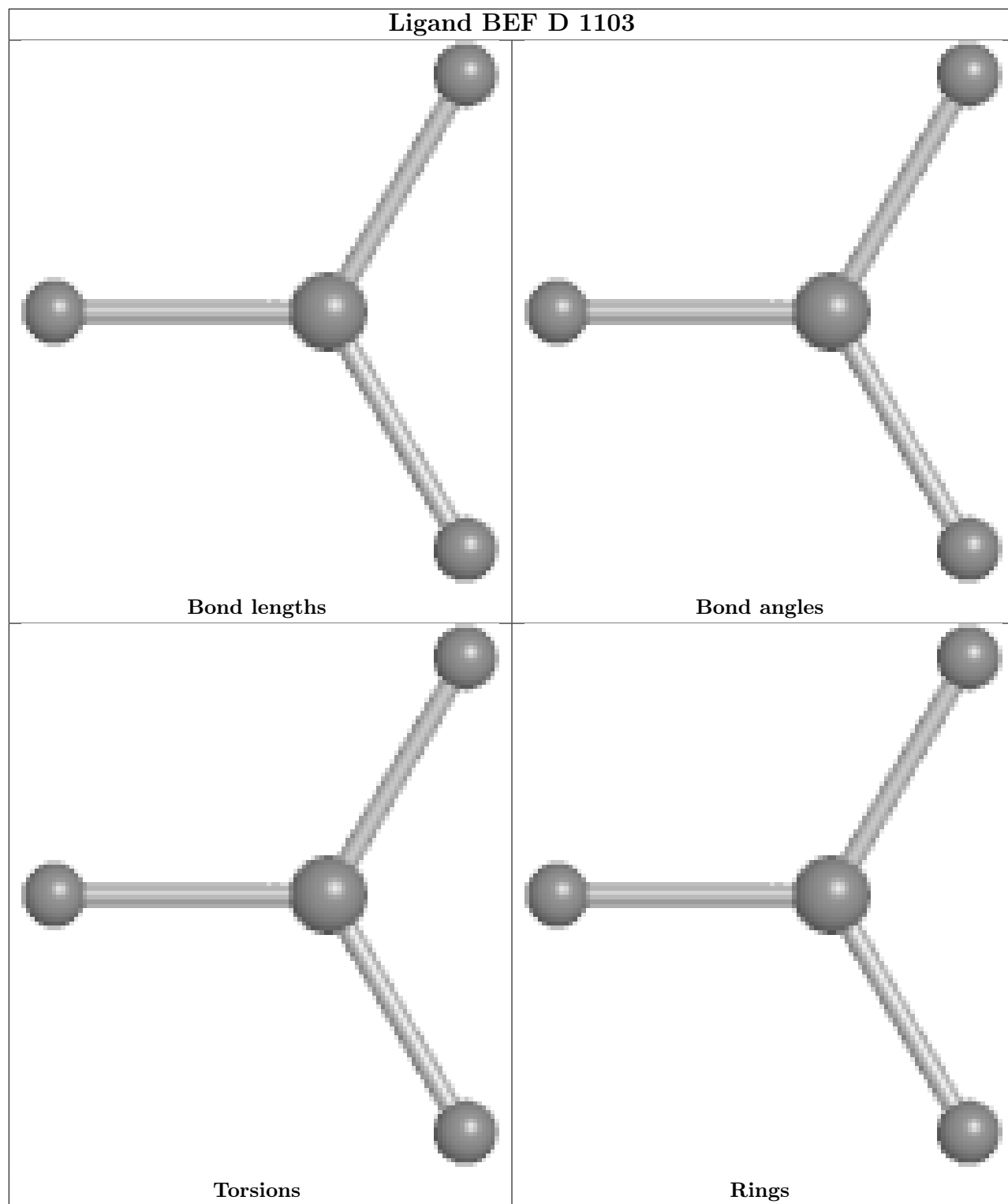


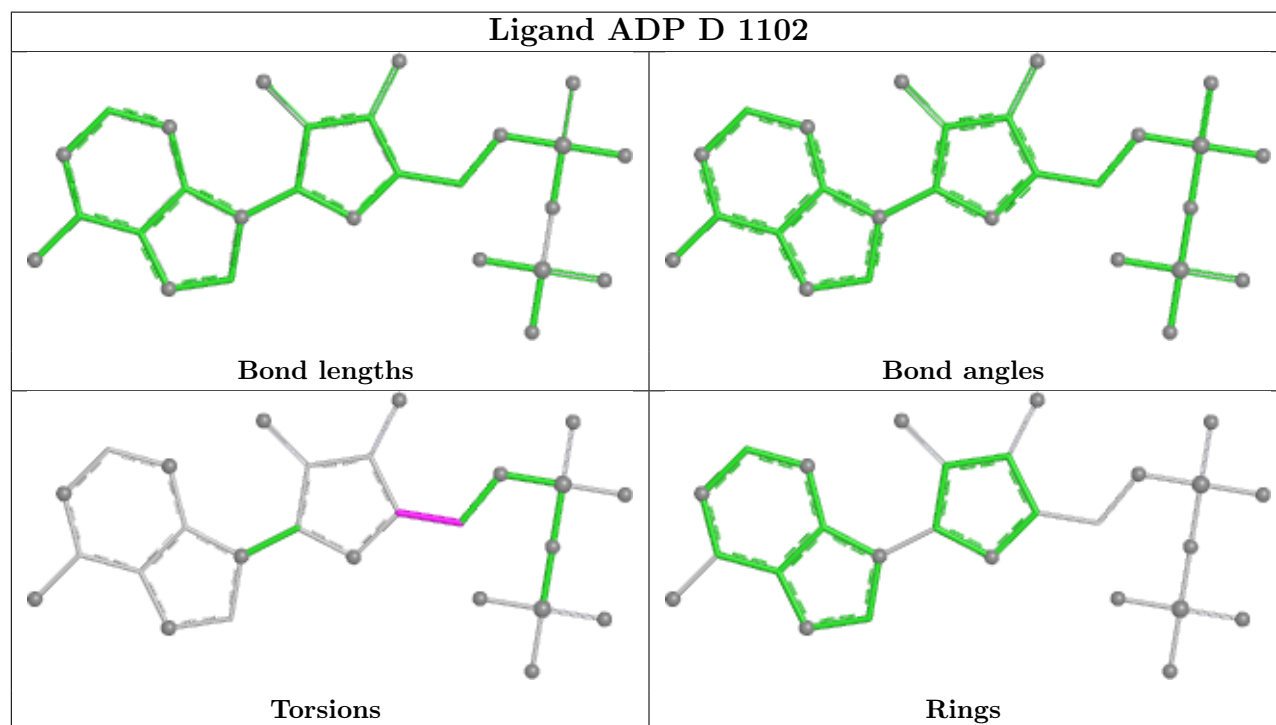
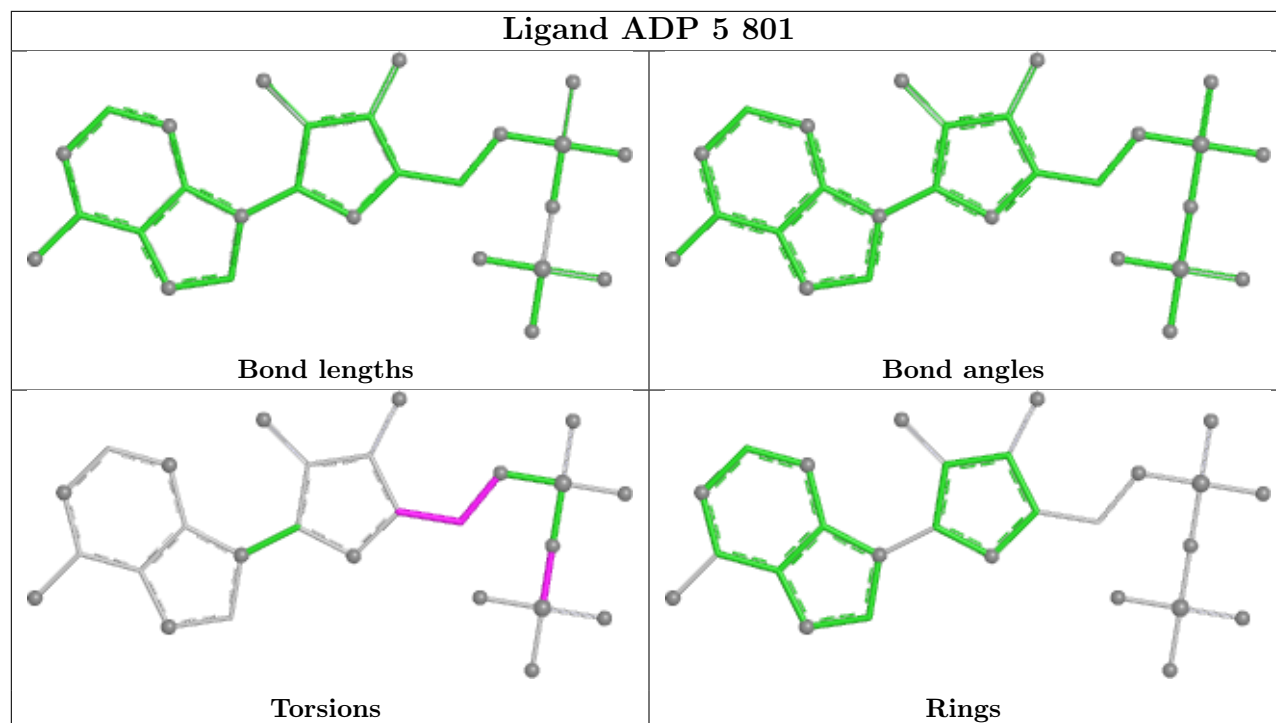


