



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:24 AM UTC

PDB ID : 7WBX / pdb_00007wbx
EMDB ID : EMD-32409
Title : RNA polymerase II elongation complex bound with Elf1 and Spt4/5, stalled at SHL(-3) of the nucleosome
Authors : Osumi, K.; Kujirai, T.; Ehara, H.; Sekine, S.; Takizawa, Y.; Kurumizaka, H.
Deposited on : 2021-12-17
Resolution : 4.00 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

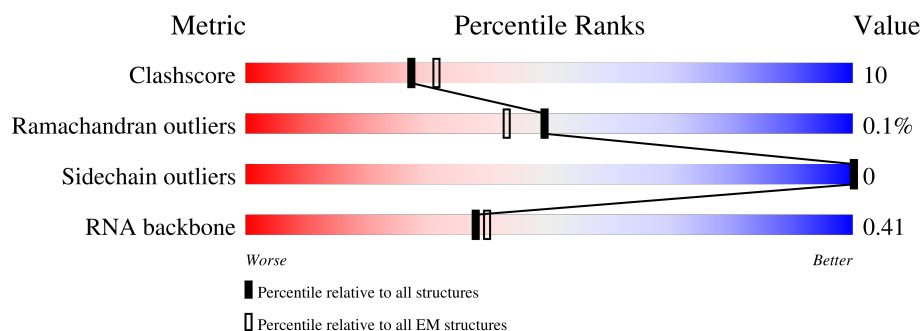
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.



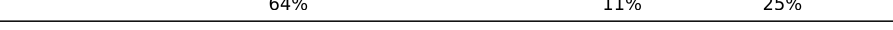
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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	1743	63% 18% 19%
2	B	1227	73% 21% 6%
3	C	304	65% 22% 13%
4	D	186	65% 25% 10%
5	E	214	74% 25%
6	F	155	39% 15% 46%
7	G	171	78% 22%

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Mol	Chain	Length	Quality of chain
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	M	113	
14	N	198	
15	P	16	
16	T	198	
17	V	108	
18	W	911	
19	a	139	
19	e	139	
20	b	106	
20	f	106	
21	c	133	
21	g	133	
22	d	129	
22	h	129	

2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 91763 atoms, of which 44620 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.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1412	Total	C	H	N	O	S	0	0
			22279	7014	11156	1938	2101	70		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1157	Total	C	H	N	O	S	0	0
			18471	5816	9243	1630	1724	58		

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	263	Total	C	H	N	O	S	0	0
			4160	1319	2062	354	413	12		

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	168	Total	C	H	N	O	S	0	0
			2631	812	1317	237	263	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	213	Total	C	H	N	O	S	0	0
			3495	1094	1755	312	324	10		

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	84	Total	C	H	N	O	S	0	0
			1371	429	694	114	131	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	171	Total	C	H	N	O	S	0	0
			2666	858	1342	214	247	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	133	Total	C	H	N	O	S	0	0
			2104	671	1052	169	208	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	111	Total	C	H	N	O	S	0	0
			1790	565	873	161	180	11		

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	66	Total	C	H	N	O	S	0	0
			1109	349	564	95	95	6		

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	113	Total	C	H	N	O	S	0	0
			1876	599	944	160	169	4		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	45	Total	C	H	N	O	S	0	0
			722	221	363	72	61	5		

- Molecule 13 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	64	Total	C	H	N	O	S	0	0
			1005	318	500	82	99	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLY	-	expression tag	UNP C4QZ45
M	-1	PRO	-	expression tag	UNP C4QZ45
M	0	GLY	-	expression tag	UNP C4QZ45

- Molecule 14 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	145	Total	C	H	N	O	P	0	0
			4617	1415	1639	526	892	145		

- Molecule 15 is a RNA chain called RNA (5'-R(P*UP*CP*GP*UP*UP*GP*UP*UP*UP*UP*UP*UP*UP*CP*UP*G)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	16	Total	C	H	N	O	P	0	0
			494	147	165	43	123	16		

- Molecule 16 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
16	T	150	Total	C	H	N	O	P	0	0
			4738	1452	1672	591	874	149		

- Molecule 17 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	V	102	Total	C	H	N	O	S	0	0
			1554	492	762	143	150	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	7	MET	-	initiating methionine	UNP C4R0E6

- Molecule 18 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	W	275	Total	C	H	N	O	S	0	0
			4503	1425	2277	397	403	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-2	GLY	-	expression tag	UNP C4R370
W	-1	PRO	-	expression tag	UNP C4R370
W	0	GLY	-	expression tag	UNP C4R370

- Molecule 19 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	a	97	Total	C	H	N	O	S	0	0
			1632	503	835	155	137	2		
19	e	97	Total	C	H	N	O	S	0	0
			1629	501	833	155	138	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-3	GLY	-	expression tag	UNP P84243
a	-2	SER	-	expression tag	UNP P84243
a	-1	HIS	-	expression tag	UNP P84243
e	-3	GLY	-	expression tag	UNP P84243
e	-2	SER	-	expression tag	UNP P84243
e	-1	HIS	-	expression tag	UNP P84243

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	b	80	Total	C	H	N	O	S	0	0
			1315	401	677	125	111	1		
20	f	78	Total	C	H	N	O	S	0	0
			1279	391	660	120	107	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805

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Chain	Residue	Modelled	Actual	Comment	Reference
b	0	MET	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805
f	0	MET	-	expression tag	UNP P62805

- Molecule 21 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	103	Total	C	H	N	O	0	0
			1645	502	849	155	139		
21	g	105	Total	C	H	N	O	0	0
			1677	511	867	158	141		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908
c	-1	HIS	-	expression tag	UNP P04908
c	0	MET	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908
g	0	MET	-	expression tag	UNP P04908

- Molecule 22 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	d	95	Total	C	H	N	O S	0	0
			1518	468	772	136	140 2		
22	h	93	Total	C	H	N	O S	0	0
			1472	456	747	130	137 2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-6	GLY	-	expression tag	UNP P06899
d	-5	SER	-	expression tag	UNP P06899
d	-4	HIS	-	expression tag	UNP P06899
d	-3	MET	-	expression tag	UNP P06899
h	-6	GLY	-	expression tag	UNP P06899

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Chain	Residue	Modelled	Actual	Comment	Reference
h	-5	SER	-	expression tag	UNP P06899
h	-4	HIS	-	expression tag	UNP P06899
h	-3	MET	-	expression tag	UNP P06899

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

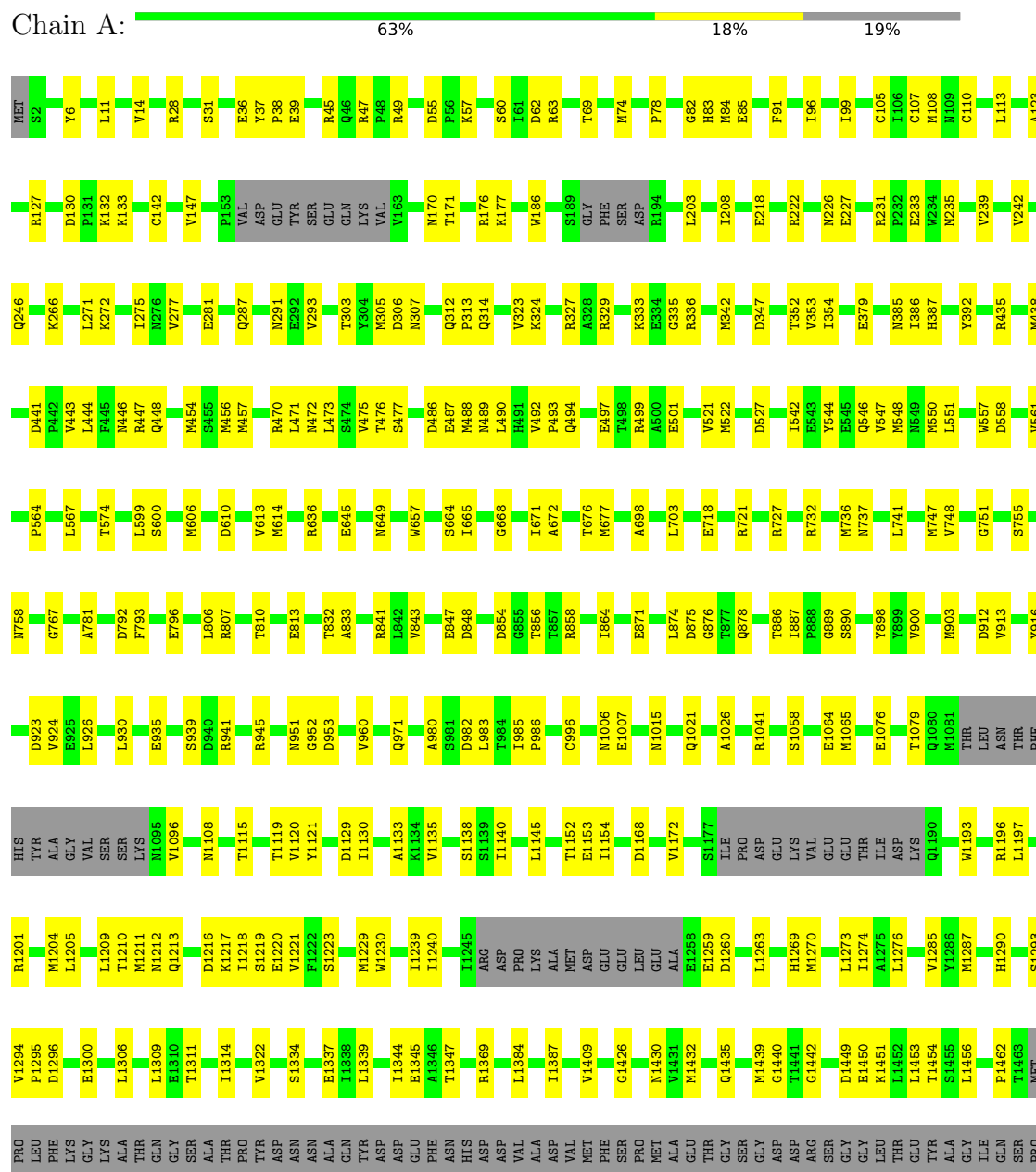
- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

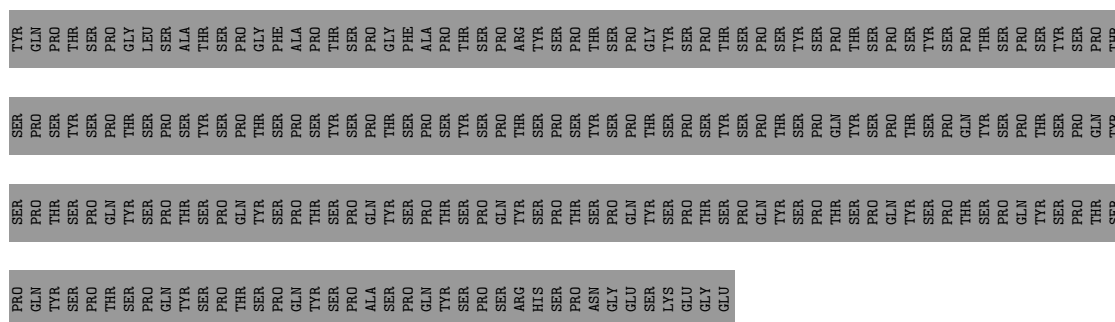
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total 1	Mg 1	0

