



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 01:59 AM UTC

PDB ID : 7Q4U / pdb_00007q4u
EMDB ID : EMD-13817
Title : Cryo-EM structure of Mycobacterium tuberculosis RNA polymerase holoenzyme octamer comprising sigma factor SigB
Authors : Brodolin, K.
Deposited on : 2021-11-02
Resolution : 4.39 Å(reported)
Based on initial model : 7PP4

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

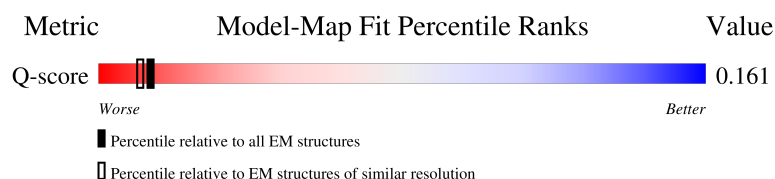
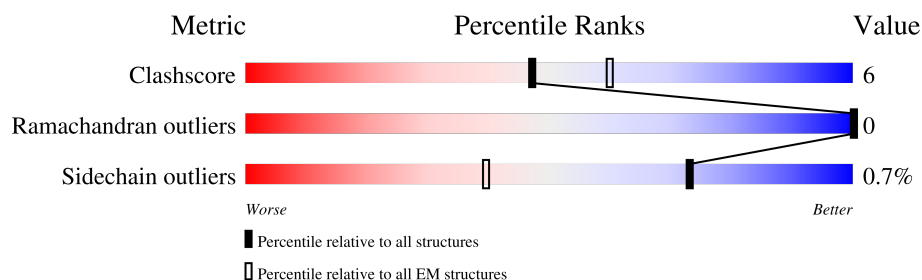
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

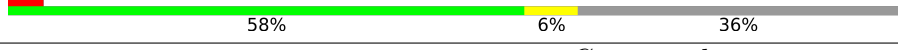
The reported resolution of this entry is 4.39 Å.

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



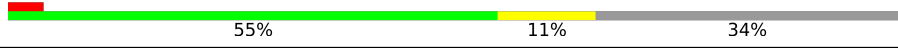
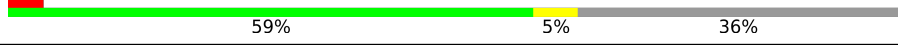
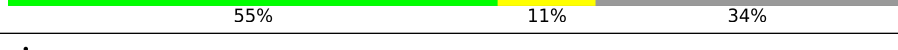
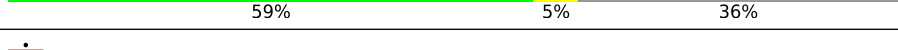
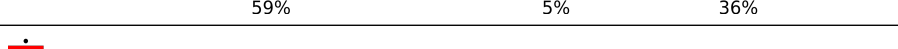
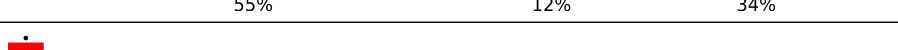
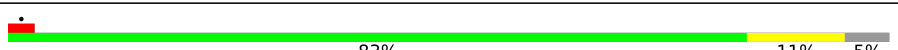
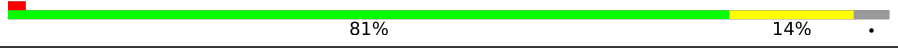
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3667 (3.89 - 4.88)

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	347	
1	AA	347	
1	B	347	
1	FA	347	

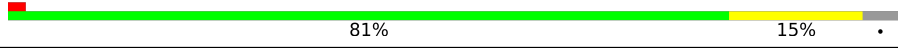
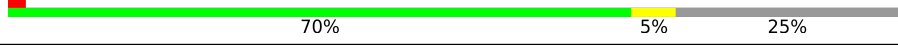
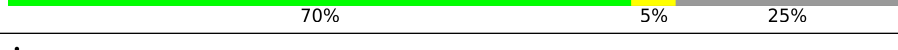
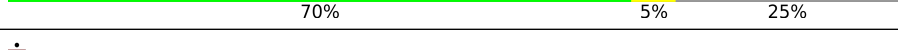
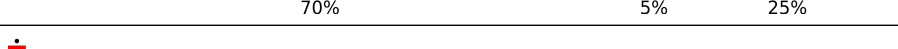
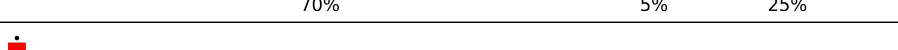
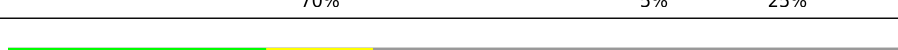
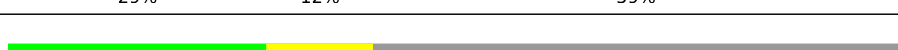
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Mol	Chain	Length	Quality of chain
1	G	347	
1	GA	347	
1	H	347	
1	LA	347	
1	M	347	
1	MA	347	
1	N	347	
1	RA	347	
1	S	347	
1	SA	347	
1	T	347	
1	Z	347	
2	BA	1174	
2	C	1174	
2	HA	1174	
2	I	1174	
2	NA	1174	
2	O	1174	
2	TA	1174	
2	V	1174	
3	CA	1319	
3	D	1319	
3	IA	1319	
3	J	1319	
3	OA	1319	

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Mol	Chain	Length	Quality of chain
3	P	1319	
3	UA	1319	
3	W	1319	
4	DA	110	
4	E	110	
4	JA	110	
4	K	110	
4	PA	110	
4	Q	110	
4	VA	110	
4	X	110	
5	EA	343	
5	F	343	
5	KA	343	
5	L	343	
5	QA	343	
5	R	343	
5	WA	343	
5	Y	343	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 190528 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	B	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		
1	G	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	H	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		
1	M	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	N	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		
1	S	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	T	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		
1	Z	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	AA	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		
1	FA	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	GA	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		
1	LA	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	MA	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		
1	RA	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	SA	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		
2	I	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		
2	O	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		
2	V	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		
2	BA	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		
2	HA	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		
2	NA	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		
2	TA	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5	MET	-	initiating methionine	UNP P9WGY9
C	6	VAL	ILE	conflict	UNP P9WGY9
I	5	MET	-	initiating methionine	UNP P9WGY9
I	6	VAL	ILE	conflict	UNP P9WGY9
O	5	MET	-	initiating methionine	UNP P9WGY9
O	6	VAL	ILE	conflict	UNP P9WGY9
V	5	MET	-	initiating methionine	UNP P9WGY9
V	6	VAL	ILE	conflict	UNP P9WGY9
BA	5	MET	-	initiating methionine	UNP P9WGY9
BA	6	VAL	ILE	conflict	UNP P9WGY9
HA	5	MET	-	initiating methionine	UNP P9WGY9
HA	6	VAL	ILE	conflict	UNP P9WGY9
NA	5	MET	-	initiating methionine	UNP P9WGY9
NA	6	VAL	ILE	conflict	UNP P9WGY9
TA	5	MET	-	initiating methionine	UNP P9WGY9
TA	6	VAL	ILE	conflict	UNP P9WGY9

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1269	Total	C	N	O	S	0	0
			9951	6231	1805	1874	41		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1269	Total 9951	C 6231	N 1805	O 1874	S 41	0	0
3	P	1269	Total 9951	C 6231	N 1805	O 1874	S 41	0	0
3	W	1269	Total 9951	C 6231	N 1805	O 1874	S 41	0	0
3	CA	1269	Total 9951	C 6231	N 1805	O 1874	S 41	0	0
3	IA	1269	Total 9951	C 6231	N 1805	O 1874	S 41	0	0
3	OA	1269	Total 9951	C 6231	N 1805	O 1874	S 41	0	0
3	UA	1269	Total 9951	C 6231	N 1805	O 1874	S 41	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP P9WGY7
D	1318	HIS	-	expression tag	UNP P9WGY7
D	1319	HIS	-	expression tag	UNP P9WGY7
D	1320	HIS	-	expression tag	UNP P9WGY7
D	1321	HIS	-	expression tag	UNP P9WGY7
D	1322	HIS	-	expression tag	UNP P9WGY7
J	1317	HIS	-	expression tag	UNP P9WGY7
J	1318	HIS	-	expression tag	UNP P9WGY7
J	1319	HIS	-	expression tag	UNP P9WGY7
J	1320	HIS	-	expression tag	UNP P9WGY7
J	1321	HIS	-	expression tag	UNP P9WGY7
J	1322	HIS	-	expression tag	UNP P9WGY7
P	1317	HIS	-	expression tag	UNP P9WGY7
P	1318	HIS	-	expression tag	UNP P9WGY7
P	1319	HIS	-	expression tag	UNP P9WGY7
P	1320	HIS	-	expression tag	UNP P9WGY7
P	1321	HIS	-	expression tag	UNP P9WGY7
P	1322	HIS	-	expression tag	UNP P9WGY7
W	1317	HIS	-	expression tag	UNP P9WGY7
W	1318	HIS	-	expression tag	UNP P9WGY7
W	1319	HIS	-	expression tag	UNP P9WGY7
W	1320	HIS	-	expression tag	UNP P9WGY7
W	1321	HIS	-	expression tag	UNP P9WGY7
W	1322	HIS	-	expression tag	UNP P9WGY7
CA	1317	HIS	-	expression tag	UNP P9WGY7

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Chain	Residue	Modelled	Actual	Comment	Reference
CA	1318	HIS	-	expression tag	UNP P9WGY7
CA	1319	HIS	-	expression tag	UNP P9WGY7
CA	1320	HIS	-	expression tag	UNP P9WGY7
CA	1321	HIS	-	expression tag	UNP P9WGY7
CA	1322	HIS	-	expression tag	UNP P9WGY7
IA	1317	HIS	-	expression tag	UNP P9WGY7
IA	1318	HIS	-	expression tag	UNP P9WGY7
IA	1319	HIS	-	expression tag	UNP P9WGY7
IA	1320	HIS	-	expression tag	UNP P9WGY7
IA	1321	HIS	-	expression tag	UNP P9WGY7
IA	1322	HIS	-	expression tag	UNP P9WGY7
OA	1317	HIS	-	expression tag	UNP P9WGY7
OA	1318	HIS	-	expression tag	UNP P9WGY7
OA	1319	HIS	-	expression tag	UNP P9WGY7
OA	1320	HIS	-	expression tag	UNP P9WGY7
OA	1321	HIS	-	expression tag	UNP P9WGY7
OA	1322	HIS	-	expression tag	UNP P9WGY7
UA	1317	HIS	-	expression tag	UNP P9WGY7
UA	1318	HIS	-	expression tag	UNP P9WGY7
UA	1319	HIS	-	expression tag	UNP P9WGY7
UA	1320	HIS	-	expression tag	UNP P9WGY7
UA	1321	HIS	-	expression tag	UNP P9WGY7
UA	1322	HIS	-	expression tag	UNP P9WGY7

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			654	417	108	129		
4	K	83	Total	C	N	O	0	0
			654	417	108	129		
4	Q	83	Total	C	N	O	0	0
			654	417	108	129		
4	X	83	Total	C	N	O	0	0
			654	417	108	129		
4	DA	83	Total	C	N	O	0	0
			654	417	108	129		
4	JA	83	Total	C	N	O	0	0
			654	417	108	129		
4	PA	83	Total	C	N	O	0	0
			654	417	108	129		
4	VA	83	Total	C	N	O	0	0
			654	417	108	129		

- Molecule 5 is a protein called RNA polymerase sigma factor SigB.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	142	Total	C	N	O	S	0	0
			1119	705	210	201	3		
5	L	142	Total	C	N	O	S	0	0
			1119	705	210	201	3		
5	R	142	Total	C	N	O	S	0	0
			1119	705	210	201	3		
5	Y	142	Total	C	N	O	S	0	0
			1119	705	210	201	3		
5	EA	142	Total	C	N	O	S	0	0
			1119	705	210	201	3		
5	KA	142	Total	C	N	O	S	0	0
			1119	705	210	201	3		
5	QA	142	Total	C	N	O	S	0	0
			1119	705	210	201	3		
5	WA	142	Total	C	N	O	S	0	0
			1119	705	210	201	3		

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP P9WGI5
F	-18	GLY	-	expression tag	UNP P9WGI5
F	-17	SER	-	expression tag	UNP P9WGI5
F	-16	SER	-	expression tag	UNP P9WGI5
F	-15	HIS	-	expression tag	UNP P9WGI5
F	-14	HIS	-	expression tag	UNP P9WGI5
F	-13	HIS	-	expression tag	UNP P9WGI5
F	-12	HIS	-	expression tag	UNP P9WGI5
F	-11	HIS	-	expression tag	UNP P9WGI5
F	-10	HIS	-	expression tag	UNP P9WGI5
F	-9	SER	-	expression tag	UNP P9WGI5
F	-8	SER	-	expression tag	UNP P9WGI5
F	-7	GLY	-	expression tag	UNP P9WGI5
F	-6	LEU	-	expression tag	UNP P9WGI5
F	-5	VAL	-	expression tag	UNP P9WGI5
F	-4	PRO	-	expression tag	UNP P9WGI5
F	-3	ARG	-	expression tag	UNP P9WGI5
F	-2	GLY	-	expression tag	UNP P9WGI5
F	-1	SER	-	expression tag	UNP P9WGI5
F	0	HIS	-	expression tag	UNP P9WGI5
L	-19	MET	-	initiating methionine	UNP P9WGI5
L	-18	GLY	-	expression tag	UNP P9WGI5

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-17	SER	-	expression tag	UNP P9WGI5
L	-16	SER	-	expression tag	UNP P9WGI5
L	-15	HIS	-	expression tag	UNP P9WGI5
L	-14	HIS	-	expression tag	UNP P9WGI5
L	-13	HIS	-	expression tag	UNP P9WGI5
L	-12	HIS	-	expression tag	UNP P9WGI5
L	-11	HIS	-	expression tag	UNP P9WGI5
L	-10	HIS	-	expression tag	UNP P9WGI5
L	-9	SER	-	expression tag	UNP P9WGI5
L	-8	SER	-	expression tag	UNP P9WGI5
L	-7	GLY	-	expression tag	UNP P9WGI5
L	-6	LEU	-	expression tag	UNP P9WGI5
L	-5	VAL	-	expression tag	UNP P9WGI5
L	-4	PRO	-	expression tag	UNP P9WGI5
L	-3	ARG	-	expression tag	UNP P9WGI5
L	-2	GLY	-	expression tag	UNP P9WGI5
L	-1	SER	-	expression tag	UNP P9WGI5
L	0	HIS	-	expression tag	UNP P9WGI5
R	-19	MET	-	initiating methionine	UNP P9WGI5
R	-18	GLY	-	expression tag	UNP P9WGI5
R	-17	SER	-	expression tag	UNP P9WGI5
R	-16	SER	-	expression tag	UNP P9WGI5
R	-15	HIS	-	expression tag	UNP P9WGI5
R	-14	HIS	-	expression tag	UNP P9WGI5
R	-13	HIS	-	expression tag	UNP P9WGI5
R	-12	HIS	-	expression tag	UNP P9WGI5
R	-11	HIS	-	expression tag	UNP P9WGI5
R	-10	HIS	-	expression tag	UNP P9WGI5
R	-9	SER	-	expression tag	UNP P9WGI5
R	-8	SER	-	expression tag	UNP P9WGI5
R	-7	GLY	-	expression tag	UNP P9WGI5
R	-6	LEU	-	expression tag	UNP P9WGI5
R	-5	VAL	-	expression tag	UNP P9WGI5
R	-4	PRO	-	expression tag	UNP P9WGI5
R	-3	ARG	-	expression tag	UNP P9WGI5
R	-2	GLY	-	expression tag	UNP P9WGI5
R	-1	SER	-	expression tag	UNP P9WGI5
R	0	HIS	-	expression tag	UNP P9WGI5
Y	-19	MET	-	initiating methionine	UNP P9WGI5
Y	-18	GLY	-	expression tag	UNP P9WGI5
Y	-17	SER	-	expression tag	UNP P9WGI5
Y	-16	SER	-	expression tag	UNP P9WGI5

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-15	HIS	-	expression tag	UNP P9WGI5
Y	-14	HIS	-	expression tag	UNP P9WGI5
Y	-13	HIS	-	expression tag	UNP P9WGI5
Y	-12	HIS	-	expression tag	UNP P9WGI5
Y	-11	HIS	-	expression tag	UNP P9WGI5
Y	-10	HIS	-	expression tag	UNP P9WGI5
Y	-9	SER	-	expression tag	UNP P9WGI5
Y	-8	SER	-	expression tag	UNP P9WGI5
Y	-7	GLY	-	expression tag	UNP P9WGI5
Y	-6	LEU	-	expression tag	UNP P9WGI5
Y	-5	VAL	-	expression tag	UNP P9WGI5
Y	-4	PRO	-	expression tag	UNP P9WGI5
Y	-3	ARG	-	expression tag	UNP P9WGI5
Y	-2	GLY	-	expression tag	UNP P9WGI5
Y	-1	SER	-	expression tag	UNP P9WGI5
Y	0	HIS	-	expression tag	UNP P9WGI5
EA	-19	MET	-	initiating methionine	UNP P9WGI5
EA	-18	GLY	-	expression tag	UNP P9WGI5
EA	-17	SER	-	expression tag	UNP P9WGI5
EA	-16	SER	-	expression tag	UNP P9WGI5
EA	-15	HIS	-	expression tag	UNP P9WGI5
EA	-14	HIS	-	expression tag	UNP P9WGI5
EA	-13	HIS	-	expression tag	UNP P9WGI5
EA	-12	HIS	-	expression tag	UNP P9WGI5
EA	-11	HIS	-	expression tag	UNP P9WGI5
EA	-10	HIS	-	expression tag	UNP P9WGI5
EA	-9	SER	-	expression tag	UNP P9WGI5
EA	-8	SER	-	expression tag	UNP P9WGI5
EA	-7	GLY	-	expression tag	UNP P9WGI5
EA	-6	LEU	-	expression tag	UNP P9WGI5
EA	-5	VAL	-	expression tag	UNP P9WGI5
EA	-4	PRO	-	expression tag	UNP P9WGI5
EA	-3	ARG	-	expression tag	UNP P9WGI5
EA	-2	GLY	-	expression tag	UNP P9WGI5
EA	-1	SER	-	expression tag	UNP P9WGI5
EA	0	HIS	-	expression tag	UNP P9WGI5
KA	-19	MET	-	initiating methionine	UNP P9WGI5
KA	-18	GLY	-	expression tag	UNP P9WGI5
KA	-17	SER	-	expression tag	UNP P9WGI5
KA	-16	SER	-	expression tag	UNP P9WGI5
KA	-15	HIS	-	expression tag	UNP P9WGI5
KA	-14	HIS	-	expression tag	UNP P9WGI5

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Chain	Residue	Modelled	Actual	Comment	Reference
KA	-13	HIS	-	expression tag	UNP P9WGI5
KA	-12	HIS	-	expression tag	UNP P9WGI5
KA	-11	HIS	-	expression tag	UNP P9WGI5
KA	-10	HIS	-	expression tag	UNP P9WGI5
KA	-9	SER	-	expression tag	UNP P9WGI5
KA	-8	SER	-	expression tag	UNP P9WGI5
KA	-7	GLY	-	expression tag	UNP P9WGI5
KA	-6	LEU	-	expression tag	UNP P9WGI5
KA	-5	VAL	-	expression tag	UNP P9WGI5
KA	-4	PRO	-	expression tag	UNP P9WGI5
KA	-3	ARG	-	expression tag	UNP P9WGI5
KA	-2	GLY	-	expression tag	UNP P9WGI5
KA	-1	SER	-	expression tag	UNP P9WGI5
KA	0	HIS	-	expression tag	UNP P9WGI5
QA	-19	MET	-	initiating methionine	UNP P9WGI5
QA	-18	GLY	-	expression tag	UNP P9WGI5
QA	-17	SER	-	expression tag	UNP P9WGI5
QA	-16	SER	-	expression tag	UNP P9WGI5
QA	-15	HIS	-	expression tag	UNP P9WGI5
QA	-14	HIS	-	expression tag	UNP P9WGI5
QA	-13	HIS	-	expression tag	UNP P9WGI5
QA	-12	HIS	-	expression tag	UNP P9WGI5
QA	-11	HIS	-	expression tag	UNP P9WGI5
QA	-10	HIS	-	expression tag	UNP P9WGI5
QA	-9	SER	-	expression tag	UNP P9WGI5
QA	-8	SER	-	expression tag	UNP P9WGI5
QA	-7	GLY	-	expression tag	UNP P9WGI5
QA	-6	LEU	-	expression tag	UNP P9WGI5
QA	-5	VAL	-	expression tag	UNP P9WGI5
QA	-4	PRO	-	expression tag	UNP P9WGI5
QA	-3	ARG	-	expression tag	UNP P9WGI5
QA	-2	GLY	-	expression tag	UNP P9WGI5
QA	-1	SER	-	expression tag	UNP P9WGI5
QA	0	HIS	-	expression tag	UNP P9WGI5
WA	-19	MET	-	initiating methionine	UNP P9WGI5
WA	-18	GLY	-	expression tag	UNP P9WGI5
WA	-17	SER	-	expression tag	UNP P9WGI5
WA	-16	SER	-	expression tag	UNP P9WGI5
WA	-15	HIS	-	expression tag	UNP P9WGI5
WA	-14	HIS	-	expression tag	UNP P9WGI5
WA	-13	HIS	-	expression tag	UNP P9WGI5
WA	-12	HIS	-	expression tag	UNP P9WGI5

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Chain	Residue	Modelled	Actual	Comment	Reference
WA	-11	HIS	-	expression tag	UNP P9WGI5
WA	-10	HIS	-	expression tag	UNP P9WGI5
WA	-9	SER	-	expression tag	UNP P9WGI5
WA	-8	SER	-	expression tag	UNP P9WGI5
WA	-7	GLY	-	expression tag	UNP P9WGI5
WA	-6	LEU	-	expression tag	UNP P9WGI5
WA	-5	VAL	-	expression tag	UNP P9WGI5
WA	-4	PRO	-	expression tag	UNP P9WGI5
WA	-3	ARG	-	expression tag	UNP P9WGI5
WA	-2	GLY	-	expression tag	UNP P9WGI5
WA	-1	SER	-	expression tag	UNP P9WGI5
WA	0	HIS	-	expression tag	UNP P9WGI5

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	D	2	Total 2	Zn 2	0
6	J	2	Total 2	Zn 2	0
6	P	2	Total 2	Zn 2	0
6	W	2	Total 2	Zn 2	0
6	CA	2	Total 2	Zn 2	0
6	IA	2	Total 2	Zn 2	0
6	OA	2	Total 2	Zn 2	0
6	UA	2	Total 2	Zn 2	0

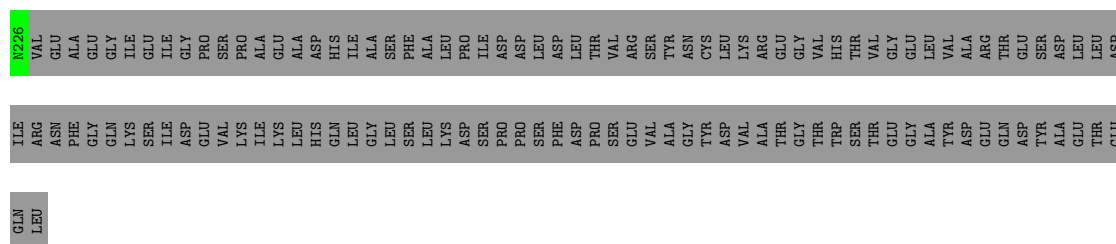
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total 1	Mg 1	0
7	J	1	Total 1	Mg 1	0

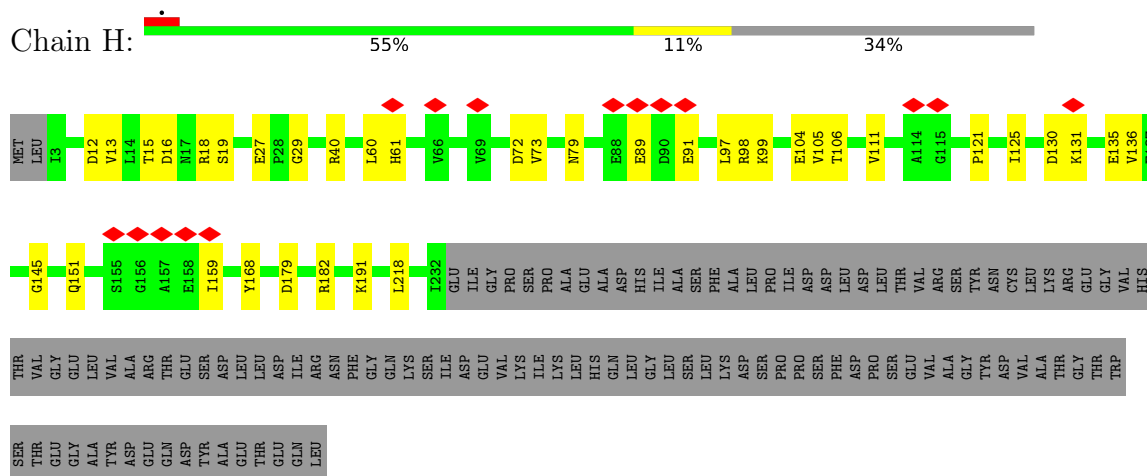
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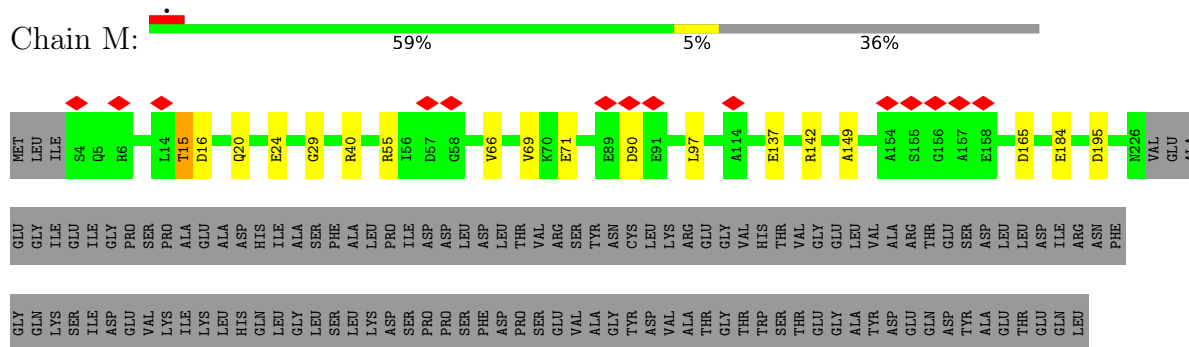
Mol	Chain	Residues	Atoms		AltConf
7	P	1	Total 1	Mg 1	0
7	W	1	Total 1	Mg 1	0
7	CA	1	Total 1	Mg 1	0
7	IA	1	Total 1	Mg 1	0
7	OA	1	Total 1	Mg 1	0
7	UA	1	Total 1	Mg 1	0



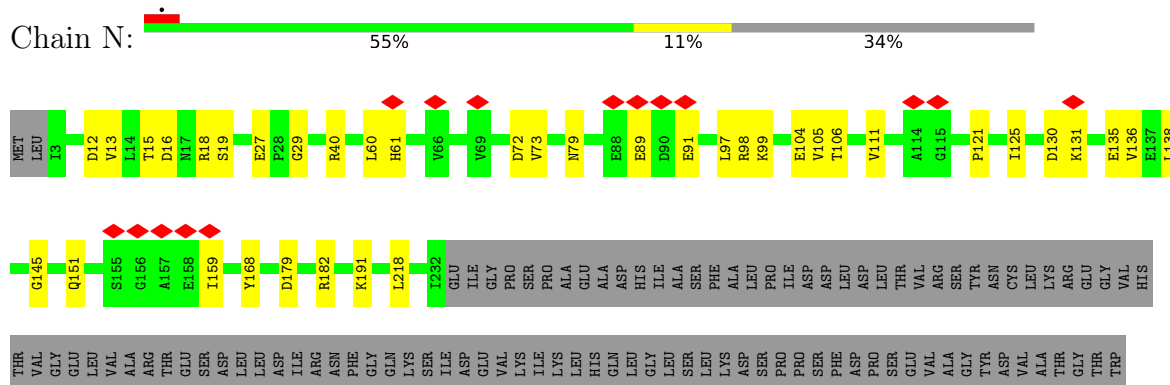
• Molecule 1: DNA-directed RNA polymerase subunit alpha

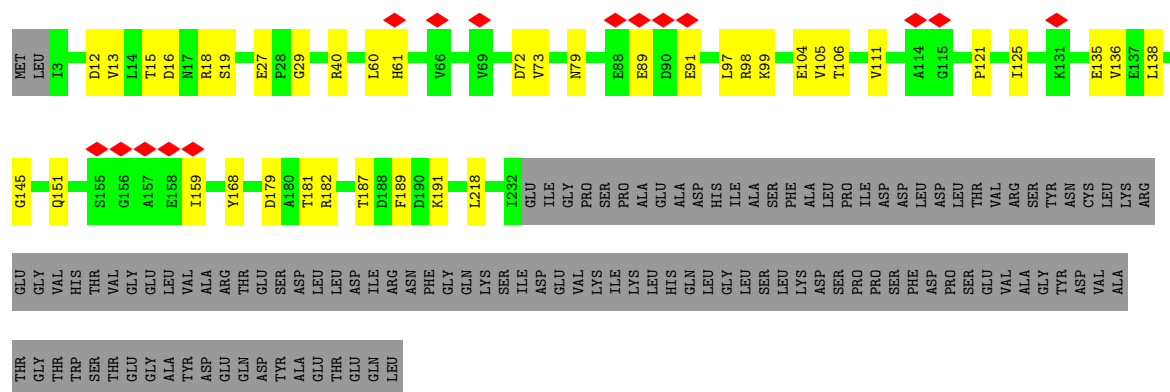


• Molecule 1: DNA-directed RNA polymerase subunit alpha

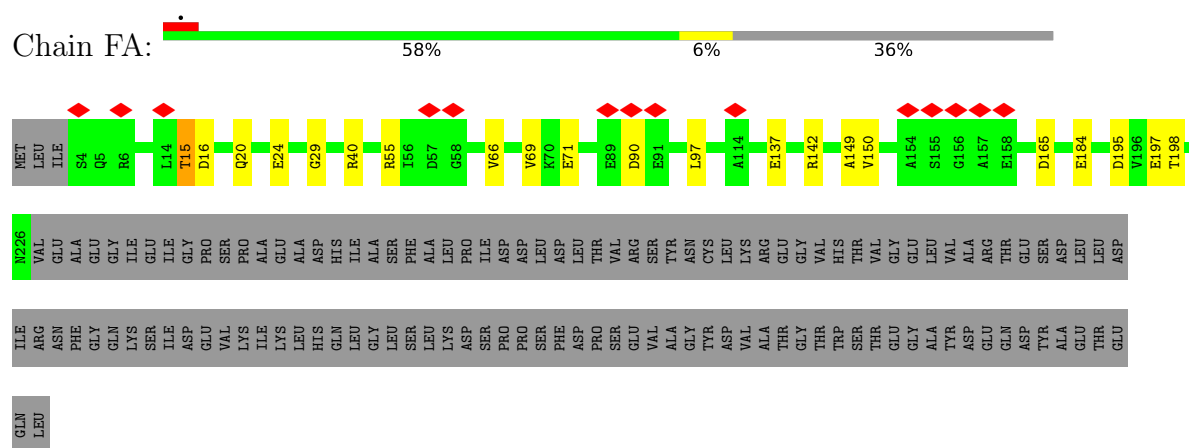


• Molecule 1: DNA-directed RNA polymerase subunit alpha

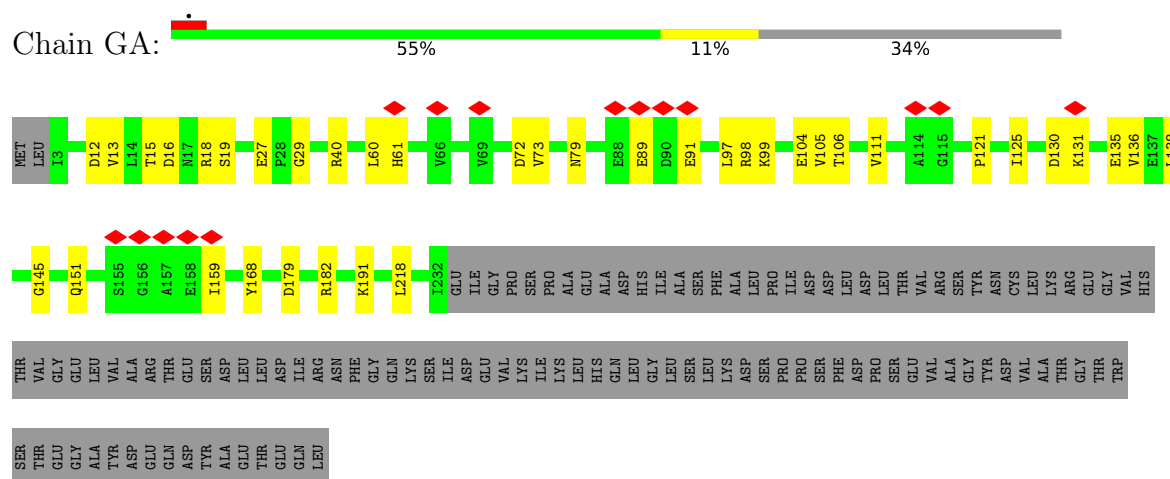




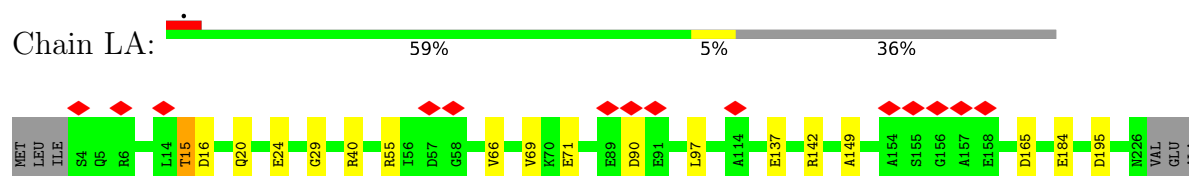
- Molecule 1: DNA-directed RNA polymerase subunit alpha

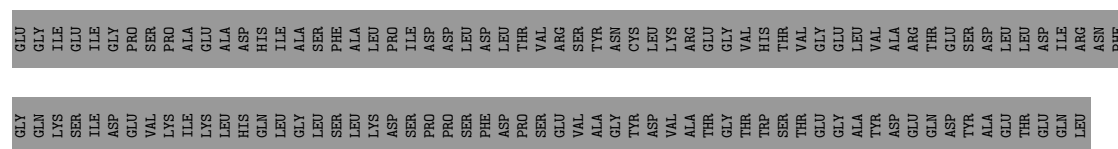


- Molecule 1: DNA-directed RNA polymerase subunit alpha

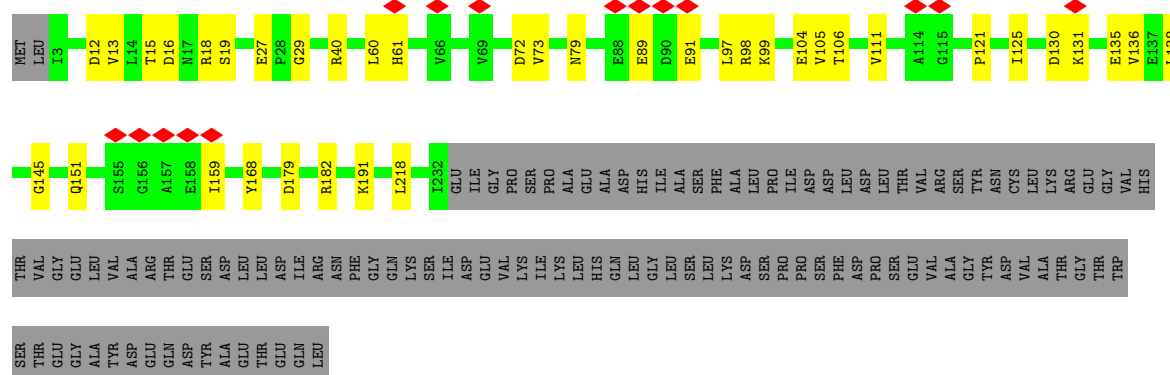


- Molecule 1: DNA-directed RNA polymerase subunit alpha

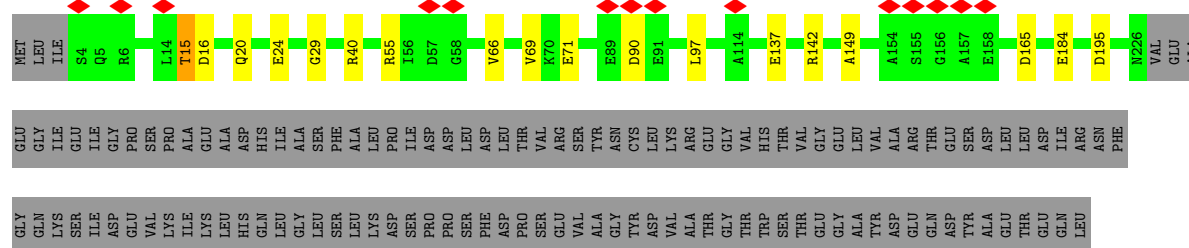




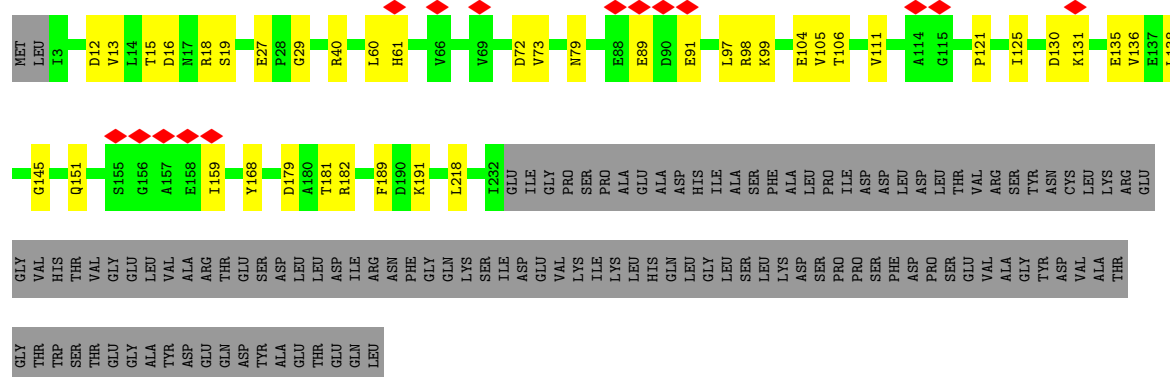
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha

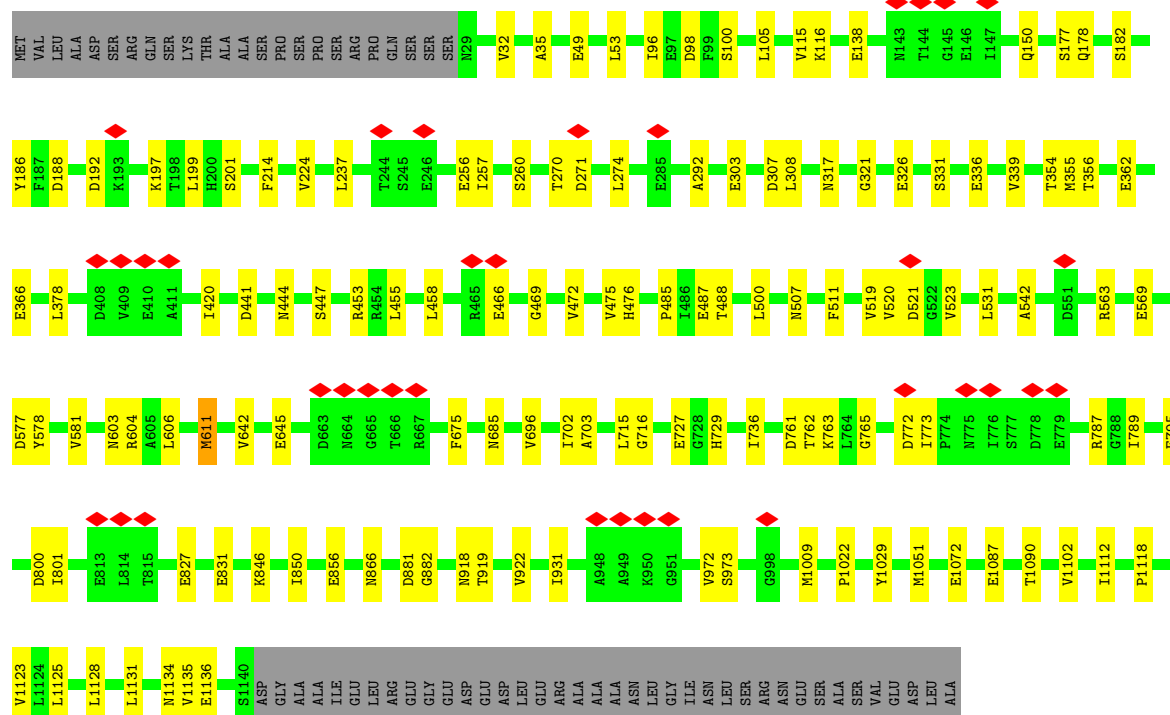


• Molecule 1: DNA-directed RNA polymerase subunit alpha



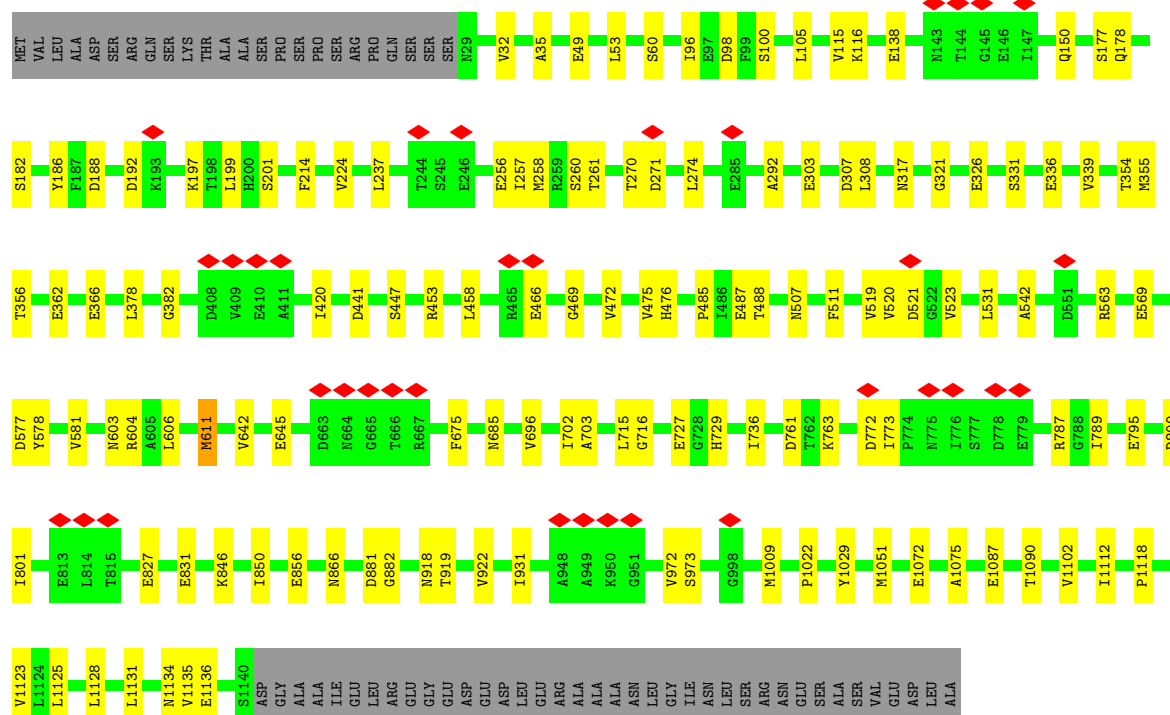
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:  83% 11% 5%