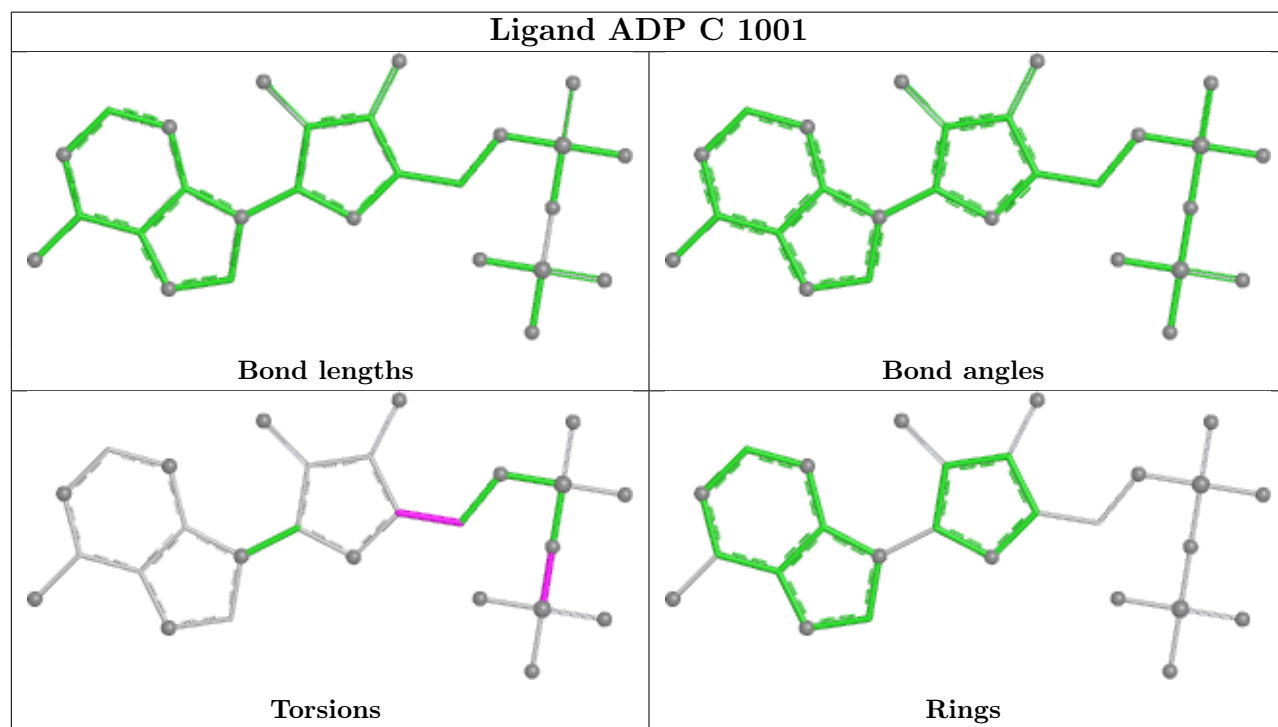
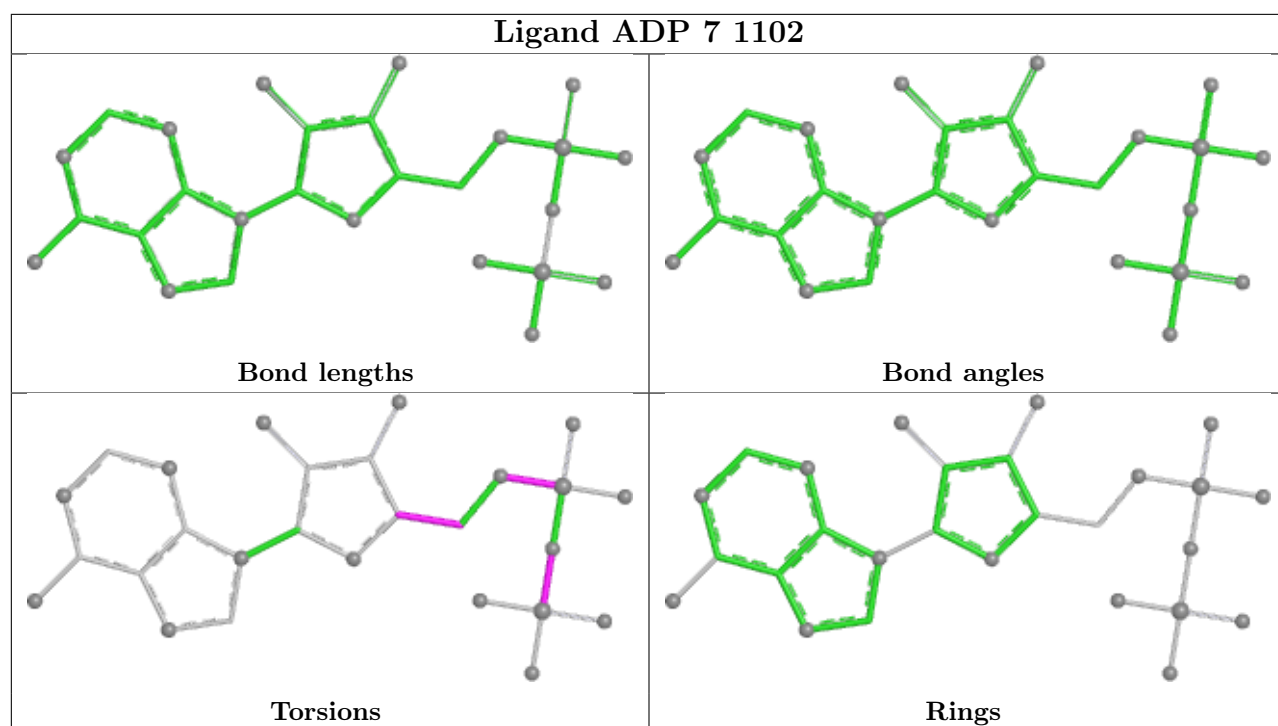


