



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:13 AM UTC

PDB ID : 9L5R / pdb_00009l5r
EMDB ID : EMD-62841
Title : Cryo-EM structure of the thermophile spliceosome (state ILS)
Authors : Li, Y.; Fischer, P.; Wang, M.; Yuan, R.; Meng, W.; Luehrmann, R.; Lau, B.; Hurt, E.; Cheng, J.
Deposited on : 2024-12-23
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

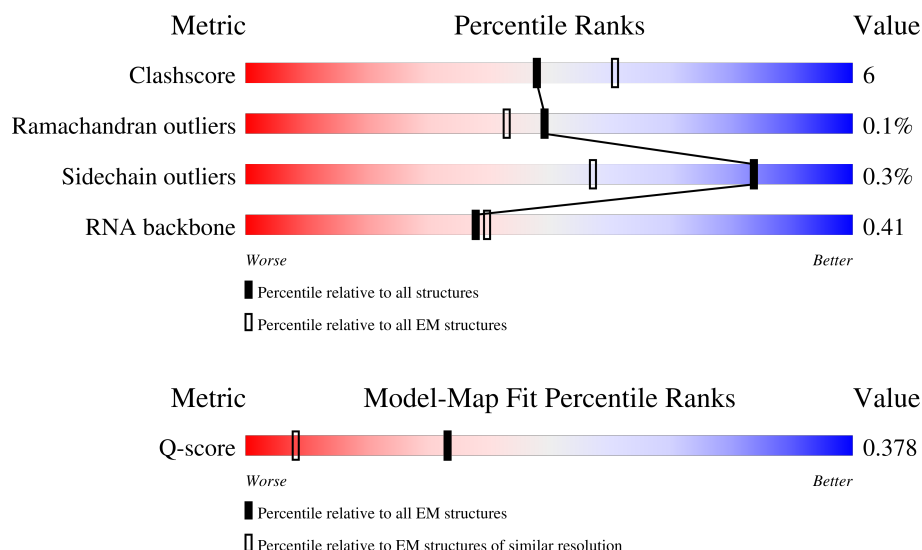
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	2	193	
2	5	116	
3	6	101	

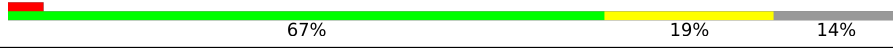
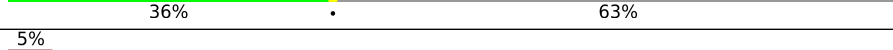
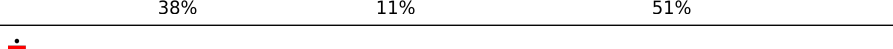
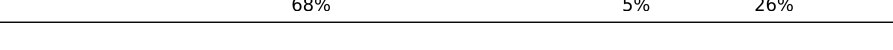
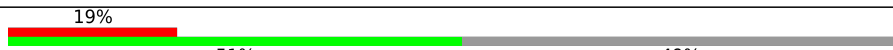
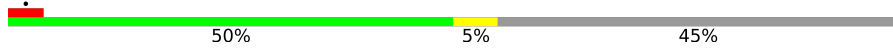
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Mol	Chain	Length	Quality of chain
4	A	2463	
5	B	326	
6	C	1011	
7	D	325	
8	E	352	
9	F	233	
10	I	839	
11	J	687	
12	L	768	
13	K	231	
14	q	480	
14	r	480	
14	s	480	
14	t	480	
15	N	148	
16	S	167	
17	T	496	
18	U	757	
19	M	395	
20	o	408	
21	R	578	
22	W	547	
23	P	260	
24	Y	1416	
25	a	98	

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Mol	Chain	Length	Quality of chain
25	j	98	
26	b	94	
26	l	94	
27	c	592	
27	m	592	
28	d	118	
28	o	118	
29	e	211	
29	p	211	
30	f	114	
30	u	114	
31	g	82	
31	k	82	
32	h	242	
33	i	201	
34	CY	510	
35	Cb	975	
36	Cc	764	
37	7	101	
38	Ci	153	
39	H	22	

2 Entry composition [i](#)

There are 44 unique types of molecules in this entry. The entry contains 104144 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 RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	106	Total	C	N	O	P	0	0
			2224	994	357	767	106		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	111	Total	C	N	O	P	0	0
			2343	1048	398	786	111		

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	98	Total	C	N	O	P	0	0
			2090	935	379	678	98		

- Molecule 4 is a protein called PRP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	2006	Total	C	N	O	S	0	0
			16540	10628	2874	2976	62		

- Molecule 5 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	258	Total	C	N	O	S	0	0
			2071	1273	388	405	5		

- Molecule 6 is a protein called SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	922	Total	C	N	O	S	0	0
			7301	4668	1229	1368	36		

- Molecule 7 is a protein called SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	95	Total	C	N	O	S	0	0
			786	477	150	154	5		

- Molecule 8 is a protein called Anaphase-promoting complex subunit 4-like WD40 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	310	Total	C	N	O	S	0	0
			2379	1493	414	462	10		

- Molecule 9 is a protein called CCDC12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	110	Total	C	N	O	S	0	0
			879	544	166	167	2		

- Molecule 10 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	738	Total	C	N	O	S	0	0
			6135	3924	1071	1112	28		

- Molecule 11 is a protein called Suppressor of forked domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	608	Total	C	N	O	S	0	0
			5176	3297	937	929	13		

- Molecule 12 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	637	Total	C	N	O	S	0	0
			5052	3111	952	974	15		

- Molecule 13 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	231	Total	C	N	O	S	0	0
			1797	1122	317	354	4		

- Molecule 14 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	q	139	Total	C	N	O	S	0	0
			1110	699	195	214	2		
14	t	141	Total	C	N	O	S	0	0
			1122	707	197	216	2		
14	r	143	Total	C	N	O	S	0	0
			1132	713	199	218	2		
14	s	140	Total	C	N	O	S	0	0
			1115	702	196	215	2		

- Molecule 15 is a protein called Putative bud site selection protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	148	Total	C	N	O	S	0	0
			1200	755	213	220	12		

- Molecule 16 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	157	Total	C	N	O	S	0	0
			1209	763	217	223	6		

- Molecule 17 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	328	Total	C	N	O	S	0	0
			2565	1621	461	469	14		

- Molecule 18 is a protein called Cell cycle control protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	348	Total	C	N	O	S	0	0
			2821	1770	516	524	11		

- Molecule 19 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	248	Total	C	N	O	S	0	0
			1964	1238	355	354	17		

- Molecule 20 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	0	276	Total	C	N	O	S	0	0
			2224	1381	424	412	7		

- Molecule 21 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	340	Total	C	N	O	P S	0	0
			2686	1664	509	503	2 8		

- Molecule 22 is a protein called PRP17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	397	Total	C	N	O	S	0	0
			2224	1336	444	440	4		

- Molecule 23 is a protein called Putative pre-mRNA splicing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	114	Total	C	N	O	S	0	0
			925	577	182	165	1		

- Molecule 24 is a protein called Pre-mRNA-splicing factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	1344	Total	C	N	O	S	0	0
			10819	6892	1900	2002	25		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	86	Total	C	N	O		0	0
			426	253	86	87			
25	j	88	Total	C	N	O	S	0	0
			704	456	121	126	1		

- Molecule 26 is a protein called Sm protein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	71	Total	C	N	O		0	0
			351	209	71	71			
26	l	81	Total	C	N	O	S	0	0
			649	412	114	120	3		

- Molecule 27 is a protein called Delta(14)-sterol reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	84	Total	C	N	O		0	0
			416	247	84	85			
27	m	86	Total	C	N	O	S	0	0
			678	427	129	118	4		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	81	Total	C	N	O		0	0
			401	239	81	81			
28	o	87	Total	C	N	O	S	0	0
			679	433	114	128	4		

- Molecule 29 is a protein called Sm protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	79	Total	C	N	O		0	0
			388	230	79	79			
29	p	103	Total	C	N	O	S	0	0
			788	490	148	145	5		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	84	Total	C	N	O		0	0
			414	246	84	84			
30	u	90	Total	C	N	O	S	0	0
			716	449	132	131	4		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	72	Total	C	N	O		0	0
			354	210	72	72			
31	k	73	Total	C	N	O	S	0	0
			577	369	101	105	2		

- Molecule 32 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	h	122	Total	C	N	O	0	0
			605	361	122	122		

- Molecule 33 is a protein called U2 small nuclear ribonucleoprotein B'-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	i	102	Total	C	N	O	0	0
			504	300	102	102		

- Molecule 34 is a protein called Nineteen complex-related protein 2-domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	CY	91	Total	C	N	O	0	0
			444	262	91	91		

- Molecule 35 is a protein called G-patch domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Cb	505	Total	C	N	O	0	0
			2496	1486	505	505		

- Molecule 36 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Cc	714	Total	C	N	O	0	0
			3541	2112	714	715		

- Molecule 37 is a RNA chain called Unknown mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	7	26	Total	C	N	O	P	0	0
			494	241	68	159	26		

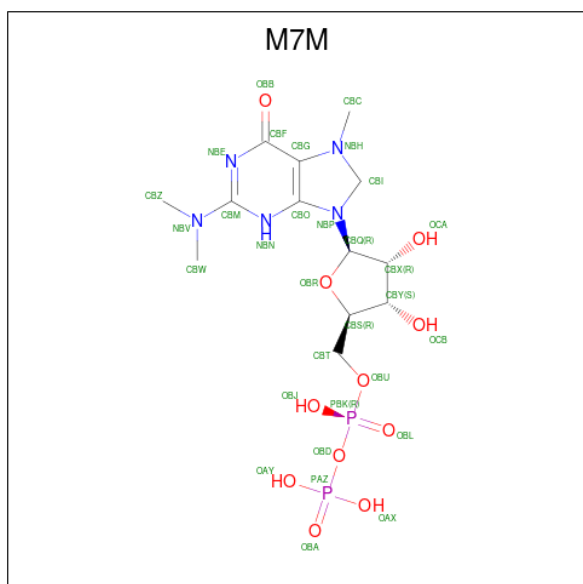
- Molecule 38 is a protein called Putative cyclophilin protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	Ci	84	Total	C	N	O	0	0
			415	247	84	84		

- Molecule 39 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	H	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 40 is N,N,7-trimethylguanosine 5'-(trihydrogen diphosphate) (CCD ID: M7M) (formula: $\text{C}_{13}\text{H}_{23}\text{N}_5\text{O}_{11}\text{P}_2$).

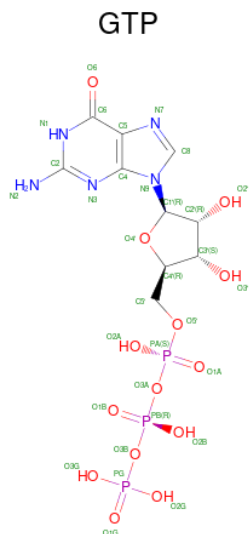


Mol	Chain	Residues	Atoms					AltConf
40	B	1	Total	C	N	O	P	0
			30	13	5	10	2	

- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

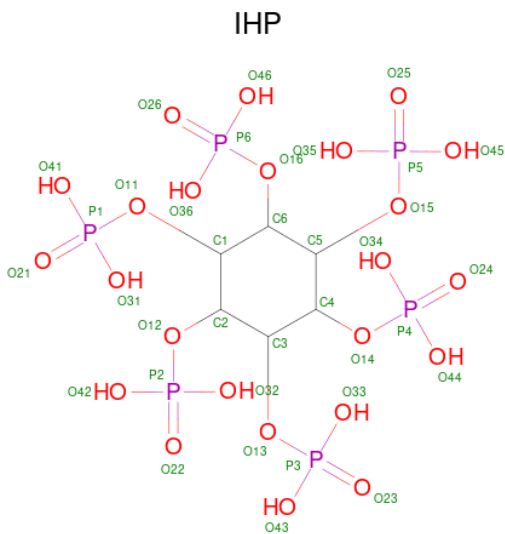
Mol	Chain	Residues	Atoms		AltConf
41	C	1	Total 1	Mg 1	0

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
42	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 43 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $\text{C}_6\text{H}_{18}\text{O}_{24}\text{P}_6$).



Mol	Chain	Residues	Atoms				AltConf
43	J	1	Total	C	O	P	0
			36	6	24	6	

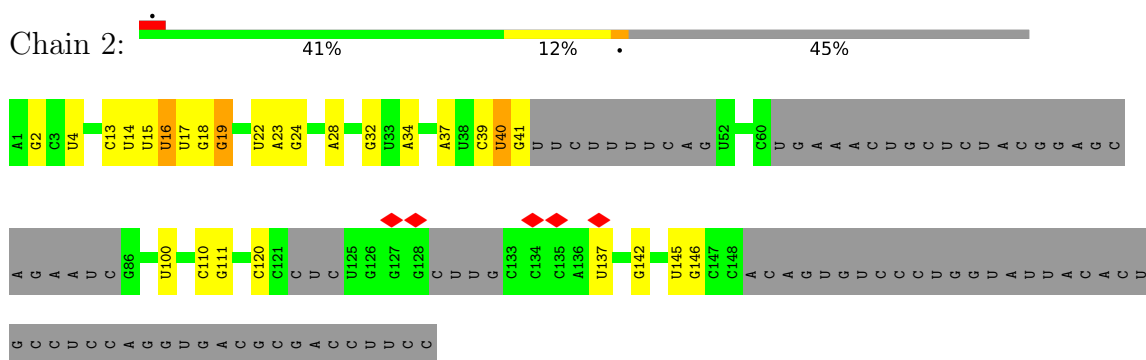
- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
44	N	3	Total 3	Zn 3	0
44	U	1	Total 1	Zn 1	0
44	M	2	Total 2	Zn 2	0

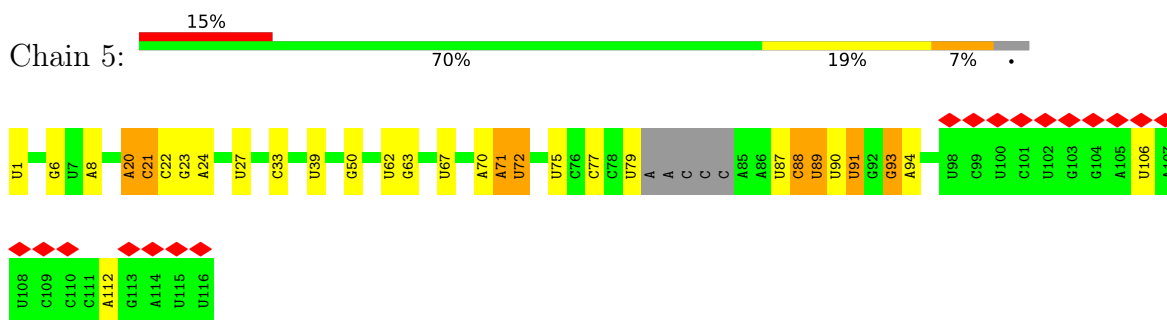
3 Residue-property plots [i](#)

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

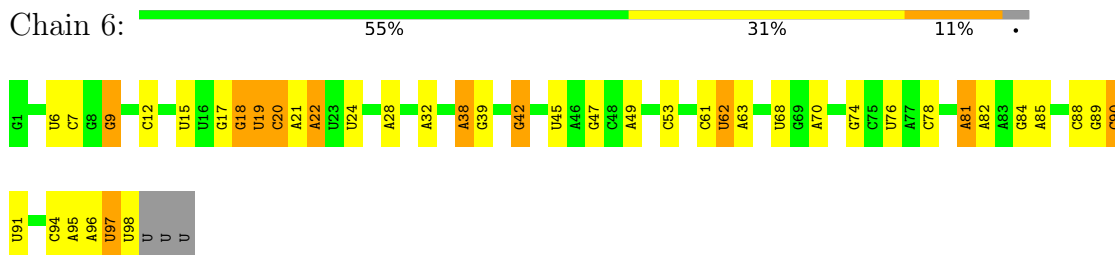
• Molecule 1: U2 snRNA



• Molecule 2: U5 snRNA



• Molecule 3: U6 snRNA



• Molecule 4: PRP8

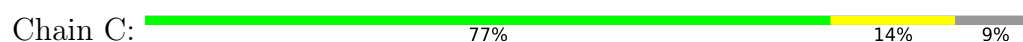




- Molecule 5: Pre-mRNA-splicing factor SYF2

[illegible]

- Molecule 6: SNU114



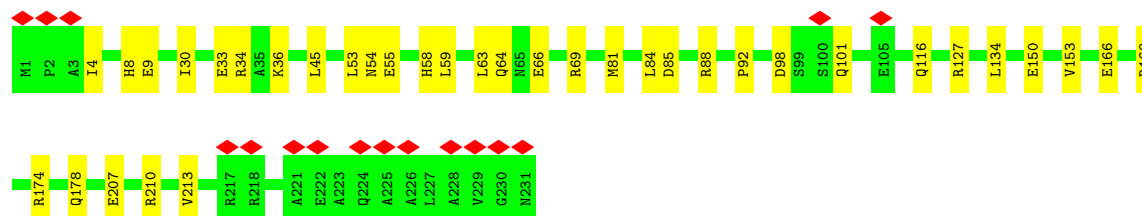
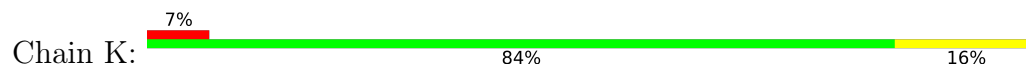
V884	A761	V553	K238	GLY	THR
V887	Y768	D561	D252	TYR	GLN
M889	A775	F575	D255	ALA	ARG
S892	A780	P589	E256	ASP	THR
R893	L791	L595	V264	GLU	ARG
R894	Q792	V604	D265	VAL	LEU
L899	D793	K605	C268	ASP	LEU
S900	K802	I609	D292	GLU	GLY
V912	L805	D619	K301	PRO	SER
N913	A806	L634	R304	ALA	SER
G914	T807	K635	E308	GLU	THR
P917	V808	L309	L309	GLN	THR
D920	K809	I641	I311	ASP	ASP
E810	S811	N642	I311	NET	SER
Q935	I812	E645	I335	ASN	ASN
A936	R813	E662	I335	ILE	HIS
M937	C826	K655	R338	ASP	THR
L940	T833	P661	S341	GLU	PHE
V941	L837	L662	K397	PRO	PRO
T959	V840	E668	P404	LEU	ASP
T966	F843	G671	E405	PRO	ALA
D973	W846	I674	E407	SER	ALA
F974	W847	E680	G408	ASP	ALA
V975	P848	L681	A409	LEU	LEU
R979	N849	Y882	Y422	TYR	ASP
R980	Y850	M683	K423	GLY	GLY
R981	S851	R691	K491	H172	ASN
L984	D852	R853	L518	K177	ASN
S985	C856	E698	V522	ILE	PHE
L994	L860	V705	V522	GLY	GLY
Y999	F861	V706	L525	GLU	GLU
P1011	L862	Q713	F526	ALA	ALA
	D863	T718	N527	R203	SER
	R867	Y721	F534	R208	GLU
	M872	Y873	Y535	E216	GLU
	Y873	I731	A536	R219	SER
	M877	T732	R539	M228	HIS
	Q881	A734	I544	M228	GLY
			A545	S229	ALA
				L230	ASN
					ALA

- Molecule 7: SDE2

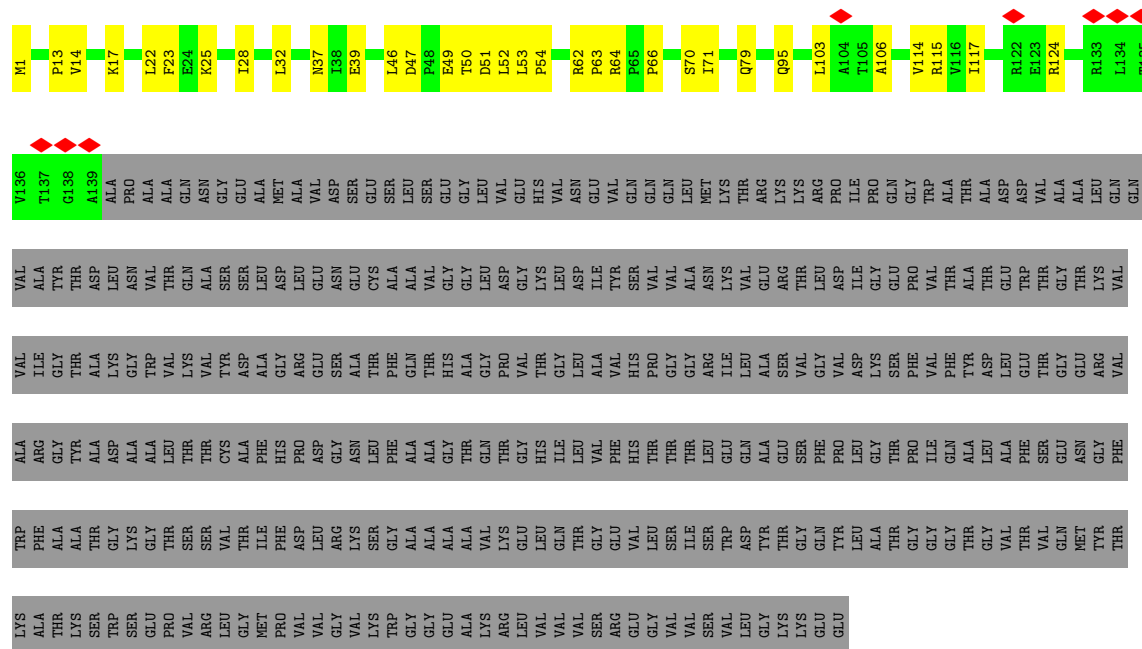
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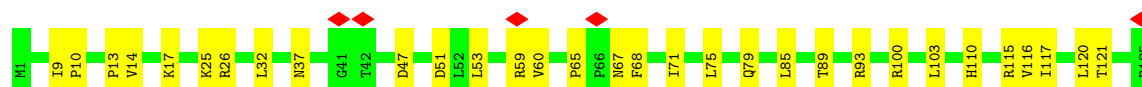
- Molecule 13: Pre-mRNA-splicing factor SPF27



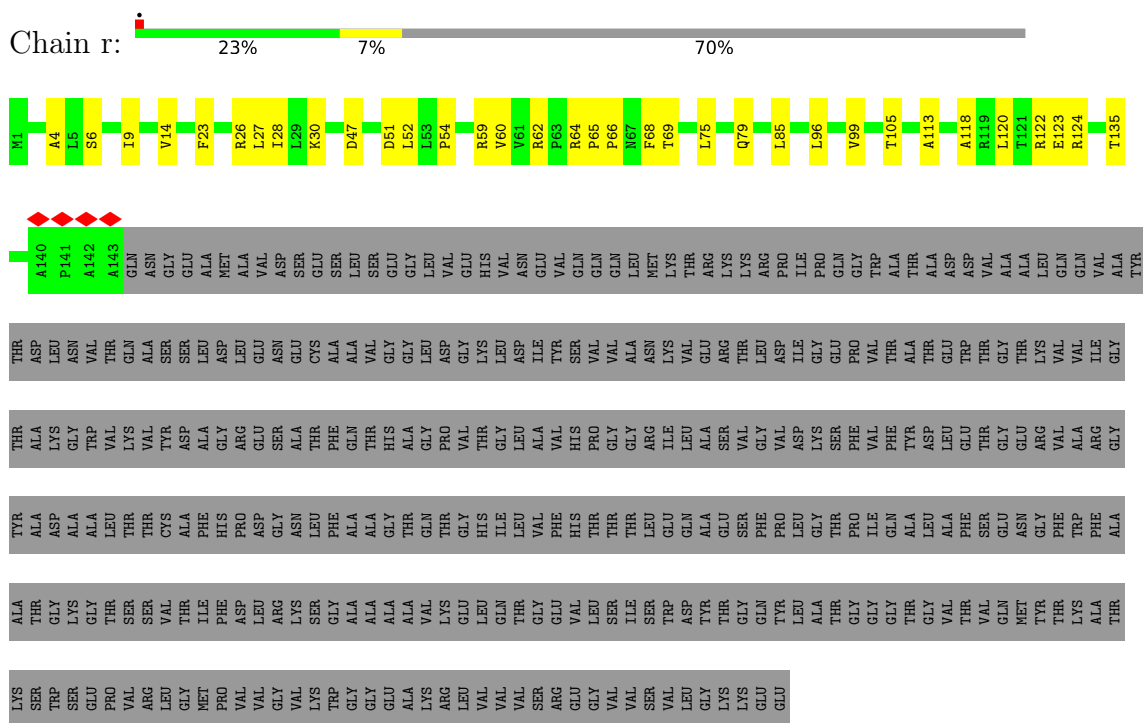
- Molecule 14: Pre-mRNA-processing factor 19



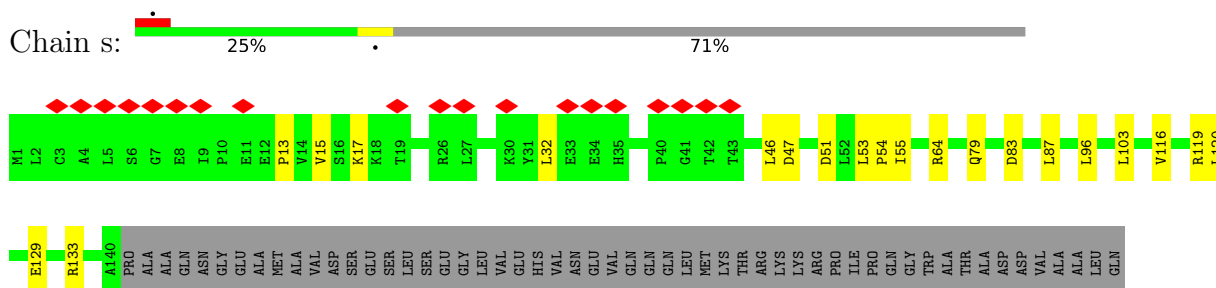
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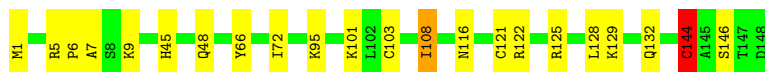
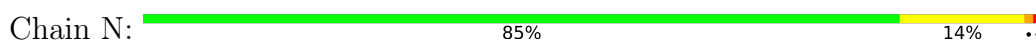


- Molecule 14: Pre-mRNA-processing factor 19

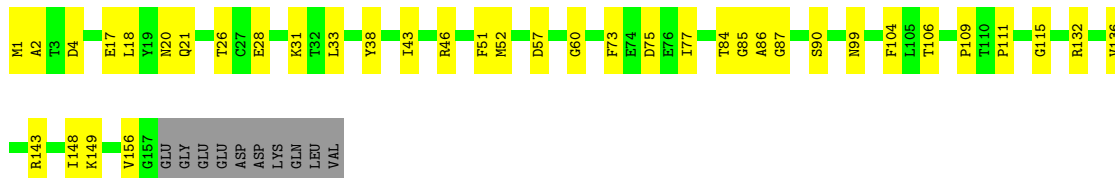




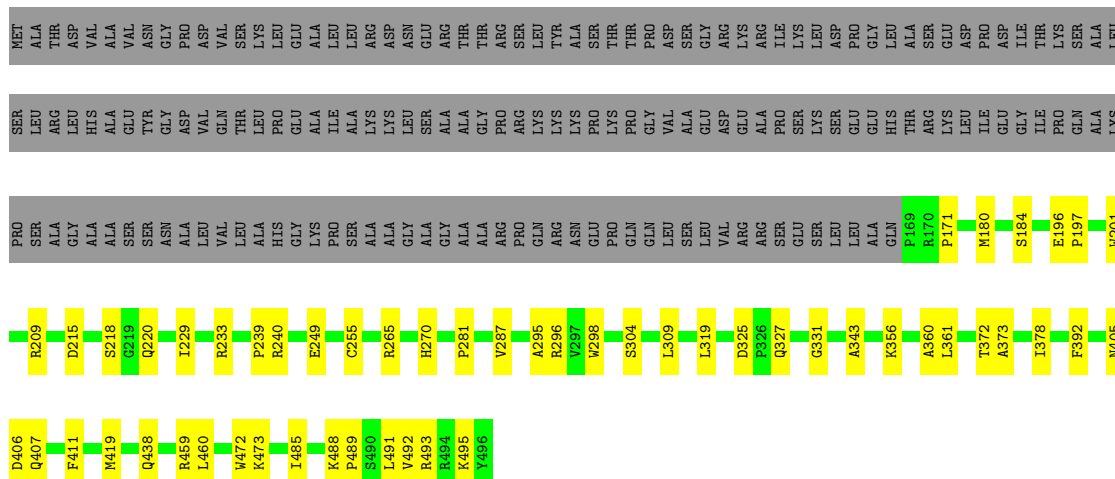
- Molecule 15: Putative bud site selection protein



- Molecule 16: Peptidyl-prolyl cis-trans isomerase



- Molecule 17: Pre-mRNA-splicing factor PRP46



- Molecule 18: Cell cycle control protein

[illegible]

