



Full wwPDB EM Validation Report ⓘ

Jun 4, 2025 – 12:26 PM EDT

PDB ID : 7RLI / pdb_00007rli
EMDB ID : EMD-24531
Title : Cryo-EM structure of human p97 bound to CB-5083 and ADP.
Authors : Caffrey, B.; Zhu, X.; Berezuk, A.; Tuttle, K.; Chittori, S.; Subramaniam, S.
Deposited on : 2021-07-23
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

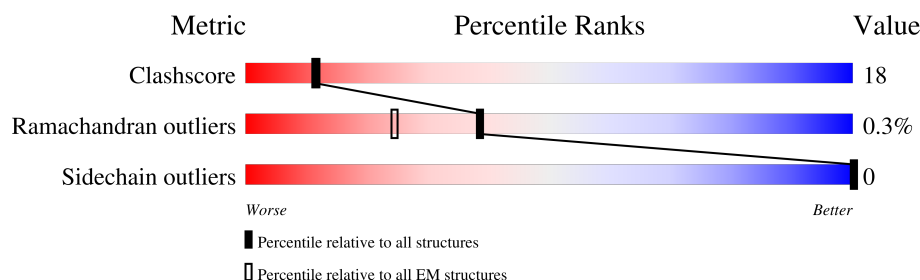
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	821	<div> <div>26%</div> <div>60%</div> <div>29%</div> <div>10%</div> </div>
1	B	821	<div> <div>26%</div> <div>60%</div> <div>29%</div> <div>10%</div> </div>
1	C	821	<div> <div>25%</div> <div>60%</div> <div>29%</div> <div>10%</div> </div>
1	D	821	<div> <div>26%</div> <div>60%</div> <div>29%</div> <div>10%</div> </div>
1	E	821	<div> <div>26%</div> <div>60%</div> <div>30%</div> <div>10%</div> </div>
1	F	821	<div> <div>26%</div> <div>60%</div> <div>29%</div> <div>10%</div> </div>
1	G	821	<div> <div>26%</div> <div>60%</div> <div>29%</div> <div>10%</div> </div>
1	H	821	<div> <div>26%</div> <div>60%</div> <div>29%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	821	<div><div></div><div>26%</div><div>61%</div><div>29%</div><div>10%</div></div>
1	J	821	<div><div></div><div>26%</div><div>60%</div><div>29%</div><div>10%</div></div>
1	K	821	<div><div></div><div>26%</div><div>59%</div><div>30%</div><div>10%</div></div>
1	L	821	<div><div></div><div>26%</div><div>60%</div><div>29%</div><div>10%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 69768 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	735	Total	C	N	O	S	0	0
			5756	3623	1015	1088	30		
1	B	735	Total	C	N	O	S	0	0
			5756	3623	1015	1088	30		
1	C	735	Total	C	N	O	S	0	0
			5756	3623	1015	1088	30		
1	D	735	Total	C	N	O	S	0	0
			5756	3623	1015	1088	30		
1	E	735	Total	C	N	O	S	0	0
			5756	3623	1015	1088	30		
1	F	735	Total	C	N	O	S	0	0
			5756	3623	1015	1088	30		
1	G	735	Total	C	N	O	S	0	0
			5756	3623	1015	1088	30		
1	H	735	Total	C	N	O	S	0	0
			5756	3623	1015	1088	30		
1	I	735	Total	C	N	O	S	0	0
			5756	3623	1015	1088	30		
1	J	735	Total	C	N	O	S	0	0
			5756	3623	1015	1088	30		
1	K	735	Total	C	N	O	S	0	0
			5756	3623	1015	1088	30		
1	L	735	Total	C	N	O	S	0	0
			5756	3623	1015	1088	30		

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP P55072
A	-13	HIS	-	expression tag	UNP P55072
A	-12	HIS	-	expression tag	UNP P55072
A	-11	HIS	-	expression tag	UNP P55072
A	-10	HIS	-	expression tag	UNP P55072
A	-9	HIS	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP P55072
A	-7	THR	-	expression tag	UNP P55072
A	-6	SER	-	expression tag	UNP P55072
A	-5	GLU	-	expression tag	UNP P55072
A	-4	ASN	-	expression tag	UNP P55072
A	-3	LEU	-	expression tag	UNP P55072
A	-2	TYR	-	expression tag	UNP P55072
A	-1	PHE	-	expression tag	UNP P55072
A	0	GLN	-	expression tag	UNP P55072
A	1	GLY	-	expression tag	UNP P55072
B	-14	HIS	-	expression tag	UNP P55072
B	-13	HIS	-	expression tag	UNP P55072
B	-12	HIS	-	expression tag	UNP P55072
B	-11	HIS	-	expression tag	UNP P55072
B	-10	HIS	-	expression tag	UNP P55072
B	-9	HIS	-	expression tag	UNP P55072
B	-8	GLY	-	expression tag	UNP P55072
B	-7	THR	-	expression tag	UNP P55072
B	-6	SER	-	expression tag	UNP P55072
B	-5	GLU	-	expression tag	UNP P55072
B	-4	ASN	-	expression tag	UNP P55072
B	-3	LEU	-	expression tag	UNP P55072
B	-2	TYR	-	expression tag	UNP P55072
B	-1	PHE	-	expression tag	UNP P55072
B	0	GLN	-	expression tag	UNP P55072
B	1	GLY	-	expression tag	UNP P55072
C	-14	HIS	-	expression tag	UNP P55072
C	-13	HIS	-	expression tag	UNP P55072
C	-12	HIS	-	expression tag	UNP P55072
C	-11	HIS	-	expression tag	UNP P55072
C	-10	HIS	-	expression tag	UNP P55072
C	-9	HIS	-	expression tag	UNP P55072
C	-8	GLY	-	expression tag	UNP P55072
C	-7	THR	-	expression tag	UNP P55072
C	-6	SER	-	expression tag	UNP P55072
C	-5	GLU	-	expression tag	UNP P55072
C	-4	ASN	-	expression tag	UNP P55072
C	-3	LEU	-	expression tag	UNP P55072
C	-2	TYR	-	expression tag	UNP P55072
C	-1	PHE	-	expression tag	UNP P55072
C	0	GLN	-	expression tag	UNP P55072
C	1	GLY	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	HIS	-	expression tag	UNP P55072
D	-13	HIS	-	expression tag	UNP P55072
D	-12	HIS	-	expression tag	UNP P55072
D	-11	HIS	-	expression tag	UNP P55072
D	-10	HIS	-	expression tag	UNP P55072
D	-9	HIS	-	expression tag	UNP P55072
D	-8	GLY	-	expression tag	UNP P55072
D	-7	THR	-	expression tag	UNP P55072
D	-6	SER	-	expression tag	UNP P55072
D	-5	GLU	-	expression tag	UNP P55072
D	-4	ASN	-	expression tag	UNP P55072
D	-3	LEU	-	expression tag	UNP P55072
D	-2	TYR	-	expression tag	UNP P55072
D	-1	PHE	-	expression tag	UNP P55072
D	0	GLN	-	expression tag	UNP P55072
D	1	GLY	-	expression tag	UNP P55072
E	-14	HIS	-	expression tag	UNP P55072
E	-13	HIS	-	expression tag	UNP P55072
E	-12	HIS	-	expression tag	UNP P55072
E	-11	HIS	-	expression tag	UNP P55072
E	-10	HIS	-	expression tag	UNP P55072
E	-9	HIS	-	expression tag	UNP P55072
E	-8	GLY	-	expression tag	UNP P55072
E	-7	THR	-	expression tag	UNP P55072
E	-6	SER	-	expression tag	UNP P55072
E	-5	GLU	-	expression tag	UNP P55072
E	-4	ASN	-	expression tag	UNP P55072
E	-3	LEU	-	expression tag	UNP P55072
E	-2	TYR	-	expression tag	UNP P55072
E	-1	PHE	-	expression tag	UNP P55072
E	0	GLN	-	expression tag	UNP P55072
E	1	GLY	-	expression tag	UNP P55072
F	-14	HIS	-	expression tag	UNP P55072
F	-13	HIS	-	expression tag	UNP P55072
F	-12	HIS	-	expression tag	UNP P55072
F	-11	HIS	-	expression tag	UNP P55072
F	-10	HIS	-	expression tag	UNP P55072
F	-9	HIS	-	expression tag	UNP P55072
F	-8	GLY	-	expression tag	UNP P55072
F	-7	THR	-	expression tag	UNP P55072
F	-6	SER	-	expression tag	UNP P55072
F	-5	GLU	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	ASN	-	expression tag	UNP P55072
F	-3	LEU	-	expression tag	UNP P55072
F	-2	TYR	-	expression tag	UNP P55072
F	-1	PHE	-	expression tag	UNP P55072
F	0	GLN	-	expression tag	UNP P55072
F	1	GLY	-	expression tag	UNP P55072
G	-14	HIS	-	expression tag	UNP P55072
G	-13	HIS	-	expression tag	UNP P55072
G	-12	HIS	-	expression tag	UNP P55072
G	-11	HIS	-	expression tag	UNP P55072
G	-10	HIS	-	expression tag	UNP P55072
G	-9	HIS	-	expression tag	UNP P55072
G	-8	GLY	-	expression tag	UNP P55072
G	-7	THR	-	expression tag	UNP P55072
G	-6	SER	-	expression tag	UNP P55072
G	-5	GLU	-	expression tag	UNP P55072
G	-4	ASN	-	expression tag	UNP P55072
G	-3	LEU	-	expression tag	UNP P55072
G	-2	TYR	-	expression tag	UNP P55072
G	-1	PHE	-	expression tag	UNP P55072
G	0	GLN	-	expression tag	UNP P55072
G	1	GLY	-	expression tag	UNP P55072
H	-14	HIS	-	expression tag	UNP P55072
H	-13	HIS	-	expression tag	UNP P55072
H	-12	HIS	-	expression tag	UNP P55072
H	-11	HIS	-	expression tag	UNP P55072
H	-10	HIS	-	expression tag	UNP P55072
H	-9	HIS	-	expression tag	UNP P55072
H	-8	GLY	-	expression tag	UNP P55072
H	-7	THR	-	expression tag	UNP P55072
H	-6	SER	-	expression tag	UNP P55072
H	-5	GLU	-	expression tag	UNP P55072
H	-4	ASN	-	expression tag	UNP P55072
H	-3	LEU	-	expression tag	UNP P55072
H	-2	TYR	-	expression tag	UNP P55072
H	-1	PHE	-	expression tag	UNP P55072
H	0	GLN	-	expression tag	UNP P55072
H	1	GLY	-	expression tag	UNP P55072
I	-14	HIS	-	expression tag	UNP P55072
I	-13	HIS	-	expression tag	UNP P55072
I	-12	HIS	-	expression tag	UNP P55072
I	-11	HIS	-	expression tag	UNP P55072

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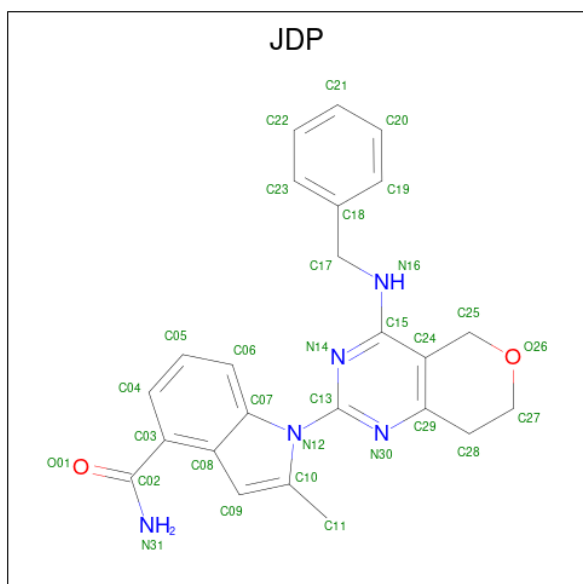
Chain	Residue	Modelled	Actual	Comment	Reference
I	-10	HIS	-	expression tag	UNP P55072
I	-9	HIS	-	expression tag	UNP P55072
I	-8	GLY	-	expression tag	UNP P55072
I	-7	THR	-	expression tag	UNP P55072
I	-6	SER	-	expression tag	UNP P55072
I	-5	GLU	-	expression tag	UNP P55072
I	-4	ASN	-	expression tag	UNP P55072
I	-3	LEU	-	expression tag	UNP P55072
I	-2	TYR	-	expression tag	UNP P55072
I	-1	PHE	-	expression tag	UNP P55072
I	0	GLN	-	expression tag	UNP P55072
I	1	GLY	-	expression tag	UNP P55072
J	-14	HIS	-	expression tag	UNP P55072
J	-13	HIS	-	expression tag	UNP P55072
J	-12	HIS	-	expression tag	UNP P55072
J	-11	HIS	-	expression tag	UNP P55072
J	-10	HIS	-	expression tag	UNP P55072
J	-9	HIS	-	expression tag	UNP P55072
J	-8	GLY	-	expression tag	UNP P55072
J	-7	THR	-	expression tag	UNP P55072
J	-6	SER	-	expression tag	UNP P55072
J	-5	GLU	-	expression tag	UNP P55072
J	-4	ASN	-	expression tag	UNP P55072
J	-3	LEU	-	expression tag	UNP P55072
J	-2	TYR	-	expression tag	UNP P55072
J	-1	PHE	-	expression tag	UNP P55072
J	0	GLN	-	expression tag	UNP P55072
J	1	GLY	-	expression tag	UNP P55072
K	-14	HIS	-	expression tag	UNP P55072
K	-13	HIS	-	expression tag	UNP P55072
K	-12	HIS	-	expression tag	UNP P55072
K	-11	HIS	-	expression tag	UNP P55072
K	-10	HIS	-	expression tag	UNP P55072
K	-9	HIS	-	expression tag	UNP P55072
K	-8	GLY	-	expression tag	UNP P55072
K	-7	THR	-	expression tag	UNP P55072
K	-6	SER	-	expression tag	UNP P55072
K	-5	GLU	-	expression tag	UNP P55072
K	-4	ASN	-	expression tag	UNP P55072
K	-3	LEU	-	expression tag	UNP P55072
K	-2	TYR	-	expression tag	UNP P55072
K	-1	PHE	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLN	-	expression tag	UNP P55072
K	1	GLY	-	expression tag	UNP P55072
L	-14	HIS	-	expression tag	UNP P55072
L	-13	HIS	-	expression tag	UNP P55072
L	-12	HIS	-	expression tag	UNP P55072
L	-11	HIS	-	expression tag	UNP P55072
L	-10	HIS	-	expression tag	UNP P55072
L	-9	HIS	-	expression tag	UNP P55072
L	-8	GLY	-	expression tag	UNP P55072
L	-7	THR	-	expression tag	UNP P55072
L	-6	SER	-	expression tag	UNP P55072
L	-5	GLU	-	expression tag	UNP P55072
L	-4	ASN	-	expression tag	UNP P55072
L	-3	LEU	-	expression tag	UNP P55072
L	-2	TYR	-	expression tag	UNP P55072
L	-1	PHE	-	expression tag	UNP P55072
L	0	GLN	-	expression tag	UNP P55072
L	1	GLY	-	expression tag	UNP P55072

- Molecule 2 is 1-[4-(benzylamino)-7,8-dihydro-5H-pyrano[4,3-d]pyrimidin-2-yl]-2-methyl-1H-indole-4-carboxamide (CCD ID: JDP) (formula: C₂₄H₂₃N₅O₂) (labeled as "Ligand of Interest" by depositor).



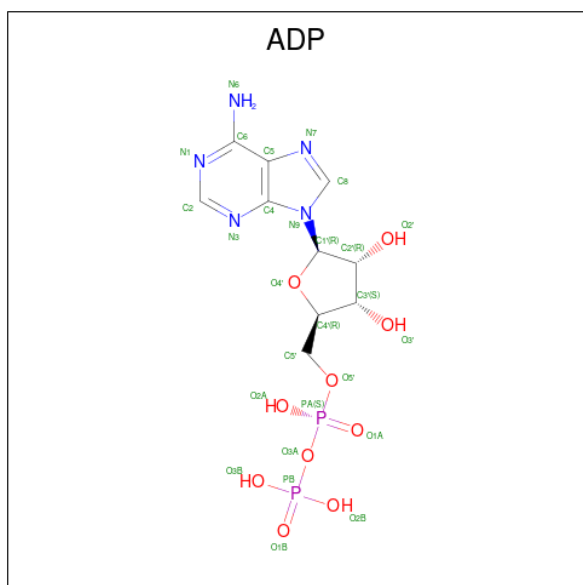
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			31	24	5	2	

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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			31	24	5	2	
2	C	1	Total	C	N	O	0
			31	24	5	2	
2	D	1	Total	C	N	O	0
			31	24	5	2	
2	E	1	Total	C	N	O	0
			31	24	5	2	
2	F	1	Total	C	N	O	0
			31	24	5	2	
2	G	1	Total	C	N	O	0
			31	24	5	2	
2	H	1	Total	C	N	O	0
			31	24	5	2	
2	I	1	Total	C	N	O	0
			31	24	5	2	
2	J	1	Total	C	N	O	0
			31	24	5	2	
2	K	1	Total	C	N	O	0
			31	24	5	2	
2	L	1	Total	C	N	O	0
			31	24	5	2	

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

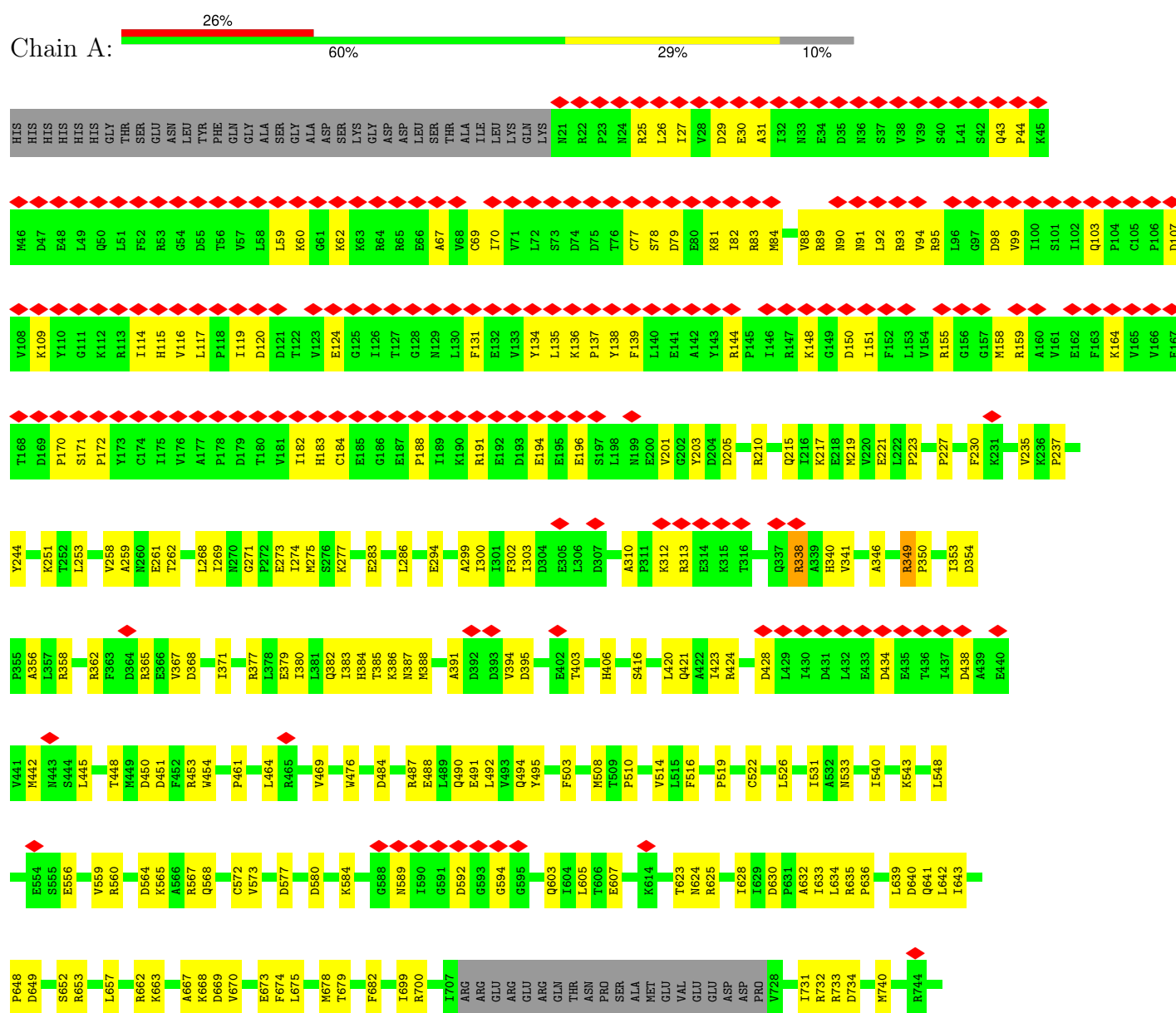


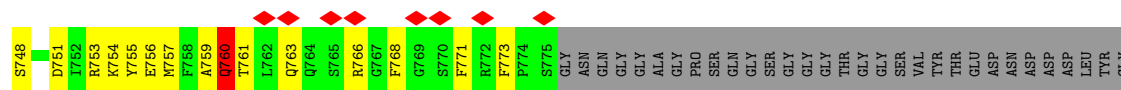
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0
3	G	1	Total 27	C 10	N 5	O 10	P 2	0
3	H	1	Total 27	C 10	N 5	O 10	P 2	0
3	I	1	Total 27	C 10	N 5	O 10	P 2	0
3	J	1	Total 27	C 10	N 5	O 10	P 2	0
3	K	1	Total 27	C 10	N 5	O 10	P 2	0
3	L	1	Total 27	C 10	N 5	O 10	P 2	0

3 Residue-property plots

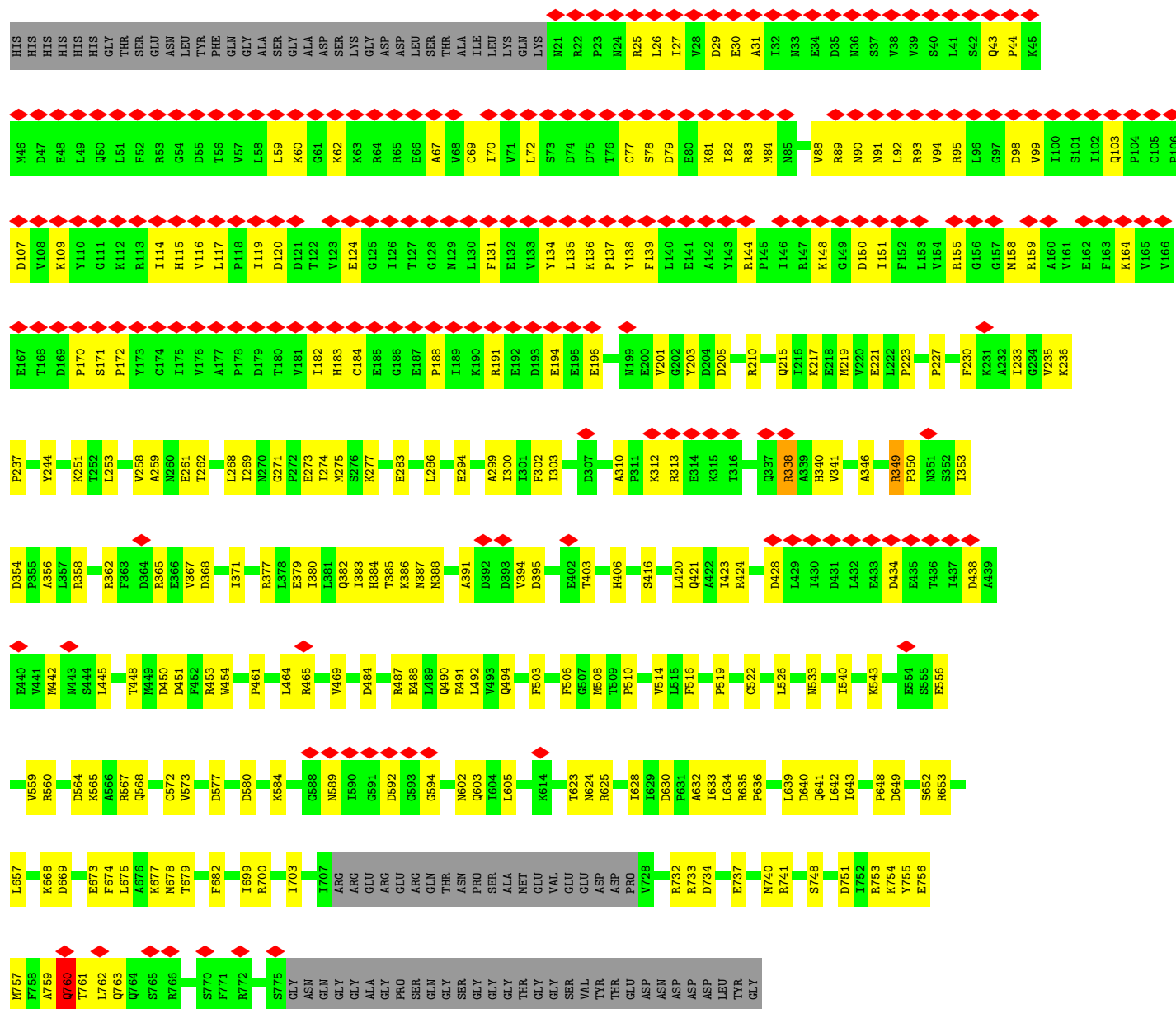
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Transitional endoplasmic reticulum ATPase



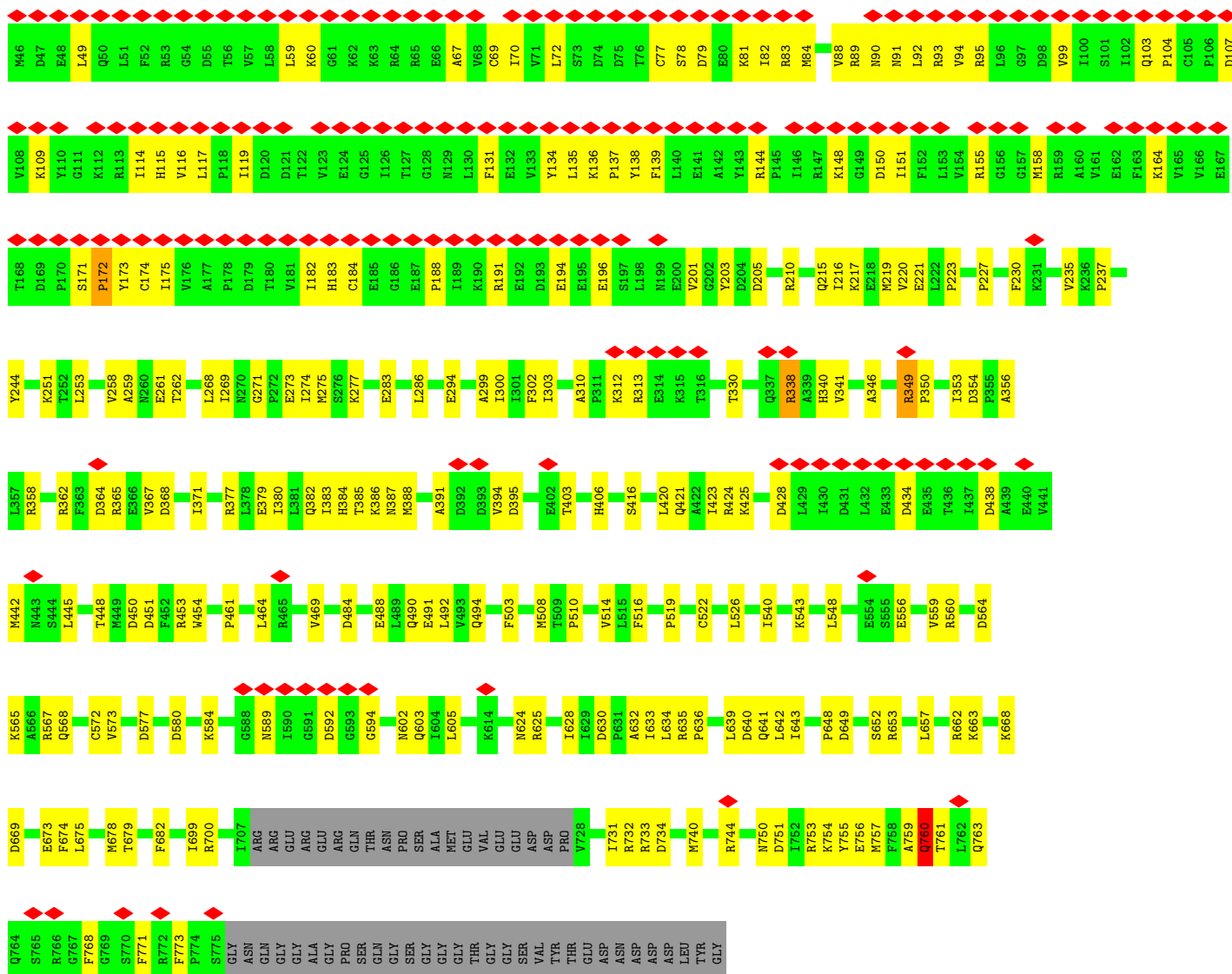


• Molecule 1: Transitional endoplasmic reticulum ATPase

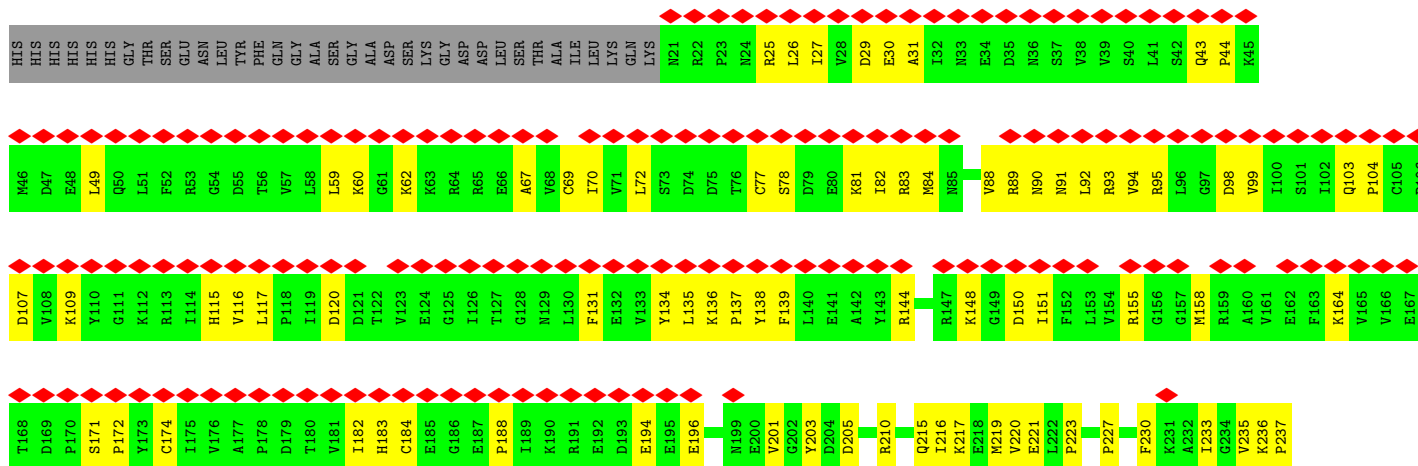


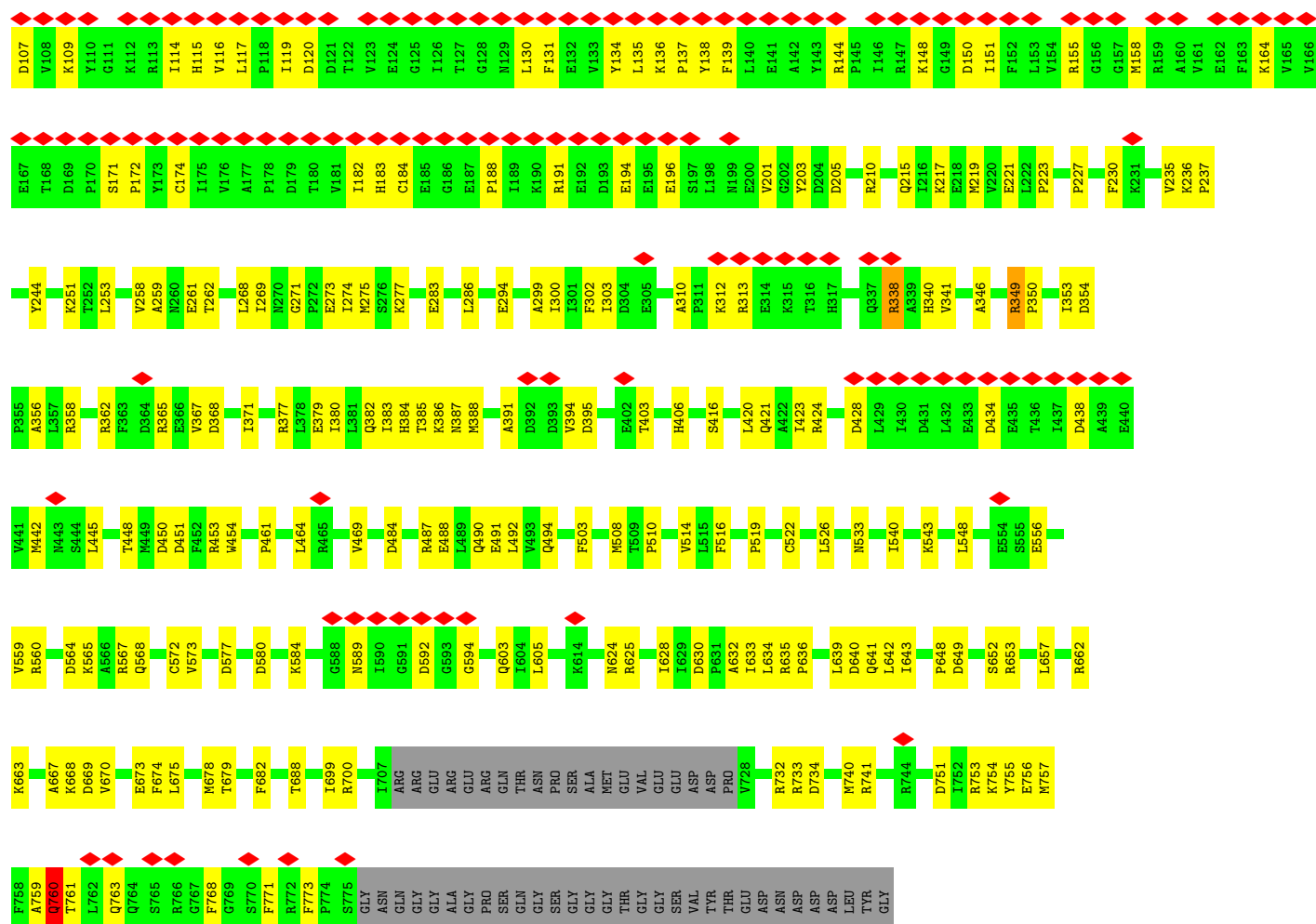
• Molecule 1: Transitional endoplasmic reticulum ATPase



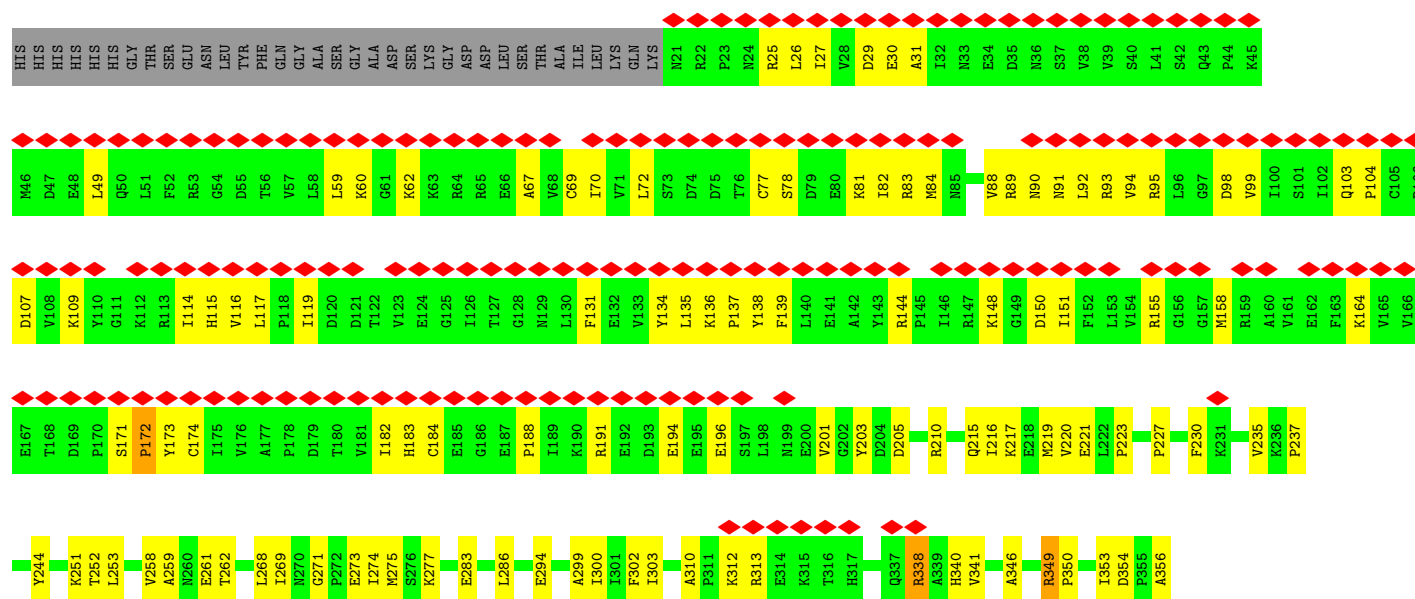


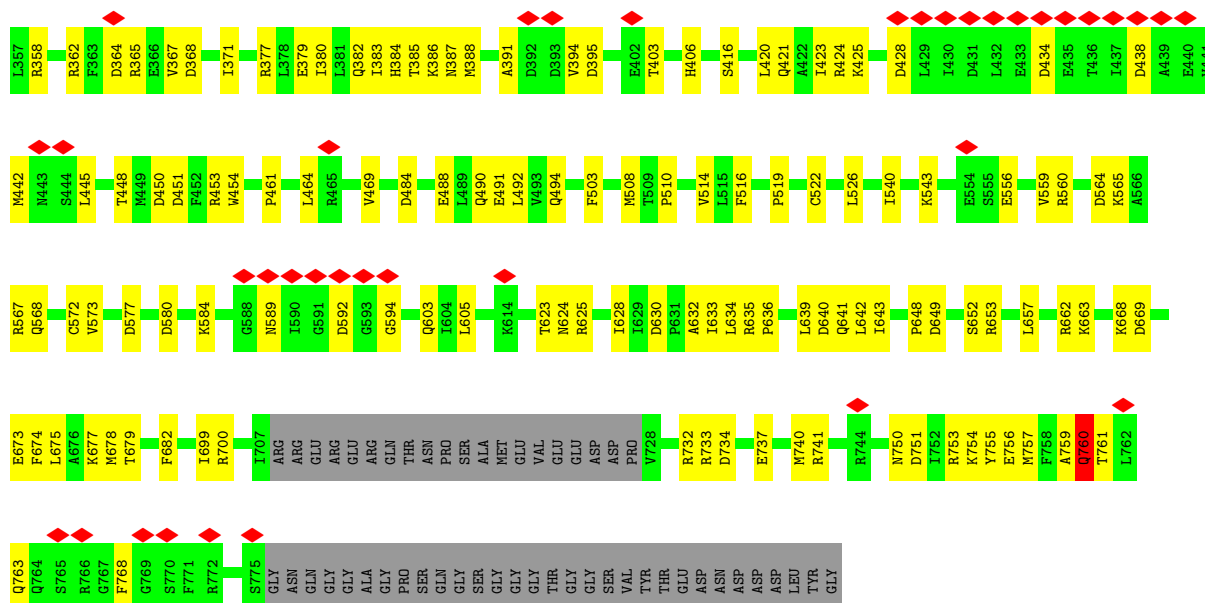
● Molecule 1: Transitional endoplasmic reticulum ATPase



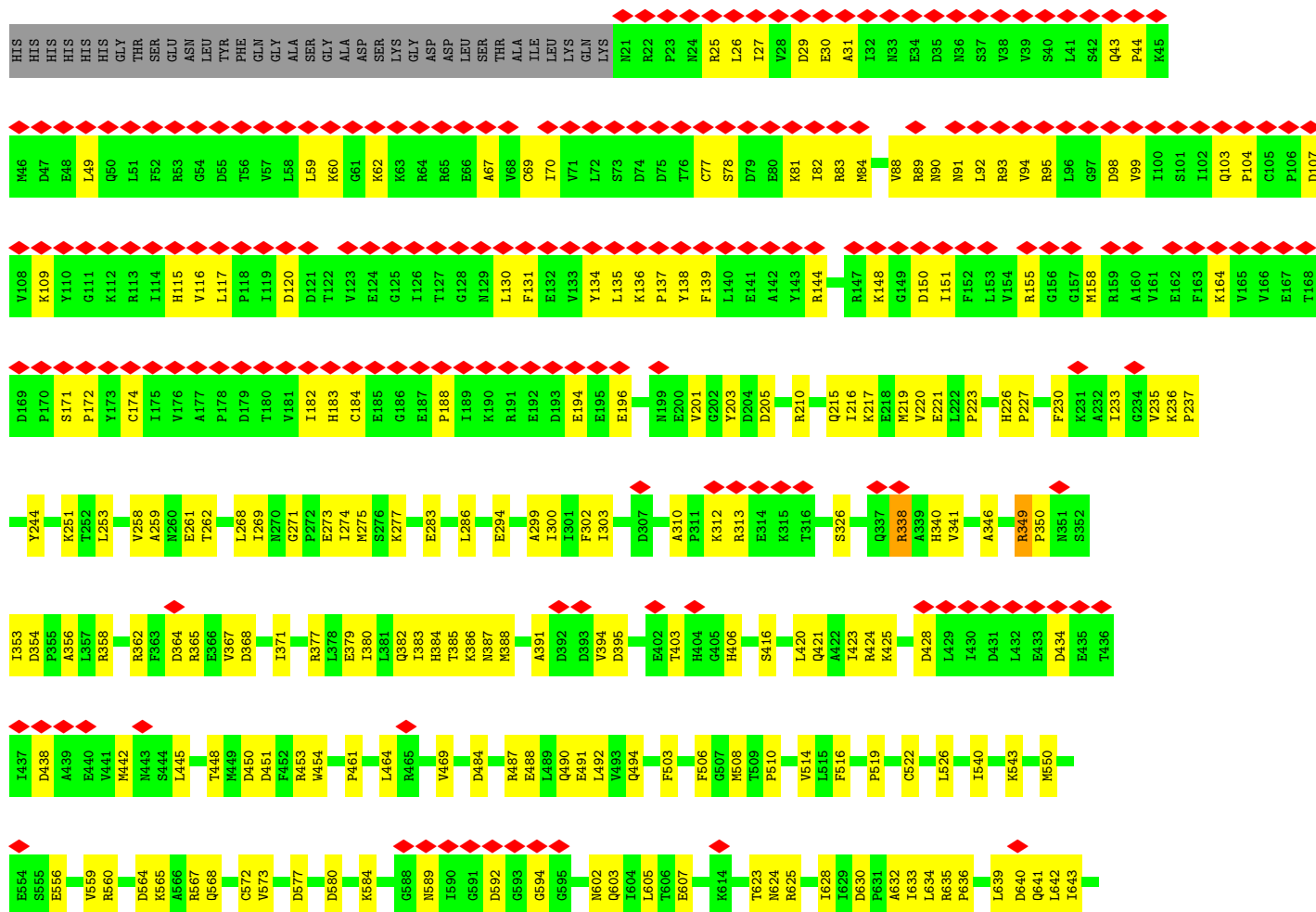


• Molecule 1: Transitional endoplasmic reticulum ATPase





• Molecule 1: Transitional endoplasmic reticulum ATPase





R753	P648	L548	I437	I353	P237	T168	V108	M46	HIS
K754	D649	E554	D438	D354	Y244	D169	K109	D47	HIS
W755	S655	S655	A439	P355	P247	P170	Y110	E48	HIS
M757	R652	E556	E440	A356	K251	S171	G111	L49	HIS
A759	L657	V559	M442	L357	L252	P172	K112	Q50	GLY
Q760	R560	R560	N443	R362	L253	Y173	R113	L51	THR
L762	D668	D564	S444	F363	T258	C174	I114	F52	THR
Q763	K669	K565	L445	D364	A259	I175	H115	R53	GLU
Q764	A666	A666	T448	R365	V258	V176	V116	R54	ASN
S765	E673	Q567	M449	E366	M260	A177	L117	D55	LEU
R766	F674	Q568	D450	E261	E261	P178	P118	T56	PHE
G767	L675	D451	F452	D368	T262	D179	I119	V57	GLN
F768	M678	C572	R453	I371	L268	T180	D120	L58	ALA
G769	V673	V673	W454	R377	L269	D181	D121	L59	ALA
S770	D577	D577	P461	L378	M270	I182	T122	K60	SER
F771	D580	D580	L464	E379	G271	H183	T123	G61	GLY
R772	K584	K584	R465	I380	E273	C184	E124	K62	ASP
S775	G588	G588	V469	Q382	M275	E185	G125	K63	SER
ASN	N589	N589	D484	I383	K277	G186	G126	R64	GLY
GLN	I590	I590	R487	H384	E283	E187	I127	R65	ASP
GLY	G591	G591	E488	T385	L286	G192	G128	A66	ASP
ALA	D592	D592	L489	K386	E294	E193	N129	E67	LEU
GLY	G593	G593	Q490	M387	A391	E194	L130	V68	SER
PRO	G594	G594	E491	M388	E299	E195	F131	C69	THR
SER	G595	G595	V493	A392	I300	E196	E132	L70	ALA
GLN	Q603	Q603	D392	D392	A299	S197	V133	V71	LEU
ALA	I604	I604	D393	D393	I301	L198	Y134	L72	TLE
GLY	T606	T606	E402	D395	F302	L199	L135	S73	GLN
THR	E607	E607	T403	D395	I303	E199	L136	D74	LYS
GLY	K614	K614	H406	E403	A310	E199	P137	D75	LYS
GLU	T608	T608	S416	T403	P311	E200	Y138	T76	LYS
VAL	M624	M624	L420	H406	K312	E201	F139	C77	LYS
ASP	R625	R625	Q421	S416	R313	G202	L140	L26	LYS
ASP	I628	I628	A423	L420	E314	Y203	L27	L26	LYS
ASP	D630	D630	R424	Q421	K315	D204	F80	V28	LYS
ASP	F631	F631	K425	A423	T316	D205	K81	D29	LYS
ASP	I632	I632	D428	R425	H317	R210	R83	E30	LYS
ASP	I633	I633	L429	L428	S326	Q215	M84	A31	LYS
ASP	L634	L634	L429	L428	Q337	I216	V88	I32	LYS
ASP	R635	R635	A532	L429	R338	K217	R89	N33	LYS
ASP	P636	P636	N533	I430	A339	E218	N90	E34	LYS
LEU	L639	L639	I540	D431	H340	D220	N91	D35	LYS
TYR	D640	D640	K543	L432	V341	E221	L92	N36	LYS
GLY	Q641	Q641	E433	L432	A346	L222	V94	V38	LYS
	L642	L642	D434	E433	R349	P223	R95	V39	LYS
	I643	I643	E435	T436	P350	P227	L96	S40	LYS
						F230	G97	L41	LYS
						K231	D98	S42	LYS
						A232	V99	Q43	LYS
						I233	I100	P44	LYS
						Q234	I102	R45	LYS
						V235	Q103	P104	LYS
						R236	C105	P106	LYS
							E167	D107	LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85876	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.283	Depositor
Minimum map value	-0.308	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.25	Depositor
Map size (\AA)	400.0, 400.0, 400.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/5852	0.45	2/7901 (0.0%)
1	B	0.17	0/5852	0.45	2/7901 (0.0%)
1	C	0.17	0/5852	0.45	2/7901 (0.0%)
1	D	0.17	0/5852	0.45	2/7901 (0.0%)
1	E	0.17	0/5852	0.45	2/7901 (0.0%)
1	F	0.17	0/5852	0.45	2/7901 (0.0%)
1	G	0.17	0/5852	0.45	2/7901 (0.0%)
1	H	0.17	0/5852	0.45	2/7901 (0.0%)
1	I	0.17	0/5852	0.45	2/7901 (0.0%)
1	J	0.17	0/5852	0.45	2/7901 (0.0%)
1	K	0.17	0/5852	0.45	2/7901 (0.0%)
1	L	0.17	0/5852	0.45	2/7901 (0.0%)
All	All	0.17	0/70224	0.45	24/94812 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	24

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	349	ARG	CG-CD-NE	7.24	127.92	112.00
1	J	349	ARG	CG-CD-NE	7.23	127.90	112.00
1	K	349	ARG	CG-CD-NE	7.23	127.90	112.00
1	C	349	ARG	CG-CD-NE	7.23	127.90	112.00
1	E	349	ARG	CG-CD-NE	7.22	127.89	112.00
1	B	349	ARG	CG-CD-NE	7.22	127.88	112.00
1	D	349	ARG	CG-CD-NE	7.22	127.88	112.00
1	F	349	ARG	CG-CD-NE	7.21	127.87	112.00
1	A	349	ARG	CG-CD-NE	7.21	127.86	112.00
1	H	349	ARG	CG-CD-NE	7.21	127.85	112.00
1	L	349	ARG	CG-CD-NE	7.21	127.86	112.00
1	G	349	ARG	CG-CD-NE	7.20	127.84	112.00
1	D	760	GLN	CA-CB-CG	6.10	126.30	114.10
1	H	760	GLN	CA-CB-CG	6.09	126.28	114.10
1	B	760	GLN	CA-CB-CG	6.09	126.28	114.10
1	J	760	GLN	CA-CB-CG	6.08	126.26	114.10
1	K	760	GLN	CA-CB-CG	6.08	126.26	114.10
1	L	760	GLN	CA-CB-CG	6.08	126.26	114.10
1	I	760	GLN	CA-CB-CG	6.08	126.26	114.10
1	G	760	GLN	CA-CB-CG	6.08	126.25	114.10
1	E	760	GLN	CA-CB-CG	6.08	126.25	114.10
1	F	760	GLN	CA-CB-CG	6.07	126.24	114.10
1	A	760	GLN	CA-CB-CG	6.06	126.21	114.10
1	C	760	GLN	CA-CB-CG	6.06	126.22	114.10

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	ARG	Sidechain
1	A	760	GLN	Peptide
1	B	349	ARG	Sidechain
1	B	760	GLN	Peptide
1	C	349	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	760	GLN	Peptide
1	D	349	ARG	Sidechain
1	D	760	GLN	Peptide
1	E	349	ARG	Sidechain
1	E	760	GLN	Peptide
1	F	349	ARG	Sidechain
1	F	760	GLN	Peptide
1	G	349	ARG	Sidechain
1	G	760	GLN	Peptide
1	H	349	ARG	Sidechain
1	H	760	GLN	Peptide
1	I	349	ARG	Sidechain
1	I	760	GLN	Peptide
1	J	349	ARG	Sidechain
1	J	760	GLN	Peptide
1	K	349	ARG	Sidechain
1	K	760	GLN	Peptide
1	L	349	ARG	Sidechain
1	L	760	GLN	Peptide

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	A	5756	0	5819	241	0
1	B	5756	0	5819	240	0
1	C	5756	0	5820	213	0
1	D	5756	0	5820	211	0
1	E	5756	0	5820	212	0
1	F	5756	0	5820	219	0
1	G	5756	0	5820	212	0
1	H	5756	0	5820	218	0
1	I	5756	0	5820	211	0
1	J	5756	0	5819	213	0
1	K	5756	0	5819	220	0
1	L	5756	0	5820	238	0
2	A	31	0	0	1	0
2	B	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	0	1	0
2	D	31	0	0	1	0
2	E	31	0	0	1	0
2	F	31	0	0	1	0
2	G	31	0	0	1	0
2	H	31	0	0	2	0
2	I	31	0	0	1	0
2	J	31	0	0	1	0
2	K	31	0	0	1	0
2	L	31	0	0	1	0
3	A	27	0	12	2	0
3	B	27	0	12	0	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	E	27	0	12	0	0
3	F	27	0	12	3	0
3	G	27	0	12	3	0
3	H	27	0	12	1	0
3	I	27	0	12	2	0
3	J	27	0	12	0	0
3	K	27	0	12	1	0
3	L	27	0	12	3	0
All	All	69768	0	69980	2450	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 18.

