



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:52 AM UTC

PDB ID : 8OF0 / pdb_00008of0
EMDB ID : EMD-16840
Title : Structure of the mammalian Pol II-SPT6-Elongin complex, Structure 1
Authors : Chen, Y.; Kokic, G.; Dienemann, C.; Dybkov, O.; Urlaub, H.; Cramer, P.
Deposited on : 2023-03-13
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

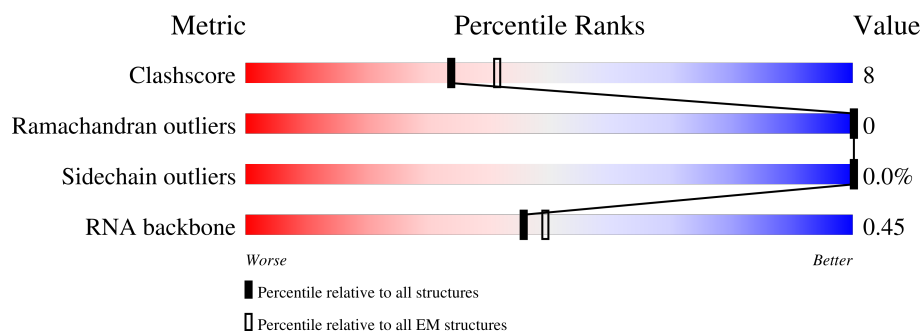
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 Å.

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



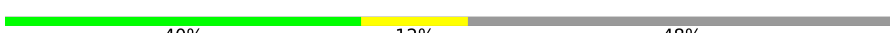
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1970	58% (green), 14% (yellow), 28% (grey)
2	B	1251	73% (green), 17% (yellow), 10% (grey)
3	C	275	79% (green), 15% (yellow), 6% (grey)
4	D	184	48% (green), 16% (yellow), 36% (grey)
5	E	210	85% (green), 14% (yellow)
6	F	127	54% (green), 8% (yellow), 39% (grey)
7	G	172	76% (green), 23% (yellow), . (grey)

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Mol	Chain	Length	Quality of chain
8	H	150	 83% 15% .
9	I	125	 64% 29% 7%
10	J	67	 87% 12% .
11	K	117	 80% 18% .
12	L	58	 55% 21% 24%
13	N	48	 40% 12% 48%
14	P	46	 20% 7% . 72%
15	T	48	 58% 19% 23%
16	Q	118	 59% 15% 25%
17	M	801	 14% . 83%
18	O	112	 63% 27% 10%
19	S	1729	 34% 13% 53%

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 41700 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1409	Total	C	N	O	S	0	0
			11159	7024	2000	2064	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1131	Total	C	N	O	S	0	0
			9047	5721	1592	1670	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	258	Total	C	N	O	S	0	0
			2072	1300	356	410	6		

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	118	Total	C	N	O	S	0	0
			967	608	167	188	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	78	Total	C	N	O	S	0	0
			626	401	106	114	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1347	872	218	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			932	577	165	179	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			367	228	69	64	6		

- Molecule 13 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	25	Total	C	N	O	P	0	0
			527	245	112	145	25		

- Molecule 14 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	13	Total	C	N	O	P	0	0
			280	125	54	88	13		

- Molecule 15 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	37	Total	C	N	O	P	0	0
			750	356	127	230	37		

- Molecule 16 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	88	Total	C	N	O	S	0	0
			696	437	121	135	3		

- Molecule 17 is a protein called Elongin-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	140	Total	C	N	O	S	0	0
			1149	724	214	204	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q14241
M	-1	ASN	-	expression tag	UNP Q14241
M	0	ALA	-	expression tag	UNP Q14241

- Molecule 18 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	101	Total	C	N	O	S	0	0
			792	506	127	153	6		

- Molecule 19 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	818	Total	C	N	O	S	0	0
			6629	4221	1144	1232	32		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	expression tag	UNP Q7KZ85
S	-1	ASN	-	expression tag	UNP Q7KZ85
S	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total Mg 1 1	0

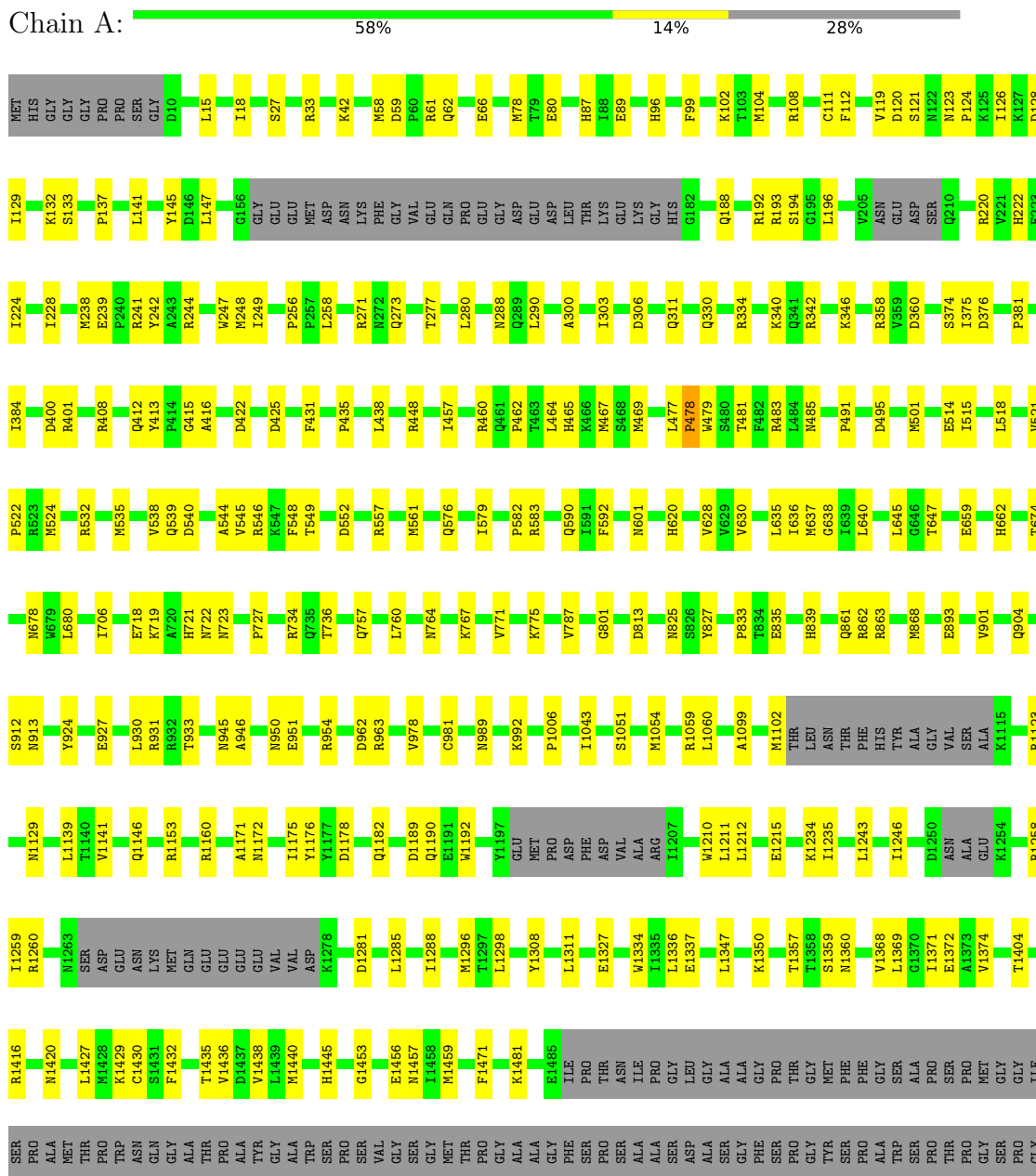
- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
21	A	2	Total Zn 2 2	0
21	B	1	Total Zn 1 1	0
21	C	1	Total Zn 1 1	0
21	I	2	Total Zn 2 2	0
21	J	1	Total Zn 1 1	0
21	L	1	Total Zn 1 1	0

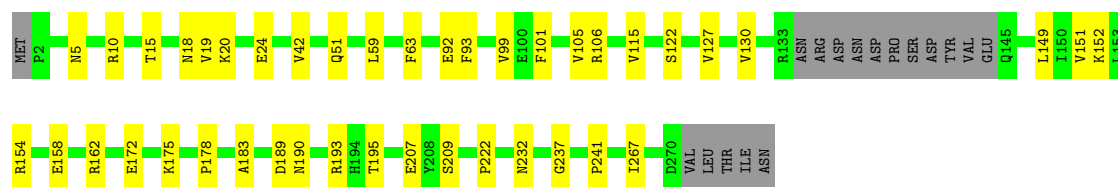
3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

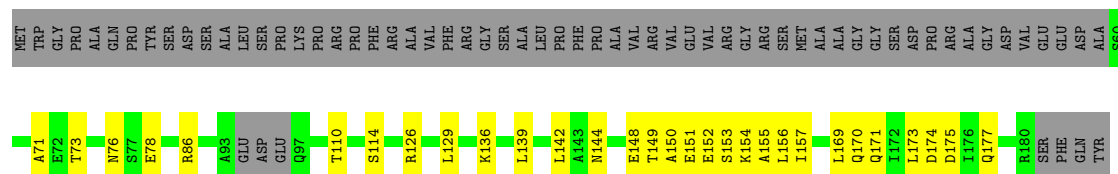


Chain C:  79% 15% 6%



• Molecule 4: RNA polymerase II subunit D

Chain D:  48% 16% 36%



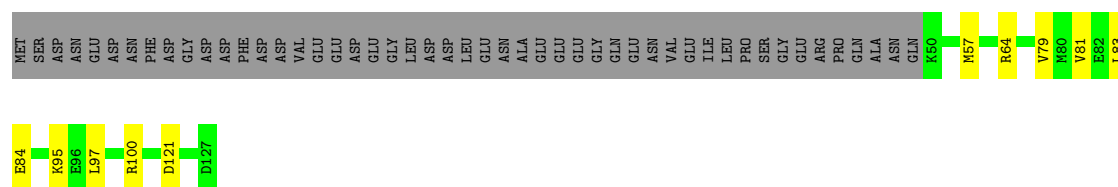
• Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E:  85% 14%



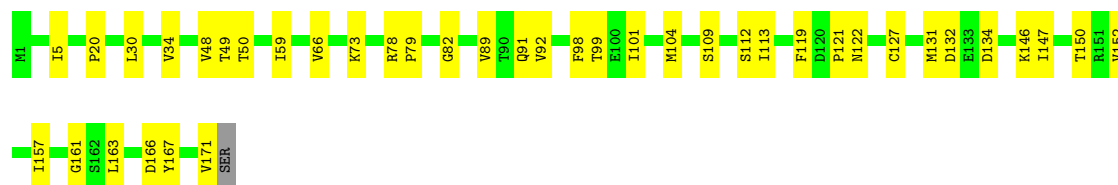
• Molecule 6: DNA-directed RNA polymerase II subunit F

