



## Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 06:49 AM UTC

PDB ID : 5MPS / pdb\_00005mps  
EMDB ID : EMD-3539  
Title : Structure of a spliceosome remodeled for exon ligation  
Authors : Fica, S.M.; Oubridge, C.; Galej, W.P.; Wilkinson, M.E.; Newman, A.J.; Bai, X.-C.; Nagai, K.  
Deposited on : 2016-12-18  
Resolution : 3.85 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](mailto: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>.

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

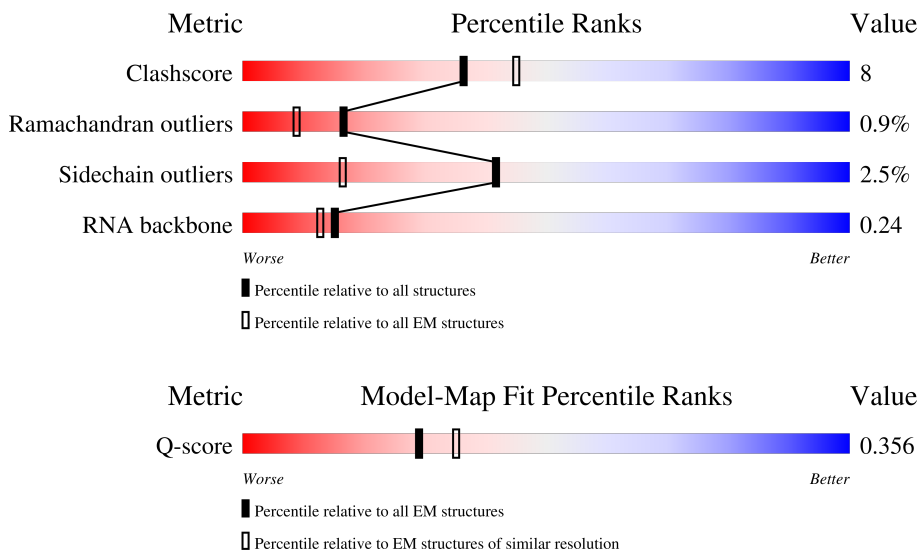
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.85 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.




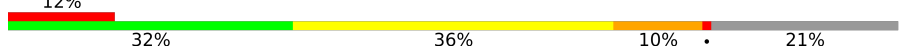

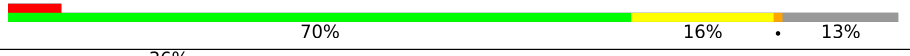
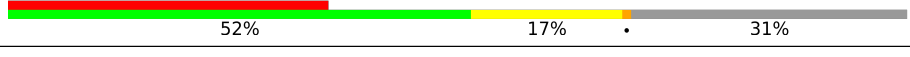



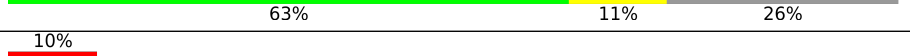
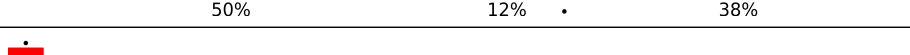
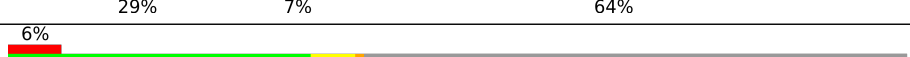
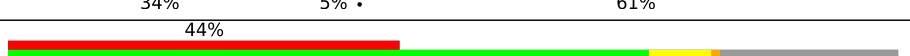

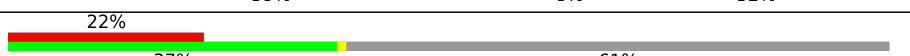
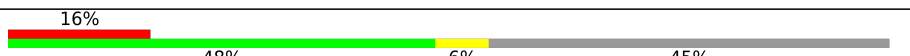


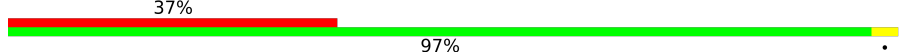







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8989 ( 3.35 - 4.35 )

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  $\geq 3$ , 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	I	95	
2	E	20	
3	2	1175	



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Mol	Chain	Length	Quality of chain
4	6	112	
5	5	179	
6	A	2413	
7	C	1008	
8	H	577	
9	J	451	
10	K	379	
11	L	157	
12	M	339	
13	N	364	
14	O	590	
15	P	175	
16	R	135	
17	S	687	
18	T	877	
19	a	251	
20	c	382	
21	o	455	
22	X	68	
23	y	215	
24	b	196	
25	d	101	
26	e	94	
27	f	86	
28	g	77	

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Mol	Chain	Length	Quality of chain
29	h	146	
30	j	110	

## 2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 58929 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 Yeast UBC4 gene for ubiquitin-conjugating enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	I	34	714	321	118	241	34	0	0

- Molecule 2 is a RNA chain called UBC4 gene exon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	E	16	346	155	66	109	16	0	0

- Molecule 3 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	2	49	1025	459	161	356	49	0	0

- Molecule 4 is a RNA chain called Saccharomyces cerevisiae strain T.52\_2H chromosome XII sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	6	99	2108	944	375	690	99	0	0

- Molecule 5 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	5	141	2999	1342	530	986	141	0	0

- Molecule 6 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	1914	15199	9832	2669	2645	53	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	874	6562	4265	1104	1168	25	0	0

- Molecule 8 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	401	3261	2104	544	595	18	0	0

- Molecule 9 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	342	2690	1699	475	506	10	0	0

- Molecule 10 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	187	1458	908	269	276	5	0	0

- Molecule 11 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	155	1162	737	217	198	10	0	0

- Molecule 12 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	252	2016	1281	356	368	11	0	0

- Molecule 13 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	227	1798	1139	309	335	15	0	0

- Molecule 14 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	211	Total	C	N	O	S	0	0
			1755	1102	320	327	6		

- Molecule 15 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	69	Total	C	N	O	S	0	0
			565	358	112	94	1		

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	108	Total	C	N	O	S	0	0
			614	369	121	124			

- Molecule 17 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	468	Total	C	N	O	S	0	0
			3229	2025	599	598	7		

- Molecule 18 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	338	Total	C	N	O	S	0	0
			1684	1008	338	338			

- Molecule 19 is a protein called Pre-mRNA-splicing factor 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	137	Total	C	N	O	S	0	0
			1119	726	194	196	3		

- Molecule 20 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	103	Total	C	N	O	S	0	0
			786	498	142	144	2		

- Molecule 21 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	o	313	Total	C	N	O	S	0	0
			2425	1537	429	451	8		

- Molecule 22 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	68	Total	C	N	O	0	0
			338	202	68	68		

- Molecule 23 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	y	83	Total	C	N	O	S	0	0
			679	420	125	133	1		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	80	Total	C	N	O	S	0	0
			631	403	114	111	3		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	82	Total	C	N	O	S	0	0
			625	399	109	115	2		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	e	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	f	72	Total	C	N	O	S	0	0
			573	368	101	103	1		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		

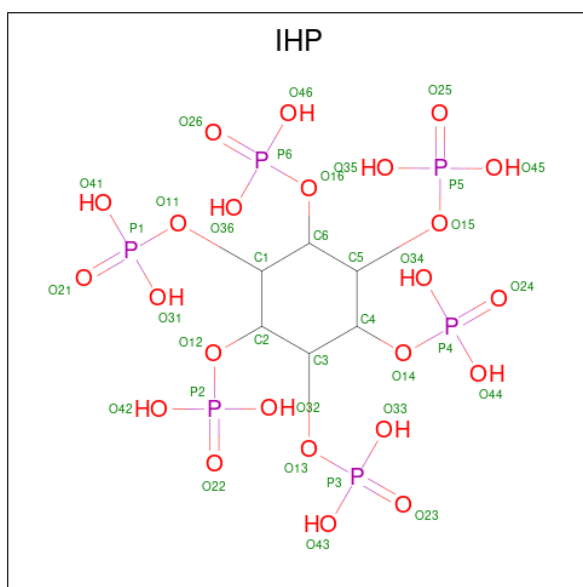
- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
31	6	3	Total	Mg	0
			3	3	

- Molecule 32 is POTASSIUM ION (CCD ID: K) (formula: K).

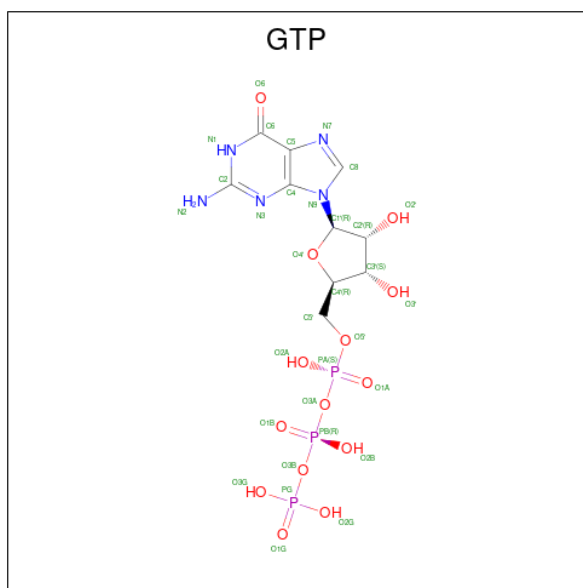
Mol	Chain	Residues	Atoms		AltConf
32	6	2	Total	K	0
			2	2	

- Molecule 33 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C<sub>6</sub>H<sub>18</sub>O<sub>24</sub>P<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	A	1	36	6	24	6	0

- Molecule 34 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
35	L	3	Total 3	Zn 3	0
35	M	1	Total 1	Zn 1	0
35	N	2	Total 2	Zn 2	0



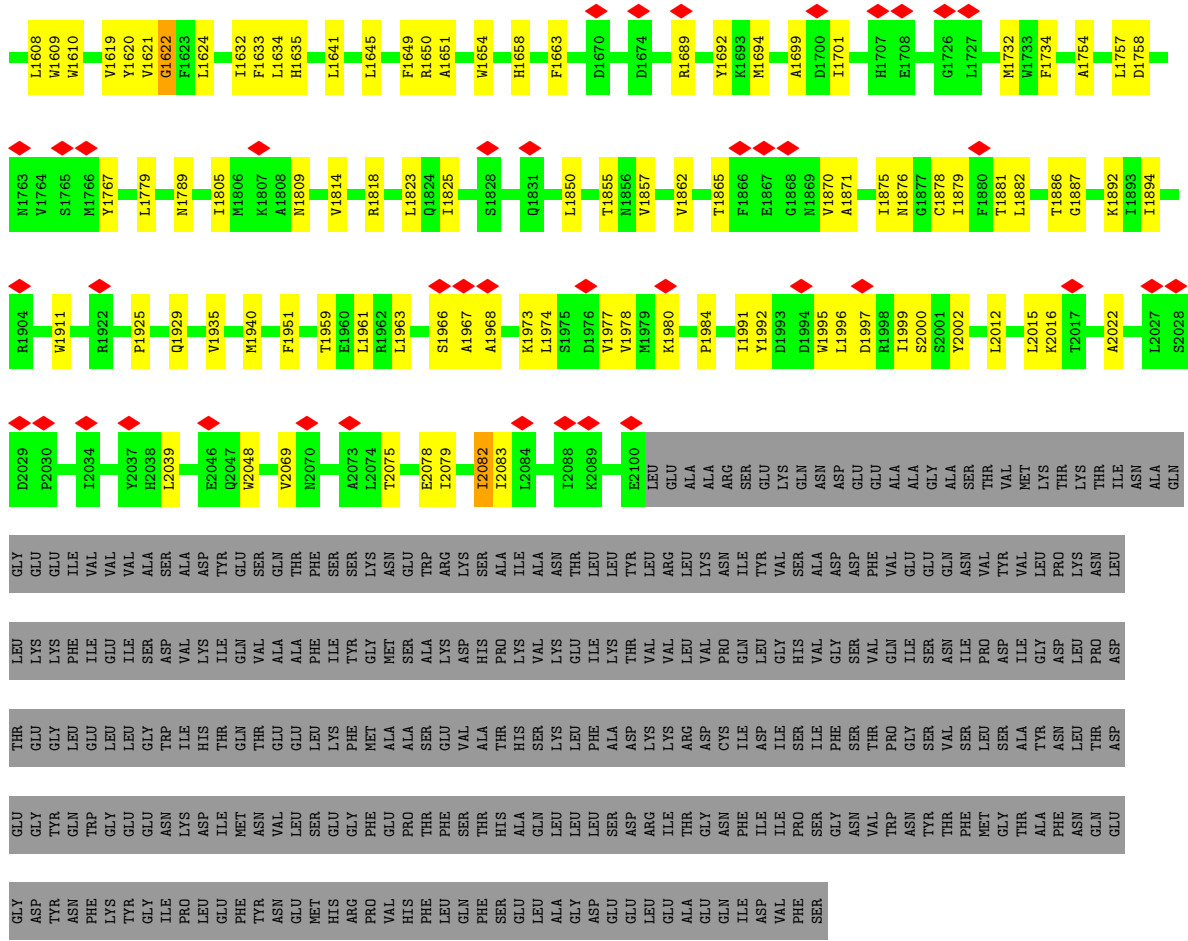


• Molecule 6: Pre-mRNA-splicing factor 8

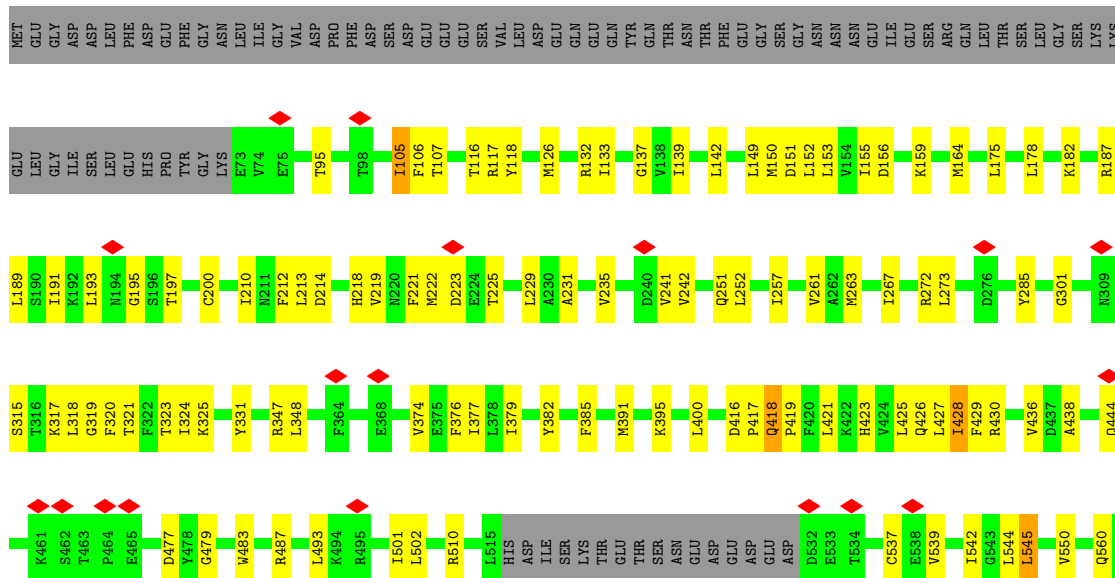
Chain A:



MET	ILE	LYS	F239	Y391	N487	1632	R720	H839	L1023	M1170	V1351	R1486
SER	ASN	ALA	F240	N392	F506	L721	L721	H839	W1028	L1171	A1352	G1487
GLY	ALA	ARG	D244	V398	L507	D634	F723	E941	M1033	F1172	E1353	T1353
PRO	GLU	ARG	T255	N404	D511	T635	R724	M944	A1047	L1182	E1354	P1355
PRO	VAL	ASN	L127	N413	V518	H636	I725	V945	L1050	R1204	L1356	L1356
PRO	ASP	PHE	E137	N413	Y522	L641	I730	L849	L1054	W1207	V1361	R1511
PRO	THR	THR	H138	Y417	S521	L653	T731	L852	L1054	R1212	N1369	F1514
GLY	LEU	LEU	L139	D418	Y522	H654	R732	T853	M1057	I1230	K1372	R1521
GLU	PRO	PRO	W301	F423	L525	H654	R737	R854	A1058	I1230	L1373	N1522
GLU	PRO	PRO	S302	L305	L525	H656	R737	W856	M1057	Y1251	G1374	N1522
ASP	ASP	PRO	D304	F423	L526	L657	W742	W856	L1066	Y1251	L1375	W1537
SER	SER	PRO	L305	F424	K527	L657	Y756	I957	M1067	M1257	N1376	M1537
PRO	PRO	PRO	S315	N428	Y529	H659	R756	Q868	R1068	L1258	K1377	R1543
LEU	ALA	LEU	S315	N428	V530	L660	L756	M886	L1069	L1259	K1378	M1379
LEU	LEU	GLY	Y167	L428	W530	L660	L756	M886	V1074	F1280	M1379	I1547
PRO	LEU	LEU	Y167	L428	V530	L660	L756	M886	V1074	F1280	F1383	I1547
PRO	GLU	ASP	L168	P169	W530	L660	N760	W889	I1082	M1262	V1387	I1553
PRO	GLU	ASP	P169	N326	T537	G665	N760	W889	T1083	V1267	V1387	L1557
PRO	GLU	LEU	L173	N326	L548	T666	S761	R893	T1083	R1268	P1391	L1557
PRO	THR	THR	L173	L330	L548	T666	W762	R893	M1087	I1288	P1391	T1560
PRO	THR	LYS	L176	L330	Y556	Y671	I766	I898	M1087	I1288	I1400	T1560
PRO	ALA	ALA	L176	F336	Y556	Y671	I766	I898	V1088	L1270	I1400	T1560
PRO	GLY	GLU	M179	F336	Y559	K672	W770	Y905	V1088	L1270	I1400	T1560
GLY	GLY	LYS	F180	N338	Y559	V673	P771	Y905	V1089	V1278	I1405	T1565
TYR	LYS	LYS	H181	F180	Y559	M674	F771	K906	F1092	L1406	I1405	N1568
GLU	LYS	LYS	P182	P182	Y559	H675	E772	N907	K1093	S1280	I1406	S1569
ILE	VAL	VAL	P182	N343	Y559	H675	S773	D908	K1093	M1281	I1407	S1569
GLU	GLU	GLU	P182	N343	Y559	H675	I774	D908	D1094	M1281	I1407	W1570
GLU	GLU	GLU	V191	N343	Y559	H675	I774	D908	D1094	D1282	G1421	G1421
GLU	GLU	GLU	V191	N343	Y559	H675	I774	D908	D1094	E1282	I1422	I1422
GLU	HIS	HIS	V191	N343	Y559	H675	R775	A915	V1098	E1283	F1425	F1425
GLU	GLY	GLY	Y193	N355	Y559	H675	R775	L916	M1099	W1286	R1426	R1426
ASP	ASP	ASP	H194	Y356	Y559	H675	R775	L916	M1099	D1287	R1426	R1426
ARG	ARG	ARG	H194	Y356	Y559	H675	R775	L916	M1099	L1288	D1433	D1433
PRO	ARG	ARG	T195	P357	Y559	H675	R775	S925	L1107	L1107	L1436	L1436
PRO	LYS	LYS	T195	P357	Y559	H675	R775	S925	L1107	L1107	I1440	I1440
MET	LYS	LYS	S196	P357	Y559	H675	R775	S925	L1107	L1107	F1441	F1441
VAL	LEU	LEU	A198	P357	Y559	H675	R775	S925	L1107	L1107	R1442	R1442
PRO	ASP	ASP	I199	P357	Y559	H675	R775	S925	L1107	L1107	Y1443	Y1443
SER	ILE	ILE	I199	P357	Y559	H675	R775	S925	L1107	L1107	Y1443	Y1443
SER	GLY	GLY	T200	P357	Y559	H675	R775	S925	L1107	L1107	I1444	I1444
VAL	LYS	LYS	T200	P357	Y559	H675	R775	S925	L1107	L1107	F1451	F1451
ASN	ASP	ASP	N203	P357	Y559	H675	R775	S925	L1107	L1107	S1454	S1454
GLU	THR	THR	N203	P357	Y559	H675	R775	S925	L1107	L1107	A1468	A1468
GLU	PHE	PHE	R207	P357	Y559	H675	R775	S925	L1107	L1107	M1472	M1472
ASP	VAL	VAL	W208	P357	Y559	H675	R775	S925	L1107	L1107	R1473	R1473
THR	VAL	VAL	W208	P357	Y559	H675	R775	S925	L1107	L1107	R1474	R1474
THR	THR	THR	W208	P357	Y559	H675	R775	S925	L1107	L1107	L1475	L1475
LEU	THR	THR	W208	P357	Y559	H675	R775	S925	L1107	L1107	D1485	D1485
PRO	LYS	LYS	V212	P357	Y559	H675	R775	S925	L1107	L1107		
PRO	SER	SER	V212	P357	Y559	H675	R775	S925	L1107	L1107		
PRO	ARG	ARG	S218	P357	Y559	H675	R775	S925	L1107	L1107		
PRO	LYS	LYS	S218	P357	Y559	H675	R775	S925	L1107	L1107		
PRO	ARG	ARG	R226	P357	Y559	H675	R775	S925	L1107	L1107		
PRO	ARG	ARG	R226	P357	Y559	H675	R775	S925	L1107	L1107		
PRO	ALA	ALA	E227	P357	Y559	H675	R775	S925	L1107	L1107		
PRO	ALA	ALA	E227	P357	Y559	H675	R775	S925	L1107	L1107		
PRO	LYS	LYS	R228	P357	Y559	H675	R775	S925	L1107	L1107		
SER	LYS	LYS	R228	P357	Y559	H675	R775	S925	L1107	L1107		
ASN	MET	MET	K235	P357	Y559	H675	R775	S925	L1107	L1107		
PHE	THR	THR	K235	P357	Y559	H675	R775	S925	L1107	L1107		
GLU	THR	THR	K235	P357	Y559	H675	R775	S925	L1107	L1107		
			R238	P357	Y559	H675	R775	S925	L1107	L1107		



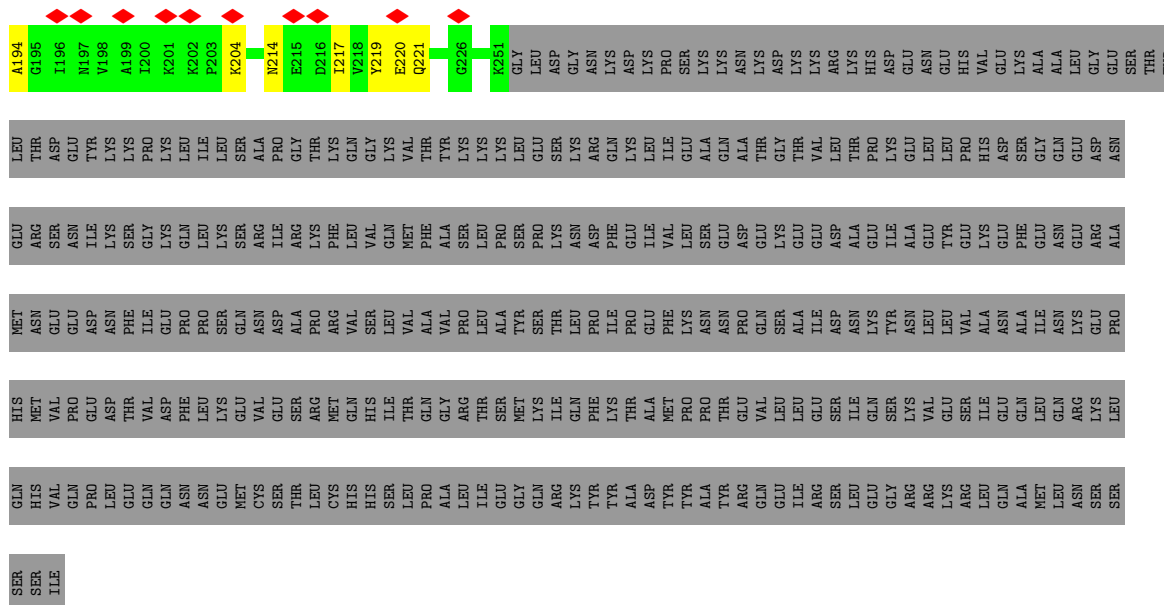
• Molecule 7: Pre-mRNA-splicing factor SNU114



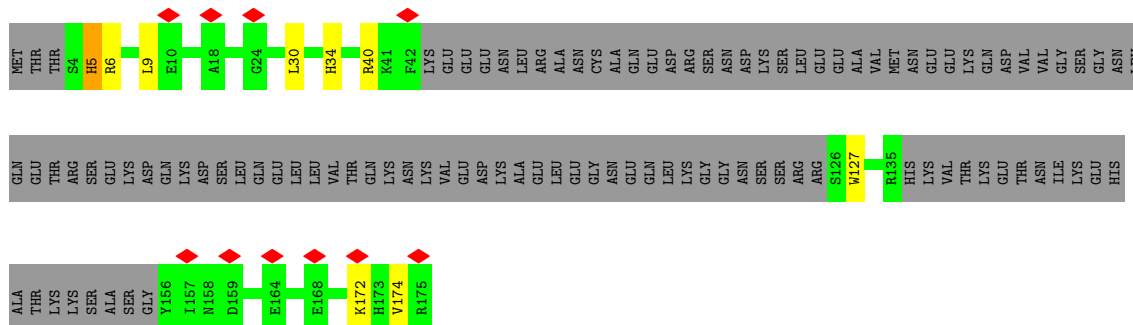




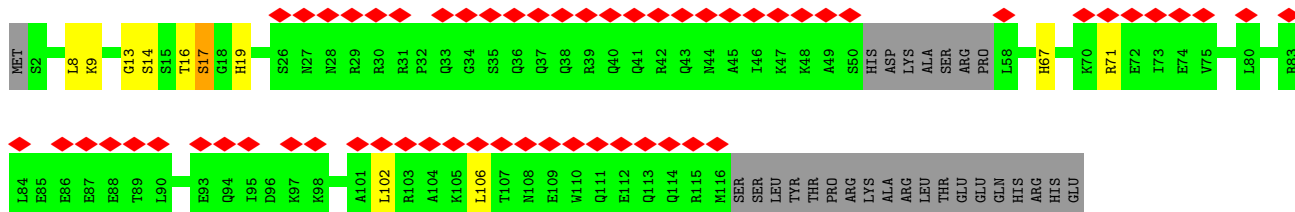
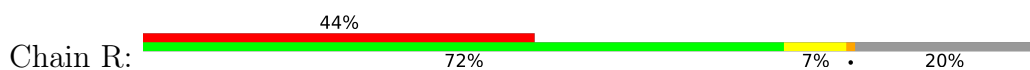




● Molecule 15: Pre-mRNA-splicing factor CWC15



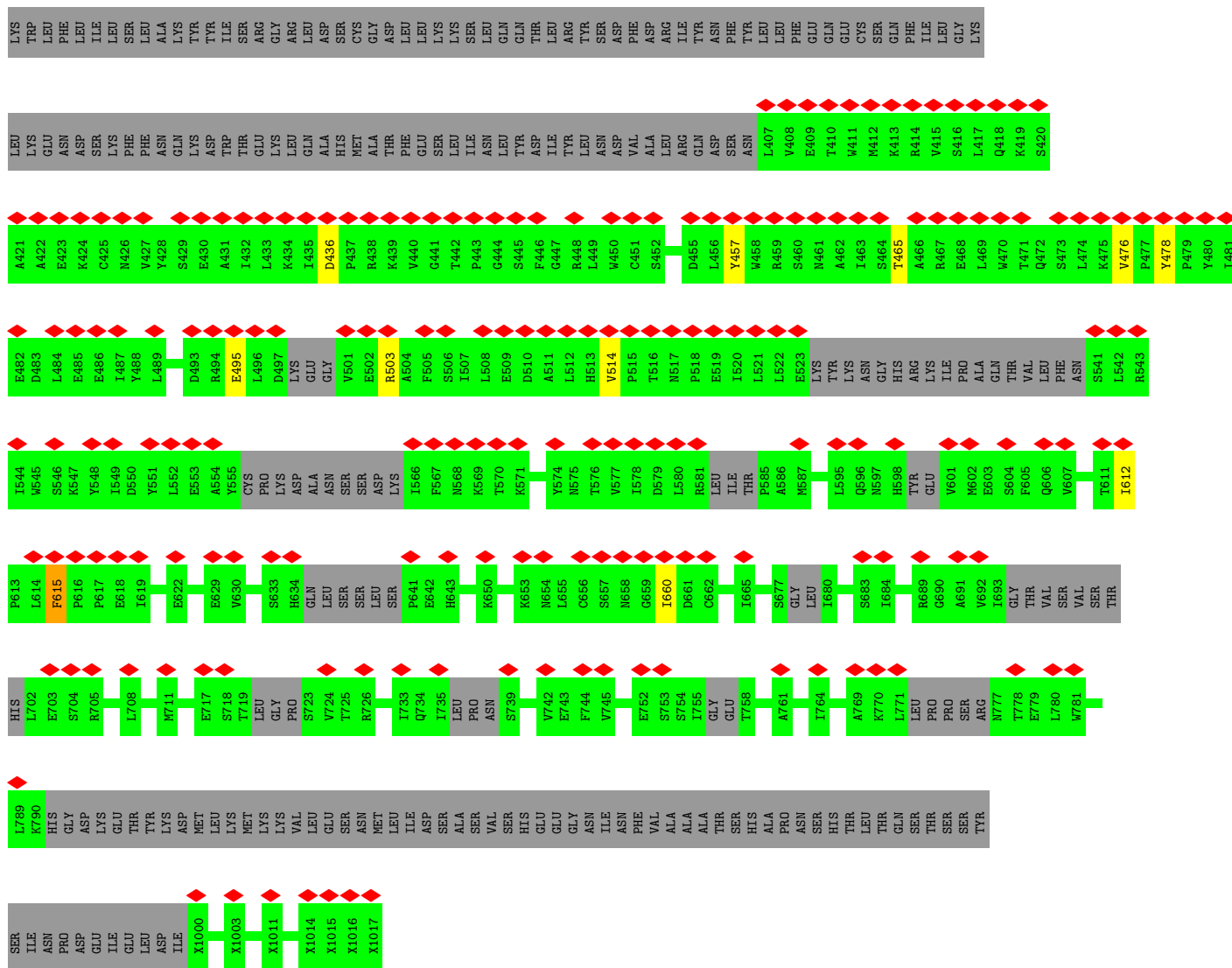
● Molecule 16: Pre-mRNA-splicing factor CWC21