All (2450) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:NZ	1:A:171:SER:H	1.03	1.46
1:B:675:LEU:CD1	1:B:740:MET:HE1	1.45	1.46
1:H:675:LEU:CD1	1:H:740:MET:HE1	1.46	1.46
1:L:148:LYS:NZ	1:L:171:SER:H	1.04	1.46
1:F:760:GLN:HE21	1:L:760:GLN:NE2	0.97	1.45
1:A:675:LEU:CD1	1:A:740:MET:HE1	1.46	1.44
1:L:675:LEU:CD1	1:L:740:MET:HE1	1.45	1.44
1:C:675:LEU:CD1	1:C:740:MET:HE1	1.46	1.44
1:F:675:LEU:CD1	1:F:740:MET:HE1	1.46	1.44
1:I:675:LEU:CD1	1:I:740:MET:HE1	1.46	1.44
1:G:675:LEU:CD1	1:G:740:MET:HE1	1.45	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:675:LEU:CD1	1:E:740:MET:HE1	1.45	1.43
1:K:675:LEU:CD1	1:K:740:MET:HE1	1.46	1.43
1:B:148:LYS:NZ	1:B:171:SER:H	1.04	1.42
1:A:760:GLN:NE2	1:K:760:GLN:NE2	1.61	1.42
1:D:675:LEU:CD1	1:D:740:MET:HE1	1.45	1.42
1:F:760:GLN:NE2	1:L:760:GLN:HE21	0.93	1.42
1:J:675:LEU:CD1	1:J:740:MET:HE1	1.45	1.42
1:E:760:GLN:NE2	1:G:760:GLN:HE21	0.91	1.41
1:D:760:GLN:HE21	1:H:760:GLN:NE2	0.96	1.41
1:C:760:GLN:NE2	1:I:760:GLN:HE21	0.94	1.41
1:E:760:GLN:HE21	1:G:760:GLN:NE2	0.94	1.41
1:C:760:GLN:HE21	1:I:760:GLN:NE2	0.93	1.38
1:B:148:LYS:HZ1	1:B:171:SER:N	1.22	1.36
1:D:760:GLN:NE2	1:H:760:GLN:HE21	0.90	1.35
1:A:148:LYS:HZ1	1:A:171:SER:N	1.22	1.34
1:F:135:LEU:HA	1:F:138:TYR:CE2	1.63	1.33
1:L:148:LYS:HZ1	1:L:171:SER:N	1.23	1.33
1:A:135:LEU:HA	1:A:138:TYR:CE2	1.63	1.32
1:L:135:LEU:HA	1:L:138:TYR:CE2	1.64	1.32
1:E:135:LEU:HA	1:E:138:TYR:CE2	1.64	1.32
1:G:135:LEU:HA	1:G:138:TYR:CE2	1.64	1.32
1:K:135:LEU:HA	1:K:138:TYR:CE2	1.64	1.32
1:J:135:LEU:HA	1:J:138:TYR:CE2	1.63	1.32
1:B:135:LEU:HA	1:B:138:TYR:CE2	1.63	1.31
1:D:135:LEU:HA	1:D:138:TYR:CE2	1.63	1.31
1:H:135:LEU:HA	1:H:138:TYR:CE2	1.63	1.31
1:C:135:LEU:HA	1:C:138:TYR:CE2	1.64	1.30
1:I:135:LEU:HA	1:I:138:TYR:CE2	1.63	1.30
1:A:148:LYS:CE	1:A:171:SER:N	1.95	1.30
1:C:675:LEU:CD1	1:C:740:MET:CE	2.10	1.29
1:E:675:LEU:CD1	1:E:740:MET:CE	2.10	1.29
1:I:675:LEU:CD1	1:I:740:MET:CE	2.10	1.29
1:K:675:LEU:CD1	1:K:740:MET:CE	2.10	1.29
1:B:148:LYS:CE	1:B:171:SER:N	1.95	1.29
1:A:675:LEU:CD1	1:A:740:MET:CE	2.10	1.28
1:J:675:LEU:CD1	1:J:740:MET:CE	2.10	1.28
1:L:148:LYS:CE	1:L:171:SER:N	1.95	1.28
1:D:675:LEU:CD1	1:D:740:MET:CE	2.10	1.28
1:G:675:LEU:CD1	1:G:740:MET:CE	2.10	1.28
1:F:675:LEU:CD1	1:F:740:MET:CE	2.10	1.27
1:L:148:LYS:HE3	1:L:171:SER:N	1.49	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:675:LEU:CD1	1:L:740:MET:CE	2.10	1.27
1:H:675:LEU:CD1	1:H:740:MET:CE	2.10	1.27
1:B:675:LEU:CD1	1:B:740:MET:CE	2.10	1.26
1:B:148:LYS:HE3	1:B:171:SER:N	1.49	1.25
1:H:675:LEU:HD11	1:H:740:MET:CE	1.67	1.25
1:B:675:LEU:HD11	1:B:740:MET:CE	1.68	1.24
1:D:675:LEU:HD11	1:D:740:MET:CE	1.67	1.24
1:J:675:LEU:HD11	1:J:740:MET:CE	1.68	1.24
1:A:675:LEU:HD11	1:A:740:MET:CE	1.67	1.24
1:G:675:LEU:HD11	1:G:740:MET:CE	1.67	1.23
1:A:148:LYS:HE3	1:A:171:SER:N	1.49	1.23
1:H:130:LEU:HG	1:H:134:TYR:CE2	1.73	1.23
1:L:675:LEU:HD11	1:L:740:MET:CE	1.67	1.22
1:F:675:LEU:HD11	1:F:740:MET:CE	1.68	1.22
1:C:675:LEU:HD11	1:C:740:MET:CE	1.68	1.21
1:I:675:LEU:HD11	1:I:740:MET:CE	1.67	1.21
1:E:675:LEU:HD11	1:E:740:MET:CE	1.67	1.20
1:K:675:LEU:HD11	1:K:740:MET:CE	1.67	1.20
1:L:148:LYS:CE	1:L:171:SER:H	1.55	1.18
1:A:148:LYS:CE	1:A:171:SER:H	1.55	1.17
1:B:148:LYS:CE	1:B:171:SER:H	1.56	1.16
1:A:148:LYS:HE3	1:A:171:SER:CA	1.76	1.14
1:L:148:LYS:HE3	1:L:171:SER:CA	1.76	1.14
1:B:148:LYS:HE3	1:B:171:SER:CA	1.76	1.13
1:A:508:MET:HE2	1:B:699:ILE:CD1	1.82	1.09
1:A:148:LYS:CD	1:A:171:SER:HB2	1.84	1.08
1:L:148:LYS:CD	1:L:171:SER:HB2	1.84	1.07
1:B:148:LYS:CD	1:B:171:SER:HB2	1.84	1.06
1:C:383:ILE:CD1	1:C:384:HIS:CD2	2.39	1.05
1:G:383:ILE:CD1	1:G:384:HIS:CD2	2.39	1.04
1:L:383:ILE:CD1	1:L:384:HIS:CD2	2.39	1.04
1:G:383:ILE:CD1	1:G:384:HIS:HD2	1.70	1.03
1:H:130:LEU:O	1:H:130:LEU:HD23	1.59	1.03
1:H:508:MET:HE2	1:I:699:ILE:CD1	1.89	1.03
1:L:383:ILE:CD1	1:L:384:HIS:HD2	1.70	1.03
1:C:383:ILE:CD1	1:C:384:HIS:HD2	1.70	1.01
1:I:135:LEU:HG	1:I:138:TYR:OH	1.61	1.00
1:C:135:LEU:HG	1:C:138:TYR:OH	1.62	1.00
1:G:135:LEU:HG	1:G:138:TYR:OH	1.61	0.99
1:B:135:LEU:HG	1:B:138:TYR:OH	1.61	0.99
1:J:135:LEU:HG	1:J:138:TYR:OH	1.62	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:LEU:HG	1:D:138:TYR:OH	1.61	0.99
1:L:135:LEU:HG	1:L:138:TYR:OH	1.61	0.99
1:F:135:LEU:HG	1:F:138:TYR:OH	1.61	0.99
1:A:135:LEU:HG	1:A:138:TYR:OH	1.62	0.99
1:H:135:LEU:HG	1:H:138:TYR:OH	1.61	0.99
1:L:383:ILE:HD11	1:L:384:HIS:HD2	1.26	0.99
1:G:383:ILE:HD11	1:G:384:HIS:HD2	1.25	0.98
1:E:135:LEU:HG	1:E:138:TYR:OH	1.61	0.98
1:E:675:LEU:HD13	1:E:740:MET:CE	1.93	0.98
1:A:508:MET:CE	1:B:699:ILE:HD12	1.92	0.98
1:G:699:ILE:CD1	1:L:508:MET:HE2	1.93	0.98
1:K:675:LEU:HD13	1:K:740:MET:CE	1.94	0.98
1:K:135:LEU:HG	1:K:138:TYR:OH	1.62	0.98
1:J:508:MET:HE2	1:K:699:ILE:CD1	1.94	0.97
1:D:675:LEU:HD13	1:D:740:MET:CE	1.93	0.97
1:C:383:ILE:HD11	1:C:384:HIS:HD2	1.26	0.97
1:G:383:ILE:HD12	1:G:384:HIS:CD2	2.00	0.97
1:J:675:LEU:HD13	1:J:740:MET:CE	1.93	0.97
1:G:383:ILE:HD11	1:G:384:HIS:CD2	1.99	0.96
1:B:675:LEU:HD13	1:B:740:MET:CE	1.93	0.96
1:I:508:MET:HE2	1:J:699:ILE:CD1	1.95	0.96
1:B:448:THR:OG1	1:B:450:ASP:OD1	1.83	0.96
1:H:448:THR:OG1	1:H:450:ASP:OD1	1.83	0.96
1:H:675:LEU:HD13	1:H:740:MET:CE	1.93	0.96
1:A:383:ILE:CD1	1:A:384:HIS:ND1	2.29	0.96
1:A:448:THR:OG1	1:A:450:ASP:OD1	1.83	0.96
1:F:383:ILE:CD1	1:F:384:HIS:ND1	2.29	0.96
1:A:148:LYS:HZ3	1:A:170:PRO:HA	1.30	0.96
1:G:448:THR:OG1	1:G:450:ASP:OD1	1.83	0.96
1:F:448:THR:OG1	1:F:450:ASP:OD1	1.83	0.96
1:L:383:ILE:HD11	1:L:384:HIS:CD2	1.99	0.96
1:L:448:THR:OG1	1:L:450:ASP:OD1	1.83	0.96
1:C:383:ILE:HD12	1:C:384:HIS:CD2	2.00	0.96
1:L:148:LYS:HZ3	1:L:170:PRO:HA	1.30	0.96
1:H:383:ILE:CD1	1:H:384:HIS:ND1	2.29	0.95
1:B:383:ILE:CD1	1:B:384:HIS:ND1	2.29	0.95
1:D:383:ILE:CD1	1:D:384:HIS:ND1	2.29	0.95
1:J:383:ILE:CD1	1:J:384:HIS:ND1	2.29	0.95
1:L:383:ILE:HD12	1:L:384:HIS:CD2	2.00	0.95
1:B:508:MET:HE2	1:C:699:ILE:CD1	1.95	0.95
1:E:383:ILE:CD1	1:E:384:HIS:ND1	2.29	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:675:LEU:HD13	1:I:740:MET:CE	1.94	0.95
1:K:383:ILE:CD1	1:K:384:HIS:ND1	2.29	0.95
1:B:148:LYS:HZ3	1:B:170:PRO:HA	1.30	0.95
1:C:448:THR:OG1	1:C:450:ASP:OD1	1.84	0.95
1:I:448:THR:OG1	1:I:450:ASP:OD1	1.83	0.95
1:D:448:THR:OG1	1:D:450:ASP:OD1	1.83	0.95
1:J:448:THR:OG1	1:J:450:ASP:OD1	1.83	0.95
1:B:134:TYR:O	1:B:138:TYR:CD2	2.20	0.94
1:B:148:LYS:NZ	1:B:170:PRO:HA	1.82	0.94
1:C:675:LEU:HD13	1:C:740:MET:CE	1.94	0.94
1:F:134:TYR:O	1:F:138:TYR:CD2	2.21	0.94
1:K:448:THR:OG1	1:K:450:ASP:OD1	1.83	0.94
1:E:134:TYR:O	1:E:138:TYR:CD2	2.20	0.94
1:E:448:THR:OG1	1:E:450:ASP:OD1	1.83	0.94
1:H:134:TYR:O	1:H:138:TYR:CD2	2.20	0.94
1:I:383:ILE:CD1	1:I:384:HIS:ND1	2.29	0.94
1:L:134:TYR:O	1:L:138:TYR:CD2	2.21	0.94
1:C:383:ILE:HD11	1:C:384:HIS:CD2	1.99	0.94
1:A:675:LEU:HD13	1:A:740:MET:CE	1.93	0.94
1:G:134:TYR:O	1:G:138:TYR:CD2	2.21	0.94
1:I:134:TYR:O	1:I:138:TYR:CD2	2.21	0.94
1:C:134:TYR:O	1:C:138:TYR:CD2	2.21	0.94
1:F:675:LEU:HD13	1:F:740:MET:CE	1.94	0.94
1:K:134:TYR:O	1:K:138:TYR:CD2	2.21	0.94
1:L:675:LEU:HD13	1:L:740:MET:CE	1.93	0.94
1:G:675:LEU:HD13	1:G:740:MET:CE	1.93	0.93
1:A:134:TYR:O	1:A:138:TYR:CD2	2.21	0.93
1:D:134:TYR:O	1:D:138:TYR:CD2	2.20	0.93
1:J:134:TYR:O	1:J:138:TYR:CD2	2.21	0.93
1:L:148:LYS:NZ	1:L:170:PRO:HA	1.82	0.93
1:C:508:MET:HE2	1:D:699:ILE:CD1	1.99	0.93
1:L:148:LYS:NZ	1:L:171:SER:N	1.80	0.93
1:H:508:MET:CE	1:I:699:ILE:HD12	1.98	0.93
1:A:148:LYS:NZ	1:A:170:PRO:HA	1.82	0.92
1:B:508:MET:CE	1:C:699:ILE:HD12	2.00	0.92
1:J:508:MET:CE	1:K:699:ILE:HD12	1.99	0.92
1:C:134:TYR:O	1:C:138:TYR:HD2	1.54	0.91
1:H:135:LEU:CA	1:H:138:TYR:CE2	2.53	0.91
1:I:134:TYR:O	1:I:138:TYR:HD2	1.54	0.91
1:B:135:LEU:CA	1:B:138:TYR:CE2	2.53	0.91
1:D:135:LEU:CA	1:D:138:TYR:CE2	2.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:TYR:O	1:F:138:TYR:HD2	1.54	0.91
1:G:134:TYR:O	1:G:138:TYR:HD2	1.54	0.91
1:I:135:LEU:CA	1:I:138:TYR:CE2	2.53	0.91
1:A:134:TYR:O	1:A:138:TYR:HD2	1.54	0.91
1:C:135:LEU:CA	1:C:138:TYR:CE2	2.53	0.91
1:F:135:LEU:CA	1:F:138:TYR:CE2	2.53	0.91
1:J:135:LEU:CA	1:J:138:TYR:CE2	2.53	0.91
1:B:134:TYR:O	1:B:138:TYR:HD2	1.54	0.90
1:E:134:TYR:O	1:E:138:TYR:HD2	1.54	0.90
1:E:135:LEU:CA	1:E:138:TYR:CE2	2.53	0.90
1:H:134:TYR:O	1:H:138:TYR:HD2	1.54	0.90
1:A:148:LYS:NZ	1:A:171:SER:N	1.80	0.90
1:K:135:LEU:CA	1:K:138:TYR:CE2	2.53	0.90
1:L:134:TYR:O	1:L:138:TYR:HD2	1.54	0.90
1:A:135:LEU:CA	1:A:138:TYR:CE2	2.53	0.90
1:L:135:LEU:CA	1:L:138:TYR:CE2	2.53	0.90
1:K:134:TYR:O	1:K:138:TYR:HD2	1.54	0.90
1:D:134:TYR:O	1:D:138:TYR:HD2	1.54	0.90
1:G:135:LEU:CA	1:G:138:TYR:CE2	2.53	0.89
1:J:134:TYR:O	1:J:138:TYR:HD2	1.54	0.89
1:A:148:LYS:HD2	1:A:171:SER:HB2	1.54	0.89
1:G:699:ILE:HD12	1:L:508:MET:CE	2.02	0.89
1:H:130:LEU:CG	1:H:134:TYR:CE2	2.56	0.89
1:B:508:MET:HE2	1:C:699:ILE:HD12	1.54	0.89
1:L:148:LYS:HD2	1:L:171:SER:HB2	1.54	0.89
1:A:508:MET:CE	1:B:699:ILE:CD1	2.51	0.88
1:B:148:LYS:HD2	1:B:171:SER:HB2	1.54	0.87
1:H:383:ILE:HD12	1:H:384:HIS:ND1	1.90	0.87
1:K:383:ILE:HD12	1:K:384:HIS:ND1	1.90	0.87
1:E:383:ILE:HD12	1:E:384:HIS:ND1	1.90	0.87
1:A:383:ILE:HD12	1:A:384:HIS:ND1	1.90	0.86
1:B:383:ILE:HD12	1:B:384:HIS:ND1	1.90	0.86
1:I:383:ILE:HD11	1:I:384:HIS:ND1	1.90	0.86
1:J:383:ILE:HD12	1:J:384:HIS:ND1	1.90	0.86
1:D:383:ILE:HD12	1:D:384:HIS:ND1	1.90	0.86
1:L:251:LYS:N	3:L:902:ADP:O2B	2.07	0.86
1:B:592:ASP:OD1	1:B:594:GLY:N	2.09	0.86
1:I:508:MET:CE	1:J:699:ILE:HD12	2.05	0.86
1:B:383:ILE:HD11	1:B:384:HIS:ND1	1.90	0.85
1:G:508:MET:HE2	1:H:699:ILE:CD1	2.05	0.85
1:H:592:ASP:OD1	1:H:594:GLY:N	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:383:ILE:HD12	1:I:384:HIS:ND1	1.90	0.85
1:I:592:ASP:OD1	1:I:594:GLY:N	2.09	0.85
1:C:592:ASP:OD1	1:C:594:GLY:N	2.09	0.85
1:I:508:MET:HE2	1:J:699:ILE:HD12	1.57	0.85
1:D:592:ASP:OD1	1:D:594:GLY:N	2.09	0.85
1:H:383:ILE:HD11	1:H:384:HIS:ND1	1.90	0.85
1:H:130:LEU:HG	1:H:134:TYR:CD2	2.11	0.85
1:J:592:ASP:OD1	1:J:594:GLY:N	2.09	0.85
1:L:148:LYS:HE3	1:L:171:SER:CB	2.07	0.85
1:A:383:ILE:HD11	1:A:384:HIS:ND1	1.90	0.85
1:H:508:MET:HE2	1:I:699:ILE:HD12	1.56	0.85
1:K:592:ASP:OD1	1:K:594:GLY:N	2.09	0.85
1:B:148:LYS:HE3	1:B:171:SER:CB	2.07	0.85
1:E:592:ASP:OD1	1:E:594:GLY:N	2.09	0.85
1:G:592:ASP:OD1	1:G:594:GLY:N	2.09	0.84
1:A:592:ASP:OD1	1:A:594:GLY:N	2.09	0.84
1:F:383:ILE:HD11	1:F:384:HIS:ND1	1.90	0.84
1:F:592:ASP:OD1	1:F:594:GLY:N	2.09	0.84
1:L:592:ASP:OD1	1:L:594:GLY:N	2.09	0.84
1:J:508:MET:HE2	1:K:699:ILE:HD12	1.59	0.84
1:C:403:THR:OG1	1:C:406:HIS:ND1	2.11	0.84
1:E:383:ILE:HD11	1:E:384:HIS:ND1	1.90	0.84
1:F:383:ILE:HD12	1:F:384:HIS:ND1	1.90	0.84
1:E:403:THR:OG1	1:E:406:HIS:ND1	2.11	0.84
1:I:403:THR:OG1	1:I:406:HIS:ND1	2.11	0.84
1:K:383:ILE:HD11	1:K:384:HIS:ND1	1.90	0.84
1:A:148:LYS:HE3	1:A:171:SER:CB	2.07	0.84
1:K:403:THR:OG1	1:K:406:HIS:ND1	2.11	0.84
1:K:508:MET:HE2	1:L:699:ILE:CD1	2.07	0.84
1:L:403:THR:OG1	1:L:406:HIS:ND1	2.11	0.84
1:A:403:THR:OG1	1:A:406:HIS:ND1	2.11	0.83
1:F:403:THR:OG1	1:F:406:HIS:ND1	2.11	0.83
1:H:403:THR:OG1	1:H:406:HIS:ND1	2.11	0.83
1:B:403:THR:OG1	1:B:406:HIS:ND1	2.11	0.83
1:G:403:THR:OG1	1:G:406:HIS:ND1	2.11	0.83
1:D:383:ILE:HD11	1:D:384:HIS:ND1	1.90	0.83
1:D:403:THR:OG1	1:D:406:HIS:ND1	2.11	0.83
1:J:403:THR:OG1	1:J:406:HIS:ND1	2.11	0.83
1:J:383:ILE:HD11	1:J:384:HIS:ND1	1.91	0.82
1:D:508:MET:HE2	1:E:699:ILE:CD1	2.09	0.82
1:H:130:LEU:CD1	1:H:134:TYR:HE2	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:MET:CE	1:D:699:ILE:HD12	2.10	0.82
1:E:760:GLN:NE2	1:G:760:GLN:NE2	1.72	0.82
1:G:699:ILE:HD12	1:L:508:MET:HE2	1.59	0.82
1:E:508:MET:HE2	1:F:699:ILE:CD1	2.10	0.81
1:B:148:LYS:HZ1	1:B:170:PRO:C	1.89	0.81
1:B:148:LYS:NZ	1:B:171:SER:N	1.80	0.81
1:L:148:LYS:HZ1	1:L:170:PRO:C	1.89	0.81
1:K:508:MET:HE2	1:L:699:ILE:HD12	1.63	0.80
1:A:148:LYS:HZ1	1:A:170:PRO:C	1.89	0.80
1:F:675:LEU:HD11	1:F:740:MET:HE1	0.81	0.80
1:G:675:LEU:HD11	1:G:740:MET:HE1	0.80	0.80
1:E:135:LEU:HA	1:E:138:TYR:CZ	2.17	0.80
1:E:675:LEU:HD11	1:E:740:MET:HE1	0.81	0.80
1:L:675:LEU:HD11	1:L:740:MET:HE1	0.80	0.80
1:A:675:LEU:HD11	1:A:740:MET:HE1	0.80	0.80
1:D:135:LEU:HA	1:D:138:TYR:CZ	2.17	0.80
1:E:383:ILE:HD11	1:E:384:HIS:CE1	2.17	0.80
1:H:675:LEU:HD11	1:H:740:MET:HE1	0.81	0.80
1:K:675:LEU:HD11	1:K:740:MET:HE1	0.80	0.80
1:J:135:LEU:HA	1:J:138:TYR:CZ	2.17	0.79
1:D:383:ILE:HD11	1:D:384:HIS:CE1	2.17	0.79
1:K:135:LEU:HA	1:K:138:TYR:CZ	2.18	0.79
1:K:383:ILE:HD11	1:K:384:HIS:CE1	2.18	0.79
1:B:675:LEU:HD11	1:B:740:MET:HE1	0.80	0.79
1:F:135:LEU:HA	1:F:138:TYR:CZ	2.17	0.79
1:J:383:ILE:HD11	1:J:384:HIS:CE1	2.18	0.79
1:L:135:LEU:HA	1:L:138:TYR:CZ	2.17	0.79
1:A:148:LYS:CE	1:A:171:SER:HB2	2.13	0.79
1:B:135:LEU:HA	1:B:138:TYR:CZ	2.17	0.79
1:H:130:LEU:HG	1:H:134:TYR:HE2	1.42	0.79
1:I:135:LEU:HA	1:I:138:TYR:CZ	2.17	0.79
1:A:699:ILE:CD1	1:F:508:MET:HE2	2.13	0.79
1:D:675:LEU:HD11	1:D:740:MET:HE1	0.80	0.79
1:J:675:LEU:HD11	1:J:740:MET:HE1	0.81	0.79
1:H:135:LEU:HA	1:H:138:TYR:CZ	2.17	0.79
1:C:135:LEU:HA	1:C:138:TYR:CZ	2.17	0.79
1:C:675:LEU:HD11	1:C:740:MET:HE1	0.81	0.79
1:F:383:ILE:HD11	1:F:384:HIS:CE1	2.17	0.79
1:G:135:LEU:HA	1:G:138:TYR:CZ	2.17	0.78
1:I:675:LEU:HD11	1:I:740:MET:HE1	0.81	0.78
1:L:148:LYS:CE	1:L:171:SER:HB2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HA	1:A:138:TYR:CZ	2.17	0.78
1:K:508:MET:CE	1:L:699:ILE:HD12	2.13	0.78
1:I:383:ILE:HD11	1:I:384:HIS:CE1	2.18	0.78
1:B:148:LYS:CE	1:B:171:SER:HB2	2.13	0.78
1:A:383:ILE:HD11	1:A:384:HIS:CE1	2.18	0.78
1:B:383:ILE:HD11	1:B:384:HIS:CE1	2.18	0.78
1:G:508:MET:CE	1:H:699:ILE:HD12	2.14	0.77
1:A:508:MET:HE1	1:B:699:ILE:HD12	1.65	0.77
1:H:383:ILE:HD11	1:H:384:HIS:CE1	2.18	0.77
1:A:148:LYS:CE	1:A:171:SER:CB	2.62	0.77
1:E:508:MET:CE	1:F:699:ILE:HD12	2.14	0.77
1:K:235:VAL:HG13	1:L:416:SER:HB2	1.67	0.77
1:G:508:MET:HE2	1:H:699:ILE:HD12	1.65	0.77
1:H:508:MET:CE	1:I:699:ILE:CD1	2.61	0.77
1:H:130:LEU:CG	1:H:134:TYR:HE2	1.97	0.77
1:L:148:LYS:CE	1:L:171:SER:CB	2.63	0.76
1:B:148:LYS:CE	1:B:171:SER:CB	2.63	0.76
1:L:148:LYS:HD2	1:L:171:SER:CB	2.16	0.76
1:L:675:LEU:CD1	1:L:740:MET:HE3	2.16	0.76
1:E:675:LEU:CD1	1:E:740:MET:HE3	2.16	0.76
1:D:760:GLN:NE2	1:H:760:GLN:NE2	1.75	0.76
1:F:675:LEU:CD1	1:F:740:MET:HE3	2.16	0.76
1:K:675:LEU:CD1	1:K:740:MET:HE3	2.16	0.76
1:G:675:LEU:CD1	1:G:740:MET:HE3	2.16	0.76
1:A:675:LEU:CD1	1:A:740:MET:HE3	2.16	0.75
1:C:508:MET:HE2	1:D:699:ILE:HD12	1.65	0.75
1:B:148:LYS:CD	1:B:171:SER:CB	2.65	0.75
1:B:148:LYS:HD2	1:B:171:SER:CB	2.16	0.75
1:C:675:LEU:CD1	1:C:740:MET:HE3	2.16	0.75
1:I:675:LEU:CD1	1:I:740:MET:HE3	2.16	0.75
1:A:148:LYS:HD2	1:A:171:SER:CB	2.16	0.75
1:I:251:LYS:N	3:I:902:ADP:O2B	2.20	0.75
1:L:148:LYS:CD	1:L:171:SER:CB	2.65	0.74
1:D:383:ILE:CD1	1:D:384:HIS:CE1	2.70	0.74
1:H:675:LEU:CD1	1:H:740:MET:HE3	2.16	0.74
1:J:383:ILE:CD1	1:J:384:HIS:CE1	2.70	0.74
1:J:508:MET:HE1	1:K:699:ILE:HD12	1.69	0.74
1:D:155:ARG:HH21	1:D:386:LYS:HZ3	1.34	0.74
1:E:383:ILE:CD1	1:E:384:HIS:CE1	2.70	0.74
1:I:383:ILE:CD1	1:I:384:HIS:CE1	2.70	0.74
1:A:383:ILE:CD1	1:A:384:HIS:CE1	2.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:LEU:CD1	1:B:740:MET:HE3	2.16	0.74
1:H:383:ILE:CD1	1:H:384:HIS:CE1	2.70	0.74
1:K:383:ILE:CD1	1:K:384:HIS:CE1	2.70	0.74
1:B:148:LYS:CG	1:B:171:SER:HB2	2.17	0.74
1:B:383:ILE:CD1	1:B:384:HIS:CE1	2.70	0.74
1:F:383:ILE:CD1	1:F:384:HIS:CE1	2.70	0.74
1:J:155:ARG:HH21	1:J:386:LYS:HZ3	1.35	0.73
1:L:148:LYS:CG	1:L:171:SER:HB2	2.17	0.73
1:D:675:LEU:CD1	1:D:740:MET:HE3	2.16	0.73
1:J:675:LEU:CD1	1:J:740:MET:HE3	2.16	0.73
1:E:350:PRO:O	1:E:358:ARG:NH2	2.22	0.73
1:K:350:PRO:O	1:K:358:ARG:NH2	2.22	0.73
1:H:350:PRO:O	1:H:358:ARG:NH2	2.22	0.73
1:A:148:LYS:CG	1:A:171:SER:HB2	2.17	0.73
1:B:350:PRO:O	1:B:358:ARG:NH2	2.22	0.73
1:I:350:PRO:O	1:I:358:ARG:NH2	2.22	0.73
1:D:508:MET:CE	1:E:699:ILE:HD12	2.18	0.72
1:C:350:PRO:O	1:C:358:ARG:NH2	2.22	0.72
1:L:148:LYS:NZ	1:L:170:PRO:CA	2.52	0.72
1:E:675:LEU:HD13	1:E:740:MET:HE3	1.72	0.72
1:A:350:PRO:O	1:A:358:ARG:NH2	2.22	0.72
1:I:675:LEU:HD13	1:I:740:MET:HE3	1.72	0.72
1:K:675:LEU:HD13	1:K:740:MET:HE3	1.72	0.72
1:F:350:PRO:O	1:F:358:ARG:NH2	2.22	0.72
1:L:350:PRO:O	1:L:358:ARG:NH2	2.22	0.72
1:C:675:LEU:HD13	1:C:740:MET:HE3	1.72	0.72
1:G:350:PRO:O	1:G:358:ARG:NH2	2.22	0.71
1:D:508:MET:HE2	1:E:699:ILE:HD12	1.71	0.71
1:A:699:ILE:HD12	1:F:508:MET:CE	2.19	0.71
1:A:148:LYS:NZ	1:A:170:PRO:CA	2.52	0.71
1:L:675:LEU:HD13	1:L:740:MET:HE3	1.72	0.71
1:J:675:LEU:HD13	1:J:740:MET:HE3	1.72	0.71
1:J:350:PRO:O	1:J:358:ARG:NH2	2.22	0.71
1:D:675:LEU:HD13	1:D:740:MET:HE3	1.72	0.70
1:D:350:PRO:O	1:D:358:ARG:NH2	2.22	0.70
1:F:675:LEU:HD13	1:F:740:MET:HE3	1.72	0.70
1:E:487:ARG:HE	1:F:700:ARG:CZ	2.04	0.70
1:A:148:LYS:CD	1:A:171:SER:CB	2.65	0.70
1:B:148:LYS:NZ	1:B:170:PRO:CA	2.52	0.69
1:C:760:GLN:NE2	1:I:760:GLN:NE2	1.76	0.69
1:F:760:GLN:NE2	1:L:760:GLN:NE2	1.77	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:148:LYS:HE3	1:L:171:SER:HB2	1.74	0.69
1:H:636:PRO:HA	1:H:640:ASP:HB3	1.75	0.69
1:C:636:PRO:HA	1:C:640:ASP:HB3	1.75	0.69
1:H:508:MET:HE1	1:I:699:ILE:HD12	1.74	0.69
1:A:636:PRO:HA	1:A:640:ASP:HB3	1.75	0.69
1:D:636:PRO:HA	1:D:640:ASP:HB3	1.75	0.69
1:J:636:PRO:HA	1:J:640:ASP:HB3	1.75	0.69
1:B:90:ASN:ND2	1:B:196:GLU:O	2.26	0.69
1:H:90:ASN:ND2	1:H:196:GLU:O	2.26	0.69
1:G:675:LEU:HD13	1:G:740:MET:HE3	1.72	0.68
1:B:636:PRO:HA	1:B:640:ASP:HB3	1.75	0.68
1:G:90:ASN:ND2	1:G:196:GLU:O	2.26	0.68
1:J:508:MET:CE	1:K:699:ILE:CD1	2.64	0.68
1:A:90:ASN:ND2	1:A:196:GLU:O	2.26	0.68
1:C:90:ASN:ND2	1:C:196:GLU:O	2.26	0.68
1:I:90:ASN:ND2	1:I:196:GLU:O	2.26	0.68
1:L:90:ASN:ND2	1:L:196:GLU:O	2.26	0.68
1:A:699:ILE:HD12	1:F:508:MET:HE2	1.76	0.68
1:F:90:ASN:ND2	1:F:196:GLU:O	2.26	0.68
1:A:675:LEU:HD13	1:A:740:MET:HE3	1.72	0.68
1:E:636:PRO:HA	1:E:640:ASP:HB3	1.75	0.68
1:G:699:ILE:CD1	1:L:508:MET:CE	2.65	0.68
1:K:636:PRO:HA	1:K:640:ASP:HB3	1.74	0.68
1:B:508:MET:HE1	1:C:699:ILE:HD12	1.76	0.68
1:F:636:PRO:HA	1:F:640:ASP:HB3	1.75	0.68
1:L:636:PRO:HA	1:L:640:ASP:HB3	1.75	0.68
1:A:155:ARG:HH21	1:A:386:LYS:HZ3	1.42	0.68
1:G:155:ARG:HH21	1:G:386:LYS:HZ3	1.42	0.68
1:E:90:ASN:ND2	1:E:196:GLU:O	2.26	0.67
1:D:90:ASN:ND2	1:D:196:GLU:O	2.26	0.67
1:K:90:ASN:ND2	1:K:196:GLU:O	2.26	0.67
1:G:636:PRO:HA	1:G:640:ASP:HB3	1.75	0.67
1:I:636:PRO:HA	1:I:640:ASP:HB3	1.75	0.67
1:H:675:LEU:HD13	1:H:740:MET:HE3	1.72	0.67
1:J:90:ASN:ND2	1:J:196:GLU:O	2.26	0.67
1:A:148:LYS:NZ	1:A:170:PRO:C	2.52	0.67
1:C:640:ASP:OD1	1:C:641:GLN:HG2	1.94	0.67
1:B:235:VAL:HG13	1:C:416:SER:HB2	1.77	0.67
1:B:675:LEU:HD13	1:B:740:MET:HE3	1.72	0.67
1:H:640:ASP:OD1	1:H:641:GLN:HG2	1.94	0.67
1:E:640:ASP:OD1	1:E:641:GLN:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:233:ILE:HB	1:K:158:MET:HE3	1.76	0.66
1:F:640:ASP:OD1	1:F:641:GLN:HG2	1.94	0.66
1:L:640:ASP:OD1	1:L:641:GLN:HG2	1.94	0.66
1:B:148:LYS:NZ	1:B:170:PRO:C	2.52	0.66
1:D:640:ASP:OD1	1:D:641:GLN:HG2	1.94	0.66
1:J:640:ASP:OD1	1:J:641:GLN:HG2	1.94	0.66
1:B:148:LYS:HE3	1:B:171:SER:HB2	1.74	0.66
1:E:155:ARG:HH21	1:E:386:LYS:HZ3	1.43	0.66
1:E:508:MET:HE1	1:F:699:ILE:HD12	1.77	0.66
1:K:155:ARG:HH21	1:K:386:LYS:HZ3	1.43	0.66
1:L:148:LYS:HZ1	1:L:171:SER:H	0.67	0.66
1:A:640:ASP:OD1	1:A:641:GLN:HG2	1.94	0.66
1:A:148:LYS:HZ1	1:A:171:SER:H	0.67	0.65
1:I:491:GLU:HB3	1:J:700:ARG:HH21	1.62	0.65
1:A:148:LYS:HE3	1:A:171:SER:HB2	1.74	0.65
1:A:416:SER:HB2	1:F:235:VAL:HG13	1.78	0.65
1:J:235:VAL:HG13	1:K:416:SER:HB2	1.79	0.65
1:E:95:ARG:HH11	1:E:95:ARG:HG3	1.62	0.65
1:J:95:ARG:HH11	1:J:95:ARG:HG3	1.62	0.65
1:K:95:ARG:HH11	1:K:95:ARG:HG3	1.62	0.65
1:D:95:ARG:HG3	1:D:95:ARG:HH11	1.62	0.65
1:B:624:ASN:O	1:B:755:TYR:OH	2.12	0.64
1:B:508:MET:CE	1:C:699:ILE:CD1	2.68	0.64
1:H:95:ARG:HH11	1:H:95:ARG:HG3	1.62	0.64
1:I:95:ARG:HH11	1:I:95:ARG:HG3	1.62	0.64
1:B:95:ARG:HH11	1:B:95:ARG:HG3	1.62	0.64
1:A:95:ARG:HG3	1:A:95:ARG:HH11	1.62	0.64
1:C:95:ARG:HH11	1:C:95:ARG:HG3	1.62	0.64
1:G:95:ARG:HG3	1:G:95:ARG:HH11	1.62	0.64
1:L:95:ARG:HG3	1:L:95:ARG:HH11	1.62	0.64
1:F:95:ARG:HH11	1:F:95:ARG:HG3	1.63	0.64
1:A:148:LYS:HG3	1:A:171:SER:HB2	1.79	0.64
1:C:155:ARG:HH21	1:C:386:LYS:HZ3	1.46	0.63
1:D:235:VAL:HG13	1:E:416:SER:HB2	1.79	0.63
1:C:559:VAL:HG21	1:C:603:GLN:HB3	1.81	0.63
1:B:148:LYS:HG3	1:B:171:SER:HB2	1.79	0.63
1:G:699:ILE:HD12	1:L:508:MET:HE1	1.77	0.63
1:D:450:ASP:HA	1:D:453:ARG:HG2	1.81	0.63
1:E:592:ASP:OD1	1:E:592:ASP:C	2.42	0.63
1:J:450:ASP:HA	1:J:453:ARG:HG2	1.81	0.63
1:I:559:VAL:HG21	1:I:603:GLN:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:592:ASP:OD1	1:K:592:ASP:C	2.42	0.63
1:L:148:LYS:HG3	1:L:171:SER:HB2	1.79	0.63
1:D:592:ASP:OD1	1:D:592:ASP:C	2.42	0.63
1:A:674:PHE:CE1	1:A:678:MET:SD	2.92	0.63
1:B:559:VAL:HG21	1:B:603:GLN:HB3	1.81	0.63
1:C:450:ASP:HA	1:C:453:ARG:HG2	1.81	0.63
1:F:592:ASP:OD1	1:F:592:ASP:C	2.42	0.62
1:I:674:PHE:CE1	1:I:678:MET:SD	2.92	0.62
1:J:592:ASP:OD1	1:J:592:ASP:C	2.42	0.62
1:L:592:ASP:OD1	1:L:592:ASP:C	2.42	0.62
1:B:674:PHE:CE1	1:B:678:MET:SD	2.92	0.62
1:G:624:ASN:O	1:G:755:TYR:OH	2.12	0.62
1:H:559:VAL:HG21	1:H:603:GLN:HB3	1.81	0.62
1:H:674:PHE:CE1	1:H:678:MET:SD	2.92	0.62
1:I:450:ASP:HA	1:I:453:ARG:HG2	1.80	0.62
1:J:559:VAL:HG21	1:J:603:GLN:HB3	1.81	0.62
1:K:674:PHE:CE1	1:K:678:MET:SD	2.92	0.62
1:L:674:PHE:CE1	1:L:678:MET:SD	2.92	0.62
1:A:450:ASP:HA	1:A:453:ARG:HG2	1.80	0.62
1:C:674:PHE:CE1	1:C:678:MET:SD	2.93	0.62
1:D:559:VAL:HG21	1:D:603:GLN:HB3	1.81	0.62
1:E:674:PHE:CE1	1:E:678:MET:SD	2.92	0.62
1:G:450:ASP:HA	1:G:453:ARG:HG2	1.80	0.62
1:G:674:PHE:CE1	1:G:678:MET:SD	2.93	0.62
1:C:592:ASP:OD1	1:C:592:ASP:C	2.42	0.62
1:F:674:PHE:CE1	1:F:678:MET:SD	2.93	0.62
1:E:450:ASP:HA	1:E:453:ARG:HG2	1.80	0.62
1:G:251:LYS:N	3:G:902:ADP:O2B	2.32	0.62
1:H:450:ASP:HA	1:H:453:ARG:HG2	1.80	0.62
1:K:450:ASP:HA	1:K:453:ARG:HG2	1.80	0.62
1:I:592:ASP:OD1	1:I:592:ASP:C	2.42	0.62
1:D:674:PHE:CE1	1:D:678:MET:SD	2.92	0.62
1:A:592:ASP:OD1	1:A:592:ASP:C	2.42	0.62
1:B:450:ASP:HA	1:B:453:ARG:HG2	1.81	0.62
1:J:674:PHE:CE1	1:J:678:MET:SD	2.93	0.61
1:B:592:ASP:OD1	1:B:592:ASP:C	2.42	0.61
1:G:592:ASP:OD1	1:G:592:ASP:C	2.42	0.61
1:L:559:VAL:HG21	1:L:603:GLN:HB3	1.81	0.61
1:F:450:ASP:HA	1:F:453:ARG:HG2	1.80	0.61
1:F:559:VAL:HG21	1:F:603:GLN:HB3	1.81	0.61
1:G:559:VAL:HG21	1:G:603:GLN:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:450:ASP:HA	1:L:453:ARG:HG2	1.80	0.61
1:E:559:VAL:HG21	1:E:603:GLN:HB3	1.81	0.61
1:H:592:ASP:OD1	1:H:592:ASP:C	2.42	0.61
1:K:559:VAL:HG21	1:K:603:GLN:HB3	1.81	0.61
1:L:252:THR:OG1	3:L:902:ADP:O1B	2.16	0.61
1:A:559:VAL:HG21	1:A:603:GLN:HB3	1.81	0.61
1:H:757:MET:O	1:H:761:THR:OG1	2.16	0.61
1:B:148:LYS:HZ1	1:B:170:PRO:CA	2.14	0.61
1:B:757:MET:O	1:B:761:THR:OG1	2.16	0.61
1:C:564:ASP:OD1	1:C:567:ARG:NH1	2.34	0.60
1:I:564:ASP:OD1	1:I:567:ARG:NH1	2.34	0.60
1:E:158:MET:HG3	1:E:158:MET:O	2.02	0.60
1:F:158:MET:HG3	1:F:158:MET:O	2.02	0.60
1:G:131:PHE:HE2	1:G:184:CYS:HB3	1.67	0.60
1:G:235:VAL:HG13	1:H:416:SER:HB2	1.84	0.60
1:G:491:GLU:HB3	1:H:700:ARG:HH21	1.66	0.60
1:I:158:MET:HG3	1:I:158:MET:O	2.02	0.60
1:A:131:PHE:HE2	1:A:184:CYS:HB3	1.67	0.60
1:K:233:ILE:HB	1:L:158:MET:HE3	1.83	0.60
1:C:158:MET:HG3	1:C:158:MET:O	2.02	0.60
1:D:158:MET:HG3	1:D:158:MET:O	2.02	0.60
1:I:757:MET:O	1:I:761:THR:OG1	2.16	0.60
1:J:158:MET:HG3	1:J:158:MET:O	2.02	0.60
1:K:158:MET:HG3	1:K:158:MET:O	2.02	0.60
1:L:131:PHE:HE2	1:L:184:CYS:HB3	1.67	0.60
1:L:158:MET:HG3	1:L:158:MET:O	2.02	0.60
1:B:131:PHE:HE2	1:B:184:CYS:HB3	1.67	0.60
1:C:757:MET:O	1:C:761:THR:OG1	2.16	0.60
1:K:201:VAL:HG21	1:K:253:LEU:HB2	1.84	0.60
1:A:148:LYS:HZ1	1:A:170:PRO:CA	2.14	0.60
1:D:757:MET:O	1:D:761:THR:OG1	2.16	0.60
1:F:131:PHE:HE2	1:F:184:CYS:HB3	1.67	0.60
1:H:131:PHE:HE2	1:H:184:CYS:HB3	1.67	0.60
1:H:158:MET:O	1:H:158:MET:HG3	2.02	0.60
1:K:491:GLU:HB3	1:L:700:ARG:HH21	1.67	0.60
1:B:158:MET:HG3	1:B:158:MET:O	2.02	0.60
1:E:201:VAL:HG21	1:E:253:LEU:HB2	1.84	0.60
1:D:201:VAL:HG21	1:D:253:LEU:HB2	1.84	0.60
1:J:757:MET:O	1:J:761:THR:OG1	2.16	0.60
1:A:668:LYS:HA	1:A:668:LYS:HE3	1.84	0.60
1:D:564:ASP:OD1	1:D:567:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:668:LYS:HA	1:F:668:LYS:HE3	1.84	0.60
1:H:148:LYS:NZ	1:H:174:CYS:SG	2.75	0.60
1:C:131:PHE:HE2	1:C:184:CYS:HB3	1.67	0.59
1:E:131:PHE:HE2	1:E:184:CYS:HB3	1.67	0.59
1:F:93:ARG:NH2	1:F:194:GLU:OE1	2.35	0.59
1:I:425:LYS:NZ	1:I:451:ASP:OD1	2.30	0.59
1:J:564:ASP:OD1	1:J:567:ARG:NH1	2.34	0.59
1:K:131:PHE:HE2	1:K:184:CYS:HB3	1.67	0.59
1:L:93:ARG:NH2	1:L:194:GLU:OE1	2.35	0.59
1:B:668:LYS:HE3	1:B:668:LYS:HA	1.84	0.59
1:C:425:LYS:NZ	1:C:451:ASP:OD1	2.30	0.59
1:G:148:LYS:NZ	1:G:174:CYS:SG	2.75	0.59
1:H:668:LYS:HA	1:H:668:LYS:HE3	1.84	0.59
1:J:201:VAL:HG21	1:J:253:LEU:HB2	1.84	0.59
1:L:668:LYS:HA	1:L:668:LYS:HE3	1.84	0.59
1:A:768:PHE:O	1:B:741:ARG:HA	2.02	0.59
1:D:148:LYS:NZ	1:D:174:CYS:SG	2.75	0.59
1:F:564:ASP:OD1	1:F:567:ARG:NH1	2.34	0.59
1:G:668:LYS:HA	1:G:668:LYS:HE3	1.84	0.59
1:H:564:ASP:OD1	1:H:567:ARG:NH1	2.34	0.59
1:I:131:PHE:HE2	1:I:184:CYS:HB3	1.67	0.59
1:J:148:LYS:NZ	1:J:174:CYS:SG	2.75	0.59
1:J:668:LYS:HE3	1:J:668:LYS:HA	1.84	0.59
1:B:564:ASP:OD1	1:B:567:ARG:NH1	2.34	0.59
1:D:131:PHE:HE2	1:D:184:CYS:HB3	1.67	0.59
1:D:668:LYS:HA	1:D:668:LYS:HE3	1.84	0.59
1:E:93:ARG:NH2	1:E:194:GLU:OE1	2.35	0.59
1:H:93:ARG:NH2	1:H:194:GLU:OE1	2.35	0.59
1:L:148:LYS:NZ	1:L:170:PRO:C	2.52	0.59
1:L:148:LYS:HZ1	1:L:170:PRO:CA	2.14	0.59
1:L:564:ASP:OD1	1:L:567:ARG:NH1	2.34	0.59
1:K:93:ARG:NH2	1:K:194:GLU:OE1	2.35	0.59
1:A:564:ASP:OD1	1:A:567:ARG:NH1	2.34	0.59
1:B:93:ARG:NH2	1:B:194:GLU:OE1	2.35	0.59
1:E:508:MET:CE	1:F:699:ILE:CD1	2.75	0.59
1:I:93:ARG:NH2	1:I:194:GLU:OE1	2.35	0.59
1:J:131:PHE:HE2	1:J:184:CYS:HB3	1.67	0.59
1:C:93:ARG:NH2	1:C:194:GLU:OE1	2.35	0.59
1:E:148:LYS:NZ	1:E:174:CYS:SG	2.75	0.59
1:G:564:ASP:OD1	1:G:567:ARG:NH1	2.34	0.59
1:K:148:LYS:NZ	1:K:174:CYS:SG	2.75	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:MET:HE1	1:K:677:LYS:HG2	1.84	0.59
1:E:669:ASP:O	1:E:733:ARG:NH2	2.36	0.59
1:J:624:ASN:O	1:J:755:TYR:OH	2.12	0.59
1:K:669:ASP:O	1:K:733:ARG:NH2	2.36	0.59
1:A:93:ARG:NH2	1:A:194:GLU:OE1	2.35	0.59
1:C:148:LYS:NZ	1:C:174:CYS:SG	2.75	0.59
1:D:624:ASN:O	1:D:755:TYR:OH	2.12	0.59
1:H:491:GLU:HB3	1:I:700:ARG:HH21	1.68	0.59
1:I:148:LYS:NZ	1:I:174:CYS:SG	2.75	0.59
1:K:425:LYS:NZ	1:K:451:ASP:OD1	2.30	0.59
1:B:677:LYS:HG2	1:K:678:MET:HE1	1.84	0.58
1:C:732:ARG:HH12	1:C:734:ASP:HB3	1.68	0.58
1:E:732:ARG:HH12	1:E:734:ASP:HB3	1.69	0.58
1:F:669:ASP:O	1:F:733:ARG:NH2	2.36	0.58
1:I:732:ARG:HH12	1:I:734:ASP:HB3	1.68	0.58
1:K:732:ARG:HH12	1:K:734:ASP:HB3	1.68	0.58
1:A:201:VAL:HG21	1:A:253:LEU:HB2	1.84	0.58
1:B:201:VAL:HG21	1:B:253:LEU:HB2	1.84	0.58
1:C:201:VAL:HG21	1:C:253:LEU:HB2	1.84	0.58
1:C:668:LYS:HA	1:C:668:LYS:HE3	1.84	0.58
1:E:605:LEU:HD21	1:E:633:ILE:HA	1.85	0.58
1:G:158:MET:HG3	1:G:158:MET:O	2.02	0.58
1:H:201:VAL:HG21	1:H:253:LEU:HB2	1.84	0.58
1:I:201:VAL:HG21	1:I:253:LEU:HB2	1.84	0.58
1:L:669:ASP:O	1:L:733:ARG:NH2	2.36	0.58
1:A:299:ALA:HB3	1:A:341:VAL:HG12	1.86	0.58
1:C:416:SER:O	1:C:420:LEU:HD22	2.04	0.58
1:C:669:ASP:O	1:C:733:ARG:NH2	2.36	0.58
1:D:299:ALA:HB3	1:D:341:VAL:HG12	1.85	0.58
1:F:148:LYS:NZ	1:F:174:CYS:SG	2.75	0.58
1:G:201:VAL:HG21	1:G:253:LEU:HB2	1.84	0.58
1:G:299:ALA:HB3	1:G:341:VAL:HG12	1.85	0.58
1:G:732:ARG:HH12	1:G:734:ASP:HB3	1.68	0.58
1:I:416:SER:O	1:I:420:LEU:HD22	2.04	0.58
1:I:669:ASP:O	1:I:733:ARG:NH2	2.36	0.58
1:K:605:LEU:HD21	1:K:633:ILE:HA	1.85	0.58
1:L:69:CYS:SG	1:L:70:ILE:N	2.76	0.58
1:A:158:MET:HG3	1:A:158:MET:O	2.02	0.58
1:A:732:ARG:HH12	1:A:734:ASP:HB3	1.69	0.58
1:B:233:ILE:HB	1:C:158:MET:HE3	1.83	0.58
1:E:425:LYS:NZ	1:E:451:ASP:OD1	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:416:SER:O	1:H:420:LEU:HD22	2.04	0.58
1:J:605:LEU:HD21	1:J:633:ILE:HA	1.85	0.58
1:J:669:ASP:O	1:J:733:ARG:NH2	2.36	0.58
1:B:416:SER:O	1:B:420:LEU:HD22	2.03	0.58
1:B:669:ASP:O	1:B:733:ARG:NH2	2.36	0.58
1:D:605:LEU:HD21	1:D:633:ILE:HA	1.85	0.58
1:D:669:ASP:O	1:D:733:ARG:NH2	2.36	0.58
1:F:69:CYS:SG	1:F:70:ILE:N	2.76	0.58
1:J:299:ALA:HB3	1:J:341:VAL:HG12	1.86	0.58
1:B:148:LYS:HZ1	1:B:171:SER:H	0.67	0.58
1:D:416:SER:O	1:D:420:LEU:HD22	2.04	0.58
1:E:640:ASP:OD1	1:E:641:GLN:N	2.37	0.58
1:F:640:ASP:OD1	1:F:641:GLN:N	2.37	0.58
1:H:299:ALA:HB3	1:H:341:VAL:HG12	1.85	0.58
1:H:669:ASP:O	1:H:733:ARG:NH2	2.36	0.58
1:I:668:LYS:HA	1:I:668:LYS:HE3	1.84	0.58
1:J:416:SER:O	1:J:420:LEU:HD22	2.04	0.58
1:K:668:LYS:HA	1:K:668:LYS:HE3	1.84	0.58
1:A:757:MET:O	1:A:761:THR:OG1	2.16	0.58
1:F:201:VAL:HG21	1:F:253:LEU:HB2	1.84	0.58
1:G:93:ARG:NH2	1:G:194:GLU:OE1	2.35	0.58
1:G:757:MET:O	1:G:761:THR:OG1	2.16	0.58
1:K:273:GLU:OE1	1:K:273:GLU:N	2.31	0.58
1:K:624:ASN:O	1:K:755:TYR:OH	2.12	0.58
1:L:640:ASP:OD1	1:L:641:GLN:N	2.37	0.58
1:A:669:ASP:O	1:A:733:ARG:NH2	2.36	0.58
1:B:299:ALA:HB3	1:B:341:VAL:HG12	1.85	0.58
1:D:93:ARG:NH2	1:D:194:GLU:OE1	2.35	0.58
1:E:273:GLU:OE1	1:E:273:GLU:N	2.31	0.58
1:E:624:ASN:O	1:E:755:TYR:OH	2.12	0.58
1:E:668:LYS:HA	1:E:668:LYS:HE3	1.84	0.58
1:G:416:SER:O	1:G:420:LEU:HD22	2.03	0.58
1:J:93:ARG:NH2	1:J:194:GLU:OE1	2.35	0.58
1:L:201:VAL:HG21	1:L:253:LEU:HB2	1.84	0.58
1:B:491:GLU:HB3	1:C:700:ARG:HH21	1.68	0.58
1:D:732:ARG:HH12	1:D:734:ASP:HB3	1.69	0.58
1:J:732:ARG:HH12	1:J:734:ASP:HB3	1.69	0.58
1:L:416:SER:O	1:L:420:LEU:HD22	2.03	0.58
1:L:605:LEU:HD21	1:L:633:ILE:HA	1.85	0.58
1:A:416:SER:O	1:A:420:LEU:HD22	2.04	0.58
1:F:155:ARG:HH21	1:F:386:LYS:HZ3	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:MET:HA	1:F:445:LEU:HG	1.85	0.58
1:F:605:LEU:HD21	1:F:633:ILE:HA	1.85	0.58
1:G:669:ASP:O	1:G:733:ARG:NH2	2.36	0.58
1:K:564:ASP:OD1	1:K:567:ARG:NH1	2.34	0.58
1:E:564:ASP:OD1	1:E:567:ARG:NH1	2.34	0.57
1:F:416:SER:O	1:F:420:LEU:HD22	2.03	0.57
1:H:69:CYS:SG	1:H:70:ILE:N	2.76	0.57
1:B:69:CYS:SG	1:B:70:ILE:N	2.76	0.57
1:C:69:CYS:SG	1:C:70:ILE:N	2.76	0.57
1:C:299:ALA:HB3	1:C:341:VAL:HG12	1.85	0.57
1:C:640:ASP:OD1	1:C:641:GLN:N	2.37	0.57
1:H:640:ASP:OD1	1:H:641:GLN:N	2.37	0.57
1:L:442:MET:HA	1:L:445:LEU:HG	1.85	0.57
1:A:605:LEU:HD21	1:A:633:ILE:HA	1.85	0.57
1:B:732:ARG:HH12	1:B:734:ASP:HB3	1.69	0.57
1:H:732:ARG:HH12	1:H:734:ASP:HB3	1.68	0.57
1:L:227:PRO:HA	1:L:340:HIS:CE1	2.39	0.57
1:A:219:MET:SD	1:A:365:ARG:NH1	2.78	0.57
1:D:442:MET:HA	1:D:445:LEU:HG	1.85	0.57
1:E:299:ALA:HB3	1:E:341:VAL:HG12	1.85	0.57
1:E:487:ARG:HE	1:F:700:ARG:NH1	2.02	0.57
1:F:219:MET:SD	1:F:365:ARG:NH1	2.78	0.57
1:F:227:PRO:HA	1:F:340:HIS:CE1	2.39	0.57
1:G:605:LEU:HD21	1:G:633:ILE:HA	1.85	0.57
1:J:227:PRO:HA	1:J:340:HIS:CE1	2.39	0.57
1:J:442:MET:HA	1:J:445:LEU:HG	1.85	0.57
1:C:605:LEU:HD21	1:C:633:ILE:HA	1.85	0.57
1:D:227:PRO:HA	1:D:340:HIS:CE1	2.39	0.57
1:I:605:LEU:HD21	1:I:633:ILE:HA	1.85	0.57
1:K:299:ALA:HB3	1:K:341:VAL:HG12	1.86	0.57
1:A:640:ASP:OD1	1:A:641:GLN:N	2.37	0.57
1:B:227:PRO:HA	1:B:340:HIS:CE1	2.39	0.57
1:D:640:ASP:OD1	1:D:641:GLN:N	2.37	0.57
1:G:219:MET:SD	1:G:365:ARG:NH1	2.78	0.57
1:G:227:PRO:HA	1:G:340:HIS:CE1	2.39	0.57
1:J:640:ASP:OD1	1:J:641:GLN:N	2.37	0.57
1:K:271:GLY:H	1:K:273:GLU:CD	2.13	0.57
1:L:219:MET:SD	1:L:365:ARG:NH1	2.78	0.57
1:E:271:GLY:H	1:E:273:GLU:CD	2.13	0.57
1:H:227:PRO:HA	1:H:340:HIS:CE1	2.39	0.57
1:I:299:ALA:HB3	1:I:341:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:634:LEU:HD22	1:J:642:LEU:HD11	1.87	0.57
1:L:673:GLU:N	1:L:673:GLU:OE1	2.38	0.57
1:C:442:MET:HA	1:C:445:LEU:HG	1.85	0.57
1:C:673:GLU:OE1	1:C:673:GLU:N	2.38	0.57
1:D:634:LEU:HD22	1:D:642:LEU:HD11	1.87	0.57
1:F:203:TYR:HE2	1:F:261:GLU:HB2	1.70	0.57
1:F:673:GLU:OE1	1:F:673:GLU:N	2.38	0.57
1:H:130:LEU:O	1:H:130:LEU:CD2	2.43	0.57
1:H:442:MET:HA	1:H:445:LEU:HG	1.85	0.57
1:I:442:MET:HA	1:I:445:LEU:HG	1.85	0.57
1:I:673:GLU:OE1	1:I:673:GLU:N	2.38	0.57
1:L:271:GLY:H	1:L:273:GLU:CD	2.13	0.57
1:A:227:PRO:HA	1:A:340:HIS:CE1	2.39	0.57
1:A:258:VAL:O	1:A:262:THR:OG1	2.21	0.57
1:A:442:MET:HA	1:A:445:LEU:HG	1.85	0.57
1:C:219:MET:SD	1:C:365:ARG:NH1	2.78	0.57
1:E:227:PRO:HA	1:E:340:HIS:CE1	2.39	0.57
1:E:416:SER:O	1:E:420:LEU:HD22	2.03	0.57
1:F:271:GLY:H	1:F:273:GLU:CD	2.13	0.57
1:F:299:ALA:HB3	1:F:341:VAL:HG12	1.85	0.57
1:G:203:TYR:HE2	1:G:261:GLU:HB2	1.70	0.57
1:G:565:LYS:HA	1:G:568:GLN:HG3	1.86	0.57
1:H:605:LEU:HD21	1:H:633:ILE:HA	1.85	0.57
1:I:219:MET:SD	1:I:365:ARG:NH1	2.78	0.57
1:J:487:ARG:HE	1:K:700:ARG:CZ	2.17	0.57
1:K:219:MET:SD	1:K:365:ARG:NH1	2.78	0.57
1:K:227:PRO:HA	1:K:340:HIS:CE1	2.39	0.57
1:K:757:MET:O	1:K:761:THR:OG1	2.16	0.57
1:L:203:TYR:HE2	1:L:261:GLU:HB2	1.70	0.57
1:A:203:TYR:HE2	1:A:261:GLU:HB2	1.70	0.57
1:D:219:MET:SD	1:D:365:ARG:NH1	2.78	0.57
1:D:271:GLY:H	1:D:273:GLU:CD	2.13	0.57
1:G:442:MET:HA	1:G:445:LEU:HG	1.85	0.57
1:I:227:PRO:HA	1:I:340:HIS:CE1	2.39	0.57
1:I:273:GLU:OE1	1:I:273:GLU:N	2.31	0.57
1:J:271:GLY:H	1:J:273:GLU:CD	2.13	0.57
1:K:416:SER:O	1:K:420:LEU:HD22	2.04	0.57
1:K:565:LYS:HA	1:K:568:GLN:HG3	1.86	0.57
1:A:565:LYS:HA	1:A:568:GLN:HG3	1.86	0.56
1:B:273:GLU:OE1	1:B:273:GLU:N	2.31	0.56
1:B:565:LYS:HA	1:B:568:GLN:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:PRO:HA	1:C:340:HIS:CE1	2.39	0.56
1:C:273:GLU:OE1	1:C:273:GLU:N	2.31	0.56
1:E:203:TYR:HE2	1:E:261:GLU:HB2	1.70	0.56
1:E:442:MET:HA	1:E:445:LEU:HG	1.85	0.56
1:E:757:MET:O	1:E:761:THR:OG1	2.16	0.56
1:H:219:MET:SD	1:H:365:ARG:NH1	2.78	0.56
1:J:219:MET:SD	1:J:365:ARG:NH1	2.78	0.56
1:K:634:LEU:HD22	1:K:642:LEU:HD11	1.87	0.56
1:B:605:LEU:HD21	1:B:633:ILE:HA	1.85	0.56
1:C:508:MET:HE1	1:D:699:ILE:HD12	1.88	0.56
1:C:565:LYS:HA	1:C:568:GLN:HG3	1.86	0.56
1:E:219:MET:SD	1:E:365:ARG:NH1	2.78	0.56
1:E:565:LYS:HA	1:E:568:GLN:HG3	1.86	0.56
1:E:634:LEU:HD22	1:E:642:LEU:HD11	1.87	0.56
1:I:565:LYS:HA	1:I:568:GLN:HG3	1.87	0.56
1:K:442:MET:HA	1:K:445:LEU:HG	1.85	0.56
1:L:299:ALA:HB3	1:L:341:VAL:HG12	1.86	0.56
1:A:274:ILE:HA	1:A:277:LYS:HE2	1.88	0.56
1:A:773:PHE:HB3	1:B:733:ARG:HH11	1.70	0.56
1:B:219:MET:SD	1:B:365:ARG:NH1	2.78	0.56
1:B:442:MET:HA	1:B:445:LEU:HG	1.85	0.56
1:B:673:GLU:OE1	1:B:673:GLU:N	2.38	0.56
1:D:673:GLU:N	1:D:673:GLU:OE1	2.38	0.56
1:E:69:CYS:SG	1:E:70:ILE:N	2.76	0.56
1:G:271:GLY:H	1:G:273:GLU:CD	2.13	0.56
1:H:565:LYS:HA	1:H:568:GLN:HG3	1.86	0.56
1:I:271:GLY:H	1:I:273:GLU:CD	2.13	0.56
1:K:69:CYS:SG	1:K:70:ILE:N	2.76	0.56
1:K:203:TYR:HE2	1:K:261:GLU:HB2	1.70	0.56
1:L:155:ARG:HH21	1:L:386:LYS:HZ3	1.52	0.56
1:I:258:VAL:O	1:I:262:THR:OG1	2.21	0.56
1:A:271:GLY:H	1:A:273:GLU:CD	2.13	0.56
1:B:203:TYR:HE2	1:B:261:GLU:HB2	1.70	0.56
1:C:258:VAL:O	1:C:262:THR:OG1	2.21	0.56
1:E:235:VAL:HG13	1:F:416:SER:HB2	1.87	0.56
1:F:565:LYS:HA	1:F:568:GLN:HG3	1.86	0.56
1:G:274:ILE:HA	1:G:277:LYS:HE2	1.88	0.56
1:G:673:GLU:N	1:G:673:GLU:OE1	2.38	0.56
1:H:673:GLU:OE1	1:H:673:GLU:N	2.38	0.56
1:I:634:LEU:HD22	1:I:642:LEU:HD11	1.87	0.56
1:J:565:LYS:HA	1:J:568:GLN:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:673:GLU:OE1	1:J:673:GLU:N	2.38	0.56
1:K:673:GLU:OE1	1:K:673:GLU:N	2.38	0.56
1:L:565:LYS:HA	1:L:568:GLN:HG3	1.86	0.56
1:B:274:ILE:HA	1:B:277:LYS:HE2	1.88	0.56
1:C:271:GLY:H	1:C:273:GLU:CD	2.13	0.56
1:E:673:GLU:OE1	1:E:673:GLU:N	2.38	0.56
1:F:624:ASN:O	1:F:755:TYR:OH	2.12	0.56
1:G:516:PHE:HB3	1:G:643:ILE:HG13	1.88	0.56
1:H:203:TYR:HE2	1:H:261:GLU:HB2	1.70	0.56
1:H:273:GLU:OE1	1:H:273:GLU:N	2.31	0.56
1:H:274:ILE:HA	1:H:277:LYS:HE2	1.88	0.56
1:A:673:GLU:N	1:A:673:GLU:OE1	2.38	0.56
1:C:634:LEU:HD22	1:C:642:LEU:HD11	1.87	0.56
1:F:273:GLU:OE1	1:F:273:GLU:N	2.31	0.56
1:F:634:LEU:HD22	1:F:642:LEU:HD11	1.87	0.56
1:H:271:GLY:H	1:H:273:GLU:CD	2.13	0.56
1:L:273:GLU:OE1	1:L:273:GLU:N	2.31	0.56
1:L:624:ASN:O	1:L:755:TYR:OH	2.12	0.56
1:L:634:LEU:HD22	1:L:642:LEU:HD11	1.87	0.56
1:B:516:PHE:HB3	1:B:643:ILE:HG13	1.88	0.56
1:D:89:ARG:HA	1:D:94:VAL:HG12	1.88	0.56
1:D:203:TYR:HE2	1:D:261:GLU:HB2	1.70	0.56
1:D:565:LYS:HA	1:D:568:GLN:HG3	1.86	0.56
1:F:274:ILE:HA	1:F:277:LYS:HE2	1.88	0.56
1:A:516:PHE:HB3	1:A:643:ILE:HG13	1.88	0.56
1:B:271:GLY:H	1:B:273:GLU:CD	2.13	0.56
1:H:516:PHE:HB3	1:H:643:ILE:HG13	1.88	0.56
1:I:89:ARG:HA	1:I:94:VAL:HG12	1.88	0.56
1:J:89:ARG:HA	1:J:94:VAL:HG12	1.88	0.56
1:A:69:CYS:SG	1:A:70:ILE:N	2.76	0.56
1:C:203:TYR:HE2	1:C:261:GLU:HB2	1.70	0.56
1:C:768:PHE:O	1:D:741:ARG:HA	2.06	0.56
1:G:69:CYS:SG	1:G:70:ILE:N	2.76	0.56
1:I:203:TYR:HE2	1:I:261:GLU:HB2	1.70	0.56
1:J:203:TYR:HE2	1:J:261:GLU:HB2	1.70	0.56
1:L:274:ILE:HA	1:L:277:LYS:HE2	1.88	0.56
1:A:634:LEU:HD22	1:A:642:LEU:HD11	1.87	0.55
1:D:273:GLU:OE1	1:D:273:GLU:N	2.31	0.55
1:F:516:PHE:HB3	1:F:643:ILE:HG13	1.88	0.55
1:G:634:LEU:HD22	1:G:642:LEU:HD11	1.87	0.55
1:L:516:PHE:HB3	1:L:643:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ALA:O	1:A:362:ARG:NH1	2.36	0.55
1:C:89:ARG:HA	1:C:94:VAL:HG12	1.88	0.55
1:F:258:VAL:O	1:F:262:THR:OG1	2.21	0.55
1:H:244:TYR:HB2	1:H:368:ASP:HA	1.89	0.55
1:J:506:PHE:HE1	1:K:731:ILE:HG13	1.71	0.55
1:B:244:TYR:HB2	1:B:368:ASP:HA	1.89	0.55
1:C:274:ILE:HA	1:C:277:LYS:HE2	1.88	0.55
1:J:273:GLU:OE1	1:J:273:GLU:N	2.31	0.55
1:K:648:PRO:O	1:K:653:ARG:NH1	2.40	0.55
1:L:425:LYS:NZ	1:L:451:ASP:OD1	2.30	0.55
1:A:244:TYR:HB2	1:A:368:ASP:HA	1.88	0.55
1:B:89:ARG:HA	1:B:94:VAL:HG12	1.88	0.55
1:B:634:LEU:HD22	1:B:642:LEU:HD11	1.87	0.55
1:E:648:PRO:O	1:E:653:ARG:NH1	2.40	0.55
1:H:634:LEU:HD22	1:H:642:LEU:HD11	1.87	0.55
1:I:516:PHE:HB3	1:I:643:ILE:HG13	1.88	0.55
1:F:425:LYS:NZ	1:F:451:ASP:OD1	2.30	0.55
1:A:395:ASP:OD1	1:A:395:ASP:N	2.40	0.55
1:C:356:ALA:O	1:C:362:ARG:NH1	2.36	0.55
1:C:516:PHE:HB3	1:C:643:ILE:HG13	1.88	0.55
1:E:274:ILE:HA	1:E:277:LYS:HE2	1.88	0.55
1:G:244:TYR:HB2	1:G:368:ASP:HA	1.89	0.55
1:H:89:ARG:HA	1:H:94:VAL:HG12	1.88	0.55
1:I:274:ILE:HA	1:I:277:LYS:HE2	1.88	0.55
1:K:89:ARG:HA	1:K:94:VAL:HG12	1.88	0.55
1:A:648:PRO:O	1:A:653:ARG:NH1	2.40	0.55
1:E:89:ARG:HA	1:E:94:VAL:HG12	1.88	0.55
1:E:244:TYR:HB2	1:E:368:ASP:HA	1.89	0.55
1:G:395:ASP:OD1	1:G:395:ASP:N	2.40	0.55
1:G:648:PRO:O	1:G:653:ARG:NH1	2.40	0.55
1:I:69:CYS:SG	1:I:70:ILE:N	2.76	0.55
1:K:274:ILE:HA	1:K:277:LYS:HE2	1.88	0.55
1:L:757:MET:O	1:L:761:THR:OG1	2.16	0.55
1:A:84:MET:HE1	1:A:88:VAL:HG23	1.88	0.55
1:C:491:GLU:HB3	1:D:700:ARG:HH21	1.72	0.55
1:F:84:MET:HE1	1:F:88:VAL:HG23	1.88	0.55
1:F:395:ASP:OD1	1:F:395:ASP:N	2.40	0.55
1:G:84:MET:HE1	1:G:88:VAL:HG23	1.88	0.55
1:H:648:PRO:O	1:H:653:ARG:NH1	2.40	0.55
1:I:84:MET:HE1	1:I:88:VAL:HG23	1.88	0.55
1:K:31:ALA:HA	1:K:83:ARG:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:244:TYR:HB2	1:K:368:ASP:HA	1.89	0.55
1:A:548:LEU:HB3	1:F:602:ASN:ND2	2.22	0.55
1:B:648:PRO:O	1:B:653:ARG:NH1	2.40	0.55
1:C:84:MET:HE1	1:C:88:VAL:HG23	1.89	0.55
1:D:330:THR:HG21	1:E:273:GLU:HA	1.87	0.55
1:F:648:PRO:O	1:F:653:ARG:NH1	2.40	0.55
1:I:648:PRO:O	1:I:653:ARG:NH1	2.40	0.55
1:L:395:ASP:OD1	1:L:395:ASP:N	2.40	0.55
1:L:648:PRO:O	1:L:653:ARG:NH1	2.40	0.55
1:C:648:PRO:O	1:C:653:ARG:NH1	2.40	0.55
1:D:274:ILE:HA	1:D:277:LYS:HE2	1.88	0.55
1:E:31:ALA:HA	1:E:83:ARG:HD2	1.89	0.55
1:J:648:PRO:O	1:J:653:ARG:NH1	2.40	0.55
1:K:506:PHE:HE1	1:L:731:ILE:HG13	1.71	0.55
1:K:516:PHE:HB3	1:K:643:ILE:HG13	1.88	0.55
1:E:516:PHE:HB3	1:E:643:ILE:HG13	1.88	0.54
1:F:757:MET:O	1:F:761:THR:OG1	2.16	0.54
1:G:700:ARG:HH21	1:L:491:GLU:HB3	1.72	0.54
1:J:274:ILE:HA	1:J:277:LYS:HE2	1.88	0.54
1:J:516:PHE:HB3	1:J:643:ILE:HG13	1.88	0.54
1:L:84:MET:HE1	1:L:88:VAL:HG23	1.89	0.54
1:L:244:TYR:HB2	1:L:368:ASP:HA	1.89	0.54
1:B:395:ASP:OD1	1:B:395:ASP:N	2.40	0.54
1:D:244:TYR:HB2	1:D:368:ASP:HA	1.89	0.54
1:D:516:PHE:HB3	1:D:643:ILE:HG13	1.88	0.54
1:D:648:PRO:O	1:D:653:ARG:NH1	2.40	0.54
1:G:89:ARG:HA	1:G:94:VAL:HG12	1.88	0.54
1:F:244:TYR:HB2	1:F:368:ASP:HA	1.89	0.54
1:H:395:ASP:OD1	1:H:395:ASP:N	2.40	0.54
1:K:84:MET:HE1	1:K:88:VAL:HG23	1.88	0.54
1:D:31:ALA:HA	1:D:83:ARG:HD2	1.89	0.54
1:E:84:MET:HE1	1:E:88:VAL:HG23	1.89	0.54
1:E:751:ASP:HA	1:E:754:LYS:HG2	1.89	0.54
1:F:155:ARG:HH22	1:F:387:ASN:HB3	1.73	0.54
1:J:244:TYR:HB2	1:J:368:ASP:HA	1.89	0.54
1:K:602:ASN:ND2	1:L:548:LEU:HB3	2.21	0.54
1:L:155:ARG:HH22	1:L:387:ASN:HB3	1.73	0.54
1:L:751:ASP:HA	1:L:754:LYS:HG2	1.89	0.54
1:A:89:ARG:HA	1:A:94:VAL:HG12	1.88	0.54
1:F:751:ASP:HA	1:F:754:LYS:HG2	1.89	0.54
1:J:31:ALA:HA	1:J:83:ARG:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:395:ASP:OD1	1:K:395:ASP:N	2.40	0.54
1:E:395:ASP:OD1	1:E:395:ASP:N	2.40	0.54
1:E:492:LEU:HD11	1:E:641:GLN:HG3	1.90	0.54
1:H:31:ALA:HA	1:H:83:ARG:HD2	1.89	0.54
1:I:751:ASP:HA	1:I:754:LYS:HG2	1.89	0.54
1:K:751:ASP:HA	1:K:754:LYS:HG2	1.89	0.54
1:A:155:ARG:HH22	1:A:387:ASN:HB3	1.73	0.54
1:E:155:ARG:HH22	1:E:387:ASN:HB3	1.73	0.54
1:H:751:ASP:HA	1:H:754:LYS:HG2	1.89	0.54
1:K:492:LEU:HD11	1:K:641:GLN:HG3	1.90	0.54
1:B:31:ALA:HA	1:B:83:ARG:HD2	1.89	0.54
1:C:244:TYR:HB2	1:C:368:ASP:HA	1.89	0.54
1:C:395:ASP:OD1	1:C:395:ASP:N	2.40	0.54
1:E:773:PHE:HB3	1:F:733:ARG:HH11	1.72	0.54
1:G:155:ARG:HH22	1:G:387:ASN:HB3	1.73	0.54
1:K:155:ARG:HH22	1:K:387:ASN:HB3	1.73	0.54
1:B:751:ASP:HA	1:B:754:LYS:HG2	1.89	0.54
1:C:508:MET:CE	1:D:699:ILE:CD1	2.72	0.54
1:C:751:ASP:HA	1:C:754:LYS:HG2	1.89	0.54
1:D:155:ARG:HH22	1:D:387:ASN:HB3	1.73	0.54
1:F:310:ALA:HB1	1:F:354:ASP:HB2	1.90	0.54
1:G:416:SER:HB2	1:L:235:VAL:HG13	1.90	0.54
1:J:155:ARG:HH22	1:J:387:ASN:HB3	1.73	0.54
1:J:630:ASP:O	1:J:633:ILE:HG22	2.08	0.54
1:L:310:ALA:HB1	1:L:354:ASP:HB2	1.90	0.54
1:L:492:LEU:HD11	1:L:641:GLN:HG3	1.90	0.54
1:A:751:ASP:HA	1:A:754:LYS:HG2	1.89	0.54
1:D:630:ASP:O	1:D:633:ILE:HG22	2.08	0.54
1:G:385:THR:HA	1:G:388:MET:HE3	1.90	0.54
1:H:84:MET:HE1	1:H:88:VAL:HG23	1.88	0.54
1:I:31:ALA:HA	1:I:83:ARG:HD2	1.89	0.54
1:I:244:TYR:HB2	1:I:368:ASP:HA	1.88	0.54
1:L:31:ALA:HA	1:L:83:ARG:HD2	1.89	0.54
1:L:89:ARG:HA	1:L:94:VAL:HG12	1.88	0.54
1:C:630:ASP:O	1:C:633:ILE:HG22	2.08	0.53
1:F:492:LEU:HD11	1:F:641:GLN:HG3	1.90	0.53
1:F:649:ASP:OD1	1:F:652:SER:OG	2.23	0.53
1:I:395:ASP:OD1	1:I:395:ASP:N	2.40	0.53
1:J:69:CYS:SG	1:J:70:ILE:N	2.76	0.53
1:L:377:ARG:O	1:L:380:ILE:HG22	2.09	0.53
1:B:155:ARG:HH22	1:B:387:ASN:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ARG:O	1:C:380:ILE:HG22	2.09	0.53
1:D:492:LEU:HD11	1:D:641:GLN:HG3	1.90	0.53
1:E:630:ASP:O	1:E:633:ILE:HG22	2.08	0.53
1:F:89:ARG:HA	1:F:94:VAL:HG12	1.88	0.53
1:I:630:ASP:O	1:I:633:ILE:HG22	2.08	0.53
1:J:377:ARG:O	1:J:380:ILE:HG22	2.09	0.53
1:J:487:ARG:HE	1:K:700:ARG:NH1	2.07	0.53
1:J:624:ASN:OD1	1:J:624:ASN:N	2.42	0.53
1:K:438:ASP:N	1:K:438:ASP:OD1	2.42	0.53
1:K:630:ASP:O	1:K:633:ILE:HG22	2.08	0.53
1:A:107:ASP:HB3	1:A:109:LYS:HZ2	1.73	0.53
1:A:273:GLU:HA	1:F:330:THR:HG21	1.90	0.53
1:B:84:MET:HE1	1:B:88:VAL:HG23	1.89	0.53
1:D:377:ARG:O	1:D:380:ILE:HG22	2.09	0.53
1:D:624:ASN:OD1	1:D:624:ASN:N	2.42	0.53
1:D:751:ASP:HA	1:D:754:LYS:HG2	1.89	0.53
1:F:31:ALA:HA	1:F:83:ARG:HD2	1.89	0.53
1:F:107:ASP:HB3	1:F:109:LYS:HZ2	1.73	0.53
1:F:377:ARG:O	1:F:380:ILE:HG22	2.09	0.53
1:G:751:ASP:HA	1:G:754:LYS:HG2	1.89	0.53
1:I:377:ARG:O	1:I:380:ILE:HG22	2.09	0.53
1:J:492:LEU:HD11	1:J:641:GLN:HG3	1.90	0.53
1:K:356:ALA:O	1:K:362:ARG:NH1	2.36	0.53
1:A:487:ARG:HE	1:B:700:ARG:NH1	2.07	0.53
1:C:31:ALA:HA	1:C:83:ARG:HD2	1.89	0.53
1:E:377:ARG:O	1:E:380:ILE:HG22	2.09	0.53
1:G:107:ASP:HB3	1:G:109:LYS:HZ2	1.73	0.53
1:G:438:ASP:OD1	1:G:438:ASP:N	2.42	0.53
1:J:751:ASP:HA	1:J:754:LYS:HG2	1.89	0.53
1:K:377:ARG:O	1:K:380:ILE:HG22	2.09	0.53
1:L:107:ASP:HB3	1:L:109:LYS:HZ2	1.74	0.53
1:A:273:GLU:OE1	1:A:273:GLU:N	2.31	0.53
1:A:438:ASP:OD1	1:A:438:ASP:N	2.42	0.53
1:A:492:LEU:HD11	1:A:641:GLN:HG3	1.90	0.53
1:C:155:ARG:HH22	1:C:387:ASN:HB3	1.73	0.53
1:E:356:ALA:O	1:E:362:ARG:NH1	2.36	0.53
1:E:438:ASP:N	1:E:438:ASP:OD1	2.42	0.53
1:J:385:THR:HA	1:J:388:MET:HE3	1.90	0.53
1:L:438:ASP:OD1	1:L:438:ASP:N	2.42	0.53
1:B:377:ARG:O	1:B:380:ILE:HG22	2.09	0.53
1:D:84:MET:HE1	1:D:88:VAL:HG23	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:385:THR:HA	1:E:388:MET:HE3	1.90	0.53
1:F:438:ASP:OD1	1:F:438:ASP:N	2.42	0.53
1:G:649:ASP:OD1	1:G:652:SER:OG	2.23	0.53
1:H:377:ARG:O	1:H:380:ILE:HG22	2.09	0.53
1:I:155:ARG:HH22	1:I:387:ASN:HB3	1.73	0.53
1:A:771:PHE:HD2	1:B:737:GLU:HG3	1.74	0.53
1:D:438:ASP:OD1	1:D:438:ASP:N	2.42	0.53
1:E:107:ASP:HB3	1:E:109:LYS:HZ2	1.74	0.53
1:J:84:MET:HE1	1:J:88:VAL:HG23	1.89	0.53
1:A:385:THR:HA	1:A:388:MET:HE3	1.91	0.53
1:A:508:MET:HE2	1:B:699:ILE:HD13	1.85	0.53
1:B:503:PHE:HE1	1:C:699:ILE:HG21	1.73	0.53
1:B:630:ASP:O	1:B:633:ILE:HG22	2.08	0.53
1:D:69:CYS:SG	1:D:70:ILE:N	2.76	0.53
1:D:385:THR:HA	1:D:388:MET:HE3	1.91	0.53
1:G:31:ALA:HA	1:G:83:ARG:HD2	1.89	0.53
1:G:273:GLU:OE1	1:G:273:GLU:N	2.31	0.53
1:H:385:THR:HA	1:H:388:MET:HE3	1.90	0.53
1:K:107:ASP:HB3	1:K:109:LYS:HZ2	1.74	0.53
1:A:31:ALA:HA	1:A:83:ARG:HD2	1.89	0.53
1:B:385:THR:HA	1:B:388:MET:HE3	1.90	0.53
1:D:395:ASP:OD1	1:D:395:ASP:N	2.40	0.53
1:G:492:LEU:HD11	1:G:641:GLN:HG3	1.90	0.53
1:H:155:ARG:HH21	1:H:386:LYS:HZ3	1.57	0.53
1:H:155:ARG:HH22	1:H:387:ASN:HB3	1.73	0.53
1:H:630:ASP:O	1:H:633:ILE:HG22	2.08	0.53
1:I:310:ALA:HB1	1:I:354:ASP:HB2	1.90	0.53
1:B:492:LEU:HD11	1:B:641:GLN:HG3	1.90	0.53
1:C:492:LEU:HD11	1:C:641:GLN:HG3	1.90	0.53
1:D:107:ASP:HB3	1:D:109:LYS:HZ2	1.73	0.53
1:I:492:LEU:HD11	1:I:641:GLN:HG3	1.90	0.53
1:J:377:ARG:NH2	1:J:403:THR:O	2.42	0.53
1:J:395:ASP:OD1	1:J:395:ASP:N	2.40	0.53
1:C:310:ALA:HB1	1:C:354:ASP:HB2	1.90	0.52
1:D:377:ARG:NH2	1:D:403:THR:O	2.42	0.52
1:D:488:GLU:HA	1:D:491:GLU:HG2	1.91	0.52
1:G:377:ARG:O	1:G:380:ILE:HG22	2.09	0.52
1:G:630:ASP:O	1:G:633:ILE:HG22	2.08	0.52
1:H:438:ASP:OD1	1:H:438:ASP:N	2.42	0.52
1:H:492:LEU:HD11	1:H:641:GLN:HG3	1.90	0.52
1:J:488:GLU:HA	1:J:491:GLU:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:385:THR:HA	1:K:388:MET:HE3	1.90	0.52
1:A:377:ARG:O	1:A:380:ILE:HG22	2.09	0.52
1:A:630:ASP:O	1:A:633:ILE:HG22	2.08	0.52
1:A:699:ILE:HD12	1:F:508:MET:HE1	1.91	0.52
1:B:310:ALA:HB1	1:B:354:ASP:HB2	1.90	0.52
1:B:438:ASP:OD1	1:B:438:ASP:N	2.42	0.52
1:D:117:LEU:HD12	1:D:188:PRO:HA	1.91	0.52
1:F:385:THR:HA	1:F:388:MET:HE3	1.90	0.52
1:J:107:ASP:HB3	1:J:109:LYS:HZ2	1.74	0.52
1:H:107:ASP:HB3	1:H:109:LYS:HZ2	1.74	0.52
1:H:130:LEU:CD1	1:H:134:TYR:CE2	2.83	0.52
1:I:385:THR:HA	1:I:388:MET:HE3	1.90	0.52
1:J:117:LEU:HD12	1:J:188:PRO:HA	1.91	0.52
1:K:488:GLU:HA	1:K:491:GLU:HG2	1.91	0.52
1:L:760:GLN:HA	1:L:763:GLN:HB2	1.92	0.52
1:C:760:GLN:HA	1:C:763:GLN:HB2	1.92	0.52
1:D:380:ILE:HD11	3:D:902:ADP:C6	2.44	0.52
1:E:117:LEU:HD12	1:E:188:PRO:HA	1.91	0.52
1:E:488:GLU:HA	1:E:491:GLU:HG2	1.92	0.52
1:F:760:GLN:HA	1:F:763:GLN:HB2	1.92	0.52
1:H:310:ALA:HB1	1:H:354:ASP:HB2	1.90	0.52
1:I:488:GLU:HA	1:I:491:GLU:HG2	1.91	0.52
1:L:630:ASP:O	1:L:633:ILE:HG22	2.08	0.52
1:A:624:ASN:OD1	1:A:624:ASN:N	2.42	0.52
1:A:760:GLN:NE2	1:K:760:GLN:CD	2.56	0.52
1:C:385:THR:HA	1:C:388:MET:HE3	1.90	0.52
1:D:491:GLU:HB3	1:E:700:ARG:HH21	1.75	0.52
1:F:630:ASP:O	1:F:633:ILE:HG22	2.08	0.52
1:G:310:ALA:HB1	1:G:354:ASP:HB2	1.90	0.52
1:G:624:ASN:OD1	1:G:624:ASN:N	2.42	0.52
1:I:62:LYS:NZ	1:I:98:ASP:OD2	2.40	0.52
1:I:760:GLN:HA	1:I:763:GLN:HB2	1.92	0.52
1:J:310:ALA:HB1	1:J:354:ASP:HB2	1.90	0.52
1:C:488:GLU:HA	1:C:491:GLU:HG2	1.91	0.52
1:E:506:PHE:HE1	1:F:731:ILE:HG13	1.75	0.52
1:I:107:ASP:HB3	1:I:109:LYS:HZ2	1.75	0.52
1:J:607:GLU:CD	1:K:465:ARG:HH22	2.18	0.52
1:K:117:LEU:HD12	1:K:188:PRO:HA	1.91	0.52
1:L:385:THR:HA	1:L:388:MET:HE3	1.91	0.52
1:A:310:ALA:HB1	1:A:354:ASP:HB2	1.90	0.52
1:B:107:ASP:HB3	1:B:109:LYS:HZ2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HD12	1:B:188:PRO:HA	1.91	0.52
1:C:107:ASP:HB3	1:C:109:LYS:HZ2	1.75	0.52
1:C:377:ARG:NH2	1:C:403:THR:O	2.42	0.52
1:D:560:ARG:HH11	1:D:560:ARG:HA	1.74	0.52
1:F:560:ARG:HA	1:F:560:ARG:HH11	1.74	0.52
1:G:91:ASN:HD21	1:G:150:ASP:HB3	1.75	0.52
1:G:377:ARG:NH2	1:G:403:THR:O	2.42	0.52
1:G:508:MET:CE	1:H:699:ILE:CD1	2.79	0.52
1:H:251:LYS:HD2	1:H:346:ALA:HB1	1.91	0.52
1:H:488:GLU:HA	1:H:491:GLU:HG2	1.91	0.52
1:I:508:MET:HE1	1:J:699:ILE:HD12	1.86	0.52
1:A:377:ARG:NH2	1:A:403:THR:O	2.42	0.52
1:B:251:LYS:HD2	1:B:346:ALA:HB1	1.91	0.52
1:B:488:GLU:HA	1:B:491:GLU:HG2	1.92	0.52
1:D:251:LYS:HD2	1:D:346:ALA:HB1	1.91	0.52
1:D:310:ALA:HB1	1:D:354:ASP:HB2	1.90	0.52
1:E:310:ALA:HB1	1:E:354:ASP:HB2	1.90	0.52
1:I:377:ARG:NH2	1:I:403:THR:O	2.42	0.52
1:J:560:ARG:HH11	1:J:560:ARG:HA	1.74	0.52
1:K:310:ALA:HB1	1:K:354:ASP:HB2	1.90	0.52
1:A:91:ASN:HD21	1:A:150:ASP:HB3	1.75	0.52
1:D:602:ASN:ND2	1:E:548:LEU:HB3	2.24	0.52
1:E:560:ARG:HA	1:E:560:ARG:HH11	1.74	0.52
1:G:25:ARG:HB3	1:G:99:VAL:HB	1.92	0.52
1:H:25:ARG:HB3	1:H:99:VAL:HB	1.92	0.52
1:H:117:LEU:HD12	1:H:188:PRO:HA	1.91	0.52
1:I:560:ARG:HA	1:I:560:ARG:HH11	1.74	0.52
1:J:251:LYS:HD2	1:J:346:ALA:HB1	1.91	0.52
1:K:560:ARG:HA	1:K:560:ARG:HH11	1.74	0.52
1:L:560:ARG:HH11	1:L:560:ARG:HA	1.74	0.52
1:A:251:LYS:HD2	1:A:346:ALA:HB1	1.91	0.52
1:A:560:ARG:HA	1:A:560:ARG:HH11	1.74	0.52
1:B:25:ARG:HB3	1:B:99:VAL:HB	1.92	0.52
1:B:560:ARG:HH11	1:B:560:ARG:HA	1.74	0.52
1:C:560:ARG:HA	1:C:560:ARG:HH11	1.74	0.52
1:E:760:GLN:HA	1:E:763:GLN:HB2	1.92	0.52
1:F:253:LEU:HD13	3:F:902:ADP:H2'	1.91	0.52
1:F:377:ARG:NH2	1:F:403:THR:O	2.42	0.52
1:I:155:ARG:HH21	1:I:386:LYS:HZ3	1.58	0.52
1:L:117:LEU:HD12	1:L:188:PRO:HA	1.91	0.52
1:A:25:ARG:HB3	1:A:99:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:LYS:HD2	1:G:346:ALA:HB1	1.91	0.51
1:L:377:ARG:NH2	1:L:403:THR:O	2.42	0.51
1:D:760:GLN:HA	1:D:763:GLN:HB2	1.92	0.51
1:F:117:LEU:HD12	1:F:188:PRO:HA	1.91	0.51
1:H:356:ALA:O	1:H:362:ARG:NH1	2.36	0.51
1:J:760:GLN:HA	1:J:763:GLN:HB2	1.92	0.51
1:K:760:GLN:HA	1:K:763:GLN:HB2	1.92	0.51
1:L:488:GLU:HA	1:L:491:GLU:HG2	1.91	0.51
1:B:155:ARG:HH21	1:B:386:LYS:HZ3	1.58	0.51
1:C:251:LYS:HD2	1:C:346:ALA:HB1	1.91	0.51
1:F:488:GLU:HA	1:F:491:GLU:HG2	1.91	0.51
1:G:560:ARG:HH11	1:G:560:ARG:HA	1.74	0.51
1:H:560:ARG:HA	1:H:560:ARG:HH11	1.74	0.51
1:A:491:GLU:HB3	1:B:700:ARG:HH21	1.75	0.51
1:H:91:ASN:HD21	1:H:150:ASP:HB3	1.75	0.51
1:H:377:ARG:NH2	1:H:403:THR:O	2.42	0.51
1:H:753:ARG:O	1:H:757:MET:HG3	2.11	0.51
1:I:117:LEU:HD12	1:I:188:PRO:HA	1.91	0.51
1:I:251:LYS:HD2	1:I:346:ALA:HB1	1.91	0.51
1:B:506:PHE:HE1	1:C:731:ILE:HG13	1.74	0.51
1:B:753:ARG:O	1:B:757:MET:HG3	2.11	0.51
1:B:760:GLN:HA	1:B:763:GLN:HB2	1.92	0.51
1:E:602:ASN:ND2	1:F:548:LEU:HB3	2.26	0.51
1:G:488:GLU:HA	1:G:491:GLU:HG2	1.91	0.51
1:K:251:LYS:HD2	1:K:346:ALA:HB1	1.91	0.51
1:B:89:ARG:HA	1:B:94:VAL:CG1	2.41	0.51
1:B:91:ASN:HD21	1:B:150:ASP:HB3	1.75	0.51
1:B:377:ARG:NH2	1:B:403:THR:O	2.42	0.51
1:B:434:ASP:N	1:B:434:ASP:OD1	2.43	0.51
1:D:91:ASN:HD21	1:D:150:ASP:HB3	1.75	0.51
1:E:251:LYS:HD2	1:E:346:ALA:HB1	1.91	0.51
1:E:753:ARG:O	1:E:757:MET:HG3	2.11	0.51
1:F:155:ARG:HH21	1:F:386:LYS:NZ	2.09	0.51
1:G:89:ARG:HA	1:G:94:VAL:CG1	2.41	0.51
1:G:760:GLN:HA	1:G:763:GLN:HB2	1.92	0.51
1:J:91:ASN:HD21	1:J:150:ASP:HB3	1.75	0.51
1:L:155:ARG:HH21	1:L:386:LYS:NZ	2.09	0.51
1:A:488:GLU:HA	1:A:491:GLU:HG2	1.92	0.51
1:C:25:ARG:HB3	1:C:99:VAL:HB	1.92	0.51
1:C:117:LEU:HD12	1:C:188:PRO:HA	1.91	0.51
1:D:89:ARG:HA	1:D:94:VAL:CG1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:ARG:HA	1:E:94:VAL:CG1	2.41	0.51
1:E:377:ARG:NH2	1:E:403:THR:O	2.42	0.51
1:F:91:ASN:HD21	1:F:150:ASP:HB3	1.75	0.51
1:F:434:ASP:OD1	1:F:434:ASP:N	2.43	0.51
1:H:89:ARG:HA	1:H:94:VAL:CG1	2.41	0.51
1:K:377:ARG:NH2	1:K:403:THR:O	2.42	0.51
1:L:434:ASP:N	1:L:434:ASP:OD1	2.43	0.51
1:A:89:ARG:HA	1:A:94:VAL:CG1	2.41	0.51
1:A:699:ILE:CD1	1:F:508:MET:CE	2.83	0.51
1:A:760:GLN:HA	1:A:763:GLN:HB2	1.92	0.51
1:B:356:ALA:O	1:B:362:ARG:NH1	2.36	0.51
1:F:25:ARG:HB3	1:F:99:VAL:HB	1.92	0.51
1:G:117:LEU:HD12	1:G:188:PRO:HA	1.91	0.51
1:G:434:ASP:N	1:G:434:ASP:OD1	2.43	0.51
1:G:753:ARG:O	1:G:757:MET:HG3	2.11	0.51
1:H:434:ASP:OD1	1:H:434:ASP:N	2.43	0.51
1:H:760:GLN:HA	1:H:763:GLN:HB2	1.92	0.51
1:I:25:ARG:HB3	1:I:99:VAL:HB	1.92	0.51
1:K:508:MET:HE1	1:L:699:ILE:HD12	1.91	0.51
1:K:753:ARG:O	1:K:757:MET:HG3	2.11	0.51
1:A:434:ASP:N	1:A:434:ASP:OD1	2.43	0.51
1:A:753:ARG:O	1:A:757:MET:HG3	2.11	0.51
1:C:771:PHE:HD2	1:D:737:GLU:HG3	1.76	0.51
1:D:756:GLU:O	1:D:759:ALA:N	2.44	0.51
1:J:508:MET:HE2	1:K:699:ILE:HD11	1.90	0.51
1:K:602:ASN:HD21	1:L:548:LEU:HB3	1.75	0.51
1:L:25:ARG:HB3	1:L:99:VAL:HB	1.92	0.51
1:L:89:ARG:HA	1:L:94:VAL:CG1	2.41	0.51
1:C:89:ARG:HA	1:C:94:VAL:CG1	2.41	0.51
1:C:753:ARG:O	1:C:757:MET:HG3	2.11	0.51
1:F:89:ARG:HA	1:F:94:VAL:CG1	2.41	0.51
1:J:89:ARG:HA	1:J:94:VAL:CG1	2.41	0.51
1:J:753:ARG:O	1:J:757:MET:HG3	2.11	0.51
1:J:756:GLU:O	1:J:759:ALA:N	2.44	0.51
1:K:89:ARG:HA	1:K:94:VAL:CG1	2.41	0.51
1:K:91:ASN:HD21	1:K:150:ASP:HB3	1.75	0.51
1:L:251:LYS:HD2	1:L:346:ALA:HB1	1.91	0.51
1:A:117:LEU:HD12	1:A:188:PRO:HA	1.91	0.50
1:A:548:LEU:HB3	1:F:602:ASN:HD21	1.75	0.50
1:D:753:ARG:O	1:D:757:MET:HG3	2.11	0.50
1:E:91:ASN:HD21	1:E:150:ASP:HB3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:251:LYS:HD2	1:F:346:ALA:HB1	1.91	0.50
1:G:92:LEU:HD13	1:G:92:LEU:O	2.11	0.50
1:I:89:ARG:HA	1:I:94:VAL:CG1	2.41	0.50
1:I:753:ARG:O	1:I:757:MET:HG3	2.11	0.50
1:J:503:PHE:CE1	1:K:699:ILE:HD13	2.46	0.50
1:L:91:ASN:HD21	1:L:150:ASP:HB3	1.75	0.50
1:L:649:ASP:OD1	1:L:652:SER:OG	2.23	0.50
1:B:92:LEU:O	1:B:92:LEU:HD13	2.12	0.50
1:B:155:ARG:HH21	1:B:386:LYS:NZ	2.09	0.50
1:C:92:LEU:O	1:C:92:LEU:HD13	2.12	0.50
1:F:92:LEU:O	1:F:92:LEU:HD13	2.11	0.50
1:H:92:LEU:O	1:H:92:LEU:HD13	2.12	0.50
1:I:92:LEU:O	1:I:92:LEU:HD13	2.11	0.50
1:L:92:LEU:HD13	1:L:92:LEU:O	2.12	0.50
1:A:92:LEU:O	1:A:92:LEU:HD13	2.12	0.50
1:H:155:ARG:HH21	1:H:386:LYS:NZ	2.09	0.50
1:C:756:GLU:O	1:C:759:ALA:N	2.44	0.50
1:I:91:ASN:HD21	1:I:150:ASP:HB3	1.75	0.50
1:E:25:ARG:HB3	1:E:99:VAL:HB	1.92	0.50
1:I:756:GLU:O	1:I:759:ALA:N	2.45	0.50
1:K:25:ARG:HB3	1:K:99:VAL:HB	1.92	0.50
1:C:91:ASN:HD21	1:C:150:ASP:HB3	1.75	0.50
1:E:92:LEU:O	1:E:92:LEU:HD13	2.12	0.50
1:E:589:ASN:N	1:E:589:ASN:OD1	2.45	0.50
1:E:756:GLU:O	1:E:759:ALA:N	2.44	0.50
1:G:508:MET:HE1	1:H:699:ILE:HD12	1.93	0.50
1:J:506:PHE:CE1	1:K:731:ILE:HG13	2.46	0.50
1:K:92:LEU:O	1:K:92:LEU:HD13	2.11	0.50
1:K:589:ASN:N	1:K:589:ASN:OD1	2.45	0.50
1:K:756:GLU:O	1:K:759:ALA:N	2.44	0.50
1:A:760:GLN:CD	1:K:760:GLN:NE2	2.58	0.50