Chain F:  54% 8% 39%



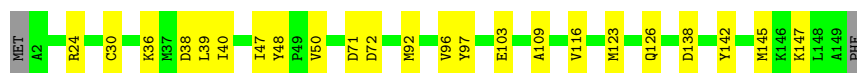
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:  76% 23%



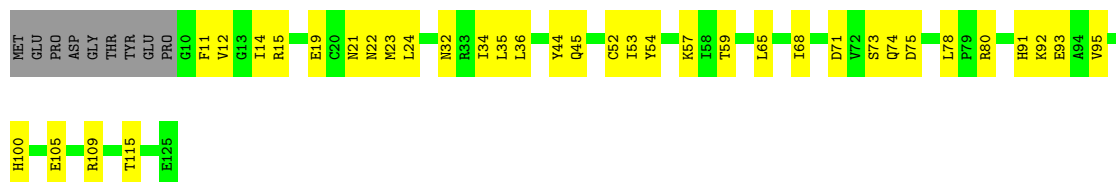
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  83% 15%



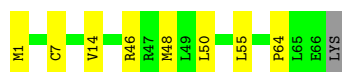
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:



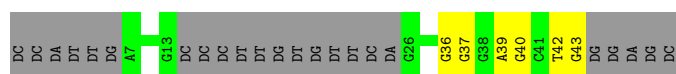
- Molecule 12: RNA polymerase II subunit K

Chain L:



- Molecule 13: Non-template DNA

Chain N:

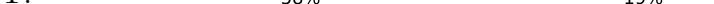


- Molecule 14: RNA

Chain P:

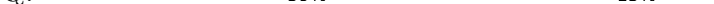


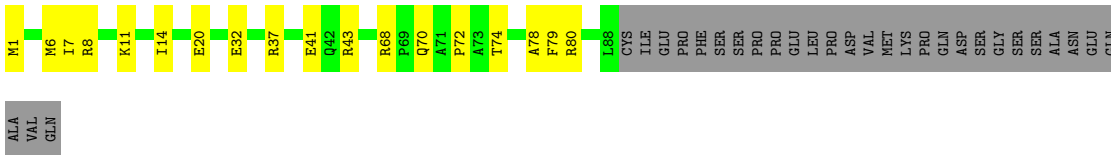
- Molecule 15: Template DNA

Chain T:  58% 19% 23%



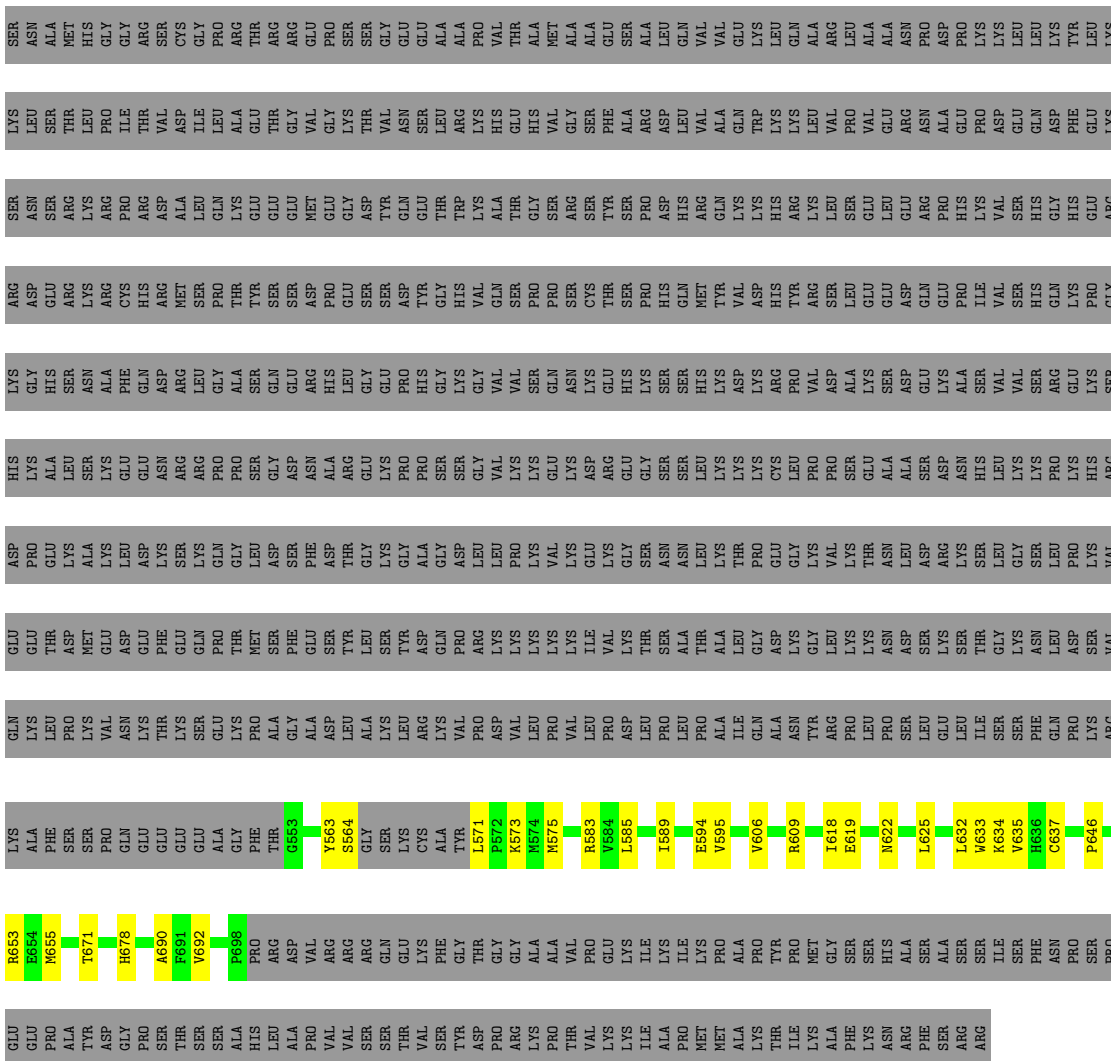
- Molecule 16: Elongin-B

Chain Q: 



- Molecule 17: Elongin-A

Chain M: 14% . 83%



- Molecule 18: Elongin-C

Chain O:  63% 27% 10%

MET	ASP	GLY	GLU	GLU	LYS	THR	TYR	GLY	GLY	CYS	E12	Y18	V19	K20	S23	G26	T30	V31	K32	H35	Q51	F52	N58	R63	E64	I65	L70	V73	C74	M75	Y76	Y79	S86	S87	I90	A96	T99	A100	L101	E102	L103	L104	M105	A106
A107	M108	C112																																										

• Molecule 19: Transcription elongation factor SPT6

Chain S:  34% 13% 53%

L1004	A890	G778	Y685	L594	GLU	L416	I303	GLU	L416	GLU	ASP	PRO	LYS	TYR	ILE	ASN	SER	ASN	ILE	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
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LEU	ARG	ALA	PRO	GLY	ALA	SER	TYR	GLN	GLN	F1107	
LEU	GLN	TYR	ALA	LYS	SER	SER	TYR	GLN	ASP	A1108	
ASP	GLN	HIS	ASN	PRO	PHE	LYS	ASP	ASN	PHE	L1111	
MET	PRO	VAL	ILE	ILE	ARG	GLU	ASP	PRO	ALA	G1117	
ASP	LYS	PRO	LEU	GLU	ASP	ASN	ALA	GLU	GLU		
SER	SER	THR	ALA	TYR	LEU	HIS	GLU	LEU	ALA		
ASN	ASN	PRO	ASP	VAL	LEU	LEU	ALA	SER	SER	H1120	
SER	SER	ALA	LEU	THR	THR	THR	THR	ASN	ALA	I1121	
HIS	ALA	GLN	THR	VAL	HIS	VAL	ASP	GLU	GLU	T1122	
ALA	ALA	PRO	ARG	PRO	THR	THR	THR	LYS	VAL	L1123	
ALA	ALA	VAL	ALA	GLY	TYR	LYS	LYS	ASN	TRP	Y1124	
ILE	ILE	ASN	ASN	GLY	GLN	VAL	GLU	HIS	ASN	D1125	
ASP	TRP	ALA	ALA	PHE	ASP	SER	GLU	PHE	ASP		
TRP	LYS	THR	LEU	ARG	TYR	ASP	GLU	ASP	SER	C1132	
LYS	MET	PRO	PRO	TYR	SER	GLY	LYS	SER	GLY	Y1133	
ALA	ALA	THR	ASN	ARG	GLY	ILE	TYR	SER	GLY	Y1134	
ALA	ALA	PRO	MET	GLN	GLY	TYR	ARG	SER	SER	K1135	
GLN	GLN	THR	THR	ILE	ASP	GLN	GLN	LYS	CYS	D1136	
TRP	TRP	TYR	SER	ILE	ARG	HIS	GLN	PRO	GLY	L1137	
LEU	SER	GLN	GLN	PRO	LYS	VAL	GLN	GLN	GLY	R1138	
GLN	GLN	TYR	MET	VAL	LEU	VAL	THR	ALA	ALA	T1139	
LYS	LYS	THR	SER	ASN	GLU	GLU	THR	ALA	Y1141	A1140	
GLU	GLU	THR	THR	VAL	THR	GLU	THR	ALA	I1142		
ALA	ALA	PRO	ALA	GLY	GLU	GLU	TYR	ALA	S1143		
ALA	ALA	ILE	ILE	LEU	LEU	GLY	ILE	LYS			
ARG	ARG	ALA	ALA	PHE	ILE	LYS	ARG	VAL	Y1149		
ARG	ARG	PRO	VAL	THR	THR	ASN	ILE	L1145			
LYS	LYS	THR	THR	PHE	LYS	ALA	ALA	SER	M1152		
GLN	GLN	THR	GLY	LYS	THR	PHE	ALA	ASP	L1153		
LYS	LYS	PRO	GLN	GLN	GLY	HIS	HIS	ASP	A1175		
GLN	GLN	GLN	GLN	ASN	PRO	LYS	LYS	VAL	ARG		
LEU	LEU	TYR	ASN	GLN	GLY	GLY	VAL	VAL	ARG		
THR	THR	GLN	PRO	ASP	THR	THR	ALA	LYS	PRO		
PRO	PRO	LEU	ASN	PRO	ILE	LEU	ASN	ARG	GLN		
ARG	ARG	GLN	ALA	VAL	PRO	TRP	ASN	F1253	GLY		
PRO	PRO	ALA	THR	PRO	THR	ILE	ILE		GLU		
SER	SER	ALA	PRO	GLY	PHE	ASN	LYS	F1275	SER		
SER	SER	THR	ALA	ILE	ILE	SER	GLN		TVR		
PRO	PRO	THR	GLN	THR	CYS	GLU	ALA	R1282	ASP		
MET	MET	GLN	TRP	PRO	ALA	GLU	GLU	THR	GLN		
ILE	ILE	ALA	ALA	SER	PHE	LYS	LYS	SER	ALA		
GLU	GLU	SER	SER	SER	GLU	GLU	LEU	LEU	ILE		
THR	THR	GLN	TYR	ARG	LEU	ASP	GLU	ASP	ARG		
PRO	PRO	ALA	GLY	THR	PRO	ASP	THR	ARG	ASN		
SER	SER	GLN	TYR	THR	GLY	GLU	GLU	ASN	GLU		
ALA	ALA	PRO	TYR	ARG	ILE	ILE	GLU	ASN	THR		
ILE	ILE	GLN	GLY	THR	PHE	VAL	LYS	GLU	GLY		
ALA	ALA	PRO	GLY	PRO	ALA	ALA	GLY	LYS	TRP		
GLY	GLY	SER	SER	ALA	LEU	LEU	ARG	VAL	LYS		
ASP	ASP	THR	GLY	ILE	TYR	VAL	TYR	VAL	LEU		
ALA	ALA	SER	GLY	ILE	GLY	VAL	ILE	ILE	PRO		
THR	THR	ARG	GLY	ASN	PRO	GLN	ILE	LYS	ASP		
PRO	PRO	GLN	SER	THR	ALA	MET	PRO	ARG	CYS		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72087	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.09	Depositor
Minimum defocus (nm)	350	Depositor
Maximum defocus (nm)	7500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	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	0.25	0/11360	0.47	1/15328 (0.0%)
2	B	0.28	0/9227	0.48	1/12454 (0.0%)
3	C	0.27	0/2115	0.42	0/2873
4	D	0.30	0/979	0.59	0/1312
5	E	0.25	0/1752	0.51	0/2366
6	F	0.26	0/636	0.52	0/859
7	G	0.22	0/1378	0.51	0/1870
8	H	0.24	0/1207	0.44	0/1628
9	I	0.23	0/954	0.51	0/1293
10	J	0.29	0/533	0.46	0/719
11	K	0.27	0/939	0.44	0/1271
12	L	0.25	0/372	0.49	0/493
13	N	0.20	0/594	0.35	0/915
14	P	0.17	0/313	0.21	0/486
15	T	0.27	0/836	0.45	0/1287
16	Q	0.22	0/707	0.62	0/952
17	M	0.30	0/1172	0.61	0/1578
18	O	0.24	0/810	0.62	0/1097
19	S	0.22	0/6750	0.52	0/9096
All	All	0.25	0/42634	0.49	2/57877 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
18	O	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	PRO	CA-C-O	-5.85	116.88	121.38
2	B	430	VAL	N-CA-C	-5.62	107.26	112.43