3 Residue-property plots

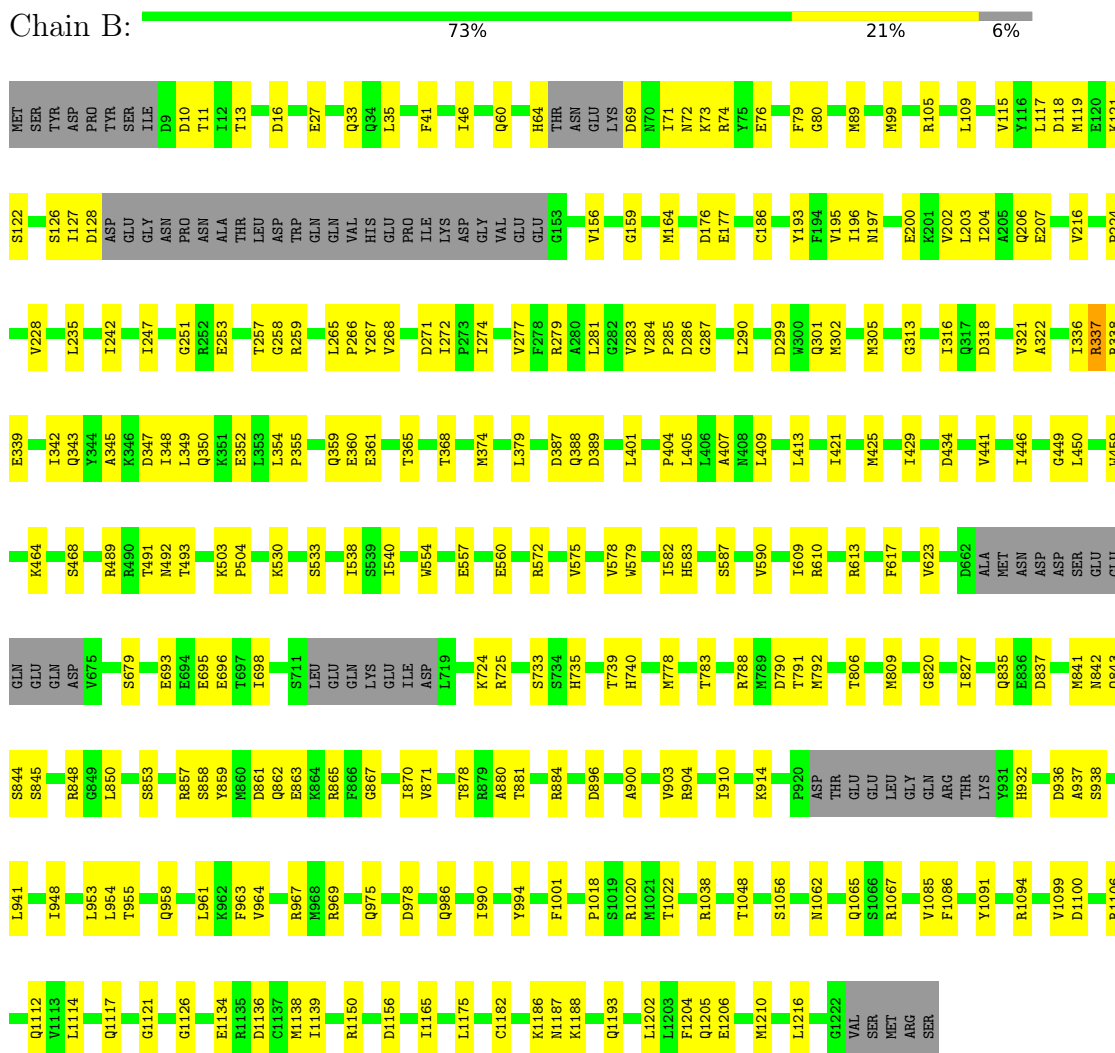
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 subunit

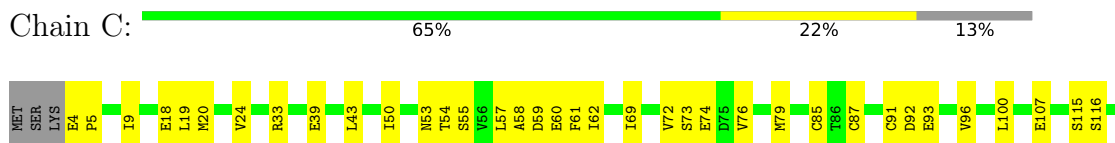


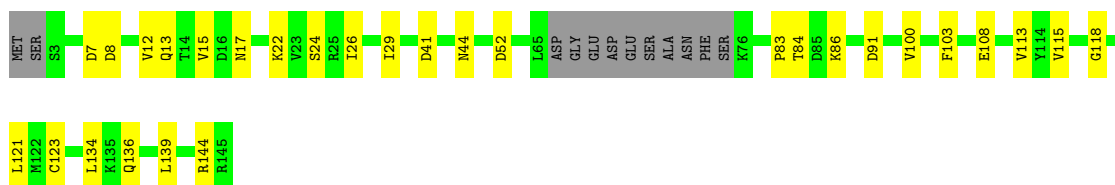


- Molecule 2: DNA-directed RNA polymerase subunit beta



- Molecule 3: RNA polymerase II third largest subunit B44, part of central core





- Molecule 9: DNA-directed RNA polymerase subunit

Chain I: 69% 28% .



- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

Chain J: 64% 28% 8%



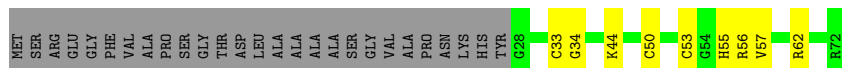
- Molecule 11: RNA polymerase II subunit B12.5

Chain K: 74% 22% .



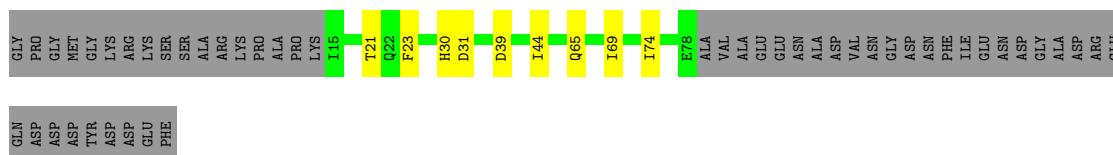
- Molecule 12: RNA polymerase subunit ABC10-alpha

Chain L: 50% 12% 38%



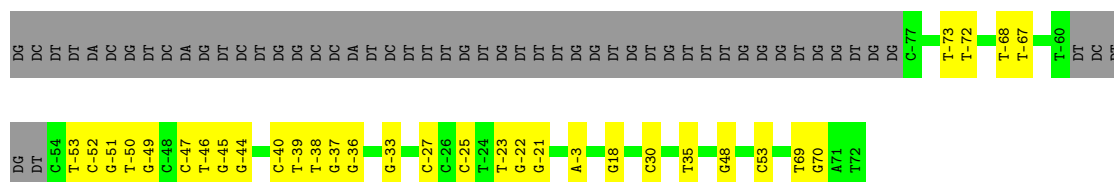
- Molecule 13: Transcription elongation factor 1 homolog

Chain M: 49% 8% 43%



- Molecule 14: DNA (198-MER)

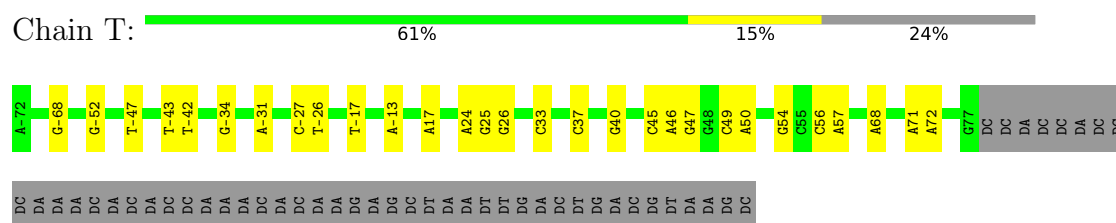
Chain N: 57% 16% 27%



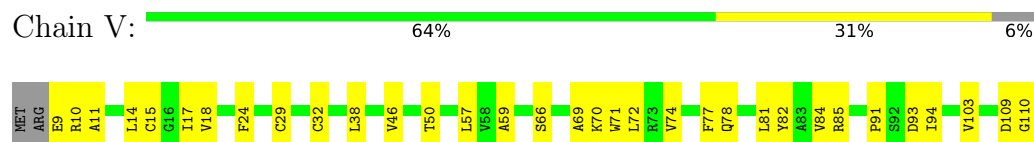
- Molecule 15: RNA (5'-R(P*UP*CP*GP*UP*UP*GP*UP*UP*UP*UP*UP*UP*UP*CP*UP*G)-3')



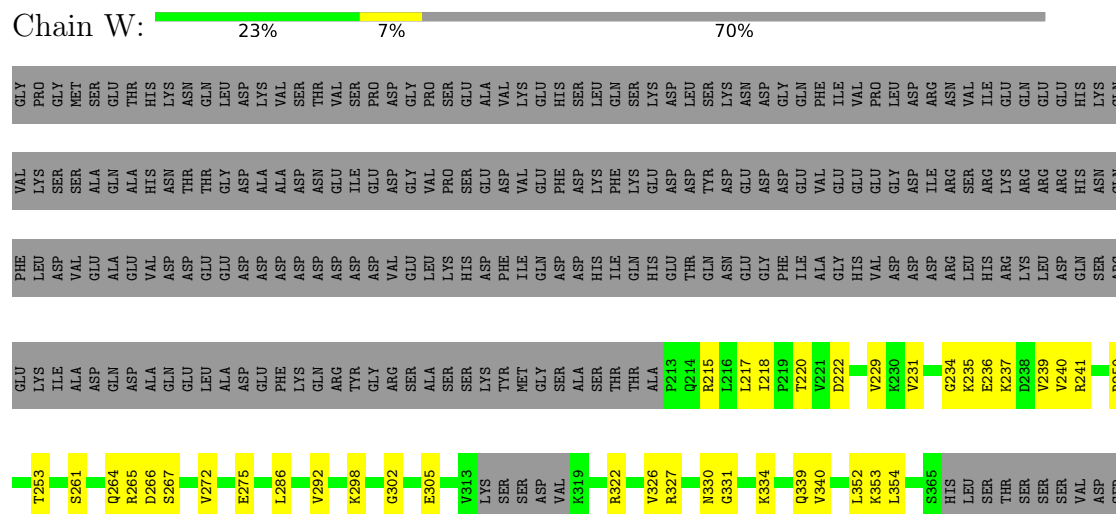
- Molecule 16: DNA (198-MER)

