



Full wwPDB EM Validation Report ⓘ

Nov 3, 2025 – 04:07 pm GMT

PDB ID : 9S3G / pdb_00009s3g
EMDB ID : EMD-54537
Title : State 1 MAP3 RNA Pol II activated elongation complex with SETD2 and upstream hexasome
Authors : Walshe, J.L.; Ochmann, M.; Dienemann, C.; Cramer, P.
Deposited on : 2025-07-24
Resolution : 6.40 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:

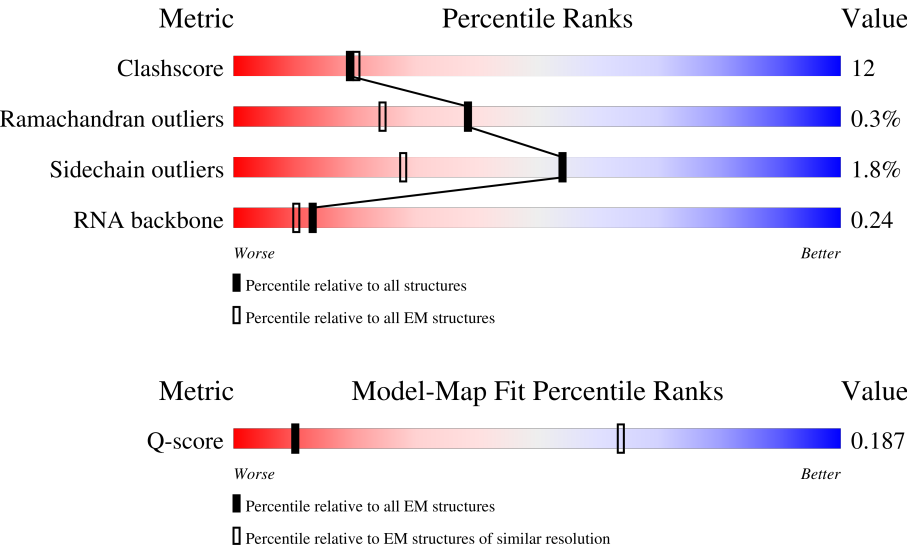
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

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 6.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	544 (5.90 - 6.90)

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

Mol	Chain	Length	Quality of chain
1	A	1970	
2	B	1174	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1729	
14	N	184	
15	O	1133	
16	P	21	
17	Q	1179	
18	R	713	
19	S	304	
20	T	184	
21	U	666	
22	V	531	
23	W	305	
24	X	531	
25	Y	121	
26	Z	1087	
27	a	136	
27	e	136	

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Mol	Chain	Length	Quality of chain
28	b	103	
28	f	103	
29	g	135	
30	h	126	
31	j	1049	
32	k	709	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 75297 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1444	Total	C	N	O	S	0	0
			11455	7198	2046	2137	74		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1136	Total	C	N	O	S	0	0
			9088	5745	1597	1682	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	126	Total	C	N	O	S	0	0
			1014	634	170	206	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 polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	78	Total	C	N	O	S	0	0
			627	401	106	115	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
			1343	871	217	247	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	149	Total	C	N	O	S	0	0
			1198	759	195	239	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			950	587	169	183	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	47	Total	C	N	O	S	0	0
			398	246	77	69	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	852	Total	C	N	O	S	0	0
			7001	4440	1219	1308	34		

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	55	Total	C	N	O	P	0	0
			1130	535	197	343	55		

- Molecule 15 is a protein called Histone-lysine N-methyltransferase SETD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	152	Total	C	N	O	S	0	0
			1228	772	209	241	6		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	1432	SER	-	expression tag	UNP Q9BYW2
O	1433	ASN	-	expression tag	UNP Q9BYW2
O	1434	ALA	-	expression tag	UNP Q9BYW2
O	1962	LEU	PRO	variant	UNP Q9BYW2

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	21	Total	C	N	O	P	0	0
			436	195	66	154	21		

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	892	Total	C	N	O	S	0	0
			7240	4587	1266	1355	32		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	1177	TYR	-	expression tag	UNP Q6PD62
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 18 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	220	Total	C	N	O	S	0	0
			1694	1063	312	312	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-262	SER	-	expression tag	UNP Q92541
R	-261	ASN	-	expression tag	UNP Q92541
R	-260	ALA	-	expression tag	UNP Q92541

- Molecule 19 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	99	Total	C	N	O	S	0	0
			795	484	147	158	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	expression tag	UNP P23193
S	-1	ASN	-	expression tag	UNP P23193
S	0	ALA	-	expression tag	UNP P23193

- Molecule 20 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	67	Total	C	N	O	P	0	0
			1369	645	273	384	67		

- Molecule 21 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	179	Total	C	N	O	S	0	0
			1469	919	262	282	6		

- Molecule 22 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	281	Total	C	N	O	S	0	0
			2310	1461	390	447	12		

- Molecule 23 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	305	Total	C	N	O	S	0	0
			2374	1507	399	463	5		

- Molecule 24 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	53	Total	C	N	O	0	0
			434	268	85	81		

- Molecule 25 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	116	Total	C	N	O	S	0	0
			912	570	159	174	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP Q4R941
Y	-2	PRO	-	expression tag	UNP Q4R941
Y	-1	GLY	-	expression tag	UNP Q4R941
Y	0	SER	-	expression tag	UNP Q4R941

- Molecule 26 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	498	Total	C	N	O	S	0	0
			3976	2529	702	728	17		

- Molecule 27 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	96	Total	C	N	O	S	0	0
			789	497	152	138	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	76	Total	C	N	O	S	0	0
			615	390	115	108	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	37	MET	LYS	engineered mutation	UNP Q71DI3
a	111	ALA	CYS	engineered mutation	UNP Q71DI3
e	37	MET	LYS	engineered mutation	UNP Q71DI3
e	111	ALA	CYS	engineered mutation	UNP Q71DI3

- Molecule 28 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
28	f	79	Total	C	N	O	S	0	0
			627	395	121	110	1		

- Molecule 29 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	g	91	Total	C	N	O	0	0
			710	444	141	125		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	-4	SER	-	expression tag	UNP P04908
g	-3	ASN	-	expression tag	UNP P04908
g	-2	ALA	-	expression tag	UNP P04908
g	-1	PRO	-	expression tag	UNP P04908
g	0	TRP	-	expression tag	UNP P04908

- Molecule 30 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	94	Total	C	N	O	S	0	0
			734	461	132	139	2		

- Molecule 31 is a protein called FACT complex subunit SPT16.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	497	Total	C	N	O	S	0	0
			4050	2560	686	787	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	-1	SER	-	expression tag	UNP Q9Y5B9
j	0	ASN	-	expression tag	UNP Q9Y5B9

- Molecule 32 is a protein called FACT complex subunit SSRP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	423	Total	C	N	O	S	0	0
			3446	2206	590	635	15		

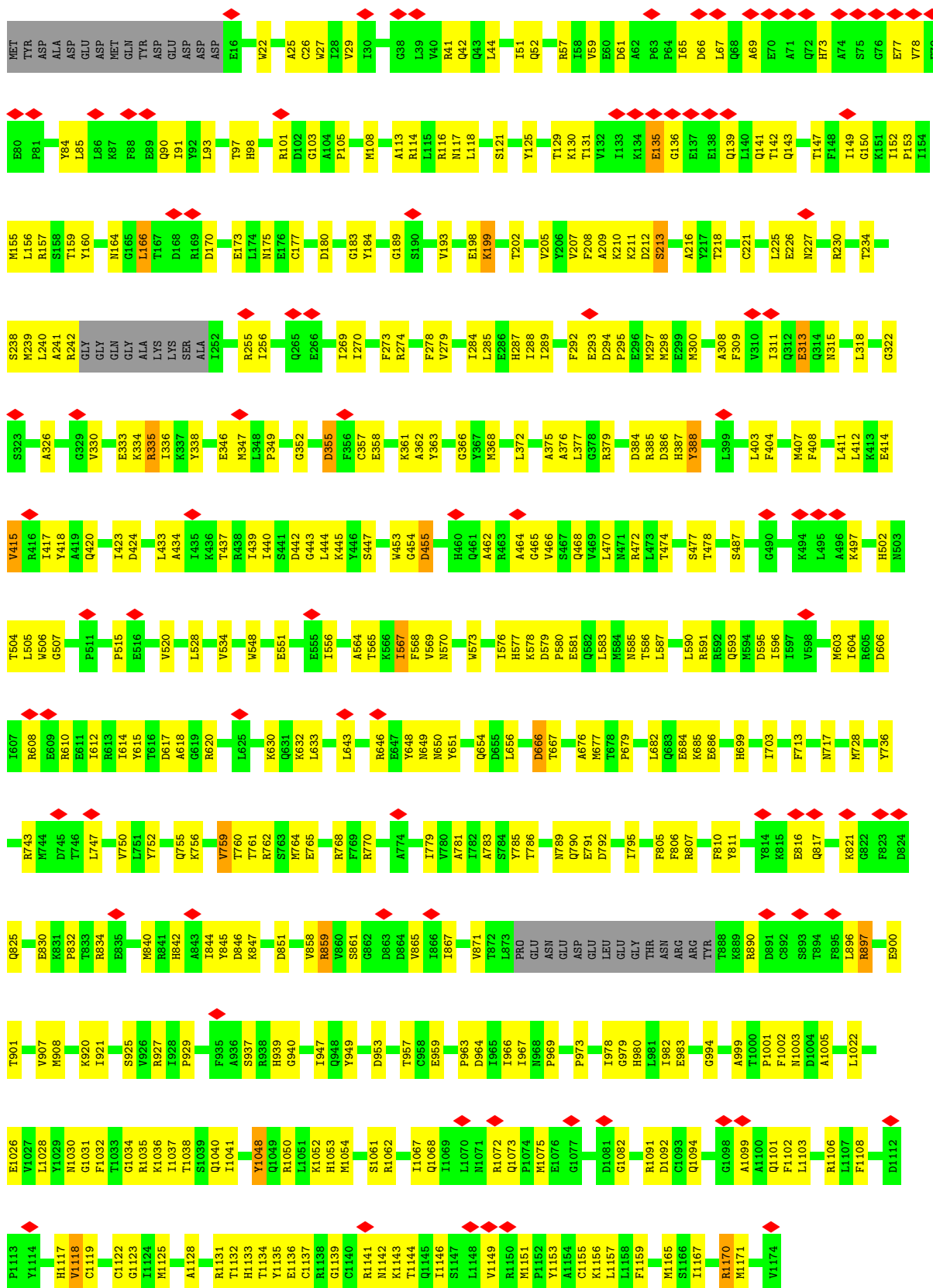
- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

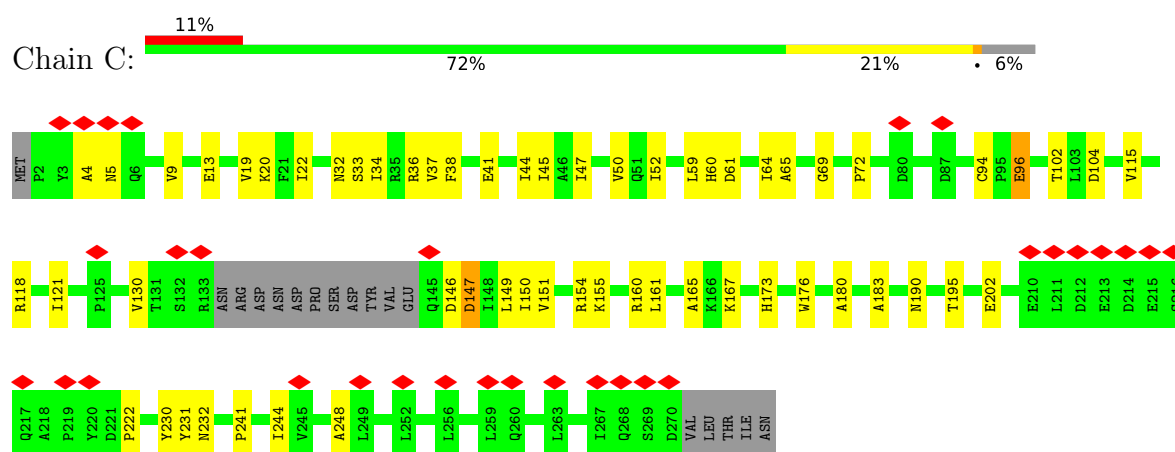
- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

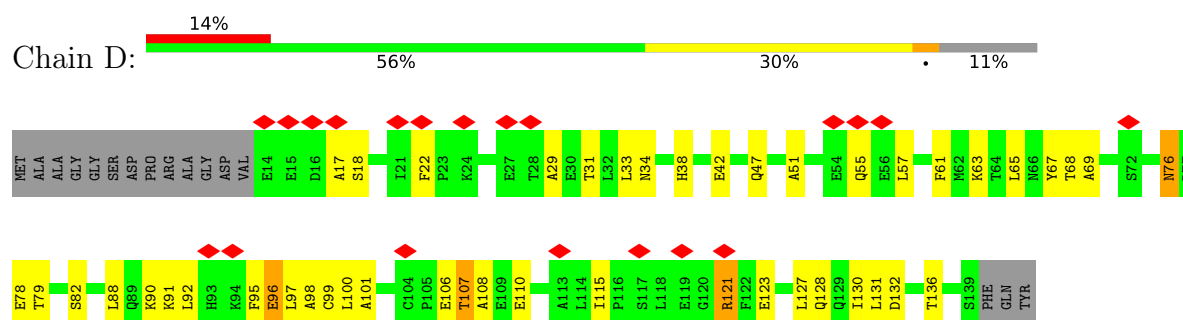




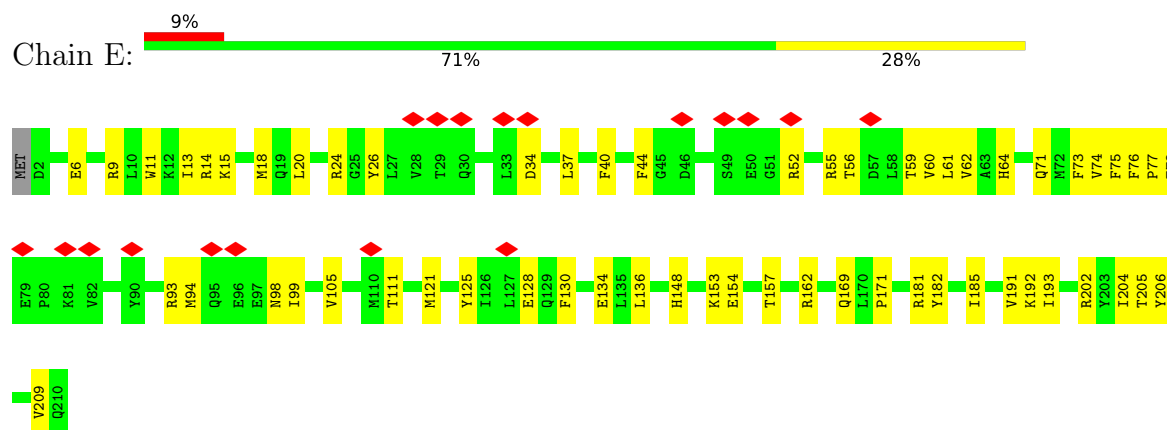
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



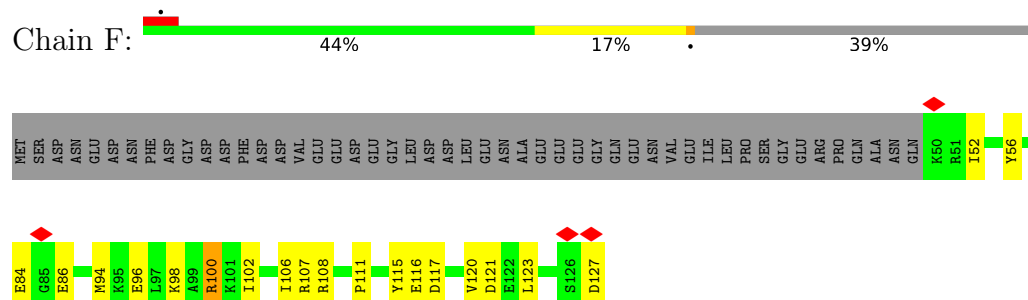
• Molecule 4: RNA polymerase II subunit D



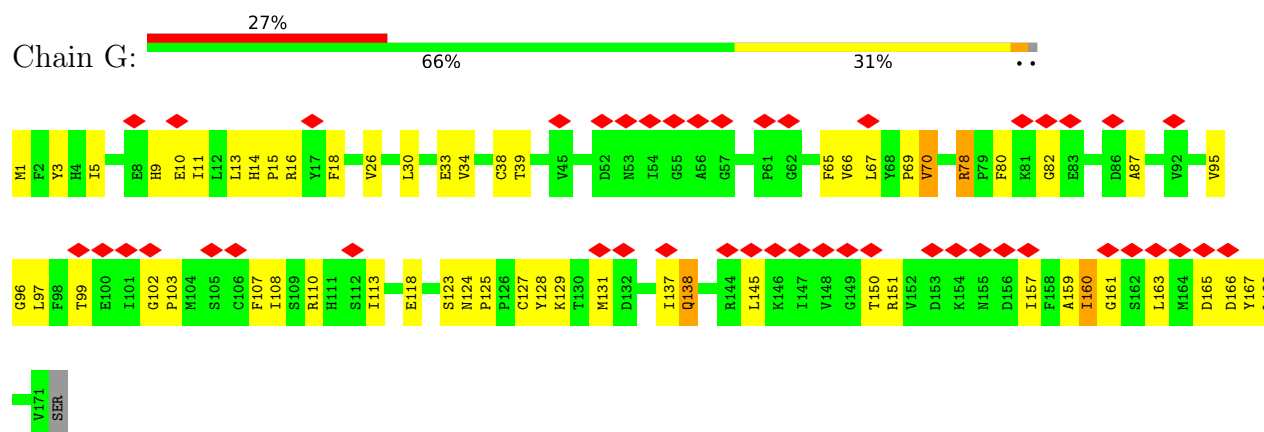
• Molecule 5: DNA-directed RNA polymerase II subunit E



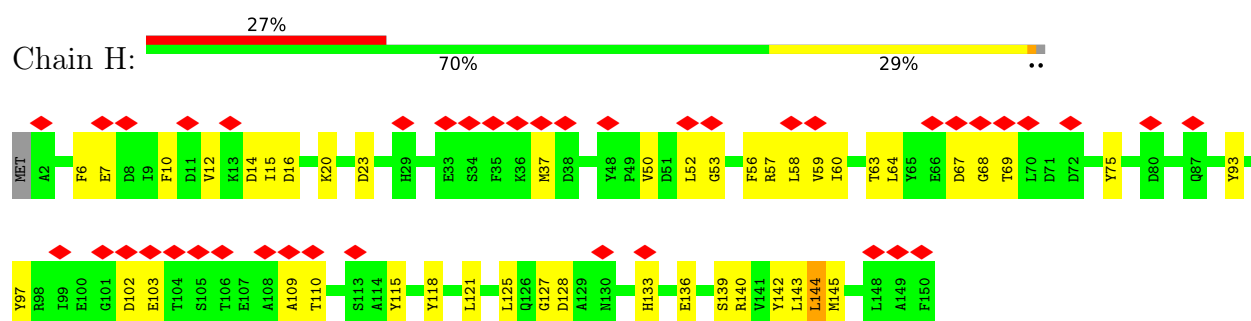
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



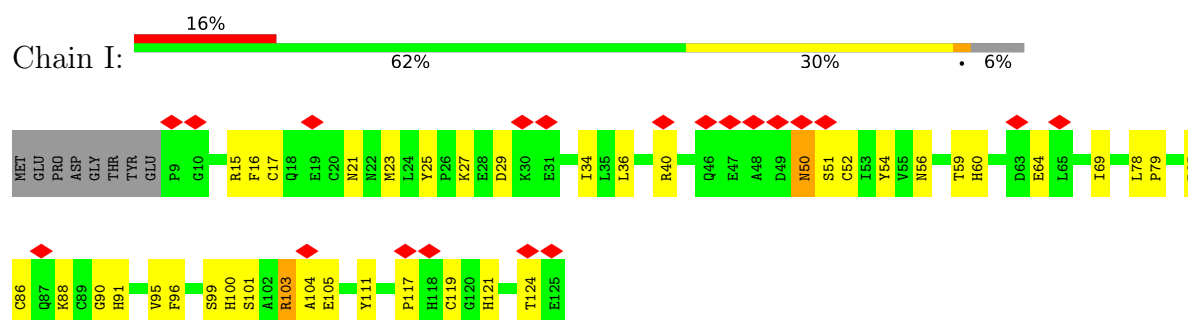
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



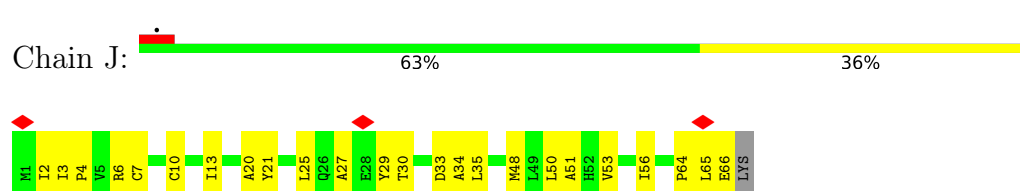
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



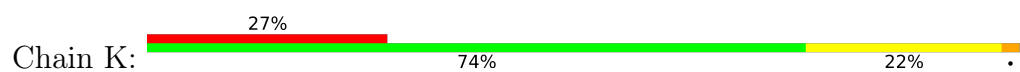
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

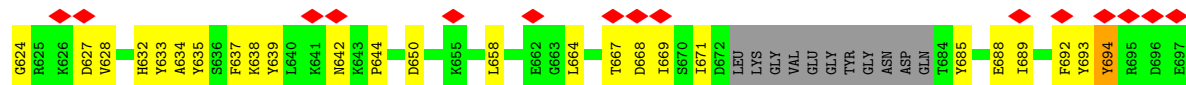


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

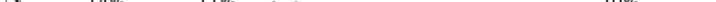


- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a





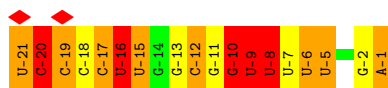


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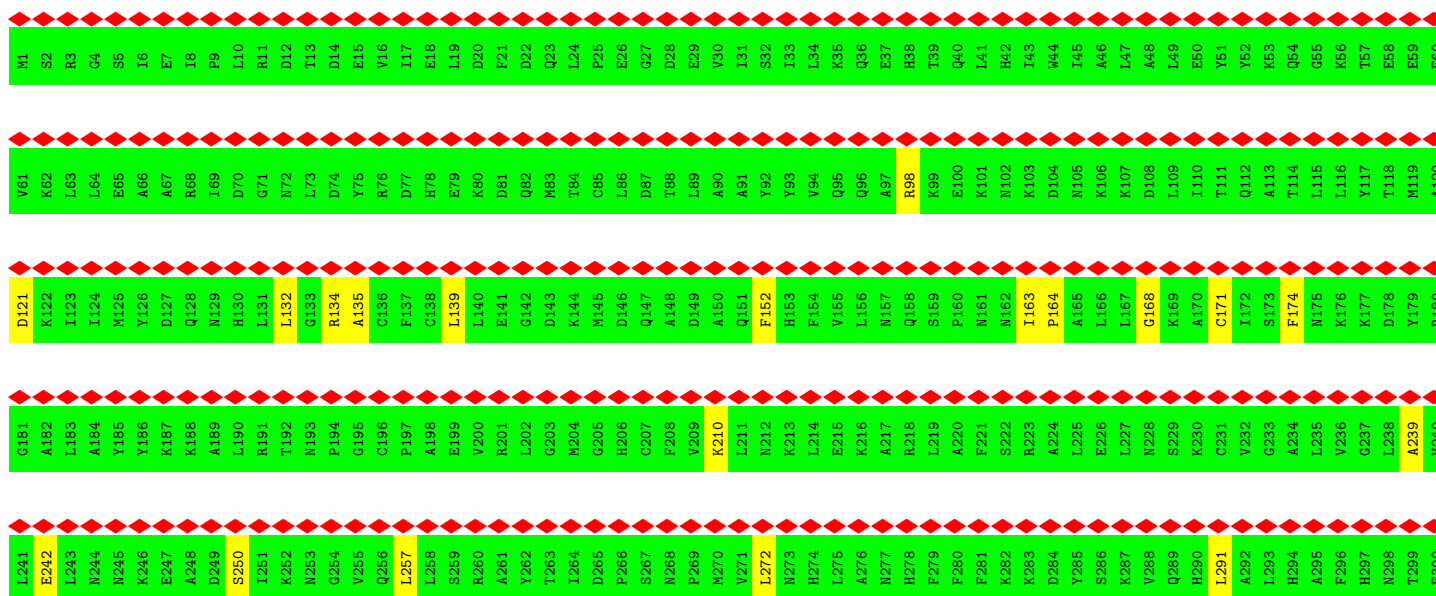
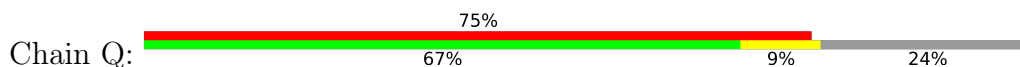


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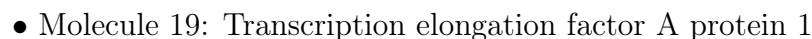
- Molecule 16: RNA



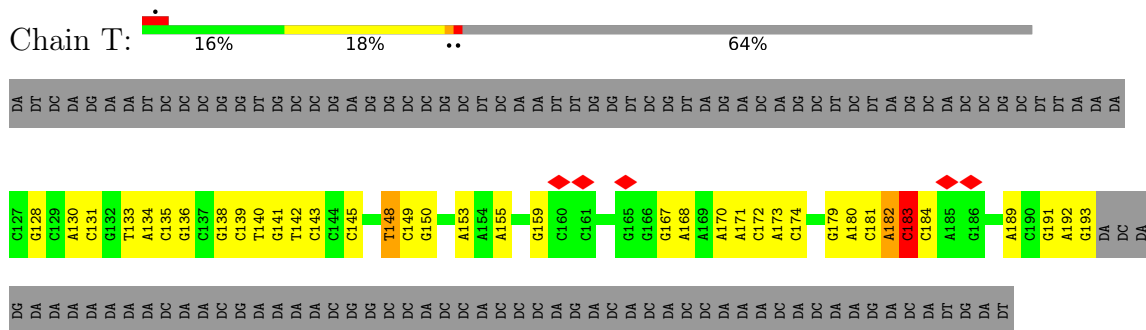
- Molecule 17: RNA polymerase-associated protein CTR9 homolog



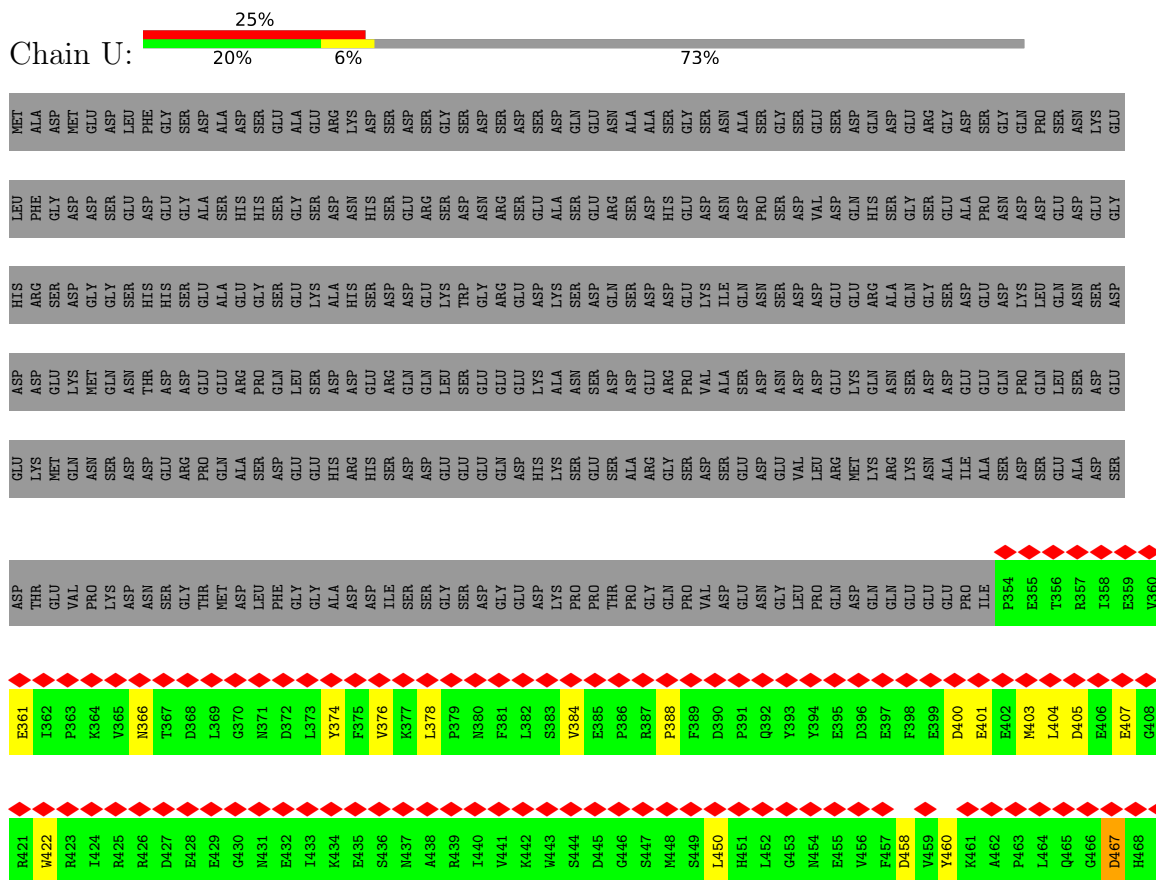
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GLN	SER	GLY	LYS	LYS	LYS	GLY	LYS	GLY	L723	F663	S603	D543	A483	E423	C363	A302
ASP	SER	GLY	LEU	GLY	GLY	GLY	GLY	GLY	A724	R664	M604	K544	E484	Q424	F364	M304
ASP	ASP	GLY	ILE	GLY	GLY	GLY	GLY	GLY	R725	E665	L605	G545	E485	T425	E365	Q305
ASN	ASP	ALA	ALA	ARG	ARG	ARG	ARG	ARG	A726	A666	A606	N546	E486	D426	K366	A306
PRO	PRO	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L727	R667	L607	F547	H487	I427	V367	E307
SER	SER	GLU	GLU	GLU	GLU	GLU	GLU	GLU	F728	D668	G608	Y548	D488	Q428	L368	S308
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	K729	V669	M609	E549	E489	G429	K369	C309
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	C730	W669	V610	A550	A490	A430	A370	Y310
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	G731	A671	W611	S551	Y491	L431	Y371	Q311
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	K732	Q672	L612	D552	Y492	S432	P372	L312
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L733	V673	Q613	W553	M493	A433	N373	A313
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	Q734	R674	T614	F554	A494	Y434	N374	R314
PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	E735	E675	L615	K555	I495	G435	Y375	S315
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	C736	A676	H616	E556	S496	T436	E376	F316
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ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	Q738	A678	P618	L558	T498	T438	M378	V318
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	K739	D679	T619	Q559	T499	R439	K379	Q319
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L740	I680	R620	I560	S500	I440	I380	E320
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L741	S681	D621	W561	S501	I441	I381	D321
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ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	A747	L687	R627	W568	E508	A447	Q327	Q327
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	P748	A688	H628	S569	A509	D448	Y328	Y328
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	S749	H689	Q629	SS69	A509	V449	S389	Y329
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	D750	I690	D630	L570	M510	P450	D390	Y330
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	T751	Y691	R631	I571	C511	P451	Q391	Q331
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	V752	V692	A632	G572	E512	E452	E392	A332
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L753	E693	L633	N573	F513	I453	K393	T333
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	W754	Q694	A634	L574	H514	L454	R394	Q334
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	F755	K695	I635	H575	E515	N455	D395	F335
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	W756	Q696	Y636	L576	A516	N456	I396	A336
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	T757	Y697	K637	L577	E517	V457	A397	S337
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	A758	I698	Q638	K578	K518	G458	K398	S338
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L759	S699	V639	Q579	L519	A459	G399	S339
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	W760	A700	L640	E580	Y520	L460	H400	F340
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L761	V701	R641	W581	K521	H461	L401	V341
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	Q762	Q702	M642	G582	N522	F462	K402	L342
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	R763	W703	D643	P583	I523	R463	K403	P343
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L764	V704	A644	G584	L524	L464	V404	F344
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	A765	W705	N646	Q585	R525	G465	T405	F345
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	T766	N706	L647	K586	E526	N466	T406	G346
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	Q767	C707	L647	K587	H527	L467	Q407	L347
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	V768	L708	Y648	F588	P528	G468	Y408	Q348
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L769	R709	A649	E589	N529	E469	P409	Q349
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	K770	W710	A650	R590	Y530	A470	D410	M350
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	D771	F711	N651	I591	V531	K471	D411	Y361
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	E772	Y712	G652	L592	D532	K472	V412	I362
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	K773	L653	I653	K593	C533	Y473	E413	Y363
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	S774	H714	G654	Q594	Y534	F474	A414	R364
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	N775	A655	V656	P595	L535	L475	W415	G365
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L776	Q715	V656	S596	R536	A476	I416	D366
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	N716	N716	L657	T597	L537	S477	E417	K367
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	E778	T718	A658	Q598	G538	L478	L418	G368
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	V779	V719	H659	S599	A539	D479	A419	N369
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L780	W720	K660	D600	M540	R480	Q420	A360
L841	R842	A843	K844	Q845	E846	Q847	E848	L849	L781	Y722	Y723	Y724	Y725	Y726	Y727	Y728
R842	A843	K844	Q845	E846	Q847	E848	L849	L850	Y729	Y730	Y731	Y732	Y733	Y734	Y735	Y736
A843	K844	Q845	E846	Q847	E848	L849	L850	L851	Y736	Y737	Y738	Y739	Y740	Y741	Y742	Y743
K844	Q845	E846	Q847	E848	L849	L850	L851	L852	Y743	Y744	Y745	Y746	Y747	Y748	Y749	Y750
Q845	E846	Q847	E848	L849	L850	L851	L852	L853	Y750	Y751	Y752	Y753	Y754	Y755	Y756	Y757
E846	Q847	E848	L849	L850	L851	L852	L853	L854	Y751	Y752	Y753	Y754	Y755	Y756	Y757	Y758
Q847	E848	L849	L850	L851	L852	L853	L854	L855	Y752	Y753	Y754	Y755	Y756	Y757	Y758	Y759
E848	L849	L850	L851	L852	L853	L854	L855	L856	Y753	Y754	Y755	Y756	Y757	Y758	Y759	Y760
L849	L850	L851	L852	L853	L854	L855	L856	L857	Y754	Y755	Y756	Y757	Y758	Y759	Y760	Y761
L850	L851	L852	L853	L854	L855	L856	L857	L858	Y755	Y756	Y757	Y758	Y759	Y760	Y761	Y762
L851	L852	L853	L854	L855	L856	L857	L858	L859	Y756	Y757	Y758	Y759	Y760	Y761	Y762	Y763
L852	L853	L854	L855	L856	L857	L858	L859	L860	Y757	Y758	Y759	Y760	Y761	Y762	Y763	Y764
L853	L854	L855	L856	L857	L858	L859	L860	L861	Y758	Y759	Y760	Y761	Y762	Y763	Y764	Y765
L854	L855	L856	L857	L858	L859	L860	L861	L862	Y759	Y760	Y761	Y762	Y763	Y764	Y765	Y766
L855	L856	L857	L858	L859	L860	L861	L862	L863	Y760	Y761	Y762	Y763	Y764	Y765	Y766	Y767
L856	L857	L858	L859	L860	L861	L862	L863	L864	Y761	Y762	Y763	Y764	Y765	Y766	Y767	Y768
L857	L858	L859	L860	L861	L862	L863	L864	L865	Y762	Y763	Y764	Y765	Y766	Y767	Y768	Y769
L858	L859	L860	L861	L862	L863	L864	L865	L866	Y763	Y764	Y765	Y766	Y767	Y768	Y769	Y770
L859	L860	L861	L862	L863	L864	L865	L866	L867	Y764	Y765	Y766	Y767	Y768	Y769	Y770	Y771
L860	L861	L862	L863	L864	L865	L866	L867	L868	Y765	Y766	Y767	Y768	Y769	Y770	Y771	Y772
L861	L862	L863	L864	L865	L866	L867	L868	L869	Y766	Y767	Y768	Y769	Y770	Y771	Y772	Y773
L862	L863	L864	L865	L866	L867	L868	L869	L870	Y767	Y768	Y769	Y770	Y771	Y772	Y773	Y774
L863	L864	L865	L866	L867	L868	L869	L870	L871	Y768	Y769	Y770	Y771	Y772	Y773	Y774	Y775
L864	L865	L866	L867	L868	L869	L870	L871	L872	Y769	Y770	Y771	Y772	Y773	Y774	Y775	Y776
L865	L866	L867	L868	L869	L870	L871	L872	L873	Y770	Y771	Y772	Y773	Y774	Y775	Y776	Y777
L866	L867	L868	L869	L870	L871	L872	L873	L874	Y771	Y772	Y773	Y774	Y775	Y776	Y777	Y778
L867	L868	L869	L870	L871	L872	L873	L874	L875	Y772	Y773	Y774	Y775	Y776	Y777	Y778	Y779
L868	L869	L870	L871	L872	L873	L874	L875	L876	Y773	Y774	Y775	Y776	Y777	Y778	Y779	Y780
L869	L870	L871	L872	L873	L874	L875	L876	L877	Y774	Y775	Y776	Y777	Y778	Y779	Y780	Y781
L870	L871	L872	L873	L874	L875	L876	L877	L878	Y775	Y776	Y777	Y778	Y779	Y780	Y781	Y782
L871	L872	L873	L874	L875	L876	L877	L878	L879	Y776	Y777	Y778	Y779	Y780	Y781	Y782	Y783
L872	L873	L874	L875	L876	L877	L878	L879	L880	Y							