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
18	O	90	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11159	0	11304	179	0
2	B	9047	0	9080	139	0
3	C	2072	0	2019	28	0
4	D	967	0	973	38	0
5	E	1721	0	1737	20	0
6	F	626	0	657	6	0
7	G	1347	0	1347	41	0
8	H	1186	0	1147	15	0
9	I	932	0	856	28	0
10	J	524	0	540	7	0
11	K	920	0	942	14	0
12	L	367	0	367	9	0
13	N	527	0	278	3	0
14	P	280	0	142	3	0
15	T	750	0	418	7	0
16	Q	696	0	694	13	0
17	M	1149	0	1127	26	0
18	O	792	0	774	21	0
19	S	6629	0	6583	166	0
20	A	1	0	0	0	0
21	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	1	0	0	0	0
21	C	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
All	All	41700	0	40985	672	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 8.

All (672) 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)
7:G:132:ASP:O	19:S:416:LEU:HD21	1.45	1.15
4:D:148:GLU:HG2	19:S:519:SER:HB2	1.13	1.12
4:D:149:THR:OG1	4:D:152:GLU:HB2	1.62	0.99
4:D:148:GLU:CG	19:S:519:SER:HB2	1.96	0.96
7:G:134:ASP:OD1	19:S:475:ILE:HG23	1.66	0.95
19:S:303:ILE:HD11	19:S:405:GLN:NE2	1.84	0.93
7:G:134:ASP:OD1	19:S:475:ILE:HD12	1.70	0.90
4:D:150:ALA:HB1	4:D:169:LEU:CB	2.05	0.86
4:D:150:ALA:HB1	4:D:169:LEU:HB2	1.58	0.83
19:S:303:ILE:CD1	19:S:405:GLN:HE21	1.94	0.80
7:G:122:ASN:O	19:S:405:GLN:HG3	1.80	0.80
7:G:132:ASP:O	19:S:416:LEU:CD2	2.28	0.77
19:S:303:ILE:CD1	19:S:405:GLN:NE2	2.47	0.77
4:D:152:GLU:HA	4:D:155:ALA:HB3	1.69	0.74
19:S:301:ARG:HD2	19:S:401:GLU:HG2	1.69	0.74
7:G:119:PHE:CD2	7:G:121:PRO:HG3	2.22	0.74
7:G:132:ASP:C	19:S:416:LEU:HD21	2.12	0.73
1:A:718:GLU:HB2	17:M:564:SER:C	2.15	0.72
4:D:149:THR:OG1	4:D:152:GLU:CB	2.37	0.72
5:E:82:VAL:HB	5:E:110:MET:HG2	1.70	0.71
18:O:20:LYS:H	18:O:58:ASN:HB3	1.55	0.71
7:G:132:ASP:O	19:S:416:LEU:HD11	1.90	0.71
1:A:950:ASN:OD1	1:A:954:ARG:NH1	2.24	0.70
19:S:795:PHE:HB3	19:S:910:LEU:HD13	1.74	0.70
17:M:573:LYS:HB3	17:M:575:MET:HE3	1.74	0.69
2:B:359:ARG:NH2	9:I:21:ASN:OD1	2.26	0.69
7:G:171:VAL:C	19:S:520:ARG:HA	2.18	0.69
17:M:563:TYR:O	17:M:564:SER:C	2.36	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:936:ARG:NH2	12:L:54:VAL:O	2.25	0.68
4:D:151:GLU:HA	4:D:154:LYS:CE	2.23	0.68
1:A:360:ASP:OD1	2:B:1139:ARG:NH1	2.27	0.68
2:B:831:PRO:HB2	2:B:850:PRO:HG2	1.76	0.67
19:S:616:LEU:HB3	19:S:643:LYS:HB3	1.76	0.67
1:A:384:ILE:HG12	2:B:1138:SER:HB3	1.76	0.67
19:S:586:GLU:OE2	19:S:715:ARG:NH1	2.28	0.67
1:A:576:GLN:O	1:A:590:GLN:NE2	2.27	0.67
19:S:589:ARG:HH21	19:S:708:GLN:HE22	1.42	0.66
6:F:100:ARG:NH2	6:F:121:ASP:O	2.28	0.66
8:H:50:VAL:HA	8:H:147:LYS:HZ1	1.60	0.66
4:D:150:ALA:HB1	4:D:169:LEU:HB3	1.78	0.65
3:C:59:LEU:HD12	3:C:151:VAL:HG23	1.79	0.65
7:G:119:PHE:CE2	7:G:121:PRO:HG3	2.31	0.65
17:M:632:LEU:O	17:M:635:VAL:HB	1.96	0.64
1:A:827:TYR:HH	1:A:839:HIS:HE2	1.46	0.64
19:S:294:LEU:HB3	19:S:299:GLN:HE21	1.61	0.64
4:D:152:GLU:HA	7:G:167:TYR:CE2	2.32	0.64
4:D:149:THR:O	4:D:152:GLU:HB3	1.98	0.64
4:D:151:GLU:HA	4:D:154:LYS:HE3	1.80	0.64
19:S:417:PHE:HB3	19:S:448:MET:HE1	1.80	0.64
4:D:86:ARG:NH1	7:G:48:VAL:O	2.31	0.63
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.79	0.63
2:B:855:SER:O	2:B:1122:PRO:HA	1.97	0.63
17:M:575:MET:O	18:O:76:TYR:OH	2.17	0.63
10:J:1:MET:HA	10:J:55:LEU:HB2	1.81	0.63
2:B:313:TRP:HB2	2:B:336:THR:HB	1.82	0.62
19:S:559:THR:O	19:S:695:ARG:NH2	2.32	0.62
19:S:558:GLU:HB3	19:S:695:ARG:HH22	1.63	0.61
19:S:1142:ARG:NH1	19:S:1143:SER:O	2.34	0.61
17:M:585:LEU:HD23	17:M:606:VAL:HG11	1.81	0.61
18:O:63:ARG:HG2	18:O:64:GLU:HG2	1.81	0.61
19:S:322:ARG:HA	19:S:326:ALA:HB3	1.81	0.61
2:B:834:PRO:HG2	2:B:841:MET:HE1	1.83	0.61
18:O:23:SER:HB3	18:O:70:LEU:HD13	1.81	0.61
1:A:1054:MET:HE1	1:A:1060:LEU:HD12	1.82	0.61
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.82	0.61
17:M:619:GLU:OE1	17:M:653:ARG:NH1	2.34	0.61
1:A:102:LYS:HZ2	1:A:141:LEU:HD23	1.65	0.61
11:K:17:LYS:O	11:K:36:ASN:ND2	2.34	0.61
19:S:849:THR:HG21	19:S:920:ILE:HG13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:622:ASN:HB3	17:M:625:LEU:HD13	1.83	0.61
1:A:120:ASP:O	1:A:123:ASN:ND2	2.33	0.61
2:B:810:MET:HE3	2:B:826:HIS:HB3	1.82	0.61
19:S:469:LEU:HB2	19:S:598:ARG:HE	1.65	0.61
1:A:862:ARG:NH2	1:A:1432:PHE:O	2.34	0.60
2:B:967:ARG:NH1	14:P:36:G:N7	2.49	0.60
2:B:1181:ARG:NH2	2:B:1186:GLU:OE1	2.34	0.60
11:K:12:LEU:HD11	11:K:18:LYS:HD3	1.83	0.60
19:S:1095:ASN:HB3	19:S:1097:GLU:HG3	1.84	0.60
4:D:155:ALA:HB1	7:G:166:ASP:OD2	2.02	0.60
18:O:102:GLU:O	18:O:105:MET:HB2	2.01	0.60
2:B:629:ASN:HB2	2:B:632:GLU:HG2	1.83	0.60
1:A:18:ILE:HG13	2:B:1248:MET:HE2	1.84	0.60
2:B:1139:ARG:NH2	2:B:1143:PRO:O	2.35	0.60
4:D:152:GLU:O	4:D:156:LEU:HG	2.01	0.60
7:G:82:GLY:HA2	7:G:146:LYS:HE2	1.84	0.60
19:S:1072:ASP:O	19:S:1098:ARG:NH2	2.35	0.60
4:D:152:GLU:HG3	7:G:167:TYR:CD2	2.38	0.59
11:K:17:LYS:HD2	11:K:20:THR:HG22	1.83	0.59
19:S:1014:ARG:NH1	19:S:1058:VAL:O	2.35	0.59
1:A:15:LEU:HD11	2:B:1227:ARG:HG3	1.83	0.59
2:B:795:GLN:HG2	2:B:797:PRO:HD2	1.85	0.59
1:A:827:TYR:OH	1:A:839:HIS:NE2	2.35	0.59
2:B:234:ARG:NH2	2:B:254:CYS:O	2.36	0.58
1:A:1427:LEU:HB2	1:A:1456:GLU:HG3	1.84	0.58
19:S:303:ILE:HD13	19:S:405:GLN:HE21	1.67	0.58
1:A:465:HIS:HD2	1:A:467:MET:HE2	1.68	0.58
1:A:1178:ASP:O	1:A:1260:ARG:NH2	2.37	0.58
18:O:70:LEU:HA	18:O:73:VAL:HG22	1.84	0.58
1:A:1210:TRP:HD1	1:A:1281:ASP:HB3	1.67	0.58
2:B:316:MET:HG3	2:B:333:ILE:HG13	1.86	0.58
3:C:106:ARG:HD2	3:C:158:GLU:HB3	1.86	0.58
3:C:190:ASN:O	3:C:193:ARG:NH1	2.37	0.58
1:A:1171:ALA:HA	9:I:59:THR:HG22	1.86	0.58
1:A:330:GLN:HG3	1:A:334:ARG:HH21	1.69	0.58
19:S:857:ALA:HA	19:S:860:LEU:HB2	1.86	0.58
2:B:533:GLN:NE2	15:T:34:DT:OP1	2.37	0.58