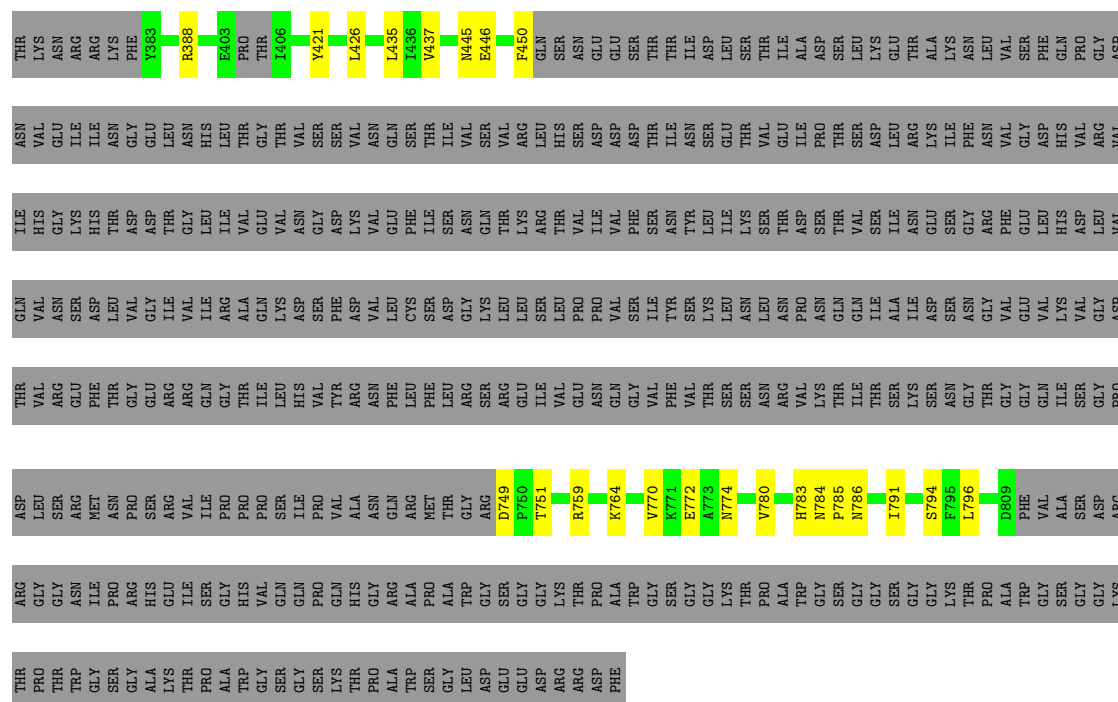


- Molecule 17: Transcription elongation factor SPT4

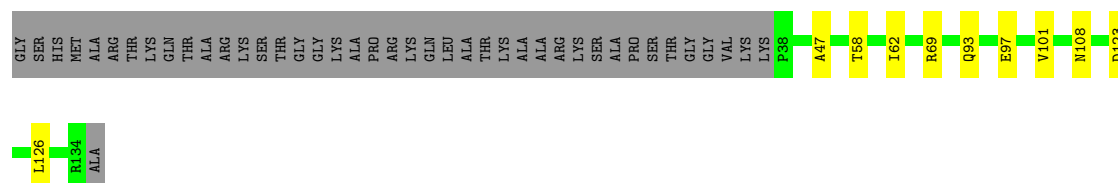


- Molecule 18: Transcription elongation factor SPT5

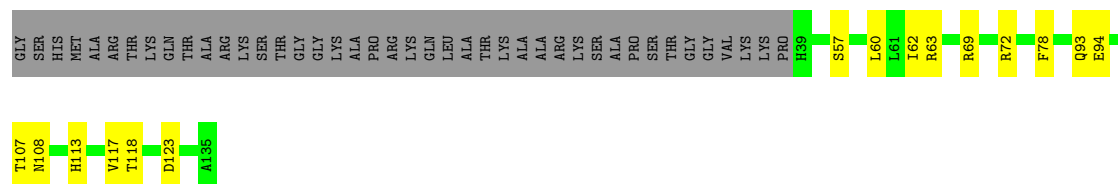




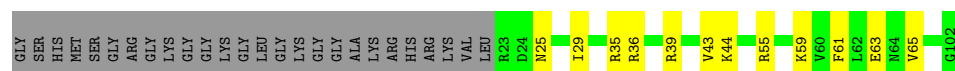
- Molecule 19: Histone H3.3



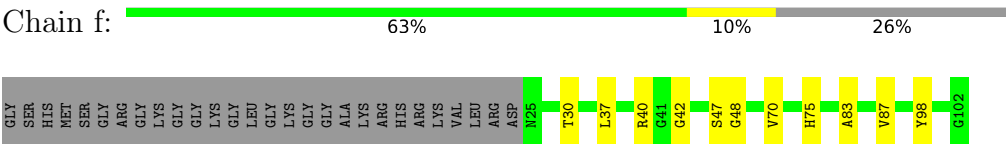
- Molecule 19: Histone H3.3



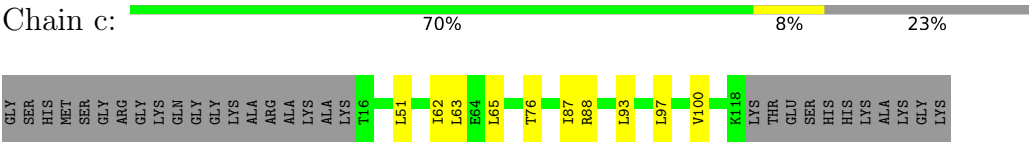
- Molecule 20: Histone H4



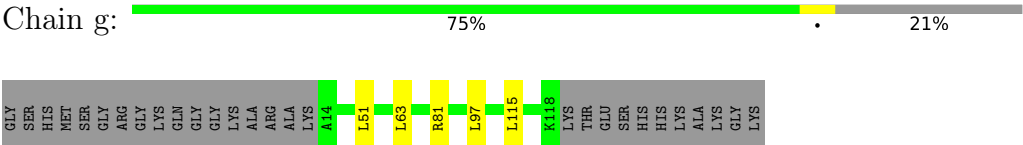
- Molecule 20: Histone H4



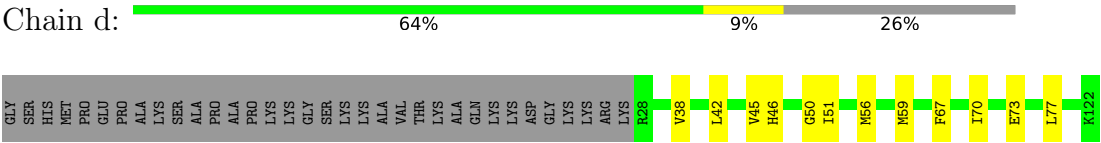
● Molecule 21: Histone H2A type 1-B/E



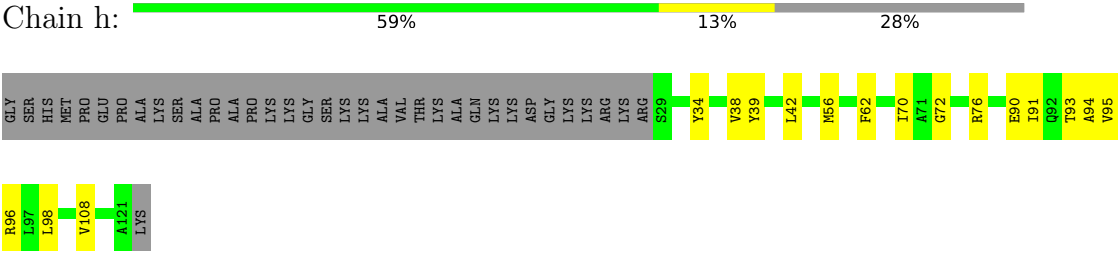
● Molecule 21: Histone H2A type 1-B/E



● Molecule 22: Histone H2B type 1-J



● Molecule 22: Histone H2B type 1-J



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38079	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 ($e^-/\text{\AA}^2$)	57.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.24	0/11329	0.35	0/15310
2	B	0.25	0/9407	0.35	0/12685
3	C	0.26	0/2139	0.35	0/2895
4	D	0.14	0/1326	0.33	0/1788
5	E	0.22	0/1772	0.30	0/2385
6	F	0.25	0/687	0.34	0/931
7	G	0.14	0/1353	0.31	0/1837
8	H	0.23	0/1069	0.31	0/1444
9	I	0.13	0/934	0.29	0/1257
10	J	0.26	0/554	0.38	0/742
11	K	0.24	0/953	0.32	0/1291
12	L	0.22	0/365	0.32	0/484
13	M	0.15	0/513	0.31	0/693
14	N	0.20	0/3333	0.42	0/5145
15	P	0.21	0/363	0.22	0/561
16	T	0.21	0/3446	0.40	0/5311
17	V	0.12	0/808	0.25	0/1097
18	W	0.12	0/2267	0.29	0/3048
19	a	0.11	0/809	0.30	0/1085
19	e	0.13	0/807	0.30	0/1081
20	b	0.14	0/645	0.34	0/862
20	f	0.15	0/626	0.28	0/837
21	c	0.13	0/806	0.32	0/1089
21	g	0.12	0/820	0.27	0/1107
22	d	0.13	0/757	0.29	0/1015
22	h	0.13	0/736	0.30	0/990
All	All	0.21	0/48624	0.35	0/66970

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	11123	11156	11146	244	0
2	B	9228	9243	9232	202	0
3	C	2098	2062	2057	55	0
4	D	1314	1317	1314	31	0
5	E	1740	1755	1754	36	0
6	F	677	694	693	22	0
7	G	1324	1342	1342	28	0
8	H	1052	1052	1050	17	0
9	I	917	873	866	27	0
10	J	545	564	560	18	0
11	K	932	944	944	22	0
12	L	359	363	358	7	0
13	M	505	500	495	6	0
14	N	2978	1639	1640	33	0
15	P	329	165	165	6	0
16	T	3066	1672	1673	35	0
17	V	792	762	757	23	0
18	W	2226	2277	2273	45	0
19	a	797	835	835	8	0
19	e	796	833	832	15	0
20	b	638	677	676	11	0
20	f	619	660	659	9	0
21	c	796	849	848	11	0
21	g	810	867	866	8	0
22	d	746	772	771	11	0
22	h	725	747	745	15	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	V	1	0	0	0	0
24	A	1	0	0	0	0
All	All	47143	44620	44551	821	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 10.