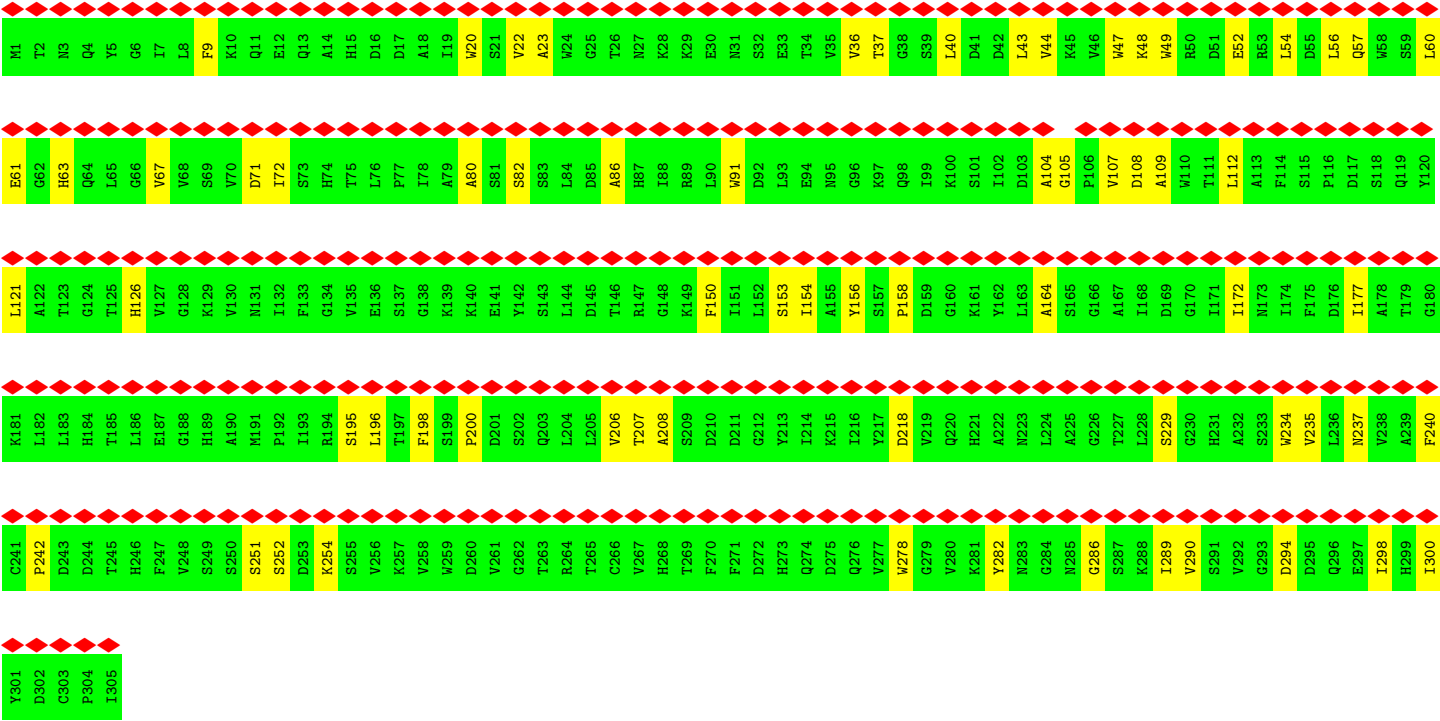


- Molecule 20: Template DNA

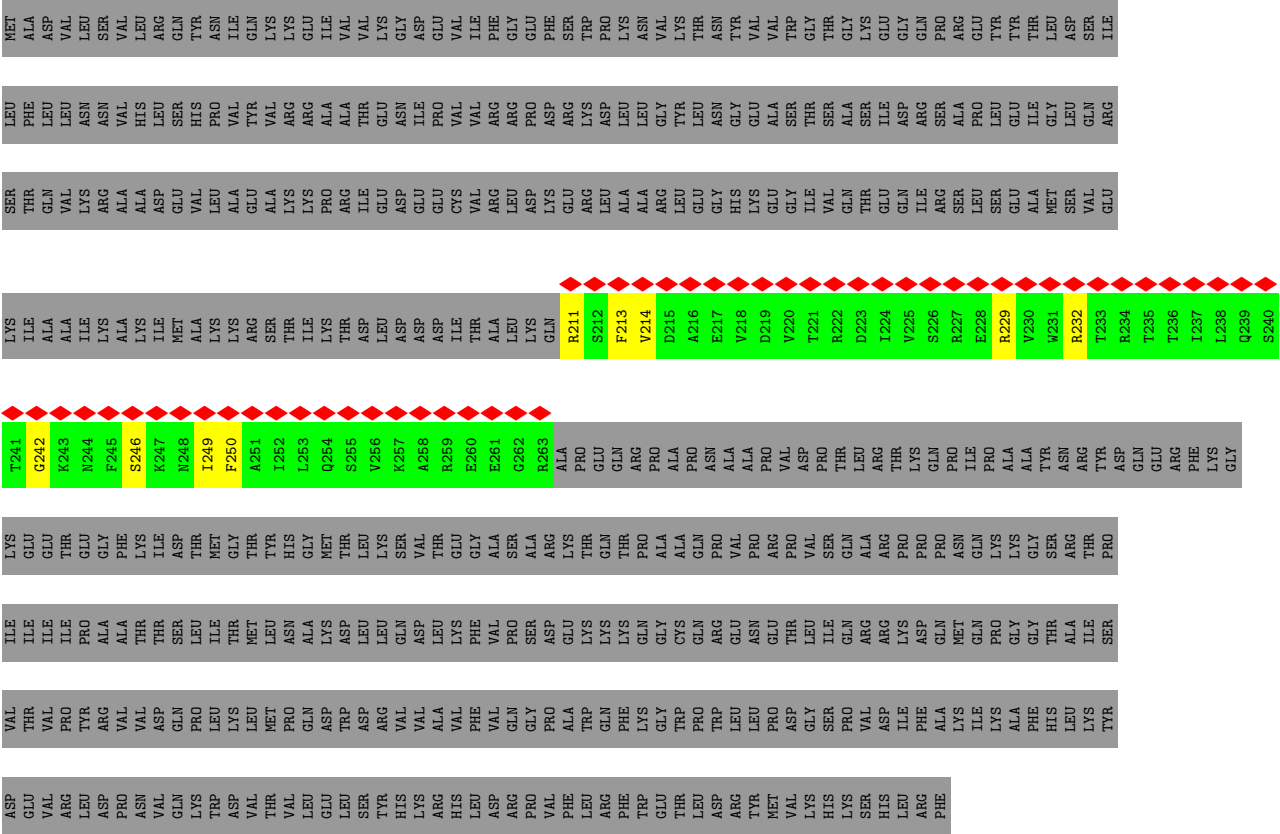


- Molecule 21: RNA polymerase-associated protein LEO1





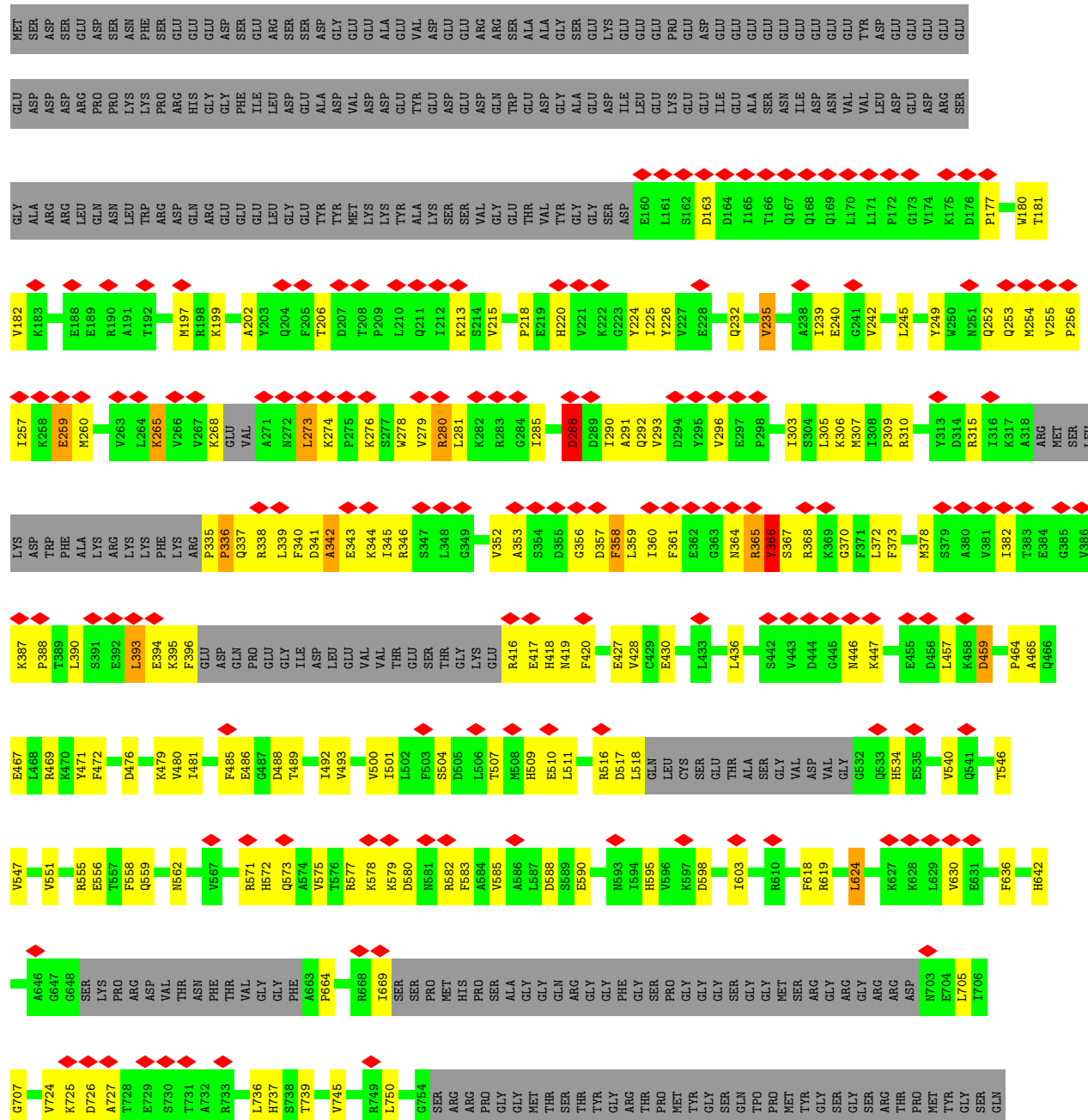
• Molecule 24: Parafibromin



• Molecule 25: Transcription elongation factor SPT4

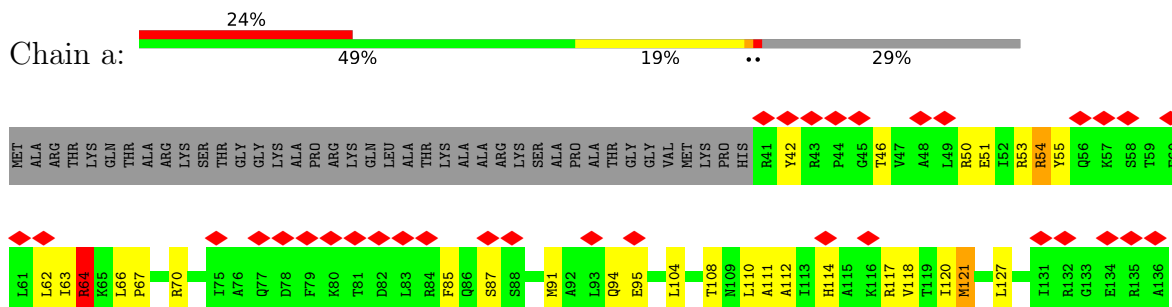


Chain Z:  14% 30% 15% 54%

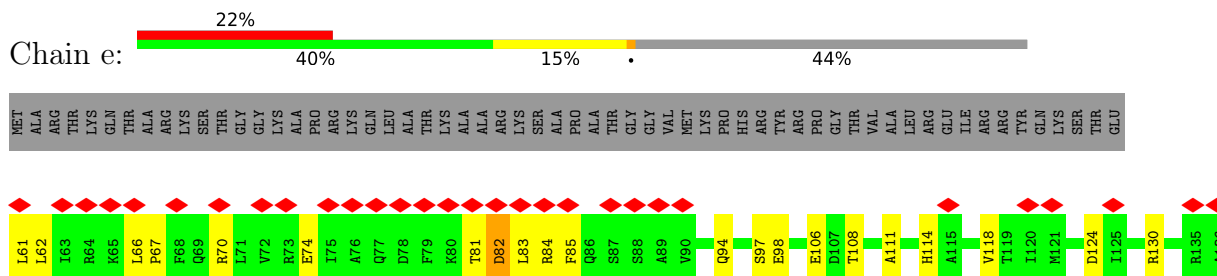




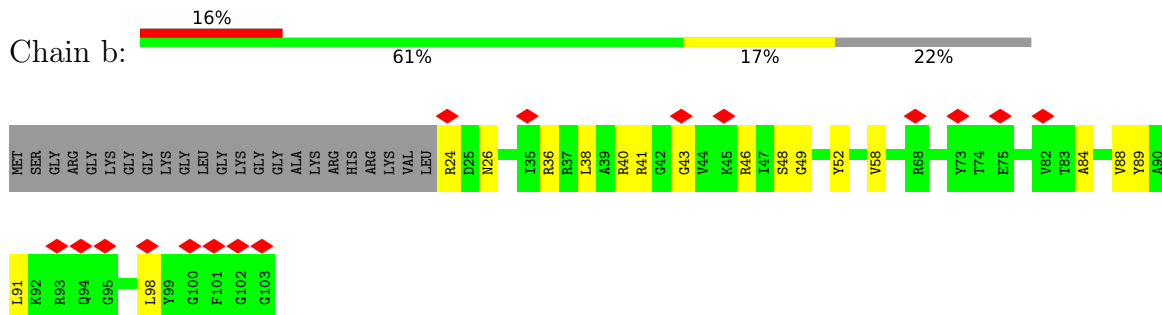
- Molecule 27: Histone H3.2



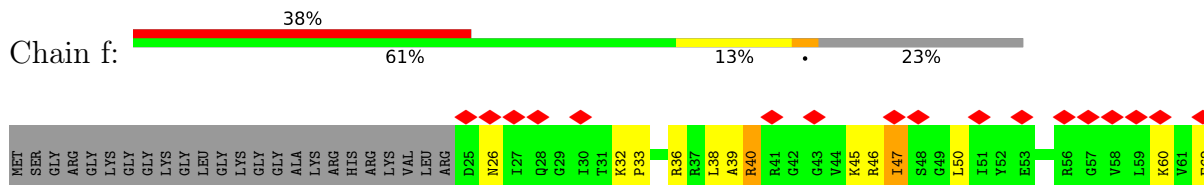
- Molecule 27: Histone H3.2

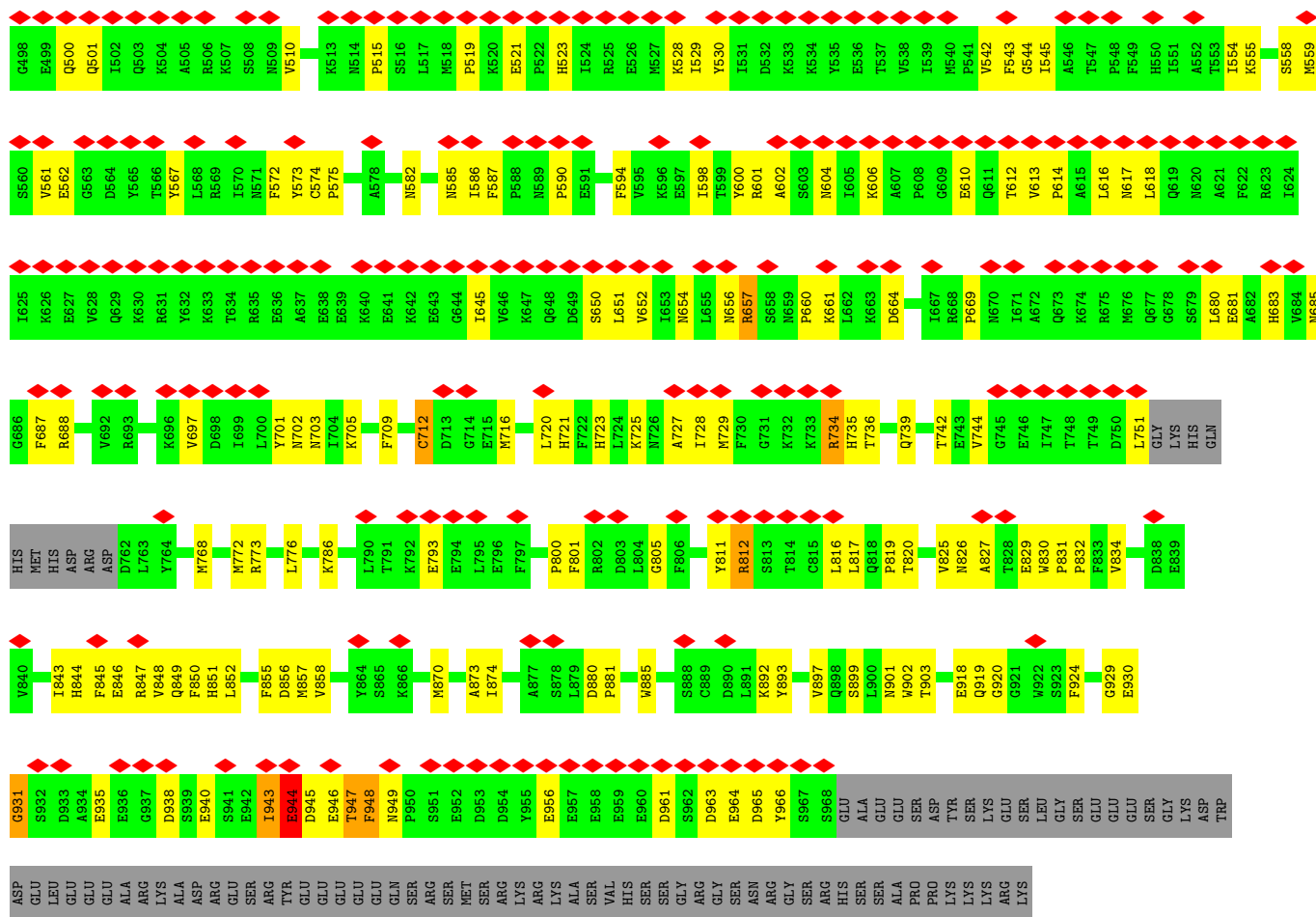


- Molecule 28: Histone H4

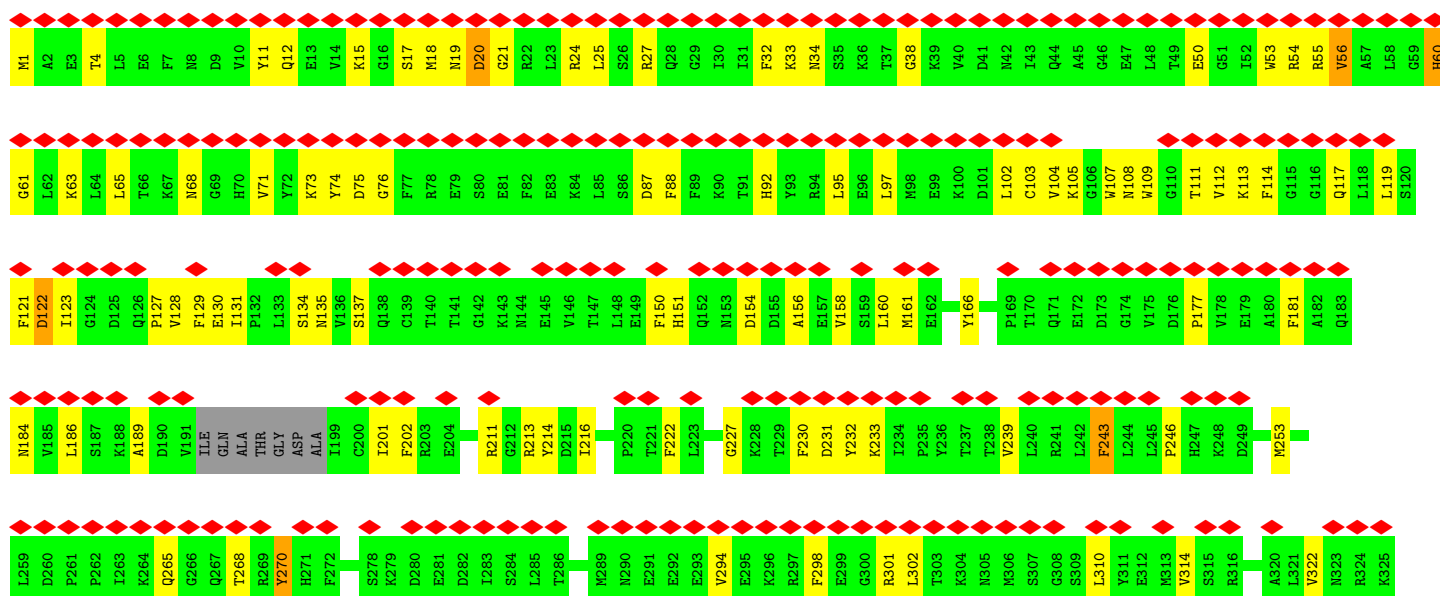


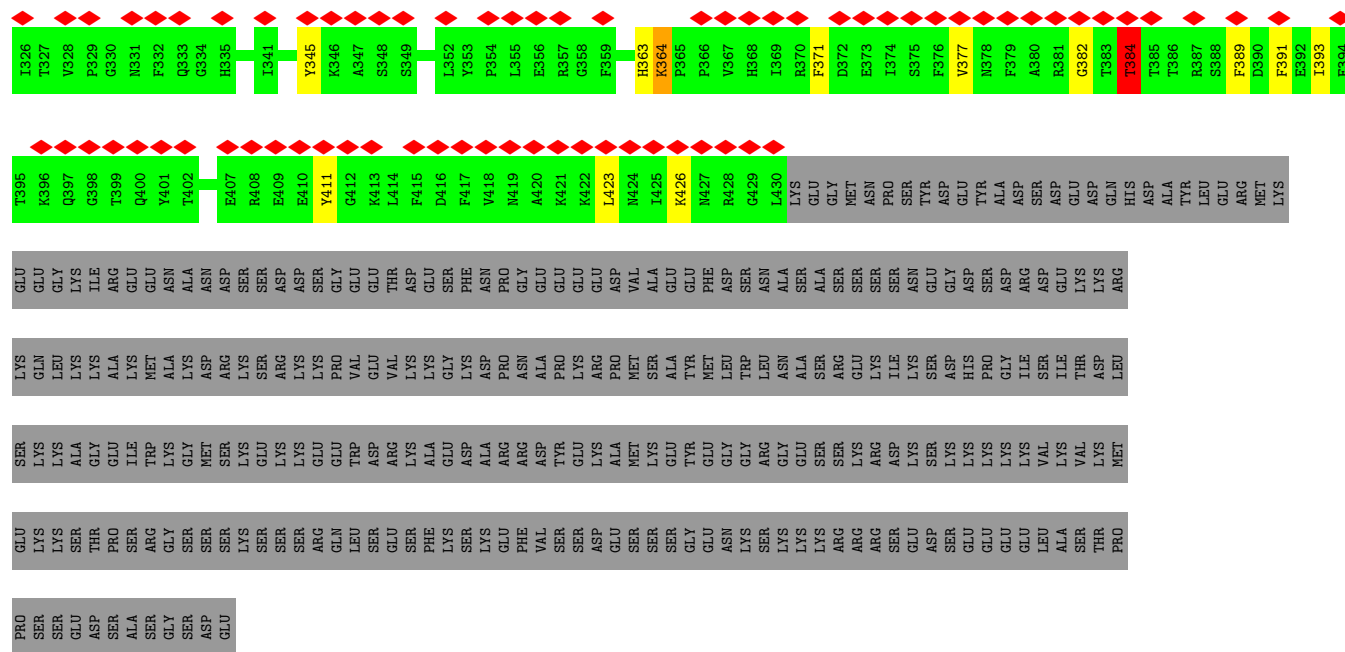
- Molecule 28: Histone H4





• Molecule 32: FACT complex subunit SSRP1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112302	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39.83	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0075	Depositor
Map size (\AA)	537.6, 537.6, 537.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.05, 1.05, 1.05	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	0.44	0/11663	0.96	6/15739 (0.0%)
2	B	0.40	0/9269	0.95	7/12512 (0.1%)
3	C	0.35	0/2115	0.86	0/2873
4	D	0.48	0/1027	1.03	1/1381 (0.1%)
5	E	0.43	0/1752	0.99	0/2366
6	F	0.49	0/637	0.92	0/859
7	G	0.43	0/1374	0.97	3/1865 (0.2%)
8	H	0.37	0/1220	0.80	0/1644
9	I	0.39	0/973	0.92	0/1316
10	J	0.33	0/533	0.88	0/719
11	K	0.38	0/939	0.77	0/1271
12	L	0.42	0/404	0.98	0/536
13	M	0.73	3/7131 (0.0%)	1.20	32/9607 (0.3%)
14	N	0.75	0/1262	1.31	10/1946 (0.5%)
15	O	0.79	0/1243	1.51	5/1672 (0.3%)
16	P	0.94	8/483 (1.7%)	1.08	1/748 (0.1%)
17	Q	0.35	0/7379	0.85	0/9945
18	R	0.34	0/1717	0.96	1/2303 (0.0%)
19	S	0.31	0/800	0.64	0/1068
20	T	0.67	0/1540	1.23	7/2370 (0.3%)
21	U	0.40	0/1498	0.98	3/2018 (0.1%)
22	V	0.38	0/2360	0.94	0/3188
23	W	0.29	0/2433	0.73	0/3311
24	X	0.34	0/438	0.87	0/587
25	Y	0.37	0/928	1.01	0/1250
26	Z	0.43	0/4045	1.15	19/5445 (0.3%)
27	a	0.78	0/799	1.20	1/1070 (0.1%)
27	e	0.37	0/622	0.91	0/833
28	b	0.59	0/645	1.11	0/862
28	f	0.33	0/634	0.99	3/848 (0.4%)
29	g	0.29	0/718	0.89	0/966
30	h	0.39	0/745	0.92	1/1000 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	j	0.40	0/4133	0.97	6/5573 (0.1%)
32	k	0.41	0/3523	0.99	3/4746 (0.1%)
All	All	0.47	11/76982 (0.0%)	1.00	109/104437 (0.1%)

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	7
2	B	0	8
4	D	0	1
6	F	0	1
7	G	0	2
9	I	0	1
10	J	0	1
12	L	0	2
13	M	0	16
14	N	0	9
16	P	0	3
17	Q	0	1
18	R	0	2
20	T	0	10
21	U	0	1
24	X	0	2
25	Y	0	2
26	Z	0	6
27	a	0	1
29	g	0	2
30	h	0	2
31	j	0	4
32	k	0	2
All	All	0	86

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	-20	C	C1'-N1	6.79	1.58	1.48
13	M	1037	ILE	CA-C	6.67	1.60	1.52
16	P	-6	U	C1'-N1	6.62	1.58	1.48
16	P	-1	A	P-OP1	6.48	1.61	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1013	SER	CA-C	-5.96	1.45	1.52
16	P	-19	C	C1'-N1	5.74	1.56	1.47
16	P	-15	U	C1'-N1	5.73	1.57	1.48
16	P	-16	U	C1'-N1	5.66	1.55	1.47
16	P	-12	C	C1'-N1	5.54	1.55	1.47
16	P	-5	U	C1'-N1	5.43	1.56	1.48
13	M	375	PHE	CA-C	-5.02	1.46	1.52

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1038	ASP	CA-CB-CG	13.18	125.78	112.60
13	M	685	TYR	N-CA-C	11.09	125.55	111.24
13	M	1036	LYS	CA-C-N	9.22	132.44	122.11
13	M	1036	LYS	C-N-CA	9.22	132.44	122.11
13	M	968	GLU	CB-CA-C	-9.18	95.25	110.85
14	N	53	DC	O3'-P-O5'	-8.49	91.27	104.00
20	T	183	DC	C3'-C2'-C1'	8.17	113.86	101.60
13	M	981	TYR	CA-CB-CG	-8.09	99.34	113.90
26	Z	393	LEU	N-CA-C	7.76	127.34	110.80
30	h	122	TYR	N-CA-C	-7.66	101.25	110.44
14	N	2	DG	O3'-P-O5'	-7.49	92.77	104.00
26	Z	394	GLU	N-CA-C	7.47	122.39	113.28
13	M	1037	ILE	O-C-N	-7.42	114.95	122.67
13	M	688	GLU	N-CA-C	7.23	119.24	111.36
27	a	118	VAL	N-CA-C	-7.19	104.77	111.45
13	M	1037	ILE	CA-C-O	-7.17	115.21	121.09
20	T	183	DC	O3'-P-O5'	-7.17	93.24	104.00
32	k	364	LYS	N-CA-C	7.10	118.31	109.57
13	M	375	PHE	CA-CB-CG	-6.96	106.84	113.80
26	Z	366	TYR	CA-CB-CG	-6.77	101.71	113.90
26	Z	288	ASP	N-CA-C	6.75	120.72	111.54
13	M	692	PHE	N-CA-C	6.72	119.96	111.69
26	Z	296	VAL	N-CA-C	6.71	117.55	107.75
14	N	54	DG	O3'-P-O5'	-6.60	94.09	104.00
14	N	52	DA	C2'-C3'-O3'	6.58	121.36	111.50
14	N	53	DC	C2'-C3'-O3'	6.57	121.36	111.50
26	Z	365	ARG	N-CA-C	-6.56	97.15	108.56
32	k	243	PHE	CA-CB-CG	6.48	120.28	113.80
20	T	145	DC	O5'-C5'-C4'	6.44	120.46	110.80
13	M	967	ASN	OD1-CG-ND2	-6.28	116.32	122.60
13	M	562	PHE	CB-CA-C	6.25	118.55	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1129	GLU	CB-CA-C	-6.24	100.24	110.85
13	M	1052	VAL	N-CA-C	6.24	119.78	111.17
2	B	443	GLY	N-CA-C	-6.18	105.01	112.49
13	M	906	TYR	N-CA-C	6.18	118.61	110.08
20	T	149	DC	C5'-C4'-C3'	-6.14	105.68	114.90
26	Z	358	PHE	N-CA-CB	-6.14	100.92	110.57
1	A	480	SER	N-CA-C	6.11	123.82	110.80
13	M	694	TYR	N-CA-CB	-6.11	101.91	111.56
1	A	1206	ARG	NE-CZ-NH2	6.09	124.68	119.20
31	j	956	GLU	N-CA-C	6.06	118.68	111.71
1	A	479	TRP	N-CA-C	6.06	119.92	111.74
21	U	403	MET	CA-C-N	6.06	129.73	120.82
21	U	403	MET	C-N-CA	6.06	129.73	120.82
26	Z	276	LYS	N-CA-C	5.96	121.85	113.56
20	T	182	DA	C3'-C2'-C1'	-5.94	92.70	101.60
7	G	166	ASP	N-CA-C	5.91	123.39	110.80
13	M	1036	LYS	N-CA-CB	-5.91	101.99	110.44
15	O	2013	LEU	N-CA-C	5.91	118.48	111.33
26	Z	417	GLU	CA-C-N	5.86	133.63	121.32
26	Z	417	GLU	C-N-CA	5.86	133.63	121.32
14	N	3	DT	C3'-C2'-C1'	-5.85	92.83	101.60
13	M	538	LYS	CA-CB-CG	-5.83	102.44	114.10
15	O	2014	ASP	N-CA-C	5.80	117.69	111.36
31	j	500	GLN	CA-C-N	5.73	131.84	121.06
31	j	500	GLN	C-N-CA	5.73	131.84	121.06
13	M	1251	LYS	CA-CB-CG	-5.68	102.74	114.10
13	M	1034	PHE	N-CA-C	5.67	120.19	113.16
7	G	165	ASP	CA-C-N	5.62	132.28	121.54
7	G	165	ASP	C-N-CA	5.62	132.28	121.54
13	M	546	PHE	CA-CB-CG	-5.60	108.20	113.80
31	j	586	ILE	CA-C-N	5.59	128.83	120.83
31	j	586	ILE	C-N-CA	5.59	128.83	120.83
13	M	1038	ASP	N-CA-CB	5.59	120.01	110.50
13	M	595	GLN	OE1-CD-NE2	-5.54	117.06	122.60
28	f	96	ARG	CA-C-N	5.50	129.50	121.31
28	f	96	ARG	C-N-CA	5.50	129.50	121.31
14	N	17	DC	N1-C1'-C2'	-5.46	105.32	113.50
13	M	1056	SER	N-CA-C	5.45	117.47	109.24
14	N	53	DC	C5'-C4'-C3'	-5.44	106.74	114.90
4	D	55	GLN	N-CA-C	-5.42	100.20	109.24
16	P	-2	G	C4'-C3'-C2'	-5.41	97.19	102.60
13	M	1036	LYS	CA-C-O	-5.41	115.72	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	j	501	GLN	N-CA-C	5.40	117.06	110.41
2	B	212	ASP	CA-C-N	5.34	132.02	122.09
2	B	212	ASP	C-N-CA	5.34	132.02	122.09
15	O	1793	ASN	OD1-CG-ND2	-5.33	117.27	122.60
2	B	227	ASN	N-CA-C	-5.33	105.58	111.71
26	Z	257	ILE	CA-C-N	5.32	132.01	122.38
26	Z	257	ILE	C-N-CA	5.32	132.01	122.38
26	Z	280	ARG	N-CA-CB	-5.30	101.61	110.83
2	B	686	GLU	N-CA-C	-5.29	105.03	112.12
15	O	1731	ASP	CA-C-N	5.28	127.36	120.28
15	O	1731	ASP	C-N-CA	5.28	127.36	120.28
28	f	97	THR	N-CA-C	5.27	117.73	110.35
13	M	1014	ARG	NE-CZ-NH2	5.25	123.93	119.20
14	N	57	DC	N1-C1'-C2'	-5.24	105.63	113.50
26	Z	336	PRO	N-CA-C	5.24	118.83	111.33
1	A	160	MET	N-CA-C	5.23	117.28	109.59
13	M	689	ILE	N-CA-C	5.23	116.70	111.00
18	R	506	PRO	N-CA-C	5.22	117.07	110.70
1	A	364	ARG	NE-CZ-NH2	5.21	123.89	119.20
26	Z	358	PHE	N-CA-C	-5.20	100.71	109.07
21	U	404	LEU	N-CA-C	5.19	116.99	110.24
2	B	213	SER	N-CA-C	-5.19	100.25	108.14
2	B	761	THR	N-CA-C	-5.18	102.81	110.48
20	T	182	DA	C4-N9-C1'	-5.17	119.30	127.05
1	A	461	GLN	N-CA-C	5.16	120.62	113.45
14	N	3	DT	C1'-O4'-C4'	-5.16	101.97	109.70
20	T	183	DC	O4'-C4'-C3'	5.15	113.13	105.40
26	Z	395	LYS	CB-CA-C	-5.11	103.03	110.95
13	M	1095	ASN	CA-C-N	5.08	124.57	119.19
13	M	1095	ASN	C-N-CA	5.08	124.57	119.19
32	k	270	TYR	N-CA-C	5.04	116.63	108.41
13	M	542	THR	N-CA-C	-5.04	103.12	110.08
26	Z	395	LYS	N-CA-C	5.03	116.61	111.03
13	M	1014	ARG	CA-CB-CG	-5.01	104.08	114.10
26	Z	359	LEU	N-CA-C	5.00	117.28	109.52
26	Z	163	ASP	N-CA-C	5.00	117.84	111.69

There are no chirality outliers.