19:S:1011:LEU:HD13	19:S:1017:LEU:HG	1.85	0.58
2:B:211:LYS:HB3	2:B:214:GLU:HB3	1.86	0.57
5:E:172:ARG:HD2	5:E:210:GLN:HB3	1.86	0.57
19:S:564:ALA:O	19:S:705:TRP:NE1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:1025:PRO:HA	19:S:1028:PHE:HB3	1.85	0.57
1:A:78:MET:O	2:B:1149:ARG:NH2	2.38	0.57
1:A:124:PRO:O	1:A:128:ASP:HB2	2.04	0.57
1:A:1212:LEU:HB2	1:A:1259:ILE:HB	1.86	0.57
5:E:104:ILE:HD11	5:E:118:LEU:HD21	1.85	0.57
9:I:71:ASP:O	9:I:74:GLN:HG2	2.05	0.57
2:B:167:GLN:NE2	2:B:168:ILE:O	2.38	0.57
19:S:424:GLN:HE22	19:S:442:ALA:HA	1.70	0.57
18:O:18:TYR:HB3	18:O:30:ILE:HD11	1.87	0.57
8:H:103:GLU:HB3	8:H:109:ALA:HB2	1.86	0.57
3:C:19:VAL:HG12	3:C:241:PRO:HB2	1.87	0.57
4:D:150:ALA:CB	4:D:170:GLN:HG3	2.35	0.57
7:G:134:ASP:OD1	19:S:475:ILE:CG2	2.47	0.57
1:A:42:LYS:O	1:A:288:ASN:ND2	2.34	0.56
5:E:116:GLN:NE2	5:E:120:ASP:OD2	2.38	0.56
19:S:785:ALA:HB1	19:S:912:GLN:HE21	1.70	0.56
2:B:984:VAL:HG22	2:B:998:ILE:HG12	1.87	0.56
12:L:19:CYS:HA	12:L:44:MET:HG2	1.86	0.56
19:S:316:GLU:OE2	19:S:367:ARG:NH1	2.38	0.56
19:S:925:ILE:HA	19:S:985:LEU:HD21	1.87	0.56
3:C:149:LEU:HD21	3:C:152:LYS:HE3	1.86	0.56
3:C:154:ARG:HD3	10:J:64:PRO:HD3	1.88	0.56
1:A:59:ASP:HB3	1:A:62:GLN:HG3	1.86	0.56
19:S:558:GLU:OE2	19:S:695:ARG:NH1	2.39	0.56
1:A:927:GLU:OE1	1:A:931:ARG:NH1	2.39	0.56
2:B:1192:GLN:HG2	2:B:1227:ARG:HG2	1.86	0.56
19:S:612:GLU:O	19:S:646:LYS:NZ	2.38	0.56
1:A:674:THR:O	1:A:678:ASN:ND2	2.38	0.56
19:S:462:ASP:HB3	19:S:603:ARG:HG3	1.88	0.56
4:D:156:LEU:O	4:D:157:ILE:C	2.48	0.55
1:A:912:SER:HB3	1:A:1327:GLU:HG2	1.87	0.55
18:O:96:ALA:HB3	18:O:99:ILE:HG12	1.88	0.55
1:A:1347:LEU:HB3	5:E:137:ILE:HD13	1.87	0.55
2:B:300:SER:OG	2:B:427:HIS:ND1	2.37	0.55
19:S:465:ASN:O	19:S:598:ARG:NH2	2.40	0.55
19:S:956:ASN:HA	19:S:959:TYR:HB3	1.88	0.55
1:A:601:ASN:HA	1:A:630:VAL:O	2.06	0.55
19:S:543:PRO:O	19:S:547:GLY:N	2.38	0.55
1:A:374:SER:OG	1:A:376:ASP:OD1	2.25	0.55
2:B:461:ASP:O	2:B:467:ASN:ND2	2.35	0.55
7:G:101:ILE:HD12	7:G:104:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:GLU:HG3	2:B:167:GLN:H	1.72	0.55
2:B:1219:ASN:HD21	2:B:1222:GLN:HB2	1.72	0.55
5:E:77:PRO:HG3	5:E:90:TYR:HE2	1.72	0.55
3:C:59:LEU:HD13	3:C:63:PHE:CE2	2.43	0.54
19:S:1032:ALA:HA	19:S:1035:LEU:HD12	1.89	0.54
1:A:1211:LEU:HD11	1:A:1258:ARG:HB3	1.88	0.54
1:A:460:ARG:HB2	1:A:501:MET:HE3	1.88	0.54
8:H:96:VAL:HG22	8:H:116:VAL:HG22	1.89	0.54
19:S:934:ASP:OD1	19:S:934:ASP:N	2.38	0.54
2:B:1130:HIS:HB3	2:B:1135:LYS:HE3	1.90	0.54
7:G:152:VAL:HA	7:G:157:ILE:HD12	1.90	0.54
3:C:51:GLN:OE1	3:C:162:ARG:NH2	2.40	0.54
13:N:42:DT:H2''	13:N:43:DG:C8	2.42	0.54
2:B:362:LEU:HD11	2:B:382:LEU:HD11	1.90	0.54
4:D:174:ASP:HA	4:D:177:GLN:HG2	1.90	0.54
19:S:782:LEU:HB3	19:S:848:VAL:HG12	1.89	0.54
19:S:474:ASP:O	19:S:478:MET:N	2.32	0.54
2:B:397:PHE:O	2:B:401:ARG:NH1	2.40	0.54
2:B:1015:ARG:NH2	2:B:1060:GLU:OE2	2.37	0.54
7:G:167:TYR:HB3	19:S:518:ALA:HB2	1.90	0.54
12:L:17:TYR:HB3	12:L:44:MET:HB3	1.88	0.54
18:O:51:GLN:HG3	18:O:52:PHE:H	1.73	0.54
1:A:549:THR:HG21	1:A:640:LEU:HD12	1.89	0.54
1:A:951:GLU:OE2	1:A:954:ARG:NH2	2.41	0.54
16:Q:1:MET:N	16:Q:20:GLU:OE2	2.40	0.54
19:S:1232:LEU:HB3	19:S:1236:VAL:HG22	1.90	0.54
1:A:80:GLU:OE2	2:B:1208:ARG:NH2	2.41	0.54
3:C:20:LYS:NZ	3:C:207:GLU:OE2	2.40	0.54
1:A:718:GLU:HA	17:M:564:SER:O	2.08	0.53
2:B:464:HIS:NE2	2:B:748:GLU:OE2	2.40	0.53
9:I:15:ARG:HB3	9:I:24:LEU:HD12	1.91	0.53
19:S:620:PRO:O	19:S:625:ARG:NH1	2.40	0.53
1:A:760:LEU:HD13	1:A:764:ASN:HD22	1.73	0.53
1:A:1311:LEU:HB2	1:A:1334:TRP:CZ3	2.44	0.53
2:B:1192:GLN:HB3	2:B:1225:LEU:HD11	1.91	0.53
2:B:918:ARG:O	14:P:35:A:N6	2.42	0.53
3:C:59:LEU:HD13	3:C:63:PHE:HE2	1.74	0.53
1:A:464:LEU:HD22	1:A:861:GLN:HE22	1.73	0.53
2:B:357:SER:OG	2:B:358:ASP:N	2.42	0.53
2:B:829:TYR:HE1	2:B:886:VAL:HG13	1.74	0.53
11:K:11:LEU:O	11:K:37:LYS:NZ	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:548:GLU:OE1	19:S:557:HIS:NE2	2.38	0.53
2:B:169:TYR:HB3	17:M:690:ALA:HB2	1.89	0.53
1:A:727:PRO:HA	1:A:736:THR:HG21	1.91	0.53
19:S:973:VAL:HG23	19:S:1010:ARG:HB2	1.91	0.53
2:B:586:VAL:HG11	2:B:601:LYS:HD3	1.91	0.52
3:C:5:ASN:OD1	11:K:52:LYS:NZ	2.42	0.52
4:D:171:GLN:NE2	4:D:175:ASP:OD2	2.42	0.52
17:M:594:GLU:HA	17:M:622:ASN:HD21	1.73	0.52
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.91	0.52
2:B:982:ASP:OD1	2:B:1001:ARG:NH1	2.42	0.52
4:D:78:GLU:OE2	4:D:126:ARG:NH1	2.43	0.52
19:S:1149:ILE:HA	19:S:1152:MET:HG2	1.91	0.52
3:C:10:ARG:NH2	3:C:24:GLU:OE2	2.40	0.52
19:S:653:PHE:HZ	19:S:730:LYS:HG2	1.75	0.52
19:S:974:ASN:HB3	19:S:1010:ARG:HG3	1.91	0.52
4:D:150:ALA:N	4:D:173:LEU:HD22	2.24	0.52
1:A:477:LEU:HB2	1:A:483:ARG:HH21	1.73	0.52
12:L:25:GLU:O	12:L:37:ARG:NH2	2.43	0.52
15:T:37:DC:H2'	15:T:38:DG:C8	2.44	0.52
18:O:23:SER:HB2	18:O:65:ILE:HB	1.92	0.52
19:S:892:LEU:HA	19:S:895:ASN:HB2	1.90	0.52
1:A:1175:ILE:HB	9:I:54:TYR:H	1.73	0.52
2:B:358:ASP:HB2	9:I:22:ASN:HA	1.92	0.52
2:B:894:GLN:HB3	2:B:995:PHE:HD1	1.75	0.52
19:S:303:ILE:HD11	19:S:405:GLN:HE22	1.71	0.52
19:S:447:ASP:OD1	19:S:450:ARG:NH2	2.40	0.52
19:S:1069:MET:HB2	19:S:1102:LEU:HD11	1.91	0.52
1:A:119:VAL:HG11	1:A:147:LEU:HB3	1.92	0.52
1:A:256:PRO:HD2	1:A:280:LEU:HD11	1.92	0.52
1:A:358:ARG:NH2	2:B:1153:GLU:OE1	2.43	0.52
2:B:371:ASP:OD2	2:B:456:ARG:NH1	2.36	0.52
2:B:429:GLY:O	2:B:438:LYS:NZ	2.34	0.52
19:S:561:GLN:HG2	19:S:702:VAL:HG22	1.91	0.52
19:S:634:ALA:HA	19:S:637:PHE:HD2	1.74	0.52
19:S:890:ALA:HB1	19:S:912:GLN:HB2	1.91	0.52
1:A:1243:LEU:HD13	1:A:1259:ILE:HG23	1.91	0.51
1:A:1430:CYS:HB2	1:A:1435:THR:HG23	1.92	0.51
2:B:499:PHE:O	2:B:503:GLY:N	2.41	0.51
7:G:119:PHE:HD2	7:G:121:PRO:HG3	1.72	0.51
9:I:19:GLU:HG2	9:I:44:TYR:HD2	1.75	0.51