- Molecule 2: DNA-directed RNA polymerase subunit beta

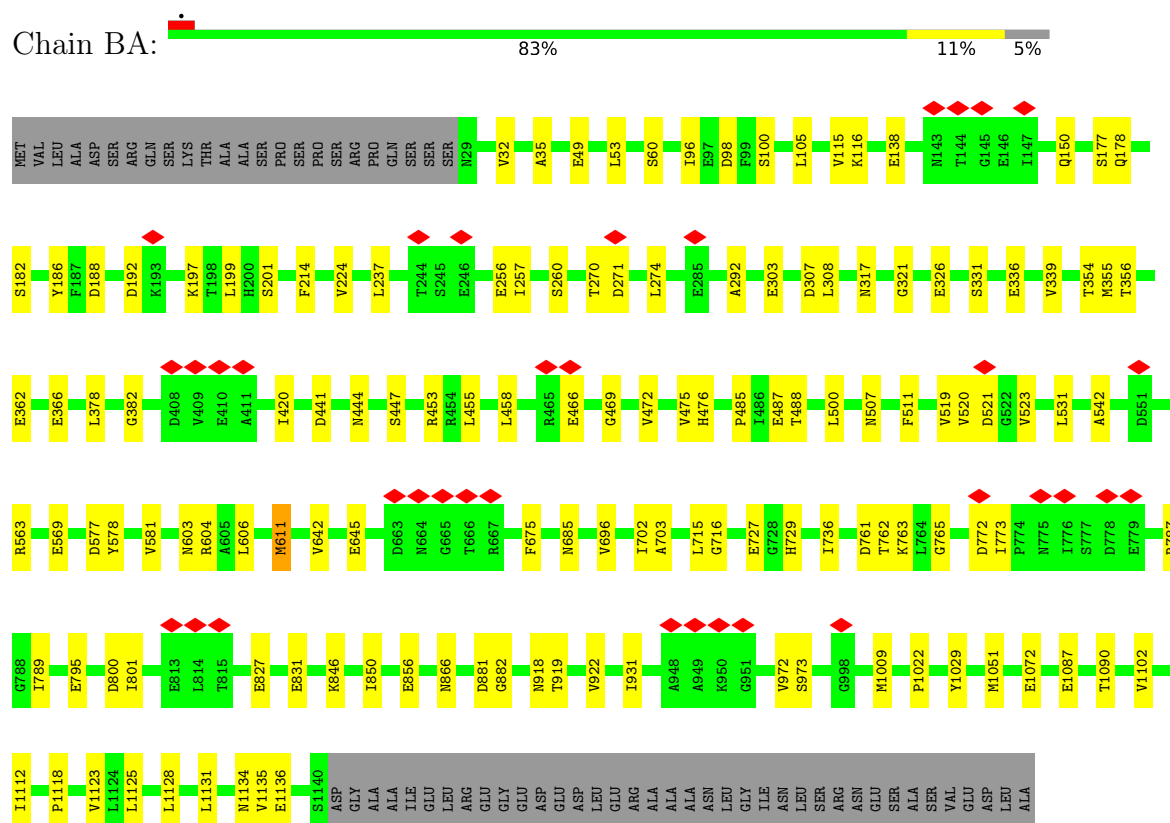
Chain I:  83% 11% 5%



- Molecule 2: DNA-directed RNA polymerase subunit beta

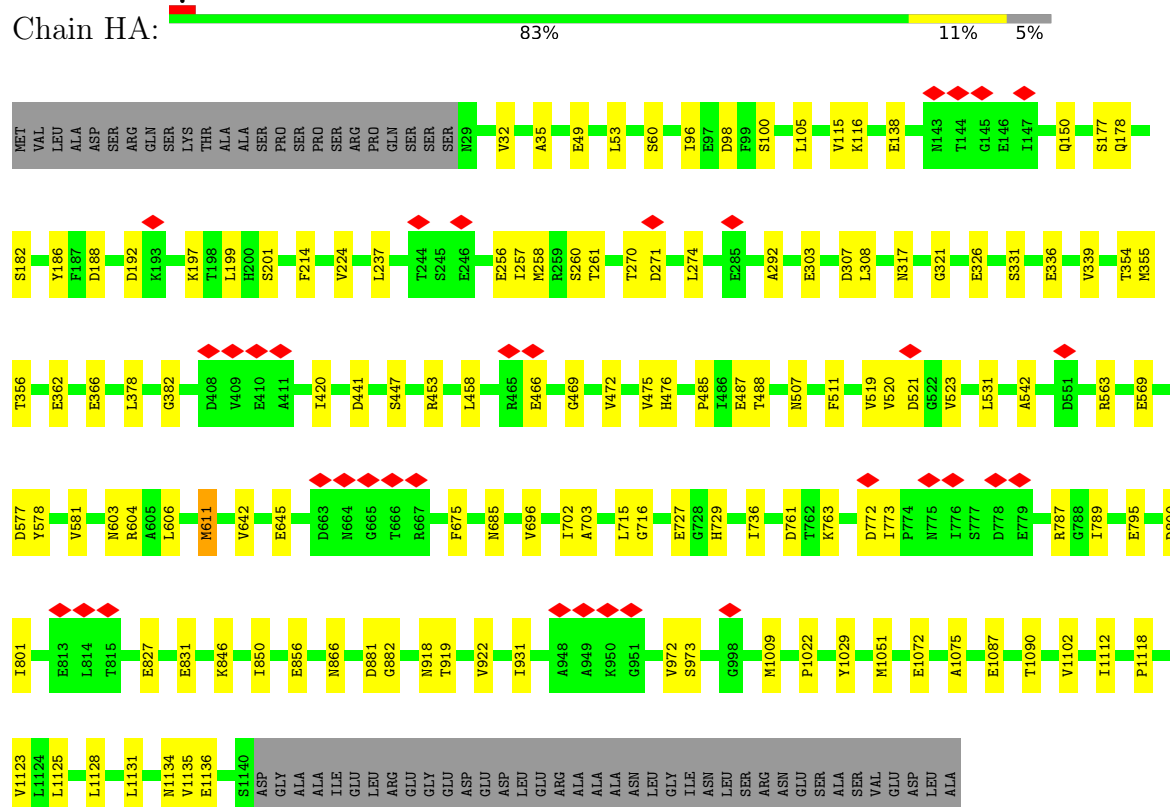


Chain BA:



- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain HA:



- Molecule 2: DNA-directed RNA polymerase subunit beta

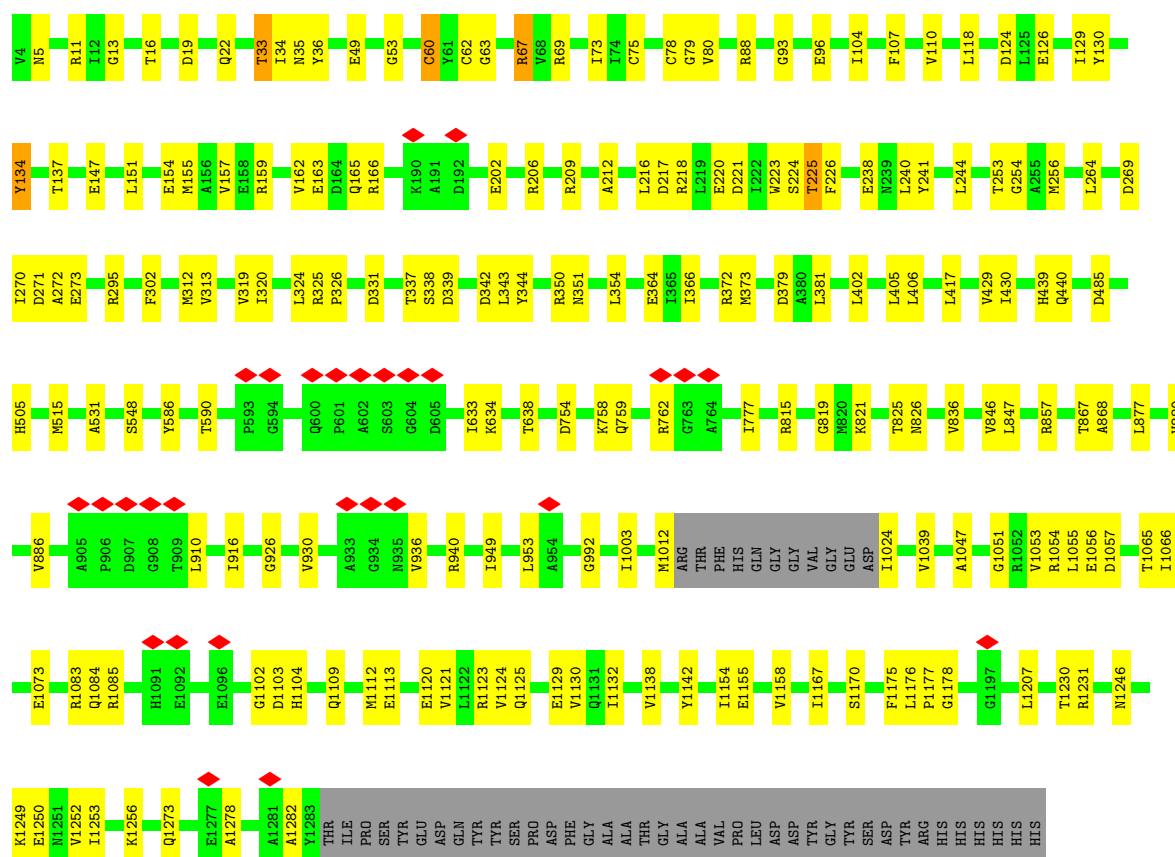
Frequency	Percentage
Daily	83%
Weekly	11%
Monthly	5%



Frequency	Percentage
Daily	83%
Weekly	11%
Monthly	5%

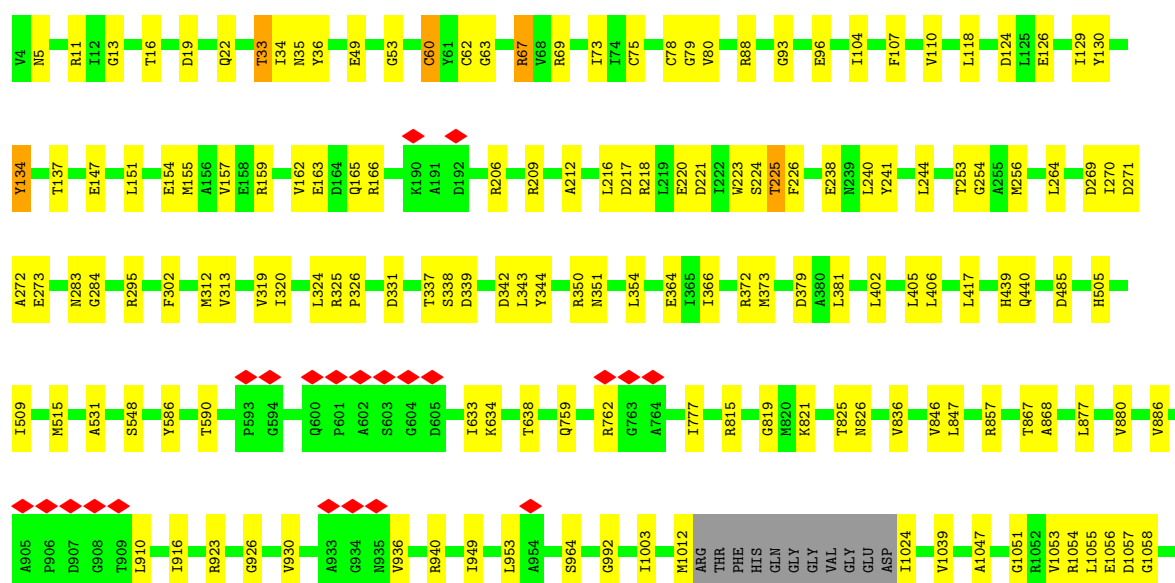


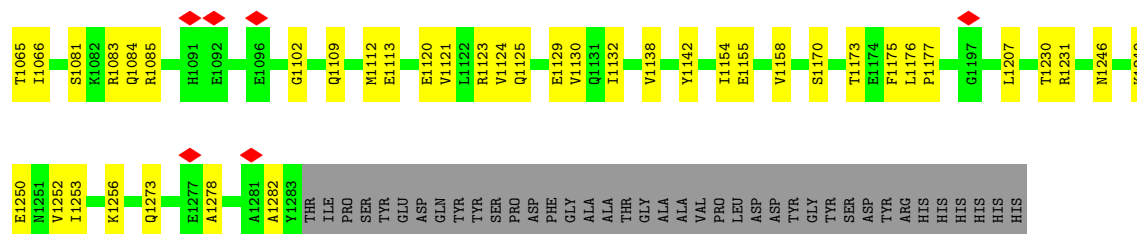
Chain D:  81% 14%



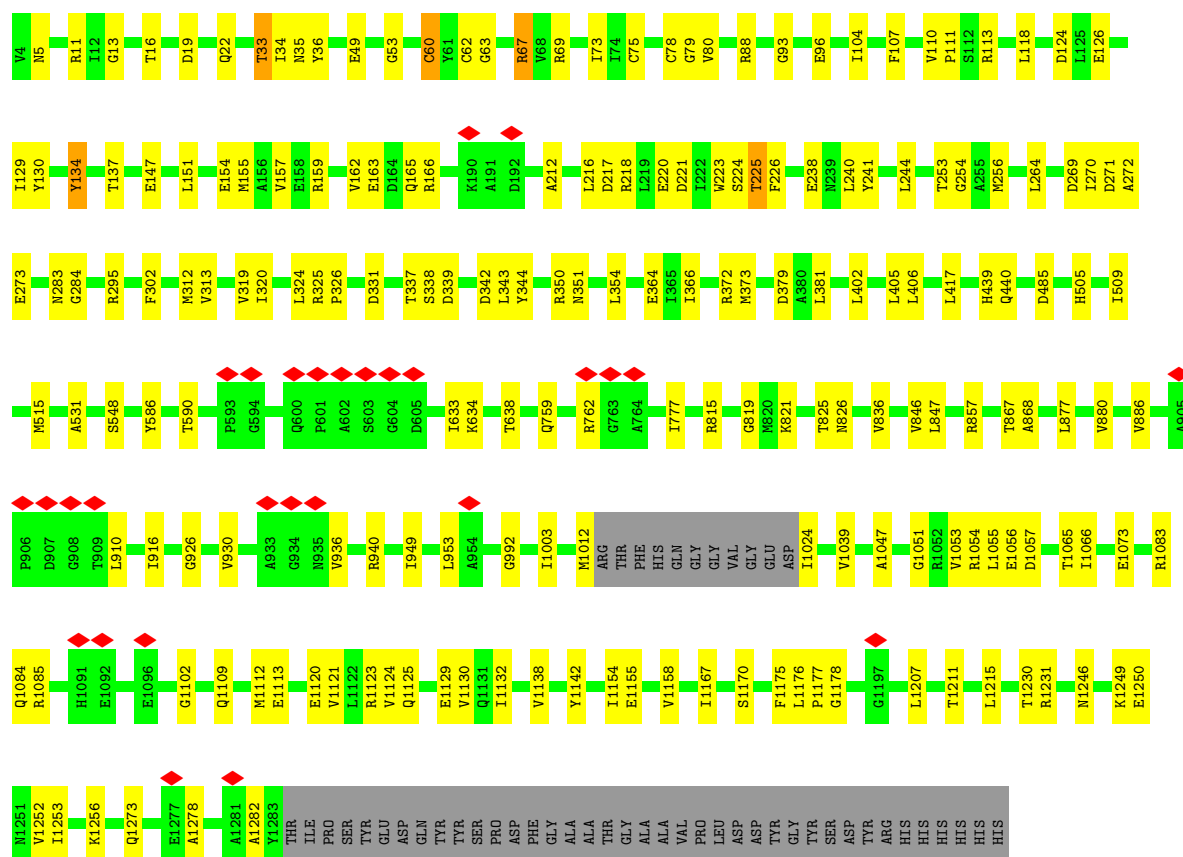
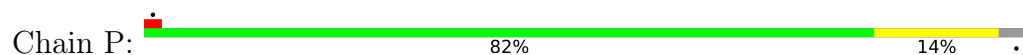
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J:  82% 14%

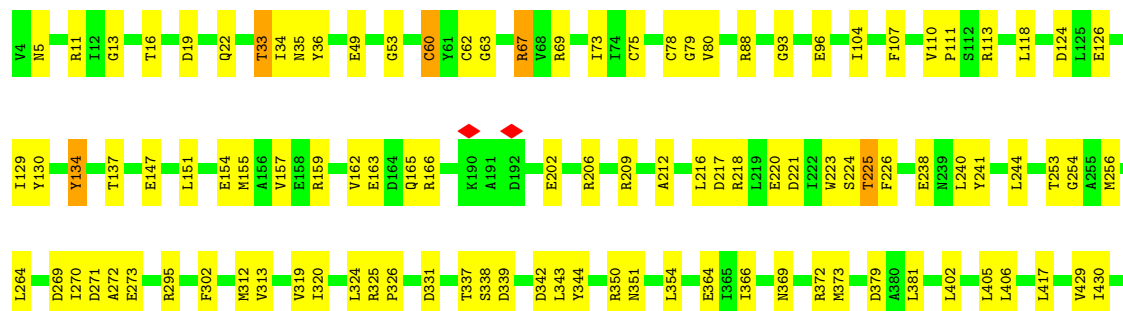
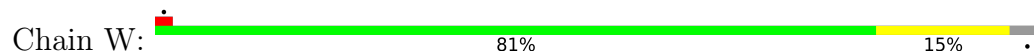


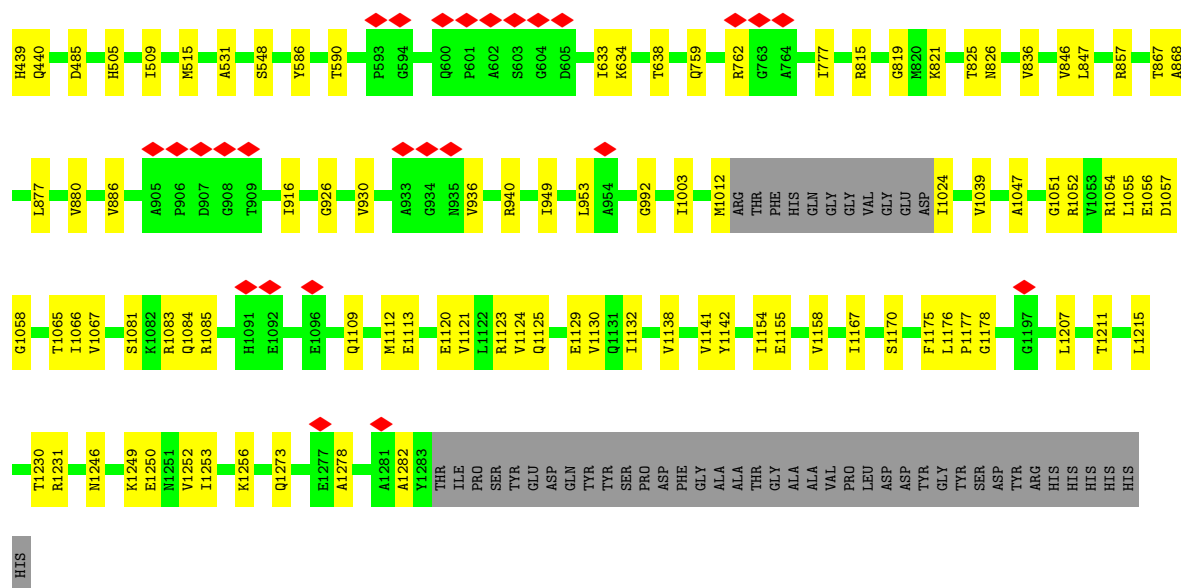


• Molecule 3: DNA-directed RNA polymerase subunit beta'



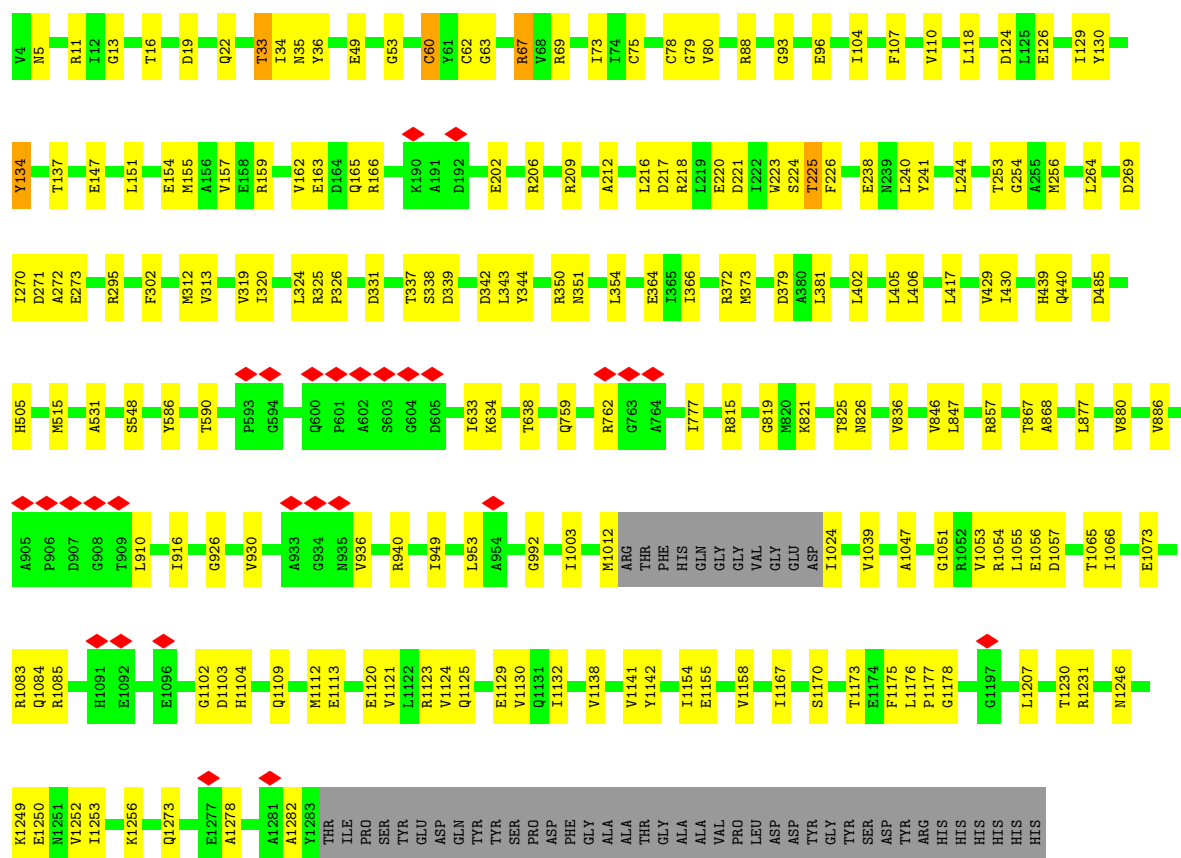
• Molecule 3: DNA-directed RNA polymerase subunit beta'





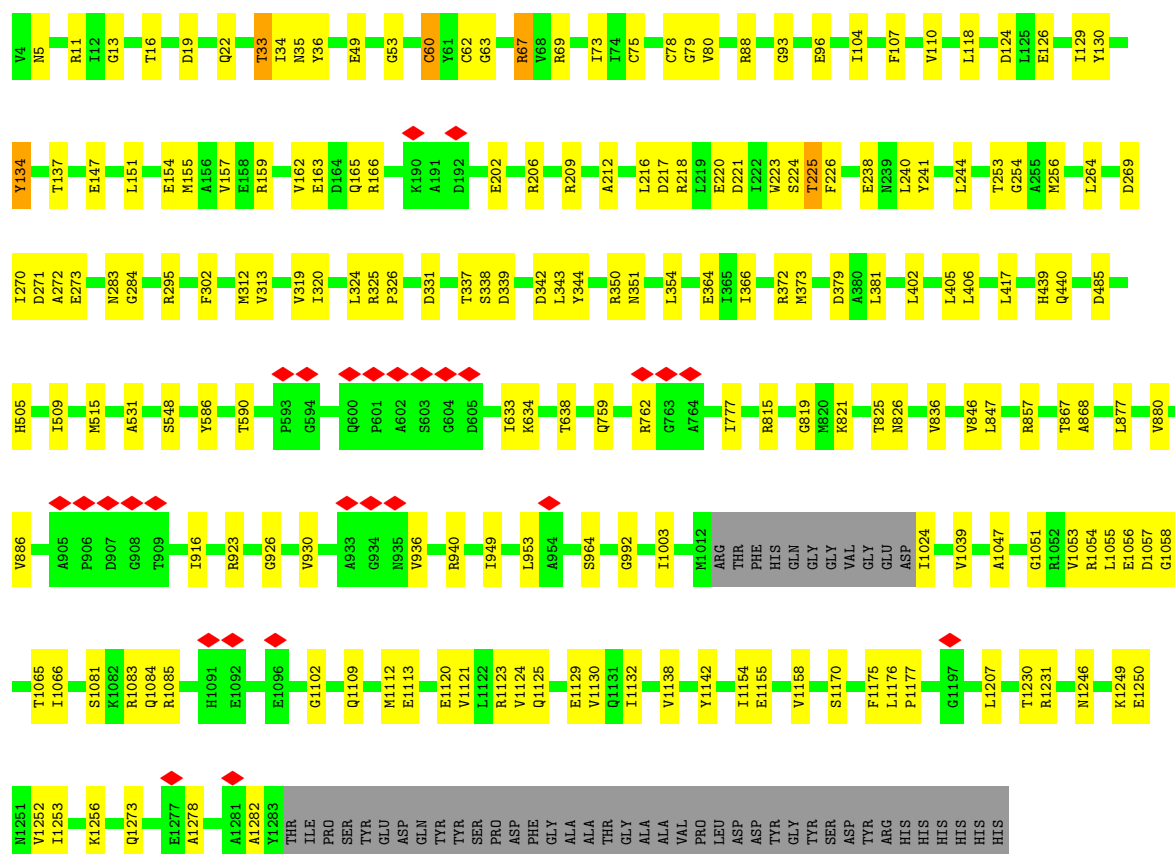
- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain CA: 81% 14%

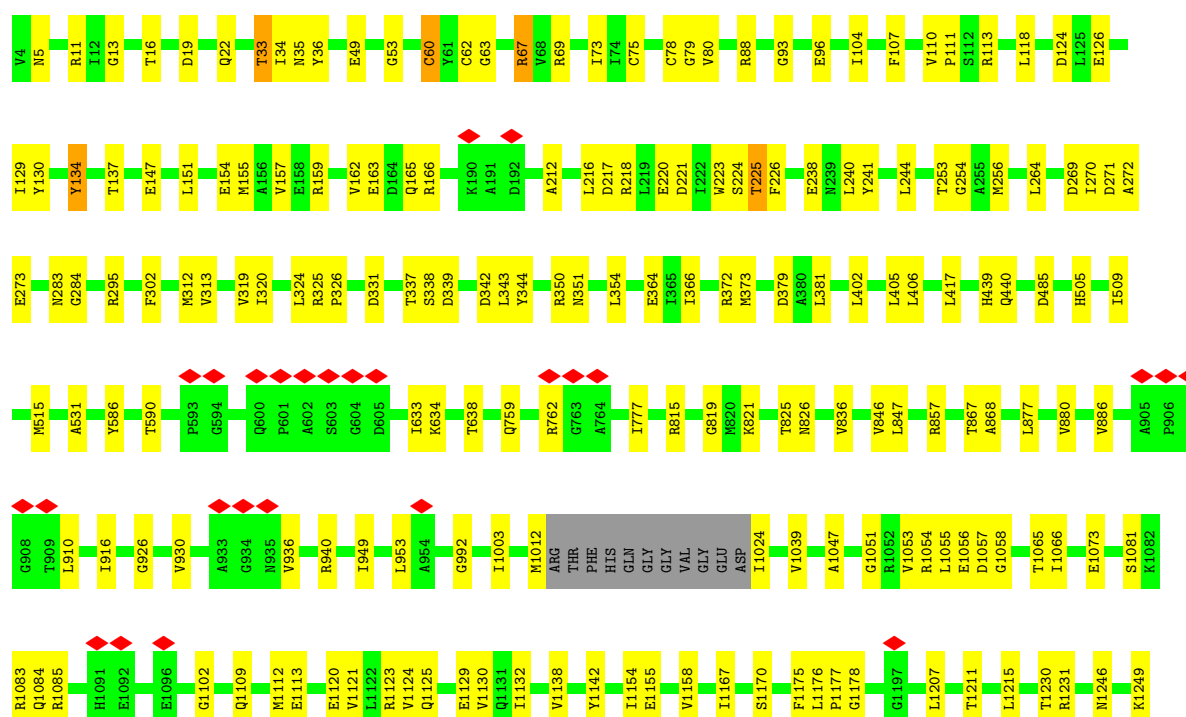
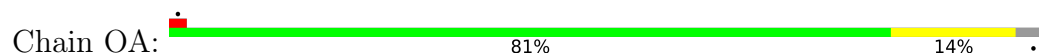


- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain IA: 82% 14%

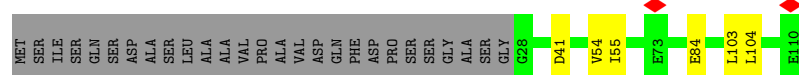


• Molecule 3: DNA-directed RNA polymerase subunit beta'



- Molecule 3: DNA-directed RNA polymerase subunit beta'

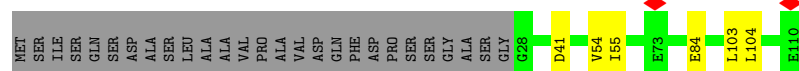
- Molecule 4: DNA-directed RNA polymerase subunit omega



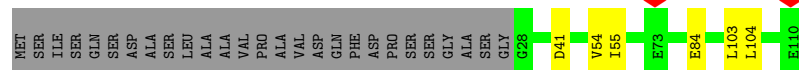
- Molecule 4: DNA-directed RNA polymerase subunit omega



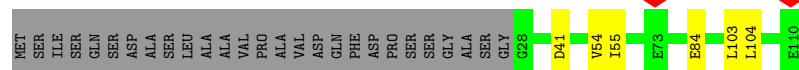
- Molecule 4: DNA-directed RNA polymerase subunit omega



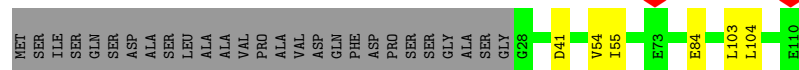
- Molecule 4: DNA-directed RNA polymerase subunit omega



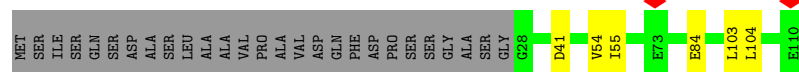
- Molecule 4: DNA-directed RNA polymerase subunit omega



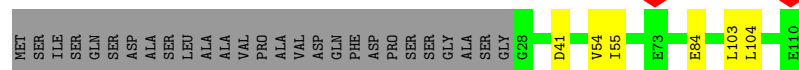
- Molecule 4: DNA-directed RNA polymerase subunit omega



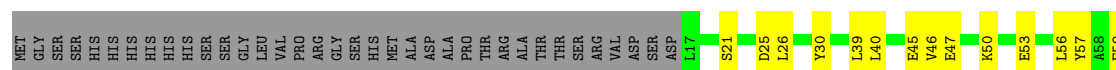
- Molecule 4: DNA-directed RNA polymerase subunit omega

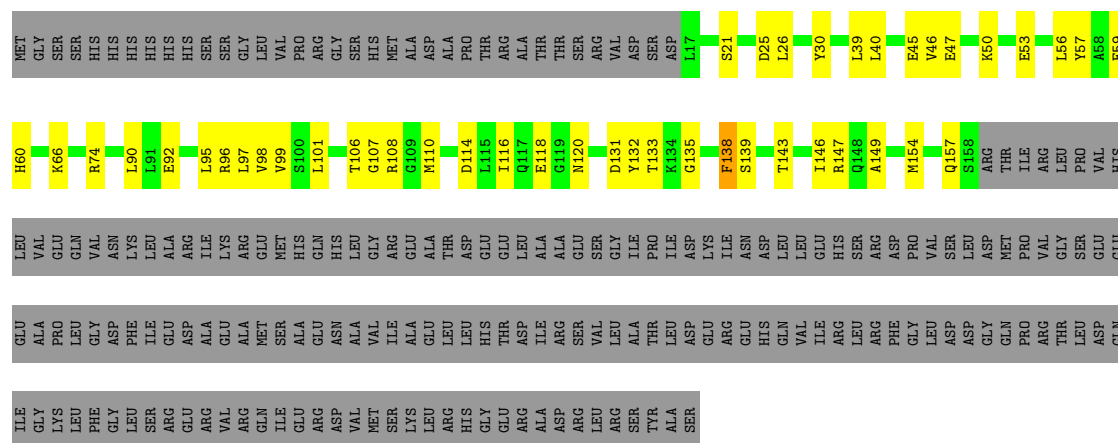


- Molecule 4: DNA-directed RNA polymerase subunit omega



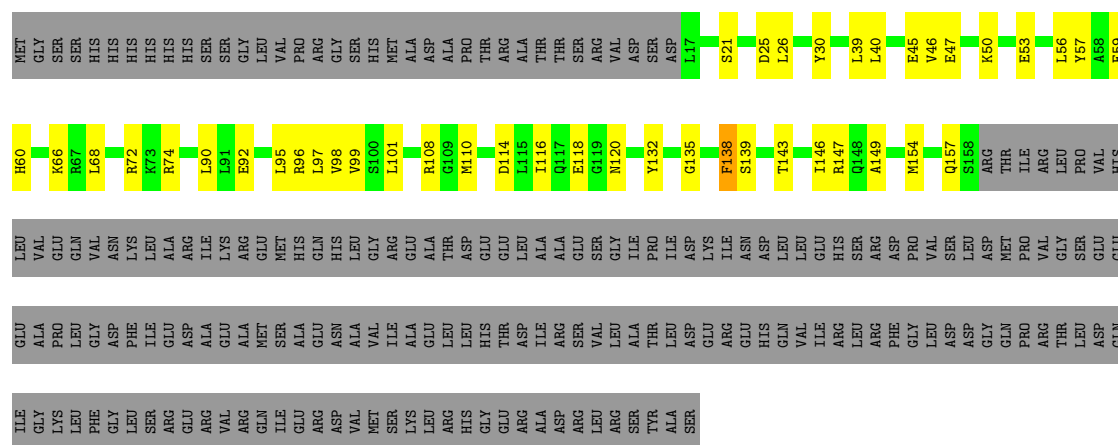
- Molecule 5: RNA polymerase sigma factor SigB





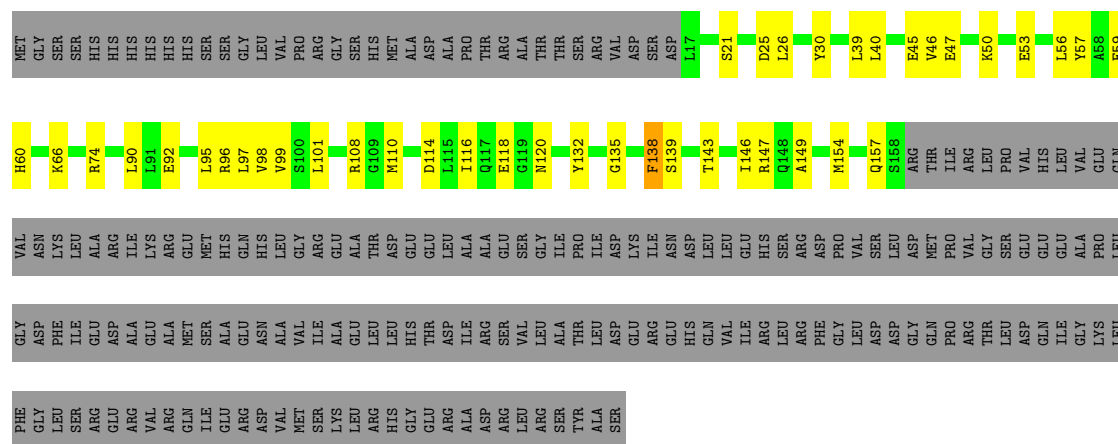
- Molecule 5: RNA polymerase sigma factor SigB

Chain EA: 29% 12% 59%



- Molecule 5: RNA polymerase sigma factor SigB

Chain KA: 29% 12% 59%



- Molecule 5: RNA polymerase sigma factor SigB

Chain QA: 28% 13% 59%

THR	LEU	SER	GLY	LEU	THR	GLY	LEU	GLY	GLY	THR	GLY	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	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● Molecule 5: RNA polymerase sigma factor SigB

Chain WA: 28% 13% 59%

ILE	GLY	ALA	GLU	LEU	H60	MET
LYS	PRO	LEU	GLU	VAL	K66	SER
PHE	GLY	ASP	GLN	VAL	R74	HIS
LEU	ASP	ASN	ASN	LYS	L90	HIS
SER	ILE	LEU	LEU	ALA	L91	HIS
ARG	GLU	ASP	ARG	ALA	E92	HIS
GLU	ARG	ALA	ILE	LYS	L95	SER
VAL	VAL	GLU	LYS	ARG	R96	SER
ARG	ALA	MET	GLU	GLU	L97	GLY
GLN	GLN	SER	MET	MET	V98	LEU
ILE	ILE	ALA	SER	HIS	V99	VAL
GLU	ARG	GLU	GLN	GLN	S100	PRO
ASP	ASN	ASN	HIS	HIS	L101	ARG
VAL	VAL	ALA	LEU	LEU	T106	GLY
MET	ILE	VAL	GLY	GLY	G107	SER
SER	LYS	ALA	GLU	GLU	R108	HIS
ARG	ARG	LEU	ALA	ALA	G109	MET
LEU	LEU	LEU	THR	THR	M110	ALA
HIS	HIS	HIS	ASP	ASP	D114	ASP
GLY	GLU	THR	GLU	GLU	L115	PRO
GLU	ARG	ASP	LEU	LEU	I116	THR
ARG	ALA	ILE	ALA	ALA	Q117	ARG
ASP	ASP	ARG	ALA	ALA	E118	ALA
ARG	ARG	SER	GLU	GLU	G119	THR
VAL	VAL	VAL	SER	SER	N120	THR
LEU	LEU	LEU	GLY	GLY	D131	ARG
SER	SER	ALA	ILE	ILE	Y132	VAL
TYR	THR	THR	PRO	PRO	T133	ASP
ALA	LEU	LEU	ILE	ILE	K134	SER
SER	ASP	ASP	ASP	ASP	G135	ASP
GLU	GLU	GLU	LYS	LYS	F138	L17
ARG	ARG	ARG	ILE	ILE	S139	S21
GLU	GLU	HIS	ASN	ASN	T143	D25
HIS	GLN	GLN	LEU	LEU	ILE	L26
ILE	VAL	VAL	LEU	LEU	GLU	Y30
ASP	ASP	ARG	GLU	GLU	I146	Y30
VAL	VAL	LEU	HIS	HIS	R147	L39
LEU	LEU	LEU	SER	SER	Q148	L40
ARG	ARG	ARG	ARG	ARG	A149	L40
PHE	PHE	ASP	ASP	ASP	M154	E45
GLY	GLY	GLY	PRO	PRO	VAL	V46
LEU	LEU	LEU	VAL	VAL	SER	E47
ASP	ASP	ASP	SER	SER	Q157	E47
GLY	GLY	GLY	ASP	ASP	S158	K50
GLN	GLN	GLN	ARG	ARG	THR	THR
PRO	PRO	PRO	PRO	PRO	ILE	E53
ARG	ARG	ARG	VAL	VAL	ARG	ARG
THR	THR	THR	VAL	VAL	LEU	L56
LEU	LEU	LEU	SER	SER	PRO	Y57
GLU	GLU	GLU	GLU	GLU	VAL	A58
GLN	GLN	GLN	VAL	VAL	HIS	E59

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D4	Depositor
Number of particles used	115457	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 ($e^-/\text{\AA}^2$)	49.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.457	Depositor
Minimum map value	-0.959	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	495.0, 495.0, 495.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.09	0/1726	0.23	0/2348
1	AA	0.11	0/1775	0.24	0/2414
1	B	0.11	0/1775	0.24	0/2414
1	FA	0.09	0/1726	0.23	0/2348
1	G	0.09	0/1726	0.23	0/2348
1	GA	0.11	0/1775	0.24	0/2414
1	H	0.11	0/1775	0.24	0/2414
1	LA	0.09	0/1726	0.23	0/2348
1	M	0.09	0/1726	0.23	0/2348
1	MA	0.11	0/1775	0.24	0/2414
1	N	0.11	0/1775	0.24	0/2414
1	RA	0.09	0/1726	0.23	0/2348
1	S	0.09	0/1726	0.23	0/2348
1	SA	0.11	0/1775	0.24	0/2414
1	T	0.11	0/1775	0.24	0/2414
1	Z	0.09	0/1726	0.23	0/2348
2	BA	0.11	0/8799	0.24	0/11929
2	C	0.11	0/8799	0.24	0/11929
2	HA	0.11	0/8799	0.24	0/11929
2	I	0.11	0/8799	0.24	0/11929
2	NA	0.11	0/8799	0.24	0/11929
2	O	0.11	0/8799	0.24	0/11929
2	TA	0.11	0/8799	0.24	0/11929
2	V	0.11	0/8799	0.24	0/11929
3	CA	0.19	0/10118	0.34	0/13675
3	D	0.19	0/10118	0.34	0/13675
3	IA	0.19	0/10118	0.34	0/13675
3	J	0.19	0/10118	0.34	0/13675
3	OA	0.19	0/10118	0.34	0/13675
3	P	0.19	0/10118	0.34	0/13675
3	UA	0.19	0/10118	0.34	0/13675
3	W	0.19	0/10118	0.34	0/13675

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	DA	0.09	0/667	0.23	0/908
4	E	0.09	0/667	0.23	0/908
4	JA	0.09	0/667	0.23	0/908
4	K	0.09	0/667	0.23	0/908
4	PA	0.09	0/667	0.23	0/908
4	Q	0.09	0/667	0.23	0/908
4	VA	0.09	0/667	0.23	0/908
4	X	0.09	0/667	0.23	0/908
5	EA	0.46	0/1134	0.80	0/1525
5	F	0.46	0/1134	0.80	0/1525
5	KA	0.46	0/1134	0.80	0/1525
5	L	0.46	0/1134	0.80	0/1525
5	QA	0.46	0/1134	0.80	0/1525
5	R	0.46	0/1134	0.80	0/1525
5	WA	0.46	0/1134	0.80	0/1525
5	Y	0.46	0/1134	0.80	0/1525
All	All	0.18	0/193752	0.33	0/262392

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1700	0	1734	13	0
1	AA	1749	0	1781	27	0
1	B	1749	0	1781	27	0
1	FA	1700	0	1734	14	0
1	G	1700	0	1734	14	0
1	GA	1749	0	1781	26	0
1	H	1749	0	1781	26	0
1	LA	1700	0	1734	13	0
1	M	1700	0	1734	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	MA	1749	0	1781	26	0
1	N	1749	0	1781	26	0
1	RA	1700	0	1734	13	0
1	S	1700	0	1734	13	0
1	SA	1749	0	1781	27	0
1	T	1749	0	1781	27	0
1	Z	1700	0	1734	13	0
2	BA	8640	0	8584	89	0
2	C	8640	0	8584	88	0
2	HA	8640	0	8584	87	0
2	I	8640	0	8584	87	0
2	NA	8640	0	8584	87	0
2	O	8640	0	8584	88	0
2	TA	8640	0	8584	87	0
2	V	8640	0	8584	86	0
3	CA	9951	0	10035	146	0
3	D	9951	0	10035	145	0
3	IA	9951	0	10035	141	0
3	J	9951	0	10035	143	0
3	OA	9951	0	10035	145	0
3	P	9951	0	10035	145	0
3	UA	9951	0	10035	148	0
3	W	9951	0	10035	149	0
4	DA	654	0	648	4	0
4	E	654	0	648	4	0
4	JA	654	0	648	4	0
4	K	654	0	648	4	0
4	PA	654	0	648	4	0
4	Q	654	0	648	4	0
4	VA	654	0	648	4	0
4	X	654	0	648	4	0
5	EA	1119	0	1155	31	0
5	F	1119	0	1155	31	0
5	KA	1119	0	1155	31	0
5	L	1119	0	1155	31	0
5	QA	1119	0	1155	34	0
5	R	1119	0	1155	33	0
5	WA	1119	0	1155	32	0
5	Y	1119	0	1155	32	0
6	CA	2	0	0	0	0
6	D	2	0	0	0	0
6	IA	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	2	0	0	0	0
6	OA	2	0	0	0	0
6	P	2	0	0	0	0
6	UA	2	0	0	0	0
6	W	2	0	0	0	0
7	CA	1	0	0	0	0
7	D	1	0	0	0	0
7	IA	1	0	0	0	0
7	J	1	0	0	0	0
7	OA	1	0	0	0	0
7	P	1	0	0	0	0
7	UA	1	0	0	0	0
7	W	1	0	0	0	0
All	All	190528	0	191496	2303	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 6.