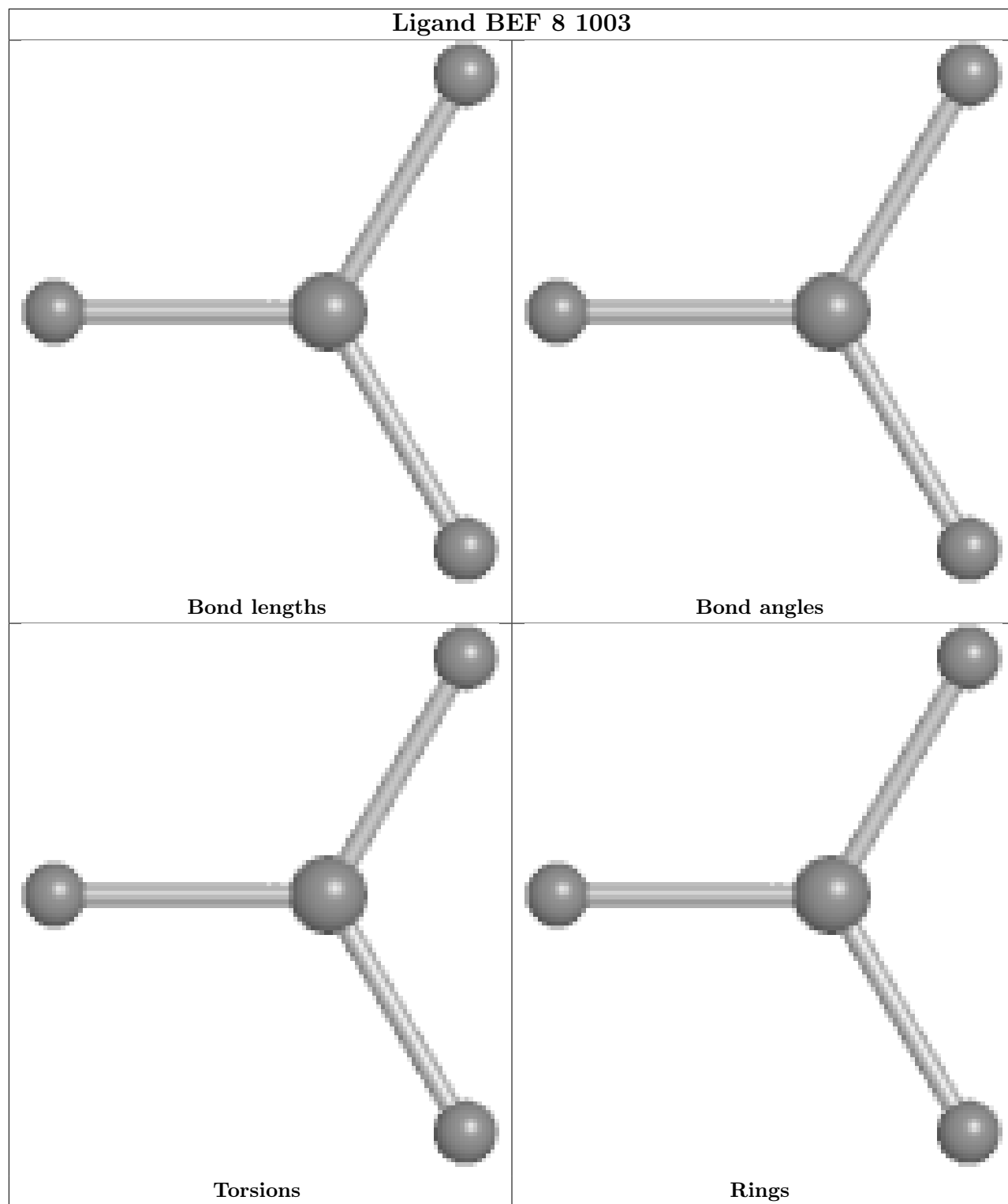


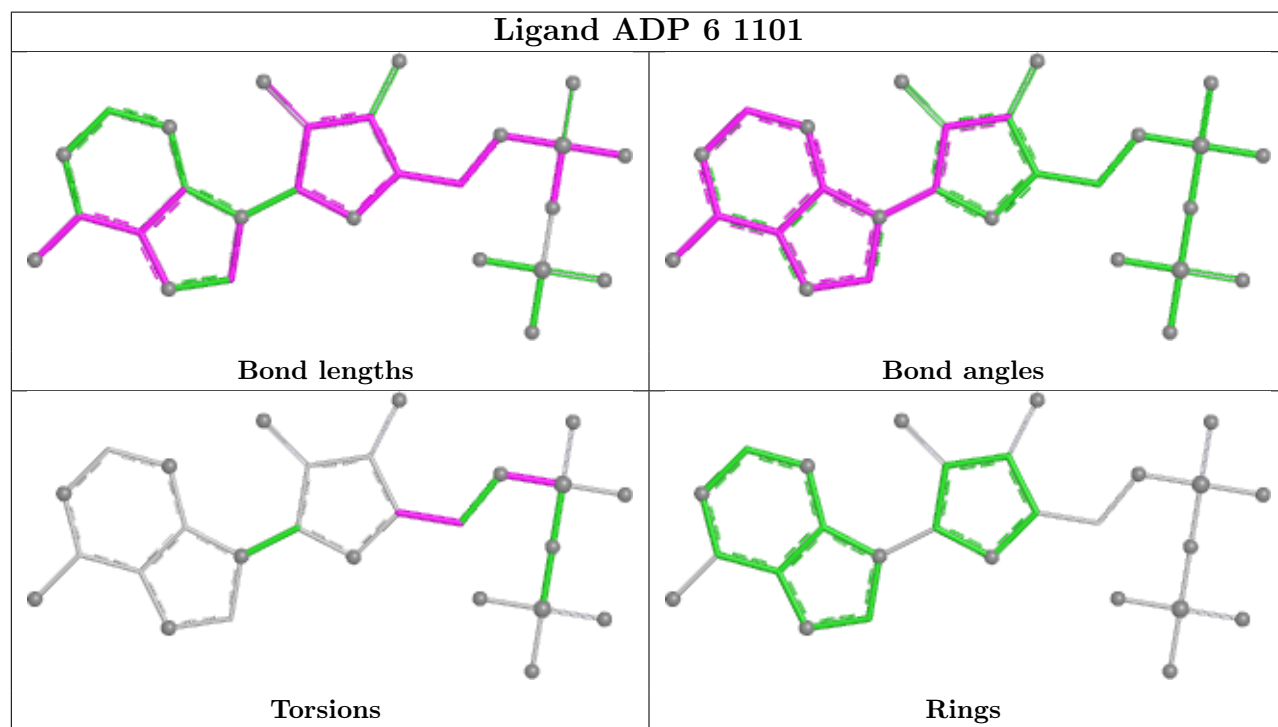
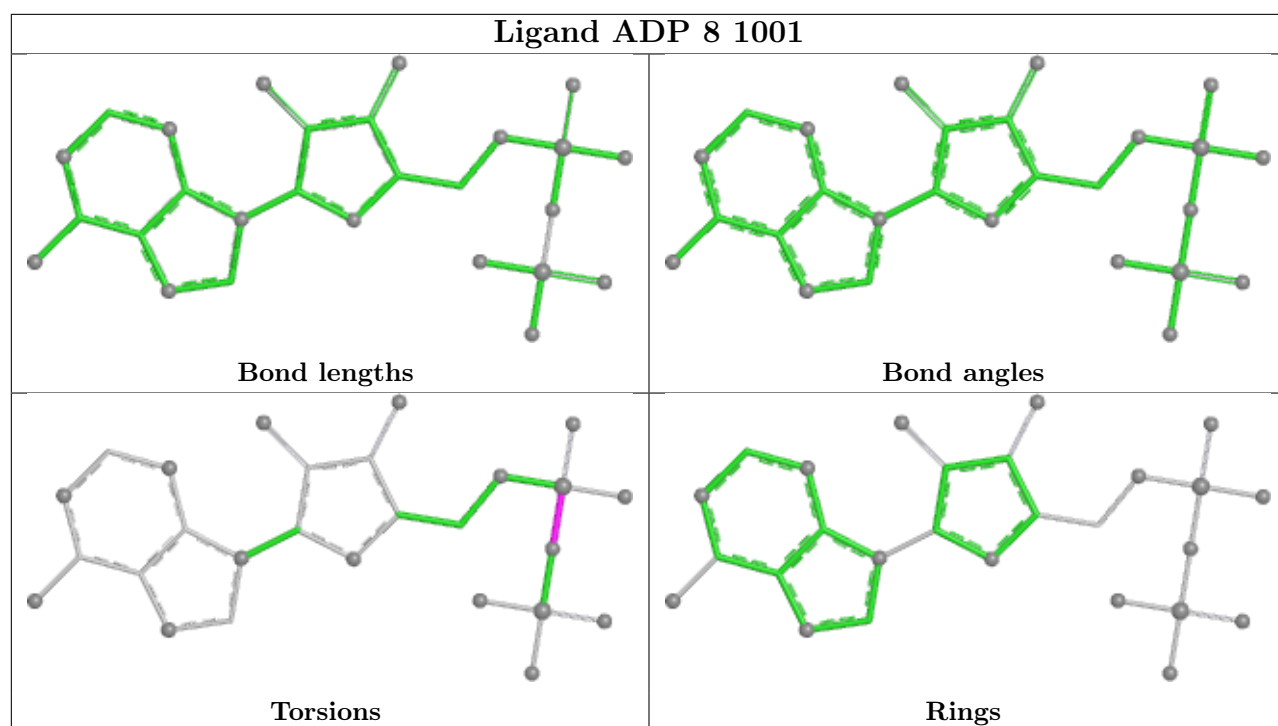