8:H:40:ILE:O	8:H:123:MET:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:810:ARG:HD3	19:S:812:PRO:HD3	1.92	0.51
1:A:1160:ARG:NH2	1:A:1350:LYS:O	2.44	0.51
19:S:704:GLU:HA	19:S:707:ARG:HB3	1.93	0.51
19:S:1004:LEU:HD11	19:S:1010:ARG:HA	1.93	0.51
1:A:66:GLU:HB3	1:A:271:ARG:HH22	1.75	0.51
2:B:927:ASP:OD1	2:B:927:ASP:N	2.41	0.51
2:B:944:ILE:HB	2:B:971:THR:HB	1.91	0.51
1:A:481:THR:O	1:A:483:ARG:NH1	2.44	0.51
2:B:209:VAL:O	2:B:216:GLN:HA	2.10	0.51
19:S:597:ALA:HA	19:S:721:LEU:HD21	1.93	0.51
19:S:1111:LEU:HB3	19:S:1117:GLY:HA2	1.91	0.51
19:S:946:GLN:O	19:S:951:LYS:NZ	2.35	0.51
1:A:416:ALA:HA	1:A:448:ARG:HA	1.93	0.51
1:A:734:ARG:HD2	9:I:105:GLU:HG2	1.92	0.51
2:B:820:ARG:O	2:B:999:ARG:NH1	2.44	0.51
19:S:355:THR:HA	19:S:358:LYS:HB2	1.92	0.51
19:S:785:ALA:HB3	19:S:795:PHE:HB2	1.93	0.51
1:A:583:ARG:NH1	3:C:222:PRO:O	2.44	0.51
17:M:690:ALA:HB1	17:M:692:VAL:HG23	1.93	0.50
1:A:721:HIS:HB2	17:M:564:SER:O	2.12	0.50
5:E:3:ASP:HB3	5:E:48:PRO:HD2	1.93	0.50
5:E:55:ARG:HA	5:E:58:LEU:HD12	1.93	0.50
16:Q:68:ARG:HG3	16:Q:70:GLN:H	1.76	0.50
2:B:703:LEU:HD23	2:B:739:VAL:HG12	1.92	0.50
2:B:1143:PRO:HB2	2:B:1152:MET:HG3	1.93	0.50
7:G:50:THR:HG22	7:G:73:LYS:HB2	1.93	0.50
19:S:303:ILE:HD11	19:S:405:GLN:HE21	1.53	0.50
19:S:355:THR:HG22	19:S:387:GLU:HB3	1.93	0.50
19:S:649:ARG:HB3	19:S:652:GLN:HB2	1.94	0.50
1:A:1453:GLY:O	1:A:1457:ASN:ND2	2.44	0.50
7:G:113:ILE:HG22	7:G:163:LEU:HD13	1.92	0.50
7:G:147:ILE:HA	7:G:161:GLY:HA2	1.94	0.50
9:I:92:LYS:HD3	17:M:609:ARG:HH12	1.76	0.50
19:S:1132:CYS:HB3	19:S:1135:LYS:HB2	1.92	0.50
3:C:154:ARG:HH11	10:J:64:PRO:HD3	1.77	0.50
19:S:672:ASP:OD1	19:S:685:TYR:N	2.38	0.50
1:A:342:ARG:NH1	2:B:1238:GLU:OE2	2.45	0.50
1:A:1371:ILE:HA	1:A:1374:VAL:HG12	1.94	0.50
19:S:618:ILE:HG23	19:S:667:THR:HG22	1.94	0.50
1:A:481:THR:H	1:A:483:ARG:NH1	2.09	0.50
3:C:175:LYS:NZ	12:L:57:ALA:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:75:ASP:O	9:I:80:ARG:NH1	2.45	0.50
2:B:825:ALA:HB3	2:B:888:TYR:HB2	1.93	0.49
2:B:1065:LYS:O	2:B:1069:ASN:ND2	2.44	0.49
19:S:887:ASN:HB2	19:S:890:ALA:HB3	1.94	0.49
1:A:96:HIS:HB3	1:A:99:PHE:HB2	1.94	0.49
1:A:545:VAL:HG11	1:A:645:LEU:HD12	1.94	0.49
1:A:1210:TRP:CD1	1:A:1281:ASP:HB3	2.46	0.49
10:J:14:VAL:HG21	10:J:48:MET:HG2	1.94	0.49
1:A:290:LEU:HD12	1:A:306:ASP:HB3	1.93	0.49
1:A:1234:LYS:NZ	1:A:1298:LEU:O	2.44	0.49
4:D:71:ALA:HB2	7:G:5:ILE:HD13	1.94	0.49
4:D:73:THR:O	4:D:126:ARG:NH2	2.39	0.49
8:H:71:ASP:OD2	8:H:142:TYR:OH	2.25	0.49
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.94	0.49
2:B:319:ARG:HB2	2:B:331:GLN:HE22	1.77	0.49
9:I:35:LEU:HD21	9:I:53:ILE:HD11	1.95	0.49
19:S:297:ARG:HH12	19:S:963:ILE:HG21	1.77	0.49
19:S:1010:ARG:NE	19:S:1012:GLU:OE2	2.44	0.49
1:A:408:ARG:HH21	1:A:412:GLN:HB3	1.77	0.49
1:A:1006:PRO:HB3	1:A:1051:SER:HB2	1.93	0.49
8:H:48:TYR:HE2	8:H:145:MET:HE2	1.78	0.49
1:A:992:LYS:NZ	8:H:138:ASP:OD2	2.36	0.49
1:A:1440:MET:HE2	2:B:1242:MET:HE2	1.95	0.49
2:B:901:ASP:O	2:B:949:THR:OG1	2.29	0.49
9:I:36:LEU:HD12	9:I:45:GLN:HB3	1.94	0.49
19:S:829:LYS:HE3	19:S:833:ILE:HD11	1.95	0.49
1:A:33:ARG:HE	2:B:1216:GLY:HA2	1.78	0.49
1:A:478:PRO:HD2	11:K:67:LEU:HB3	1.95	0.49
7:G:79:PRO:HB3	7:G:104:MET:HE1	1.93	0.49
7:G:91:GLN:HB3	7:G:98:PHE:HB2	1.93	0.49
19:S:756:ALA:HB3	19:S:1140:ALA:HA	1.93	0.49
2:B:169:TYR:N	2:B:202:TYR:O	2.38	0.49
2:B:357:SER:OG	9:I:21:ASN:ND2	2.41	0.49
4:D:151:GLU:O	4:D:155:ALA:N	2.29	0.49
7:G:132:ASP:O	19:S:416:LEU:CD1	2.59	0.48
1:A:1141:VAL:HA	1:A:1357:THR:HG23	1.95	0.48
1:A:1471:PHE:O	6:F:64:ARG:NH1	2.46	0.48
9:I:14:ILE:HD11	9:I:23:MET:HG3	1.94	0.48
1:A:933:THR:HG22	1:A:1059:ARG:HH21	1.77	0.48
2:B:670:GLN:NE2	2:B:672:ASP:OD2	2.32	0.48
4:D:136:LYS:HA	4:D:139:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:533:ASP:N	19:S:533:ASP:OD1	2.42	0.48
1:A:1427:LEU:HD22	1:A:1459:MET:HE1	1.95	0.48
19:S:616:LEU:HD11	19:S:667:THR:HB	1.94	0.48
19:S:742:ILE:HD11	19:S:949:VAL:HB	1.94	0.48
19:S:659:ALA:HB1	19:S:665:LEU:HB2	1.95	0.48
19:S:1149:ILE:HG23	19:S:1153:LEU:HD13	1.94	0.48
1:A:1481:LYS:HA	7:G:20:PRO:HA	1.96	0.48
2:B:373:GLU:OE2	2:B:456:ARG:NH2	2.46	0.48
2:B:550:LEU:HD11	2:B:1129:LYS:HD2	1.94	0.48
2:B:685:ARG:NH1	2:B:686:GLU:OE2	2.47	0.48
2:B:872:ILE:HG12	2:B:1024:ILE:HG22	1.94	0.48
5:E:134:GLU:OE1	5:E:181:ARG:NH2	2.46	0.48
16:Q:6:MET:HG3	16:Q:8:ARG:HB2	1.95	0.48
16:Q:72:PRO:HG3	18:O:75:MET:HE1	1.94	0.48
1:A:552:ASP:HB2	8:H:24:ARG:HB2	1.96	0.48
19:S:1152:MET:HG3	19:S:1153:LEU:HD12	1.94	0.48
4:D:129:LEU:HD11	4:D:142:LEU:HD11	1.95	0.48
4:D:150:ALA:HB3	4:D:170:GLN:HG3	1.95	0.48
9:I:73:SER:HB2	9:I:115:THR:HA	1.94	0.48
17:M:575:MET:SD	17:M:583:ARG:NH1	2.86	0.48
19:S:1014:ARG:NH2	19:S:1056:SER:O	2.40	0.48
2:B:1112:ARG:NH1	2:B:1113:LYS:O	2.47	0.48
7:G:30:LEU:O	7:G:34:VAL:HB	2.14	0.48
19:S:716:ALA:HA	19:S:720:PHE:HD2	1.79	0.48
1:A:121:SER:HA	1:A:126:ILE:HG21	1.94	0.48
2:B:168:ILE:HG22	2:B:203:VAL:HG23	1.95	0.48
2:B:893:GLU:OE1	2:B:971:THR:OG1	2.31	0.48
19:S:621:THR:OG1	19:S:663:GLY:O	2.28	0.48
6:F:84:GLU:OE1	6:F:95:LYS:NZ	2.47	0.47
7:G:131:MET:O	19:S:415:ARG:NH1	2.47	0.47
10:J:7:CYS:HA	10:J:48:MET:HE3	1.95	0.47
16:Q:70:GLN:NE2	18:O:79:TYR:OH	2.47	0.47
1:A:192:ARG:NH1	1:A:194:SER:OG	2.47	0.47
1:A:546:ARG:HD2	1:A:771:VAL:HG23	1.96	0.47
2:B:314:VAL:HG12	2:B:449:LEU:HD22	1.95	0.47
2:B:664:LEU:HB3	2:B:680:MET:SD	2.54	0.47
3:C:15:THR:OG1	3:C:18:ASN:OD1	2.33	0.47
16:Q:7:ILE:HB	16:Q:14:ILE:HB	1.96	0.47
19:S:409:ARG:HA	19:S:412:ASN:HD22	1.79	0.47
19:S:444:ASP:HB2	19:S:447:ASP:H	1.79	0.47
1:A:1429:LYS:HB2	1:A:1438:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:92:VAL:HG11	7:G:127:CYS:HA	1.95	0.47