All (2303) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:326:PRO:O	3:W:337:THR:OG1	1.93	0.87
3:UA:326:PRO:O	3:UA:337:THR:OG1	1.93	0.87
3:OA:326:PRO:O	3:OA:337:THR:OG1	1.93	0.87
3:P:326:PRO:O	3:P:337:THR:OG1	1.93	0.87
3:J:326:PRO:O	3:J:337:THR:OG1	1.93	0.85
3:D:326:PRO:O	3:D:337:THR:OG1	1.93	0.85
3:CA:326:PRO:O	3:CA:337:THR:OG1	1.93	0.85
3:IA:326:PRO:O	3:IA:337:THR:OG1	1.93	0.85
5:WA:97:LEU:HD21	5:WA:143:THR:HG22	1.61	0.82
5:Y:97:LEU:HD21	5:Y:143:THR:HG22	1.61	0.82
5:F:97:LEU:HD21	5:F:143:THR:HG22	1.61	0.82
5:L:97:LEU:HD21	5:L:143:THR:HG22	1.61	0.82
5:KA:97:LEU:HD21	5:KA:143:THR:HG22	1.61	0.82
5:EA:97:LEU:HD21	5:EA:143:THR:HG22	1.61	0.82
5:R:97:LEU:HD21	5:R:143:THR:HG22	1.61	0.82
5:QA:97:LEU:HD21	5:QA:143:THR:HG22	1.61	0.82
3:J:238:GLU:OE1	3:J:238:GLU:N	2.14	0.81
3:IA:238:GLU:OE1	3:IA:238:GLU:N	2.14	0.81
3:D:238:GLU:N	3:D:238:GLU:OE1	2.14	0.81
3:CA:238:GLU:OE1	3:CA:238:GLU:N	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:238:GLU:N	3:W:238:GLU:OE1	2.14	0.80
3:UA:238:GLU:OE1	3:UA:238:GLU:N	2.14	0.80
1:A:40:ARG:NH2	1:B:29:GLY:O	2.15	0.80
1:FA:40:ARG:NH2	1:GA:29:GLY:O	2.15	0.80
1:G:40:ARG:NH2	1:H:29:GLY:O	2.15	0.80
1:Z:40:ARG:NH2	1:AA:29:GLY:O	2.15	0.80
3:OA:238:GLU:N	3:OA:238:GLU:OE1	2.14	0.80
3:P:238:GLU:OE1	3:P:238:GLU:N	2.14	0.80
1:RA:40:ARG:NH2	1:SA:29:GLY:O	2.15	0.79
1:S:40:ARG:NH2	1:T:29:GLY:O	2.15	0.79
3:W:364:GLU:OE1	3:W:364:GLU:N	2.16	0.79
3:UA:364:GLU:OE1	3:UA:364:GLU:N	2.16	0.79
1:LA:40:ARG:NH2	1:MA:29:GLY:O	2.15	0.79
3:OA:364:GLU:OE1	3:OA:364:GLU:N	2.16	0.79
1:M:40:ARG:NH2	1:N:29:GLY:O	2.15	0.79
3:P:364:GLU:OE1	3:P:364:GLU:N	2.16	0.79
3:D:364:GLU:OE1	3:D:364:GLU:N	2.16	0.79
3:CA:364:GLU:OE1	3:CA:364:GLU:N	2.16	0.79
3:IA:364:GLU:OE1	3:IA:364:GLU:N	2.16	0.78
3:J:364:GLU:N	3:J:364:GLU:OE1	2.16	0.77
5:R:97:LEU:HD11	5:R:143:THR:CG2	2.15	0.76
5:QA:97:LEU:HD11	5:QA:143:THR:CG2	2.15	0.76
5:L:97:LEU:HD11	5:L:143:THR:CG2	2.15	0.76
5:Y:97:LEU:HD11	5:Y:143:THR:CG2	2.15	0.76
5:KA:97:LEU:HD11	5:KA:143:THR:CG2	2.15	0.76
5:WA:97:LEU:HD11	5:WA:143:THR:CG2	2.15	0.76
2:I:356:THR:OG1	2:I:362:GLU:OE1	2.04	0.76
5:EA:97:LEU:HD11	5:EA:143:THR:CG2	2.15	0.76
2:HA:356:THR:OG1	2:HA:362:GLU:OE1	2.04	0.76
5:F:97:LEU:HD11	5:F:143:THR:CG2	2.15	0.76
3:P:1120:GLU:OE1	3:P:1120:GLU:N	2.19	0.76
3:OA:1120:GLU:OE1	3:OA:1120:GLU:N	2.19	0.76
3:D:1120:GLU:OE1	3:D:1120:GLU:N	2.19	0.76
3:CA:1120:GLU:OE1	3:CA:1120:GLU:N	2.19	0.76
2:O:795:GLU:OE2	2:O:846:LYS:NZ	2.19	0.75
2:NA:795:GLU:OE2	2:NA:846:LYS:NZ	2.19	0.75
2:V:356:THR:OG1	2:V:362:GLU:OE1	2.04	0.75
2:O:356:THR:OG1	2:O:362:GLU:OE1	2.04	0.75
2:TA:356:THR:OG1	2:TA:362:GLU:OE1	2.04	0.75
2:BA:356:THR:OG1	2:BA:362:GLU:OE1	2.04	0.75
2:NA:356:THR:OG1	2:NA:362:GLU:OE1	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:356:THR:OG1	2:C:362:GLU:OE1	2.04	0.75
1:S:90:ASP:OD1	1:S:142:ARG:NH2	2.20	0.75
3:IA:1120:GLU:OE1	3:IA:1120:GLU:N	2.19	0.75
2:I:795:GLU:OE2	2:I:846:LYS:NZ	2.19	0.75
3:J:1120:GLU:N	3:J:1120:GLU:OE1	2.19	0.75
2:HA:795:GLU:OE2	2:HA:846:LYS:NZ	2.19	0.75
1:RA:90:ASP:OD1	1:RA:142:ARG:NH2	2.20	0.75
3:W:1120:GLU:OE1	3:W:1120:GLU:N	2.19	0.75
1:A:90:ASP:OD1	1:A:142:ARG:NH2	2.20	0.74
3:UA:1120:GLU:N	3:UA:1120:GLU:OE1	2.19	0.74
1:M:90:ASP:OD1	1:M:142:ARG:NH2	2.20	0.74
2:V:795:GLU:OE2	2:V:846:LYS:NZ	2.19	0.74
1:Z:90:ASP:OD1	1:Z:142:ARG:NH2	2.20	0.74
1:LA:90:ASP:OD1	1:LA:142:ARG:NH2	2.20	0.74
2:TA:795:GLU:OE2	2:TA:846:LYS:NZ	2.19	0.74
2:TA:563:ARG:NH1	2:TA:569:GLU:OE2	2.21	0.74
2:V:563:ARG:NH1	2:V:569:GLU:OE2	2.21	0.74
2:BA:795:GLU:OE2	2:BA:846:LYS:NZ	2.19	0.74
1:FA:90:ASP:OD1	1:FA:142:ARG:NH2	2.20	0.74
2:C:795:GLU:OE2	2:C:846:LYS:NZ	2.19	0.74
2:BA:563:ARG:NH1	2:BA:569:GLU:OE2	2.21	0.74
2:NA:563:ARG:NH1	2:NA:569:GLU:OE2	2.21	0.74
2:C:563:ARG:NH1	2:C:569:GLU:OE2	2.21	0.74
1:G:90:ASP:OD1	1:G:142:ARG:NH2	2.20	0.74
2:O:563:ARG:NH1	2:O:569:GLU:OE2	2.21	0.74
4:DA:84:GLU:N	4:DA:84:GLU:OE1	2.21	0.74
4:E:84:GLU:OE1	4:E:84:GLU:N	2.21	0.74
4:K:84:GLU:N	4:K:84:GLU:OE1	2.21	0.74
4:JA:84:GLU:OE1	4:JA:84:GLU:N	2.21	0.74
2:O:1131:LEU:HD21	3:P:402:LEU:HD22	1.70	0.73
2:V:1131:LEU:HD21	3:W:402:LEU:HD22	1.70	0.73
2:NA:1131:LEU:HD21	3:OA:402:LEU:HD22	1.70	0.73
2:C:1131:LEU:HD21	3:D:402:LEU:HD22	1.70	0.73
2:BA:1131:LEU:HD21	3:CA:402:LEU:HD22	1.70	0.73
4:VA:84:GLU:OE1	4:VA:84:GLU:N	2.21	0.73
4:X:84:GLU:OE1	4:X:84:GLU:N	2.21	0.73
2:HA:563:ARG:NH1	2:HA:569:GLU:OE2	2.21	0.73
3:IA:5:ASN:O	3:IA:1256:LYS:NZ	2.22	0.73
2:TA:1131:LEU:HD21	3:UA:402:LEU:HD22	1.70	0.73
2:I:563:ARG:NH1	2:I:569:GLU:OE2	2.21	0.73
3:J:5:ASN:O	3:J:1256:LYS:NZ	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:5:ASN:O	3:D:1256:LYS:NZ	2.22	0.73
3:OA:5:ASN:O	3:OA:1256:LYS:NZ	2.22	0.73
3:P:5:ASN:O	3:P:1256:LYS:NZ	2.22	0.72
3:UA:5:ASN:O	3:UA:1256:LYS:NZ	2.22	0.72
3:W:5:ASN:O	3:W:1256:LYS:NZ	2.22	0.72
3:CA:5:ASN:O	3:CA:1256:LYS:NZ	2.22	0.72
4:PA:84:GLU:OE1	4:PA:84:GLU:N	2.21	0.72
4:Q:84:GLU:OE1	4:Q:84:GLU:N	2.21	0.72
3:P:1057:ASP:OD2	3:P:1085:ARG:NH1	2.23	0.72
3:OA:1057:ASP:OD2	3:OA:1085:ARG:NH1	2.23	0.72
2:I:1131:LEU:HD21	3:J:402:LEU:HD22	1.70	0.72
2:HA:1131:LEU:HD21	3:IA:402:LEU:HD22	1.70	0.72
3:OA:137:THR:OG1	3:OA:253:THR:O	2.07	0.72
3:UA:1170:SER:OG	3:UA:1175:PHE:O	2.06	0.72
3:P:137:THR:OG1	3:P:253:THR:O	2.07	0.72
3:W:1170:SER:OG	3:W:1175:PHE:O	2.06	0.72
3:CA:1057:ASP:OD2	3:CA:1085:ARG:NH1	2.23	0.71
3:IA:1057:ASP:OD2	3:IA:1085:ARG:NH1	2.23	0.71
3:D:1057:ASP:OD2	3:D:1085:ARG:NH1	2.23	0.71
3:J:1057:ASP:OD2	3:J:1085:ARG:NH1	2.23	0.71
3:UA:137:THR:OG1	3:UA:253:THR:O	2.07	0.71
3:UA:1057:ASP:OD2	3:UA:1085:ARG:NH1	2.23	0.71
2:O:1072:GLU:OE1	2:O:1072:GLU:N	2.24	0.71
3:W:1057:ASP:OD2	3:W:1085:ARG:NH1	2.23	0.71
2:NA:1072:GLU:OE1	2:NA:1072:GLU:N	2.24	0.71
3:CA:1170:SER:OG	3:CA:1175:PHE:O	2.06	0.71
3:D:1170:SER:OG	3:D:1175:PHE:O	2.06	0.71
3:J:137:THR:OG1	3:J:253:THR:O	2.07	0.70
2:BA:1072:GLU:OE1	2:BA:1072:GLU:N	2.24	0.70
3:IA:137:THR:OG1	3:IA:253:THR:O	2.07	0.70
2:C:1072:GLU:OE1	2:C:1072:GLU:N	2.24	0.70
2:I:761:ASP:OD1	2:I:866:ASN:ND2	2.25	0.70
3:J:60:CYS:SG	3:J:63:GLY:N	2.64	0.70
2:HA:761:ASP:OD1	2:HA:866:ASN:ND2	2.25	0.70
2:O:761:ASP:OD1	2:O:866:ASN:ND2	2.25	0.70
2:V:1072:GLU:OE1	2:V:1072:GLU:N	2.24	0.70
2:HA:1072:GLU:OE1	2:HA:1072:GLU:N	2.24	0.70
3:IA:60:CYS:SG	3:IA:63:GLY:N	2.64	0.70
2:NA:761:ASP:OD1	2:NA:866:ASN:ND2	2.25	0.70
2:TA:1072:GLU:N	2:TA:1072:GLU:OE1	2.24	0.70
2:C:761:ASP:OD1	2:C:866:ASN:ND2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BA:761:ASP:OD1	2:BA:866:ASN:ND2	2.25	0.70
2:I:1072:GLU:N	2:I:1072:GLU:OE1	2.24	0.70
3:OA:60:CYS:SG	3:OA:63:GLY:N	2.64	0.70
3:P:60:CYS:SG	3:P:63:GLY:N	2.64	0.70
3:CA:137:THR:OG1	3:CA:253:THR:O	2.07	0.70
3:CA:1176:LEU:HD12	3:CA:1177:PRO:HD2	1.74	0.70
3:D:1176:LEU:HD12	3:D:1177:PRO:HD2	1.74	0.70
3:D:137:THR:OG1	3:D:253:THR:O	2.07	0.70
1:G:71:GLU:OE1	1:G:71:GLU:N	2.25	0.70
3:UA:1176:LEU:HD12	3:UA:1177:PRO:HD2	1.74	0.70
3:D:60:CYS:SG	3:D:63:GLY:N	2.64	0.69
3:W:1176:LEU:HD12	3:W:1177:PRO:HD2	1.74	0.69
3:CA:60:CYS:SG	3:CA:63:GLY:N	2.64	0.69
1:FA:71:GLU:N	1:FA:71:GLU:OE1	2.25	0.69
3:W:96:GLU:O	3:W:351:ASN:ND2	2.26	0.69
3:UA:96:GLU:O	3:UA:351:ASN:ND2	2.26	0.69
1:A:71:GLU:OE1	1:A:71:GLU:N	2.25	0.69
1:M:71:GLU:OE1	1:M:71:GLU:N	2.25	0.69
5:R:132:TYR:O	5:R:135:GLY:N	2.26	0.69
1:S:71:GLU:N	1:S:71:GLU:OE1	2.25	0.69
2:V:761:ASP:OD1	2:V:866:ASN:ND2	2.25	0.69
3:W:60:CYS:SG	3:W:63:GLY:N	2.64	0.69
1:LA:71:GLU:OE1	1:LA:71:GLU:N	2.25	0.69
1:RA:71:GLU:OE1	1:RA:71:GLU:N	2.25	0.69
3:UA:60:CYS:SG	3:UA:63:GLY:N	2.64	0.69
1:Z:71:GLU:OE1	1:Z:71:GLU:N	2.25	0.69
5:QA:132:TYR:O	5:QA:135:GLY:N	2.26	0.69
2:TA:761:ASP:OD1	2:TA:866:ASN:ND2	2.25	0.69
3:P:1170:SER:OG	3:P:1175:PHE:O	2.06	0.69
3:D:96:GLU:O	3:D:351:ASN:ND2	2.26	0.68
3:W:137:THR:OG1	3:W:253:THR:O	2.07	0.68
3:CA:96:GLU:O	3:CA:351:ASN:ND2	2.26	0.68
3:IA:1176:LEU:HD12	3:IA:1177:PRO:HD2	1.74	0.68
5:KA:132:TYR:O	5:KA:135:GLY:N	2.26	0.68
3:J:1176:LEU:HD12	3:J:1177:PRO:HD2	1.74	0.68
5:L:132:TYR:O	5:L:135:GLY:N	2.26	0.68
2:V:507:ASN:OD1	2:V:511:PHE:N	2.27	0.68
2:TA:507:ASN:OD1	2:TA:511:PHE:N	2.27	0.68
3:P:1121:VAL:HG23	3:P:1130:VAL:HG12	1.75	0.68
2:NA:326:GLU:OE1	2:NA:326:GLU:N	2.27	0.68
2:C:507:ASN:OD1	2:C:511:PHE:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:326:GLU:OE1	2:O:326:GLU:N	2.27	0.68
3:OA:96:GLU:O	3:OA:351:ASN:ND2	2.26	0.68
3:OA:1121:VAL:HG23	3:OA:1130:VAL:HG12	1.75	0.68
5:F:132:TYR:O	5:F:135:GLY:N	2.26	0.68
3:P:96:GLU:O	3:P:351:ASN:ND2	2.26	0.68
3:P:1176:LEU:HD12	3:P:1177:PRO:HD2	1.74	0.68
2:BA:507:ASN:OD1	2:BA:511:PHE:N	2.27	0.68
5:EA:132:TYR:O	5:EA:135:GLY:N	2.26	0.68
2:HA:326:GLU:OE1	2:HA:326:GLU:N	2.27	0.68
3:IA:96:GLU:O	3:IA:351:ASN:ND2	2.26	0.68
3:OA:1176:LEU:HD12	3:OA:1177:PRO:HD2	1.74	0.68
3:UA:1121:VAL:HG23	3:UA:1130:VAL:HG12	1.75	0.68
5:WA:132:TYR:O	5:WA:135:GLY:N	2.26	0.68
3:D:1054:ARG:O	3:D:1065:THR:OG1	2.12	0.68
2:I:326:GLU:N	2:I:326:GLU:OE1	2.27	0.68
3:J:96:GLU:O	3:J:351:ASN:ND2	2.26	0.68
2:V:326:GLU:OE1	2:V:326:GLU:N	2.27	0.68
3:W:1121:VAL:HG23	3:W:1130:VAL:HG12	1.75	0.68
5:Y:132:TYR:O	5:Y:135:GLY:N	2.26	0.68
3:CA:1054:ARG:O	3:CA:1065:THR:OG1	2.12	0.68
2:TA:326:GLU:N	2:TA:326:GLU:OE1	2.27	0.68
2:NA:507:ASN:OD1	2:NA:511:PHE:N	2.27	0.68
2:O:507:ASN:OD1	2:O:511:PHE:N	2.27	0.67
2:C:326:GLU:OE1	2:C:326:GLU:N	2.27	0.67
3:J:1121:VAL:HG23	3:J:1130:VAL:HG12	1.75	0.67
2:V:800:ASP:OD1	2:V:801:ILE:N	2.28	0.67
3:IA:1121:VAL:HG23	3:IA:1130:VAL:HG12	1.75	0.67
2:TA:800:ASP:OD1	2:TA:801:ILE:N	2.28	0.67
3:D:1121:VAL:HG23	3:D:1130:VAL:HG12	1.75	0.67
2:BA:326:GLU:OE1	2:BA:326:GLU:N	2.27	0.67
3:CA:1121:VAL:HG23	3:CA:1130:VAL:HG12	1.75	0.67
3:OA:1054:ARG:O	3:OA:1065:THR:OG1	2.12	0.67
3:P:1054:ARG:O	3:P:1065:THR:OG1	2.12	0.67
2:I:507:ASN:OD1	2:I:511:PHE:N	2.27	0.67
3:W:1054:ARG:O	3:W:1065:THR:OG1	2.12	0.67
2:HA:507:ASN:OD1	2:HA:511:PHE:N	2.27	0.67
2:NA:800:ASP:OD1	2:NA:801:ILE:N	2.28	0.67
2:I:150:GLN:N	2:I:150:GLN:OE1	2.28	0.67
2:O:800:ASP:OD1	2:O:801:ILE:N	2.28	0.67
2:HA:150:GLN:OE1	2:HA:150:GLN:N	2.28	0.67
3:UA:1054:ARG:O	3:UA:1065:THR:OG1	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:150:GLN:OE1	2:O:150:GLN:N	2.28	0.67
3:W:49:GLU:OE1	3:W:49:GLU:N	2.27	0.67
2:NA:150:GLN:OE1	2:NA:150:GLN:N	2.28	0.67
3:D:49:GLU:OE1	3:D:49:GLU:N	2.27	0.67
3:UA:49:GLU:OE1	3:UA:49:GLU:N	2.27	0.67
2:C:800:ASP:OD1	2:C:801:ILE:N	2.28	0.66
3:CA:49:GLU:N	3:CA:49:GLU:OE1	2.27	0.66
2:I:800:ASP:OD1	2:I:801:ILE:N	2.28	0.66
2:V:150:GLN:OE1	2:V:150:GLN:N	2.28	0.66
2:BA:800:ASP:OD1	2:BA:801:ILE:N	2.28	0.66
2:HA:800:ASP:OD1	2:HA:801:ILE:N	2.28	0.66
2:TA:150:GLN:N	2:TA:150:GLN:OE1	2.28	0.66
3:J:1054:ARG:O	3:J:1065:THR:OG1	2.12	0.66
3:IA:1054:ARG:O	3:IA:1065:THR:OG1	2.12	0.66
1:B:89:GLU:OE1	1:B:91:GLU:N	2.29	0.66
2:BA:150:GLN:OE1	2:BA:150:GLN:N	2.28	0.66
2:C:150:GLN:OE1	2:C:150:GLN:N	2.28	0.66
1:AA:89:GLU:OE1	1:AA:91:GLU:N	2.29	0.66
1:T:106:THR:OG1	1:T:121:PRO:O	2.14	0.66
5:Y:101:LEU:HD21	5:Y:147:ARG:NH2	2.11	0.66
3:IA:1273:GLN:N	3:IA:1273:GLN:OE1	2.29	0.66
1:SA:106:THR:OG1	1:SA:121:PRO:O	2.14	0.66
5:WA:101:LEU:HD21	5:WA:147:ARG:NH2	2.11	0.66
3:J:1273:GLN:OE1	3:J:1273:GLN:N	2.29	0.66
1:H:89:GLU:OE1	1:H:91:GLU:N	2.29	0.65
5:R:101:LEU:HD21	5:R:147:ARG:NH2	2.11	0.65
1:T:89:GLU:OE1	1:T:91:GLU:N	2.29	0.65
1:MA:89:GLU:OE1	1:MA:91:GLU:N	2.29	0.65
5:QA:101:LEU:HD21	5:QA:147:ARG:NH2	2.11	0.65
1:SA:89:GLU:OE1	1:SA:91:GLU:N	2.29	0.65
1:N:89:GLU:OE1	1:N:91:GLU:N	2.29	0.65
1:GA:89:GLU:OE1	1:GA:91:GLU:N	2.29	0.65
3:IA:1170:SER:OG	3:IA:1175:PHE:O	2.06	0.65
5:EA:101:LEU:HD21	5:EA:147:ARG:NH2	2.11	0.65
3:OA:1273:GLN:OE1	3:OA:1273:GLN:N	2.29	0.65
5:F:101:LEU:HD21	5:F:147:ARG:NH2	2.11	0.65
3:P:1273:GLN:N	3:P:1273:GLN:OE1	2.29	0.65
3:OA:49:GLU:OE1	3:OA:49:GLU:N	2.27	0.65
3:D:1273:GLN:OE1	3:D:1273:GLN:N	2.29	0.65
3:J:1170:SER:OG	3:J:1175:PHE:O	2.06	0.65
2:I:542:ALA:N	2:I:578:TYR:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:256:GLU:OE1	2:O:256:GLU:N	2.30	0.65
3:P:49:GLU:N	3:P:49:GLU:OE1	2.27	0.65
2:BA:256:GLU:OE1	2:BA:256:GLU:N	2.30	0.65
3:CA:1273:GLN:N	3:CA:1273:GLN:OE1	2.29	0.65
3:IA:49:GLU:OE1	3:IA:49:GLU:N	2.27	0.65
2:TA:542:ALA:N	2:TA:578:TYR:O	2.29	0.65
2:C:256:GLU:N	2:C:256:GLU:OE1	2.30	0.65
1:H:106:THR:OG1	1:H:121:PRO:O	2.14	0.65
3:J:49:GLU:OE1	3:J:49:GLU:N	2.27	0.65
1:N:106:THR:OG1	1:N:121:PRO:O	2.14	0.65
3:P:241:TYR:OH	3:P:254:GLY:O	2.14	0.65
2:V:542:ALA:N	2:V:578:TYR:O	2.29	0.65
1:AA:106:THR:OG1	1:AA:121:PRO:O	2.14	0.65
2:HA:542:ALA:N	2:HA:578:TYR:O	2.29	0.65
2:NA:256:GLU:N	2:NA:256:GLU:OE1	2.30	0.65
1:B:106:THR:OG1	1:B:121:PRO:O	2.14	0.64
1:GA:106:THR:OG1	1:GA:121:PRO:O	2.14	0.64
2:HA:466:GLU:N	2:HA:466:GLU:OE1	2.30	0.64
3:OA:241:TYR:OH	3:OA:254:GLY:O	2.14	0.64
5:F:110:MET:SD	5:F:157:GLN:HG2	2.37	0.64
2:I:466:GLU:OE1	2:I:466:GLU:N	2.30	0.64
5:L:101:LEU:HD21	5:L:147:ARG:NH2	2.11	0.64
5:L:110:MET:SD	5:L:157:GLN:HG2	2.37	0.64
5:EA:110:MET:SD	5:EA:157:GLN:HG2	2.37	0.64
1:MA:106:THR:OG1	1:MA:121:PRO:O	2.14	0.64
2:O:542:ALA:N	2:O:578:TYR:O	2.29	0.64
5:KA:110:MET:SD	5:KA:157:GLN:HG2	2.37	0.64
2:NA:542:ALA:N	2:NA:578:TYR:O	2.29	0.64
2:C:466:GLU:OE1	2:C:466:GLU:N	2.30	0.64
3:W:1273:GLN:OE1	3:W:1273:GLN:N	2.29	0.64
2:BA:466:GLU:OE1	2:BA:466:GLU:N	2.30	0.64
2:BA:542:ALA:N	2:BA:578:TYR:O	2.29	0.64
5:KA:101:LEU:HD21	5:KA:147:ARG:NH2	2.11	0.64
3:UA:1273:GLN:OE1	3:UA:1273:GLN:N	2.29	0.64
2:NA:466:GLU:OE1	2:NA:466:GLU:N	2.30	0.64
2:C:542:ALA:N	2:C:578:TYR:O	2.29	0.64
2:O:466:GLU:OE1	2:O:466:GLU:N	2.30	0.64
5:R:110:MET:SD	5:R:157:GLN:HG2	2.37	0.64
5:QA:110:MET:SD	5:QA:157:GLN:HG2	2.37	0.64
2:TA:466:GLU:OE1	2:TA:466:GLU:N	2.30	0.64
2:V:466:GLU:OE1	2:V:466:GLU:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:241:TYR:OH	3:W:254:GLY:O	2.14	0.64
3:D:241:TYR:OH	3:D:254:GLY:O	2.14	0.64
2:I:256:GLU:OE1	2:I:256:GLU:N	2.30	0.64
3:P:126:GLU:OE2	5:R:21:SER:OG	2.16	0.64
3:P:926:GLY:O	3:P:940:ARG:NH1	2.31	0.64
3:OA:926:GLY:O	3:OA:940:ARG:NH1	2.31	0.64
3:J:926:GLY:O	3:J:940:ARG:NH1	2.31	0.63
2:V:182:SER:O	2:V:186:TYR:OH	2.16	0.63
2:HA:256:GLU:OE1	2:HA:256:GLU:N	2.30	0.63
3:IA:926:GLY:O	3:IA:940:ARG:NH1	2.31	0.63
3:OA:126:GLU:OE2	5:QA:21:SER:OG	2.16	0.63
2:TA:256:GLU:OE1	2:TA:256:GLU:N	2.30	0.63
3:UA:241:TYR:OH	3:UA:254:GLY:O	2.14	0.63
2:I:188:ASP:N	2:I:201:SER:O	2.30	0.63
2:V:256:GLU:N	2:V:256:GLU:OE1	2.30	0.63
3:W:320:ILE:O	3:W:325:ARG:NH1	2.32	0.63
3:CA:241:TYR:OH	3:CA:254:GLY:O	2.14	0.63
2:TA:182:SER:O	2:TA:186:TYR:OH	2.16	0.63
3:UA:320:ILE:O	3:UA:325:ARG:NH1	2.32	0.63
5:WA:110:MET:SD	5:WA:157:GLN:HG2	2.37	0.63
2:O:188:ASP:N	2:O:201:SER:O	2.30	0.63
5:Y:110:MET:SD	5:Y:157:GLN:HG2	2.37	0.63
3:CA:320:ILE:O	3:CA:325:ARG:NH1	2.32	0.63
2:HA:188:ASP:N	2:HA:201:SER:O	2.30	0.63
3:IA:320:ILE:O	3:IA:325:ARG:NH1	2.32	0.63
3:D:320:ILE:O	3:D:325:ARG:NH1	2.32	0.63
3:J:320:ILE:O	3:J:325:ARG:NH1	2.32	0.63
2:NA:188:ASP:N	2:NA:201:SER:O	2.30	0.63
2:V:188:ASP:N	2:V:201:SER:O	2.30	0.63
2:BA:188:ASP:N	2:BA:201:SER:O	2.30	0.63
3:UA:926:GLY:O	3:UA:940:ARG:NH1	2.31	0.63
2:C:188:ASP:N	2:C:201:SER:O	2.30	0.63
3:W:926:GLY:O	3:W:940:ARG:NH1	2.31	0.63
3:D:926:GLY:O	3:D:940:ARG:NH1	2.31	0.63
3:P:320:ILE:O	3:P:325:ARG:NH1	2.32	0.63
2:TA:188:ASP:N	2:TA:201:SER:O	2.30	0.63
3:W:126:GLU:OE2	5:Y:21:SER:OG	2.16	0.62
3:OA:320:ILE:O	3:OA:325:ARG:NH1	2.32	0.62
3:UA:126:GLU:OE2	5:WA:21:SER:OG	2.16	0.62
3:CA:926:GLY:O	3:CA:940:ARG:NH1	2.31	0.62
3:J:271:ASP:OD1	3:J:272:ALA:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:IA:271:ASP:OD1	3:IA:272:ALA:N	2.33	0.62
2:O:182:SER:O	2:O:186:TYR:OH	2.16	0.62
2:C:182:SER:O	2:C:186:TYR:OH	2.16	0.62
2:NA:182:SER:O	2:NA:186:TYR:OH	2.16	0.62
3:J:134:TYR:CD1	3:J:256:MET:HE3	2.35	0.62
3:IA:134:TYR:CD1	3:IA:256:MET:HE3	2.35	0.62
3:UA:271:ASP:OD1	3:UA:272:ALA:N	2.33	0.62
3:W:271:ASP:OD1	3:W:272:ALA:N	2.33	0.62
2:BA:182:SER:O	2:BA:186:TYR:OH	2.16	0.62
3:D:155:MET:SD	3:D:223:TRP:CD2	2.93	0.62
3:CA:155:MET:SD	3:CA:223:TRP:CD2	2.93	0.62
3:W:134:TYR:CD1	3:W:256:MET:HE3	2.35	0.62
3:D:271:ASP:OD1	3:D:272:ALA:N	2.33	0.61
1:H:60:LEU:O	1:H:61:HIS:ND1	2.33	0.61
1:AA:60:LEU:O	1:AA:61:HIS:ND1	2.33	0.61
3:CA:271:ASP:OD1	3:CA:272:ALA:N	2.33	0.61
1:GA:60:LEU:O	1:GA:61:HIS:ND1	2.33	0.61
3:OA:271:ASP:OD1	3:OA:272:ALA:N	2.33	0.61
3:UA:134:TYR:CD1	3:UA:256:MET:HE3	2.35	0.61
1:B:60:LEU:O	1:B:61:HIS:ND1	2.33	0.61
3:P:271:ASP:OD1	3:P:272:ALA:N	2.33	0.61
3:IA:155:MET:SD	3:IA:223:TRP:CD2	2.93	0.61
3:J:155:MET:SD	3:J:223:TRP:CD2	2.93	0.61
3:J:586:TYR:O	3:J:590:THR:OG1	2.13	0.61
3:OA:155:MET:SD	3:OA:223:TRP:CD2	2.93	0.61
2:I:182:SER:O	2:I:186:TYR:OH	2.16	0.61
3:P:155:MET:SD	3:P:223:TRP:CD2	2.93	0.61
3:CA:126:GLU:OE2	5:EA:21:SER:OG	2.16	0.61
3:OA:1170:SER:OG	3:OA:1175:PHE:O	2.06	0.61
3:D:126:GLU:OE2	5:F:21:SER:OG	2.16	0.61
3:J:373:MET:HE1	5:L:114:ASP:CG	2.26	0.61
3:P:134:TYR:CD1	3:P:256:MET:HE3	2.35	0.61
3:P:373:MET:HE1	5:R:114:ASP:CG	2.26	0.61
3:W:155:MET:SD	3:W:223:TRP:CD2	2.93	0.61
3:CA:134:TYR:CD1	3:CA:256:MET:HE3	2.35	0.61
3:IA:241:TYR:OH	3:IA:254:GLY:O	2.14	0.61
3:IA:373:MET:HE1	5:KA:114:ASP:CG	2.26	0.61
3:IA:586:TYR:O	3:IA:590:THR:OG1	2.13	0.61
1:MA:15:THR:HG22	1:MA:16:ASP:H	1.66	0.61
3:UA:155:MET:SD	3:UA:223:TRP:CD2	2.93	0.61
3:D:134:TYR:CD1	3:D:256:MET:HE3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:15:THR:HG22	1:N:16:ASP:H	1.66	0.61
3:P:1083:ARG:HB3	3:P:1112:MET:HE2	1.83	0.61
3:OA:373:MET:HE1	5:QA:114:ASP:CG	2.26	0.61
1:N:60:LEU:O	1:N:61:HIS:ND1	2.33	0.60
1:T:60:LEU:O	1:T:61:HIS:ND1	2.33	0.60
2:HA:182:SER:O	2:HA:186:TYR:OH	2.16	0.60
3:IA:1083:ARG:HB3	3:IA:1112:MET:HE2	1.83	0.60
3:OA:134:TYR:CD1	3:OA:256:MET:HE3	2.35	0.60
3:OA:1083:ARG:HB3	3:OA:1112:MET:HE2	1.83	0.60
3:D:373:MET:HE1	5:F:114:ASP:CG	2.26	0.60
3:D:586:TYR:O	3:D:590:THR:OG1	2.13	0.60
3:J:73:ILE:HD11	5:EA:60:HIS:CE1	2.36	0.60
3:J:1083:ARG:HB3	3:J:1112:MET:HE2	1.83	0.60
1:MA:60:LEU:O	1:MA:61:HIS:ND1	2.33	0.60
1:SA:15:THR:HG22	1:SA:16:ASP:H	1.66	0.60
1:SA:60:LEU:O	1:SA:61:HIS:ND1	2.33	0.60
5:F:60:HIS:CE1	3:IA:73:ILE:HD11	2.36	0.60
3:J:241:TYR:OH	3:J:254:GLY:O	2.14	0.60
1:T:15:THR:HG22	1:T:16:ASP:H	1.66	0.60
3:D:73:ILE:HD11	5:KA:60:HIS:CE1	2.36	0.60
5:L:60:HIS:CE1	3:CA:73:ILE:HD11	2.36	0.60
3:P:1124:VAL:HG23	3:P:1125:GLN:HG2	1.83	0.60
3:CA:373:MET:HE1	5:EA:114:ASP:CG	2.26	0.60
3:IA:126:GLU:OE2	5:KA:21:SER:OG	2.16	0.60
3:J:126:GLU:OE2	5:L:21:SER:OG	2.16	0.60
1:GA:15:THR:HG22	1:GA:16:ASP:H	1.66	0.60
3:OA:1124:VAL:HG23	3:OA:1125:GLN:HG2	1.83	0.60
2:TA:918:ASN:OD1	2:TA:919:THR:N	2.35	0.60
3:UA:1112:MET:SD	3:UA:1113:GLU:N	2.73	0.60
3:UA:1124:VAL:HG23	3:UA:1125:GLN:HG2	1.83	0.60
1:H:15:THR:HG22	1:H:16:ASP:H	1.66	0.60
2:V:441:ASP:OD2	2:V:447:SER:OG	2.20	0.60
2:V:918:ASN:OD1	2:V:919:THR:N	2.35	0.60
3:W:1083:ARG:HB3	3:W:1112:MET:HE2	1.83	0.60
3:W:1124:VAL:HG23	3:W:1125:GLN:HG2	1.83	0.60
2:NA:49:GLU:N	2:NA:49:GLU:OE1	2.35	0.60
2:NA:441:ASP:OD2	2:NA:447:SER:OG	2.20	0.60
2:TA:441:ASP:OD2	2:TA:447:SER:OG	2.20	0.60
3:UA:1083:ARG:HB3	3:UA:1112:MET:HE2	1.83	0.60
2:C:441:ASP:OD2	2:C:447:SER:OG	2.20	0.60
2:O:49:GLU:OE1	2:O:49:GLU:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:441:ASP:OD2	2:O:447:SER:OG	2.20	0.60
3:W:373:MET:HE1	5:Y:114:ASP:CG	2.26	0.60
2:BA:441:ASP:OD2	2:BA:447:SER:OG	2.20	0.60
3:P:73:ILE:HD11	5:WA:60:HIS:CE1	2.36	0.60
3:P:586:TYR:O	3:P:590:THR:OG1	2.13	0.60
2:NA:881:ASP:OD1	2:NA:882:GLY:N	2.35	0.60
3:UA:373:MET:HE1	5:WA:114:ASP:CG	2.26	0.60
3:D:67:ARG:HG3	5:KA:53:GLU:CD	2.27	0.60
5:L:53:GLU:CD	3:CA:67:ARG:HG3	2.27	0.60
2:O:881:ASP:OD1	2:O:882:GLY:N	2.35	0.60
3:W:1112:MET:SD	3:W:1113:GLU:N	2.73	0.60
2:C:881:ASP:OD1	2:C:882:GLY:N	2.35	0.60
3:W:73:ILE:HD11	5:QA:60:HIS:CE1	2.36	0.60
1:AA:15:THR:HG22	1:AA:16:ASP:H	1.66	0.60
2:BA:881:ASP:OD1	2:BA:882:GLY:N	2.35	0.60
1:B:15:THR:HG22	1:B:16:ASP:H	1.66	0.59
3:P:1112:MET:SD	3:P:1113:GLU:N	2.73	0.59
2:V:49:GLU:OE1	2:V:49:GLU:N	2.35	0.59
5:Y:60:HIS:CE1	3:OA:73:ILE:HD11	2.36	0.59
2:BA:645:GLU:OE1	2:BA:645:GLU:N	2.35	0.59
3:CA:1112:MET:SD	3:CA:1113:GLU:N	2.73	0.59
2:HA:49:GLU:OE1	2:HA:49:GLU:N	2.35	0.59
3:OA:586:TYR:O	3:OA:590:THR:OG1	2.13	0.59
3:OA:1112:MET:SD	3:OA:1113:GLU:N	2.73	0.59
2:TA:49:GLU:OE1	2:TA:49:GLU:N	2.35	0.59
2:C:645:GLU:OE1	2:C:645:GLU:N	2.35	0.59
2:C:918:ASN:OD1	2:C:919:THR:N	2.35	0.59
3:D:1083:ARG:HB3	3:D:1112:MET:HE2	1.83	0.59
5:F:53:GLU:CD	3:IA:67:ARG:HG3	2.27	0.59
2:I:441:ASP:OD2	2:I:447:SER:OG	2.20	0.59
2:I:881:ASP:OD1	2:I:882:GLY:N	2.35	0.59
3:J:67:ARG:HG3	5:EA:53:GLU:CD	2.27	0.59
5:R:60:HIS:CE1	3:UA:73:ILE:HD11	2.37	0.59
3:W:67:ARG:HG3	5:QA:53:GLU:CD	2.27	0.59
3:CA:1083:ARG:HB3	3:CA:1112:MET:HE2	1.83	0.59
2:HA:441:ASP:OD2	2:HA:447:SER:OG	2.20	0.59
1:LA:24:GLU:OE1	1:LA:24:GLU:N	2.35	0.59
3:D:1138:VAL:HG11	3:D:1154:ILE:HG21	1.84	0.59
2:I:49:GLU:OE1	2:I:49:GLU:N	2.35	0.59
1:M:24:GLU:N	1:M:24:GLU:OE1	2.35	0.59
2:BA:918:ASN:OD1	2:BA:919:THR:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CA:1138:VAL:HG11	3:CA:1154:ILE:HG21	1.84	0.59
2:HA:881:ASP:OD1	2:HA:882:GLY:N	2.35	0.59
1:G:24:GLU:OE1	1:G:24:GLU:N	2.35	0.59
5:R:53:GLU:CD	3:UA:67:ARG:HG3	2.27	0.59
2:V:519:VAL:N	2:V:577:ASP:O	2.35	0.59
2:V:645:GLU:OE1	2:V:645:GLU:N	2.35	0.59
3:D:1112:MET:SD	3:D:1113:GLU:N	2.73	0.59
2:I:519:VAL:N	2:I:577:ASP:O	2.35	0.59
3:CA:1124:VAL:HG23	3:CA:1125:GLN:HG2	1.83	0.59
1:FA:24:GLU:OE1	1:FA:24:GLU:N	2.35	0.59
2:TA:519:VAL:N	2:TA:577:ASP:O	2.35	0.59
2:TA:645:GLU:OE1	2:TA:645:GLU:N	2.35	0.59
2:C:485:PRO:O	3:D:857:ARG:NH1	2.36	0.59
3:D:1124:VAL:HG23	3:D:1125:GLN:HG2	1.83	0.59
2:I:485:PRO:O	3:J:857:ARG:NH1	2.36	0.59
2:I:918:ASN:OD1	2:I:919:THR:N	2.35	0.59
2:O:918:ASN:OD1	2:O:919:THR:N	2.35	0.59
5:Y:53:GLU:CD	3:OA:67:ARG:HG3	2.27	0.59
2:HA:918:ASN:OD1	2:HA:919:THR:N	2.35	0.59
2:NA:918:ASN:OD1	2:NA:919:THR:N	2.35	0.59
3:UA:1138:VAL:HG11	3:UA:1154:ILE:HG21	1.84	0.59
1:A:24:GLU:OE1	1:A:24:GLU:N	2.35	0.59
3:P:67:ARG:HG3	5:WA:53:GLU:CD	2.27	0.59
3:W:1138:VAL:HG11	3:W:1154:ILE:HG21	1.84	0.59
1:Z:24:GLU:OE1	1:Z:24:GLU:N	2.35	0.59
2:BA:485:PRO:O	3:CA:857:ARG:NH1	2.36	0.59
2:HA:485:PRO:O	3:IA:857:ARG:NH1	2.36	0.59
2:HA:519:VAL:N	2:HA:577:ASP:O	2.35	0.59
2:NA:485:PRO:O	3:OA:857:ARG:NH1	2.36	0.59
1:RA:24:GLU:OE1	1:RA:24:GLU:N	2.35	0.59
3:J:1124:VAL:HG23	3:J:1125:GLN:HG2	1.83	0.59
2:O:485:PRO:O	3:P:857:ARG:NH1	2.36	0.59
1:S:24:GLU:OE1	1:S:24:GLU:N	2.35	0.59
3:IA:1124:VAL:HG23	3:IA:1125:GLN:HG2	1.83	0.59
2:C:49:GLU:OE1	2:C:49:GLU:N	2.35	0.59
2:BA:49:GLU:OE1	2:BA:49:GLU:N	2.35	0.59
2:V:881:ASP:OD1	2:V:882:GLY:N	2.35	0.58
2:TA:881:ASP:OD1	2:TA:882:GLY:N	2.35	0.58
2:I:257:ILE:O	2:I:260:SER:OG	2.19	0.58
2:V:485:PRO:O	3:W:857:ARG:NH1	2.36	0.58
2:HA:645:GLU:OE1	2:HA:645:GLU:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:IA:1112:MET:SD	3:IA:1113:GLU:N	2.73	0.58
2:TA:485:PRO:O	3:UA:857:ARG:NH1	2.36	0.58
2:O:645:GLU:OE1	2:O:645:GLU:N	2.35	0.58
3:IA:1138:VAL:HG11	3:IA:1154:ILE:HG21	1.84	0.58
2:NA:645:GLU:N	2:NA:645:GLU:OE1	2.35	0.58
2:I:645:GLU:OE1	2:I:645:GLU:N	2.35	0.58
3:J:1138:VAL:HG11	3:J:1154:ILE:HG21	1.84	0.58
1:N:27:GLU:OE1	1:N:27:GLU:N	2.37	0.58
1:MA:27:GLU:OE1	1:MA:27:GLU:N	2.37	0.58
2:TA:458:LEU:HD23	2:TA:458:LEU:H	1.68	0.58
2:O:458:LEU:HD23	2:O:458:LEU:H	1.68	0.58
2:V:458:LEU:HD23	2:V:458:LEU:H	1.68	0.58
2:HA:257:ILE:O	2:HA:260:SER:OG	2.19	0.58
2:NA:458:LEU:HD23	2:NA:458:LEU:H	1.68	0.58
2:O:257:ILE:O	2:O:260:SER:OG	2.19	0.58
3:P:78:CYS:SG	3:P:80:VAL:HG22	2.44	0.58
3:OA:78:CYS:SG	3:OA:80:VAL:HG22	2.44	0.58
3:J:1112:MET:SD	3:J:1113:GLU:N	2.73	0.58
3:P:1138:VAL:HG11	3:P:1154:ILE:HG21	1.84	0.58
1:GA:138:LEU:HD23	1:GA:138:LEU:H	1.69	0.58
3:OA:1138:VAL:HG11	3:OA:1154:ILE:HG21	1.84	0.58
3:D:350:ARG:NE	3:D:373:MET:HE2	2.19	0.58
1:H:138:LEU:H	1:H:138:LEU:HD23	1.69	0.58
1:N:138:LEU:HD23	1:N:138:LEU:H	1.69	0.58
3:CA:350:ARG:NE	3:CA:373:MET:HE2	2.19	0.58
2:NA:257:ILE:O	2:NA:260:SER:OG	2.19	0.58
1:T:27:GLU:OE1	1:T:27:GLU:N	2.37	0.58
3:IA:78:CYS:SG	3:IA:80:VAL:HG22	2.44	0.58
1:MA:138:LEU:HD23	1:MA:138:LEU:H	1.69	0.58
3:J:78:CYS:SG	3:J:80:VAL:HG22	2.44	0.58
1:SA:27:GLU:OE1	1:SA:27:GLU:N	2.37	0.58
3:D:78:CYS:SG	3:D:80:VAL:HG22	2.44	0.57
2:C:303:GLU:OE2	2:C:331:SER:OG	2.22	0.57
3:P:350:ARG:NE	3:P:373:MET:HE2	2.19	0.57
2:BA:303:GLU:OE2	2:BA:331:SER:OG	2.22	0.57
3:CA:78:CYS:SG	3:CA:80:VAL:HG22	2.44	0.57
5:F:139:SER:O	5:F:143:THR:HG23	2.05	0.57
5:EA:139:SER:O	5:EA:143:THR:HG23	2.05	0.57
3:OA:350:ARG:NE	3:OA:373:MET:HE2	2.19	0.57
5:F:25:ASP:OD1	5:F:26:LEU:N	2.37	0.57
3:W:78:CYS:SG	3:W:80:VAL:HG22	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:25:ASP:OD1	5:Y:26:LEU:N	2.37	0.57
5:EA:25:ASP:OD1	5:EA:26:LEU:N	2.37	0.57
5:QA:131:ASP:OD2	5:QA:133:THR:OG1	2.18	0.57
5:WA:25:ASP:OD1	5:WA:26:LEU:N	2.37	0.57
2:C:458:LEU:HD23	2:C:458:LEU:H	1.68	0.57
3:UA:78:CYS:SG	3:UA:80:VAL:HG22	2.44	0.57
5:WA:139:SER:O	5:WA:143:THR:HG23	2.05	0.57
2:I:603:ASN:OD1	2:I:604:ARG:N	2.38	0.57
2:O:303:GLU:OE2	2:O:331:SER:OG	2.22	0.57
5:R:25:ASP:OD1	5:R:26:LEU:N	2.37	0.57
5:Y:139:SER:O	5:Y:143:THR:HG23	2.05	0.57
2:BA:458:LEU:HD23	2:BA:458:LEU:H	1.68	0.57
2:NA:303:GLU:OE2	2:NA:331:SER:OG	2.22	0.57
3:UA:350:ARG:NE	3:UA:373:MET:HE2	2.19	0.57
3:J:350:ARG:NE	3:J:373:MET:HE2	2.19	0.57
3:W:350:ARG:NE	3:W:373:MET:HE2	2.19	0.57
2:HA:603:ASN:OD1	2:HA:604:ARG:N	2.38	0.57
5:QA:25:ASP:OD1	5:QA:26:LEU:N	2.37	0.57
1:B:138:LEU:HD23	1:B:138:LEU:H	1.69	0.57
1:H:27:GLU:N	1:H:27:GLU:OE1	2.37	0.57
1:GA:27:GLU:OE1	1:GA:27:GLU:N	2.37	0.57
3:IA:350:ARG:NE	3:IA:373:MET:HE2	2.19	0.57
2:NA:603:ASN:OD1	2:NA:604:ARG:N	2.38	0.57
2:TA:303:GLU:OE2	2:TA:331:SER:OG	2.22	0.57
3:D:60:CYS:SG	3:D:62:CYS:N	2.78	0.56
2:O:603:ASN:OD1	2:O:604:ARG:N	2.38	0.56
3:P:60:CYS:SG	3:P:62:CYS:N	2.78	0.56
1:AA:138:LEU:HD23	1:AA:138:LEU:H	1.69	0.56
3:OA:60:CYS:SG	3:OA:62:CYS:N	2.78	0.56
3:D:33:THR:HG22	3:D:34:ILE:H	1.71	0.56
2:I:303:GLU:OE2	2:I:331:SER:OG	2.22	0.56
3:J:33:THR:HG22	3:J:34:ILE:H	1.71	0.56
3:J:129:ILE:HG22	3:J:130:TYR:CD1	2.41	0.56
2:V:303:GLU:OE2	2:V:331:SER:OG	2.22	0.56
3:CA:33:THR:HG22	3:CA:34:ILE:H	1.71	0.56
3:CA:60:CYS:SG	3:CA:62:CYS:N	2.78	0.56
3:CA:273:GLU:OE2	3:CA:295:ARG:NH2	2.36	0.56
3:IA:33:THR:HG22	3:IA:34:ILE:H	1.71	0.56
3:IA:129:ILE:HG22	3:IA:130:TYR:CD1	2.41	0.56
3:D:273:GLU:OE2	3:D:295:ARG:NH2	2.36	0.56
2:O:1090:THR:HG22	2:O:1118:PRO:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:129:ILE:HG22	3:P:130:TYR:CD1	2.41	0.56
1:T:138:LEU:HD23	1:T:138:LEU:H	1.69	0.56
2:HA:303:GLU:OE2	2:HA:331:SER:OG	2.22	0.56
5:KA:25:ASP:OD1	5:KA:26:LEU:N	2.37	0.56
2:NA:1090:THR:HG22	2:NA:1118:PRO:HG3	1.87	0.56
3:OA:129:ILE:HG22	3:OA:130:TYR:CD1	2.41	0.56
1:SA:138:LEU:HD23	1:SA:138:LEU:H	1.69	0.56
3:J:1176:LEU:HD12	3:J:1177:PRO:CD	2.36	0.56
5:L:25:ASP:OD1	5:L:26:LEU:N	2.37	0.56
2:O:519:VAL:N	2:O:577:ASP:O	2.35	0.56
3:P:134:TYR:HD1	3:P:256:MET:HE3	1.71	0.56
3:P:1176:LEU:HD12	3:P:1177:PRO:CD	2.36	0.56
3:IA:1176:LEU:HD12	3:IA:1177:PRO:CD	2.36	0.56
3:OA:134:TYR:HD1	3:OA:256:MET:HE3	1.71	0.56
3:OA:1176:LEU:HD12	3:OA:1177:PRO:CD	2.36	0.56
2:I:458:LEU:HD23	2:I:458:LEU:H	1.68	0.56
5:KA:139:SER:O	5:KA:143:THR:HG23	2.05	0.56
3:P:439:HIS:ND1	3:P:439:HIS:O	2.39	0.56
3:W:439:HIS:ND1	3:W:439:HIS:O	2.39	0.56
3:W:815:ARG:O	3:W:819:GLY:N	2.38	0.56
2:BA:603:ASN:OD1	2:BA:604:ARG:N	2.38	0.56
3:CA:586:TYR:O	3:CA:590:THR:OG1	2.13	0.56
2:C:519:VAL:N	2:C:577:ASP:O	2.35	0.56
3:D:439:HIS:ND1	3:D:439:HIS:O	2.39	0.56
3:J:439:HIS:ND1	3:J:439:HIS:O	2.39	0.56
5:L:139:SER:O	5:L:143:THR:HG23	2.05	0.56
3:W:134:TYR:HD1	3:W:256:MET:HE3	1.71	0.56
3:CA:439:HIS:ND1	3:CA:439:HIS:O	2.39	0.56
2:HA:1087:GLU:OE2	3:IA:548:SER:OG	2.18	0.56
3:IA:60:CYS:SG	3:IA:62:CYS:N	2.78	0.56
3:IA:439:HIS:ND1	3:IA:439:HIS:O	2.39	0.56
2:NA:519:VAL:N	2:NA:577:ASP:O	2.35	0.56
3:OA:439:HIS:ND1	3:OA:439:HIS:O	2.39	0.56
2:TA:1090:THR:HG22	2:TA:1118:PRO:HG3	1.87	0.56
3:UA:439:HIS:ND1	3:UA:439:HIS:O	2.39	0.56
3:UA:815:ARG:O	3:UA:819:GLY:N	2.38	0.56
2:C:603:ASN:OD1	2:C:604:ARG:N	2.38	0.56
3:J:60:CYS:SG	3:J:62:CYS:N	2.78	0.56
2:V:1090:THR:HG22	2:V:1118:PRO:HG3	1.87	0.56
2:HA:458:LEU:HD23	2:HA:458:LEU:H	1.68	0.56
2:TA:603:ASN:OD1	2:TA:604:ARG:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:UA:134:TYR:HD1	3:UA:256:MET:HE3	1.71	0.56
5:R:139:SER:O	5:R:143:THR:HG23	2.05	0.56
5:QA:139:SER:O	5:QA:143:THR:HG23	2.05	0.56
1:B:27:GLU:OE1	1:B:27:GLU:N	2.37	0.56
2:V:603:ASN:OD1	2:V:604:ARG:N	2.38	0.56
3:W:129:ILE:HG22	3:W:130:TYR:CD1	2.41	0.56
2:BA:519:VAL:N	2:BA:577:ASP:O	2.35	0.56
3:UA:129:ILE:HG22	3:UA:130:TYR:CD1	2.41	0.56
1:AA:27:GLU:OE1	1:AA:27:GLU:N	2.37	0.55
3:CA:129:ILE:HG22	3:CA:130:TYR:CD1	2.41	0.55
3:UA:33:THR:HG22	3:UA:34:ILE:H	1.71	0.55
3:D:129:ILE:HG22	3:D:130:TYR:CD1	2.41	0.55
3:W:33:THR:HG22	3:W:34:ILE:H	1.71	0.55
3:D:1176:LEU:HD12	3:D:1177:PRO:CD	2.36	0.55
3:W:212:ALA:O	3:W:216:LEU:HD23	2.07	0.55
3:CA:1176:LEU:HD12	3:CA:1177:PRO:CD	2.36	0.55
3:UA:212:ALA:O	3:UA:216:LEU:HD23	2.07	0.55
5:F:101:LEU:HD21	5:F:147:ARG:HH21	1.72	0.55
1:M:149:ALA:N	1:M:165:ASP:OD1	2.40	0.55
3:P:33:THR:HG22	3:P:34:ILE:H	1.71	0.55
3:W:60:CYS:SG	3:W:62:CYS:N	2.78	0.55
5:EA:101:LEU:HD21	5:EA:147:ARG:HH21	1.72	0.55
2:HA:1090:THR:HG22	2:HA:1118:PRO:HG3	1.87	0.55
2:TA:1087:GLU:OE2	3:UA:548:SER:OG	2.18	0.55
3:UA:60:CYS:SG	3:UA:62:CYS:N	2.78	0.55
2:I:1090:THR:HG22	2:I:1118:PRO:HG3	1.87	0.55
3:P:402:LEU:HD23	3:P:402:LEU:C	2.32	0.55
3:W:402:LEU:HD23	3:W:402:LEU:C	2.32	0.55
1:LA:149:ALA:N	1:LA:165:ASP:OD1	2.40	0.55
3:OA:402:LEU:HD23	3:OA:402:LEU:C	2.32	0.55
3:D:1278:ALA:O	3:D:1282:ALA:N	2.40	0.55
3:W:1176:LEU:HD12	3:W:1177:PRO:CD	2.36	0.55
3:CA:1278:ALA:O	3:CA:1282:ALA:N	2.40	0.55
3:IA:212:ALA:O	3:IA:216:LEU:HD23	2.07	0.55
3:OA:33:THR:HG22	3:OA:34:ILE:H	1.71	0.55
3:UA:402:LEU:HD23	3:UA:402:LEU:C	2.32	0.55
3:J:212:ALA:O	3:J:216:LEU:HD23	2.07	0.54
3:IA:134:TYR:HD1	3:IA:256:MET:HE3	1.71	0.54
1:G:149:ALA:N	1:G:165:ASP:OD1	2.40	0.54
3:P:1278:ALA:O	3:P:1282:ALA:N	2.40	0.54
3:W:1278:ALA:O	3:W:1282:ALA:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BA:1090:THR:HG22	2:BA:1118:PRO:HG3	1.87	0.54
3:IA:273:GLU:OE2	3:IA:295:ARG:NH2	2.36	0.54
3:OA:1278:ALA:O	3:OA:1282:ALA:N	2.40	0.54
3:UA:440:GLN:NE2	3:UA:515:MET:SD	2.80	0.54
3:UA:1176:LEU:HD12	3:UA:1177:PRO:CD	2.36	0.54
3:D:212:ALA:O	3:D:216:LEU:HD23	2.07	0.54
3:J:134:TYR:HD1	3:J:256:MET:HE3	1.71	0.54
3:P:440:GLN:NE2	3:P:515:MET:SD	2.80	0.54
3:W:440:GLN:NE2	3:W:515:MET:SD	2.80	0.54
1:FA:149:ALA:N	1:FA:165:ASP:OD1	2.40	0.54
3:UA:1278:ALA:O	3:UA:1282:ALA:N	2.40	0.54
1:A:184:GLU:O	1:B:151:GLN:NE2	2.41	0.54
2:C:1090:THR:HG22	2:C:1118:PRO:HG3	1.87	0.54
3:D:134:TYR:HD1	3:D:256:MET:HE3	1.71	0.54
1:S:149:ALA:N	1:S:165:ASP:OD1	2.40	0.54
1:Z:184:GLU:O	1:AA:151:GLN:NE2	2.41	0.54
3:CA:212:ALA:O	3:CA:216:LEU:HD23	2.07	0.54
3:IA:402:LEU:C	3:IA:402:LEU:HD23	2.32	0.54
3:OA:440:GLN:NE2	3:OA:515:MET:SD	2.80	0.54
1:RA:149:ALA:N	1:RA:165:ASP:OD1	2.40	0.54
3:J:273:GLU:OE2	3:J:295:ARG:NH2	2.36	0.54
1:M:184:GLU:O	1:N:151:GLN:NE2	2.41	0.54
3:P:815:ARG:O	3:P:819:GLY:N	2.38	0.54
1:LA:184:GLU:O	1:MA:151:GLN:NE2	2.41	0.54
2:TA:307:ASP:OD1	2:TA:308:LEU:N	2.41	0.54
2:C:257:ILE:O	2:C:260:SER:OG	2.19	0.54
1:G:184:GLU:O	1:H:151:GLN:NE2	2.41	0.54
3:J:221:ASP:O	3:J:225:THR:OG1	2.26	0.54
3:J:402:LEU:HD23	3:J:402:LEU:C	2.32	0.54
3:J:440:GLN:NE2	3:J:515:MET:SD	2.80	0.54
2:O:307:ASP:OD1	2:O:308:LEU:N	2.41	0.54
2:V:307:ASP:OD1	2:V:308:LEU:N	2.41	0.54
3:CA:440:GLN:NE2	3:CA:515:MET:SD	2.80	0.54
1:FA:184:GLU:O	1:GA:151:GLN:NE2	2.41	0.54
3:IA:221:ASP:O	3:IA:225:THR:OG1	2.26	0.54
2:NA:307:ASP:OD1	2:NA:308:LEU:N	2.41	0.54
3:D:440:GLN:NE2	3:D:515:MET:SD	2.80	0.54
3:J:1278:ALA:O	3:J:1282:ALA:N	2.40	0.54
3:CA:134:TYR:HD1	3:CA:256:MET:HE3	1.71	0.54
3:OA:212:ALA:O	3:OA:216:LEU:HD23	2.07	0.54
3:OA:273:GLU:OE2	3:OA:295:ARG:NH2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLU:OE1	1:B:104:GLU:N	2.41	0.54
3:P:212:ALA:O	3:P:216:LEU:HD23	2.07	0.54
1:AA:104:GLU:OE1	1:AA:104:GLU:N	2.41	0.54
3:IA:440:GLN:NE2	3:IA:515:MET:SD	2.80	0.54
3:OA:815:ARG:O	3:OA:819:GLY:N	2.38	0.54
5:WA:101:LEU:HD21	5:WA:147:ARG:HH21	1.72	0.54
3:D:402:LEU:HD23	3:D:402:LEU:C	2.32	0.54
3:P:147:GLU:OE1	3:P:147:GLU:N	2.41	0.54
3:W:147:GLU:OE1	3:W:147:GLU:N	2.41	0.54
2:BA:257:ILE:O	2:BA:260:SER:OG	2.19	0.54
3:IA:1278:ALA:O	3:IA:1282:ALA:N	2.40	0.54
3:OA:147:GLU:N	3:OA:147:GLU:OE1	2.41	0.54
3:UA:147:GLU:OE1	3:UA:147:GLU:N	2.41	0.54
1:S:184:GLU:O	1:T:151:GLN:NE2	2.41	0.54
3:W:354:LEU:HD23	3:W:354:LEU:C	2.33	0.54
5:Y:101:LEU:HD21	5:Y:147:ARG:HH21	1.72	0.54
3:UA:354:LEU:C	3:UA:354:LEU:HD23	2.33	0.54
2:C:307:ASP:OD1	2:C:308:LEU:N	2.41	0.53
3:D:147:GLU:OE1	3:D:147:GLU:N	2.41	0.53
3:P:273:GLU:OE2	3:P:295:ARG:NH2	2.36	0.53
2:BA:307:ASP:OD1	2:BA:308:LEU:N	2.41	0.53
3:CA:402:LEU:HD23	3:CA:402:LEU:C	2.32	0.53
1:GA:104:GLU:N	1:GA:104:GLU:OE1	2.41	0.53
1:RA:184:GLU:O	1:SA:151:GLN:NE2	2.41	0.53
1:H:104:GLU:OE1	1:H:104:GLU:N	2.41	0.53
2:O:1123:VAL:HG13	3:P:324:LEU:HD11	1.91	0.53
3:CA:147:GLU:OE1	3:CA:147:GLU:N	2.41	0.53
3:IA:147:GLU:N	3:IA:147:GLU:OE1	2.41	0.53
2:NA:1123:VAL:HG13	3:OA:324:LEU:HD11	1.91	0.53
2:I:307:ASP:OD1	2:I:308:LEU:N	2.41	0.53
3:J:147:GLU:OE1	3:J:147:GLU:N	2.41	0.53
3:P:354:LEU:HD23	3:P:354:LEU:C	2.33	0.53
1:MA:104:GLU:OE1	1:MA:104:GLU:N	2.41	0.53
3:OA:354:LEU:HD23	3:OA:354:LEU:C	2.33	0.53
1:N:104:GLU:OE1	1:N:104:GLU:N	2.41	0.53
1:Z:149:ALA:N	1:Z:165:ASP:OD1	2.40	0.53
1:A:149:ALA:N	1:A:165:ASP:OD1	2.40	0.53
3:P:53:GLY:O	3:P:88:ARG:NH2	2.42	0.53
5:R:101:LEU:HD21	5:R:147:ARG:HH21	1.72	0.53
3:W:1120:GLU:O	3:W:1124:VAL:HG22	2.09	0.53
2:HA:307:ASP:OD1	2:HA:308:LEU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:IA:53:GLY:O	3:IA:88:ARG:NH2	2.42	0.53
3:OA:53:GLY:O	3:OA:88:ARG:NH2	2.42	0.53
2:C:856:GLU:OE1	2:C:856:GLU:N	2.41	0.53
3:J:53:GLY:O	3:J:88:ARG:NH2	2.42	0.53
3:J:110:VAL:HG23	3:J:110:VAL:O	2.09	0.53
5:L:101:LEU:HD21	5:L:147:ARG:HH21	1.72	0.53
2:V:1123:VAL:HG13	3:W:324:LEU:HD11	1.91	0.53
2:BA:856:GLU:OE1	2:BA:856:GLU:N	2.41	0.53
3:IA:110:VAL:HG23	3:IA:110:VAL:O	2.09	0.53
1:SA:104:GLU:OE1	1:SA:104:GLU:N	2.41	0.53
2:TA:1123:VAL:HG13	3:UA:324:LEU:HD11	1.91	0.53
3:UA:273:GLU:OE2	3:UA:295:ARG:NH2	2.36	0.53
3:UA:1120:GLU:O	3:UA:1124:VAL:HG22	2.09	0.53
2:I:696:VAL:HG11	2:I:702:ILE:HD11	1.90	0.53
2:I:1123:VAL:HG13	3:J:324:LEU:HD11	1.91	0.53
3:P:1120:GLU:O	3:P:1124:VAL:HG22	2.09	0.53
1:T:104:GLU:N	1:T:104:GLU:OE1	2.41	0.53
2:HA:1123:VAL:HG13	3:IA:324:LEU:HD11	1.91	0.53
5:QA:101:LEU:HD21	5:QA:147:ARG:HH21	1.72	0.53
3:J:815:ARG:O	3:J:819:GLY:N	2.38	0.53
2:O:696:VAL:HG11	2:O:702:ILE:HD11	1.90	0.53
2:O:1087:GLU:OE2	3:P:548:SER:OG	2.18	0.53
2:HA:696:VAL:HG11	2:HA:702:ILE:HD11	1.90	0.53
5:KA:101:LEU:HD21	5:KA:147:ARG:HH21	1.72	0.53
3:OA:1120:GLU:O	3:OA:1124:VAL:HG22	2.09	0.53
3:P:110:VAL:HG23	3:P:110:VAL:O	2.09	0.53
5:R:99:VAL:HG23	5:R:116:ILE:HD12	1.90	0.53
3:W:53:GLY:O	3:W:88:ARG:NH2	2.42	0.53
2:NA:696:VAL:HG11	2:NA:702:ILE:HD11	1.90	0.53
3:UA:53:GLY:O	3:UA:88:ARG:NH2	2.42	0.53
3:W:273:GLU:OE2	3:W:295:ARG:NH2	2.36	0.53
3:CA:221:ASP:O	3:CA:225:THR:OG1	2.26	0.53
3:OA:110:VAL:O	3:OA:110:VAL:HG23	2.09	0.53
5:QA:99:VAL:HG23	5:QA:116:ILE:HD12	1.90	0.53
3:D:354:LEU:HD23	3:D:354:LEU:C	2.33	0.52
5:F:99:VAL:HG23	5:F:116:ILE:HD12	1.90	0.52
3:CA:354:LEU:HD23	3:CA:354:LEU:C	2.33	0.52
1:GA:182:ARG:NH1	3:IA:485:ASP:OD1	2.43	0.52
3:IA:815:ARG:O	3:IA:819:GLY:N	2.38	0.52
1:B:182:ARG:NH1	3:D:485:ASP:OD1	2.43	0.52
3:D:221:ASP:O	3:D:225:THR:OG1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:182:ARG:NH1	3:J:485:ASP:OD1	2.43	0.52
1:AA:182:ARG:NH1	3:CA:485:ASP:OD1	2.43	0.52
5:EA:99:VAL:HG23	5:EA:116:ILE:HD12	1.90	0.52
5:L:99:VAL:HG23	5:L:116:ILE:HD12	1.90	0.52
5:Y:97:LEU:HD11	5:Y:143:THR:HG23	1.91	0.52
3:CA:110:VAL:HG23	3:CA:110:VAL:O	2.09	0.52
2:HA:1102:VAL:HG23	2:HA:1112:ILE:HG23	1.92	0.52
5:WA:97:LEU:HD11	5:WA:143:THR:HG23	1.91	0.52