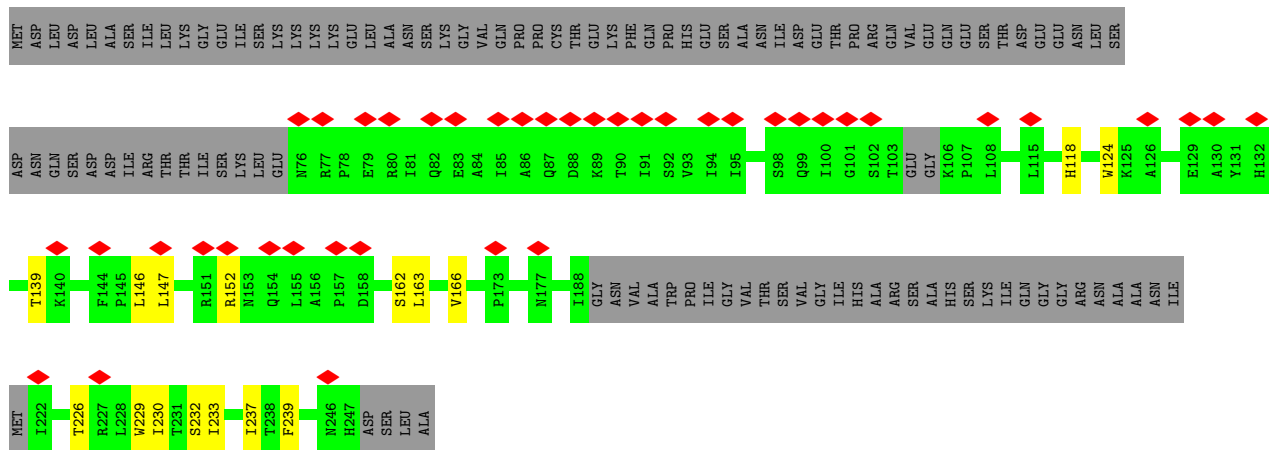
● Molecule 17: Pre-mRNA-splicing factor CLF1





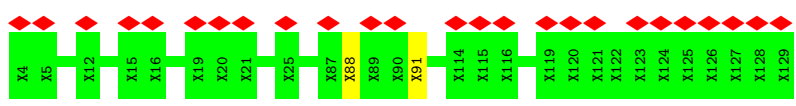


• Molecule 19: Pre-mRNA-splicing factor 18

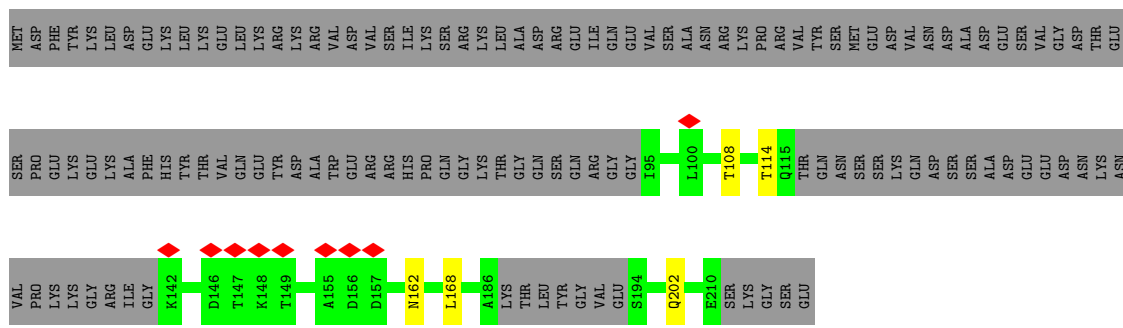


• Molecule 20: Pre-mRNA-splicing factor SLU7

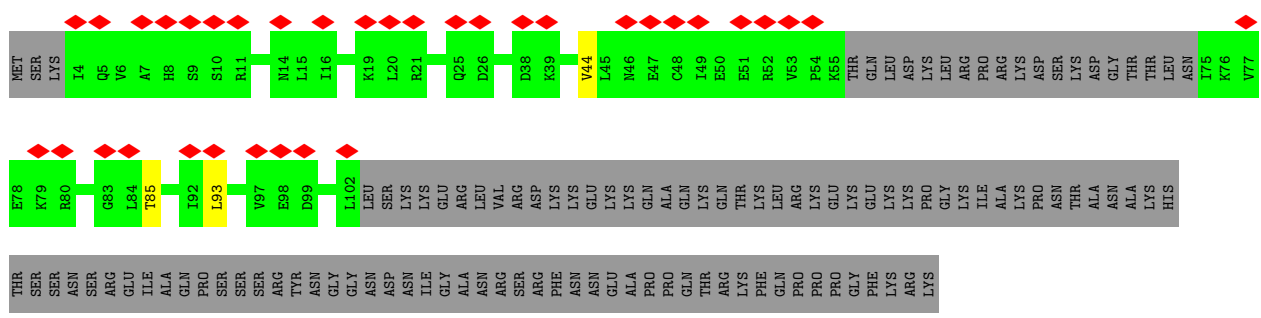
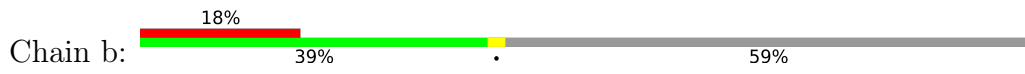




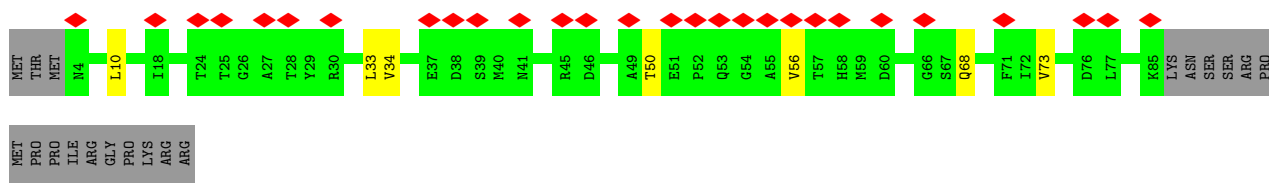
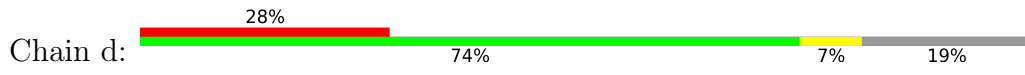
• Molecule 23: Pre-mRNA-splicing factor SYF2



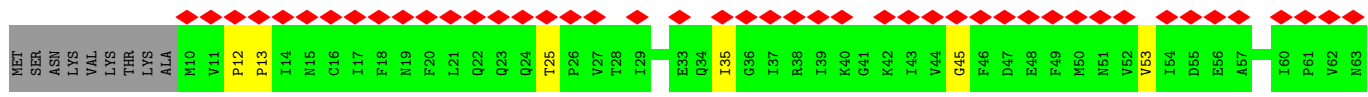
• Molecule 24: Small nuclear ribonucleoprotein-associated protein B



• Molecule 25: Small nuclear ribonucleoprotein Sm D3



• Molecule 26: Small nuclear ribonucleoprotein E





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65824	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.170	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.036	Depositor
Map size (Å)	589.16, 589.16, 589.16	wwPDB
Map dimensions	412, 412, 412	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	I	0.41	0/795	0.87	3/1231 (0.2%)
2	E	0.41	0/388	0.84	0/603
3	2	0.41	0/1140	0.78	0/1770
4	6	0.41	0/2357	0.83	6/3667 (0.2%)
5	5	0.41	0/3351	0.83	3/5213 (0.1%)
6	A	0.60	5/15598 (0.0%)	1.02	6/21212 (0.0%)
7	C	0.57	1/6703 (0.0%)	0.98	7/9138 (0.1%)
8	H	0.66	0/3314	1.16	3/4463 (0.1%)
9	J	0.61	0/2749	0.86	3/3735 (0.1%)
10	K	0.61	0/1480	1.01	1/2000 (0.1%)
11	L	0.61	0/1186	1.04	0/1606
12	M	0.54	0/2062	0.93	2/2772 (0.1%)
13	N	0.58	0/1823	0.98	0/2456
14	O	0.60	0/1781	1.11	1/2385 (0.0%)
15	P	0.49	0/580	0.82	0/776
16	R	0.57	0/617	1.24	0/848
17	S	0.63	0/3269	1.25	4/4446 (0.1%)
18	T	0.67	0/1583	1.47	9/2192 (0.4%)
19	a	0.55	0/1141	0.87	0/1546
20	c	0.60	1/798 (0.1%)	0.92	1/1074 (0.1%)
21	o	0.57	0/2491	0.82	1/3384 (0.0%)
23	y	0.44	0/681	0.76	0/902
24	b	0.54	0/636	0.75	0/856
25	d	0.54	0/634	0.77	0/859
26	e	0.68	1/585 (0.2%)	0.83	0/795
27	f	0.59	0/585	0.75	0/791
28	g	0.70	2/532 (0.4%)	0.80	0/715
29	h	0.57	0/649	0.77	0/880
30	j	0.54	0/753	0.80	0/1013
All	All	0.58	10/60261 (0.0%)	0.99	50/83328 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	0	1
9	J	0	1
15	P	0	1
21	o	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	230	SER	C-O	5.70	1.34	1.23
6	A	1658	HIS	C-O	5.68	1.30	1.24
26	e	12	PRO	CA-C	5.67	1.55	1.51
7	C	251	GLN	CD-OE1	5.33	1.33	1.23
6	A	194	HIS	ND1-CE1	5.28	1.37	1.32
28	g	18	ASN	CG-OD1	5.23	1.33	1.23
6	A	1099	ASN	CG-OD1	5.21	1.33	1.23
28	g	20	ASN	CG-OD1	5.16	1.33	1.23
6	A	705	GLN	N-CA	-5.09	1.43	1.46
6	A	705	GLN	CD-OE1	5.01	1.33	1.23

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	612	ILE	CA-C-N	12.72	132.68	119.19
18	T	612	ILE	C-N-CA	12.72	132.68	119.19
18	T	615	PHE	CA-C-N	9.90	130.57	120.38
18	T	615	PHE	C-N-CA	9.90	130.57	120.38
5	5	27	G	C4'-C3'-O3'	8.09	121.53	109.40
18	T	436	ASP	CA-C-N	8.06	128.15	119.28
18	T	436	ASP	C-N-CA	8.06	128.15	119.28
17	S	334	PHE	CA-C-N	8.03	128.11	119.28
17	S	334	PHE	C-N-CA	8.03	128.11	119.28
7	C	986	GLY	CA-C-N	8.02	129.86	119.84
7	C	986	GLY	C-N-CA	8.02	129.86	119.84
4	6	45	A	C2'-C3'-O3'	7.68	125.22	113.70
6	A	404	ASN	N-CA-C	7.62	120.65	109.07
12	M	163	VAL	N-CA-C	7.34	117.42	110.30
4	6	92	C	C2'-C3'-O3'	7.29	120.43	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	317	ILE	N-CA-CB	7.14	119.69	110.13
1	I	9	A	C4'-C3'-O3'	7.01	123.51	113.00
9	J	194	HIS	CA-C-N	6.79	128.32	119.84
9	J	194	HIS	C-N-CA	6.79	128.32	119.84
18	T	476	VAL	CA-C-N	6.75	126.69	120.21
18	T	476	VAL	C-N-CA	6.75	126.69	120.21
1	I	9	A	C2'-C3'-O3'	-6.65	103.72	113.70
6	A	194	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	I	13	U	C2'-C3'-O3'	6.35	119.03	109.50
7	C	106	PHE	N-CA-C	6.17	119.71	110.14
4	6	73	A	C4'-C3'-O3'	-6.16	103.77	113.00
7	C	379	ILE	O-C-N	6.12	124.41	120.07
4	6	92	C	C4'-C3'-O3'	6.12	118.57	109.40
18	T	514	VAL	O-C-N	6.12	124.33	120.42
8	H	316	LYS	N-CA-C	5.85	119.72	112.24
5	5	102	C	C4'-C3'-O3'	-5.82	104.27	113.00
4	6	72	C	C4'-C3'-O3'	-5.72	104.42	113.00
6	A	194	HIS	CB-CG-ND1	5.67	131.21	122.70
10	K	82	LEU	N-CA-C	5.54	117.17	111.03
17	S	420	VAL	CA-C-N	5.52	124.87	118.85
17	S	420	VAL	C-N-CA	5.52	124.87	118.85
12	M	163	VAL	N-CA-CB	5.51	116.63	110.62
4	6	77	G	C4'-C3'-O3'	-5.45	104.82	113.00
7	C	379	ILE	N-CA-CB	5.35	113.87	110.50
6	A	1421	GLY	N-CA-C	-5.31	104.32	111.54
6	A	484	PHE	N-CA-C	5.29	121.49	109.81
5	5	39	U	C2'-C3'-O3'	5.26	121.59	113.70
7	C	418	GLN	O-C-N	5.22	123.87	120.27
6	A	666	ILE	N-CA-C	-5.17	105.67	110.53
8	H	453	GLY	N-CA-C	5.15	118.87	112.64
9	J	229	THR	N-CA-C	5.10	117.13	109.23
14	O	20	ILE	CB-CA-C	-5.09	105.45	111.97
20	c	226	ASP	N-CA-C	5.05	121.56	110.80
21	o	350	TYR	N-CA-C	5.03	117.16	109.07
7	C	428	ILE	N-CA-CB	5.02	116.09	110.62

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	C	105	ILE	Peptide
9	J	194	HIS	Peptide