Chain M: 49% 13% 37%

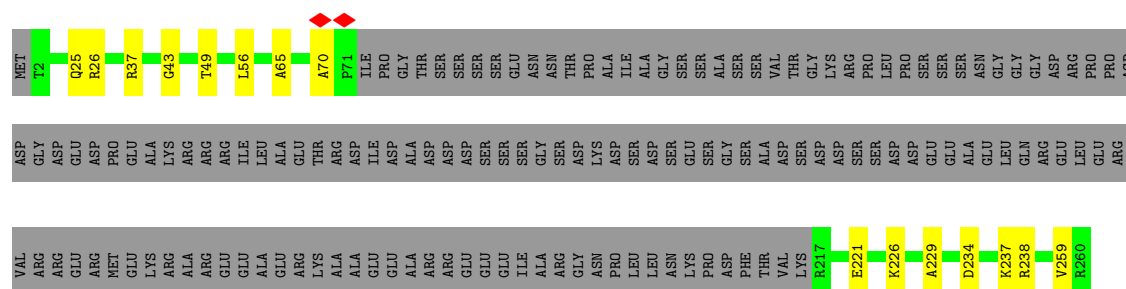
SER	D330	ALA	GLY	K138	GLY	MET
	G331	ALA	VAL		PRO	
ALA		ALA	GLU		GLU	PRO
GLY	A334	ALA	TYR		TYR	ILE
ASN	F335	ALA	GLY		GLY	GLN
	P336	ALA	ALA	K138		GLN
	GLU	ALA	ARG		ASP	
	ALA	ARG	THR	A143	LEU	ASN
	ASN	THR	GLY	R144	ARG	ALA
	LYS	GLY	ALA	L147	GLY	ALA
	SER	ALA	GLY	R148	THR	GLY
	ALA	SER				
	GLN	ALA		P155		
	LYS	ALA	ARG	TYR	PHE	SER
	ILE	ARG	GLY	PHE	ARG	THR
	GLU	GLY	LYS	LYS	GLY	D18
	ALA	PRO	GLY	ARG	F19	
	ALA	GLY		ARG	P20	
	ALA	A221	GLY	ARG	S21	
	ALA		GLU	GLU	V22	
	ALA	P228	LEU	LEU		
	GLN		ASP	ASP	P28	
	GLY		SER	SER		
	GLY	L232	GLU	GLU	A57	
	ALA		ASN	ASN	R65	
	ALA	I239	VAL	PRO	K66	
	GLY	M240	VAL	VAL		
	ALA	I244	ALA	ALA	T69	
	ALA	T245	GLY	GLY		
	GLY	G246	GLY	GLY	K79	
	GLY	I247	SER	SER		
	ALA	E248	GLY	GLY	C82	
	ALA	D249	GLY	GLY	Q83	
	ALA		SER	SER	C94	
	GLU	P252	THR	THR	C95	
	ALA	E253	VAL	VAL		
	ALA	W254	GLY	GLY	D88	
	GLN		GLY	GLY		
	ASN	F260	ASN	ASN		
	ASP		ALA	ALA	G92	
	LEU	H276	VAL	VAL	I95	
	ALA	C277	VAL	GLY		
	ASP	A278	GLY	GLY	R98	
	LEU		ALA	ALA	D99	
	ALA	R285	GLY	GLY		
	ILE		LEU	LEU	K100	
	ALA	L295	GLY	GLY	A101	
	ALA	K296	GLY	GLY	L102	
	PRO	G297	ALA	ALA	E103	
	PRO		GLY	GLY	L104	
	GLY	R307	PRO	PRO		
	ALA	I308	ILE	ILE	S111	
	ALA		ARG	ARG	E112	
	ASP	N320	THR	THR	I113	
	ASP	K321	ARG	ARG	N114	
	VAL		ASP	ASP	R115	
	GLN		THR	THR		
	TYR	M327	ARG	ARG	A123	
	ALA					

[illegible]

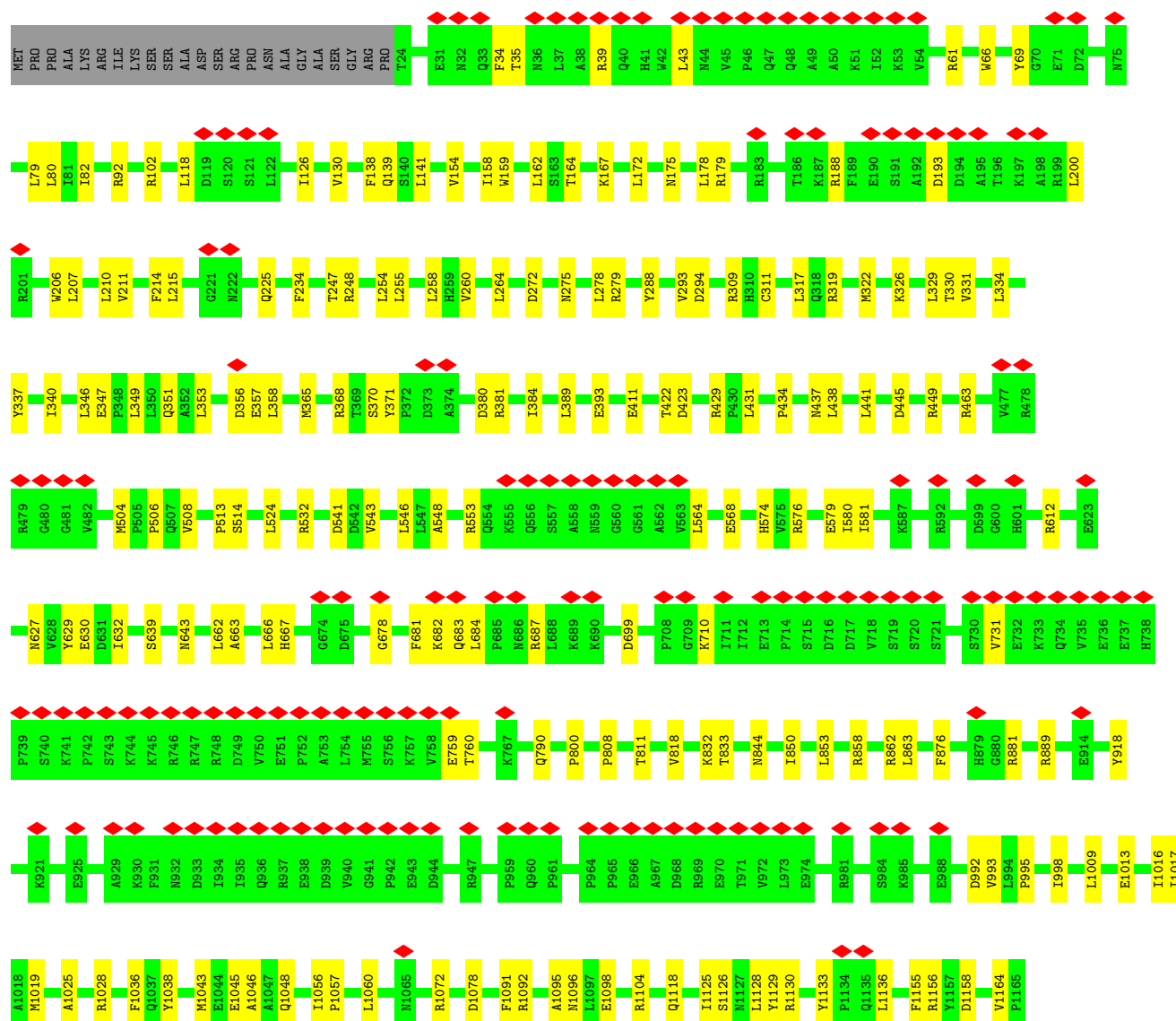
PRO	ARG	MET	ARG	ARG	A195	M1
PHE	ASP	ASP	ARG	ARG	Q196	
ASN	ARG	ARG	ARG	ARG	Q197	P13
VAL	THR	ASP	THR	THR	G198	K16
ASP	ASN	ILE	THR	THR	N199	
LYS	ALA	SER	ARG	ARG	R206	R25
PHE	GLU	GLU	GLU	SER	1207	
LEU	TYR	LYS	ARG	ARG		
SER	GLU	ILE	SER	SER	P217	I33
GLU	ASP	ALA	GLY	GLY		V34
VAL	ASP	LEU	SER	SER	S35	
GLN	GLU	GLY	TYR	TYR	K224	
LYS	GLU	ILE	SER	SER		I39
GLY	ALA	LYS	GLY	GLY	S234	T42
SER	GLY	ALA	SER	SER		GLN
ASN	GLU	PRO	GLU	GLU	S242	ILE
GLY	LYS	THR	SER	SER	P243	VAL
GLY	GLU	MET	GLY	GLY	P244	ILE
GLY	MET	SER	SER	SER		ARG
GLY	GLU	GLY	GLU	GLU	P258	ARG
LYS	THR	GLU	THR	THR	P259	ARG
ARG	ILE	SER	ASP	ASP	P260	THR
GLY	ARG	MET	GLY	GLY		GLY
TYR	LYS	TYR	SER	SER	I272	PRO
GLY	GLY	ASP	GLU	GLU		P52
LEU	ASN	SER	ARG	ARG	E299	
GLN	ARG	ARG	GLU	GLU		R57
ASP	PHE	LEU	ARG	ARG	M303	
GLU	GLY	PHE	ARG	ARG		P65
ASP	GLU	ASN	ARG	ARG	R306	
SER	ALA	GLN	ALA	ALA		F68
ARG	LEU	SER	ARG	ARG	E310	
GLN	GLY	SER	ARG	ARG		P83
ALA	ARG	GLY	GLU	GLU	R313	
LYS	GLY	PHE	LYS	LYS	Q314	K92
ARG	THR	GLY	LEU	LEU		
SER	PHE	ALA	LYS	LYS	Q329	D101
ARG	LYS	THR	GLU	GLU		
VAL	GLY	ILE	GLU	GLU	K330	K105
ASP	THR	ASN	GLU	GLU	E331	
ASP	GLU	GLU	GLU	GLU	E332	I111
ASP	ASP	ASP	LYS	LYS	H333	
GLU	ALA	ASN	LEU	LEU	R120	
ASN	GLN	PRO	ARG	ARG	L334	
ASP	PRO	TYR	GLN	GLN	R335	L132
ASP	ARG	ASP	SER	SER	Q336	
	GLU	LYS	ARG	ARG	L337	R157
	PRO	PRO	MET	GLY	A338	T158
	VAL	PHE	ALA	ALA	Q339	P175
	GLN	ALA	GLU	GLU	Q340	K176
	PHE	ALA	ARG	ARG	A341	N177
	GLU	GLN	ALA	ARG	R342	V178
	LYS	GLU	ALA	ALA	A343	
	ASP	ALA	GLN	GLN	E344	T182
	THR	ILE	VAL	VAL		
	THR	GLU	SER	LEU	R345	K190
	THR	SER	ALA	ALA	A346	Y191
	ALA	ILE	ARG	ARG		
	ASP	TYR	GLU	GLU	A347	S194
					A348	
					A349	
			ALA	SER		
			GLY	GLY		

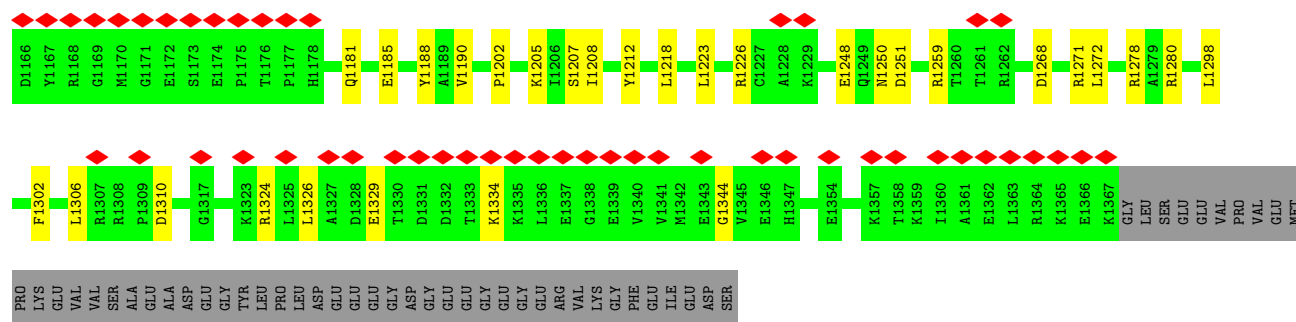
R242	LYS	V72	MET
P254	ALA	L73	PRO
I255	PRO	T74	PHE
	GLU		GLY
S272	PRO	K80	GLU
A273	ALA	T81	TYR
	ILE	I82	
	ALA		PRO
V282	ARG	K90	PRO
	ARG		ASN
R286	LYS	V101	LEU
	GLU		PRO
V409	ALA	N105	VAL
	GLU	R106	ARG
I418	GLU	E107	ASP
	MET	M108	ALA
K444	GLY		LEU
LEU	GLU	A125	ILE
TRP	GLU		LEU
ASP	ARG	Y134	ARG
	THR		GLU
	GLU	R143	SER
	PHE	ARG	GLN
	LEU	GLU	ALA
	GLY	GLU	GLN
	GLU	TYR	ALA
	SER	GLU	PRO
	GLU	VAL	THR
	TYR	VAL	ALA
	ASP	ASP	ASN
	TYR	LYS	HIS
	LEU	LYS	ALA
	GLY	GLY	VAL
	ARG	GLU	V34
	THR	GLU	P36
	TYR	GLU	Y36
	MET	ASP	
	HIS	GLY	
	VAL	ASP	N40
	PRO	GLU	P51
	GLN	TYR	F52
	ASP	GLU	ARG
	LEU	GLU	ASP
	VAL	VAL	THR
	VAL	GLU	SER
	SER	VAL	SER
	LEU	THR	SER
	ASN	ASP	SER
	LYS	GLU	ALA
	GLU	GLU	ALA
	VAL	GLU	SER
	GLY	VAL	GLY
	ILE	VAL	GLY
	THR	ILE	SER
	ASN	GLU	LEU
	TYR	GLU	LYS
	TYR	GLY	ARG
	ILE	THR	K69
	PRO	VAL	N70
	LYS	LEU	M74

Chain P:

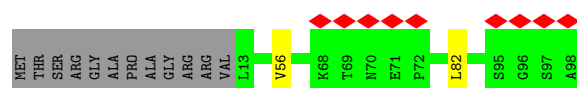
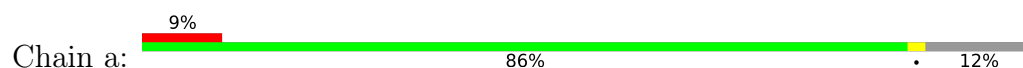


Chain Y:





• Molecule 25: Small nuclear ribonucleoprotein E



• Molecule 25: Small nuclear ribonucleoprotein E



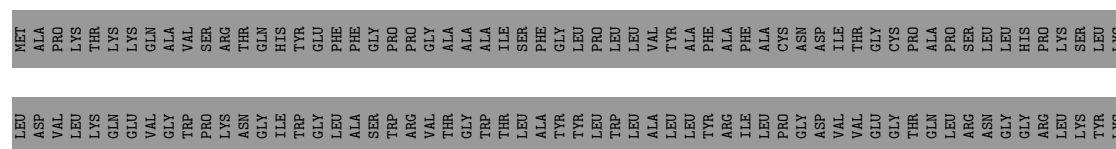
• Molecule 26: Sm protein F

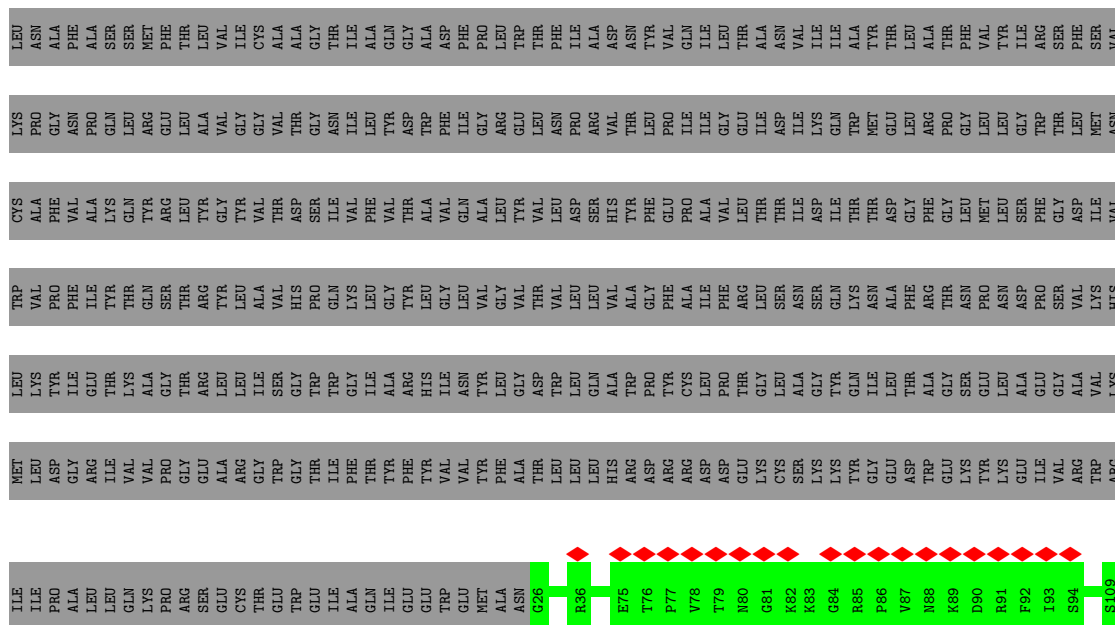


• Molecule 26: Sm protein F

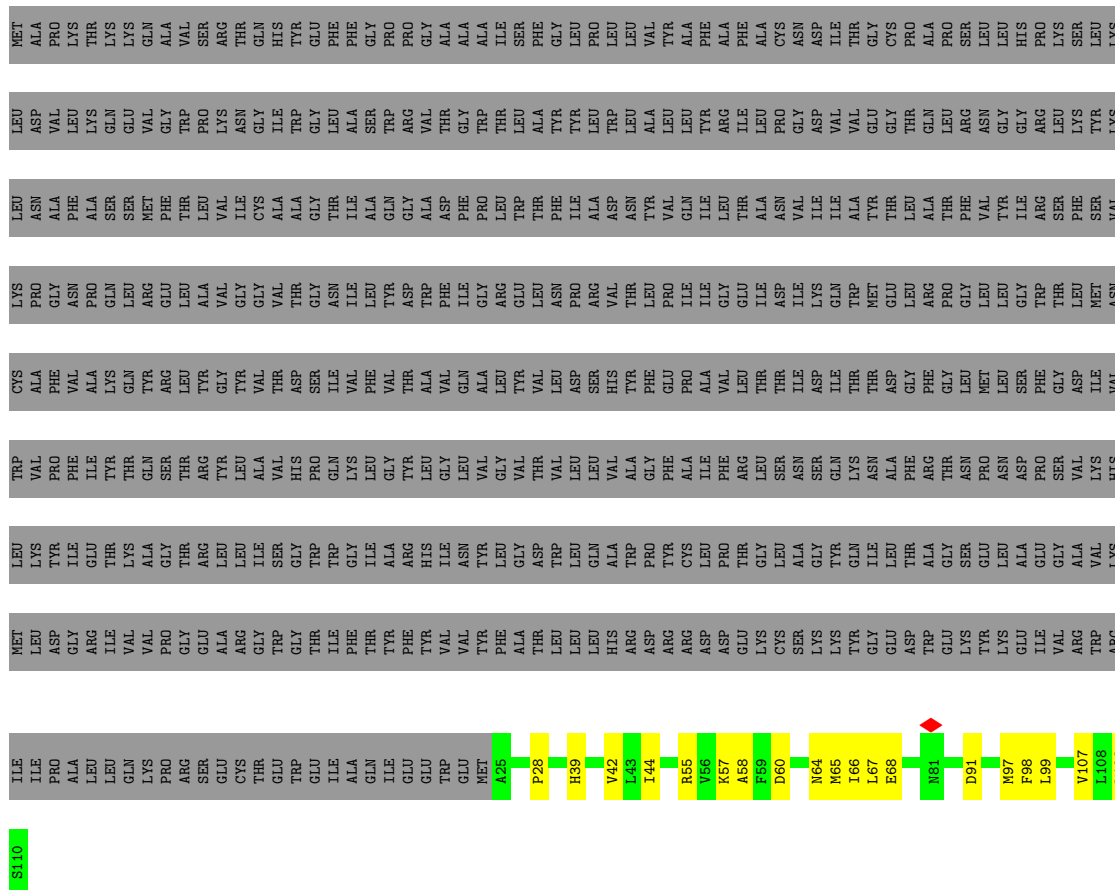


• Molecule 27: Delta(14)-sterol reductase



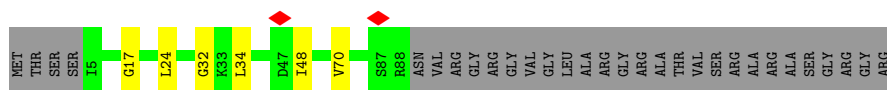


- Molecule 27: Delta(14)-sterol reductase



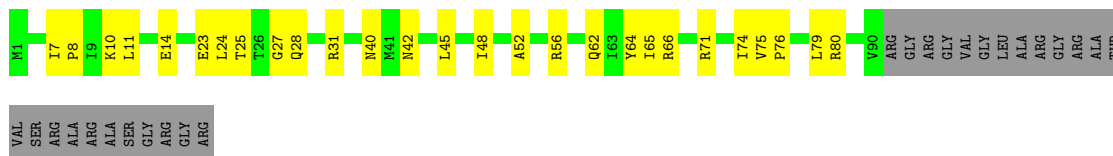
- Molecule 28: Small nuclear ribonucleoprotein Sm D1





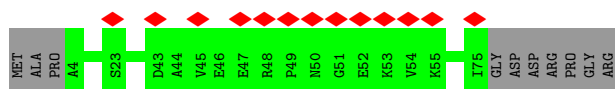
- Molecule 30: Small nuclear ribonucleoprotein Sm D3

Chain u: 55% 24% 21%



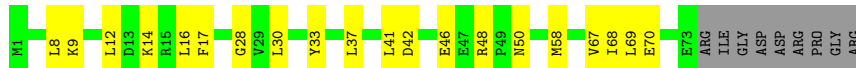
- Molecule 31: Small nuclear ribonucleoprotein G

Chain g: 16% 88% 12%



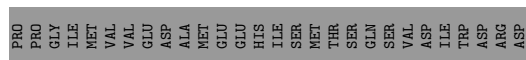
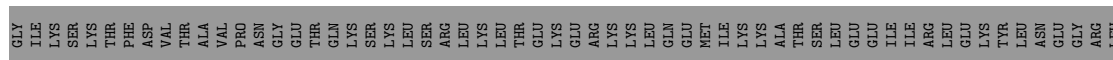
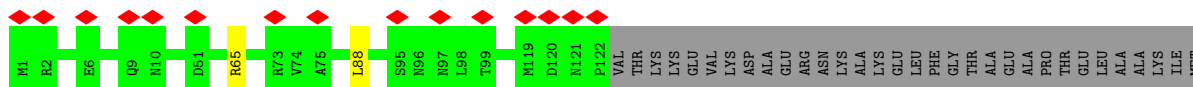
- Molecule 32: Small nuclear ribonucleoprotein G

Chain k: 65% 24% 11%



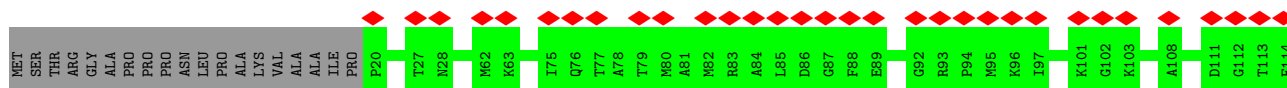
- Molecule 33: U2 small nuclear ribonucleoprotein A'

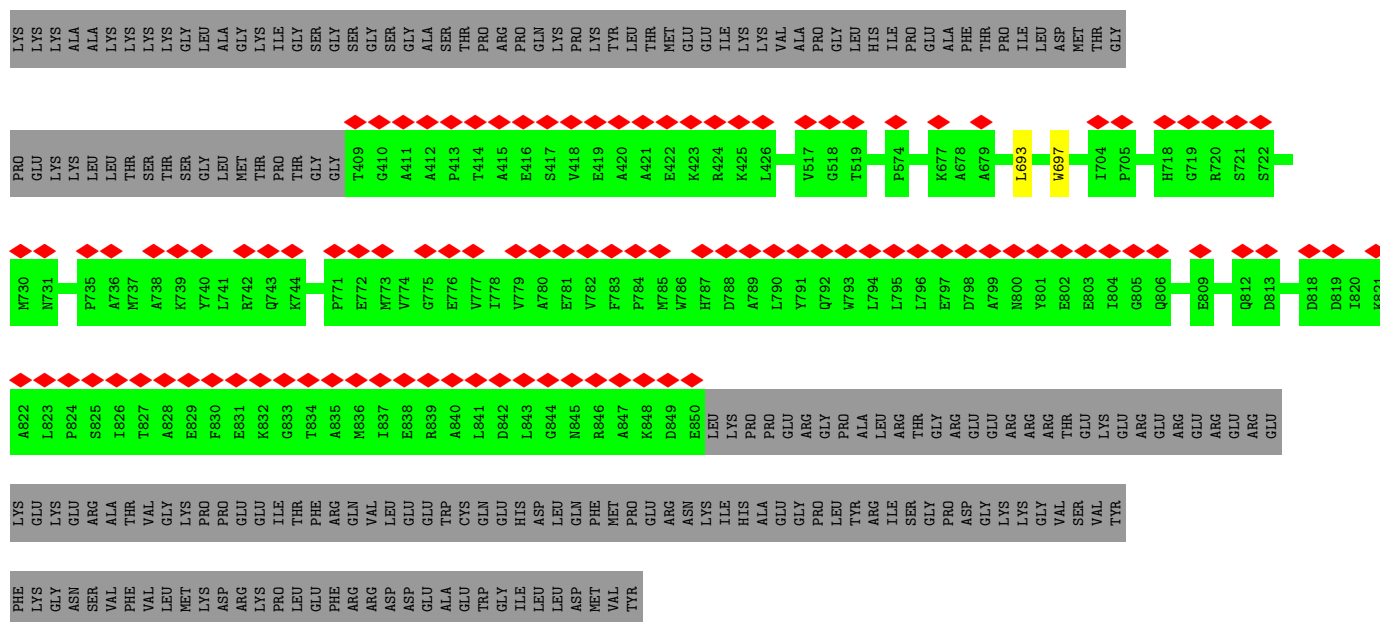
Chain h: 6% 50% 50%



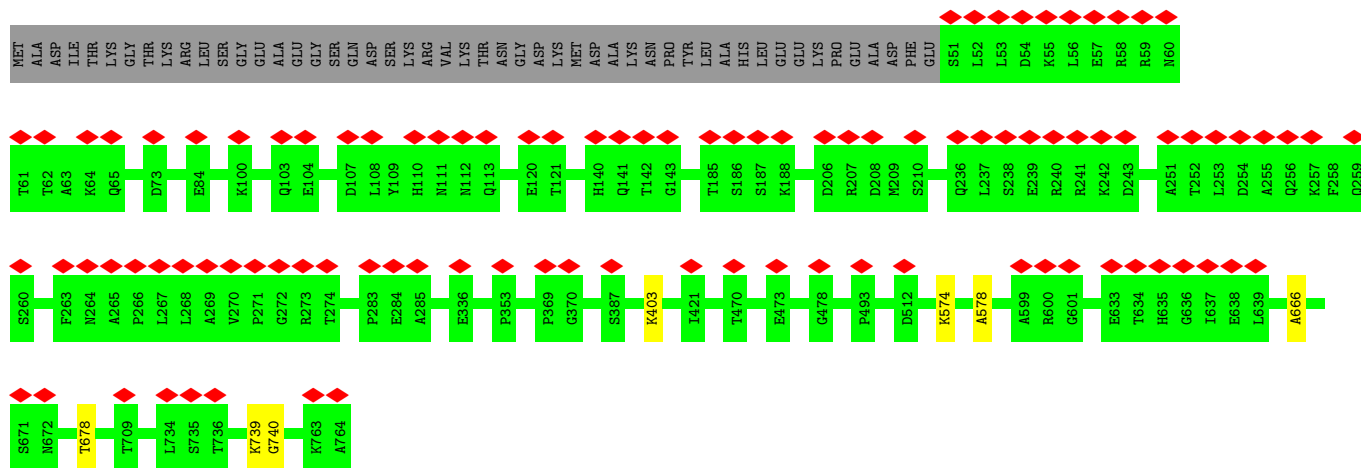
- Molecule 33: U2 small nuclear ribonucleoprotein B'-like protein

Chain i: 19% 51% 49%

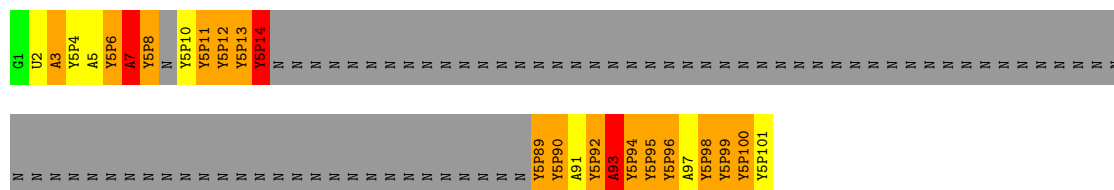




• Molecule 36: RNA helicase

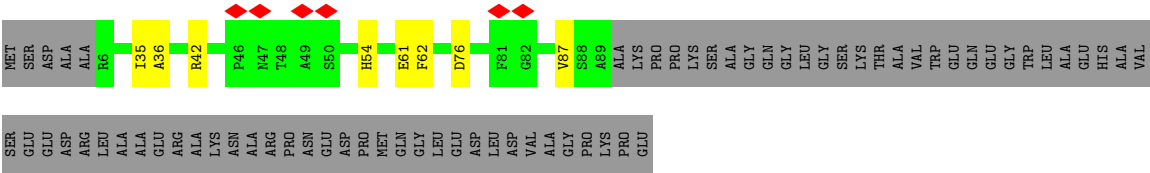


• Molecule 37: Unknown mRNA

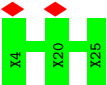


• Molecule 38: Putative cyclophilin protein





● Molecule 39: Unknown protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77668	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.259	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	447.36, 447.36, 447.36	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.932, 0.932, 0.932	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, P5P, ZN, MG, GTP, M7M, Y5P, SEP

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	2	0.26	0/2471	0.36	0/3832
2	5	0.39	0/2612	0.44	0/4059
3	6	0.48	0/2338	0.54	0/3639
4	A	0.39	0/16969	0.57	3/23006 (0.0%)
5	B	0.35	0/2099	0.53	0/2806
6	C	0.32	0/7464	0.50	0/10117
7	D	0.25	0/793	0.62	0/1051
8	E	0.31	0/2428	0.61	2/3295 (0.1%)
9	F	0.27	0/891	0.61	0/1201
10	I	0.24	0/6282	0.51	1/8491 (0.0%)
11	J	0.34	0/5301	0.50	0/7149
12	L	0.30	0/5120	0.53	0/6882
13	K	0.20	0/1833	0.46	0/2493
14	q	0.19	0/1128	0.49	0/1533
14	r	0.18	0/1151	0.42	0/1566
14	s	0.16	0/1133	0.37	0/1540
14	t	0.16	0/1141	0.41	0/1552
15	N	0.55	0/1227	0.79	3/1655 (0.2%)
16	S	0.28	0/1235	0.53	0/1671
17	T	0.54	0/2635	0.79	0/3582
18	U	0.27	0/2883	0.51	0/3895
19	M	0.31	0/2006	0.60	1/2703 (0.0%)
20	0	0.36	0/2278	0.57	0/3081
21	R	0.41	0/2724	0.60	2/3675 (0.1%)
22	W	0.24	0/2237	0.50	1/3068 (0.0%)
23	P	0.38	0/945	0.58	0/1264
24	Y	0.13	0/11057	0.33	0/14995
25	a	0.11	0/425	0.31	0/589
25	j	0.16	0/716	0.47	0/969
26	b	0.12	0/350	0.35	0/486
26	l	0.20	0/661	0.53	0/898
27	c	0.10	0/415	0.31	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	m	0.18	0/687	0.50	0/922
28	d	0.12	0/400	0.31	0/556
28	o	0.25	0/691	0.56	0/940
29	e	0.12	0/386	0.34	0/533
29	p	0.23	0/799	0.62	0/1079
30	f	0.10	0/413	0.30	0/573
30	u	0.25	0/726	0.65	0/979
31	g	0.12	0/353	0.37	0/489
31	k	0.21	0/584	0.66	0/787
32	h	0.11	0/604	0.34	0/841
33	i	0.08	0/503	0.24	0/699
34	CY	0.11	0/443	0.30	0/612
35	Cb	0.10	0/2494	0.27	0/3471
36	Cc	0.10	0/3540	0.28	0/4935
37	7	0.55	0/71	0.95	0/106
38	Ci	0.09	0/414	0.26	0/575
All	All	0.31	0/106056	0.51	13/145415 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	1
8	E	0	1
10	I	0	1
12	L	0	2
16	S	0	1
All	All	0	6