3:D:110:VAL:O	3:D:110:VAL:HG23	2.09	0.52
2:I:1102:VAL:HG23	2:I:1112:ILE:HG23	1.92	0.52
3:J:69:ARG:HH22	5:EA:53:GLU:HG2	1.75	0.52
3:P:93:GLY:O	3:P:319:VAL:N	2.41	0.52
3:W:110:VAL:HG23	3:W:110:VAL:O	2.09	0.52
5:KA:99:VAL:HG23	5:KA:116:ILE:HD12	1.90	0.52
3:OA:93:GLY:O	3:OA:319:VAL:N	2.41	0.52
3:OA:221:ASP:O	3:OA:225:THR:OG1	2.26	0.52
5:F:53:GLU:HG2	3:IA:69:ARG:HH22	1.75	0.52
2:I:827:GLU:N	2:I:827:GLU:OE1	2.43	0.52
3:J:354:LEU:C	3:J:354:LEU:HD23	2.33	0.52
2:O:1134:ASN:N	3:P:13:GLY:O	2.43	0.52
2:V:197:LYS:O	2:V:199:LEU:HD12	2.10	0.52
3:CA:53:GLY:O	3:CA:88:ARG:NH2	2.42	0.52
2:HA:827:GLU:OE1	2:HA:827:GLU:N	2.43	0.52
3:IA:354:LEU:HD23	3:IA:354:LEU:C	2.33	0.52
3:IA:1120:GLU:O	3:IA:1124:VAL:HG22	2.09	0.52
2:NA:1134:ASN:N	3:OA:13:GLY:O	2.43	0.52
2:TA:197:LYS:O	2:TA:199:LEU:HD12	2.10	0.52
3:UA:110:VAL:HG23	3:UA:110:VAL:O	2.09	0.52
3:D:53:GLY:O	3:D:88:ARG:NH2	2.42	0.52
3:P:221:ASP:O	3:P:225:THR:OG1	2.26	0.52
1:T:182:ARG:NH1	3:W:485:ASP:OD1	2.43	0.52
2:BA:1102:VAL:HG23	2:BA:1112:ILE:HG23	1.92	0.52
2:NA:1102:VAL:HG23	2:NA:1112:ILE:HG23	1.92	0.52
2:C:1102:VAL:HG23	2:C:1112:ILE:HG23	1.92	0.52
3:J:1120:GLU:O	3:J:1124:VAL:HG22	2.09	0.52
1:N:182:ARG:NH1	3:P:485:ASP:OD1	2.43	0.52
2:O:1102:VAL:HG23	2:O:1112:ILE:HG23	1.92	0.52
3:P:337:THR:OG1	3:P:338:SER:N	2.43	0.52
2:V:696:VAL:HG11	2:V:702:ILE:HD11	1.90	0.52
1:MA:182:ARG:NH1	3:OA:485:ASP:OD1	2.43	0.52
3:OA:337:THR:OG1	3:OA:338:SER:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:182:ARG:NH1	3:UA:485:ASP:OD1	2.43	0.52
2:C:696:VAL:HG11	2:C:702:ILE:HD11	1.90	0.52
2:C:1123:VAL:HG13	3:D:324:LEU:HD11	1.91	0.52
3:D:337:THR:OG1	3:D:338:SER:N	2.43	0.52
3:D:339:ASP:O	3:D:342:ASP:N	2.43	0.52
3:J:339:ASP:O	3:J:342:ASP:N	2.43	0.52
2:BA:696:VAL:HG11	2:BA:702:ILE:HD11	1.90	0.52
2:BA:1123:VAL:HG13	3:CA:324:LEU:HD11	1.91	0.52
3:CA:337:THR:OG1	3:CA:338:SER:N	2.43	0.52
3:CA:339:ASP:O	3:CA:342:ASP:N	2.43	0.52
5:KA:97:LEU:HD11	5:KA:143:THR:HG23	1.91	0.52
3:P:69:ARG:HH22	5:WA:53:GLU:HG2	1.75	0.52
3:CA:1120:GLU:O	3:CA:1124:VAL:HG22	2.09	0.52
3:IA:339:ASP:O	3:IA:342:ASP:N	2.43	0.52
2:TA:696:VAL:HG11	2:TA:702:ILE:HD11	1.90	0.52
3:UA:337:THR:OG1	3:UA:338:SER:N	2.43	0.52
5:L:97:LEU:HD11	5:L:143:THR:HG23	1.91	0.52
1:S:15:THR:HG22	1:S:16:ASP:H	1.75	0.52
3:W:337:THR:OG1	3:W:338:SER:N	2.43	0.52
5:Y:53:GLU:HG2	3:OA:69:ARG:HH22	1.75	0.52
5:Y:99:VAL:HG23	5:Y:116:ILE:HD12	1.90	0.52
2:C:177:SER:HB3	2:C:378:LEU:HD11	1.92	0.51
3:D:1120:GLU:O	3:D:1124:VAL:HG22	2.09	0.51
1:G:15:THR:HG22	1:G:16:ASP:H	1.75	0.51
3:W:586:TYR:O	3:W:590:THR:OG1	2.13	0.51
1:FA:15:THR:HG22	1:FA:16:ASP:H	1.75	0.51
2:HA:197:LYS:O	2:HA:199:LEU:HD12	2.10	0.51
1:LA:15:THR:HG22	1:LA:16:ASP:H	1.75	0.51
1:RA:15:THR:HG22	1:RA:16:ASP:H	1.75	0.51
2:I:197:LYS:O	2:I:199:LEU:HD12	2.10	0.51
2:I:1134:ASN:N	3:J:13:GLY:O	2.43	0.51
5:L:90:LEU:HD11	5:L:138:PHE:CE2	2.46	0.51
1:M:15:THR:HG22	1:M:16:ASP:H	1.75	0.51
2:V:1102:VAL:HG23	2:V:1112:ILE:HG23	1.92	0.51
2:BA:177:SER:HB3	2:BA:378:LEU:HD11	1.92	0.51
2:HA:1134:ASN:N	3:IA:13:GLY:O	2.43	0.51
5:KA:90:LEU:HD11	5:KA:138:PHE:CE2	2.46	0.51
2:TA:1102:VAL:HG23	2:TA:1112:ILE:HG23	1.92	0.51
5:WA:99:VAL:HG23	5:WA:116:ILE:HD12	1.90	0.51
1:A:15:THR:HG22	1:A:16:ASP:H	1.75	0.51
3:D:1056:GLU:OE1	3:D:1056:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:197:LYS:O	2:O:199:LEU:HD12	2.10	0.51
2:V:257:ILE:O	2:V:260:SER:OG	2.19	0.51
2:V:1134:ASN:N	3:W:13:GLY:O	2.43	0.51
3:CA:1056:GLU:N	3:CA:1056:GLU:OE1	2.44	0.51
2:O:177:SER:HB3	2:O:378:LEU:HD11	1.92	0.51
5:R:53:GLU:HG2	3:UA:69:ARG:HH22	1.75	0.51
2:V:1087:GLU:OE2	3:W:548:SER:OG	2.18	0.51
1:Z:15:THR:HG22	1:Z:16:ASP:H	1.75	0.51
2:NA:197:LYS:O	2:NA:199:LEU:HD12	2.10	0.51
3:D:815:ARG:O	3:D:819:GLY:N	2.38	0.51
2:NA:177:SER:HB3	2:NA:378:LEU:HD11	1.92	0.51
2:TA:1134:ASN:N	3:UA:13:GLY:O	2.43	0.51
2:C:197:LYS:O	2:C:199:LEU:HD12	2.10	0.51
2:I:177:SER:HB3	2:I:378:LEU:HD11	1.92	0.51
2:O:827:GLU:OE1	2:O:827:GLU:N	2.43	0.51
3:P:354:LEU:HD23	3:P:354:LEU:O	2.11	0.51
2:V:827:GLU:N	2:V:827:GLU:OE1	2.43	0.51
3:W:69:ARG:HH22	5:QA:53:GLU:HG2	1.75	0.51
2:HA:177:SER:HB3	2:HA:378:LEU:HD11	1.92	0.51
3:OA:354:LEU:HD23	3:OA:354:LEU:O	2.11	0.51
5:QA:90:LEU:HD11	5:QA:138:PHE:CE2	2.46	0.51
2:C:827:GLU:OE1	2:C:827:GLU:N	2.43	0.51
2:C:1134:ASN:N	3:D:13:GLY:O	2.43	0.51
3:D:69:ARG:HH22	5:KA:53:GLU:HG2	1.75	0.51
3:J:354:LEU:HD23	3:J:354:LEU:O	2.11	0.51
5:R:90:LEU:HD11	5:R:138:PHE:CE2	2.46	0.51
3:CA:354:LEU:HD23	3:CA:354:LEU:O	2.11	0.51
3:IA:354:LEU:HD23	3:IA:354:LEU:O	2.11	0.51
2:TA:257:ILE:O	2:TA:260:SER:OG	2.19	0.51
2:TA:827:GLU:N	2:TA:827:GLU:OE1	2.43	0.51
3:UA:586:TYR:O	3:UA:590:THR:OG1	2.13	0.51
2:C:237:LEU:O	2:C:237:LEU:HD23	2.11	0.51
3:D:354:LEU:HD23	3:D:354:LEU:O	2.11	0.51
3:J:1056:GLU:N	3:J:1056:GLU:OE1	2.44	0.51
5:L:53:GLU:HG2	3:CA:69:ARG:HH22	1.75	0.51
2:BA:197:LYS:O	2:BA:199:LEU:HD12	2.10	0.51
2:BA:237:LEU:HD23	2:BA:237:LEU:O	2.11	0.51
2:BA:827:GLU:OE1	2:BA:827:GLU:N	2.43	0.51
2:BA:1134:ASN:N	3:CA:13:GLY:O	2.43	0.51
2:NA:827:GLU:OE1	2:NA:827:GLU:N	2.43	0.51
2:I:237:LEU:O	2:I:237:LEU:HD23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:75:CYS:O	3:P:79:GLY:N	2.43	0.51
3:W:354:LEU:HD23	3:W:354:LEU:O	2.11	0.51
3:W:1056:GLU:OE1	3:W:1056:GLU:N	2.44	0.51
4:X:103:LEU:C	4:X:104:LEU:HD12	2.36	0.51
3:CA:815:ARG:O	3:CA:819:GLY:N	2.38	0.51
3:IA:1056:GLU:OE1	3:IA:1056:GLU:N	2.44	0.51
3:OA:75:CYS:O	3:OA:79:GLY:N	2.43	0.51
3:OA:269:ASP:OD1	3:OA:270:ILE:N	2.44	0.51
3:UA:1056:GLU:OE1	3:UA:1056:GLU:N	2.44	0.51
4:VA:103:LEU:C	4:VA:104:LEU:HD12	2.36	0.51
5:L:95:LEU:HA	5:L:98:VAL:HG12	1.93	0.51
3:P:269:ASP:OD1	3:P:270:ILE:N	2.44	0.51
2:V:611:MET:HE2	2:V:611:MET:HA	1.93	0.51
5:KA:95:LEU:HA	5:KA:98:VAL:HG12	1.93	0.51
2:TA:611:MET:HE2	2:TA:611:MET:HA	1.93	0.51
3:UA:354:LEU:HD23	3:UA:354:LEU:O	2.11	0.51
2:I:531:LEU:HD21	2:I:578:TYR:CZ	2.46	0.50
3:J:269:ASP:OD1	3:J:270:ILE:N	2.44	0.50
2:V:237:LEU:O	2:V:237:LEU:HD23	2.11	0.50
2:HA:237:LEU:HD23	2:HA:237:LEU:O	2.11	0.50
2:HA:531:LEU:HD21	2:HA:578:TYR:CZ	2.46	0.50
3:IA:269:ASP:OD1	3:IA:270:ILE:N	2.44	0.50
2:TA:237:LEU:O	2:TA:237:LEU:HD23	2.11	0.50
3:UA:339:ASP:O	3:UA:342:ASP:N	2.43	0.50
5:F:90:LEU:HD11	5:F:138:PHE:CE2	2.46	0.50
2:V:856:GLU:OE1	2:V:856:GLU:N	2.41	0.50
3:W:339:ASP:O	3:W:342:ASP:N	2.43	0.50
5:EA:90:LEU:HD11	5:EA:138:PHE:CE2	2.46	0.50
2:HA:611:MET:HE2	2:HA:611:MET:HA	1.93	0.50
3:OA:1056:GLU:OE1	3:OA:1056:GLU:N	2.44	0.50
1:B:145:GLY:N	1:B:168:TYR:O	2.45	0.50
2:C:611:MET:HE2	2:C:611:MET:HA	1.93	0.50
2:I:611:MET:HE2	2:I:611:MET:HA	1.93	0.50
3:J:223:TRP:O	3:J:226:PHE:N	2.45	0.50
5:L:57:TYR:CZ	3:IA:157:VAL:HG21	2.47	0.50
2:O:531:LEU:HD21	2:O:578:TYR:CZ	2.46	0.50
3:P:157:VAL:HG21	5:EA:57:TYR:CZ	2.47	0.50
3:P:1056:GLU:N	3:P:1056:GLU:OE1	2.44	0.50
2:V:177:SER:HB3	2:V:378:LEU:HD11	1.92	0.50
1:AA:145:GLY:N	1:AA:168:TYR:O	2.45	0.50
3:IA:223:TRP:O	3:IA:226:PHE:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:TA:177:SER:HB3	2:TA:378:LEU:HD11	1.92	0.50
2:TA:856:GLU:OE1	2:TA:856:GLU:N	2.41	0.50
3:J:157:VAL:HG21	5:KA:57:TYR:CZ	2.47	0.50
3:P:339:ASP:O	3:P:342:ASP:N	2.43	0.50
1:T:145:GLY:N	1:T:168:TYR:O	2.45	0.50
3:W:157:VAL:HG21	5:WA:57:TYR:CZ	2.47	0.50
3:W:759:GLN:OE1	3:W:762:ARG:NE	2.40	0.50
5:Y:90:LEU:HD11	5:Y:138:PHE:CE2	2.46	0.50
2:BA:611:MET:HA	2:BA:611:MET:HE2	1.93	0.50
2:NA:531:LEU:HD21	2:NA:578:TYR:CZ	2.46	0.50
3:OA:339:ASP:O	3:OA:342:ASP:N	2.43	0.50
1:SA:145:GLY:N	1:SA:168:TYR:O	2.45	0.50
5:WA:90:LEU:HD11	5:WA:138:PHE:CE2	2.46	0.50
3:D:402:LEU:HD23	3:D:402:LEU:O	2.11	0.50
5:F:57:TYR:CZ	3:OA:157:VAL:HG21	2.47	0.50
2:I:856:GLU:OE1	2:I:856:GLU:N	2.41	0.50
3:J:337:THR:OG1	3:J:338:SER:N	2.43	0.50
2:BA:531:LEU:HD21	2:BA:578:TYR:CZ	2.46	0.50
2:NA:237:LEU:O	2:NA:237:LEU:HD23	2.11	0.50
5:QA:97:LEU:HD11	5:QA:143:THR:HG23	1.91	0.50
2:C:531:LEU:HD21	2:C:578:TYR:CZ	2.46	0.50
4:K:103:LEU:C	4:K:104:LEU:HD12	2.36	0.50
1:N:145:GLY:N	1:N:168:TYR:O	2.45	0.50
2:O:237:LEU:HD23	2:O:237:LEU:O	2.11	0.50
2:O:611:MET:HA	2:O:611:MET:HE2	1.93	0.50
3:P:886:VAL:O	3:P:886:VAL:HG23	2.12	0.50
3:CA:402:LEU:HD23	3:CA:402:LEU:O	2.11	0.50
2:HA:856:GLU:OE1	2:HA:856:GLU:N	2.41	0.50
4:JA:103:LEU:C	4:JA:104:LEU:HD12	2.36	0.50
1:LA:29:GLY:O	1:MA:40:ARG:NH1	2.43	0.50
1:MA:145:GLY:N	1:MA:168:TYR:O	2.45	0.50
3:OA:886:VAL:HG23	3:OA:886:VAL:O	2.12	0.50
3:UA:759:GLN:OE1	3:UA:762:ARG:NE	2.40	0.50
3:P:402:LEU:HD23	3:P:402:LEU:O	2.11	0.50
5:Y:57:TYR:CZ	3:UA:157:VAL:HG21	2.47	0.50
3:CA:886:VAL:O	3:CA:886:VAL:HG23	2.12	0.50
3:IA:337:THR:OG1	3:IA:338:SER:N	2.43	0.50
2:NA:611:MET:HE2	2:NA:611:MET:HA	1.93	0.50
2:TA:531:LEU:HD21	2:TA:578:TYR:CZ	2.46	0.50
2:C:1087:GLU:OE2	3:D:548:SER:OG	2.18	0.50
3:D:886:VAL:HG23	3:D:886:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:29:GLY:O	1:N:40:ARG:NH1	2.43	0.50
5:R:97:LEU:HD11	5:R:143:THR:HG23	1.91	0.50
3:W:93:GLY:O	3:W:319:VAL:N	2.41	0.50
3:W:402:LEU:HD23	3:W:402:LEU:O	2.11	0.50
5:QA:95:LEU:HA	5:QA:98:VAL:HG12	1.93	0.50
3:UA:886:VAL:HG23	3:UA:886:VAL:O	2.12	0.50
5:WA:131:ASP:OD2	5:WA:133:THR:OG1	2.18	0.50
2:O:420:ILE:HD12	2:O:420:ILE:N	2.27	0.50
5:R:95:LEU:HA	5:R:98:VAL:HG12	1.93	0.50
2:V:531:LEU:HD21	2:V:578:TYR:CZ	2.46	0.50
3:W:886:VAL:HG23	3:W:886:VAL:O	2.12	0.50
2:NA:420:ILE:N	2:NA:420:ILE:HD12	2.27	0.50
3:OA:402:LEU:HD23	3:OA:402:LEU:O	2.11	0.50
5:F:97:LEU:HD11	5:F:143:THR:HG23	1.91	0.49
2:O:856:GLU:OE1	2:O:856:GLU:N	2.41	0.49
5:R:57:TYR:CZ	3:CA:157:VAL:HG21	2.47	0.49
5:EA:95:LEU:HA	5:EA:98:VAL:HG12	1.93	0.49
1:GA:145:GLY:N	1:GA:168:TYR:O	2.45	0.49
3:UA:402:LEU:HD23	3:UA:402:LEU:O	2.11	0.49
3:D:157:VAL:HG21	5:QA:57:TYR:CZ	2.47	0.49
5:F:95:LEU:HA	5:F:98:VAL:HG12	1.93	0.49
1:H:145:GLY:N	1:H:168:TYR:O	2.45	0.49
2:O:789:ILE:HD12	2:O:850:ILE:HD12	1.94	0.49
2:V:789:ILE:HD12	2:V:850:ILE:HD12	1.94	0.49
5:Y:95:LEU:HA	5:Y:98:VAL:HG12	1.93	0.49
4:DA:103:LEU:C	4:DA:104:LEU:HD12	2.36	0.49
5:EA:97:LEU:HD11	5:EA:143:THR:HG23	1.91	0.49
2:NA:789:ILE:HD12	2:NA:850:ILE:HD12	1.94	0.49
2:TA:789:ILE:HD12	2:TA:850:ILE:HD12	1.94	0.49
3:UA:93:GLY:O	3:UA:319:VAL:N	2.41	0.49
3:UA:269:ASP:OD1	3:UA:270:ILE:N	2.44	0.49
5:WA:95:LEU:HA	5:WA:98:VAL:HG12	1.93	0.49
4:E:103:LEU:C	4:E:104:LEU:HD12	2.36	0.49
2:I:727:GLU:N	2:I:727:GLU:OE1	2.46	0.49
4:Q:103:LEU:C	4:Q:104:LEU:HD12	2.36	0.49
3:W:269:ASP:OD1	3:W:270:ILE:N	2.44	0.49
5:Y:131:ASP:OD2	5:Y:133:THR:OG1	2.18	0.49
2:HA:727:GLU:OE1	2:HA:727:GLU:N	2.46	0.49
2:NA:1051:MET:SD	2:NA:1051:MET:N	2.79	0.49
4:PA:103:LEU:C	4:PA:104:LEU:HD12	2.36	0.49
3:UA:221:ASP:O	3:UA:225:THR:OG1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:402:LEU:HD23	3:J:402:LEU:O	2.11	0.49
3:W:223:TRP:O	3:W:226:PHE:N	2.45	0.49
2:BA:1087:GLU:OE2	3:CA:548:SER:OG	2.18	0.49
3:CA:1084:GLN:OE1	3:CA:1084:GLN:N	2.45	0.49
2:NA:856:GLU:OE1	2:NA:856:GLU:N	2.41	0.49
3:UA:223:TRP:O	3:UA:226:PHE:N	2.45	0.49
3:UA:1084:GLN:OE1	3:UA:1084:GLN:N	2.45	0.49
2:C:789:ILE:HD12	2:C:850:ILE:HD12	1.94	0.49
3:D:1084:GLN:OE1	3:D:1084:GLN:N	2.45	0.49
2:I:420:ILE:HD12	2:I:420:ILE:N	2.27	0.49
2:O:727:GLU:OE1	2:O:727:GLU:N	2.46	0.49
3:W:221:ASP:O	3:W:225:THR:OG1	2.26	0.49
3:W:1084:GLN:OE1	3:W:1084:GLN:N	2.45	0.49
2:BA:789:ILE:HD12	2:BA:850:ILE:HD12	1.94	0.49
3:IA:402:LEU:HD23	3:IA:402:LEU:O	2.11	0.49
2:NA:727:GLU:OE1	2:NA:727:GLU:N	2.46	0.49
2:C:727:GLU:OE1	2:C:727:GLU:N	2.46	0.49
3:D:269:ASP:OD1	3:D:270:ILE:N	2.44	0.49
3:J:886:VAL:HG23	3:J:886:VAL:O	2.12	0.49
3:CA:269:ASP:OD1	3:CA:270:ILE:N	2.44	0.49
2:HA:420:ILE:HD12	2:HA:420:ILE:N	2.27	0.49
2:C:420:ILE:N	2:C:420:ILE:HD12	2.27	0.49
3:D:381:LEU:HD23	3:D:381:LEU:C	2.38	0.49
2:I:789:ILE:HD12	2:I:850:ILE:HD12	1.94	0.49
3:W:75:CYS:O	3:W:79:GLY:N	2.43	0.49
2:BA:420:ILE:HD12	2:BA:420:ILE:N	2.27	0.49
2:BA:727:GLU:OE1	2:BA:727:GLU:N	2.46	0.49
3:CA:381:LEU:HD23	3:CA:381:LEU:C	2.38	0.49
2:C:1136:GLU:OE1	3:D:11:ARG:NE	2.46	0.49
1:H:12:ASP:OD1	1:H:13:VAL:N	2.46	0.49
3:J:1084:GLN:OE1	3:J:1084:GLN:N	2.45	0.49
2:V:420:ILE:N	2:V:420:ILE:HD12	2.27	0.49
2:HA:789:ILE:HD12	2:HA:850:ILE:HD12	1.94	0.49
3:IA:886:VAL:HG23	3:IA:886:VAL:O	2.12	0.49
2:NA:521:ASP:OD1	2:NA:523:VAL:HG12	2.13	0.49
3:OA:381:LEU:HD23	3:OA:381:LEU:C	2.38	0.49
3:UA:75:CYS:O	3:UA:79:GLY:N	2.43	0.49
5:F:90:LEU:HD11	5:F:138:PHE:HE2	1.78	0.49
5:L:90:LEU:HD11	5:L:138:PHE:HE2	1.78	0.49
2:O:521:ASP:OD1	2:O:523:VAL:HG12	2.13	0.49
3:P:381:LEU:HD23	3:P:381:LEU:C	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:12:ASP:OD1	1:T:13:VAL:N	2.46	0.49
2:V:727:GLU:N	2:V:727:GLU:OE1	2.46	0.49
2:BA:1136:GLU:OE1	3:CA:11:ARG:NE	2.46	0.49
3:CA:223:TRP:O	3:CA:226:PHE:N	2.45	0.49
1:GA:12:ASP:OD1	1:GA:13:VAL:N	2.46	0.49
3:IA:1084:GLN:N	3:IA:1084:GLN:OE1	2.45	0.49
4:JA:41:ASP:OD1	4:JA:41:ASP:N	2.45	0.49
2:TA:420:ILE:HD12	2:TA:420:ILE:N	2.27	0.49
3:UA:118:LEU:HD21	3:UA:264:LEU:HD23	1.95	0.49
3:J:118:LEU:HD21	3:J:264:LEU:HD23	1.95	0.49
3:W:118:LEU:HD21	3:W:264:LEU:HD23	1.95	0.49
5:EA:90:LEU:HD11	5:EA:138:PHE:HE2	1.78	0.49
5:KA:90:LEU:HD11	5:KA:138:PHE:HE2	1.78	0.49
1:SA:12:ASP:OD1	1:SA:13:VAL:N	2.46	0.49
2:TA:727:GLU:N	2:TA:727:GLU:OE1	2.46	0.49
3:D:223:TRP:O	3:D:226:PHE:N	2.45	0.48
3:J:75:CYS:O	3:J:79:GLY:N	2.43	0.48
3:J:93:GLY:O	3:J:319:VAL:N	2.41	0.48
4:K:41:ASP:N	4:K:41:ASP:OD1	2.45	0.48
3:P:1084:GLN:OE1	3:P:1084:GLN:N	2.45	0.48
5:R:90:LEU:HD11	5:R:138:PHE:HE2	1.78	0.48
2:V:521:ASP:OD1	2:V:523:VAL:HG12	2.13	0.48
5:Y:108:ARG:CB	5:Y:154:MET:HE2	2.43	0.48
4:DA:41:ASP:OD1	4:DA:41:ASP:N	2.45	0.48
3:IA:118:LEU:HD21	3:IA:264:LEU:HD23	1.95	0.48
2:NA:1136:GLU:OE1	3:OA:11:ARG:NE	2.46	0.48
3:OA:505:HIS:NE2	3:OA:531:ALA:O	2.46	0.48
3:OA:1084:GLN:OE1	3:OA:1084:GLN:N	2.45	0.48
2:TA:831:GLU:OE1	2:TA:831:GLU:N	2.44	0.48
2:C:521:ASP:OD1	2:C:523:VAL:HG12	2.13	0.48
3:J:759:GLN:OE1	3:J:762:ARG:NE	2.40	0.48
3:P:505:HIS:NE2	3:P:531:ALA:O	2.46	0.48
2:BA:521:ASP:OD1	2:BA:523:VAL:HG12	2.13	0.48
3:CA:505:HIS:NE2	3:CA:531:ALA:O	2.46	0.48
5:QA:90:LEU:HD11	5:QA:138:PHE:HE2	1.78	0.48
2:TA:521:ASP:OD1	2:TA:523:VAL:HG12	2.13	0.48
3:UA:381:LEU:HD23	3:UA:381:LEU:C	2.38	0.48
5:WA:108:ARG:CB	5:WA:154:MET:HE2	2.43	0.48
2:C:831:GLU:OE1	2:C:831:GLU:N	2.44	0.48
3:D:505:HIS:NE2	3:D:531:ALA:O	2.46	0.48
3:D:759:GLN:OE1	3:D:762:ARG:NE	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:41:ASP:N	4:E:41:ASP:OD1	2.45	0.48
5:F:108:ARG:CB	5:F:154:MET:HE2	2.43	0.48
2:V:831:GLU:OE1	2:V:831:GLU:N	2.44	0.48
3:W:381:LEU:HD23	3:W:381:LEU:C	2.38	0.48
5:Y:46:VAL:HG23	5:Y:47:GLU:N	2.29	0.48
5:Y:90:LEU:HD11	5:Y:138:PHE:HE2	1.78	0.48
3:CA:759:GLN:OE1	3:CA:762:ARG:NE	2.40	0.48
5:EA:108:ARG:CB	5:EA:154:MET:HE2	2.43	0.48
3:IA:75:CYS:O	3:IA:79:GLY:N	2.43	0.48
5:KA:46:VAL:HG23	5:KA:47:GLU:N	2.29	0.48
1:B:12:ASP:OD1	1:B:13:VAL:N	2.46	0.48
5:L:46:VAL:HG23	5:L:47:GLU:N	2.29	0.48
1:N:12:ASP:OD1	1:N:13:VAL:N	2.46	0.48
3:P:886:VAL:HG23	3:P:992:GLY:H	1.79	0.48
3:IA:381:LEU:C	3:IA:381:LEU:HD23	2.38	0.48
1:MA:12:ASP:OD1	1:MA:13:VAL:N	2.46	0.48
3:OA:886:VAL:HG23	3:OA:992:GLY:H	1.79	0.48
2:TA:716:GLY:N	2:TA:1029:TYR:OH	2.43	0.48
5:WA:46:VAL:HG23	5:WA:47:GLU:N	2.29	0.48
5:WA:90:LEU:HD11	5:WA:138:PHE:HE2	1.78	0.48
2:C:520:VAL:HG23	2:C:521:ASP:N	2.29	0.48
2:I:1136:GLU:OE1	3:J:11:ARG:NE	2.46	0.48
3:J:381:LEU:HD23	3:J:381:LEU:C	2.38	0.48
3:P:217:ASP:OD1	3:P:218:ARG:N	2.47	0.48
1:AA:12:ASP:OD1	1:AA:13:VAL:N	2.46	0.48
2:BA:520:VAL:HG23	2:BA:521:ASP:N	2.29	0.48
3:IA:93:GLY:O	3:IA:319:VAL:N	2.41	0.48
3:OA:217:ASP:OD1	3:OA:218:ARG:N	2.47	0.48
2:C:606:LEU:HD23	2:C:606:LEU:C	2.39	0.48
2:C:763:LYS:NZ	3:D:331:ASP:O	2.46	0.48
3:D:75:CYS:O	3:D:79:GLY:N	2.43	0.48
3:D:118:LEU:HD21	3:D:264:LEU:HD23	1.95	0.48
3:D:217:ASP:OD1	3:D:218:ARG:N	2.47	0.48
4:Q:41:ASP:OD1	4:Q:41:ASP:N	2.45	0.48
5:R:46:VAL:HG23	5:R:47:GLU:N	2.29	0.48
2:V:716:GLY:N	2:V:1029:TYR:OH	2.43	0.48
2:V:763:LYS:NZ	3:W:331:ASP:O	2.46	0.48
2:BA:763:LYS:NZ	3:CA:331:ASP:O	2.46	0.48
3:CA:118:LEU:HD21	3:CA:264:LEU:HD23	1.95	0.48
3:CA:217:ASP:OD1	3:CA:218:ARG:N	2.47	0.48
2:HA:716:GLY:N	2:HA:1029:TYR:OH	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HA:1136:GLU:OE1	3:IA:11:ARG:NE	2.46	0.48
3:IA:759:GLN:OE1	3:IA:762:ARG:NE	2.40	0.48
5:F:46:VAL:HG23	5:F:47:GLU:N	2.29	0.48
2:I:716:GLY:N	2:I:1029:TYR:OH	2.43	0.48
2:I:787:ARG:NH2	2:I:789:ILE:HD11	2.29	0.48
3:P:118:LEU:HD21	3:P:264:LEU:HD23	1.95	0.48
2:V:520:VAL:HG23	2:V:521:ASP:N	2.29	0.48
3:W:240:LEU:O	3:W:244:LEU:HD23	2.14	0.48
2:BA:606:LEU:HD23	2:BA:606:LEU:C	2.39	0.48
5:EA:46:VAL:HG23	5:EA:47:GLU:N	2.29	0.48
2:HA:521:ASP:OD1	2:HA:523:VAL:HG12	2.13	0.48
2:HA:787:ARG:NH2	2:HA:789:ILE:HD11	2.29	0.48
3:IA:886:VAL:HG23	3:IA:992:GLY:H	1.79	0.48
3:OA:223:TRP:O	3:OA:226:PHE:N	2.45	0.48
2:TA:520:VAL:HG23	2:TA:521:ASP:N	2.29	0.48
2:TA:763:LYS:NZ	3:UA:331:ASP:O	2.46	0.48
2:C:729:HIS:HB2	2:C:736:ILE:HD11	1.96	0.48
2:I:521:ASP:OD1	2:I:523:VAL:HG12	2.13	0.48
5:L:108:ARG:CB	5:L:154:MET:HE2	2.43	0.48
2:O:366:GLU:OE1	2:O:366:GLU:N	2.47	0.48
2:V:606:LEU:HD23	2:V:606:LEU:C	2.39	0.48
4:X:41:ASP:OD1	4:X:41:ASP:N	2.45	0.48
5:KA:108:ARG:CB	5:KA:154:MET:HE2	2.43	0.48
3:OA:118:LEU:HD21	3:OA:264:LEU:HD23	1.95	0.48
4:PA:41:ASP:N	4:PA:41:ASP:OD1	2.45	0.48
2:TA:606:LEU:C	2:TA:606:LEU:HD23	2.39	0.48
3:UA:240:LEU:O	3:UA:244:LEU:HD23	2.14	0.48
4:VA:41:ASP:OD1	4:VA:41:ASP:N	2.45	0.48
3:J:217:ASP:OD1	3:J:218:ARG:N	2.47	0.48
3:J:886:VAL:HG23	3:J:992:GLY:H	1.79	0.48
3:P:223:TRP:O	3:P:226:PHE:N	2.45	0.48
2:BA:729:HIS:HB2	2:BA:736:ILE:HD11	1.96	0.48
3:CA:75:CYS:O	3:CA:79:GLY:N	2.43	0.48
3:IA:217:ASP:OD1	3:IA:218:ARG:N	2.47	0.48
2:NA:366:GLU:N	2:NA:366:GLU:OE1	2.47	0.48
2:C:366:GLU:OE1	2:C:366:GLU:N	2.47	0.48
2:I:469:GLY:O	2:I:472:VAL:HG12	2.14	0.48
2:O:729:HIS:HB2	2:O:736:ILE:HD11	1.96	0.48
2:V:53:LEU:O	2:V:453:ARG:NH2	2.47	0.48
2:BA:366:GLU:OE1	2:BA:366:GLU:N	2.47	0.48
3:CA:240:LEU:O	3:CA:244:LEU:HD23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HA:469:GLY:O	2:HA:472:VAL:HG12	2.14	0.48
2:NA:729:HIS:HB2	2:NA:736:ILE:HD11	1.96	0.48
2:TA:53:LEU:O	2:TA:453:ARG:NH2	2.47	0.48
2:TA:366:GLU:OE1	2:TA:366:GLU:N	2.47	0.48
2:TA:729:HIS:HB2	2:TA:736:ILE:HD11	1.96	0.48
3:D:240:LEU:O	3:D:244:LEU:HD23	2.14	0.47
3:D:1167:ILE:O	3:D:1178:GLY:N	2.45	0.47
2:I:307:ASP:C	2:I:308:LEU:HD12	2.39	0.47
2:I:763:LYS:NZ	3:J:331:ASP:O	2.46	0.47
3:J:240:LEU:O	3:J:244:LEU:HD23	2.14	0.47
2:O:520:VAL:HG23	2:O:521:ASP:N	2.29	0.47
2:O:763:LYS:NZ	3:P:331:ASP:O	2.46	0.47
2:V:366:GLU:OE1	2:V:366:GLU:N	2.47	0.47
2:V:729:HIS:HB2	2:V:736:ILE:HD11	1.96	0.47
2:HA:729:HIS:HB2	2:HA:736:ILE:HD11	1.96	0.47
3:IA:240:LEU:O	3:IA:244:LEU:HD23	2.14	0.47
2:NA:520:VAL:HG23	2:NA:521:ASP:N	2.29	0.47
2:NA:606:LEU:HD23	2:NA:606:LEU:C	2.39	0.47
2:TA:787:ARG:NH2	2:TA:789:ILE:HD11	2.29	0.47
2:I:729:HIS:HB2	2:I:736:ILE:HD11	1.96	0.47
2:O:606:LEU:HD23	2:O:606:LEU:C	2.39	0.47
2:V:787:ARG:NH2	2:V:789:ILE:HD11	2.29	0.47
2:BA:53:LEU:O	2:BA:453:ARG:NH2	2.47	0.47
2:HA:763:LYS:NZ	3:IA:331:ASP:O	2.46	0.47
2:NA:763:LYS:NZ	3:OA:331:ASP:O	2.46	0.47
2:NA:787:ARG:NH2	2:NA:789:ILE:HD11	2.29	0.47
3:UA:217:ASP:OD1	3:UA:218:ARG:N	2.47	0.47
2:C:53:LEU:O	2:C:453:ARG:NH2	2.47	0.47
2:I:675:PHE:N	2:I:685:ASN:OD1	2.41	0.47
5:L:97:LEU:HD21	5:L:143:THR:CG2	2.41	0.47
2:O:469:GLY:O	2:O:472:VAL:HG12	2.14	0.47
2:O:675:PHE:N	2:O:685:ASN:OD1	2.41	0.47
2:O:787:ARG:NH2	2:O:789:ILE:HD11	2.29	0.47
3:W:217:ASP:OD1	3:W:218:ARG:N	2.47	0.47
3:CA:877:LEU:O	3:CA:880:VAL:HG12	2.15	0.47
2:HA:307:ASP:C	2:HA:308:LEU:HD12	2.39	0.47
2:TA:1136:GLU:OE1	3:UA:11:ARG:NE	2.46	0.47
3:D:877:LEU:O	3:D:880:VAL:HG12	2.15	0.47
2:I:487:GLU:O	2:I:488:THR:OG1	2.31	0.47
2:I:520:VAL:HG23	2:I:521:ASP:N	2.29	0.47
5:L:101:LEU:HD12	5:L:146:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:101:LEU:HD12	5:R:146:ILE:HD11	1.97	0.47
5:R:108:ARG:CB	5:R:154:MET:HE2	2.43	0.47
3:W:343:LEU:HD13	3:W:381:LEU:HA	1.97	0.47
3:W:1003:ILE:HD11	3:W:1142:TYR:CE2	2.50	0.47
3:CA:886:VAL:HG23	3:CA:992:GLY:H	1.79	0.47
5:KA:97:LEU:HD21	5:KA:143:THR:CG2	2.41	0.47
5:KA:101:LEU:HD12	5:KA:146:ILE:HD11	1.97	0.47
2:NA:307:ASP:C	2:NA:308:LEU:HD12	2.39	0.47
2:NA:469:GLY:O	2:NA:472:VAL:HG12	2.14	0.47
3:OA:319:VAL:HG12	3:OA:344:TYR:CE1	2.50	0.47
5:QA:108:ARG:CB	5:QA:154:MET:HE2	2.43	0.47
3:UA:343:LEU:HD13	3:UA:381:LEU:HA	1.97	0.47
3:UA:1003:ILE:HD11	3:UA:1142:TYR:CE2	2.50	0.47
3:D:1003:ILE:HD11	3:D:1142:TYR:CE2	2.50	0.47
3:J:366:ILE:HG12	5:L:120:ASN:OD1	2.15	0.47
3:J:877:LEU:O	3:J:880:VAL:HG12	2.15	0.47
3:J:1003:ILE:HD11	3:J:1142:TYR:CE2	2.50	0.47
2:O:53:LEU:O	2:O:453:ARG:NH2	2.47	0.47
2:O:307:ASP:C	2:O:308:LEU:HD12	2.39	0.47
3:P:111:PRO:O	3:P:113:ARG:NH1	2.43	0.47
3:P:319:VAL:HG12	3:P:344:TYR:CE1	2.50	0.47
3:CA:1003:ILE:HD11	3:CA:1142:TYR:CE2	2.50	0.47
2:HA:366:GLU:N	2:HA:366:GLU:OE1	2.47	0.47
2:HA:520:VAL:HG23	2:HA:521:ASP:N	2.29	0.47
2:HA:606:LEU:HD23	2:HA:606:LEU:C	2.39	0.47
2:HA:675:PHE:N	2:HA:685:ASN:OD1	2.41	0.47
3:IA:877:LEU:O	3:IA:880:VAL:HG12	2.15	0.47
3:IA:1003:ILE:HD11	3:IA:1142:TYR:CE2	2.50	0.47
5:KA:97:LEU:HD11	5:KA:143:THR:HG22	1.96	0.47
2:NA:675:PHE:N	2:NA:685:ASN:OD1	2.41	0.47
2:NA:716:GLY:N	2:NA:1029:TYR:OH	2.43	0.47
5:QA:101:LEU:HD12	5:QA:146:ILE:HD11	1.97	0.47
3:D:886:VAL:HG23	3:D:992:GLY:H	1.79	0.47
2:I:366:GLU:OE1	2:I:366:GLU:N	2.47	0.47
5:L:97:LEU:HD11	5:L:143:THR:HG22	1.96	0.47
2:O:716:GLY:N	2:O:1029:TYR:OH	2.43	0.47
3:IA:366:ILE:HG12	5:KA:120:ASN:OD1	2.15	0.47
2:NA:53:LEU:O	2:NA:453:ARG:NH2	2.47	0.47
3:OA:111:PRO:O	3:OA:113:ARG:NH1	2.43	0.47
2:C:307:ASP:C	2:C:308:LEU:HD12	2.39	0.47
2:C:787:ARG:NH2	2:C:789:ILE:HD11	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:343:LEU:HD13	3:D:381:LEU:HA	1.97	0.47
3:D:366:ILE:HG12	5:F:120:ASN:OD1	2.15	0.47
3:D:1024:ILE:HD12	3:D:1024:ILE:N	2.30	0.47
2:I:606:LEU:C	2:I:606:LEU:HD23	2.39	0.47
2:I:772:ASP:OD1	2:I:773:ILE:N	2.48	0.47
3:J:1024:ILE:HD12	3:J:1024:ILE:N	2.30	0.47
2:O:1051:MET:SD	2:O:1051:MET:N	2.79	0.47
3:P:759:GLN:OE1	3:P:762:ARG:NE	2.40	0.47
3:W:886:VAL:HG23	3:W:992:GLY:H	1.79	0.47
2:BA:307:ASP:C	2:BA:308:LEU:HD12	2.39	0.47
2:BA:787:ARG:NH2	2:BA:789:ILE:HD11	2.29	0.47
3:CA:343:LEU:HD13	3:CA:381:LEU:HA	1.97	0.47
3:CA:366:ILE:HG12	5:EA:120:ASN:OD1	2.15	0.47
3:CA:1024:ILE:HD12	3:CA:1024:ILE:N	2.30	0.47
2:HA:53:LEU:O	2:HA:453:ARG:NH2	2.47	0.47
3:IA:1024:ILE:N	3:IA:1024:ILE:HD12	2.30	0.47
3:UA:886:VAL:HG23	3:UA:992:GLY:H	1.79	0.47
2:I:53:LEU:O	2:I:453:ARG:NH2	2.47	0.47
3:P:366:ILE:HG12	5:R:120:ASN:OD1	2.15	0.47
3:P:1155:GLU:HA	3:P:1158:VAL:HG22	1.97	0.47
2:V:307:ASP:C	2:V:308:LEU:HD12	2.39	0.47
2:HA:772:ASP:OD1	2:HA:773:ILE:N	2.48	0.47
3:OA:877:LEU:O	3:OA:880:VAL:HG12	2.15	0.47
3:P:877:LEU:O	3:P:880:VAL:HG12	2.15	0.47
2:V:1136:GLU:OE1	3:W:11:ARG:NE	2.46	0.47
3:W:1155:GLU:HA	3:W:1158:VAL:HG22	1.97	0.47
2:NA:831:GLU:OE1	2:NA:831:GLU:N	2.44	0.47
2:NA:1136:GLU:OE1	3:OA:11:ARG:NH2	2.47	0.47
3:OA:240:LEU:O	3:OA:244:LEU:HD23	2.14	0.47
3:OA:366:ILE:HG12	5:QA:120:ASN:OD1	2.15	0.47
3:OA:1024:ILE:HD12	3:OA:1024:ILE:N	2.30	0.47
3:OA:1155:GLU:HA	3:OA:1158:VAL:HG22	1.97	0.47
2:TA:307:ASP:C	2:TA:308:LEU:HD12	2.39	0.47
3:P:104:ILE:HB	3:P:379:ASP:OD1	2.15	0.47
3:P:1024:ILE:N	3:P:1024:ILE:HD12	2.30	0.47
5:R:97:LEU:HD21	5:R:143:THR:CG2	2.41	0.47
3:CA:93:GLY:O	3:CA:319:VAL:N	2.41	0.47
1:FA:29:GLY:O	1:GA:40:ARG:NH1	2.43	0.47
3:OA:104:ILE:HB	3:OA:379:ASP:OD1	2.15	0.47
3:UA:1155:GLU:HA	3:UA:1158:VAL:HG22	1.97	0.47
3:D:93:GLY:O	3:D:319:VAL:N	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:101:LEU:HD12	5:F:146:ILE:HD11	1.97	0.46
2:O:1131:LEU:CD2	3:P:402:LEU:HD22	2.44	0.46
2:O:1136:GLU:OE1	3:P:11:ARG:NH2	2.47	0.46
3:P:240:LEU:O	3:P:244:LEU:HD23	2.14	0.46
3:W:319:VAL:HG12	3:W:344:TYR:CE1	2.50	0.46
5:Y:101:LEU:HD12	5:Y:146:ILE:HD11	1.97	0.46
3:CA:319:VAL:HG12	3:CA:344:TYR:CE1	2.50	0.46
1:GA:18:ARG:O	1:GA:19:SER:OG	2.30	0.46
3:OA:759:GLN:OE1	3:OA:762:ARG:NE	2.40	0.46
5:QA:97:LEU:HD21	5:QA:143:THR:CG2	2.41	0.46
3:UA:319:VAL:HG12	3:UA:344:TYR:CE1	2.50	0.46
5:WA:101:LEU:HD12	5:WA:146:ILE:HD11	1.97	0.46
3:D:319:VAL:HG12	3:D:344:TYR:CE1	2.50	0.46
1:H:18:ARG:O	1:H:19:SER:OG	2.30	0.46
2:O:831:GLU:OE1	2:O:831:GLU:N	2.44	0.46
2:V:772:ASP:OD1	2:V:773:ILE:N	2.48	0.46
3:W:159:ARG:HA	3:W:162:VAL:HG12	1.98	0.46
3:CA:104:ILE:HB	3:CA:379:ASP:OD1	2.15	0.46
3:CA:1155:GLU:HA	3:CA:1158:VAL:HG22	1.97	0.46
5:EA:101:LEU:HD12	5:EA:146:ILE:HD11	1.97	0.46
3:OA:134:TYR:CD1	3:OA:134:TYR:N	2.83	0.46
5:QA:46:VAL:HG23	5:QA:47:GLU:N	2.29	0.46
2:TA:772:ASP:OD1	2:TA:773:ILE:N	2.48	0.46
1:B:72:ASP:OD1	1:B:73:VAL:N	2.46	0.46
3:D:104:ILE:HB	3:D:379:ASP:OD1	2.15	0.46
3:D:821:LYS:HB3	3:D:836:VAL:HG21	1.97	0.46
3:D:1155:GLU:HA	3:D:1158:VAL:HG22	1.97	0.46
1:G:29:GLY:O	1:H:40:ARG:NH1	2.43	0.46
3:P:134:TYR:CD1	3:P:134:TYR:N	2.83	0.46
1:AA:72:ASP:OD1	1:AA:73:VAL:N	2.46	0.46
2:BA:469:GLY:O	2:BA:472:VAL:HG12	2.14	0.46
3:CA:159:ARG:HA	3:CA:162:VAL:HG12	1.98	0.46
3:CA:821:LYS:HB3	3:CA:836:VAL:HG21	1.97	0.46
2:NA:1131:LEU:CD2	3:OA:402:LEU:HD22	2.44	0.46
3:UA:159:ARG:HA	3:UA:162:VAL:HG12	1.98	0.46
3:UA:1024:ILE:HD12	3:UA:1024:ILE:N	2.30	0.46
2:C:469:GLY:O	2:C:472:VAL:HG12	2.14	0.46
3:D:159:ARG:HA	3:D:162:VAL:HG12	1.98	0.46
2:O:772:ASP:OD1	2:O:773:ILE:N	2.48	0.46
3:W:1024:ILE:HD12	3:W:1024:ILE:N	2.30	0.46
3:IA:134:TYR:CD1	3:IA:134:TYR:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:IA:505:HIS:NE2	3:IA:531:ALA:O	2.46	0.46
3:IA:1155:GLU:HA	3:IA:1158:VAL:HG22	1.97	0.46
2:NA:772:ASP:OD1	2:NA:773:ILE:N	2.48	0.46
3:J:134:TYR:CD1	3:J:134:TYR:N	2.83	0.46
3:J:343:LEU:HD13	3:J:381:LEU:HA	1.97	0.46
3:J:1155:GLU:HA	3:J:1158:VAL:HG22	1.97	0.46
3:P:821:LYS:HB3	3:P:836:VAL:HG21	1.97	0.46
3:P:1003:ILE:HD11	3:P:1142:TYR:CE2	2.50	0.46
3:P:1246:ASN:N	3:P:1250:GLU:OE2	2.49	0.46
5:R:97:LEU:HD11	5:R:143:THR:HG22	1.96	0.46
3:IA:343:LEU:HD13	3:IA:381:LEU:HA	1.97	0.46
5:QA:97:LEU:HD11	5:QA:143:THR:HG22	1.96	0.46
5:F:108:ARG:CB	5:F:154:MET:CE	2.94	0.46
3:J:159:ARG:HA	3:J:162:VAL:HG12	1.98	0.46
3:J:505:HIS:NE2	3:J:531:ALA:O	2.46	0.46
5:EA:108:ARG:CB	5:EA:154:MET:CE	2.94	0.46
2:HA:1136:GLU:OE1	3:IA:11:ARG:NH2	2.47	0.46
3:IA:159:ARG:HA	3:IA:162:VAL:HG12	1.98	0.46
3:OA:343:LEU:HD13	3:OA:381:LEU:HA	1.97	0.46
3:OA:821:LYS:HB3	3:OA:836:VAL:HG21	1.97	0.46
3:OA:1246:ASN:N	3:OA:1250:GLU:OE2	2.49	0.46
2:I:1087:GLU:OE2	3:J:548:SER:OG	2.18	0.46
3:P:343:LEU:HD13	3:P:381:LEU:HA	1.97	0.46
3:W:104:ILE:HD12	3:W:379:ASP:HB3	1.98	0.46
1:MA:72:ASP:OD1	1:MA:73:VAL:N	2.46	0.46
3:OA:1003:ILE:HD11	3:OA:1142:TYR:CE2	2.50	0.46
3:UA:877:LEU:O	3:UA:880:VAL:HG12	2.15	0.46
1:B:99:LYS:HD2	1:B:105:VAL:HG12	1.98	0.46
2:C:675:PHE:N	2:C:685:ASN:OD1	2.41	0.46
2:I:1112:ILE:HD12	2:I:1112:ILE:N	2.31	0.46
3:J:319:VAL:HG12	3:J:344:TYR:CE1	2.50	0.46
5:L:108:ARG:CB	5:L:154:MET:CE	2.94	0.46
2:O:1136:GLU:OE1	3:P:11:ARG:NE	2.46	0.46
3:W:877:LEU:O	3:W:880:VAL:HG12	2.15	0.46
3:W:1246:ASN:N	3:W:1250:GLU:OE2	2.49	0.46
1:AA:99:LYS:HD2	1:AA:105:VAL:HG12	1.98	0.46
2:BA:772:ASP:OD1	2:BA:773:ILE:N	2.48	0.46
5:KA:108:ARG:CB	5:KA:154:MET:CE	2.94	0.46
3:UA:104:ILE:HD12	3:UA:379:ASP:HB3	1.98	0.46
3:UA:1246:ASN:N	3:UA:1250:GLU:OE2	2.49	0.46
2:C:772:ASP:OD1	2:C:773:ILE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.98	0.46
5:F:97:LEU:HD11	5:F:143:THR:HG22	1.96	0.46
2:I:1136:GLU:OE1	3:J:11:ARG:NH2	2.47	0.46
1:N:72:ASP:OD1	1:N:73:VAL:N	2.46	0.46
2:O:32:VAL:CG2	2:O:35:ALA:HB2	2.46	0.46
3:P:1123:ARG:HG3	3:P:1124:VAL:HG13	1.98	0.46
2:V:32:VAL:CG2	2:V:35:ALA:HB2	2.46	0.46
2:V:675:PHE:N	2:V:685:ASN:OD1	2.41	0.46
3:W:104:ILE:HB	3:W:379:ASP:OD1	2.15	0.46
3:W:134:TYR:CD1	3:W:134:TYR:N	2.83	0.46
2:BA:675:PHE:N	2:BA:685:ASN:OD1	2.41	0.46
3:CA:104:ILE:HD12	3:CA:379:ASP:HB3	1.98	0.46
2:HA:1112:ILE:HD12	2:HA:1112:ILE:N	2.31	0.46
3:OA:1123:ARG:HG3	3:OA:1124:VAL:HG13	1.98	0.46
2:TA:32:VAL:CG2	2:TA:35:ALA:HB2	2.46	0.46
3:UA:104:ILE:HB	3:UA:379:ASP:OD1	2.15	0.46
3:D:134:TYR:CD1	3:D:134:TYR:N	2.83	0.46
3:J:821:LYS:HB3	3:J:836:VAL:HG21	1.97	0.46
3:CA:134:TYR:CD1	3:CA:134:TYR:N	2.83	0.46
2:HA:831:GLU:OE1	2:HA:831:GLU:N	2.44	0.46
3:IA:319:VAL:HG12	3:IA:344:TYR:CE1	2.50	0.46
3:IA:821:LYS:HB3	3:IA:836:VAL:HG21	1.97	0.46
2:NA:32:VAL:CG2	2:NA:35:ALA:HB2	2.46	0.46
2:TA:469:GLY:O	2:TA:472:VAL:HG12	2.14	0.46
2:TA:675:PHE:N	2:TA:685:ASN:OD1	2.41	0.46
3:UA:134:TYR:CD1	3:UA:134:TYR:N	2.83	0.46
1:G:55:ARG:N	1:G:137:GLU:O	2.50	0.45
2:I:831:GLU:OE1	2:I:831:GLU:N	2.44	0.45
2:O:1112:ILE:HD12	2:O:1112:ILE:N	2.31	0.45
2:V:469:GLY:O	2:V:472:VAL:HG12	2.14	0.45
3:W:223:TRP:O	3:W:224:SER:C	2.59	0.45
3:CA:1167:ILE:O	3:CA:1178:GLY:N	2.45	0.45
5:EA:97:LEU:HD11	5:EA:143:THR:HG22	1.96	0.45
1:FA:55:ARG:N	1:FA:137:GLU:O	2.50	0.45
3:OA:159:ARG:HA	3:OA:162:VAL:HG12	1.98	0.45
3:UA:366:ILE:HG12	5:WA:120:ASN:OD1	2.15	0.45
3:J:104:ILE:HB	3:J:379:ASP:OD1	2.15	0.45
3:P:159:ARG:HA	3:P:162:VAL:HG12	1.98	0.45
1:GA:72:ASP:OD1	1:GA:73:VAL:N	2.46	0.45
2:NA:1112:ILE:N	2:NA:1112:ILE:HD12	2.31	0.45
3:UA:223:TRP:O	3:UA:224:SER:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1136:GLU:OE1	3:D:11:ARG:NH2	2.47	0.45
2:I:475:VAL:HG12	2:I:476:HIS:N	2.32	0.45
3:W:162:VAL:O	3:W:165:GLN:HG3	2.17	0.45
3:W:366:ILE:HG12	5:Y:120:ASN:OD1	2.15	0.45
5:Y:108:ARG:CB	5:Y:154:MET:CE	2.94	0.45
2:HA:475:VAL:HG12	2:HA:476:HIS:N	2.32	0.45
3:IA:104:ILE:HB	3:IA:379:ASP:OD1	2.15	0.45
3:IA:1246:ASN:N	3:IA:1250:GLU:OE2	2.49	0.45
3:UA:162:VAL:O	3:UA:165:GLN:HG3	2.17	0.45
1:B:97:LEU:HD23	1:B:98:ARG:N	2.32	0.45
2:C:1112:ILE:N	2:C:1112:ILE:HD12	2.31	0.45
1:H:72:ASP:OD1	1:H:73:VAL:N	2.46	0.45
2:I:32:VAL:CG2	2:I:35:ALA:HB2	2.46	0.45
3:J:93:GLY:O	3:J:319:VAL:HG22	2.16	0.45
2:O:317:ASN:O	2:O:321:GLY:N	2.50	0.45
3:P:162:VAL:O	3:P:165:GLN:HG3	2.17	0.45
3:P:633:ILE:HG22	3:P:634:LYS:N	2.31	0.45
1:AA:97:LEU:HD23	1:AA:98:ARG:N	2.32	0.45
2:BA:1112:ILE:HD12	2:BA:1112:ILE:N	2.31	0.45
2:BA:1136:GLU:OE1	3:CA:11:ARG:NH2	2.47	0.45
3:CA:163:GLU:O	3:CA:166:ARG:HG3	2.17	0.45
3:IA:93:GLY:O	3:IA:319:VAL:HG22	2.16	0.45
1:MA:99:LYS:HD2	1:MA:105:VAL:HG12	1.98	0.45
2:NA:317:ASN:O	2:NA:321:GLY:N	2.50	0.45
3:OA:162:VAL:O	3:OA:165:GLN:HG3	2.17	0.45
3:OA:633:ILE:HG22	3:OA:634:LYS:N	2.31	0.45
1:SA:72:ASP:OD1	1:SA:73:VAL:N	2.46	0.45
3:UA:821:LYS:HB3	3:UA:836:VAL:HG21	1.97	0.45
5:WA:108:ARG:CB	5:WA:154:MET:CE	2.94	0.45
3:D:16:THR:N	3:D:19:ASP:OD2	2.50	0.45
3:D:22:GLN:NE2	3:D:22:GLN:O	2.50	0.45
3:D:163:GLU:O	3:D:166:ARG:HG3	2.17	0.45
3:J:1246:ASN:N	3:J:1250:GLU:OE2	2.49	0.45
1:N:99:LYS:HD2	1:N:105:VAL:HG12	1.98	0.45
2:O:475:VAL:HG12	2:O:476:HIS:N	2.32	0.45
5:R:108:ARG:CB	5:R:154:MET:CE	2.94	0.45
2:V:1131:LEU:CD2	3:W:402:LEU:HD22	2.44	0.45
3:W:633:ILE:HG22	3:W:634:LYS:N	2.31	0.45
3:W:821:LYS:HB3	3:W:836:VAL:HG21	1.97	0.45
3:CA:22:GLN:O	3:CA:22:GLN:NE2	2.50	0.45
2:HA:32:VAL:CG2	2:HA:35:ALA:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:56:LEU:O	5:F:59:GLU:HB3	2.17	0.45
3:J:163:GLU:O	3:J:166:ARG:HG3	2.17	0.45
3:P:104:ILE:HD12	3:P:379:ASP:HB3	1.98	0.45
3:P:1054:ARG:N	3:P:1065:THR:O	2.42	0.45
1:T:72:ASP:OD1	1:T:73:VAL:N	2.46	0.45
5:Y:97:LEU:HD11	5:Y:143:THR:HG22	1.96	0.45
3:CA:16:THR:N	3:CA:19:ASP:OD2	2.50	0.45
3:CA:1170:SER:O	3:CA:1173:THR:OG1	2.29	0.45
5:EA:56:LEU:O	5:EA:59:GLU:HB3	2.17	0.45
3:IA:163:GLU:O	3:IA:166:ARG:HG3	2.17	0.45
2:NA:475:VAL:HG12	2:NA:476:HIS:N	2.32	0.45
3:OA:16:THR:N	3:OA:19:ASP:OD2	2.50	0.45
3:OA:217:ASP:HA	3:OA:220:GLU:HG3	1.98	0.45
5:QA:108:ARG:CB	5:QA:154:MET:CE	2.94	0.45
2:TA:1112:ILE:N	2:TA:1112:ILE:HD12	2.31	0.45
3:UA:505:HIS:NE2	3:UA:531:ALA:O	2.46	0.45
3:UA:633:ILE:HG22	3:UA:634:LYS:N	2.31	0.45
2:C:32:VAL:CG2	2:C:35:ALA:HB2	2.46	0.45
3:D:93:GLY:O	3:D:319:VAL:HG22	2.16	0.45
3:D:1123:ARG:HG3	3:D:1124:VAL:HG13	1.98	0.45
3:J:223:TRP:O	3:J:224:SER:C	2.59	0.45
3:P:16:THR:N	3:P:19:ASP:OD2	2.50	0.45
3:P:217:ASP:HA	3:P:220:GLU:HG3	1.98	0.45
3:P:867:THR:HG23	3:P:868:ALA:N	2.32	0.45
2:V:1112:ILE:N	2:V:1112:ILE:HD12	2.31	0.45
2:BA:32:VAL:CG2	2:BA:35:ALA:HB2	2.46	0.45
3:CA:1123:ARG:HG3	3:CA:1124:VAL:HG13	1.98	0.45
3:IA:223:TRP:O	3:IA:224:SER:C	2.59	0.45
3:OA:163:GLU:O	3:OA:166:ARG:HG3	2.17	0.45
5:WA:97:LEU:HD11	5:WA:143:THR:HG22	1.96	0.45
3:J:104:ILE:HD12	3:J:379:ASP:HB3	1.98	0.45
3:J:633:ILE:HG22	3:J:634:LYS:N	2.31	0.45
3:J:867:THR:HG23	3:J:868:ALA:N	2.32	0.45
3:P:163:GLU:O	3:P:166:ARG:HG3	2.17	0.45
1:T:99:LYS:HD2	1:T:105:VAL:HG12	1.98	0.45
3:W:93:GLY:O	3:W:319:VAL:HG22	2.16	0.45
2:BA:716:GLY:N	2:BA:1029:TYR:OH	2.43	0.45
3:CA:93:GLY:O	3:CA:319:VAL:HG22	2.16	0.45
1:GA:97:LEU:HD23	1:GA:98:ARG:N	2.32	0.45
3:IA:633:ILE:HG22	3:IA:634:LYS:N	2.31	0.45
3:OA:104:ILE:HD12	3:OA:379:ASP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:OA:1054:ARG:N	3:OA:1065:THR:O	2.42	0.45
2:TA:1131:LEU:CD2	3:UA:402:LEU:HD22	2.44	0.45
3:UA:93:GLY:O	3:UA:319:VAL:HG22	2.16	0.45
2:C:270:THR:HG23	2:C:271:ASP:N	2.32	0.45
2:C:317:ASN:O	2:C:321:GLY:N	2.50	0.45
2:C:475:VAL:HG12	2:C:476:HIS:N	2.32	0.45
2:C:1051:MET:SD	2:C:1051:MET:N	2.79	0.45
3:D:1230:THR:HG23	3:D:1231:ARG:N	2.32	0.45
3:D:1246:ASN:N	3:D:1250:GLU:OE2	2.49	0.45
1:H:97:LEU:HD23	1:H:98:ARG:N	2.32	0.45
2:I:922:VAL:HG11	2:I:931:ILE:HD11	1.99	0.45
3:J:1230:THR:HG23	3:J:1231:ARG:N	2.32	0.45
5:L:118:GLU:OE2	5:L:149:ALA:HB1	2.17	0.45
3:P:22:GLN:O	3:P:22:GLN:NE2	2.50	0.45
3:W:505:HIS:NE2	3:W:531:ALA:O	2.46	0.45
2:BA:270:THR:HG23	2:BA:271:ASP:N	2.32	0.45
2:BA:475:VAL:HG12	2:BA:476:HIS:N	2.32	0.45
2:BA:1051:MET:SD	2:BA:1051:MET:N	2.79	0.45
3:CA:1230:THR:HG23	3:CA:1231:ARG:N	2.32	0.45
3:CA:1246:ASN:N	3:CA:1250:GLU:OE2	2.49	0.45
3:IA:104:ILE:HD12	3:IA:379:ASP:HB3	1.98	0.45
3:IA:867:THR:HG23	3:IA:868:ALA:N	2.32	0.45
3:IA:1230:THR:HG23	3:IA:1231:ARG:N	2.32	0.45
5:KA:118:GLU:OE2	5:KA:149:ALA:HB1	2.17	0.45
1:MA:97:LEU:HD23	1:MA:98:ARG:N	2.32	0.45
3:OA:867:THR:HG23	3:OA:868:ALA:N	2.32	0.45
1:RA:29:GLY:O	1:SA:40:ARG:NH1	2.43	0.45
1:SA:97:LEU:HD23	1:SA:98:ARG:N	2.32	0.45
1:SA:99:LYS:HD2	1:SA:105:VAL:HG12	1.98	0.45
2:TA:270:THR:HG23	2:TA:271:ASP:N	2.32	0.45
2:TA:1136:GLU:OE1	3:UA:11:ARG:NH2	2.47	0.45
2:I:270:THR:HG23	2:I:271:ASP:N	2.32	0.45
1:M:55:ARG:N	1:M:137:GLU:O	2.50	0.45
1:N:97:LEU:HD23	1:N:98:ARG:N	2.32	0.45
3:P:350:ARG:CZ	3:P:373:MET:HE2	2.47	0.45
5:R:56:LEU:O	5:R:59:GLU:HB3	2.17	0.45
1:T:97:LEU:HD23	1:T:98:ARG:N	2.32	0.45
2:V:270:THR:HG23	2:V:271:ASP:N	2.32	0.45
2:V:1128:LEU:HD23	2:V:1135:VAL:HG21	1.99	0.45
2:BA:317:ASN:O	2:BA:321:GLY:N	2.50	0.45
3:CA:217:ASP:HA	3:CA:220:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CA:223:TRP:O	3:CA:224:SER:C	2.59	0.45
2:HA:922:VAL:HG11	2:HA:931:ILE:HD11	1.99	0.45
3:IA:1112:MET:HE3	3:IA:1113:GLU:HB2	2.00	0.45
3:OA:22:GLN:NE2	3:OA:22:GLN:O	2.50	0.45
3:OA:93:GLY:O	3:OA:319:VAL:HG22	2.16	0.45
3:OA:350:ARG:CZ	3:OA:373:MET:HE2	2.47	0.45
2:TA:317:ASN:O	2:TA:321:GLY:N	2.50	0.45
2:TA:1128:LEU:HD23	2:TA:1135:VAL:HG21	1.99	0.45
1:B:79:ASN:ND2	1:B:125:ILE:O	2.50	0.44
2:C:716:GLY:N	2:C:1029:TYR:OH	2.43	0.44
3:D:223:TRP:O	3:D:224:SER:C	2.59	0.44
1:H:99:LYS:HD2	1:H:105:VAL:HG12	1.98	0.44
3:J:1112:MET:HE3	3:J:1113:GLU:HB2	2.00	0.44
2:O:336:GLU:HA	2:O:339:VAL:HG22	1.99	0.44
3:P:93:GLY:O	3:P:319:VAL:HG22	2.16	0.44
1:S:29:GLY:O	1:T:40:ARG:NH1	2.43	0.44
2:V:317:ASN:O	2:V:321:GLY:N	2.50	0.44
2:V:1136:GLU:OE1	3:W:11:ARG:NH2	2.47	0.44
1:GA:99:LYS:HD2	1:GA:105:VAL:HG12	1.98	0.44
2:HA:270:THR:HG23	2:HA:271:ASP:N	2.32	0.44
1:LA:55:ARG:N	1:LA:137:GLU:O	2.50	0.44
2:NA:336:GLU:HA	2:NA:339:VAL:HG22	1.99	0.44
2:TA:475:VAL:HG12	2:TA:476:HIS:N	2.32	0.44
2:C:336:GLU:HA	2:C:339:VAL:HG22	1.99	0.44
2:C:1128:LEU:HD23	2:C:1135:VAL:HG21	1.99	0.44
3:W:350:ARG:CZ	3:W:373:MET:HE2	2.47	0.44
3:W:867:THR:HG23	3:W:868:ALA:N	2.32	0.44
1:AA:79:ASN:ND2	1:AA:125:ILE:O	2.50	0.44
2:BA:336:GLU:HA	2:BA:339:VAL:HG22	1.99	0.44
2:HA:317:ASN:O	2:HA:321:GLY:N	2.50	0.44
2:HA:1128:LEU:HD23	2:HA:1135:VAL:HG21	1.99	0.44
2:NA:922:VAL:HG11	2:NA:931:ILE:HD11	1.99	0.44
2:NA:1009:MET:HE3	2:NA:1022:PRO:HB3	1.99	0.44
3:OA:223:TRP:O	3:OA:224:SER:C	2.59	0.44
3:OA:1230:THR:HG23	3:OA:1231:ARG:N	2.32	0.44