1:E:649:ASP:N	1:E:652:SER:OG	2.45	0.50
1:K:649:ASP:N	1:K:652:SER:OG	2.45	0.50
1:C:434:ASP:OD1	1:C:434:ASP:N	2.43	0.50
1:E:313:ARG:NH2	1:E:353:ILE:O	2.44	0.50
1:E:773:PHE:HB3	1:F:733:ARG:NH1	2.27	0.50
1:H:773:PHE:HB3	1:I:733:ARG:HH11	1.77	0.50
1:K:313:ARG:NH2	1:K:353:ILE:O	2.44	0.50
1:B:95:ARG:HG3	1:B:95:ARG:NH1	2.27	0.50
1:D:589:ASN:OD1	1:D:589:ASN:N	2.45	0.50
1:D:649:ASP:N	1:D:652:SER:OG	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:624:ASN:OD1	1:F:624:ASN:N	2.42	0.50
1:F:753:ARG:O	1:F:757:MET:HG3	2.11	0.50
1:G:756:GLU:O	1:G:759:ALA:N	2.44	0.50
1:H:95:ARG:HG3	1:H:95:ARG:NH1	2.27	0.50
1:L:624:ASN:OD1	1:L:624:ASN:N	2.42	0.50
1:L:649:ASP:N	1:L:652:SER:OG	2.45	0.50
1:L:753:ARG:O	1:L:757:MET:HG3	2.11	0.50
1:F:589:ASN:N	1:F:589:ASN:OD1	2.45	0.49
1:F:649:ASP:N	1:F:652:SER:OG	2.45	0.49
1:H:768:PHE:O	1:I:741:ARG:HA	2.12	0.49
1:I:434:ASP:OD1	1:I:434:ASP:N	2.43	0.49
1:J:25:ARG:HB3	1:J:99:VAL:HB	1.92	0.49
1:J:649:ASP:N	1:J:652:SER:OG	2.45	0.49
1:A:756:GLU:O	1:A:759:ALA:N	2.44	0.49
1:B:756:GLU:O	1:B:759:ALA:N	2.44	0.49
1:D:25:ARG:HB3	1:D:99:VAL:HB	1.92	0.49
1:E:259:ALA:HB2	1:E:300:ILE:HG21	1.95	0.49
1:I:155:ARG:HH21	1:I:386:LYS:NZ	2.09	0.49
1:J:589:ASN:OD1	1:J:589:ASN:N	2.45	0.49
1:K:259:ALA:HB2	1:K:300:ILE:HG21	1.95	0.49
1:L:95:ARG:HG3	1:L:95:ARG:NH1	2.27	0.49
1:L:589:ASN:OD1	1:L:589:ASN:N	2.45	0.49
1:A:487:ARG:HE	1:B:700:ARG:CZ	2.26	0.49
1:B:640:ASP:OD1	1:B:640:ASP:N	2.45	0.49
1:C:438:ASP:N	1:C:438:ASP:OD1	2.42	0.49
1:D:602:ASN:HD21	1:E:548:LEU:HB3	1.77	0.49
1:F:210:ARG:NH1	1:F:379:GLU:OE1	2.45	0.49
1:H:380:ILE:HD11	3:H:902:ADP:C6	2.46	0.49
1:H:469:VAL:HG22	1:H:540:ILE:HG12	1.95	0.49
1:I:210:ARG:NH1	1:I:379:GLU:OE1	2.45	0.49
1:I:438:ASP:OD1	1:I:438:ASP:N	2.42	0.49
1:J:210:ARG:NH1	1:J:379:GLU:OE1	2.45	0.49
1:J:438:ASP:OD1	1:J:438:ASP:N	2.42	0.49
1:L:210:ARG:NH1	1:L:379:GLU:OE1	2.45	0.49
1:B:469:VAL:HG22	1:B:540:ILE:HG12	1.95	0.49
1:C:649:ASP:N	1:C:652:SER:OG	2.45	0.49
1:D:210:ARG:NH1	1:D:379:GLU:OE1	2.45	0.49
1:F:95:ARG:HG3	1:F:95:ARG:NH1	2.27	0.49
1:I:356:ALA:O	1:I:362:ARG:NH1	2.36	0.49
1:I:580:ASP:OD1	1:I:623:THR:OG1	2.29	0.49
1:I:589:ASN:OD1	1:I:589:ASN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:649:ASP:N	1:I:652:SER:OG	2.45	0.49
1:J:313:ARG:NH2	1:J:353:ILE:O	2.45	0.49
1:A:210:ARG:NH1	1:A:379:GLU:OE1	2.46	0.49
1:A:649:ASP:N	1:A:652:SER:OG	2.45	0.49
1:C:210:ARG:NH1	1:C:379:GLU:OE1	2.46	0.49
1:C:526:LEU:HD12	2:C:901:JDP:C06	2.43	0.49
1:C:589:ASN:N	1:C:589:ASN:OD1	2.45	0.49
1:D:313:ARG:NH2	1:D:353:ILE:O	2.45	0.49
1:E:364:ASP:OD1	1:E:364:ASP:N	2.38	0.49
1:F:756:GLU:O	1:F:759:ALA:N	2.44	0.49
1:G:210:ARG:NH1	1:G:379:GLU:OE1	2.46	0.49
1:G:649:ASP:N	1:G:652:SER:OG	2.45	0.49
1:H:756:GLU:O	1:H:759:ALA:N	2.44	0.49
1:A:95:ARG:HG3	1:A:95:ARG:NH1	2.27	0.49
1:B:259:ALA:HB2	1:B:300:ILE:HG21	1.95	0.49
1:C:624:ASN:O	1:C:755:TYR:OH	2.12	0.49
1:F:130:LEU:HD12	1:F:130:LEU:C	2.37	0.49
1:F:207:GLY:H	3:F:902:ADP:H2	1.61	0.49
1:H:210:ARG:NH1	1:H:379:GLU:OE1	2.45	0.49
1:H:428:ASP:N	1:H:428:ASP:OD1	2.46	0.49
1:I:313:ARG:NH2	1:I:353:ILE:O	2.44	0.49
1:I:526:LEU:HD12	2:I:901:JDP:C06	2.43	0.49
1:J:503:PHE:HE1	1:K:699:ILE:HG21	1.77	0.49
1:L:130:LEU:C	1:L:130:LEU:HD12	2.37	0.49
1:L:756:GLU:O	1:L:759:ALA:N	2.44	0.49
1:A:469:VAL:HG22	1:A:540:ILE:HG12	1.95	0.49
1:A:700:ARG:CZ	1:F:487:ARG:HE	2.24	0.49
1:A:731:ILE:HG13	1:F:506:PHE:HE1	1.77	0.49
1:B:649:ASP:N	1:B:652:SER:OG	2.45	0.49
1:C:469:VAL:HG22	1:C:540:ILE:HG12	1.95	0.49
1:D:92:LEU:HD13	1:D:92:LEU:O	2.12	0.49
1:D:155:ARG:HH21	1:D:386:LYS:NZ	2.09	0.49
1:F:215:GLN:OE1	1:F:367:VAL:HG13	2.12	0.49
1:H:259:ALA:HB2	1:H:300:ILE:HG21	1.95	0.49
1:J:155:ARG:HH21	1:J:386:LYS:NZ	2.09	0.49
1:J:215:GLN:OE1	1:J:367:VAL:HG13	2.12	0.49
1:B:210:ARG:NH1	1:B:379:GLU:OE1	2.45	0.49
1:B:442:MET:N	1:B:442:MET:SD	2.86	0.49
1:F:26:LEU:HD23	1:F:82:ILE:HG22	1.95	0.49
1:G:469:VAL:HG22	1:G:540:ILE:HG12	1.95	0.49
1:H:258:VAL:O	1:H:262:THR:OG1	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:442:MET:N	1:H:442:MET:SD	2.86	0.49
1:H:649:ASP:N	1:H:652:SER:OG	2.45	0.49
1:I:640:ASP:N	1:I:640:ASP:OD1	2.45	0.49
1:C:313:ARG:NH2	1:C:353:ILE:O	2.45	0.49
1:E:434:ASP:N	1:E:434:ASP:OD1	2.43	0.49
1:E:633:ILE:HG13	1:E:639:LEU:HD12	1.95	0.49
1:G:215:GLN:OE1	1:G:367:VAL:HG13	2.13	0.49
1:I:469:VAL:HG22	1:I:540:ILE:HG12	1.95	0.49
1:J:92:LEU:O	1:J:92:LEU:HD13	2.12	0.49
1:J:130:LEU:C	1:J:130:LEU:HD12	2.37	0.49
1:K:434:ASP:OD1	1:K:434:ASP:N	2.43	0.49
1:K:526:LEU:HD12	2:K:901:JDP:C06	2.43	0.49
1:L:26:LEU:HD23	1:L:82:ILE:HG22	1.95	0.49
1:L:215:GLN:OE1	1:L:367:VAL:HG13	2.13	0.49
1:L:356:ALA:O	1:L:362:ARG:NH1	2.36	0.49
1:A:215:GLN:OE1	1:A:367:VAL:HG13	2.13	0.49
1:A:589:ASN:OD1	1:A:589:ASN:N	2.45	0.49
1:C:155:ARG:HH21	1:C:386:LYS:NZ	2.09	0.49
1:D:259:ALA:HB2	1:D:300:ILE:HG21	1.95	0.49
1:F:259:ALA:HB2	1:F:300:ILE:HG21	1.95	0.49
1:F:633:ILE:HG13	1:F:639:LEU:HD12	1.95	0.49
1:I:95:ARG:HG3	1:I:95:ARG:NH1	2.27	0.49
1:K:633:ILE:HG13	1:K:639:LEU:HD12	1.95	0.49
1:L:259:ALA:HB2	1:L:300:ILE:HG21	1.95	0.49
1:L:380:ILE:HD11	3:L:902:ADP:C6	2.48	0.49
1:L:633:ILE:HG13	1:L:639:LEU:HD12	1.95	0.49
1:C:95:ARG:HG3	1:C:95:ARG:NH1	2.27	0.48
1:C:442:MET:N	1:C:442:MET:SD	2.86	0.48
1:D:215:GLN:OE1	1:D:367:VAL:HG13	2.13	0.48
1:D:633:ILE:HG13	1:D:639:LEU:HD12	1.95	0.48
1:D:768:PHE:O	1:E:741:ARG:HA	2.14	0.48
1:E:526:LEU:HD12	2:E:901:JDP:C06	2.43	0.48
1:F:356:ALA:O	1:F:362:ARG:NH1	2.36	0.48
1:J:633:ILE:HG13	1:J:639:LEU:HD12	1.95	0.48
1:K:210:ARG:NH1	1:K:379:GLU:OE1	2.45	0.48
1:A:259:ALA:HB2	1:A:300:ILE:HG21	1.95	0.48
1:A:428:ASP:OD1	1:A:428:ASP:N	2.46	0.48
1:A:633:ILE:HG13	1:A:639:LEU:HD12	1.95	0.48
1:C:382:GLN:HA	1:C:385:THR:HG22	1.96	0.48
1:D:469:VAL:HG22	1:D:540:ILE:HG12	1.95	0.48
1:E:210:ARG:NH1	1:E:379:GLU:OE1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:GLU:OE1	1:F:89:ARG:NH2	2.47	0.48
1:J:259:ALA:HB2	1:J:300:ILE:HG21	1.95	0.48
1:L:30:GLU:OE1	1:L:89:ARG:NH2	2.47	0.48
1:B:602:ASN:ND2	1:C:548:LEU:HB3	2.28	0.48
1:B:762:LEU:HA	1:C:744:ARG:NH1	2.28	0.48
1:C:624:ASN:OD1	1:C:624:ASN:N	2.42	0.48
1:G:428:ASP:OD1	1:G:428:ASP:N	2.46	0.48
1:G:589:ASN:OD1	1:G:589:ASN:N	2.45	0.48
1:G:741:ARG:HA	1:L:768:PHE:O	2.13	0.48
1:I:30:GLU:OE1	1:I:89:ARG:NH2	2.47	0.48
1:I:382:GLN:HA	1:I:385:THR:HG22	1.96	0.48
1:I:442:MET:N	1:I:442:MET:SD	2.86	0.48
1:I:633:ILE:HG13	1:I:639:LEU:HD12	1.95	0.48
1:L:135:LEU:HA	1:L:138:TYR:HE2	1.60	0.48
1:A:251:LYS:N	3:A:902:ADP:O2B	2.46	0.48
1:B:215:GLN:OE1	1:B:367:VAL:HG13	2.13	0.48
1:B:503:PHE:CE1	1:C:699:ILE:HD13	2.49	0.48
1:B:633:ILE:HG13	1:B:639:LEU:HD12	1.95	0.48
1:C:30:GLU:OE1	1:C:89:ARG:NH2	2.47	0.48
1:C:633:ILE:HG13	1:C:639:LEU:HD12	1.95	0.48
1:D:526:LEU:HD12	2:D:901:JDP:C06	2.43	0.48
1:F:135:LEU:HA	1:F:138:TYR:HE2	1.60	0.48
1:G:26:LEU:HD23	1:G:82:ILE:HG22	1.95	0.48
1:G:633:ILE:HG13	1:G:639:LEU:HD12	1.95	0.48
1:H:30:GLU:OE1	1:H:89:ARG:NH2	2.47	0.48
1:H:215:GLN:OE1	1:H:367:VAL:HG13	2.12	0.48
1:J:27:ILE:O	1:J:81:LYS:NZ	2.45	0.48
1:J:469:VAL:HG22	1:J:540:ILE:HG12	1.95	0.48
1:B:526:LEU:HD12	2:B:901:JDP:C06	2.43	0.48
1:D:27:ILE:O	1:D:81:LYS:NZ	2.45	0.48
1:D:428:ASP:OD1	1:D:428:ASP:N	2.46	0.48
1:D:508:MET:HE1	1:E:699:ILE:HD12	1.94	0.48
1:F:469:VAL:HG22	1:F:540:ILE:HG12	1.95	0.48
1:H:633:ILE:HG13	1:H:639:LEU:HD12	1.95	0.48
1:I:215:GLN:OE1	1:I:367:VAL:HG13	2.13	0.48
1:I:259:ALA:HB2	1:I:300:ILE:HG21	1.95	0.48
1:J:356:ALA:O	1:J:362:ARG:NH1	2.36	0.48
1:J:428:ASP:OD1	1:J:428:ASP:N	2.46	0.48
1:K:67:ALA:HB2	1:K:92:LEU:HD23	1.96	0.48
1:K:640:ASP:N	1:K:640:ASP:OD1	2.45	0.48
1:A:26:LEU:HD23	1:A:82:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:GLU:OE1	1:B:89:ARG:NH2	2.47	0.48
1:C:27:ILE:O	1:C:81:LYS:NZ	2.45	0.48
1:C:215:GLN:OE1	1:C:367:VAL:HG13	2.13	0.48
1:E:67:ALA:HB2	1:E:92:LEU:HD23	1.96	0.48
1:E:215:GLN:OE1	1:E:367:VAL:HG13	2.12	0.48
1:G:158:MET:HE3	1:L:233:ILE:HB	1.94	0.48
1:J:526:LEU:HD12	2:J:901:JDP:C06	2.43	0.48
1:L:67:ALA:HB2	1:L:92:LEU:HD23	1.96	0.48
1:L:469:VAL:HG22	1:L:540:ILE:HG12	1.95	0.48
1:B:223:PRO:O	1:B:340:HIS:ND1	2.47	0.48
1:B:503:PHE:HD2	1:B:510:PRO:HG3	1.79	0.48
1:C:259:ALA:HB2	1:C:300:ILE:HG21	1.95	0.48
1:D:223:PRO:O	1:D:340:HIS:ND1	2.47	0.48
1:D:356:ALA:O	1:D:362:ARG:NH1	2.36	0.48
1:F:67:ALA:HB2	1:F:92:LEU:HD23	1.96	0.48
1:G:259:ALA:HB2	1:G:300:ILE:HG21	1.95	0.48
1:H:223:PRO:O	1:H:340:HIS:ND1	2.47	0.48
1:I:27:ILE:O	1:I:81:LYS:NZ	2.45	0.48
1:I:624:ASN:OD1	1:I:624:ASN:N	2.42	0.48
1:J:223:PRO:O	1:J:340:HIS:ND1	2.47	0.48
1:J:226:HIS:CD2	1:K:427:MET:HE1	2.49	0.48
1:K:215:GLN:OE1	1:K:367:VAL:HG13	2.12	0.48
1:A:442:MET:N	1:A:442:MET:SD	2.86	0.48
1:C:556:GLU:HG2	1:C:603:GLN:HG3	1.96	0.48
1:D:434:ASP:N	1:D:434:ASP:OD1	2.43	0.48
1:D:556:GLU:HG2	1:D:603:GLN:HG3	1.96	0.48
1:E:469:VAL:HG22	1:E:540:ILE:HG12	1.95	0.48
1:E:632:ALA:HA	1:E:635:ARG:HG3	1.96	0.48
1:G:356:ALA:O	1:G:362:ARG:NH1	2.36	0.48
1:G:640:ASP:OD1	1:G:640:ASP:N	2.45	0.48
1:H:27:ILE:O	1:H:81:LYS:NZ	2.45	0.48
1:H:313:ARG:NH2	1:H:353:ILE:O	2.45	0.48
1:H:503:PHE:HD2	1:H:510:PRO:HG3	1.79	0.48
1:H:526:LEU:HD12	2:H:901:JDP:C06	2.43	0.48
1:J:382:GLN:HA	1:J:385:THR:HG22	1.96	0.48
1:J:434:ASP:N	1:J:434:ASP:OD1	2.43	0.48
1:J:556:GLU:HG2	1:J:603:GLN:HG3	1.96	0.48
1:K:223:PRO:O	1:K:340:HIS:ND1	2.47	0.48
1:K:469:VAL:HG22	1:K:540:ILE:HG12	1.95	0.48
1:A:67:ALA:HB2	1:A:92:LEU:HD23	1.96	0.48
1:A:503:PHE:HD2	1:A:510:PRO:HG3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:PRO:O	1:C:340:HIS:ND1	2.47	0.48
1:D:30:GLU:OE1	1:D:89:ARG:NH2	2.47	0.48
1:E:30:GLU:OE1	1:E:89:ARG:NH2	2.47	0.48
1:F:382:GLN:HA	1:F:385:THR:HG22	1.96	0.48
1:G:442:MET:SD	1:G:442:MET:N	2.86	0.48
1:G:526:LEU:HD12	2:G:901:JDP:C06	2.43	0.48
1:I:223:PRO:O	1:I:340:HIS:ND1	2.47	0.48
1:I:556:GLU:HG2	1:I:603:GLN:HG3	1.96	0.48
1:I:653:ARG:O	1:I:657:LEU:HD23	2.14	0.48
1:K:30:GLU:OE1	1:K:89:ARG:NH2	2.47	0.48
1:L:382:GLN:HA	1:L:385:THR:HG22	1.96	0.48
1:B:653:ARG:O	1:B:657:LEU:HD23	2.14	0.48
1:D:653:ARG:O	1:D:657:LEU:HD23	2.14	0.48
1:E:223:PRO:O	1:E:340:HIS:ND1	2.47	0.48
1:G:30:GLU:OE1	1:G:89:ARG:NH2	2.47	0.48
1:G:67:ALA:HB2	1:G:92:LEU:HD23	1.96	0.48
1:H:653:ARG:O	1:H:657:LEU:HD23	2.14	0.48
1:J:30:GLU:OE1	1:J:89:ARG:NH2	2.47	0.48
1:J:653:ARG:O	1:J:657:LEU:HD23	2.14	0.48
1:A:30:GLU:OE1	1:A:89:ARG:NH2	2.47	0.47
1:B:134:TYR:C	1:B:138:TYR:CE2	2.92	0.47
1:B:382:GLN:HA	1:B:385:THR:HG22	1.95	0.47
1:B:624:ASN:OD1	1:B:624:ASN:N	2.42	0.47
1:C:653:ARG:O	1:C:657:LEU:HD23	2.14	0.47
1:D:382:GLN:HA	1:D:385:THR:HG22	1.96	0.47
1:E:556:GLU:HG2	1:E:603:GLN:HG3	1.96	0.47
1:F:223:PRO:O	1:F:340:HIS:ND1	2.47	0.47
1:G:503:PHE:HD2	1:G:510:PRO:HG3	1.79	0.47
1:I:26:LEU:HD23	1:I:82:ILE:HG22	1.95	0.47
1:I:632:ALA:HA	1:I:635:ARG:HG3	1.96	0.47
1:K:556:GLU:HG2	1:K:603:GLN:HG3	1.96	0.47
1:K:632:ALA:HA	1:K:635:ARG:HG3	1.97	0.47
1:A:526:LEU:HD12	2:A:901:JDP:C06	2.43	0.47
1:C:26:LEU:HD23	1:C:82:ILE:HG22	1.95	0.47
1:C:503:PHE:HD2	1:C:510:PRO:HG3	1.79	0.47
1:C:632:ALA:HA	1:C:635:ARG:HG3	1.96	0.47
1:E:653:ARG:O	1:E:657:LEU:HD23	2.14	0.47
1:F:526:LEU:HD12	2:F:901:JDP:C06	2.43	0.47
1:H:556:GLU:HG2	1:H:603:GLN:HG3	1.96	0.47
1:J:67:ALA:HB2	1:J:92:LEU:HD23	1.95	0.47
1:K:653:ARG:O	1:K:657:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:526:LEU:HD12	2:L:901:JDP:C06	2.43	0.47
1:A:313:ARG:NH2	1:A:353:ILE:O	2.45	0.47
1:B:135:LEU:HG	1:B:138:TYR:CZ	2.49	0.47
1:B:313:ARG:NH2	1:B:353:ILE:O	2.45	0.47
1:B:632:ALA:HA	1:B:635:ARG:HG3	1.96	0.47
1:C:649:ASP:OD1	1:C:652:SER:OG	2.23	0.47
1:D:67:ALA:HB2	1:D:92:LEU:HD23	1.96	0.47
1:F:503:PHE:HD2	1:F:510:PRO:HG3	1.79	0.47
1:G:95:ARG:HG3	1:G:95:ARG:NH1	2.27	0.47
1:J:235:VAL:HG23	1:K:158:MET:HE1	1.96	0.47
1:L:223:PRO:O	1:L:340:HIS:ND1	2.47	0.47
1:B:26:LEU:HD23	1:B:82:ILE:HG22	1.95	0.47
1:B:556:GLU:HG2	1:B:603:GLN:HG3	1.96	0.47
1:D:26:LEU:HD23	1:D:82:ILE:HG22	1.95	0.47
1:D:134:TYR:C	1:D:138:TYR:CE2	2.93	0.47
1:D:632:ALA:HA	1:D:635:ARG:HG3	1.96	0.47
1:E:442:MET:N	1:E:442:MET:SD	2.86	0.47
1:F:428:ASP:N	1:F:428:ASP:OD1	2.46	0.47
1:G:313:ARG:NH2	1:G:353:ILE:O	2.45	0.47
1:H:382:GLN:HA	1:H:385:THR:HG22	1.96	0.47
1:H:632:ALA:HA	1:H:635:ARG:HG3	1.96	0.47
1:I:503:PHE:HD2	1:I:510:PRO:HG3	1.79	0.47
1:J:26:LEU:HD23	1:J:82:ILE:HG22	1.95	0.47
1:J:95:ARG:HG3	1:J:95:ARG:NH1	2.27	0.47
1:K:382:GLN:HA	1:K:385:THR:HG22	1.96	0.47
1:L:428:ASP:OD1	1:L:428:ASP:N	2.46	0.47
1:A:223:PRO:O	1:A:340:HIS:ND1	2.47	0.47
1:A:653:ARG:O	1:A:657:LEU:HD23	2.14	0.47
1:F:252:THR:OG1	3:F:902:ADP:O3B	2.26	0.47
1:G:223:PRO:O	1:G:340:HIS:ND1	2.47	0.47
1:H:134:TYR:C	1:H:138:TYR:CE2	2.93	0.47
1:I:134:TYR:C	1:I:138:TYR:CE2	2.93	0.47
1:J:134:TYR:C	1:J:138:TYR:CE2	2.93	0.47
1:J:632:ALA:HA	1:J:635:ARG:HG3	1.96	0.47
1:L:632:ALA:HA	1:L:635:ARG:HG3	1.96	0.47
1:C:134:TYR:C	1:C:138:TYR:CE2	2.93	0.47
1:E:26:LEU:HD23	1:E:82:ILE:HG22	1.95	0.47
1:E:382:GLN:HA	1:E:385:THR:HG22	1.96	0.47
1:E:403:THR:OG1	1:E:406:HIS:CE1	2.68	0.47
1:F:556:GLU:HG2	1:F:603:GLN:HG3	1.96	0.47
1:F:632:ALA:HA	1:F:635:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:556:GLU:HG2	1:G:603:GLN:HG3	1.96	0.47
1:H:26:LEU:HD23	1:H:82:ILE:HG22	1.95	0.47
1:H:135:LEU:HG	1:H:138:TYR:CZ	2.49	0.47
1:H:624:ASN:OD1	1:H:624:ASN:N	2.42	0.47
1:K:442:MET:N	1:K:442:MET:SD	2.86	0.47
1:L:580:ASP:OD1	1:L:623:THR:OG1	2.29	0.47
1:A:62:LYS:NZ	1:A:98:ASP:OD2	2.40	0.47
1:A:155:ARG:HH21	1:A:386:LYS:NZ	2.09	0.47
1:A:556:GLU:HG2	1:A:603:GLN:HG3	1.96	0.47
1:B:67:ALA:HB2	1:B:92:LEU:HD23	1.96	0.47
1:D:95:ARG:HG3	1:D:95:ARG:NH1	2.27	0.47
1:D:442:MET:SD	1:D:442:MET:N	2.86	0.47
1:D:543:LYS:HA	1:D:577:ASP:HB3	1.97	0.47
1:E:155:ARG:HH21	1:E:386:LYS:NZ	2.09	0.47
1:F:134:TYR:C	1:F:138:TYR:CE2	2.93	0.47
1:F:580:ASP:OD1	1:F:623:THR:OG1	2.29	0.47
1:G:62:LYS:NZ	1:G:98:ASP:OD2	2.40	0.47
1:G:653:ARG:O	1:G:657:LEU:HD23	2.14	0.47
1:H:67:ALA:HB2	1:H:92:LEU:HD23	1.95	0.47
1:J:543:LYS:HA	1:J:577:ASP:HB3	1.97	0.47
1:K:26:LEU:HD23	1:K:82:ILE:HG22	1.95	0.47
1:K:155:ARG:HH21	1:K:386:LYS:NZ	2.09	0.47
1:L:503:PHE:HD2	1:L:510:PRO:HG3	1.79	0.47
1:L:556:GLU:HG2	1:L:603:GLN:HG3	1.96	0.47
1:L:732:ARG:HH12	1:L:734:ASP:HB3	1.79	0.47
1:C:131:PHE:HD1	1:C:135:LEU:HD13	1.80	0.47
1:D:275:MET:SD	1:D:275:MET:N	2.88	0.47
1:D:678:MET:HE1	1:I:677:LYS:HG2	1.96	0.47
1:E:428:ASP:N	1:E:428:ASP:OD1	2.46	0.47
1:F:732:ARG:HH12	1:F:734:ASP:HB3	1.79	0.47
1:G:134:TYR:C	1:G:138:TYR:CE2	2.93	0.47
1:G:155:ARG:HH21	1:G:386:LYS:NZ	2.09	0.47
1:J:275:MET:N	1:J:275:MET:SD	2.88	0.47
1:J:442:MET:N	1:J:442:MET:SD	2.86	0.47
1:K:403:THR:OG1	1:K:406:HIS:CE1	2.68	0.47
1:K:428:ASP:N	1:K:428:ASP:OD1	2.46	0.47
1:L:442:MET:SD	1:L:442:MET:N	2.86	0.47
1:A:514:VAL:HG23	1:A:641:GLN:O	2.15	0.47
1:A:632:ALA:HA	1:A:635:ARG:HG3	1.97	0.47
1:C:217:LYS:H	1:C:217:LYS:HG2	1.58	0.47
1:E:503:PHE:HD2	1:E:510:PRO:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:607:GLU:CD	1:F:465:ARG:HH22	2.22	0.47
1:G:514:VAL:HG23	1:G:641:GLN:O	2.15	0.47
1:I:67:ALA:HB2	1:I:92:LEU:HD23	1.95	0.47
1:I:649:ASP:OD1	1:I:652:SER:OG	2.23	0.47
1:J:491:GLU:HB3	1:K:700:ARG:HH21	1.79	0.47
1:L:134:TYR:C	1:L:138:TYR:CE2	2.93	0.47
1:L:403:THR:OG1	1:L:406:HIS:CE1	2.68	0.47
1:L:653:ARG:O	1:L:657:LEU:HD23	2.14	0.47
1:A:134:TYR:C	1:A:138:TYR:CE2	2.93	0.47
1:A:382:GLN:HA	1:A:385:THR:HG22	1.95	0.47
1:C:67:ALA:HB2	1:C:92:LEU:HD23	1.95	0.47
1:D:131:PHE:HD1	1:D:135:LEU:HD13	1.80	0.47
1:E:134:TYR:C	1:E:138:TYR:CE2	2.93	0.47
1:E:514:VAL:HG23	1:E:641:GLN:O	2.15	0.47
1:F:403:THR:OG1	1:F:406:HIS:CE1	2.68	0.47
1:F:653:ARG:O	1:F:657:LEU:HD23	2.14	0.47
1:G:131:PHE:HD1	1:G:135:LEU:HD13	1.80	0.47
1:G:632:ALA:HA	1:G:635:ARG:HG3	1.96	0.47
1:I:131:PHE:HD1	1:I:135:LEU:HD13	1.80	0.47
1:J:503:PHE:HD2	1:J:510:PRO:HG3	1.79	0.47
1:K:275:MET:N	1:K:275:MET:SD	2.88	0.47
1:K:506:PHE:CE1	1:L:731:ILE:HG13	2.50	0.47
1:K:514:VAL:HG23	1:K:641:GLN:O	2.15	0.47
1:L:275:MET:SD	1:L:275:MET:N	2.88	0.47
1:A:543:LYS:HA	1:A:577:ASP:HB3	1.97	0.46
1:D:503:PHE:HD2	1:D:510:PRO:HG3	1.79	0.46
1:E:275:MET:N	1:E:275:MET:SD	2.88	0.46
1:E:543:LYS:HA	1:E:577:ASP:HB3	1.97	0.46
1:E:761:THR:O	1:F:744:ARG:NH1	2.45	0.46
1:F:275:MET:N	1:F:275:MET:SD	2.88	0.46
1:F:442:MET:N	1:F:442:MET:SD	2.86	0.46
1:G:382:GLN:HA	1:G:385:THR:HG22	1.96	0.46
1:H:235:VAL:HG13	1:I:416:SER:HB2	1.97	0.46
1:J:514:VAL:HG23	1:J:641:GLN:O	2.15	0.46
1:K:503:PHE:HD2	1:K:510:PRO:HG3	1.79	0.46
1:K:543:LYS:HA	1:K:577:ASP:HB3	1.97	0.46
1:A:131:PHE:HD1	1:A:135:LEU:HD13	1.80	0.46
1:C:602:ASN:ND2	1:D:548:LEU:HB3	2.30	0.46
1:D:514:VAL:HG23	1:D:641:GLN:O	2.15	0.46
1:F:79:ASP:OD1	1:F:79:ASP:N	2.42	0.46
1:F:131:PHE:HD1	1:F:135:LEU:HD13	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:543:LYS:HA	1:G:577:ASP:HB3	1.97	0.46
1:I:543:LYS:HA	1:I:577:ASP:HB3	1.97	0.46
1:J:131:PHE:HD1	1:J:135:LEU:HD13	1.80	0.46
1:C:275:MET:N	1:C:275:MET:SD	2.88	0.46
1:C:364:ASP:OD1	1:C:364:ASP:N	2.38	0.46
1:D:403:THR:OG1	1:D:406:HIS:CE1	2.68	0.46
1:E:330:THR:HG21	1:F:273:GLU:HA	1.97	0.46
1:E:580:ASP:OD1	1:E:623:THR:OG1	2.29	0.46
1:I:514:VAL:HG23	1:I:641:GLN:O	2.15	0.46
1:L:79:ASP:OD1	1:L:79:ASP:N	2.42	0.46
1:B:134:TYR:O	1:B:138:TYR:CE2	2.68	0.46
1:F:543:LYS:HA	1:F:577:ASP:HB3	1.97	0.46
1:G:79:ASP:OD1	1:G:79:ASP:N	2.42	0.46
1:G:135:LEU:HG	1:G:138:TYR:CZ	2.49	0.46
1:I:217:LYS:H	1:I:217:LYS:HG2	1.57	0.46
1:I:275:MET:N	1:I:275:MET:SD	2.88	0.46
1:J:326:SER:HB2	1:K:272:PRO:O	2.16	0.46
1:J:403:THR:OG1	1:J:406:HIS:CE1	2.68	0.46
1:K:580:ASP:OD1	1:K:623:THR:OG1	2.29	0.46
1:L:131:PHE:HD1	1:L:135:LEU:HD13	1.80	0.46
1:A:135:LEU:HG	1:A:138:TYR:CZ	2.49	0.46
1:C:514:VAL:HG23	1:C:641:GLN:O	2.16	0.46
1:C:543:LYS:HA	1:C:577:ASP:HB3	1.97	0.46
1:G:217:LYS:H	1:G:217:LYS:HG2	1.57	0.46
1:H:131:PHE:HD1	1:H:135:LEU:HD13	1.80	0.46
1:I:252:THR:OG1	3:I:902:ADP:O1B	2.20	0.46
1:I:674:PHE:CZ	1:I:678:MET:SD	3.09	0.46
1:K:134:TYR:C	1:K:138:TYR:CE2	2.93	0.46
1:A:79:ASP:OD1	1:A:79:ASP:N	2.42	0.46
1:A:158:MET:HE3	1:F:233:ILE:HB	1.96	0.46
1:A:649:ASP:OD1	1:A:652:SER:OG	2.23	0.46
1:B:217:LYS:H	1:B:217:LYS:HG2	1.58	0.46
1:B:514:VAL:HG23	1:B:641:GLN:O	2.15	0.46
1:C:428:ASP:N	1:C:428:ASP:OD1	2.46	0.46
1:C:674:PHE:CZ	1:C:678:MET:SD	3.09	0.46
1:D:134:TYR:O	1:D:138:TYR:CE2	2.68	0.46
1:D:135:LEU:HG	1:D:138:TYR:CZ	2.49	0.46
1:H:134:TYR:O	1:H:138:TYR:CE2	2.68	0.46
1:H:514:VAL:HG23	1:H:641:GLN:O	2.16	0.46
1:H:589:ASN:N	1:H:589:ASN:OD1	2.45	0.46
1:L:543:LYS:HA	1:L:577:ASP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:GLU:OE1	1:K:766:ARG:NH1	2.49	0.46
1:B:275:MET:N	1:B:275:MET:SD	2.88	0.46
1:B:589:ASN:OD1	1:B:589:ASN:N	2.45	0.46
1:D:461:PRO:HB2	1:D:464:LEU:HD21	1.98	0.46
1:E:461:PRO:HB2	1:E:464:LEU:HD21	1.98	0.46
1:F:268:LEU:HD23	1:F:302:PHE:HD2	1.81	0.46
1:F:294:GLU:HG3	1:F:338:ARG:HD2	1.98	0.46
1:H:275:MET:N	1:H:275:MET:SD	2.88	0.46
1:H:543:LYS:HA	1:H:577:ASP:HB3	1.97	0.46
1:J:134:TYR:O	1:J:138:TYR:CE2	2.69	0.46
1:L:294:GLU:HG3	1:L:338:ARG:HD2	1.98	0.46
1:L:674:PHE:CZ	1:L:678:MET:SD	3.09	0.46
1:A:674:PHE:CZ	1:A:678:MET:SD	3.09	0.46
1:B:131:PHE:HD1	1:B:135:LEU:HD13	1.80	0.46
1:B:543:LYS:HA	1:B:577:ASP:HB3	1.97	0.46
1:E:674:PHE:CZ	1:E:678:MET:SD	3.09	0.46
1:G:134:TYR:O	1:G:138:TYR:CE2	2.68	0.46
1:G:275:MET:N	1:G:275:MET:SD	2.88	0.46
1:I:364:ASP:OD1	1:I:364:ASP:N	2.38	0.46
1:I:428:ASP:OD1	1:I:428:ASP:N	2.46	0.46
1:J:425:LYS:NZ	1:J:451:ASP:OD1	2.30	0.46
1:J:461:PRO:HB2	1:J:464:LEU:HD21	1.98	0.46
1:K:461:PRO:HB2	1:K:464:LEU:HD21	1.98	0.46
1:K:674:PHE:CZ	1:K:678:MET:SD	3.09	0.46
1:L:62:LYS:NZ	1:L:98:ASP:OD2	2.40	0.46
1:L:268:LEU:HD23	1:L:302:PHE:HD2	1.81	0.46
1:A:275:MET:N	1:A:275:MET:SD	2.88	0.46
1:B:506:PHE:CE1	1:C:731:ILE:HG13	2.50	0.46
1:F:514:VAL:HG23	1:F:641:GLN:O	2.15	0.46
1:F:674:PHE:CZ	1:F:678:MET:SD	3.09	0.46
1:G:27:ILE:O	1:G:81:LYS:NZ	2.45	0.46
1:I:508:MET:CE	1:J:699:ILE:CD1	2.70	0.46
1:D:425:LYS:NZ	1:D:451:ASP:OD1	2.30	0.46
1:E:131:PHE:HD1	1:E:135:LEU:HD13	1.80	0.46
1:G:252:THR:OG1	3:G:902:ADP:O1B	2.25	0.46
1:H:674:PHE:CZ	1:H:678:MET:SD	3.09	0.46
1:J:135:LEU:HG	1:J:138:TYR:CZ	2.49	0.46
1:L:461:PRO:HB2	1:L:464:LEU:HD21	1.98	0.46
1:L:514:VAL:HG23	1:L:641:GLN:O	2.15	0.46
1:A:751:ASP:O	1:A:755:TYR:HD1	1.99	0.45
1:B:674:PHE:CZ	1:B:678:MET:SD	3.09	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:674:PHE:CZ	1:D:678:MET:SD	3.09	0.45
1:E:258:VAL:O	1:E:262:THR:OG1	2.21	0.45
1:F:461:PRO:HB2	1:F:464:LEU:HD21	1.98	0.45
1:G:120:ASP:OD1	1:G:120:ASP:N	2.48	0.45
1:I:134:TYR:O	1:I:138:TYR:CE2	2.68	0.45
1:K:131:PHE:HD1	1:K:135:LEU:HD13	1.80	0.45
1:A:27:ILE:O	1:A:81:LYS:NZ	2.45	0.45
1:A:120:ASP:OD1	1:A:120:ASP:N	2.48	0.45
1:A:268:LEU:HD23	1:A:302:PHE:HD2	1.81	0.45
1:C:27:ILE:HG22	1:C:81:LYS:HE2	1.99	0.45
1:D:364:ASP:OD1	1:D:364:ASP:N	2.38	0.45
1:D:677:LYS:HG2	1:I:678:MET:HE1	1.99	0.45
1:G:674:PHE:CZ	1:G:678:MET:SD	3.09	0.45
1:G:751:ASP:O	1:G:755:TYR:HD1	1.99	0.45
1:A:134:TYR:O	1:A:138:TYR:CE2	2.69	0.45
1:E:95:ARG:HG3	1:E:95:ARG:NH1	2.27	0.45
1:E:268:LEU:HD23	1:E:302:PHE:HD2	1.81	0.45
1:E:294:GLU:HG3	1:E:338:ARG:HD2	1.98	0.45
1:F:135:LEU:HG	1:F:138:TYR:CZ	2.49	0.45
1:G:268:LEU:HD23	1:G:302:PHE:HD2	1.81	0.45
1:G:294:GLU:HG3	1:G:338:ARG:HD2	1.98	0.45
1:I:27:ILE:HG22	1:I:81:LYS:HE2	1.99	0.45
1:K:268:LEU:HD23	1:K:302:PHE:HD2	1.81	0.45
1:A:294:GLU:HG3	1:A:338:ARG:HD2	1.98	0.45
1:B:27:ILE:HG22	1:B:81:LYS:HE2	1.99	0.45
1:B:268:LEU:HD23	1:B:302:PHE:HD2	1.81	0.45
1:B:751:ASP:O	1:B:755:TYR:HD1	1.99	0.45
1:C:134:TYR:O	1:C:138:TYR:CE2	2.69	0.45
1:D:233:ILE:HB	1:E:158:MET:HE3	1.97	0.45
1:H:27:ILE:HG22	1:H:81:LYS:HE2	1.99	0.45
1:H:268:LEU:HD23	1:H:302:PHE:HD2	1.81	0.45
1:H:751:ASP:O	1:H:755:TYR:HD1	1.99	0.45
1:K:258:VAL:O	1:K:262:THR:OG1	2.21	0.45
1:K:624:ASN:OD1	1:K:624:ASN:N	2.42	0.45
1:E:624:ASN:OD1	1:E:624:ASN:N	2.42	0.45
1:G:465:ARG:HH22	1:L:607:GLU:CD	2.24	0.45
1:H:217:LYS:H	1:H:217:LYS:HG2	1.57	0.45
1:I:403:THR:OG1	1:I:406:HIS:CE1	2.68	0.45
1:K:95:ARG:HG3	1:K:95:ARG:NH1	2.27	0.45
1:K:294:GLU:HG3	1:K:338:ARG:HD2	1.98	0.45
1:L:148:LYS:HE3	1:L:171:SER:HA	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:450:ASP:OD1	1:L:451:ASP:N	2.50	0.45
1:A:277:LYS:H	1:A:277:LYS:HG2	1.55	0.45
1:B:580:ASP:OD1	1:B:623:THR:OG1	2.29	0.45
1:E:135:LEU:HG	1:E:138:TYR:CZ	2.49	0.45
1:E:450:ASP:OD1	1:E:451:ASP:N	2.50	0.45
1:J:674:PHE:CZ	1:J:678:MET:SD	3.09	0.45
1:K:62:LYS:NZ	1:K:98:ASP:OD2	2.40	0.45
1:K:312:LYS:HE2	1:K:312:LYS:HA	1.99	0.45
1:L:751:ASP:O	1:L:755:TYR:HD1	1.99	0.45
1:C:268:LEU:HD23	1:C:302:PHE:HD2	1.81	0.45
1:E:62:LYS:NZ	1:E:98:ASP:OD2	2.40	0.45
1:E:312:LYS:HE2	1:E:312:LYS:HA	1.99	0.45
1:F:450:ASP:OD1	1:F:451:ASP:N	2.50	0.45
1:I:421:GLN:HB2	1:I:454:TRP:CZ3	2.52	0.45
1:I:491:GLU:HB3	1:J:700:ARG:NH2	2.29	0.45
1:J:27:ILE:HG22	1:J:81:LYS:HE2	1.99	0.45
1:L:135:LEU:HG	1:L:138:TYR:CZ	2.49	0.45
1:C:403:THR:OG1	1:C:406:HIS:CE1	2.68	0.45
1:C:751:ASP:O	1:C:755:TYR:HD1	1.99	0.45
1:D:27:ILE:HG22	1:D:81:LYS:HE2	1.99	0.45
1:F:751:ASP:O	1:F:755:TYR:HD1	1.99	0.45
1:G:421:GLN:HB2	1:G:454:TRP:CZ3	2.52	0.45
1:I:461:PRO:HB2	1:I:464:LEU:HD21	1.98	0.45
1:K:450:ASP:OD1	1:K:451:ASP:N	2.50	0.45
1:A:421:GLN:HB2	1:A:454:TRP:CZ3	2.52	0.45
1:A:519:PRO:HG2	1:A:522:CYS:SG	2.57	0.45
1:B:148:LYS:CE	1:B:170:PRO:C	2.81	0.45
1:C:421:GLN:HB2	1:C:454:TRP:CZ3	2.52	0.45
1:D:560:ARG:HA	1:D:560:ARG:NH1	2.32	0.45
1:G:519:PRO:HG2	1:G:522:CYS:SG	2.57	0.45
1:J:148:LYS:HD3	1:J:148:LYS:HA	1.78	0.45
1:L:312:LYS:HE2	1:L:312:LYS:HA	1.99	0.45
1:B:62:LYS:NZ	1:B:98:ASP:OD2	2.40	0.45
1:D:59:LEU:O	1:D:67:ALA:N	2.50	0.45
1:D:751:ASP:O	1:D:755:TYR:HD1	1.99	0.45
1:E:217:LYS:H	1:E:217:LYS:HG2	1.58	0.45
1:E:519:PRO:HG2	1:E:522:CYS:SG	2.57	0.45
1:F:312:LYS:HE2	1:F:312:LYS:HA	1.99	0.45
1:F:313:ARG:NH2	1:F:353:ILE:O	2.45	0.45
1:H:421:GLN:HB2	1:H:454:TRP:CZ3	2.52	0.45
1:I:268:LEU:HD23	1:I:302:PHE:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:751:ASP:O	1:I:755:TYR:HD1	1.99	0.45
1:J:59:LEU:O	1:J:67:ALA:N	2.50	0.45
1:J:560:ARG:HA	1:J:560:ARG:NH1	2.32	0.45
1:K:135:LEU:HG	1:K:138:TYR:CZ	2.50	0.45
1:L:27:ILE:O	1:L:81:LYS:NZ	2.45	0.45
1:L:421:GLN:HB2	1:L:454:TRP:CZ3	2.52	0.45
1:A:450:ASP:OD1	1:A:451:ASP:N	2.50	0.44
1:B:294:GLU:HG3	1:B:338:ARG:HD2	1.98	0.44
1:B:421:GLN:HB2	1:B:454:TRP:CZ3	2.52	0.44
1:C:59:LEU:O	1:C:67:ALA:N	2.50	0.44
1:C:235:VAL:HG13	1:D:416:SER:HB2	1.99	0.44
1:C:450:ASP:OD1	1:C:451:ASP:N	2.50	0.44
1:C:461:PRO:HB2	1:C:464:LEU:HD21	1.98	0.44
1:D:268:LEU:HD23	1:D:302:PHE:HD2	1.81	0.44
1:D:421:GLN:HB2	1:D:454:TRP:CZ3	2.52	0.44
1:D:584:LYS:HD3	1:D:625:ARG:HD3	1.99	0.44
1:F:62:LYS:NZ	1:F:98:ASP:OD2	2.41	0.44
1:F:421:GLN:HB2	1:F:454:TRP:CZ3	2.52	0.44
1:G:27:ILE:HG22	1:G:81:LYS:HE2	1.99	0.44
1:G:277:LYS:H	1:G:277:LYS:HG2	1.55	0.44
1:G:450:ASP:OD1	1:G:451:ASP:N	2.50	0.44
1:H:403:THR:OG1	1:H:406:HIS:CE1	2.68	0.44
1:H:519:PRO:HG2	1:H:522:CYS:SG	2.57	0.44
1:I:450:ASP:OD1	1:I:451:ASP:N	2.50	0.44
1:I:768:PHE:O	1:J:741:ARG:HA	2.17	0.44
1:J:268:LEU:HD23	1:J:302:PHE:HD2	1.81	0.44
1:J:294:GLU:HG3	1:J:338:ARG:HD2	1.98	0.44
1:J:751:ASP:O	1:J:755:TYR:HD1	1.99	0.44
1:K:519:PRO:HG2	1:K:522:CYS:SG	2.57	0.44
1:L:313:ARG:NH2	1:L:353:ILE:O	2.45	0.44
1:A:27:ILE:HG22	1:A:81:LYS:HE2	1.99	0.44
1:A:461:PRO:HB2	1:A:464:LEU:HD21	1.98	0.44
1:B:403:THR:OG1	1:B:406:HIS:CE1	2.68	0.44
1:C:60:LYS:HZ2	1:C:103:GLN:HG2	1.83	0.44
1:F:27:ILE:O	1:F:81:LYS:NZ	2.45	0.44
1:G:461:PRO:HB2	1:G:464:LEU:HD21	1.98	0.44
1:H:62:LYS:NZ	1:H:98:ASP:OD2	2.40	0.44
1:I:59:LEU:O	1:I:67:ALA:N	2.51	0.44
1:J:421:GLN:HB2	1:J:454:TRP:CZ3	2.52	0.44
1:J:584:LYS:HD3	1:J:625:ARG:HD3	1.99	0.44
1:A:403:THR:OG1	1:A:406:HIS:CE1	2.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:ARG:HA	1:A:560:ARG:NH1	2.32	0.44
1:A:700:ARG:HH21	1:F:491:GLU:HB3	1.82	0.44
1:B:519:PRO:HG2	1:B:522:CYS:SG	2.57	0.44
1:D:294:GLU:HG3	1:D:338:ARG:HD2	1.98	0.44
1:D:312:LYS:HE2	1:D:312:LYS:HA	1.99	0.44
1:E:151:ILE:HG12	1:E:164:LYS:HD3	2.00	0.44
1:G:403:THR:OG1	1:G:406:HIS:CE1	2.68	0.44
1:G:560:ARG:HA	1:G:560:ARG:NH1	2.33	0.44
1:G:602:ASN:ND2	1:H:548:LEU:HB3	2.33	0.44
1:H:120:ASP:OD1	1:H:120:ASP:N	2.48	0.44
1:H:560:ARG:HA	1:H:560:ARG:NH1	2.32	0.44
1:K:151:ILE:HG12	1:K:164:LYS:HD3	1.99	0.44
1:K:217:LYS:H	1:K:217:LYS:HG2	1.58	0.44
1:K:516:PHE:HB3	1:K:643:ILE:CG1	2.48	0.44
1:K:751:ASP:O	1:K:755:TYR:HD1	1.99	0.44
1:B:120:ASP:OD1	1:B:120:ASP:N	2.48	0.44
1:B:461:PRO:HB2	1:B:464:LEU:HD21	1.98	0.44
1:B:560:ARG:HA	1:B:560:ARG:NH1	2.32	0.44
1:C:294:GLU:HG3	1:C:338:ARG:HD2	1.98	0.44
1:C:584:LYS:HD3	1:C:625:ARG:HD3	2.00	0.44
1:D:116:VAL:HG22	1:D:182:ILE:HD11	2.00	0.44
1:E:27:ILE:HG22	1:E:81:LYS:HE2	1.99	0.44
1:E:516:PHE:HB3	1:E:643:ILE:CG1	2.48	0.44
1:F:116:VAL:HG22	1:F:182:ILE:HD11	2.00	0.44
1:G:139:PHE:HE1	1:G:144:ARG:HH11	1.65	0.44
1:H:294:GLU:HG3	1:H:338:ARG:HD2	1.98	0.44
1:I:294:GLU:HG3	1:I:338:ARG:HD2	1.98	0.44
1:I:519:PRO:HG2	1:I:522:CYS:SG	2.57	0.44
1:I:584:LYS:HD3	1:I:625:ARG:HD3	2.00	0.44
1:J:312:LYS:HA	1:J:312:LYS:HE2	1.99	0.44
1:J:364:ASP:OD1	1:J:364:ASP:N	2.38	0.44
1:K:27:ILE:HG22	1:K:81:LYS:HE2	1.99	0.44
1:K:584:LYS:HD3	1:K:625:ARG:HD3	2.00	0.44
1:A:380:ILE:HD11	3:A:902:ADP:C6	2.52	0.44
1:B:428:ASP:OD1	1:B:428:ASP:N	2.46	0.44
1:C:277:LYS:H	1:C:277:LYS:HG2	1.55	0.44
1:E:584:LYS:HD3	1:E:625:ARG:HD3	2.00	0.44
1:E:751:ASP:O	1:E:755:TYR:HD1	1.99	0.44
1:F:59:LEU:O	1:F:67:ALA:N	2.50	0.44
1:G:116:VAL:HG22	1:G:182:ILE:HD11	2.00	0.44
1:G:233:ILE:HB	1:H:158:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:516:PHE:HB3	1:H:643:ILE:CG1	2.48	0.44
1:J:519:PRO:HG2	1:J:522:CYS:SG	2.57	0.44
1:K:421:GLN:HB2	1:K:454:TRP:CZ3	2.52	0.44
1:L:59:LEU:O	1:L:67:ALA:N	2.51	0.44
1:L:519:PRO:HG2	1:L:522:CYS:SG	2.57	0.44
1:A:116:VAL:HG22	1:A:182:ILE:HD11	2.00	0.44
1:B:516:PHE:HB3	1:B:643:ILE:CG1	2.48	0.44
1:C:519:PRO:HG2	1:C:522:CYS:SG	2.57	0.44
1:D:62:LYS:NZ	1:D:98:ASP:OD2	2.40	0.44
1:D:519:PRO:HG2	1:D:522:CYS:SG	2.57	0.44
1:H:461:PRO:HB2	1:H:464:LEU:HD21	1.98	0.44
1:J:116:VAL:HG22	1:J:182:ILE:HD11	2.00	0.44
1:J:580:ASP:OD1	1:J:623:THR:OG1	2.29	0.44
1:K:330:THR:HG21	1:L:273:GLU:HA	2.00	0.44
1:L:116:VAL:HG22	1:L:182:ILE:HD11	2.00	0.44
1:L:139:PHE:HE1	1:L:144:ARG:HH11	1.65	0.44
1:A:139:PHE:HE1	1:A:144:ARG:HH11	1.65	0.44
1:A:607:GLU:CD	1:B:465:ARG:HH22	2.25	0.44
1:B:391:ALA:HB3	1:B:394:VAL:HG23	1.99	0.44
1:D:148:LYS:HD3	1:D:148:LYS:HA	1.78	0.44
1:D:516:PHE:HB3	1:D:643:ILE:CG1	2.48	0.44
1:E:391:ALA:HB3	1:E:394:VAL:HG23	1.99	0.44
1:E:421:GLN:HB2	1:E:454:TRP:CZ3	2.52	0.44
1:F:560:ARG:HA	1:F:560:ARG:NH1	2.32	0.44
1:H:391:ALA:HB3	1:H:394:VAL:HG23	1.99	0.44
1:H:491:GLU:HB3	1:I:700:ARG:NH2	2.31	0.44
1:J:516:PHE:HB3	1:J:643:ILE:CG1	2.48	0.44
1:K:503:PHE:HE1	1:L:699:ILE:HG21	1.82	0.44
1:L:560:ARG:HA	1:L:560:ARG:NH1	2.32	0.44
1:B:27:ILE:O	1:B:81:LYS:NZ	2.45	0.44
1:B:148:LYS:HE3	1:B:171:SER:HA	1.86	0.44
1:B:312:LYS:HA	1:B:312:LYS:HE2	1.99	0.44
1:C:116:VAL:HG22	1:C:182:ILE:HD11	2.00	0.44
1:C:391:ALA:HB3	1:C:394:VAL:HG23	2.00	0.44
1:C:560:ARG:HA	1:C:560:ARG:NH1	2.32	0.44
1:F:484:ASP:OD1	1:F:484:ASP:N	2.49	0.44
1:F:519:PRO:HG2	1:F:522:CYS:SG	2.57	0.44
1:I:148:LYS:HA	1:I:148:LYS:HD3	1.78	0.44
1:K:391:ALA:HB3	1:K:394:VAL:HG23	1.99	0.44
1:K:560:ARG:HA	1:K:560:ARG:NH1	2.33	0.44
1:L:484:ASP:OD1	1:L:484:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASP:OD1	1:B:79:ASP:N	2.42	0.44
1:B:277:LYS:H	1:B:277:LYS:HG2	1.55	0.44
1:B:450:ASP:OD1	1:B:451:ASP:N	2.50	0.44
1:E:116:VAL:HG22	1:E:182:ILE:HD11	2.00	0.44
1:E:560:ARG:HA	1:E:560:ARG:NH1	2.33	0.44
1:F:27:ILE:HG22	1:F:81:LYS:HE2	1.99	0.44
1:F:139:PHE:HE1	1:F:144:ARG:HH11	1.65	0.44
1:F:391:ALA:HB3	1:F:394:VAL:HG23	1.99	0.44
1:H:139:PHE:HE1	1:H:144:ARG:HH11	1.65	0.44
1:H:450:ASP:OD1	1:H:451:ASP:N	2.50	0.44
1:H:487:ARG:HE	1:I:700:ARG:CZ	2.31	0.44
1:I:277:LYS:H	1:I:277:LYS:HG2	1.55	0.44
1:I:391:ALA:HB3	1:I:394:VAL:HG23	2.00	0.44
1:I:516:PHE:HB3	1:I:643:ILE:CG1	2.48	0.44
1:I:560:ARG:HA	1:I:560:ARG:NH1	2.32	0.44
1:I:649:ASP:N	1:I:649:ASP:OD1	2.42	0.44
1:J:450:ASP:OD1	1:J:451:ASP:N	2.50	0.44
1:K:116:VAL:HG22	1:K:182:ILE:HD11	2.00	0.44
1:L:27:ILE:HG22	1:L:81:LYS:HE2	1.99	0.44
1:A:516:PHE:HB3	1:A:643:ILE:CG1	2.48	0.43
1:B:72:LEU:HD12	1:B:72:LEU:HA	1.89	0.43
1:B:139:PHE:HE1	1:B:144:ARG:HH11	1.65	0.43
1:D:450:ASP:OD1	1:D:451:ASP:N	2.50	0.43
1:G:700:ARG:CZ	1:L:487:ARG:HE	2.30	0.43
1:H:312:LYS:HE2	1:H:312:LYS:HA	1.99	0.43
1:I:116:VAL:HG22	1:I:182:ILE:HD11	2.00	0.43
1:J:62:LYS:NZ	1:J:98:ASP:OD2	2.40	0.43
1:L:391:ALA:HB3	1:L:394:VAL:HG23	2.00	0.43
1:L:584:LYS:HD3	1:L:625:ARG:HD3	1.99	0.43
1:A:625:ARG:HH11	1:A:625:ARG:HG2	1.84	0.43
1:B:625:ARG:HG2	1:B:625:ARG:HH11	1.83	0.43
1:C:625:ARG:HG2	1:C:625:ARG:HH11	1.84	0.43
1:D:580:ASP:OD1	1:D:623:THR:OG1	2.29	0.43
1:H:59:LEU:O	1:H:67:ALA:N	2.51	0.43
1:H:135:LEU:CA	1:H:138:TYR:HE2	2.25	0.43
1:I:235:VAL:HG11	1:J:420:LEU:HD11	1.99	0.43
1:K:139:PHE:HE1	1:K:144:ARG:HH11	1.65	0.43
1:K:649:ASP:OD1	1:K:652:SER:OG	2.23	0.43
1:A:59:LEU:O	1:A:67:ALA:N	2.50	0.43
1:B:59:LEU:O	1:B:67:ALA:N	2.51	0.43
1:D:60:LYS:HZ2	1:D:103:GLN:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:VAL:O	1:D:262:THR:OG1	2.21	0.43
1:E:139:PHE:HE1	1:E:144:ARG:HH11	1.65	0.43
1:E:625:ARG:HG2	1:E:625:ARG:HH11	1.84	0.43
1:F:584:LYS:HD3	1:F:625:ARG:HD3	2.00	0.43
1:G:625:ARG:HG2	1:G:625:ARG:HH11	1.84	0.43
1:H:79:ASP:OD1	1:H:79:ASP:N	2.42	0.43
1:H:584:LYS:HD3	1:H:625:ARG:HD3	2.00	0.43
1:H:625:ARG:HG2	1:H:625:ARG:HH11	1.84	0.43
1:I:625:ARG:HH11	1:I:625:ARG:HG2	1.84	0.43
1:L:516:PHE:HB3	1:L:643:ILE:CG1	2.48	0.43
1:A:773:PHE:CE2	1:B:733:ARG:HG2	2.53	0.43
1:B:116:VAL:HG22	1:B:182:ILE:HD11	2.00	0.43
1:D:649:ASP:OD1	1:D:652:SER:OG	2.23	0.43
1:E:533:ASN:HD22	1:E:533:ASN:HA	1.61	0.43
1:F:136:LYS:HB2	1:F:137:PRO:HD3	2.01	0.43
1:F:151:ILE:HG12	1:F:164:LYS:HD3	2.00	0.43
1:G:59:LEU:O	1:G:67:ALA:N	2.51	0.43
1:H:116:VAL:HG22	1:H:182:ILE:HD11	2.00	0.43
1:H:487:ARG:HE	1:I:700:ARG:NH1	2.17	0.43
1:J:139:PHE:HE1	1:J:144:ARG:HH11	1.65	0.43
1:K:625:ARG:HG2	1:K:625:ARG:HH11	1.84	0.43
1:L:151:ILE:HG12	1:L:164:LYS:HD3	2.00	0.43
1:A:484:ASP:OD1	1:A:484:ASP:N	2.49	0.43
1:A:580:ASP:HB2	1:A:628:ILE:HD11	2.00	0.43
1:C:148:LYS:HD3	1:C:148:LYS:HA	1.78	0.43
1:C:649:ASP:N	1:C:649:ASP:OD1	2.42	0.43
1:E:59:LEU:O	1:E:67:ALA:N	2.51	0.43
1:E:602:ASN:HD21	1:F:548:LEU:HB3	1.82	0.43
1:F:516:PHE:HB3	1:F:643:ILE:CG1	2.48	0.43
1:G:484:ASP:OD1	1:G:484:ASP:N	2.49	0.43
1:H:151:ILE:HG12	1:H:164:LYS:HD3	2.00	0.43
1:I:139:PHE:HE1	1:I:144:ARG:HH11	1.65	0.43
1:I:312:LYS:HE2	1:I:312:LYS:HA	1.99	0.43
1:J:136:LYS:HB2	1:J:137:PRO:HD3	2.01	0.43
1:J:258:VAL:O	1:J:262:THR:OG1	2.21	0.43
1:K:59:LEU:O	1:K:67:ALA:N	2.51	0.43
1:A:148:LYS:HE3	1:A:171:SER:HA	1.86	0.43
1:A:491:GLU:HB3	1:B:700:ARG:NH2	2.34	0.43
1:A:584:LYS:HD3	1:A:625:ARG:HD3	2.00	0.43
1:B:584:LYS:HD3	1:B:625:ARG:HD3	2.00	0.43
1:D:277:LYS:H	1:D:277:LYS:HG2	1.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:649:ASP:OD1	1:E:652:SER:OG	2.23	0.43
1:F:625:ARG:HG2	1:F:625:ARG:HH11	1.84	0.43
1:G:312:LYS:HE2	1:G:312:LYS:HA	1.99	0.43
1:G:580:ASP:HB2	1:G:628:ILE:HD11	2.00	0.43
1:H:277:LYS:H	1:H:277:LYS:HG2	1.55	0.43
1:H:580:ASP:HB2	1:H:628:ILE:HD11	2.00	0.43
1:I:235:VAL:HG13	1:J:416:SER:HB2	2.01	0.43
1:L:136:LYS:HB2	1:L:137:PRO:HD3	2.01	0.43
1:A:151:ILE:HG12	1:A:164:LYS:HD3	2.00	0.43
1:A:495:TYR:CD2	1:B:703:ILE:HD12	2.53	0.43
1:B:151:ILE:HG12	1:B:164:LYS:HD3	2.00	0.43
1:B:491:GLU:HB3	1:C:700:ARG:NH2	2.34	0.43
1:B:580:ASP:HB2	1:B:628:ILE:HD11	2.00	0.43
1:C:139:PHE:HE1	1:C:144:ARG:HH11	1.65	0.43
1:C:312:LYS:HE2	1:C:312:LYS:HA	1.99	0.43
1:C:516:PHE:HB3	1:C:643:ILE:CG1	2.48	0.43
1:D:136:LYS:HB2	1:D:137:PRO:HD3	2.01	0.43
1:D:139:PHE:HE1	1:D:144:ARG:HH11	1.65	0.43
1:H:60:LYS:HZ2	1:H:103:GLN:HG2	1.83	0.43
1:H:72:LEU:HD12	1:H:72:LEU:HA	1.89	0.43
1:H:130:LEU:CG	1:H:134:TYR:CD2	2.90	0.43
1:J:77:CYS:SG	1:J:78:SER:N	2.92	0.43
1:K:359:ARG:HD2	1:L:247:PRO:HG2	2.00	0.43
1:A:77:CYS:SG	1:A:78:SER:N	2.92	0.43
1:A:136:LYS:HB2	1:A:137:PRO:HD3	2.01	0.43
1:A:312:LYS:HE2	1:A:312:LYS:HA	1.99	0.43
1:C:79:ASP:OD1	1:C:79:ASP:N	2.42	0.43
1:G:584:LYS:HD3	1:G:625:ARG:HD3	2.00	0.43
1:K:533:ASN:HD22	1:K:533:ASN:HA	1.61	0.43
1:A:148:LYS:CE	1:A:170:PRO:C	2.81	0.43
1:B:77:CYS:SG	1:B:78:SER:N	2.92	0.43
1:C:77:CYS:SG	1:C:78:SER:N	2.92	0.43
1:C:151:ILE:HG12	1:C:164:LYS:HD3	2.00	0.43
1:D:77:CYS:SG	1:D:78:SER:N	2.92	0.43
1:D:391:ALA:HB3	1:D:394:VAL:HG23	2.00	0.43
1:D:625:ARG:HG2	1:D:625:ARG:HH11	1.84	0.43
1:G:77:CYS:SG	1:G:78:SER:N	2.92	0.43
1:G:136:LYS:HB2	1:G:137:PRO:HD3	2.01	0.43
1:I:77:CYS:SG	1:I:78:SER:N	2.92	0.43
1:J:391:ALA:HB3	1:J:394:VAL:HG23	1.99	0.43
1:J:649:ASP:OD1	1:J:652:SER:OG	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:625:ARG:HG2	1:L:625:ARG:HH11	1.84	0.43
1:B:135:LEU:CA	1:B:138:TYR:HE2	2.25	0.43
1:C:572:CYS:SG	1:C:573:VAL:N	2.92	0.43
1:F:580:ASP:HB2	1:F:628:ILE:HD11	2.00	0.43
1:G:151:ILE:HG12	1:G:164:LYS:HD3	2.00	0.43
1:H:77:CYS:SG	1:H:78:SER:N	2.92	0.43
1:H:572:CYS:SG	1:H:573:VAL:N	2.92	0.43
1:I:423:ILE:HD12	1:I:424:ARG:N	2.34	0.43
1:I:572:CYS:SG	1:I:573:VAL:N	2.92	0.43
1:J:277:LYS:H	1:J:277:LYS:HG2	1.55	0.43
1:J:625:ARG:HG2	1:J:625:ARG:HH11	1.83	0.43
1:L:580:ASP:HB2	1:L:628:ILE:HD11	2.00	0.43
1:A:391:ALA:HB3	1:A:394:VAL:HG23	1.99	0.42
1:B:533:ASN:HD22	1:B:533:ASN:HA	1.61	0.42
1:B:572:CYS:SG	1:B:573:VAL:N	2.92	0.42
1:C:136:LYS:HB2	1:C:137:PRO:HD3	2.01	0.42
1:D:269:ILE:HD11	1:D:303:ILE:HG12	2.01	0.42
1:E:134:TYR:O	1:E:138:TYR:CE2	2.68	0.42
1:E:148:LYS:HA	1:E:148:LYS:HD3	1.78	0.42
1:F:77:CYS:SG	1:F:78:SER:N	2.92	0.42
1:F:364:ASP:OD1	1:F:364:ASP:N	2.38	0.42
1:G:391:ALA:HB3	1:G:394:VAL:HG23	2.00	0.42
1:I:60:LYS:HZ2	1:I:103:GLN:HG2	1.84	0.42
1:J:60:LYS:HZ2	1:J:103:GLN:HG2	1.84	0.42
1:J:572:CYS:SG	1:J:573:VAL:N	2.92	0.42
1:K:572:CYS:SG	1:K:573:VAL:N	2.92	0.42
1:A:572:CYS:SG	1:A:573:VAL:N	2.92	0.42
1:B:423:ILE:HD12	1:B:424:ARG:N	2.34	0.42
1:B:487:ARG:HE	1:C:700:ARG:CZ	2.31	0.42
1:C:423:ILE:HD12	1:C:424:ARG:N	2.34	0.42
1:D:572:CYS:SG	1:D:573:VAL:N	2.92	0.42
1:E:60:LYS:HZ2	1:E:103:GLN:HG2	1.84	0.42
1:E:81:LYS:HD2	1:E:81:LYS:HA	1.78	0.42
1:G:572:CYS:SG	1:G:573:VAL:N	2.92	0.42
1:I:151:ILE:HG12	1:I:164:LYS:HD3	2.00	0.42
1:I:624:ASN:O	1:I:755:TYR:OH	2.12	0.42
1:K:60:LYS:HZ2	1:K:103:GLN:HG2	1.84	0.42
1:L:77:CYS:SG	1:L:78:SER:N	2.92	0.42
1:C:580:ASP:HB2	1:C:628:ILE:HD11	2.00	0.42
1:D:219:MET:SD	1:D:365:ARG:CZ	3.07	0.42
1:D:423:ILE:HD12	1:D:424:ARG:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:572:CYS:SG	1:E:573:VAL:N	2.92	0.42
1:I:580:ASP:HB2	1:I:628:ILE:HD11	2.00	0.42
1:J:269:ILE:HD11	1:J:303:ILE:HG12	2.01	0.42
1:J:423:ILE:HD12	1:J:424:ARG:N	2.34	0.42
1:A:679:THR:HB	1:A:682:PHE:CG	2.55	0.42
1:D:151:ILE:HG12	1:D:164:LYS:HD3	2.00	0.42
1:D:508:MET:CE	1:E:699:ILE:CD1	2.82	0.42
1:D:679:THR:HB	1:D:682:PHE:CG	2.55	0.42
1:D:750:ASN:HD22	1:I:750:ASN:HD22	1.67	0.42
1:E:27:ILE:O	1:E:81:LYS:NZ	2.45	0.42
1:F:750:ASN:HD22	1:G:750:ASN:HD22	1.68	0.42
1:G:679:THR:HB	1:G:682:PHE:CG	2.55	0.42
1:H:423:ILE:HD12	1:H:424:ARG:N	2.34	0.42
1:H:533:ASN:HD22	1:H:533:ASN:HA	1.61	0.42
1:I:219:MET:SD	1:I:365:ARG:CZ	3.08	0.42
1:J:679:THR:HB	1:J:682:PHE:CG	2.55	0.42
1:K:148:LYS:HA	1:K:148:LYS:HD3	1.78	0.42
1:L:364:ASP:OD1	1:L:364:ASP:N	2.38	0.42
1:A:219:MET:SD	1:A:365:ARG:CZ	3.07	0.42
1:A:624:ASN:O	1:A:755:TYR:OH	2.12	0.42
1:C:219:MET:SD	1:C:365:ARG:CZ	3.08	0.42
1:E:269:ILE:HD11	1:E:303:ILE:HG12	2.01	0.42
1:E:580:ASP:HB2	1:E:628:ILE:HD11	2.00	0.42
1:G:258:VAL:O	1:G:262:THR:OG1	2.21	0.42
1:G:423:ILE:HD12	1:G:424:ARG:N	2.34	0.42
1:I:136:LYS:HB2	1:I:137:PRO:HD3	2.01	0.42
1:J:151:ILE:HG12	1:J:164:LYS:HD3	2.00	0.42
1:J:219:MET:SD	1:J:365:ARG:CZ	3.08	0.42
1:K:27:ILE:O	1:K:81:LYS:NZ	2.45	0.42
1:K:580:ASP:HB2	1:K:628:ILE:HD11	2.00	0.42
1:L:216:ILE:H	1:L:216:ILE:HG12	1.69	0.42
1:A:423:ILE:HD12	1:A:424:ARG:N	2.34	0.42
1:C:148:LYS:HE2	1:C:171:SER:HB2	2.02	0.42
1:D:580:ASP:HB2	1:D:628:ILE:HD11	2.00	0.42
1:E:77:CYS:SG	1:E:78:SER:N	2.92	0.42
1:F:572:CYS:SG	1:F:573:VAL:N	2.92	0.42
1:G:219:MET:SD	1:G:365:ARG:CZ	3.07	0.42
1:G:283:GLU:O	1:G:286:LEU:HD23	2.20	0.42
1:G:580:ASP:OD1	1:G:623:THR:OG1	2.29	0.42
1:H:136:LYS:HB2	1:H:137:PRO:HD3	2.01	0.42
1:H:269:ILE:HD11	1:H:303:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:148:LYS:HE2	1:I:171:SER:HB2	2.02	0.42
1:K:269:ILE:HD11	1:K:303:ILE:HG12	2.01	0.42
1:A:283:GLU:O	1:A:286:LEU:HD23	2.20	0.42
1:B:269:ILE:HD11	1:B:303:ILE:HG12	2.00	0.42
1:E:135:LEU:CA	1:E:138:TYR:HE2	2.26	0.42
1:E:217:LYS:O	1:E:221:GLU:HB2	2.20	0.42
1:E:762:LEU:HA	1:F:744:ARG:NH1	2.34	0.42
1:F:217:LYS:O	1:F:221:GLU:HB2	2.20	0.42
1:H:679:THR:HB	1:H:682:PHE:CG	2.55	0.42
1:K:77:CYS:SG	1:K:78:SER:N	2.92	0.42
1:K:81:LYS:HD2	1:K:81:LYS:HA	1.78	0.42
1:L:217:LYS:O	1:L:221:GLU:HB2	2.20	0.42
1:L:258:VAL:O	1:L:262:THR:OG1	2.21	0.42
1:B:136:LYS:HB2	1:B:137:PRO:HD3	2.01	0.42
1:B:201:VAL:HA	1:B:205:ASP:OD2	2.20	0.42
1:B:679:THR:HB	1:B:682:PHE:CG	2.55	0.42
1:E:679:THR:HB	1:E:682:PHE:CG	2.55	0.42
1:H:732:ARG:NH1	1:H:734:ASP:HB3	2.34	0.42
1:H:771:PHE:HD2	1:I:737:GLU:HG3	1.85	0.42
1:I:135:LEU:HG	1:I:138:TYR:CZ	2.49	0.42
1:I:732:ARG:NH1	1:I:734:ASP:HB3	2.34	0.42
1:J:120:ASP:OD1	1:J:120:ASP:N	2.48	0.42
1:J:580:ASP:HB2	1:J:628:ILE:HD11	2.00	0.42
1:K:49:LEU:HB3	1:K:104:PRO:HD3	2.02	0.42
1:K:219:MET:SD	1:K:365:ARG:CZ	3.07	0.42
1:K:251:LYS:N	3:K:902:ADP:O2B	2.52	0.42
1:L:148:LYS:CE	1:L:170:PRO:C	2.81	0.42
1:L:572:CYS:SG	1:L:573:VAL:N	2.92	0.42
1:A:217:LYS:O	1:A:221:GLU:HB2	2.20	0.42
1:A:230:PHE:CE2	1:A:237:PRO:HB3	2.55	0.42
1:C:72:LEU:HD12	1:C:72:LEU:HA	1.89	0.42
1:C:135:LEU:HG	1:C:138:TYR:CZ	2.49	0.42
1:C:330:THR:HG21	1:D:273:GLU:HA	2.02	0.42
1:C:732:ARG:NH1	1:C:734:ASP:HB3	2.34	0.42
1:E:233:ILE:HB	1:F:158:MET:HE3	2.01	0.42
1:F:148:LYS:HE2	1:F:171:SER:HB2	2.02	0.42
1:F:216:ILE:H	1:F:216:ILE:HG12	1.69	0.42
1:G:217:LYS:O	1:G:221:GLU:HB2	2.20	0.42
1:G:230:PHE:CE2	1:G:237:PRO:HB3	2.55	0.42
1:G:516:PHE:HB3	1:G:643:ILE:CG1	2.48	0.42
1:G:602:ASN:HD21	1:H:548:LEU:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:VAL:HA	1:H:205:ASP:OD2	2.20	0.42
1:H:283:GLU:O	1:H:286:LEU:HD23	2.20	0.42
1:I:29:ASP:OD2	1:I:81:LYS:HE3	2.20	0.42
1:K:29:ASP:OD2	1:K:81:LYS:HE3	2.20	0.42
1:K:134:TYR:O	1:K:138:TYR:CE2	2.69	0.42
1:K:217:LYS:O	1:K:221:GLU:HB2	2.20	0.42
1:K:679:THR:HB	1:K:682:PHE:CG	2.55	0.42
1:L:269:ILE:HD11	1:L:303:ILE:HG12	2.00	0.42
1:A:490:GLN:O	1:A:494:GLN:HB3	2.20	0.42
1:B:283:GLU:O	1:B:286:LEU:HD23	2.20	0.42
1:C:490:GLN:O	1:C:494:GLN:HB3	2.20	0.42
1:C:679:THR:HB	1:C:682:PHE:CG	2.55	0.42
1:C:750:ASN:HD22	1:J:750:ASN:HD22	1.68	0.42
1:D:29:ASP:OD2	1:D:81:LYS:HE3	2.20	0.42
1:D:120:ASP:OD1	1:D:120:ASP:N	2.48	0.42
1:E:29:ASP:OD2	1:E:81:LYS:HE3	2.20	0.42
1:E:49:LEU:HB3	1:E:104:PRO:HD3	2.02	0.42
1:E:115:HIS:ND1	1:E:183:HIS:O	2.53	0.42
1:E:219:MET:SD	1:E:365:ARG:CZ	3.08	0.42
1:F:219:MET:SD	1:F:365:ARG:CZ	3.07	0.42
1:F:748:SER:OG	1:F:751:ASP:OD2	2.38	0.42
1:G:380:ILE:HD11	3:G:902:ADP:C6	2.55	0.42
1:G:490:GLN:O	1:G:494:GLN:HB3	2.20	0.42
1:H:230:PHE:CE2	1:H:237:PRO:HB3	2.55	0.42
1:H:490:GLN:O	1:H:494:GLN:HB3	2.20	0.42
1:J:29:ASP:OD2	1:J:81:LYS:HE3	2.20	0.42
1:J:49:LEU:HB3	1:J:104:PRO:HD3	2.02	0.42
1:K:115:HIS:ND1	1:K:183:HIS:O	2.53	0.42
1:K:136:LYS:HB2	1:K:137:PRO:HD3	2.01	0.42
1:A:235:VAL:HG13	1:B:416:SER:HB2	2.02	0.41
1:A:580:ASP:OD1	1:A:623:THR:OG1	2.29	0.41
1:B:490:GLN:O	1:B:494:GLN:HB3	2.20	0.41
1:B:732:ARG:NH1	1:B:734:ASP:HB3	2.34	0.41
1:C:29:ASP:OD2	1:C:81:LYS:HE3	2.20	0.41
1:C:773:PHE:HB3	1:D:733:ARG:HH11	1.85	0.41
1:D:49:LEU:HB3	1:D:104:PRO:HD3	2.02	0.41
1:D:148:LYS:HE2	1:D:171:SER:HB2	2.02	0.41
1:E:508:MET:HE2	1:F:699:ILE:HD12	1.79	0.41
1:F:230:PHE:CE2	1:F:237:PRO:HB3	2.55	0.41
1:F:679:THR:HB	1:F:682:PHE:CG	2.55	0.41
1:I:490:GLN:O	1:I:494:GLN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:679:THR:HB	1:I:682:PHE:CG	2.55	0.41
1:J:148:LYS:HE2	1:J:171:SER:HB2	2.02	0.41
1:J:313:ARG:HH22	1:J:353:ILE:C	2.28	0.41
1:J:371:ILE:N	1:J:371:ILE:HD13	2.36	0.41
1:L:679:THR:HB	1:L:682:PHE:CG	2.55	0.41
1:B:219:MET:SD	1:B:365:ARG:CZ	3.08	0.41
1:B:230:PHE:CE2	1:B:237:PRO:HB3	2.55	0.41
1:D:115:HIS:ND1	1:D:183:HIS:O	2.53	0.41
1:D:217:LYS:O	1:D:221:GLU:HB2	2.20	0.41
1:D:313:ARG:HH22	1:D:353:ILE:C	2.28	0.41
1:D:371:ILE:N	1:D:371:ILE:HD13	2.36	0.41
1:F:134:TYR:O	1:F:138:TYR:CE2	2.68	0.41
1:F:269:ILE:HD11	1:F:303:ILE:HG12	2.01	0.41
1:G:269:ILE:HD11	1:G:303:ILE:HG12	2.00	0.41
1:G:768:PHE:O	1:H:741:ARG:HA	2.19	0.41
1:H:29:ASP:OD2	1:H:81:LYS:HE3	2.20	0.41
1:H:219:MET:SD	1:H:365:ARG:CZ	3.08	0.41
1:H:669:ASP:N	1:H:669:ASP:OD1	2.53	0.41
1:J:135:LEU:HA	1:J:138:TYR:HE2	1.60	0.41
1:K:135:LEU:CA	1:K:138:TYR:HE2	2.26	0.41
1:L:230:PHE:CE2	1:L:237:PRO:HB3	2.55	0.41
1:L:490:GLN:O	1:L:494:GLN:HB3	2.20	0.41
1:L:531:ILE:HD12	1:L:531:ILE:HA	1.92	0.41
1:L:748:SER:OG	1:L:751:ASP:OD2	2.38	0.41
1:A:508:MET:HE2	1:B:699:ILE:HD11	1.85	0.41
1:B:81:LYS:HA	1:B:81:LYS:HD2	1.78	0.41
1:B:217:LYS:O	1:B:221:GLU:HB2	2.20	0.41
1:B:669:ASP:N	1:B:669:ASP:OD1	2.53	0.41
1:D:43:GLN:HB3	1:D:44:PRO:HD3	2.03	0.41
1:D:81:LYS:HD2	1:D:81:LYS:HA	1.78	0.41
1:D:669:ASP:OD1	1:D:669:ASP:N	2.53	0.41
1:F:490:GLN:O	1:F:494:GLN:HB3	2.20	0.41
1:G:115:HIS:ND1	1:G:183:HIS:O	2.53	0.41
1:G:148:LYS:HE2	1:G:171:SER:HB2	2.02	0.41
1:J:81:LYS:HD2	1:J:81:LYS:HA	1.78	0.41
1:J:115:HIS:ND1	1:J:183:HIS:O	2.53	0.41
1:J:201:VAL:HA	1:J:205:ASP:OD2	2.20	0.41
1:J:662:ARG:HG3	1:J:663:LYS:HG2	2.02	0.41
1:J:669:ASP:OD1	1:J:669:ASP:N	2.53	0.41
1:A:269:ILE:HD11	1:A:303:ILE:HG12	2.01	0.41
1:B:29:ASP:OD2	1:B:81:LYS:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LYS:HZ2	1:B:103:GLN:HG2	1.85	0.41
1:B:371:ILE:HD13	1:B:371:ILE:N	2.36	0.41
1:C:269:ILE:HD11	1:C:303:ILE:HG12	2.01	0.41
1:D:201:VAL:HA	1:D:205:ASP:OD2	2.20	0.41
1:E:136:LYS:HB2	1:E:137:PRO:HD3	2.01	0.41
1:E:148:LYS:HE2	1:E:171:SER:HB2	2.02	0.41
1:F:29:ASP:OD2	1:F:81:LYS:HE3	2.20	0.41
1:F:114:ILE:HG13	1:F:182:ILE:HG13	2.03	0.41
1:F:115:HIS:ND1	1:F:183:HIS:O	2.53	0.41
1:F:283:GLU:O	1:F:286:LEU:HD23	2.20	0.41
1:F:313:ARG:HH22	1:F:353:ILE:C	2.28	0.41
1:F:371:ILE:HD13	1:F:371:ILE:N	2.36	0.41
1:G:148:LYS:HD3	1:G:148:LYS:HA	1.78	0.41
1:H:313:ARG:HH22	1:H:353:ILE:C	2.28	0.41
1:J:43:GLN:HB3	1:J:44:PRO:HD3	2.03	0.41
1:J:217:LYS:O	1:J:221:GLU:HB2	2.20	0.41
1:K:148:LYS:HE2	1:K:171:SER:HB2	2.02	0.41
1:K:230:PHE:CE2	1:K:237:PRO:HB3	2.55	0.41
1:K:423:ILE:HD12	1:K:424:ARG:N	2.34	0.41
1:L:114:ILE:HG13	1:L:182:ILE:HG13	2.03	0.41
1:L:134:TYR:O	1:L:138:TYR:CE2	2.68	0.41
1:L:283:GLU:O	1:L:286:LEU:HD23	2.20	0.41
1:L:313:ARG:HH22	1:L:353:ILE:C	2.28	0.41
1:L:371:ILE:HD13	1:L:371:ILE:N	2.36	0.41
1:L:423:ILE:HD12	1:L:424:ARG:N	2.34	0.41
1:A:115:HIS:ND1	1:A:183:HIS:O	2.53	0.41
1:A:313:ARG:HH22	1:A:353:ILE:C	2.28	0.41
1:A:766:ARG:NH1	1:K:756:GLU:OE1	2.53	0.41
1:B:756:GLU:OE1	1:J:766:ARG:NH1	2.54	0.41
1:C:283:GLU:O	1:C:286:LEU:HD23	2.20	0.41
1:C:371:ILE:HD13	1:C:371:ILE:N	2.36	0.41
1:D:662:ARG:HG3	1:D:663:LYS:HG2	2.02	0.41
1:E:423:ILE:HD12	1:E:424:ARG:N	2.34	0.41
1:E:490:GLN:O	1:E:494:GLN:HB3	2.20	0.41
1:F:423:ILE:HD12	1:F:424:ARG:N	2.34	0.41
1:F:533:ASN:HD22	1:F:533:ASN:HA	1.61	0.41
1:G:114:ILE:HG13	1:G:182:ILE:HG13	2.03	0.41
1:H:115:HIS:ND1	1:H:183:HIS:O	2.53	0.41
1:I:72:LEU:HD12	1:I:72:LEU:HA	1.89	0.41
1:I:269:ILE:HD11	1:I:303:ILE:HG12	2.01	0.41
1:I:283:GLU:O	1:I:286:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:371:ILE:HD13	1:I:371:ILE:N	2.36	0.41
1:L:29:ASP:OD2	1:L:81:LYS:HE3	2.20	0.41
1:L:49:LEU:HB3	1:L:104:PRO:HD3	2.02	0.41
1:L:219:MET:SD	1:L:365:ARG:CZ	3.08	0.41
1:A:114:ILE:HG13	1:A:182:ILE:HG13	2.03	0.41
1:A:662:ARG:HG3	1:A:663:LYS:HG2	2.02	0.41
1:B:43:GLN:HB3	1:B:44:PRO:HD3	2.03	0.41
1:B:115:HIS:ND1	1:B:183:HIS:O	2.53	0.41
1:B:313:ARG:HH22	1:B:353:ILE:C	2.28	0.41
1:C:380:ILE:HD11	3:C:902:ADP:C6	2.56	0.41
1:C:669:ASP:OD1	1:C:669:ASP:N	2.54	0.41
1:D:135:LEU:HA	1:D:138:TYR:HE2	1.60	0.41
1:D:490:GLN:O	1:D:494:GLN:HB3	2.20	0.41
1:E:230:PHE:CE2	1:E:237:PRO:HB3	2.55	0.41
1:G:313:ARG:HH22	1:G:353:ILE:C	2.28	0.41
1:G:662:ARG:HG3	1:G:663:LYS:HG2	2.02	0.41
1:H:371:ILE:HD13	1:H:371:ILE:N	2.36	0.41
1:J:602:ASN:ND2	1:K:548:LEU:HB3	2.36	0.41
1:K:490:GLN:O	1:K:494:GLN:HB3	2.20	0.41
1:L:115:HIS:ND1	1:L:183:HIS:O	2.53	0.41
1:A:201:VAL:HA	1:A:205:ASP:OD2	2.20	0.41
1:B:258:VAL:O	1:B:262:THR:OG1	2.21	0.41
1:C:662:ARG:HG3	1:C:663:LYS:HG2	2.02	0.41
1:D:216:ILE:O	1:D:220:VAL:HG22	2.21	0.41
1:F:49:LEU:HB3	1:F:104:PRO:HD3	2.02	0.41
1:H:43:GLN:HB3	1:H:44:PRO:HD3	2.03	0.41
1:H:217:LYS:O	1:H:221:GLU:HB2	2.20	0.41
1:I:662:ARG:HG3	1:I:663:LYS:HG2	2.02	0.41
1:I:669:ASP:OD1	1:I:669:ASP:N	2.53	0.41
1:J:216:ILE:O	1:J:220:VAL:HG22	2.21	0.41
1:J:230:PHE:CE2	1:J:237:PRO:HB3	2.55	0.41
1:J:490:GLN:O	1:J:494:GLN:HB3	2.20	0.41
1:K:43:GLN:HB3	1:K:44:PRO:HD3	2.03	0.41
1:C:114:ILE:HG13	1:C:182:ILE:HG13	2.03	0.41
1:C:115:HIS:ND1	1:C:183:HIS:O	2.53	0.41
1:C:119:ILE:HD13	1:C:191:ARG:HB3	2.03	0.41
1:C:217:LYS:O	1:C:221:GLU:HB2	2.20	0.41
1:E:43:GLN:HB3	1:E:44:PRO:HD3	2.03	0.41
1:F:531:ILE:HD12	1:F:531:ILE:HA	1.92	0.41
1:G:272:PRO:O	1:L:326:SER:HB2	2.21	0.41
1:H:84:MET:CE	1:H:88:VAL:HG23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:ILE:HD13	1:H:191:ARG:HB3	2.03	0.41
1:I:115:HIS:ND1	1:I:183:HIS:O	2.53	0.41
1:A:217:LYS:H	1:A:217:LYS:HG2	1.57	0.41
1:A:748:SER:OG	1:A:751:ASP:OD2	2.38	0.41
1:B:84:MET:CE	1:B:88:VAL:HG23	2.51	0.41
1:B:114:ILE:HG13	1:B:182:ILE:HG13	2.03	0.41
1:B:119:ILE:HD13	1:B:191:ARG:HB3	2.03	0.41
1:C:201:VAL:HA	1:C:205:ASP:OD2	2.20	0.41
1:C:484:ASP:OD1	1:C:484:ASP:N	2.49	0.41
1:D:230:PHE:CE2	1:D:237:PRO:HB3	2.55	0.41
1:D:484:ASP:OD1	1:D:484:ASP:N	2.49	0.41
1:D:550:MET:H	1:D:550:MET:HG2	1.74	0.41
1:E:201:VAL:HA	1:E:205:ASP:OD2	2.20	0.41
1:E:216:ILE:O	1:E:220:VAL:HG22	2.21	0.41
1:E:371:ILE:N	1:E:371:ILE:HD13	2.36	0.41
1:E:662:ARG:HG3	1:E:663:LYS:HG2	2.02	0.41
1:E:669:ASP:N	1:E:669:ASP:OD1	2.53	0.41
1:G:201:VAL:HA	1:G:205:ASP:OD2	2.20	0.41
1:G:732:ARG:NH1	1:G:734:ASP:HB3	2.34	0.41
1:H:81:LYS:HA	1:H:81:LYS:HD2	1.78	0.41
1:H:148:LYS:HE2	1:H:171:SER:HB2	2.02	0.41
1:H:565:LYS:HB2	1:H:565:LYS:HE3	1.95	0.41
1:I:49:LEU:HB3	1:I:104:PRO:HD3	2.02	0.41
1:I:119:ILE:HD13	1:I:191:ARG:HB3	2.03	0.41
1:I:217:LYS:O	1:I:221:GLU:HB2	2.20	0.41
1:I:484:ASP:OD1	1:I:484:ASP:N	2.49	0.41
1:I:503:PHE:HE1	1:J:699:ILE:HG21	1.86	0.41
1:J:236:LYS:HA	1:J:236:LYS:HD3	1.86	0.41
1:K:201:VAL:HA	1:K:205:ASP:OD2	2.20	0.41
1:K:371:ILE:HD13	1:K:371:ILE:N	2.36	0.41
1:K:662:ARG:HG3	1:K:663:LYS:HG2	2.02	0.41
1:K:669:ASP:N	1:K:669:ASP:OD1	2.53	0.41
1:A:43:GLN:HB3	1:A:44:PRO:HD3	2.03	0.41
1:A:84:MET:CE	1:A:88:VAL:HG23	2.51	0.41
1:D:732:ARG:NH1	1:D:734:ASP:HB3	2.34	0.41
1:E:531:ILE:HD12	1:E:531:ILE:HA	1.92	0.41
1:G:43:GLN:HB3	1:G:44:PRO:HD3	2.03	0.41
1:G:748:SER:OG	1:G:751:ASP:OD2	2.38	0.41
1:H:148:LYS:HA	1:H:148:LYS:HD3	1.78	0.41
1:I:114:ILE:HG13	1:I:182:ILE:HG13	2.03	0.41
1:I:216:ILE:O	1:I:220:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:484:ASP:OD1	1:J:484:ASP:N	2.49	0.41
1:J:732:ARG:NH1	1:J:734:ASP:HB3	2.34	0.41
1:L:201:VAL:HA	1:L:205:ASP:OD2	2.20	0.41
1:L:533:ASN:HD22	1:L:533:ASN:HA	1.61	0.41
1:A:155:ARG:NH2	1:A:387:ASN:HB3	2.36	0.40
1:A:667:ALA:HB3	1:A:670:VAL:HG23	2.04	0.40
1:A:732:ARG:NH1	1:A:734:ASP:HB3	2.34	0.40
1:B:580:ASP:O	1:B:584:LYS:HG3	2.21	0.40
1:C:580:ASP:O	1:C:584:LYS:HG3	2.21	0.40
1:D:283:GLU:O	1:D:286:LEU:HD23	2.20	0.40
1:F:201:VAL:HA	1:F:205:ASP:OD2	2.20	0.40
1:G:84:MET:CE	1:G:88:VAL:HG23	2.51	0.40
1:G:667:ALA:HB3	1:G:670:VAL:HG23	2.04	0.40
1:I:201:VAL:HA	1:I:205:ASP:OD2	2.20	0.40
1:J:283:GLU:O	1:J:286:LEU:HD23	2.20	0.40
1:K:216:ILE:O	1:K:220:VAL:HG22	2.21	0.40
1:K:283:GLU:O	1:K:286:LEU:HD23	2.20	0.40
1:K:531:ILE:HD12	1:K:531:ILE:HA	1.92	0.40
1:L:130:LEU:HD12	1:L:130:LEU:O	2.21	0.40
1:L:216:ILE:O	1:L:220:VAL:HG22	2.21	0.40
1:L:565:LYS:HB2	1:L:565:LYS:HE3	1.95	0.40
1:A:773:PHE:CD2	1:B:733:ARG:HG2	2.55	0.40
1:C:175:ILE:HD13	1:C:175:ILE:HA	1.96	0.40
1:C:216:ILE:H	1:C:216:ILE:HG12	1.69	0.40
1:C:216:ILE:O	1:C:220:VAL:HG22	2.21	0.40
1:E:155:ARG:HH12	1:E:387:ASN:HB3	1.87	0.40
1:E:283:GLU:O	1:E:286:LEU:HD23	2.20	0.40
1:E:667:ALA:HB3	1:E:670:VAL:HG23	2.04	0.40
1:F:148:LYS:HD3	1:F:148:LYS:HA	1.78	0.40
1:F:155:ARG:NH2	1:F:387:ASN:HB3	2.36	0.40
1:F:565:LYS:HB2	1:F:565:LYS:HE3	1.95	0.40
1:G:119:ILE:HD13	1:G:191:ARG:HB3	2.03	0.40
1:G:155:ARG:NH2	1:G:387:ASN:HB3	2.37	0.40
1:G:371:ILE:HD13	1:G:371:ILE:N	2.36	0.40
1:G:533:ASN:HD22	1:G:533:ASN:HA	1.61	0.40
1:H:484:ASP:O	1:H:488:GLU:HG2	2.22	0.40
1:H:580:ASP:O	1:H:584:LYS:HG3	2.22	0.40
1:I:84:MET:CE	1:I:88:VAL:HG23	2.51	0.40
1:I:230:PHE:CE2	1:I:237:PRO:HB3	2.55	0.40
1:I:580:ASP:O	1:I:584:LYS:HG3	2.22	0.40
1:J:607:GLU:OE1	1:K:465:ARG:NH2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:667:ALA:HB3	1:K:670:VAL:HG23	2.04	0.40
1:A:119:ILE:HD13	1:A:191:ARG:HB3	2.03	0.40
1:A:124:GLU:O	1:A:159:ARG:NH2	2.55	0.40
1:A:533:ASN:HD22	1:A:533:ASN:HA	1.61	0.40
1:A:580:ASP:O	1:A:584:LYS:HG3	2.22	0.40
1:B:484:ASP:O	1:B:488:GLU:HG2	2.22	0.40
1:B:565:LYS:HB2	1:B:565:LYS:HE3	1.95	0.40
1:C:49:LEU:HB3	1:C:104:PRO:HD3	2.02	0.40
1:C:84:MET:CE	1:C:88:VAL:HG23	2.51	0.40
1:C:230:PHE:CE2	1:C:237:PRO:HB3	2.55	0.40
1:C:313:ARG:HH22	1:C:353:ILE:C	2.28	0.40
1:D:72:LEU:HD12	1:D:72:LEU:HA	1.89	0.40
1:D:580:ASP:O	1:D:584:LYS:HG3	2.22	0.40
1:E:476:TRP:HZ2	1:E:531:ILE:HD13	1.87	0.40
1:E:732:ARG:NH1	1:E:734:ASP:HB3	2.34	0.40
1:F:124:GLU:O	1:F:159:ARG:NH2	2.55	0.40
1:F:130:LEU:HD12	1:F:130:LEU:O	2.21	0.40
1:F:216:ILE:O	1:F:220:VAL:HG22	2.21	0.40
1:F:217:LYS:H	1:F:217:LYS:HG2	1.57	0.40
1:G:124:GLU:O	1:G:159:ARG:NH2	2.55	0.40
1:G:580:ASP:O	1:G:584:LYS:HG3	2.22	0.40
1:H:114:ILE:HG13	1:H:182:ILE:HG13	2.03	0.40
1:I:216:ILE:H	1:I:216:ILE:HG12	1.69	0.40
1:J:580:ASP:O	1:J:584:LYS:HG3	2.21	0.40
1:K:155:ARG:HH12	1:K:387:ASN:HB3	1.87	0.40
1:K:732:ARG:NH1	1:K:734:ASP:HB3	2.34	0.40
1:L:124:GLU:O	1:L:159:ARG:NH2	2.55	0.40
1:L:155:ARG:HH12	1:L:387:ASN:HB3	1.87	0.40
1:L:155:ARG:NH2	1:L:387:ASN:HB3	2.36	0.40
1:A:371:ILE:HD13	1:A:371:ILE:N	2.36	0.40
1:A:476:TRP:HZ2	1:A:531:ILE:HD13	1.87	0.40
1:B:236:LYS:HA	1:B:236:LYS:HD3	1.86	0.40
1:B:748:SER:OG	1:B:751:ASP:OD2	2.38	0.40
1:C:172:PRO:HB2	1:C:173:TYR:H	1.62	0.40
1:D:236:LYS:HA	1:D:236:LYS:HD3	1.87	0.40
1:F:155:ARG:HH12	1:F:387:ASN:HB3	1.87	0.40
1:G:60:LYS:HZ2	1:G:103:GLN:HG2	1.86	0.40
1:G:476:TRP:HZ2	1:G:531:ILE:HD13	1.87	0.40
1:G:700:ARG:NH2	1:L:491:GLU:HB3	2.36	0.40
1:I:172:PRO:HB2	1:I:173:TYR:H	1.62	0.40
1:I:313:ARG:HH22	1:I:353:ILE:C	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:550:MET:H	1:J:550:MET:HG2	1.74	0.40
1:K:476:TRP:HZ2	1:K:531:ILE:HD13	1.87	0.40
1:L:43:GLN:HB3	1:L:44:PRO:HD3	2.03	0.40
1:A:29:ASP:OD2	1:A:81:LYS:HE3	2.20	0.40
1:A:60:LYS:HZ2	1:A:103:GLN:HG2	1.86	0.40
1:B:124:GLU:O	1:B:159:ARG:NH2	2.55	0.40
1:D:667:ALA:HB3	1:D:670:VAL:HG23	2.03	0.40
1:E:124:GLU:O	1:E:159:ARG:NH2	2.55	0.40
1:E:484:ASP:OD1	1:E:484:ASP:N	2.49	0.40
1:F:84:MET:CE	1:F:88:VAL:HG23	2.51	0.40
1:G:29:ASP:OD2	1:G:81:LYS:HE3	2.20	0.40
1:G:565:LYS:HB2	1:G:565:LYS:HE3	1.95	0.40
1:G:737:GLU:HG3	1:L:771:PHE:HD2	1.87	0.40
1:H:236:LYS:HA	1:H:236:LYS:HD3	1.87	0.40
1:H:662:ARG:HG3	1:H:663:LYS:HG2	2.02	0.40
1:H:667:ALA:HB3	1:H:670:VAL:HG23	2.03	0.40
1:H:688:THR:OG1	2:H:901:JDP:O01	2.38	0.40
1:K:124:GLU:O	1:K:159:ARG:NH2	2.55	0.40
1:K:484:ASP:OD1	1:K:484:ASP:N	2.49	0.40
1:L:81:LYS:HD2	1:L:81:LYS:HA	1.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	731/821 (89%)	691 (94%)	38 (5%)	2 (0%)	37 68
1	B	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37 68
1	C	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37 68
1	D	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	F	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	G	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	H	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	I	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	J	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	K	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	L	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
All	All	8772/9852 (89%)	8281 (94%)	467 (5%)	24 (0%)	38	68