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	144	CYS	CB-CA-C	-8.33	95.08	109.07
4	A	833	VAL	N-CA-C	-7.05	107.01	113.71
22	W	108	MET	CA-CB-CG	6.49	127.08	114.10
15	N	108	ILE	N-CA-C	-6.46	106.69	112.90
8	E	92	ASP	CA-C-N	5.99	132.99	121.54
8	E	92	ASP	C-N-CA	5.99	132.99	121.54
21	R	190	LYS	CA-C-N	5.85	132.72	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	R	190	LYS	C-N-CA	5.85	132.72	121.54
15	N	116	ASN	CB-CA-C	5.74	119.56	111.86
10	I	424	ILE	CG1-CB-CG2	-5.40	94.49	110.70
4	A	1028	ASN	CA-C-N	5.31	131.68	121.54
4	A	1028	ASN	C-N-CA	5.31	131.68	121.54
19	M	144	ARG	CA-CB-CG	5.05	124.21	114.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1437	ARG	Peptide
8	E	92	ASP	Peptide
10	I	416	GLY	Peptide
12	L	505	LEU	Peptide
12	L	539	LEU	Peptide
16	S	51	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2224	0	1130	15	0
2	5	2343	0	1190	14	0
3	6	2090	0	1058	18	0
4	A	16540	0	16528	217	0
5	B	2071	0	2054	23	0
6	C	7301	0	7338	94	0
7	D	786	0	782	15	0
8	E	2379	0	2343	46	0
9	F	879	0	899	15	0
10	I	6135	0	6049	106	0
11	J	5176	0	5069	56	0
12	L	5052	0	5108	62	0
13	K	1797	0	1783	28	0
14	q	1110	0	1136	27	0
14	r	1132	0	1158	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	s	1115	0	1141	18	0
14	t	1122	0	1148	26	0
15	N	1200	0	1184	11	0
16	S	1209	0	1207	23	0
17	T	2565	0	2516	33	0
18	U	2821	0	2773	51	0
19	M	1964	0	1969	37	0
20	0	2224	0	2131	38	0
21	R	2686	0	2686	39	0
22	W	2224	0	1400	18	0
23	P	925	0	918	12	0
24	Y	10819	0	10842	137	0
25	a	426	0	182	1	0
25	j	704	0	743	13	0
26	b	351	0	152	3	0
26	l	649	0	652	12	0
27	c	416	0	178	0	0
27	m	678	0	723	14	0
28	d	401	0	175	0	0
28	o	679	0	711	20	0
29	e	388	0	180	2	0
29	p	788	0	816	20	0
30	f	414	0	182	4	0
30	u	716	0	738	22	0
31	g	354	0	152	0	0
31	k	577	0	611	12	0
32	h	605	0	265	1	0
33	i	504	0	238	0	0
34	CY	444	0	199	0	0
35	Cb	2496	0	1148	1	0
36	Cc	3541	0	1590	4	0
37	7	494	0	301	23	0
38	Ci	415	0	199	4	0
39	H	110	0	24	0	0
40	B	30	0	19	0	0
41	C	1	0	0	0	0
42	C	32	0	12	0	0
43	J	36	0	6	4	0
44	M	2	0	0	0	0
44	N	3	0	0	0	0
44	U	1	0	0	0	0
All	All	104144	0	93736	1161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1161) 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)
28:o:14:THR:HA	28:o:27:GLY:O	1.23	1.29
19:M:297:GLY:HA2	19:M:308:ILE:O	1.37	1.18
19:M:99:ASP:O	19:M:103:GLU:HA	1.64	0.97
4:A:1532:LEU:O	4:A:1536:GLU:HB2	1.67	0.94
28:o:14:THR:CA	28:o:27:GLY:O	2.19	0.85
20:0:86:ARG:NH2	37:7:8:Y5P:HB	1.93	0.83
19:M:297:GLY:CA	19:M:308:ILE:O	2.25	0.83
20:0:208:ARG:NH1	37:7:13:Y5P:HC	1.94	0.82
1:2:40:U:H3	37:7:89:Y5P:H5	1.46	0.79
20:0:86:ARG:HH21	37:7:8:Y5P:HB	1.44	0.79
6:C:121:ALA:HB2	17:T:220:GLN:HE22	1.48	0.78
1:2:34:A:N1	37:7:95:Y5P:N3	2.33	0.77
20:0:213:ARG:NH2	37:7:12:Y5P:HB2	2.01	0.76
37:7:99:Y5P:H4A	37:7:100:Y5P:H4	1.66	0.75
4:A:1912:VAL:O	4:A:1932:GLY:HA3	1.86	0.75
17:T:327:GLN:HE22	21:R:158:THR:HG21	1.52	0.74
4:A:1692:LYS:HD2	18:U:477:GLU:HG2	1.70	0.74
24:Y:358:LEU:HD13	24:Y:384:ILE:HG21	1.71	0.73
24:Y:889:ARG:HB2	24:Y:993:VAL:HG11	1.71	0.72
9:F:94:LEU:O	9:F:97:LYS:O	2.07	0.71
1:2:40:U:N3	37:7:89:Y5P:H5	2.05	0.71
1:2:2:G:H1	3:6:90:C:H42	1.39	0.71
5:B:107:THR:O	5:B:110:SER:O	2.07	0.71
4:A:1671:ARG:HD2	4:A:1798:TYR:HB3	1.73	0.71
10:I:476:ASP:HB3	10:I:479:ASP:HB2	1.73	0.71
30:u:31:ARG:O	30:u:48:ILE:HA	1.90	0.70
5:B:107:THR:O	5:B:111:GLN:HB2	1.90	0.70
8:E:154:THR:HG22	8:E:195:VAL:HG11	1.74	0.69
24:Y:800:PRO:HA	24:Y:1072:ARG:HG2	1.75	0.69
29:p:49:GLU:O	29:p:73:LYS:HA	1.92	0.69
6:C:634:LEU:HD22	6:C:683:MET:HG3	1.74	0.69
27:m:67:LEU:HB2	27:m:97:MET:HB3	1.75	0.69
14:q:103:LEU:HB2	14:t:103:LEU:HD21	1.74	0.69
10:I:44:LYS:HG3	10:I:56:VAL:HG21	1.74	0.69
3:6:17:G:H4'	3:6:18:G:H21	1.59	0.68
24:Y:524:LEU:HD13	24:Y:532:ARG:HG3	1.75	0.68
3:6:20:C:N3	20:0:130:LYS:NZ	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:r:64:ARG:HE	14:r:69:THR:HA	1.58	0.68
6:C:849:ASN:O	6:C:853:ARG:NH1	2.27	0.68
24:Y:639:SER:O	24:Y:643:ASN:HB2	1.94	0.68
19:M:82:CYS:HB3	19:M:85:CYS:SG	2.33	0.68
6:C:335:ILE:HD12	6:C:338:ARG:HG3	1.76	0.67
1:2:34:A:H61	37:7:95:Y5P:H4	1.59	0.67
4:A:1914:ARG:HH12	4:A:2021:GLN:HE22	1.41	0.67
4:A:1263:ARG:O	4:A:1266:ARG:O	2.12	0.67
18:U:512:CYS:SG	18:U:562:HIS:HE1	2.14	0.66
29:e:16:ASN:HA	29:e:33:MET:O	1.94	0.66
20:0:204:ILE:HG21	20:0:207:ILE:HG13	1.76	0.66
6:C:238:LYS:HA	30:u:14:GLU:HG2	1.77	0.66
6:C:877:MET:HG2	6:C:887:VAL:HG21	1.75	0.66
10:I:277:ARG:NH1	24:Y:311:CYS:SG	2.68	0.66
24:Y:1126:SER:O	24:Y:1130:ARG:HB2	1.95	0.66
4:A:450:GLN:O	6:C:304:ARG:NH2	2.29	0.66
6:C:780:ALA:HB3	6:C:791:LEU:HB3	1.77	0.66
11:J:351:ALA:HB1	11:J:370:LEU:HD21	1.77	0.65
6:C:397:LYS:HZ1	6:C:405:ILE:HG12	1.61	0.65
17:T:378:ILE:HB	17:T:392:PHE:HB2	1.78	0.65
4:A:304:GLU:OE1	15:N:9:LYS:NZ	2.29	0.65
21:R:207:ILE:HG23	22:W:80:MET:HE1	1.77	0.65
31:k:67:VAL:HG12	31:k:68:ILE:HG13	1.79	0.65
4:A:2019:PRO:HG2	4:A:2067:LEU:HB3	1.79	0.65
6:C:721:TYR:HA	6:C:731:ILE:O	1.96	0.65
7:D:148:ARG:NH2	10:I:741:ASN:OD1	2.30	0.65
10:I:101:ALA:O	10:I:105:LEU:HB2	1.96	0.65
17:T:459:ARG:HG2	23:P:56:LEU:HD21	1.79	0.65
4:A:1859:LYS:O	4:A:1863:ALA:HB3	1.97	0.65
10:I:253:ARG:HH22	24:Y:508:VAL:HA	1.62	0.65
5:B:265:ASP:OD2	11:J:148:TYR:OH	2.13	0.64
19:M:99:ASP:O	19:M:103:GLU:CA	2.42	0.64
3:6:19:U:OP1	19:M:65:ARG:NH1	2.29	0.64
8:E:245:LEU:HD13	8:E:294:ILE:HD11	1.78	0.64
29:p:28:GLN:HB3	29:p:50:PHE:HB2	1.80	0.64
1:2:15:U:OP2	3:6:76:U:O2'	2.15	0.64
4:A:1904:GLN:HG2	4:A:1987:GLN:HB3	1.80	0.64
24:Y:504:MET:SD	24:Y:514:SER:OG	2.56	0.64
4:A:1265:SER:O	4:A:1311:ASN:ND2	2.31	0.64
5:B:105:GLU:HA	5:B:108:LYS:HE2	1.80	0.63
21:R:190:LYS:O	21:R:206:ARG:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:541:ASP:N	24:Y:580:ILE:O	2.32	0.63
4:A:1711:LYS:HZ3	18:U:438:ILE:HD13	1.62	0.63
19:M:246:GLY:HA3	19:M:331:GLY:HA3	1.80	0.63
4:A:402:PRO:O	4:A:405:GLU:C	2.42	0.63
4:A:1339:SER:HA	4:A:1403:GLU:HB3	1.80	0.63
10:I:278:ALA:O	10:I:282:PHE:HB2	1.98	0.63
12:L:17:LEU:HB2	12:L:36:LEU:HD11	1.81	0.63
10:I:82:LEU:HD11	10:I:94:VAL:HG21	1.79	0.63
27:m:44:ILE:HG12	27:m:107:VAL:HG23	1.80	0.62
4:A:386:ALA:HB2	4:A:392:ARG:HD3	1.80	0.62
3:6:81:A:OP1	5:B:191:ARG:NH1	2.32	0.62
25:j:84:LYS:NZ	26:l:44:MET:SD	2.73	0.62
19:M:69:THR:HB	19:M:83:GLN:HG2	1.80	0.62
4:A:594:MET:C	4:A:596:LYS:H	2.07	0.62
4:A:1659:ARG:HH11	18:U:459:LEU:HD22	1.64	0.62
4:A:1957:GLN:HB3	4:A:1963:LEU:HD21	1.82	0.62
11:J:475:GLN:NE2	12:L:339:MET:SD	2.68	0.62
6:C:196:ASP:O	6:C:203:ARG:NH1	2.33	0.62
28:o:18:GLU:HB2	28:o:67:TYR:HB2	1.79	0.62
1:2:32:G:H22	37:7:98:Y5P:H2	1.65	0.61
4:A:432:TYR:O	6:C:691:ARG:NH1	2.29	0.61
4:A:1911:ASN:OD1	4:A:1914:ARG:NH2	2.33	0.61
17:T:209:ARG:HH21	17:T:229:ILE:HG22	1.64	0.61
4:A:1263:ARG:O	4:A:1266:ARG:C	2.43	0.61
14:r:27:LEU:HA	14:r:30:LYS:HE2	1.82	0.61
24:Y:850:ILE:O	24:Y:853:LEU:C	2.43	0.61
9:F:137:LYS:NZ	43:J:1001:IHP:O35	2.34	0.61
24:Y:553:ARG:HH22	24:Y:568:GLU:HG2	1.65	0.61
4:A:566:GLN:HB2	4:A:571:ARG:HE	1.66	0.61
4:A:1123:LEU:HD13	4:A:1174:ILE:HD13	1.81	0.61
11:J:408:LYS:NZ	43:J:1001:IHP:O34	2.34	0.61
20:0:208:ARG:HH22	37:7:14:Y5P:C5'	2.13	0.61
36:Cc:574:LYS:O	36:Cc:578:ALA:HB2	1.99	0.61
4:A:1508:ASP:OD1	4:A:1541:ARG:NH1	2.34	0.61
4:A:1894:ASN:HA	4:A:1897:GLU:HB2	1.83	0.61
4:A:1996:LEU:O	4:A:2000:GLU:HB2	2.01	0.61
4:A:884:ASN:OD1	4:A:887:ARG:NH1	2.34	0.61
4:A:1251:ASN:O	4:A:1255:PHE:HB2	2.00	0.61
11:J:28:GLU:OE1	12:L:167:ARG:NH1	2.34	0.61
11:J:373:PHE:HA	11:J:376:ILE:HG22	1.83	0.61
14:r:14:VAL:HA	14:r:54:PRO:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:o:47:PRO:HG2	28:o:50:GLU:HB2	1.83	0.61
14:t:65:PRO:HD2	14:t:68:PHE:HB2	1.83	0.60
4:A:1557:LEU:HD11	4:A:1586:ARG:HB3	1.83	0.60
30:u:25:THR:HA	30:u:71:ARG:HD2	1.82	0.60
4:A:529:ILE:HG21	6:C:310:LYS:HD3	1.84	0.60
12:L:399:ALA:O	21:R:306:ARG:NH2	2.34	0.60
24:Y:158:ILE:HG21	24:Y:207:LEU:HD23	1.83	0.60
24:Y:627:ASN:HB3	24:Y:630:GLU:HB2	1.82	0.60
18:U:458:ARG:NH2	18:U:487:VAL:O	2.35	0.60
4:A:1056:GLN:OE1	4:A:1060:ARG:NH1	2.34	0.60
16:S:87:GLY:N	16:S:106:THR:O	2.34	0.60
14:q:71:ILE:HD12	14:r:85:LEU:HD21	1.82	0.60
10:I:336:ILE:HD13	24:Y:322:MET:HE1	1.84	0.60
31:k:16:LEU:HD21	31:k:30:LEU:HD23	1.84	0.60
13:K:88:ARG:O	13:K:116:GLN:NE2	2.35	0.59
24:Y:833:THR:HB	24:Y:1016:ILE:HG12	1.84	0.59
6:C:208:ARG:NH2	6:C:216:GLU:O	2.35	0.59
1:2:37:A:N1	37:7:92:Y5P:N3	2.51	0.59
6:C:894:ARG:NH1	6:C:920:ASP:O	2.36	0.59
19:M:297:GLY:O	19:M:307:ARG:HA	2.02	0.59
15:N:125:ARG:HD3	15:N:128:LEU:HD12	1.84	0.59
21:R:313:ARG:NH2	21:R:314:GLN:OE1	2.31	0.59
2:5:20:A:H2'	2:5:21:C:H5	1.68	0.59
8:E:259:ARG:HD3	8:E:261:PHE:H	1.67	0.59
26:b:19:ASN:N	26:b:37:LEU:O	2.35	0.59
24:Y:543:VAL:O	24:Y:643:ASN:ND2	2.36	0.59
31:k:42:ASP:HA	31:k:58:MET:HA	1.83	0.59
4:A:1250:GLU:O	4:A:1253:ILE:C	2.45	0.59
20:0:201:TRP:NE1	20:0:233:MET:SD	2.76	0.59
24:Y:1272:LEU:HD22	24:Y:1298:LEU:HD22	1.84	0.59
4:A:574:TYR:OH	4:A:742:ARG:NH2	2.36	0.59
6:C:255:ASP:HB3	6:C:662:LEU:HB2	1.85	0.59
24:Y:662:LEU:HD11	24:Y:666:LEU:HD23	1.84	0.58
29:p:22:THR:HB	29:p:88:ALA:HB3	1.85	0.58
4:A:1436:SER:OG	4:A:1673:ASN:O	2.22	0.58
20:0:99:ARG:NH2	20:0:237:SER:O	2.36	0.58
14:t:17:LYS:HE3	14:t:53:LEU:HB2	1.86	0.58
19:M:20:PRO:HB2	19:M:22:VAL:HG23	1.86	0.58
24:Y:579:GLU:HB2	24:Y:612:ARG:HB3	1.85	0.58
26:l:25:ARG:NH1	26:l:26:LEU:O	2.34	0.58
1:2:34:A:H61	37:7:95:Y5P:C4	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:q:47:ASP:H	14:q:51:ASP:HB2	1.67	0.58
4:A:1758:LEU:HB2	4:A:1787:PHE:HB3	1.85	0.58
18:U:660:MET:O	18:U:664:ARG:HB2	2.04	0.58
10:I:202:LEU:HB3	24:Y:508:VAL:HG21	1.84	0.58
17:T:361:LEU:HG	17:T:372:THR:HG22	1.84	0.58
28:o:12:ASN:H	28:o:29:ILE:HB	1.69	0.58
11:J:264:GLU:OE1	21:R:16:LYS:NZ	2.36	0.58
24:Y:172:LEU:HB3	24:Y:179:ARG:HD2	1.85	0.58
24:Y:844:ASN:OD1	24:Y:862:ARG:NH1	2.37	0.58
18:U:526:LEU:O	18:U:723:ARG:NH2	2.37	0.58
5:B:101:GLN:HA	5:B:104:LYS:HD2	1.85	0.58
10:I:228:GLU:O	10:I:271:ARG:NH2	2.37	0.58
24:Y:423:ASP:OD2	24:Y:463:ARG:NH1	2.37	0.58
10:I:387:ASP:O	10:I:391:ALA:HB2	2.04	0.57
12:L:571:LEU:HD22	12:L:592:VAL:HG11	1.84	0.57
18:U:578:ARG:HH11	18:U:659:ARG:HD3	1.69	0.57
4:A:1873:ARG:NH1	18:U:445:GLU:OE2	2.37	0.57
10:I:247:ILE:HG21	10:I:265:LEU:HB2	1.85	0.57
16:S:26:THR:HG22	16:S:73:PHE:HE2	1.69	0.57
17:T:180:MET:HG3	17:T:473:LYS:HE2	1.86	0.57
3:6:12:C:OP2	4:A:154:ARG:NH1	2.31	0.57
16:S:28:GLU:HA	16:S:31:LYS:HG3	1.86	0.57
2:5:90:U:OP1	28:o:63:ASN:ND2	2.37	0.57
12:L:746:GLU:OE2	12:L:750:GLN:NE2	2.38	0.57
9:F:162:ARG:HH22	11:J:453:LEU:HD22	1.69	0.57
12:L:721:ARG:HD3	13:K:174:ARG:HG3	1.86	0.57
17:T:411:PHE:HE1	17:T:419:MET:HB3	1.69	0.57
6:C:713:GLN:OE1	6:C:867:ARG:NH1	2.37	0.57
17:T:233:ARG:NH1	17:T:249:GLU:OE2	2.37	0.57
4:A:443:LEU:HD22	6:C:219:ARG:HH11	1.69	0.57
14:r:59:ARG:NH1	14:r:60:VAL:O	2.37	0.57
24:Y:317:LEU:HD12	24:Y:365:MET:HE1	1.87	0.57
27:m:98:PHE:HB3	28:o:68:TYR:HB3	1.87	0.57
29:p:80:ILE:HD11	30:u:11:LEU:HD22	1.87	0.57
16:S:17:GLU:OE2	21:R:57:ARG:NH2	2.36	0.57
18:U:516:TYR:HD1	18:U:527:PRO:HD3	1.69	0.57
19:M:79:LYS:HD3	19:M:95:ILE:HG21	1.85	0.57
24:Y:272:ASP:O	24:Y:279:ARG:NH1	2.38	0.57
8:E:163:SER:O	8:E:170:ILE:HA	2.05	0.56
24:Y:629:TYR:HA	24:Y:632:ILE:HD12	1.87	0.56
12:L:614:LYS:HE3	14:q:115:ARG:HH12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:660:MET:HE1	18:U:663:ARG:HH21	1.69	0.56
24:Y:506:PRO:HB3	24:Y:513:PRO:HA	1.86	0.56
1:2:22:U:H3	4:A:900:LYS:HE3	1.69	0.56
2:5:93:G:O6	25:j:37:GLN:NE2	2.37	0.56
4:A:1402:ARG:NH1	4:A:1500:ILE:O	2.33	0.56
4:A:1767:THR:HA	4:A:1779:ILE:HA	1.88	0.56
6:C:527:ASN:C	6:C:527:ASN:HD22	2.14	0.56
10:I:387:ASP:O	10:I:391:ALA:CB	2.52	0.56
12:L:578:ALA:HA	12:L:589:VAL:HB	1.87	0.56
14:r:4:ALA:HB3	14:r:23:PHE:HE1	1.70	0.56
16:S:111:PRO:HB3	20:0:304:LEU:HD13	1.87	0.56
21:R:175:PRO:HD2	23:P:25:GLN:HG2	1.86	0.56
24:Y:353:LEU:O	24:Y:381:ARG:NH2	2.38	0.56
6:C:881:GLN:HA	6:C:884:VAL:HG12	1.87	0.56
4:A:1307:LYS:HA	4:A:1328:ARG:HH22	1.70	0.56
6:C:979:ARG:NH2	6:C:985:SER:OG	2.39	0.56
17:T:343:ALA:HB2	21:R:158:THR:HG22	1.87	0.56
19:M:88:ASP:OD1	19:M:98:ARG:NH1	2.39	0.56
20:0:312:ALA:O	20:0:316:ALA:HB2	2.06	0.56
30:u:76:PRO:HD2	30:u:79:LEU:HD12	1.88	0.56
12:L:66:ASP:OD2	12:L:97:ARG:NH2	2.38	0.56
20:0:208:ARG:HH11	37:7:13:Y5P:HC	1.67	0.56
4:A:971:GLU:OE2	4:A:998:TYR:OH	2.23	0.56
14:r:47:ASP:HB3	14:r:51:ASP:H	1.71	0.56
17:T:255:CYS:HB3	17:T:265:ARG:HB2	1.88	0.56
22:W:409:VAL:O	22:W:418:ILE:N	2.38	0.56
38:Ci:36:ALA:N	38:Ci:61:GLU:O	2.38	0.56
4:A:788:GLU:HA	21:R:224:LYS:HA	1.88	0.56
10:I:483:SER:HB3	10:I:486:GLN:HG3	1.88	0.56
10:I:219:TRP:HA	10:I:222:MET:HE2	1.88	0.56
13:K:207:GLU:OE2	13:K:210:ARG:NH2	2.39	0.56
14:t:89:THR:HG22	14:t:93:ARG:HE	1.70	0.56
17:T:360:ALA:HB3	17:T:373:ALA:HB3	1.88	0.56
24:Y:66:TRP:O	24:Y:102:ARG:NH1	2.39	0.56
4:A:1464:ALA:HA	4:A:1467:LYS:HB2	1.87	0.56
6:C:808:VAL:HG21	6:C:843:PHE:HB3	1.87	0.56
4:A:824:MET:O	17:T:356:LYS:NZ	2.36	0.55
5:B:212:ILE:HD11	21:R:33:ILE:HD11	1.87	0.55
10:I:247:ILE:HD12	10:I:265:LEU:HD13	1.87	0.55
10:I:699:GLN:HE22	12:L:309:LYS:HG2	1.71	0.55
16:S:90:SER:HB2	16:S:104:PHE:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:209:ARG:HE	17:T:229:ILE:HA	1.69	0.55
24:Y:389:LEU:O	24:Y:393:GLU:HB2	2.05	0.55
1:2:110:C:N4	1:2:146:G:N7	2.54	0.55
4:A:835:THR:HG23	21:R:260:PRO:HD3	1.87	0.55
4:A:1042:GLU:HB3	4:A:1139:LYS:NZ	2.21	0.55
14:r:124:ARG:HG3	14:s:120:LEU:HD22	1.87	0.55
4:A:2028:LYS:HZ3	4:A:2094:ILE:HG23	1.70	0.55
19:M:244:ILE:HB	19:M:278:ALA:HB3	1.87	0.55
27:m:58:ALA:HB3	27:m:66:ILE:HD12	1.88	0.55
6:C:873:TYR:HA	6:C:941:VAL:O	2.06	0.55
18:U:580:PHE:HD1	18:U:740:TRP:HE1	1.54	0.55
24:Y:1025:ALA:HA	24:Y:1056:ILE:HG21	1.88	0.55
26:l:18:VAL:HA	26:l:37:LEU:HD22	1.89	0.55
1:2:40:U:C5	37:7:90:Y5P:H4	2.42	0.55
10:I:313:LEU:HD11	10:I:334:LEU:HD13	1.88	0.55
17:T:325:ASP:OD2	21:R:157:ARG:NH2	2.40	0.55
4:A:1748:LYS:NZ	4:A:1751:SER:OG	2.38	0.55
6:C:172:HIS:O	6:C:177:LYS:NZ	2.39	0.55
11:J:16:ALA:HA	12:L:153:ILE:HD13	1.87	0.55
14:r:123:GLU:OE1	14:r:124:ARG:NH1	2.40	0.55
19:M:239:ILE:O	19:M:285:ARG:NH1	2.38	0.55
2:5:89:U:H1'	29:p:82:ARG:HH12	1.72	0.55
10:I:267:THR:HA	10:I:270:ILE:HG12	1.89	0.55
14:s:15:VAL:HG23	14:s:55:ILE:HD11	1.89	0.55
14:s:47:ASP:HB3	14:s:51:ASP:H	1.72	0.55
4:A:1494:ASN:HB3	4:A:1497:ARG:HG2	1.89	0.55
8:E:154:THR:OG1	8:E:160:LEU:N	2.39	0.55
10:I:246:ILE:HD11	24:Y:508:VAL:HG12	1.89	0.55
24:Y:1181:GLN:HB3	24:Y:1218:LEU:HD22	1.89	0.55
24:Y:1326:LEU:HA	24:Y:1329:GLU:HB2	1.88	0.55
4:A:1772:LEU:HD21	4:A:1854:GLN:HG3	1.88	0.55
18:U:661:ALA:O	18:U:665:SER:HB2	2.06	0.55
27:m:42:VAL:HG12	27:m:109:LEU:HA	1.88	0.55
28:o:15:VAL:HG12	28:o:71:PRO:HD3	1.88	0.55
9:F:116:ALA:O	9:F:119:ALA:C	2.50	0.55
10:I:580:GLU:HG3	11:J:334:LEU:HD13	1.88	0.55
13:K:53:LEU:O	13:K:64:GLN:NE2	2.39	0.55
24:Y:138:PHE:HA	24:Y:141:LEU:HG	1.89	0.55
10:I:363:ASN:HB3	10:I:366:GLU:HB2	1.87	0.54
27:m:39:HIS:O	27:m:55:ARG:NH1	2.40	0.54
4:A:1724:PHE:HB3	4:A:1736:VAL:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:l:41:ASP:OD2	26:l:45:ASN:ND2	2.39	0.54
2:5:112:A:O2'	29:p:55:ARG:NH2	2.40	0.54
4:A:1252:VAL:HG23	4:A:1269:LEU:HD12	1.89	0.54
9:F:122:LEU:HD11	10:I:684:LEU:HA	1.90	0.54
10:I:580:GLU:OE2	10:I:583:ARG:NH1	2.41	0.54
13:K:85:ASP:H	14:t:79:GLN:HE22	1.55	0.54
24:Y:411:GLU:OE1	24:Y:576:ARG:NH2	2.41	0.54
4:A:392:ARG:NH1	4:A:393:PHE:O	2.39	0.54
13:K:9:GLU:O	14:s:119:ARG:NH1	2.40	0.54
18:U:419:VAL:HB	18:U:424:GLY:HA3	1.90	0.54
18:U:630:ARG:HD3	18:U:646:VAL:HG21	1.88	0.54
8:E:127:LEU:HB2	8:E:141:TYR:HB2	1.89	0.54
7:D:168:GLU:OE1	7:D:172:ARG:NH2	2.40	0.54
24:Y:118:LEU:HD21	24:Y:206:TRP:HA	1.89	0.54
28:o:62:GLY:HA2	28:o:65:ILE:HD12	1.90	0.54
18:U:736:ARG:O	18:U:742:ARG:NH1	2.40	0.54
24:Y:1188:TYR:HE2	24:Y:1344:GLY:HA2	1.73	0.54
4:A:1374:ILE:O	4:A:1378:SER:CB	2.56	0.54
14:q:124:ARG:HD3	14:t:120:LEU:HD22	1.89	0.54
16:S:46:ARG:HB3	16:S:52:MET:HE1	1.89	0.54
18:U:523:PRO:O	18:U:723:ARG:NH2	2.41	0.54
37:7:95:Y5P:H4A	37:7:96:Y5P:H4	1.88	0.54
8:E:45:ARG:NH2	8:E:49:LEU:O	2.42	0.53
31:k:37:LEU:HD21	30:u:66:ARG:HH12	1.73	0.53
2:5:1:U:H3	2:5:79:U:H2'	1.73	0.53
10:I:88:ALA:HA	10:I:91:TYR:HB2	1.90	0.53
11:J:165:ARG:HA	11:J:168:LYS:HE2	1.88	0.53
24:Y:1130:ARG:HG3	24:Y:1136:LEU:HB2	1.90	0.53
24:Y:1251:ASP:HA	24:Y:1280:ARG:HB2	1.90	0.53
29:p:47:THR:HG21	29:p:79:THR:HG23	1.88	0.53
38:Ci:76:ASP:HA	38:Ci:87:VAL:H	1.73	0.53
4:A:1680:VAL:HG23	4:A:1689:LEU:HB2	1.90	0.53
5:B:115:THR:HB	5:B:120:LEU:HD21	1.91	0.53
8:E:167:ASP:OD1	8:E:167:ASP:N	2.40	0.53
12:L:397:GLU:OE2	21:R:313:ARG:NH1	2.42	0.53
13:K:4:ILE:HG23	13:K:45:LEU:HD11	1.89	0.53
24:Y:818:VAL:HG12	24:Y:853:LEU:HD12	1.90	0.53
12:L:630:GLU:O	12:L:634:ASN:HA	2.09	0.53
4:A:647:TYR:O	4:A:682:LYS:NZ	2.41	0.53
4:A:1250:GLU:O	4:A:1253:ILE:O	2.27	0.53
4:A:1980:PRO:HD2	4:A:1983:GLU:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:234:THR:HG22	8:E:247:TYR:HB3	1.89	0.53
10:I:420:THR:HA	10:I:423:ILE:HG22	1.90	0.53
27:m:57:LYS:HZ2	27:m:68:GLU:HG3	1.74	0.53
24:Y:248:ARG:NH1	24:Y:288:TYR:O	2.36	0.53
2:5:89:U:O2	29:p:82:ARG:NH1	2.42	0.53
4:A:962:ASP:OD1	4:A:1048:TYR:OH	2.27	0.53
5:B:221:LEU:HD22	5:B:233:ALA:HB1	1.91	0.53
8:E:318:PRO:HB3	29:p:128:ALA:HB2	1.90	0.53
10:I:69:LYS:HG2	10:I:73:MET:HE1	1.90	0.53
10:I:517:ARG:NH1	10:I:520:GLU:OE1	2.41	0.53
12:L:20:ALA:HB2	12:L:35:LEU:HD22	1.90	0.53
13:K:210:ARG:HA	13:K:213:VAL:HG12	1.91	0.53
14:q:17:LYS:HE3	14:q:53:LEU:HB2	1.91	0.52
2:5:88:C:N3	30:u:40:ASN:ND2	2.58	0.52
4:A:1737:GLN:HB3	4:A:1757:GLN:HB3	1.91	0.52
18:U:740:TRP:HA	18:U:743:VAL:HG22	1.90	0.52
20:O:208:ARG:HH12	37:7:13:Y5P:HC	1.74	0.52
4:A:1104:ILE:HD13	4:A:1284:LEU:HD12	1.91	0.52
4:A:1381:THR:OG1	4:A:1382:THR:N	2.41	0.52
8:E:152:ASP:OD1	8:E:153:VAL:N	2.41	0.52
11:J:422:ASN:HB3	11:J:425:ALA:HB3	1.91	0.52
12:L:679:GLU:OE1	13:K:127:ARG:NH2	2.43	0.52
18:U:514:LEU:HD22	18:U:558:VAL:HG11	1.91	0.52
4:A:1039:GLU:OE1	12:L:42:LYS:NZ	2.29	0.52
19:M:247:ILE:H	19:M:276:HIS:HB3	1.74	0.52
24:Y:548:ALA:HB3	24:Y:574:HIS:HB2	1.90	0.52
12:L:177:LYS:O	12:L:181:LYS:HG2	2.10	0.52
13:K:166:GLU:OE1	13:K:169:ARG:NH2	2.40	0.52
19:M:111:SER:HB3	19:M:114:ASN:HD22	1.74	0.52
24:Y:347:GLU:OE2	24:Y:351:GLN:NE2	2.42	0.52
25:j:54:ASN:OD1	25:j:85:GLY:N	2.43	0.52
4:A:415:ARG:HE	6:C:981:ARG:HA	1.75	0.52
4:A:897:THR:HA	4:A:900:LYS:HE2	1.92	0.52
6:C:255:ASP:HB2	6:C:661:PRO:HB2	1.91	0.52
24:Y:1057:PRO:HA	24:Y:1060:LEU:HG	1.92	0.52
3:6:94:C:O2	7:D:190:ARG:NH2	2.42	0.52
4:A:1631:GLU:O	4:A:1660:ARG:NH1	2.42	0.52
4:A:1649:GLN:NE2	18:U:466:ASP:O	2.36	0.52
24:Y:1009:LEU:HD12	24:Y:1013:GLU:HB3	1.91	0.52
4:A:262:MET:HB3	4:A:266:MET:HE3	1.92	0.52
6:C:228:MET:HE2	6:C:230:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:286:ILE:HG23	10:I:295:PHE:HE1	1.75	0.52
10:I:334:LEU:HD11	10:I:338:MET:HE3	1.91	0.52
12:L:682:LEU:HD22	14:r:66:PRO:HB3	1.90	0.52
17:T:287:VAL:HG12	17:T:319:LEU:HD11	1.91	0.52
28:o:20:LYS:HA	28:o:66:ARG:HB2	1.91	0.52
4:A:420:ASN:C	4:A:420:ASN:HD22	2.17	0.52
6:C:265:ASP:OD1	6:C:539:ARG:NH1	2.38	0.52
11:J:508:MET:HE3	11:J:510:GLU:HB2	1.92	0.52
4:A:1936:ILE:HB	4:A:1945:PHE:HB2	1.92	0.51
6:C:553:VAL:HG22	6:C:609:ILE:HG12	1.92	0.51
9:F:131:LYS:NZ	43:J:1001:IHP:O25	2.41	0.51
11:J:361:LYS:HA	11:J:364:TRP:HB2	1.92	0.51
11:J:472:ALA:HB2	11:J:505:VAL:HG12	1.91	0.51
10:I:311:GLY:HA2	10:I:314:MET:HG2	1.92	0.51
14:r:65:PRO:HG2	14:r:68:PHE:HB2	1.92	0.51
17:T:405:ASN:HB3	17:T:407:GLN:H	1.75	0.51
24:Y:678:GLY:O	24:Y:683:GLN:NE2	2.43	0.51
24:Y:832:LYS:HB2	24:Y:1038:TYR:HA	1.92	0.51
4:A:342:TRP:HD1	4:A:545:MET:HG2	1.76	0.51
4:A:955:PRO:HB2	4:A:1009:LYS:HE2	1.93	0.51
8:E:131:ASP:HB2	8:E:138:ILE:HD11	1.91	0.51
12:L:717:PHE:O	12:L:721:ARG:HG2	2.09	0.51
20:O:237:SER:OG	20:O:242:GLU:O	2.27	0.51
4:A:2015:GLU:OE2	18:U:664:ARG:NH1	2.41	0.51
13:K:8:HIS:HB3	14:s:116:VAL:HG21	1.92	0.51
19:M:104:LEU:HD11	19:M:143:ALA:HB2	1.92	0.51
23:P:65:ALA:HB1	23:P:70:ALA:HB3	1.91	0.51
24:Y:39:ARG:HG2	24:Y:43:LEU:HD12	1.93	0.51
35:Cb:693:LEU:O	35:Cb:697:TRP:CB	2.58	0.51
13:K:81:MET:HE2	14:t:75:LEU:HD12	1.93	0.51
13:K:134:LEU:HD21	14:r:64:ARG:HB3	1.91	0.51
30:u:42:ASN:HD22	30:u:66:ARG:HA	1.75	0.51
14:q:106:ALA:HB1	14:t:110:HIS:CE1	2.46	0.51
17:T:240:ARG:NH1	17:T:281:PRO:O	2.44	0.51
24:Y:188:ARG:HH11	24:Y:200:LEU:HD11	1.76	0.51
24:Y:790:GLN:NE2	24:Y:811:THR:O	2.43	0.51
24:Y:1043:MET:HE1	24:Y:1046:ALA:HA	1.93	0.51
24:Y:1248:GLU:O	24:Y:1278:ARG:NH1	2.41	0.51
2:5:90:U:H5''	2:5:91:U:H5'	1.91	0.51
4:A:1215:TYR:HD1	4:A:1224:VAL:HG22	1.75	0.51
6:C:404:PRO:HB3	6:C:409:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:131:ASP:OD2	8:E:133:THR:OG1	2.26	0.51
9:F:60:PRO:O	9:F:64:HIS:ND1	2.41	0.51
12:L:155:LEU:O	12:L:160:LYS:NZ	2.43	0.51
14:q:106:ALA:HB1	14:t:110:HIS:HE1	1.76	0.51
26:l:53:GLU:OE1	26:l:60:THR:OG1	2.29	0.51
29:p:80:ILE:HG23	30:u:8:PRO:HB3	1.93	0.51
4:A:1402:ARG:HG3	4:A:1502:TRP:CD1	2.46	0.51
8:E:267:HIS:NE2	8:E:270:THR:OG1	2.40	0.51
19:M:307:ARG:NH1	19:M:330:ASP:OD1	2.44	0.51
20:O:208:ARG:HH22	37:7:14:Y5P:HA1	1.75	0.51
24:Y:92:ARG:NH2	24:Y:1092:ARG:O	2.44	0.51
24:Y:858:ARG:NH1	24:Y:992:ASP:OD2	2.44	0.51
24:Y:1208:ILE:HD12	24:Y:1223:LEU:HD11	1.92	0.51
4:A:1884:GLU:HB2	18:U:664:ARG:HA	1.92	0.50
10:I:525:THR:HB	10:I:528:THR:HG23	1.93	0.50
12:L:528:ARG:NE	12:L:580:TYR:OH	2.44	0.50
13:K:98:ASP:HB3	13:K:101:GLN:HB2	1.91	0.50
4:A:1374:ILE:O	4:A:1378:SER:HB3	2.12	0.50
6:C:959:THR:HG21	6:C:973:ASP:HB2	1.93	0.50
13:K:66:GLU:OE1	13:K:69:ARG:NH2	2.44	0.50
14:q:79:GLN:OE1	14:t:26:ARG:NH2	2.45	0.50
28:o:58:LEU:HD11	29:p:88:ALA:HB1	1.94	0.50
4:A:1042:GLU:HB3	4:A:1139:LYS:HZ1	1.77	0.50
9:F:135:ASP:OD1	9:F:136:LEU:N	2.44	0.50
12:L:559:ASP:HB3	12:L:562:ARG:HB2	1.93	0.50
24:Y:34:PHE:HB3	24:Y:80:LEU:HD21	1.94	0.50
6:C:619:ASP:OD1	6:C:619:ASP:N	2.42	0.50
6:C:979:ARG:HG2	6:C:984:LEU:HD12	1.94	0.50
12:L:527:GLU:OE1	12:L:528:ARG:NH2	2.44	0.50
14:t:59:ARG:HE	14:t:60:VAL:H	1.58	0.50
20:O:109:THR:HG23	20:O:111:ALA:H	1.76	0.50
24:Y:275:ASN:HB3	24:Y:278:LEU:HB3	1.93	0.50
4:A:2112:ASP:O	4:A:2116:ASN:ND2	2.44	0.50
6:C:561:ASP:N	6:C:561:ASP:OD1	2.44	0.50
30:u:11:LEU:HD21	30:u:75:VAL:HG21	1.94	0.50
4:A:1015:GLN:O	4:A:1016:ARG:NH1	2.43	0.50
10:I:420:THR:O	10:I:424:ILE:HB	2.12	0.50
13:K:174:ARG:O	13:K:178:GLN:HB2	2.12	0.50
18:U:542:LEU:HD13	18:U:728:VAL:HG22	1.94	0.50
19:M:307:ARG:HH21	19:M:334:ALA:HA	1.77	0.50
24:Y:682:LYS:HD3	24:Y:687:ARG:HH12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1320:GLU:HG2	4:A:1360:THR:HG22	1.93	0.50
10:I:163:ALA:HA	10:I:166:ILE:HD12	1.93	0.50
16:S:2:ALA:HA	16:S:18:LEU:O	2.12	0.50
16:S:43:ILE:HA	16:S:149:LYS:HA	1.93	0.50
18:U:565:ASN:ND2	18:U:668:LYS:O	2.44	0.50
24:Y:1155:PHE:O	24:Y:1324:ARG:NH2	2.44	0.50
5:B:151:ALA:HA	5:B:154:TRP:CD1	2.47	0.49
6:C:238:LYS:HG3	30:u:14:GLU:HA	1.93	0.49
6:C:405:ILE:HG23	6:C:406:GLU:HG3	1.94	0.49
6:C:718:THR:OG1	6:C:863:ASP:OD2	2.30	0.49
7:D:227:MET:HE1	10:I:309:VAL:HG12	1.94	0.49
10:I:665:LEU:HD13	10:I:669:GLU:HB3	1.94	0.49
12:L:318:VAL:HG12	12:L:323:LEU:HD22	1.94	0.49
14:t:85:LEU:HD12	14:s:64:ARG:HH12	1.77	0.49
18:U:468:ARG:NH2	18:U:470:GLU:OE2	2.45	0.49
4:A:1656:ILE:O	4:A:1659:ARG:HG2	2.11	0.49
6:C:641:ILE:HD12	6:C:698:GLU:HB3	1.94	0.49
11:J:352:ILE:O	11:J:367:TYR:OH	2.26	0.49
11:J:551:GLN:HA	11:J:554:ILE:HD12	1.92	0.49
12:L:16:ILE:HD11	12:L:163:LEU:HD23	1.93	0.49
14:r:75:LEU:O	14:r:79:GLN:NE2	2.45	0.49
16:S:60:GLY:O	16:S:143:ARG:NH2	2.38	0.49
18:U:538:THR:N	18:U:576:GLU:OE2	2.44	0.49
24:Y:319:ARG:HA	24:Y:322:MET:HE2	1.93	0.49
24:Y:329:LEU:HD11	24:Y:353:LEU:HD11	1.93	0.49
14:q:64:ARG:NH2	14:r:6:SER:O	2.45	0.49
28:o:3:LEU:HA	28:o:6:PHE:HB2	1.94	0.49
4:A:594:MET:C	4:A:596:LYS:N	2.71	0.49
12:L:665:LEU:HD21	13:K:92:PRO:HG2	1.93	0.49
14:s:13:PRO:HB2	14:s:55:ILE:HD12	1.94	0.49
24:Y:225:GLN:OE1	24:Y:429:ARG:NH2	2.44	0.49
4:A:278:ARG:NH1	4:A:703:ASP:OD2	2.45	0.49
4:A:427:ARG:HD3	4:A:434:TYR:HB3	1.94	0.49
4:A:739:ILE:HD11	4:A:759:PRO:HG2	1.94	0.49
4:A:2098:LEU:HB3	4:A:2102:ASP:HB3	1.94	0.49
10:I:374:TRP:HE3	10:I:377:ASN:HD21	1.60	0.49
10:I:405:TRP:NE1	10:I:428:ALA:HB2	2.28	0.49
18:U:652:LYS:HB3	18:U:657:LEU:HD13	1.95	0.49
24:Y:139:GLN:HA	24:Y:437:ASN:HD21	1.77	0.49
31:k:46:GLU:OE2	31:k:48:ARG:NH1	2.45	0.49
4:A:986:SER:HA	4:A:989:GLU:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1636:PHE:HA	4:A:1639:SER:HB2	1.95	0.49
11:J:578:LYS:HE2	11:J:615:HIS:HB3	1.94	0.49
24:Y:293:VAL:HG11	24:Y:441:LEU:HD13	1.95	0.49
25:j:75:LYS:O	26:l:87:THR:OG1	2.31	0.49
12:L:608:GLN:HA	12:L:611:MET:HE2	1.95	0.49
14:s:32:LEU:HD21	14:s:46:LEU:HD23	1.94	0.49
4:A:1545:ARG:HB2	4:A:1548:THR:HG23	1.95	0.49
4:A:1756:ILE:HB	4:A:1789:ILE:HB	1.94	0.49
7:D:166:LYS:HA	7:D:169:MET:HE2	1.94	0.49
10:I:526:PRO:HB3	10:I:564:LEU:HD11	1.95	0.49
14:r:30:LYS:NZ	14:s:83:ASP:OD1	2.36	0.49
1:2:37:A:C2	37:7:93:P5P:C2	2.96	0.49
4:A:728:GLN:HG2	4:A:767:PHE:HB2	1.94	0.49
4:A:1225:PHE:HE2	4:A:1312:LEU:HD21	1.78	0.49
4:A:1419:GLU:OE2	4:A:1444:TYR:OH	2.31	0.49
6:C:826:CYS:HB3	6:C:975:VAL:HG23	1.94	0.49
24:Y:663:ALA:O	24:Y:667:HIS:HB3	2.13	0.49
24:Y:1125:ILE:HA	24:Y:1128:LEU:HB2	1.95	0.49
6:C:169:LEU:HD23	6:C:268:CYS:HB2	1.95	0.48
8:E:212:LYS:HG2	8:E:224:THR:HG22	1.95	0.48
8:E:281:ASN:ND2	8:E:325:ASN:OD1	2.39	0.48
11:J:25:LEU:HD21	12:L:163:LEU:HD22	1.94	0.48
24:Y:445:ASP:OD2	24:Y:449:ARG:NH2	2.46	0.48
6:C:304:ARG:HA	6:C:308:GLU:HG3	1.94	0.48
11:J:553:GLU:HA	11:J:556:ILE:HD12	1.94	0.48
20:O:213:ARG:CZ	37:7:12:Y5P:HB2	2.43	0.48
24:Y:434:PRO:HB2	24:Y:449:ARG:HB2	1.94	0.48
24:Y:699:ASP:N	24:Y:699:ASP:OD1	2.45	0.48
28:o:38:THR:HG22	28:o:65:ILE:HD11	1.95	0.48
4:A:740:TYR:CE1	4:A:744:ASN:ND2	2.82	0.48
4:A:1787:PHE:HA	4:A:1826:THR:O	2.13	0.48
8:E:278:LEU:HB2	22:W:90:LYS:HE3	1.95	0.48
31:k:9:LYS:HA	31:k:12:LEU:HD23	1.95	0.48
3:6:53:C:C4	11:J:66:ARG:HD2	2.49	0.48
4:A:1395:ILE:O	4:A:1399:THR:OG1	2.25	0.48
4:A:1742:HIS:HB3	4:A:1745:LYS:HB2	1.95	0.48
6:C:734:ALA:HA	6:C:860:LEU:HD11	1.94	0.48
4:A:2001:VAL:HA	4:A:2004:VAL:HG23	1.96	0.48
6:C:635:LYS:HE2	6:C:674:ILE:HG21	1.96	0.48
6:C:899:LEU:H	6:C:914:GLY:HA2	1.79	0.48
11:J:361:LYS:O	11:J:365:ARG:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:q:62:ARG:HD2	14:q:63:PRO:HD2	1.95	0.48
24:Y:215:LEU:HD21	24:Y:260:VAL:HG13	1.96	0.48
38:Ci:42:ARG:HA	38:Ci:54:HIS:HA	1.94	0.48
4:A:265:THR:HA	4:A:268:LYS:HE2	1.96	0.48
4:A:1996:LEU:O	4:A:2000:GLU:CB	2.60	0.48
6:C:103:THR:HG21	23:P:238:ARG:HH21	1.79	0.48
7:D:149:ARG:HB2	7:D:152:THR:HG23	1.96	0.48
10:I:303:VAL:O	10:I:307:GLU:HB2	2.13	0.48
15:N:129:LYS:HB2	15:N:132:GLN:HB2	1.96	0.48
22:W:255:ILE:HA	22:W:272:SER:HA	1.96	0.48
4:A:148:LYS:NZ	8:E:207:ILE:O	2.46	0.48
4:A:1039:GLU:HB3	4:A:1042:GLU:HG3	1.96	0.48
4:A:1512:VAL:HG23	4:A:1538:SER:HB2	1.95	0.48
8:E:236:ARG:NH2	8:E:328:GLU:OE2	2.42	0.48
24:Y:731:VAL:HB	24:Y:760:THR:HB	1.95	0.48
26:l:77:THR:OG1	26:l:82:LYS:NZ	2.46	0.48
10:I:371:VAL:HG11	10:I:385:TYR:CE1	2.49	0.48
12:L:328:LYS:HA	12:L:331:MET:HE2	1.95	0.48
14:r:118:ALA:HB1	14:r:122:ARG:HH12	1.78	0.48
19:M:240:MET:HE1	19:M:285:ARG:HB2	1.96	0.48
22:W:282:VAL:HA	22:W:286:ARG:HA	1.95	0.48
4:A:450:GLN:NE2	6:C:935:GLN:O	2.44	0.48
4:A:1079:VAL:HG22	4:A:1316:MET:HB3	1.96	0.48
11:J:130:ASP:HB3	21:R:111:ILE:HD13	1.94	0.48
11:J:450:GLU:HA	11:J:453:LEU:HB2	1.95	0.48
14:r:47:ASP:H	14:r:51:ASP:HB2	1.79	0.48
16:S:1:MET:HB3	16:S:20:ASN:HB2	1.96	0.48
21:R:52:PRO:HB2	21:R:57:ARG:HG2	1.96	0.48
29:p:33:MET:HA	29:p:44:LEU:HA	1.95	0.48
8:E:191:THR:OG1	8:E:232:ILE:O	2.29	0.47
14:r:120:LEU:HD22	14:r:124:ARG:HH12	1.78	0.47
23:P:37:ARG:HD3	23:P:43:GLY:HA3	1.95	0.47
29:e:16:ASN:CA	29:e:33:MET:O	2.61	0.47
4:A:501:GLU:HA	4:A:504:ALA:HB2	1.95	0.47
4:A:1073:GLU:HB2	4:A:1077:LEU:HB3	1.96	0.47
4:A:1786:LYS:O	4:A:1826:THR:OG1	2.29	0.47
6:C:850:TYR:HA	6:C:853:ARG:NH1	2.29	0.47
20:0:269:ALA:O	20:0:273:ILE:HG12	2.13	0.47
3:6:62:U:OP2	23:P:26:ARG:NH1	2.47	0.47
7:D:215:MET:HE1	10:I:297:MET:HB2	1.96	0.47
10:I:155:ALA:HB2	10:I:166:ILE:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:408:TYR:CD2	10:I:424:ILE:HD11	2.48	0.47
12:L:562:ARG:HE	14:q:114:VAL:HG21	1.78	0.47
13:K:54:ASN:OD1	13:K:55:GLU:N	2.47	0.47
14:t:9:ILE:HG21	14:t:60:VAL:HG21	1.96	0.47
25:j:20:LEU:HD23	25:j:23:LEU:HD21	1.95	0.47
8:E:113:ARG:HA	8:E:155:GLN:HE22	1.80	0.47
12:L:181:LYS:HA	12:L:184:GLU:HG2	1.96	0.47
12:L:692:ARG:NH2	13:K:150:GLU:OE1	2.48	0.47
21:R:178:VAL:HG13	21:R:217:PRO:HB3	1.96	0.47
24:Y:164:THR:HG22	24:Y:167:LYS:H	1.80	0.47
24:Y:564:LEU:HB3	24:Y:568:GLU:HB2	1.95	0.47
6:C:168:ALA:HB2	6:C:264:VAL:HG11	1.97	0.47
11:J:50:LEU:HD22	12:L:254:PRO:HG3	1.97	0.47