All (86) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1052	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1196	TYR	Sidechain
1	A	244	ARG	Sidechain
1	A	327	ARG	Sidechain
1	A	349	ARG	Sidechain
1	A	408	ARG	Sidechain
1	A	583	ARG	Sidechain
2	B	101	ARG	Sidechain
2	B	1131	ARG	Sidechain
2	B	1170	ARG	Sidechain
2	B	242	ARG	Sidechain
2	B	335	ARG	Sidechain
2	B	41	ARG	Sidechain
2	B	859	ARG	Sidechain
2	B	890	ARG	Sidechain
4	D	121	ARG	Sidechain
6	F	100	ARG	Sidechain
7	G	151	ARG	Sidechain
7	G	78	ARG	Sidechain
9	I	103	ARG	Sidechain
10	J	6	ARG	Sidechain
12	L	31	ARG	Sidechain
12	L	42	ARG	Sidechain
13	M	1014	ARG	Sidechain
13	M	1063	TYR	Sidechain
13	M	1134	TYR	Sidechain
13	M	1138	ARG	Sidechain
13	M	1266	ARG	Sidechain
13	M	297	ARG	Sidechain
13	M	450	ARG	Sidechain
13	M	551	ARG	Sidechain
13	M	589	ARG	Sidechain
13	M	693	TYR	Sidechain
13	M	694	TYR	Sidechain
13	M	715	ARG	Sidechain
13	M	810	ARG	Sidechain
13	M	904	ARG	Sidechain
13	M	911	ARG	Sidechain
13	M	995	ARG	Sidechain
14	N	2	DG	Sidechain
14	N	3	DT	Sidechain
14	N	4	DC	Sidechain
14	N	5	DT	Sidechain

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Mol	Chain	Res	Type	Group
14	N	52	DA	Sidechain
14	N	53	DC	Sidechain
14	N	54	DG	Sidechain
14	N	57	DC	Sidechain
14	N	6	DT	Sidechain
16	P	-10	G	Sidechain
16	P	-8	U	Sidechain
16	P	-9	U	Sidechain
17	Q	98	ARG	Sidechain
18	R	11	ARG	Sidechain
18	R	503	ARG	Sidechain
20	T	135	DC	Sidechain
20	T	136	DG	Sidechain
20	T	148	DT	Sidechain
20	T	150	DG	Sidechain
20	T	155	DA	Sidechain
20	T	159	DG	Sidechain
20	T	170	DA	Sidechain
20	T	171	DA	Sidechain
20	T	182	DA	Sidechain
20	T	183	DC	Sidechain
21	U	492	ARG	Sidechain
24	X	229	ARG	Sidechain
24	X	232	ARG	Sidechain
25	Y	111	ARG	Sidechain
25	Y	46	ARG	Sidechain
26	Z	315	ARG	Sidechain
26	Z	366	TYR	Sidechain
26	Z	416	ARG	Sidechain
26	Z	516	ARG	Sidechain
26	Z	571	ARG	Sidechain
26	Z	582	ARG	Sidechain
27	a	64	ARG	Sidechain
29	g	18	ARG	Sidechain
29	g	78	ARG	Sidechain
30	h	34	ARG	Sidechain
30	h	93	ARG	Sidechain
31	j	657	ARG	Sidechain
31	j	734	ARG	Sidechain
31	j	773	ARG	Sidechain
31	j	812	ARG	Sidechain
32	k	270	TYR	Sidechain