1:A:1212:LEU:HG	1:A:1285:LEU:HD11	1.96	0.47
4:D:151:GLU:O	4:D:152:GLU:C	2.57	0.47
12:L:40:GLY:O	12:L:42:ARG:NH1	2.48	0.47
19:S:919:ARG:HB2	19:S:926:GLU:HG2	1.97	0.47
1:A:400:ASP:OD1	1:A:401:ARG:N	2.47	0.47
2:B:375:MET:HA	2:B:378:VAL:HG22	1.96	0.47
2:B:1199:CYS:HB3	2:B:1217:CYS:SG	2.53	0.47
6:F:57:MET:HE1	6:F:97:LEU:HD11	1.96	0.47
19:S:535:LEU:HA	19:S:538:LYS:HB2	1.97	0.47
19:S:756:ALA:N	19:S:1139:THR:O	2.41	0.47
19:S:989:VAL:HB	19:S:992:LEU:HB2	1.96	0.47
1:A:544:ALA:O	1:A:548:PHE:HB2	2.15	0.47
19:S:394:TRP:NE1	19:S:964:ASN:OD1	2.48	0.47
1:A:495:ASP:OD1	1:A:495:ASP:N	2.45	0.47
1:A:1416:ARG:O	1:A:1420:ASN:HB2	2.15	0.47
19:S:316:GLU:HG2	19:S:403:TRP:CE2	2.50	0.47
5:E:60:VAL:HB	5:E:74:VAL:HB	1.96	0.46
9:I:32:ASN:HB2	9:I:34:ILE:HG12	1.98	0.46
9:I:80:ARG:HG3	9:I:95:VAL:HG12	1.96	0.46
1:A:1099:ALA:HA	1:A:1102:MET:HE2	1.96	0.46
1:A:1139:LEU:HD23	1:A:1359:SER:HB2	1.97	0.46
2:B:359:ARG:O	2:B:363:GLU:HB2	2.15	0.46
2:B:704:ILE:HD11	2:B:740:GLU:HB2	1.97	0.46
3:C:99:VAL:HG21	3:C:127:VAL:HG21	1.98	0.46
10:J:46:ARG:O	10:J:50:LEU:HB2	2.15	0.46
19:S:915:SER:O	19:S:919:ARG:N	2.47	0.46
1:A:59:ASP:OD2	1:A:61:ARG:NH2	2.46	0.46
1:A:241:ARG:NH1	1:A:242:TYR:OH	2.48	0.46
1:A:413:TYR:O	1:A:415:GLY:N	2.48	0.46
19:S:645:VAL:HG23	19:S:646:LYS:HD3	1.96	0.46
2:B:1127:ARG:NH2	2:B:1131:MET:SD	2.88	0.46
4:D:110:THR:O	4:D:114:SER:OG	2.30	0.46
18:O:100:ALA:HA	18:O:103:LEU:HB3	1.98	0.46
19:S:330:ILE:HD11	19:S:611:GLN:HG2	1.97	0.46
19:S:420:MET:O	19:S:424:GLN:N	2.45	0.46
19:S:591:MET:O	19:S:594:LEU:HG	2.16	0.46
19:S:1014:ARG:HA	19:S:1017:LEU:HD13	1.98	0.46
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.86	0.46
2:B:936:ARG:HG2	2:B:980:ILE:HG12	1.98	0.46
5:E:71:GLN:HB2	5:E:99:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:649:ARG:HG3	19:S:650:ASP:H	1.81	0.46
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.98	0.46
19:S:706:ASN:O	19:S:710:THR:N	2.47	0.46
1:A:539:GLN:HE22	1:A:775:LYS:HE2	1.80	0.46
4:D:76:ASN:O	4:D:110:THR:OG1	2.32	0.46
19:S:905:ASP:OD1	19:S:905:ASP:N	2.49	0.46
2:B:812:VAL:HG23	2:B:831:PRO:HG3	1.98	0.46
9:I:65:LEU:HD13	9:I:68:ILE:HD12	1.98	0.46
16:Q:6:MET:HG2	16:Q:74:THR:HG23	1.98	0.46
19:S:1057:ARG:HG3	19:S:1134:TYR:HE1	1.81	0.46
1:A:1192:TRP:HZ3	1:A:1246:ILE:HG22	1.82	0.45
2:B:303:GLU:HG3	2:B:647:ASN:HD22	1.81	0.45
3:C:130:VAL:HG11	3:C:237:GLY:HA3	1.98	0.45
19:S:351:LYS:HA	19:S:351:LYS:HD2	1.80	0.45
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	1.97	0.45
2:B:142:ILE:HB	2:B:163:LEU:HB2	1.98	0.45
4:D:152:GLU:CA	4:D:155:ALA:HB3	2.42	0.45
19:S:285:GLN:NE2	19:S:288:GLU:OE1	2.49	0.45
1:A:108:ARG:NE	1:A:145:TYR:OH	2.49	0.45
1:A:465:HIS:CD2	1:A:467:MET:HE2	2.50	0.45
8:H:38:ASP:HB3	8:H:126:GLN:HG3	1.98	0.45
1:A:467:MET:HG3	1:A:524:MET:HB3	1.98	0.45
2:B:234:ARG:HH21	2:B:248:LEU:HD13	1.81	0.45
2:B:312:ILE:HD12	2:B:424:MET:HG2	1.97	0.45
4:D:129:LEU:HB3	4:D:139:LEU:HG	1.99	0.45
1:A:27:SER:HB3	1:A:247:TRP:CE2	2.52	0.45
1:A:722:ASN:OD1	17:M:564:SER:C	2.59	0.45
1:A:813:ASP:OD1	9:I:100:HIS:NE2	2.49	0.45
2:B:107:ILE:HD13	2:B:779:MET:HE3	1.98	0.45
19:S:1057:ARG:NH1	19:S:1135:LYS:O	2.42	0.45
1:A:945:ASN:OD1	1:A:946:ALA:N	2.49	0.45
2:B:644:ILE:HD11	2:B:654:HIS:HB2	1.99	0.45
2:B:682:ARG:NH2	9:I:74:GLN:HE22	2.15	0.45
19:S:924:LEU:HD21	19:S:965:ARG:HG2	1.99	0.45
1:A:706:ILE:HD11	1:A:787:VAL:HG21	1.99	0.45
2:B:394:ALA:O	2:B:398:ILE:HG13	2.16	0.45
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.99	0.45
3:C:115:VAL:HB	3:C:151:VAL:HG12	1.98	0.45
4:D:150:ALA:HB2	4:D:170:GLN:HG3	1.98	0.45
19:S:996:LYS:O	19:S:999:HIS:ND1	2.50	0.45
1:A:126:ILE:HD13	1:A:126:ILE:HA	1.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:389:HIS:O	19:S:393:LEU:N	2.42	0.45
1:A:1182:GLN:O	1:A:1190:GLN:NE2	2.50	0.44
2:B:1197:ASN:HB2	2:B:1222:GLN:HB3	1.98	0.44
6:F:79:VAL:HG11	6:F:83:LEU:HD23	1.99	0.44
2:B:476:LEU:HB3	2:B:530:TRP:CZ2	2.52	0.44
12:L:15:MET:N	12:L:28:ILE:O	2.50	0.44
7:G:59:ILE:HG12	7:G:66:VAL:HG22	2.00	0.44
1:A:129:ILE:O	1:A:133:SER:N	2.48	0.44
1:A:462:PRO:HG3	15:T:24:DG:H21	1.83	0.44
1:A:868:MET:HG2	1:A:1404:THR:HG21	1.99	0.44
19:S:424:GLN:NE2	19:S:441:ARG:O	2.46	0.44
19:S:1236:VAL:HG12	19:S:1275:PHE:HD2	1.82	0.44
1:A:104:MET:HE3	1:A:193:ARG:HB2	1.99	0.44
1:A:491:PRO:HG3	1:A:535:MET:SD	2.57	0.44
1:A:863:ARG:NH2	1:A:1129:ASN:OD1	2.51	0.44
2:B:127:PHE:HB2	2:B:474:GLY:HA2	1.98	0.44
2:B:578:LEU:HD12	2:B:582:LEU:HD12	2.00	0.44
5:E:55:ARG:HB2	5:E:78:GLU:HG2	1.98	0.44
19:S:469:LEU:HD11	19:S:594:LEU:HD13	1.98	0.44
2:B:142:ILE:HD11	2:B:489:LEU:HD22	1.99	0.44
2:B:884:ARG:HH12	12:L:58:ARG:C	2.26	0.44
3:C:267:ILE:HG12	11:K:84:GLN:HG2	2.00	0.44
4:D:154:LYS:HE3	4:D:154:LYS:HB2	1.84	0.44
5:E:174:GLN:HG3	5:E:210:GLN:HE21	1.82	0.44
7:G:49:THR:N	7:G:73:LYS:O	2.51	0.44
7:G:134:ASP:CG	19:S:475:ILE:HG23	2.38	0.44
11:K:61:TYR:HA	11:K:72:ILE:O	2.17	0.44
1:A:1123:ARG:NH2	1:A:1360:ASN:O	2.37	0.44
4:D:76:ASN:OD1	4:D:144:ASN:ND2	2.51	0.44
17:M:595:VAL:HA	18:O:101:LEU:HD21	1.99	0.44
19:S:695:ARG:H	19:S:706:ASN:HD21	1.66	0.44
1:A:723:ASN:HD21	9:I:109:ARG:HG2	1.83	0.44
1:A:228:ILE:O	1:A:244:ARG:NH2	2.41	0.44
1:A:1210:TRP:HH2	9:I:35:LEU:HD13	1.82	0.44
18:O:86:SER:OG	18:O:87:SER:N	2.51	0.44
1:A:42:LYS:HE3	1:A:42:LYS:HB2	1.79	0.43
17:M:646:PRO:HG3	17:M:655:MET:HE3	1.99	0.43
19:S:913:ALA:HA	19:S:916:LEU:HB2	1.99	0.43
1:A:425:ASP:OD1	1:A:425:ASP:N	2.46	0.43
2:B:388:ILE:HG23	2:B:393:VAL:HG12	2.00	0.43
15:T:24:DG:H2'	15:T:25:DA:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:68:ARG:HG3	16:Q:70:GLN:N	2.33	0.43
19:S:297:ARG:NH1	19:S:963:ILE:HD13	2.33	0.43