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Mol	Chain	Res	Type	Group
15	P	5	HIS	Peptide
21	o	239	LYS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	714	0	361	6	0
2	E	346	0	173	11	0
3	2	1025	0	518	14	0
4	6	2108	0	1063	27	0
5	5	2999	0	1515	35	0
6	A	15199	0	14954	279	0
7	C	6562	0	6486	112	0
8	H	3261	0	3323	94	0
9	J	2690	0	2690	89	0
10	K	1458	0	1468	24	0
11	L	1162	0	1111	19	0
12	M	2016	0	1985	34	0
13	N	1798	0	1842	40	0
14	O	1755	0	1794	29	0
15	P	565	0	555	7	0
16	R	614	0	390	8	0
17	S	3229	0	2573	43	0
18	T	1684	0	716	2	0
19	a	1119	0	1164	11	0
20	c	786	0	719	9	0
21	o	2425	0	2253	41	0
22	X	338	0	70	1	0
23	y	679	0	706	4	0
24	b	631	0	670	3	0
25	d	625	0	647	5	0
26	e	575	0	597	8	0
27	f	573	0	572	7	0
28	g	529	0	557	10	0
29	h	644	0	686	10	0
30	j	741	0	778	16	0
31	6	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	6	2	0	0	0	0
33	A	36	0	6	1	0
34	C	32	0	12	0	0
35	L	3	0	0	0	0
35	M	1	0	0	0	0
35	N	2	0	0	0	0
All	All	58929	0	52954	865	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (865) 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)
8:H:312:LEU:HA	8:H:315:LEU:CD2	1.64	1.27
8:H:311:LYS:O	8:H:315:LEU:CD2	1.85	1.24
8:H:311:LYS:O	8:H:315:LEU:HD22	1.38	1.24
8:H:312:LEU:C	8:H:315:LEU:HD23	1.61	1.22
8:H:312:LEU:CA	8:H:315:LEU:HD23	1.72	1.19
12:M:108:VAL:CG1	13:N:59:LEU:HD22	1.72	1.19
8:H:312:LEU:CA	8:H:315:LEU:CD2	2.21	1.18
8:H:312:LEU:O	8:H:315:LEU:HD23	1.44	1.18
12:M:108:VAL:CG1	13:N:59:LEU:CD2	2.21	1.17
8:H:312:LEU:HA	8:H:315:LEU:HD21	1.39	1.04
8:H:315:LEU:HD22	8:H:315:LEU:H	1.22	1.03
12:M:108:VAL:HG13	13:N:59:LEU:HD22	1.40	1.03
8:H:317:ILE:HD11	8:H:322:LYS:HG2	1.42	1.01
8:H:312:LEU:C	8:H:315:LEU:CD2	2.35	0.98
12:M:108:VAL:HG13	13:N:59:LEU:CD2	1.91	0.96
8:H:312:LEU:HA	8:H:315:LEU:HD23	1.31	0.95
12:M:108:VAL:HG11	13:N:59:LEU:HD22	1.47	0.93
8:H:311:LYS:O	8:H:315:LEU:HD21	1.66	0.91
12:M:108:VAL:CG1	13:N:59:LEU:HD21	1.97	0.91
8:H:317:ILE:HD11	8:H:322:LYS:CG	1.99	0.90
8:H:311:LYS:C	8:H:315:LEU:HD21	2.00	0.86
8:H:312:LEU:CA	8:H:315:LEU:HD21	1.99	0.85
9:J:355:THR:HG21	9:J:404:CYS:HA	1.59	0.83
9:J:156:ILE:HD13	9:J:197:LEU:HD21	1.59	0.82
7:C:142:LEU:HD11	7:C:189:LEU:HD22	1.61	0.82
21:o:319:ILE:HG21	21:o:368:LYS:CB	2.09	0.82
12:M:108:VAL:HG21	13:N:73:CYS:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:312:LEU:O	8:H:315:LEU:CD2	2.25	0.81
7:C:139:ILE:HD12	7:C:225:THR:HG23	1.62	0.79
9:J:240:ALA:HB1	9:J:248:ILE:HD11	1.65	0.78
12:M:108:VAL:HG12	13:N:59:LEU:HD21	1.65	0.78
6:A:139:LEU:HD12	6:A:193:TYR:CG	2.18	0.78
8:H:311:LYS:C	8:H:315:LEU:CD2	2.56	0.78
11:L:41:LEU:HD23	11:L:44:LYS:HB2	1.65	0.78
3:2:25:A:OP1	6:A:854:ARG:HD2	1.83	0.77
14:O:16:VAL:HG22	14:O:152:LEU:HD21	1.66	0.77
8:H:136:LEU:HD22	8:H:169:THR:HG21	1.66	0.77
9:J:342:LEU:HD21	10:K:55:VAL:HG21	1.66	0.77
6:A:856:TRP:CD1	15:P:174:VAL:HG21	2.19	0.77
6:A:1350:ILE:HG23	6:A:1356:LEU:HD23	1.67	0.77
8:H:317:ILE:O	8:H:317:ILE:HD12	1.85	0.76
8:H:315:LEU:CD2	8:H:315:LEU:H	1.98	0.76
8:H:317:ILE:CD1	8:H:322:LYS:HG3	2.15	0.76
9:J:248:ILE:HG23	9:J:262:LEU:HB2	1.68	0.75
7:C:493:LEU:HD22	7:C:542:ILE:HD11	1.68	0.75
7:C:257:ILE:HD11	7:C:263:MET:HE2	1.70	0.74
6:A:1020:ILE:HG22	6:A:1022:PRO:HD2	1.71	0.73
21:o:177:LEU:HD11	21:o:189:ILE:HG23	1.69	0.73
7:C:539:VAL:HG13	7:C:564:ILE:HG23	1.71	0.73
8:H:315:LEU:HD22	8:H:315:LEU:N	2.02	0.72
6:A:1391:PRO:HG2	6:A:1547:ILE:HD11	1.70	0.72
8:H:316:LYS:HG3	8:H:316:LYS:O	1.90	0.71
17:S:140:LEU:HD21	17:S:155:LEU:HD22	1.71	0.71
6:A:1082:ILE:HD13	6:A:1113:ILE:HD11	1.72	0.71
8:H:317:ILE:HD12	8:H:317:ILE:C	2.15	0.71
8:H:317:ILE:CD1	8:H:322:LYS:CG	2.66	0.71
12:M:104:LEU:HD21	13:N:16:CYS:HA	1.73	0.70
17:S:209:GLU:HB3	17:S:218:THR:HG22	1.71	0.70
6:A:1634:LEU:HD21	6:A:1641:LEU:HD12	1.73	0.70
6:A:518:VAL:HG21	6:A:689:TYR:CD2	2.26	0.70
6:A:377:VAL:HG11	7:C:912:ALA:HB3	1.73	0.69
9:J:403:LEU:HD11	9:J:419:ALA:HB2	1.74	0.69
6:A:621:LEU:HD23	6:A:722:LEU:HD21	1.73	0.69
9:J:164:MET:HE2	9:J:185:VAL:HG11	1.76	0.68
7:C:633:ILE:HB	7:C:645:LEU:HD12	1.76	0.68
5:5:101:C:OP1	6:A:672:LYS:N	2.26	0.68
4:6:79:A:OP1	4:6:81:G:O2'	2.12	0.67
9:J:230:VAL:HG22	9:J:241:THR:HG22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:108:VAL:HG11	13:N:59:LEU:CD2	2.09	0.67
6:A:1067:ASN:HB2	6:A:1083:THR:HG21	1.76	0.67
9:J:164:MET:HE1	9:J:199:SER:CB	2.25	0.67
6:A:857:ILE:HD11	6:A:969:ILE:HD11	1.76	0.67
9:J:144:CYS:SG	9:J:188:VAL:N	2.68	0.66
6:A:1092:PHE:CZ	6:A:1093:LYS:HG3	2.31	0.66
7:C:193:LEU:HD12	7:C:213:LEU:HB3	1.78	0.66
14:O:37:ALA:HB2	14:O:45:ALA:HA	1.76	0.66
25:d:50:THR:HG22	25:d:56:VAL:HG12	1.78	0.66
7:C:142:LEU:HD13	7:C:218:HIS:HB2	1.78	0.65
5:5:38:A:H2'	5:5:39:U:O4'	1.96	0.65
9:J:333:SER:HB2	9:J:343:THR:HG23	1.79	0.65
21:o:266:GLY:HA3	21:o:296:ILE:HD11	1.78	0.65
7:C:155:ILE:HD11	7:C:175:LEU:HD23	1.78	0.65
8:H:132:GLU:HB2	8:H:135:ILE:HD11	1.78	0.64
8:H:330:ILE:O	8:H:334:LEU:HD23	1.97	0.64
6:A:1092:PHE:O	6:A:1093:LYS:C	2.39	0.64
12:M:250:MET:SD	13:N:139:LEU:HD21	2.37	0.64
6:A:228:LYS:HG3	6:A:695:LEU:HD11	1.80	0.64
7:C:197:THR:HG21	7:C:544:LEU:HD22	1.78	0.64
5:5:45:A:H61	5:5:74:U:H3	1.46	0.64
6:A:569:LEU:HD21	6:A:637:VAL:HG21	1.80	0.64
6:A:1961:LEU:HD13	6:A:2083:ILE:HG21	1.78	0.63
8:H:49:ILE:HB	8:H:56:ILE:HD13	1.80	0.63
8:H:334:LEU:HD21	8:H:384:LEU:HD12	1.81	0.63
12:M:250:MET:HB2	13:N:139:LEU:HD11	1.81	0.62
2:E:-3:A:H2'	2:E:-2:A:O4'	2.00	0.62
10:K:202:MET:HE2	14:O:79:GLU:CD	2.24	0.62
27:f:72:PHE:HB2	30:j:33:LEU:HD23	1.82	0.62
6:A:1375:LEU:HD12	6:A:1383:PHE:CZ	2.35	0.61
6:A:1422:ILE:HD12	6:A:1422:ILE:O	2.00	0.61
21:o:266:GLY:CA	21:o:296:ILE:HD11	2.30	0.61
30:j:82:LYS:HG2	30:j:82:LYS:O	2.00	0.61
6:A:388:PRO:HB2	6:A:398:VAL:HG11	1.82	0.61
7:C:839:ILE:HB	7:C:840:PRO:HD3	1.81	0.61
14:O:16:VAL:CG2	14:O:152:LEU:HD21	2.31	0.61
9:J:145:VAL:HG22	9:J:157:THR:HG22	1.82	0.61
7:C:605:ILE:HB	7:C:652:MET:HE2	1.82	0.61
7:C:483:TRP:CH2	7:C:550:VAL:HG11	2.36	0.61
14:O:24:ALA:HB2	14:O:39:LEU:HD23	1.83	0.61
6:A:664:THR:O	6:A:666:ILE:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:j:85:ILE:HG22	30:j:85:ILE:O	2.02	0.60
6:A:2048:TRP:CD1	20:c:334:THR:HG21	2.37	0.60
7:C:691:VAL:HG12	7:C:841:LEU:HD22	1.83	0.59
29:h:7:LEU:HD11	30:j:95:PHE:CZ	2.37	0.59
6:A:585:ARG:HD3	12:M:33:TRP:CE2	2.38	0.59
5:5:45:A:N6	5:5:74:U:H3	2.00	0.59
6:A:677:ILE:HG21	6:A:1621:VAL:HG12	1.85	0.59
9:J:164:MET:HE1	9:J:199:SER:HB2	1.84	0.59
9:J:277:VAL:HG22	9:J:278:ASP:H	1.67	0.59
6:A:1126:LEU:HD11	6:A:1161:TYR:CD2	2.36	0.59
7:C:391:MET:HE2	7:C:395:LYS:HB3	1.83	0.59
30:j:79:LYS:O	30:j:80:LYS:HG3	2.03	0.59
7:C:241:VAL:HG11	7:C:273:LEU:CD2	2.33	0.59
4:6:2:U:H2'	4:6:3:U:O4'	2.03	0.59
6:A:966:PRO:HB3	6:A:1089:VAL:HB	1.84	0.59
8:H:421:LYS:HB2	8:H:468:ILE:HD11	1.84	0.59
14:O:214:ASN:ND2	17:S:44:ARG:O	2.35	0.59
8:H:312:LEU:N	8:H:315:LEU:HD21	2.17	0.59
21:o:209:ILE:HG12	21:o:212:LEU:HD21	1.85	0.59
6:A:374:ILE:HG22	6:A:376:ARG:HG2	1.84	0.58
7:C:222:MET:HE1	7:C:252:LEU:HD21	1.85	0.58
19:a:146:LEU:HD11	19:a:229:TRP:CZ3	2.38	0.58
9:J:373:LEU:HD13	9:J:389:THR:CG2	2.33	0.58
6:A:1023:LEU:HD13	6:A:1451:PHE:CE1	2.38	0.58
6:A:1632:ILE:HD11	6:A:1649:PHE:CE2	2.38	0.58
17:S:65:MET:HE3	17:S:95:ASP:CB	2.34	0.58
6:A:779:ALA:HA	6:A:782:ILE:HD12	1.85	0.58
6:A:660:ILE:HG21	6:A:711:TRP:CH2	2.39	0.58
6:A:1422:ILE:HD13	6:A:1425:PHE:CZ	2.38	0.58
6:A:671:TYR:CZ	6:A:674:MET:HG3	2.39	0.57
8:H:61:VAL:HG23	8:H:101:MET:SD	2.44	0.57
6:A:585:ARG:HD3	12:M:33:TRP:CD2	2.40	0.57
9:J:200:VAL:HG11	9:J:230:VAL:HG23	1.87	0.57
9:J:265:HIS:CE1	9:J:291:ARG:HG2	2.40	0.57
17:S:270:ALA:HB1	17:S:280:LEU:HD11	1.85	0.57
4:6:63:G:H2'	4:6:64:U:C6	2.39	0.57
6:A:1286:TRP:CE2	6:A:1302:LEU:HD11	2.40	0.57
6:A:1350:ILE:HD12	6:A:1356:LEU:CD2	2.34	0.57
7:C:562:VAL:HG23	7:C:564:ILE:HD11	1.87	0.57
8:H:334:LEU:HD12	8:H:380:GLN:HB3	1.87	0.57
6:A:1968:ALA:HA	6:A:2012:LEU:HD22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1426:ARG:HD2	16:R:8:LEU:HD12	1.87	0.57
6:A:1814:VAL:O	6:A:1818:ARG:HG2	2.04	0.57
7:C:191:ILE:HG23	7:C:221:PHE:CE1	2.40	0.57
19:a:226:THR:HG22	19:a:230:ILE:HD12	1.87	0.57
21:o:179:LEU:HD21	21:o:212:LEU:HD13	1.87	0.57
19:a:139:THR:HG23	19:a:232:SER:OG	2.05	0.56
2:E:-4:A:OP1	6:A:668:ARG:NE	2.38	0.56
8:H:200:ILE:O	8:H:204:ASP:N	2.35	0.56
7:C:323:THR:CG2	7:C:438:ALA:HB2	2.36	0.56
21:o:233:TRP:HA	21:o:240:VAL:HG11	1.86	0.56
6:A:176:LEU:HD22	6:A:632:ILE:HD11	1.86	0.56
6:A:1023:LEU:HA	6:A:1451:PHE:CZ	2.40	0.56
14:O:182:ILE:HD12	21:o:356:MET:HB3	1.86	0.56
6:A:1422:ILE:HD11	8:H:306:ASP:CG	2.31	0.56
8:H:351:ILE:HG21	8:H:395:GLU:HB3	1.85	0.56
12:M:108:VAL:HG22	13:N:75:MET:HG2	1.86	0.56
14:O:20:ILE:HD11	14:O:152:LEU:HD22	1.86	0.56
1:I:3:A:C2	1:I:4:U:C2	2.94	0.56
8:H:151:VAL:HG22	8:H:155:MET:HE3	1.88	0.56
5:5:110:U:H2'	5:5:111:C:O4'	2.06	0.56
6:A:1309:ILE:HG12	6:A:1356:LEU:HD13	1.88	0.56
6:A:1882:LEU:HD11	6:A:1991:ILE:HG21	1.88	0.55
7:C:687:ALA:HB3	7:C:852:THR:HG21	1.88	0.55
1:I:67:C:H2'	1:I:68:U:O4'	2.06	0.55
6:A:1980:LYS:HA	21:o:323:GLN:HE22	1.71	0.55
9:J:324:ALA:HB3	9:J:356:LEU:HD21	1.89	0.55
17:S:250:PHE:CE2	17:S:266:LEU:HD13	2.42	0.55
6:A:1543:ARG:O	6:A:1547:ILE:HD12	2.06	0.55
17:S:149:VAL:HA	17:S:152:VAL:HG12	1.89	0.55
14:O:17:GLU:HA	14:O:20:ILE:HD12	1.88	0.55
26:e:91:THR:HB	28:g:61:THR:HG22	1.89	0.55
3:2:34:G:O2'	3:2:35:U:H6	1.90	0.55
5:5:23:C:O2	5:5:23:C:O4'	2.25	0.55
6:A:343:ASN:HD21	6:A:354:PRO:HA	1.72	0.55
8:H:25:VAL:HG23	8:H:44:LEU:HD13	1.89	0.55
19:a:146:LEU:HD21	19:a:229:TRP:CE3	2.41	0.55
6:A:255:ILE:HD11	6:A:637:VAL:HG13	1.89	0.55
7:C:655:LEU:C	7:C:655:LEU:HD23	2.32	0.55
17:S:193:VAL:HG11	17:S:202:TRP:CZ2	2.42	0.55
19:a:118:HIS:CE1	19:a:147:LEU:HD11	2.41	0.55
6:A:1973:LYS:HB3	6:A:2039:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:29:GLN:HB3	11:L:55:LEU:HD11	1.88	0.55
28:g:15:ILE:HG21	28:g:71:LEU:HD13	1.88	0.55
6:A:742:VAL:HG21	9:J:224:LEU:HA	1.89	0.55
6:A:2002:TYR:HB2	20:c:299:LEU:HD12	1.88	0.55
7:C:900:LEU:O	7:C:902:VAL:N	2.39	0.55
4:6:35:A:H2'	12:M:75:PHE:CE1	2.42	0.54
4:6:61:C:H2'	4:6:62:A:O4'	2.07	0.54
4:6:70:U:OP2	6:A:737:ARG:NH2	2.40	0.54
9:J:194:HIS:CD2	9:J:253:MET:HE1	2.41	0.54
6:A:615:LEU:HD13	6:A:619:PHE:CD2	2.41	0.54
6:A:624:GLU:HB3	6:A:666:ILE:HG12	1.89	0.54
10:K:198:ASN:HB3	10:K:202:MET:HE1	1.89	0.54
17:S:251:ALA:HB1	17:S:267:TYR:OH	2.07	0.54
5:5:173:U:O2'	27:f:74:ARG:NH2	2.40	0.54
6:A:1158:ILE:HG12	6:A:1172:PHE:CE1	2.43	0.54
13:N:240:LEU:HD13	13:N:251:LEU:HD13	1.89	0.54
29:h:3:LEU:HD11	30:j:60:ALA:HB1	1.88	0.54
6:A:898:ILE:HB	6:A:1074:VAL:HG12	1.89	0.54
8:H:309:ALA:O	8:H:313:LEU:HD13	2.07	0.54
5:5:65:U:H2'	5:5:66:A:C8	2.43	0.54
7:C:823:ILE:CG2	7:C:825:VAL:HG23	2.37	0.54
8:H:21:ILE:HG22	8:H:47:VAL:HG23	1.88	0.54
8:H:60:VAL:HG13	8:H:76:LEU:HD21	1.89	0.54
21:o:311:SER:HB3	21:o:317:VAL:HG22	1.89	0.54
6:A:1379:MET:HE1	6:A:1619:VAL:CG2	2.38	0.54
11:L:30:LEU:HD13	11:L:55:LEU:HD22	1.89	0.54
6:A:857:ILE:HD11	6:A:969:ILE:CD1	2.38	0.54
9:J:321:PHE:HB2	10:K:57:LEU:HD12	1.90	0.54
17:S:99:ILE:N	17:S:100:PRO:CD	2.71	0.54
6:A:1624:LEU:HD21	6:A:1635:HIS:CE1	2.43	0.54
7:C:116:THR:HG21	7:C:118:TYR:CZ	2.42	0.54
13:N:16:CYS:HB2	13:N:74:CYS:SG	2.47	0.54
4:6:62:A:H61	15:P:5:HIS:HB2	1.73	0.53
6:A:673:VAL:HG22	6:A:714:PHE:CE1	2.44	0.53
5:5:39:U:H2'	5:5:40:C:C6	2.43	0.53
6:A:1632:ILE:HG21	6:A:1645:LEU:HD13	1.90	0.53
13:N:13:CYS:SG	13:N:16:CYS:HB2	2.48	0.53
6:A:1699:ALA:HB2	6:A:1767:TYR:CD1	2.43	0.53
3:2:34:G:HO2'	3:2:35:U:H6	1.55	0.53
14:O:76:LEU:HD12	14:O:91:MET:HE3	1.89	0.53
5:5:43:G:N2	5:5:46:C:OP1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:123:U:H2'	5:5:124:C:C6	2.43	0.53
7:C:155:ILE:HG23	7:C:164:MET:HE1	1.90	0.53
9:J:277:VAL:HG11	9:J:321:PHE:HZ	1.74	0.53
6:A:1283:GLU:N	8:H:345:ILE:HD11	2.24	0.53
8:H:351:ILE:HD11	8:H:361:TYR:CB	2.39	0.53
21:o:349:ASN:O	21:o:365:LEU:N	2.38	0.53
30:j:79:LYS:O	30:j:80:LYS:CG	2.57	0.53
7:C:324:ILE:HD12	7:C:325:LYS:N	2.24	0.53
17:S:65:MET:SD	17:S:65:MET:N	2.81	0.53
8:H:73:ILE:HG13	8:H:74:PRO:HD3	1.90	0.53
9:J:257:ILE:CD1	10:K:78:VAL:HG23	2.39	0.53
9:J:359:ASN:OD1	9:J:360:GLN:N	2.41	0.53
14:O:186:GLN:HG3	21:o:356:MET:HE2	1.91	0.53
21:o:323:GLN:O	21:o:325:ASN:OD1	2.27	0.53
6:A:615:LEU:HD13	6:A:619:PHE:CE2	2.44	0.53
14:O:30:THR:O	14:O:33:TRP:NE1	2.42	0.52
4:6:35:A:N1	12:M:81:CYS:HA	2.24	0.52
4:6:41:A:H2'	4:6:42:A:O4'	2.09	0.52
6:A:165:LEU:HD21	6:A:578:MET:HB3	1.91	0.52
6:A:1375:LEU:HD12	6:A:1383:PHE:HZ	1.72	0.52
9:J:200:VAL:HG21	9:J:227:VAL:CG1	2.39	0.52
8:H:51:ILE:HG22	8:H:245:CYS:SG	2.49	0.52
17:S:225:ALA:O	17:S:228:THR:HG22	2.09	0.52
6:A:1372:LYS:HB3	6:A:1378:LYS:HA	1.91	0.52
6:A:915:ALA:HB1	6:A:993:ALA:HB1	1.90	0.52
6:A:889:TRP:O	6:A:893:ARG:HG2	2.09	0.52
11:L:90:LEU:HB2	11:L:106:LEU:HD11	1.91	0.52
6:A:1257:ASN:OD1	6:A:1270:LEU:HD13	2.09	0.52
7:C:323:THR:HG21	7:C:438:ALA:HB2	1.91	0.52
1:I:58:U:H2'	1:I:59:C:O4'	2.09	0.52
11:L:104:CYS:SG	11:L:105:CYS:N	2.83	0.52
6:A:868:GLN:O	10:K:197:ILE:HA	2.10	0.52
7:C:539:VAL:HG13	7:C:564:ILE:CG2	2.39	0.52
8:H:58:LYS:HA	8:H:61:VAL:HG12	1.92	0.52
5:5:62:G:H2'	5:5:63:C:O4'	2.10	0.52
7:C:242:VAL:HG21	7:C:272:ARG:HE	1.74	0.52
7:C:318:LEU:HD22	7:C:421:LEU:CD2	2.40	0.52
9:J:200:VAL:CG2	9:J:227:VAL:HB	2.40	0.51
21:o:356:MET:HA	21:o:356:MET:HE3	1.90	0.51
5:5:30:A:H2'	5:5:31:G:O4'	2.10	0.51
9:J:144:CYS:SG	9:J:187:ASP:HA	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:290:VAL:HG11	9:J:334:TRP:CZ3	2.45	0.51
6:A:1067:ASN:CB	6:A:1083:THR:HG21	2.40	0.51
7:C:823:ILE:HG22	7:C:825:VAL:HG23	1.92	0.51
8:H:83:LEU:HD21	8:H:90:ILE:HB	1.93	0.51
6:A:168:LEU:N	6:A:169:PRO:HD2	2.26	0.51
9:J:284:SER:OG	9:J:311:VAL:O	2.28	0.51
6:A:627:LYS:HG2	6:A:664:THR:HB	1.92	0.51
7:C:139:ILE:CG2	7:C:252:LEU:HD22	2.40	0.51
7:C:241:VAL:HG11	7:C:273:LEU:HD23	1.92	0.51
9:J:145:VAL:N	9:J:404:CYS:SG	2.84	0.51
19:a:162:SER:O	19:a:166:VAL:HG23	2.11	0.51
6:A:1624:LEU:HD22	6:A:1633:PHE:HB3	1.93	0.51
6:A:1823:LEU:O	6:A:1825:ILE:HG23	2.10	0.51
6:A:849:LEU:HD23	6:A:978:ILE:HG21	1.92	0.51
17:S:63:LEU:HB2	17:S:65:MET:HE1	1.93	0.51
6:A:355:LEU:HD23	6:A:356:TYR:CE2	2.46	0.51
7:C:116:THR:HG21	7:C:118:TYR:CE1	2.46	0.51
6:A:687:ILE:HD11	6:A:706:PRO:HG3	1.93	0.51
6:A:1407:ILE:HG21	6:A:1426:ARG:NH2	2.26	0.51
8:H:74:PRO:HA	8:H:123:ILE:HD12	1.92	0.51
14:O:20:ILE:HD11	14:O:152:LEU:CD2	2.41	0.51
17:S:81:MET:HE3	17:S:112:VAL:HG11	1.92	0.51
29:h:16:THR:HB	29:h:96:ILE:HB	1.93	0.51
6:A:1400:ILE:HG21	6:A:1440:ILE:HD12	1.93	0.51
6:A:1732:MET:HE1	6:A:1789:ASN:HB2	1.93	0.51
7:C:385:PHE:CE1	7:C:425:LEU:HD11	2.46	0.50
2:E:-9:U:H2'	2:E:-9:U:O2	2.11	0.50
8:H:312:LEU:N	8:H:315:LEU:CD2	2.74	0.50
6:A:1454:SER:HA	6:A:1487:GLY:HA2	1.93	0.50
7:C:324:ILE:HG22	7:C:377:ILE:HD13	1.92	0.50
7:C:418:GLN:HB3	7:C:419:PRO:HD3	1.92	0.50
1:I:14:U:C6	12:M:229:ASP:HB3	2.47	0.50
6:A:138:HIS:HB2	11:L:52:ILE:HD11	1.92	0.50
6:A:687:ILE:HD11	6:A:706:PRO:CG	2.41	0.50
8:H:181:LEU:HD13	8:H:194:LEU:HD22	1.92	0.50
21:o:222:LEU:HD13	21:o:253:VAL:HB	1.93	0.50
6:A:806:ALA:N	6:A:807:PRO:HD2	2.26	0.50
13:N:34:CYS:SG	13:N:37:CYS:N	2.83	0.50
6:A:338:ASN:O	6:A:342:LEU:HG	2.11	0.50
6:A:522:TYR:CZ	6:A:686:ILE:HD12	2.47	0.50
9:J:324:ALA:CB	9:J:364:LEU:HD11	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:33:ALA:HB1	11:L:52:ILE:HG22	1.93	0.50
6:A:1387:VAL:HG12	6:A:1610:TRP:CD2	2.47	0.50
8:H:94:LEU:HA	8:H:97:GLU:HG2	1.94	0.50
9:J:269:ILE:HA	9:J:285:SER:HA	1.94	0.50
6:A:194:HIS:CD2	10:K:122:LEU:HD23	2.46	0.50
6:A:1379:MET:HE1	6:A:1619:VAL:HG22	1.93	0.50
6:A:1925:PRO:O	6:A:1929:GLN:N	2.45	0.50
7:C:241:VAL:HG22	7:C:267:ILE:CG2	2.42	0.50
6:A:1212:ARG:HA	6:A:1259:LEU:HD11	1.93	0.49
9:J:277:VAL:HG11	9:J:321:PHE:CZ	2.47	0.49
17:S:285:LEU:HD21	17:S:302:SER:CB	2.41	0.49
21:o:385:TYR:HB3	21:o:431:GLN:HA	1.93	0.49
30:j:96:LEU:HD21	30:j:101:VAL:CG2	2.42	0.49
7:C:314:ALA:CB	7:C:321:THR:HG22	2.42	0.49
9:J:242:ALA:HB2	9:J:248:ILE:HA	1.92	0.49
9:J:357:SER:O	9:J:365:PHE:HB3	2.11	0.49
5:5:103:A:OP2	6:A:675:HIS:NE2	2.44	0.49
6:A:139:LEU:HD13	6:A:562:ILE:HD11	1.94	0.49
6:A:173:LEU:HD13	6:A:715:LEU:HB2	1.94	0.49
6:A:468:LEU:HD21	7:C:382:TYR:HB3	1.95	0.49
20:c:315:ILE:HG22	20:c:316:ARG:HG2	1.94	0.49
6:A:165:LEU:HD12	6:A:622:MET:HG2	1.94	0.49
6:A:660:ILE:HG21	6:A:711:TRP:CZ2	2.48	0.49
6:A:1407:ILE:HG21	6:A:1426:ARG:HH21	1.77	0.49
9:J:242:ALA:HB1	9:J:269:ILE:CG2	2.43	0.49
11:L:29:GLN:CB	11:L:55:LEU:HD11	2.43	0.49
6:A:1426:ARG:CD	16:R:8:LEU:HD12	2.43	0.49
6:A:1855:THR:HG21	6:A:1966:SER:HB3	1.93	0.49
9:J:334:TRP:HD1	9:J:341:LEU:HA	1.78	0.49
6:A:461:LEU:HD11	7:C:331:TYR:HB3	1.95	0.49
6:A:834:ILE:HD13	6:A:845:VAL:HG23	1.93	0.49
6:A:1391:PRO:CG	6:A:1547:ILE:HD11	2.42	0.49
10:K:174:ASN:HD21	10:K:185:ARG:HH22	1.60	0.49
9:J:403:LEU:CD1	9:J:419:ALA:HB2	2.42	0.49
21:o:222:LEU:HD13	21:o:253:VAL:CG1	2.42	0.49
3:2:3:G:H2'	3:2:4:A:O4'	2.13	0.49
6:A:1754:ALA:O	6:A:1758:ASP:HB2	2.12	0.49
7:C:800:TYR:O	7:C:803:VAL:HG12	2.13	0.49
12:M:74:LEU:HA	12:M:112:PHE:CE1	2.47	0.49
7:C:493:LEU:CD2	7:C:542:ILE:HD11	2.40	0.49
9:J:200:VAL:CG1	9:J:230:VAL:HG23	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:327:CYS:SG	9:J:328:THR:N	2.86	0.49
10:K:182:LEU:HD11	14:O:22:LYS:CG	2.43	0.49
10:K:202:MET:N	10:K:202:MET:HE3	2.28	0.49
6:A:168:LEU:HB2	6:A:578:MET:HE1	1.93	0.49
8:H:47:VAL:HG13	8:H:49:ILE:HG23	1.94	0.49
6:A:166:LYS:HE3	6:A:730:ILE:HD11	1.95	0.48
6:A:343:ASN:HD21	6:A:354:PRO:CA	2.25	0.48
21:o:170:PHE:CZ	21:o:443:ILE:HD12	2.47	0.48
9:J:289:THR:HG22	9:J:305:THR:HG22	1.95	0.48
12:M:246:SER:C	12:M:250:MET:HE3	2.38	0.48
14:O:14:THR:HG23	14:O:17:GLU:HB2	1.95	0.48
17:S:185:VAL:O	17:S:188:ILE:HG13	2.13	0.48
6:A:1862:VAL:HG13	6:A:1870:VAL:HG13	1.95	0.48
8:H:58:LYS:O	8:H:61:VAL:HG12	2.13	0.48
14:O:30:THR:HG23	14:O:31:HIS:CE1	2.48	0.48
6:A:336:PHE:HB3	6:A:530:VAL:HG21	1.93	0.48
6:A:1267:VAL:HG22	6:A:1302:LEU:CD2	2.44	0.48
7:C:315:SER:HB3	7:C:320:PHE:CE1	2.48	0.48
29:h:3:LEU:HD13	30:j:62:ASP:HB3	1.95	0.48
6:A:480:TYR:OH	7:C:317:LYS:NZ	2.46	0.48
6:A:632:ILE:HG22	6:A:656:ILE:HG21	1.95	0.48
6:A:766:ILE:HG21	6:A:782:ILE:HD13	1.95	0.48
6:A:1967:ALA:HB1	6:A:2015:LEU:HB3	1.96	0.48
9:J:238:LEU:HD21	9:J:250:LEU:HD22	1.94	0.48
13:N:25:MET:CB	13:N:46:PHE:HB3	2.44	0.48
6:A:355:LEU:HD23	6:A:356:TYR:CZ	2.49	0.48
7:C:318:LEU:HD13	7:C:421:LEU:HD21	1.95	0.48
7:C:801:TRP:HB3	7:C:843:LYS:HD3	1.96	0.48
7:C:862:TYR:CE2	7:C:908:VAL:HG13	2.48	0.48
12:M:250:MET:CG	13:N:139:LEU:HD11	2.43	0.48
17:S:141:ILE:HG21	23:y:108:THR:CG2	2.43	0.48
21:o:181:GLY:HA3	21:o:212:LEU:HD11	1.95	0.48
22:X:88:UNK:O	22:X:91:UNK:N	2.46	0.48
27:f:71:ILE:HG22	30:j:105:LEU:HB3	1.95	0.48
1:I:3:A:N6	4:6:51:A:O4'	2.47	0.48
6:A:238:ARG:NH2	6:A:1694:MET:O	2.46	0.48
8:H:143:LEU:HD11	8:H:151:VAL:HG11	1.95	0.48
12:M:99:ILE:HD13	12:M:188:TYR:CD2	2.49	0.48
12:M:249:MET:HE1	13:N:86:LEU:HD11	1.96	0.48
17:S:140:LEU:CD2	17:S:155:LEU:HD22	2.41	0.48
6:A:1033:ASN:HB2	6:A:1288:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:276:PRO:HB2	10:K:63:ILE:HD12	1.94	0.48
9:J:344:ASN:HD22	10:K:45:PRO:HG3	1.78	0.48
17:S:107:ASP:O	17:S:111:LYS:HG2	2.14	0.48
3:2:46:C:H2'	3:2:47:U:C6	2.49	0.48
4:6:70:U:H2'	4:6:71:G:O4'	2.14	0.48
6:A:182:PRO:HB2	6:A:264:ILE:HD11	1.95	0.48
6:A:379:ILE:HD11	6:A:391:TYR:CD1	2.49	0.48
8:H:44:LEU:O	8:H:47:VAL:HG12	2.13	0.48
29:h:96:ILE:HG23	30:j:91:ILE:CG2	2.44	0.48
12:M:250:MET:CB	13:N:139:LEU:HD11	2.44	0.48
6:A:209:ILE:HG21	6:A:303:PHE:HE2	1.79	0.47
8:H:135:ILE:HD12	8:H:162:LEU:HD21	1.95	0.47
9:J:376:TYR:HD1	9:J:383:LYS:HA	1.79	0.47
10:K:185:ARG:NH1	14:O:26:GLN:O	2.43	0.47
8:H:80:ILE:HD12	8:H:94:LEU:HD13	1.96	0.47
6:A:239:PHE:HA	6:A:240:PRO:C	2.39	0.47
7:C:150:MET:HB3	7:C:178:LEU:HD22	1.95	0.47
8:H:351:ILE:HD11	8:H:361:TYR:HB2	1.95	0.47
17:S:140:LEU:HD22	17:S:152:VAL:HG23	1.95	0.47
6:A:1565:THR:HG21	6:A:1825:ILE:HD11	1.95	0.47
17:S:65:MET:HE3	17:S:95:ASP:HB3	1.97	0.47
6:A:636:HIS:CE1	6:A:653:ILE:HD11	2.49	0.47
7:C:150:MET:HG3	7:C:214:ASP:CB	2.44	0.47
16:R:8:LEU:HD23	16:R:9:LYS:N	2.30	0.47
21:o:209:ILE:HD11	21:o:223:SER:HB2	1.97	0.47
7:C:149:LEU:HD23	7:C:150:MET:HE2	1.95	0.47
7:C:195:GLY:C	7:C:545:LEU:HD13	2.39	0.47
27:f:52:GLN:HG3	30:j:33:LEU:HD22	1.96	0.47
3:2:34:G:O2'	3:2:35:U:C6	2.66	0.47
6:A:625:LEU:HD22	6:A:715:LEU:HD21	1.96	0.47
6:A:1168:ILE:HD12	6:A:1170:MET:HE2	1.96	0.47
6:A:1344:THR:HG21	6:A:1537:TRP:CD2	2.49	0.47
6:A:1991:ILE:HG23	6:A:1992:TYR:CD2	2.50	0.47
33:A:3001:IHP:O21	20:c:170:ARG:NH1	2.47	0.47
9:J:147:ILE:HD11	9:J:169:LEU:HD11	1.97	0.47
13:N:116:LYS:HB3	13:N:118:VAL:HG22	1.96	0.47
14:O:88:ALA:HB2	14:O:95:ALA:HA	1.96	0.47