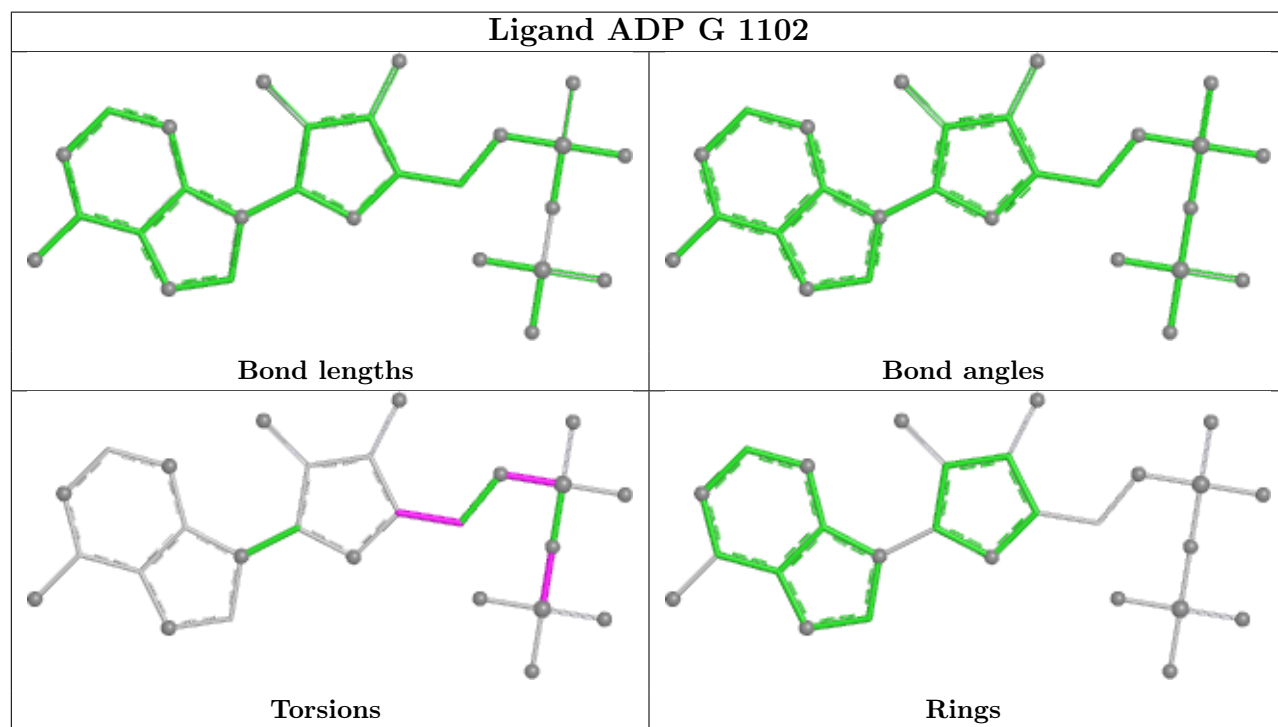
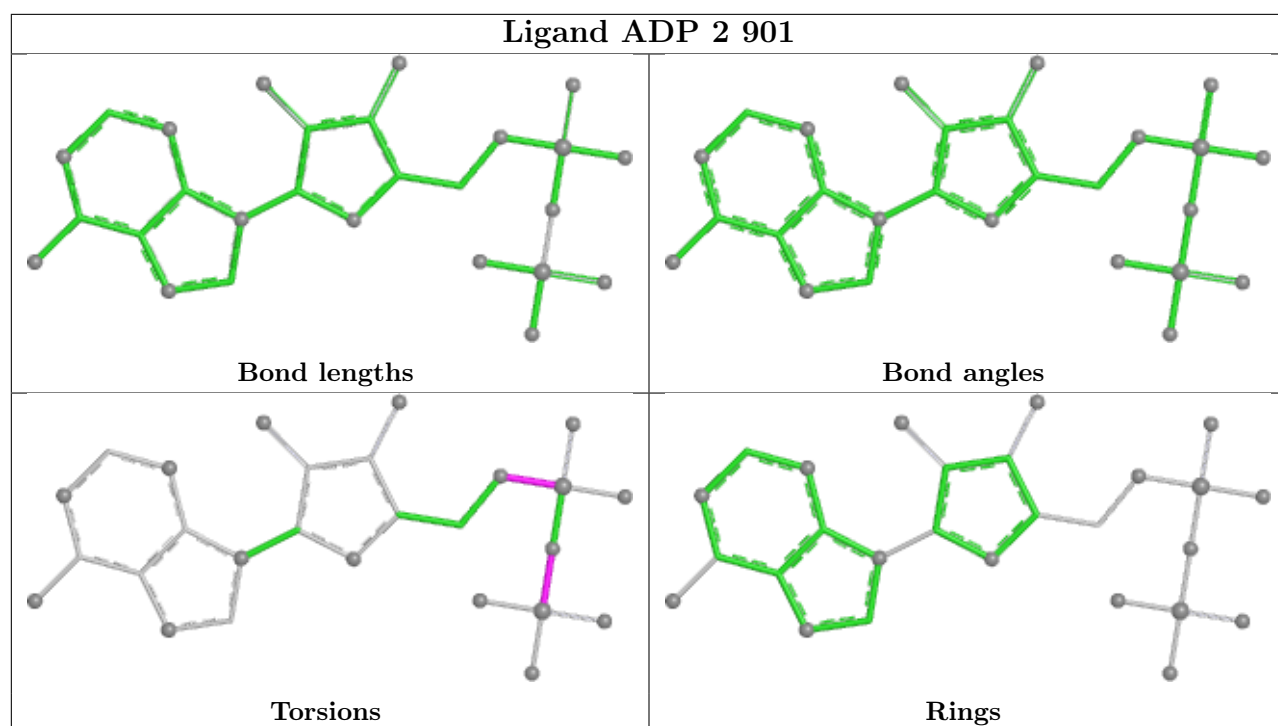