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	PRO
1	B	172	PRO
1	C	172	PRO
1	D	172	PRO
1	E	172	PRO
1	F	172	PRO
1	G	172	PRO
1	H	172	PRO
1	I	172	PRO
1	J	172	PRO
1	K	172	PRO
1	L	172	PRO
1	A	338	ARG
1	B	338	ARG
1	C	338	ARG
1	D	338	ARG
1	E	338	ARG
1	F	338	ARG
1	G	338	ARG
1	H	338	ARG
1	I	338	ARG
1	J	338	ARG
1	K	338	ARG
1	L	338	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	625/691 (90%)	625 (100%)	0	100	100
1	B	625/691 (90%)	625 (100%)	0	100	100
1	C	625/691 (90%)	625 (100%)	0	100	100
1	D	625/691 (90%)	625 (100%)	0	100	100
1	E	625/691 (90%)	625 (100%)	0	100	100
1	F	625/691 (90%)	625 (100%)	0	100	100
1	G	625/691 (90%)	625 (100%)	0	100	100
1	H	625/691 (90%)	625 (100%)	0	100	100
1	I	625/691 (90%)	625 (100%)	0	100	100
1	J	625/691 (90%)	625 (100%)	0	100	100
1	K	625/691 (90%)	625 (100%)	0	100	100
1	L	625/691 (90%)	625 (100%)	0	100	100
All	All	7500/8292 (90%)	7500 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	285	ASN
1	A	337	GLN
1	A	536	GLN
1	B	43	GLN
1	B	285	ASN
1	B	536	GLN
1	B	538	ASN
1	B	602	ASN
1	B	692	GLN
1	C	43	GLN