24:Y:154:VAL:HG21	24:Y:247:THR:HG22	1.95	0.47
24:Y:326:LYS:O	24:Y:330:THR:OG1	2.29	0.47
27:m:65:MET:HB3	27:m:99:LEU:HB3	1.96	0.47
29:p:39:HIS:O	29:p:39:HIS:ND1	2.46	0.47
2:5:39:U:OP1	4:A:1425:ARG:NH1	2.45	0.47
8:E:77:SER:HB3	8:E:346:MET:HE1	1.97	0.47
10:I:525:THR:HG22	10:I:527:GLN:H	1.79	0.47
11:J:405:THR:HG1	11:J:410:TRP:HE1	1.63	0.47
12:L:745:ARG:HH21	14:r:135:THR:HG22	1.78	0.47
21:R:65:PRO:HA	21:R:68:PHE:HD2	1.80	0.47
24:Y:581:ILE:HD11	24:Y:612:ARG:HB2	1.96	0.47
30:u:45:LEU:O	30:u:62:GLN:HA	2.15	0.47
4:A:1893:GLN:O	4:A:1896:SER:OG	2.29	0.47
6:C:745:ASP:OD2	6:C:768:TYR:OH	2.33	0.47
8:E:125:MET:HE2	8:E:146:GLU:HA	1.97	0.47
10:I:276:ASP:OD1	10:I:276:ASP:N	2.47	0.47
10:I:310:ILE:HA	10:I:313:LEU:HG	1.95	0.47
10:I:686:GLU:HG2	10:I:689:ARG:HD3	1.97	0.47
14:q:39:GLU:HB2	14:q:46:LEU:HG	1.96	0.47
18:U:553:GLY:O	18:U:588:TYR:OH	2.32	0.47
3:6:17:G:H4'	3:6:18:G:N2	2.27	0.47
4:A:670:ALA:HB2	4:A:778:TRP:HB3	1.97	0.47
4:A:1524:GLN:HE22	4:A:1525:GLN:HE21	1.63	0.47
11:J:444:ARG:NH2	43:J:1001:IHP:O46	2.48	0.47
21:R:310:GLU:OE2	21:R:313:ARG:NH1	2.47	0.47
24:Y:79:LEU:HD13	24:Y:126:ILE:HG23	1.97	0.47
24:Y:206:TRP:O	24:Y:210:LEU:HB2	2.14	0.47
25:j:62:GLU:OE2	25:j:76:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:515:PHE:O	4:A:517:ASP:N	2.47	0.47
6:C:847:TRP:HZ2	6:C:852:ASP:HB3	1.80	0.47
8:E:343:ASP:HB3	8:E:345:THR:HG22	1.96	0.47
11:J:135:ARG:HG3	11:J:136:LEU:HG	1.97	0.47
14:q:14:VAL:HA	14:q:54:PRO:HA	1.97	0.47
17:T:215:ASP:OD2	17:T:218:SER:OG	2.27	0.47
20:0:111:ALA:HB1	20:0:137:LEU:HD12	1.95	0.47
10:I:595:PRO:HB2	10:I:630:ALA:HB2	1.97	0.47
4:A:1788:TRP:CD2	4:A:1827:GLY:HA3	2.50	0.46
17:T:197:PRO:HG3	17:T:239:PRO:HA	1.98	0.46
17:T:331:GLY:HA3	17:T:361:LEU:HD11	1.97	0.46
18:U:401:LEU:HA	18:U:405:TYR:HD2	1.79	0.46
25:j:47:ARG:HB3	25:j:56:VAL:HG23	1.97	0.46
4:A:1199:LEU:HD22	4:A:1214:LEU:HD22	1.97	0.46
6:C:833:THR:HG21	6:C:861:PHE:HE1	1.80	0.46
10:I:248:ARG:NH2	10:I:284:GLU:OE1	2.48	0.46
10:I:421:ALA:O	10:I:424:ILE:HG22	2.16	0.46
12:L:22:SER:OG	21:R:272:ILE:O	2.28	0.46
24:Y:1251:ASP:OD1	24:Y:1280:ARG:NH1	2.47	0.46
4:A:1095:THR:OG1	4:A:1328:ARG:NH2	2.48	0.46
4:A:1508:ASP:HA	4:A:1511:ARG:HG2	1.97	0.46
4:A:1914:ARG:NH2	4:A:2021:GLN:OE1	2.46	0.46
8:E:288:SER:HB2	8:E:293:LYS:HB2	1.97	0.46
14:s:79:GLN:O	14:s:83:ASP:HB2	2.15	0.46
23:P:221:GLU:HA	23:P:226:LYS:HZ1	1.79	0.46
37:7:6:Y5P:H2'	37:7:7:P5P:H8	1.96	0.46
5:B:262:LEU:HD21	11:J:117:LEU:HD22	1.98	0.46
10:I:119:LEU:HD13	10:I:128:THR:HA	1.98	0.46
18:U:540:LEU:HB2	18:U:580:PHE:CE2	2.50	0.46
31:k:14:LYS:HB3	31:k:16:LEU:HD23	1.98	0.46
6:C:847:TRP:CD1	6:C:849:ASN:H	2.33	0.46
11:J:336:GLU:OE2	11:J:348:TYR:OH	2.31	0.46
16:S:77:ILE:HG21	16:S:115:GLY:HA2	1.98	0.46
4:A:915:GLN:HG2	4:A:1151:HIS:HB3	1.98	0.46
9:F:163:LEU:HD22	9:F:166:LYS:HZ1	1.80	0.46
10:I:447:ALA:HB2	10:I:463:MET:HE3	1.98	0.46
11:J:188:GLU:HB3	11:J:191:ARG:HB2	1.96	0.46
12:L:65:GLU:OE1	12:L:89:ARG:NH2	2.46	0.46
14:r:99:VAL:HG13	14:s:103:LEU:HD22	1.97	0.46
15:N:66:TYR:HB2	15:N:72:ILE:HD11	1.97	0.46
22:W:72:VAL:HG12	22:W:74:THR:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:331:VAL:HA	24:Y:334:LEU:HD12	1.98	0.46
27:m:91:ASP:OD1	27:m:91:ASP:N	2.47	0.46
4:A:434:TYR:OH	6:C:680:GLU:OE2	2.33	0.46
4:A:1203:ASP:OD1	4:A:1203:ASP:N	2.44	0.46
4:A:1509:SER:HA	4:A:1542:GLY:HA2	1.97	0.46
4:A:1859:LYS:O	4:A:1863:ALA:CB	2.64	0.46
14:q:70:SER:OG	14:r:62:ARG:NH2	2.49	0.46
31:k:28:GLY:HA3	31:k:41:LEU:HD13	1.97	0.46
4:A:1493:PRO:HD2	4:A:1601:VAL:HG22	1.97	0.46
6:C:301:LYS:HD3	6:C:304:ARG:HD2	1.98	0.46
6:C:847:TRP:HE1	6:C:849:ASN:HB2	1.80	0.46
11:J:388:ALA:HA	11:J:391:ILE:HD12	1.98	0.46
18:U:427:ARG:HD2	18:U:429:GLN:HE22	1.81	0.46
18:U:538:THR:HA	18:U:559:PRO:HA	1.98	0.46
24:Y:710:LYS:HD3	24:Y:759:GLU:HB2	1.97	0.46
24:Y:1045:GLU:HB3	24:Y:1048:GLN:HB2	1.98	0.46
30:f:32:GLY:HA3	30:f:48:ILE:HA	1.98	0.46
26:l:32:GLU:HG3	26:l:54:PHE:HB2	1.97	0.46
2:5:71:A:H5'	2:5:72:U:C6	2.50	0.46
4:A:406:ASP:HA	4:A:1263:ARG:HH22	1.80	0.46
16:S:57:ASP:OD2	16:S:60:GLY:N	2.48	0.46
27:m:97:MET:HE1	28:o:67:TYR:HB3	1.98	0.46
3:6:9:G:OP2	22:W:106:ARG:NH1	2.42	0.46
4:A:486:SER:OG	4:A:488:GLU:OE1	2.34	0.46
4:A:1767:THR:HG22	4:A:1779:ILE:HG12	1.98	0.46
10:I:242:ASP:N	10:I:242:ASP:OD1	2.48	0.46
11:J:20:ILE:HG21	12:L:12:ILE:HD13	1.97	0.46
16:S:75:ASP:OD1	16:S:99:ASN:ND2	2.49	0.46
24:Y:92:ARG:HH22	24:Y:1096:ASN:HA	1.81	0.46
24:Y:564:LEU:HD13	24:Y:568:GLU:HB3	1.98	0.46
27:m:60:ASP:OD1	27:m:64:ASN:N	2.47	0.46
28:o:72:ASP:OD1	28:o:72:ASP:N	2.48	0.46
30:u:24:LEU:HD21	30:u:65:ILE:HD12	1.98	0.46
4:A:1632:LYS:HZ3	4:A:1634:SER:HG	1.61	0.45
5:B:234:VAL:HG11	21:R:39:ILE:HD11	1.98	0.45
10:I:279:ARG:NH2	10:I:306:GLU:OE1	2.49	0.45
11:J:265:ARG:NH1	21:R:13:PRO:O	2.46	0.45
14:q:66:PRO:HB3	14:r:9:ILE:HG12	1.97	0.45
21:R:194:SER:OG	22:W:70:ASN:OD1	2.34	0.45
24:Y:358:LEU:HD13	24:Y:384:ILE:HD13	1.99	0.45
24:Y:1310:ASP:OD1	24:Y:1310:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:l:14:LEU:HD13	26:l:40:ILE:HD13	1.98	0.45
4:A:342:TRP:HB3	4:A:545:MET:HE2	1.97	0.45
4:A:1374:ILE:O	4:A:1378:SER:OG	2.33	0.45
4:A:1552:LYS:NZ	18:U:702:GLU:OE1	2.41	0.45
10:I:179:GLU:HA	10:I:182:ILE:HD12	1.98	0.45
10:I:244:GLU:OE2	10:I:269:TRP:NE1	2.37	0.45
14:q:14:VAL:HG21	14:q:25:LYS:HB3	1.98	0.45
18:U:703:VAL:O	18:U:707:MET:HG3	2.16	0.45
22:W:105:ASN:O	22:W:108:MET:HB2	2.16	0.45
24:Y:1190:VAL:HG11	24:Y:1226:ARG:HD2	1.98	0.45
4:A:1912:VAL:HG12	4:A:1954:TRP:HZ2	1.81	0.45
6:C:252:ASP:HB3	6:C:682:TYR:HB2	1.99	0.45
6:C:733:MET:HG3	6:C:860:LEU:HD22	1.97	0.45
6:C:805:LEU:O	6:C:809:LYS:CB	2.65	0.45
10:I:457:ASP:OD1	10:I:457:ASP:N	2.49	0.45
12:L:67:GLU:OE2	12:L:375:HIS:ND1	2.46	0.45
14:t:14:VAL:HG11	14:t:25:LYS:HD3	1.98	0.45
14:r:28:ILE:HG12	14:r:52:LEU:HD21	1.97	0.45
15:N:122:ARG:HH11	15:N:144:CYS:HB3	1.80	0.45
25:j:50:ASP:OD1	25:j:50:ASP:N	2.48	0.45
10:I:577:ILE:HG13	10:I:582:LEU:HG	1.98	0.45
18:U:705:GLY:O	18:U:708:LEU:O	2.35	0.45
20:0:102:ILE:HG12	20:0:140:LEU:HD23	1.98	0.45
30:f:17:GLY:CA	30:f:34:LEU:O	2.64	0.45
4:A:1274:VAL:O	4:A:1278:ARG:HG3	2.16	0.45
6:C:338:ARG:O	6:C:341:SER:OG	2.27	0.45
8:E:149:ASN:ND2	8:E:166:ASP:OD1	2.34	0.45
8:E:208:ASP:N	8:E:208:ASP:OD1	2.47	0.45
10:I:226:LEU:HD23	10:I:233:ILE:HG13	1.97	0.45
16:S:84:THR:HA	20:0:304:LEU:HD21	1.98	0.45
16:S:136:VAL:HG11	16:S:148:ILE:HD11	1.98	0.45
17:T:171:PRO:HG2	17:T:485:ILE:HG21	1.99	0.45
24:Y:329:LEU:HD21	24:Y:353:LEU:HG	1.98	0.45
24:Y:1212:TYR:OH	24:Y:1259:ARG:NE	2.44	0.45
2:5:89:U:O2'	29:p:39:HIS:NE2	2.36	0.45
4:A:533:TRP:CZ2	6:C:308:GLU:HG2	2.52	0.45
4:A:1103:ILE:HG12	4:A:1225:PHE:HD2	1.82	0.45
16:S:4:ASP:HB2	16:S:156:VAL:HB	1.98	0.45
19:M:148:ARG:HH22	20:0:285:ILE:HD13	1.80	0.45
21:R:191:TYR:HB3	21:R:206:ARG:O	2.16	0.45
24:Y:258:LEU:O	24:Y:371:TYR:OH	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:995:PRO:HA	24:Y:998:ILE:HD12	1.98	0.45
38:Ci:35:ILE:HA	38:Ci:62:PHE:HA	1.98	0.45
6:C:802:LYS:O	6:C:806:ALA:N	2.50	0.45
10:I:688:ASP:OD1	10:I:688:ASP:N	2.48	0.45
16:S:109:PRO:HB2	20:O:307:TYR:CE1	2.52	0.45
19:M:252:PRO:HB2	19:M:254:TRP:CD1	2.52	0.45
28:o:70:LEU:HD22	28:o:74:LEU:HD22	1.98	0.45
4:A:1111:VAL:O	4:A:1115:ILE:HG13	2.17	0.45
6:C:525:LEU:HD23	6:C:534:PHE:HB3	1.99	0.45
8:E:249:MET:HB3	8:E:276:LEU:HD22	1.97	0.45
12:L:561:ALA:HB1	14:q:117:ILE:HG23	1.97	0.45
23:P:234:ASP:O	23:P:237:LYS:NZ	2.36	0.45
24:Y:422:THR:HG22	24:Y:431:LEU:HD13	1.97	0.45
29:p:37:ASP:OD1	29:p:41:ASN:N	2.49	0.45
30:u:24:LEU:O	30:u:27:GLY:N	2.50	0.45
4:A:293:TRP:O	4:A:298:GLU:N	2.50	0.45
4:A:1582:TRP:H	4:A:1582:TRP:CD1	2.33	0.45
6:C:158:MET:HE3	6:C:589:PRO:HD2	1.99	0.45
6:C:889:ASN:O	6:C:892:SER:OG	2.34	0.45
9:F:136:LEU:HG	11:J:369:PHE:CZ	2.52	0.45
10:I:167:TRP:HE1	10:I:171:MET:HE2	1.81	0.45
12:L:700:LEU:HB2	13:K:153:VAL:HG22	1.99	0.45
20:O:72:THR:N	20:O:82:SER:O	2.50	0.45
21:R:176:LYS:O	21:R:178:VAL:N	2.50	0.45
4:A:1524:GLN:NE2	4:A:1525:GLN:HE21	2.15	0.45
11:J:513:TRP:HB3	11:J:536:LEU:HD22	1.99	0.45
14:q:117:ILE:HD11	14:t:116:VAL:HG12	1.99	0.45
20:O:54:ARG:NE	20:O:105:ASP:OD1	2.42	0.45
20:O:101:ASN:N	20:O:105:ASP:OD2	2.49	0.45
20:O:120:CYS:HB3	20:O:123:PHE:HB3	1.99	0.45
21:R:120:ARG:NH2	21:R:234:SEP:O2P	2.33	0.45
4:A:409:GLU:O	4:A:415:ARG:NH1	2.49	0.44
4:A:1310:PRO:HB3	4:A:1328:ARG:NH1	2.32	0.44
6:C:255:ASP:OD1	6:C:256:GLU:N	2.48	0.44
10:I:103:ILE:HG12	24:Y:918:TYR:CG	2.52	0.44
14:q:32:LEU:HD22	14:q:37:ASN:HA	1.98	0.44
15:N:103:CYS:N	15:N:144:CYS:SG	2.90	0.44
28:o:16:THR:HB	28:o:69:ILE:HB	1.99	0.44
2:5:67:U:OP1	15:N:95:LYS:NZ	2.49	0.44
4:A:311:ASP:HB3	4:A:315:ASP:H	1.81	0.44
4:A:401:ASP:OD2	4:A:403:ASN:ND2	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:83:ASN:HB3	10:I:86:ILE:HG13	2.00	0.44
14:t:10:PRO:HG2	14:t:13:PRO:HB3	2.00	0.44
16:S:1:MET:HE2	16:S:21:GLN:HB2	1.99	0.44
25:j:50:ASP:OD1	25:j:54:ASN:N	2.50	0.44
4:A:351:ASN:C	4:A:351:ASN:HD22	2.26	0.44
4:A:1630:TRP:HB3	4:A:1660:ARG:HH22	1.83	0.44
4:A:1829:MET:O	4:A:1841:ALA:HA	2.17	0.44
4:A:2046:LEU:HB3	4:A:2063:LEU:HD11	1.99	0.44
8:E:116:ASP:OD1	8:E:116:ASP:N	2.51	0.44
10:I:197:LYS:HZ3	10:I:201:ILE:HG13	1.82	0.44
11:J:13:LYS:HD2	12:L:152:THR:HG21	1.98	0.44
19:M:101:ALA:HB1	19:M:147:LEU:HD11	1.98	0.44
24:Y:1028:ARG:HG3	24:Y:1056:ILE:HG23	2.00	0.44
31:k:69:LEU:HB2	30:u:64:TYR:HB3	2.00	0.44
4:A:1828:LEU:HD11	4:A:1841:ALA:HB1	1.99	0.44
5:B:215:ALA:HB3	5:B:221:LEU:HD12	1.98	0.44
10:I:405:TRP:HZ2	10:I:427:LYS:HG3	1.83	0.44
10:I:439:LEU:HB3	10:I:488:VAL:HG11	1.99	0.44
24:Y:850:ILE:O	24:Y:853:LEU:O	2.34	0.44
4:A:1261:TRP:O	4:A:1266:ARG:NH1	2.50	0.44
8:E:59:HIS:CE1	8:E:79:SER:HB3	2.52	0.44
11:J:459:CYS:HA	11:J:462:LEU:HD12	1.99	0.44
17:T:406:ASP:OD2	23:P:49:THR:OG1	2.25	0.44
24:Y:175:ASN:HB3	24:Y:178:LEU:HB2	1.99	0.44
24:Y:663:ALA:O	24:Y:667:HIS:CB	2.66	0.44
3:6:53:C:N4	11:J:66:ARG:HD2	2.32	0.44
4:A:718:MET:SD	4:A:725:LEU:HD11	2.57	0.44
4:A:1466:ASP:O	4:A:1614:HIS:NE2	2.49	0.44
5:B:324:THR:OG1	5:B:325:MET:N	2.50	0.44
6:C:900:SER:OG	6:C:913:ASN:ND2	2.44	0.44
21:R:207:ILE:HD12	22:W:80:MET:HE1	2.00	0.44
24:Y:1092:ARG:HG3	24:Y:1098:GLU:HG3	1.99	0.44
4:A:1641:GLN:HE22	4:A:1645:LEU:HB2	1.83	0.44
6:C:761:ALA:HA	6:C:775:ALA:HB1	2.00	0.44
8:E:203:TYR:HD1	8:E:213:VAL:HG22	1.83	0.44
11:J:411:ILE:HG23	11:J:415:HIS:CE1	2.52	0.44
12:L:134:LEU:HB2	12:L:138:GLU:HB3	2.00	0.44
26:b:19:ASN:CA	26:b:37:LEU:O	2.66	0.44
4:A:736:LYS:HA	4:A:736:LYS:HD2	1.86	0.44
6:C:994:LEU:HD13	6:C:999:TYR:HA	2.00	0.44
11:J:362:ARG:NH2	12:L:324:ASP:OD2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:215:LYS:HB3	12:L:215:LYS:HE3	1.75	0.44
13:K:84:LEU:HD21	14:t:75:LEU:HB3	1.98	0.44
14:q:1:MET:H1	14:r:60:VAL:HG22	1.83	0.44
15:N:101:LYS:HD2	15:N:146:SER:HA	2.00	0.44
24:Y:294:ASP:OD2	24:Y:309:ARG:NH2	2.50	0.44
26:l:44:MET:HE3	26:l:70:CYS:HB2	2.00	0.44
8:E:207:ILE:HA	8:E:231:THR:HG22	2.00	0.44
10:I:393:ASN:HB3	10:I:396:LYS:HB2	1.99	0.44
12:L:376:ILE:O	12:L:380:ILE:HD12	2.17	0.44
14:t:67:ASN:OD1	14:t:68:PHE:N	2.51	0.44
19:M:104:LEU:HB2	21:R:92:LYS:HZ1	1.83	0.44
24:Y:541:ASP:CA	24:Y:580:ILE:O	2.66	0.44
27:m:60:ASP:OD1	27:m:60:ASP:N	2.51	0.44
5:B:189:TYR:O	5:B:193:ILE:HG12	2.18	0.43
13:K:33:GLU:HA	13:K:36:LYS:HG3	2.00	0.43
14:r:30:LYS:NZ	14:s:87:LEU:HG	2.34	0.43
16:S:33:LEU:HD22	16:S:38:TYR:CD2	2.53	0.43
17:T:209:ARG:NE	17:T:229:ILE:HA	2.32	0.43
24:Y:546:LEU:HB3	24:Y:632:ILE:HG21	2.00	0.43
31:k:50:ASN:OD1	31:k:50:ASN:N	2.51	0.43
4:A:1553:ASP:OD1	4:A:1553:ASP:N	2.42	0.43
10:I:161:ILE:HA	10:I:164:VAL:HG22	1.99	0.43
10:I:364:VAL:HB	10:I:399:GLY:HA3	1.99	0.43
19:M:19:PHE:CD1	19:M:20:PRO:HD2	2.53	0.43
22:W:125:ALA:HA	22:W:134:TYR:HB2	1.99	0.43
36:Cc:739:LYS:HA	36:Cc:740:GLY:HA2	1.75	0.43
3:6:42:G:OP2	12:L:24:TYR:OH	2.33	0.43
4:A:1784:THR:HG21	4:A:1826:THR:HG21	2.01	0.43
4:A:1791:VAL:HA	4:A:1830:ILE:O	2.18	0.43
6:C:544:ILE:HG12	6:C:589:PRO:HA	2.00	0.43
6:C:853:ARG:HA	6:C:856:CYS:SG	2.59	0.43
12:L:610:LEU:HA	12:L:613:MET:HG2	1.99	0.43
19:M:245:THR:HA	19:M:327:MET:HE3	2.01	0.43
20:O:210:LEU:HD23	20:O:212:ASN:HD21	1.83	0.43
24:Y:1156:ARG:NH2	24:Y:1334:LYS:O	2.50	0.43
1:2:19:G:O2'	4:A:809:ASP:OD2	2.30	0.43
4:A:216:LYS:HD2	4:A:216:LYS:HA	1.73	0.43
5:B:263:VAL:HG21	11:J:120:ARG:HG2	1.99	0.43
8:E:278:LEU:HD12	22:W:90:LYS:HE3	2.00	0.43
10:I:148:TRP:HH2	10:I:169:ARG:HB3	1.81	0.43
14:q:49:GLU:HG2	14:q:50:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:196:GLU:HG2	17:T:201:TRP:CE2	2.53	0.43
18:U:556:VAL:HG21	18:U:721:TRP:HH2	1.83	0.43
19:M:244:ILE:HD11	19:M:260:PHE:HE2	1.84	0.43
21:R:34:VAL:HG22	21:R:35:SER:H	1.83	0.43
24:Y:337:TYR:HA	24:Y:340:ILE:HG12	2.01	0.43
24:Y:876:PHE:HA	24:Y:881:ARG:HE	1.83	0.43
4:A:605:GLN:OE1	21:R:182:THR:OG1	2.35	0.43
4:A:1033:ASN:ND2	4:A:1571:ILE:HD12	2.34	0.43
4:A:1093:TRP:CE3	4:A:1325:PRO:HG3	2.54	0.43
8:E:317:LEU:HD23	22:W:36:TYR:HB2	1.99	0.43
9:F:108:LYS:NZ	10:I:647:SER:OG	2.40	0.43
10:I:362:ASN:HA	10:I:392:ILE:HG23	2.00	0.43
13:K:59:LEU:HD23	13:K:63:LEU:HD13	2.00	0.43
14:s:129:GLU:OE2	14:s:133:ARG:NE	2.52	0.43
4:A:270:LYS:NZ	4:A:749:GLY:O	2.52	0.43
4:A:1072:SER:OG	4:A:1073:GLU:OE1	2.30	0.43
4:A:1733:ILE:HD13	4:A:1758:LEU:HD22	2.00	0.43
4:A:2073:ASN:HD21	4:A:2113:LEU:HD11	1.83	0.43
5:B:127:HIS:NE2	7:D:189:GLU:OE2	2.46	0.43
6:C:793:ASP:HA	6:C:837:LEU:HB2	1.99	0.43
8:E:127:LEU:HD12	8:E:148:ILE:HD13	2.01	0.43
14:s:53:LEU:HD12	14:s:54:PRO:HD2	1.99	0.43
16:S:86:ALA:HB3	21:R:83:PRO:HD2	2.00	0.43
18:U:419:VAL:O	18:U:425:ARG:NH1	2.52	0.43
19:M:228:PRO:O	19:M:232:LEU:HB2	2.19	0.43
23:P:237:LYS:HA	23:P:237:LYS:HD3	1.86	0.43
26:b:52:GLU:HA	26:b:62:HIS:HA	2.00	0.43
30:u:24:LEU:HD21	30:u:65:ILE:HG23	2.00	0.43
4:A:549:GLN:O	4:A:762:ARG:NE	2.50	0.43
6:C:575:PHE:HB2	6:C:595:LEU:HB3	2.01	0.43
10:I:189:GLY:HA2	10:I:191:TYR:CZ	2.54	0.43
10:I:675:LEU:HD21	10:I:709:PHE:HD1	1.83	0.43
11:J:340:ASP:HB3	11:J:343:ARG:HB2	2.00	0.43
12:L:572:LEU:HG	14:t:115:ARG:HH21	1.83	0.43
14:q:23:PHE:HB3	14:q:28:ILE:HG21	2.01	0.43
24:Y:210:LEU:HG	24:Y:234:PHE:HE2	1.82	0.43
24:Y:1202:PRO:HG2	24:Y:1205:LYS:HD2	2.01	0.43
29:p:76:LEU:HD23	30:u:74:ILE:HG13	2.00	0.43
3:6:22:A:H61	20:0:130:LYS:NZ	2.17	0.43
4:A:346:LEU:HD12	4:A:531:LEU:HD12	2.01	0.43
10:I:167:TRP:CD1	10:I:181:PHE:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:686:GLU:HB3	10:I:689:ARG:HB2	2.00	0.43
19:M:249:ASP:OD1	20:O:260:ARG:NH1	2.50	0.43
24:Y:69:TYR:O	24:Y:102:ARG:NH2	2.48	0.43
24:Y:863:LEU:HB2	24:Y:1019:MET:HB3	2.01	0.43
4:A:1613:GLU:OE2	4:A:1801:HIS:NE2	2.51	0.43
8:E:234:THR:HG21	8:E:285:GLY:H	1.83	0.43
8:E:245:LEU:HD22	8:E:294:ILE:HG13	2.00	0.43
14:t:32:LEU:HD22	14:t:37:ASN:HA	2.01	0.43
30:f:24:LEU:HA	30:f:70:VAL:HA	2.00	0.43
26:l:25:ARG:HD2	26:l:75:TRP:NE1	2.34	0.43
28:o:74:LEU:HD23	28:o:76:LEU:HD23	2.01	0.43
30:u:52:ALA:HB3	30:u:56:ARG:HB3	2.00	0.43
4:A:1433:LYS:HE3	4:A:1433:LYS:HB3	1.93	0.43
4:A:1914:ARG:NH2	4:A:2024:MET:SD	2.89	0.43
8:E:73:THR:HG23	8:E:74:LEU:HG	1.99	0.43
10:I:132:PHE:CE1	10:I:147:ILE:HG22	2.53	0.43
12:L:252:PHE:CZ	12:L:257:GLN:HG2	2.54	0.43
13:K:58:HIS:ND1	14:s:87:LEU:HB3	2.34	0.43
13:K:81:MET:HE1	14:t:71:ILE:HG13	2.01	0.43
18:U:712:PRO:O	18:U:716:LYS:HG2	2.18	0.43
21:R:243:PRO:HA	21:R:244:PRO:HD3	1.92	0.43
24:Y:255:LEU:HD22	24:Y:260:VAL:HG21	2.00	0.43
30:f:17:GLY:HA2	30:f:34:LEU:O	2.19	0.43
7:D:185:ILE:O	7:D:188:THR:OG1	2.24	0.42
14:q:117:ILE:HD13	14:t:117:ILE:HG13	2.01	0.42
20:O:313:VAL:HG13	22:W:51:PRO:HB2	2.00	0.42
22:W:80:MET:HE3	22:W:82:ILE:HG12	2.01	0.42
36:Cc:666:ALA:HA	36:Cc:678:THR:HA	2.00	0.42
37:7:7:P5P:H8	37:7:7:P5P:OP2	2.19	0.42
8:E:177:THR:HG22	8:E:179:ASN:H	1.82	0.42
10:I:113:GLU:HG2	10:I:150:LEU:HD12	2.00	0.42
18:U:444:GLU:OE2	18:U:486:ARG:NH1	2.52	0.42
19:M:244:ILE:HG12	19:M:308:ILE:HG22	2.00	0.42
19:M:320:ASN:OD1	19:M:321:LYS:N	2.52	0.42
3:6:78:C:H3'	11:J:111:ARG:HH21	1.84	0.42
4:A:251:ILE:HG22	4:A:253:PRO:HD2	2.00	0.42
4:A:709:PHE:HB3	4:A:760:SER:HB3	2.01	0.42
4:A:1803:ILE:HG23	4:A:1840:SER:HB3	2.01	0.42
6:C:522:VAL:HG11	6:C:536:ALA:HB1	2.00	0.42
14:q:95:GLN:HG3	14:t:100:ARG:HH21	1.83	0.42
24:Y:1078:ASP:OD2	24:Y:1133:TYR:OH	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:k:8:LEU:HB2	31:k:33:TYR:CE1	2.54	0.42
4:A:1934:ILE:HB	4:A:1947:LYS:HB3	2.02	0.42
6:C:668:GLU:O	6:C:671:GLY:N	2.49	0.42
6:C:810:GLU:O	6:C:813:ARG:HB2	2.18	0.42
10:I:44:LYS:O	10:I:53:GLN:NE2	2.49	0.42
11:J:163:PHE:CD1	11:J:179:TYR:HB2	2.54	0.42
11:J:335:GLU:HB3	11:J:344:VAL:HG22	2.01	0.42
17:T:184:SER:OG	17:T:438:GLN:OE1	2.17	0.42
18:U:618:PRO:HD2	18:U:621:LEU:HD21	2.01	0.42
20:O:193:ILE:HG22	20:O:238:LEU:HD22	2.01	0.42
24:Y:193:ASP:OD1	24:Y:193:ASP:N	2.53	0.42
8:E:350:GLU:HG3	8:E:352:ILE:HG23	2.01	0.42
11:J:160:ARG:HD3	11:J:191:ARG:HH21	1.84	0.42
13:K:30:ILE:HD12	14:r:113:ALA:HA	2.01	0.42
19:M:57:ALA:HB2	19:M:66:LYS:HE3	2.01	0.42
24:Y:159:TRP:HA	24:Y:162:LEU:HG	2.00	0.42
24:Y:380:ASP:OD1	24:Y:380:ASP:N	2.52	0.42
27:m:57:LYS:HE3	28:o:76:LEU:HD13	2.02	0.42
4:A:797:LYS:HB3	4:A:797:LYS:HE3	1.91	0.42
4:A:886:GLU:OE1	4:A:889:ARG:NH2	2.40	0.42
4:A:1542:GLY:O	4:A:1545:ARG:NH1	2.49	0.42
4:A:1742:HIS:ND1	4:A:1753:CYS:SG	2.79	0.42
18:U:468:ARG:HH21	18:U:470:GLU:HG2	1.84	0.42
24:Y:35:THR:OG1	24:Y:61:ARG:NH1	2.52	0.42
25:j:58:ASP:OD1	25:j:80:GLN:NE2	2.44	0.42
4:A:1907:ILE:HD11	4:A:1988:LEU:HD13	2.02	0.42
6:C:292:ASP:O	6:C:491:LYS:NZ	2.48	0.42
10:I:327:ASP:OD1	10:I:327:ASP:N	2.52	0.42
18:U:530:PRO:HG2	18:U:728:VAL:HG11	2.02	0.42
6:C:301:LYS:HB3	6:C:304:ARG:HG3	2.02	0.42
9:F:144:MET:N	9:F:144:MET:SD	2.93	0.42
10:I:24:GLU:OE2	10:I:59:ARG:NH1	2.46	0.42
24:Y:356:ASP:OD1	24:Y:356:ASP:N	2.49	0.42
4:A:1184:ARG:CZ	4:A:1210:HIS:HB3	2.50	0.42
5:B:108:LYS:HB3	5:B:112:ARG:NH2	2.34	0.42
13:K:34:ARG:HH22	14:r:105:THR:HG23	1.85	0.42
19:M:112:GLU:O	19:M:115:ARG:HG2	2.20	0.42
20:O:97:LYS:HB3	20:O:97:LYS:HE3	1.81	0.42
24:Y:351:GLN:HA	24:Y:381:ARG:HH21	1.85	0.42
24:Y:438:LEU:HD23	24:Y:1104:ARG:HG3	2.01	0.42
4:A:254:VAL:HA	4:A:352:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:277:LYS:O	4:A:700:GLN:NE2	2.45	0.42
4:A:1285:LYS:HG2	23:P:229:ALA:HB2	2.02	0.42
4:A:1430:LEU:HD21	4:A:1669:ILE:HD13	2.02	0.42
7:D:234:ASP:HB3	10:I:337:ARG:HH22	1.85	0.42
15:N:121:CYS:HA	15:N:125:ARG:HH22	1.84	0.42
18:U:436:MET:HB2	18:U:440:ASP:HB2	2.02	0.42
18:U:707:MET:HE2	18:U:707:MET:HB3	1.93	0.42
20:O:89:LYS:H	20:O:89:LYS:HG2	1.65	0.42
20:O:142:THR:OG1	20:O:143:ILE:N	2.52	0.42
24:Y:211:VAL:HG11	24:Y:258:LEU:HD13	2.01	0.42
24:Y:808:PRO:HG2	24:Y:1136:LEU:HD21	2.02	0.42
24:Y:1158:ASP:OD1	24:Y:1158:ASP:N	2.46	0.42
32:h:65:ARG:HA	32:h:88:LEU:HA	2.02	0.42
29:p:78:LEU:O	30:u:74:ILE:HA	2.20	0.42
4:A:799:VAL:HB	17:T:229:ILE:HD11	2.02	0.41
7:D:163:LEU:HD23	7:D:163:LEU:HA	1.93	0.41
10:I:744:VAL:HG21	12:L:300:ARG:HE	1.84	0.41
11:J:342:ASP:OD1	11:J:343:ARG:N	2.53	0.41
11:J:405:THR:OG1	11:J:410:TRP:NE1	2.44	0.41
12:L:527:GLU:O	12:L:531:ARG:HG2	2.20	0.41
6:C:311:ILE:O	6:C:422:TYR:OH	2.31	0.41
6:C:733:MET:HB3	6:C:837:LEU:HD23	2.02	0.41
9:F:98:ALA:HA	9:F:101:LEU:HB2	2.02	0.41
11:J:42:GLN:O	11:J:43:ARG:NE	2.53	0.41
17:T:196:GLU:HG2	17:T:201:TRP:CD2	2.55	0.41
17:T:298:TRP:HA	17:T:304:SER:O	2.20	0.41
20:O:143:ILE:HD12	20:O:143:ILE:HA	1.88	0.41
25:a:56:VAL:HA	25:a:82:LEU:HA	2.01	0.41
25:j:60:ALA:HB3	25:j:81:ILE:HD13	2.00	0.41
29:p:78:LEU:HD11	30:u:80:ARG:HB2	2.01	0.41
5:B:298:ASN:C	5:B:298:ASN:HD22	2.27	0.41
10:I:282:PHE:CE2	10:I:302:TYR:HB2	2.55	0.41
11:J:360:GLU:HG2	11:J:362:ARG:H	1.85	0.41
12:L:336:ALA:HA	12:L:339:MET:HE2	2.01	0.41
14:q:13:PRO:HB3	14:q:22:LEU:HD11	2.01	0.41
14:t:128:ARG:HH21	14:t:131:LEU:HD22	1.85	0.41
19:M:295:LEU:HB2	19:M:308:ILE:HD11	2.02	0.41
22:W:80:MET:HE2	22:W:80:MET:HB3	1.76	0.41
24:Y:368:ARG:NE	24:Y:370:SER:O	2.53	0.41
3:6:38:A:H61	18:U:468:ARG:HG2	1.85	0.41
4:A:1402:ARG:HH12	4:A:1505:GLU:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1427:LYS:HG2	4:A:1438:PHE:CE2	2.55	0.41
4:A:1905:LEU:HD21	4:A:1936:ILE:HG23	2.01	0.41
6:C:877:MET:HA	6:C:937:MET:O	2.21	0.41
10:I:425:MET:HG3	10:I:446:TRP:CD1	2.55	0.41
10:I:603:LEU:HD23	10:I:603:LEU:HA	1.88	0.41
11:J:376:ILE:HD12	11:J:376:ILE:HA	1.94	0.41
12:L:323:LEU:HA	12:L:326:ILE:HG22	2.02	0.41
19:M:148:ARG:HH12	20:O:285:ILE:HB	1.86	0.41
22:W:34:VAL:O	22:W:40:ASN:ND2	2.53	0.41
24:Y:1091:PHE:HA	24:Y:1095:ALA:HB3	2.02	0.41
29:p:51:ARG:HB2	29:p:72:GLU:HG2	2.02	0.41
4:A:1514:THR:O	4:A:1518:GLN:HG3	2.20	0.41
4:A:1814:TYR:O	4:A:1820:SER:OG	2.32	0.41
4:A:1832:ILE:HD11	4:A:1857:MET:HE1	2.02	0.41
5:B:167:LYS:HE2	5:B:167:LYS:HB2	1.87	0.41
6:C:873:TYR:CD2	6:C:940:LEU:HB3	2.55	0.41
7:D:223:VAL:HG13	7:D:227:MET:HE1	2.01	0.41
12:L:541:ARG:H	12:L:541:ARG:HD3	1.86	0.41
17:T:295:ALA:HB3	17:T:309:LEU:HB2	2.01	0.41
17:T:460:LEU:HB3	17:T:472:TRP:HB2	2.01	0.41
18:U:556:VAL:HG12	18:U:613:VAL:HG22	2.03	0.41
21:R:196:GLN:HB3	21:R:199:ASN:H	1.84	0.41
24:Y:346:LEU:HD12	24:Y:349:LEU:HD12	2.02	0.41
24:Y:681:PHE:HA	24:Y:684:LEU:HB2	2.02	0.41
4:A:643:LEU:HD11	4:A:665:SER:HB2	2.02	0.41
4:A:854:LYS:HA	4:A:854:LYS:HD2	1.85	0.41
4:A:1176:ASP:OD1	4:A:1215:TYR:OH	2.29	0.41
6:C:705:VAL:HG22	6:C:706:VAL:H	1.84	0.41
6:C:872:MET:HE1	6:C:917:PRO:HG3	2.03	0.41
6:C:966:THR:O	6:C:970:THR:OG1	2.36	0.41
8:E:80:MET:HG3	8:E:105:ALA:HB2	2.03	0.41
9:F:61:VAL:HG22	10:I:451:LEU:HD23	2.02	0.41
11:J:324:ASN:HB3	11:J:327:VAL:HB	2.00	0.41
20:O:59:PRO:HA	20:O:62:VAL:HB	2.02	0.41
24:Y:158:ILE:HB	24:Y:254:LEU:HD13	2.03	0.41
25:j:33:TRP:HB2	25:j:90:LEU:HB3	2.03	0.41
28:o:79:LEU:HD23	28:o:79:LEU:HA	1.91	0.41
29:p:18:ARG:HH21	29:p:31:GLY:HA2	1.85	0.41
6:C:397:LYS:HB2	6:C:397:LYS:HE2	1.83	0.41
6:C:642:ASN:HB2	6:C:645:GLU:HB2	2.02	0.41
10:I:424:ILE:HG21	10:I:424:ILE:HD13	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:157:GLU:HA	12:L:160:LYS:HE2	2.02	0.41
14:t:117:ILE:O	14:t:121:THR:OG1	2.30	0.41
17:T:356:LYS:HA	17:T:356:LYS:HD3	1.79	0.41
24:Y:1118:GLN:OE1	24:Y:1129:TYR:OH	2.38	0.41
26:l:45:ASN:HB2	27:m:28:PRO:HG2	2.02	0.41
8:E:80:MET:C	8:E:82:ARG:H	2.29	0.41
10:I:170:TYR:HA	10:I:173:VAL:HG12	2.03	0.41
12:L:731:ARG:HD2	13:K:9:GLU:HB3	2.01	0.41
21:R:299:GLU:O	21:R:303:MET:HG2	2.20	0.41
22:W:254:PRO:O	22:W:273:ALA:N	2.54	0.41
24:Y:82:ILE:HD13	24:Y:130:VAL:HG13	2.02	0.41
4:A:311:ASP:H	4:A:315:ASP:HB2	1.85	0.41
4:A:910:TRP:CD1	23:P:259:VAL:HG11	2.56	0.41
4:A:1084:GLN:O	4:A:1088:ASN:ND2	2.53	0.41
4:A:1214:LEU:HB2	4:A:1225:PHE:HB3	2.03	0.41
4:A:1318:GLY:HA2	4:A:1363:ASP:OD2	2.20	0.41
4:A:1442:VAL:HG23	4:A:1665:TRP:CD2	2.56	0.41
5:B:108:LYS:O	5:B:112:ARG:NE	2.36	0.41
5:B:245:ASN:O	16:S:132:ARG:NH2	2.37	0.41
6:C:534:PHE:HE2	6:C:655:LYS:HG2	1.86	0.41
7:D:162:TYR:HB2	12:L:286:SER:HB2	2.03	0.41
8:E:63:ILE:HA	8:E:79:SER:HB2	2.03	0.41
8:E:259:ARG:NH2	12:L:750:GLN:HG3	2.36	0.41
10:I:185:LEU:HD13	10:I:194:ALA:HA	2.02	0.41
10:I:569:LEU:HD23	10:I:569:LEU:HA	1.88	0.41
12:L:531:ARG:HH21	12:L:576:ASP:HA	1.86	0.41
18:U:578:ARG:NH1	18:U:659:ARG:HD3	2.35	0.41
24:Y:1017:ILE:HD13	24:Y:1036:PHE:HZ	1.85	0.41
24:Y:1207:SER:OG	24:Y:1250:ASN:ND2	2.40	0.41
24:Y:1268:ASP:HB3	24:Y:1271:ARG:HB2	2.02	0.41
31:k:17:PHE:HD2	31:k:70:GLU:HB2	1.85	0.41
30:u:7:ILE:HA	30:u:10:LYS:HG2	2.03	0.41
4:A:533:TRP:HZ2	6:C:308:GLU:HG2	1.86	0.41
4:A:911:LEU:O	4:A:915:GLN:HG3	2.21	0.41
4:A:1124:LEU:HD22	4:A:1128:MET:HE3	2.03	0.41
4:A:1221:LYS:HB2	4:A:1221:LYS:HE3	1.83	0.41
12:L:292:LYS:O	12:L:296:MET:HB2	2.22	0.41
16:S:85:GLY:HA2	16:S:109:PRO:HG3	2.01	0.41
21:R:101:ASP:OD1	21:R:105:LYS:N	2.51	0.41
24:Y:1164:VAL:HG21	24:Y:1185:GLU:HG2	2.03	0.41
37:7:94:Y5P:H4A	37:7:95:Y5P:H4	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:234:ASP:OD2	10:I:279:ARG:NH1	2.53	0.40
11:J:335:GLU:HG3	11:J:347:VAL:HG21	2.03	0.40
15:N:45:HIS:O	15:N:48:GLN:HG2	2.21	0.40
17:T:270:HIS:CD2	17:T:296:ARG:HD2	2.56	0.40
19:M:28:PRO:O	21:R:206:ARG:NH2	2.49	0.40
21:R:258:PRO:HA	21:R:259:PRO:HD3	1.97	0.40
24:Y:214:PHE:HZ	24:Y:264:LEU:HD21	1.86	0.40
24:Y:353:LEU:HD22	24:Y:357:GLU:HB3	2.04	0.40
4:A:589:LYS:HE2	4:A:589:LYS:HB3	1.91	0.40
4:A:1077:LEU:HG	4:A:1081:LYS:HE2	2.04	0.40
4:A:1640:MET:SD	4:A:1653:LEU:HD21	2.61	0.40
4:A:1720:LEU:HD23	4:A:1720:LEU:HA	1.95	0.40
6:C:518:LEU:HD11	6:C:545:ALA:HA	2.04	0.40
10:I:50:LEU:HD22	10:I:81:LYS:HE2	2.02	0.40
10:I:405:TRP:CZ2	10:I:427:LYS:HG3	2.55	0.40
10:I:427:LYS:O	10:I:431:VAL:HG23	2.22	0.40
10:I:472:ARG:HE	21:R:25:ARG:NH1	2.20	0.40
14:q:14:VAL:HG12	14:q:52:LEU:HD12	2.03	0.40
14:r:26:ARG:NH1	14:s:79:GLN:OE1	2.54	0.40
14:r:96:LEU:HD13	14:s:96:LEU:HA	2.03	0.40
14:r:123:GLU:HB3	14:r:124:ARG:NH1	2.37	0.40
24:Y:1302:PHE:O	24:Y:1306:LEU:HB2	2.21	0.40
3:6:97:U:O2'	36:Cc:403:LYS:O	2.39	0.40
4:A:991:LEU:HD23	4:A:991:LEU:HA	1.85	0.40
4:A:1243:GLU:HG3	4:A:1282:TRP:CZ2	2.57	0.40
7:D:150:LEU:HD11	11:J:18:ILE:HG12	2.02	0.40
8:E:240:ASP:N	8:E:240:ASP:OD1	2.53	0.40
10:I:251:ILE:HG23	10:I:258:ARG:HG2	2.03	0.40
12:L:80:TRP:CE2	12:L:95:LEU:HD13	2.57	0.40
18:U:670:MET:HE3	18:U:670:MET:HB3	1.95	0.40
18:U:739:ASP:HB3	18:U:742:ARG:HB2	2.03	0.40
30:u:23:GLU:HA	30:u:28:GLN:O	2.20	0.40
1:2:16:U:H5	5:B:304:LYS:HB2	1.87	0.40
6:C:181:MET:HE1	6:C:228:MET:HB2	2.03	0.40
6:C:811:SER:O	6:C:853:ARG:NH2	2.47	0.40
8:E:310:THR:OG1	8:E:311:GLY:N	2.55	0.40
9:F:94:LEU:O	9:F:97:LYS:C	2.64	0.40
10:I:256:ASP:OD1	10:I:256:ASP:N	2.53	0.40
10:I:423:ILE:HD12	10:I:423:ILE:HA	1.96	0.40
10:I:673:MET:HE3	10:I:673:MET:HB3	1.80	0.40
11:J:365:ARG:HA	11:J:406:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:s:17:LYS:HE2	14:s:53:LEU:HD13	2.03	0.40
15:N:1:MET:HE2	15:N:5:ARG:HG2	2.02	0.40
18:U:711:GLU:HB2	18:U:714:VAL:HG23	2.04	0.40
19:M:92:GLY:HA2	21:R:197:MET:HG2	2.03	0.40
25:j:35:TYR:CE1	25:j:87:ASN:HA	2.56	0.40
2:5:62:U:H2'	2:5:63:G:C8	2.56	0.40
4:A:282:PRO:HA	4:A:283:PRO:HD3	1.93	0.40
4:A:520:LEU:HA	6:C:423:LYS:HG2	2.03	0.40
4:A:837:LEU:HD23	4:A:837:LEU:HA	1.92	0.40
6:C:604:VAL:HG12	6:C:605:LYS:HG2	2.04	0.40
6:C:884:VAL:HG23	6:C:912:VAL:HG21	2.03	0.40
10:I:332:PHE:HE2	24:Y:322:MET:HE3	1.86	0.40
10:I:371:VAL:HG11	10:I:385:TYR:HE1	1.85	0.40
10:I:407:ASN:HA	10:I:410:LYS:HG2	2.02	0.40
10:I:458:GLU:HA	10:I:461:ARG:HG2	2.04	0.40
14:t:47:ASP:HB3	14:t:51:ASP:H	1.85	0.40
18:U:621:LEU:HD23	18:U:621:LEU:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	2004/2463 (81%)	1911 (95%)	90 (4%)	3 (0%)	48	77
5	B	256/326 (78%)	249 (97%)	6 (2%)	1 (0%)	30	60
6	C	920/1011 (91%)	889 (97%)	29 (3%)	2 (0%)	43	72
7	D	91/325 (28%)	90 (99%)	1 (1%)	0	100	100
8	E	308/352 (88%)	285 (92%)	23 (8%)	0	100	100
9	F	108/233 (46%)	104 (96%)	3 (3%)	1 (1%)	14	41
10	I	736/839 (88%)	705 (96%)	29 (4%)	2 (0%)	36	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	J	604/687 (88%)	592 (98%)	12 (2%)	0	100	100
12	L	629/768 (82%)	602 (96%)	26 (4%)	1 (0%)	43	72
13	K	229/231 (99%)	224 (98%)	5 (2%)	0	100	100
14	q	137/480 (28%)	135 (98%)	2 (2%)	0	100	100
14	r	141/480 (29%)	140 (99%)	1 (1%)	0	100	100
14	s	138/480 (29%)	137 (99%)	1 (1%)	0	100	100
14	t	139/480 (29%)	136 (98%)	3 (2%)	0	100	100
15	N	146/148 (99%)	136 (93%)	8 (6%)	2 (1%)	9	30
16	S	155/167 (93%)	148 (96%)	7 (4%)	0	100	100
17	T	326/496 (66%)	311 (95%)	14 (4%)	1 (0%)	36	66
18	U	346/757 (46%)	321 (93%)	23 (7%)	2 (1%)	21	51
19	M	242/395 (61%)	225 (93%)	17 (7%)	0	100	100
20	0	274/408 (67%)	261 (95%)	13 (5%)	0	100	100
21	R	334/578 (58%)	312 (93%)	21 (6%)	1 (0%)	36	66
22	W	391/547 (72%)	376 (96%)	14 (4%)	1 (0%)	36	66
23	P	110/260 (42%)	102 (93%)	8 (7%)	0	100	100
24	Y	1342/1416 (95%)	1315 (98%)	27 (2%)	0	100	100
25	a	84/98 (86%)	83 (99%)	1 (1%)	0	100	100
25	j	86/98 (88%)	84 (98%)	2 (2%)	0	100	100
26	b	69/94 (73%)	69 (100%)	0	0	100	100
26	l	79/94 (84%)	77 (98%)	2 (2%)	0	100	100
27	c	82/592 (14%)	80 (98%)	2 (2%)	0	100	100
27	m	84/592 (14%)	80 (95%)	4 (5%)	0	100	100
28	d	79/118 (67%)	76 (96%)	3 (4%)	0	100	100
28	o	85/118 (72%)	78 (92%)	7 (8%)	0	100	100
29	e	75/211 (36%)	73 (97%)	2 (3%)	0	100	100
29	p	99/211 (47%)	92 (93%)	7 (7%)	0	100	100
30	f	82/114 (72%)	79 (96%)	3 (4%)	0	100	100
30	u	88/114 (77%)	83 (94%)	5 (6%)	0	100	100
31	g	70/82 (85%)	69 (99%)	1 (1%)	0	100	100
31	k	71/82 (87%)	68 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	h	120/242 (50%)	117 (98%)	3 (2%)	0	100	100
33	i	100/201 (50%)	100 (100%)	0	0	100	100
34	CY	89/510 (18%)	88 (99%)	1 (1%)	0	100	100
35	Cb	501/975 (51%)	495 (99%)	6 (1%)	0	100	100
36	Cc	712/764 (93%)	694 (98%)	18 (2%)	0	100	100
38	Ci	82/153 (54%)	82 (100%)	0	0	100	100
All	All	12843/19790 (65%)	12373 (96%)	453 (4%)	17 (0%)	49	77