5:5:110:U:C2	5:5:111:C:C6	3.03	0.47
6:A:2015:LEU:HD22	6:A:2022:ALA:HB1	1.96	0.47
5:5:93:G:C2	5:5:102:C:C2	3.03	0.47
6:A:1347:ARG:HD3	6:A:1444:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:216:ILE:HD12	9:J:216:ILE:C	2.39	0.47
11:L:41:LEU:HD21	12:M:83:LEU:HD21	1.96	0.47
13:N:8:PRO:HB2	13:N:62:VAL:HG11	1.97	0.47
21:o:311:SER:CB	21:o:317:VAL:HG22	2.45	0.47
6:A:611:LYS:O	6:A:614:ARG:HG2	2.16	0.47
9:J:156:ILE:HG22	9:J:166:VAL:HG13	1.97	0.47
9:J:290:VAL:HG12	9:J:304:LEU:HB2	1.96	0.46
14:O:217:ILE:HD11	17:S:82:ARG:CZ	2.45	0.46
5:5:25:G:H2'	5:5:25:G:N3	2.30	0.46
6:A:161:PHE:CE1	6:A:198:ALA:HA	2.50	0.46
6:A:637:VAL:O	6:A:641:LEU:N	2.46	0.46
7:C:241:VAL:HG11	7:C:273:LEU:HD22	1.97	0.46
7:C:319:GLY:O	7:C:426:GLN:NE2	2.48	0.46
10:K:180:VAL:HG12	10:K:185:ARG:NH1	2.30	0.46
5:5:88:U:O2'	9:J:216:ILE:HD11	2.15	0.46
6:A:228:LYS:CG	6:A:695:LEU:HD11	2.42	0.46
6:A:522:TYR:CE1	6:A:686:ILE:HD12	2.50	0.46
6:A:1107:LEU:HB2	6:A:1110:ALA:HB2	1.98	0.46
6:A:1282:ASP:C	8:H:345:ILE:HD11	2.40	0.46
16:R:67:HIS:O	16:R:71:ARG:CB	2.63	0.46
21:o:319:ILE:CD1	21:o:368:LYS:O	2.63	0.46
6:A:1354:GLU:N	6:A:1355:PRO:CD	2.79	0.46
14:O:76:LEU:O	14:O:80:LEU:N	2.43	0.46
21:o:273:LEU:HD23	21:o:288:THR:HG22	1.97	0.46
1:I:64:U:H2'	1:I:65:U:O4'	2.16	0.46
6:A:165:LEU:HD13	6:A:578:MET:HE2	1.97	0.46
11:L:22:THR:HG21	11:L:62:TYR:CE1	2.50	0.46
6:A:1204:ARG:NH2	6:A:1260:PHE:HA	2.31	0.46
8:H:60:VAL:HG13	8:H:76:LEU:HD11	1.98	0.46
9:J:277:VAL:HG22	9:J:278:ASP:N	2.29	0.46
9:J:365:PHE:CE1	9:J:373:LEU:HG	2.50	0.46
9:J:407:PHE:CZ	9:J:414:LEU:HD13	2.51	0.46
11:L:78:TYR:OH	11:L:92:ILE:HG21	2.16	0.46
13:N:139:LEU:HD13	13:N:139:LEU:C	2.40	0.46
14:O:214:ASN:HD22	17:S:44:ARG:HG3	1.80	0.46
17:S:128:THR:HB	17:S:129:LEU:HD12	1.96	0.46
5:5:106:A:O2'	9:J:213:LYS:NZ	2.30	0.46
6:A:209:ILE:HB	6:A:212:VAL:HB	1.97	0.46
6:A:1961:LEU:HD12	6:A:1963:LEU:HG	1.98	0.46
8:H:45:PHE:CZ	8:H:258:LEU:HB3	2.50	0.46
8:H:402:LEU:HD22	8:H:420:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:67:TYR:HE1	11:L:75:LYS:HA	1.80	0.46
29:h:96:ILE:HG23	30:j:91:ILE:HG23	1.98	0.46
6:A:191:VAL:O	6:A:559:GLN:HA	2.16	0.46
6:A:789:ALA:HB2	6:A:799:TRP:CE2	2.51	0.46
6:A:831:ARG:HG3	6:A:852:LEU:CD1	2.46	0.46
7:C:347:ARG:O	7:C:348:LEU:C	2.58	0.46
17:S:72:ALA:HB1	17:S:88:PHE:CZ	2.50	0.46
6:A:719:ILE:N	6:A:720:PRO:CD	2.79	0.46
6:A:1082:ILE:HG23	6:A:1109:PHE:HE1	1.81	0.46
7:C:222:MET:CE	7:C:252:LEU:HD21	2.45	0.46
12:M:121:ARG:O	12:M:123:ASP:N	2.48	0.46
12:M:146:LEU:HD13	12:M:151:LEU:HD12	1.96	0.46
14:O:194:ALA:C	21:o:183:ASN:HD21	2.24	0.46
19:a:118:HIS:NE2	19:a:147:LEU:HD11	2.31	0.46
24:b:85:THR:HG22	25:d:73:VAL:HA	1.97	0.46
4:6:39:G:C6	12:M:117:PHE:HD2	2.33	0.46
6:A:1701:ILE:HB	6:A:1734:PHE:HB2	1.99	0.46
8:H:148:LEU:HA	8:H:151:VAL:HG12	1.97	0.46
9:J:198:PHE:CD1	9:J:239:ILE:HD13	2.50	0.46
14:O:189:ARG:NE	17:S:38:LEU:HD12	2.31	0.46
6:A:1165:LEU:HD21	6:A:1514:PHE:CE1	2.51	0.45
19:a:146:LEU:HD11	19:a:229:TRP:CE3	2.50	0.45
21:o:212:LEU:HD23	21:o:223:SER:HA	1.97	0.45
28:g:28:ILE:HG22	28:g:41:ASP:HB3	1.99	0.45
6:A:995:LEU:O	6:A:999:LEU:HG	2.16	0.45
6:A:1651:ALA:HB2	6:A:1911:TRP:CH2	2.51	0.45
9:J:227:VAL:HA	9:J:243:GLY:HA3	1.98	0.45
11:L:52:ILE:C	11:L:52:ILE:HD12	2.42	0.45
17:S:285:LEU:HD22	17:S:299:GLU:HA	1.99	0.45
17:S:300:THR:O	17:S:304:LYS:CB	2.64	0.45
6:A:518:VAL:HG21	6:A:689:TYR:CE2	2.51	0.45
6:A:1165:LEU:HD21	6:A:1514:PHE:HE1	1.81	0.45
7:C:152:LEU:HD21	7:C:319:GLY:HA2	1.97	0.45
11:L:61:ARG:O	11:L:61:ARG:HD3	2.16	0.45
17:S:199:MET:HB2	17:S:242:GLU:HB3	1.98	0.45
6:A:674:MET:HA	6:A:677:ILE:HD12	1.98	0.45
6:A:831:ARG:HG3	6:A:852:LEU:HD13	1.99	0.45
6:A:1850:LEU:HD11	6:A:1881:THR:HG22	1.97	0.45
6:A:1875:ILE:HG22	6:A:1876:ASN:N	2.31	0.45
9:J:341:LEU:HD23	9:J:342:LEU:N	2.31	0.45
10:K:134:VAL:HG11	13:N:115:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:344:GLU:O	20:c:348:THR:HG23	2.17	0.45
26:e:35:ILE:HD11	28:g:21:GLY:HA3	1.98	0.45
27:f:36:THR:HG23	27:f:60:VAL:HA	1.98	0.45
5:5:35:A:H2'	5:5:36:A:C8	2.52	0.45
9:J:291:ARG:HD3	9:J:303:VAL:HG23	1.99	0.45
7:C:235:VAL:HG23	7:C:261:VAL:HG11	1.99	0.45
7:C:879:LEU:HD11	7:C:921:SER:OG	2.16	0.45
6:A:1865:THR:CG2	6:A:1871:ALA:HB2	2.46	0.45
8:H:463:ASN:O	8:H:466:THR:OG1	2.29	0.45
13:N:94:VAL:HG23	13:N:142:ILE:HD12	1.99	0.45
3:2:5:A:H5'	23:y:114:THR:HG22	1.98	0.45
6:A:330:LEU:HD21	6:A:386:ALA:HB2	1.98	0.45
6:A:721:LEU:HD11	6:A:725:TYR:CZ	2.52	0.45
17:S:155:LEU:C	17:S:155:LEU:HD23	2.42	0.45
6:A:376:ARG:NH1	7:C:957:ALA:O	2.49	0.45
7:C:126:MET:SD	7:C:132:ARG:NH2	2.90	0.45
9:J:209:TRP:HA	9:J:216:ILE:HA	1.99	0.45
12:M:12:GLN:HE22	12:M:58:HIS:HB3	1.81	0.45
12:M:121:ARG:O	12:M:124:MET:N	2.49	0.45
21:o:209:ILE:CG1	21:o:212:LEU:HD21	2.46	0.45
29:h:7:LEU:HD11	30:j:95:PHE:CE1	2.51	0.45
5:5:80:G:C4	5:5:82:A:C2	3.05	0.45
7:C:152:LEU:HD11	7:C:319:GLY:HA2	1.97	0.45
7:C:200:CYS:HB3	7:C:436:VAL:HG21	1.99	0.45
7:C:493:LEU:HD21	7:C:539:VAL:HG21	1.98	0.45
9:J:198:PHE:CE1	9:J:239:ILE:HD13	2.51	0.45
13:N:67:GLN:HG2	13:N:120:LEU:HD23	1.99	0.45
21:o:181:GLY:HA2	21:o:187:ILE:HA	1.98	0.45
6:A:1047:ALA:HB3	6:A:1251:TYR:HB3	1.99	0.44
7:C:691:VAL:CG1	7:C:841:LEU:HD22	2.46	0.44
9:J:242:ALA:HB1	9:J:269:ILE:HG21	1.99	0.44
10:K:112:ILE:HD13	13:N:25:MET:HE3	1.99	0.44
21:o:177:LEU:HD13	21:o:178:ILE:N	2.31	0.44
19:a:152:ARG:HD3	20:c:218:LEU:HD11	1.98	0.44
20:c:220:LYS:HA	20:c:223:LEU:HG	1.99	0.44
4:6:69:C:C2	4:6:78:G:C2	3.05	0.44
6:A:138:HIS:CE1	11:L:49:LEU:HD11	2.52	0.44
9:J:296:VAL:HG23	10:K:73:TYR:CG	2.52	0.44
13:N:43:LEU:HD21	13:N:57:LYS:HB2	1.99	0.44
14:O:22:LYS:HB2	14:O:56:LEU:HD11	1.99	0.44
5:5:15:A:N7	5:5:133:C:N4	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:461:LEU:HD11	7:C:331:TYR:CB	2.46	0.44
6:A:660:ILE:HD12	6:A:660:ILE:HA	1.94	0.44
8:H:346:LEU:HD21	8:H:350:MET:HE3	1.99	0.44
18:T:457:TYR:CB	18:T:465:THR:HA	2.48	0.44
30:j:79:LYS:C	30:j:80:LYS:HG3	2.43	0.44
4:6:62:A:C4	4:6:63:G:C8	3.06	0.44
6:A:756:LEU:C	6:A:756:LEU:HD12	2.43	0.44
6:A:1050:LEU:HD22	6:A:1170:MET:HE3	1.99	0.44
6:A:1182:LEU:HD11	15:P:127:TRP:HZ2	1.81	0.44
7:C:257:ILE:CD1	7:C:263:MET:HE2	2.44	0.44
7:C:416:ASP:HB3	7:C:417:PRO:HD2	1.99	0.44
21:o:166:THR:HA	21:o:182:GLY:HA2	1.99	0.44
6:A:203:ASN:HA	6:A:548:LEU:HD23	1.99	0.44
6:A:1689:ARG:NH1	6:A:1692:TYR:OH	2.51	0.44
7:C:318:LEU:HD22	7:C:421:LEU:HD22	1.98	0.44
24:b:93:LEU:HA	29:h:91:THR:HG21	1.98	0.44
6:A:1328:PHE:CD2	6:A:1603:ASN:HB2	2.53	0.44
6:A:1624:LEU:HD21	6:A:1635:HIS:ND1	2.32	0.44
7:C:150:MET:SD	7:C:212:PHE:HB3	2.58	0.44
7:C:155:ILE:CD1	7:C:175:LEU:HD23	2.47	0.44
8:H:73:ILE:CG1	8:H:74:PRO:HD3	2.48	0.44
8:H:317:ILE:CD1	8:H:317:ILE:C	2.86	0.44
12:M:48:VAL:HG22	12:M:220:GLY:N	2.33	0.44
13:N:60:ILE:HG13	13:N:72:GLN:HG3	1.98	0.44
16:R:102:LEU:O	16:R:106:LEU:CB	2.66	0.44
2:E:-15:A:N3	2:E:-15:A:H2'	2.32	0.44
5:5:103:A:C4	5:5:104:G:C8	3.06	0.44
6:A:137:GLU:HG3	11:L:30:LEU:HD23	2.00	0.44
6:A:1082:ILE:HG23	6:A:1109:PHE:CE1	2.53	0.44
8:H:355:ARG:O	8:H:359:THR:HG23	2.18	0.44
13:N:68:ARG:HB3	13:N:84:ILE:HD12	2.00	0.44
6:A:1054:LEU:HD13	6:A:1121:ILE:HD13	1.99	0.44
6:A:1508:HIS:O	6:A:1511:ARG:HG2	2.17	0.44
9:J:181:HIS:CE1	9:J:201:SER:HG	2.36	0.44
9:J:229:THR:HG21	9:J:271:GLN:HA	1.99	0.44
9:J:324:ALA:CB	9:J:356:LEU:HD21	2.48	0.44
19:a:233:ILE:O	19:a:237:ILE:HD12	2.17	0.44
3:2:20:G:C2	15:P:6:ARG:HD3	2.52	0.43
6:A:181:HIS:HB3	6:A:182:PRO:HD2	2.00	0.43
7:C:231:ALA:O	7:C:487:ARG:NH1	2.51	0.43
8:H:298:VAL:HG13	8:H:311:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:44:VAL:HG11	25:d:10:LEU:HD13	2.00	0.43
6:A:996:ASP:OD2	6:A:1511:ARG:NH1	2.49	0.43
6:A:1974:LEU:O	6:A:1977:VAL:HG12	2.18	0.43
7:C:501:ILE:HD13	7:C:567:ILE:HG23	2.00	0.43
7:C:760:LEU:HD23	7:C:764:ASN:HD21	1.82	0.43
8:H:189:THR:O	8:H:192:GLU:HG2	2.18	0.43
9:J:181:HIS:CG	9:J:201:SER:HG	2.34	0.43
4:6:1:G:H2'	4:6:2:U:C6	2.53	0.43
7:C:105:ILE:HG22	7:C:182:LYS:HB3	2.00	0.43
7:C:187:ARG:NH2	7:C:653:ASP:OD2	2.51	0.43
13:N:71:CYS:SG	13:N:72:GLN:N	2.92	0.43
7:C:423:HIS:CE1	7:C:427:LEU:HD11	2.53	0.43
8:H:98:LEU:O	8:H:101:MET:HG2	2.18	0.43
2:E:-14:A:O2'	2:E:-13:G:O4'	2.25	0.43
25:d:68:GLN:HG3	28:g:69:ILE:HA	2.00	0.43
26:e:45:GLY:HA3	26:e:53:VAL:HG12	2.01	0.43
3:2:43:G:H2'	3:2:44:U:H5'	2.01	0.43
5:5:111:C:H2'	5:5:112:C:C6	2.54	0.43
7:C:151:ASP:CB	7:C:175:LEU:O	2.67	0.43
27:f:26:ARG:HA	27:f:41:THR:HA	2.01	0.43
29:h:16:THR:HB	29:h:96:ILE:HD12	2.00	0.43
6:A:342:LEU:HD22	6:A:392:ASN:ND2	2.34	0.43
6:A:1353:THR:HG23	6:A:1356:LEU:HB3	1.99	0.43
6:A:1999:ILE:HG22	6:A:2000:SER:N	2.34	0.43
7:C:567:ILE:HG22	7:C:571:TYR:CE1	2.53	0.43
7:C:866:ILE:HG22	7:C:868:VAL:HG13	2.00	0.43
9:J:250:LEU:HD11	9:J:262:LEU:HD11	2.00	0.43
17:S:534:TYR:HA	17:S:551:PHE:CB	2.49	0.43
3:2:17:U:O2'	23:y:202:GLN:OE1	2.35	0.43
4:6:78:G:O2'	6:A:611:LYS:HD3	2.19	0.43
5:5:74:U:O2	5:5:78:A:C4	2.72	0.43
5:5:112:C:H1'	6:A:716:ARG:HG3	1.99	0.43
9:J:341:LEU:HD22	10:K:45:PRO:HA	2.01	0.43
17:S:126:ILE:HD12	17:S:136:TRP:CD2	2.53	0.43
3:2:36:A:H2'	3:2:37:G:C8	2.54	0.43
6:A:137:GLU:OE1	11:L:34:GLN:NE2	2.52	0.43
6:A:521:SER:HB2	6:A:682:ASP:HA	2.00	0.43
6:A:905:TYR:HB2	6:A:908:ASP:HB2	2.01	0.43
6:A:1069:LEU:HB3	6:A:1116:TYR:CE2	2.54	0.43
7:C:444:GLN:N	7:C:445:PRO:CD	2.82	0.43
7:C:622:LEU:HD21	7:C:644:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:217:ILE:HG23	15:P:34:HIS:CG	2.54	0.43
13:N:71:CYS:SG	13:N:73:CYS:N	2.80	0.43
21:o:399:CYS:SG	21:o:409:THR:HG22	2.58	0.43
6:A:226:ARG:O	6:A:229:ARG:HB2	2.19	0.43
6:A:845:VAL:HG11	6:A:1321:MET:HE1	2.00	0.43
6:A:1069:LEU:HB3	6:A:1116:TYR:HE2	1.84	0.43
7:C:107:THR:HG21	7:C:479:GLY:HA2	2.01	0.43
7:C:137:GLY:HA2	7:C:213:LEU:HB2	2.01	0.43
8:H:17:ASN:O	8:H:20:MET:HG2	2.19	0.43
9:J:271:GLN:HB3	9:J:314:THR:HG22	2.01	0.43
13:N:214:ILE:O	13:N:244:HIS:NE2	2.43	0.43
21:o:214:PHE:CD1	21:o:221:PHE:HB3	2.54	0.43
21:o:431:GLN:HB2	21:o:445:SER:HB3	2.01	0.43
4:6:72:C:OP2	6:A:732:ARG:NH2	2.52	0.42
5:5:102:C:OP1	6:A:675:HIS:NE2	2.52	0.42
6:A:1087:ASN:HD21	6:A:1098:VAL:CG1	2.32	0.42
6:A:1886:THR:O	6:A:1996:LEU:HD11	2.18	0.42
8:H:351:ILE:HD13	8:H:358:GLN:HA	2.00	0.42
9:J:282:VAL:HG11	9:J:323:VAL:HG21	2.01	0.42
28:g:38:VAL:HG23	28:g:68:ILE:HD11	2.00	0.42
6:A:637:VAL:O	6:A:641:LEU:HB2	2.19	0.42
6:A:1278:VAL:HG23	6:A:1278:VAL:O	2.19	0.42
6:A:1351:VAL:HA	8:H:303:LEU:HD21	2.01	0.42
7:C:602:VAL:HG11	7:C:860:PRO:HG3	2.01	0.42
7:C:825:VAL:HG22	7:C:834:MET:SD	2.59	0.42
8:H:143:LEU:CD1	8:H:151:VAL:HG21	2.49	0.42
8:H:423:LEU:HD23	8:H:427:LEU:HD13	2.01	0.42
13:N:39:LEU:HD13	13:N:40:PRO:HD2	2.01	0.42
4:6:35:A:O2'	11:L:40:LYS:HE2	2.19	0.42
5:5:74:U:O2	5:5:78:A:C2	2.72	0.42
6:A:1033:ASN:HD22	6:A:1288:LEU:HB3	1.85	0.42
6:A:1207:TRP:CZ2	6:A:1268:ARG:HB2	2.55	0.42
6:A:1621:VAL:O	6:A:1622:GLY:C	2.62	0.42
7:C:928:CYS:SG	7:C:929:GLN:N	2.92	0.42
8:H:44:LEU:HD23	8:H:79:LEU:HD21	2.01	0.42
9:J:334:TRP:CD1	9:J:341:LEU:HA	2.54	0.42
10:K:75:GLN:O	10:K:78:VAL:HG12	2.18	0.42
13:N:101:THR:HG22	13:N:120:LEU:HB3	2.01	0.42
6:A:229:ARG:HG2	6:A:695:LEU:HD23	2.01	0.42
6:A:460:PRO:HB3	7:C:376:PHE:HA	2.01	0.42
6:A:1400:ILE:CG2	6:A:1440:ILE:HB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:314:ALA:HB2	7:C:321:THR:HG22	2.01	0.42
7:C:617:LYS:HB3	7:C:666:ILE:HD11	2.01	0.42
8:H:28:ILE:HG12	8:H:43:ASP:HB3	2.02	0.42
9:J:142:VAL:CG1	9:J:157:THR:HB	2.50	0.42
6:A:165:LEU:CD2	6:A:578:MET:HB3	2.49	0.42
6:A:834:ILE:CD1	6:A:845:VAL:HG23	2.50	0.42
6:A:1280:SER:O	6:A:1281:ASN:C	2.62	0.42
6:A:1608:LEU:HG	6:A:1823:LEU:HD21	2.01	0.42
8:H:312:LEU:HD13	8:H:350:MET:HE1	2.02	0.42
2:E:-8:C:H2'	2:E:-7:U:O4'	2.20	0.42
6:A:654:HIS:CE1	6:A:658:ASN:OD1	2.72	0.42
6:A:688:TYR:O	6:A:692:ASN:N	2.53	0.42
6:A:1082:ILE:HG21	6:A:1113:ILE:CD1	2.50	0.42
6:A:1634:LEU:HD21	6:A:1641:LEU:CD1	2.46	0.42
4:6:71:G:N2	4:6:74:U:OP2	2.47	0.42
7:C:178:LEU:HD12	7:C:178:LEU:N	2.35	0.42
7:C:229:LEU:HD22	7:C:235:VAL:HG21	2.02	0.42
9:J:326:ALA:HB2	9:J:356:LEU:HD13	2.01	0.42
10:K:110:HIS:NE2	13:N:20:GLU:O	2.52	0.42
12:M:173:ILE:HG12	12:M:184:VAL:HG13	2.02	0.42
25:d:33:LEU:HD23	25:d:34:VAL:N	2.35	0.42
26:e:77:LEU:HD21	26:e:80:ILE:CD1	2.50	0.42
2:E:-13:G:C2	8:H:316:LYS:HD2	2.55	0.42
6:A:200:THR:OG1	6:A:574:GLN:NE2	2.53	0.42
6:A:556:TYR:CG	10:K:120:ASP:HB3	2.54	0.42
6:A:754:TYR:HA	9:J:183:MET:CE	2.49	0.42
6:A:1369:ASN:O	6:A:1373:LEU:CB	2.67	0.42
6:A:1553:ILE:HG21	6:A:1570:TRP:CE3	2.54	0.42
17:S:140:LEU:HD13	17:S:156:TYR:CZ	2.54	0.42
20:c:299:LEU:C	20:c:299:LEU:HD23	2.44	0.42
4:6:30:G:OP1	11:L:115:ASN:N	2.44	0.42
6:A:139:LEU:HD12	6:A:193:TYR:CD2	2.55	0.42
6:A:168:LEU:HD21	6:A:626:LEU:HD11	2.00	0.42
6:A:719:ILE:N	6:A:720:PRO:HD2	2.34	0.42
6:A:780:ARG:HA	6:A:780:ARG:NE	2.35	0.42
6:A:1887:GLY:O	6:A:1991:ILE:HG22	2.20	0.42
6:A:2078:GLU:O	6:A:2082:ILE:HD12	2.19	0.42
8:H:98:LEU:HA	8:H:101:MET:HE3	2.02	0.42
8:H:462:ILE:HG23	8:H:473:LEU:HD13	2.02	0.42
9:J:250:LEU:CD1	9:J:295:VAL:HG23	2.50	0.42
3:2:20:G:O4'	6:A:780:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:841:GLU:HB2	6:A:844:MET:CB	2.50	0.42
9:J:187:ASP:O	9:J:200:VAL:HG12	2.20	0.42
9:J:327:CYS:SG	9:J:330:ASP:N	2.93	0.42
21:o:210:LYS:HD2	21:o:226:PHE:CZ	2.55	0.42
4:6:52:G:H2'	4:6:53:A:C8	2.55	0.41
4:6:91:A:C2	17:S:99:ILE:HG21	2.55	0.41
6:A:330:LEU:HD12	7:C:920:LEU:HD21	2.01	0.41
6:A:1805:ILE:HG23	6:A:1809:ASN:HB2	2.02	0.41
6:A:1999:ILE:HD11	20:c:338:TYR:CE1	2.54	0.41
7:C:200:CYS:SG	7:C:210:ILE:HD12	2.60	0.41
7:C:870:ALA:N	7:C:871:PRO:HD2	2.35	0.41
8:H:334:LEU:CD1	8:H:380:GLN:HB3	2.48	0.41
9:J:223:HIS:CG	9:J:227:VAL:CG2	3.03	0.41
26:e:77:LEU:HD21	26:e:80:ILE:HD12	2.02	0.41
6:A:165:LEU:HD11	6:A:579:LEU:HD23	2.02	0.41
6:A:207:ARG:HD2	6:A:298:TYR:O	2.19	0.41
6:A:209:ILE:HG23	6:A:301:TRP:CE2	2.55	0.41
6:A:708:TRP:CZ2	6:A:712:LEU:HD11	2.54	0.41
6:A:1442:ARG:HG3	8:H:300:LYS:O	2.20	0.41
6:A:1974:LEU:O	6:A:1978:VAL:HG23	2.20	0.41
9:J:244:ARG:HA	9:J:268:PRO:HB3	2.01	0.41
12:M:156:ILE:HG21	12:M:175:TYR:CE1	2.54	0.41
2:E:-9:U:O4'	16:R:19:HIS:HB2	2.20	0.41
2:E:-5:G:OP2	6:A:1377:SER:O	2.38	0.41
6:A:2075:THR:O	6:A:2079:ILE:HG12	2.20	0.41
8:H:42:ARG:O	8:H:45:PHE:HB3	2.20	0.41
9:J:111:ILE:HG22	17:S:194:MET:O	2.19	0.41
4:6:57:U:H2'	4:6:58:C:O4'	2.20	0.41
6:A:714:PHE:CE1	6:A:718:THR:HG21	2.56	0.41
6:A:886:MET:HE3	6:A:1120:VAL:HG22	2.01	0.41
6:A:1468:ALA:O	6:A:1472:ASN:N	2.53	0.41
7:C:152:LEU:HD21	7:C:319:GLY:CA	2.50	0.41
8:H:373:ILE:HD11	8:H:419:PHE:CD2	2.55	0.41
9:J:213:LYS:HZ2	9:J:215:GLN:HG3	1.85	0.41
14:O:39:LEU:HD11	14:O:155:ALA:CB	2.50	0.41
16:R:16:THR:OG1	16:R:17:SER:N	2.53	0.41
21:o:213:ARG:NH1	21:o:299:LEU:O	2.53	0.41
5:5:169:U:O2	28:g:66:ASN:N	2.53	0.41
6:A:766:ILE:CG2	6:A:782:ILE:HD13	2.50	0.41
6:A:818:SER:HB3	9:J:141:TRP:CZ2	2.55	0.41
6:A:1107:LEU:HD23	6:A:1109:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1879:ILE:HD11	6:A:1894:ILE:HD11	2.02	0.41
7:C:95:THR:HG21	15:P:40:ARG:NH2	2.35	0.41
9:J:311:VAL:HA	9:J:326:ALA:O	2.20	0.41
9:J:358:ILE:HG22	9:J:359:ASN:O	2.20	0.41
13:N:84:ILE:O	13:N:87:ARG:HG3	2.20	0.41
17:S:47:GLN:HG2	17:S:51:ARG:HE	1.85	0.41
17:S:140:LEU:CD2	17:S:152:VAL:HG23	2.51	0.41
17:S:185:VAL:HG22	17:S:189:TYR:CE2	2.55	0.41
26:e:13:PRO:HG2	28:g:37:ASN:HB2	2.03	0.41
6:A:1609:TRP:HE3	6:A:1823:LEU:HD13	1.85	0.41
8:H:49:ILE:CG2	8:H:56:ILE:HG21	2.51	0.41
8:H:50:LEU:HB2	8:H:251:LEU:HD22	2.02	0.41
29:h:17:ILE:O	29:h:24:THR:HA	2.20	0.41
3:2:15:C:HO2'	3:2:18:U:H3	1.68	0.41
5:5:167:A:N6	30:j:63:ARG:O	2.54	0.41
6:A:583:ILE:HD11	6:A:619:PHE:CZ	2.55	0.41
10:K:112:ILE:HD11	13:N:23:ILE:HB	2.02	0.41
14:O:219:TYR:O	14:O:221:GLN:N	2.54	0.41
17:S:367:TRP:O	17:S:371:ILE:N	2.44	0.41
26:e:91:THR:HG21	28:g:58:GLY:HA3	2.03	0.41
4:6:31:G:N1	13:N:53:ASN:O	2.54	0.41
6:A:1935:VAL:O	6:A:1959:THR:HG22	2.21	0.41
7:C:212:PHE:O	7:C:213:LEU:HD23	2.20	0.41
14:O:163:GLN:HB3	14:O:167:ALA:HB3	2.02	0.41
21:o:177:LEU:HD21	21:o:189:ILE:CG2	2.50	0.41
21:o:285:LEU:HD13	21:o:288:THR:HG23	2.02	0.41
28:g:10:TYR:HE1	28:g:73:ALA:HB2	1.86	0.41
5:5:130:A:H2'	5:5:131:A:C8	2.56	0.41
6:A:305:LEU:HD21	6:A:476:ALA:HB2	2.02	0.41
6:A:762:VAL:HG22	6:A:815:TYR:CG	2.56	0.41
6:A:1857:VAL:HG22	6:A:1878:CYS:O	2.21	0.41
7:C:133:ILE:HD13	7:C:560:GLN:HB3	2.01	0.41
7:C:139:ILE:CD1	7:C:225:THR:HG23	2.40	0.41
7:C:677:PHE:CD1	7:C:857:LEU:HD11	2.56	0.41
17:S:81:MET:HE3	17:S:112:VAL:HG21	2.02	0.41
17:S:185:VAL:HG22	17:S:189:TYR:CZ	2.56	0.41
17:S:199:MET:SD	17:S:246:LEU:HD22	2.60	0.41
26:e:91:THR:O	26:e:91:THR:HG23	2.20	0.41
3:2:5:A:C5'	23:y:114:THR:HG22	2.51	0.41
6:A:218:SER:CB	6:A:315:SER:HA	2.51	0.41
6:A:695:LEU:HD13	6:A:696:GLY:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1066:LEU:HD21	6:A:1113:ILE:HG21	2.03	0.41
6:A:1632:ILE:HD11	6:A:1649:PHE:CD2	2.56	0.41
7:C:117:ARG:NH1	7:C:156:ASP:O	2.54	0.41
8:H:65:LEU:HD12	8:H:117:ILE:HD11	2.03	0.41
8:H:391:LEU:HD23	8:H:391:LEU:HA	1.95	0.41
9:J:146:ALA:HB3	9:J:188:VAL:HG23	2.03	0.41
2:E:-5:G:O3'	6:A:667:TYR:HE1	2.04	0.40
4:6:42:A:H2'	4:6:43:C:O4'	2.21	0.40
4:6:69:C:C2	4:6:78:G:N2	2.89	0.40
5:5:93:G:H4'	16:R:13:GLY:HA2	2.03	0.40
6:A:179:MET:HE1	6:A:653:ILE:HG21	2.03	0.40
6:A:506:PHE:CD2	6:A:525:LEU:HD13	2.56	0.40
6:A:1654:TRP:CZ3	6:A:1779:LEU:HD12	2.55	0.40
6:A:1995:TRP:CD1	6:A:1995:TRP:N	2.89	0.40
7:C:126:MET:SD	7:C:132:ARG:HG2	2.60	0.40
7:C:320:PHE:HB2	7:C:429:PHE:HD2	1.86	0.40
7:C:502:LEU:HD21	7:C:510:ARG:HH21	1.85	0.40
7:C:813:ILE:HD13	7:C:818:TYR:OH	2.21	0.40
8:H:151:VAL:O	8:H:154:VAL:HG12	2.21	0.40
8:H:333:SER:HA	8:H:343:TYR:CE2	2.55	0.40
8:H:474:THR:HA	8:H:477:MET:HG2	2.03	0.40
10:K:170:SER:O	10:K:185:ARG:NH2	2.48	0.40
12:M:73:CYS:O	12:M:76:PHE:HB3	2.21	0.40
18:T:495:GLU:CB	18:T:503:ARG:CB	2.98	0.40
6:A:593:LEU:HD23	6:A:593:LEU:HA	1.94	0.40
6:A:1028:TRP:HA	6:A:1145:MET:HE1	2.03	0.40
6:A:1230:ILE:HD13	6:A:1230:ILE:HA	1.85	0.40
6:A:1379:MET:HE1	6:A:1619:VAL:HG23	2.03	0.40
6:A:1967:ALA:HB2	6:A:2016:LYS:HA	2.03	0.40
21:o:309:ILE:HG21	21:o:351:PHE:CZ	2.56	0.40
21:o:319:ILE:HD12	21:o:368:LYS:O	2.20	0.40
5:5:103:A:O2'	5:5:104:G:H5''	2.20	0.40
6:A:507:LEU:HD21	6:A:529:TYR:CD2	2.55	0.40
6:A:1028:TRP:CG	6:A:1262:MET:HE1	2.56	0.40
6:A:1632:ILE:HG21	6:A:1645:LEU:CD1	2.50	0.40
6:A:1879:ILE:HD12	6:A:1892:LYS:HB3	2.02	0.40
9:J:198:PHE:HZ	9:J:253:MET:HE3	1.87	0.40
9:J:200:VAL:HG21	9:J:227:VAL:HG12	2.03	0.40
10:K:146:VAL:N	17:S:128:THR:O	2.52	0.40
14:O:91:MET:HA	14:O:91:MET:HE2	2.03	0.40
21:o:213:ARG:NH2	21:o:339:MET:HE1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:o:250:PRO:HA	21:o:267:LEU:HA	2.04	0.40
21:o:338:SER:HB2	21:o:356:MET:HE1	2.03	0.40
27:f:45:THR:HG22	27:f:51:LEU:HD23	2.04	0.40
2:E:-5:G:C4	6:A:671:TYR:CE1	3.10	0.40
6:A:781:THR:O	6:A:785:HIS:HB2	2.22	0.40
6:A:1553:ILE:HG21	6:A:1570:TRP:CZ3	2.57	0.40
6:A:1557:LEU:HA	6:A:1560:THR:HG23	2.03	0.40
7:C:331:TYR:OH	7:C:428:ILE:O	2.33	0.40
7:C:602:VAL:HG21	7:C:932:PHE:CE2	2.56	0.40
4:6:85:C:O2	14:O:167:ALA:HA	2.22	0.40
5:5:45:A:N6	5:5:74:U:N3	2.56	0.40
5:5:104:G:OP2	6:A:531:LEU:HD11	2.22	0.40
6:A:239:PHE:HE1	6:A:635:THR:HG22	1.87	0.40
6:A:377:VAL:HG11	7:C:912:ALA:CB	2.48	0.40
6:A:1369:ASN:O	6:A:1373:LEU:N	2.41	0.40
7:C:285:TYR:HB2	7:C:374:VAL:HG22	2.04	0.40
9:J:150:VAL:HG11	15:P:40:ARG:NH2	2.37	0.40
19:a:124:TRP:HA	19:a:239:PHE:CZ	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	A	1906/2413 (79%)	1733 (91%)	161 (8%)	12 (1%)	21	55
7	C	864/1008 (86%)	771 (89%)	87 (10%)	6 (1%)	18	53
8	H	393/577 (68%)	353 (90%)	36 (9%)	4 (1%)	12	45
9	J	340/451 (75%)	295 (87%)	39 (12%)	6 (2%)	6	34
10	K	183/379 (48%)	163 (89%)	17 (9%)	3 (2%)	7	36
11	L	153/157 (98%)	136 (89%)	16 (10%)	1 (1%)	18	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	250/339 (74%)	236 (94%)	12 (5%)	2 (1%)	16	50
13	N	217/364 (60%)	191 (88%)	22 (10%)	4 (2%)	6	34
14	O	207/590 (35%)	193 (93%)	11 (5%)	3 (1%)	9	38
15	P	63/175 (36%)	56 (89%)	7 (11%)	0	100	100
16	R	104/135 (77%)	91 (88%)	12 (12%)	1 (1%)	12	45
17	S	438/687 (64%)	415 (95%)	20 (5%)	3 (1%)	18	53
18	T	294/877 (34%)	279 (95%)	12 (4%)	3 (1%)	12	45
19	a	131/251 (52%)	123 (94%)	8 (6%)	0	100	100
20	c	97/382 (25%)	87 (90%)	8 (8%)	2 (2%)	5	32
21	o	305/455 (67%)	251 (82%)	46 (15%)	8 (3%)	4	28
23	y	77/215 (36%)	76 (99%)	1 (1%)	0	100	100
24	b	76/196 (39%)	74 (97%)	2 (3%)	0	100	100
25	d	80/101 (79%)	73 (91%)	7 (9%)	0	100	100
26	e	71/94 (76%)	62 (87%)	9 (13%)	0	100	100
27	f	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
28	g	65/77 (84%)	63 (97%)	2 (3%)	0	100	100
29	h	78/146 (53%)	71 (91%)	7 (9%)	0	100	100
30	j	92/110 (84%)	83 (90%)	9 (10%)	0	100	100
All	All	6554/10265 (64%)	5936 (91%)	560 (8%)	58 (1%)	16	47