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Mol	Chain	Res	Type
1	C	285	ASN
1	C	337	GLN
1	C	384	HIS
1	C	536	GLN
1	C	538	ASN
1	C	602	ASN
1	C	692	GLN
1	D	43	GLN
1	D	285	ASN
1	D	337	GLN
1	D	536	GLN
1	D	692	GLN
1	D	750	ASN
1	D	760	GLN
1	E	43	GLN
1	E	285	ASN
1	E	337	GLN
1	E	536	GLN
1	E	602	ASN
1	E	750	ASN
1	F	43	GLN
1	F	285	ASN
1	F	536	GLN
1	F	538	ASN
1	F	750	ASN
1	F	760	GLN
1	G	43	GLN
1	G	285	ASN
1	G	337	GLN
1	G	384	HIS
1	G	536	GLN
1	G	692	GLN
1	G	760	GLN
1	H	43	GLN
1	H	285	ASN
1	H	337	GLN
1	H	536	GLN
1	H	538	ASN
1	H	764	GLN
1	I	43	GLN
1	I	285	ASN
1	I	327	GLN

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Mol	Chain	Res	Type
1	I	337	GLN
1	I	536	GLN
1	I	692	GLN
1	I	760	GLN
1	I	764	GLN
1	J	43	GLN
1	J	285	ASN
1	J	337	GLN
1	J	536	GLN
1	J	602	ASN
1	J	692	GLN
1	J	750	ASN
1	J	764	GLN
1	K	43	GLN
1	K	285	ASN
1	K	337	GLN
1	K	536	GLN
1	K	692	GLN
1	K	764	GLN
1	L	43	GLN
1	L	285	ASN
1	L	337	GLN
1	L	384	HIS
1	L	536	GLN
1	L	538	ASN
1	L	602	ASN
1	L	750	ASN
1	L	764	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ADP	A	902	-	24,29,29	0.87	0	29,45,45	1.16	2 (6%)
3	ADP	K	902	-	24,29,29	0.88	0	29,45,45	1.17	2 (6%)
2	JDP	I	901	-	33,35,35	2.17	6 (18%)	32,50,50	3.13	7 (21%)
3	ADP	I	902	-	24,29,29	0.89	0	29,45,45	1.16	2 (6%)
2	JDP	B	901	-	33,35,35	2.19	6 (18%)	32,50,50	3.12	7 (21%)
3	ADP	F	902	-	24,29,29	0.88	0	29,45,45	1.17	2 (6%)
3	ADP	B	902	-	24,29,29	0.88	0	29,45,45	1.17	2 (6%)
2	JDP	E	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.12	8 (25%)
2	JDP	A	901	-	33,35,35	2.19	6 (18%)	32,50,50	3.13	7 (21%)
3	ADP	E	902	-	24,29,29	0.87	0	29,45,45	1.17	2 (6%)
2	JDP	J	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.12	7 (21%)
2	JDP	F	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.12	7 (21%)
3	ADP	L	902	-	24,29,29	0.87	0	29,45,45	1.17	2 (6%)
3	ADP	G	902	-	24,29,29	0.89	0	29,45,45	1.17	2 (6%)
2	JDP	K	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.13	7 (21%)
3	ADP	D	902	-	24,29,29	0.88	0	29,45,45	1.16	2 (6%)
2	JDP	D	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.13	7 (21%)
2	JDP	H	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.12	7 (21%)
3	ADP	H	902	-	24,29,29	0.88	0	29,45,45	1.16	2 (6%)
2	JDP	L	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.12	7 (21%)
2	JDP	G	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.12	7 (21%)
3	ADP	J	902	-	24,29,29	0.86	0	29,45,45	1.16	2 (6%)
3	ADP	C	902	-	24,29,29	0.87	0	29,45,45	1.17	2 (6%)
2	JDP	C	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.12	7 (21%)