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	494	LYS
4	A	1219	ILE
5	B	111	GLN
6	C	840	VAL
9	F	98	ALA
15	N	7	ALA
18	U	400	VAL
21	R	177	ASN
4	A	595	GLN
12	L	390	GLN
6	C	846	TRP
10	I	558	TYR
22	W	101	VAL
18	U	399	ILE
15	N	6	PRO
10	I	416	GLY
17	T	489	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1813/2212 (82%)	1809 (100%)	4 (0%)	87	96
5	B	208/270 (77%)	208 (100%)	0	100	100
6	C	809/884 (92%)	808 (100%)	1 (0%)	88	97
7	D	80/276 (29%)	80 (100%)	0	100	100
8	E	254/287 (88%)	254 (100%)	0	100	100
9	F	92/179 (51%)	92 (100%)	0	100	100
10	I	646/729 (89%)	646 (100%)	0	100	100
11	J	525/592 (89%)	525 (100%)	0	100	100
12	L	520/635 (82%)	518 (100%)	2 (0%)	84	94
13	K	186/186 (100%)	186 (100%)	0	100	100
14	q	122/385 (32%)	122 (100%)	0	100	100
14	r	123/385 (32%)	123 (100%)	0	100	100
14	s	122/385 (32%)	122 (100%)	0	100	100
14	t	123/385 (32%)	123 (100%)	0	100	100
15	N	131/131 (100%)	129 (98%)	2 (2%)	57	84
16	S	126/135 (93%)	126 (100%)	0	100	100
17	T	276/408 (68%)	271 (98%)	5 (2%)	51	82
18	U	294/649 (45%)	293 (100%)	1 (0%)	86	95
19	M	210/293 (72%)	210 (100%)	0	100	100
20	0	227/335 (68%)	219 (96%)	8 (4%)	32	67
21	R	278/476 (58%)	277 (100%)	1 (0%)	84	94
22	W	73/459 (16%)	73 (100%)	0	100	100
23	P	91/213 (43%)	91 (100%)	0	100	100
24	Y	1173/1231 (95%)	1173 (100%)	0	100	100
25	j	79/85 (93%)	79 (100%)	0	100	100
26	l	72/84 (86%)	72 (100%)	0	100	100
27	m	77/497 (16%)	77 (100%)	0	100	100
28	o	78/95 (82%)	78 (100%)	0	100	100
29	p	84/152 (55%)	84 (100%)	0	100	100
30	u	80/94 (85%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	k	64/71 (90%)	64 (100%)	0	100	100
All	All	9036/13198 (68%)	9012 (100%)	24 (0%)	84	95