19:S:979:HIS:HB3	19:S:981:TYR:HB3	1.98	0.43
4:D:153:SER:OG	4:D:154:LYS:N	2.51	0.43
19:S:697:GLU:HG2	19:S:699:SER:H	1.82	0.43
19:S:1053:LEU:O	19:S:1056:SER:OG	2.30	0.43
1:A:300:ALA:HA	1:A:303:ILE:HG22	2.01	0.43
1:A:1368:VAL:HG12	1:A:1369:LEU:HG	2.00	0.43
2:B:470:LEU:HD22	2:B:562:LEU:HD22	1.99	0.43
19:S:909:VAL:O	19:S:912:GLN:HG2	2.19	0.43
1:A:196:LEU:HD13	1:A:311:GLN:HG3	2.01	0.43
2:B:171:SER:OG	2:B:172:LYS:N	2.51	0.43
8:H:36:LYS:HA	8:H:36:LYS:HD3	1.76	0.43
17:M:589:ILE:HD12	17:M:589:ILE:H	1.83	0.43
19:S:629:ASP:OD1	19:S:632:HIS:ND1	2.40	0.43
1:A:137:PRO:HB2	1:A:1445:HIS:HB3	2.01	0.43
2:B:169:TYR:HB2	2:B:202:TYR:HB2	2.00	0.43
11:K:42:LEU:HD13	11:K:45:ILE:HD11	2.00	0.43
13:N:36:DG:H2'	13:N:37:DG:C8	2.53	0.43
19:S:868:VAL:HG11	19:S:881:GLY:HA2	2.00	0.43
1:A:431:PHE:HZ	14:P:34:G:H2'	1.83	0.43
1:A:757:GLN:HA	1:A:760:LEU:HG	2.00	0.43
1:A:1235:ILE:HG13	1:A:1296:MET:HE1	2.01	0.43
2:B:703:LEU:HG	2:B:775:ILE:HG12	2.00	0.43
2:B:915:GLN:HB3	2:B:964:TYR:CG	2.53	0.43
5:E:35:GLN:HE21	5:E:35:GLN:HB3	1.62	0.43
19:S:378:PHE:O	19:S:381:LYS:NZ	2.47	0.43
19:S:1136:ASP:OD2	19:S:1138:ARG:NH2	2.52	0.43
2:B:208:THR:HG22	2:B:218:GLN:HG2	2.01	0.43
8:H:30:CYS:HB2	8:H:39:LEU:HB3	2.01	0.43
19:S:445:THR:O	19:S:449:GLU:N	2.45	0.43
19:S:906:TYR:CZ	19:S:910:LEU:HG	2.53	0.43
19:S:1108:ALA:HA	19:S:1111:LEU:HD12	2.00	0.43
2:B:1115:THR:HA	3:C:195:THR:HA	2.00	0.43
18:O:18:TYR:O	18:O:58:ASN:ND2	2.51	0.43
19:S:1057:ARG:HG3	19:S:1134:TYR:CE1	2.54	0.43
19:S:1120:HIS:CD2	19:S:1121:ILE:HG12	2.54	0.43
3:C:172:GLU:OE2	12:L:58:ARG:NH2	2.41	0.43
7:G:89:VAL:HA	7:G:99:THR:HA	2.01	0.43
13:N:39:DA:H2'	13:N:40:DG:C8	2.54	0.43
1:A:273:GLN:HB3	1:A:277:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:PRO:HB2	1:A:662:HIS:HB2	2.01	0.42
1:A:1372:GLU:HG3	5:E:193:ILE:HD13	2.01	0.42
2:B:1137:HIS:NE2	2:B:1159:GLY:O	2.47	0.42
9:I:12:VAL:HG11	9:I:52:CYS:HB3	2.01	0.42
16:Q:11:LYS:HD2	18:O:26:GLY:HA2	2.01	0.42
16:Q:79:PHE:O	16:Q:80:ARG:NE	2.43	0.42
19:S:320:ILE:HG12	19:S:399:TRP:HB3	1.99	0.42
1:A:346:LYS:NZ	15:T:24:DG:OP1	2.46	0.42
1:A:636:ILE:HG22	1:A:637:MET:HG2	2.01	0.42
1:A:1176:TYR:HB2	1:A:1211:LEU:HD23	2.01	0.42
1:A:1372:GLU:HG3	5:E:193:ILE:HG21	2.00	0.42
2:B:673:ILE:HD11	17:M:671:THR:HA	2.00	0.42
16:Q:43:ARG:HB3	16:Q:78:ALA:HB3	2.01	0.42
19:S:532:LEU:HB3	19:S:591:MET:HE3	2.01	0.42
1:A:620:HIS:O	8:H:97:TYR:OH	2.35	0.42
17:M:634:LYS:HA	17:M:637:CYS:HB2	2.02	0.42
1:A:557:ARG:O	1:A:561:MET:HG3	2.20	0.42
1:A:1172:ASN:HB2	1:A:1215:GLU:CD	2.45	0.42
2:B:172:LYS:HA	2:B:172:LYS:HD2	1.82	0.42
2:B:417:LYS:O	2:B:421:GLN:HB2	2.18	0.42
2:B:787:ILE:HG23	2:B:841:MET:HE3	2.01	0.42
7:G:78:ARG:HH12	7:G:150:THR:HG21	1.84	0.42
19:S:707:ARG:HH21	19:S:708:GLN:HG2	1.83	0.42
1:A:132:LYS:HB3	1:A:132:LYS:HE2	1.91	0.42
2:B:1052:ARG:HB3	2:B:1054:THR:HG23	2.02	0.42
9:I:78:LEU:HD23	9:I:78:LEU:HA	1.89	0.42
1:A:375:ILE:HD12	1:A:521:VAL:HG12	2.01	0.42
1:A:479:TRP:CD1	2:B:1008:ILE:HD12	2.54	0.42
1:A:514:GLU:O	1:A:518:LEU:HB2	2.20	0.42
2:B:618:ILE:HG12	2:B:674:ILE:HD13	2.01	0.42
2:B:1185:PHE:HZ	2:B:1227:ARG:HB3	1.84	0.42
7:G:166:ASP:CG	7:G:167:TYR:CE2	2.98	0.42
19:S:523:MET:O	19:S:524:TYR:C	2.63	0.42
19:S:618:ILE:HG21	19:S:665:LEU:HD13	2.01	0.42
1:A:239:GLU:HG2	1:A:242:TYR:CD2	2.54	0.42
1:A:422:ASP:OD1	1:A:422:ASP:N	2.51	0.42
2:B:1011:LYS:HG2	2:B:1128:LEU:HD12	2.01	0.42
19:S:754:ARG:O	19:S:1139:THR:N	2.53	0.42
1:A:220:ARG:O	1:A:224:ILE:HD12	2.19	0.42
2:B:451:LEU:HB3	2:B:457:ARG:HB2	2.02	0.42
3:C:189:ASP:OD1	3:C:209:SER:OG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:46:ARG:O	10:J:50:LEU:CB	2.68	0.42
18:O:32:LYS:HB2	18:O:35:HIS:HB2	2.02	0.42
19:S:851:ALA:HB1	19:S:887:ASN:ND2	2.35	0.42
19:S:1121:ILE:O	19:S:1125:ASP:N	2.48	0.42
1:A:111:CYS:SG	1:A:112:PHE:N	2.93	0.42
2:B:171:SER:HB3	2:B:200:PRO:HG2	2.01	0.42
11:K:57:LEU:N	11:K:76:GLN:O	2.52	0.42
19:S:1107:PHE:HB2	19:S:1123:LEU:HD13	2.02	0.42
1:A:579:ILE:HG12	8:H:92:MET:HG2	2.01	0.42
2:B:445:MET:HE2	2:B:445:MET:HB3	1.92	0.42
2:B:616:SER:O	2:B:619:LEU:N	2.51	0.42
19:S:570:ALA:O	19:S:574:VAL:HG13	2.20	0.42
19:S:637:PHE:HE1	19:S:652:GLN:HG2	1.85	0.42
19:S:753:LEU:HD22	19:S:924:LEU:HD13	2.02	0.42
1:A:435:PRO:HA	1:A:438:LEU:HB2	2.00	0.41
2:B:617:PRO:HG3	17:M:678:HIS:CD2	2.55	0.41
11:K:41:THR:O	11:K:45:ILE:HG12	2.20	0.41
1:A:539:GLN:H	1:A:539:GLN:HG2	1.58	0.41
1:A:1146:GLN:HB3	1:A:1153:ARG:NH2	2.34	0.41
2:B:376:GLU:HA	2:B:379:LYS:HE3	2.02	0.41
1:A:544:ALA:HB2	1:A:680:LEU:HD13	2.02	0.41
1:A:893:GLU:OE1	5:E:197:SER:OG	2.33	0.41
7:G:119:PHE:C	7:G:121:PRO:HD3	2.46	0.41
19:S:319:TRP:NE1	19:S:455:GLN:O	2.42	0.41
19:S:542:THR:HB	19:S:545:GLN:HB2	2.02	0.41
2:B:162:LEU:HB3	2:B:208:THR:OG1	2.20	0.41
2:B:257:ASP:HA	2:B:258:PRO:HD3	1.92	0.41
11:K:109:ILE:HD13	11:K:109:ILE:HA	1.90	0.41
17:M:633:TRP:CD1	17:M:653:ARG:HB2	2.56	0.41
18:O:20:LYS:HE2	18:O:30:ILE:HD12	2.03	0.41
19:S:522:ASP:C	19:S:524:TYR:N	2.78	0.41
19:S:585:LEU:O	19:S:589:ARG:HG3	2.20	0.41
19:S:1013:SER:HB3	19:S:1016:GLN:HB2	2.01	0.41
1:A:58:MET:HA	1:A:258:LEU:HD21	2.01	0.41
1:A:87:HIS:CD2	1:A:89:GLU:HG3	2.55	0.41
2:B:720:LEU:HD11	2:B:733:LEU:HD11	2.01	0.41
2:B:792:ASP:OD1	2:B:792:ASP:N	2.45	0.41
2:B:857:VAL:HG21	2:B:1125:TYR:CE1	2.56	0.41
2:B:898:LYS:HB2	2:B:902:GLN:HB2	2.01	0.41
2:B:1171:GLN:HB2	2:B:1180:LEU:HD13	2.01	0.41
5:E:90:TYR:O	5:E:94:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:707:ARG:CZ	19:S:708:GLN:HE21	2.33	0.41
1:A:540:ASP:HB2	2:B:867:GLN:CD	2.45	0.41
1:A:592:PHE:HZ	1:A:645:LEU:HD11	1.85	0.41
1:A:1189:ASP:OD1	1:A:1189:ASP:N	2.53	0.41
2:B:477:LEU:HD21	2:B:525:LEU:HD11	2.02	0.41