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
3	ADP	A	902	-	-	0/12/32/32	0/3/3/3
3	ADP	K	902	-	-	1/12/32/32	0/3/3/3
2	JDP	I	901	-	-	4/9/20/20	0/5/5/5
3	ADP	I	902	-	-	1/12/32/32	0/3/3/3
2	JDP	B	901	-	-	4/9/20/20	0/5/5/5
3	ADP	F	902	-	-	0/12/32/32	0/3/3/3
3	ADP	B	902	-	-	0/12/32/32	0/3/3/3
2	JDP	E	901	-	-	4/9/20/20	0/5/5/5
2	JDP	A	901	-	-	4/9/20/20	0/5/5/5
3	ADP	E	902	-	-	0/12/32/32	0/3/3/3
2	JDP	J	901	-	-	4/9/20/20	0/5/5/5
2	JDP	F	901	-	-	4/9/20/20	0/5/5/5
3	ADP	L	902	-	-	1/12/32/32	0/3/3/3
3	ADP	G	902	-	-	1/12/32/32	0/3/3/3
2	JDP	K	901	-	-	4/9/20/20	0/5/5/5
3	ADP	D	902	-	-	0/12/32/32	0/3/3/3
2	JDP	D	901	-	-	4/9/20/20	0/5/5/5
2	JDP	H	901	-	-	4/9/20/20	0/5/5/5
3	ADP	H	902	-	-	1/12/32/32	0/3/3/3
2	JDP	L	901	-	-	4/9/20/20	0/5/5/5
2	JDP	G	901	-	-	4/9/20/20	0/5/5/5
3	ADP	J	902	-	-	1/12/32/32	0/3/3/3
3	ADP	C	902	-	-	0/12/32/32	0/3/3/3
2	JDP	C	901	-	-	4/9/20/20	0/5/5/5

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	JDP	C15-N16	7.06	1.45	1.34
2	B	901	JDP	C15-N16	7.05	1.45	1.34
2	H	901	JDP	C15-N16	7.05	1.45	1.34
2	G	901	JDP	C15-N16	7.03	1.45	1.34
2	C	901	JDP	C15-N16	7.02	1.45	1.34
2	E	901	JDP	C15-N16	7.02	1.45	1.34
2	J	901	JDP	C15-N16	7.00	1.45	1.34
2	F	901	JDP	C15-N16	7.00	1.45	1.34
2	K	901	JDP	C15-N16	6.99	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	901	JDP	C15-N16	6.98	1.45	1.34
2	D	901	JDP	C15-N16	6.97	1.45	1.34
2	L	901	JDP	C15-N16	6.95	1.45	1.34
2	J	901	JDP	C02-N31	6.86	1.45	1.33
2	A	901	JDP	C02-N31	6.85	1.45	1.33
2	F	901	JDP	C02-N31	6.85	1.45	1.33
2	D	901	JDP	C02-N31	6.84	1.45	1.33
2	I	901	JDP	C02-N31	6.83	1.45	1.33
2	L	901	JDP	C02-N31	6.82	1.45	1.33
2	B	901	JDP	C02-N31	6.81	1.45	1.33
2	K	901	JDP	C02-N31	6.81	1.45	1.33
2	H	901	JDP	C02-N31	6.80	1.45	1.33
2	G	901	JDP	C02-N31	6.79	1.45	1.33
2	C	901	JDP	C02-N31	6.78	1.45	1.33
2	E	901	JDP	C02-N31	6.78	1.45	1.33
2	B	901	JDP	C25-C24	4.39	1.57	1.51
2	A	901	JDP	C25-C24	4.36	1.57	1.51
2	K	901	JDP	C25-C24	4.34	1.57	1.51
2	E	901	JDP	C25-C24	4.34	1.57	1.51
2	H	901	JDP	C25-C24	4.33	1.57	1.51
2	C	901	JDP	C25-C24	4.31	1.57	1.51
2	L	901	JDP	C25-C24	4.31	1.57	1.51
2	I	901	JDP	C25-C24	4.31	1.57	1.51
2	G	901	JDP	C25-C24	4.30	1.57	1.51
2	J	901	JDP	C25-C24	4.29	1.57	1.51
2	D	901	JDP	C25-C24	4.28	1.57	1.51
2	F	901	JDP	C25-C24	4.26	1.57	1.51
2	L	901	JDP	C24-C29	-4.01	1.34	1.40
2	A	901	JDP	C24-C29	-3.97	1.34	1.40
2	C	901	JDP	C24-C29	-3.96	1.34	1.40
2	F	901	JDP	C24-C29	-3.96	1.34	1.40
2	G	901	JDP	C24-C29	-3.94	1.34	1.40
2	E	901	JDP	C24-C29	-3.93	1.34	1.40
2	I	901	JDP	C24-C29	-3.92	1.34	1.40
2	B	901	JDP	C24-C29	-3.92	1.34	1.40
2	D	901	JDP	C24-C29	-3.91	1.34	1.40
2	H	901	JDP	C24-C29	-3.91	1.34	1.40
2	K	901	JDP	C24-C29	-3.90	1.34	1.40
2	J	901	JDP	C24-C29	-3.87	1.34	1.40
2	F	901	JDP	O01-C02	-2.92	1.18	1.24
2	C	901	JDP	O01-C02	-2.92	1.18	1.24
2	L	901	JDP	O01-C02	-2.91	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	JDP	O01-C02	-2.90	1.18	1.24
2	B	901	JDP	O01-C02	-2.89	1.18	1.24
2	I	901	JDP	O01-C02	-2.88	1.18	1.24
2	H	901	JDP	O01-C02	-2.88	1.18	1.24
2	A	901	JDP	O01-C02	-2.88	1.18	1.24
2	G	901	JDP	O01-C02	-2.87	1.18	1.24
2	K	901	JDP	O01-C02	-2.87	1.18	1.24
2	J	901	JDP	O01-C02	-2.87	1.18	1.24
2	E	901	JDP	O01-C02	-2.85	1.18	1.24
2	E	901	JDP	C24-C15	-2.33	1.37	1.42
2	J	901	JDP	C24-C15	-2.33	1.37	1.42
2	B	901	JDP	C24-C15	-2.32	1.37	1.42
2	I	901	JDP	C24-C15	-2.32	1.37	1.42
2	K	901	JDP	C24-C15	-2.31	1.37	1.42
2	G	901	JDP	C24-C15	-2.31	1.37	1.42
2	H	901	JDP	C24-C15	-2.30	1.38	1.42
2	F	901	JDP	C24-C15	-2.30	1.38	1.42
2	A	901	JDP	C24-C15	-2.30	1.38	1.42
2	L	901	JDP	C24-C15	-2.29	1.38	1.42
2	C	901	JDP	C24-C15	-2.29	1.38	1.42
2	D	901	JDP	C24-C15	-2.29	1.38	1.42

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	901	JDP	C11-C10-C09	-15.42	100.95	128.71
2	A	901	JDP	C11-C10-C09	-15.41	100.95	128.71
2	E	901	JDP	C11-C10-C09	-15.39	100.99	128.71
2	C	901	JDP	C11-C10-C09	-15.39	100.99	128.71
2	K	901	JDP	C11-C10-C09	-15.39	100.99	128.71
2	D	901	JDP	C11-C10-C09	-15.39	101.00	128.71
2	J	901	JDP	C11-C10-C09	-15.38	101.01	128.71
2	B	901	JDP	C11-C10-C09	-15.38	101.02	128.71
2	H	901	JDP	C11-C10-C09	-15.38	101.02	128.71
2	F	901	JDP	C11-C10-C09	-15.37	101.03	128.71
2	L	901	JDP	C11-C10-C09	-15.37	101.04	128.71
2	G	901	JDP	C11-C10-C09	-15.37	101.04	128.71
2	A	901	JDP	C24-C29-N30	-4.63	119.91	123.48
2	D	901	JDP	C24-C29-N30	-4.62	119.92	123.48
2	I	901	JDP	C24-C29-N30	-4.61	119.93	123.48
2	K	901	JDP	C24-C29-N30	-4.60	119.94	123.48
2	L	901	JDP	C24-C29-N30	-4.58	119.95	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	JDP	C24-C29-N30	-4.58	119.95	123.48
2	C	901	JDP	C24-C29-N30	-4.57	119.96	123.48
2	E	901	JDP	C24-C29-N30	-4.56	119.97	123.48
2	H	901	JDP	C24-C29-N30	-4.55	119.98	123.48
2	F	901	JDP	C24-C29-N30	-4.54	119.98	123.48
2	G	901	JDP	C24-C29-N30	-4.53	119.99	123.48
2	J	901	JDP	C24-C29-N30	-4.53	119.99	123.48
2	K	901	JDP	C28-C29-N30	3.72	120.90	115.85
2	H	901	JDP	C28-C29-N30	3.69	120.87	115.85
2	J	901	JDP	C28-C29-N30	3.68	120.85	115.85
2	D	901	JDP	C28-C29-N30	3.68	120.85	115.85
2	E	901	JDP	C28-C29-N30	3.67	120.84	115.85
2	B	901	JDP	C28-C29-N30	3.67	120.84	115.85
2	I	901	JDP	C28-C29-N30	3.67	120.83	115.85
2	A	901	JDP	C28-C29-N30	3.66	120.83	115.85
2	G	901	JDP	C28-C29-N30	3.66	120.82	115.85
2	L	901	JDP	C28-C29-N30	3.65	120.81	115.85
2	C	901	JDP	C28-C29-N30	3.64	120.81	115.85
2	F	901	JDP	C28-C29-N30	3.61	120.76	115.85
3	F	902	ADP	N3-C2-N1	-3.58	123.81	128.67
3	C	902	ADP	N3-C2-N1	-3.55	123.85	128.67
3	K	902	ADP	N3-C2-N1	-3.55	123.86	128.67
3	B	902	ADP	N3-C2-N1	-3.55	123.86	128.67
3	E	902	ADP	N3-C2-N1	-3.54	123.86	128.67
3	H	902	ADP	N3-C2-N1	-3.54	123.87	128.67
3	A	902	ADP	N3-C2-N1	-3.53	123.88	128.67
3	L	902	ADP	N3-C2-N1	-3.52	123.89	128.67
3	J	902	ADP	N3-C2-N1	-3.52	123.89	128.67
3	G	902	ADP	N3-C2-N1	-3.51	123.91	128.67
3	D	902	ADP	N3-C2-N1	-3.50	123.92	128.67
3	I	902	ADP	N3-C2-N1	-3.49	123.94	128.67
2	H	901	JDP	C27-C28-C29	2.82	116.78	111.62
2	K	901	JDP	C27-C28-C29	2.81	116.75	111.62
2	J	901	JDP	C27-C28-C29	2.80	116.75	111.62
2	L	901	JDP	C27-C28-C29	2.80	116.74	111.62
2	E	901	JDP	C27-C28-C29	2.79	116.72	111.62
2	I	901	JDP	C27-C28-C29	2.79	116.72	111.62
2	G	901	JDP	C27-C28-C29	2.78	116.71	111.62
2	B	901	JDP	C27-C28-C29	2.78	116.71	111.62
2	A	901	JDP	C27-C28-C29	2.78	116.70	111.62
2	D	901	JDP	C27-C28-C29	2.77	116.69	111.62
2	C	901	JDP	C27-C28-C29	2.77	116.69	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	901	JDP	C27-C28-C29	2.77	116.69	111.62
3	B	902	ADP	C4-C5-N7	-2.65	106.53	109.34
3	G	902	ADP	C4-C5-N7	-2.65	106.54	109.34
3	I	902	ADP	C4-C5-N7	-2.65	106.54	109.34
3	L	902	ADP	C4-C5-N7	-2.64	106.55	109.34
3	K	902	ADP	C4-C5-N7	-2.63	106.56	109.34
3	J	902	ADP	C4-C5-N7	-2.62	106.57	109.34
3	C	902	ADP	C4-C5-N7	-2.62	106.57	109.34
3	D	902	ADP	C4-C5-N7	-2.61	106.58	109.34
3	A	902	ADP	C4-C5-N7	-2.61	106.58	109.34
3	F	902	ADP	C4-C5-N7	-2.61	106.58	109.34
3	E	902	ADP	C4-C5-N7	-2.61	106.58	109.34
3	H	902	ADP	C4-C5-N7	-2.55	106.64	109.34
2	I	901	JDP	C08-C03-C02	2.52	124.41	120.82
2	B	901	JDP	C08-C03-C02	2.51	124.39	120.82
2	K	901	JDP	C08-C03-C02	2.50	124.38	120.82
2	G	901	JDP	C08-C03-C02	2.49	124.36	120.82
2	C	901	JDP	C08-C03-C02	2.48	124.36	120.82
2	L	901	JDP	C08-C03-C02	2.48	124.36	120.82
2	E	901	JDP	C08-C03-C02	2.48	124.35	120.82
2	D	901	JDP	C08-C03-C02	2.47	124.34	120.82
2	F	901	JDP	C08-C03-C02	2.47	124.34	120.82
2	H	901	JDP	C08-C03-C02	2.46	124.32	120.82
2	J	901	JDP	C08-C03-C02	2.46	124.32	120.82
2	A	901	JDP	C08-C03-C02	2.45	124.31	120.82
2	G	901	JDP	C17-N16-C15	-2.41	119.96	123.08
2	J	901	JDP	C17-N16-C15	-2.38	120.00	123.08
2	L	901	JDP	C17-N16-C15	-2.37	120.02	123.08
2	F	901	JDP	C17-N16-C15	-2.36	120.03	123.08
2	A	901	JDP	C17-N16-C15	-2.36	120.04	123.08
2	D	901	JDP	C17-N16-C15	-2.34	120.05	123.08
2	B	901	JDP	C17-N16-C15	-2.33	120.07	123.08
2	E	901	JDP	C17-N16-C15	-2.33	120.07	123.08
2	I	901	JDP	C17-N16-C15	-2.33	120.07	123.08
2	H	901	JDP	C17-N16-C15	-2.32	120.08	123.08
2	C	901	JDP	C17-N16-C15	-2.32	120.09	123.08
2	K	901	JDP	C17-N16-C15	-2.30	120.11	123.08
2	H	901	JDP	C28-C29-C24	-2.19	119.15	121.40
2	J	901	JDP	C28-C29-C24	-2.19	119.16	121.40
2	K	901	JDP	C28-C29-C24	-2.19	119.16	121.40
2	E	901	JDP	C28-C29-C24	-2.17	119.18	121.40
2	G	901	JDP	C28-C29-C24	-2.16	119.19	121.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	JDP	C28-C29-C24	-2.14	119.20	121.40
2	D	901	JDP	C28-C29-C24	-2.12	119.22	121.40
2	C	901	JDP	C28-C29-C24	-2.11	119.23	121.40
2	I	901	JDP	C28-C29-C24	-2.11	119.24	121.40
2	L	901	JDP	C28-C29-C24	-2.11	119.24	121.40
2	F	901	JDP	C28-C29-C24	-2.10	119.25	121.40
2	A	901	JDP	C28-C29-C24	-2.09	119.26	121.40
2	E	901	JDP	C09-C08-C07	2.00	108.02	106.27

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	JDP	N14-C15-N16-C17
2	A	901	JDP	C24-C15-N16-C17
2	B	901	JDP	N14-C15-N16-C17
2	B	901	JDP	C24-C15-N16-C17
2	C	901	JDP	N14-C15-N16-C17
2	C	901	JDP	C24-C15-N16-C17
2	D	901	JDP	N14-C15-N16-C17
2	D	901	JDP	C24-C15-N16-C17
2	E	901	JDP	N14-C15-N16-C17
2	E	901	JDP	C24-C15-N16-C17
2	F	901	JDP	N14-C15-N16-C17
2	F	901	JDP	C24-C15-N16-C17
2	G	901	JDP	N14-C15-N16-C17
2	G	901	JDP	C24-C15-N16-C17
2	H	901	JDP	N14-C15-N16-C17
2	H	901	JDP	C24-C15-N16-C17
2	I	901	JDP	N14-C15-N16-C17
2	I	901	JDP	C24-C15-N16-C17
2	J	901	JDP	N14-C15-N16-C17
2	J	901	JDP	C24-C15-N16-C17
2	K	901	JDP	N14-C15-N16-C17
2	K	901	JDP	C24-C15-N16-C17
2	L	901	JDP	N14-C15-N16-C17
2	L	901	JDP	C24-C15-N16-C17
3	G	902	ADP	C5'-O5'-PA-O1A
3	H	902	ADP	C5'-O5'-PA-O1A
3	I	902	ADP	C5'-O5'-PA-O1A
3	J	902	ADP	C5'-O5'-PA-O1A
3	K	902	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	L	902	ADP	C5'-O5'-PA-O1A
2	A	901	JDP	O01-C02-C03-C08
2	B	901	JDP	O01-C02-C03-C08
2	C	901	JDP	O01-C02-C03-C08
2	D	901	JDP	O01-C02-C03-C08
2	E	901	JDP	O01-C02-C03-C08
2	F	901	JDP	O01-C02-C03-C08
2	G	901	JDP	O01-C02-C03-C08
2	H	901	JDP	O01-C02-C03-C08
2	I	901	JDP	O01-C02-C03-C08
2	J	901	JDP	O01-C02-C03-C08
2	K	901	JDP	O01-C02-C03-C08
2	L	901	JDP	O01-C02-C03-C08
2	A	901	JDP	N31-C02-C03-C08
2	B	901	JDP	N31-C02-C03-C08
2	C	901	JDP	N31-C02-C03-C08
2	D	901	JDP	N31-C02-C03-C08
2	E	901	JDP	N31-C02-C03-C08
2	F	901	JDP	N31-C02-C03-C08
2	G	901	JDP	N31-C02-C03-C08
2	H	901	JDP	N31-C02-C03-C08
2	I	901	JDP	N31-C02-C03-C08
2	J	901	JDP	N31-C02-C03-C08
2	K	901	JDP	N31-C02-C03-C08
2	L	901	JDP	N31-C02-C03-C08

There are no ring outliers.