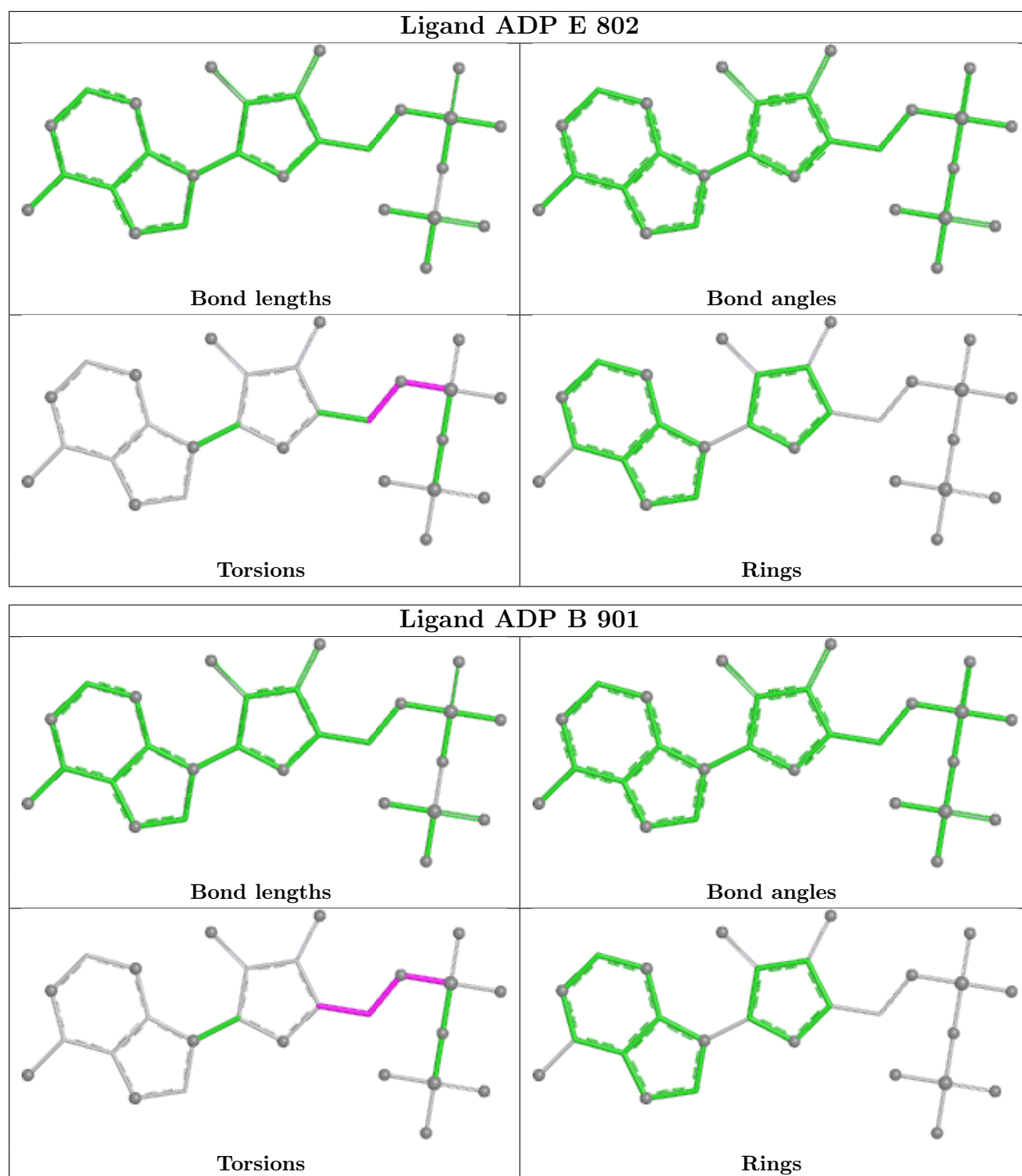












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

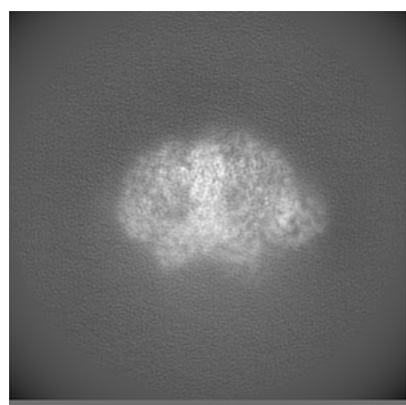
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13620. These allow visual inspection of the internal detail of the map and identification of artifacts.

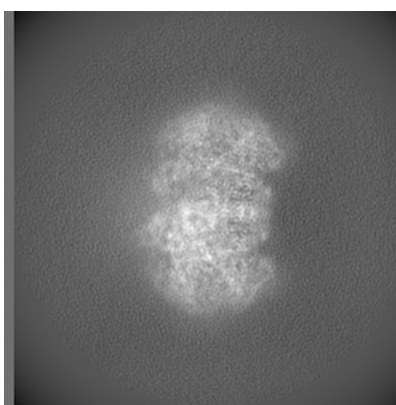
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

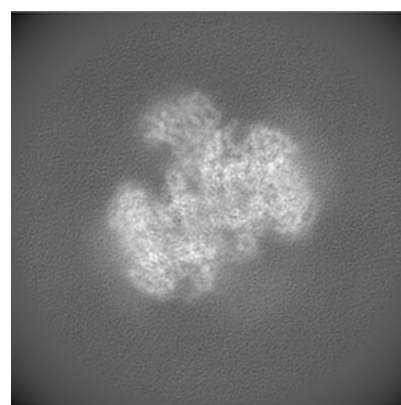
6.1.1 Primary map



X



Y

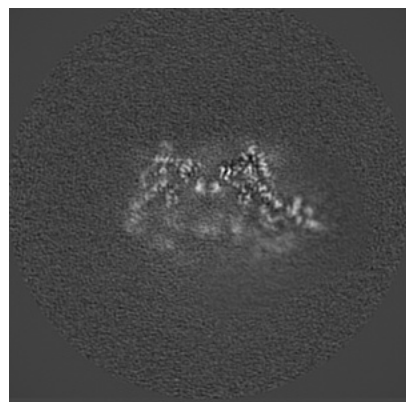


Z

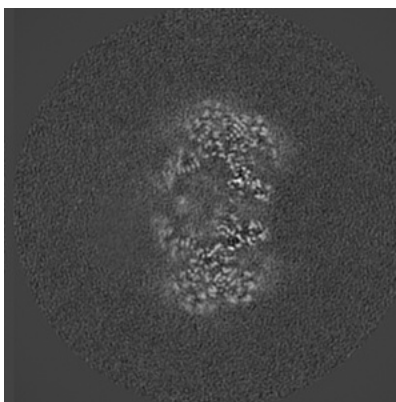
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

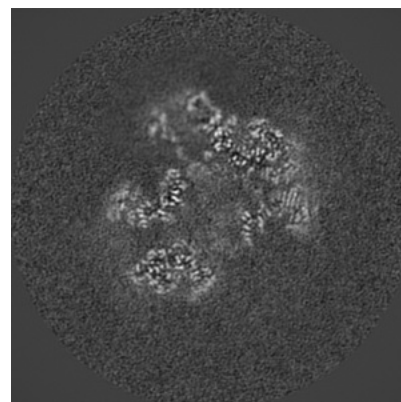
6.2.1 Primary map



X Index: 180



Y Index: 180

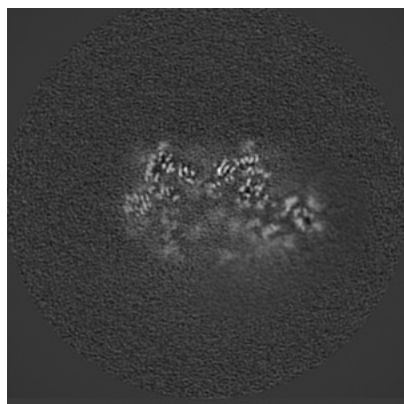


Z Index: 180

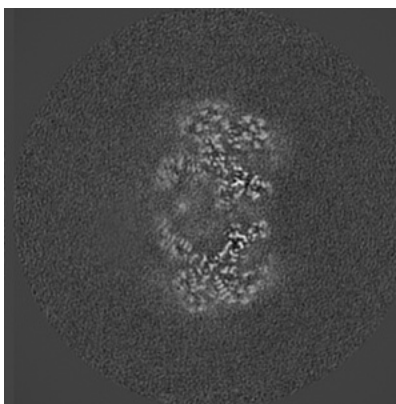
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