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	420	ASN
4	A	589	LYS
4	A	593	SER
4	A	638	LYS
6	C	527	ASN
12	L	209	ILE
12	L	210	LYS
15	N	108	ILE
15	N	144	CYS
17	T	488	LYS
17	T	491	LEU
17	T	492	VAL
17	T	493	ARG
17	T	495	LYS
18	U	468	ARG
20	0	85	ASP
20	0	88	ASP
20	0	89	LYS
20	0	91	LEU
20	0	208	ARG
20	0	209	VAL
20	0	212	ASN
20	0	213	ARG
21	R	132	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	156	GLN
4	A	471	ASN
4	A	644	HIS
4	A	711	HIS
4	A	830	GLN
4	A	1026	ASN
4	A	1028	ASN

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Mol	Chain	Res	Type
4	A	1088	ASN
4	A	1130	HIS
4	A	1141	ASN
4	A	1309	ASN
4	A	1368	ASN
4	A	1486	HIS
4	A	1525	GLN
4	A	1547	ASN
4	A	1593	ASN
4	A	1595	ASN
4	A	1737	GLN
4	A	1837	ASN
4	A	1864	ASN
4	A	2002	ASN
4	A	2090	GLN
4	A	2093	HIS
4	A	2116	ASN
5	B	111	GLN
6	C	106	GLN
6	C	243	ASN
6	C	250	HIS
6	C	527	ASN
6	C	582	ASN
6	C	849	ASN
6	C	897	HIS
7	D	144	ASN
7	D	182	GLN
9	F	88	ASN
9	F	128	GLN
9	F	142	GLN
10	I	77	ASN
10	I	485	GLN
10	I	706	ASN
11	J	73	GLN
11	J	80	GLN
11	J	104	ASN
11	J	177	ASN
11	J	194	GLN
11	J	276	ASN
11	J	284	GLN
12	L	11	ASN
12	L	208	ASN

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Mol	Chain	Res	Type
12	L	218	GLN
13	K	65	ASN
13	K	121	GLN
13	K	146	ASN
14	q	110	HIS
14	s	110	HIS
15	N	83	ASN
15	N	116	ASN
15	N	127	GLN
16	S	99	ASN
17	T	220	GLN
18	U	591	GLN
18	U	642	GLN
19	M	90	GLN
20	0	175	GLN
20	0	240	HIS
20	0	258	GLN
24	Y	175	ASN
24	Y	271	ASN
24	Y	310	HIS
24	Y	324	HIS
24	Y	437	ASN
24	Y	653	GLN
24	Y	1048	GLN
24	Y	1141	HIS
24	Y	1350	GLN
26	l	50	ASN
26	l	72	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	101/193 (52%)	18 (17%)	2 (1%)
2	5	109/116 (93%)	21 (19%)	1 (0%)
3	6	97/101 (96%)	36 (37%)	2 (2%)
37	7	23/101 (22%)	7 (30%)	0
All	All	330/511 (64%)	82 (24%)	5 (1%)

All (82) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	4	U
1	2	14	U
1	2	16	U
1	2	17	U
1	2	18	G
1	2	19	G
1	2	23	A
1	2	24	G
1	2	28	A
1	2	39	C
1	2	40	U
1	2	41	G
1	2	100	U
1	2	111	G
1	2	120	C
1	2	137	U
1	2	142	G
1	2	145	U
2	5	6	G
2	5	8	A
2	5	20	A
2	5	21	C
2	5	22	C
2	5	23	G
2	5	24	A
2	5	27	U
2	5	33	C
2	5	50	G
2	5	71	A
2	5	72	U
2	5	75	U
2	5	77	C
2	5	87	U
2	5	88	C
2	5	89	U
2	5	91	U
2	5	93	G
2	5	94	A
2	5	106	U
3	6	6	U
3	6	7	C
3	6	9	G
3	6	15	U

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Mol	Chain	Res	Type
3	6	18	G
3	6	19	U
3	6	20	C
3	6	21	A
3	6	22	A
3	6	24	U
3	6	28	A
3	6	32	A
3	6	38	A
3	6	39	G
3	6	42	G
3	6	45	U
3	6	47	G
3	6	49	A
3	6	61	C
3	6	62	U
3	6	63	A
3	6	68	U
3	6	70	A
3	6	74	G
3	6	81	A
3	6	82	A
3	6	84	G
3	6	85	A
3	6	88	C
3	6	89	G
3	6	90	C
3	6	91	U
3	6	95	A
3	6	96	A
3	6	97	U
3	6	98	U
37	7	2	U
37	7	3	P5P
37	7	7	P5P
37	7	11	Y5P
37	7	14	Y5P
37	7	93	P5P
37	7	97	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	13	C
1	2	23	A
2	5	70	A
3	6	15	U
3	6	38	A

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

25 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
37	Y5P	7	90	37	14,19,20	4.58	2 (14%)	18,26,29	1.34	2 (11%)
21	SEP	R	242	21	8,9,10	0.70	0	7,12,14	1.24	1 (14%)
37	Y5P	7	12	37	14,19,20	4.20	2 (14%)	18,26,29	1.05	1 (5%)
37	Y5P	7	10	37	14,19,20	4.22	2 (14%)	18,26,29	1.03	1 (5%)
37	P5P	7	5	37	20,23,24	1.00	2 (10%)	27,33,36	1.87	3 (11%)
37	P5P	7	3	3,37	20,23,24	0.43	0	27,33,36	0.70	1 (3%)
37	Y5P	7	98	37	14,19,20	4.15	2 (14%)	18,26,29	1.00	1 (5%)
21	SEP	R	234	21	8,9,10	1.42	1 (12%)	7,12,14	0.84	0
37	Y5P	7	100	37	14,19,20	4.59	2 (14%)	18,26,29	1.37	2 (11%)
37	Y5P	7	89	37	14,19,20	4.26	2 (14%)	18,26,29	0.99	1 (5%)
37	Y5P	7	14	37	14,19,20	4.18	2 (14%)	18,26,29	1.06	1 (5%)
37	Y5P	7	96	37	14,19,20	4.17	2 (14%)	18,26,29	1.05	1 (5%)
37	Y5P	7	101	37	14,19,20	4.23	2 (14%)	18,26,29	1.05	1 (5%)
37	Y5P	7	4	37	14,19,20	4.24	2 (14%)	18,26,29	1.15	1 (5%)
37	Y5P	7	95	37	14,19,20	4.19	2 (14%)	18,26,29	1.02	1 (5%)
37	Y5P	7	99	37	14,19,20	4.61	2 (14%)	18,26,29	1.38	2 (11%)
37	P5P	7	91	1,37	20,23,24	0.46	0	27,33,36	0.68	1 (3%)
37	P5P	7	7	3,37	20,23,24	0.90	1 (5%)	27,33,36	1.89	4 (14%)
37	P5P	7	93	1,37	20,23,24	0.48	0	27,33,36	0.70	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	Y5P	7	94	37	14,19,20	4.58	2 (14%)	18,26,29	1.38	2 (11%)
37	Y5P	7	13	37	14,19,20	4.19	2 (14%)	18,26,29	1.03	1 (5%)
37	Y5P	7	6	37	14,19,20	4.16	2 (14%)	18,26,29	0.97	1 (5%)
37	Y5P	7	8	37	14,19,20	4.55	2 (14%)	18,26,29	1.37	2 (11%)
37	Y5P	7	92	37	14,19,20	4.25	2 (14%)	18,26,29	0.98	1 (5%)
37	Y5P	7	11	37	14,19,20	4.23	2 (14%)	18,26,29	1.02	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	Y5P	7	90	37	-	2/7/33/34	0/2/2/2
21	SEP	R	242	21	-	3/6/8/10	-
37	Y5P	7	12	37	-	4/7/33/34	0/2/2/2
37	Y5P	7	10	37	-	3/7/33/34	0/2/2/2
37	P5P	7	5	37	-	0/7/25/26	0/3/3/3
37	P5P	7	3	3,37	-	2/7/25/26	0/3/3/3
37	Y5P	7	98	37	-	1/7/33/34	0/2/2/2
21	SEP	R	234	21	-	2/6/8/10	-
37	Y5P	7	100	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	89	37	-	3/7/33/34	0/2/2/2
37	Y5P	7	14	37	-	2/7/33/34	0/2/2/2
37	Y5P	7	96	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	101	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	4	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	95	37	-	4/7/33/34	0/2/2/2
37	Y5P	7	99	37	-	1/7/33/34	0/2/2/2
37	P5P	7	91	1,37	-	1/7/25/26	0/3/3/3
37	P5P	7	7	3,37	-	2/7/25/26	0/3/3/3
37	P5P	7	93	1,37	-	1/7/25/26	0/3/3/3
37	Y5P	7	94	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	13	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	6	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	8	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	92	37	-	1/7/33/34	0/2/2/2
37	Y5P	7	11	37	-	4/7/33/34	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	7	99	Y5P	C4-N3	-13.78	1.33	1.46
37	7	94	Y5P	C4-N3	-13.56	1.33	1.46
37	7	92	Y5P	C2-N3	13.47	1.37	1.27
37	7	89	Y5P	C2-N3	13.45	1.37	1.27
37	7	101	Y5P	C2-N3	13.45	1.37	1.27
37	7	100	Y5P	C4-N3	-13.45	1.33	1.46
37	7	90	Y5P	C4-N3	-13.33	1.33	1.46
37	7	4	Y5P	C2-N3	13.22	1.37	1.27
37	7	11	Y5P	C2-N3	13.20	1.37	1.27
37	7	95	Y5P	C2-N3	13.20	1.37	1.27
37	7	8	Y5P	C4-N3	-13.14	1.33	1.46
37	7	10	Y5P	C2-N3	13.14	1.37	1.27
37	7	14	Y5P	C2-N3	13.10	1.37	1.27
37	7	6	Y5P	C2-N3	13.00	1.37	1.27
37	7	13	Y5P	C2-N3	12.99	1.37	1.27
37	7	12	Y5P	C2-N3	12.99	1.37	1.27
37	7	98	Y5P	C2-N3	12.81	1.37	1.27
37	7	96	Y5P	C2-N3	12.77	1.37	1.27
37	7	8	Y5P	C2-N3	10.73	1.35	1.27
37	7	90	Y5P	C2-N3	10.67	1.35	1.27
37	7	100	Y5P	C2-N3	10.58	1.35	1.27
37	7	94	Y5P	C2-N3	10.40	1.35	1.27
37	7	99	Y5P	C2-N3	10.29	1.35	1.27
37	7	96	Y5P	C4-N3	-8.87	1.37	1.46
37	7	12	Y5P	C4-N3	-8.77	1.38	1.46
37	7	98	Y5P	C4-N3	-8.72	1.38	1.46
37	7	13	Y5P	C4-N3	-8.69	1.38	1.46
37	7	10	Y5P	C4-N3	-8.67	1.38	1.46
37	7	4	Y5P	C4-N3	-8.67	1.38	1.46
37	7	11	Y5P	C4-N3	-8.65	1.38	1.46
37	7	14	Y5P	C4-N3	-8.51	1.38	1.46
37	7	6	Y5P	C4-N3	-8.47	1.38	1.46
37	7	89	Y5P	C4-N3	-8.44	1.38	1.46
37	7	92	Y5P	C4-N3	-8.36	1.38	1.46
37	7	95	Y5P	C4-N3	-8.34	1.38	1.46
37	7	101	Y5P	C4-N3	-8.28	1.38	1.46
21	R	234	SEP	P-O1P	3.17	1.60	1.50
37	7	5	P5P	C6-N1	2.29	1.39	1.34
37	7	7	P5P	C6-N1	2.23	1.39	1.34
37	7	5	P5P	C6-C5	2.03	1.42	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7	7	P5P	C6-N1-C2	7.84	125.06	115.80
37	7	5	P5P	C6-N1-C2	7.75	124.94	115.80
37	7	94	Y5P	C5-C4-N3	4.92	122.08	114.15
37	7	99	Y5P	C5-C4-N3	4.91	122.06	114.15
37	7	100	Y5P	C5-C4-N3	4.88	122.02	114.15
37	7	8	Y5P	C5-C4-N3	4.78	121.86	114.15
37	7	90	Y5P	C5-C4-N3	4.69	121.72	114.15
37	7	7	P5P	C5-C6-N1	-4.10	111.68	121.90
37	7	5	P5P	C5-C6-N1	-4.08	111.74	121.90
37	7	101	Y5P	N1-C2-N3	-3.91	114.56	125.39
37	7	10	Y5P	N1-C2-N3	-3.83	114.76	125.39
37	7	11	Y5P	N1-C2-N3	-3.82	114.79	125.39
37	7	12	Y5P	N1-C2-N3	-3.82	114.80	125.39
37	7	4	Y5P	N1-C2-N3	-3.82	114.81	125.39
37	7	95	Y5P	N1-C2-N3	-3.81	114.81	125.39
37	7	13	Y5P	N1-C2-N3	-3.81	114.84	125.39
37	7	14	Y5P	N1-C2-N3	-3.80	114.84	125.39
37	7	98	Y5P	N1-C2-N3	-3.74	115.03	125.39
37	7	89	Y5P	N1-C2-N3	-3.72	115.07	125.39
37	7	92	Y5P	N1-C2-N3	-3.72	115.07	125.39
37	7	6	Y5P	N1-C2-N3	-3.65	115.26	125.39
37	7	96	Y5P	N1-C2-N3	-3.60	115.40	125.39
21	R	242	SEP	OG-CB-CA	2.74	110.81	108.14
37	7	7	P5P	C6-C5-C4	2.56	119.04	116.24
37	7	91	P5P	C6-N1-C2	2.39	118.62	115.80
37	7	8	Y5P	N1-C2-N3	-2.35	118.88	125.39
37	7	3	P5P	C6-N1-C2	2.33	118.55	115.80
37	7	93	P5P	C6-N1-C2	2.28	118.50	115.80
37	7	100	Y5P	N1-C2-N3	-2.19	119.31	125.39
37	7	90	Y5P	N1-C2-N3	-2.17	119.37	125.39
37	7	94	Y5P	N1-C2-N3	-2.16	119.40	125.39
37	7	99	Y5P	N1-C2-N3	-2.11	119.54	125.39
37	7	5	P5P	C6-C5-C4	2.10	118.53	116.24
37	7	7	P5P	N1-C2-N3	-2.03	123.88	127.33

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	R	234	SEP	N-CA-CB-OG
21	R	234	SEP	C-CA-CB-OG
21	R	242	SEP	C-CA-CB-OG
37	7	6	Y5P	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
37	7	11	Y5P	O4'-C1'-N1-C2
37	7	89	Y5P	O4'-C1'-N1-C2
37	7	94	Y5P	O4'-C1'-N1-C2
37	7	96	Y5P	O4'-C1'-N1-C2
37	7	98	Y5P	O4'-C1'-N1-C2
37	7	99	Y5P	O4'-C1'-N1-C2
37	7	100	Y5P	O4'-C1'-N1-C2
37	7	4	Y5P	O4'-C1'-N1-C2
37	7	8	Y5P	O4'-C1'-N1-C2
37	7	10	Y5P	O4'-C1'-N1-C2
37	7	14	Y5P	O4'-C1'-N1-C2
37	7	90	Y5P	O4'-C1'-N1-C2
37	7	92	Y5P	O4'-C1'-N1-C2
37	7	95	Y5P	O4'-C1'-N1-C2
37	7	3	P5P	C3'-C4'-C5'-O5'
37	7	11	Y5P	O4'-C4'-C5'-O5'
37	7	89	Y5P	C4'-C5'-O5'-P
37	7	11	Y5P	C3'-C4'-C5'-O5'
37	7	12	Y5P	C2'-C1'-N1-C2
37	7	12	Y5P	C2'-C1'-N1-C6
37	7	3	P5P	O4'-C4'-C5'-O5'
37	7	95	Y5P	C3'-C4'-C5'-O5'
37	7	12	Y5P	O4'-C1'-N1-C6
37	7	7	P5P	C3'-C4'-C5'-O5'
37	7	12	Y5P	O4'-C1'-N1-C2
37	7	13	Y5P	O4'-C1'-N1-C2
37	7	95	Y5P	O4'-C4'-C5'-O5'
21	R	242	SEP	CB-OG-P-O1P
37	7	10	Y5P	C4'-C5'-O5'-P
21	R	242	SEP	N-CA-CB-OG
37	7	11	Y5P	C4'-C5'-O5'-P
37	7	93	P5P	C4'-C5'-O5'-P
37	7	95	Y5P	C4'-C5'-O5'-P
37	7	101	Y5P	O4'-C1'-N1-C2
37	7	14	Y5P	C4'-C5'-O5'-P
37	7	7	P5P	O4'-C4'-C5'-O5'
37	7	89	Y5P	O4'-C4'-C5'-O5'
37	7	10	Y5P	O4'-C4'-C5'-O5'
37	7	90	Y5P	C4'-C5'-O5'-P
37	7	91	P5P	O4'-C4'-C5'-O5'

There are no ring outliers.