21 monomers are involved in 30 short contacts:

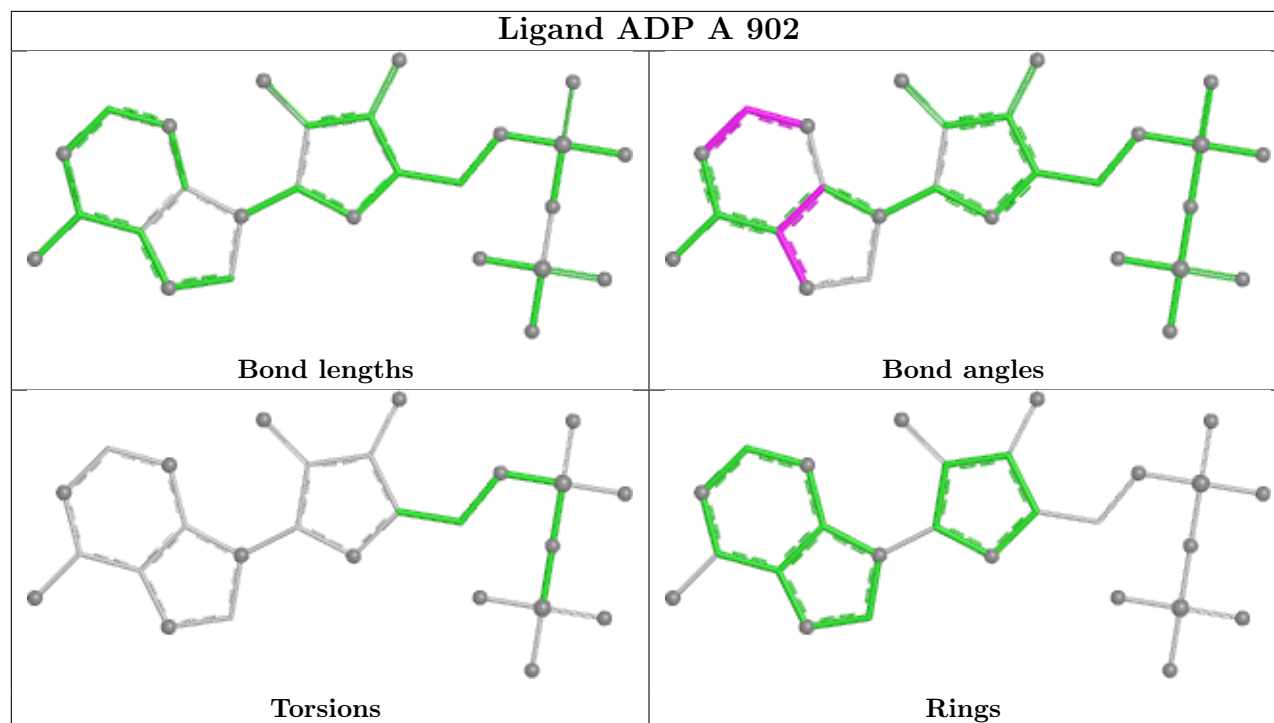
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	ADP	2	0
3	K	902	ADP	1	0
2	I	901	JDP	1	0
3	I	902	ADP	2	0
2	B	901	JDP	1	0
3	F	902	ADP	3	0
2	E	901	JDP	1	0
2	A	901	JDP	1	0
2	J	901	JDP	1	0
2	F	901	JDP	1	0
3	L	902	ADP	3	0
3	G	902	ADP	3	0

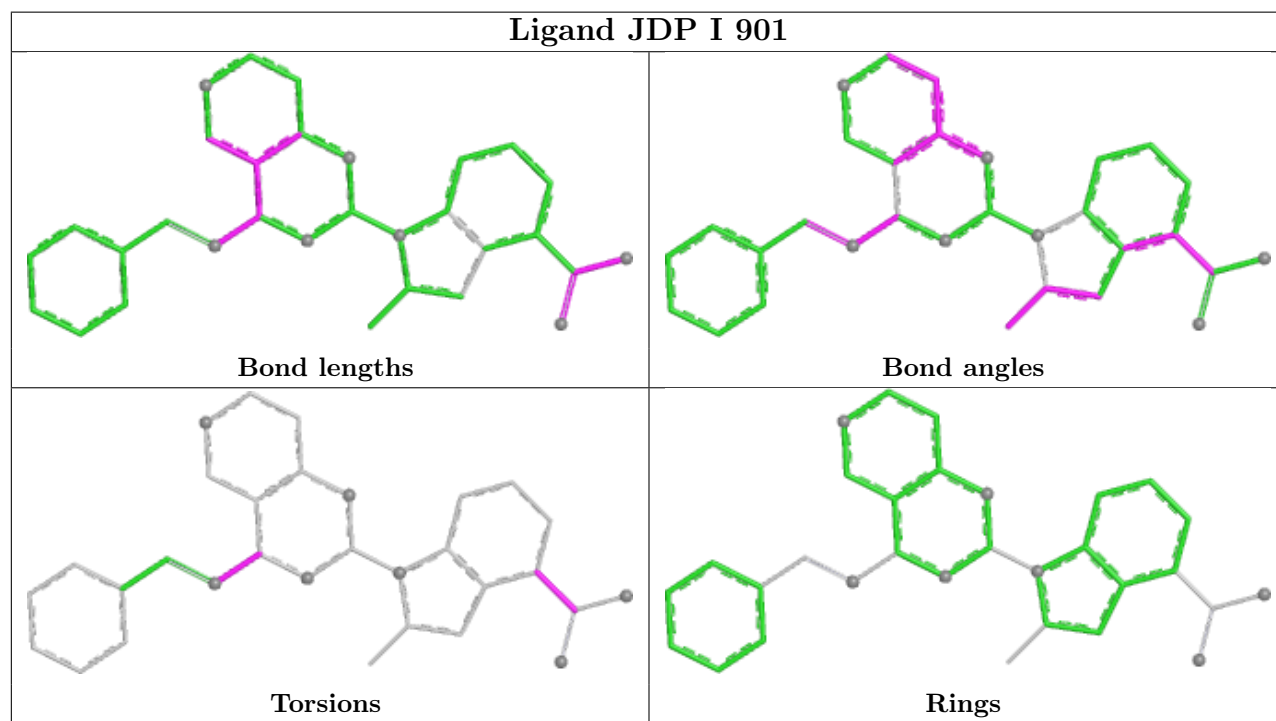
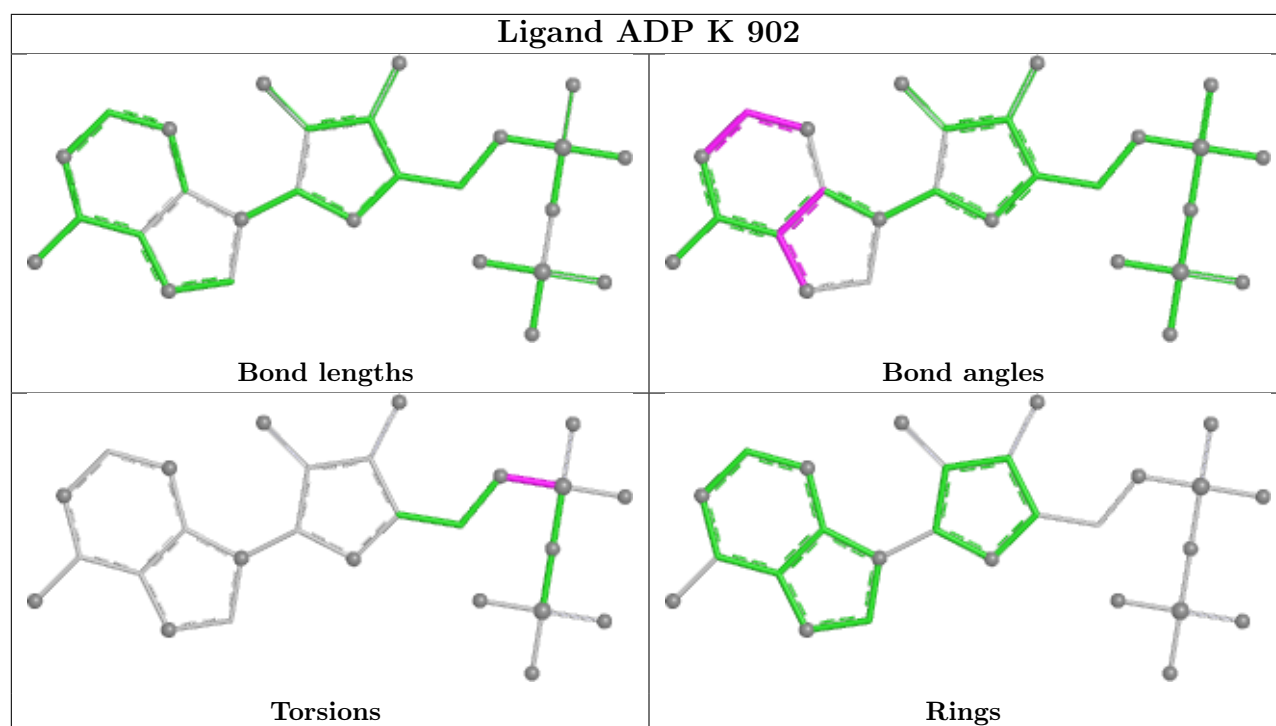
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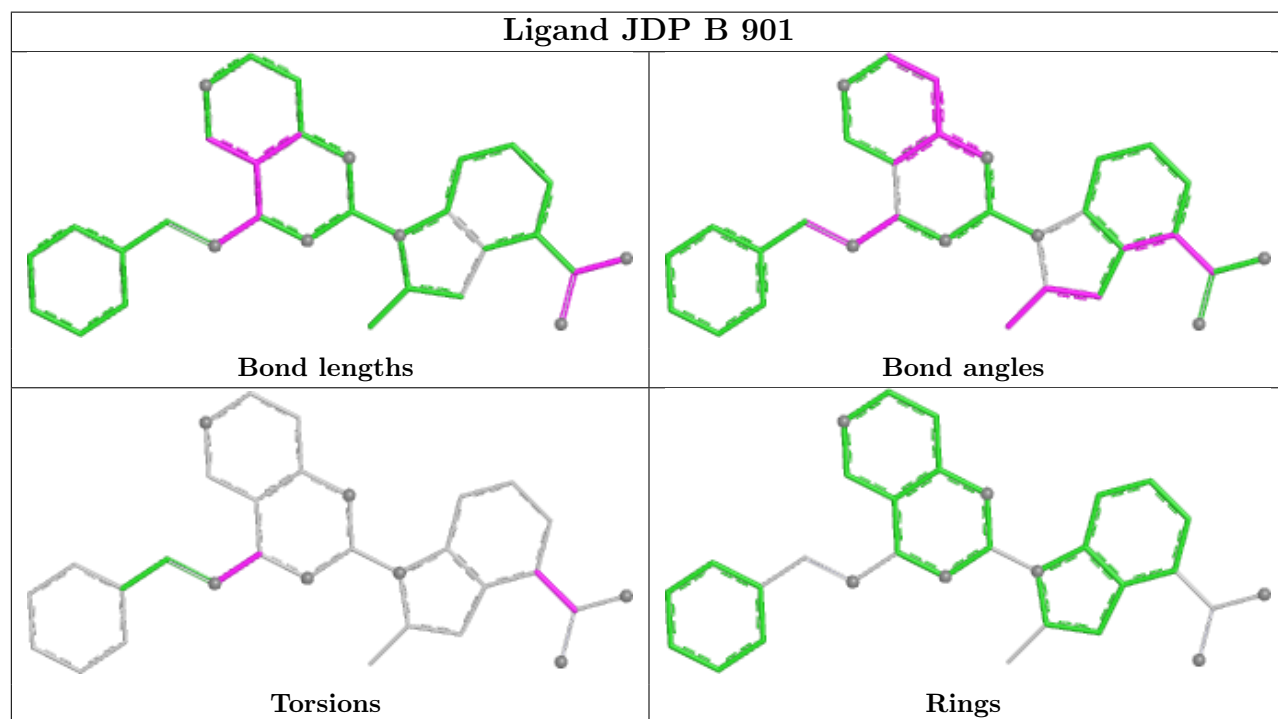
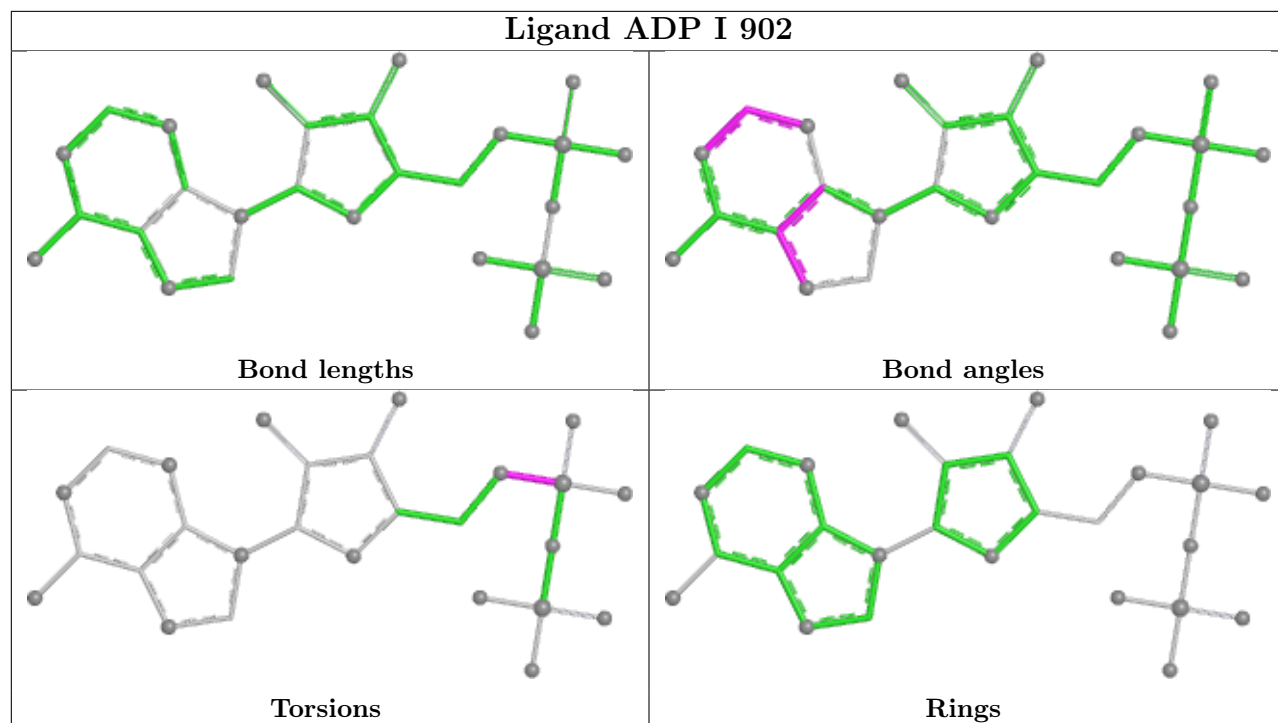
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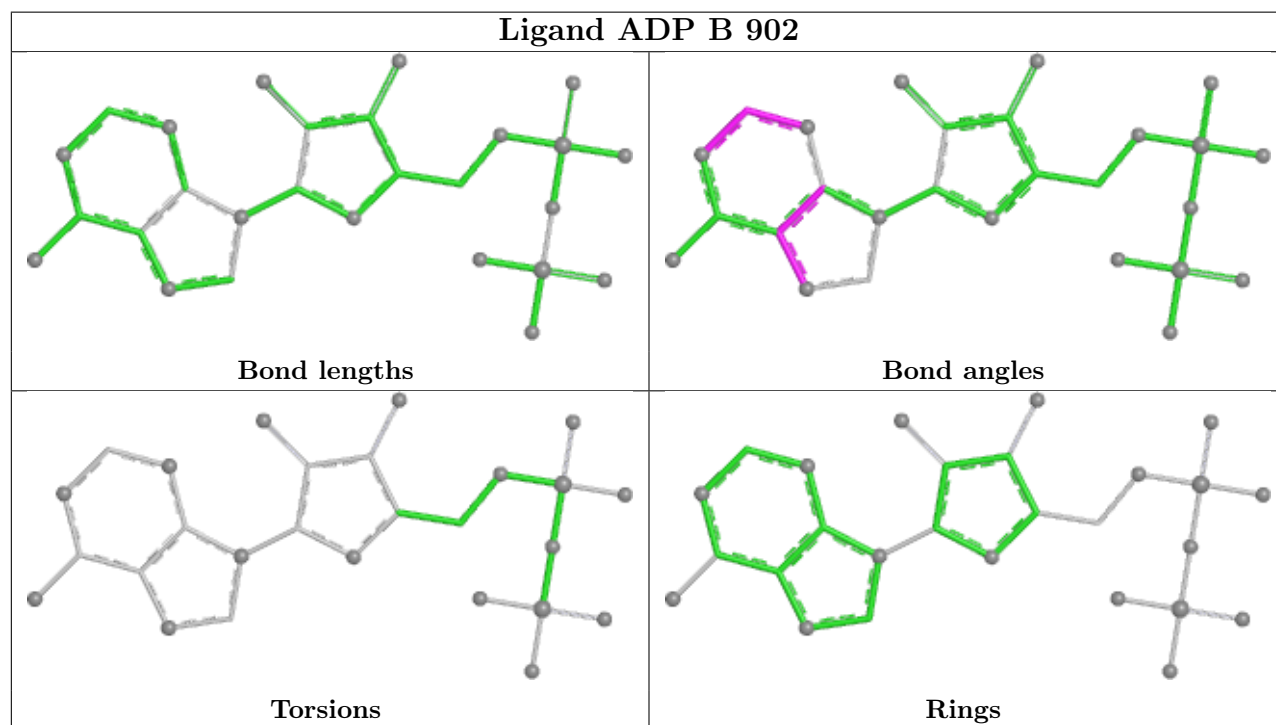
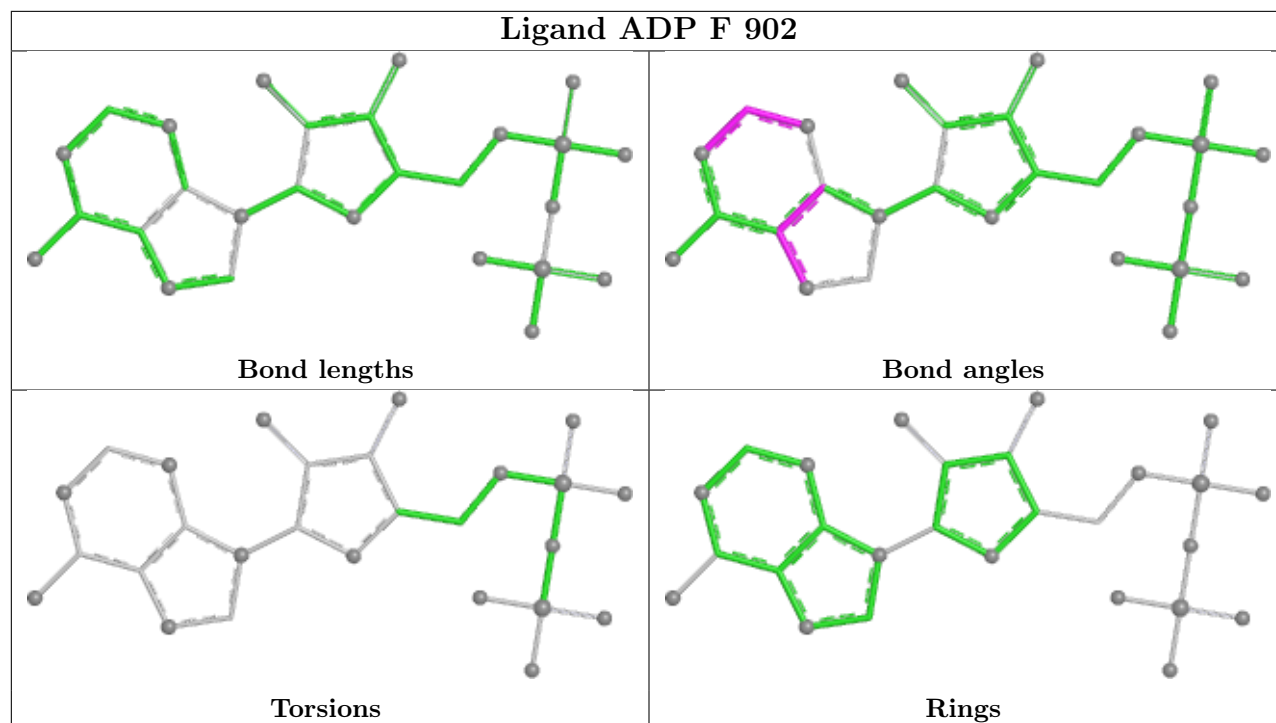
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	901	JDP	1	0
3	D	902	ADP	1	0
2	D	901	JDP	1	0
2	H	901	JDP	2	0
3	H	902	ADP	1	0
2	L	901	JDP	1	0
2	G	901	JDP	1	0
3	C	902	ADP	1	0
2	C	901	JDP	1	0

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.

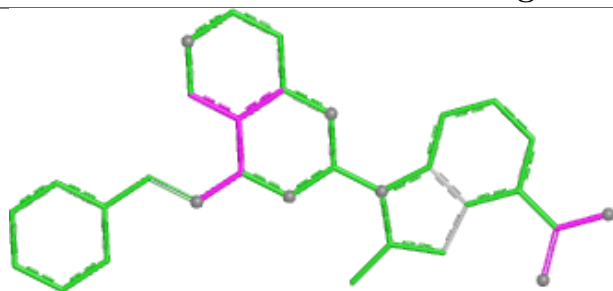




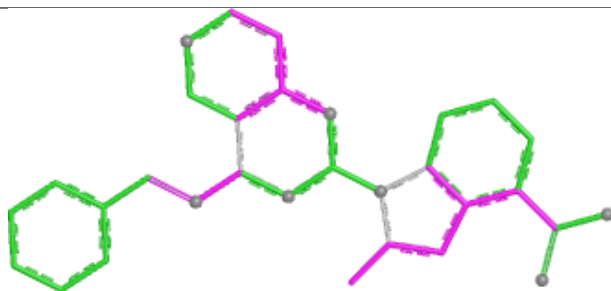




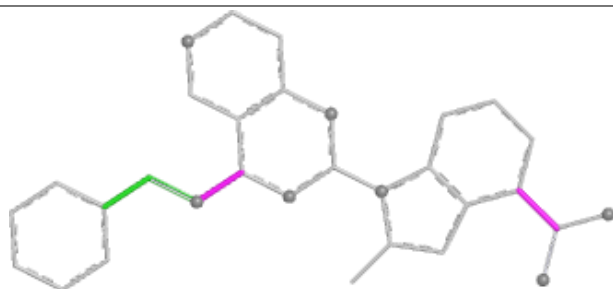
Ligand JDP E 901



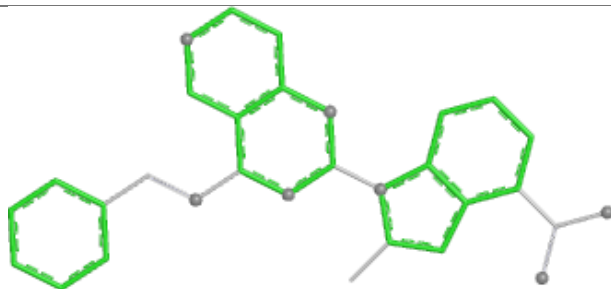
Bond lengths



Bond angles

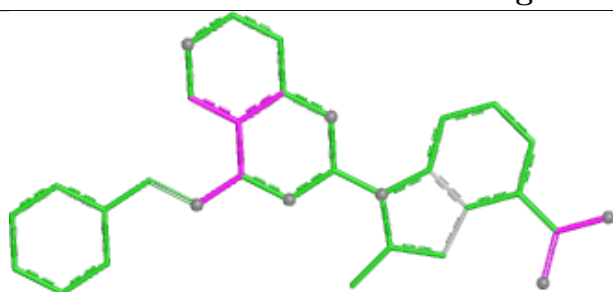


Torsions

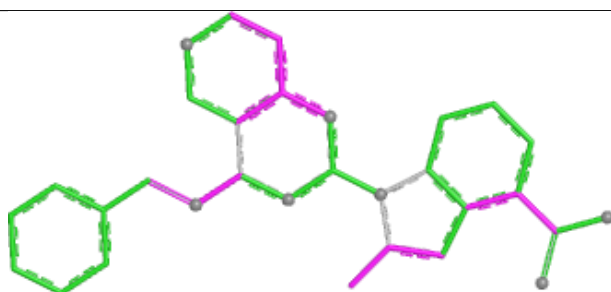


Rings

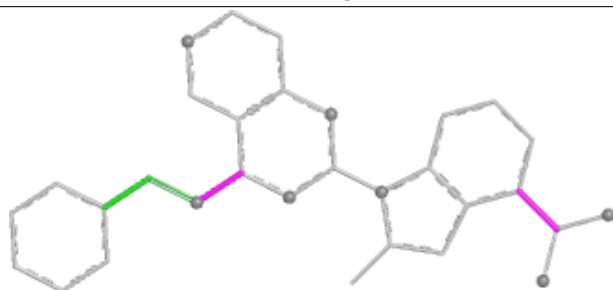
Ligand JDP A 901



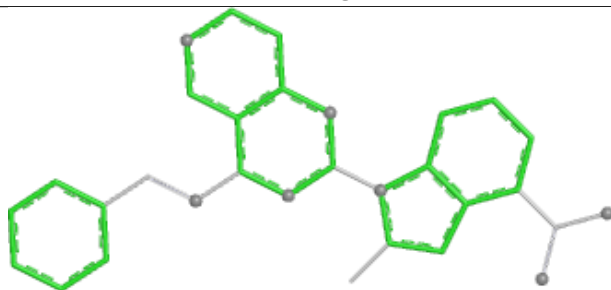
Bond lengths



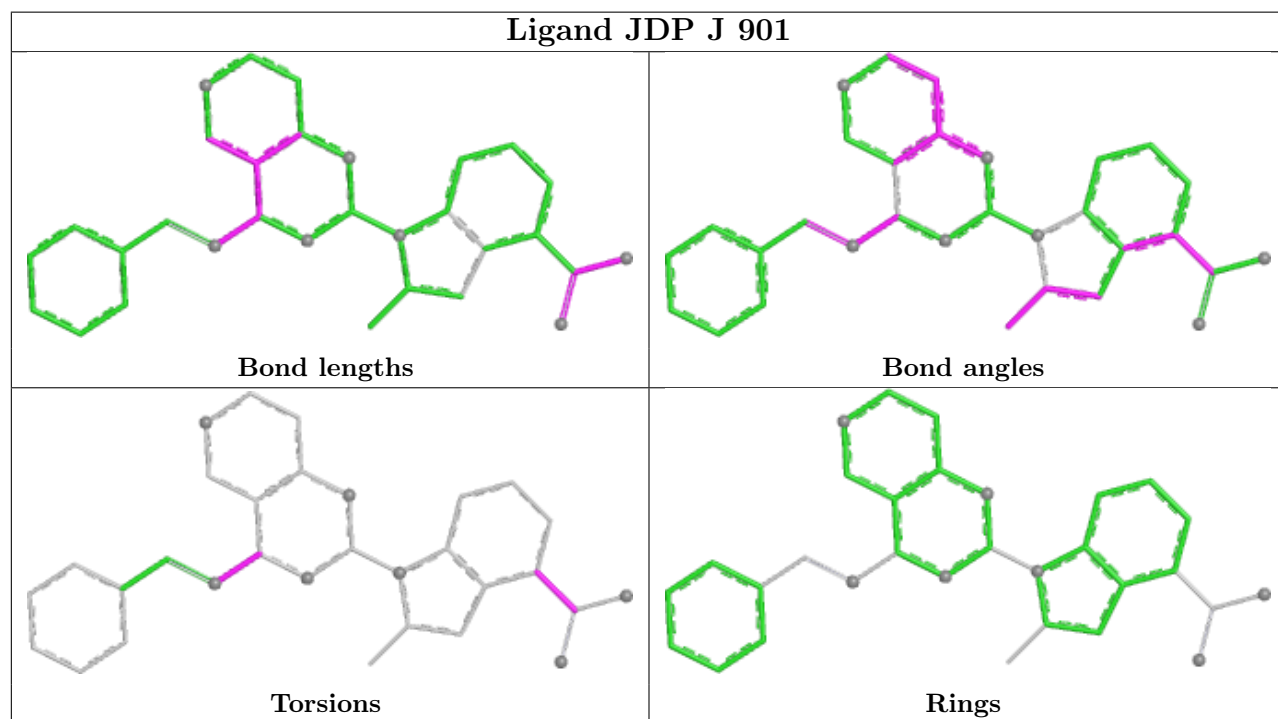
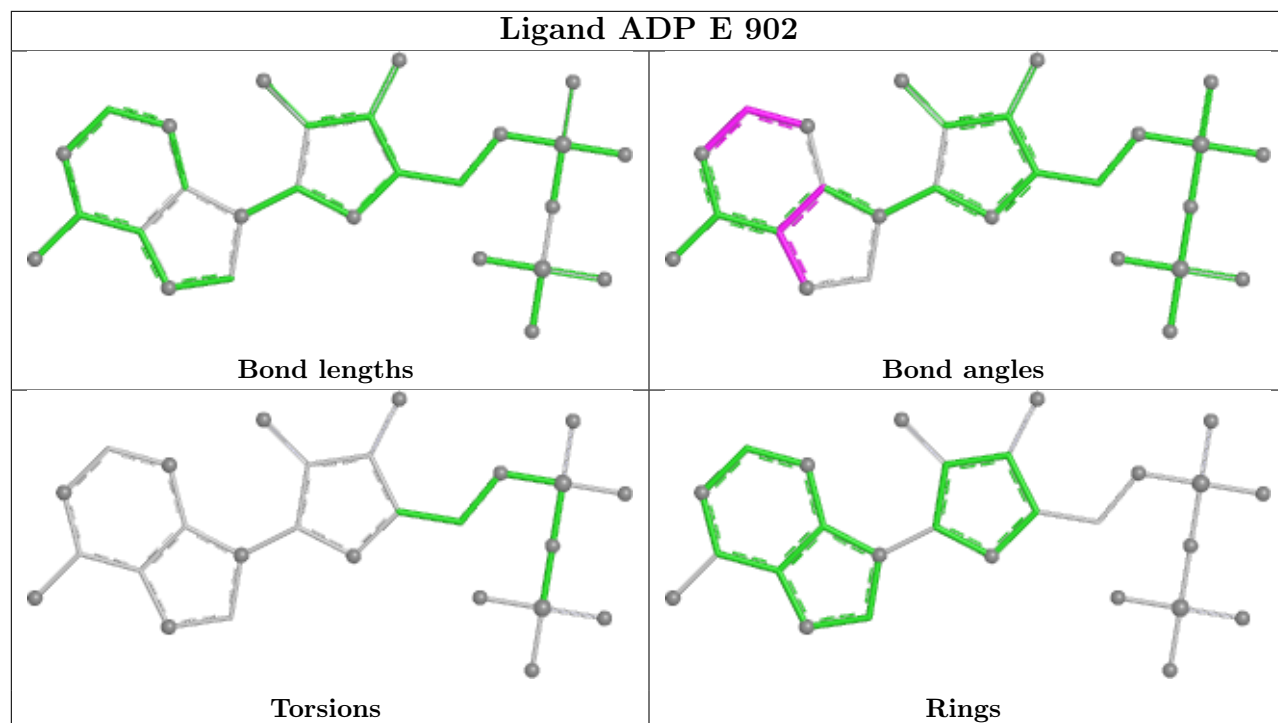
Bond angles



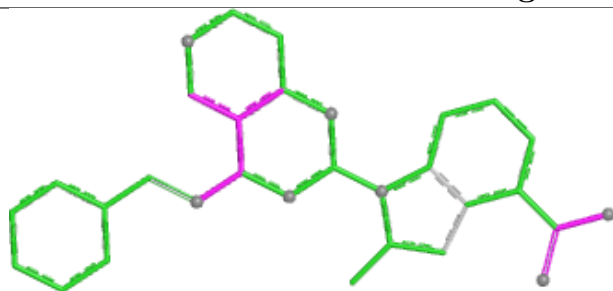
Torsions



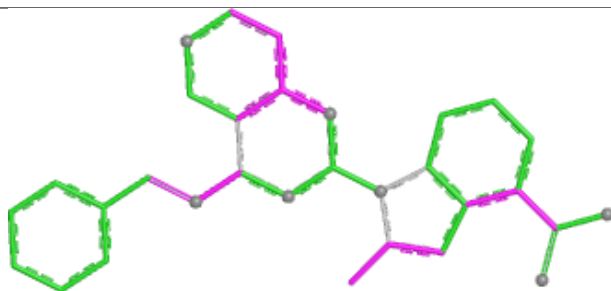
Rings



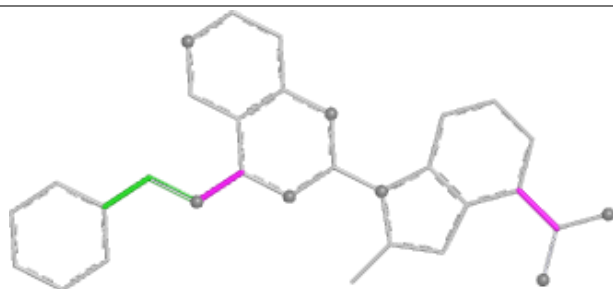
Ligand JDP F 901



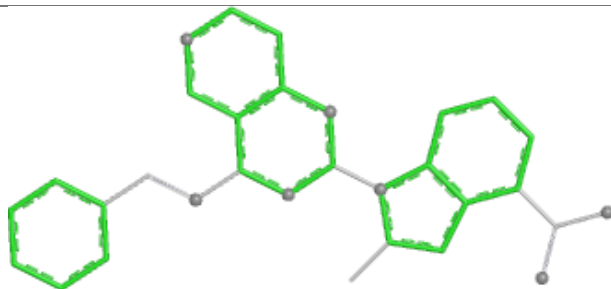
Bond lengths



Bond angles

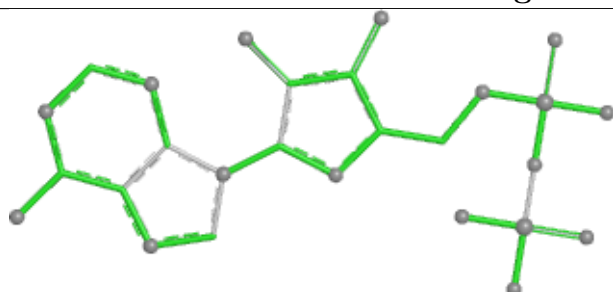


Torsions

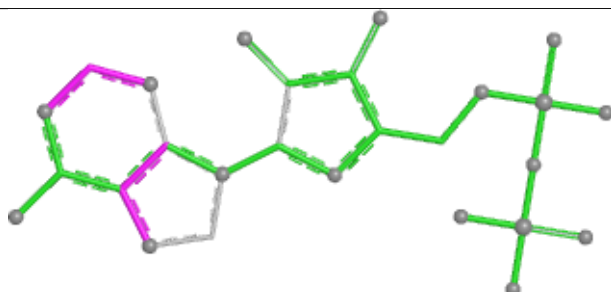


Rings

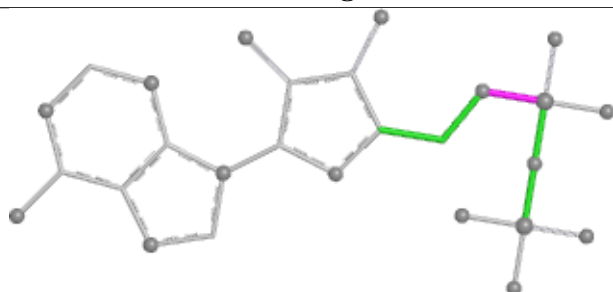
Ligand ADP L 902



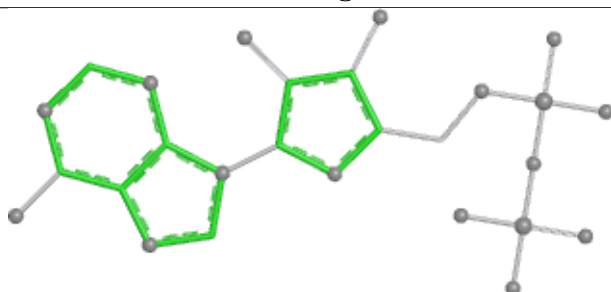
Bond lengths



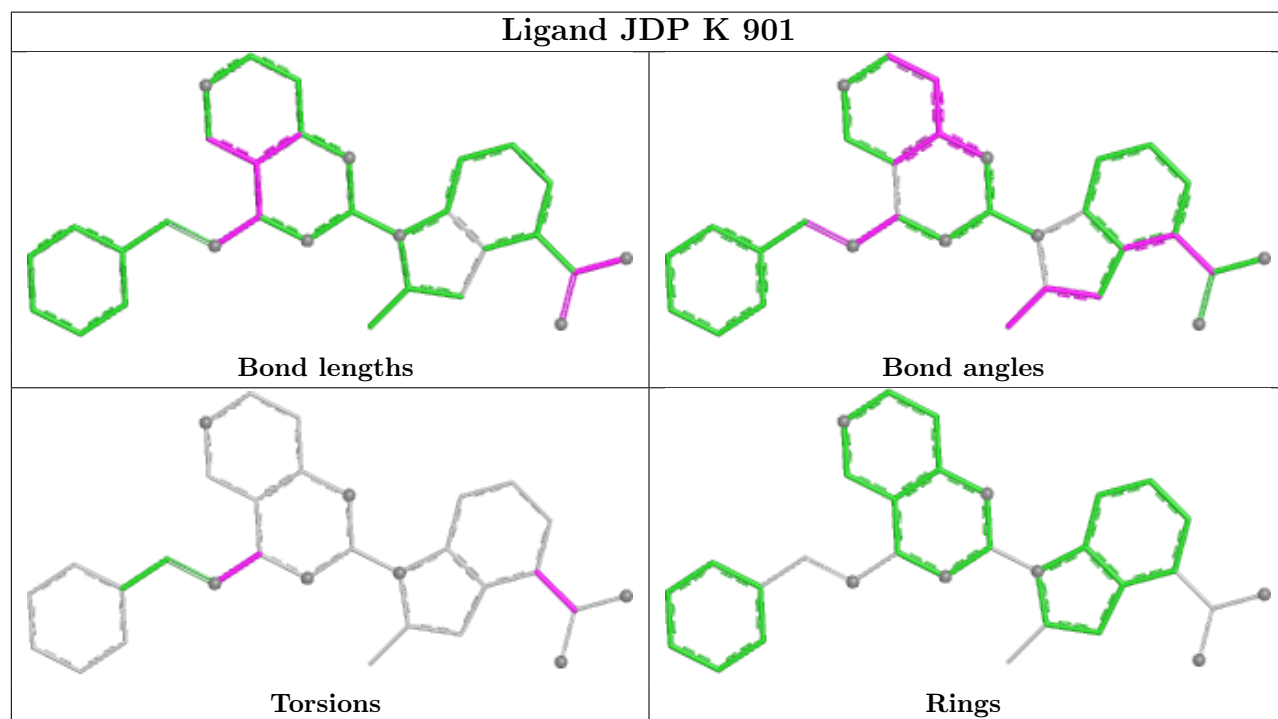
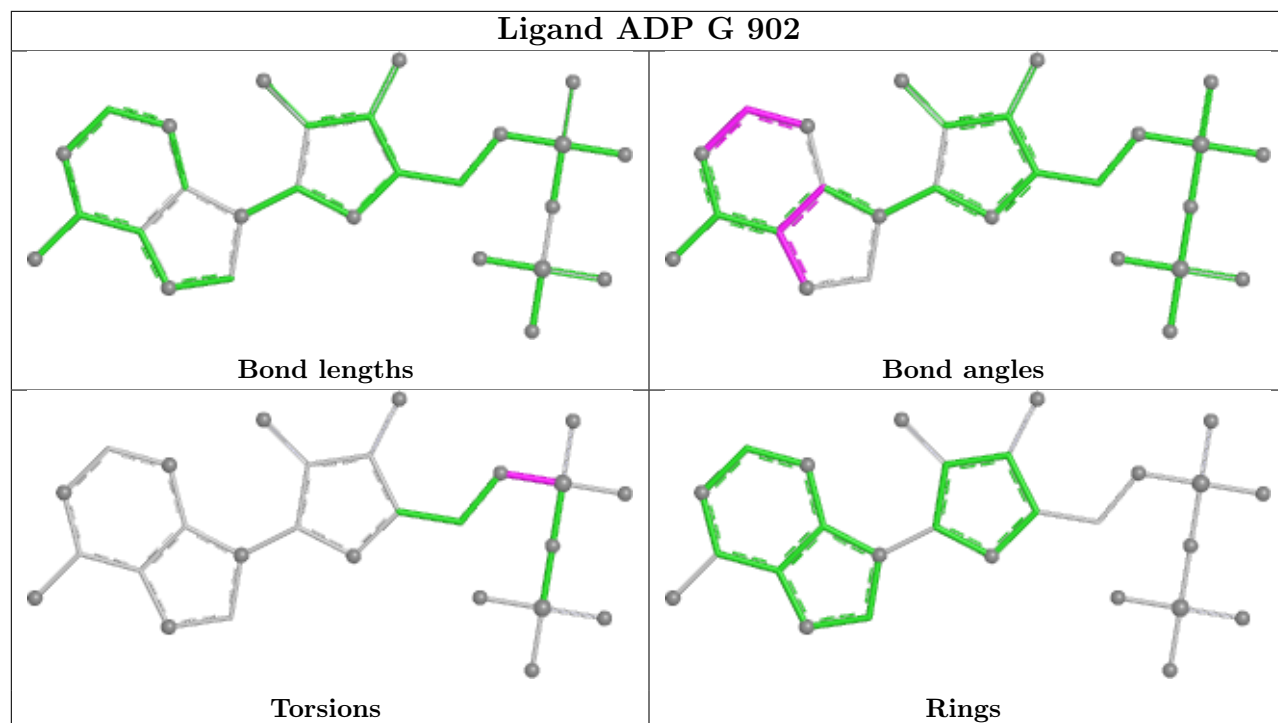
Bond angles

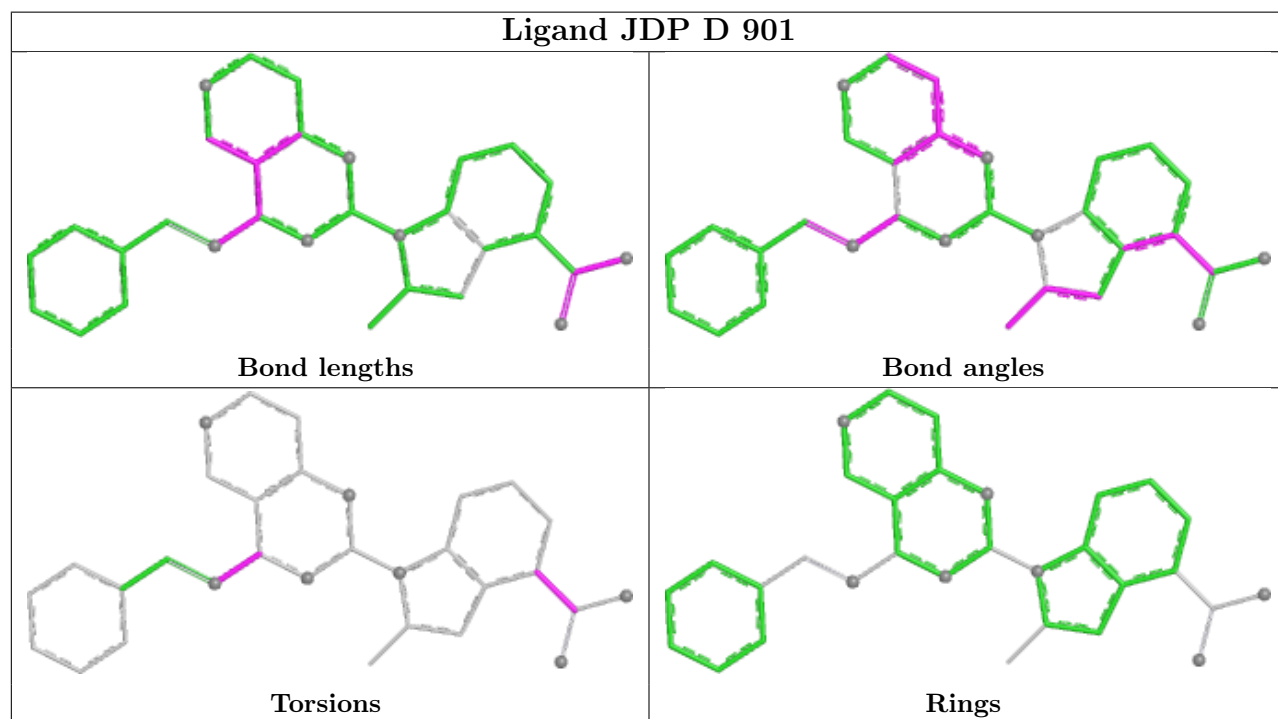
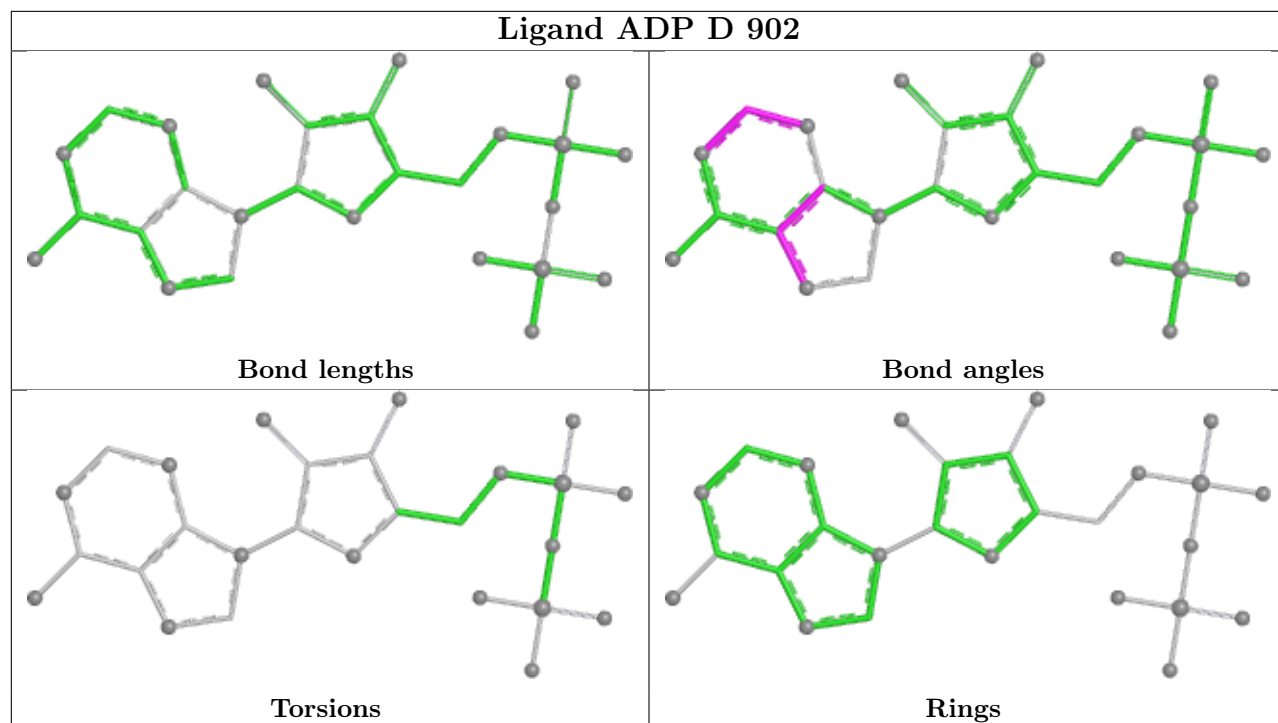