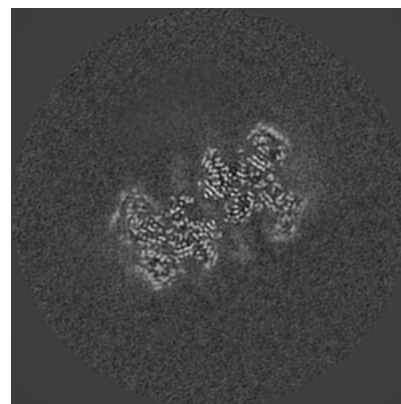
6.3.1 Primary map



X Index: 175



Y Index: 176

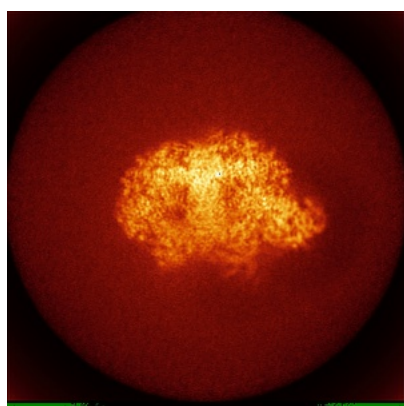


Z Index: 214

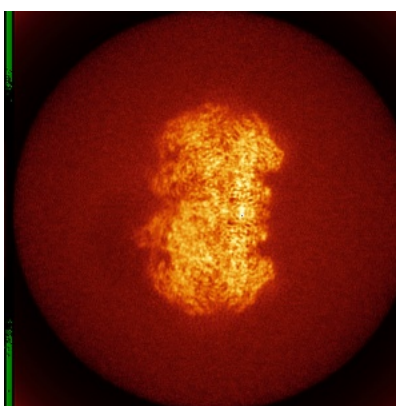
The images above show the largest variance slices of the map in three orthogonal directions.

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

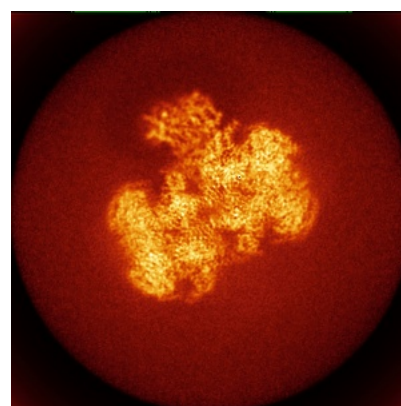
6.4.1 Primary map



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.

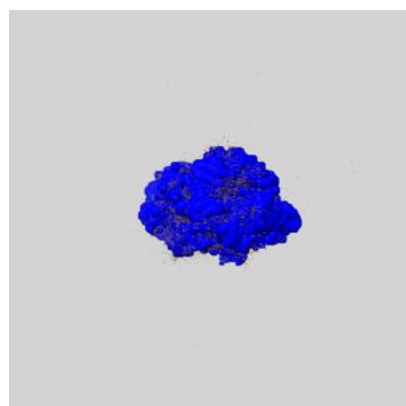
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

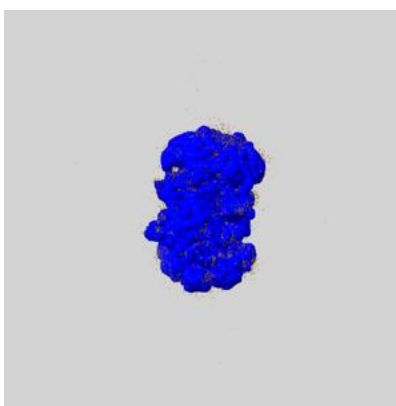
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

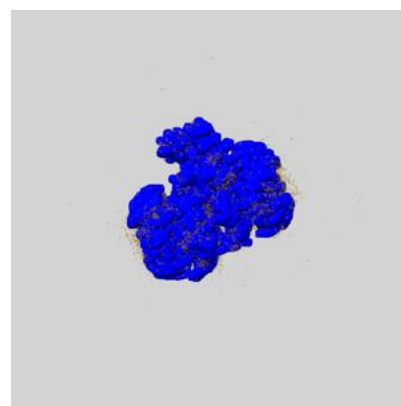
6.6.1 emd_13620_msk_1.map [i](#)