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Mol	Chain	Res	Type	Group
32	k	345	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	11455	0	11554	347	0
2	B	9088	0	9112	307	0
3	C	2072	0	2020	49	0
4	D	1014	0	988	45	0
5	E	1721	0	1737	46	0
6	F	627	0	657	18	0
7	G	1343	0	1340	50	0
8	H	1198	0	1156	29	0
9	I	950	0	879	33	0
10	J	524	0	540	21	0
11	K	920	0	942	25	0
12	L	398	0	401	13	0
13	M	7001	0	6979	248	0
14	N	1130	0	619	60	0
15	O	1228	0	1260	11	0
16	P	436	0	222	33	0
17	Q	7240	0	7186	67	0
18	R	1694	0	1626	23	0
19	S	795	0	798	29	0
20	T	1369	0	740	84	0
21	U	1469	0	1441	37	0
22	V	2310	0	2247	29	0
23	W	2374	0	2290	46	0
24	X	434	0	444	4	0
25	Y	912	0	904	30	0
26	Z	3976	0	4048	160	0
27	a	789	0	827	35	0
27	e	615	0	646	24	0
28	b	638	0	676	23	0
28	f	627	0	663	28	0
29	g	710	0	750	21	0
30	h	734	0	756	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	j	4050	0	3970	134	0
32	k	3446	0	3418	87	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	C	1	0	0	0	0
33	I	2	0	0	0	0
33	J	1	0	0	0	0
33	L	1	0	0	0	0
33	Y	1	0	0	0	0
34	A	1	0	0	0	0
All	All	75297	0	73836	1853	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1853) 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)
14:N:-6:DT:OP1	27:a:64:ARG:HD2	1.25	1.25
20:T:173:DA:OP1	28:f:45:LYS:NZ	1.68	1.25
14:N:1:DT:OP1	31:j:582:ASN:ND2	1.69	1.24
1:A:1251:ASN:CB	19:S:228:MET:HG3	1.67	1.23
20:T:173:DA:P	28:f:45:LYS:NZ	2.12	1.22
20:T:173:DA:C5'	28:f:45:LYS:HZ2	1.58	1.14
1:A:1417:HIS:CE1	14:N:44:DC:H5'	1.66	1.13
20:T:173:DA:H3'	27:e:118:VAL:CG1	1.72	1.10
16:P:-1:A:N6	20:T:148:DT:O4	1.83	1.10
20:T:139:DC:H2''	20:T:140:DT:H71	1.23	1.10
13:M:1229:LYS:NZ	16:P:-20:C:OP2	1.84	1.10
20:T:173:DA:C5'	28:f:45:LYS:NZ	2.15	1.10
20:T:173:DA:P	28:f:45:LYS:HZ2	1.69	1.09
16:P:-1:A:N1	20:T:148:DT:N3	2.04	1.06
14:N:-6:DT:OP1	27:a:64:ARG:CD	2.05	1.05
1:A:1417:HIS:NE2	14:N:43:DA:H4'	1.74	1.02
1:A:1417:HIS:CD2	14:N:43:DA:H4'	1.95	1.00
13:M:1231:ARG:HH12	16:P:-19:C:H3'	1.23	1.00
20:T:192:DA:OP1	28:b:24:ARG:HD2	1.59	1.00
1:A:1251:ASN:HB3	19:S:228:MET:HG3	1.39	1.00
16:P:-1:A:N1	20:T:148:DT:C4	2.30	0.99
16:P:-1:A:N1	20:T:148:DT:O4	1.95	0.97
20:T:141:DG:C2'	20:T:142:DT:H72	1.94	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:-1:A:C6	20:T:148:DT:O4	2.18	0.97
20:T:141:DG:H2'	20:T:142:DT:H72	1.44	0.97
1:A:1251:ASN:HB2	19:S:228:MET:CG	1.98	0.93
14:N:48:DG:N3	20:T:138:DG:N2	2.17	0.93
20:T:173:DA:H5'	28:f:45:LYS:NZ	1.84	0.92
1:A:1251:ASN:ND2	19:S:228:MET:HE3	1.83	0.92
1:A:1251:ASN:HD22	19:S:228:MET:CE	1.81	0.92
1:A:1251:ASN:CB	19:S:228:MET:CG	2.47	0.91
31:j:656:ASN:OD1	31:j:657:ARG:NH2	2.03	0.91
20:T:173:DA:H3'	27:e:118:VAL:HG11	1.54	0.89
20:T:193:DG:O5'	27:a:66:LEU:HD23	1.74	0.88
20:T:139:DC:H2''	20:T:140:DT:C7	2.03	0.87
20:T:192:DA:OP1	28:b:24:ARG:CD	2.23	0.87
4:D:76:ASN:OD1	4:D:78:GLU:N	2.08	0.87
1:A:1251:ASN:ND2	19:S:228:MET:SD	2.47	0.87
20:T:139:DC:C2'	20:T:140:DT:H71	2.03	0.87
20:T:173:DA:H5''	28:f:45:LYS:HZ2	1.40	0.86
1:A:1421:ARG:HH12	14:N:44:DC:H5''	1.40	0.86
20:T:184:DC:OP2	28:b:36:ARG:NH2	2.09	0.85
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.10	0.84
20:T:141:DG:C2'	20:T:142:DT:C7	2.57	0.83
20:T:184:DC:OP2	28:b:52:TYR:OH	1.97	0.83
26:Z:366:TYR:CD1	26:Z:366:TYR:C	2.57	0.82
13:M:1094:GLU:OE2	31:j:657:ARG:NE	2.11	0.82
20:T:173:DA:H5''	28:f:45:LYS:HD3	1.60	0.82
20:T:173:DA:H5'	28:f:45:LYS:HZ3	1.41	0.81
1:A:1417:HIS:CD2	14:N:43:DA:C4'	2.61	0.81
1:A:355:MET:HE3	1:A:1431:SER:OG	1.81	0.81
32:k:63:LYS:HE2	32:k:65:LEU:HD11	1.61	0.81
1:A:1251:ASN:HD22	19:S:228:MET:CG	1.94	0.80
26:Z:358:PHE:CD1	26:Z:366:TYR:OH	2.34	0.80
1:A:1251:ASN:ND2	19:S:197:ASN:CG	2.40	0.80
2:B:783:ALA:O	2:B:789:ASN:ND2	2.13	0.80
13:M:889:LEU:HD11	13:M:930:VAL:HG11	1.64	0.80
14:N:58:DG:C2	20:T:128:DG:C2	2.69	0.79
27:a:127:LEU:HD22	27:e:114:HIS:CG	2.16	0.79
13:M:308:ALA:CB	13:M:313:LEU:HD13	2.12	0.79
20:T:184:DC:H3'	28:b:40:ARG:NH1	1.97	0.79
1:A:1417:HIS:HE1	14:N:44:DC:H5'	1.42	0.79
13:M:385:GLU:OE1	13:M:1121:ILE:CD1	2.30	0.79
1:A:99:PHE:O	1:A:103:THR:HG23	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:173:DA:P	28:f:45:LYS:HZ1	1.92	0.78
20:T:174:DC:OP2	27:e:118:VAL:HG13	1.83	0.78
16:P:-1:A:C2	20:T:148:DT:N3	2.48	0.77
20:T:141:DG:H2''	20:T:142:DT:C7	2.15	0.77
14:N:48:DG:C2	20:T:138:DG:C2	2.73	0.77
1:A:1251:ASN:HD22	19:S:228:MET:HE3	1.44	0.77
2:B:666:ASP:OD1	2:B:667:THR:N	2.17	0.77
1:A:1251:ASN:HB2	19:S:228:MET:SD	2.24	0.76
13:M:469:LEU:HB2	13:M:598:ARG:HG3	1.67	0.76
23:W:86:ALA:HB3	23:W:105:GLY:O	1.86	0.76
1:A:1251:ASN:ND2	19:S:228:MET:CE	2.45	0.76
26:Z:285:ILE:HG21	26:Z:335:PRO:HG2	1.64	0.76
13:M:1231:ARG:NH1	16:P:-19:C:H3'	2.01	0.75
20:T:173:DA:H5''	28:f:45:LYS:NZ	2.00	0.75
27:a:54:ARG:NH1	31:j:935:GLU:OE1	2.18	0.75
30:h:122:TYR:CG	30:h:122:TYR:O	2.38	0.75
14:N:-6:DT:P	27:a:64:ARG:HD2	2.27	0.75
26:Z:705:LEU:HD11	26:Z:727:ALA:HB2	1.69	0.74
1:A:360:ASP:OD1	2:B:1062:ARG:NE	2.12	0.74
20:T:184:DC:P	28:b:36:ARG:NH2	2.61	0.73
13:M:455:GLN:N	13:M:459:GLU:OE2	2.22	0.73
14:N:58:DG:N3	20:T:128:DG:N2	2.37	0.73
13:M:1094:GLU:CD	31:j:657:ARG:HH11	1.97	0.72
13:M:1018:VAL:HG13	13:M:1028:PHE:CD1	2.25	0.72
31:j:856:ASP:OD1	31:j:857:MET:N	2.23	0.72
13:M:469:LEU:HD13	13:M:594:LEU:HD12	1.69	0.72
2:B:593:GLN:NE2	21:U:467:ASP:OD2	2.22	0.72
1:A:42:LYS:O	1:A:288:ASN:ND2	2.22	0.72
20:T:173:DA:H3'	27:e:118:VAL:HG13	1.69	0.72
2:B:207:VAL:HG13	2:B:372:LEU:HD12	1.71	0.72
10:J:2:ILE:HD12	10:J:56:ILE:HD13	1.72	0.71
20:T:179:DG:H21	32:k:211:ARG:NH1	1.88	0.71
13:M:319:TRP:O	13:M:323:ASN:ND2	2.24	0.71
13:M:700:HIS:HA	13:M:703:GLN:HG2	1.74	0.70
2:B:274:ARG:NH2	2:B:279:VAL:O	2.21	0.69
16:P:-16:U:H5	26:Z:583:PHE:CE1	2.10	0.69
20:T:172:DC:O3'	28:f:45:LYS:NZ	2.26	0.69
13:M:610:PHE:CE1	13:M:671:ILE:HD11	2.28	0.69
1:A:106:VAL:CG2	1:A:238:MET:HE1	2.23	0.69
1:A:699:TYR:O	1:A:703:GLN:NE2	2.24	0.69
16:P:-16:U:C5	26:Z:583:PHE:CE1	2.81	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:173:DA:H5''	28:f:45:LYS:CD	2.23	0.69
13:M:1094:GLU:OE2	31:j:657:ARG:NH1	2.25	0.69
1:A:140:ARG:O	1:A:144:VAL:HG13	1.94	0.68
13:M:297:ARG:NE	13:M:372:GLU:OE2	2.27	0.68
1:A:1417:HIS:CE1	14:N:44:DC:C5'	2.53	0.68
2:B:953:ASP:OD1	3:C:36:ARG:NH1	2.26	0.68
1:A:464:LEU:HD11	1:A:1100:THR:HG21	1.74	0.68
1:A:83:GLY:HA3	1:A:257:PRO:HB2	1.75	0.68
13:M:889:LEU:HD11	13:M:930:VAL:CG1	2.24	0.68
26:Z:540:VAL:HB	26:Z:575:VAL:CG2	2.24	0.67
1:A:1417:HIS:NE2	14:N:43:DA:C4'	2.53	0.67
14:N:-5:DG:H2''	14:N:-4:DC:C5	2.29	0.67
14:N:11:DG:H2''	14:N:12:DT:H72	1.76	0.67
15:O:1742:MET:HE3	15:O:1782:TRP:CH2	2.29	0.67
1:A:565:MET:HE3	11:K:60:GLY:C	2.19	0.67
1:A:1419:VAL:HG23	1:A:1432:PHE:CE1	2.29	0.67
5:E:56:THR:HG23	5:E:78:GLU:HG3	1.77	0.67
17:Q:419:ALA:HB2	17:Q:433:ALA:HB3	1.76	0.67
2:B:861:SER:HA	2:B:901:THR:HA	1.77	0.67
14:N:-5:DG:C2	20:T:189:DA:C2	2.82	0.67
1:A:1454:VAL:HG12	1:A:1458:ILE:HD12	1.77	0.67
4:D:42:GLU:HG2	4:D:65:LEU:HD11	1.77	0.67
1:A:565:MET:HE1	11:K:58:PHE:HE1	1.60	0.67
2:B:455:ASP:OD1	2:B:455:ASP:N	2.28	0.67
26:Z:232:GLN:O	26:Z:235:VAL:HG22	1.95	0.67
1:A:886:VAL:HG12	5:E:169:GLN:O	1.95	0.66
1:A:1022:ILE:HG21	1:A:1037:ALA:HB1	1.77	0.66
14:N:48:DG:C2	20:T:138:DG:N2	2.62	0.66
1:A:115:SER:HB2	1:A:227:ARG:HB2	1.76	0.66
1:A:228:ILE:O	1:A:244:ARG:NH1	2.28	0.66
14:N:58:DG:C2	20:T:128:DG:N2	2.64	0.66
20:T:183:DC:P	28:b:49:GLY:H	2.19	0.66
1:A:1429:LYS:HA	1:A:1432:PHE:CE2	2.32	0.65
26:Z:215:VAL:CG1	26:Z:225:ILE:HD12	2.27	0.65
2:B:285:LEU:O	2:B:289:ILE:N	2.29	0.65
2:B:1031:GLY:O	3:C:36:ARG:NE	2.29	0.65
16:P:-16:U:C5	26:Z:583:PHE:HE1	2.14	0.65
26:Z:291:ALA:HB3	26:Z:305:LEU:HG	1.79	0.65
2:B:1151:MET:HE1	2:B:1159:PHE:CD2	2.31	0.65
7:G:131:MET:O	13:M:412:ASN:ND2	2.29	0.65
32:k:363:HIS:CD2	32:k:364:LYS:H	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:HIS:CG	2:B:677:MET:HE2	2.32	0.65
2:B:157:ARG:NH1	2:B:177:CYS:O	2.28	0.65
13:M:1094:GLU:HG2	31:j:657:ARG:NH1	2.11	0.65
1:A:110:VAL:HG11	1:A:228:ILE:CD1	2.27	0.64
4:D:107:THR:HG23	4:D:110:GLU:CB	2.26	0.64
4:D:107:THR:HG23	4:D:110:GLU:HB3	1.79	0.64
20:T:184:DC:H3'	28:b:40:ARG:HH12	1.61	0.64
1:A:115:SER:CB	1:A:227:ARG:HB2	2.28	0.64
14:N:58:DG:C4	20:T:128:DG:N2	2.66	0.64
13:M:669:ILE:HG21	13:M:729:LEU:HD23	1.80	0.64
13:M:986:ILE:HD12	13:M:997:GLY:C	2.23	0.64
31:j:825:VAL:HG12	31:j:834:VAL:HA	1.79	0.64
2:B:470:LEU:HD11	2:B:478:THR:HG23	1.79	0.64
2:B:832:PRO:HB2	2:B:840:MET:SD	2.38	0.64
13:M:746:SER:OG	13:M:961:GLU:OE2	2.16	0.63
27:a:63:ILE:O	27:a:94:GLN:NE2	2.31	0.63
2:B:677:MET:H	2:B:682:LEU:CD1	2.11	0.63
1:A:244:ARG:HB3	1:A:247:TRP:CE2	2.33	0.63
1:A:413:TYR:OH	1:A:450:MET:O	2.12	0.63
13:M:469:LEU:CD1	13:M:594:LEU:HD12	2.28	0.63
1:A:106:VAL:HG22	1:A:238:MET:HE1	1.79	0.63
12:L:19:CYS:SG	12:L:20:GLY:N	2.71	0.63
1:A:18:ILE:HD12	2:B:1171:MET:HB3	1.80	0.62
1:A:1251:ASN:CG	19:S:228:MET:HG3	2.24	0.62
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.80	0.62
13:M:1229:LYS:HZ2	16:P:-20:C:P	2.18	0.62
13:M:606:LEU:HD23	13:M:721:LEU:HB3	1.80	0.62
13:M:852:GLY:HA2	13:M:884:LEU:HD11	1.81	0.62
26:Z:291:ALA:CB	26:Z:305:LEU:HG	2.29	0.62
6:F:100:ARG:NH1	6:F:121:ASP:O	2.32	0.62
13:M:1246:SER:C	13:M:1282:ARG:HG3	2.25	0.62
31:j:661:LYS:NZ	31:j:681:GLU:OE2	2.30	0.62
27:e:130:ARG:NH1	31:j:873:ALA:O	2.32	0.62
2:B:77:GLU:C	26:Z:202:ALA:HB1	2.26	0.61
13:M:986:ILE:HD13	13:M:1001:LEU:HD12	1.80	0.61
20:T:173:DA:C3'	27:e:118:VAL:CG1	2.65	0.61
20:T:183:DC:H2''	20:T:184:DC:C6	2.35	0.61
2:B:408:PHE:HA	2:B:440:ILE:HD11	1.81	0.61
25:Y:45:ASN:O	25:Y:49:VAL:HG23	2.00	0.61
2:B:270:ILE:HG23	2:B:284:ILE:HD13	1.82	0.61
8:H:10:PHE:HB2	8:H:56:PHE:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:292:THR:HG23	13:M:299:GLN:HE21	1.65	0.61
2:B:216:ALA:HB2	2:B:241:ALA:HA	1.82	0.61
13:M:986:ILE:HD13	13:M:1001:LEU:CD1	2.31	0.61
16:P:-1:A:H2	20:T:148:DT:H3	1.43	0.61
13:M:385:GLU:OE1	13:M:1121:ILE:HD13	1.99	0.61
18:R:387:VAL:HG13	18:R:405:ILE:HD11	1.81	0.61
20:T:184:DC:P	28:b:52:TYR:OH	2.58	0.61
4:D:29:ALA:HB1	7:G:3:TYR:CD2	2.36	0.61
13:M:624:GLY:HA2	13:M:627:ASP:OD1	2.00	0.61
5:E:55:ARG:NE	5:E:77:PRO:O	2.34	0.61
25:Y:94:PRO:HD2	25:Y:97:ILE:HD11	1.82	0.61
5:E:56:THR:HG23	5:E:78:GLU:CG	2.31	0.61
2:B:412:LEU:O	2:B:415:VAL:HG22	2.02	0.60
26:Z:356:GLY:HA2	31:j:772:MET:HE2	1.82	0.60
2:B:1119:CYS:HA	2:B:1146:ILE:HD13	1.83	0.60
2:B:651:TYR:HD1	21:U:460:TYR:CG	2.19	0.60
19:S:194:ARG:NH2	19:S:226:GLU:OE1	2.35	0.60
14:N:2:DG:C4'	28:b:46:ARG:HH11	2.14	0.60
1:A:1251:ASN:ND2	19:S:228:MET:CG	2.62	0.60
5:E:60:VAL:O	5:E:74:VAL:N	2.34	0.60
13:M:308:ALA:HB2	13:M:313:LEU:HD13	1.82	0.60
14:N:11:DG:H2''	14:N:12:DT:C7	2.31	0.60
27:e:106:GLU:OE1	32:k:384:THR:N	2.35	0.60
9:I:17:CYS:O	9:I:21:ASN:N	2.33	0.60
13:M:851:ALA:HB2	13:M:916:LEU:CD1	2.32	0.60
13:M:1173:GLY:O	13:M:1229:LYS:N	2.33	0.60
23:W:172:ILE:HD13	23:W:207:THR:HG21	1.82	0.59
2:B:418:TYR:CD1	2:B:434:ALA:HB2	2.37	0.59
7:G:18:PHE:CE1	7:G:66:VAL:HG12	2.38	0.59
8:H:7:GLU:OE2	8:H:57:ARG:NH1	2.31	0.59
13:M:552:ASP:OD2	13:M:556:ARG:NE	2.31	0.59
14:N:48:DG:N2	20:T:138:DG:N3	2.51	0.59
1:A:809:HIS:CD2	2:B:677:MET:HE2	2.38	0.59
2:B:507:GLY:HA2	2:B:703:ILE:HG22	1.84	0.59
13:M:467:PHE:HE1	13:M:475:ILE:HD11	1.66	0.59
17:Q:674:ARG:HH21	17:Q:674:ARG:HG2	1.68	0.59
1:A:21:VAL:HG22	1:A:1449:ASP:HB3	1.84	0.59
20:T:173:DA:OP1	28:f:45:LYS:CE	2.51	0.59
1:A:1251:ASN:HD21	19:S:197:ASN:CG	2.10	0.59
2:B:388:TYR:H	2:B:504:THR:HG21	1.68	0.59
2:B:465:GLY:HA3	16:P:-5:U:H4'	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:781:ALA:HB2	2:B:963:PRO:HB3	1.83	0.59
7:G:96:GLY:H	7:G:110:ARG:HB2	1.67	0.59
13:M:832:ASP:O	13:M:835:THR:HG22	2.03	0.59
26:Z:310:ARG:NH1	26:Z:337:GLN:OE1	2.36	0.59
7:G:145:LEU:HD12	7:G:145:LEU:C	2.28	0.59
17:Q:135:ALA:HB1	17:Q:152:PHE:CZ	2.38	0.59
1:A:1417:HIS:HE2	14:N:43:DA:H4'	1.64	0.59
9:I:27:LYS:O	9:I:36:LEU:N	2.30	0.59
13:M:1094:GLU:OE2	31:j:657:ARG:CZ	2.50	0.59
3:C:94:CYS:SG	3:C:96:GLU:HB3	2.43	0.58
4:D:96:GLU:OE1	4:D:96:GLU:N	2.36	0.58
1:A:421:ARG:NE	1:A:425:ASP:OD2	2.31	0.58
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.85	0.58
13:M:1094:GLU:CD	31:j:657:ARG:NH1	2.60	0.58
14:N:54:DG:H1'	14:N:55:DT:C6	2.38	0.58
1:A:1420:ASN:OD1	1:A:1432:PHE:CE1	2.56	0.58
2:B:568:PHE:CE2	2:B:573:TRP:HB2	2.38	0.58
26:Z:353:ALA:HB3	26:Z:360:ILE:HB	1.85	0.58
26:Z:479:LYS:HA	26:Z:489:THR:HG22	1.84	0.58
5:E:73:PHE:CE2	5:E:99:ILE:HB	2.39	0.58
9:I:17:CYS:O	9:I:21:ASN:HA	2.02	0.58
13:M:467:PHE:CE1	13:M:475:ILE:HD11	2.38	0.58
1:A:1036:ASN:OD1	5:E:202:ARG:NH2	2.34	0.58
9:I:86:CYS:O	9:I:90:GLY:N	2.35	0.58
20:T:174:DC:OP2	27:e:118:VAL:CG1	2.41	0.58
26:Z:285:ILE:O	26:Z:310:ARG:CZ	2.52	0.58
3:C:149:LEU:HG	10:J:2:ILE:HD11	1.86	0.58
31:j:846:GLU:OE2	31:j:902:TRP:NE1	2.31	0.58
3:C:4:ALA:HB1	11:K:97:GLU:CG	2.34	0.58
13:M:793:PRO:HA	13:M:812:PRO:HA	1.85	0.58
2:B:654:GLN:HB2	21:U:492:ARG:NH1	2.18	0.58
20:T:173:DA:H5''	28:f:45:LYS:CE	2.34	0.58
26:Z:292:GLN:HG2	26:Z:293:VAL:H	1.68	0.58
13:M:294:LEU:O	13:M:299:GLN:NE2	2.35	0.57
13:M:385:GLU:OE1	13:M:1121:ILE:HD11	2.01	0.57
13:M:1062:THR:HB	13:M:1126:ILE:HD11	1.86	0.57
17:Q:152:PHE:CZ	17:Q:168:GLY:HA3	2.37	0.57
17:Q:416:ILE:HG21	22:V:51:TYR:HB2	1.85	0.57
17:Q:860:GLN:OE1	17:Q:864:ARG:NH2	2.35	0.57
26:Z:366:TYR:C	26:Z:366:TYR:HD1	2.09	0.57
13:M:1265:CYS:SG	13:M:1279:LEU:HD13	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:407:GLU:HG3	21:U:520:ILE:HD12	1.86	0.57
1:A:904:GLN:CD	1:A:982:ASN:HA	2.29	0.57
1:A:609:HIS:ND1	1:A:626:THR:OG1	2.33	0.57
2:B:1094:GLN:HB2	2:B:1103:LEU:HD13	1.87	0.57
20:T:183:DC:H5"	28:b:48:SER:HA	1.87	0.57
1:A:413:TYR:O	1:A:449:HIS:ND1	2.37	0.57
2:B:821:LYS:HD3	2:B:871:VAL:HG21	1.87	0.57
2:B:1091:ARG:HG3	2:B:1103:LEU:HD11	1.85	0.57
2:B:1122:CYS:HB2	2:B:1170:ARG:HH11	1.69	0.57
26:Z:366:TYR:O	26:Z:372:LEU:HD23	2.04	0.57
2:B:564:ALA:HB2	2:B:578:LYS:HD3	1.86	0.57
2:B:713:PHE:CZ	2:B:982:ILE:HG22	2.39	0.57
2:B:816:GLU:HG2	2:B:867:ILE:HG21	1.86	0.57
31:j:845:PHE:HB3	31:j:848:VAL:CG2	2.35	0.57
1:A:353:ASN:O	2:B:1073:GLN:NE2	2.33	0.57
7:G:127:CYS:HB3	7:G:138:GLN:HB3	1.87	0.57
14:N:-7:DG:N2	20:T:191:DG:N3	2.52	0.57
26:Z:546:THR:HG22	26:Z:547:VAL:N	2.20	0.57
27:a:70:ARG:HB3	28:b:26:ASN:OD1	2.05	0.57
29:g:74:ASN:HA	31:j:929:GLY:O	2.04	0.57
5:E:24:ARG:HH12	5:E:128:GLU:CD	2.13	0.57
6:F:98:LYS:NZ	6:F:127:ASP:OXT	2.38	0.57
13:M:793:PRO:HG2	13:M:795:PHE:CE2	2.39	0.57
31:j:848:VAL:O	31:j:897:VAL:HG22	2.05	0.57
1:A:863:ARG:NH1	1:A:1129:ASN:OD1	2.38	0.56
2:B:152:ILE:HD11	2:B:404:PHE:CE1	2.40	0.56
3:C:180:ALA:O	10:J:10:CYS:HB2	2.05	0.56
13:M:539:PHE:CG	13:M:592:VAL:HG21	2.40	0.56
26:Z:340:PHE:O	26:Z:370:GLY:HA2	2.05	0.56
13:M:628:VAL:HG21	13:M:664:LEU:HD13	1.86	0.56
27:a:114:HIS:NE2	27:e:111:ALA:HB1	2.20	0.56
31:j:739:GLN:NE2	31:j:827:ALA:O	2.31	0.56
13:M:911:ARG:O	13:M:914:VAL:HG22	2.05	0.56
18:R:402:VAL:HG23	18:R:451:GLU:HG2	1.88	0.56
26:Z:555:ARG:NH2	26:Z:556:GLU:OE2	2.39	0.56
28:f:50:LEU:HG	31:j:716:MET:HG2	1.87	0.56
29:g:89:ARG:NH1	31:j:850:PHE:O	2.38	0.56
31:j:485:LEU:HD23	31:j:485:LEU:C	2.30	0.56
20:T:181:DC:OP1	32:k:213:ARG:N	2.38	0.56
26:Z:540:VAL:HB	26:Z:575:VAL:HG21	1.87	0.56
2:B:103:GLY:O	21:U:526:ARG:HA	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:100:LEU:HD21	4:D:115:ILE:HD13	1.88	0.56
13:M:1258:LYS:HD2	26:Z:669:ILE:HG23	1.88	0.56
14:N:2:DG:H4'	28:b:46:ARG:HH11	1.71	0.56
14:N:50:DG:H2'	14:N:51:DT:C6	2.40	0.56
25:Y:30:TYR:CD1	32:k:426:LYS:HE3	2.41	0.56
32:k:21:GLY:HA3	32:k:32:PHE:CZ	2.41	0.56
32:k:63:LYS:CE	32:k:65:LEU:HD11	2.33	0.56
1:A:154:CYS:SG	1:A:183:GLY:HA3	2.46	0.56
1:A:440:LEU:HD12	1:A:440:LEU:O	2.06	0.56
13:M:1231:ARG:HH12	16:P:-19:C:C3'	2.08	0.56
20:T:183:DC:C2'	20:T:184:DC:C6	2.88	0.56
26:Z:366:TYR:CD1	26:Z:367:SER:N	2.74	0.56
32:k:50:GLU:HB3	32:k:65:LEU:HD13	1.87	0.56
4:D:76:ASN:OD1	4:D:76:ASN:C	2.49	0.56
4:D:47:GLN:O	4:D:51:ALA:HB3	2.05	0.56
26:Z:745:VAL:HG11	26:Z:750:LEU:HD21	1.87	0.56
1:A:695:ASP:OD1	1:A:697:LYS:N	2.34	0.55
2:B:287:HIS:O	2:B:366:GLY:HA3	2.06	0.55
13:M:301:ARG:HD3	13:M:397:TRP:CZ2	2.42	0.55
13:M:311:ASP:OD1	13:M:312:GLU:N	2.37	0.55
25:Y:48:MET:HA	25:Y:48:MET:HE3	1.88	0.55
26:Z:485:PHE:CD2	26:Z:511:LEU:HD21	2.41	0.55
1:A:948:ILE:HG23	1:A:1007:ILE:HD13	1.89	0.55
7:G:14:HIS:CD2	7:G:16:ARG:NE	2.74	0.55
13:M:546:PHE:CE1	13:M:550:LEU:HD21	2.42	0.55
13:M:1274:LYS:HE2	16:P:-21:U:H4'	1.89	0.55
2:B:97:THR:OG1	21:U:523:MET:HG2	2.06	0.55
5:E:55:ARG:NH1	5:E:105:VAL:O	2.40	0.55
14:N:-3:DC:H2'	14:N:-2:DT:H71	1.89	0.55
17:Q:740:LEU:HD12	17:Q:760:VAL:HG21	1.88	0.55
20:T:181:DC:H3'	32:k:213:ARG:HE	1.71	0.55
27:e:94:GLN:HA	27:e:97:SER:OG	2.07	0.55
32:k:137:SER:HB2	32:k:151:HIS:HA	1.88	0.55
1:A:919:LYS:C	1:A:1052:ARG:HD3	2.32	0.55
6:F:56:TYR:O	6:F:108:ARG:NH1	2.40	0.55
13:M:373:VAL:HG13	13:M:393:LEU:CB	2.36	0.55
26:Z:281:LEU:H	26:Z:288:ASP:HA	1.71	0.55
2:B:1142:ASN:ND2	2:B:1144:THR:O	2.40	0.55
5:E:130:PHE:CZ	5:E:181:ARG:HB3	2.42	0.55
14:N:48:DG:C4	20:T:138:DG:N2	2.74	0.55
23:W:208:ALA:HB1	23:W:235:VAL:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:306:LYS:HG2	26:Z:373:PHE:CE2	2.42	0.55
1:A:154:CYS:SG	1:A:183:GLY:CA	2.95	0.55
2:B:515:PRO:O	2:B:520:VAL:HA	2.05	0.55
8:H:128:ASP:C	8:H:128:ASP:OD1	2.49	0.55
13:M:650:ASP:HB2	13:M:740:TYR:CG	2.41	0.55
2:B:288:ILE:HG12	2:B:366:GLY:HA2	1.88	0.55
13:M:375:PHE:CD1	13:M:375:PHE:C	2.84	0.55
18:R:366:ARG:N	18:R:444:ASN:OD1	2.40	0.55
1:A:359:VAL:HG23	1:A:362:SER:OG	2.06	0.55
1:A:385:ALA:HB1	1:A:413:TYR:CE1	2.42	0.55
4:D:123:GLU:OE1	4:D:123:GLU:N	2.40	0.55
8:H:93:TYR:OH	8:H:140:ARG:HD2	2.07	0.55
23:W:164:ALA:HB2	23:W:198:PHE:CZ	2.41	0.55
26:Z:199:LYS:NZ	26:Z:240:GLU:O	2.40	0.55
1:A:487:SER:OG	1:A:673:GLN:NE2	2.40	0.55
1:A:520:MET:HG3	1:A:522:PRO:HD2	1.89	0.55
13:M:310:ASP:HA	13:M:313:LEU:HB3	1.89	0.55
14:N:48:DG:N2	20:T:138:DG:C2	2.74	0.55
19:S:203:ASN:ND2	19:S:205:ASN:OD1	2.40	0.55
31:j:543:PHE:HZ	32:k:150:PHE:CE2	2.25	0.55
21:U:366:ASN:ND2	22:V:280:ASP:OD1	2.35	0.54
1:A:823:VAL:CG1	1:A:831:LEU:HD22	2.37	0.54
1:A:982:ASN:ND2	1:A:985:ARG:HB2	2.21	0.54
5:E:185:ILE:HD13	5:E:191:VAL:HG21	1.88	0.54
1:A:578:ALA:N	1:A:590:GLN:OE1	2.35	0.54
20:T:184:DC:P	28:b:36:ARG:HH22	2.29	0.54
26:Z:291:ALA:CB	26:Z:306:LYS:O	2.55	0.54
1:A:83:GLY:HA3	1:A:257:PRO:CB	2.38	0.54
2:B:211:LYS:C	2:B:213:SER:H	2.15	0.54
7:G:14:HIS:HA	7:G:65:PHE:CD2	2.42	0.54
17:Q:416:ILE:HG21	22:V:51:TYR:CB	2.38	0.54
2:B:583:LEU:O	2:B:587:LEU:HD23	2.06	0.54
13:M:980:PRO:HA	13:M:983:GLN:HG3	1.89	0.54
13:M:1239:PHE:CD1	16:P:-21:U:OP2	2.61	0.54
26:Z:361:PHE:CE2	26:Z:367:SER:HB2	2.42	0.54
27:e:66:LEU:HB3	27:e:67:PRO:HD3	1.88	0.54
1:A:515:ILE:HD11	2:B:1102:PHE:CD1	2.43	0.54
1:A:1440:MET:HG2	2:B:1167:ILE:HD11	1.89	0.54
2:B:84:TYR:C	2:B:85:LEU:HD12	2.33	0.54
2:B:677:MET:H	2:B:682:LEU:HD12	1.72	0.54
2:B:825:GLN:HB3	2:B:871:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:859:ARG:HG2	26:Z:737:HIS:HA	1.89	0.54
2:B:859:ARG:H	26:Z:737:HIS:CE1	2.26	0.54
17:Q:272:LEU:HD22	17:Q:291:LEU:CD2	2.36	0.54
17:Q:416:ILE:HD13	22:V:51:TYR:CD1	2.42	0.54
26:Z:279:VAL:O	26:Z:290:ILE:HG23	2.08	0.54
31:j:858:VAL:HG22	31:j:870:MET:CE	2.37	0.54
1:A:511:THR:HG23	2:B:1102:PHE:HA	1.89	0.54
2:B:274:ARG:NE	2:B:311:ILE:O	2.41	0.54
13:M:1000:LEU:C	13:M:1000:LEU:HD23	2.32	0.54
15:O:1786:LEU:HD21	15:O:1796:LEU:HD23	1.90	0.54
26:Z:336:PRO:HB3	26:Z:338:ARG:HH12	1.73	0.54
27:a:95:GLU:OE1	29:g:105:GLN:N	2.41	0.54
32:k:391:PHE:CE2	32:k:393:ILE:HD11	2.43	0.54
1:A:788:VAL:HG12	1:A:791:GLN:NE2	2.22	0.54
2:B:269:ILE:HD12	2:B:270:ILE:N	2.22	0.54
5:E:121:MET:HE3	5:E:125:TYR:CD1	2.42	0.54
7:G:127:CYS:HB2	7:G:137:ILE:O	2.07	0.54
23:W:112:LEU:HD11	23:W:121:LEU:HD21	1.90	0.54
31:j:529:ILE:HD11	31:j:600:TYR:CD2	2.43	0.54
2:B:93:LEU:O	21:U:520:ILE:HA	2.08	0.54
12:L:24:THR:HG21	12:L:38:GLU:OE2	2.08	0.54
19:S:200:ASP:HB3	19:S:228:MET:HE1	1.90	0.54
27:a:127:LEU:HD22	27:e:114:HIS:CD2	2.43	0.54
31:j:844:HIS:CD2	31:j:846:GLU:HG2	2.42	0.54
13:M:1239:PHE:CG	16:P:-21:U:OP2	2.61	0.54
22:V:251:ASP:OD1	22:V:254:GLY:N	2.41	0.54
26:Z:418:HIS:CD2	26:Z:465:ALA:CB	2.91	0.54
1:A:93:PRO:HA	1:A:250:VAL:O	2.08	0.53
2:B:834:ARG:NH2	16:P:-15:U:O2	2.42	0.53
2:B:1151:MET:HE2	2:B:1155:CYS:C	2.32	0.53
9:I:27:LYS:N	9:I:36:LEU:O	2.31	0.53
1:A:33:ARG:HB3	2:B:1139:GLY:HA2	1.90	0.53
1:A:289:GLN:NE2	1:A:306:ASP:OD2	2.34	0.53
1:A:1415:THR:O	1:A:1419:VAL:HG22	2.08	0.53
4:D:99:CYS:SG	4:D:115:ILE:HG12	2.49	0.53
13:M:527:CYS:CB	13:M:591:MET:SD	2.96	0.53
13:M:1094:GLU:CG	31:j:657:ARG:NH1	2.71	0.53
14:N:1:DT:H2"	14:N:2:DG:C8	2.44	0.53
28:b:49:GLY:HA2	28:b:52:TYR:CE2	2.43	0.53
32:k:239:VAL:HB	32:k:322:VAL:HG11	1.90	0.53
8:H:64:LEU:HD21	8:H:142:TYR:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:64:GLU:HG2	9:I:111:TYR:CZ	2.43	0.53
2:B:1030:ASN:O	2:B:1034:GLY:N	2.39	0.53
3:C:45:ILE:HD13	3:C:167:LYS:HA	1.91	0.53
4:D:127:LEU:O	4:D:131:LEU:HD13	2.07	0.53
10:J:35:LEU:HD11	10:J:50:LEU:HG	1.90	0.53
13:M:917:ALA:O	13:M:920:ILE:HG22	2.07	0.53
2:B:157:ARG:NE	2:B:180:ASP:O	2.41	0.53
31:j:562:GLU:OE1	32:k:233:LYS:NZ	2.33	0.53
32:k:102:LEU:HA	32:k:127:PRO:O	2.09	0.53
1:A:90:LEU:HD21	1:A:253:LEU:HB2	1.90	0.53
1:A:1421:ARG:NH1	14:N:44:DC:H5"	2.17	0.53
2:B:608:ARG:HA	9:I:69:ILE:HD11	1.88	0.53
13:M:301:ARG:CZ	13:M:305:VAL:HG22	2.39	0.53
25:Y:62:ALA:HB1	26:Z:197:MET:SD	2.48	0.53
26:Z:180:TRP:CZ3	26:Z:254:MET:HB2	2.44	0.53
31:j:529:ILE:HD11	31:j:600:TYR:CG	2.43	0.53
31:j:545:ILE:HA	32:k:56:VAL:HA	1.90	0.53
1:A:73:THR:HB	1:A:84:HIS:CD2	2.43	0.53
1:A:1022:ILE:HD11	1:A:1076:PHE:CZ	2.44	0.53
8:H:37:MET:SD	8:H:127:GLY:HA3	2.49	0.53
18:R:390:GLY:H	18:R:441:PHE:HB3	1.74	0.53
1:A:565:MET:HE3	11:K:60:GLY:CA	2.39	0.53
26:Z:273:LEU:HG	26:Z:378:MET:HE3	1.91	0.53
1:A:1251:ASN:ND2	19:S:228:MET:HG3	2.24	0.53
2:B:595:ASP:OD1	2:B:596:ILE:N	2.40	0.53
3:C:190:ASN:ND2	3:C:195:THR:O	2.22	0.53
5:E:192:LYS:HG3	5:E:206:TYR:CE1	2.44	0.53
9:I:101:SER:O	9:I:105:GLU:N	2.25	0.53
13:M:527:CYS:HB2	13:M:591:MET:SD	2.49	0.53
23:W:158:PRO:HG2	23:W:200:PRO:HA	1.89	0.53
1:A:18:ILE:HG21	1:A:21:VAL:HG12	1.90	0.53
1:A:965:VAL:O	1:A:968:VAL:HG22	2.09	0.53
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.90	0.53
17:Q:412:VAL:HG13	17:Q:437:ALA:HB1	1.91	0.53
23:W:47:TRP:CZ3	23:W:56:LEU:HB2	2.44	0.53
29:g:86:LEU:O	29:g:90:ASN:ND2	2.36	0.53
1:A:694:ALA:HB3	1:A:699:TYR:CE1	2.44	0.52
1:A:834:THR:HG23	2:B:677:MET:HE3	1.90	0.52
15:O:1736:LEU:HD21	18:R:38:GLU:HG2	1.91	0.52
26:Z:480:VAL:HG12	26:Z:486:GLU:HA	1.91	0.52
1:A:381:PRO:HG2	1:A:384:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:PRO:CG	1:A:384:ILE:HD12	2.38	0.52
13:M:807:ASP:N	13:M:807:ASP:OD1	2.42	0.52
26:Z:274:LYS:N	26:Z:378:MET:SD	2.82	0.52
1:A:920:PHE:CE1	1:A:1053:ARG:HD2	2.44	0.52
14:N:-6:DT:OP1	27:a:64:ARG:CG	2.58	0.52
26:Z:340:PHE:CE1	26:Z:344:LYS:HG2	2.44	0.52
1:A:62:GLN:CG	1:A:84:HIS:O	2.58	0.52
2:B:403:LEU:HD11	2:B:453:TRP:CZ2	2.44	0.52
4:D:76:ASN:HB3	4:D:79:THR:HG23	1.90	0.52
11:K:93:ASP:OD1	11:K:94:LEU:N	2.43	0.52
14:N:4:DC:H1'	14:N:5:DT:C6	2.45	0.52
20:T:193:DG:P	27:a:66:LEU:HD23	2.49	0.52
27:a:111:ALA:HB1	27:a:127:LEU:HD23	1.90	0.52
1:A:565:MET:HE1	11:K:58:PHE:CE1	2.42	0.52
1:A:1054:MET:SD	1:A:1060:LEU:HD12	2.49	0.52
1:A:1440:MET:CG	2:B:1167:ILE:HD11	2.40	0.52
26:Z:340:PHE:CZ	26:Z:341:ASP:O	2.63	0.52
1:A:31:LEU:HD21	1:A:254:PRO:HB3	1.90	0.52
1:A:833:PRO:HG3	2:B:1002:PHE:CG	2.45	0.52
3:C:34:ILE:HG22	3:C:38:PHE:CZ	2.45	0.52
4:D:91:LYS:CB	4:D:121:ARG:HH11	2.23	0.52
13:M:308:ALA:HB1	13:M:313:LEU:HD13	1.90	0.52
21:U:458:ASP:OD1	22:V:194:TYR:CZ	2.63	0.52
31:j:529:ILE:HD12	31:j:618:LEU:CD2	2.40	0.52
31:j:602:ALA:HB1	31:j:614:PRO:HB2	1.90	0.52
2:B:386:ASP:OD2	2:B:497:LYS:HB3	2.10	0.52
2:B:1040:GLN:NE2	3:C:195:THR:OG1	2.43	0.52
20:T:181:DC:O5'	32:k:213:ARG:HD2	2.10	0.52
1:A:1317:LYS:HD3	1:A:1335:ILE:HD11	1.92	0.52
2:B:939:HIS:CE1	2:B:979:GLY:C	2.88	0.52
7:G:78:ARG:HG3	7:G:80:PHE:CZ	2.44	0.52
17:Q:650:ALA:HB1	24:X:249:ILE:CD1	2.40	0.52
20:T:139:DC:C2'	20:T:140:DT:C7	2.75	0.52
1:A:348:GLY:O	1:A:352:GLY:N	2.42	0.52
1:A:354:LEU:HA	1:A:357:LYS:HE2	1.91	0.52
1:A:355:MET:HE2	1:A:1459:MET:HG2	1.91	0.52
13:M:824:GLU:HG3	13:M:825:GLU:H	1.74	0.52
20:T:183:DC:H2'	20:T:184:DC:C5	2.45	0.52
13:M:757:PRO:HB3	13:M:921:GLN:O	2.10	0.52
26:Z:501:ILE:HD11	26:Z:510:GLU:HB2	1.91	0.52
27:e:74:GLU:OE1	28:f:26:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:j:944:GLU:O	31:j:944:GLU:HG2	2.10	0.52
2:B:333:GLU:H	2:B:333:GLU:CD	2.18	0.51
5:E:11:TRP:CE3	5:E:37:LEU:HB2	2.44	0.51
9:I:50:ASN:C	9:I:52:CYS:H	2.18	0.51
13:M:294:LEU:O	13:M:996:LYS:HE3	2.10	0.51
13:M:373:VAL:HG13	13:M:393:LEU:HB2	1.91	0.51
2:B:52:GLN:CG	2:B:160:TYR:OH	2.59	0.51
2:B:411:LEU:HD22	2:B:440:ILE:HD13	1.91	0.51
2:B:747:LEU:HD11	20:T:153:DA:H5'	1.92	0.51
32:k:246:PRO:HB3	32:k:253:MET:HE1	1.92	0.51
2:B:953:ASP:HA	3:C:36:ARG:NH1	2.25	0.51
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.45	0.51
17:Q:451:PRO:HD3	17:Q:484:GLU:HG3	1.93	0.51
26:Z:305:LEU:O	26:Z:373:PHE:HA	2.11	0.51
26:Z:624:LEU:HB2	26:Z:636:PHE:CE2	2.46	0.51
29:g:103:ILE:H	31:j:851:HIS:HE2	1.57	0.51
5:E:111:THR:HG21	14:N:53:DC:H5''	1.92	0.51
31:j:856:ASP:OD2	31:j:870:MET:HE3	2.11	0.51
1:A:1171:ALA:HA	9:I:59:THR:HG23	1.93	0.51
13:M:758:TYR:CG	13:M:759:ARG:N	2.78	0.51
26:Z:215:VAL:HG11	26:Z:225:ILE:HD12	1.91	0.51
2:B:121:SER:HA	2:B:153:PRO:HA	1.92	0.51
4:D:31:THR:HG22	7:G:1:MET:HE3	1.92	0.51
13:M:1264:HIS:O	13:M:1286:LEU:HD11	2.11	0.51
26:Z:547:VAL:HG21	26:Z:618:PHE:CD1	2.45	0.51
28:b:91:LEU:CD1	28:b:98:LEU:HD22	2.40	0.51
32:k:112:VAL:HG11	32:k:181:PHE:CZ	2.46	0.51
2:B:346:GLU:O	2:B:349:PRO:HD3	2.10	0.51
13:M:845:PRO:O	13:M:880:ILE:HG23	2.10	0.51
20:T:141:DG:H2''	20:T:142:DT:H73	1.90	0.51
1:A:972:THR:HA	1:A:1320:ILE:HG21	1.92	0.51
6:F:98:LYS:HE2	6:F:98:LYS:HA	1.92	0.51
13:M:836:LEU:HD23	13:M:867:ILE:HD13	1.92	0.51
13:M:907:PRO:HD2	13:M:910:LEU:HD12	1.93	0.51
23:W:60:LEU:HD13	23:W:91:TRP:HB3	1.92	0.51
31:j:468:MET:HE3	31:j:473:LYS:HG2	1.93	0.51
32:k:122:ASP:HA	32:k:127:PRO:HA	1.91	0.51
1:A:1422:GLN:O	1:A:1429:LYS:HE2	2.10	0.51
2:B:939:HIS:CD2	2:B:980:HIS:HA	2.46	0.51
4:D:88:LEU:HB3	4:D:97:LEU:CD1	2.41	0.51
13:M:802:GLU:HB3	13:M:979:HIS:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:462:PHE:CG	22:V:46:PRO:HG2	2.46	0.51
23:W:37:THR:HG21	23:W:298:ILE:HD13	1.93	0.51
29:g:74:ASN:CA	31:j:929:GLY:O	2.59	0.51
31:j:712:CYS:HB2	31:j:744:VAL:HG21	1.91	0.51
1:A:71:CYS:O	1:A:75:ALA:N	2.42	0.51
1:A:154:CYS:SG	1:A:184:CYS:N	2.77	0.51
2:B:44:LEU:HD23	2:B:155:MET:HE3	1.94	0.51
2:B:959:GLU:HA	3:C:183:ALA:HA	1.93	0.51
5:E:6:GLU:OE1	5:E:9:ARG:NH1	2.42	0.51
13:M:1250:VAL:HG21	13:M:1256:ARG:HG3	1.92	0.51
31:j:602:ALA:HB1	31:j:614:PRO:CB	2.41	0.51
2:B:25:ALA:O	2:B:29:VAL:HG23	2.11	0.50
2:B:51:ILE:HG21	2:B:160:TYR:CD2	2.46	0.50
13:M:632:HIS:CE1	13:M:633:TYR:CE2	2.99	0.50
23:W:63:HIS:CD2	23:W:67:VAL:HG22	2.46	0.50
26:Z:546:THR:CG2	26:Z:547:VAL:N	2.74	0.50
1:A:205:VAL:HG12	1:A:207:GLU:O	2.11	0.50
1:A:440:LEU:HA	1:A:444:TYR:CD2	2.46	0.50
1:A:962:ASP:HB3	1:A:1043:ILE:HG23	1.94	0.50
1:A:1400:LEU:O	1:A:1404:THR:HG23	2.11	0.50
2:B:1151:MET:HE2	2:B:1156:LYS:N	2.26	0.50
13:M:456:SER:N	13:M:459:GLU:OE2	2.44	0.50
13:M:594:LEU:CD2	13:M:720:PHE:CZ	2.94	0.50
13:M:851:ALA:HB2	13:M:916:LEU:HD13	1.92	0.50
27:a:62:LEU:HD12	28:b:38:LEU:HD23	1.93	0.50
1:A:1163:HIS:HB2	1:A:1301:ILE:O	2.10	0.50
2:B:846:ASP:O	12:L:51:ARG:NH1	2.45	0.50
9:I:17:CYS:O	9:I:21:ASN:CA	2.59	0.50
20:T:133:DT:H2'	20:T:134:DA:C8	2.47	0.50
31:j:947:THR:O	31:j:947:THR:HG22	2.11	0.50
1:A:106:VAL:HG22	1:A:238:MET:CE	2.41	0.50
1:A:286:ILE:HD11	1:A:313:HIS:CE1	2.45	0.50
2:B:22:TRP:CZ2	2:B:679:PRO:HD2	2.46	0.50
13:M:373:VAL:HG12	13:M:390:ILE:HD12	1.94	0.50
31:j:585:ASN:HB3	31:j:590:PRO:CG	2.42	0.50
31:j:845:PHE:HB3	31:j:848:VAL:HG21	1.92	0.50
32:k:34:ASN:O	32:k:38:GLY:N	2.44	0.50
1:A:1139:LEU:HD23	1:A:1359:SER:HA	1.94	0.50
2:B:156:LEU:HD22	2:B:184:TYR:CE2	2.46	0.50
8:H:60:ILE:HD12	8:H:125:LEU:HD22	1.92	0.50
13:M:754:ARG:HD2	13:M:754:ARG:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:783:VAL:HG22	17:Q:824:ALA:HB1	1.94	0.50
26:Z:281:LEU:HD11	26:Z:307:MET:SD	2.52	0.50
26:Z:551:VAL:HG22	26:Z:559:GLN:O	2.11	0.50
1:A:832:THR:HG23	1:A:833:PRO:HD2	1.92	0.50
2:B:269:ILE:HD12	2:B:270:ILE:H	1.77	0.50
3:C:4:ALA:HB1	11:K:97:GLU:HG2	1.93	0.50
13:M:566:PRO:HD2	13:M:704:GLU:HB3	1.94	0.50
13:M:700:HIS:HA	13:M:703:GLN:CG	2.41	0.50
25:Y:63:MET:CE	25:Y:77:VAL:HG23	2.42	0.50
27:a:87:SER:O	27:a:91:MET:HG2	2.12	0.50
1:A:345:GLY:O	1:A:348:GLY:N	2.36	0.50
1:A:350:VAL:HG23	1:A:351:ARG:H	1.76	0.50
2:B:939:HIS:NE2	2:B:980:HIS:HA	2.27	0.50
13:M:395:ARG:O	13:M:398:GLN:HB2	2.11	0.50
26:Z:249:TYR:O	26:Z:252:GLN:NE2	2.41	0.50
31:j:606:LYS:HB2	31:j:613:VAL:HG22	1.93	0.50
1:A:282:ASP:HB3	1:A:313:HIS:CE1	2.47	0.50
5:E:61:LEU:HD11	5:E:71:GLN:HB3	1.94	0.50
26:Z:293:VAL:CG2	26:Z:303:ILE:CG1	2.90	0.50
31:j:555:LYS:HA	31:j:573:TYR:CZ	2.47	0.50
1:A:370:ASP:CG	11:K:65:HIS:HE2	2.20	0.50
2:B:414:GLU:HG3	2:B:439:ILE:HD11	1.93	0.50
13:M:973:VAL:HB	13:M:1011:LEU:HD12	1.94	0.50
16:P:-7:U:H2'	16:P:-6:U:C6	2.47	0.50
25:Y:30:TYR:CE1	32:k:426:LYS:HE3	2.47	0.50
26:Z:459:ASP:N	26:Z:459:ASP:OD1	2.44	0.50
31:j:946:GLU:OE2	31:j:949:ASN:HB2	2.12	0.50
1:A:191:ILE:HA	1:A:199:TYR:O	2.12	0.49
1:A:880:ARG:HA	1:A:885:GLN:O	2.12	0.49
2:B:604:ILE:O	2:B:612:ILE:HA	2.12	0.49
2:B:1119:CYS:HB2	2:B:1137:CYS:HB2	1.94	0.49
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.47	0.49
17:Q:419:ALA:HB2	17:Q:433:ALA:CB	2.42	0.49
31:j:598:ILE:HG23	32:k:160:LEU:HD13	1.93	0.49
13:M:473:ARG:HD2	13:M:525:THR:HG23	1.94	0.49
25:Y:18:LEU:HD23	25:Y:18:LEU:C	2.37	0.49
1:A:125:LYS:O	1:A:129:ILE:HG12	2.12	0.49
1:A:958:ARG:HD2	1:A:1046:ARG:HD2	1.94	0.49
2:B:821:LYS:CD	2:B:871:VAL:HG21	2.42	0.49
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.47	0.49
13:M:618:ILE:HG23	13:M:667:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:35:ARG:HH12	31:j:793:GLU:C	2.19	0.49
26:Z:419:ASN:HB3	26:Z:481:ILE:HD12	1.93	0.49
1:A:106:VAL:HG21	1:A:238:MET:HE1	1.94	0.49
1:A:609:HIS:HA	1:A:626:THR:HG21	1.95	0.49
8:H:136:GLU:HG3	8:H:139:SER:HB3	1.94	0.49
14:N:57:DC:H2'	14:N:58:DG:C8	2.47	0.49
22:V:312:PHE:CZ	22:V:324:ASN:HB3	2.47	0.49
31:j:510:VAL:HG13	32:k:105:LYS:HG2	1.95	0.49
6:F:96:GLU:O	6:F:100:ARG:N	2.45	0.49
13:M:527:CYS:HB3	13:M:532:LEU:HD12	1.94	0.49
2:B:149:ILE:HG22	2:B:150:GLY:N	2.28	0.49
13:M:802:GLU:OE1	13:M:802:GLU:N	2.46	0.49
14:N:4:DC:H3'	27:a:117:ARG:HD3	1.95	0.49
17:Q:163:ILE:HB	17:Q:164:PRO:HD3	1.94	0.49
19:S:231:ASP:O	19:S:232:GLU:HG3	2.12	0.49
1:A:413:TYR:O	1:A:415:GLY:N	2.40	0.49
1:A:909:LEU:C	1:A:911:PRO:HD3	2.38	0.49
2:B:1151:MET:HE1	2:B:1159:PHE:CE2	2.48	0.49
7:G:129:LYS:HE2	13:M:409:ARG:HD3	1.93	0.49
8:H:52:LEU:HD23	8:H:53:GLY:N	2.27	0.49
12:L:29:LYS:HB2	12:L:32:ASP:OD2	2.13	0.49
13:M:758:TYR:CD2	13:M:847:VAL:HG21	2.48	0.49
13:M:807:ASP:OD2	13:M:843:LYS:NZ	2.46	0.49
13:M:824:GLU:CD	16:P:-18:C:H41	2.20	0.49
14:N:-7:DG:C2	20:T:191:DG:C2	3.01	0.49
17:Q:787:GLU:HA	17:Q:821:LEU:HD11	1.93	0.49
23:W:126:HIS:HA	23:W:150:PHE:CD2	2.47	0.49
2:B:728:MET:CE	2:B:940:GLY:HA2	2.43	0.49
2:B:1034:GLY:HA3	3:C:32:ASN:HB2	1.94	0.49
8:H:67:ASP:CG	8:H:69:THR:HG23	2.38	0.49
23:W:172:ILE:CD1	23:W:207:THR:HG21	2.42	0.49
29:g:42:GLU:HB2	30:h:88:SER:HB2	1.95	0.49
1:A:123:ASN:OD1	1:A:125:LYS:HG2	2.12	0.49
2:B:897:ARG:HB2	2:B:900:GLU:HG3	1.95	0.49
3:C:59:LEU:HB2	3:C:64:ILE:HD11	1.95	0.49
3:C:102:THR:O	3:C:121:ILE:HB	2.13	0.49
7:G:10:GLU:HA	7:G:69:PRO:HA	1.93	0.49
13:M:851:ALA:HB2	13:M:916:LEU:HD11	1.94	0.49
15:O:1742:MET:HE3	15:O:1782:TRP:CZ3	2.47	0.49
22:V:51:TYR:CD1	22:V:52:PRO:HD2	2.48	0.49
31:j:482:ALA:HB2	31:j:892:LYS:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:j:618:LEU:HD21	32:k:158:VAL:HG13	1.95	0.49
32:k:11:TYR:CE2	32:k:20:ASP:HB3	2.48	0.49
32:k:382:GLY:HA3	32:k:389:PHE:CA	2.42	0.49
1:A:111:CYS:O	1:A:115:SER:N	2.42	0.49
1:A:542:LEU:O	1:A:545:VAL:HG12	2.13	0.49
1:A:909:LEU:O	1:A:911:PRO:HD3	2.13	0.49
2:B:67:LEU:O	2:B:84:TYR:N	2.46	0.49
2:B:210:LYS:O	2:B:213:SER:OG	2.20	0.49
2:B:646:ARG:HA	2:B:649:ASN:O	2.13	0.49
6:F:108:ARG:O	6:F:115:TYR:HA	2.13	0.49
17:Q:139:LEU:HD13	17:Q:171:CYS:SG	2.52	0.49
26:Z:361:PHE:CD1	26:Z:365:ARG:HB2	2.48	0.49
26:Z:547:VAL:HG21	26:Z:618:PHE:CG	2.48	0.49
27:e:108:THR:HG23	27:e:124:ASP:CB	2.42	0.49
31:j:542:VAL:HG11	32:k:129:PHE:CG	2.48	0.49
31:j:575:PRO:HB2	32:k:166:TYR:CE1	2.47	0.49
2:B:384:ASP:HB3	2:B:387:HIS:HB2	1.94	0.48
2:B:779:ILE:O	2:B:964:ASP:N	2.42	0.48
4:D:38:HIS:CE1	4:D:69:ALA:HB2	2.48	0.48
4:D:63:LYS:HG3	7:G:103:PRO:HA	1.94	0.48
9:I:79:PRO:HB2	9:I:96:PHE:CE1	2.48	0.48
11:K:5:PRO:HB2	11:K:7:PHE:CE2	2.48	0.48
13:M:441:ARG:HD3	13:M:470:TYR:CD1	2.48	0.48
13:M:1012:GLU:H	13:M:1012:GLU:CD	2.20	0.48
15:O:1736:LEU:CD2	18:R:38:GLU:HG2	2.43	0.48
17:Q:523:ILE:O	17:Q:527:HIS:N	2.38	0.48
17:Q:610:VAL:O	17:Q:614:THR:HG23	2.13	0.48
17:Q:863:LYS:HE3	17:Q:863:LYS:HA	1.94	0.48
26:Z:446:ASN:O	26:Z:464:PRO:HA	2.13	0.48
26:Z:476:ASP:HB2	26:Z:492:ILE:HD12	1.95	0.48
27:a:46:THR:O	27:a:50:ARG:HB2	2.13	0.48
1:A:133:SER:OG	1:A:140:ARG:HD3	2.12	0.48
1:A:141:LEU:HD23	1:A:141:LEU:C	2.38	0.48
1:A:561:MET:SD	11:K:58:PHE:HA	2.52	0.48
2:B:209:ALA:HB1	2:B:216:ALA:O	2.12	0.48
2:B:472:ARG:HD2	2:B:736:TYR:CD1	2.48	0.48
4:D:92:LEU:HD23	4:D:100:LEU:HD12	1.94	0.48
14:N:45:DA:C2	14:N:46:DG:C2	3.01	0.48
16:P:-17:C:N4	16:P:-15:U:O4	2.46	0.48
23:W:60:LEU:HD13	23:W:91:TRP:CG	2.48	0.48
31:j:855:PHE:O	31:j:874:ILE:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:LEU:C	1:A:911:PRO:CD	2.86	0.48
1:A:1027:ASP:C	1:A:1027:ASP:OD1	2.56	0.48
1:A:1251:ASN:HD21	19:S:228:MET:HE3	1.74	0.48
2:B:69:ALA:HA	2:B:423:ILE:HD12	1.94	0.48
8:H:15:ILE:O	8:H:16:ASP:C	2.56	0.48
8:H:103:GLU:HG3	8:H:109:ALA:HB2	1.95	0.48
25:Y:46:ARG:HA	25:Y:49:VAL:HB	1.94	0.48
26:Z:181:THR:OG1	26:Z:253:GLN:HB2	2.13	0.48
26:Z:342:ALA:HB2	26:Z:361:PHE:HD2	1.78	0.48
1:A:465:HIS:NE2	1:A:467:MET:HB2	2.28	0.48
2:B:155:MET:HE3	2:B:183:GLY:HA2	1.95	0.48
2:B:193:VAL:HG11	2:B:470:LEU:HD13	1.95	0.48
2:B:534:VAL:O	2:B:618:ALA:HB2	2.13	0.48
9:I:85:PRO:HA	9:I:91:HIS:O	2.14	0.48
10:J:7:CYS:HA	10:J:48:MET:HE2	1.95	0.48
30:h:99:VAL:HG13	30:h:103:LEU:HD12	1.95	0.48
1:A:62:GLN:HG3	1:A:84:HIS:O	2.14	0.48
1:A:481:THR:O	1:A:483:ARG:NH1	2.41	0.48
1:A:511:THR:HG23	2:B:1102:PHE:HB2	1.95	0.48
1:A:766:PHE:HB3	1:A:781:ILE:HG12	1.96	0.48
1:A:955:GLU:HA	1:A:958:ARG:CZ	2.43	0.48
1:A:1162:GLU:O	1:A:1300:GLY:HA3	2.12	0.48
2:B:90:GLN:HA	21:U:516:GLN:OE1	2.14	0.48
2:B:117:ASN:HA	2:B:189:GLY:HA3	1.95	0.48
2:B:957:THR:HG22	2:B:1028:LEU:CD2	2.44	0.48
4:D:33:LEU:CD2	4:D:98:ALA:HA	2.43	0.48
4:D:76:ASN:HB3	4:D:79:THR:CG2	2.43	0.48
8:H:102:ASP:OD1	8:H:110:THR:N	2.47	0.48
11:K:64:PRO:HG3	11:K:72:ILE:HD12	1.96	0.48
13:M:562:PHE:CD2	13:M:563:PRO:HD2	2.48	0.48
13:M:824:GLU:OE1	16:P:-18:C:N4	2.39	0.48
13:M:894:MET:SD	13:M:912:GLN:HG3	2.54	0.48
26:Z:346:ARG:HG2	26:Z:352:VAL:HG22	1.94	0.48
32:k:265:GLN:N	32:k:268:THR:O	2.47	0.48
3:C:33:SER:O	3:C:37:VAL:HG23	2.14	0.48
3:C:72:PRO:HD3	10:J:13:ILE:HG12	1.96	0.48
5:E:34:ASP:C	5:E:34:ASP:OD1	2.56	0.48
13:M:658:LEU:HD11	13:M:948:HIS:CD2	2.48	0.48
13:M:799:VAL:HG13	13:M:804:GLU:O	2.13	0.48
13:M:847:VAL:HA	13:M:881:GLY:O	2.13	0.48
13:M:851:ALA:HB1	13:M:887:ASN:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:934:ASP:OD1	13:M:934:ASP:N	2.45	0.48
26:Z:182:VAL:HG22	26:Z:225:ILE:O	2.14	0.48
26:Z:342:ALA:HB2	26:Z:361:PHE:CD2	2.48	0.48
31:j:858:VAL:HG22	31:j:870:MET:HE1	1.96	0.48
32:k:131:ILE:HG21	32:k:150:PHE:CE1	2.48	0.48
1:A:95:PHE:CE1	1:A:218:PRO:HA	2.49	0.48
1:A:413:TYR:CD1	1:A:413:TYR:C	2.88	0.48
2:B:630:LYS:C	2:B:632:LYS:H	2.21	0.48
7:G:95:VAL:O	7:G:95:VAL:HG13	2.14	0.48
13:M:852:GLY:CA	13:M:884:LEU:HD11	2.43	0.48
14:N:4:DC:H3'	27:a:121:MET:HE1	1.96	0.48
17:Q:754:MET:HE1	17:Q:795:TYR:CD2	2.48	0.48
26:Z:556:GLU:HA	26:Z:572:HIS:CE1	2.49	0.48
30:h:39:SER:HB3	31:j:948:PHE:CZ	2.48	0.48
1:A:23:PHE:O	1:A:1446:GLY:HA2	2.13	0.48
1:A:1429:LYS:HA	1:A:1432:PHE:CZ	2.49	0.48
17:Q:342:LEU:HD11	22:V:70:HIS:CE1	2.48	0.48
18:R:370:GLU:HA	18:R:373:CYS:SG	2.53	0.48
21:U:527:ASP:OD2	21:U:531:GLN:NE2	2.46	0.48
25:Y:75:GLN:NE2	25:Y:87:VAL:HA	2.28	0.48
28:b:41:ARG:C	28:b:43:GLY:H	2.20	0.48
31:j:601:ARG:NH1	32:k:154:ASP:OD1	2.42	0.48
32:k:75:ASP:OD1	32:k:76:GLY:N	2.39	0.48
7:G:97:LEU:N	7:G:108:ILE:O	2.39	0.48
9:I:101:SER:HB3	9:I:104:ALA:HB3	1.94	0.48
13:M:650:ASP:HB2	13:M:740:TYR:CD1	2.49	0.48
17:Q:416:ILE:HG23	17:Q:434:TYR:CE1	2.48	0.48
17:Q:508:GLU:OE2	17:Q:520:TYR:OH	2.28	0.48
26:Z:558:PHE:CE2	26:Z:572:HIS:HA	2.48	0.48
1:A:1030:SER:HB2	5:E:162:ARG:HE	1.78	0.48
7:G:14:HIS:CD2	7:G:16:ARG:H	2.32	0.48
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.49	0.48
13:M:668:ASP:OD1	13:M:668:ASP:N	2.45	0.48
13:M:855:ARG:CD	13:M:1275:PHE:CD2	2.97	0.48
17:Q:716:ASN:O	17:Q:720:VAL:HG23	2.14	0.48
26:Z:293:VAL:HG22	26:Z:303:ILE:HG12	1.96	0.48
1:A:288:ASN:O	1:A:291:ARG:HG2	2.14	0.47
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.96	0.47
13:M:462:ASP:CG	13:M:607:ARG:HH12	2.21	0.47
13:M:827:GLU:HG2	13:M:828:LYS:HG3	1.96	0.47
23:W:86:ALA:HA	23:W:109:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:j:819:PRO:HB3	31:j:885:TRP:CZ2	2.49	0.47
32:k:73:LYS:NZ	32:k:130:GLU:O	2.43	0.47
1:A:1301:ILE:HB	1:A:1304:ILE:HD12	1.96	0.47
5:E:93:ARG:HG3	17:Q:891:PHE:CZ	2.48	0.47
13:M:589:ARG:HD2	13:M:711:MET:HG3	1.95	0.47
1:A:569:THR:HG23	1:A:667:LEU:HB3	1.96	0.47
1:A:1405:MET:HA	1:A:1412:MET:HE3	1.96	0.47
2:B:352:GLY:O	2:B:361:LYS:NZ	2.42	0.47
4:D:132:ASP:O	4:D:136:THR:HG23	2.15	0.47
13:M:1257:VAL:O	13:M:1258:LYS:HE2	2.15	0.47
14:N:-7:DG:N2	20:T:191:DG:C2	2.83	0.47
14:N:11:DG:C2'	14:N:12:DT:H72	2.43	0.47
1:A:350:VAL:HG11	1:A:1430:CYS:SG	2.54	0.47
1:A:1139:LEU:HG	1:A:1341:VAL:HG12	1.96	0.47
2:B:73:HIS:CG	26:Z:199:LYS:HA	2.49	0.47
2:B:433:LEU:HD11	21:U:535:MET:O	2.14	0.47
9:I:117:PRO:C	9:I:119:CYS:H	2.22	0.47
26:Z:361:PHE:CE2	26:Z:367:SER:CB	2.97	0.47
28:f:39:ALA:CB	28:f:47:ILE:HD11	2.45	0.47
31:j:543:PHE:CZ	32:k:150:PHE:CE2	3.02	0.47
31:j:943:ILE:HG22	31:j:944:GLU:OE1	2.15	0.47
1:A:1366:PHE:CD2	1:A:1411:LEU:HD12	2.50	0.47
7:G:9:HIS:O	7:G:70:VAL:N	2.43	0.47
7:G:38:CYS:SG	7:G:39:THR:N	2.87	0.47
11:K:31:CYS:SG	11:K:84:GLN:NE2	2.87	0.47
27:a:50:ARG:CG	31:j:924:PHE:CD1	2.98	0.47
1:A:110:VAL:HG11	1:A:228:ILE:HD11	1.97	0.47
1:A:566:PHE:HB2	1:A:675:VAL:HG22	1.95	0.47
1:A:1482:TYR:N	1:A:1482:TYR:CD1	2.81	0.47
13:M:375:PHE:CD2	13:M:1030:ASN:HA	2.49	0.47
13:M:413:LEU:HD12	13:M:460:LEU:HD11	1.95	0.47
13:M:486:ARG:HB3	13:M:514:GLU:OE2	2.15	0.47
13:M:742:ILE:HD13	13:M:953:GLU:HB3	1.97	0.47
14:N:4:DC:C3'	27:a:121:MET:HE1	2.45	0.47
21:U:378:LEU:CD1	21:U:384:VAL:HG23	2.45	0.47
25:Y:64:MET:HE1	26:Z:215:VAL:CG2	2.44	0.47
32:k:1:MET:CE	32:k:87:ASP:HB3	2.43	0.47
32:k:310:LEU:HD12	32:k:314:VAL:HG23	1.96	0.47
1:A:375:ILE:O	1:A:488:VAL:HG21	2.15	0.47
1:A:464:LEU:CD1	1:A:1100:THR:HG21	2.44	0.47
1:A:1317:LYS:CD	1:A:1335:ILE:HD11	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:PHE:O	2:B:218:THR:N	2.38	0.47
2:B:352:GLY:HA3	2:B:357:CYS:SG	2.54	0.47
2:B:786:THR:HG21	2:B:949:TYR:CE2	2.49	0.47
4:D:79:THR:HA	4:D:82:SER:OG	2.15	0.47
6:F:121:ASP:OD1	6:F:121:ASP:N	2.44	0.47
13:M:303:ILE:HG21	13:M:404:THR:HG21	1.95	0.47
13:M:566:PRO:HD2	13:M:704:GLU:CB	2.45	0.47
13:M:1244:PHE:HA	13:M:1282:ARG:HD2	1.96	0.47
17:Q:415:TRP:CE2	17:Q:436:THR:HG21	2.49	0.47
17:Q:422:LEU:HD22	17:Q:426:ASP:HB3	1.96	0.47
26:Z:292:GLN:O	26:Z:306:LYS:HG3	2.15	0.47
26:Z:479:LYS:CA	26:Z:489:THR:HG22	2.45	0.47
27:a:42:TYR:OH	31:j:918:GLU:OE1	2.26	0.47
32:k:201:ILE:HA	32:k:216:ILE:O	2.15	0.47
32:k:216:ILE:O	32:k:216:ILE:HG22	2.13	0.47
1:A:233:CYS:SG	1:A:240:PRO:HB3	2.55	0.47
1:A:1067:TRP:CE3	1:A:1067:TRP:C	2.93	0.47
1:A:1148:ALA:O	1:A:1334:TRP:N	2.45	0.47
1:A:1251:ASN:ND2	19:S:197:ASN:OD1	2.48	0.47
2:B:238:SER:O	2:B:256:ILE:HG23	2.14	0.47
5:E:20:LEU:HA	5:E:182:TYR:CZ	2.50	0.47
13:M:799:VAL:HG12	13:M:921:GLN:NE2	2.29	0.47
17:Q:174:PHE:CZ	17:Q:210:LYS:HG3	2.50	0.47
20:T:173:DA:C3'	27:e:118:VAL:HG13	2.40	0.47
26:Z:291:ALA:HB2	26:Z:306:LYS:O	2.15	0.47
27:e:108:THR:HG23	27:e:124:ASP:HB3	1.95	0.47
29:g:58:TYR:OH	30:h:110:HIS:HB2	2.14	0.47
1:A:1251:ASN:ND2	19:S:197:ASN:ND2	2.62	0.47
26:Z:281:LEU:N	26:Z:288:ASP:HA	2.29	0.47
27:a:51:GLU:HB3	27:a:55:TYR:CE1	2.49	0.47
30:h:119:VAL:O	30:h:123:THR:OG1	2.26	0.47
31:j:515:PRO:HA	32:k:104:VAL:HG11	1.96	0.47
31:j:705:LYS:HA	31:j:725:LYS:HE3	1.97	0.47
1:A:1053:ARG:HB3	1:A:1058:PHE:CE2	2.50	0.47
1:A:1189:ASP:HA	1:A:1192:TRP:CD1	2.50	0.47
2:B:551:GLU:HB3	2:B:556:ILE:HD13	1.96	0.47
2:B:1091:ARG:CG	2:B:1103:LEU:HD11	2.45	0.47
3:C:4:ALA:HB1	11:K:97:GLU:HG3	1.98	0.47
3:C:22:ILE:HD13	3:C:230:TYR:CE2	2.50	0.47
9:I:23:MET:HE3	9:I:25:TYR:CZ	2.49	0.47
17:Q:590:ARG:HH22	17:Q:594:GLN:HG3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1119:CYS:HB2	2:B:1137:CYS:SG	2.55	0.46
4:D:33:LEU:HD22	4:D:101:ALA:HB3	1.97	0.46
5:E:13:ILE:HG23	5:E:136:LEU:HD23	1.97	0.46
5:E:121:MET:HE3	5:E:125:TYR:CG	2.50	0.46
13:M:1036:LYS:O	13:M:1037:ILE:HG13	2.15	0.46
14:N:54:DG:H2"	14:N:55:DT:H71	1.97	0.46
21:U:411:ARG:NH1	21:U:510:ASP:OD2	2.39	0.46
23:W:242:PRO:HD2	23:W:286:GLY:CA	2.45	0.46
31:j:685:ASN:C	31:j:701:TYR:CD2	2.92	0.46
32:k:12:GLN:O	32:k:19:ASN:N	2.46	0.46
1:A:863:ARG:HH11	1:A:1128:ILE:CG2	2.28	0.46
5:E:148:HIS:CD2	5:E:193:ILE:HG12	2.50	0.46
13:M:784:ILE:HG13	13:M:796:CYS:HB3	1.97	0.46
26:Z:291:ALA:HB3	26:Z:305:LEU:CG	2.44	0.46
31:j:543:PHE:HZ	32:k:150:PHE:CD2	2.34	0.46
31:j:618:LEU:HD21	32:k:158:VAL:CG1	2.45	0.46
31:j:880:ASP:HB3	31:j:881:PRO:HD3	1.97	0.46
32:k:27:ARG:HG2	32:k:92:HIS:CE1	2.50	0.46
32:k:53:TRP:CE3	32:k:97:LEU:HD23	2.49	0.46
13:M:786:PHE:CZ	13:M:853:GLU:HB2	2.51	0.46
13:M:1036:LYS:HG2	13:M:1134:TYR:CD2	2.51	0.46
17:Q:242:GLU:O	17:Q:250:SER:HB3	2.15	0.46
19:S:145:ARG:HB3	19:S:173:GLU:CB	2.46	0.46
23:W:196:LEU:HA	23:W:206:VAL:O	2.16	0.46
27:a:50:ARG:HD2	31:j:924:PHE:CG	2.50	0.46
32:k:222:PHE:CE1	32:k:233:LYS:HD3	2.50	0.46
2:B:752:TYR:CE2	2:B:807:ARG:HD2	2.51	0.46
4:D:76:ASN:O	4:D:79:THR:OG1	2.24	0.46
5:E:73:PHE:HE2	5:E:99:ILE:HB	1.81	0.46
13:M:469:LEU:HD22	13:M:598:ARG:HG2	1.97	0.46
14:N:0:DG:H2"	14:N:1:DT:C6	2.50	0.46
17:Q:585:GLN:NE2	17:Q:589:GLU:OE2	2.40	0.46
18:R:25:LEU:HD13	31:j:801:PHE:CE2	2.51	0.46
27:a:70:ARG:CB	28:b:26:ASN:OD1	2.64	0.46
27:e:82:ASP:N	27:e:82:ASP:OD1	2.47	0.46
31:j:598:ILE:HG23	32:k:160:LEU:CD1	2.46	0.46
1:A:565:MET:HE3	11:K:60:GLY:HA3	1.97	0.46
1:A:733:LEU:O	1:A:736:THR:HG22	2.15	0.46
1:A:1141:VAL:HG13	1:A:1352:VAL:HG13	1.98	0.46
2:B:581:GLU:O	2:B:585:ASN:ND2	2.48	0.46
2:B:760:THR:HB	2:B:764:MET:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:94:MET:HE3	6:F:98:LYS:HE3	1.97	0.46
13:M:754:ARG:O	13:M:754:ARG:CD	2.64	0.46
16:P:-16:U:C6	26:Z:583:PHE:CE1	3.03	0.46