All (821) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:900:VAL:HG21	1:A:930:LEU:HD23	1.33	1.05
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.37	1.04
3:C:69:ILE:HD11	3:C:144:LEU:HD21	1.50	0.94
14:N:-44:DG:N2	16:T:45:DC:O2	2.01	0.94
1:A:39:GLU:O	1:A:49:ARG:NH2	2.07	0.88
1:A:996:CYS:O	1:A:1021:GLN:NE2	2.06	0.88
1:A:333:LYS:NZ	16:T:56:DC:OP2	2.06	0.88
1:A:889:GLY:O	1:A:941:ARG:NH2	2.07	0.87
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.56	0.87
2:B:27:GLU:OE2	2:B:679:SER:OG	1.91	0.87
3:C:85:CYS:O	18:W:764:LYS:NZ	2.08	0.86
1:A:60:SER:O	1:A:74:MET:HE1	1.75	0.85
1:A:108:MET:SD	1:A:170:ASN:ND2	2.50	0.84
2:B:299:ASP:HB3	2:B:302:MET:HE2	1.60	0.83
19:a:69:ARG:NH1	20:b:25:ASN:OD1	2.12	0.83
11:K:57:THR:OG1	11:K:76:GLN:O	1.97	0.83
1:A:930:LEU:HD11	1:A:985:ILE:HG21	1.60	0.82
2:B:305:MET:HE3	2:B:379:LEU:HD12	1.61	0.82
2:B:1038:ARG:NH1	2:B:1062:ASN:OD1	2.12	0.82
8:H:91:ASP:O	8:H:144:ARG:NH1	2.12	0.82
1:A:916:TYR:OH	1:A:983:LEU:O	1.98	0.81
1:A:287:GLN:O	1:A:291:ASN:ND2	2.12	0.81
2:B:355:PRO:O	2:B:359:GLN:NE2	2.13	0.81
14:N:-25:DC:O2	16:T:25:DG:N2	2.13	0.81
17:V:46:VAL:O	17:V:50:THR:OG1	1.98	0.81
2:B:318:ASP:OD1	2:B:321:VAL:HG22	1.82	0.80
1:A:676:THR:OG1	1:A:737:ASN:ND2	2.14	0.80
1:A:636:ARG:NH1	1:A:878:GLN:OE1	2.15	0.79
5:E:21:MET:HE3	5:E:25:ARG:HD2	1.64	0.79
2:B:186:CYS:SG	2:B:783:THR:OG1	2.39	0.79
2:B:207:GLU:OE2	2:B:493:THR:OG1	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ASN:OD1	1:A:447:ARG:N	2.16	0.79
1:A:218:GLU:OE2	1:A:222:ARG:NH2	2.16	0.78
1:A:444:LEU:HD21	1:A:456:MET:CE	2.13	0.78
2:B:613:ARG:NH2	9:I:57:GLY:O	2.17	0.78
1:A:1172:VAL:HG12	1:A:1229:MET:HE2	1.65	0.78
2:B:35:LEU:HD23	2:B:164:MET:HE3	1.67	0.78
14:N:-49:DG:O6	16:T:49:DC:N4	2.16	0.77
1:A:718:GLU:OE1	1:A:721:ARG:NH2	2.18	0.77
1:A:1462:PRO:O	7:G:21:GLN:NE2	2.18	0.77
2:B:121:LYS:NZ	2:B:434:ASP:OD1	2.18	0.77
6:F:81:THR:OG1	6:F:144:GLU:OE2	2.02	0.77
7:G:152:THR:HG23	7:G:157:ILE:HG22	1.65	0.77
4:D:110:ASN:O	4:D:116:LYS:NZ	2.18	0.76
2:B:733:SER:OG	2:B:735:HIS:O	2.03	0.76
5:E:28:PHE:HB2	5:E:64:THR:HG22	1.67	0.76
1:A:807:ARG:NE	2:B:724:LYS:O	2.19	0.76
14:N:-40:DC:O2	16:T:40:DG:N2	2.13	0.76
5:E:47:ASP:OD2	5:E:53:GLN:NE2	2.18	0.75
1:A:887:ILE:O	1:A:945:ARG:NH2	2.20	0.75
14:N:-37:DG:O6	16:T:37:DC:N4	2.20	0.74
4:D:169:VAL:O	4:D:171:LEU:HD12	1.87	0.74
1:A:1450:GLU:O	1:A:1454:THR:HG23	1.87	0.74
1:A:951:ASN:ND2	1:A:953:ASP:OD2	2.21	0.74
8:H:7:ASP:OD1	8:H:8:ASP:N	2.20	0.73
18:W:327:ARG:NH2	18:W:446:GLU:OE2	2.21	0.73
9:I:19:ASP:O	9:I:23:GLN:N	2.21	0.73
1:A:755:SER:N	1:A:758:ASN:OD1	2.21	0.73
1:A:62:ASP:OD1	1:A:63:ARG:N	2.21	0.73
2:B:489:ARG:NH2	2:B:533:SER:O	2.20	0.73
5:E:190:LYS:N	5:E:193:GLN:OE1	2.20	0.73
19:e:62:ILE:O	19:e:93:GLN:NE2	2.22	0.72
2:B:464:LYS:O	2:B:468:SER:OG	2.06	0.72
2:B:492:ASN:OD1	2:B:493:THR:N	2.23	0.72
1:A:982:ASP:O	1:A:1041:ARG:NH2	2.22	0.72
4:D:118:GLU:OE2	4:D:122:THR:OG1	2.07	0.72
5:E:213:CYS:SG	5:E:214:LEU:N	2.63	0.72
1:A:99:ILE:HG13	1:A:235:MET:HE2	1.71	0.72
1:A:1450:GLU:N	1:A:1450:GLU:OE1	2.23	0.72
3:C:93:GLU:N	3:C:93:GLU:OE1	2.23	0.72
16:T:17:DA:OP2	19:e:69:ARG:NH2	2.22	0.71
10:J:57:GLU:OE1	10:J:57:GLU:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1210:THR:OG1	1:A:1212:ASN:OD1	2.09	0.71
2:B:413:LEU:HD21	2:B:449:GLY:HA3	1.72	0.71
17:V:69:ALA:HB1	17:V:74:VAL:HG23	1.72	0.71
1:A:874:LEU:O	1:A:1369:ARG:NH1	2.23	0.71
1:A:379:GLU:OE1	1:A:435:ARG:NE	2.23	0.71
2:B:251:GLY:O	2:B:259:ARG:NH2	2.23	0.71
6:F:140:ASP:OD1	6:F:141:GLY:N	2.24	0.71
8:H:83:PRO:O	8:H:86:LYS:NZ	2.23	0.70
18:W:235:LYS:O	18:W:239:VAL:HG23	1.91	0.70
1:A:354:ILE:HD13	1:A:488:MET:HE2	1.74	0.70
1:A:1296:ASP:N	1:A:1300:GLU:O	2.24	0.70
1:A:1076:GLU:O	1:A:1079:THR:OG1	2.10	0.70
18:W:330:ASN:OD1	18:W:331:GLY:N	2.25	0.70
19:e:57:SER:O	20:f:40:ARG:NH2	2.25	0.70
22:h:72:GLY:O	22:h:76:ARG:NE	2.25	0.70
8:H:13:GLN:OE1	8:H:29:ILE:HD13	1.92	0.70
2:B:421:ILE:HD11	2:B:441:VAL:HG12	1.74	0.70
3:C:57:LEU:HB2	3:C:62:ILE:HD11	1.74	0.70
3:C:181:ASP:OD1	3:C:184:ASN:N	2.25	0.70
9:I:87:GLN:NE2	9:I:96:ASN:O	2.24	0.70
1:A:732:ARG:O	1:A:736:MET:HE2	1.92	0.69
2:B:590:VAL:HG12	2:B:617:PHE:CE1	2.27	0.69
1:A:781:ALA:N	2:B:696:GLU:OE2	2.25	0.69
2:B:247:ILE:CD1	2:B:374:MET:HE1	2.22	0.69
1:A:492:VAL:O	2:B:1150:ARG:NH2	2.25	0.69
2:B:841:MET:HE3	2:B:990:ILE:HD11	1.75	0.69
8:H:41:ASP:OD2	8:H:121:LEU:N	2.26	0.68
3:C:74:GLU:OE1	3:C:128:ASN:ND2	2.27	0.68
3:C:116:SER:OG	3:C:140:GLN:O	2.05	0.68
2:B:896:ASP:O	12:L:44:LYS:NZ	2.17	0.68
3:C:53:ASN:OD1	3:C:54:THR:N	2.27	0.68
14:N:35:DT:O2	16:T:-34:DG:N2	2.26	0.68
18:W:749:ASP:OD1	18:W:751:THR:OG1	2.09	0.68
1:A:854:ASP:OD2	1:A:858:ARG:NH2	2.27	0.68
2:B:865:ARG:HG3	2:B:871:VAL:HG12	1.76	0.68
4:D:3:VAL:HG12	7:G:9:LEU:HD11	1.76	0.68
17:V:78:GLN:O	17:V:82:TYR:OH	2.08	0.68
1:A:843:VAL:HG11	2:B:1136:ASP:OD2	1.94	0.68
2:B:13:THR:N	2:B:16:ASP:OD2	2.26	0.68
6:F:103:MET:SD	7:G:15:PRO:HG2	2.34	0.68
20:b:59:LYS:NZ	20:b:63:GLU:OE2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ASN:OD1	1:A:227:GLU:N	2.27	0.67
14:N:-68:DT:O4	16:T:68:DA:N6	2.27	0.67
19:a:62:ILE:O	19:a:93:GLN:NE2	2.28	0.67
1:A:281:GLU:N	1:A:281:GLU:OE1	2.27	0.67
3:C:242:GLN:OE1	3:C:246:ARG:NH2	2.28	0.67
2:B:842:ASN:OD1	2:B:844:SER:N	2.28	0.67
18:W:770:VAL:HA	18:W:780:VAL:HG22	1.76	0.67
18:W:264:GLN:NE2	18:W:265:ARG:O	2.28	0.67
3:C:107:GLU:OE1	3:C:149:ASN:ND2	2.28	0.67
21:c:88:ARG:NH1	21:c:97:LEU:O	2.27	0.67
2:B:861:ASP:OD1	2:B:862:GLN:N	2.27	0.66
2:B:560:GLU:N	2:B:560:GLU:OE1	2.29	0.66
2:B:579:TRP:HZ2	2:B:582:ILE:HD11	1.59	0.66
5:E:101:GLU:OE2	5:E:102:LYS:NZ	2.29	0.66
18:W:215:ARG:O	18:W:218:ILE:HG23	1.95	0.66
22:d:51:ILE:HD13	22:d:56:MET:HE2	1.77	0.66
2:B:72:ASN:ND2	2:B:128:ASP:OD1	2.28	0.66
14:N:-23:DT:OP1	19:e:72:ARG:NH2	2.27	0.66
1:A:1064:GLU:OE1	6:F:88:TYR:OH	2.07	0.65
6:F:112:GLU:OE1	6:F:112:GLU:N	2.28	0.65
6:F:111:ILE:HD11	6:F:114:GLU:HB3	1.79	0.65
5:E:19:LYS:NZ	5:E:33:GLU:O	2.29	0.65
7:G:101:ALA:O	7:G:108:VAL:N	2.27	0.65
11:K:107:GLU:O	11:K:111:ILE:HD12	1.97	0.65
4:D:114:ARG:NH1	4:D:147:SER:O	2.29	0.65
1:A:447:ARG:NH2	15:P:10:G:O2'	2.30	0.65
2:B:848:ARG:NH2	10:J:10:CYS:O	2.29	0.65
3:C:69:ILE:CD1	3:C:144:LEU:HD21	2.26	0.65
1:A:1145:LEU:HD11	1:A:1270:MET:O	1.96	0.65
1:A:441:ASP:OD1	1:A:499:ARG:NH1	2.30	0.65
4:D:13:ARG:NH1	4:D:14:ARG:O	2.30	0.65
10:J:10:CYS:SG	10:J:11:GLY:N	2.70	0.64
8:H:108:GLU:N	8:H:108:GLU:OE1	2.30	0.64
18:W:231:VAL:HG11	18:W:272:VAL:HG21	1.80	0.64
2:B:778:MET:HE2	2:B:1094:ARG:HD3	1.77	0.64
17:V:74:VAL:HG12	17:V:77:PHE:HD2	1.62	0.64
10:J:47:ARG:O	10:J:51:THR:OG1	2.11	0.64
21:c:62:ILE:HD12	21:c:87:ILE:CD1	2.27	0.64
1:A:900:VAL:HG21	1:A:930:LEU:CD2	2.18	0.64
10:J:10:CYS:SG	10:J:42:ARG:NH2	2.70	0.64
2:B:958:GLN:NE2	2:B:958:GLN:O	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:GLU:OE1	1:A:847:GLU:N	2.30	0.63
2:B:788:ARG:O	2:B:967:ARG:NH1	2.32	0.63
22:d:38:VAL:HG21	22:d:59:MET:SD	2.39	0.63
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.30	0.63
5:E:114:ASN:OD1	5:E:115:ILE:N	2.31	0.63
1:A:930:LEU:HD11	1:A:985:ILE:CG2	2.26	0.63
2:B:247:ILE:HD12	2:B:374:MET:HE1	1.81	0.63
2:B:350:GLN:OE1	2:B:361:GLU:N	2.32	0.63
1:A:82:GLY:O	1:A:242:VAL:N	2.30	0.63
1:A:546:GLN:HG2	1:A:550:MET:HE3	1.79	0.62
1:A:890:SER:N	1:A:1300:GLU:OE1	2.31	0.62
1:A:74:MET:HE2	1:A:74:MET:HA	1.81	0.62
1:A:810:THR:OG1	1:A:813:GLU:OE1	2.16	0.62
9:I:100:PHE:HB3	9:I:109:THR:HG23	1.81	0.62
1:A:1218:ILE:O	1:A:1221:VAL:HG12	1.98	0.62
1:A:557:TRP:O	11:K:26:ARG:NH2	2.33	0.62
3:C:39:GLU:OE1	3:C:254:LYS:NZ	2.30	0.62
18:W:421:TYR:HE1	18:W:426:LEU:HD13	1.65	0.62
7:G:23:ASN:ND2	7:G:56:VAL:HG21	2.15	0.62
1:A:796:GLU:OE1	1:A:796:GLU:N	2.28	0.61
1:A:1339:LEU:HD22	1:A:1384:LEU:HD23	1.82	0.61
7:G:144:ARG:N	7:G:169:GLY:O	2.34	0.61
1:A:1449:ASP:OD1	1:A:1450:GLU:N	2.32	0.61
1:A:841:ARG:NH2	1:A:1108:ASN:OD1	2.34	0.61
1:A:1426:GLY:O	1:A:1430:ASN:ND2	2.32	0.61
1:A:107:CYS:CB	1:A:110:CYS:SG	2.89	0.61
2:B:491:THR:OG1	2:B:530:LYS:O	2.19	0.61
11:K:29:ASN:ND2	11:K:77:THR:O	2.33	0.61
4:D:61:ARG:HA	4:D:89:LEU:HD21	1.82	0.61
5:E:93:ARG:O	5:E:97:LEU:HD23	2.00	0.61
14:N:-72:DT:O4	16:T:71:DA:N6	2.33	0.60
22:h:39:TYR:OH	22:h:56:MET:SD	2.49	0.60
1:A:698:ALA:HB2	1:A:703:LEU:HD13	1.82	0.60
2:B:35:LEU:CD2	2:B:164:MET:HE3	2.30	0.60
1:A:1334:SER:OG	1:A:1337:GLU:OE1	2.10	0.60
18:W:334:LYS:O	18:W:388:ARG:NH1	2.34	0.60
17:V:14:LEU:HD11	17:V:103:VAL:HG11	1.83	0.60
11:K:103:HIS:NE2	11:K:107:GLU:OE2	2.34	0.60
1:A:1439:MET:O	1:A:1442:GLY:N	2.34	0.59
2:B:867:GLY:N	2:B:870:ILE:O	2.36	0.59
4:D:40:ASP:OD1	4:D:44:ASN:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:354:LEU:O	18:W:426:LEU:N	2.33	0.59
1:A:574:THR:OG1	8:H:118:GLY:O	2.10	0.59
2:B:1202:LEU:O	2:B:1206:GLU:OE1	2.21	0.59
3:C:9:ILE:HD11	11:K:105:PHE:CE1	2.38	0.59
11:K:14:ASP:OD2	11:K:15:ASP:N	2.35	0.59
17:V:85:ARG:NH2	17:V:109:ASP:O	2.36	0.59
1:A:1210:THR:OG1	1:A:1213:GLN:OE1	2.20	0.59
1:A:550:MET:HE1	1:A:657:TRP:HD1	1.68	0.59
2:B:955:THR:OG1	12:L:56:ARG:O	2.09	0.59
1:A:1212:ASN:OD1	1:A:1213:GLN:N	2.36	0.59
2:B:936:ASP:OD1	2:B:937:ALA:N	2.36	0.59
5:E:94:ASN:OD1	5:E:95:PHE:N	2.36	0.58
2:B:279:ARG:NH1	2:B:313:GLY:O	2.35	0.58
3:C:137:ASP:OD1	3:C:138:TYR:N	2.36	0.58
1:A:1347:THR:HG21	1:A:1384:LEU:HD21	1.84	0.58
8:H:22:LYS:O	8:H:44:ASN:N	2.36	0.58
14:N:-53:DT:O2	16:T:54:DG:N2	2.35	0.58