X



Y

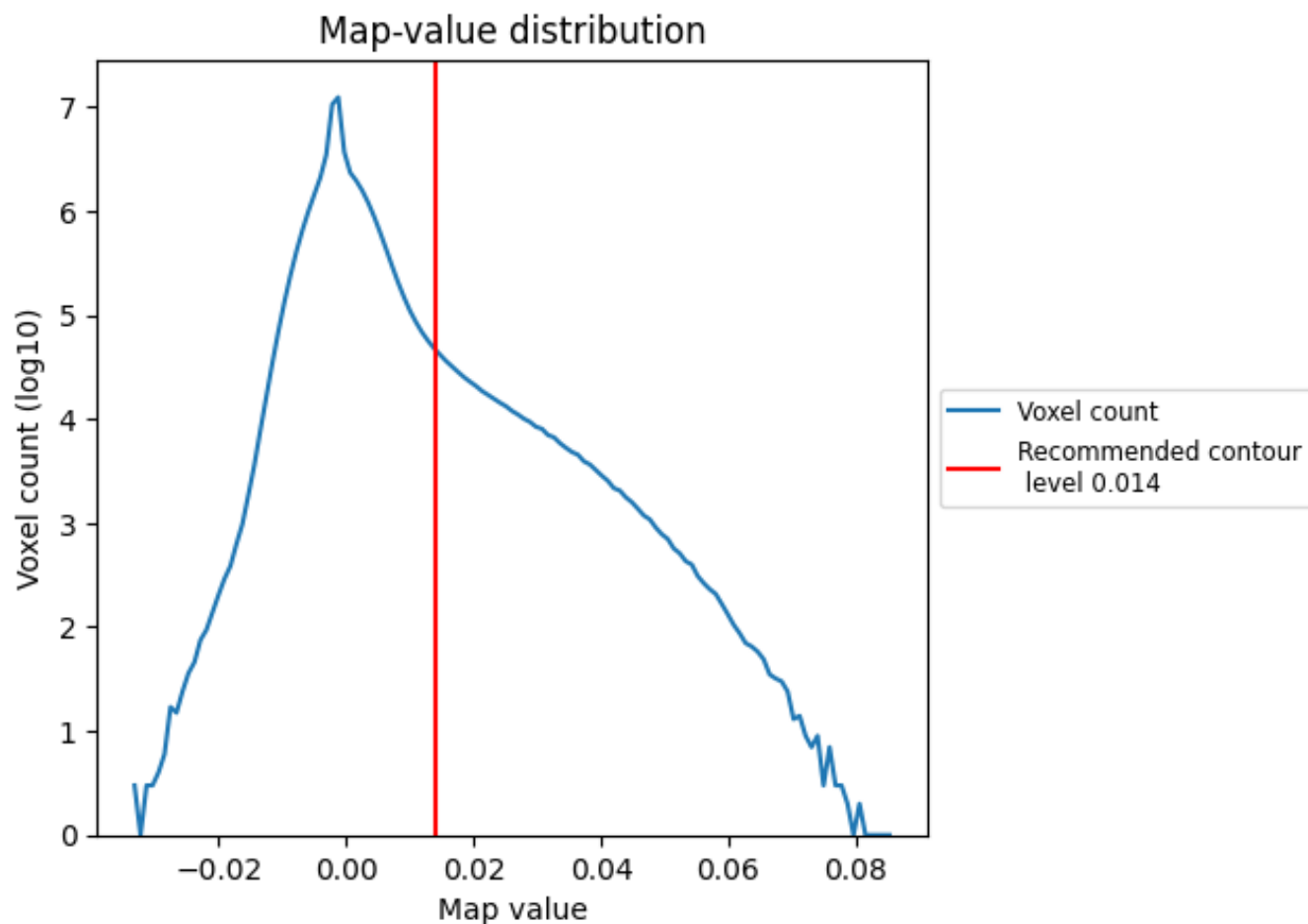


Z

7 Map analysis [i](#)

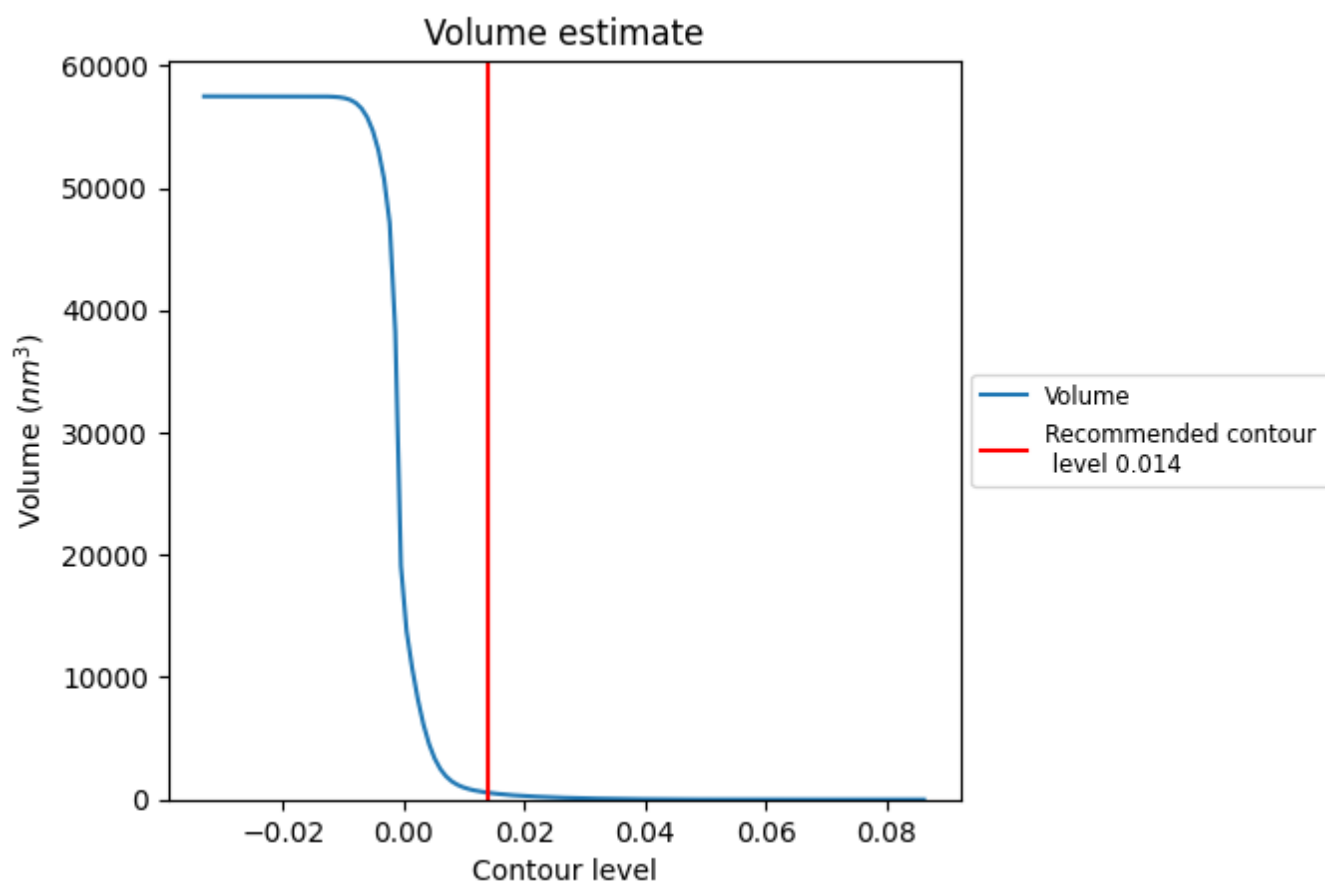
This section contains the results of statistical analysis of the map.

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.

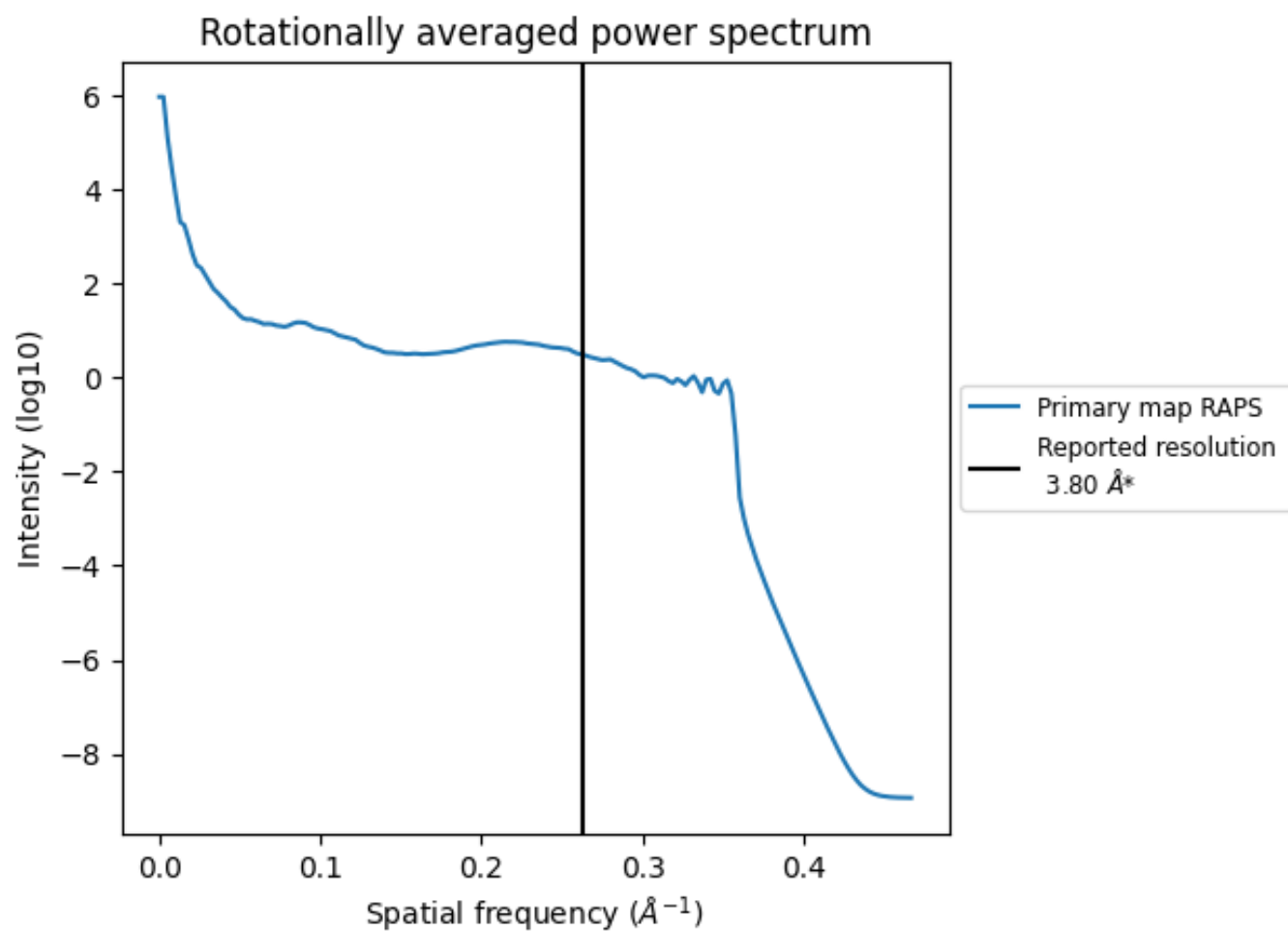
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 557 nm³; this corresponds to an approximate mass of 504 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 0.263 Å⁻¹