5:QA:56:LEU:O	5:QA:59:GLU:HB3	2.17	0.44
2:TA:60:SER:OG	2:TA:382:GLY:N	2.46	0.44
2:TA:487:GLU:O	2:TA:488:THR:OG1	2.31	0.44
3:UA:22:GLN:NE2	3:UA:22:GLN:O	2.50	0.44
3:UA:350:ARG:CZ	3:UA:373:MET:HE2	2.47	0.44
3:D:217:ASP:HA	3:D:220:GLU:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1112:MET:HE3	3:D:1113:GLU:HB2	2.00	0.44
2:I:317:ASN:O	2:I:321:GLY:N	2.50	0.44
2:I:336:GLU:HA	2:I:339:VAL:HG22	1.99	0.44
2:I:1128:LEU:HD23	2:I:1135:VAL:HG21	1.99	0.44
3:J:1123:ARG:HG3	3:J:1124:VAL:HG13	1.98	0.44
2:O:922:VAL:HG11	2:O:931:ILE:HD11	1.99	0.44
2:O:1009:MET:HE3	2:O:1022:PRO:HB3	1.99	0.44
3:P:223:TRP:O	3:P:224:SER:C	2.59	0.44
3:P:1230:THR:HG23	3:P:1231:ARG:N	2.32	0.44
2:V:475:VAL:HG12	2:V:476:HIS:N	2.32	0.44
3:W:16:THR:N	3:W:19:ASP:OD2	2.50	0.44
3:W:22:GLN:NE2	3:W:22:GLN:O	2.50	0.44
3:W:1123:ARG:HG3	3:W:1124:VAL:HG13	1.98	0.44
5:Y:56:LEU:O	5:Y:59:GLU:HB3	2.17	0.44
2:BA:1128:LEU:HD23	2:BA:1135:VAL:HG21	1.99	0.44
3:CA:633:ILE:HG22	3:CA:634:LYS:N	2.31	0.44
2:HA:336:GLU:HA	2:HA:339:VAL:HG22	1.99	0.44
3:IA:16:THR:N	3:IA:19:ASP:OD2	2.50	0.44
3:UA:163:GLU:O	3:UA:166:ARG:HG3	2.17	0.44
3:UA:867:THR:HG23	3:UA:868:ALA:N	2.32	0.44
5:WA:56:LEU:O	5:WA:59:GLU:HB3	2.17	0.44
3:D:134:TYR:HD1	3:D:134:TYR:N	2.16	0.44
3:D:633:ILE:HG22	3:D:634:LYS:N	2.31	0.44
2:I:192:ASP:HB2	2:I:199:LEU:HD11	2.00	0.44
3:J:16:THR:N	3:J:19:ASP:OD2	2.50	0.44
2:V:336:GLU:HA	2:V:339:VAL:HG22	1.99	0.44
3:W:163:GLU:O	3:W:166:ARG:HG3	2.17	0.44
3:W:1112:MET:HE3	3:W:1113:GLU:HB2	2.00	0.44
3:CA:134:TYR:HD1	3:CA:134:TYR:N	2.16	0.44
3:CA:350:ARG:CZ	3:CA:373:MET:HE2	2.47	0.44
3:CA:1112:MET:HE3	3:CA:1113:GLU:HB2	2.00	0.44
2:HA:1009:MET:HE3	2:HA:1022:PRO:HB3	1.99	0.44
3:IA:162:VAL:O	3:IA:165:GLN:HG3	2.17	0.44
2:NA:192:ASP:HB2	2:NA:199:LEU:HD11	2.00	0.44
2:NA:270:THR:HG23	2:NA:271:ASP:N	2.32	0.44
3:UA:16:THR:N	3:UA:19:ASP:OD2	2.50	0.44
3:UA:1112:MET:HE3	3:UA:1113:GLU:HB2	2.00	0.44
3:UA:1123:ARG:HG3	3:UA:1124:VAL:HG13	1.98	0.44
2:C:487:GLU:O	2:C:488:THR:OG1	2.31	0.44
3:D:350:ARG:CZ	3:D:373:MET:HE2	2.47	0.44
3:D:867:THR:HG23	3:D:868:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:118:GLU:OE2	5:F:149:ALA:HB1	2.17	0.44
1:H:111:VAL:O	1:H:111:VAL:HG13	2.18	0.44
3:J:162:VAL:O	3:J:165:GLN:HG3	2.17	0.44
3:J:350:ARG:CZ	3:J:373:MET:HE2	2.47	0.44
2:O:192:ASP:HB2	2:O:199:LEU:HD11	2.00	0.44
2:O:270:THR:HG23	2:O:271:ASP:N	2.32	0.44
1:S:55:ARG:N	1:S:137:GLU:O	2.50	0.44
2:V:60:SER:OG	2:V:382:GLY:N	2.46	0.44
2:HA:192:ASP:HB2	2:HA:199:LEU:HD11	2.00	0.44
3:IA:350:ARG:CZ	3:IA:373:MET:HE2	2.47	0.44
3:IA:1123:ARG:HG3	3:IA:1124:VAL:HG13	1.98	0.44
5:KA:56:LEU:O	5:KA:59:GLU:HB3	2.17	0.44
2:TA:336:GLU:HA	2:TA:339:VAL:HG22	1.99	0.44
3:UA:124:ASP:N	3:UA:124:ASP:OD1	2.51	0.44
3:UA:1167:ILE:O	3:UA:1178:GLY:N	2.45	0.44
5:WA:118:GLU:OE2	5:WA:149:ALA:HB1	2.17	0.44
2:I:1009:MET:HE3	2:I:1022:PRO:HB3	1.99	0.44
3:J:217:ASP:HA	3:J:220:GLU:HG3	1.98	0.44
5:L:56:LEU:O	5:L:59:GLU:HB3	2.17	0.44
3:W:124:ASP:OD1	3:W:124:ASP:N	2.51	0.44
5:Y:118:GLU:OE2	5:Y:149:ALA:HB1	2.17	0.44
2:BA:487:GLU:O	2:BA:488:THR:OG1	2.31	0.44
3:CA:867:THR:HG23	3:CA:868:ALA:N	2.32	0.44
5:EA:118:GLU:OE2	5:EA:149:ALA:HB1	2.17	0.44
1:GA:111:VAL:HG13	1:GA:111:VAL:O	2.18	0.44
3:IA:217:ASP:HA	3:IA:220:GLU:HG3	1.98	0.44
2:NA:1128:LEU:HD23	2:NA:1135:VAL:HG21	1.99	0.44
5:QA:118:GLU:OE2	5:QA:149:ALA:HB1	2.17	0.44
1:RA:55:ARG:N	1:RA:137:GLU:O	2.50	0.44
1:SA:111:VAL:O	1:SA:111:VAL:HG13	2.18	0.44
2:TA:1009:MET:HE3	2:TA:1022:PRO:HB3	1.99	0.44
1:B:111:VAL:O	1:B:111:VAL:HG13	2.18	0.44
3:J:147:GLU:O	3:J:151:LEU:HD23	2.18	0.44
2:O:1128:LEU:HD23	2:O:1135:VAL:HG21	1.99	0.44
5:R:118:GLU:OE2	5:R:149:ALA:HB1	2.17	0.44
1:T:111:VAL:HG13	1:T:111:VAL:O	2.18	0.44
2:V:192:ASP:HB2	2:V:199:LEU:HD11	2.00	0.44
3:W:111:PRO:O	3:W:113:ARG:NH1	2.43	0.44
3:W:1230:THR:HG23	3:W:1231:ARG:N	2.32	0.44
1:Z:29:GLY:O	1:AA:40:ARG:NH1	2.43	0.44
1:AA:111:VAL:HG13	1:AA:111:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HA:274:LEU:HD13	2:HA:292:ALA:HB3	1.99	0.44
2:TA:192:ASP:HB2	2:TA:199:LEU:HD11	2.00	0.44
2:TA:274:LEU:HD13	2:TA:292:ALA:HB3	1.99	0.44
3:UA:134:TYR:HD1	3:UA:134:TYR:N	2.16	0.44
1:A:29:GLY:O	1:B:40:ARG:NH1	2.43	0.44
1:B:18:ARG:O	1:B:19:SER:OG	2.30	0.44
2:I:274:LEU:HD13	2:I:292:ALA:HB3	1.99	0.44
3:J:846:VAL:HG13	3:J:847:LEU:HD22	2.00	0.44
1:N:79:ASN:ND2	1:N:125:ILE:O	2.50	0.44
2:V:274:LEU:HD13	2:V:292:ALA:HB3	1.99	0.44
2:V:1009:MET:HE3	2:V:1022:PRO:HB3	1.99	0.44
3:W:134:TYR:HD1	3:W:134:TYR:N	2.16	0.44
3:W:217:ASP:HA	3:W:220:GLU:HG3	1.98	0.44
3:W:1167:ILE:O	3:W:1178:GLY:N	2.45	0.44
1:AA:18:ARG:O	1:AA:19:SER:OG	2.30	0.44
2:BA:831:GLU:OE1	2:BA:831:GLU:N	2.44	0.44
3:CA:130:TYR:O	3:CA:372:ARG:HD3	2.18	0.44
3:CA:846:VAL:HG13	3:CA:847:LEU:HD22	2.00	0.44
3:IA:147:GLU:O	3:IA:151:LEU:HD23	2.18	0.44
2:TA:96:ILE:HD11	2:TA:105:LEU:HD23	2.00	0.44
2:C:715:LEU:HD12	2:C:715:LEU:N	2.33	0.44
3:D:130:TYR:O	3:D:372:ARG:HD3	2.18	0.44
3:D:846:VAL:HG13	3:D:847:LEU:HD22	2.00	0.44
1:N:18:ARG:O	1:N:19:SER:OG	2.30	0.44
3:P:1112:MET:HE3	3:P:1113:GLU:HB2	2.00	0.44
2:V:96:ILE:HD11	2:V:105:LEU:HD23	2.00	0.44
2:V:922:VAL:HG11	2:V:931:ILE:HD11	1.99	0.44
3:W:1207:LEU:C	3:W:1207:LEU:HD12	2.43	0.44
3:IA:22:GLN:O	3:IA:22:GLN:NE2	2.50	0.44
3:IA:846:VAL:HG13	3:IA:847:LEU:HD22	2.00	0.44
1:MA:79:ASN:ND2	1:MA:125:ILE:O	2.50	0.44
3:OA:124:ASP:OD1	3:OA:124:ASP:N	2.51	0.44
3:UA:217:ASP:HA	3:UA:220:GLU:HG3	1.98	0.44
3:UA:1207:LEU:C	3:UA:1207:LEU:HD12	2.43	0.44
3:UA:1230:THR:HG23	3:UA:1231:ARG:N	2.32	0.44
2:C:274:LEU:HD13	2:C:292:ALA:HB3	1.99	0.43
1:G:97:LEU:HD23	1:G:97:LEU:C	2.43	0.43
3:J:22:GLN:NE2	3:J:22:GLN:O	2.50	0.43
3:J:134:TYR:HD1	3:J:134:TYR:N	2.16	0.43
3:P:124:ASP:N	3:P:124:ASP:OD1	2.51	0.43
1:Z:97:LEU:HD23	1:Z:97:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BA:274:LEU:HD13	2:BA:292:ALA:HB3	1.99	0.43
2:BA:715:LEU:N	2:BA:715:LEU:HD12	2.33	0.43
3:CA:124:ASP:N	3:CA:124:ASP:OD1	2.51	0.43
1:FA:97:LEU:C	1:FA:97:LEU:HD23	2.43	0.43
3:IA:134:TYR:HD1	3:IA:134:TYR:N	2.16	0.43
1:MA:18:ARG:O	1:MA:19:SER:OG	2.30	0.43
2:NA:274:LEU:HD13	2:NA:292:ALA:HB3	1.99	0.43
3:OA:1112:MET:HE3	3:OA:1113:GLU:HB2	2.00	0.43
2:TA:922:VAL:HG11	2:TA:931:ILE:HD11	1.99	0.43
1:A:55:ARG:N	1:A:137:GLU:O	2.50	0.43
1:A:97:LEU:HD23	1:A:97:LEU:C	2.43	0.43
3:D:124:ASP:OD1	3:D:124:ASP:N	2.51	0.43
3:D:147:GLU:O	3:D:151:LEU:HD23	2.18	0.43
3:D:162:VAL:O	3:D:165:GLN:HG3	2.17	0.43
1:H:79:ASN:ND2	1:H:125:ILE:O	2.50	0.43
3:J:1058:GLY:O	3:J:1081:SER:OG	2.35	0.43
1:N:111:VAL:O	1:N:111:VAL:HG13	2.18	0.43
3:P:1207:LEU:C	3:P:1207:LEU:HD12	2.43	0.43
2:V:178:GLN:O	2:V:378:LEU:HD12	2.18	0.43
3:CA:147:GLU:O	3:CA:151:LEU:HD23	2.18	0.43
1:GA:79:ASN:ND2	1:GA:125:ILE:O	2.50	0.43
1:MA:111:VAL:O	1:MA:111:VAL:HG13	2.18	0.43
3:OA:1207:LEU:C	3:OA:1207:LEU:HD12	2.43	0.43
2:TA:178:GLN:O	2:TA:378:LEU:HD12	2.18	0.43
3:UA:111:PRO:O	3:UA:113:ARG:NH1	2.43	0.43
2:C:178:GLN:O	2:C:378:LEU:HD12	2.18	0.43
3:D:1207:LEU:C	3:D:1207:LEU:HD12	2.43	0.43
2:O:274:LEU:HD13	2:O:292:ALA:HB3	1.99	0.43
3:W:130:TYR:O	3:W:372:ARG:HD3	2.18	0.43
2:BA:178:GLN:O	2:BA:378:LEU:HD12	2.18	0.43
2:BA:1009:MET:HE3	2:BA:1022:PRO:HB3	1.99	0.43
3:IA:130:TYR:O	3:IA:372:ARG:HD3	2.18	0.43
3:OA:134:TYR:HD1	3:OA:134:TYR:N	2.16	0.43
3:J:124:ASP:N	3:J:124:ASP:OD1	2.51	0.43
3:J:130:TYR:O	3:J:372:ARG:HD3	2.18	0.43
1:N:135:GLU:N	1:N:135:GLU:OE1	2.52	0.43
1:Z:55:ARG:N	1:Z:137:GLU:O	2.50	0.43
2:BA:192:ASP:HB2	2:BA:199:LEU:HD11	2.00	0.43
2:BA:922:VAL:HG11	2:BA:931:ILE:HD11	1.99	0.43
3:CA:162:VAL:O	3:CA:165:GLN:HG3	2.17	0.43
3:CA:1207:LEU:C	3:CA:1207:LEU:HD12	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:IA:124:ASP:OD1	3:IA:124:ASP:N	2.51	0.43
3:IA:1058:GLY:O	3:IA:1081:SER:OG	2.35	0.43
1:MA:135:GLU:OE1	1:MA:135:GLU:N	2.52	0.43
2:NA:715:LEU:HD12	2:NA:715:LEU:N	2.33	0.43
3:UA:130:TYR:O	3:UA:372:ARG:HD3	2.18	0.43
2:C:192:ASP:HB2	2:C:199:LEU:HD11	2.00	0.43
2:C:922:VAL:HG11	2:C:931:ILE:HD11	1.99	0.43
2:C:1009:MET:HE3	2:C:1022:PRO:HB3	1.99	0.43
5:F:40:LEU:HD12	5:F:45:GLU:OE1	2.19	0.43
2:I:60:SER:OG	2:I:382:GLY:N	2.46	0.43
3:J:825:THR:HG22	3:J:826:ASN:N	2.34	0.43
1:M:66:VAL:O	1:M:69:VAL:HG22	2.19	0.43
2:O:715:LEU:N	2:O:715:LEU:HD12	2.33	0.43
3:P:134:TYR:HD1	3:P:134:TYR:N	2.16	0.43
2:V:115:VAL:HG12	2:V:116:LYS:N	2.34	0.43
2:V:715:LEU:HD12	2:V:715:LEU:N	2.33	0.43
3:CA:1121:VAL:HG23	3:CA:1130:VAL:CG1	2.47	0.43
2:HA:60:SER:OG	2:HA:382:GLY:N	2.46	0.43
3:IA:825:THR:HG22	3:IA:826:ASN:N	2.34	0.43
3:IA:1207:LEU:C	3:IA:1207:LEU:HD12	2.43	0.43
1:LA:66:VAL:O	1:LA:69:VAL:HG22	2.19	0.43
2:TA:115:VAL:HG12	2:TA:116:LYS:N	2.34	0.43
2:TA:715:LEU:HD12	2:TA:715:LEU:N	2.33	0.43
2:C:98:ASP:OD2	2:C:100:SER:OG	2.37	0.43
2:C:214:PHE:CE1	2:C:224:VAL:HG12	2.54	0.43
3:D:1121:VAL:HG23	3:D:1130:VAL:CG1	2.47	0.43
3:J:1207:LEU:C	3:J:1207:LEU:HD12	2.43	0.43
1:N:97:LEU:HD23	1:N:97:LEU:C	2.44	0.43
1:N:130:ASP:OD2	1:N:131:LYS:NZ	2.51	0.43
2:O:214:PHE:CE1	2:O:224:VAL:HG12	2.54	0.43
3:P:825:THR:HG22	3:P:826:ASN:N	2.34	0.43
3:W:1054:ARG:N	3:W:1065:THR:O	2.42	0.43
2:BA:98:ASP:OD2	2:BA:100:SER:OG	2.37	0.43
2:BA:214:PHE:CE1	2:BA:224:VAL:HG12	2.54	0.43
5:EA:40:LEU:HD12	5:EA:45:GLU:OE1	2.19	0.43
2:HA:214:PHE:CE1	2:HA:224:VAL:HG12	2.54	0.43
1:MA:130:ASP:OD2	1:MA:131:LYS:NZ	2.51	0.43
2:NA:214:PHE:CE1	2:NA:224:VAL:HG12	2.54	0.43
3:OA:825:THR:HG22	3:OA:826:ASN:N	2.34	0.43
1:RA:97:LEU:HD23	1:RA:97:LEU:C	2.43	0.43
1:B:97:LEU:HD23	1:B:97:LEU:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:214:PHE:CE1	2:I:224:VAL:HG12	2.54	0.43
1:S:97:LEU:C	1:S:97:LEU:HD23	2.43	0.43
1:AA:97:LEU:HD23	1:AA:97:LEU:C	2.44	0.43
3:OA:130:TYR:O	3:OA:372:ARG:HD3	2.18	0.43
3:UA:1054:ARG:N	3:UA:1065:THR:O	2.42	0.43
3:P:147:GLU:O	3:P:151:LEU:HD23	2.18	0.43
1:MA:97:LEU:HD23	1:MA:97:LEU:C	2.44	0.43
3:UA:1121:VAL:HG23	3:UA:1130:VAL:CG1	2.47	0.43
1:H:179:ASP:O	1:H:191:LYS:N	2.52	0.43
2:I:115:VAL:HG12	2:I:116:LYS:N	2.34	0.43
1:M:97:LEU:HD23	1:M:97:LEU:C	2.43	0.43
2:O:96:ILE:HD11	2:O:105:LEU:HD23	2.00	0.43
2:O:98:ASP:OD2	2:O:100:SER:OG	2.37	0.43
3:P:130:TYR:O	3:P:372:ARG:HD3	2.18	0.43
3:P:846:VAL:HG13	3:P:847:LEU:HD22	2.00	0.43
3:P:1053:VAL:O	3:P:1102:GLY:N	2.49	0.43
1:S:66:VAL:O	1:S:69:VAL:HG22	2.19	0.43
1:T:135:GLU:OE1	1:T:135:GLU:N	2.52	0.43
5:Y:40:LEU:HD12	5:Y:45:GLU:OE1	2.19	0.43
3:CA:825:THR:HG22	3:CA:826:ASN:N	2.34	0.43
1:GA:179:ASP:O	1:GA:191:LYS:N	2.52	0.43
2:NA:98:ASP:OD2	2:NA:100:SER:OG	2.37	0.43
2:NA:487:GLU:O	2:NA:488:THR:OG1	2.31	0.43
3:OA:846:VAL:HG13	3:OA:847:LEU:HD22	2.00	0.43
1:SA:135:GLU:OE1	1:SA:135:GLU:N	2.52	0.43
2:C:96:ILE:HD11	2:C:105:LEU:HD23	2.00	0.43
3:D:825:THR:HG22	3:D:826:ASN:N	2.34	0.43
1:H:97:LEU:HD23	1:H:97:LEU:C	2.44	0.43
1:H:159:ILE:HD12	1:H:159:ILE:N	2.34	0.43
5:L:40:LEU:HD12	5:L:45:GLU:OE1	2.19	0.43
2:O:487:GLU:O	2:O:488:THR:OG1	2.31	0.43
3:P:405:LEU:C	3:P:406:LEU:HD12	2.44	0.43
3:P:417:LEU:HD21	3:P:1253:ILE:CG1	2.49	0.43
1:T:218:LEU:C	1:T:218:LEU:HD23	2.44	0.43
3:W:107:PHE:CD1	3:W:107:PHE:C	2.97	0.43
3:W:1121:VAL:HG23	3:W:1130:VAL:CG1	2.47	0.43
1:AA:179:ASP:O	1:AA:191:LYS:N	2.52	0.43
2:BA:96:ILE:HD11	2:BA:105:LEU:HD23	2.00	0.43
1:GA:159:ILE:N	1:GA:159:ILE:HD12	2.34	0.43
2:HA:115:VAL:HG12	2:HA:116:LYS:N	2.34	0.43
5:KA:40:LEU:HD12	5:KA:45:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:NA:96:ILE:HD11	2:NA:105:LEU:HD23	2.00	0.43
3:OA:147:GLU:O	3:OA:151:LEU:HD23	2.18	0.43
3:OA:405:LEU:C	3:OA:406:LEU:HD12	2.44	0.43
3:OA:417:LEU:HD21	3:OA:1253:ILE:CG1	2.49	0.43
3:OA:1053:VAL:O	3:OA:1102:GLY:N	2.49	0.43
1:SA:79:ASN:ND2	1:SA:125:ILE:O	2.50	0.43
1:SA:218:LEU:HD23	1:SA:218:LEU:C	2.44	0.43
3:UA:107:PHE:CD1	3:UA:107:PHE:C	2.97	0.43
5:WA:40:LEU:HD12	5:WA:45:GLU:OE1	2.19	0.43
1:B:179:ASP:O	1:B:191:LYS:N	2.52	0.42
1:T:79:ASN:ND2	1:T:125:ILE:O	2.50	0.42
1:GA:97:LEU:HD23	1:GA:97:LEU:C	2.44	0.42
1:GA:135:GLU:OE1	1:GA:135:GLU:N	2.52	0.42
1:LA:97:LEU:HD23	1:LA:97:LEU:C	2.43	0.42
1:RA:66:VAL:O	1:RA:69:VAL:HG22	2.19	0.42
3:UA:147:GLU:O	3:UA:151:LEU:HD23	2.18	0.42
3:D:949:ILE:O	3:D:953:LEU:HD23	2.19	0.42
5:F:108:ARG:HB2	5:F:154:MET:CE	2.50	0.42
1:H:135:GLU:OE1	1:H:135:GLU:N	2.52	0.42
2:I:715:LEU:HD12	2:I:715:LEU:N	2.33	0.42
3:J:405:LEU:C	3:J:406:LEU:HD12	2.44	0.42
1:N:218:LEU:HD23	1:N:218:LEU:C	2.44	0.42
3:W:1066:ILE:HG23	3:W:1066:ILE:O	2.19	0.42
5:EA:108:ARG:HB2	5:EA:154:MET:CE	2.50	0.42
1:MA:218:LEU:HD23	1:MA:218:LEU:C	2.44	0.42
1:G:66:VAL:O	1:G:69:VAL:HG22	2.19	0.42
2:I:98:ASP:OD2	2:I:100:SER:OG	2.37	0.42
2:I:138:GLU:N	2:I:138:GLU:OE1	2.53	0.42
2:I:178:GLN:O	2:I:378:LEU:HD12	2.18	0.42
3:J:417:LEU:HD21	3:J:1253:ILE:CG1	2.49	0.42
2:O:115:VAL:HG12	2:O:116:LYS:N	2.34	0.42
3:P:366:ILE:H	3:P:366:ILE:HD12	1.85	0.42
3:W:147:GLU:O	3:W:151:LEU:HD23	2.18	0.42
3:CA:949:ILE:O	3:CA:953:LEU:HD23	2.19	0.42
2:HA:96:ILE:HD11	2:HA:105:LEU:HD23	2.00	0.42
2:HA:138:GLU:OE1	2:HA:138:GLU:N	2.53	0.42
2:HA:178:GLN:O	2:HA:378:LEU:HD12	2.18	0.42
2:HA:715:LEU:N	2:HA:715:LEU:HD12	2.33	0.42
3:IA:405:LEU:C	3:IA:406:LEU:HD12	2.44	0.42
3:IA:417:LEU:HD21	3:IA:1253:ILE:CG1	2.49	0.42
3:IA:949:ILE:O	3:IA:953:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:OA:366:ILE:H	3:OA:366:ILE:HD12	1.85	0.42
3:UA:1066:ILE:HG23	3:UA:1066:ILE:O	2.19	0.42
2:C:1131:LEU:CD2	3:D:402:LEU:HD22	2.44	0.42
3:J:949:ILE:O	3:J:953:LEU:HD23	2.19	0.42
1:N:159:ILE:HD12	1:N:159:ILE:N	2.34	0.42
5:R:108:ARG:HB2	5:R:154:MET:CE	2.50	0.42
1:T:97:LEU:HD23	1:T:97:LEU:C	2.44	0.42
1:AA:135:GLU:N	1:AA:135:GLU:OE1	2.52	0.42
2:BA:115:VAL:HG12	2:BA:116:LYS:N	2.34	0.42
3:CA:302:PHE:HZ	3:CA:312:MET:HE3	1.85	0.42
1:FA:66:VAL:O	1:FA:69:VAL:HG22	2.19	0.42
2:HA:98:ASP:OD2	2:HA:100:SER:OG	2.37	0.42
1:MA:159:ILE:N	1:MA:159:ILE:HD12	2.34	0.42
2:NA:115:VAL:HG12	2:NA:116:LYS:N	2.34	0.42
3:OA:1167:ILE:O	3:OA:1178:GLY:N	2.45	0.42
4:PA:54:VAL:HG13	4:PA:55:ILE:N	2.35	0.42
1:B:135:GLU:OE1	1:B:135:GLU:N	2.52	0.42
2:C:138:GLU:OE1	2:C:138:GLU:N	2.53	0.42
3:D:302:PHE:HZ	3:D:312:MET:HE3	1.85	0.42
3:D:313:VAL:O	3:D:313:VAL:HG23	2.20	0.42
2:I:96:ILE:HD11	2:I:105:LEU:HD23	2.00	0.42
3:J:313:VAL:HG23	3:J:313:VAL:O	2.20	0.42
3:J:366:ILE:HD12	3:J:366:ILE:H	1.85	0.42
3:P:1066:ILE:O	3:P:1066:ILE:HG23	2.19	0.42
3:P:1167:ILE:O	3:P:1178:GLY:N	2.45	0.42
4:Q:54:VAL:HG13	4:Q:55:ILE:N	2.35	0.42
2:V:214:PHE:CE1	2:V:224:VAL:HG12	2.54	0.42
3:W:417:LEU:HD21	3:W:1253:ILE:CG1	2.49	0.42
3:W:825:THR:HG22	3:W:826:ASN:N	2.34	0.42
2:BA:138:GLU:N	2:BA:138:GLU:OE1	2.53	0.42
3:CA:313:VAL:HG23	3:CA:313:VAL:O	2.20	0.42
3:CA:417:LEU:HD21	3:CA:1253:ILE:CG1	2.49	0.42
3:IA:313:VAL:HG23	3:IA:313:VAL:O	2.20	0.42
3:IA:366:ILE:H	3:IA:366:ILE:HD12	1.85	0.42
3:IA:1121:VAL:CG2	3:IA:1130:VAL:HG12	2.46	0.42
5:QA:108:ARG:HB2	5:QA:154:MET:CE	2.50	0.42
3:UA:417:LEU:HD21	3:UA:1253:ILE:CG1	2.49	0.42
3:D:417:LEU:HD21	3:D:1253:ILE:CG1	2.49	0.42
3:D:1066:ILE:HG23	3:D:1066:ILE:O	2.19	0.42
2:I:354:THR:OG1	2:I:362:GLU:OE2	2.38	0.42
3:J:107:PHE:CD1	3:J:107:PHE:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1066:ILE:HG23	3:J:1066:ILE:O	2.19	0.42
5:L:108:ARG:HB2	5:L:154:MET:CE	2.50	0.42
3:P:1047:ALA:N	3:P:1109:GLN:O	2.53	0.42
5:R:40:LEU:HD12	5:R:45:GLU:OE1	2.19	0.42
1:Z:66:VAL:O	1:Z:69:VAL:HG22	2.19	0.42
3:CA:1066:ILE:O	3:CA:1066:ILE:HG23	2.19	0.42
2:HA:354:THR:OG1	2:HA:362:GLU:OE2	2.38	0.42
3:IA:1066:ILE:HG23	3:IA:1066:ILE:O	2.19	0.42
3:OA:1047:ALA:N	3:OA:1109:GLN:O	2.53	0.42
3:OA:1066:ILE:HG23	3:OA:1066:ILE:O	2.19	0.42
3:OA:1121:VAL:CG2	3:OA:1130:VAL:HG12	2.46	0.42
5:QA:40:LEU:HD12	5:QA:45:GLU:OE1	2.19	0.42
1:SA:97:LEU:HD23	1:SA:97:LEU:C	2.44	0.42
2:TA:214:PHE:CE1	2:TA:224:VAL:HG12	2.54	0.42
3:UA:825:THR:HG22	3:UA:826:ASN:N	2.34	0.42
1:H:218:LEU:HD23	1:H:218:LEU:C	2.44	0.42
4:K:54:VAL:HG13	4:K:55:ILE:N	2.35	0.42
3:P:930:VAL:HG22	3:P:936:VAL:HG12	2.01	0.42
3:P:1121:VAL:CG2	3:P:1130:VAL:HG12	2.46	0.42
2:V:354:THR:OG1	2:V:362:GLU:OE2	2.38	0.42
3:W:405:LEU:C	3:W:406:LEU:HD12	2.44	0.42
3:W:846:VAL:HG13	3:W:847:LEU:HD22	2.00	0.42
1:AA:159:ILE:HD12	1:AA:159:ILE:N	2.34	0.42
2:BA:1131:LEU:CD2	3:CA:402:LEU:HD22	2.44	0.42
3:CA:107:PHE:CD1	3:CA:107:PHE:C	2.97	0.42
1:GA:218:LEU:C	1:GA:218:LEU:HD23	2.44	0.42
3:IA:107:PHE:CD1	3:IA:107:PHE:C	2.97	0.42
5:KA:108:ARG:HB2	5:KA:154:MET:CE	2.50	0.42
3:UA:405:LEU:C	3:UA:406:LEU:HD12	2.44	0.42
3:UA:1052:ARG:N	3:UA:1067:VAL:O	2.47	0.42
3:UA:1055:LEU:C	3:UA:1055:LEU:HD23	2.45	0.42
1:A:66:VAL:O	1:A:69:VAL:HG22	2.19	0.42
1:B:159:ILE:HD12	1:B:159:ILE:N	2.34	0.42
3:D:405:LEU:C	3:D:406:LEU:HD12	2.44	0.42
3:D:1055:LEU:HD23	3:D:1055:LEU:C	2.45	0.42
2:I:258:MET:O	2:I:261:THR:OG1	2.32	0.42
3:J:1121:VAL:CG2	3:J:1130:VAL:HG12	2.46	0.42
3:J:1249:LYS:O	3:J:1252:VAL:HG12	2.20	0.42
1:N:179:ASP:O	1:N:191:LYS:N	2.52	0.42
2:O:642:VAL:HG22	2:O:703:ALA:HB3	2.02	0.42
3:P:1249:LYS:O	3:P:1252:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:179:ASP:O	1:T:191:LYS:N	2.52	0.42
2:V:98:ASP:OD2	2:V:100:SER:OG	2.37	0.42
2:V:138:GLU:OE1	2:V:138:GLU:N	2.53	0.42
3:W:366:ILE:H	3:W:366:ILE:HD12	1.85	0.42
3:W:930:VAL:HG22	3:W:936:VAL:HG12	2.01	0.42
3:W:949:ILE:O	3:W:953:LEU:HD23	2.19	0.42
3:W:1055:LEU:C	3:W:1055:LEU:HD23	2.45	0.42
3:CA:405:LEU:C	3:CA:406:LEU:HD12	2.44	0.42
3:CA:1055:LEU:HD23	3:CA:1055:LEU:C	2.45	0.42
1:GA:130:ASP:OD2	1:GA:131:LYS:NZ	2.51	0.42
3:IA:1249:LYS:O	3:IA:1252:VAL:HG12	2.20	0.42
4:JA:54:VAL:HG13	4:JA:55:ILE:N	2.35	0.42
1:MA:179:ASP:O	1:MA:191:LYS:N	2.52	0.42
2:NA:60:SER:OG	2:NA:382:GLY:N	2.46	0.42
3:OA:930:VAL:HG22	3:OA:936:VAL:HG12	2.01	0.42
3:OA:1249:LYS:O	3:OA:1252:VAL:HG12	2.20	0.42
2:TA:354:THR:OG1	2:TA:362:GLU:OE2	2.38	0.42
2:TA:642:VAL:HG22	2:TA:703:ALA:HB3	2.02	0.42
2:TA:696:VAL:HG11	2:TA:702:ILE:CD1	2.50	0.42
3:UA:846:VAL:HG13	3:UA:847:LEU:HD22	2.00	0.42
3:UA:930:VAL:HG22	3:UA:936:VAL:HG12	2.01	0.42
1:B:218:LEU:HD23	1:B:218:LEU:C	2.44	0.42
3:D:35:ASN:OD1	3:D:36:TYR:N	2.53	0.42
3:D:107:PHE:CD1	3:D:107:PHE:C	2.97	0.42
2:O:60:SER:OG	2:O:382:GLY:N	2.46	0.42
2:O:178:GLN:O	2:O:378:LEU:HD12	2.18	0.42
2:V:642:VAL:HG22	2:V:703:ALA:HB3	2.02	0.42
2:V:696:VAL:HG11	2:V:702:ILE:CD1	2.50	0.42
3:W:1052:ARG:N	3:W:1067:VAL:O	2.47	0.42
4:X:54:VAL:HG13	4:X:55:ILE:N	2.35	0.42
1:AA:218:LEU:HD23	1:AA:218:LEU:C	2.44	0.42
3:CA:916:ILE:HD11	3:CA:949:ILE:HD12	2.02	0.42
3:IA:916:ILE:HD11	3:IA:949:ILE:HD12	2.02	0.42
2:NA:138:GLU:OE1	2:NA:138:GLU:N	2.53	0.42
2:NA:178:GLN:O	2:NA:378:LEU:HD12	2.18	0.42
2:NA:642:VAL:HG22	2:NA:703:ALA:HB3	2.02	0.42
3:OA:35:ASN:OD1	3:OA:36:TYR:N	2.53	0.42
3:OA:949:ILE:O	3:OA:953:LEU:HD23	2.19	0.42
1:SA:179:ASP:O	1:SA:191:LYS:N	2.52	0.42
2:TA:98:ASP:OD2	2:TA:100:SER:OG	2.37	0.42
2:TA:138:GLU:OE1	2:TA:138:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:UA:949:ILE:O	3:UA:953:LEU:HD23	2.19	0.42
4:VA:54:VAL:HG13	4:VA:55:ILE:N	2.35	0.42
3:D:916:ILE:HD11	3:D:949:ILE:HD12	2.02	0.42
3:D:930:VAL:HG22	3:D:936:VAL:HG12	2.01	0.42
1:H:130:ASP:OD2	1:H:131:LYS:NZ	2.51	0.42
3:J:302:PHE:HZ	3:J:312:MET:HE3	1.85	0.42
3:J:916:ILE:HD11	3:J:949:ILE:HD12	2.02	0.42
3:J:1039:VAL:O	3:J:1039:VAL:HG23	2.20	0.42
3:J:1051:GLY:H	3:J:1066:ILE:HD11	1.85	0.42
2:O:138:GLU:N	2:O:138:GLU:OE1	2.53	0.42
3:P:35:ASN:OD1	3:P:36:TYR:N	2.53	0.42
3:P:949:ILE:O	3:P:953:LEU:HD23	2.19	0.42
3:P:1039:VAL:O	3:P:1039:VAL:HG23	2.20	0.42
3:P:1051:GLY:H	3:P:1066:ILE:HD11	1.85	0.42
3:W:313:VAL:O	3:W:313:VAL:HG23	2.20	0.42
3:CA:35:ASN:OD1	3:CA:36:TYR:N	2.53	0.42
3:CA:366:ILE:H	3:CA:366:ILE:HD12	1.85	0.42
3:CA:930:VAL:HG22	3:CA:936:VAL:HG12	2.01	0.42
3:IA:283:ASN:OD1	3:IA:284:GLY:N	2.46	0.42
3:IA:302:PHE:HZ	3:IA:312:MET:HE3	1.85	0.42
3:IA:1039:VAL:HG23	3:IA:1039:VAL:O	2.20	0.42
3:IA:1051:GLY:H	3:IA:1066:ILE:HD11	1.85	0.42
3:OA:1039:VAL:O	3:OA:1039:VAL:HG23	2.20	0.42
3:OA:1051:GLY:H	3:OA:1066:ILE:HD11	1.85	0.42
3:UA:313:VAL:O	3:UA:313:VAL:HG23	2.20	0.42
3:UA:366:ILE:H	3:UA:366:ILE:HD12	1.85	0.42
2:C:115:VAL:HG12	2:C:116:LYS:N	2.34	0.41
3:D:1047:ALA:N	3:D:1109:GLN:O	2.53	0.41
5:R:96:ARG:O	5:R:99:VAL:HG12	2.20	0.41
1:T:159:ILE:N	1:T:159:ILE:HD12	2.34	0.41
3:W:35:ASN:OD1	3:W:36:TYR:N	2.53	0.41
3:W:1051:GLY:H	3:W:1066:ILE:HD11	1.85	0.41
2:BA:354:THR:OG1	2:BA:362:GLU:OE2	2.38	0.41
2:BA:696:VAL:HG11	2:BA:702:ILE:CD1	2.50	0.41
5:QA:96:ARG:O	5:QA:99:VAL:HG12	2.20	0.41
3:UA:35:ASN:OD1	3:UA:36:TYR:N	2.53	0.41
3:UA:1051:GLY:H	3:UA:1066:ILE:HD11	1.85	0.41
2:C:354:THR:OG1	2:C:362:GLU:OE2	2.38	0.41
3:D:366:ILE:H	3:D:366:ILE:HD12	1.85	0.41
3:D:1039:VAL:O	3:D:1039:VAL:HG23	2.20	0.41
3:D:1051:GLY:H	3:D:1066:ILE:HD11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:642:VAL:HG22	2:I:703:ALA:HB3	2.02	0.41
3:J:1055:LEU:C	3:J:1055:LEU:HD23	2.45	0.41
3:P:302:PHE:HZ	3:P:312:MET:HE3	1.85	0.41
3:CA:1047:ALA:N	3:CA:1109:GLN:O	2.53	0.41
3:CA:1051:GLY:H	3:CA:1066:ILE:HD11	1.85	0.41
2:HA:258:MET:O	2:HA:261:THR:OG1	2.32	0.41
2:HA:487:GLU:O	2:HA:488:THR:OG1	2.31	0.41
2:HA:642:VAL:HG22	2:HA:703:ALA:HB3	2.02	0.41
3:IA:1055:LEU:HD23	3:IA:1055:LEU:C	2.45	0.41
5:KA:96:ARG:O	5:KA:99:VAL:HG12	2.20	0.41
3:OA:107:PHE:CD1	3:OA:107:PHE:C	2.97	0.41
1:SA:97:LEU:HB3	1:SA:136:VAL:HG22	2.02	0.41
1:SA:159:ILE:HD12	1:SA:159:ILE:N	2.34	0.41
3:UA:1249:LYS:O	3:UA:1252:VAL:HG12	2.20	0.41
2:C:696:VAL:HG11	2:C:702:ILE:CD1	2.50	0.41
5:F:96:ARG:O	5:F:99:VAL:HG12	2.20	0.41
3:J:159:ARG:O	3:J:162:VAL:HG12	2.21	0.41
5:L:96:ARG:O	5:L:99:VAL:HG12	2.20	0.41
1:M:20:GLN:NE2	1:M:195:ASP:OD2	2.54	0.41
1:T:97:LEU:HB3	1:T:136:VAL:HG22	2.02	0.41
2:BA:355:MET:SD	2:BA:356:THR:N	2.94	0.41
3:CA:1039:VAL:O	3:CA:1039:VAL:HG23	2.20	0.41
5:EA:96:ARG:O	5:EA:99:VAL:HG12	2.20	0.41
3:IA:159:ARG:O	3:IA:162:VAL:HG12	2.21	0.41
3:IA:638:THR:O	3:IA:638:THR:HG22	2.20	0.41
1:LA:20:GLN:NE2	1:LA:195:ASP:OD2	2.54	0.41
3:UA:1047:ALA:N	3:UA:1109:GLN:O	2.53	0.41
2:C:355:MET:SD	2:C:356:THR:N	2.94	0.41
2:I:1051:MET:SD	2:I:1051:MET:N	2.79	0.41
3:J:283:ASN:OD1	3:J:284:GLY:N	2.46	0.41
3:J:638:THR:O	3:J:638:THR:HG22	2.20	0.41
3:P:107:PHE:CD1	3:P:107:PHE:C	2.97	0.41
3:W:302:PHE:HZ	3:W:312:MET:HE3	1.85	0.41
3:W:1047:ALA:N	3:W:1109:GLN:O	2.53	0.41
3:W:1051:GLY:N	3:W:1066:ILE:HD11	2.35	0.41
3:W:1249:LYS:O	3:W:1252:VAL:HG12	2.20	0.41
2:HA:1051:MET:SD	2:HA:1051:MET:N	2.79	0.41
2:NA:696:VAL:HG11	2:NA:702:ILE:CD1	2.50	0.41
3:OA:302:PHE:HZ	3:OA:312:MET:HE3	1.85	0.41
3:OA:1121:VAL:HG23	3:OA:1130:VAL:CG1	2.47	0.41
5:WA:108:ARG:HB2	5:WA:154:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:GLN:NE2	1:G:195:ASP:OD2	2.54	0.41
3:J:1047:ALA:N	3:J:1109:GLN:O	2.53	0.41
2:O:696:VAL:HG11	2:O:702:ILE:CD1	2.50	0.41
5:Y:108:ARG:HB2	5:Y:154:MET:CE	2.50	0.41
3:IA:1047:ALA:N	3:IA:1109:GLN:O	2.53	0.41
3:UA:302:PHE:HZ	3:UA:312:MET:HE3	1.85	0.41
3:UA:638:THR:O	3:UA:638:THR:HG22	2.20	0.41
3:UA:1051:GLY:N	3:UA:1066:ILE:HD11	2.35	0.41
3:D:159:ARG:O	3:D:162:VAL:HG12	2.21	0.41
3:J:930:VAL:HG22	3:J:936:VAL:HG12	2.01	0.41
3:P:1121:VAL:HG23	3:P:1130:VAL:CG1	2.47	0.41
3:W:638:THR:O	3:W:638:THR:HG22	2.20	0.41
3:W:916:ILE:HD11	3:W:949:ILE:HD12	2.02	0.41
3:CA:159:ARG:O	3:CA:162:VAL:HG12	2.21	0.41
1:FA:20:GLN:NE2	1:FA:195:ASP:OD2	2.54	0.41
3:IA:930:VAL:HG22	3:IA:936:VAL:HG12	2.01	0.41
2:NA:354:THR:OG1	2:NA:362:GLU:OE2	2.38	0.41
2:TA:355:MET:SD	2:TA:356:THR:N	2.94	0.41
3:UA:916:ILE:HD11	3:UA:949:ILE:HD12	2.02	0.41
1:B:97:LEU:HB3	1:B:136:VAL:HG22	2.02	0.41
2:C:972:VAL:HG12	2:C:973:SER:N	2.36	0.41
2:O:354:THR:OG1	2:O:362:GLU:OE2	2.38	0.41
2:O:1075:ALA:HB3	3:P:509:ILE:HD12	2.02	0.41
3:P:159:ARG:O	3:P:162:VAL:HG12	2.21	0.41
3:P:1051:GLY:N	3:P:1066:ILE:HD11	2.35	0.41
1:S:16:ASP:OD1	1:S:16:ASP:N	2.54	0.41
1:T:18:ARG:O	1:T:19:SER:OG	2.30	0.41
2:V:355:MET:SD	2:V:356:THR:N	2.94	0.41
2:V:1075:ALA:HB3	3:W:509:ILE:HD12	2.02	0.41
5:Y:106:THR:OG1	5:Y:107:GLY:N	2.54	0.41
1:AA:97:LEU:HB3	1:AA:136:VAL:HG22	2.02	0.41
2:BA:972:VAL:HG12	2:BA:973:SER:N	2.36	0.41
3:IA:1053:VAL:O	3:IA:1102:GLY:N	2.49	0.41
3:OA:159:ARG:O	3:OA:162:VAL:HG12	2.21	0.41
3:OA:283:ASN:OD1	3:OA:284:GLY:N	2.46	0.41
1:RA:16:ASP:OD1	1:RA:16:ASP:N	2.54	0.41
3:J:1051:GLY:N	3:J:1066:ILE:HD11	2.35	0.41
2:O:355:MET:SD	2:O:356:THR:N	2.94	0.41
1:T:130:ASP:OD2	1:T:131:LYS:NZ	2.51	0.41
3:W:1129:GLU:OE1	3:W:1132:ILE:HD11	2.21	0.41
1:Z:20:GLN:NE2	1:Z:195:ASP:OD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:197:GLU:OE1	1:FA:198:THR:N	2.50	0.41
2:HA:696:VAL:HG11	2:HA:702:ILE:CD1	2.50	0.41
3:OA:1051:GLY:N	3:OA:1066:ILE:HD11	2.35	0.41
3:OA:1058:GLY:O	3:OA:1081:SER:OG	2.35	0.41
1:SA:18:ARG:O	1:SA:19:SER:OG	2.30	0.41
1:SA:130:ASP:OD2	1:SA:131:LYS:NZ	2.51	0.41
5:WA:106:THR:OG1	5:WA:107:GLY:N	2.54	0.41
1:A:20:GLN:NE2	1:A:195:ASP:OD2	2.54	0.41
2:C:642:VAL:HG22	2:C:703:ALA:HB3	2.02	0.41
3:D:638:THR:O	3:D:638:THR:HG22	2.20	0.41
3:D:910:LEU:HD21	3:D:953:LEU:HD13	2.03	0.41
3:D:1012:MET:N	3:D:1012:MET:SD	2.94	0.41
3:D:1051:GLY:N	3:D:1066:ILE:HD11	2.35	0.41
3:D:1053:VAL:O	3:D:1102:GLY:N	2.49	0.41
3:D:1249:LYS:O	3:D:1252:VAL:HG12	2.20	0.41
4:E:54:VAL:HG13	4:E:55:ILE:N	2.35	0.41
1:G:150:VAL:O	1:G:150:VAL:HG22	2.21	0.41
1:G:197:GLU:OE1	1:G:198:THR:N	2.50	0.41
1:H:97:LEU:HB3	1:H:136:VAL:HG22	2.02	0.41
2:I:696:VAL:HG11	2:I:702:ILE:CD1	2.50	0.41
3:J:1053:VAL:O	3:J:1102:GLY:N	2.49	0.41
1:N:97:LEU:HB3	1:N:136:VAL:HG22	2.02	0.41
3:P:283:ASN:OD1	3:P:284:GLY:N	2.46	0.41
3:P:313:VAL:O	3:P:313:VAL:HG23	2.20	0.41
3:P:1211:THR:O	3:P:1215:LEU:HD13	2.21	0.41
1:S:20:GLN:NE2	1:S:195:ASP:OD2	2.54	0.41
2:V:972:VAL:HG12	2:V:973:SER:N	2.36	0.41
3:W:202:GLU:O	3:W:206:ARG:HG2	2.21	0.41
3:W:1012:MET:SD	3:W:1012:MET:N	2.94	0.41
3:W:1039:VAL:O	3:W:1039:VAL:HG23	2.20	0.41
3:W:1211:THR:O	3:W:1215:LEU:HD13	2.21	0.41
2:BA:642:VAL:HG22	2:BA:703:ALA:HB3	2.02	0.41
3:CA:638:THR:O	3:CA:638:THR:HG22	2.20	0.41
3:CA:910:LEU:HD21	3:CA:953:LEU:HD13	2.03	0.41
3:CA:1012:MET:N	3:CA:1012:MET:SD	2.94	0.41
3:CA:1051:GLY:N	3:CA:1066:ILE:HD11	2.35	0.41
3:CA:1053:VAL:O	3:CA:1102:GLY:N	2.49	0.41
4:DA:54:VAL:HG13	4:DA:55:ILE:N	2.35	0.41
1:FA:150:VAL:O	1:FA:150:VAL:HG22	2.21	0.41
3:IA:1051:GLY:N	3:IA:1066:ILE:HD11	2.35	0.41
1:MA:97:LEU:HB3	1:MA:136:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:NA:355:MET:SD	2:NA:356:THR:N	2.94	0.41
2:NA:1075:ALA:HB3	3:OA:509:ILE:HD12	2.02	0.41
3:OA:313:VAL:HG23	3:OA:313:VAL:O	2.20	0.41
2:TA:972:VAL:HG12	2:TA:973:SER:N	2.36	0.41
2:TA:1075:ALA:HB3	3:UA:509:ILE:HD12	2.02	0.41
3:UA:202:GLU:O	3:UA:206:ARG:HG2	2.21	0.41
3:UA:1012:MET:SD	3:UA:1012:MET:N	2.94	0.41
3:UA:1129:GLU:OE1	3:UA:1132:ILE:HD11	2.21	0.41
3:UA:1211:THR:O	3:UA:1215:LEU:HD13	2.21	0.41
3:D:206:ARG:HE	3:D:209:ARG:NH1	2.19	0.41
3:D:331:ASP:N	3:D:331:ASP:OD1	2.54	0.41
3:J:35:ASN:OD1	3:J:36:TYR:N	2.53	0.41
3:J:331:ASP:OD1	3:J:331:ASP:N	2.54	0.41
2:O:972:VAL:HG12	2:O:973:SER:N	2.36	0.41
3:P:638:THR:HG22	3:P:638:THR:O	2.20	0.41
3:P:1055:LEU:HD23	3:P:1055:LEU:C	2.45	0.41
5:R:68:LEU:HD21	5:R:72:ARG:HD3	2.03	0.41
3:W:1058:GLY:O	3:W:1081:SER:OG	2.35	0.41
5:Y:96:ARG:O	5:Y:99:VAL:HG12	2.20	0.41
1:Z:197:GLU:OE1	1:Z:198:THR:N	2.50	0.41
3:CA:206:ARG:HE	3:CA:209:ARG:NH1	2.19	0.41
3:CA:331:ASP:N	3:CA:331:ASP:OD1	2.54	0.41
3:CA:1103:ASP:OD1	3:CA:1104:HIS:N	2.47	0.41
1:GA:97:LEU:HB3	1:GA:136:VAL:HG22	2.02	0.41
3:IA:331:ASP:OD1	3:IA:331:ASP:N	2.54	0.41
3:OA:1055:LEU:HD23	3:OA:1055:LEU:C	2.45	0.41
3:OA:1211:THR:O	3:OA:1215:LEU:HD13	2.21	0.41
1:RA:20:GLN:NE2	1:RA:195:ASP:OD2	2.54	0.41
3:UA:331:ASP:OD1	3:UA:331:ASP:N	2.54	0.41
3:UA:1039:VAL:O	3:UA:1039:VAL:HG23	2.20	0.41
3:D:429:VAL:HG12	3:D:430:ILE:N	2.36	0.40
5:F:68:LEU:HD21	5:F:72:ARG:HD3	2.03	0.40
2:I:1075:ALA:HB3	3:J:509:ILE:HD12	2.02	0.40
3:J:206:ARG:HE	3:J:209:ARG:NH1	2.19	0.40
3:P:910:LEU:HD21	3:P:953:LEU:HD13	2.03	0.40
3:P:1012:MET:SD	3:P:1012:MET:N	2.94	0.40
3:W:331:ASP:OD1	3:W:331:ASP:N	2.54	0.40
3:CA:429:VAL:HG12	3:CA:430:ILE:N	2.36	0.40
3:CA:1249:LYS:O	3:CA:1252:VAL:HG12	2.20	0.40
5:EA:68:LEU:HD21	5:EA:72:ARG:HD3	2.03	0.40
2:HA:355:MET:SD	2:HA:356:THR:N	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:IA:35:ASN:OD1	3:IA:36:TYR:N	2.53	0.40
2:NA:972:VAL:HG12	2:NA:973:SER:N	2.36	0.40
3:OA:1012:MET:SD	3:OA:1012:MET:N	2.94	0.40
5:QA:68:LEU:HD21	5:QA:72:ARG:HD3	2.03	0.40
3:UA:1058:GLY:O	3:UA:1081:SER:OG	2.35	0.40
3:D:202:GLU:O	3:D:206:ARG:HG2	2.21	0.40
2:I:355:MET:SD	2:I:356:THR:N	2.94	0.40
3:J:1129:GLU:OE1	3:J:1132:ILE:HD11	2.21	0.40
3:P:1129:GLU:OE1	3:P:1132:ILE:HD11	2.21	0.40
5:R:106:THR:OG1	5:R:107:GLY:N	2.54	0.40
2:V:455:LEU:HD11	2:V:500:LEU:HD22	2.04	0.40
3:W:429:VAL:HG12	3:W:430:ILE:N	2.36	0.40
3:CA:1129:GLU:OE1	3:CA:1132:ILE:HD11	2.21	0.40
2:HA:1075:ALA:HB3	3:IA:509:ILE:HD12	2.02	0.40
3:IA:206:ARG:HE	3:IA:209:ARG:NH1	2.19	0.40
3:IA:1129:GLU:OE1	3:IA:1132:ILE:HD11	2.21	0.40
3:OA:638:THR:O	3:OA:638:THR:HG22	2.20	0.40
3:OA:910:LEU:HD21	3:OA:953:LEU:HD13	2.03	0.40
5:QA:106:THR:OG1	5:QA:107:GLY:N	2.54	0.40
2:TA:455:LEU:HD11	2:TA:500:LEU:HD22	2.04	0.40
3:UA:429:VAL:HG12	3:UA:430:ILE:N	2.36	0.40
3:UA:1121:VAL:CG2	3:UA:1130:VAL:HG12	2.46	0.40
5:WA:96:ARG:O	5:WA:99:VAL:HG12	2.20	0.40
1:A:197:GLU:OE1	1:A:198:THR:N	2.50	0.40
1:B:182:ARG:HA	1:B:187:THR:HA	2.04	0.40
2:C:444:ASN:OD1	2:C:444:ASN:N	2.55	0.40
2:C:762:THR:OG1	2:C:765:GLY:O	2.34	0.40
3:D:1103:ASP:OD1	3:D:1104:HIS:N	2.47	0.40
3:D:1129:GLU:OE1	3:D:1132:ILE:HD11	2.21	0.40
2:I:972:VAL:HG12	2:I:973:SER:N	2.36	0.40
3:P:1073:GLU:OE1	3:P:1073:GLU:N	2.55	0.40
3:W:159:ARG:O	3:W:162:VAL:HG12	2.21	0.40
3:W:1121:VAL:CG2	3:W:1130:VAL:HG12	2.46	0.40
1:AA:182:ARG:HA	1:AA:187:THR:HA	2.04	0.40
2:BA:444:ASN:OD1	2:BA:444:ASN:N	2.55	0.40
3:CA:202:GLU:O	3:CA:206:ARG:HG2	2.21	0.40
3:CA:1073:GLU:OE1	3:CA:1073:GLU:N	2.55	0.40
1:LA:16:ASP:OD1	1:LA:16:ASP:N	2.54	0.40
3:OA:1073:GLU:N	3:OA:1073:GLU:OE1	2.55	0.40
3:OA:1129:GLU:OE1	3:OA:1132:ILE:HD11	2.21	0.40
3:UA:159:ARG:O	3:UA:162:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:THR:N	1:B:189:PHE:O	2.55	0.40
2:C:455:LEU:HD11	2:C:500:LEU:HD22	2.04	0.40
3:D:1073:GLU:OE1	3:D:1073:GLU:N	2.55	0.40
3:J:910:LEU:HD21	3:J:953:LEU:HD13	2.03	0.40
3:J:923:ARG:NH1	3:J:964:SER:OG	2.54	0.40
3:J:1170:SER:O	3:J:1173:THR:OG1	2.29	0.40
1:M:16:ASP:OD1	1:M:16:ASP:N	2.54	0.40
3:P:916:ILE:HD11	3:P:949:ILE:HD12	2.02	0.40
1:T:181:THR:N	1:T:189:PHE:O	2.55	0.40
1:AA:181:THR:N	1:AA:189:PHE:O	2.55	0.40
2:BA:60:SER:OG	2:BA:382:GLY:N	2.46	0.40
2:BA:455:LEU:HD11	2:BA:500:LEU:HD22	2.04	0.40
2:NA:455:LEU:HD11	2:NA:500:LEU:HD22	2.04	0.40
1:SA:181:THR:N	1:SA:189:PHE:O	2.55	0.40
3:D:754:ASP:O	3:D:758:LYS:HG2	2.21	0.40
3:J:1012:MET:N	3:J:1012:MET:SD	2.94	0.40
2:O:455:LEU:HD11	2:O:500:LEU:HD22	2.04	0.40
3:W:206:ARG:HE	3:W:209:ARG:NH1	2.19	0.40
3:W:369:ASN:ND2	3:W:372:ARG:HH22	2.20	0.40
3:W:1138:VAL:HA	3:W:1141:VAL:HG12	2.04	0.40
2:BA:762:THR:OG1	2:BA:765:GLY:O	2.34	0.40
3:CA:1138:VAL:HA	3:CA:1141:VAL:HG12	2.04	0.40
2:HA:972:VAL:HG12	2:HA:973:SER:N	2.36	0.40
3:IA:202:GLU:O	3:IA:206:ARG:HG2	2.21	0.40
3:IA:923:ARG:NH1	3:IA:964:SER:OG	2.54	0.40
3:OA:916:ILE:HD11	3:OA:949:ILE:HD12	2.02	0.40
3:UA:206:ARG:HE	3:UA:209:ARG:NH1	2.19	0.40
3:UA:1138:VAL:HA	3:UA:1141:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/347 (64%)	212 (96%)	9 (4%)	0	100	100
1	AA	228/347 (66%)	222 (97%)	6 (3%)	0	100	100
1	B	228/347 (66%)	222 (97%)	6 (3%)	0	100	100
1	FA	221/347 (64%)	212 (96%)	9 (4%)	0	100	100
1	G	221/347 (64%)	212 (96%)	9 (4%)	0	100	100
1	GA	228/347 (66%)	222 (97%)	6 (3%)	0	100	100
1	H	228/347 (66%)	222 (97%)	6 (3%)	0	100	100
1	LA	221/347 (64%)	212 (96%)	9 (4%)	0	100	100
1	M	221/347 (64%)	212 (96%)	9 (4%)	0	100	100
1	MA	228/347 (66%)	222 (97%)	6 (3%)	0	100	100
1	N	228/347 (66%)	222 (97%)	6 (3%)	0	100	100
1	RA	221/347 (64%)	212 (96%)	9 (4%)	0	100	100
1	S	221/347 (64%)	212 (96%)	9 (4%)	0	100	100
1	SA	228/347 (66%)	222 (97%)	6 (3%)	0	100	100
1	T	228/347 (66%)	222 (97%)	6 (3%)	0	100	100
1	Z	221/347 (64%)	212 (96%)	9 (4%)	0	100	100
2	BA	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100	100
2	C	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100	100
2	HA	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100	100
2	I	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100	100
2	NA	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100	100
2	O	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100	100
2	TA	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100	100
2	V	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100	100
3	CA	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100	100
3	D	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100	100
3	IA	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100	100
3	J	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100	100
3	OA	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100	100
3	P	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100	100
3	UA	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100	100
3	W	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	DA	81/110 (74%)	75 (93%)	6 (7%)	0	100	100
4	E	81/110 (74%)	75 (93%)	6 (7%)	0	100	100
4	JA	81/110 (74%)	75 (93%)	6 (7%)	0	100	100
4	K	81/110 (74%)	75 (93%)	6 (7%)	0	100	100
4	PA	81/110 (74%)	75 (93%)	6 (7%)	0	100	100
4	Q	81/110 (74%)	75 (93%)	6 (7%)	0	100	100
4	VA	81/110 (74%)	75 (93%)	6 (7%)	0	100	100
4	X	81/110 (74%)	75 (93%)	6 (7%)	0	100	100
5	EA	140/343 (41%)	136 (97%)	4 (3%)	0	100	100
5	F	140/343 (41%)	136 (97%)	4 (3%)	0	100	100
5	KA	140/343 (41%)	136 (97%)	4 (3%)	0	100	100
5	L	140/343 (41%)	136 (97%)	4 (3%)	0	100	100
5	QA	140/343 (41%)	136 (97%)	4 (3%)	0	100	100
5	R	140/343 (41%)	136 (97%)	4 (3%)	0	100	100
5	WA	140/343 (41%)	136 (97%)	4 (3%)	0	100	100
5	Y	140/343 (41%)	136 (97%)	4 (3%)	0	100	100
All	All	24360/29120 (84%)	23496 (96%)	864 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/297 (65%)	191 (100%)	1 (0%)	81	81
1	AA	197/297 (66%)	197 (100%)	0	100	100
1	B	197/297 (66%)	197 (100%)	0	100	100
1	FA	192/297 (65%)	191 (100%)	1 (0%)	81	81
1	G	192/297 (65%)	191 (100%)	1 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GA	197/297 (66%)	197 (100%)	0	100	100
1	H	197/297 (66%)	197 (100%)	0	100	100
1	LA	192/297 (65%)	191 (100%)	1 (0%)	81	81
1	M	192/297 (65%)	191 (100%)	1 (0%)	81	81
1	MA	197/297 (66%)	197 (100%)	0	100	100
1	N	197/297 (66%)	197 (100%)	0	100	100
1	RA	192/297 (65%)	191 (100%)	1 (0%)	81	81
1	S	192/297 (65%)	191 (100%)	1 (0%)	81	81
1	SA	197/297 (66%)	197 (100%)	0	100	100
1	T	197/297 (66%)	197 (100%)	0	100	100
1	Z	192/297 (65%)	191 (100%)	1 (0%)	81	81
2	BA	946/995 (95%)	943 (100%)	3 (0%)	86	84
2	C	946/995 (95%)	943 (100%)	3 (0%)	86	84
2	HA	946/995 (95%)	943 (100%)	3 (0%)	86	84
2	I	946/995 (95%)	943 (100%)	3 (0%)	86	84
2	NA	946/995 (95%)	943 (100%)	3 (0%)	86	84
2	O	946/995 (95%)	943 (100%)	3 (0%)	86	84
2	TA	946/995 (95%)	943 (100%)	3 (0%)	86	84
2	V	946/995 (95%)	943 (100%)	3 (0%)	86	84
3	CA	1058/1098 (96%)	1051 (99%)	7 (1%)	76	79
3	D	1058/1098 (96%)	1051 (99%)	7 (1%)	76	79
3	IA	1058/1098 (96%)	1051 (99%)	7 (1%)	76	79
3	J	1058/1098 (96%)	1051 (99%)	7 (1%)	76	79
3	OA	1058/1098 (96%)	1051 (99%)	7 (1%)	76	79
3	P	1058/1098 (96%)	1051 (99%)	7 (1%)	76	79
3	UA	1058/1098 (96%)	1051 (99%)	7 (1%)	76	79
3	W	1058/1098 (96%)	1051 (99%)	7 (1%)	76	79
4	DA	70/90 (78%)	70 (100%)	0	100	100
4	E	70/90 (78%)	70 (100%)	0	100	100
4	JA	70/90 (78%)	70 (100%)	0	100	100
4	K	70/90 (78%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	PA	70/90 (78%)	70 (100%)	0	100	100
4	Q	70/90 (78%)	70 (100%)	0	100	100
4	VA	70/90 (78%)	70 (100%)	0	100	100
4	X	70/90 (78%)	70 (100%)	0	100	100
5	EA	111/284 (39%)	104 (94%)	7 (6%)	16	38
5	F	111/284 (39%)	104 (94%)	7 (6%)	16	38
5	KA	111/284 (39%)	104 (94%)	7 (6%)	16	38
5	L	111/284 (39%)	104 (94%)	7 (6%)	16	38
5	QA	111/284 (39%)	104 (94%)	7 (6%)	16	38
5	R	111/284 (39%)	104 (94%)	7 (6%)	16	38
5	WA	111/284 (39%)	104 (94%)	7 (6%)	16	38
5	Y	111/284 (39%)	104 (94%)	7 (6%)	16	38
All	All	20592/24488 (84%)	20448 (99%)	144 (1%)	73	79