17:V:93:ASP:OD1	17:V:94:ILE:N	2.35	0.58
4:D:86:ASP:O	4:D:90:ALA:N	2.37	0.58
1:A:57:LYS:O	1:A:69:THR:OG1	2.16	0.58
5:E:160:LYS:NZ	5:E:192:GLY:O	2.34	0.58
10:J:30:GLN:OE1	10:J:32:GLY:N	2.34	0.58
6:F:103:MET:HE1	7:G:14:HIS:CE1	2.38	0.58
17:V:10:ARG:C	17:V:18:VAL:HG23	2.29	0.58
22:h:96:ARG:HE	22:h:108:VAL:HG21	1.68	0.57
6:F:112:GLU:OE1	6:F:123:LYS:NZ	2.38	0.57
1:A:493:PRO:O	1:A:494:GLN:NE2	2.38	0.57
1:A:1172:VAL:HG12	1:A:1229:MET:CE	2.35	0.57
2:B:299:ASP:CB	2:B:302:MET:HE2	2.32	0.57
1:A:732:ARG:HG2	1:A:736:MET:HE1	1.86	0.57
2:B:316:ILE:HG21	2:B:322:ALA:HB2	1.86	0.57
2:B:792:MET:HE1	2:B:857:ARG:CZ	2.34	0.57
2:B:1085:VAL:HG12	2:B:1086:PHE:O	2.04	0.57
1:A:1216:ASP:O	1:A:1220:GLU:OE1	2.22	0.57
3:C:149:ASN:OD1	3:C:150:HIS:ND1	2.37	0.57
18:W:229:VAL:HG22	18:W:298:LYS:HB3	1.86	0.57
14:N:18:DG:N2	16:T:-17:DT:O2	2.38	0.56
17:V:109:ASP:OD1	17:V:110:GLY:N	2.38	0.56
2:B:204:ILE:O	2:B:206:GLN:NE2	2.33	0.56
2:B:554:TRP:O	2:B:583:HIS:NE2	2.34	0.56
14:N:-46:DT:O2	16:T:47:DG:N2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:VAL:HG23	2:B:283:VAL:O	2.05	0.56
2:B:290:LEU:HD22	9:I:6:PHE:CZ	2.41	0.56
4:D:58:LEU:HD11	4:D:121:CYS:SG	2.45	0.56
17:V:72:LEU:O	17:V:74:VAL:HG13	2.04	0.56
2:B:790:ASP:O	2:B:858:SER:OG	2.14	0.56
1:A:470:ARG:C	1:A:471:LEU:HD12	2.31	0.56
1:A:1006:ASN:OD1	1:A:1007:GLU:N	2.39	0.56
2:B:79:PHE:CE1	2:B:119:MET:HE1	2.40	0.56
7:G:133:ASN:O	7:G:134:ASP:OD2	2.24	0.56
13:M:39:ASP:HB2	13:M:44:ILE:HG23	1.87	0.56
2:B:955:THR:O	2:B:963:PHE:N	2.38	0.56
1:A:672:ALA:O	1:A:677:MET:HE1	2.06	0.56
2:B:405:LEU:HB3	2:B:459:TRP:CZ2	2.41	0.56
4:D:85:ASP:O	4:D:89:LEU:N	2.35	0.56
14:N:-49:DG:N1	16:T:49:DC:N3	2.49	0.56
9:I:92:ARG:O	9:I:95:THR:OG1	2.13	0.56
1:A:521:VAL:HG13	1:A:522:MET:HG3	1.87	0.56
5:E:21:MET:HE3	5:E:25:ARG:CD	2.36	0.56
6:F:103:MET:SD	6:F:103:MET:O	2.64	0.56
1:A:492:VAL:HG12	1:A:493:PRO:O	2.05	0.55
2:B:413:LEU:HD23	2:B:446:ILE:HA	1.86	0.55
2:B:365:THR:O	2:B:368:THR:OG1	2.24	0.55
2:B:820:GLY:N	2:B:1091:TYR:OH	2.39	0.55
1:A:354:ILE:HG21	1:A:488:MET:CE	2.37	0.55
3:C:53:ASN:OD1	3:C:55:SER:N	2.34	0.55
7:G:40:GLY:HA2	7:G:152:THR:HG21	1.88	0.55
21:c:62:ILE:HD11	21:c:93:LEU:HD22	1.89	0.55
2:B:274:ILE:O	2:B:277:VAL:HG22	2.07	0.55
5:E:84:GLU:OE1	5:E:91:THR:OG1	2.20	0.55
17:V:71:TRP:NE1	18:W:217:LEU:O	2.40	0.55
1:A:875:ASP:OD1	1:A:876:GLY:N	2.40	0.55
2:B:791:THR:O	2:B:792:MET:HE2	2.06	0.55
3:C:115:SER:OG	3:C:142:ILE:N	2.39	0.55
14:N:-37:DG:N1	16:T:37:DC:N3	2.55	0.55
22:h:72:GLY:C	22:h:76:ARG:HE	2.14	0.55
1:A:14:VAL:N	1:A:1435:GLN:OE1	2.40	0.54
4:D:127:LEU:HD22	4:D:177:GLU:HG2	1.89	0.54
6:F:78:GLU:O	6:F:80:THR:HG23	2.06	0.54
5:E:87:VAL:HB	5:E:115:ILE:HG23	1.89	0.54
9:I:26:LEU:HD13	9:I:35:THR:CG2	2.37	0.54
1:A:176:ARG:NH1	14:N:-46:DT:OP2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5:THR:OG1	7:G:8:SER:O	2.23	0.54
1:A:1152:THR:OG1	9:I:46:HIS:O	2.22	0.54
2:B:287:GLY:N	9:I:11:ASN:OD1	2.39	0.54
6:F:78:GLU:N	6:F:78:GLU:OE1	2.38	0.54
14:N:-67:DT:N3	16:T:68:DA:N1	2.55	0.54
19:a:123:ASP:OD1	19:e:113:HIS:NE2	2.40	0.54
1:A:935:GLU:OE2	1:A:939:SER:OG	2.24	0.54
9:I:68:LEU:O	9:I:70:ARG:NH1	2.40	0.54
2:B:336:ILE:O	2:B:337:ARG:O	2.25	0.54
17:V:9:GLU:HB2	17:V:18:VAL:HG22	1.88	0.54
1:A:130:ASP:OD1	1:A:133:LYS:N	2.32	0.54
1:A:983:LEU:HD13	1:A:1041:ARG:HA	1.89	0.54
3:C:72:VAL:HG22	3:C:133:VAL:HG22	1.89	0.54
1:A:448:GLN:OE1	1:A:489:ASN:ND2	2.41	0.54
1:A:1015:ASN:OD1	5:E:206:ARG:NH1	2.40	0.54
15:P:1:U:O2'	15:P:2:U:O4'	2.24	0.54
22:d:42:LEU:O	22:d:46:HIS:N	2.41	0.53
3:C:149:ASN:OD1	3:C:150:HIS:N	2.42	0.53
4:D:19:VAL:O	4:D:29:ARG:NH2	2.41	0.53
1:A:113:LEU:HD11	1:A:142:CYS:SG	2.48	0.53
3:C:79:MET:HE1	3:C:96:VAL:HG23	1.90	0.53
7:G:49:LEU:HD11	7:G:77:VAL:HG23	1.89	0.53
8:H:134:LEU:O	8:H:136:GLN:N	2.40	0.53
1:A:74:MET:HE2	1:A:74:MET:CA	2.38	0.53
22:h:90:GLU:OE1	22:h:90:GLU:N	2.41	0.53
2:B:739:THR:HG1	2:B:740:HIS:CE1	2.23	0.53
2:B:948:ILE:HD13	3:C:60:GLU:OE2	2.09	0.53
11:K:60:ALA:O	11:K:74:ARG:N	2.40	0.53
17:V:59:ALA:HB2	18:W:240:VAL:HG13	1.91	0.53
18:W:250:ARG:O	18:W:253:THR:OG1	2.23	0.53
21:c:76:THR:O	22:d:50:GLY:N	2.41	0.53
22:d:38:VAL:HG11	22:d:59:MET:SD	2.48	0.53
18:W:231:VAL:HG11	18:W:272:VAL:CG2	2.39	0.53
2:B:572:ARG:HA	2:B:582:ILE:HD13	1.91	0.53
1:A:96:ILE:HG21	1:A:177:LYS:HE2	1.91	0.53
1:A:336:ARG:HE	2:B:1202:LEU:HD22	1.74	0.53
16:T:-13:DA:OP1	20:b:36:ARG:NH1	2.40	0.52
1:A:810:THR:HG22	2:B:725:ARG:HD3	1.91	0.52
7:G:101:ALA:HB3	7:G:108:VAL:HB	1.90	0.52
21:g:97:LEU:HD11	22:h:62:PHE:CE1	2.44	0.52
7:G:152:THR:HG22	7:G:154:VAL:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-33:DG:N1	16:T:33:DC:O2	2.42	0.52
2:B:64:HIS:N	2:B:69:ASP:OD1	2.42	0.52
7:G:62:ILE:HD11	7:G:69:GLU:HB2	1.91	0.52
2:B:89:MET:CE	2:B:109:LEU:HD13	2.40	0.52
2:B:74:ARG:NH1	2:B:126:SER:OG	2.37	0.52
1:A:912:ASP:O	1:A:980:ALA:HB2	2.10	0.52
2:B:409:LEU:HD23	2:B:450:LEU:HD23	1.91	0.52
7:G:94:VAL:HG11	7:G:121:TYR:CE1	2.45	0.52
3:C:43:LEU:HD12	3:C:160:LYS:O	2.10	0.52
3:C:72:VAL:CG2	3:C:133:VAL:HG22	2.40	0.52
1:A:1456:LEU:HD21	6:F:108:LEU:HD22	1.92	0.52
5:E:60:LEU:HD12	5:E:77:LEU:O	2.09	0.52
1:A:614:MET:N	1:A:614:MET:HE2	2.25	0.52
3:C:148:ARG:N	3:C:151:GLN:OE1	2.35	0.52
4:D:115:PHE:CZ	4:D:124:VAL:HG21	2.44	0.52
14:N:-3:DA:OP1	19:e:118:THR:N	2.40	0.51
1:A:1096:VAL:HA	1:A:1115:THR:HG21	1.92	0.51
2:B:265:LEU:O	2:B:268:VAL:HG22	2.10	0.51
2:B:575:VAL:O	2:B:578:VAL:HG12	2.09	0.51
9:I:113:GLU:N	9:I:113:GLU:OE1	2.42	0.51
12:L:33:CYS:SG	12:L:34:GLY:N	2.83	0.51
14:N:69:DT:O2	16:T:-68:DG:N2	2.43	0.51
1:A:105:CYS:O	1:A:113:LEU:HD12	2.11	0.51
4:D:58:LEU:HD11	4:D:121:CYS:CB	2.40	0.51
21:g:63:LEU:HD22	22:h:42:LEU:HD13	1.92	0.51
1:A:60:SER:C	1:A:74:MET:HE1	2.36	0.51
1:A:443:VAL:HG21	1:A:490:LEU:HD11	1.91	0.51
2:B:284:VAL:N	2:B:285:PRO:CD	2.74	0.51
18:W:234:GLY:N	18:W:236:GLU:OE2	2.43	0.51
18:W:339:GLN:O	18:W:353:LYS:N	2.44	0.51
20:b:44:LYS:CB	21:g:115:LEU:HD22	2.41	0.51
1:A:606:MET:HE2	1:A:606:MET:HA	1.93	0.51
6:F:103:MET:SD	7:G:15:PRO:CG	2.97	0.51
9:I:65:ASP:OD2	9:I:68:LEU:HD23	2.11	0.51
18:W:446:GLU:O	18:W:450:PHE:N	2.42	0.51
1:A:354:ILE:HG21	1:A:488:MET:HE2	1.93	0.51
4:D:54:SER:OG	4:D:115:PHE:N	2.37	0.51
18:W:326:VAL:HG12	18:W:437:VAL:HA	1.92	0.51
2:B:387:ASP:OD1	2:B:388:GLN:N	2.44	0.51
17:V:14:LEU:HD22	17:V:32:CYS:SG	2.51	0.51
1:A:923:ASP:OD1	1:A:924:VAL:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:557:GLU:O	2:B:582:ILE:N	2.40	0.51
2:B:590:VAL:HG11	2:B:610:ARG:HD2	1.92	0.51
2:B:739:THR:OG1	2:B:740:HIS:ND1	2.31	0.51
3:C:58:ALA:O	3:C:62:ILE:HD12	2.11	0.51
1:A:347:ASP:OD1	2:B:1106:ARG:NE	2.38	0.51
2:B:33:GLN:OE1	2:B:33:GLN:N	2.41	0.51
8:H:103:PHE:CD1	8:H:113:VAL:HG22	2.45	0.51
3:C:9:ILE:HD11	11:K:105:PHE:HE1	1.75	0.50
2:B:936:ASP:OD1	2:B:938:SER:N	2.44	0.50
3:C:53:ASN:O	12:L:62:ARG:NH2	2.37	0.50
2:B:725:ARG:NH1	2:B:1048:THR:O	2.43	0.50
4:D:115:PHE:HD1	4:D:120:THR:HG22	1.76	0.50
1:A:108:MET:SD	1:A:186:TRP:NE1	2.75	0.50
2:B:336:ILE:C	2:B:337:ARG:HD3	2.36	0.50
4:D:157:ILE:HG23	4:D:164:ALA:HA	1.93	0.50
5:E:89:ILE:HD13	5:E:119:ALA:HA	1.92	0.50
18:W:326:VAL:HG12	18:W:437:VAL:HG23	1.91	0.50
19:e:108:ASN:ND2	20:f:42:GLY:O	2.44	0.50
1:A:36:GLU:O	1:A:275:ILE:HD11	2.11	0.50
2:B:71:ILE:HA	2:B:127:ILE:HG22	1.94	0.50
2:B:253:GLU:OE2	2:B:259:ARG:NH1	2.44	0.50
3:C:145:CYS:SG	3:C:146:LYS:N	2.85	0.50
22:h:34:TYR:O	22:h:38:VAL:HG23	2.11	0.50
11:K:59:VAL:HG23	11:K:75:LEU:HD13	1.92	0.50
19:a:97:GLU:O	19:a:101:VAL:HG23	2.12	0.50
21:c:100:VAL:HG11	20:f:98:TYR:CZ	2.47	0.50
2:B:880:ALA:O	2:B:932:HIS:ND1	2.44	0.50
1:A:78:PRO:O	2:B:1205:GLN:NE2	2.38	0.49
2:B:863:GLU:O	2:B:961:LEU:HD13	2.12	0.49
2:B:969:ARG:NH1	3:C:60:GLU:OE1	2.39	0.49
18:W:229:VAL:HG11	18:W:286:LEU:HD22	1.94	0.49
1:A:305:MET:HE3	2:B:1210:MET:CE	2.42	0.49
1:A:792:ASP:OD1	1:A:793:PHE:N	2.45	0.49
3:C:87:CYS:SG	3:C:91:CYS:N	2.84	0.49
14:N:53:DC:O2	16:T:-52:DG:N2	2.45	0.49
2:B:1138:MET:HE2	2:B:1138:MET:HA	1.95	0.49
1:A:473:LEU:HD13	2:B:835:GLN:CD	2.37	0.49
18:W:772:GLU:OE2	18:W:774:ASN:ND2	2.43	0.49
3:C:123:GLY:O	3:C:125:GLY:N	2.46	0.49
2:B:425:MET:HG3	2:B:429:ILE:HD12	1.93	0.49
5:E:30:SER:OG	5:E:32:GLU:OE2	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:136:GLN:HB2	8:H:139:LEU:HD21	1.94	0.49
21:g:51:LEU:CD1	22:h:70:ILE:HG21	2.43	0.49
2:B:778:MET:HE1	2:B:853:SER:OG	2.12	0.49
3:C:19:LEU:HD21	3:C:244:PHE:HE2	1.78	0.49
20:b:39:ARG:NH1	20:b:44:LYS:O	2.41	0.49
2:B:79:PHE:CD1	2:B:119:MET:HE1	2.47	0.48
3:C:19:LEU:HD12	3:C:19:LEU:C	2.38	0.48
1:A:1285:VAL:HG13	1:A:1311:THR:HG22	1.94	0.48
2:B:338:ARG:NH1	2:B:342:ILE:HD12	2.28	0.48
11:K:56:VAL:HG22	11:K:77:THR:HG22	1.95	0.48
22:d:73:GLU:O	22:d:77:LEU:HD23	2.13	0.48
1:A:392:TYR:OH	1:A:438:MET:HE1	2.13	0.48
2:B:316:ILE:HG23	2:B:321:VAL:CG2	2.38	0.48
5:E:180:GLU:N	5:E:180:GLU:OE1	2.47	0.48
6:F:118:LEU:HG	6:F:122:MET:HE2	1.94	0.48
19:e:78:PHE:HB3	20:f:70:VAL:HG11	1.95	0.48
22:h:96:ARG:NE	22:h:108:VAL:HG21	2.28	0.48
2:B:195:VAL:C	2:B:196:ILE:HD12	2.39	0.48
3:C:57:LEU:CB	3:C:62:ILE:HD11	2.42	0.48
5:E:181:ASP:O	5:E:184:ALA:N	2.46	0.48
14:N:-3:DA:OP1	19:e:117:VAL:N	2.41	0.48
18:W:784:ASN:HB2	18:W:785:PRO:CD	2.44	0.48
19:e:107:THR:HG23	19:e:123:ASP:HB2	1.96	0.48
1:A:336:ARG:NH2	2:B:1114:LEU:HD21	2.28	0.48
2:B:540:ILE:C	2:B:623:VAL:HG23	2.38	0.48
9:I:108:LYS:NZ	9:I:110:PHE:HB3	2.29	0.48