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	487	ASN
6	A	742	VAL
6	A	1620	TYR
7	C	568	SER
7	C	901	GLU
8	H	414	PRO
10	K	108	ASN
10	K	188	LYS
17	S	238	TRP
18	T	478	TYR
20	c	226	ASP
21	o	173	LYS
21	o	418	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	A	2069	VAL
7	C	927	MET
9	J	226	GLY
9	J	287	ASP
9	J	400	ARG
10	K	193	GLU
12	M	84	GLY
12	M	122	GLU
14	O	204	LYS
14	O	220	GLU
20	c	172	ASP
21	o	164	GLY
21	o	181	GLY
21	o	381	SER
6	A	511	ASP
6	A	1622	GLY
8	H	109	LYS
9	J	162	THR
13	N	16	CYS
13	N	249	GLY
16	R	14	SER
6	A	418	ASP
7	C	159	LYS
8	H	67	LYS
9	J	277	VAL
13	N	38	THR
14	O	92	ALA
18	T	615	PHE
21	o	306	SER
6	A	322	VAL
6	A	1093	LYS
6	A	1405	ILE
9	J	318	PRO
17	S	235	LEU
8	H	353	PHE
18	T	660	ILE
21	o	297	LEU
21	o	448	ALA
6	A	1984	PRO
6	A	665	GLY
11	L	152	GLY
13	N	121	GLY