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
2	C	581	VAL
2	C	611	MET
2	C	1125	LEU
3	D	33	THR
3	D	60	CYS
3	D	67	ARG
3	D	134	TYR
3	D	154	GLU
3	D	225	THR
3	D	777	ILE
5	F	30	TYR
5	F	39	LEU
5	F	50	LYS
5	F	66	LYS
5	F	74	ARG
5	F	92	GLU
5	F	138	PHE
1	G	15	THR
2	I	581	VAL
2	I	611	MET

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Mol	Chain	Res	Type
2	I	1125	LEU
3	J	33	THR
3	J	60	CYS
3	J	67	ARG
3	J	134	TYR
3	J	154	GLU
3	J	225	THR
3	J	777	ILE
5	L	30	TYR
5	L	39	LEU
5	L	50	LYS
5	L	66	LYS
5	L	74	ARG
5	L	92	GLU
5	L	138	PHE
1	M	15	THR
2	O	581	VAL
2	O	611	MET
2	O	1125	LEU
3	P	33	THR
3	P	60	CYS
3	P	67	ARG
3	P	134	TYR
3	P	154	GLU
3	P	225	THR
3	P	777	ILE
5	R	30	TYR
5	R	39	LEU
5	R	50	LYS
5	R	66	LYS
5	R	74	ARG
5	R	92	GLU
5	R	138	PHE
1	S	15	THR
2	V	581	VAL
2	V	611	MET
2	V	1125	LEU
3	W	33	THR
3	W	60	CYS
3	W	67	ARG
3	W	134	TYR
3	W	154	GLU