20:T:184:DC:OP1	28:b:36:ARG:NH2	2.48	0.46
26:Z:309:PRO:HD2	26:Z:339:LEU:HA	1.98	0.46
26:Z:360:ILE:HG23	26:Z:364:ASN:HA	1.95	0.46
30:h:122:TYR:O	30:h:122:TYR:CD1	2.68	0.46
1:A:64:VAL:CG1	1:A:78:MET:HA	2.45	0.46
1:A:189:PRO:HB3	1:A:202:TRP:CE2	2.50	0.46
2:B:149:ILE:HG22	2:B:150:GLY:H	1.80	0.46
2:B:420:GLN:HG3	2:B:424:ASP:OD2	2.16	0.46
2:B:789:ASN:ND2	2:B:966:ILE:HG22	2.31	0.46
2:B:1119:CYS:O	2:B:1123:GLY:N	2.45	0.46
13:M:316:GLU:CD	13:M:403:TRP:CD1	2.94	0.46
13:M:1281:CYS:O	13:M:1282:ARG:C	2.57	0.46
15:O:1801:ILE:HG21	15:O:2008:LEU:HB3	1.98	0.46
17:Q:751:THR:HG21	17:Q:801:ASP:H	1.79	0.46
19:S:219:LEU:N	19:S:219:LEU:HD12	2.30	0.46
25:Y:14:ARG:HB3	25:Y:53:THR:HG22	1.97	0.46
26:Z:705:LEU:C	26:Z:705:LEU:HD12	2.41	0.46
27:e:62:LEU:HD12	28:f:38:LEU:HG	1.97	0.46
1:A:96:HIS:CE1	2:B:1165:MET:O	2.68	0.46
1:A:753:GLY:O	1:A:757:GLN:HG2	2.16	0.46
1:A:790:GLN:HA	1:A:822:PHE:HA	1.97	0.46
2:B:65:ILE:N	2:B:65:ILE:HD12	2.31	0.46
2:B:615:TYR:HB3	2:B:620:ARG:HD3	1.97	0.46
2:B:1136:GLU:HA	2:B:1143:LYS:HA	1.97	0.46
13:M:316:GLU:HG2	13:M:403:TRP:CE2	2.51	0.46
13:M:862:GLU:HA	13:M:865:LYS:HD2	1.98	0.46
17:Q:415:TRP:O	17:Q:433:ALA:HB1	2.15	0.46
21:U:450:LEU:HD22	21:U:491:PHE:CE2	2.50	0.46
23:W:154:ILE:HA	23:W:164:ALA:O	2.15	0.46
31:j:702:ASN:OD1	31:j:703:ASN:N	2.49	0.46
1:A:1175:ILE:HA	1:A:1211:LEU:O	2.15	0.46
1:A:1323:THR:N	1:A:1327:GLU:O	2.22	0.46
2:B:59:VAL:HG21	2:B:91:ILE:HD11	1.97	0.46
4:D:107:THR:HG23	4:D:110:GLU:HB2	1.97	0.46
7:G:30:LEU:O	7:G:34:VAL:HG22	2.15	0.46
9:I:79:PRO:O	9:I:95:VAL:HA	2.15	0.46
21:U:405:ASP:HB2	21:U:520:ILE:O	2.15	0.46
25:Y:19:CYS:HB2	25:Y:80:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:278:TRP:CZ2	26:Z:292:GLN:NE2	2.84	0.46
27:a:112:ALA:HB2	27:a:120:ILE:HG22	1.98	0.46
1:A:244:ARG:HE	1:A:246:GLU:CD	2.24	0.46
1:A:902:GLU:OE2	1:A:985:ARG:NH1	2.49	0.46
2:B:570:ASN:N	2:B:614:ILE:O	2.38	0.46
2:B:595:ASP:CG	2:B:596:ILE:H	2.23	0.46
5:E:11:TRP:CZ2	5:E:15:LYS:HE3	2.51	0.46
7:G:87:ALA:HB1	7:G:99:THR:OG1	2.16	0.46
7:G:96:GLY:CA	7:G:108:ILE:O	2.63	0.46
9:I:25:TYR:CD1	9:I:40:ARG:HG2	2.51	0.46
12:L:39:CYS:SG	12:L:41:TYR:HB2	2.56	0.46
13:M:896:SER:HA	26:Z:573:GLN:HE22	1.81	0.46
13:M:1086:ALA:HA	13:M:1089:LEU:HD12	1.98	0.46
13:M:1286:LEU:CD2	26:Z:664:PRO:HB2	2.46	0.46
26:Z:360:ILE:HD13	26:Z:366:TYR:CD2	2.51	0.46
31:j:594:PHE:CE2	32:k:109:TRP:HB3	2.50	0.46
2:B:240:LEU:HD12	2:B:255:ARG:HB2	1.98	0.46
2:B:289:ILE:HD13	2:B:298:MET:HG2	1.98	0.46
2:B:1038:THR:HA	3:C:195:THR:HA	1.98	0.46
4:D:17:ALA:HA	4:D:22:PHE:CE1	2.50	0.46
4:D:29:ALA:HA	7:G:5:ILE:HG22	1.98	0.46
5:E:26:TYR:HA	5:E:64:HIS:HA	1.98	0.46
13:M:1241:PRO:HB2	13:M:1244:PHE:HD2	1.81	0.46
14:N:-7:DG:O3'	27:a:64:ARG:NE	2.49	0.46
26:Z:273:LEU:HD12	26:Z:378:MET:HB2	1.98	0.46
31:j:721:HIS:CE1	31:j:832:PRO:HB2	2.51	0.46
1:A:101:VAL:HG23	1:A:102:LYS:N	2.31	0.45
2:B:193:VAL:HG22	2:B:468:GLN:O	2.16	0.45
2:B:1137:CYS:O	2:B:1141:ARG:N	2.47	0.45
3:C:41:GLU:OE2	11:K:41:THR:HG21	2.16	0.45
7:G:9:HIS:CD2	7:G:11:ILE:HG22	2.52	0.45
13:M:466:HIS:HA	13:M:598:ARG:HB3	1.97	0.45
13:M:986:ILE:HD12	13:M:997:GLY:O	2.15	0.45
27:a:110:LEU:O	27:a:114:HIS:N	2.43	0.45
1:A:883:ILE:HD13	1:A:1423:ASP:OD1	2.15	0.45
13:M:522:ASP:O	13:M:525:THR:N	2.50	0.45
13:M:853:GLU:HG2	13:M:887:ASN:HD22	1.81	0.45
13:M:868:VAL:C	13:M:870:GLU:H	2.23	0.45
13:M:949:VAL:HG21	13:M:954:LEU:HB2	1.98	0.45
17:Q:121:ASP:OD2	17:Q:134:ARG:NH1	2.49	0.45
18:R:433:ASP:OD2	18:R:435:ARG:NH2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:281:TYR:OH	22:V:355:ASP:OD1	2.32	0.45
26:Z:242:VAL:HB	26:Z:245:LEU:HB2	1.99	0.45
31:j:558:SER:CB	32:k:230:PHE:HA	2.47	0.45
1:A:709:ALA:O	1:A:713:VAL:HG23	2.17	0.45
1:A:1420:ASN:OD1	1:A:1432:PHE:HE1	1.98	0.45
2:B:300:MET:HE1	2:B:376:ALA:HB1	1.98	0.45
5:E:121:MET:CE	5:E:125:TYR:CD1	2.99	0.45
10:J:21:TYR:CE1	10:J:34:ALA:HB3	2.51	0.45
13:M:562:PHE:CG	13:M:563:PRO:HD2	2.51	0.45
13:M:920:ILE:CD1	13:M:1141:TYR:CE2	2.99	0.45
13:M:1265:CYS:HB3	13:M:1281:CYS:SG	2.56	0.45
20:T:173:DA:C5'	28:f:45:LYS:CE	2.92	0.45
26:Z:578:LYS:HG3	26:Z:579:LYS:H	1.81	0.45
26:Z:618:PHE:CE2	26:Z:619:ARG:HD2	2.52	0.45
2:B:205:VAL:HG22	2:B:368:MET:HG2	1.98	0.45
2:B:896:LEU:CD2	2:B:900:GLU:HB2	2.47	0.45
2:B:994:GLY:HA2	10:J:50:LEU:HD11	1.97	0.45
7:G:38:CYS:SG	7:G:157:ILE:HG13	2.56	0.45
13:M:620:PRO:HD2	13:M:639:TYR:CE2	2.51	0.45
29:g:54:ALA:CB	30:h:118:ALA:CB	2.95	0.45
1:A:62:GLN:HG2	1:A:84:HIS:O	2.17	0.45
1:A:1065:PHE:CZ	1:A:1069:LEU:HD21	2.51	0.45
7:G:78:ARG:CG	7:G:80:PHE:CZ	3.00	0.45
17:Q:376:GLU:CD	22:V:65:SER:H	2.24	0.45
18:R:485:TYR:OH	18:R:489:ASP:OD2	2.33	0.45
18:R:492:ILE:H	18:R:492:ILE:HD12	1.80	0.45
2:B:1068:GLN:O	2:B:1072:ARG:HA	2.17	0.45
2:B:1118:VAL:HG11	2:B:1171:MET:HE3	1.99	0.45
3:C:118:ARG:NH2	3:C:147:ASP:OD1	2.44	0.45
13:M:758:TYR:CD2	13:M:759:ARG:N	2.85	0.45
13:M:758:TYR:CE2	13:M:847:VAL:HG21	2.52	0.45
17:Q:313:ALA:HB1	17:Q:329:TYR:CE2	2.52	0.45
23:W:20:TRP:CH2	23:W:40:LEU:HD13	2.52	0.45
23:W:82:SER:HB3	23:W:112:LEU:HD13	1.99	0.45
25:Y:64:MET:HE1	26:Z:215:VAL:HG23	1.99	0.45
26:Z:368:ARG:HB3	26:Z:373:PHE:CE1	2.52	0.45
32:k:294:VAL:HG13	32:k:298:PHE:CD2	2.51	0.45
1:A:18:ILE:HD11	2:B:1149:VAL:HG11	1.98	0.45
1:A:865:ILE:HG21	2:B:1092:ASP:CG	2.41	0.45
1:A:1370:GLY:O	1:A:1374:VAL:HG23	2.17	0.45
2:B:42:GLN:OE1	2:B:42:GLN:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:TYR:CE1	2:B:505:LEU:HD21	2.52	0.45
2:B:1075:MET:O	2:B:1082:GLY:CA	2.65	0.45
13:M:589:ARG:HD2	13:M:711:MET:CG	2.46	0.45
13:M:898:LYS:NZ	13:M:929:GLN:O	2.47	0.45
14:N:56:DG:C2	14:N:57:DC:C2	3.05	0.45
16:P:-16:U:H5	26:Z:583:PHE:HE1	1.50	0.45
23:W:195:SER:CB	23:W:237:ASN:HA	2.47	0.45
31:j:721:HIS:CE1	31:j:832:PRO:CB	2.99	0.45
1:A:511:THR:HG23	2:B:1102:PHE:CA	2.47	0.45
1:A:700:GLN:O	1:A:704:ASN:CG	2.60	0.45
1:A:866:LYS:CE	1:A:1432:PHE:HB3	2.46	0.45
2:B:453:TRP:HB2	2:B:466:VAL:HG21	1.97	0.45
8:H:93:TYR:CD2	8:H:142:TYR:CZ	3.05	0.45
9:I:54:TYR:OH	9:I:56:ASN:HB2	2.17	0.45
13:M:976:ALA:HA	13:M:982:SER:HB2	1.99	0.45
17:Q:537:LEU:HD23	17:Q:540:MET:CE	2.47	0.45
20:T:173:DA:H4'	28:f:46:ARG:HD2	1.98	0.45
26:Z:427:GLU:OE1	26:Z:469:ARG:NH1	2.40	0.45
1:A:367:ILE:HA	1:A:482:PHE:O	2.17	0.45
1:A:832:THR:CG2	1:A:833:PRO:HD2	2.46	0.45
1:A:1376:LYS:O	1:A:1379:GLU:HG2	2.16	0.45
4:D:110:GLU:HG3	7:G:167:TYR:CD2	2.52	0.45
8:H:64:LEU:HG	8:H:142:TYR:CE2	2.52	0.45
13:M:855:ARG:HD2	13:M:1275:PHE:CD2	2.52	0.45
22:V:208:PHE:O	22:V:322:TYR:HA	2.17	0.45
26:Z:180:TRP:CH2	26:Z:232:GLN:HB2	2.52	0.45
30:h:47:LYS:O	30:h:51:PRO:HG3	2.17	0.45
32:k:121:PHE:O	32:k:128:VAL:N	2.49	0.45
1:A:280:LEU:O	1:A:284:VAL:HG23	2.17	0.45
1:A:388:MET:HG3	2:B:1061:SER:OG	2.16	0.45
1:A:413:TYR:HB3	1:A:414:PRO:HD3	1.99	0.45
1:A:548:PHE:HD1	1:A:679:TRP:CE2	2.34	0.45
1:A:566:PHE:CD1	1:A:674:THR:HG22	2.52	0.45
1:A:1178:ASP:OD2	1:A:1260:ARG:NH1	2.49	0.45
2:B:221:CYS:HB2	2:B:368:MET:HE3	1.99	0.45
2:B:713:PHE:CE2	2:B:982:ILE:HG22	2.52	0.45
2:B:755:GLN:HB3	10:J:51:ALA:HB1	1.98	0.45
3:C:149:LEU:HD23	10:J:3:ILE:HG22	1.99	0.45
13:M:1028:PHE:CD2	13:M:1028:PHE:C	2.95	0.45
17:Q:436:THR:HG22	17:Q:440:ILE:CD1	2.47	0.45
18:R:366:ARG:HB3	18:R:444:ASN:CG	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:414:LEU:CD1	21:U:507:SER:HB2	2.47	0.45
29:g:74:ASN:O	29:g:76:LYS:HG2	2.15	0.45
31:j:544:GLY:HA3	32:k:18:MET:HE2	1.98	0.45
31:j:688:ARG:HA	31:j:697:VAL:O	2.17	0.45
1:A:904:GLN:NE2	1:A:982:ASN:HA	2.32	0.44
2:B:125:TYR:HA	2:B:147:THR:O	2.17	0.44
2:B:795:ILE:HG12	2:B:947:ILE:CG2	2.47	0.44
2:B:861:SER:C	2:B:896:LEU:HD23	2.41	0.44
13:M:319:TRP:CZ3	13:M:403:TRP:HB2	2.51	0.44
13:M:989:VAL:HB	13:M:992:LEU:HD12	1.99	0.44
14:N:-5:DG:C2'	14:N:-4:DC:C5	2.98	0.44
14:N:2:DG:H2''	14:N:3:DT:C6	2.52	0.44
20:T:130:DA:H2''	20:T:131:DC:C5	2.51	0.44
25:Y:16:CYS:O	25:Y:20:SER:HA	2.16	0.44
26:Z:428:VAL:HG23	26:Z:436:LEU:O	2.17	0.44
31:j:669:PRO:HG3	31:j:735:HIS:CE1	2.53	0.44
32:k:12:GLN:N	32:k:19:ASN:O	2.41	0.44
1:A:231:GLU:O	1:A:235:VAL:HG23	2.16	0.44
1:A:663:ASP:O	1:A:666:ARG:HB3	2.18	0.44
1:A:917:GLU:HG3	1:A:921:ARG:HB2	1.99	0.44
1:A:985:ARG:HD2	1:A:989:ASN:HD21	1.82	0.44
1:A:1170:THR:HA	1:A:1216:LEU:HD23	1.99	0.44
1:A:1347:LEU:CD2	1:A:1354:PRO:HA	2.47	0.44
2:B:93:LEU:N	21:U:519:ARG:O	2.41	0.44
2:B:270:ILE:HB	2:B:308:ALA:HB3	1.99	0.44
2:B:591:ARG:CZ	2:B:603:MET:HE1	2.47	0.44
2:B:633:LEU:HD21	2:B:679:PRO:HB3	1.98	0.44
2:B:1067:ILE:HG13	2:B:1072:ARG:C	2.42	0.44
2:B:1151:MET:HE3	2:B:1155:CYS:SG	2.57	0.44
3:C:72:PRO:HG3	10:J:13:ILE:HG12	1.99	0.44
7:G:18:PHE:N	7:G:18:PHE:CD1	2.85	0.44
9:I:86:CYS:SG	9:I:121:HIS:HB3	2.57	0.44
13:M:928:ALA:HB2	13:M:962:PHE:HE2	1.82	0.44
13:M:1142:ARG:HH21	13:M:1142:ARG:CG	2.29	0.44
17:Q:329:TYR:O	17:Q:333:THR:HG23	2.17	0.44
21:U:412:LEU:HD23	21:U:412:LEU:C	2.42	0.44
22:V:232:THR:HG21	22:V:240:MET:SD	2.58	0.44
23:W:23:ALA:CB	23:W:71:ASP:HA	2.48	0.44
23:W:282:TYR:CZ	23:W:289:ILE:HD11	2.52	0.44
26:Z:180:TRP:CD1	26:Z:235:VAL:HG11	2.52	0.44
27:a:50:ARG:NH1	31:j:919:GLN:OE1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:ASP:OD1	1:A:1029:LEU:N	2.42	0.44
2:B:135:GLU:CG	2:B:136:GLY:H	2.29	0.44
4:D:110:GLU:HG3	7:G:167:TYR:CG	2.52	0.44
6:F:102:ILE:HB	6:F:120:VAL:HG11	2.00	0.44
13:M:373:VAL:HG12	13:M:390:ILE:CD1	2.48	0.44
17:Q:347:LEU:HD23	17:Q:363:CYS:SG	2.58	0.44
21:U:483:ALA:HA	22:V:242:SER:HB3	1.98	0.44
22:V:289:TYR:O	22:V:349:LEU:N	2.47	0.44
23:W:49:TRP:CZ2	23:W:52:GLU:HA	2.53	0.44
30:h:122:TYR:O	30:h:122:TYR:CD2	2.67	0.44
31:j:964:GLU:OE1	31:j:966:TYR:OH	2.30	0.44
1:A:95:PHE:CD2	1:A:218:PRO:HG3	2.52	0.44
1:A:484:LEU:HD12	1:A:485:ASN:O	2.16	0.44
1:A:694:ALA:HB3	1:A:699:TYR:CZ	2.53	0.44
1:A:1460:LEU:HD22	1:A:1460:LEU:N	2.32	0.44
1:A:1461:GLY:HA3	2:B:1108:PHE:CD2	2.52	0.44
2:B:851:ASP:OD2	12:L:17:TYR:OH	2.31	0.44
3:C:13:GLU:HB3	3:C:20:LYS:HB2	1.99	0.44
13:M:468:LEU:O	13:M:472:GLY:HA3	2.17	0.44
13:M:639:TYR:O	13:M:1301:TYR:HA	2.18	0.44
20:T:180:DA:H2"	20:T:181:DC:C5	2.53	0.44
31:j:562:GLU:HB3	32:k:233:LYS:HD2	1.99	0.44
1:A:497:ASP:OD1	1:A:497:ASP:C	2.59	0.44
1:A:1195:VAL:HG11	19:S:196:SER:HB2	2.00	0.44
2:B:506:TRP:CD1	2:B:506:TRP:C	2.95	0.44
8:H:6:PHE:CZ	8:H:37:MET:HG3	2.52	0.44
10:J:30:THR:HG22	10:J:33:ASP:OD2	2.17	0.44
13:M:385:GLU:CD	13:M:1121:ILE:HD13	2.42	0.44
13:M:589:ARG:CD	13:M:711:MET:CG	2.96	0.44
13:M:594:LEU:HD22	13:M:720:PHE:CZ	2.53	0.44
13:M:628:VAL:CG2	13:M:664:LEU:HD13	2.47	0.44
13:M:940:LEU:HB2	13:M:942:PHE:CZ	2.53	0.44
17:Q:272:LEU:HD22	17:Q:291:LEU:HD23	2.00	0.44
26:Z:291:ALA:HB1	26:Z:306:LYS:N	2.32	0.44
26:Z:293:VAL:HG22	26:Z:303:ILE:CG1	2.48	0.44
26:Z:595:HIS:N	26:Z:598:ASP:OD2	2.33	0.44
28:b:84:ALA:O	28:b:88:VAL:HG23	2.17	0.44
28:f:40:ARG:HG2	31:j:751:LEU:HB3	1.98	0.44
31:j:610:GLU:OE1	31:j:614:PRO:HD3	2.18	0.44
32:k:111:THR:OG1	32:k:113:LYS:HE3	2.17	0.44
2:B:676:ALA:HB1	2:B:682:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:36:CYS:SG	12:L:38:GLU:HG2	2.58	0.44
13:M:370:HIS:ND1	13:M:1026:LYS:HE3	2.32	0.44
13:M:1282:ARG:O	13:M:1286:LEU:N	2.48	0.44
26:Z:177:PRO:HG3	26:Z:213:LYS:HG3	2.00	0.44
26:Z:181:THR:HG23	26:Z:255:VAL:CG1	2.48	0.44
1:A:991:GLN:HA	1:A:996:ILE:CG1	2.47	0.44
1:A:1228:MET:HE3	1:A:1247:PHE:HB2	2.00	0.44
1:A:1428:MET:HB2	1:A:1456:GLU:OE2	2.17	0.44
2:B:98:HIS:NE2	2:B:116:ARG:NH2	2.66	0.44
2:B:273:PHE:HB3	2:B:284:ILE:HG12	2.00	0.44
2:B:278:PHE:CD1	2:B:287:HIS:CE1	3.06	0.44
2:B:606:ASP:O	2:B:610:ARG:N	2.51	0.44
2:B:648:TYR:HA	22:V:195:SER:HB3	1.99	0.44
2:B:907:VAL:HG22	2:B:921:ILE:HG23	1.99	0.44
2:B:1128:ALA:HB1	2:B:1135:TYR:HD2	1.82	0.44
4:D:29:ALA:CB	7:G:3:TYR:CD2	3.01	0.44
4:D:29:ALA:HB2	7:G:5:ILE:CG2	2.47	0.44
4:D:95:PHE:CD2	7:G:1:MET:HE1	2.52	0.44
6:F:52:ILE:N	6:F:116:GLU:OE2	2.39	0.44
13:M:929:GLN:HA	13:M:984:ALA:HB2	1.99	0.44
15:O:1811:THR:HA	15:O:2019:LEU:HB3	2.00	0.44
21:U:388:PRO:HA	21:U:422:TRP:O	2.17	0.44
25:Y:2:ALA:HB3	25:Y:4:GLU:OE1	2.18	0.44
27:e:84:ARG:C	27:e:85:PHE:CD1	2.96	0.44
31:j:901:ASN:OD1	31:j:903:THR:N	2.50	0.44
1:A:112:PHE:HD1	1:A:113:PHE:CD1	2.35	0.44
1:A:540:ASP:HB3	2:B:790:GLN:HE22	1.83	0.44
2:B:207:VAL:HG11	2:B:375:ALA:HB3	2.00	0.44
2:B:326:ALA:HA	2:B:338:TYR:CD2	2.53	0.44
2:B:1117:HIS:O	2:B:1125:MET:HA	2.18	0.44
6:F:106:ILE:O	6:F:117:ASP:HA	2.18	0.44
13:M:443:LEU:HD21	13:M:471:TYR:CE2	2.52	0.44
13:M:620:PRO:CD	13:M:639:TYR:CE2	3.01	0.44
17:Q:748:PRO:HB2	23:W:150:PHE:CE2	2.53	0.44
17:Q:854:GLN:OE1	17:Q:854:GLN:HA	2.18	0.44
26:Z:534:HIS:NE2	26:Z:577:ARG:HB2	2.33	0.44
26:Z:736:LEU:HD12	26:Z:739:THR:OG1	2.18	0.44
31:j:612:THR:HB	31:j:616:LEU:HD23	2.00	0.44
31:j:709:PHE:CD1	31:j:720:LEU:HD23	2.53	0.44
32:k:294:VAL:HG13	32:k:298:PHE:HD2	1.83	0.44
1:A:369:PRO:HB3	1:A:496:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:GLN:HG2	1:A:823:VAL:HG23	1.98	0.44
2:B:677:MET:N	2:B:682:LEU:HD12	2.33	0.44
2:B:811:TYR:OH	3:C:60:HIS:CE1	2.71	0.44
2:B:1142:ASN:CG	2:B:1144:THR:O	2.60	0.44
4:D:34:ASN:O	4:D:68:THR:CG2	2.65	0.44
23:W:234:TRP:O	23:W:251:SER:OG	2.32	0.44
26:Z:447:LYS:HA	26:Z:464:PRO:HA	1.99	0.44
29:g:80:ILE:HG12	29:g:83:HIS:CE1	2.53	0.44
31:j:523:HIS:HB2	31:j:530:TYR:HB2	1.99	0.44
31:j:772:MET:HE3	31:j:776:LEU:HD11	2.00	0.44
1:A:1165:THR:HA	1:A:1296:MET:O	2.17	0.43
2:B:51:ILE:HG23	2:B:93:LEU:HD22	2.00	0.43
2:B:278:PHE:CE2	2:B:362:ALA:HB2	2.53	0.43
2:B:617:ASP:O	2:B:620:ARG:NH1	2.49	0.43
2:B:756:LYS:HE2	2:B:770:ARG:HG3	1.99	0.43
3:C:155:LYS:O	10:J:64:PRO:HB2	2.18	0.43
8:H:6:PHE:CG	8:H:7:GLU:N	2.86	0.43
13:M:893:TYR:O	13:M:899:SER:HB3	2.18	0.43
13:M:1271:ASP:OD1	13:M:1273:GLU:CD	2.60	0.43
25:Y:6:VAL:HG22	25:Y:7:PRO:HD2	2.00	0.43
26:Z:256:PRO:HD2	26:Z:259:GLU:OE1	2.18	0.43
32:k:15:LYS:HA	32:k:135:ASN:CG	2.43	0.43
32:k:214:TYR:CE2	32:k:227:GLY:HA3	2.53	0.43
1:A:880:ARG:HH21	5:E:169:GLN:NE2	2.16	0.43
1:A:945:ASN:CG	1:A:948:ILE:HG12	2.43	0.43
1:A:967:ARG:HH21	1:A:1322:ILE:HD13	1.83	0.43
2:B:285:LEU:HD22	9:I:16:PHE:HZ	1.84	0.43
2:B:363:TYR:HB3	2:B:573:TRP:CZ3	2.53	0.43
2:B:795:ILE:HG12	2:B:947:ILE:HG22	1.98	0.43
11:K:104:ARG:HA	11:K:107:VAL:HG22	2.00	0.43
13:M:704:GLU:OE1	13:M:704:GLU:N	2.51	0.43
25:Y:25:ILE:HG23	25:Y:26:ASP:N	2.33	0.43
26:Z:291:ALA:HB1	26:Z:306:LYS:H	1.83	0.43
1:A:355:MET:HE3	1:A:1431:SER:CB	2.48	0.43
1:A:570:TRP:CZ2	1:A:572:GLY:C	2.96	0.43
1:A:1347:LEU:HD22	1:A:1354:PRO:HA	2.00	0.43
2:B:113:ALA:HA	2:B:118:LEU:HB2	2.01	0.43
2:B:300:MET:CE	2:B:376:ALA:HB1	2.49	0.43
2:B:845:TYR:HA	2:B:865:VAL:HG11	2.01	0.43
5:E:185:ILE:HD12	5:E:209:VAL:CG2	2.49	0.43
6:F:107:ARG:HG3	6:F:115:TYR:CD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:756:ALA:N	13:M:1138:ARG:HB3	2.32	0.43
13:M:1291:ASN:OD1	13:M:1294:LYS:HD2	2.18	0.43
18:R:492:ILE:O	18:R:496:VAL:HG22	2.18	0.43
25:Y:45:ASN:CG	25:Y:48:MET:HB3	2.42	0.43
1:A:604:ARG:O	1:A:628:VAL:N	2.51	0.43
2:B:66:ASP:OD1	2:B:85:LEU:HG	2.18	0.43
2:B:216:ALA:N	2:B:239:MET:O	2.51	0.43
2:B:322:GLY:HA3	2:B:335:ARG:HG2	1.99	0.43
2:B:464:ALA:HB1	16:P:-6:U:O2'	2.18	0.43
2:B:502:HIS:HB3	2:B:504:THR:HG22	2.01	0.43
2:B:1003:ASN:C	2:B:1005:ALA:H	2.27	0.43
2:B:1037:ILE:HD11	2:B:1041:ILE:CG1	2.48	0.43
4:D:29:ALA:CB	7:G:5:ILE:CG2	2.96	0.43
5:E:153:LYS:O	5:E:157:THR:HG23	2.19	0.43
7:G:145:LEU:HD13	7:G:161:GLY:HA3	1.99	0.43
8:H:12:VAL:HG11	8:H:15:ILE:HD11	2.01	0.43
15:O:1718:GLU:HB2	15:O:1741:LEU:HD21	1.99	0.43
17:Q:329:TYR:CZ	17:Q:346:GLY:HA3	2.52	0.43
21:U:374:TYR:HA	21:U:487:THR:O	2.18	0.43
21:U:405:ASP:OD2	21:U:519:ARG:HG2	2.18	0.43
23:W:22:VAL:HG23	23:W:37:THR:HG22	1.99	0.43
25:Y:45:ASN:ND2	25:Y:48:MET:HB2	2.33	0.43
25:Y:116:LYS:HD3	26:Z:268:LYS:HB3	2.00	0.43
26:Z:310:ARG:HA	26:Z:337:GLN:HA	2.00	0.43
26:Z:342:ALA:O	26:Z:346:ARG:HG3	2.17	0.43
26:Z:356:GLY:CA	31:j:772:MET:HE2	2.47	0.43
26:Z:705:LEU:CD1	26:Z:724:VAL:HG11	2.49	0.43
31:j:805:GLY:HA2	31:j:817:LEU:O	2.19	0.43
1:A:427:ILE:HD13	1:A:437:ASP:O	2.17	0.43
1:A:1071:GLU:HA	1:A:1071:GLU:OE1	2.19	0.43
2:B:205:VAL:CG2	2:B:368:MET:HG2	2.49	0.43
4:D:34:ASN:O	4:D:68:THR:HG21	2.18	0.43
17:Q:667:ARG:HB2	17:Q:690:ILE:HG21	2.01	0.43
22:V:282:ALA:HB3	22:V:285:ASP:HB2	1.99	0.43
25:Y:15:ALA:HB2	25:Y:22:VAL:HG22	2.01	0.43
29:g:27:PRO:HG3	30:h:41:TYR:CE2	2.53	0.43
1:A:408:ARG:NH2	1:A:412:GLN:OE1	2.51	0.43
1:A:557:ARG:O	1:A:561:MET:HG3	2.19	0.43
1:A:894:ASP:OD1	1:A:1396:ARG:NH1	2.52	0.43
1:A:1323:THR:HG22	1:A:1324:GLU:N	2.34	0.43
2:B:551:GLU:CB	2:B:556:ILE:HD13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:929:PRO:HA	2:B:1050:ARG:NH1	2.33	0.43
7:G:118:GLU:HG2	7:G:129:LYS:O	2.18	0.43
7:G:163:LEU:HA	7:G:168:LEU:HD13	2.01	0.43
9:I:78:LEU:HG	9:I:79:PRO:HD2	2.00	0.43
11:K:58:PHE:HB3	11:K:76:GLN:HB3	2.01	0.43
17:Q:132:LEU:HD13	17:Q:164:PRO:HB2	2.01	0.43
17:Q:373:ASN:HA	17:Q:378:MET:SD	2.58	0.43
22:V:251:ASP:OD1	22:V:251:ASP:C	2.62	0.43
32:k:377:VAL:HB	32:k:391:PHE:CE1	2.53	0.43
1:A:1085:GLU:HA	6:F:60:TYR:OH	2.19	0.43
2:B:565:THR:CG2	2:B:580:PRO:HB3	2.49	0.43
3:C:173:HIS:HB3	3:C:176:TRP:CZ3	2.54	0.43
3:C:241:PRO:HA	3:C:244:ILE:HD12	2.01	0.43
12:L:35:ARG:CZ	18:R:492:ILE:HG21	2.49	0.43
13:M:896:SER:HA	26:Z:573:GLN:NE2	2.33	0.43
13:M:1150:PHE:CD2	13:M:1272:ILE:HA	2.54	0.43
14:N:5:DT:H2'	14:N:6:DT:C6	2.54	0.43
17:Q:524:LEU:HD21	17:Q:533:CYS:HB2	2.00	0.43
17:Q:695:LYS:HA	17:Q:697:TYR:CE1	2.53	0.43
26:Z:181:THR:HG22	26:Z:226:TYR:CE2	2.54	0.43
26:Z:341:ASP:O	26:Z:343:GLU:N	2.41	0.43
26:Z:579:LYS:HE3	26:Z:580:ASP:OD2	2.18	0.43
31:j:645:ILE:CD1	31:j:729:MET:HG3	2.48	0.43
31:j:654:ASN:OD1	31:j:657:ARG:HG3	2.19	0.43
1:A:421:ARG:CZ	1:A:427:ILE:HD11	2.49	0.43
1:A:804:HIS:CE1	9:I:100:HIS:CG	3.06	0.43
2:B:465:GLY:CA	16:P:-5:U:H4'	2.48	0.43
2:B:759:VAL:HG23	2:B:999:ALA:HB2	2.00	0.43
2:B:908:MET:HG3	2:B:920:LYS:O	2.19	0.43
4:D:106:GLU:OE2	13:M:521:ARG:NH2	2.45	0.43
7:G:87:ALA:CB	7:G:145:LEU:HD23	2.49	0.43
8:H:7:GLU:HB2	8:H:59:VAL:HG13	2.01	0.43
13:M:373:VAL:HG13	13:M:393:LEU:HB3	1.99	0.43
13:M:783:GLY:O	13:M:796:CYS:HA	2.19	0.43
13:M:803:GLY:HA2	13:M:921:GLN:NE2	2.33	0.43
16:P:-21:U:O2	16:P:-21:U:C2'	2.66	0.43
18:R:507:PRO:HA	18:R:508:ASN:HA	1.73	0.43
26:Z:430:GLU:HB2	26:Z:467:GLU:HA	2.01	0.43
30:h:60:MET:HE3	31:j:948:PHE:CD2	2.54	0.43
32:k:177:PRO:O	32:k:181:PHE:CB	2.67	0.43
1:A:823:VAL:HG22	1:A:835:GLU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:THR:HG23	2:B:141:GLN:HB3	1.99	0.43
2:B:355:ASP:OD1	2:B:355:ASP:N	2.52	0.43
2:B:415:VAL:HA	2:B:434:ALA:HB1	1.99	0.43
13:M:868:VAL:C	13:M:870:GLU:N	2.76	0.43
13:M:1288:ASP:OD2	13:M:1294:LYS:N	2.48	0.43
21:U:527:ASP:HB3	21:U:528:PRO:HD3	2.01	0.43
25:Y:72:SER:OG	25:Y:78:SER:HA	2.18	0.43
26:Z:472:PHE:CZ	26:Z:518:LEU:HB2	2.54	0.43
31:j:727:ALA:HB2	31:j:736:THR:HG23	2.00	0.43
31:j:901:ASN:OD1	31:j:901:ASN:C	2.62	0.43
1:A:503:LEU:HD23	1:A:503:LEU:C	2.44	0.43
1:A:511:THR:CG2	2:B:1102:PHE:HA	2.48	0.43
1:A:733:LEU:O	1:A:733:LEU:HD23	2.19	0.43
1:A:945:ASN:OD1	1:A:947:HIS:HB3	2.19	0.43
1:A:1027:ASP:OD1	1:A:1028:PRO:N	2.51	0.43
2:B:586:THR:O	2:B:590:LEU:HD13	2.19	0.43
4:D:67:TYR:CG	7:G:102:GLY:HA2	2.54	0.43
5:E:193:ILE:N	5:E:205:THR:O	2.48	0.43
9:I:99:SER:HB3	9:I:111:TYR:CE1	2.54	0.43
22:V:296:ASN:OD1	22:V:335:ARG:HG3	2.19	0.43
25:Y:14:ARG:HB2	25:Y:53:THR:CG2	2.49	0.43
26:Z:357:ASP:OD2	31:j:768:MET:HE2	2.18	0.43
26:Z:588:ASP:OD1	26:Z:588:ASP:C	2.61	0.43
28:f:62:PHE:CE2	28:f:96:ARG:HD3	2.53	0.43
1:A:540:ASP:OD1	1:A:680:LEU:CD2	2.67	0.42
1:A:892:GLY:C	1:A:894:ASP:H	2.27	0.42
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.84	0.42
1:A:965:VAL:O	1:A:969:ILE:HG12	2.19	0.42
2:B:130:LYS:N	2:B:142:THR:O	2.52	0.42
3:C:115:VAL:O	3:C:150:ILE:HB	2.19	0.42
5:E:40:PHE:CD2	5:E:44:PHE:CD2	3.07	0.42
8:H:143:LEU:HD23	8:H:145:MET:HB3	2.00	0.42
17:Q:604:MET:O	17:Q:635:ILE:HG21	2.18	0.42
18:R:30:GLU:OE1	18:R:30:GLU:HA	2.18	0.42
18:R:366:ARG:HB3	18:R:444:ASN:OD1	2.18	0.42
22:V:193:HIS:CE1	22:V:194:TYR:CE2	3.06	0.42
23:W:43:LEU:CD2	23:W:61:GLU:HG2	2.48	0.42
26:Z:181:THR:HG22	26:Z:226:TYR:CD2	2.53	0.42
26:Z:285:ILE:CG2	26:Z:335:PRO:HG2	2.40	0.42
31:j:559:MET:HA	31:j:567:TYR:O	2.19	0.42
1:A:115:SER:OG	1:A:227:ARG:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:ARG:HG3	1:A:1222:THR:HG23	2.00	0.42
2:B:114:ARG:NH1	2:B:743:ARG:NH1	2.68	0.42
2:B:569:VAL:HA	2:B:614:ILE:O	2.19	0.42
2:B:785:TYR:O	2:B:786:THR:HG22	2.19	0.42
3:C:47:ILE:HA	3:C:165:ALA:HA	2.01	0.42
3:C:52:ILE:HD12	3:C:61:ASP:HA	2.01	0.42
5:E:94:MET:O	5:E:98:ASN:N	2.53	0.42
7:G:96:GLY:HA3	7:G:107:PHE:CZ	2.54	0.42
11:K:43:GLY:HA3	11:K:61:TYR:CE2	2.54	0.42
13:M:379:TYR:CE1	13:M:1059:HIS:HB2	2.54	0.42
13:M:539:PHE:O	13:M:709:ARG:HD3	2.18	0.42
17:Q:795:TYR:CZ	23:W:107:VAL:HG11	2.54	0.42
21:U:485:PHE:CE1	22:V:312:PHE:CB	3.02	0.42
24:X:211:ARG:HB2	24:X:214:VAL:HB	2.01	0.42
26:Z:358:PHE:HD1	26:Z:368:ARG:NH2	2.17	0.42
30:h:104:PRO:HD2	30:h:107:LEU:HD12	1.99	0.42
31:j:721:HIS:HE1	31:j:832:PRO:CB	2.32	0.42
32:k:17:SER:CB	32:k:156:ALA:HB2	2.49	0.42
32:k:202:PHE:CZ	32:k:314:VAL:HG22	2.54	0.42
32:k:301:ARG:O	32:k:302:LEU:HD23	2.18	0.42
1:A:59:ASP:OD1	1:A:59:ASP:C	2.62	0.42
1:A:896:LEU:CD1	1:A:980:PRO:HG3	2.49	0.42
2:B:26:CYS:SG	2:B:699:HIS:HB2	2.59	0.42
6:F:115:TYR:CD1	6:F:115:TYR:C	2.97	0.42
7:G:150:THR:HA	7:G:159:ALA:HA	2.01	0.42
13:M:1282:ARG:NE	13:M:1285:ASP:OD2	2.48	0.42
14:N:-5:DG:C4	14:N:-4:DC:C4	3.07	0.42
26:Z:418:HIS:CG	26:Z:420:PHE:CD2	3.07	0.42
1:A:1371:ILE:HG23	1:A:1372:GLU:N	2.34	0.42
2:B:129:THR:HA	2:B:143:GLN:HA	2.02	0.42
2:B:474:THR:HG23	2:B:477:SER:H	1.85	0.42
3:C:65:ALA:O	12:L:57:ALA:HB1	2.19	0.42
5:E:14:ARG:O	5:E:18:MET:HG2	2.19	0.42
7:G:113:ILE:HD11	7:G:128:TYR:CE2	2.55	0.42
11:K:63:VAL:HG13	11:K:70:LYS:O	2.19	0.42
13:M:967:ASN:OD1	13:M:989:VAL:HA	2.19	0.42
14:N:45:DA:C6	14:N:46:DG:C6	3.07	0.42
18:R:369:LEU:CD1	18:R:439:LEU:HD23	2.49	0.42
23:W:107:VAL:HB	23:W:126:HIS:HB3	2.01	0.42
25:Y:70:TRP:CH2	26:Z:260:MET:HB3	2.54	0.42
26:Z:239:ILE:HD11	26:Z:249:TYR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:340:PHE:HZ	26:Z:345:ILE:H	1.66	0.42
29:g:75:LYS:HG2	31:j:931:GLY:N	2.34	0.42
31:j:528:LYS:HB3	31:j:617:ASN:ND2	2.35	0.42
31:j:858:VAL:HG22	31:j:870:MET:SD	2.59	0.42
1:A:567:LEU:HD12	1:A:675:VAL:HG21	2.00	0.42
2:B:805:PHE:CZ	2:B:806:PHE:CE2	3.07	0.42
2:B:1133:HIS:CD2	26:Z:630:VAL:HA	2.54	0.42
3:C:9:VAL:HG11	11:K:105:PHE:CD2	2.55	0.42
3:C:44:ILE:HD11	3:C:176:TRP:HA	2.00	0.42
13:M:522:ASP:OD1	13:M:523:MET:N	2.53	0.42
13:M:539:PHE:CD2	13:M:592:VAL:HG21	2.55	0.42
13:M:1141:TYR:CD1	13:M:1141:TYR:C	2.97	0.42
13:M:1166:LEU:HD23	13:M:1266:ARG:HG3	2.01	0.42
20:T:141:DG:H2"	20:T:142:DT:C6	2.55	0.42
21:U:400:ASP:OD1	21:U:401:GLU:N	2.53	0.42
23:W:54:LEU:HD11	23:W:300:ILE:HD11	2.00	0.42
23:W:153:SER:CB	23:W:195:SER:HA	2.49	0.42
25:Y:14:ARG:CB	25:Y:53:THR:CG2	2.97	0.42
26:Z:562:ASN:C	26:Z:562:ASN:OD1	2.61	0.42
29:g:68:GLY:HA3	30:h:50:HIS:CD2	2.55	0.42
31:j:554:ILE:HG12	31:j:572:PHE:CE1	2.55	0.42
1:A:458:PHE:CE2	1:A:501:MET:SD	3.13	0.42
2:B:270:ILE:HB	2:B:308:ALA:CB	2.49	0.42
13:M:635:TYR:CE2	13:M:1295:LEU:HB2	2.54	0.42
17:Q:452:GLU:HG3	17:Q:495:ILE:HD13	2.01	0.42
17:Q:641:ARG:CG	24:X:250:PHE:CZ	3.02	0.42
19:S:197:ASN:CB	19:S:228:MET:HE3	2.50	0.42
26:Z:285:ILE:HG13	26:Z:310:ARG:HD3	2.01	0.42
32:k:24:ARG:NH1	32:k:33:LYS:HB2	2.34	0.42
1:A:511:THR:HG23	2:B:1102:PHE:CB	2.49	0.42
1:A:828:LEU:HD12	2:B:978:ILE:HG21	2.01	0.42
1:A:866:LYS:NZ	2:B:1091:ARG:HH12	2.18	0.42
1:A:1012:GLY:HA3	1:A:1069:LEU:HD11	2.01	0.42
2:B:78:VAL:HG21	26:Z:206:THR:HG21	2.02	0.42
2:B:313:GLU:OE1	2:B:315:ASN:HB2	2.20	0.42
2:B:789:ASN:HD21	2:B:967:ILE:C	2.27	0.42
2:B:969:PRO:O	2:B:973:PRO:CD	2.68	0.42
2:B:1102:PHE:CZ	2:B:1106:ARG:HG3	2.55	0.42
7:G:13:LEU:HD12	7:G:26:VAL:HG22	2.01	0.42
13:M:395:ARG:O	13:M:399:TRP:HD1	2.02	0.42
13:M:849:THR:HB	13:M:885:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:856:ASP:O	13:M:859:MET:HG2	2.19	0.42
14:N:4:DC:C4'	27:a:121:MET:HE1	2.49	0.42
15:O:1729:LEU:HD11	15:O:1738:LEU:CD2	2.49	0.42
15:O:1776:LEU:HD21	15:O:1809:ILE:HD11	2.01	0.42
18:R:373:CYS:HA	18:R:378:PHE:CE1	2.55	0.42
21:U:526:ARG:HD2	21:U:529:GLU:OE1	2.20	0.42
27:e:81:THR:C	27:e:83:LEU:H	2.27	0.42
29:g:63:ILE:HG12	29:g:94:LEU:HD11	2.01	0.42
31:j:519:PRO:HB3	31:j:521:GLU:OE2	2.20	0.42
31:j:561:VAL:HG13	31:j:604:ASN:HD21	1.84	0.42
31:j:940:GLU:N	31:j:940:GLU:OE1	2.53	0.42
1:A:117:LEU:O	1:A:181:HIS:NE2	2.53	0.42
1:A:121:SER:HB2	1:A:235:VAL:HG21	2.02	0.42
1:A:141:LEU:HD13	1:A:1445:HIS:CE1	2.54	0.42
1:A:264:VAL:HG21	16:P:-10:G:O2'	2.19	0.42
1:A:600:ILE:H	1:A:633:GLY:CA	2.33	0.42
1:A:1085:GLU:OE1	6:F:60:TYR:OH	2.35	0.42
2:B:294:ASP:OD2	2:B:379:ARG:NH2	2.53	0.42
2:B:442:ASP:HA	2:B:445:LYS:HB3	2.02	0.42
4:D:63:LYS:HG3	7:G:102:GLY:O	2.20	0.42
5:E:26:TYR:CD2	5:E:62:VAL:HG13	2.55	0.42
5:E:162:ARG:C	5:E:162:ARG:HD3	2.45	0.42
8:H:118:TYR:HB2	8:H:121:LEU:HB2	2.02	0.42
13:M:369:GLN:HB3	13:M:371:PHE:CZ	2.54	0.42
13:M:452:LYS:HD2	13:M:452:LYS:N	2.34	0.42
13:M:918:ARG:NH1	13:M:981:TYR:CZ	2.88	0.42
28:f:60:LYS:HE2	28:f:64:GLU:OE2	2.20	0.42
31:j:811:TYR:C	31:j:812:ARG:HG3	2.45	0.42
1:A:44:PRO:CG	1:A:285:LYS:HG3	2.49	0.42
1:A:320:ASN:O	1:A:327:ARG:HD2	2.19	0.42
1:A:490:THR:HB	1:A:491:PRO:HD3	2.01	0.42
1:A:531:ASN:OD1	1:A:531:ASN:C	2.63	0.42
1:A:811:ILE:HD13	9:I:79:PRO:HA	2.01	0.42
1:A:880:ARG:NH2	6:F:111:PRO:HB2	2.34	0.42
2:B:565:THR:O	2:B:576:ILE:HA	2.20	0.42
3:C:50:VAL:N	12:L:55:PHE:O	2.48	0.42
13:M:323:ASN:HB3	13:M:399:TRP:CH2	2.55	0.42
13:M:918:ARG:NH1	13:M:981:TYR:OH	2.53	0.42
13:M:1036:LYS:HG2	13:M:1134:TYR:CE2	2.54	0.42
23:W:48:LYS:HD2	23:W:57:GLN:OE1	2.20	0.42
32:k:112:VAL:CG1	32:k:119:LEU:HD11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:THR:O	1:A:52:PRO:HA	2.20	0.42
1:A:389:THR:HG21	1:A:417:LYS:HB3	2.02	0.42
1:A:921:ARG:NH1	1:A:953:GLU:OE2	2.50	0.42
2:B:27:TRP:CZ2	2:B:762:ARG:HB2	2.55	0.42
2:B:330:VAL:HG13	2:B:334:LYS:HB3	2.02	0.42
2:B:472:ARG:NH1	2:B:743:ARG:NH1	2.67	0.42
11:K:5:PRO:HG2	11:K:8:GLU:HG3	2.02	0.42
13:M:642:ASN:O	13:M:644:PRO:HD3	2.20	0.42
21:U:526:ARG:O	21:U:528:PRO:N	2.53	0.42
22:V:259:ALA:HB1	22:V:291:ILE:CD1	2.50	0.42
23:W:60:LEU:HD13	23:W:91:TRP:CB	2.50	0.42
23:W:278:TRP:NE1	23:W:294:ASP:OD1	2.40	0.42
26:Z:292:GLN:HG2	26:Z:293:VAL:N	2.33	0.42
26:Z:726:ASP:OD1	26:Z:727:ALA:N	2.52	0.42
26:Z:745:VAL:CG1	26:Z:750:LEU:HD21	2.48	0.42
27:e:70:ARG:HB3	28:f:26:ASN:CG	2.45	0.42
31:j:664:ASP:O	31:j:742:THR:HB	2.20	0.42
32:k:4:THR:HA	32:k:25:LEU:O	2.20	0.42
1:A:514:GLU:OE2	2:B:1101:GLN:N	2.53	0.41
1:A:903:PHE:HA	1:A:977:VAL:O	2.20	0.41
1:A:1067:TRP:CE3	1:A:1068:LEU:HA	2.55	0.41
1:A:1371:ILE:HG13	1:A:1406:THR:HB	2.02	0.41
2:B:1030:ASN:ND2	2:B:1032:PHE:H	2.18	0.41
2:B:1052:LYS:HE3	2:B:1053:HIS:CE1	2.54	0.41
2:B:1153:TYR:CD1	2:B:1153:TYR:C	2.98	0.41
3:C:38:PHE:HD1	3:C:248:ALA:HB2	1.85	0.41
7:G:9:HIS:NE2	7:G:33:GLU:CD	2.78	0.41
9:I:54:TYR:CZ	9:I:56:ASN:HB2	2.55	0.41
13:M:301:ARG:CZ	13:M:401:GLU:HG2	2.50	0.41
13:M:421:GLN:HG2	13:M:443:LEU:HB2	2.02	0.41
13:M:779:ILE:O	13:M:801:GLY:HA2	2.20	0.41
17:Q:612:LEU:HA	17:Q:615:LEU:HG	2.01	0.41
23:W:164:ALA:HB3	23:W:196:LEU:HD13	2.02	0.41
26:Z:310:ARG:NH2	26:Z:337:GLN:HB2	2.34	0.41
26:Z:603:ILE:HG22	26:Z:642:HIS:O	2.20	0.41
27:a:64:ARG:HB2	27:a:67:PRO:HG2	2.02	0.41
29:g:45:GLY:O	29:g:49:PRO:HD2	2.20	0.41
32:k:114:PHE:CZ	32:k:184:ASN:HB3	2.55	0.41
1:A:54:LEU:HD12	1:A:60:PRO:HD2	2.00	0.41
1:A:90:LEU:HD21	1:A:253:LEU:CB	2.51	0.41
1:A:540:ASP:CB	2:B:790:GLN:HE22	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:PRO:O	8:H:75:TYR:HB2	2.19	0.41
1:A:696:SER:O	1:A:700:GLN:HG2	2.20	0.41
2:B:225:LEU:O	2:B:226:GLU:HG3	2.20	0.41
2:B:278:PHE:CE2	2:B:362:ALA:CB	3.03	0.41
2:B:297:MET:HE3	2:B:377:LEU:HD12	2.01	0.41
2:B:318:LEU:HD23	2:B:336:ILE:HG23	2.00	0.41
2:B:567:ILE:HD12	2:B:567:ILE:N	2.35	0.41
2:B:643:LEU:HD13	2:B:651:TYR:CD2	2.55	0.41
2:B:765:GLU:CD	2:B:770:ARG:HE	2.28	0.41
2:B:791:GLU:O	2:B:792:ASP:HB2	2.20	0.41
3:C:161:LEU:C	3:C:161:LEU:HD12	2.45	0.41
4:D:90:LYS:HE3	4:D:130:ILE:HG12	2.02	0.41
5:E:193:ILE:O	5:E:204:ILE:HA	2.19	0.41
6:F:59:LYS:HE2	6:F:60:TYR:CZ	2.55	0.41
9:I:88:LYS:HE2	9:I:121:HIS:ND1	2.35	0.41
12:L:15:MET:HB3	12:L:28:ILE:O	2.21	0.41
12:L:29:LYS:N	12:L:32:ASP:OD2	2.53	0.41
13:M:441:ARG:HD3	13:M:470:TYR:CG	2.54	0.41
13:M:474:ASP:O	13:M:475:ILE:C	2.63	0.41
13:M:902:GLU:OE2	13:M:918:ARG:NH2	2.45	0.41
21:U:470:HIS:CD2	21:U:484:VAL:HG22	2.54	0.41
25:Y:14:ARG:CB	25:Y:53:THR:HG22	2.50	0.41
26:Z:310:ARG:HB3	26:Z:336:PRO:O	2.19	0.41
29:g:81:PRO:HB3	30:h:62:ILE:CD1	2.50	0.41
1:A:428:ASP:OD2	1:A:430:ARG:NH1	2.49	0.41
1:A:1285:LEU:HD23	1:A:1285:LEU:HA	1.96	0.41
2:B:166:LEU:HD23	2:B:170:ASP:HB3	2.02	0.41
2:B:347:MET:C	2:B:349:PRO:HD3	2.45	0.41
2:B:844:ILE:HD11	26:Z:724:VAL:O	2.20	0.41
4:D:100:LEU:CD2	4:D:115:ILE:HD13	2.49	0.41
4:D:108:ALA:N	4:D:128:GLN:OE1	2.50	0.41
9:I:60:HIS:CB	9:I:103:ARG:HE	2.34	0.41
10:J:65:LEU:O	10:J:66:GLU:C	2.62	0.41
13:M:301:ARG:HD2	13:M:401:GLU:OE2	2.20	0.41
14:N:0:DG:H2'	14:N:1:DT:H71	2.03	0.41
18:R:22:MET:HG3	18:R:26:LYS:HE3	2.02	0.41
23:W:36:VAL:N	23:W:72:ILE:HD11	2.36	0.41
23:W:80:ALA:HB1	23:W:112:LEU:HD21	2.01	0.41
25:Y:34:ASP:OD1	25:Y:34:ASP:N	2.52	0.41
26:Z:480:VAL:CG1	26:Z:486:GLU:HA	2.50	0.41
27:a:53:ARG:NH1	31:j:899:SER:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:48:SER:O	28:b:49:GLY:C	2.64	0.41
31:j:542:VAL:N	31:j:545:ILE:O	2.45	0.41
31:j:918:GLU:C	31:j:920:GLY:H	2.27	0.41
32:k:137:SER:HB2	32:k:151:HIS:CA	2.50	0.41
1:A:713:VAL:HG11	1:A:817:PRO:HG3	2.03	0.41
1:A:915:ALA:HA	1:A:918:LYS:HG2	2.02	0.41
1:A:1020:LEU:O	1:A:1034:GLN:NE2	2.50	0.41
1:A:1228:MET:HG3	1:A:1248:ASN:O	2.20	0.41
2:B:728:MET:HE1	2:B:940:GLY:HA2	2.02	0.41
2:B:810:PHE:O	2:B:925:SER:N	2.53	0.41
4:D:63:LYS:CG	7:G:103:PRO:HA	2.50	0.41
8:H:97:TYR:CE1	8:H:115:TYR:HB3	2.56	0.41
13:M:650:ASP:HB2	13:M:740:TYR:CD2	2.55	0.41
13:M:886:ASP:HA	13:M:1152:MET:SD	2.61	0.41
14:N:2:DG:H4'	14:N:3:DT:OP1	2.19	0.41
14:N:58:DG:N2	20:T:128:DG:N3	2.68	0.41
23:W:44:VAL:HB	23:W:60:LEU:HB2	2.02	0.41
25:Y:9:ASP:OD1	25:Y:10:LEU:N	2.54	0.41
26:Z:278:TRP:CZ3	26:Z:388:PRO:HG3	2.55	0.41
27:e:62:LEU:HD12	28:f:38:LEU:CD2	2.50	0.41
31:j:844:HIS:HD2	31:j:846:GLU:HG2	1.83	0.41
32:k:61:GLY:HA3	32:k:74:TYR:O	2.20	0.41
32:k:371:PHE:CD1	32:k:423:LEU:HD11	2.56	0.41
32:k:389:PHE:HB3	32:k:411:TYR:CD1	2.56	0.41
1:A:18:ILE:HG21	1:A:21:VAL:CG1	2.51	0.41
1:A:32:LYS:HE3	1:A:252:VAL:CG2	2.50	0.41
1:A:87:HIS:HB2	1:A:252:VAL:CG1	2.50	0.41
1:A:94:VAL:HA	1:A:218:PRO:HG2	2.02	0.41
1:A:514:GLU:OE2	2:B:1099:ALA:C	2.63	0.41
1:A:609:HIS:CE1	1:A:613:GLU:HB3	2.56	0.41
1:A:1423:ASP:OD1	1:A:1423:ASP:N	2.42	0.41
2:B:108:MET:CE	2:B:121:SER:O	2.69	0.41
2:B:454:GLY:HA3	2:B:462:ALA:HB2	2.03	0.41
2:B:567:ILE:HA	2:B:612:ILE:O	2.21	0.41
3:C:154:ARG:NE	10:J:64:PRO:HD3	2.36	0.41
13:M:861:ILE:HG13	13:M:862:GLU:N	2.35	0.41
13:M:1287:MET:HE1	13:M:1289:ARG:HB2	2.02	0.41
16:P:-9:U:H2'	16:P:-8:U:C6	2.56	0.41
17:Q:503:LEU:HG	17:Q:507:TYR:CE2	2.56	0.41
21:U:400:ASP:OD2	22:V:172:ARG:N	2.53	0.41
23:W:156:TYR:CE1	23:W:177:ILE:HD13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:595:HIS:O	26:Z:598:ASP:CG	2.63	0.41
27:a:46:THR:O	27:a:50:ARG:CB	2.69	0.41
27:a:104:LEU:HD22	28:b:58:VAL:HG11	2.03	0.41
29:g:58:TYR:CZ	30:h:110:HIS:HB2	2.56	0.41
29:g:75:LYS:HE2	31:j:930:GLU:O	2.21	0.41
31:j:471:GLU:O	31:j:475:ARG:N	2.49	0.41
31:j:816:LEU:O	31:j:826:ASN:ND2	2.39	0.41
32:k:54:ARG:HA	32:k:60:HIS:CE1	2.56	0.41
1:A:196:LEU:HD21	1:A:315:ALA:CB	2.51	0.41
1:A:322:LEU:HD23	1:A:322:LEU:N	2.35	0.41
1:A:586:TRP:HZ2	8:H:75:TYR:CG	2.38	0.41
1:A:713:VAL:HG21	1:A:745:LEU:HD21	2.03	0.41
3:C:20:LYS:HA	3:C:231:TYR:O	2.20	0.41
5:E:52:ARG:HG3	5:E:52:ARG:HH21	1.85	0.41
6:F:107:ARG:NE	6:F:115:TYR:CE1	2.89	0.41
10:J:27:ALA:HB3	10:J:29:TYR:HD1	1.86	0.41
13:M:742:ILE:CG2	13:M:957:ALA:CB	2.98	0.41
13:M:1018:VAL:HG12	13:M:1023:MET:HG2	2.03	0.41
13:M:1166:LEU:HD23	13:M:1266:ARG:CG	2.50	0.41
17:Q:562:GLN:O	17:Q:568:TRP:NE1	2.52	0.41
17:Q:611:TRP:O	17:Q:615:LEU:HG	2.21	0.41
21:U:522:PRO:C	21:U:524:ALA:H	2.29	0.41
26:Z:280:ARG:HB2	26:Z:382:ILE:HG23	2.02	0.41
30:h:55:ILE:O	31:j:947:THR:C	2.63	0.41
31:j:574:CYS:CA	31:j:587:PHE:CZ	3.04	0.41
31:j:680:LEU:HD11	31:j:687:PHE:HB3	2.02	0.41
31:j:683:HIS:N	31:j:701:TYR:OH	2.54	0.41
32:k:11:TYR:HA	32:k:20:ASP:HA	2.03	0.41
32:k:34:ASN:O	32:k:38:GLY:CA	2.69	0.41
32:k:310:LEU:HD12	32:k:314:VAL:CG2	2.50	0.41
1:A:343:LEU:HD23	1:A:349:ARG:CG	2.50	0.41
1:A:440:LEU:HA	1:A:444:TYR:CE2	2.56	0.41
1:A:556:GLU:N	1:A:559:GLU:OE1	2.39	0.41
1:A:611:ASP:OD1	1:A:611:ASP:N	2.53	0.41
1:A:983:LEU:CD1	1:A:1045:LEU:HA	2.51	0.41
1:A:1005:HIS:NE2	1:A:1007:ILE:HB	2.36	0.41
2:B:159:THR:HA	2:B:164:ASN:CG	2.46	0.41
2:B:198:GLU:HG2	2:B:487:SER:HA	2.03	0.41
2:B:603:MET:N	2:B:603:MET:SD	2.94	0.41
2:B:969:PRO:O	2:B:973:PRO:HD3	2.20	0.41
2:B:1132:THR:OG1	2:B:1134:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:134:GLU:OE1	5:E:181:ARG:NH1	2.41	0.41
8:H:20:LYS:HE2	8:H:23:ASP:HA	2.03	0.41
10:J:3:ILE:HD12	10:J:4:PRO:HD2	2.03	0.41
13:M:357:GLN:O	13:M:358:LYS:C	2.63	0.41
20:T:141:DG:H2'	20:T:142:DT:C7	2.25	0.41
31:j:800:PRO:HA	31:j:820:THR:HG22	2.03	0.41
31:j:843:ILE:O	31:j:893:TYR:HA	2.20	0.41
1:A:230:ASP:HB3	1:A:240:PRO:HG3	2.02	0.41
1:A:766:PHE:HB3	1:A:781:ILE:CG1	2.51	0.41
1:A:959:MET:SD	1:A:1050:CYS:HB3	2.61	0.41
1:A:1178:ASP:OD1	1:A:1184:THR:HA	2.21	0.41
1:A:1427:LEU:HB3	1:A:1459:MET:SD	2.61	0.41
2:B:199:LYS:HE2	2:B:202:THR:HG23	2.03	0.41
2:B:208:PHE:CZ	2:B:385:ARG:HG2	2.56	0.41
3:C:47:ILE:HB	3:C:69:GLY:HA2	2.02	0.41
8:H:143:LEU:O	8:H:144:LEU:C	2.63	0.41
12:L:26:ASN:OD1	12:L:36:CYS:HA	2.21	0.41
13:M:285:GLN:H	13:M:285:GLN:CD	2.28	0.41
13:M:321:TYR:HB2	13:M:359:ILE:HD12	2.02	0.41
13:M:742:ILE:HD13	13:M:953:GLU:CB	2.50	0.41
13:M:1268:MET:N	13:M:1278:ASP:O	2.46	0.41
13:M:1271:ASP:CG	13:M:1274:LYS:HB3	2.46	0.41
14:N:52:DA:H1'	14:N:53:DC:O5'	2.20	0.41
15:O:1770:PHE:CZ	15:O:1775:GLY:HA2	2.56	0.41
26:Z:182:VAL:O	26:Z:224:TYR:CB	2.68	0.41
26:Z:585:VAL:HG22	26:Z:595:HIS:CD2	2.56	0.41
27:a:108:THR:HG22	27:a:120:ILE:CG2	2.51	0.41
28:f:32:LYS:HB2	28:f:33:PRO:HD3	2.02	0.41
31:j:585:ASN:HB3	31:j:590:PRO:HB3	2.03	0.41
31:j:723:HIS:CG	31:j:834:VAL:HG11	2.55	0.41
32:k:117:GLN:OE1	32:k:134:SER:N	2.53	0.41
1:A:811:ILE:HG21	9:I:79:PRO:HB3	2.02	0.41
1:A:886:VAL:HG13	5:E:171:PRO:HD3	2.03	0.41
1:A:1304:ILE:HA	1:A:1339:ASP:O	2.21	0.41
2:B:22:TRP:CZ2	2:B:679:PRO:CD	3.04	0.41
2:B:52:GLN:HG3	2:B:160:TYR:OH	2.21	0.41
2:B:59:VAL:HG21	2:B:91:ILE:CD1	2.51	0.41
2:B:173:GLU:C	2:B:175:ASN:H	2.29	0.41
2:B:293:GLU:O	2:B:295:PRO:HD3	2.21	0.41
2:B:407:MET:SD	2:B:444:LEU:HD22	2.61	0.41
2:B:684:GLU:OE1	2:B:684:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:844:ILE:HD13	26:Z:707:GLY:HA2	2.02	0.41
2:B:927:ARG:HB3	2:B:1054:MET:SD	2.61	0.41
2:B:1134:THR:HG23	2:B:1134:THR:O	2.21	0.41
5:E:59:THR:HA	5:E:76:PHE:CE1	2.56	0.41
7:G:123:SER:O	7:G:125:PRO:C	2.64	0.41
7:G:160:ILE:HD11	26:Z:493:VAL:HG12	2.02	0.41
10:J:53:VAL:HG13	10:J:53:VAL:O	2.21	0.41
13:M:836:LEU:O	13:M:837:LYS:C	2.63	0.41
13:M:868:VAL:O	13:M:870:GLU:N	2.53	0.41
13:M:1274:LYS:CE	16:P:-21:U:H4'	2.50	0.41
19:S:224:THR:HG22	19:S:225:ALA:N	2.35	0.41
23:W:9:PHE:CE2	23:W:54:LEU:HB2	2.55	0.41
23:W:218:ASP:OD1	23:W:218:ASP:C	2.63	0.41
26:Z:218:PRO:HB3	26:Z:220:HIS:CE1	2.55	0.41
26:Z:265:LYS:HE3	26:Z:265:LYS:HA	2.02	0.41
26:Z:360:ILE:CD1	26:Z:366:TYR:HD2	2.33	0.41
26:Z:588:ASP:OD1	26:Z:590:GLU:N	2.51	0.41
28:f:36:ARG:HG2	31:j:751:LEU:HD22	2.03	0.41
29:g:29:GLY:HA3	31:j:961:ASP:OD1	2.20	0.41
31:j:468:MET:HE3	31:j:473:LYS:CG	2.51	0.41
31:j:601:ARG:HD3	32:k:161:MET:HG3	2.03	0.41
31:j:654:ASN:CG	31:j:657:ARG:HG3	2.46	0.41
32:k:25:LEU:HB3	32:k:88:PHE:CE1	2.56	0.41
32:k:55:ARG:O	32:k:102:LEU:HD11	2.20	0.41
32:k:65:LEU:HG	32:k:71:VAL:HG13	2.03	0.41
1:A:110:VAL:HG11	1:A:228:ILE:HD13	2.01	0.41
1:A:112:PHE:C	1:A:114:CYS:H	2.29	0.41
1:A:353:ASN:O	1:A:357:LYS:HE2	2.20	0.41
1:A:565:MET:HG3	11:K:62:LYS:HD2	2.03	0.41
2:B:817:GLN:OE1	2:B:817:GLN:N	2.54	0.41
5:E:11:TRP:CZ3	5:E:37:LEU:HB2	2.56	0.41
8:H:58:LEU:HD21	8:H:60:ILE:HG13	2.03	0.41
8:H:63:THR:HG21	8:H:68:GLY:HA2	2.03	0.41
9:I:25:TYR:CD1	9:I:40:ARG:CG	3.04	0.41
13:M:289:ILE:HD13	13:M:300:LEU:HD21	2.02	0.41
13:M:293:ASP:CG	13:M:1024:GLY:HA3	2.46	0.41
13:M:638:LYS:HB3	13:M:1301:TYR:OH	2.20	0.41
13:M:824:GLU:CD	16:P:-18:C:N4	2.79	0.41
27:e:61:LEU:HA	27:e:98:GLU:OE2	2.21	0.41
31:j:572:PHE:CG	32:k:108:ASN:ND2	2.89	0.41
31:j:728:ILE:O	31:j:734:ARG:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:k:88:PHE:CZ	32:k:92:HIS:CD2	3.09	0.41
32:k:186:LEU:HA	32:k:189:ALA:HB3	2.02	0.41
1:A:43:TYR:O	1:A:56:GLY:HA2	2.21	0.40
1:A:45:GLU:CD	1:A:45:GLU:H	2.29	0.40
1:A:59:ASP:OD2	1:A:61:ARG:NH1	2.53	0.40
1:A:83:GLY:O	1:A:257:PRO:HG3	2.21	0.40
1:A:566:PHE:HB3	1:A:674:THR:HG22	2.04	0.40
1:A:1407:CYS:HG	1:A:1408:ARG:HH11	1.69	0.40
2:B:57:ARG:O	2:B:61:ASP:CG	2.65	0.40
2:B:844:ILE:HG13	26:Z:725:LYS:HE3	2.02	0.40
2:B:847:LYS:HG2	2:B:858:VAL:HG11	2.03	0.40
2:B:957:THR:HB	2:B:1026:GLU:OE1	2.21	0.40
4:D:57:LEU:HD13	4:D:61:PHE:CE1	2.56	0.40
13:M:450:ARG:HB3	13:M:463:VAL:HG22	2.03	0.40
13:M:824:GLU:HG2	13:M:826:ARG:NH1	2.36	0.40
17:Q:485:ALA:HA	17:Q:492:TYR:HB2	2.03	0.40
17:Q:513:PHE:CD2	23:W:229:SER:HB2	2.56	0.40
17:Q:697:TYR:CZ	17:Q:729:LYS:HB3	2.56	0.40
24:X:246:SER:O	24:X:250:PHE:CD2	2.74	0.40
26:Z:360:ILE:HD12	26:Z:364:ASN:OD1	2.21	0.40
26:Z:419:ASN:HB3	26:Z:481:ILE:CD1	2.51	0.40
29:g:52:LEU:HD21	30:h:71:PHE:CD1	2.57	0.40
31:j:542:VAL:HG11	32:k:129:PHE:CD1	2.55	0.40
32:k:107:TRP:CD2	32:k:109:TRP:CZ2	3.10	0.40
1:A:189:PRO:HG3	1:A:202:TRP:CZ2	2.56	0.40
1:A:328:ALA:C	1:A:336:LEU:HD23	2.47	0.40
1:A:485:ASN:HB3	1:A:488:VAL:HG23	2.02	0.40
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	2.03	0.40
2:B:292:PHE:CE1	9:I:16:PHE:CE2	3.08	0.40
2:B:643:LEU:HD13	2:B:651:TYR:HD2	1.86	0.40
2:B:650:ASN:C	21:U:460:TYR:OH	2.64	0.40
2:B:830:GLU:O	2:B:832:PRO:HD3	2.21	0.40
5:E:154:GLU:O	5:E:157:THR:OG1	2.39	0.40
9:I:29:ASP:HB3	9:I:34:ILE:H	1.87	0.40
11:K:35:ILE:HB	11:K:71:ILE:HG12	2.03	0.40
17:Q:419:ALA:HB1	17:Q:434:TYR:CE2	2.57	0.40
18:R:455:TRP:CD1	18:R:459:MET:HE3	2.57	0.40
20:T:167:DG:C6	20:T:168:DA:C6	3.09	0.40
21:U:473:ILE:HD13	22:V:216:ASN:HB3	2.03	0.40
22:V:199:VAL:HG12	22:V:200:THR:N	2.37	0.40
26:Z:278:TRP:CD1	26:Z:396:PHE:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:481:ILE:HG12	26:Z:517:ASP:C	2.46	0.40
26:Z:504:SER:OG	26:Z:507:THR:HG22	2.22	0.40
31:j:845:PHE:O	31:j:848:VAL:HG23	2.22	0.40
32:k:103:CYS:SG	32:k:123:ILE:HB	2.60	0.40
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.98	0.40
1:A:566:PHE:CZ	1:A:678:ASN:OD1	2.75	0.40
1:A:1172:ASN:H	1:A:1215:GLU:HG2	1.86	0.40
2:B:417:ILE:HG13	2:B:418:TYR:N	2.37	0.40
2:B:1022:LEU:CD2	3:C:202:GLU:HB3	2.51	0.40
9:I:50:ASN:O	9:I:51:SER:HB2	2.21	0.40
13:M:321:TYR:O	13:M:325:PHE:HB2	2.21	0.40
13:M:574:VAL:HG13	13:M:579:PRO:HA	2.02	0.40
13:M:620:PRO:HG3	13:M:639:TYR:CZ	2.56	0.40
13:M:634:ALA:HA	13:M:637:PHE:CZ	2.57	0.40
13:M:781:VAL:HG11	13:M:920:ILE:HG21	2.03	0.40
17:Q:350:MET:N	17:Q:350:MET:HE2	2.37	0.40
20:T:142:DT:C2	20:T:143:DC:C4	3.09	0.40
23:W:22:VAL:HG21	23:W:290:VAL:CG2	2.51	0.40
23:W:86:ALA:C	23:W:109:ALA:HB3	2.46	0.40
23:W:252:SER:C	23:W:254:LYS:H	2.29	0.40
25:Y:7:PRO:HB3	25:Y:13:LEU:HD21	2.04	0.40
1:A:286:ILE:HD11	1:A:309:LEU:HG	2.03	0.40
1:A:545:VAL:O	1:A:549:THR:HG23	2.21	0.40
1:A:618:TYR:N	1:A:618:TYR:CD1	2.88	0.40
1:A:631:GLU:HG2	1:A:988:TRP:HZ2	1.86	0.40
1:A:1228:MET:HE3	1:A:1257:LEU:HD23	2.03	0.40
2:B:51:ILE:HG21	2:B:160:TYR:CE2	2.56	0.40
2:B:105:PRO:HD3	21:U:526:ARG:HG2	2.03	0.40
2:B:717:ASN:OD1	2:B:979:GLY:N	2.54	0.40
2:B:844:ILE:HG21	26:Z:707:GLY:HA2	2.03	0.40
2:B:1035:ARG:NH2	2:B:1036:LYS:O	2.54	0.40
4:D:18:SER:OG	7:G:82:GLY:HA3	2.22	0.40
5:E:24:ARG:NH1	5:E:181:ARG:O	2.54	0.40
5:E:73:PHE:CG	5:E:75:PHE:CZ	3.09	0.40
13:M:621:THR:O	13:M:622:LYS:C	2.64	0.40
17:Q:239:ALA:HB2	17:Q:257:LEU:HB2	2.04	0.40
17:Q:314:ARG:HD2	22:V:67:GLU:OE2	2.21	0.40
19:S:144:CYS:HB2	19:S:191:VAL:HG11	2.02	0.40
21:U:376:VAL:O	22:V:311:TYR:HB2	2.21	0.40
23:W:104:ALA:HB1	23:W:108:ASP:HB2	2.03	0.40
26:Z:293:VAL:CG2	26:Z:303:ILE:HG13	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:346:ARG:HG2	26:Z:352:VAL:CG2	2.51	0.40
31:j:574:CYS:C	31:j:587:PHE:CZ	2.99	0.40
31:j:660:PRO:HG3	31:j:786:LYS:HB3	2.02	0.40
1:A:896:LEU:HB2	1:A:1396:ARG:NH1	2.37	0.40
1:A:948:ILE:HD12	1:A:1007:ILE:HD13	2.02	0.40
1:A:1227:THR:HG22	1:A:1230:GLN:CD	2.46	0.40
2:B:403:LEU:HD13	2:B:447:SER:OG	2.21	0.40
2:B:506:TRP:CH2	2:B:677:MET:HE1	2.56	0.40
2:B:577:HIS:CE1	2:B:579:ASP:C	3.00	0.40
2:B:651:TYR:HA	21:U:460:TYR:CZ	2.56	0.40
2:B:937:SER:HB2	2:B:1048:TYR:CE1	2.57	0.40
3:C:45:ILE:HG22	3:C:165:ALA:HB1	2.03	0.40
3:C:104:ASP:HA	3:C:160:ARG:HA	2.04	0.40
3:C:146:ASP:OD2	10:J:20:ALA:HB2	2.22	0.40
3:C:180:ALA:O	10:J:10:CYS:CB	2.70	0.40
7:G:124:ASN:HA	7:G:125:PRO:HA	1.91	0.40
11:K:26:LYS:O	11:K:27:VAL:HG13	2.21	0.40
13:M:285:GLN:HA	13:M:288:GLU:CD	2.45	0.40
13:M:330:ILE:O	13:M:332:LEU:HD23	2.22	0.40
13:M:699:SER:OG	13:M:702:VAL:HG22	2.22	0.40
13:M:719:GLN:NE2	13:M:720:PHE:CZ	2.89	0.40
13:M:779:ILE:H	13:M:801:GLY:HA2	1.87	0.40
18:R:366:ARG:NH2	18:R:442:VAL:O	2.55	0.40
21:U:361:GLU:HA	22:V:352:LYS:O	2.22	0.40
26:Z:504:SER:HG	26:Z:509:HIS:H	1.69	0.40
31:j:830:TRP:HA	31:j:831:PRO:C	2.46	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	1436/1970 (73%)	1368 (95%)	65 (4%)	3 (0%)	44	78
2	B	1130/1174 (96%)	1052 (93%)	77 (7%)	1 (0%)	48	83
3	C	254/275 (92%)	239 (94%)	13 (5%)	2 (1%)	16	55
4	D	124/142 (87%)	123 (99%)	1 (1%)	0	100	100
5	E	207/210 (99%)	202 (98%)	5 (2%)	0	100	100
6	F	76/127 (60%)	75 (99%)	1 (1%)	0	100	100
7	G	169/172 (98%)	159 (94%)	10 (6%)	0	100	100
8	H	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	19	56
9	I	115/125 (92%)	106 (92%)	9 (8%)	0	100	100
10	J	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	45/58 (78%)	41 (91%)	4 (9%)	0	100	100
13	M	832/1729 (48%)	792 (95%)	37 (4%)	3 (0%)	30	68
15	O	148/1133 (13%)	140 (95%)	8 (5%)	0	100	100
17	Q	890/1179 (76%)	877 (98%)	13 (2%)	0	100	100
18	R	214/713 (30%)	208 (97%)	6 (3%)	0	100	100
19	S	95/304 (31%)	90 (95%)	5 (5%)	0	100	100
21	U	175/666 (26%)	166 (95%)	8 (5%)	1 (1%)	22	60
22	V	275/531 (52%)	264 (96%)	11 (4%)	0	100	100
23	W	303/305 (99%)	295 (97%)	8 (3%)	0	100	100
24	X	51/531 (10%)	50 (98%)	0	1 (2%)	6	31
25	Y	114/121 (94%)	106 (93%)	7 (6%)	1 (1%)	14	51
26	Z	484/1087 (44%)	457 (94%)	24 (5%)	3 (1%)	22	60
27	a	94/136 (69%)	88 (94%)	6 (6%)	0	100	100
27	e	74/136 (54%)	71 (96%)	3 (4%)	0	100	100
28	b	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
28	f	77/103 (75%)	75 (97%)	2 (3%)	0	100	100
29	g	89/135 (66%)	86 (97%)	3 (3%)	0	100	100
30	h	92/126 (73%)	90 (98%)	1 (1%)	1 (1%)	12	47
31	j	493/1049 (47%)	447 (91%)	35 (7%)	11 (2%)	5	29
32	k	419/709 (59%)	392 (94%)	26 (6%)	1 (0%)	44	78
All	All	8877/15383 (58%)	8445 (95%)	403 (4%)	29 (0%)	38	72