17 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	7	90	Y5P	1	0
37	7	12	Y5P	2	0
37	7	98	Y5P	1	0
21	R	234	SEP	1	0
37	7	100	Y5P	1	0
37	7	89	Y5P	2	0
37	7	14	Y5P	2	0
37	7	96	Y5P	1	0
37	7	95	Y5P	5	0
37	7	99	Y5P	1	0
37	7	7	P5P	2	0
37	7	93	P5P	1	0
37	7	94	Y5P	1	0
37	7	13	Y5P	3	0
37	7	6	Y5P	1	0
37	7	8	Y5P	2	0
37	7	92	Y5P	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
42	GTP	C	1102	41	33,34,34	0.99	2 (6%)	50,54,54	1.63	10 (20%)
40	M7M	B	401	-	28,32,33	3.94	16 (57%)	31,49,52	1.19	3 (9%)
43	IHP	J	1001	-	36,36,36	1.53	6 (16%)	60,60,60	1.13	6 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	GTP	C	1102	41	-	6/22/38/38	0/3/3/3
40	M7M	B	401	-	-	2/17/47/48	0/3/3/3
43	IHP	J	1001	-	-	10/30/54/54	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B	401	M7M	CBY-CBS	-7.16	1.34	1.53
40	B	401	M7M	CBG-NBH	7.09	1.44	1.35
40	B	401	M7M	CBI-NBP	7.05	1.50	1.45
40	B	401	M7M	OBR-CBS	6.95	1.60	1.45
40	B	401	M7M	CBO-NBP	5.73	1.44	1.35
40	B	401	M7M	CBM-NBE	5.52	1.45	1.32
40	B	401	M7M	CBM-NBV	5.43	1.45	1.35
40	B	401	M7M	OBR-CBQ	-5.39	1.29	1.42
40	B	401	M7M	CBO-NBN	5.38	1.46	1.37
40	B	401	M7M	CBM-NBN	4.84	1.47	1.36
43	J	1001	IHP	P4-O14	3.72	1.66	1.59
43	J	1001	IHP	P3-O13	3.27	1.65	1.59
43	J	1001	IHP	P5-O15	3.23	1.65	1.59
40	B	401	M7M	CBF-NBE	3.21	1.43	1.38
43	J	1001	IHP	P1-O11	3.09	1.64	1.59
40	B	401	M7M	OCB-CBY	3.08	1.50	1.43
43	J	1001	IHP	P2-O12	3.02	1.64	1.59
43	J	1001	IHP	P6-O16	3.01	1.64	1.59
40	B	401	M7M	OCA-CBX	-3.00	1.35	1.43
40	B	401	M7M	OBG-CBF	-2.88	1.18	1.23
40	B	401	M7M	CBG-CBO	2.66	1.43	1.36
42	C	1102	GTP	O4'-C4'	-2.08	1.40	1.45
42	C	1102	GTP	C5-N7	-2.07	1.34	1.39
40	B	401	M7M	PBK-OBV	2.02	1.67	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	C	1102	GTP	C5-C4-N3	-4.87	120.64	128.39
42	C	1102	GTP	C2-N3-C4	4.44	119.94	112.30
43	J	1001	IHP	C5-C4-C3	-3.73	102.25	110.43
43	J	1001	IHP	O15-C5-C4	3.36	115.91	108.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B	401	M7M	CBO-CBG-NBH	3.31	109.30	106.86
42	C	1102	GTP	C2-N1-C6	-3.10	119.50	125.11
42	C	1102	GTP	N9-C4-N3	3.08	132.12	125.95
42	C	1102	GTP	N9-C8-N7	-2.82	108.18	113.40
42	C	1102	GTP	C5-C6-N1	2.62	119.91	113.25
42	C	1102	GTP	C8-N7-C5	2.57	108.85	104.26
42	C	1102	GTP	O2A-PA-O3A	2.46	113.92	107.27
42	C	1102	GTP	O2G-PG-O3B	2.38	112.60	104.64
40	B	401	M7M	NBP-CBI-NBH	2.36	106.71	103.37
40	B	401	M7M	CBY-CBX-CBQ	2.23	105.68	101.46
42	C	1102	GTP	O6-C6-C5	-2.22	120.67	126.53
43	J	1001	IHP	P3-O13-C3	-2.15	117.68	123.43
43	J	1001	IHP	P2-O12-C2	-2.15	117.68	123.43
43	J	1001	IHP	O13-C3-C4	2.15	113.33	108.76
43	J	1001	IHP	C6-C1-C2	2.05	114.94	110.43

There are no chirality outliers.

All (18) torsion outliers are listed below:

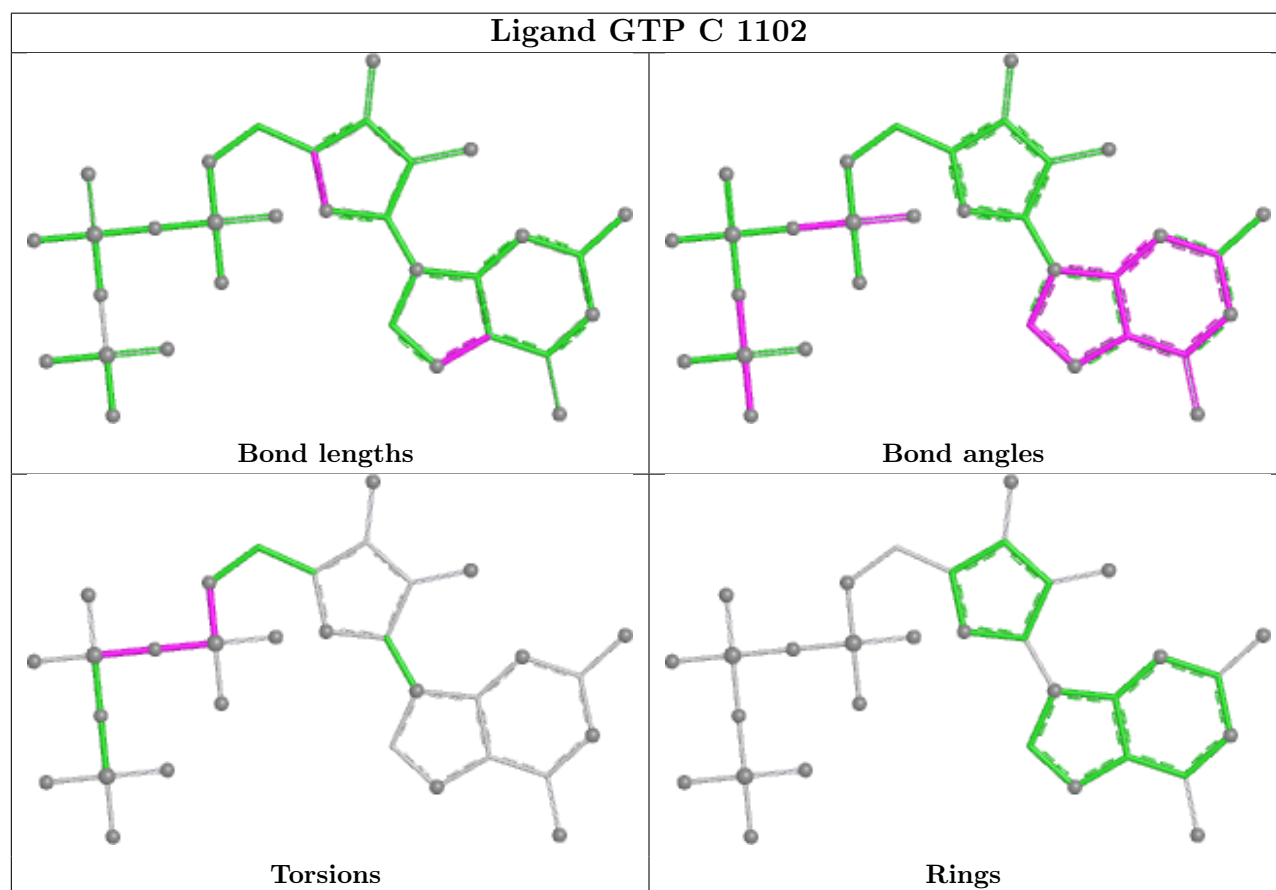
Mol	Chain	Res	Type	Atoms
42	C	1102	GTP	C5'-O5'-PA-O3A
42	C	1102	GTP	C5'-O5'-PA-O1A
42	C	1102	GTP	C5'-O5'-PA-O2A
43	J	1001	IHP	C4-C5-O15-P5
42	C	1102	GTP	PA-O3A-PB-O1B
40	B	401	M7M	OBR-CBS-CBT-OBV
43	J	1001	IHP	C6-C5-O15-P5
43	J	1001	IHP	C3-O13-P3-O23
40	B	401	M7M	CBT-OBV-PBK-OBL
42	C	1102	GTP	PB-O3A-PA-O2A
43	J	1001	IHP	C5-O15-P5-O35
43	J	1001	IHP	C1-O11-P1-O21
42	C	1102	GTP	PB-O3A-PA-O1A
43	J	1001	IHP	C1-O11-P1-O31
43	J	1001	IHP	C1-O11-P1-O41
43	J	1001	IHP	C3-O13-P3-O43
43	J	1001	IHP	C4-O14-P4-O44
43	J	1001	IHP	C4-O14-P4-O24

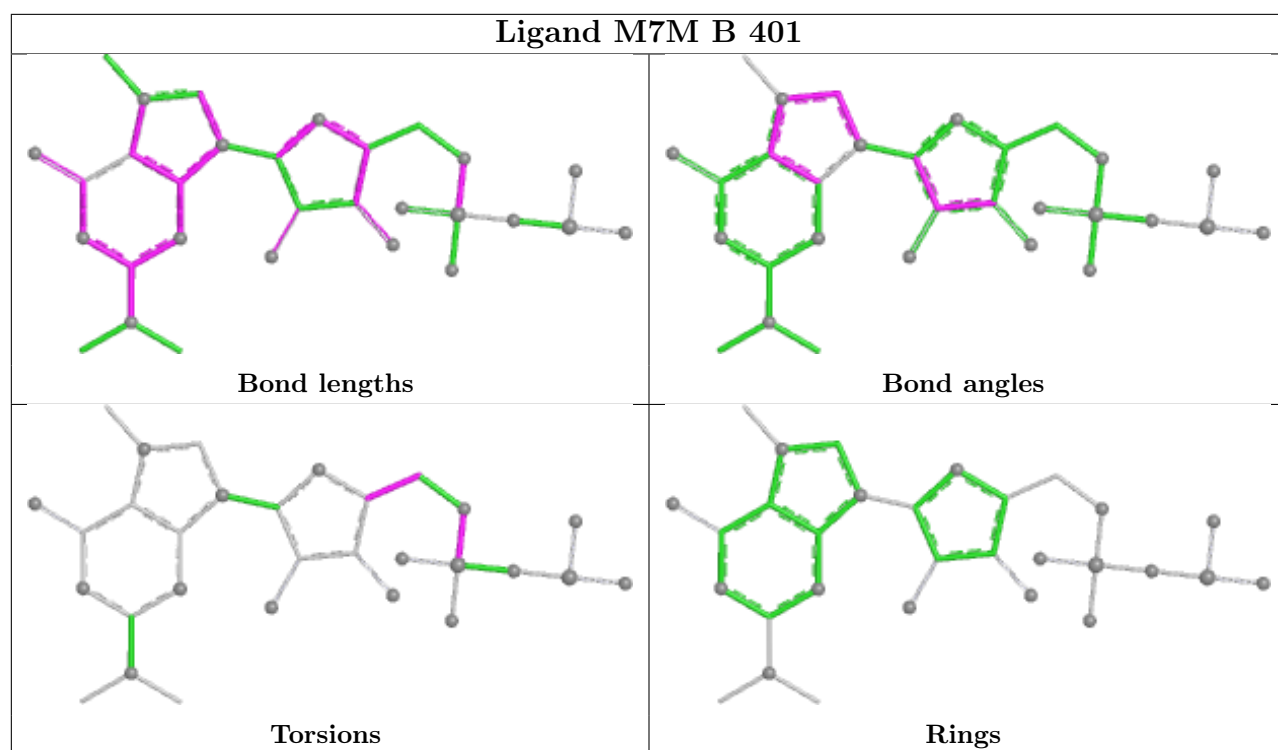
There are no ring outliers.

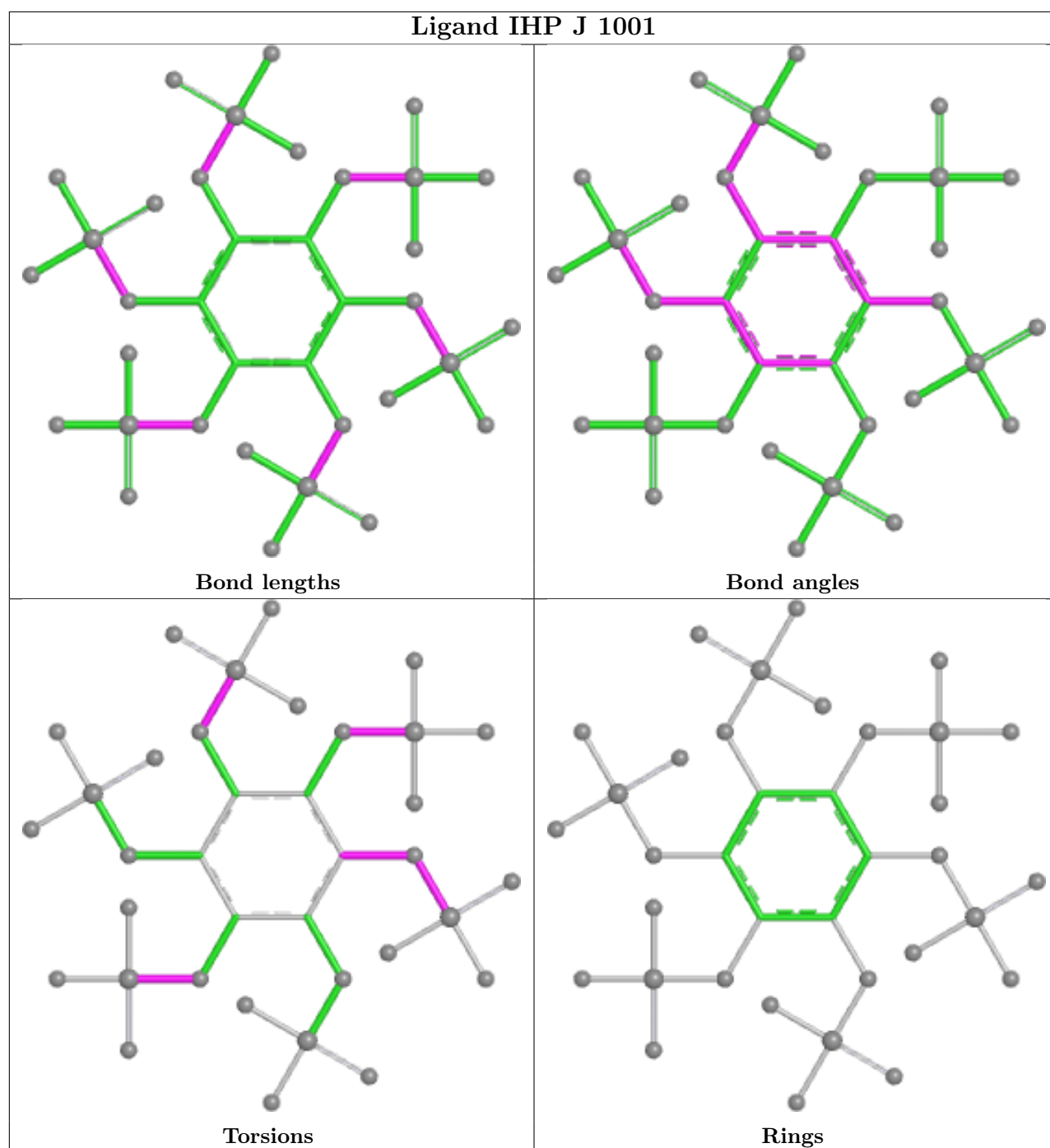
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	J	1001	IHP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

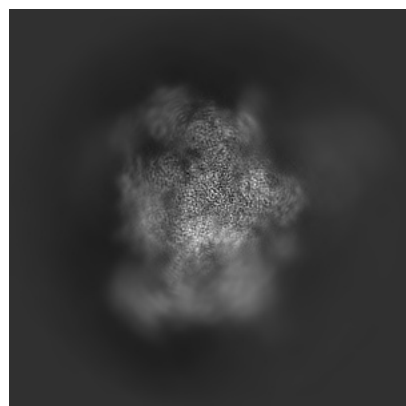
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62841. These allow visual inspection of the internal detail of the map and identification of artifacts.

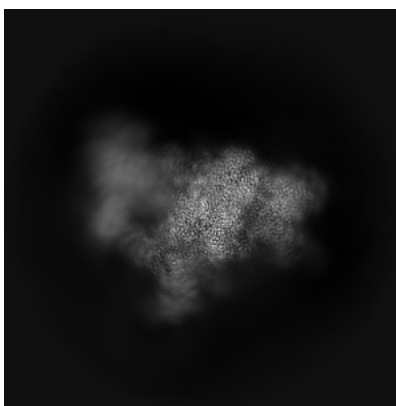
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

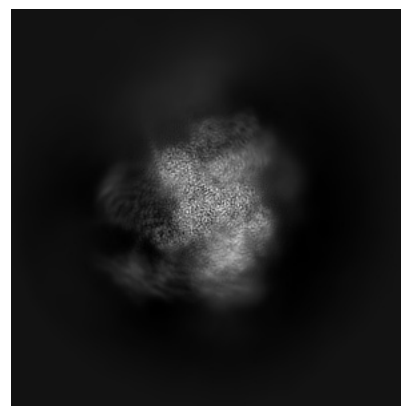
6.1.1 Primary map



X

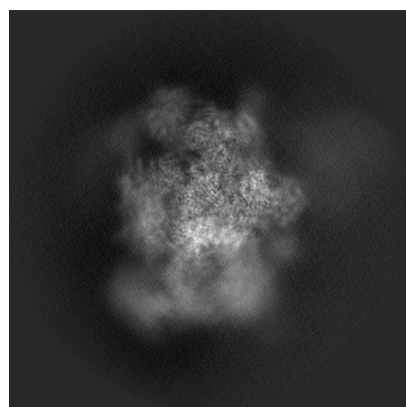


Y

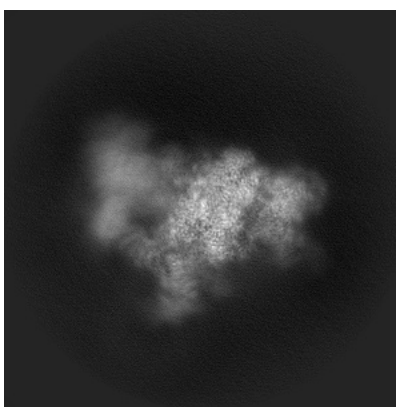


Z

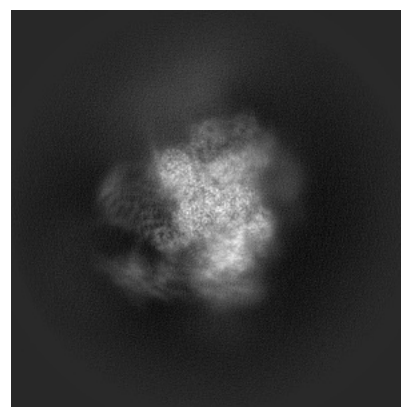
6.1.2 Raw map



X



Y

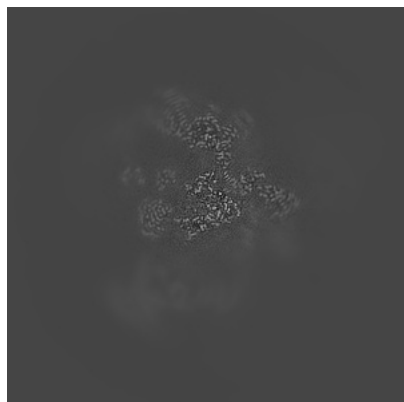


Z

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

6.2 Central slices [i](#)

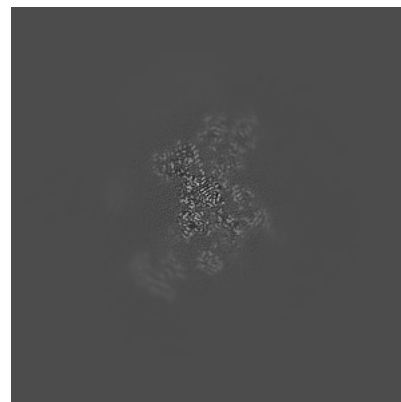
6.2.1 Primary map



X Index: 240

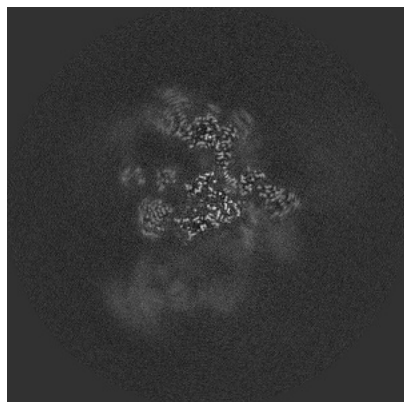


Y Index: 240

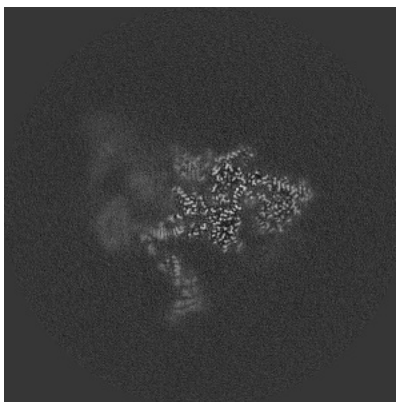


Z Index: 240

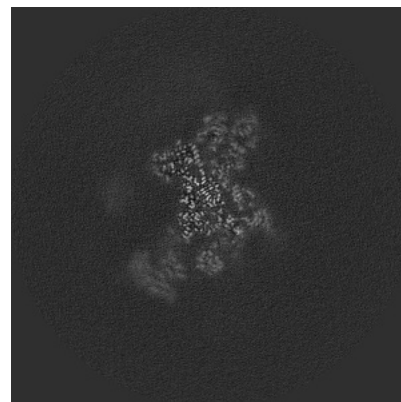
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

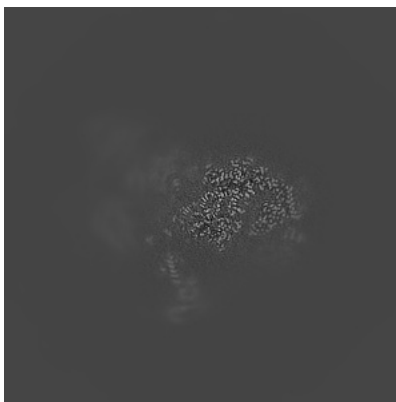
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

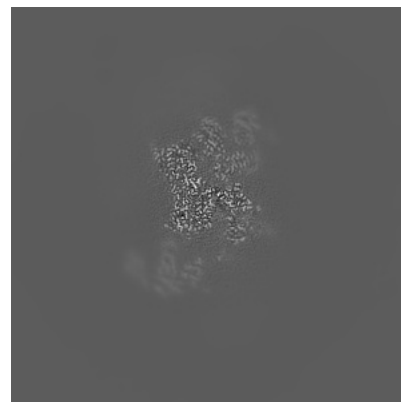
6.3.1 Primary map



X Index: 215

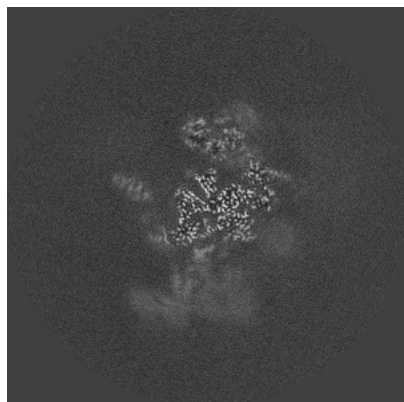


Y Index: 249



Z Index: 253

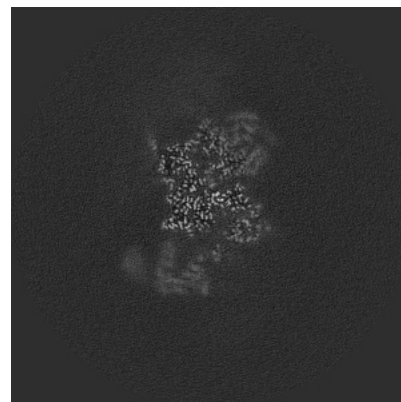
6.3.2 Raw map



X Index: 215



Y Index: 238

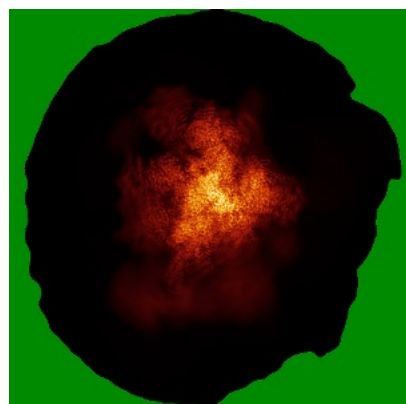


Z Index: 258

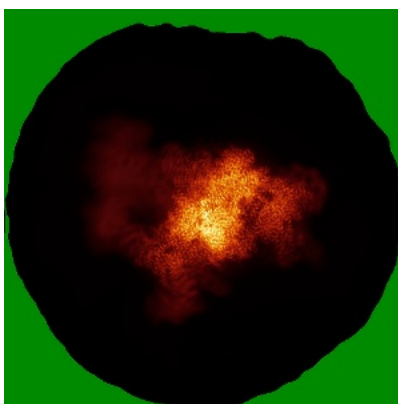
The images above show the largest variance slices of the map in three orthogonal directions.