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Mol	Chain	Res	Type
3	W	225	THR
3	W	777	ILE
5	Y	30	TYR
5	Y	39	LEU
5	Y	50	LYS
5	Y	66	LYS
5	Y	74	ARG
5	Y	92	GLU
5	Y	138	PHE
1	Z	15	THR
2	BA	581	VAL
2	BA	611	MET
2	BA	1125	LEU
3	CA	33	THR
3	CA	60	CYS
3	CA	67	ARG
3	CA	134	TYR
3	CA	154	GLU
3	CA	225	THR
3	CA	777	ILE
5	EA	30	TYR
5	EA	39	LEU
5	EA	50	LYS
5	EA	66	LYS
5	EA	74	ARG
5	EA	92	GLU
5	EA	138	PHE
1	FA	15	THR
2	HA	581	VAL
2	HA	611	MET
2	HA	1125	LEU
3	IA	33	THR
3	IA	60	CYS
3	IA	67	ARG
3	IA	134	TYR
3	IA	154	GLU
3	IA	225	THR
3	IA	777	ILE
5	KA	30	TYR
5	KA	39	LEU
5	KA	50	LYS
5	KA	66	LYS

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Mol	Chain	Res	Type
5	KA	74	ARG
5	KA	92	GLU
5	KA	138	PHE
1	LA	15	THR
2	NA	581	VAL
2	NA	611	MET
2	NA	1125	LEU
3	OA	33	THR
3	OA	60	CYS
3	OA	67	ARG
3	OA	134	TYR
3	OA	154	GLU
3	OA	225	THR
3	OA	777	ILE
5	QA	30	TYR
5	QA	39	LEU
5	QA	50	LYS
5	QA	66	LYS
5	QA	74	ARG
5	QA	92	GLU
5	QA	138	PHE
1	RA	15	THR
2	TA	581	VAL
2	TA	611	MET
2	TA	1125	LEU
3	UA	33	THR
3	UA	60	CYS
3	UA	67	ARG
3	UA	134	TYR
3	UA	154	GLU
3	UA	225	THR
3	UA	777	ILE
5	WA	30	TYR
5	WA	39	LEU
5	WA	50	LYS
5	WA	66	LYS
5	WA	74	ARG
5	WA	92	GLU
5	WA	138	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	352	GLN
2	C	614	GLN
2	C	718	ASN
2	C	841	HIS
2	C	935	HIS
3	D	262	GLN
3	D	368	ASN
3	D	369	ASN
3	D	465	HIS
3	D	748	HIS
3	D	787	GLN
1	G	226	ASN
2	I	352	GLN
2	I	585	GLN
2	I	614	GLN
2	I	718	ASN
2	I	841	HIS
2	I	935	HIS
2	I	986	GLN
2	I	1034	HIS
3	J	146	ASN
3	J	165	GLN
3	J	262	GLN
3	J	368	ASN
3	J	369	ASN
3	J	465	HIS
3	J	494	HIS
3	J	787	GLN
1	M	20	GLN
1	M	119	HIS
2	O	352	GLN
2	O	599	HIS
2	O	614	GLN
2	O	718	ASN
2	O	841	HIS
2	O	935	HIS
2	O	986	GLN
2	O	1034	HIS
3	P	262	GLN
3	P	368	ASN
3	P	369	ASN
3	P	465	HIS
3	P	748	HIS