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	Z	342	ALA
26	Z	393	LEU
30	h	105	GLY
31	j	948	PHE
31	j	963	ASP
21	U	527	ASP
31	j	650	SER
31	j	651	LEU
31	j	931	GLY
31	j	943	ILE
31	j	947	THR
31	j	965	ASP
24	X	242	GLY
31	j	944	GLU
32	k	384	THR
1	A	695	ASP
31	j	652	VAL
1	A	442	THR
31	j	712	CYS
1	A	910	LYS
8	H	144	LEU
13	M	1134	TYR
3	C	222	PRO
26	Z	387	LYS
25	Y	96	GLY
2	B	1001	PRO
13	M	980	PRO
3	C	130	VAL
13	M	563	PRO

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	1274/1747 (73%)	1253 (98%)	21 (2%)	58 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	996/1027 (97%)	968 (97%)	28 (3%)	38	57
3	C	235/252 (93%)	231 (98%)	4 (2%)	56	72
4	D	112/126 (89%)	109 (97%)	3 (3%)	40	58
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	65 (96%)	3 (4%)	24	45
7	G	149/153 (97%)	145 (97%)	4 (3%)	40	58
8	H	130/131 (99%)	127 (98%)	3 (2%)	45	64
9	I	105/112 (94%)	102 (97%)	3 (3%)	37	56
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	102 (98%)	2 (2%)	52	69
12	L	44/55 (80%)	44 (100%)	0	100	100
13	M	758/1524 (50%)	743 (98%)	15 (2%)	50	68
15	O	143/1017 (14%)	142 (99%)	1 (1%)	81	87
17	Q	763/1011 (76%)	758 (99%)	5 (1%)	81	87
18	R	163/625 (26%)	162 (99%)	1 (1%)	84	88
19	S	86/268 (32%)	84 (98%)	2 (2%)	45	64
21	U	163/590 (28%)	162 (99%)	1 (1%)	84	88
22	V	255/462 (55%)	251 (98%)	4 (2%)	58	73
23	W	260/260 (100%)	259 (100%)	1 (0%)	89	91
24	X	48/467 (10%)	47 (98%)	1 (2%)	48	66
25	Y	102/105 (97%)	100 (98%)	2 (2%)	50	68
26	Z	438/939 (47%)	426 (97%)	12 (3%)	40	58
27	a	82/110 (74%)	78 (95%)	4 (5%)	21	42
27	e	64/110 (58%)	63 (98%)	1 (2%)	58	73
28	b	65/79 (82%)	64 (98%)	1 (2%)	60	75
28	f	64/79 (81%)	62 (97%)	2 (3%)	35	54
29	g	72/104 (69%)	71 (99%)	1 (1%)	62	75
30	h	80/105 (76%)	80 (100%)	0	100	100
31	j	446/929 (48%)	438 (98%)	8 (2%)	54	71
32	k	380/631 (60%)	370 (97%)	10 (3%)	41	59
All	All	7895/13483 (59%)	7752 (98%)	143 (2%)	54	71