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

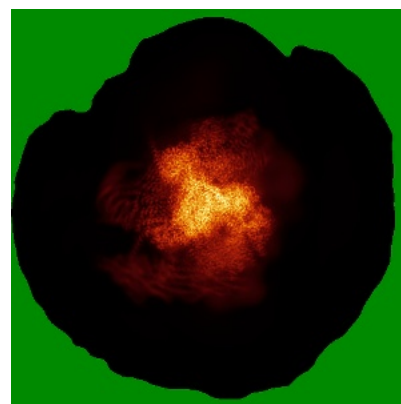
6.4.1 Primary map



X

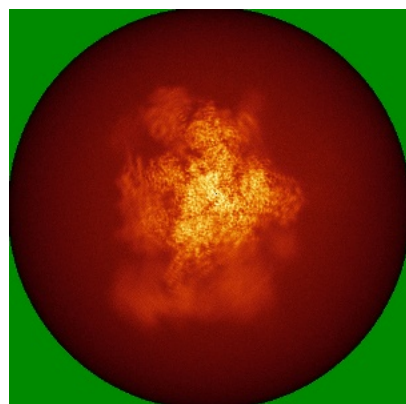


Y

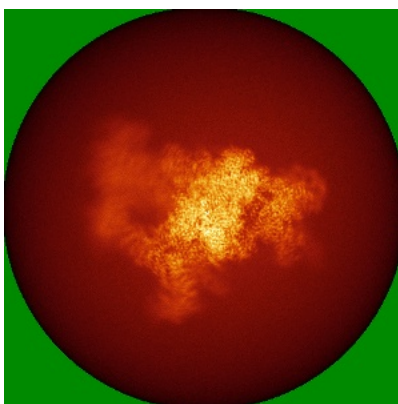


Z

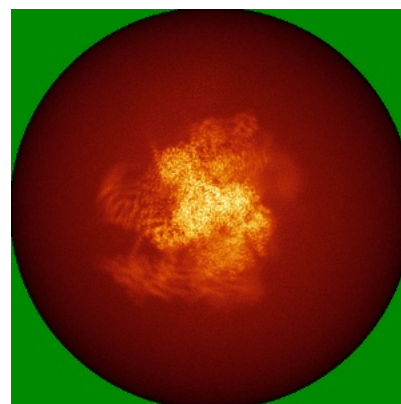
6.4.2 Raw map



X



Y

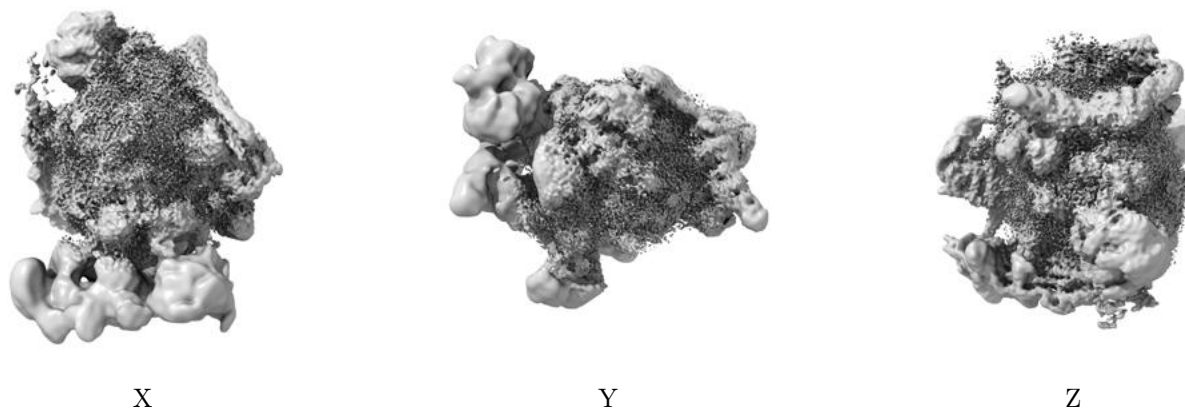


Z

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.

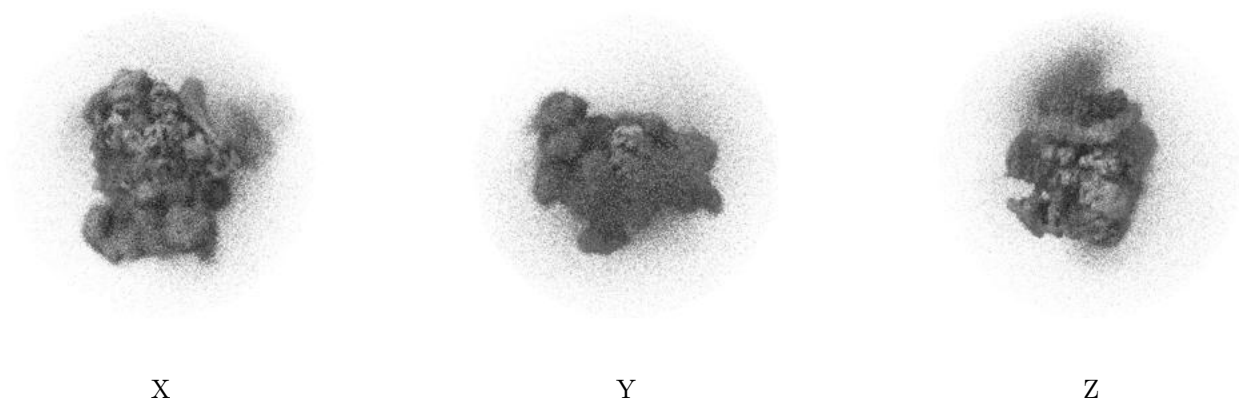
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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



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.

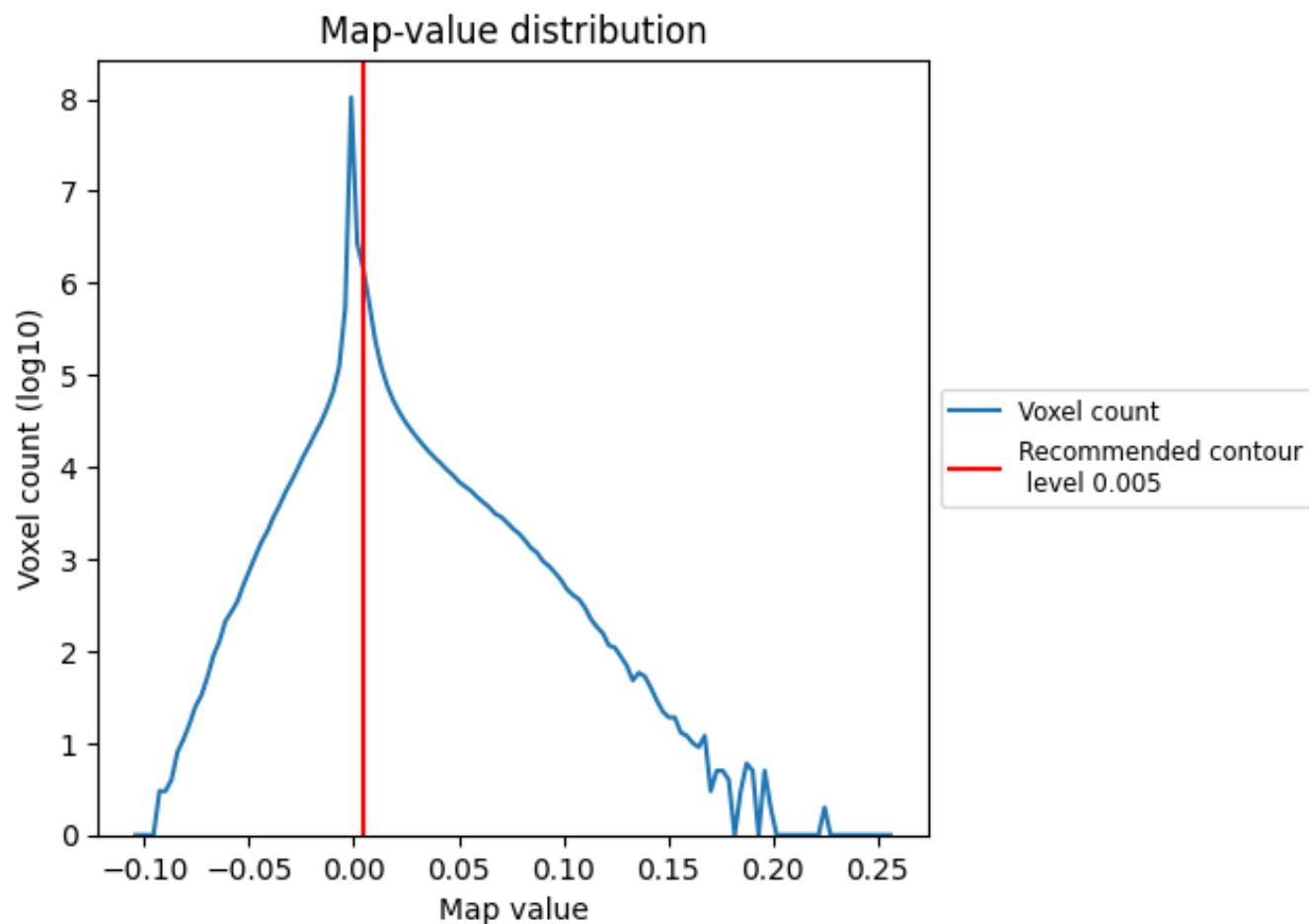
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

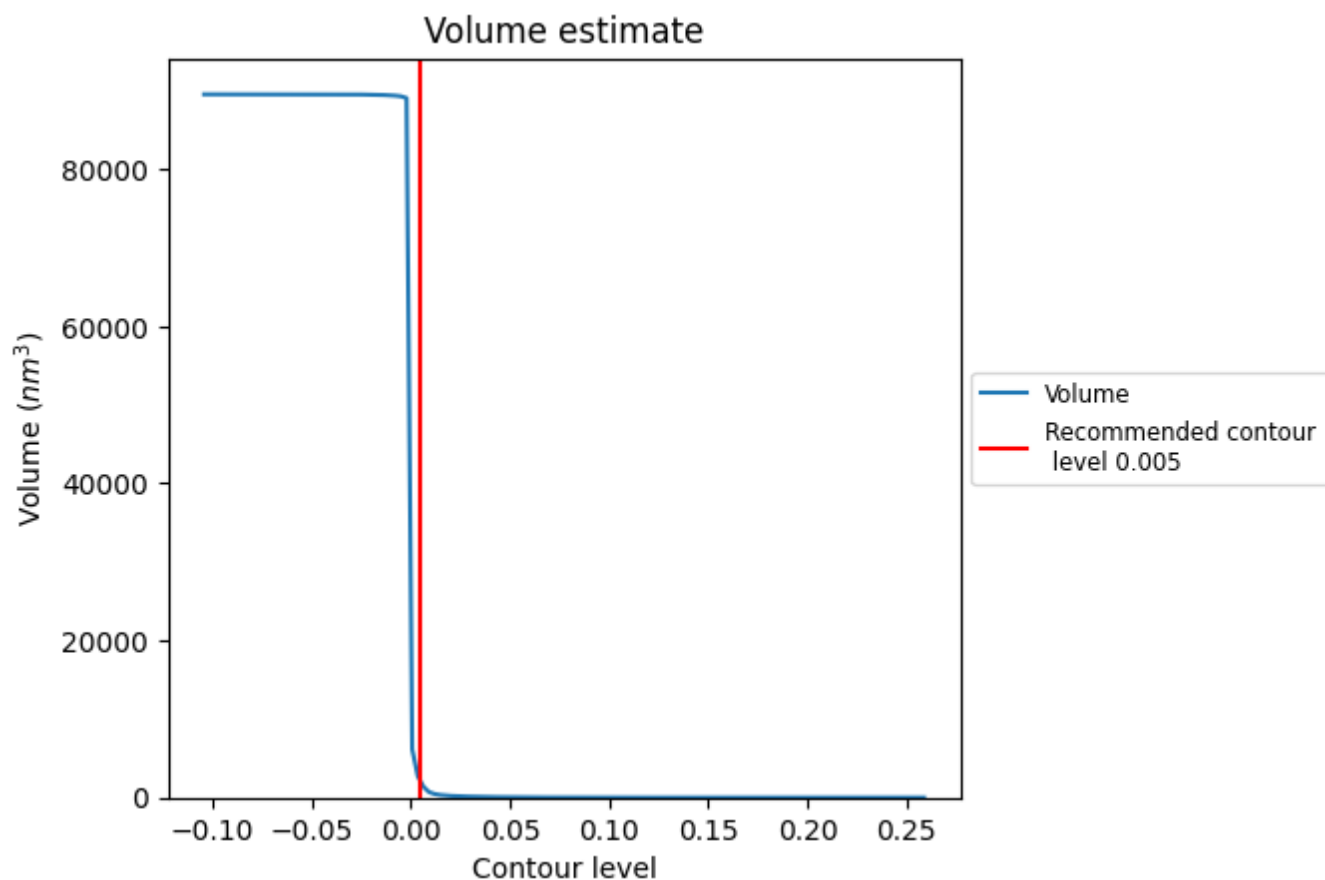
This section contains the results of statistical analysis of the map.

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.

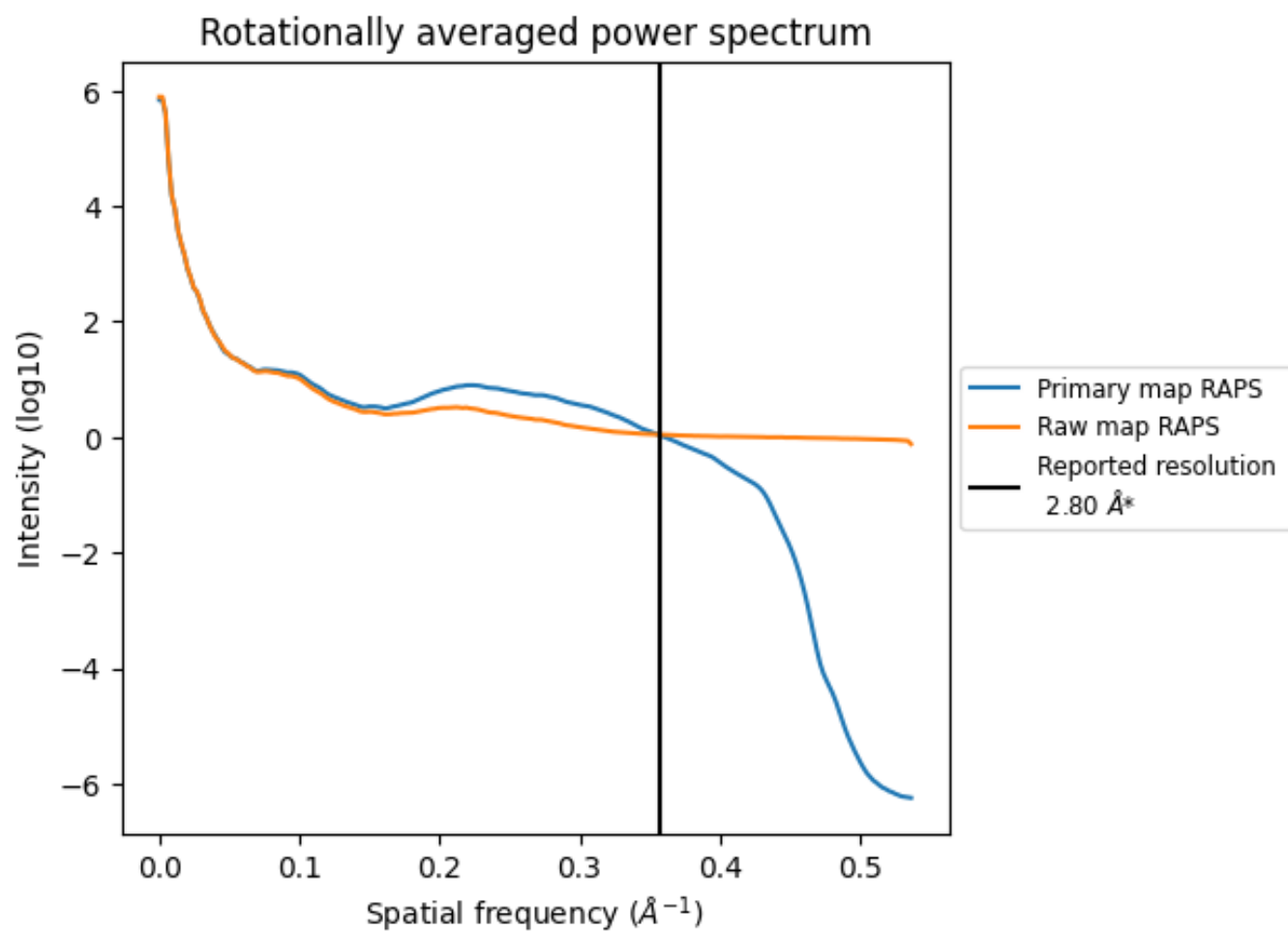
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2080 nm^3 ; this corresponds to an approximate mass of 1879 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 ⓘ

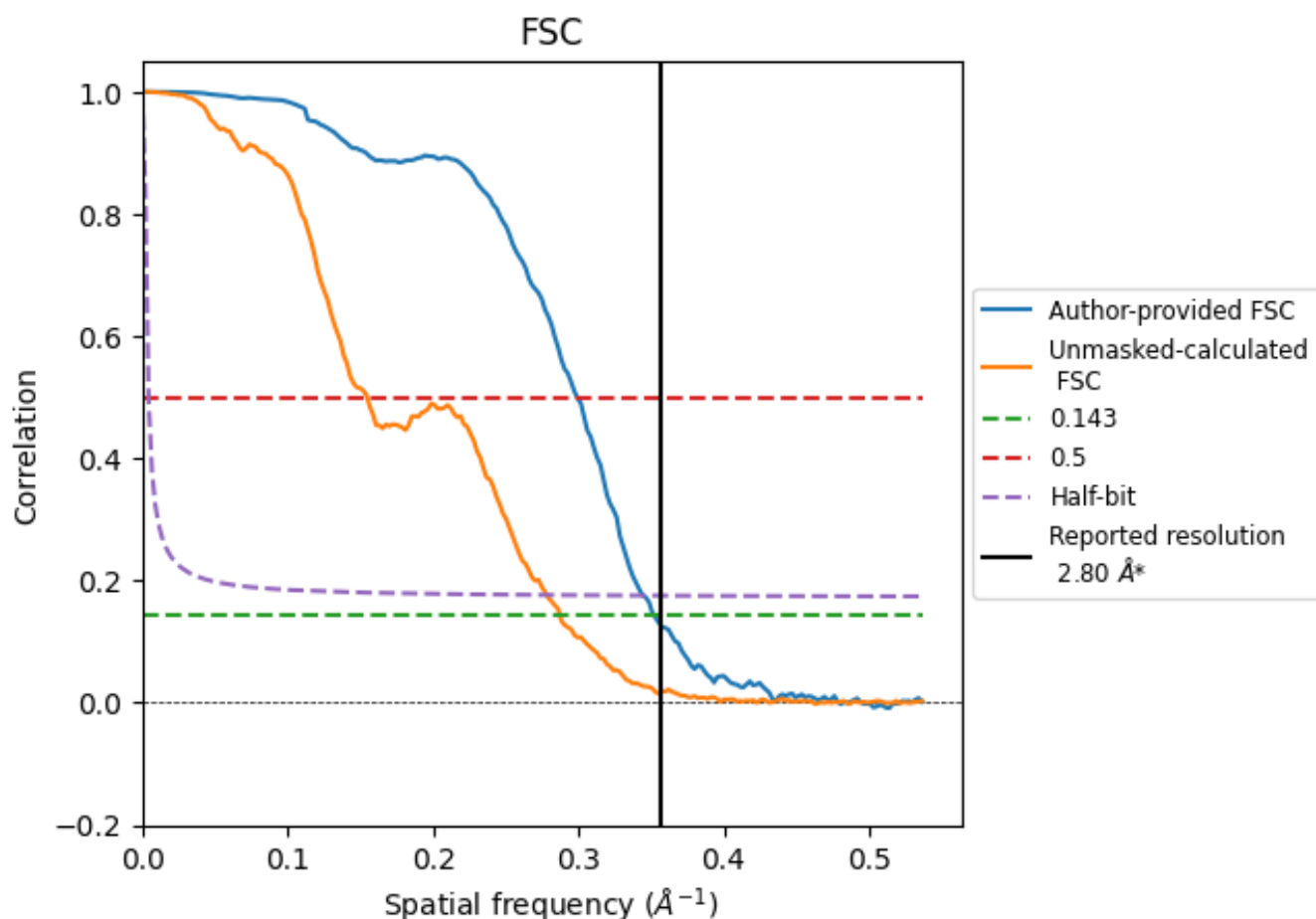


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

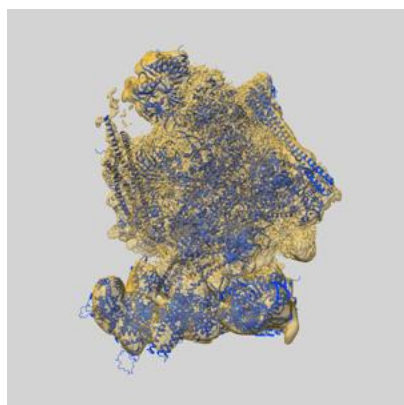
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.84	3.34	2.90
Unmasked-calculated*	3.48	6.46	3.59

*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 3.48 differs from the reported value 2.8 by more than 10 %

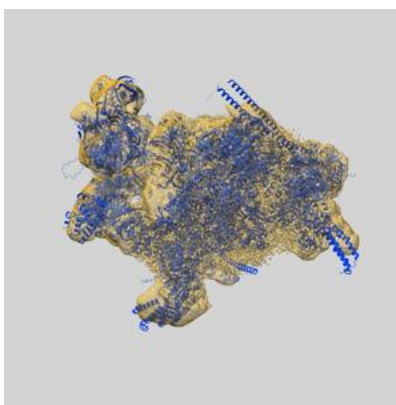
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62841 and PDB model 9L5R. Per-residue inclusion information can be found in section [3](#) on page [14](#).

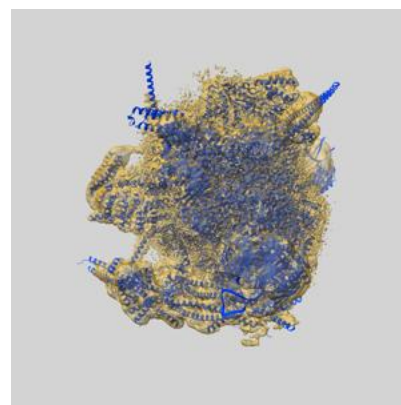
9.1 Map-model overlay [i](#)



X



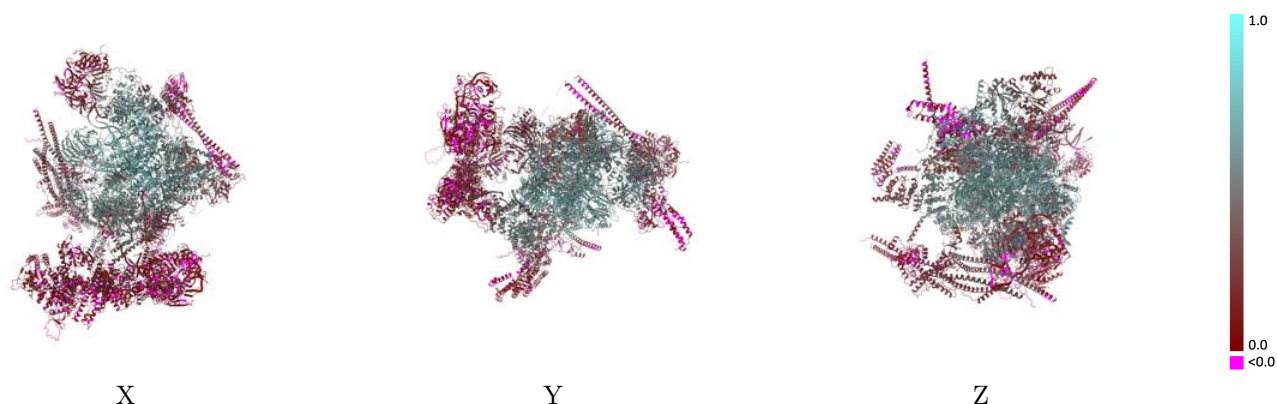
Y



Z

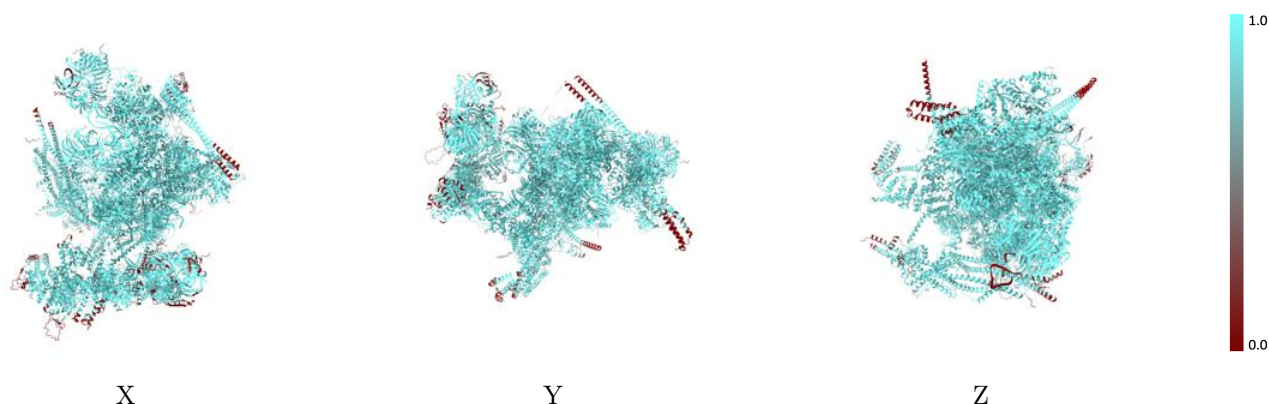
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



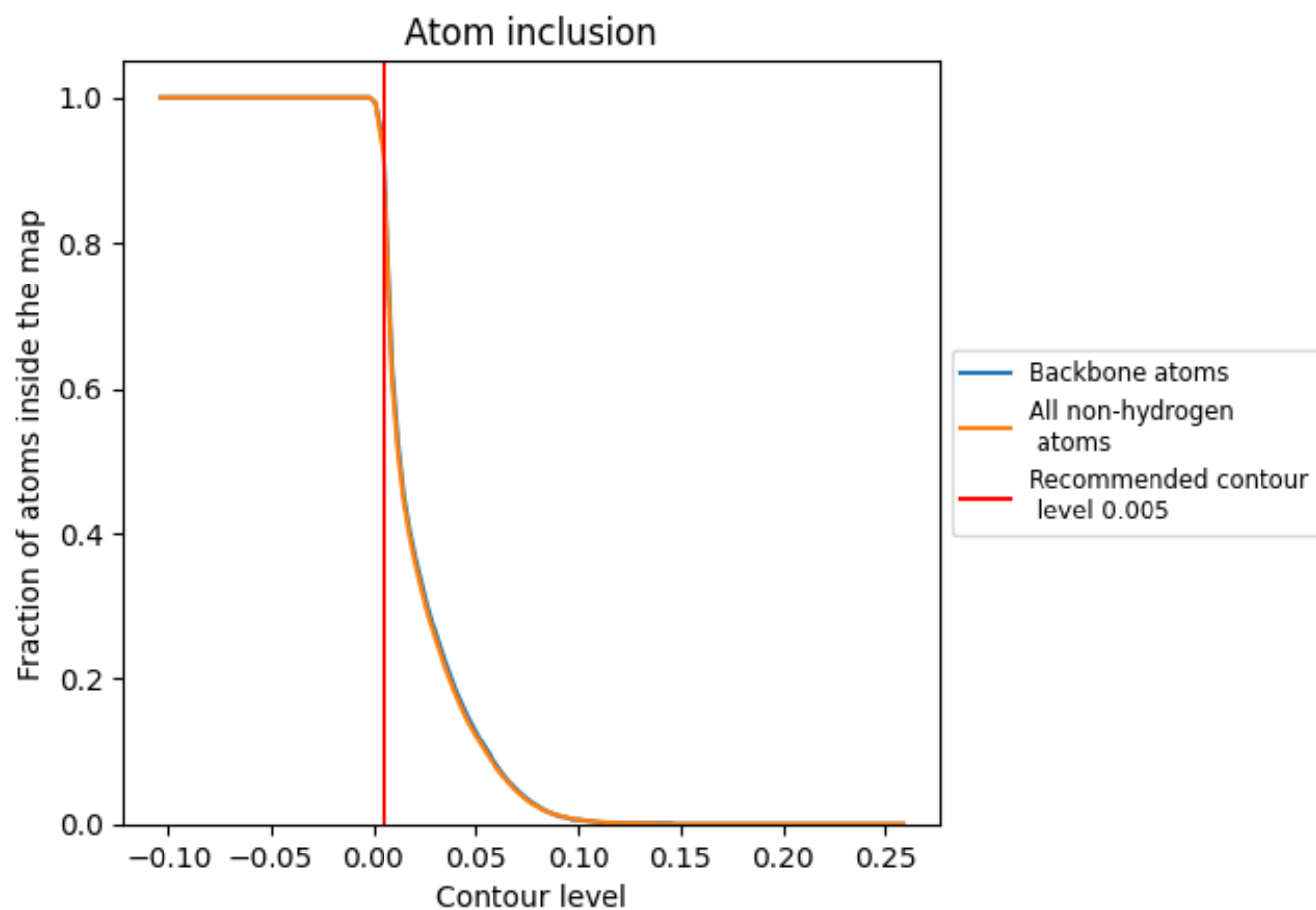
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.3780
0	 0.9860	 0.5070
2	 0.9400	 0.2700
5	 0.8500	 0.4260
6	 0.9960	 0.5910
7	 0.9980	 0.4500
A	 0.9730	 0.5640
B	 0.9430	 0.5100
C	 0.9770	 0.5260
CY	 0.6760	 0.1490
Cb	 0.7170	 0.1570
Cc	 0.8480	 0.1140
Ci	 0.9370	 0.1060
D	 0.9220	 0.3380
E	 0.9940	 0.5630
F	 0.9450	 0.3960
H	 0.8640	 0.3100
I	 0.9620	 0.3230
J	 0.9060	 0.4120
K	 0.8850	 0.2530
L	 0.8810	 0.3730
M	 0.9720	 0.4620
N	 0.9960	 0.6200
P	 0.9700	 0.6030
R	 0.9170	 0.5450
S	 0.9870	 0.5530
T	 0.9990	 0.7070
U	 0.9690	 0.4820
W	 0.9940	 0.3670
Y	 0.8110	 0.0880
a	 0.8830	 0.0680
b	 0.9520	 0.0560
c	 0.7570	 0.0630
d	 0.7950	 0.1020
e	 0.8790	 0.0950



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Chain	Atom inclusion	Q-score
f	 0.9640	 0.1220
g	 0.7910	 0.0450
h	 0.8690	 0.0980
i	 0.6390	 0.1040
j	 0.9100	 0.1980
k	 0.9610	 0.2850
l	 0.9120	 0.1370
m	 0.9440	 0.1390
o	 0.9220	 0.1580
p	 0.8590	 0.3260
q	 0.9110	 0.2090
r	 0.9060	 0.2140
s	 0.8240	 0.1680
t	 0.8410	 0.1250
u	 0.9640	 0.4050