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Mol	Chain	Res	Type
17	S	237	ILE
7	C	301	GLY
7	C	987	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	A	1577/2182 (72%)	1551 (98%)	26 (2%)	55	69
7	C	681/910 (75%)	664 (98%)	17 (2%)	42	62
8	H	366/538 (68%)	356 (97%)	10 (3%)	39	60
9	J	299/397 (75%)	280 (94%)	19 (6%)	16	42
10	K	159/328 (48%)	153 (96%)	6 (4%)	29	53
11	L	112/141 (79%)	106 (95%)	6 (5%)	20	46
12	M	214/296 (72%)	209 (98%)	5 (2%)	44	64
13	N	211/332 (64%)	207 (98%)	4 (2%)	50	66
14	O	187/525 (36%)	180 (96%)	7 (4%)	30	54
15	P	56/151 (37%)	53 (95%)	3 (5%)	20	46
16	R	25/121 (21%)	24 (96%)	1 (4%)	28	52
17	S	230/633 (36%)	223 (97%)	7 (3%)	36	57
18	T	1/786 (0%)	1 (100%)	0	100	100
19	a	125/225 (56%)	124 (99%)	1 (1%)	73	77
20	c	71/346 (20%)	70 (99%)	1 (1%)	59	70
21	o	256/413 (62%)	247 (96%)	9 (4%)	32	55
23	y	76/193 (39%)	74 (97%)	2 (3%)	40	61
24	b	70/176 (40%)	70 (100%)	0	100	100
25	d	69/89 (78%)	69 (100%)	0	100	100
26	e	65/83 (78%)	63 (97%)	2 (3%)	35	57
27	f	63/77 (82%)	63 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	g	58/66 (88%)	57 (98%)	1 (2%)	53	68
29	h	77/129 (60%)	76 (99%)	1 (1%)	61	71
30	j	79/103 (77%)	79 (100%)	0	100	100
All	All	5127/9240 (56%)	4999 (98%)	128 (2%)	42	62