Torsions

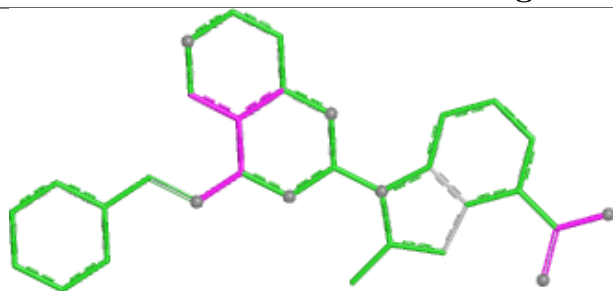


Rings

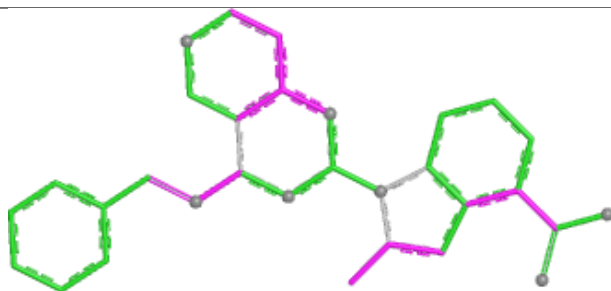




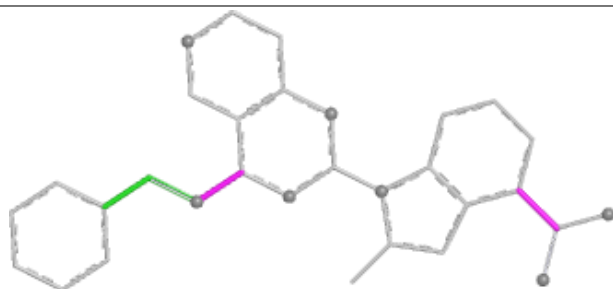
Ligand JDP H 901



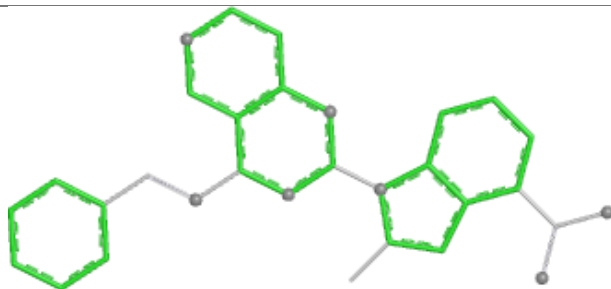
Bond lengths



Bond angles

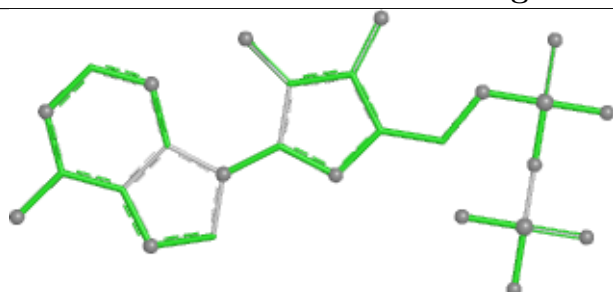


Torsions

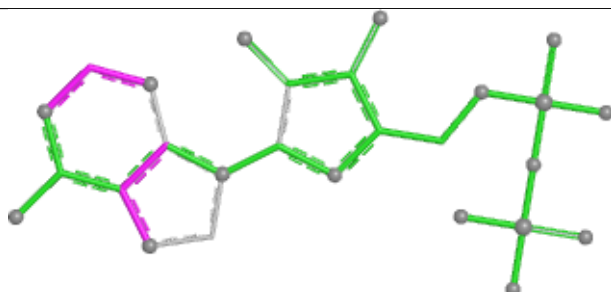


Rings

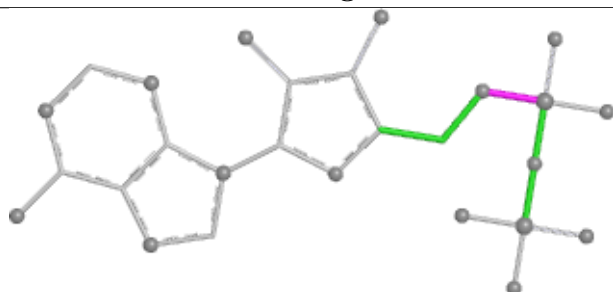
Ligand ADP H 902



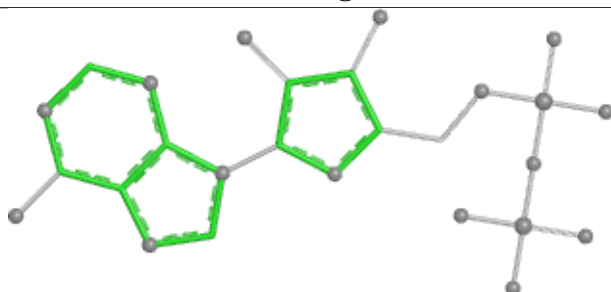
Bond lengths



Bond angles

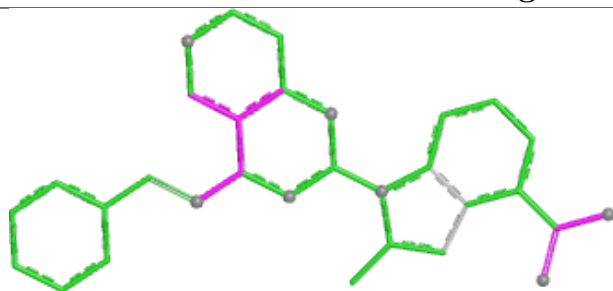


Torsions

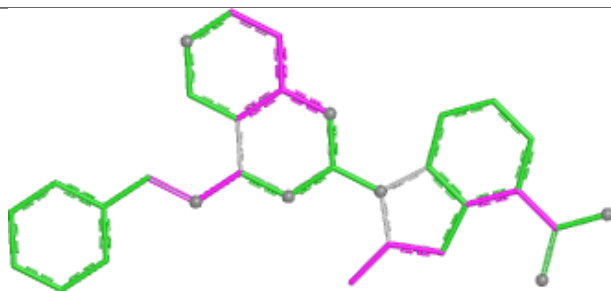


Rings

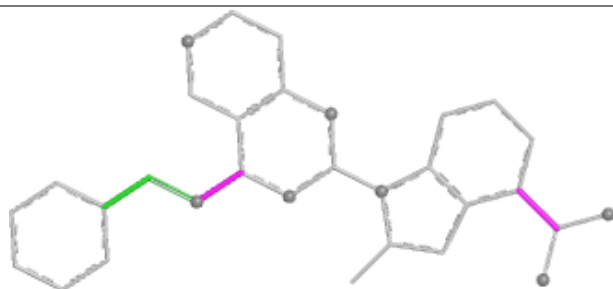
Ligand JDP L 901



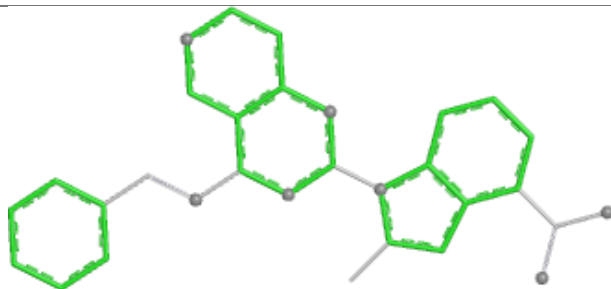
Bond lengths



Bond angles

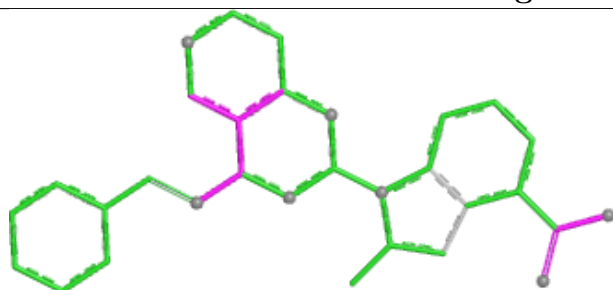


Torsions

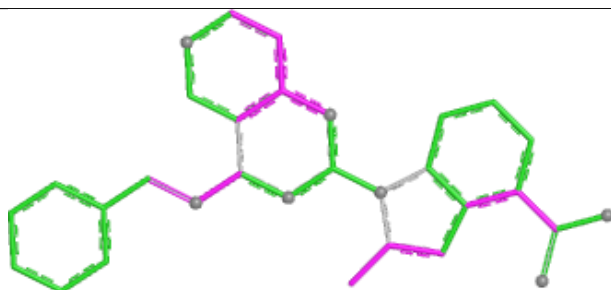


Rings

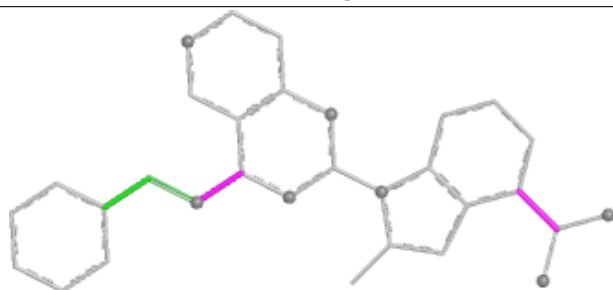
Ligand JDP G 901



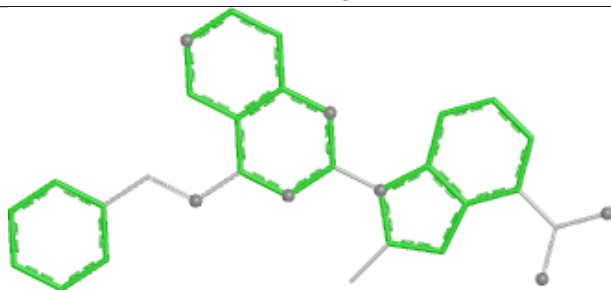
Bond lengths



Bond angles

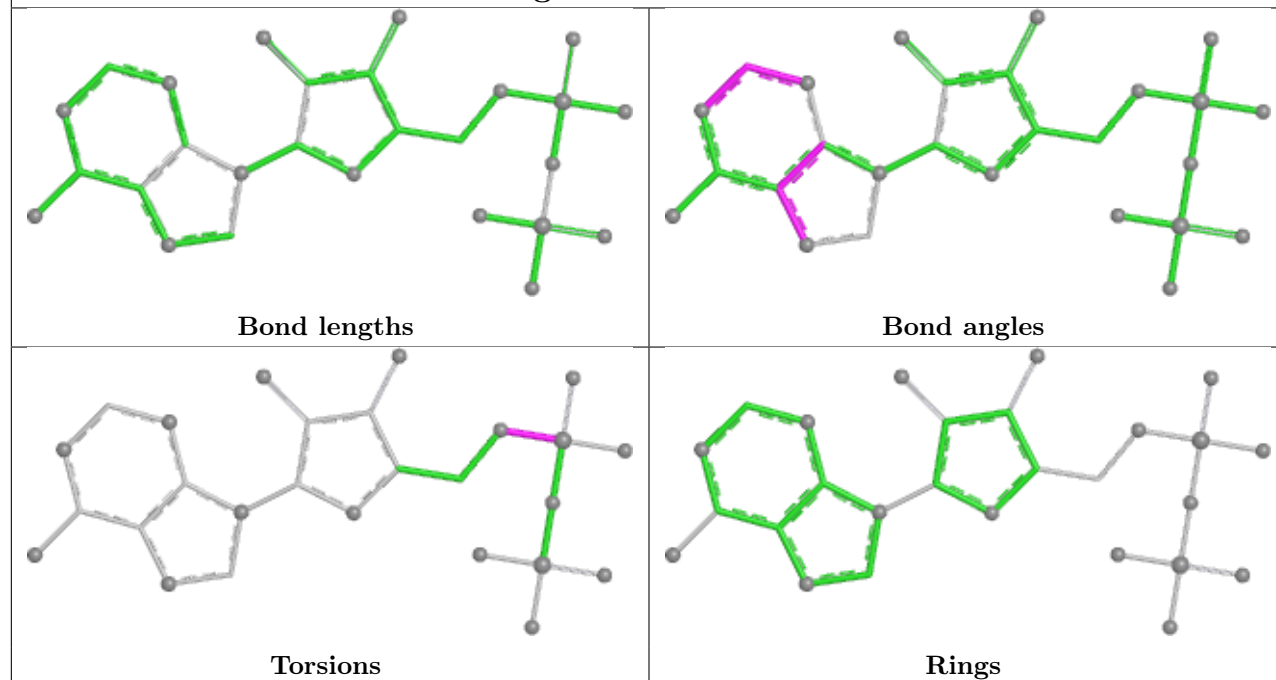


Torsions

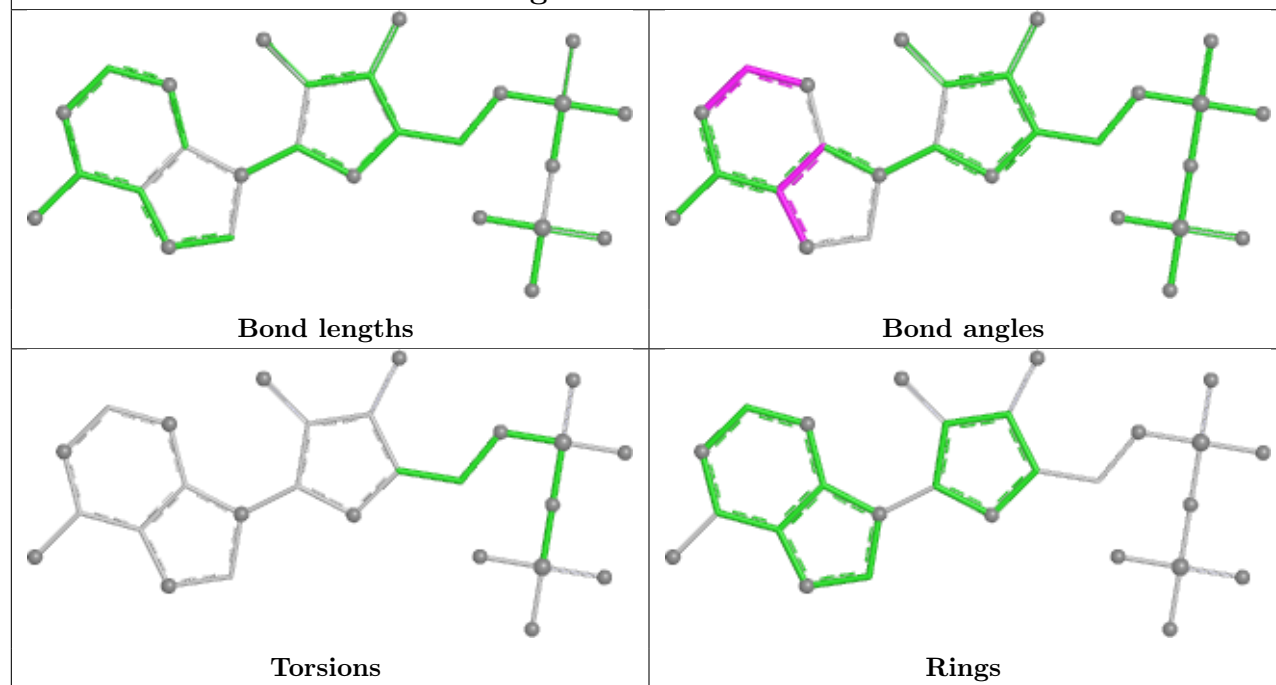


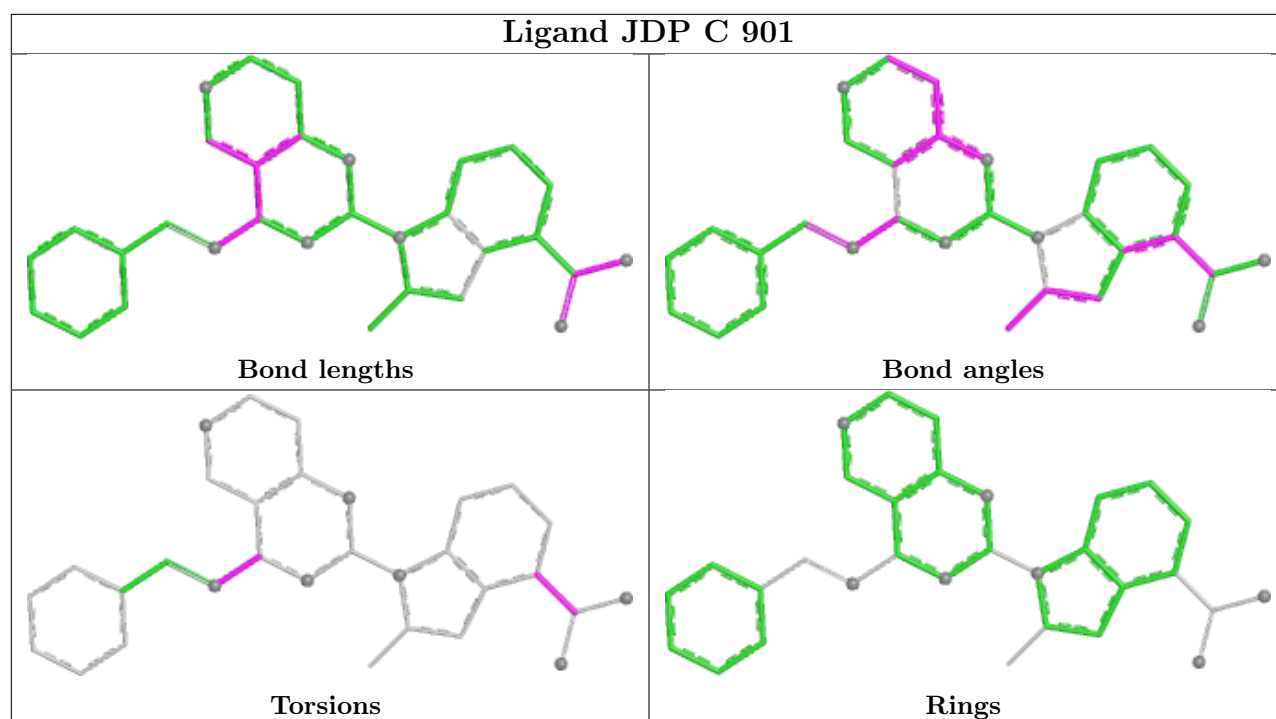
Rings

Ligand ADP J 902



Ligand ADP C 902





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

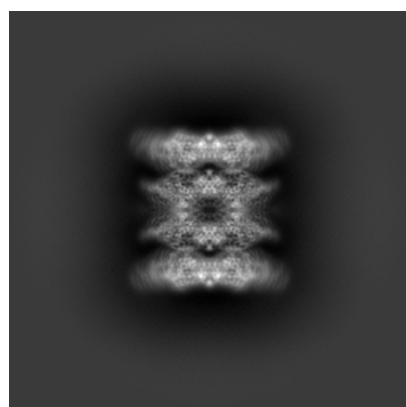
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24531. These allow visual inspection of the internal detail of the map and identification of artifacts.

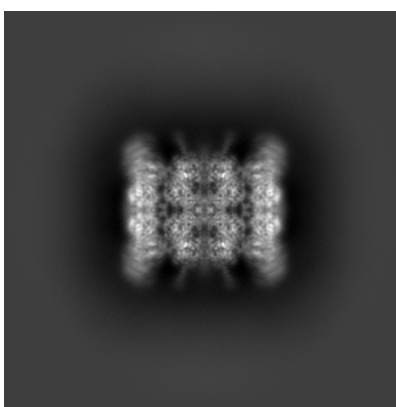
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

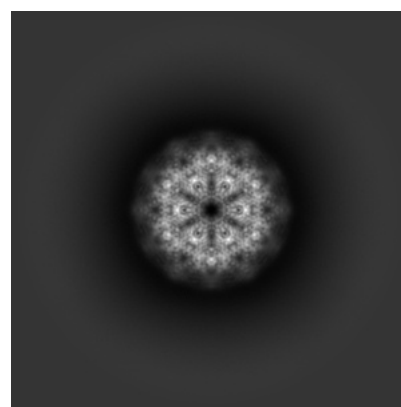
6.1.1 Primary map



X



Y

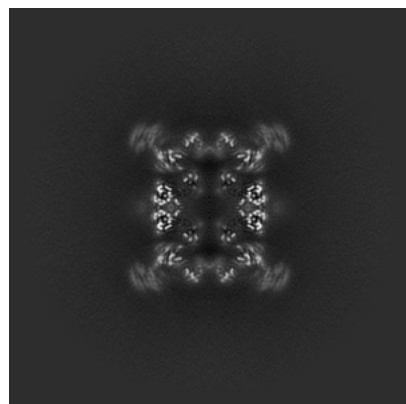


Z

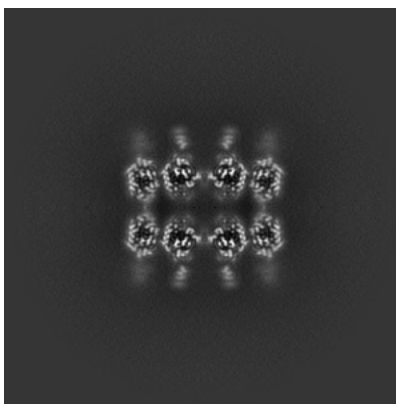
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

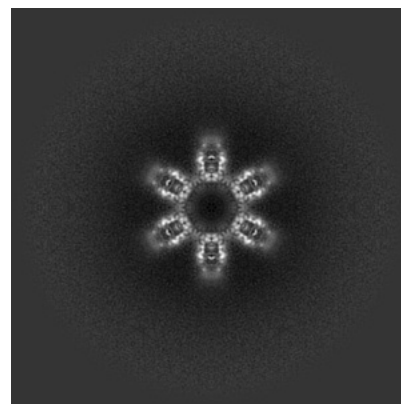
6.2.1 Primary map



X Index: 200



Y Index: 200

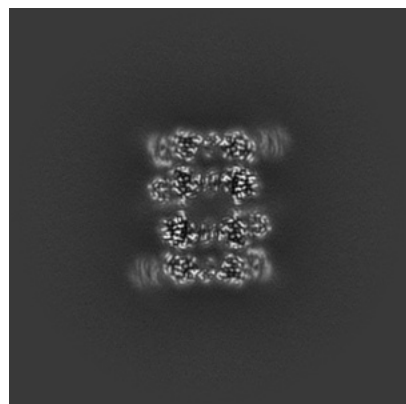


Z Index: 200

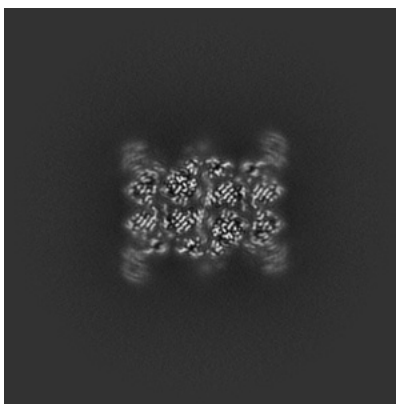
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

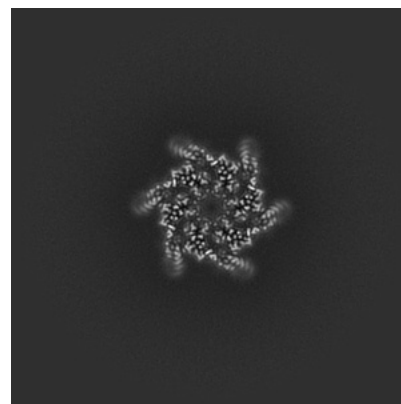
6.3.1 Primary map



X Index: 185



Y Index: 171

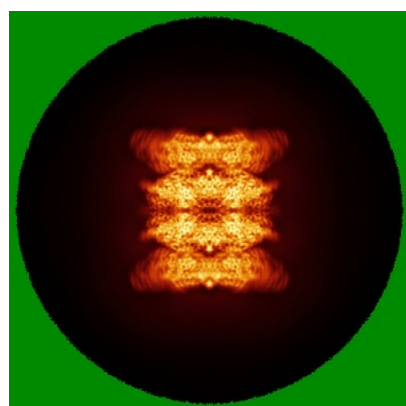


Z Index: 179

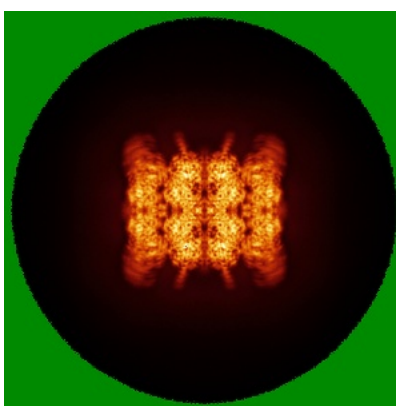
The images above show the largest variance slices of the map in three orthogonal directions.

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

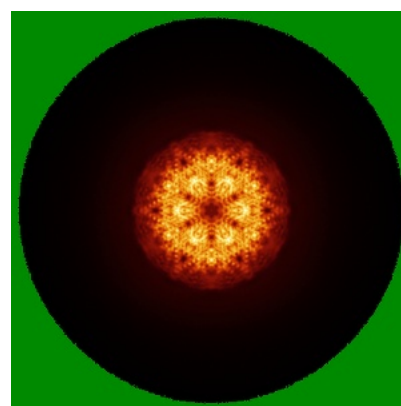
6.4.1 Primary map



X



Y

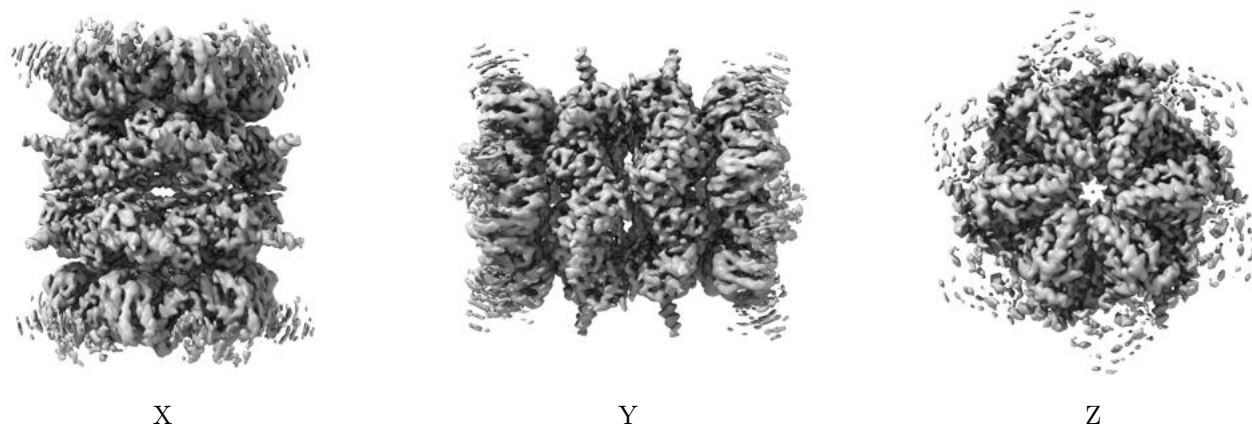


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

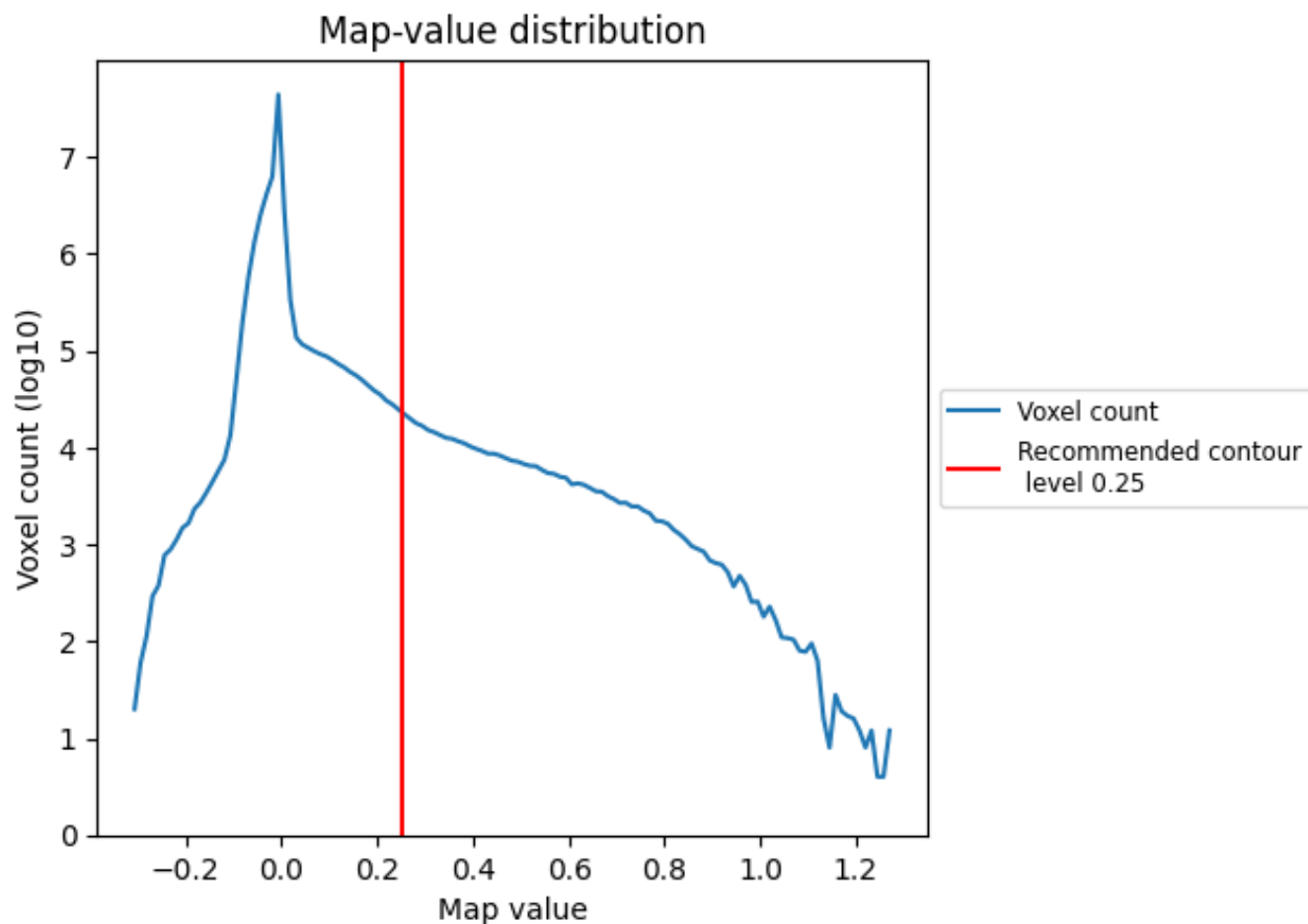
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

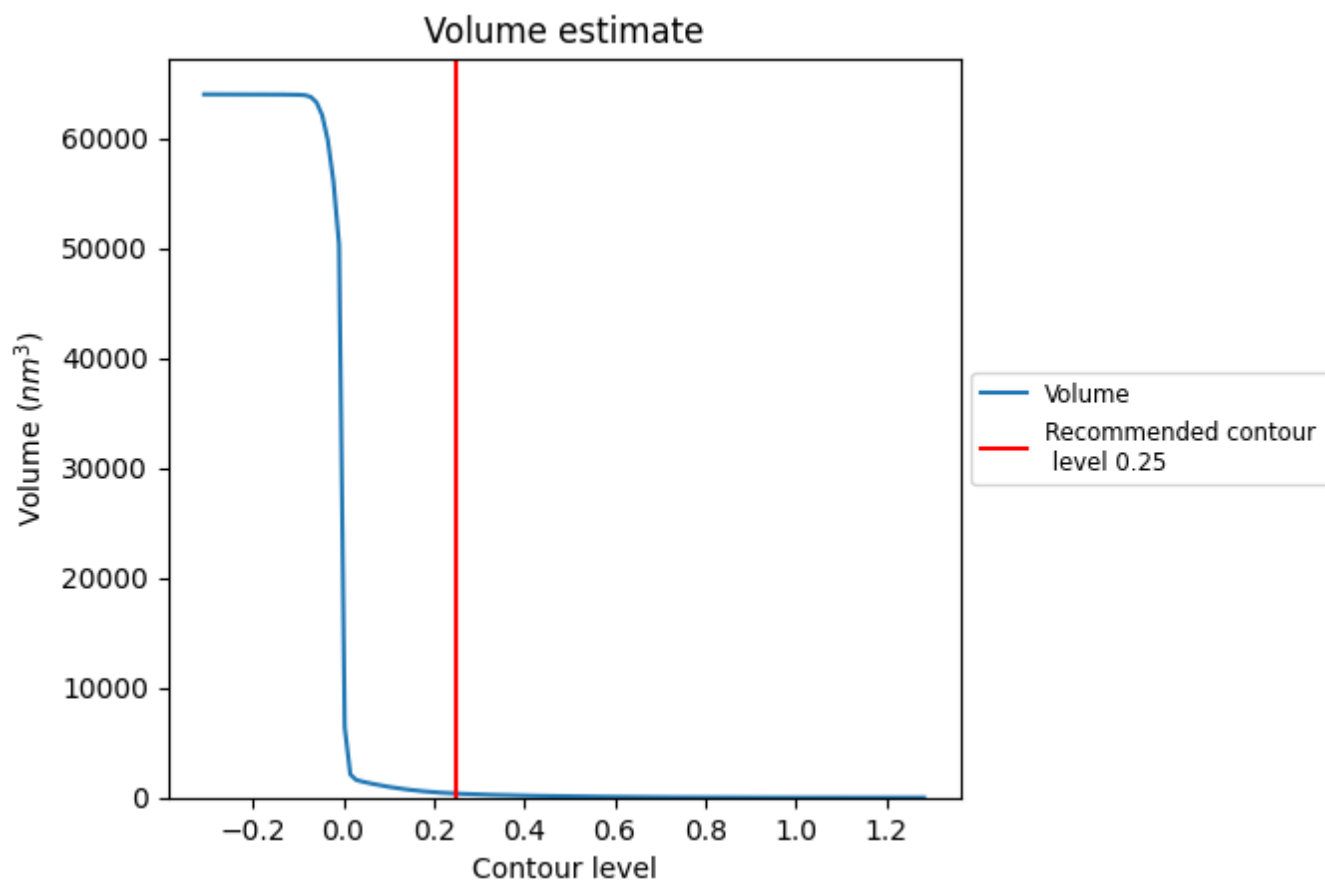
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

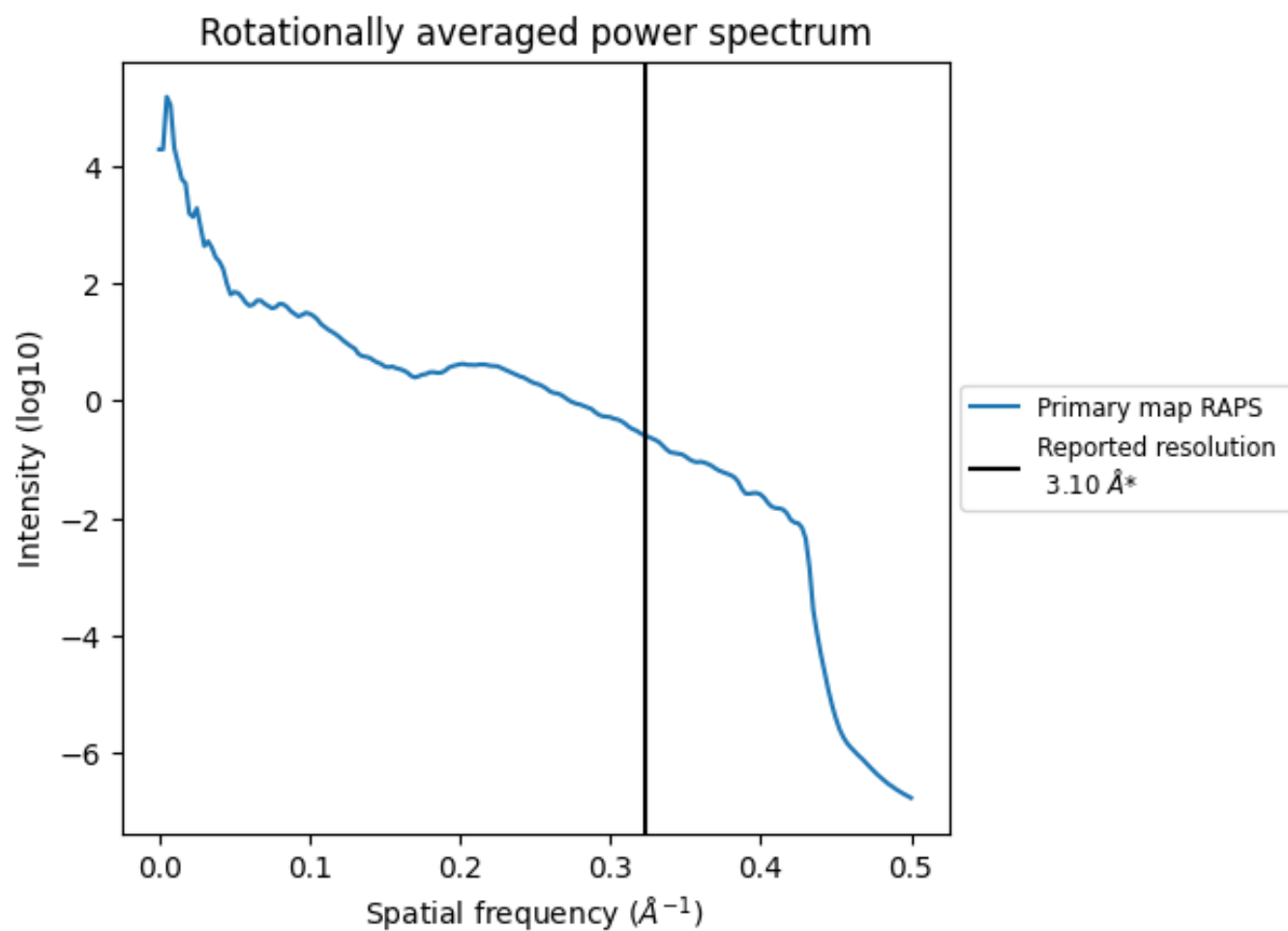
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 364 nm^3 ; this corresponds to an approximate mass of 329 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 ⓘ

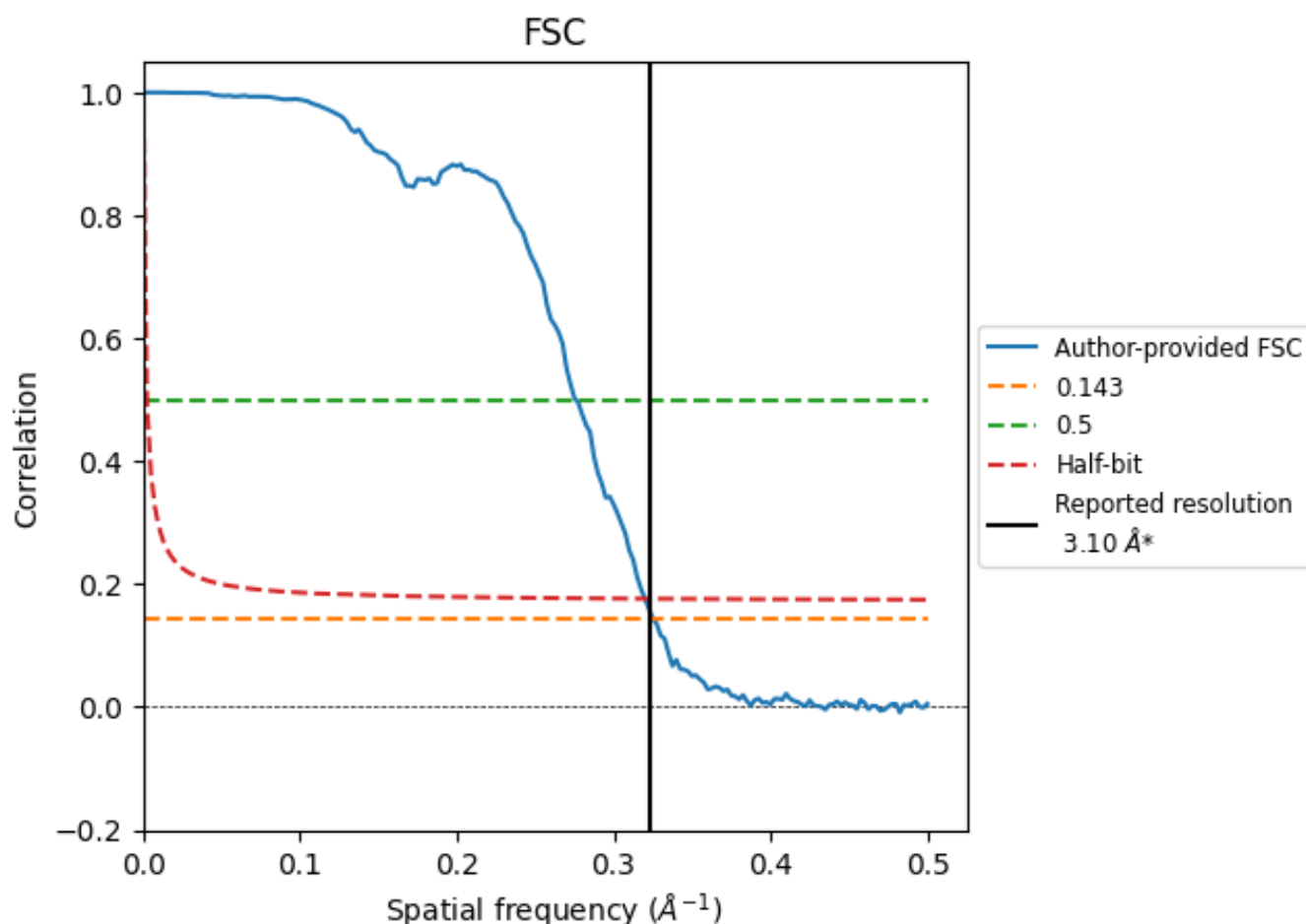


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

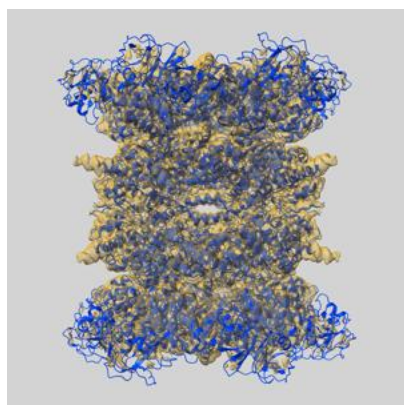
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.62	3.13
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

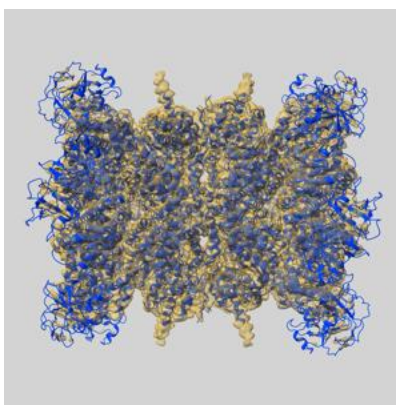
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24531 and PDB model 7RLI. Per-residue inclusion information can be found in section [3](#) on page [12](#).

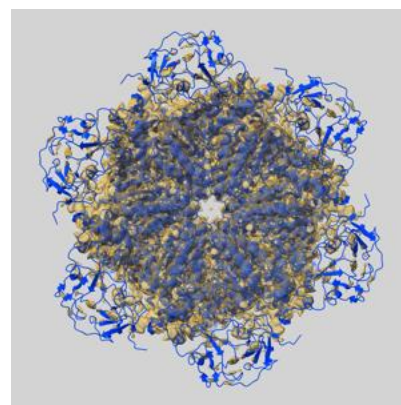
9.1 Map-model overlay [i](#)



X



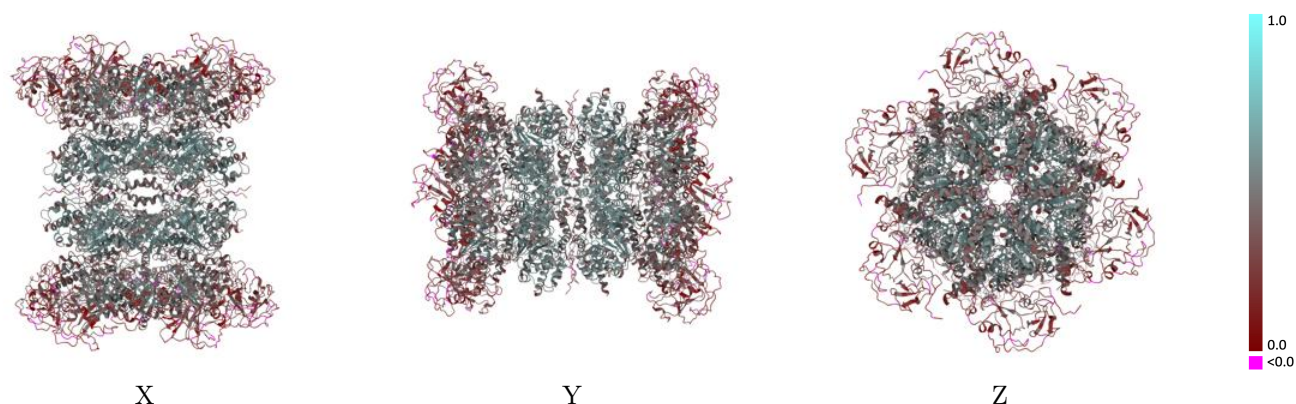
Y



Z

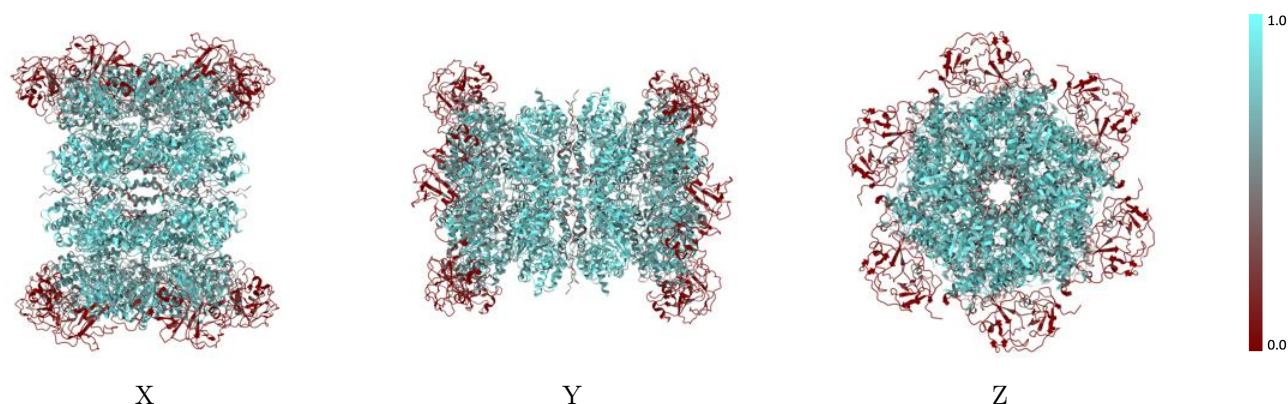
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



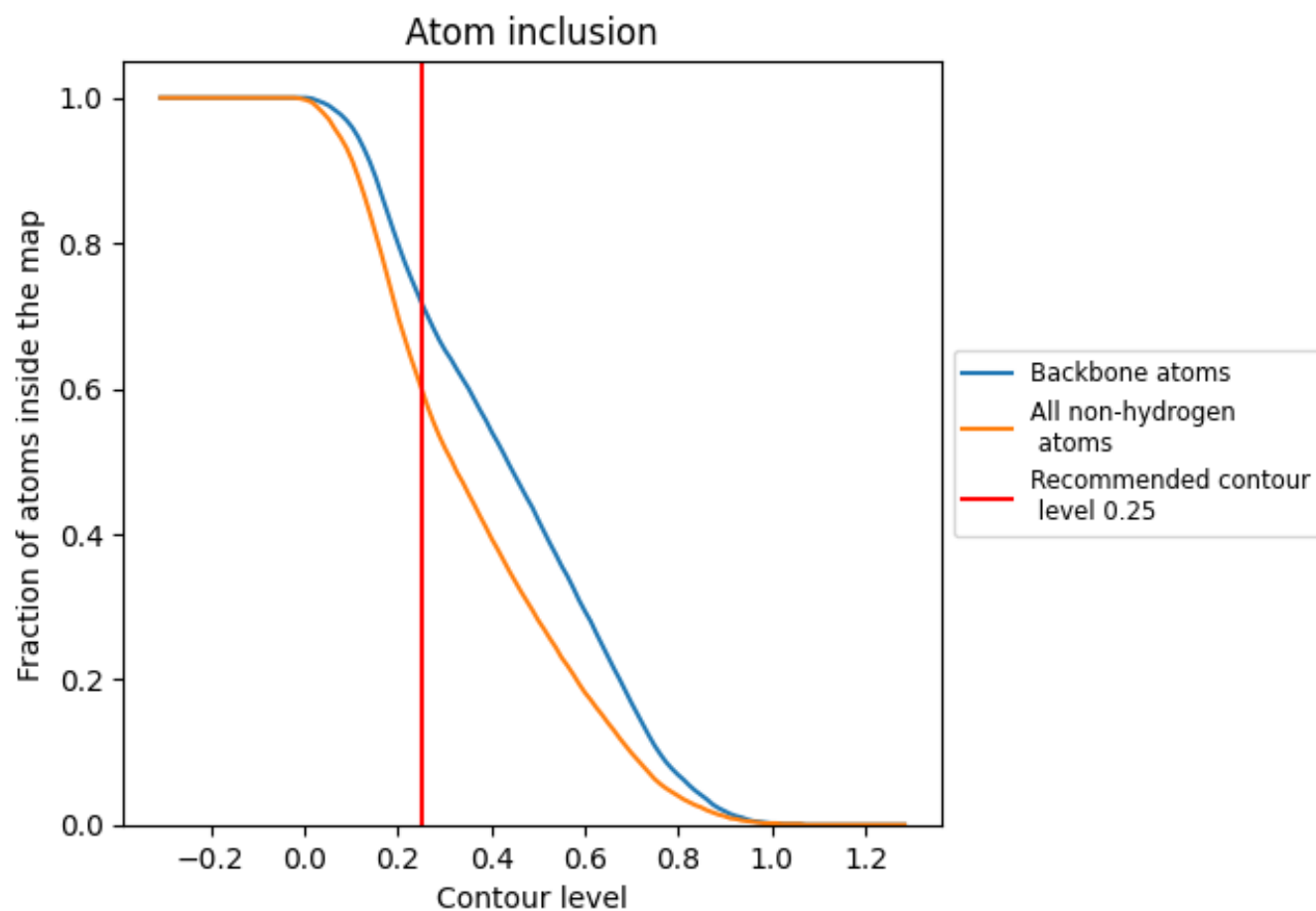
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion ⓘ



At the recommended contour level, 72% of all backbone atoms, 60% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.6000</div>	<div><div></div>0.3930</div>
A	<div><div></div>0.6010</div>	<div><div></div>0.3940</div>
B	<div><div></div>0.6000</div>	<div><div></div>0.3950</div>
C	<div><div></div>0.6000</div>	<div><div></div>0.3940</div>
D	<div><div></div>0.5990</div>	<div><div></div>0.3930</div>
E	<div><div></div>0.6000</div>	<div><div></div>0.3920</div>
F	<div><div></div>0.5990</div>	<div><div></div>0.3970</div>
G	<div><div></div>0.6000</div>	<div><div></div>0.3950</div>
H	<div><div></div>0.5990</div>	<div><div></div>0.3870</div>
I	<div><div></div>0.5990</div>	<div><div></div>0.3900</div>
J	<div><div></div>0.6000</div>	<div><div></div>0.3910</div>
K	<div><div></div>0.5990</div>	<div><div></div>0.3980</div>
L	<div><div></div>0.6010</div>	<div><div></div>0.3920</div>

1.0

0.0

<0.0