18:W:326:VAL:CG1	18:W:437:VAL:HG23	2.44	0.48
1:A:1285:VAL:HG22	1:A:1311:THR:CG2	2.44	0.48
18:W:759:ARG:NH2	18:W:794:SER:O	2.47	0.48
2:B:290:LEU:HD22	9:I:6:PHE:CE2	2.48	0.48
10:J:8:PHE:N	10:J:48:MET:HE1	2.29	0.48
20:b:44:LYS:HB2	21:g:115:LEU:HD22	1.95	0.48
1:A:610:ASP:OD1	1:A:971:GLN:NE2	2.47	0.48
5:E:111:TYR:CD2	5:E:115:ILE:HD11	2.48	0.48
8:H:100:VAL:HG22	8:H:115:VAL:HG22	1.96	0.48
13:M:21:THR:HG21	13:M:23:PHE:CE2	2.49	0.48
19:a:58:THR:HG22	21:g:81:ARG:HD3	1.95	0.48
21:g:97:LEU:HD11	22:h:62:PHE:HE1	1.79	0.48
1:A:1451:LYS:O	1:A:1454:THR:OG1	2.28	0.48
2:B:76:GLU:OE1	2:B:122:SER:OG	2.32	0.48
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:ILE:O	2:B:337:ARG:HD3	2.13	0.48
2:B:1065:GLN:OE1	2:B:1067:ARG:N	2.34	0.48
20:f:83:ALA:O	20:f:87:VAL:HG23	2.14	0.48
4:D:90:ALA:HB1	4:D:102:VAL:HG13	1.96	0.48
4:D:180:ARG:HG3	4:D:181:LEU:HD22	1.95	0.48
11:K:77:THR:OG1	11:K:81:THR:O	2.31	0.48
22:h:91:ILE:O	22:h:95:VAL:HG23	2.13	0.48
2:B:343:GLN:NE2	2:B:347:ASP:OD1	2.46	0.47
2:B:878:THR:HG1	2:B:881:THR:HG1	1.51	0.47
3:C:18:GLU:OE2	3:C:206:TYR:OH	2.30	0.47
22:d:45:VAL:O	22:d:46:HIS:ND1	2.47	0.47
1:A:903:MET:N	1:A:903:MET:HE2	2.28	0.47
2:B:1204:PHE:CE2	2:B:1216:LEU:HD11	2.50	0.47
14:N:-45:DG:N2	16:T:46:DA:C2	2.82	0.47
1:A:1290:HIS:N	1:A:1306:LEU:O	2.40	0.47
2:B:305:MET:CE	2:B:379:LEU:HD12	2.39	0.47
1:A:38:PRO:HG3	1:A:275:ILE:HD12	1.97	0.47
2:B:109:LEU:O	2:B:197:ASN:N	2.47	0.47
2:B:1156:ASP:OD1	2:B:1156:ASP:N	2.47	0.47
6:F:140:ASP:OD1	6:F:142:SER:N	2.45	0.47
21:c:51:LEU:HD13	22:d:70:ILE:HG21	1.97	0.47
1:A:848:ASP:OD1	1:A:848:ASP:N	2.44	0.47
2:B:10:ASP:OD1	2:B:11:THR:N	2.48	0.47
6:F:116:ASP:OD2	6:F:119:GLN:N	2.37	0.47
1:A:130:ASP:OD1	1:A:132:LYS:N	2.47	0.47
1:A:470:ARG:O	1:A:471:LEU:HD12	2.15	0.47
1:A:558:ASP:OD1	1:A:558:ASP:N	2.48	0.47
2:B:156:VAL:CG1	2:B:441:VAL:HG21	2.44	0.47
9:I:7:CYS:SG	9:I:8:LEU:N	2.88	0.47
1:A:74:MET:HE2	1:A:74:MET:N	2.30	0.47
1:A:444:LEU:HD21	1:A:456:MET:HE2	1.96	0.47
1:A:1145:LEU:N	1:A:1145:LEU:HD23	2.30	0.47
1:A:1145:LEU:HA	1:A:1276:LEU:HD11	1.97	0.47
2:B:105:ARG:NH2	2:B:193:TYR:OH	2.47	0.47
2:B:609:ILE:HD13	2:B:693:GLU:CG	2.45	0.47
2:B:975:GLN:N	2:B:978:ASP:OD2	2.39	0.47
3:C:92:ASP:OD1	3:C:123:GLY:N	2.47	0.47
4:D:85:ASP:OD1	4:D:86:ASP:N	2.46	0.47
9:I:47:GLU:OE1	9:I:47:GLU:N	2.47	0.47
9:I:54:GLU:N	9:I:54:GLU:OE1	2.47	0.47
18:W:322:ARG:NH1	18:W:340:VAL:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLN:OE1	1:A:246:GLN:N	2.43	0.47
1:A:1168:ASP:O	1:A:1172:VAL:HG13	2.14	0.47
2:B:128:ASP:OD1	2:B:128:ASP:N	2.47	0.47
2:B:235:LEU:HD12	2:B:242:ILE:HD11	1.97	0.47
3:C:142:ILE:HD13	10:J:16:ASP:HB3	1.95	0.47
19:a:108:ASN:OD1	20:b:43:VAL:HG22	2.15	0.47
1:A:645:GLU:O	1:A:649:ASN:ND2	2.48	0.47
1:A:912:ASP:OD1	1:A:913:VAL:N	2.48	0.47
2:B:271:ASP:OD1	2:B:272:ILE:N	2.48	0.47
2:B:587:SER:O	2:B:590:VAL:HG22	2.15	0.47
5:E:156:SER:N	5:E:159:GLU:OE1	2.41	0.47
1:A:747:MET:HE3	2:B:1018:PRO:HG3	1.96	0.47
1:A:1344:ILE:HG23	1:A:1345:GLU:N	2.29	0.47
4:D:151:GLU:OE1	4:D:151:GLU:N	2.46	0.47
3:C:50:ILE:HD12	3:C:59:ASP:HB3	1.97	0.46
1:A:55:ASP:OD1	1:A:57:LYS:N	2.44	0.46
16:T:49:DC:H2"	16:T:50:DA:H8	1.79	0.46
17:V:15:CYS:SG	17:V:17:ILE:HG22	2.56	0.46
1:A:542:ILE:HG22	1:A:547:VAL:HG23	1.97	0.46
1:A:564:PRO:HG2	1:A:567:LEU:HD23	1.97	0.46
1:A:147:VAL:HG23	1:A:171:THR:HA	1.97	0.46
1:A:456:MET:HE2	2:B:1138:MET:CE	2.45	0.46
1:A:926:LEU:O	1:A:930:LEU:HD13	2.16	0.46
14:N:-27:DC:N4	16:T:26:DG:O6	2.48	0.46
22:d:42:LEU:HD22	22:d:51:ILE:HD12	1.97	0.46
1:A:342:MET:HE1	1:A:1432:MET:HE3	1.97	0.46
6:F:75:LEU:N	6:F:78:GLU:OE2	2.48	0.46
10:J:8:PHE:H	10:J:48:MET:HE1	1.81	0.46
1:A:1168:ASP:OD2	1:A:1239:ILE:HG21	2.16	0.46
2:B:859:TYR:CE2	2:B:941:LEU:HD12	2.50	0.46
8:H:17:ASN:ND2	8:H:24:SER:OG	2.40	0.46
19:e:63:ARG:HH22	20:f:30:THR:HG21	1.81	0.46
1:A:548:MET:CE	11:K:59:VAL:H	2.28	0.46
13:M:65:GLN:O	13:M:69:ILE:HD12	2.16	0.46
17:V:57:LEU:HD11	17:V:81:LEU:HD22	1.97	0.46
1:A:323:VAL:HG12	1:A:324:LYS:N	2.30	0.46
1:A:871:GLU:OE1	5:E:201:SER:OG	2.24	0.46
1:A:1145:LEU:HD22	1:A:1274:ILE:HB	1.97	0.46
1:A:1314:ILE:HG21	1:A:1337:GLU:HG2	1.98	0.46
2:B:115:VAL:N	2:B:159:GLY:O	2.46	0.46
18:W:352:LEU:HD11	18:W:435:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:NE	1:A:85:GLU:OE2	2.48	0.46
1:A:1229:MET:SD	1:A:1230:TRP:N	2.89	0.46
2:B:986:GLN:OE1	2:B:1022:THR:HG21	2.15	0.46
19:e:62:ILE:HD11	20:f:37:LEU:HD11	1.98	0.46
1:A:900:VAL:CG2	1:A:930:LEU:HD23	2.25	0.45
7:G:4:LEU:HA	7:G:77:VAL:HG22	1.97	0.45
7:G:91:VAL:HA	7:G:101:ALA:HA	1.98	0.45
1:A:31:SER:OG	1:A:83:HIS:N	2.43	0.45
2:B:338:ARG:HH11	2:B:342:ILE:HD12	1.81	0.45
2:B:348:ILE:HG23	2:B:349:LEU:HD22	1.97	0.45
11:K:59:VAL:HG13	11:K:59:VAL:O	2.16	0.45
1:A:123:ALA:O	1:A:127:ARG:NH1	2.49	0.45
1:A:336:ARG:HH22	2:B:1114:LEU:HD21	1.81	0.45
7:G:83:LYS:HB2	7:G:148:VAL:HA	1.99	0.45
12:L:53:CYS:SG	12:L:55:HIS:ND1	2.88	0.45
14:N:-36:DG:N2	16:T:37:DC:O2	2.49	0.45
2:B:228:VAL:HG13	2:B:247:ILE:O	2.16	0.45
2:B:910:ILE:HD12	2:B:910:ILE:H	1.82	0.45
3:C:24:VAL:HG23	3:C:228:PHE:HE2	1.82	0.45
7:G:35:GLU:OE2	7:G:48:VAL:HG23	2.17	0.45
9:I:26:LEU:C	9:I:26:LEU:HD12	2.42	0.45
14:N:48:DG:N2	16:T:-47:DT:O2	2.49	0.45
2:B:1206:GLU:O	2:B:1210:MET:N	2.50	0.45
2:B:1121:GLY:O	2:B:1126:GLY:N	2.48	0.45
5:E:181:ASP:O	5:E:182:PRO:C	2.57	0.45
7:G:152:THR:CG2	7:G:157:ILE:HG22	2.41	0.45
11:K:49:GLU:HB2	11:K:94:ILE:HD11	1.97	0.45
18:W:354:LEU:N	18:W:426:LEU:O	2.40	0.45
1:A:1439:MET:O	1:A:1440:GLY:C	2.60	0.45
2:B:845:SER:HB3	2:B:850:LEU:HD22	1.98	0.45
2:B:954:LEU:HD13	2:B:964:VAL:HG12	1.99	0.45
4:D:13:ARG:O	4:D:14:ARG:NE	2.44	0.45
5:E:37:SER:N	5:E:40:GLU:OE2	2.38	0.45
1:A:886:THR:HG23	1:A:1026:ALA:CB	2.47	0.45
1:A:1204:MET:O	1:A:1209:LEU:HD23	2.17	0.45
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.52	0.45
3:C:57:LEU:HD22	10:J:1:MET:HE3	1.99	0.45
7:G:23:ASN:HD22	7:G:56:VAL:HG21	1.81	0.45
18:W:445:ASN:OD1	18:W:446:GLU:N	2.50	0.45
19:a:47:ALA:HB1	20:b:39:ARG:NH1	2.31	0.45
1:A:472:ASN:O	1:A:475:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:GLY:HA3	9:I:11:ASN:OD1	2.17	0.45
10:J:7:CYS:HA	10:J:48:MET:SD	2.57	0.45
2:B:72:ASN:O	2:B:74:ARG:NH1	2.49	0.45
2:B:72:ASN:N	2:B:126:SER:O	2.40	0.45
2:B:1112:GLN:N	2:B:1117:GLN:O	2.40	0.45
5:E:126:VAL:HG12	5:E:126:VAL:O	2.17	0.45
17:V:66:SER:O	17:V:70:LYS:N	2.45	0.45
20:b:61:PHE:CZ	20:b:65:VAL:HG21	2.52	0.45
1:A:550:MET:HE1	1:A:657:TRP:CD1	2.49	0.44
2:B:953:LEU:HD11	12:L:57:VAL:HG13	1.99	0.44
10:J:7:CYS:O	10:J:8:PHE:C	2.60	0.44
1:A:307:ASN:O	1:A:314:GLN:NE2	2.39	0.44
2:B:842:ASN:OD1	2:B:842:ASN:C	2.60	0.44
2:B:117:LEU:HD12	2:B:118:ASP:H	1.82	0.44
5:E:111:TYR:CE2	5:E:115:ILE:HD11	2.53	0.44
20:b:29:ILE:O	20:b:55:ARG:NH2	2.47	0.44
1:A:454:MET:O	1:A:457:MET:HE2	2.17	0.44
2:B:279:ARG:NE	2:B:284:VAL:O	2.46	0.44
1:A:668:GLY:HA2	1:A:671:ILE:HD12	1.99	0.44
2:B:266:PRO:HG3	2:B:352:GLU:O	2.17	0.44
18:W:784:ASN:HB2	18:W:785:PRO:HD3	1.99	0.44
1:A:1209:LEU:HD23	1:A:1209:LEU:H	1.82	0.44
1:A:1210:THR:N	1:A:1213:GLN:OE1	2.51	0.44
2:B:89:MET:HE2	2:B:99:MET:HE1	1.99	0.44
2:B:1187:ASN:OD1	2:B:1188:LYS:N	2.51	0.44
7:G:79:TRP:HZ3	7:G:106:LEU:HD23	1.82	0.44
22:h:94:ALA:O	22:h:98:LEU:HD13	2.18	0.44
1:A:231:ARG:HG3	1:A:233:GLU:OE1	2.17	0.44
1:A:832:THR:HG23	1:A:833:ALA:N	2.32	0.44
2:B:337:ARG:NH1	2:B:339:GLU:HB3	2.33	0.44
19:a:126:LEU:HD22	19:e:113:HIS:CD2	2.52	0.44
2:B:224:PRO:O	2:B:251:GLY:N	2.51	0.44
6:F:112:GLU:HG2	6:F:113:GLY:N	2.33	0.44
9:I:111:ARG:HB2	9:I:113:GLU:OE1	2.18	0.44
10:J:22:LEU:O	10:J:26:GLU:OE1	2.36	0.44
1:A:444:LEU:HD21	1:A:456:MET:HE1	1.97	0.43
1:A:1453:LEU:CD1	7:G:22:MET:HE1	2.47	0.43
15:P:1:U:H2'	15:P:2:U:C6	2.53	0.43
2:B:695:GLU:HA	2:B:698:ILE:HD11	1.99	0.43
2:B:1165:ILE:HD12	2:B:1187:ASN:HB2	2.00	0.43
17:V:91:PRO:HD2	17:V:94:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:ILE:N	1:A:986:PRO:HD2	2.33	0.43
5:E:125:THR:HG22	5:E:125:THR:O	2.18	0.43
1:A:476:THR:O	1:A:477:SER:C	2.60	0.43
2:B:281:LEU:HD23	2:B:368:THR:HG22	1.99	0.43
5:E:87:VAL:O	5:E:116:THR:HG22	2.18	0.43
5:E:92:MET:SD	5:E:119:ALA:HB1	2.59	0.43
9:I:17:LYS:N	9:I:26:LEU:O	2.43	0.43
1:A:327:ARG:HG3	1:A:1409:VAL:HG11	2.01	0.43
1:A:613:VAL:C	1:A:614:MET:HE2	2.44	0.43
2:B:105:ARG:NE	2:B:200:GLU:OE2	2.52	0.43
2:B:778:MET:HE1	2:B:853:SER:CB	2.49	0.43
1:A:226:ASN:OD1	1:A:226:ASN:C	2.62	0.43
1:A:1293:SER:O	1:A:1294:VAL:HG23	2.19	0.43
3:C:4:GLU:N	3:C:5:PRO:CD	2.82	0.43
16:T:17:DA:H5"	19:e:63:ARG:HE	1.83	0.43
3:C:20:MET:SD	3:C:20:MET:C	3.02	0.43
5:E:28:PHE:O	5:E:29:ILE:HD13	2.19	0.43
1:A:6:TYR:O	2:B:1175:LEU:HD12	2.18	0.43
2:B:354:LEU:N	2:B:355:PRO:CD	2.82	0.43
2:B:405:LEU:HB3	2:B:459:TRP:CH2	2.54	0.43
2:B:1001:PHE:CE1	3:C:33:ARG:CZ	3.02	0.43
21:c:62:ILE:HD12	21:c:87:ILE:HD11	2.01	0.43
1:A:741:LEU:C	1:A:741:LEU:HD12	2.44	0.43
1:A:1337:GLU:OE1	1:A:1337:GLU:N	2.48	0.43
21:c:63:LEU:HD13	22:d:42:LEU:HB2	2.00	0.43
1:A:557:TRP:CD1	1:A:558:ASP:OD1	2.72	0.43
1:A:748:VAL:O	1:A:751:GLY:N	2.52	0.43
1:A:874:LEU:HD23	1:A:1058:SER:O	2.19	0.43
1:A:1129:ASP:OD1	1:A:1130:ILE:N	2.51	0.43
1:A:1135:VAL:O	1:A:1138:SER:OG	2.32	0.43
1:A:1269:HIS:NE2	1:A:1273:LEU:HD23	2.33	0.43
3:C:43:LEU:HD12	3:C:160:LYS:C	2.44	0.43
3:C:69:ILE:HD11	3:C:144:LEU:CD2	2.34	0.43
21:c:62:ILE:HG23	21:c:87:ILE:HD11	2.00	0.43
19:e:60:LEU:HD21	19:e:94:GLU:OE2	2.19	0.43
1:A:448:GLN:NE2	2:B:1134:GLU:OE2	2.45	0.42