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	67	ARG
1	A	81	CYS
1	A	144	VAL
1	A	205	VAL
1	A	216	LEU
1	A	365	THR
1	A	382	ARG
1	A	406	VAL
1	A	546	ARG
1	A	567	LEU
1	A	811	ILE
1	A	883	ILE
1	A	1007	ILE
1	A	1038	THR
1	A	1128	ILE
1	A	1140	THR
1	A	1155	LYS
1	A	1227	THR
1	A	1264	SER
1	A	1456	GLU
2	B	135	GLU
2	B	139	GLN
2	B	166	LEU
2	B	199	LYS
2	B	230	ARG
2	B	234	THR
2	B	309	PHE
2	B	313	GLU
2	B	355	ASP
2	B	358	GLU
2	B	388	TYR
2	B	415	VAL
2	B	437	THR
2	B	455	ASP
2	B	528	LEU
2	B	548	TRP
2	B	567	ILE
2	B	656	LEU
2	B	666	ASP
2	B	685	LYS
2	B	750	VAL

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Mol	Chain	Res	Type
2	B	759	VAL
2	B	768	ARG
2	B	842	HIS
2	B	897	ARG
2	B	1048	TYR
2	B	1118	VAL
2	B	1157	LEU
3	C	5	ASN
3	C	96	GLU
3	C	147	ASP
3	C	151	VAL
4	D	76	ASN
4	D	96	GLU
4	D	107	THR
6	F	84	GLU
6	F	86	GLU
6	F	123	LEU
7	G	67	LEU
7	G	70	VAL
7	G	138	GLN
7	G	160	ILE
8	H	14	ASP
8	H	50	VAL
8	H	133	HIS
9	I	15	ARG
9	I	50	ASN
9	I	124	THR
11	K	27	VAL
11	K	71	ILE
13	M	594	LEU
13	M	612	GLU
13	M	792	HIS
13	M	806	THR
13	M	910	LEU
13	M	990	CYS
13	M	1015	THR
13	M	1038	ASP
13	M	1134	TYR
13	M	1161	PHE
13	M	1170	ASN
13	M	1171	VAL
13	M	1231	ARG

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Mol	Chain	Res	Type
13	M	1257	VAL
13	M	1264	HIS
15	O	2029	SER
17	Q	531	VAL
17	Q	854	GLN
17	Q	857	LEU
17	Q	861	GLU
17	Q	862	GLU
18	R	40	LEU
19	S	158	TYR
19	S	182	ASN
21	U	467	ASP
22	V	66	LEU
22	V	100	LEU
22	V	285	ASP
22	V	286	VAL
23	W	240	PHE
24	X	213	PHE
25	Y	6	VAL
25	Y	40	LEU
26	Z	235	VAL
26	Z	259	GLU
26	Z	265	LYS
26	Z	273	LEU
26	Z	288	ASP
26	Z	390	LEU
26	Z	457	LEU
26	Z	459	ASP
26	Z	471	TYR
26	Z	488	ASP
26	Z	500	VAL
26	Z	624	LEU
27	a	54	ARG
27	a	64	ARG
27	a	85	PHE
27	a	121	MET
28	b	89	TYR
27	e	82	ASP
28	f	40	ARG
28	f	47	ILE
29	g	102	THR
31	j	485	LEU

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Mol	Chain	Res	Type
31	j	829	GLU
31	j	847	ARG
31	j	849	GLN
31	j	852	LEU
31	j	938	ASP
31	j	944	GLU
31	j	945	ASP
32	k	20	ASP
32	k	56	VAL
32	k	60	HIS
32	k	68	ASN
32	k	95	LEU
32	k	122	ASP
32	k	231	ASP
32	k	232	TYR
32	k	243	PHE
32	k	384	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	96	HIS
1	A	410	ASN
1	A	721	HIS
1	A	783	GLN
1	A	989	ASN
1	A	1044	HIS
1	A	1251	ASN
1	A	1422	GLN
2	B	73	HIS
2	B	319	ASN
2	B	731	GLN
2	B	749	HIS
2	B	992	ASN
2	B	1003	ASN
2	B	1030	ASN
2	B	1117	HIS
3	C	18	ASN
3	C	51	GLN
3	C	111	GLN
3	C	260	GLN

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Mol	Chain	Res	Type
5	E	169	GLN
9	I	22	ASN
9	I	41	ASN
11	K	29	ASN
11	K	36	ASN
11	K	40	HIS
13	M	595	GLN
13	M	792	HIS
13	M	858	GLN
13	M	979	HIS
13	M	1007	ASN
13	M	1151	ASN
17	Q	278	HIS
17	Q	564	HIS
17	Q	651	ASN
17	Q	686	ASN
17	Q	706	ASN
18	R	367	HIS
18	R	488	ASN
19	S	189	ASN
19	S	239	ASN
21	U	451	HIS
21	U	465	GLN
21	U	468	HIS
22	V	298	ASN
23	W	98	GLN
23	W	184	HIS
25	Y	75	GLN
26	Z	232	GLN
26	Z	446	ASN
26	Z	545	GLN
26	Z	591	GLN
26	Z	592	ASN
26	Z	595	HIS
26	Z	607	HIS
29	g	105	GLN
31	j	710	GLN
31	j	818	GLN
32	k	70	HIS
32	k	92	HIS
32	k	108	ASN
32	k	271	HIS

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Mol	Chain	Res	Type
32	k	363	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	20/21 (95%)	8 (40%)	5 (25%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	-20	C
16	P	-17	C
16	P	-16	U
16	P	-13	G
16	P	-12	C
16	P	-10	G
16	P	-9	U
16	P	-8	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	-21	U
16	P	-13	G
16	P	-11	G
16	P	-10	G
16	P	-9	U

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 10 ligands modelled in this entry, 10 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.

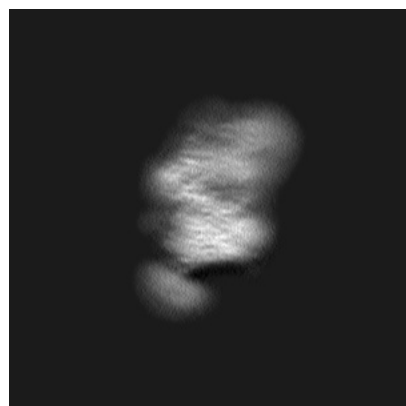
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54537. These allow visual inspection of the internal detail of the map and identification of artifacts.