9:I:92:LYS:HE2	17:M:583:ARG:HD2	2.03	0.41
19:S:907:PRO:HA	19:S:908:PRO:HD3	1.95	0.41
2:B:316:MET:HB2	2:B:449:LEU:HD21	2.01	0.41
2:B:360:ASP:O	2:B:364:HIS:ND1	2.54	0.41
8:H:72:ASP:OD1	8:H:72:ASP:N	2.54	0.41
11:K:39:ASP:N	11:K:39:ASP:OD1	2.53	0.41
17:M:618:ILE:O	17:M:622:ASN:N	2.53	0.41
19:S:546:PHE:CE1	19:S:693:TYR:HB2	2.55	0.41
1:A:222:HIS:HB2	1:A:249:ILE:HG21	2.02	0.41
1:A:376:ASP:HB3	1:A:522:PRO:HD3	2.03	0.41
1:A:767:LYS:O	1:A:771:VAL:HG22	2.21	0.41
1:A:825:ASN:ND2	1:A:835:GLU:OE1	2.53	0.41
2:B:342:GLN:HG3	2:B:401:ARG:HD2	2.02	0.41
1:A:381:PRO:HG2	1:A:384:ILE:HD12	2.02	0.41
1:A:723:ASN:OD1	9:I:109:ARG:NH1	2.54	0.41
2:B:144:LEU:HD11	2:B:493:ARG:HA	2.02	0.41
2:B:681:ILE:HG12	2:B:745:LEU:HB3	2.02	0.41
11:K:77:THR:OG1	11:K:81:TYR:O	2.35	0.41
17:M:571:LEU:HD13	17:M:583:ARG:HH21	1.86	0.41
19:S:289:ILE:HG23	19:S:299:GLN:OE1	2.21	0.41
19:S:596:ILE:HD13	19:S:713:ILE:HG22	2.02	0.41
19:S:690:LYS:HE2	19:S:690:LYS:HB3	1.83	0.41
1:A:904:GLN:NE2	1:A:981:CYS:O	2.54	0.41
1:A:1357:THR:O	5:E:142:HIS:NE2	2.40	0.41
2:B:123:SER:HB3	2:B:474:GLY:H	1.86	0.41
15:T:22:DC:H2'	15:T:23:DC:C6	2.56	0.41
16:Q:41:GLU:HG3	16:Q:80:ARG:HH21	1.85	0.41
19:S:893:TYR:CG	19:S:915:SER:HB3	2.56	0.41
1:A:532:ARG:HD2	1:A:647:THR:O	2.21	0.40
1:A:659:GLU:OE2	1:A:989:ASN:ND2	2.40	0.40
1:A:706:ILE:HD13	1:A:706:ILE:HA	1.91	0.40
1:A:801:GLY:HA3	2:B:580:ASN:HB2	2.02	0.40
1:A:913:ASN:OD1	1:A:963:ARG:NH2	2.46	0.40
1:A:924:TYR:HA	1:A:930:LEU:HD11	2.02	0.40
7:G:109:SER:HB3	7:G:112:SER:HB2	2.03	0.40
9:I:91:HIS:CE1	9:I:93:GLU:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:MET:HE1	1:A:248:MET:HE2	2.02	0.40
1:A:635:LEU:HD12	1:A:635:LEU:HA	1.91	0.40
1:A:1285:LEU:HD12	1:A:1288:ILE:HD11	2.03	0.40
4:D:152:GLU:HG3	7:G:167:TYR:CE2	2.55	0.40
7:G:132:ASP:O	19:S:416:LEU:CG	2.68	0.40
1:A:469:MET:HE1	2:B:1163:PHE:CE1	2.56	0.40
1:A:719:LYS:HB3	1:A:719:LYS:HE2	1.83	0.40
2:B:1065:LYS:HD3	2:B:1092:LEU:HD21	2.01	0.40
6:F:81:VAL:HG21	6:F:95:LYS:HG3	2.03	0.40
9:I:11:PHE:CE1	9:I:57:LYS:HG3	2.56	0.40
15:T:30:DG:H2'	15:T:31:DT:C6	2.56	0.40
18:O:103:LEU:O	18:O:106:ALA:HB3	2.22	0.40
19:S:399:TRP:CE3	19:S:402:LYS:HD2	2.56	0.40
19:S:522:ASP:CG	19:S:524:TYR:HB3	2.46	0.40
1:A:375:ILE:HG22	1:A:485:ASN:HD22	1.85	0.40
1:A:457:ILE:HD11	1:A:515:ILE:HD12	2.02	0.40
1:A:962:ASP:CG	1:A:1043:ILE:HG12	2.46	0.40
3:C:92:GLU:HG2	3:C:93:PHE:CD2	2.57	0.40
3:C:101:PHE:CE2	3:C:122:SER:HB3	2.57	0.40
18:O:105:MET:HA	18:O:108:ASN:HD22	1.86	0.40
19:S:717:LEU:HD12	19:S:717:LEU:HA	1.96	0.40
1:A:833:PRO:HG3	2:B:1079:PHE:CG	2.57	0.40
1:A:901:VAL:HB	1:A:978:VAL:HG12	2.04	0.40
1:A:1308:TYR:HB2	1:A:1337:GLU:O	2.21	0.40
2:B:440:TYR:HD2	2:B:630:LEU:HD13	1.86	0.40
2:B:513:LYS:HB3	2:B:513:LYS:HE3	1.86	0.40
2:B:1219:ASN:ND2	2:B:1222:GLN:O	2.54	0.40
5:E:102:ALA:HB3	5:E:127:LEU:HD23	2.03	0.40
16:Q:32:GLU:HA	16:Q:37:ARG:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1395/1970 (71%)	1357 (97%)	38 (3%)	0	100	100
2	B	1123/1251 (90%)	1089 (97%)	34 (3%)	0	100	100
3	C	254/275 (92%)	249 (98%)	5 (2%)	0	100	100
4	D	114/184 (62%)	104 (91%)	10 (9%)	0	100	100
5	E	207/210 (99%)	201 (97%)	6 (3%)	0	100	100
6	F	76/127 (60%)	74 (97%)	2 (3%)	0	100	100
7	G	169/172 (98%)	157 (93%)	12 (7%)	0	100	100
8	H	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
9	I	114/125 (91%)	107 (94%)	7 (6%)	0	100	100
10	J	64/67 (96%)	64 (100%)	0	0	100	100
11	K	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
12	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
16	Q	86/118 (73%)	73 (85%)	13 (15%)	0	100	100
17	M	136/801 (17%)	126 (93%)	10 (7%)	0	100	100
18	O	99/112 (88%)	92 (93%)	7 (7%)	0	100	100
19	S	792/1729 (46%)	762 (96%)	30 (4%)	0	100	100
All	All	4930/7466 (66%)	4748 (96%)	182 (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	1239/1749 (71%)	1239 (100%)	0	100	100
2	B	991/1084 (91%)	991 (100%)	0	100	100
3	C	235/252 (93%)	235 (100%)	0	100	100
4	D	109/160 (68%)	109 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	68/111 (61%)	68 (100%)	0	100	100
7	G	151/153 (99%)	151 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	102/112 (91%)	102 (100%)	0	100	100
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	40/55 (73%)	40 (100%)	0	100	100
16	Q	75/103 (73%)	75 (100%)	0	100	100
17	M	121/706 (17%)	121 (100%)	0	100	100
18	O	88/96 (92%)	88 (100%)	0	100	100
19	S	710/1524 (47%)	709 (100%)	1 (0%)	88	89
All	All	4408/6590 (67%)	4407 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	S	462	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	412	GLN
1	A	465	HIS
1	A	485	ASN
1	A	673	GLN
1	A	703	GLN
1	A	711	GLN
1	A	723	ASN
1	A	735	GLN
1	A	792	ASN
1	A	1420	ASN
2	B	222	GLN
2	B	708	GLN
2	B	726	ASN
2	B	731	GLN
2	B	802	GLN

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Mol	Chain	Res	Type
2	B	874	ASN
2	B	1063	GLN
2	B	1084	ASN
2	B	1126	GLN
2	B	1171	GLN
4	D	144	ASN
5	E	35	GLN
5	E	71	GLN
5	E	132	GLN
5	E	133	GLN
5	E	169	GLN
7	G	60	GLN
9	I	41	ASN
9	I	67	GLN
9	I	74	GLN
11	K	69	HIS
17	M	665	GLN
17	M	678	HIS
19	S	299	GLN
19	S	405	GLN
19	S	465	ASN
19	S	577	GLN
19	S	608	GLN
19	S	869	HIS
19	S	1114	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	12/46 (26%)	2 (16%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	36	G
14	P	37	G

There are no RNA pucker outliers to report.

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 9 ligands modelled in this entry, 9 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

This section contains visualisations of the EMDB entry EMD-16840. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.