1:A:864:ILE:HD12	5:E:169:LEU:HD11	2.00	0.42
2:B:441:VAL:HG23	2:B:441:VAL:O	2.19	0.42
3:C:148:ARG:HG2	3:C:149:ASN:H	1.83	0.42
3:C:262:LEU:O	11:K:84:LYS:NZ	2.41	0.42
8:H:84:THR:C	8:H:86:LYS:HZ3	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:69:ILE:HD12	13:M:69:ILE:H	1.83	0.42
1:A:1216:ASP:O	1:A:1219:SER:N	2.52	0.42
2:B:176:ASP:CG	2:B:177:GLU:H	2.28	0.42
6:F:77:GLU:OE1	6:F:77:GLU:N	2.41	0.42
13:M:30:HIS:ND1	13:M:31:ASP:O	2.50	0.42
18:W:783:HIS:O	18:W:783:HIS:ND1	2.52	0.42
2:B:405:LEU:O	2:B:459:TRP:HZ2	2.03	0.42
7:G:166:ASP:OD1	7:G:167:PHE:N	2.51	0.42
1:A:1201:ARG:O	1:A:1205:LEU:HD23	2.19	0.42
2:B:207:GLU:OE2	2:B:530:LYS:NZ	2.50	0.42
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.35	0.42
18:W:231:VAL:HG12	18:W:292:VAL:HG13	2.01	0.42
1:A:548:MET:HE2	11:K:59:VAL:H	1.85	0.42
2:B:41:PHE:CZ	2:B:46:ILE:HD11	2.55	0.42
2:B:843:GLN:N	2:B:994:TYR:O	2.37	0.42
6:F:86:THR:N	6:F:89:GLU:OE1	2.42	0.42
11:K:29:ASN:ND2	11:K:78:GLU:O	2.52	0.42
17:V:11:ALA:HA	17:V:18:VAL:HA	2.02	0.42
18:W:421:TYR:CE1	18:W:426:LEU:HD13	2.50	0.42
20:b:35:ARG:O	20:b:39:ARG:HG2	2.19	0.42
1:A:1449:ASP:OD1	1:A:1451:LYS:N	2.47	0.42
4:D:59:LEU:O	4:D:62:GLU:HG2	2.19	0.42
15:P:-1:U:H2'	15:P:0:G:H8	1.84	0.42
1:A:323:VAL:HG12	1:A:324:LYS:H	1.85	0.42
1:A:1119:THR:HG22	1:A:1121:TYR:CE1	2.54	0.42
1:A:1153:GLU:OE2	1:A:1196:ARG:NH1	2.51	0.42
1:A:951:ASN:OD1	1:A:952:GLY:N	2.53	0.42
1:A:1140:ILE:HD11	1:A:1322:VAL:HG11	2.02	0.42
7:G:24:GLN:OE1	7:G:27:ARG:NH1	2.52	0.42
16:T:49:DC:H2''	16:T:50:DA:H5''	2.01	0.42
1:A:84:MET:O	1:A:239:VAL:HG23	2.19	0.42
1:A:91:PHE:HB3	1:A:96:ILE:HD11	2.02	0.42
1:A:542:ILE:CG2	1:A:547:VAL:HG23	2.49	0.42
1:A:1065:MET:HG3	1:A:1439:MET:HE2	2.01	0.42
1:A:1197:LEU:C	1:A:1197:LEU:HD12	2.44	0.42
2:B:266:PRO:O	2:B:348:ILE:HD11	2.20	0.42
2:B:290:LEU:HD13	9:I:6:PHE:HZ	1.85	0.42
1:A:11:LEU:HD12	2:B:1193:GLN:O	2.19	0.42
2:B:884:ARG:NH2	15:P:-1:U:O2'	2.53	0.42
10:J:8:PHE:CD2	10:J:48:MET:HE2	2.55	0.42
16:T:-43:DT:H2'	16:T:-42:DT:H71	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:-27:DC:H2''	16:T:-26:DT:H71	2.01	0.42
1:A:497:GLU:O	1:A:501:GLU:OE1	2.37	0.41
1:A:544:TYR:CE2	1:A:548:MET:SD	3.13	0.41
2:B:80:GLY:N	2:B:118:ASP:O	2.53	0.41
2:B:900:ALA:O	2:B:903:VAL:HG12	2.20	0.41
2:B:1182:CYS:O	2:B:1186:LYS:N	2.53	0.41
3:C:61:PHE:CZ	10:J:1:MET:HE2	2.55	0.41
4:D:57:ARG:HB2	4:D:109:LEU:HD22	2.02	0.41
11:K:31:ILE:HD12	11:K:33:ILE:HD11	2.01	0.41
14:N:-51:DG:H2'	14:N:-50:DT:C6	2.55	0.41
1:A:38:PRO:HA	1:A:271:LEU:HD23	2.01	0.41
1:A:352:THR:C	1:A:487:GLU:OE1	2.63	0.41
1:A:854:ASP:OD1	1:A:856:THR:OG1	2.36	0.41
2:B:401:LEU:HD23	2:B:538:ILE:HG21	2.02	0.41
11:K:64:GLU:HA	11:K:64:GLU:OE2	2.19	0.41
18:W:220:THR:HG23	18:W:222:ASP:H	1.84	0.41
18:W:237:LYS:C	18:W:241:ARG:HE	2.27	0.41
1:A:385:ASN:OD1	1:A:385:ASN:N	2.52	0.41
1:A:471:LEU:CD2	1:A:488:MET:HE1	2.50	0.41
1:A:527:ASP:HB2	2:B:835:GLN:CD	2.45	0.41
1:A:599:LEU:HD21	8:H:123:CYS:HB2	2.03	0.41
1:A:1439:MET:CE	2:B:1139:ILE:HG23	2.50	0.41
2:B:257:THR:OG1	2:B:258:GLY:N	2.54	0.41
2:B:302:MET:HA	2:B:305:MET:HG2	2.03	0.41
3:C:100:LEU:C	3:C:100:LEU:HD23	2.46	0.41
4:D:25:ALA:HB1	4:D:140:PHE:CZ	2.56	0.41
5:E:161:SER:OG	5:E:165:GLN:OE1	2.35	0.41
10:J:23:ARG:HA	10:J:26:GLU:OE1	2.20	0.41
1:A:671:ILE:HG12	1:A:806:LEU:HD21	2.03	0.41
1:A:841:ARG:NE	1:A:1387:ILE:O	2.54	0.41
2:B:404:PRO:O	2:B:407:ALA:HB3	2.20	0.41
2:B:910:ILE:HD12	2:B:910:ILE:N	2.36	0.41
5:E:198:ILE:HG23	5:E:206:ARG:HG2	2.02	0.41
14:N:-47:DC:C2'	14:N:-46:DT:H71	2.50	0.41
14:N:30:DC:H42	16:T:-31:DA:N6	2.18	0.41
18:W:237:LYS:O	18:W:241:ARG:NE	2.46	0.41
1:A:664:SER:OG	1:A:665:ILE:N	2.53	0.41
3:C:33:ARG:HG3	3:C:176:ILE:HG21	2.02	0.41
6:F:119:GLN:HA	6:F:122:MET:HE3	2.03	0.41
17:V:84:VAL:HG21	18:W:265:ARG:NH1	2.34	0.41
1:A:354:ILE:HG21	1:A:488:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:ARG:NH2	1:A:1387:ILE:O	2.54	0.41
1:A:1216:ASP:O	1:A:1217:LYS:C	2.64	0.41
1:A:1260:ASP:OD1	9:I:43:VAL:HG11	2.20	0.41
1:A:1453:LEU:HD23	1:A:1453:LEU:HA	1.97	0.41
2:B:806:THR:H	2:B:809:MET:HE2	1.85	0.41
3:C:62:ILE:HD12	3:C:62:ILE:H	1.85	0.41
1:A:277:VAL:HG22	1:A:293:VAL:HG12	2.02	0.41
1:A:1193:TRP:NE1	1:A:1259:GLU:OE1	2.51	0.41
2:B:301:GLN:O	2:B:305:MET:HG2	2.20	0.41
2:B:360:GLU:OE1	2:B:360:GLU:N	2.54	0.41
2:B:579:TRP:CZ2	2:B:582:ILE:HD11	2.47	0.41
2:B:904:ARG:NH2	18:W:786:ASN:HA	2.34	0.41
3:C:174:SER:OG	3:C:175:ALA:N	2.54	0.41
10:J:20:ALA:O	10:J:24:LEU:HD13	2.21	0.41
11:K:40:HIS:CE1	11:K:63:VAL:HG21	2.56	0.41
11:K:107:GLU:O	11:K:111:ILE:CD1	2.67	0.41
14:N:-52:DC:N4	14:N:-51:DG:O6	2.54	0.41
17:V:29:CYS:HB2	17:V:38:LEU:HD12	2.01	0.41
1:A:266:LYS:HE2	1:A:303:THR:OG1	2.21	0.41
1:A:486:ASP:OD1	15:P:10:G:H4'	2.20	0.41
1:A:1168:ASP:OD2	1:A:1196:ARG:NH2	2.53	0.41
1:A:1229:MET:O	1:A:1240:ILE:HA	2.21	0.41
1:A:1294:VAL:HG12	1:A:1295:PRO:O	2.21	0.41
2:B:60:GLN:N	2:B:73:LYS:O	2.54	0.41
2:B:862:GLN:O	2:B:914:LYS:NZ	2.49	0.41
3:C:50:ILE:HG12	3:C:155:ILE:HG22	2.03	0.41
5:E:74:LEU:HD12	5:E:74:LEU:HA	1.98	0.41
9:I:108:LYS:HZ2	9:I:110:PHE:HB3	1.84	0.41
12:L:50:CYS:N	12:L:55:HIS:O	2.42	0.41
14:N:-73:DT:H72	16:T:72:DA:H61	1.85	0.41
14:N:-39:DT:H4'	14:N:-38:DT:OP1	2.21	0.41
14:N:-22:DG:H1'	14:N:-21:DG:C8	2.56	0.41
14:N:69:DT:H2''	14:N:70:DG:C8	2.56	0.41
16:T:56:DC:H2'	16:T:57:DA:C8	2.56	0.41
18:W:261:SER:O	18:W:275:GLU:N	2.50	0.41
18:W:266:ASP:OD1	18:W:267:SER:N	2.53	0.41
21:c:51:LEU:HD21	22:d:67:PHE:CD1	2.55	0.41
21:g:51:LEU:HD13	22:h:70:ILE:HG21	2.03	0.41
1:A:203:LEU:HB3	1:A:208:ILE:HD11	2.03	0.41
1:A:551:LEU:HD13	1:A:561:VAL:HG12	2.03	0.41
1:A:898:TYR:OH	1:A:1026:ALA:O	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:503:LYS:N	2:B:504:PRO:HD2	2.36	0.41
2:B:1204:PHE:HE2	2:B:1216:LEU:HD11	1.86	0.41
3:C:73:SER:O	3:C:76:VAL:HG12	2.21	0.41
6:F:99:LEU:O	6:F:103:MET:HG3	2.21	0.41
20:f:47:SER:OG	20:f:48:GLY:N	2.47	0.41
1:A:37:TYR:HB3	1:A:49:ARG:NH2	2.36	0.40
1:A:38:PRO:HB3	1:A:272:LYS:HG3	2.03	0.40
1:A:329:ARG:O	1:A:335:GLY:HA2	2.20	0.40
1:A:353:VAL:HG12	1:A:354:ILE:N	2.37	0.40
1:A:386:ILE:HG23	1:A:387:HIS:N	2.35	0.40
2:B:350:GLN:HG2	2:B:359:GLN:O	2.21	0.40
2:B:1056:SER:OG	2:B:1067:ARG:NH1	2.54	0.40
17:V:84:VAL:HG21	18:W:265:ARG:HH12	1.85	0.40
21:c:65:LEU:HD12	21:c:93:LEU:CD1	2.50	0.40
1:A:107:CYS:HB3	1:A:110:CYS:SG	2.60	0.40
1:A:303:THR:HA	1:A:306:ASP:O	2.20	0.40
1:A:599:LEU:O	1:A:600:SER:C	2.65	0.40
1:A:727:ARG:HD3	1:A:767:GLY:HA3	2.03	0.40
1:A:1211:MET:HE2	1:A:1230:TRP:HB2	2.02	0.40
1:A:1219:SER:O	1:A:1223:SER:O	2.39	0.40
2:B:216:VAL:N	2:B:389:ASP:OD2	2.48	0.40
2:B:267:TYR:HB2	2:B:348:ILE:HD11	2.03	0.40
2:B:345:ALA:O	2:B:349:LEU:HD23	2.21	0.40
2:B:954:LEU:HD12	2:B:955:THR:N	2.36	0.40
4:D:115:PHE:CD1	4:D:120:THR:HG22	2.55	0.40
7:G:30:LEU:O	7:G:34:VAL:HG12	2.21	0.40
18:W:791:ILE:HG21	18:W:796:LEU:HD21	2.03	0.40
1:A:45:ARG:HH22	1:A:47:ARG:NH2	2.19	0.40
1:A:1133:ALA:HB1	1:A:1287:MET:HE1	2.03	0.40
1:A:1285:VAL:HA	1:A:1311:THR:HG22	2.03	0.40
3:C:244:PHE:CE1	3:C:248:ILE:HD11	2.56	0.40
4:D:93:THR:OG1	4:D:102:VAL:HG11	2.21	0.40
4:D:108:TYR:HA	4:D:111:THR:HG22	2.03	0.40
9:I:25:LEU:HD22	9:I:41:PRO:HA	2.02	0.40
16:T:24:DA:H4'	16:T:25:DG:OP1	2.21	0.40
17:V:24:PHE:CZ	17:V:50:THR:HG21	2.57	0.40
20:f:75:HIS:CD2	22:h:93:THR:HG21	2.56	0.40
1:A:312:GLN:HG3	1:A:313:PRO:HD2	2.03	0.40
1:A:664:SER:OG	2:B:827:ILE:O	2.24	0.40
1:A:1120:VAL:N	1:A:1309:LEU:O	2.50	0.40
1:A:1154:ILE:HG23	1:A:1263:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:ARG:HB3	13:M:74:ILE:HG21	2.03	0.40
5:E:137:SER:HA	5:E:140:VAL:HG23	2.03	0.40
9:I:14:LEU:HD13	9:I:36:GLU:OE1	2.22	0.40
10:J:17:LYS:HB3	10:J:38:LEU:HD23	2.02	0.40
16:T:25:DG:C2	16:T:26:DG:C2	3.09	0.40
16:T:46:DA:H2''	16:T:47:DG:H8	1.87	0.40
2:B:202:VAL:HG22	2:B:203:LEU:N	2.36	0.40
4:D:141:GLU:OE1	4:D:163:LEU:HD21	2.20	0.40
8:H:12:VAL:O	8:H:52:ASP:N	2.48	0.40
9:I:79:HIS:O	9:I:79:HIS:ND1	2.50	0.40
18:W:302:GLY:N	18:W:305:GLU:OE1	2.47	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	1400/1743 (80%)	1330 (95%)	69 (5%)	1 (0%)	48	81
2	B	1145/1227 (93%)	1074 (94%)	70 (6%)	1 (0%)	48	81
3	C	261/304 (86%)	243 (93%)	18 (7%)	0	100	100
4	D	162/186 (87%)	157 (97%)	4 (2%)	1 (1%)	21	57
5	E	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
6	F	82/155 (53%)	77 (94%)	5 (6%)	0	100	100
7	G	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
8	H	129/145 (89%)	120 (93%)	9 (7%)	0	100	100
9	I	109/115 (95%)	104 (95%)	5 (5%)	0	100	100
10	J	64/72 (89%)	58 (91%)	6 (9%)	0	100	100
11	K	111/118 (94%)	109 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	43/72 (60%)	40 (93%)	3 (7%)	0	100	100
13	M	62/113 (55%)	60 (97%)	2 (3%)	0	100	100
17	V	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
18	W	265/911 (29%)	253 (96%)	12 (4%)	0	100	100
19	a	95/139 (68%)	94 (99%)	1 (1%)	0	100	100
19	e	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
20	b	78/106 (74%)	75 (96%)	3 (4%)	0	100	100
20	f	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
21	c	101/133 (76%)	101 (100%)	0	0	100	100
21	g	103/133 (77%)	100 (97%)	3 (3%)	0	100	100
22	d	93/129 (72%)	91 (98%)	2 (2%)	0	100	100
22	h	91/129 (70%)	88 (97%)	3 (3%)	0	100	100
All	All	5045/6668 (76%)	4807 (95%)	235 (5%)	3 (0%)	49	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	337	ARG
1	A	960	VAL
4	D	170	ASN