8 Fourier-Shell correlation

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

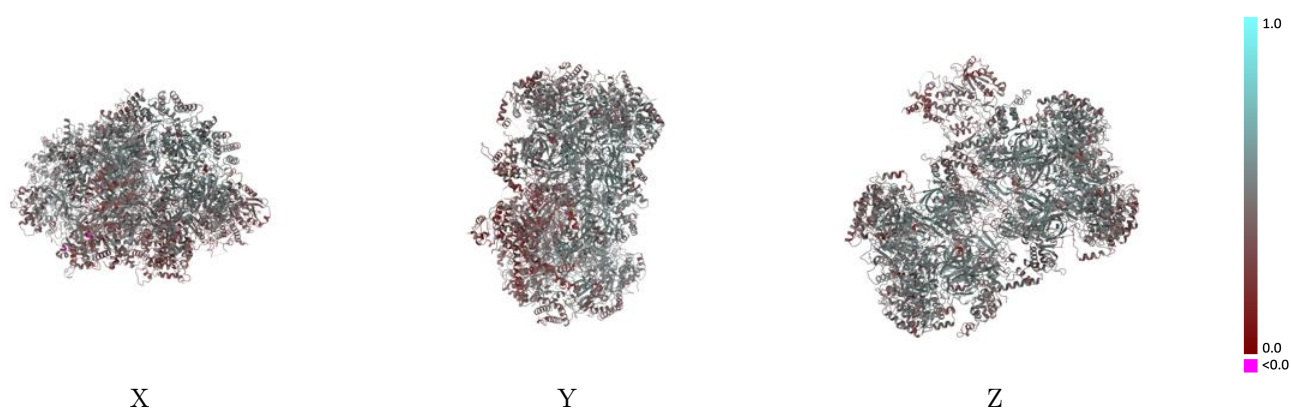
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-13620 and PDB model 7PT7. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)

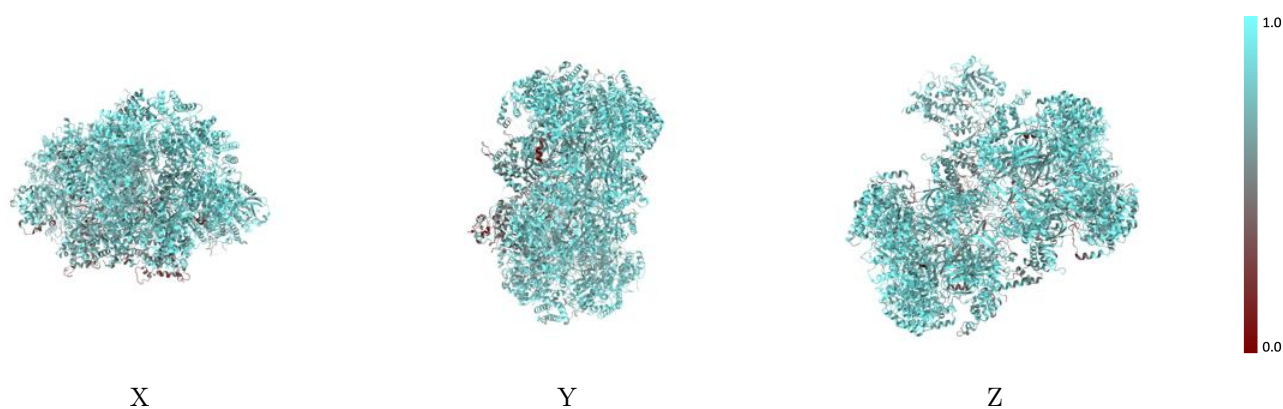
This section was not generated.

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



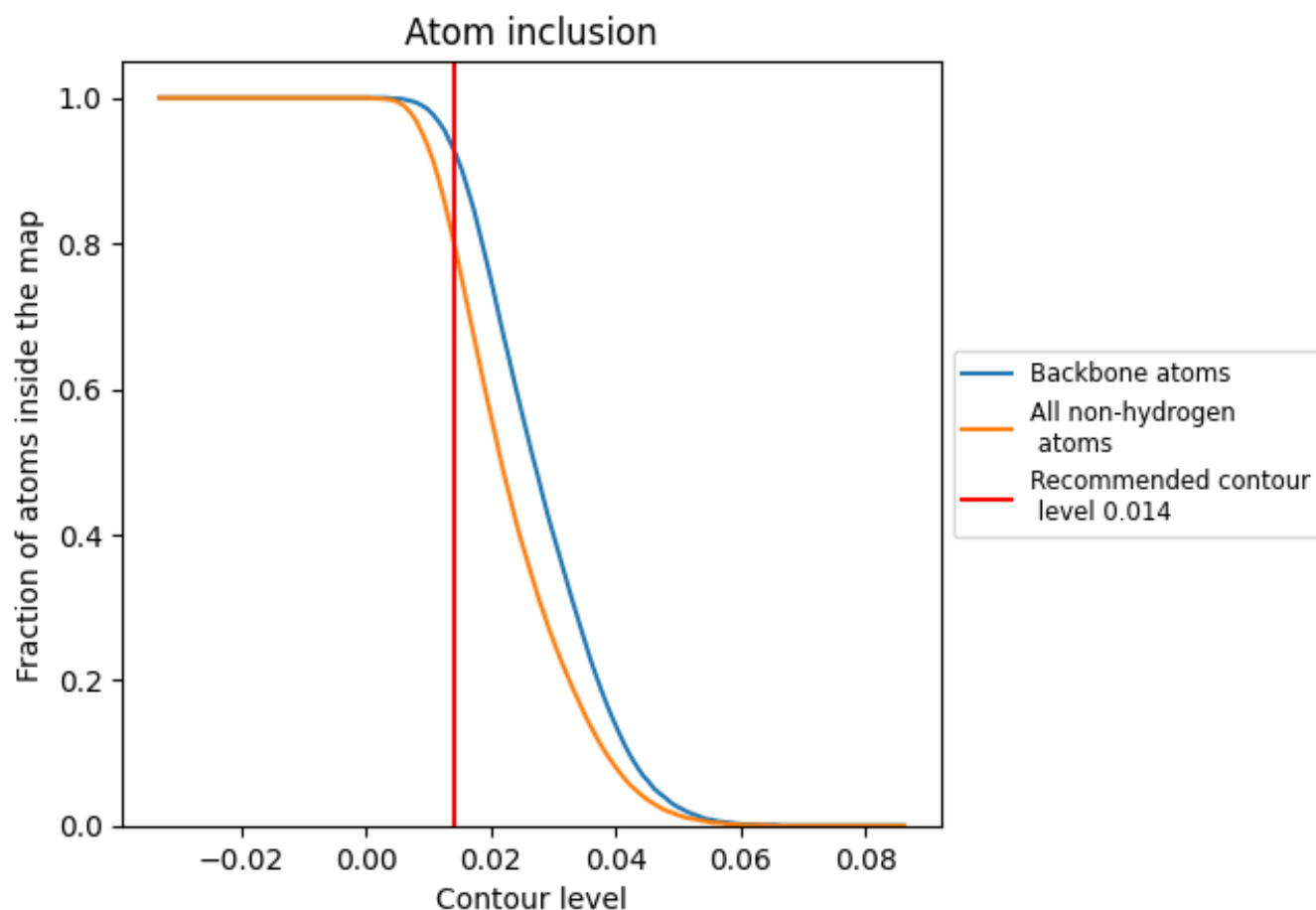
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 80% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8030	0.4450
1	0.0000	0.4240
2	0.7350	0.4080
3	0.8750	0.5000
4	0.8010	0.4490
5	0.8200	0.4650
6	0.7330	0.3940
7	0.8590	0.4870
8	0.7880	0.3500
9	0.6570	0.3090
B	0.7230	0.4050
C	0.8800	0.5050
D	0.8350	0.4750
E	0.8180	0.4590
F	0.7640	0.4160
G	0.8730	0.5010

1.0

0.0

<0.0