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Mol	Chain	Res	Type
3	P	787	GLN
1	S	119	HIS
2	V	352	GLN
2	V	599	HIS
2	V	614	GLN
2	V	718	ASN
2	V	841	HIS
2	V	935	HIS
2	V	986	GLN
2	V	1034	HIS
3	W	146	ASN
3	W	262	GLN
3	W	368	ASN
3	W	369	ASN
3	W	465	HIS
3	W	748	HIS
3	W	787	GLN
1	Z	119	HIS
2	BA	352	GLN
2	BA	614	GLN
2	BA	718	ASN
2	BA	841	HIS
2	BA	935	HIS
2	BA	1034	HIS
3	CA	262	GLN
3	CA	368	ASN
3	CA	369	ASN
3	CA	465	HIS
3	CA	494	HIS
3	CA	748	HIS
3	CA	787	GLN
1	FA	119	HIS
1	FA	226	ASN
2	HA	352	GLN
2	HA	585	GLN
2	HA	614	GLN
2	HA	718	ASN
2	HA	841	HIS
2	HA	935	HIS
2	HA	986	GLN
2	HA	1034	HIS
3	IA	165	GLN

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Mol	Chain	Res	Type
3	IA	262	GLN
3	IA	368	ASN
3	IA	369	ASN
3	IA	465	HIS
3	IA	494	HIS
3	IA	787	GLN
1	LA	119	HIS
2	NA	352	GLN
2	NA	614	GLN
2	NA	718	ASN
2	NA	841	HIS
2	NA	935	HIS
2	NA	986	GLN
2	NA	1034	HIS
3	OA	262	GLN
3	OA	368	ASN
3	OA	369	ASN
3	OA	465	HIS
3	OA	494	HIS
3	OA	748	HIS
3	OA	787	GLN
1	RA	119	HIS
2	TA	352	GLN
2	TA	599	HIS
2	TA	614	GLN
2	TA	718	ASN
2	TA	841	HIS
2	TA	935	HIS
2	TA	986	GLN
2	TA	1034	HIS
3	UA	146	ASN
3	UA	262	GLN
3	UA	368	ASN
3	UA	369	ASN
3	UA	465	HIS
3	UA	748	HIS
3	UA	787	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

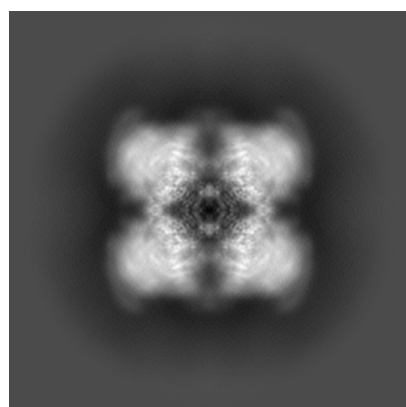
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13817. These allow visual inspection of the internal detail of the map and identification of artifacts.

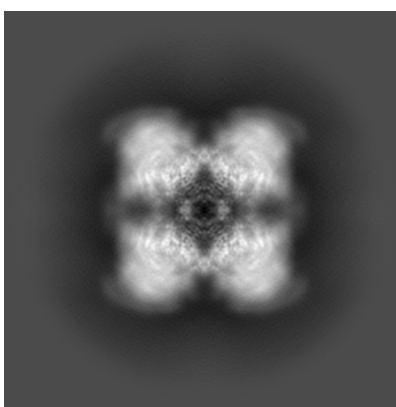
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

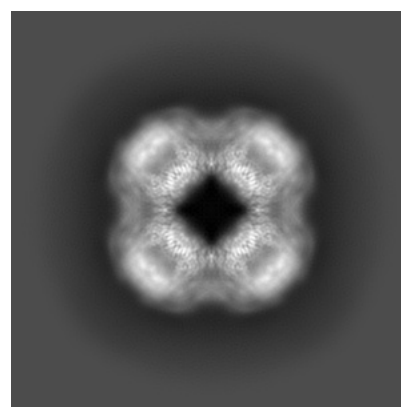
6.1.1 Primary map



X



Y

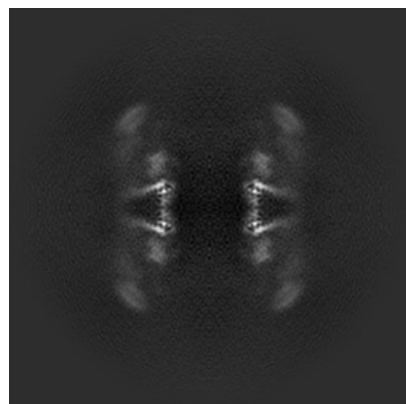


Z

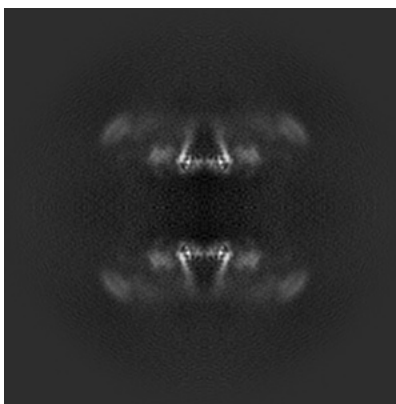
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

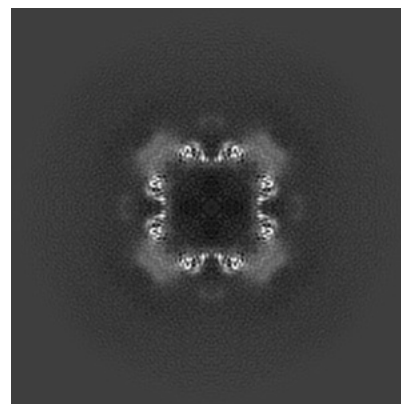
6.2.1 Primary map



X Index: 225



Y Index: 225

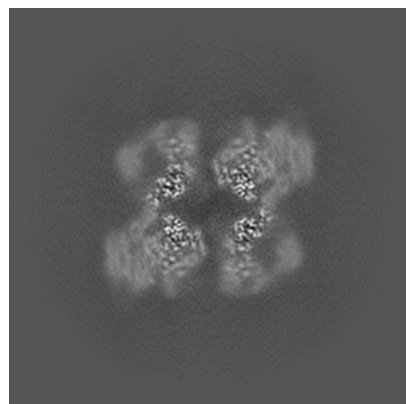


Z Index: 225

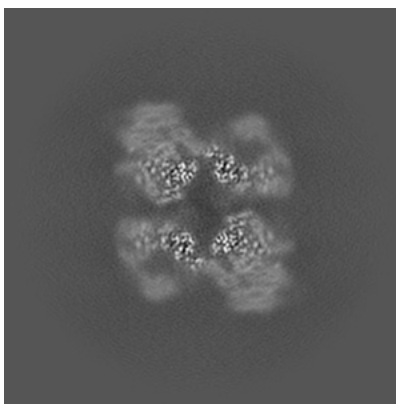
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

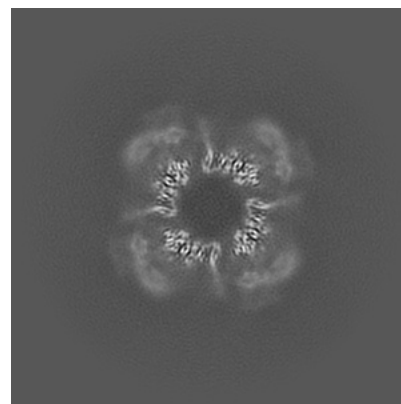
6.3.1 Primary map



X Index: 262



Y Index: 262

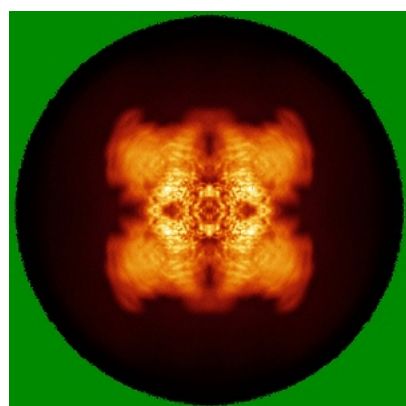


Z Index: 201

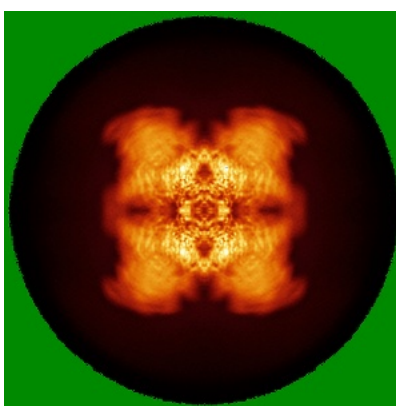
The images above show the largest variance slices of the map in three orthogonal directions.

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

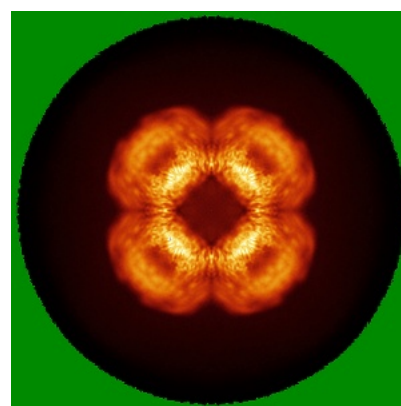
6.4.1 Primary map



X



Y

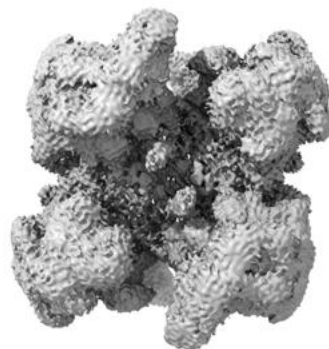


Z

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](#)

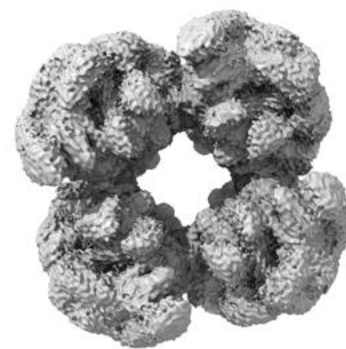
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

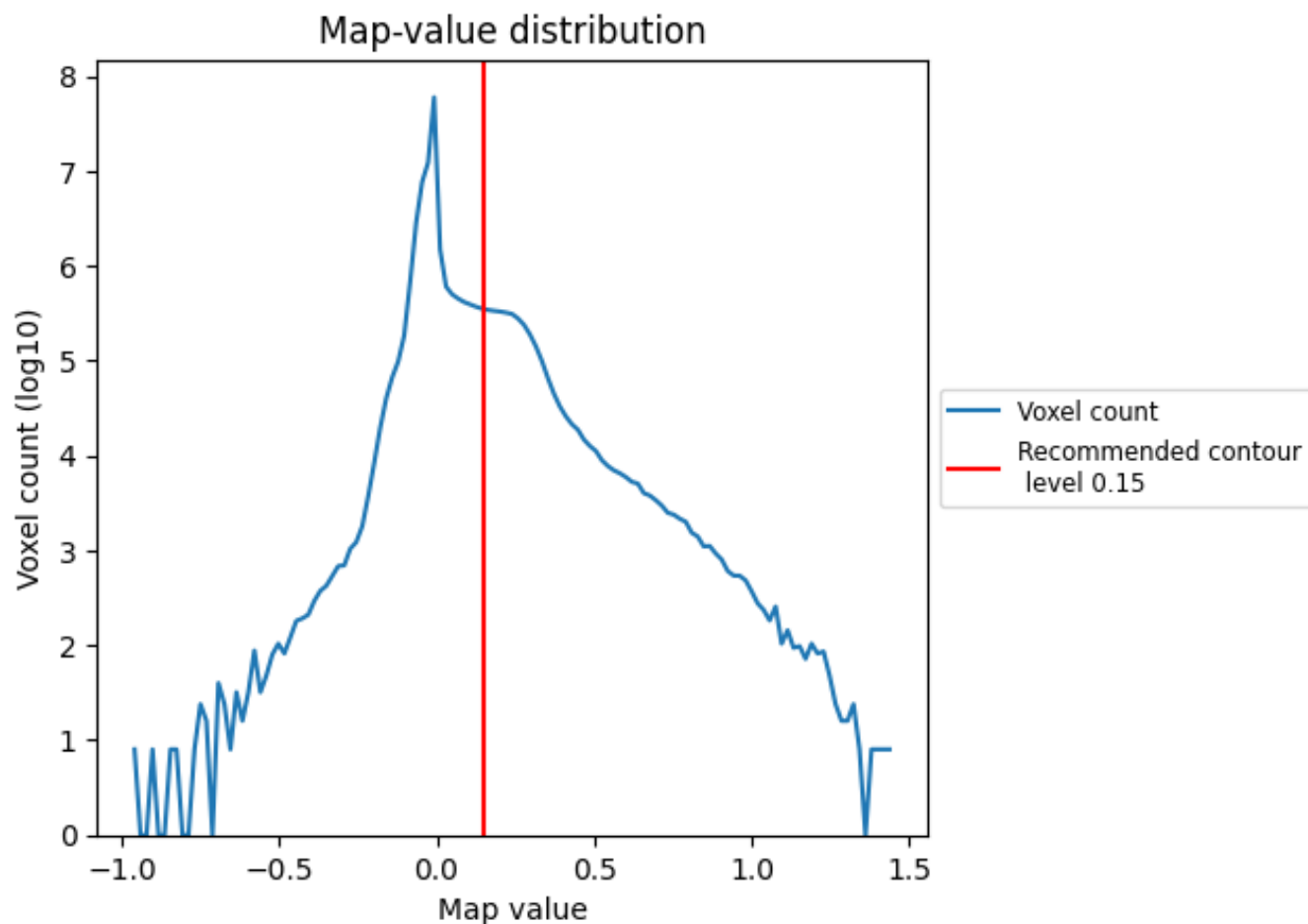
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

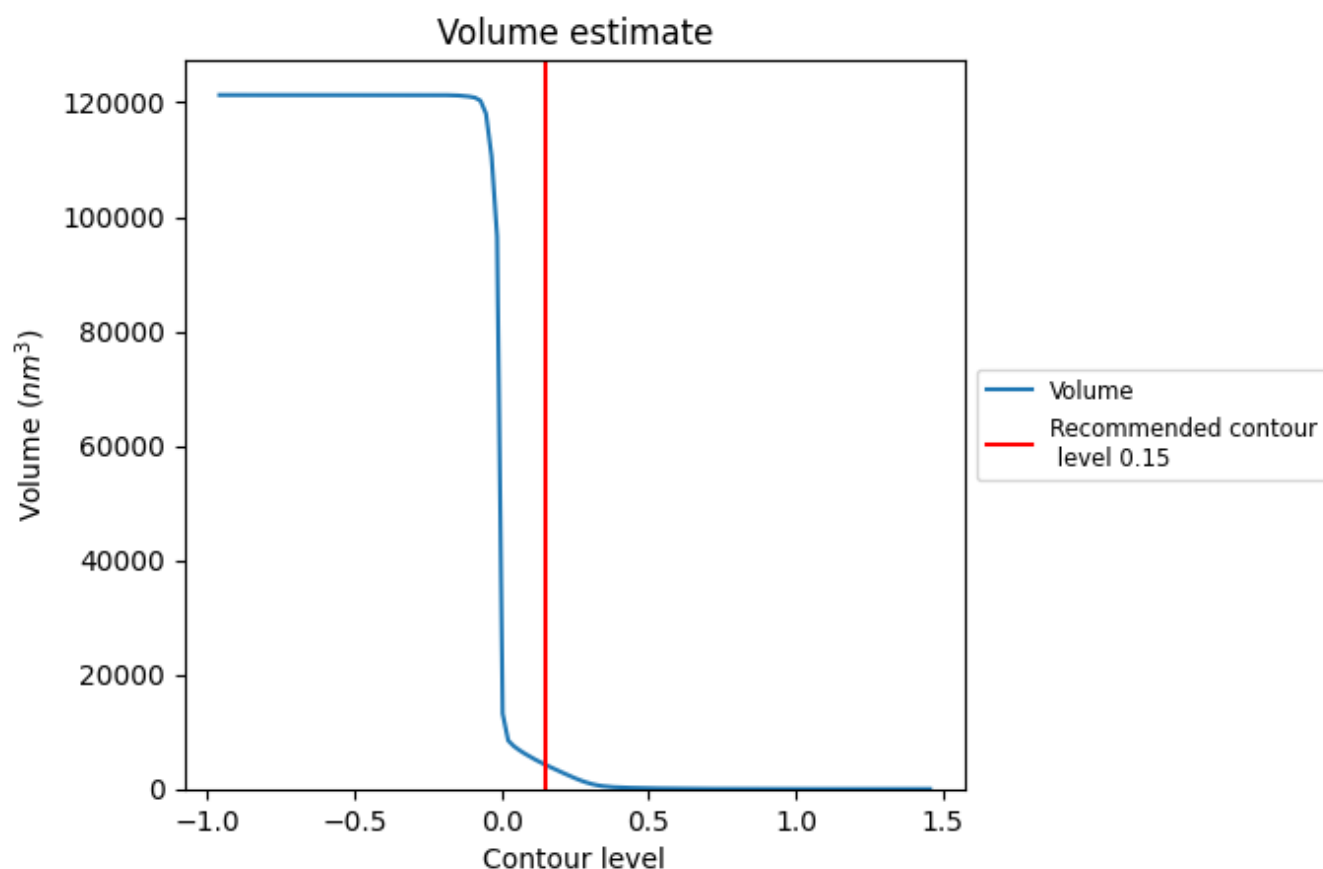
This section contains the results of statistical analysis of the map.

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.

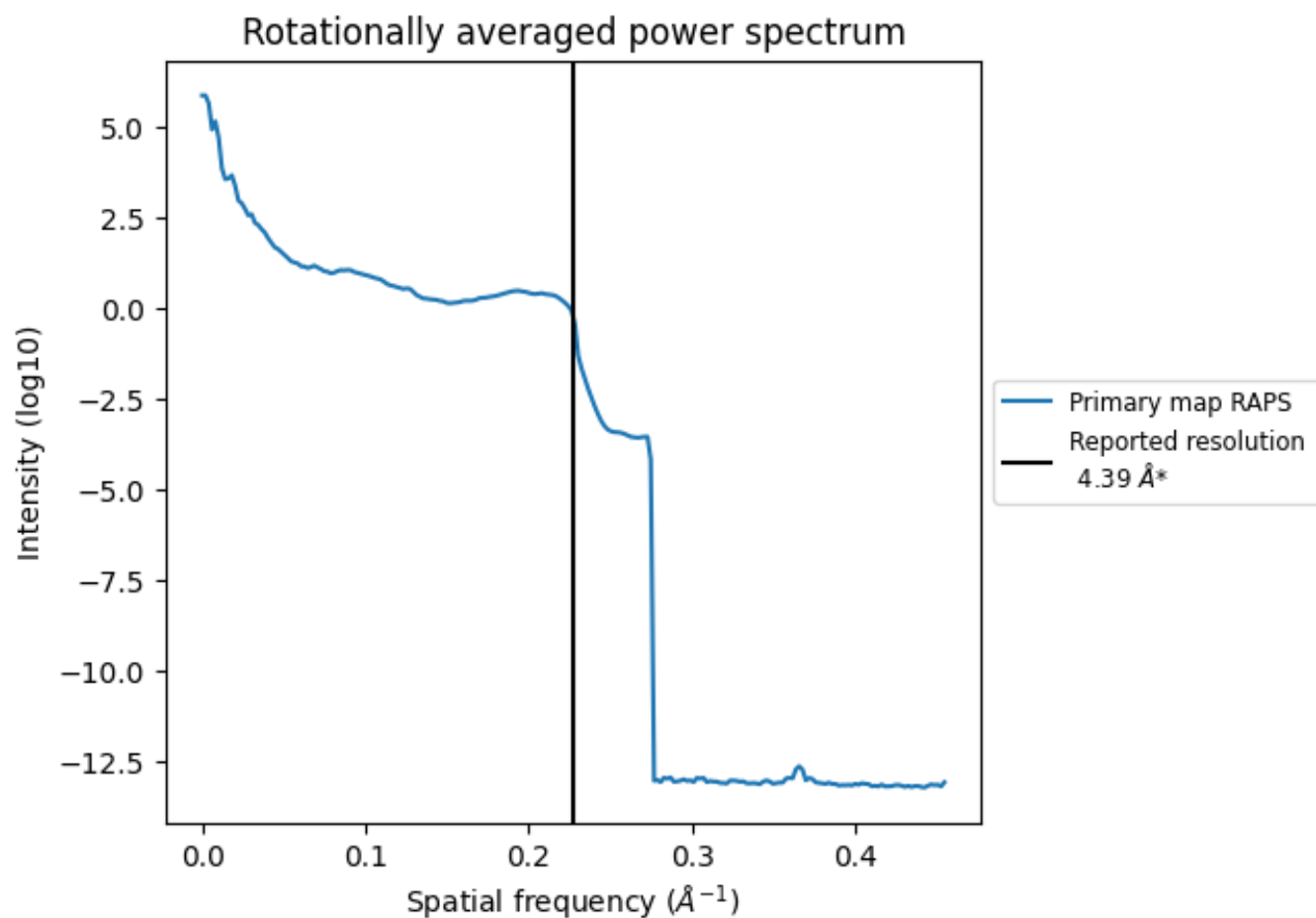
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4205 nm³; this corresponds to an approximate mass of 3799 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 ⓘ

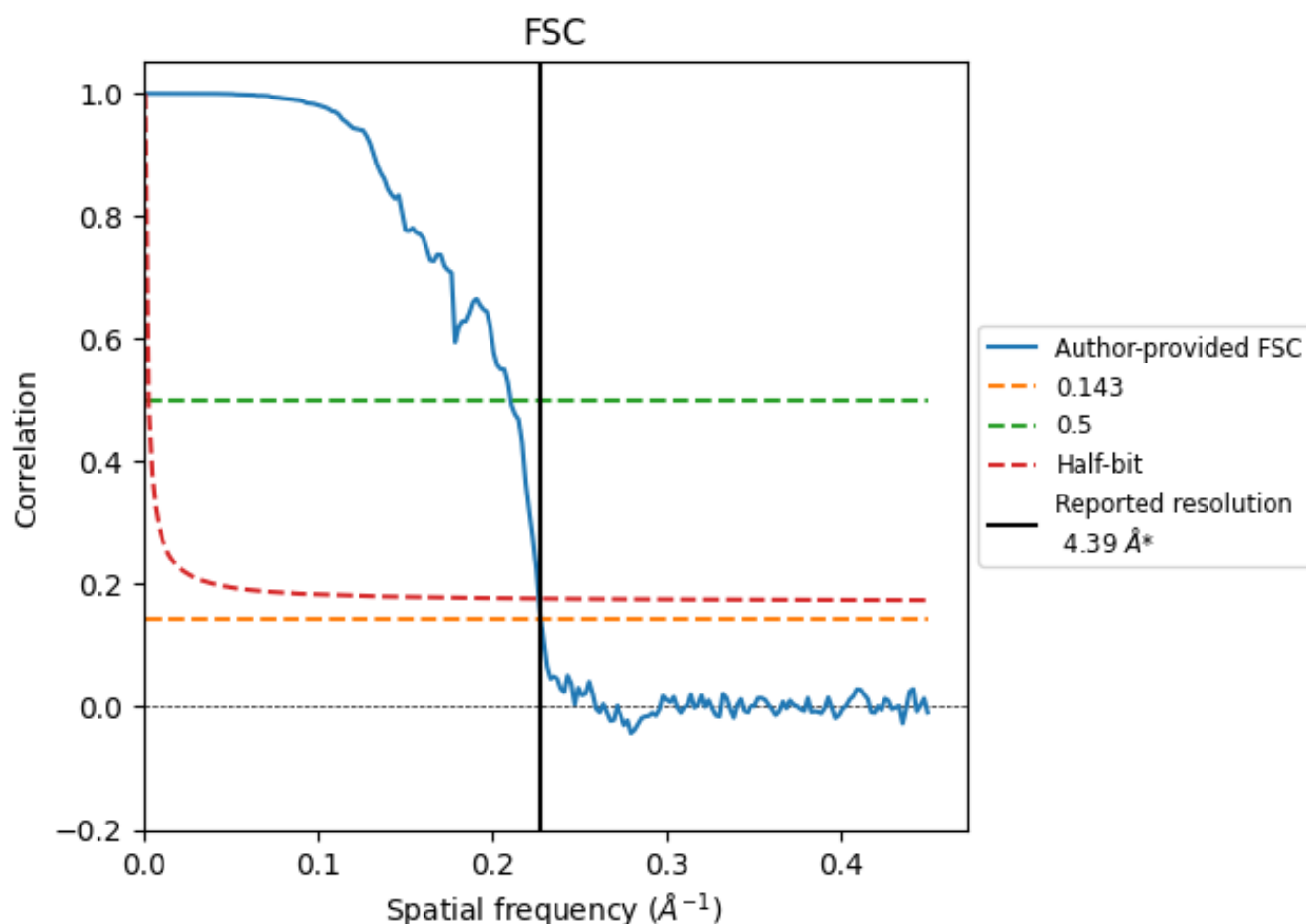


*Reported resolution corresponds to spatial frequency of 0.228 Å⁻¹

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 0.228 Å⁻¹

8.2 Resolution estimates [i](#)

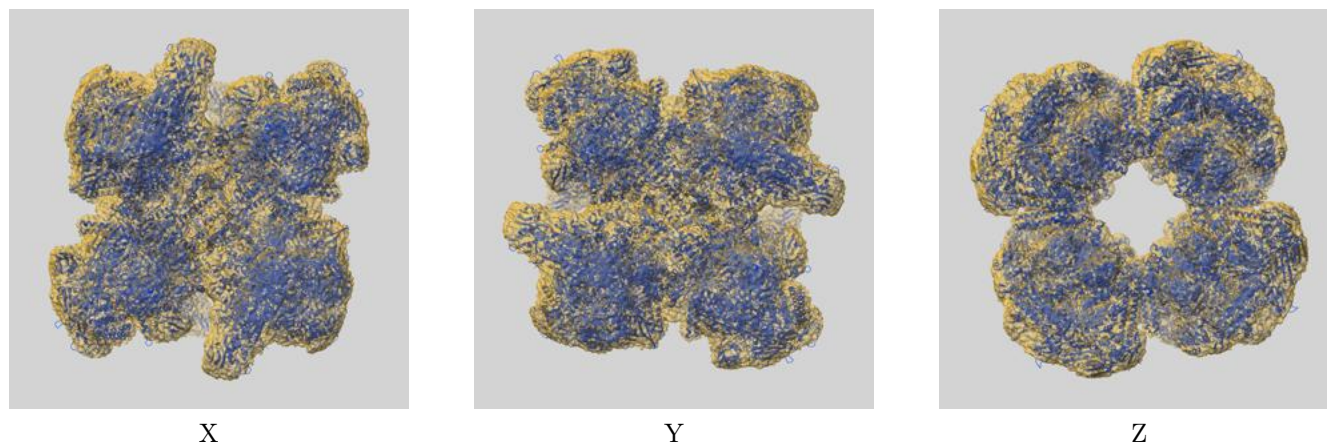
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.39	-	-
Author-provided FSC curve	4.39	4.75	4.41
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

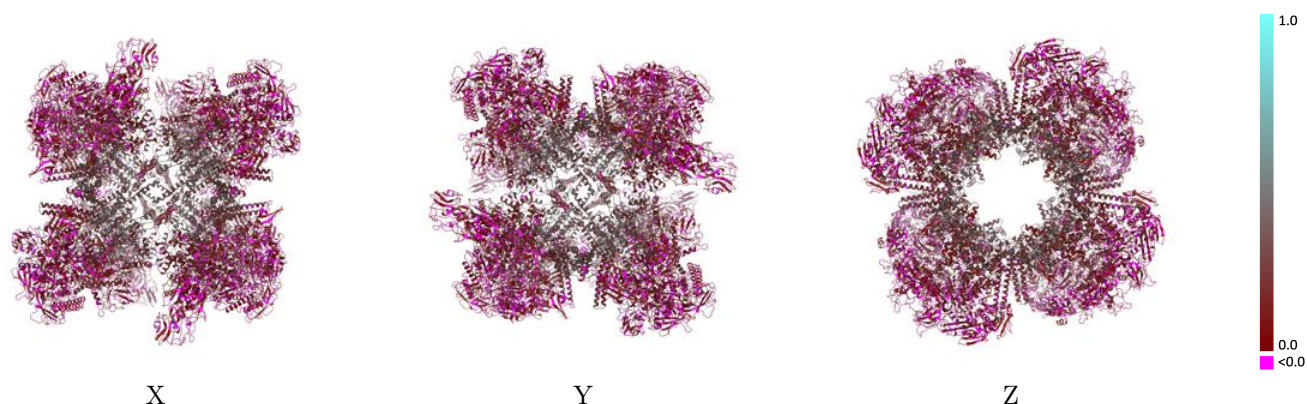
This section contains information regarding the fit between EMDB map EMD-13817 and PDB model 7Q4U. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



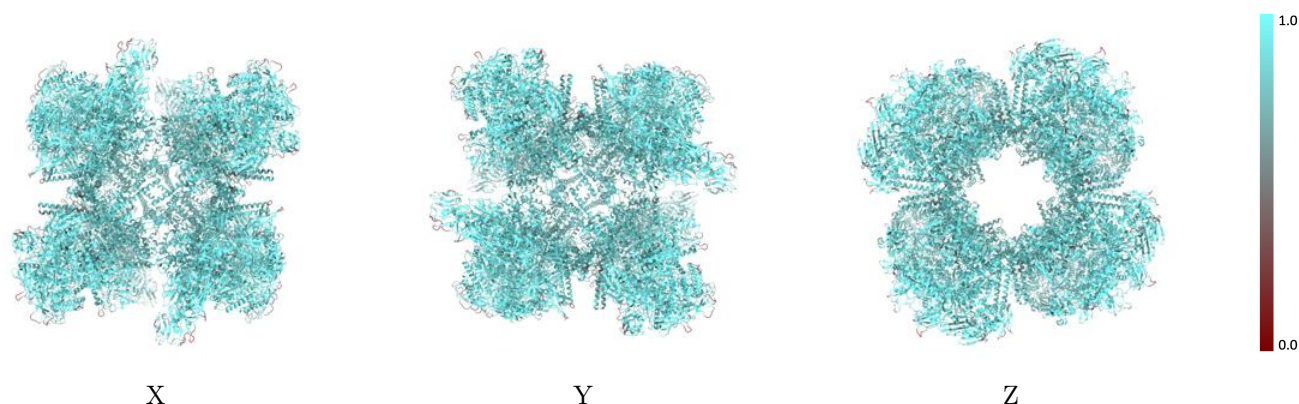
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



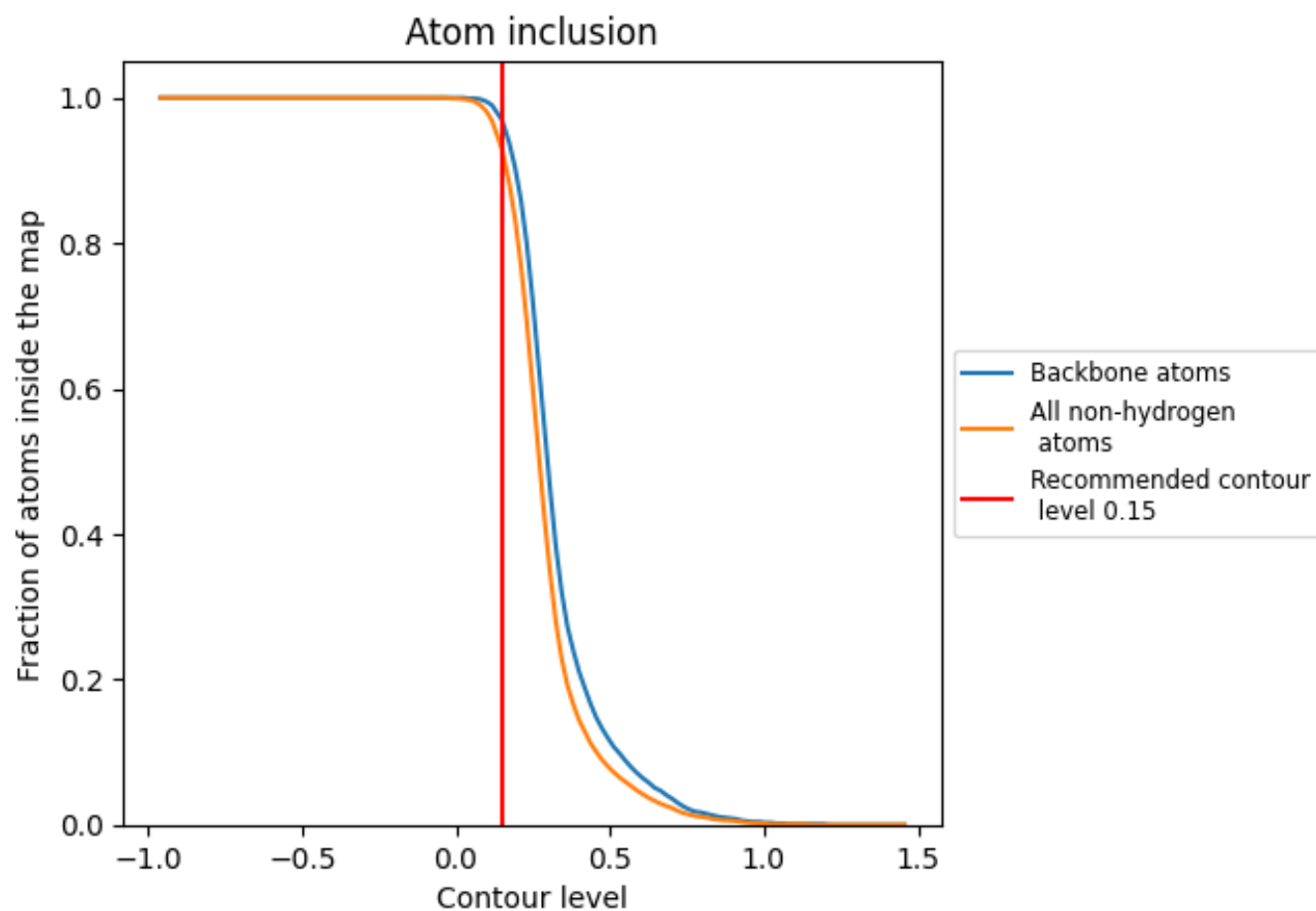
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9290	 0.1610
A	 0.9030	 0.0800
AA	 0.8760	 0.1040
B	 0.8770	 0.1050
BA	 0.9400	 0.1120
C	 0.9400	 0.1110
CA	 0.9310	 0.2080
D	 0.9320	 0.2070
DA	 0.9220	 0.1880
E	 0.9220	 0.1880
EA	 0.9450	 0.3340
F	 0.9450	 0.3330
FA	 0.9030	 0.0790
G	 0.9030	 0.0800
GA	 0.8760	 0.1010
H	 0.8760	 0.1040
HA	 0.9400	 0.1110
I	 0.9390	 0.1110
IA	 0.9310	 0.2080
J	 0.9310	 0.2080
JA	 0.9200	 0.1880
K	 0.9220	 0.1900
KA	 0.9450	 0.3350
L	 0.9450	 0.3350
LA	 0.9030	 0.0780
M	 0.9030	 0.0770
MA	 0.8780	 0.1010
N	 0.8760	 0.1030
NA	 0.9390	 0.1110
O	 0.9400	 0.1110
OA	 0.9310	 0.2070
P	 0.9310	 0.2080
PA	 0.9220	 0.1880
Q	 0.9220	 0.1920
QA	 0.9450	 0.3340



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Chain	Atom inclusion	Q-score
R	 0.9450	 0.3360
RA	 0.9030	 0.0800
S	 0.9030	 0.0780
SA	 0.8770	 0.1050
T	 0.8770	 0.1020
TA	 0.9400	 0.1120
UA	 0.9310	 0.2070
V	 0.9400	 0.1110
VA	 0.9220	 0.1880
W	 0.9310	 0.2070
WA	 0.9450	 0.3320
X	 0.9200	 0.1900
Y	 0.9450	 0.3340
Z	 0.9030	 0.0820