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	1225/1528 (80%)	1225 (100%)	0	100	100
2	B	1012/1077 (94%)	1012 (100%)	0	100	100
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	143/160 (89%)	143 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	106 (100%)	0	100	100
10	J	60/66 (91%)	60 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	38 (100%)	0	100	100
13	M	61/99 (62%)	61 (100%)	0	100	100
17	V	86/92 (94%)	86 (100%)	0	100	100
18	W	241/796 (30%)	241 (100%)	0	100	100
19	a	83/112 (74%)	83 (100%)	0	100	100
19	e	82/112 (73%)	82 (100%)	0	100	100
20	b	65/81 (80%)	65 (100%)	0	100	100
20	f	63/81 (78%)	63 (100%)	0	100	100
21	c	82/102 (80%)	82 (100%)	0	100	100
21	g	83/102 (81%)	83 (100%)	0	100	100
22	d	81/107 (76%)	81 (100%)	0	100	100
22	h	79/107 (74%)	79 (100%)	0	100	100
All	All	4469/5772 (77%)	4469 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	210	ASN
1	A	287	GLN
1	A	291	ASN
1	A	387	HIS
1	A	436	HIS
1	A	549	ASN
1	A	660	HIS
1	A	692	GLN
1	A	737	ASN

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Mol	Chain	Res	Type
1	A	936	GLN
2	B	197	ASN
2	B	770	GLN
2	B	807	GLN
4	D	41	HIS
4	D	99	ASN
7	G	155	ASN
8	H	17	ASN
8	H	44	ASN
9	I	90	GLN
13	M	42	ASN
17	V	100	GLN
19	a	113	HIS
21	c	24	GLN
21	c	68	ASN
22	d	64	ASN
22	d	81	ASN
21	g	31	HIS
22	h	64	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	15/16 (93%)	2 (13%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	-4	C
15	P	4	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 11 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32409. 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

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.