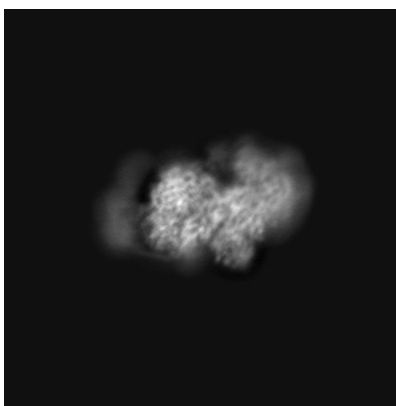
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

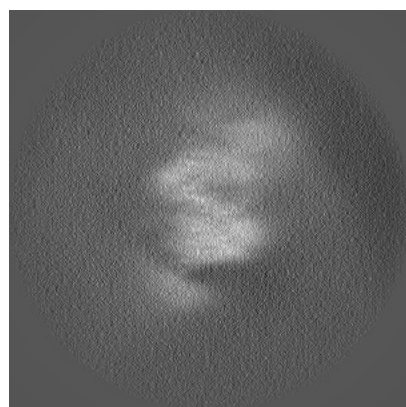


Y

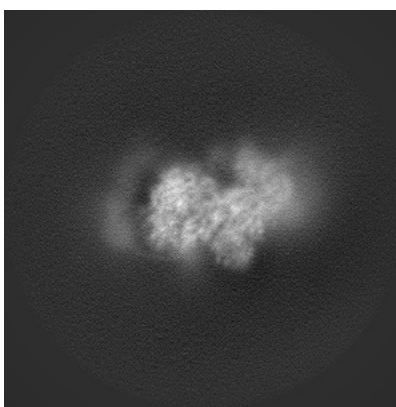


Z

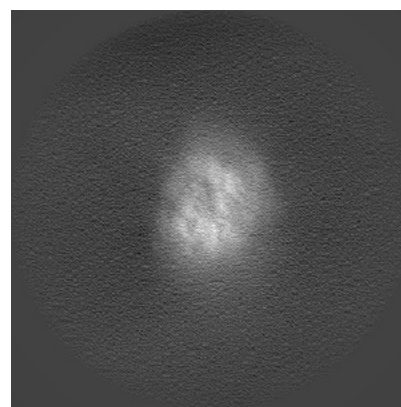
6.1.2 Raw map



X



Y

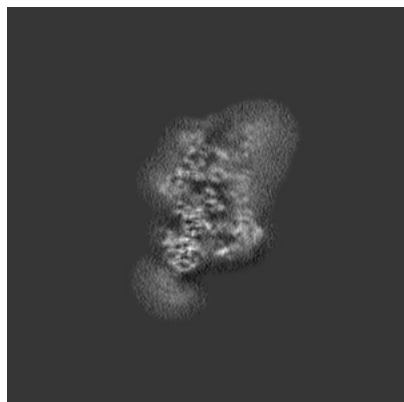


Z

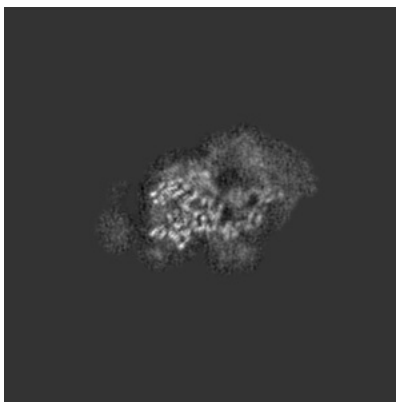
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

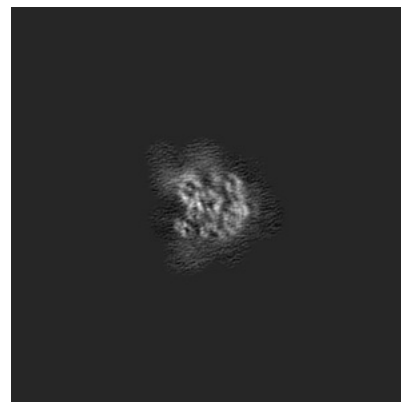
6.2.1 Primary map



X Index: 256

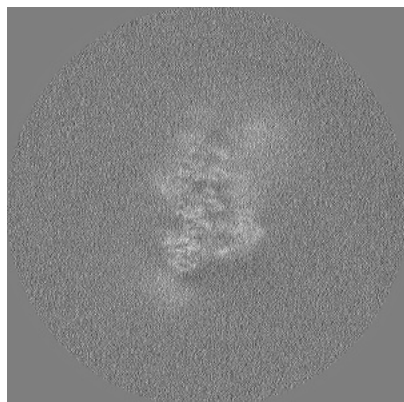


Y Index: 256

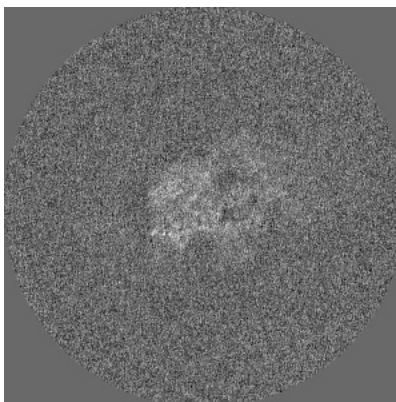


Z Index: 256

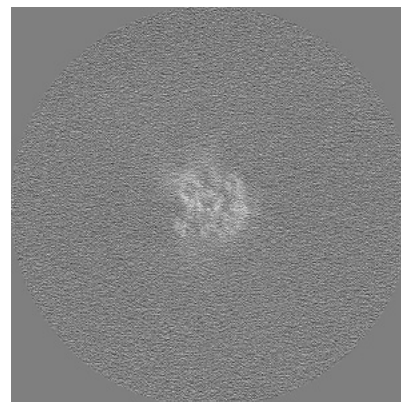
6.2.2 Raw map



X Index: 256



Y Index: 256

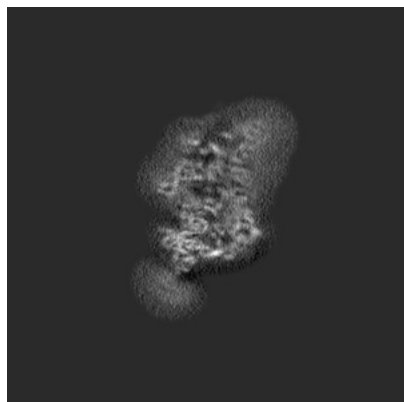


Z Index: 256

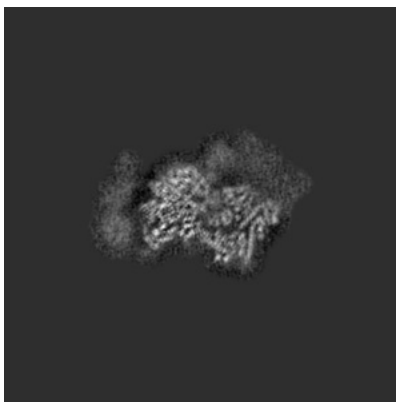
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

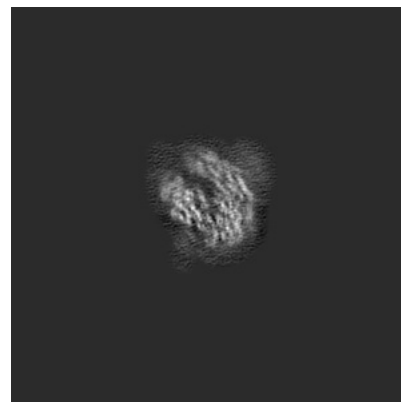
6.3.1 Primary map



X Index: 260

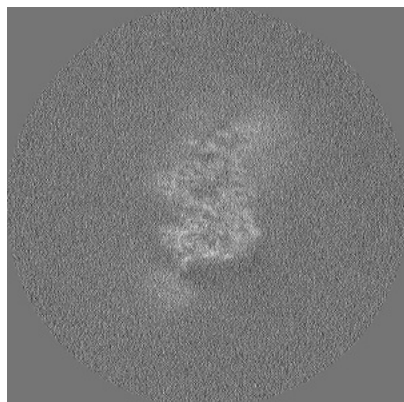


Y Index: 234

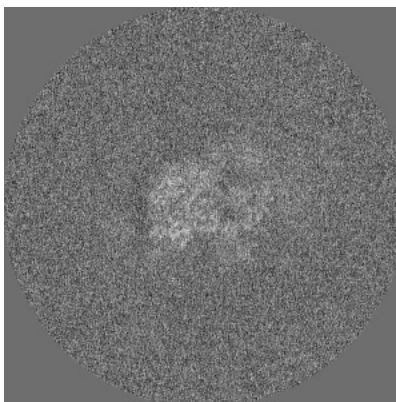


Z Index: 219

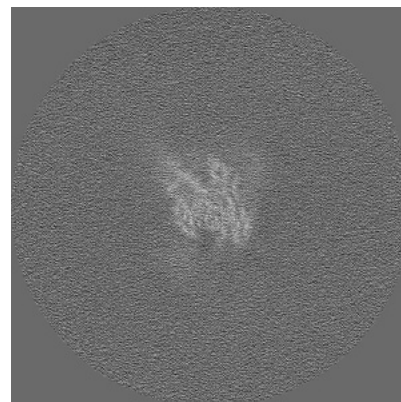
6.3.2 Raw map



X Index: 262



Y Index: 254

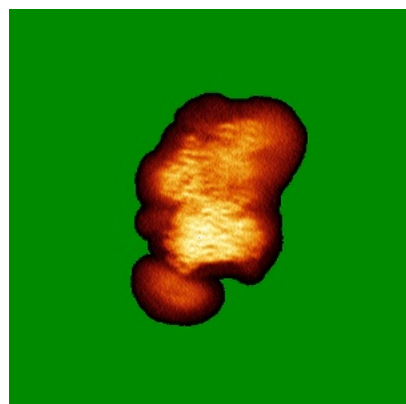


Z Index: 232

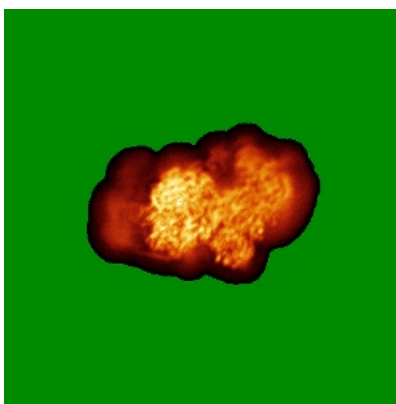
The images above show the largest variance slices of the map in three orthogonal directions.

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

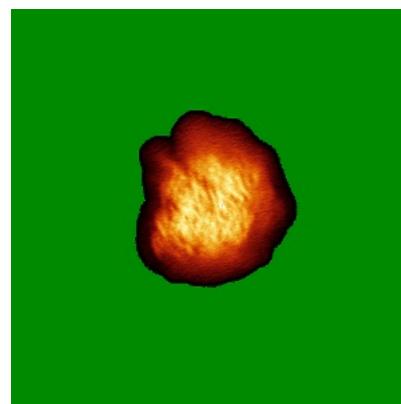
6.4.1 Primary map



X

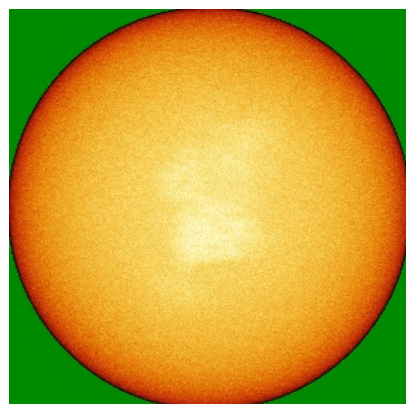


Y

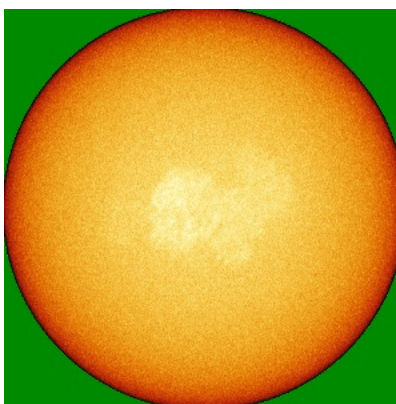


Z

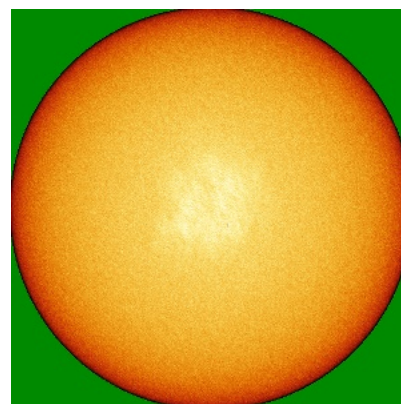
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



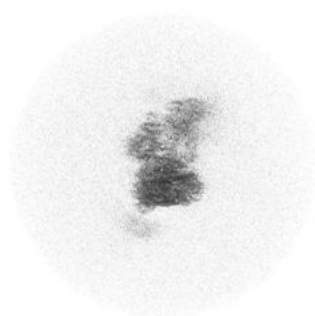
Y



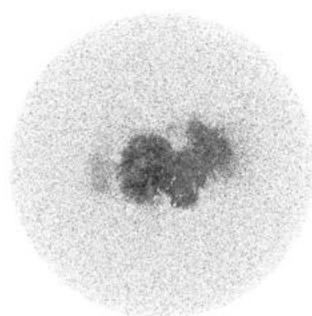
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

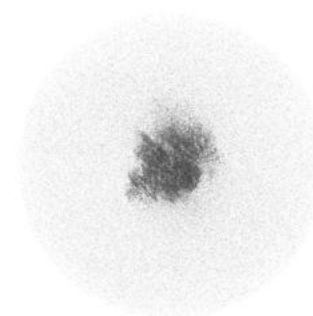
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

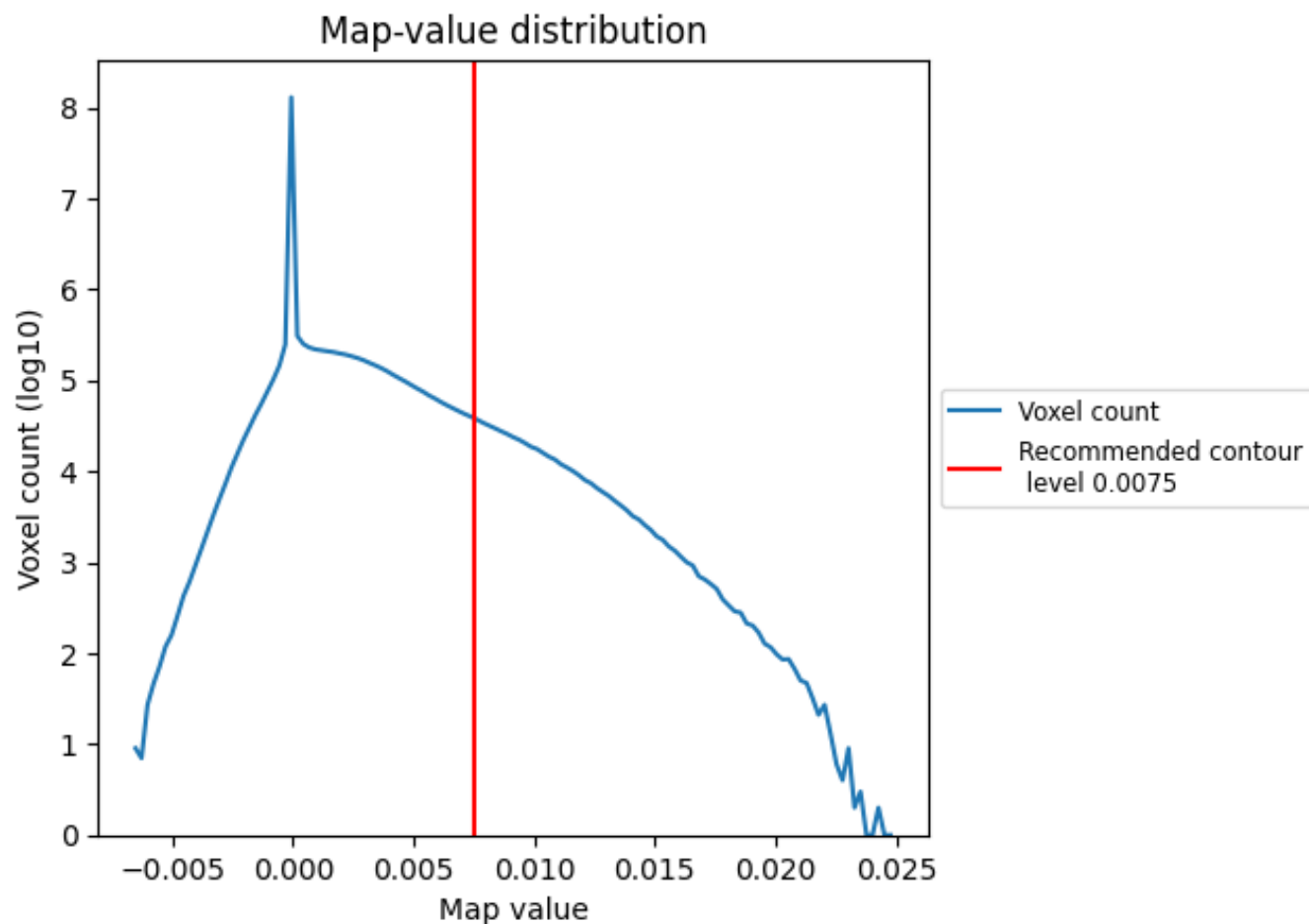
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

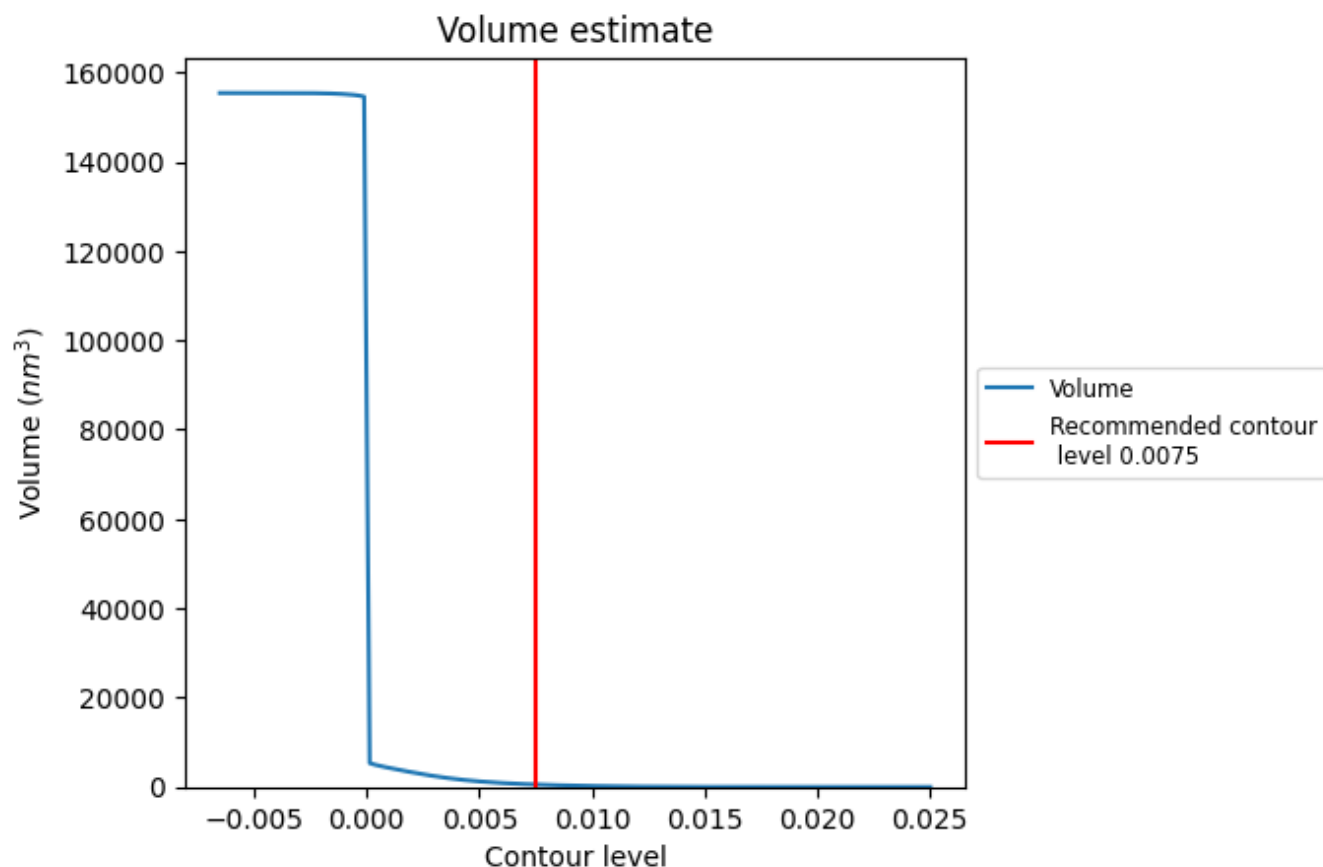
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

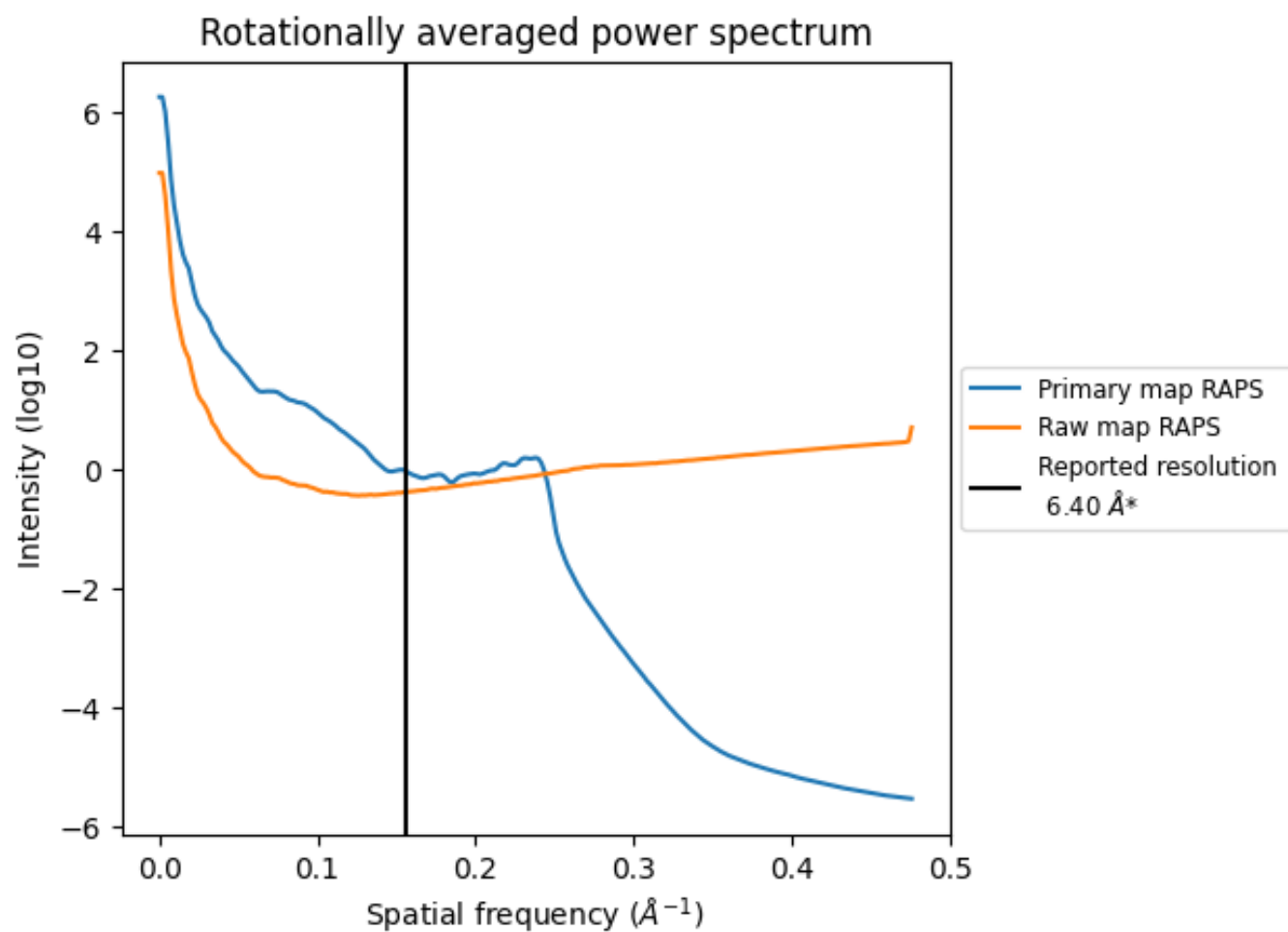
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 539 nm^3 ; this corresponds to an approximate mass of 487 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

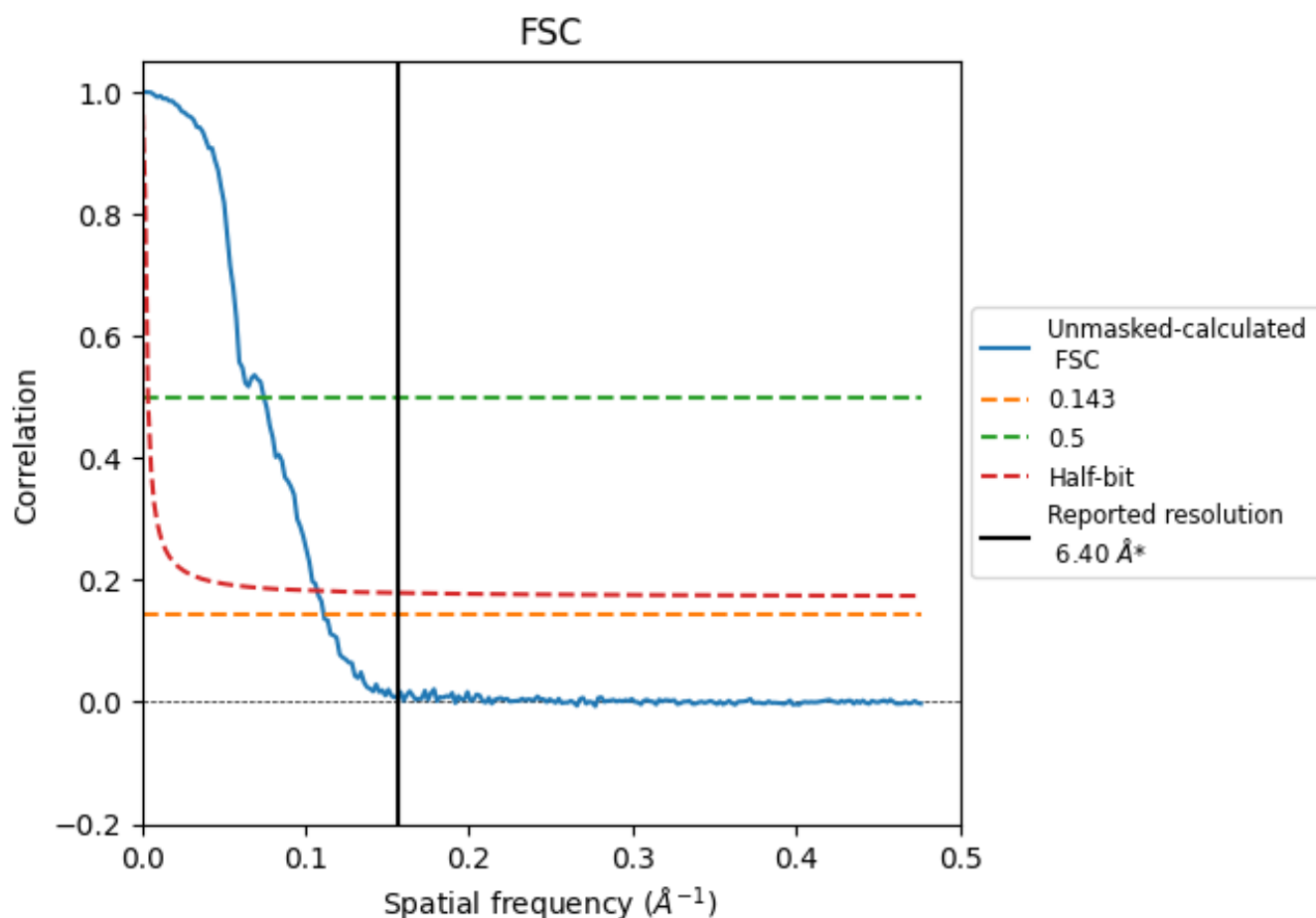


*Reported resolution corresponds to spatial frequency of 0.156 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.156 Å⁻¹

8.2 Resolution estimates [i](#)

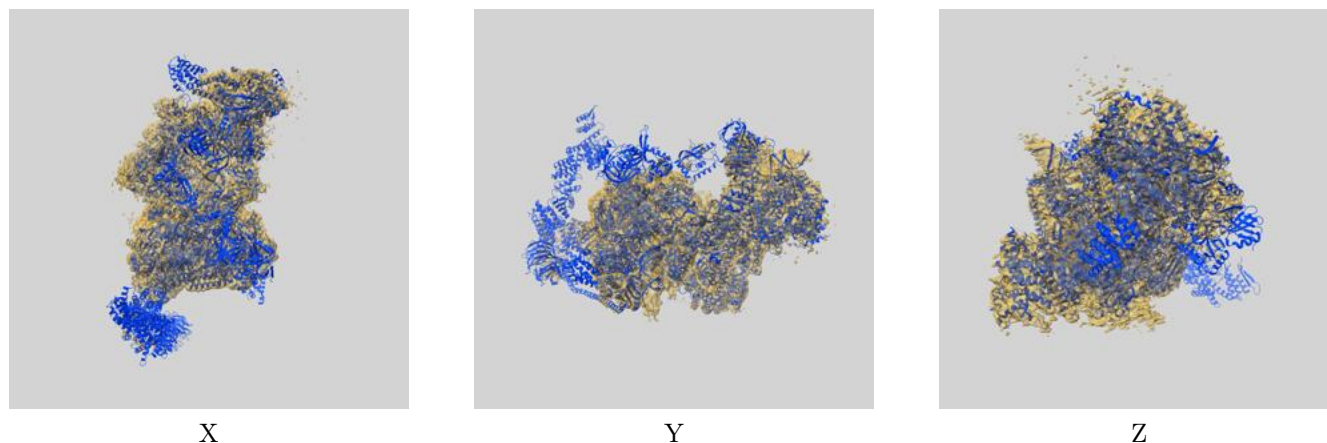
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.00	13.42	9.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.00 differs from the reported value 6.4 by more than 10 %

9 Map-model fit [i](#)

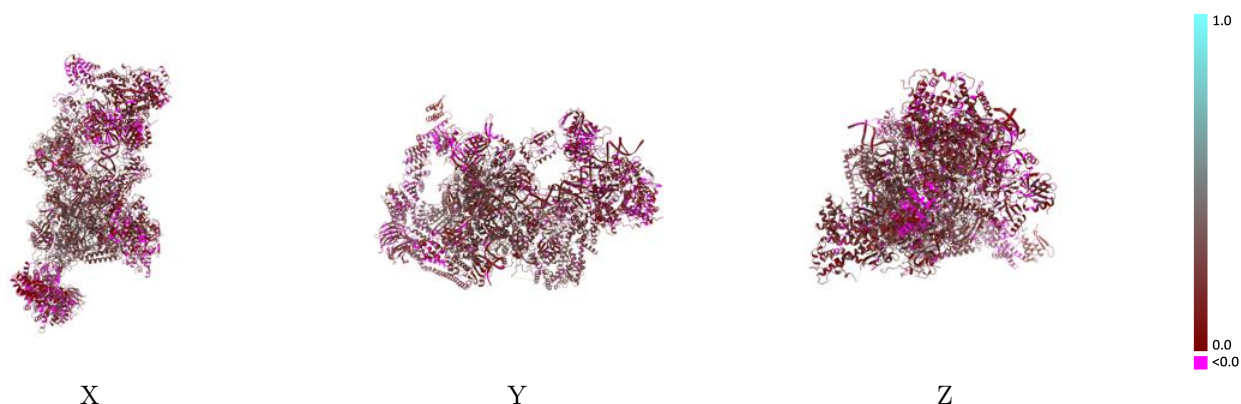
This section contains information regarding the fit between EMDB map EMD-54537 and PDB model 9S3G. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



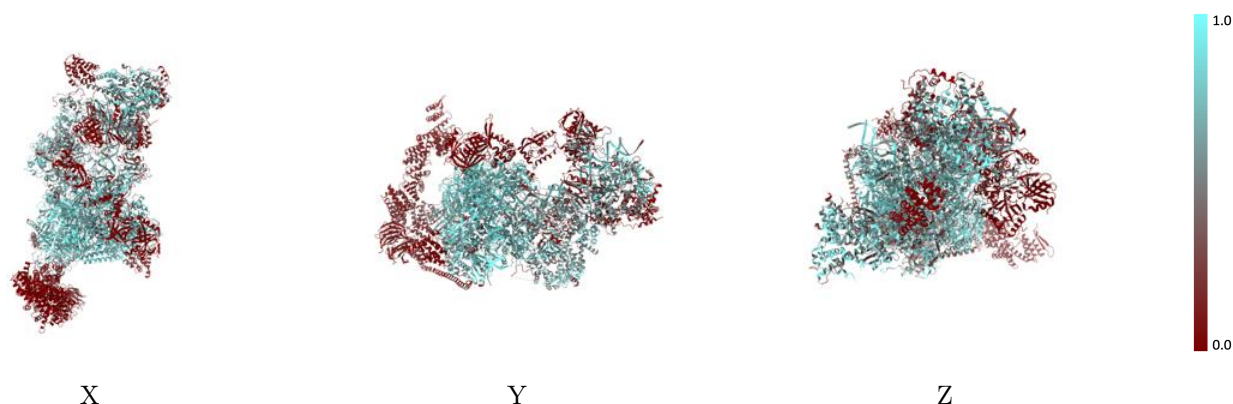
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



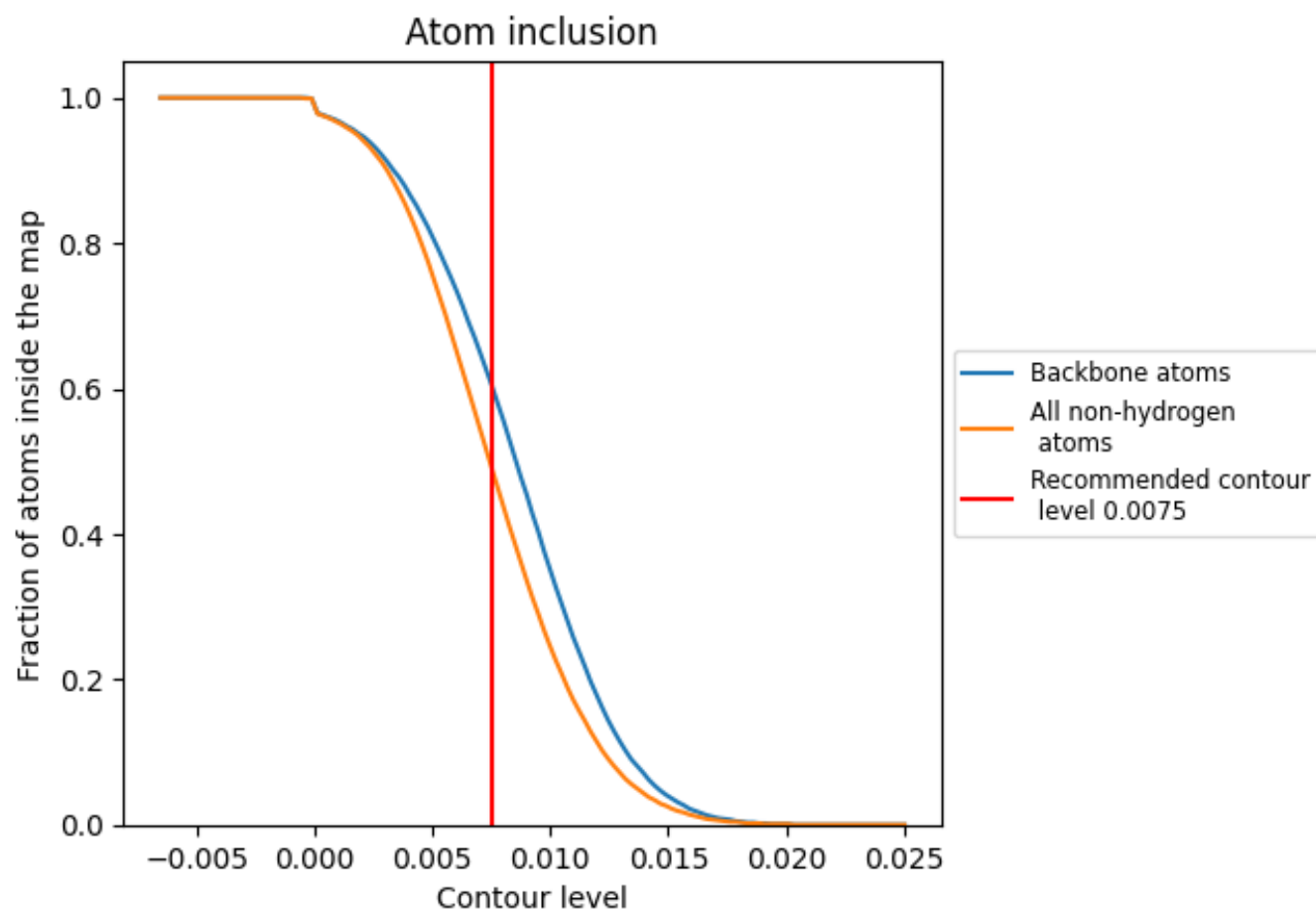
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0075).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4920	 0.1870
A	 0.7390	 0.2670
B	 0.7600	 0.2350
C	 0.7600	 0.2460
D	 0.6450	 0.2200
E	 0.7590	 0.2360
F	 0.7860	 0.2840
G	 0.5810	 0.2380
H	 0.5710	 0.2990
I	 0.6930	 0.2060
J	 0.8610	 0.2190
K	 0.6350	 0.2560
L	 0.7120	 0.1990
M	 0.6220	 0.2070
N	 0.7560	 0.1580
O	 0.0230	 0.0020
P	 0.7250	 0.2130
Q	 0.0240	 0.1120
R	 0.1120	 0.1590
S	 0.0050	 0.0430
T	 0.7810	 0.1630
U	 0.0480	 0.1170
V	 0.0060	 0.1050
W	 0.0130	 0.1270
X	 0.0190	 0.1540
Y	 0.3710	 0.1640
Z	 0.5420	 0.2020
a	 0.5380	 0.1330
b	 0.5830	 0.1500
e	 0.4330	 0.1230
f	 0.4050	 0.1280
g	 0.4670	 0.1040
h	 0.4520	 0.1130
j	 0.4520	 0.1520
k	 0.2270	 0.1030