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A	196	SER
6	A	235	LYS
6	A	326	ASN
6	A	527	LYS
6	A	537	THR
6	A	588	LEU
6	A	632	ILE
6	A	719	ILE
6	A	726	ILE
6	A	756	LEU
6	A	760	ASN
6	A	811	ILE
6	A	1094	ASP
6	A	1165	LEU
6	A	1212	ARG
6	A	1319	ILE
6	A	1337	THR
6	A	1361	VAL
6	A	1560	THR
6	A	1650	ARG
6	A	1663	PHE
6	A	1757	LEU
6	A	1940	MET
6	A	1951	PHE
6	A	1997	ASP
6	A	2082	ILE
7	C	153	LEU
7	C	219	VAL
7	C	223	ASP
7	C	400	LEU
7	C	430	ARG
7	C	477	ASP
7	C	537	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	C	545	LEU
7	C	590	LYS
7	C	602	VAL
7	C	658	ASP
7	C	774	LEU
7	C	784	SER
7	C	795	ILE
7	C	803	VAL
7	C	830	ASN
7	C	928	CYS
8	H	84	ASN
8	H	130	ILE
8	H	186	LEU
8	H	193	SER
8	H	297	LEU
8	H	315	LEU
8	H	317	ILE
8	H	357	TRP
8	H	419	PHE
8	H	421	LYS
9	J	110	LEU
9	J	139	LEU
9	J	156	ILE
9	J	162	THR
9	J	188	VAL
9	J	216	ILE
9	J	238	LEU
9	J	248	ILE
9	J	260	ILE
9	J	261	THR
9	J	274	CYS
9	J	286	THR
9	J	290	VAL
9	J	303	VAL
9	J	323	VAL
9	J	343	THR
9	J	386	SER
9	J	443	ASN
9	J	446	LEU
10	K	37	ASN
10	K	62	GLU
10	K	179	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	K	190	LEU
10	K	195	ASN
10	K	202	MET
11	L	30	LEU
11	L	52	ILE
11	L	55	LEU
11	L	142	PHE
11	L	153	CYS
11	L	155	SER
12	M	13	VAL
12	M	31	ASN
12	M	102	LEU
12	M	187	LYS
12	M	242	LEU
13	N	22	ASN
13	N	39	LEU
13	N	106	ASN
13	N	288	ILE
14	O	36	VAL
14	O	44	THR
14	O	50	LEU
14	O	53	ASN
14	O	56	LEU
14	O	98	CYS
14	O	160	LEU
15	P	9	LEU
15	P	30	LEU
15	P	172	LYS
16	R	17	SER
17	S	65	MET
17	S	124	ARG
17	S	128	THR
17	S	143	GLU
17	S	156	TYR
17	S	232	LEU
17	S	237	ILE
19	a	163	LEU
20	c	297	LEU
21	o	156	ARG
21	o	166	THR
21	o	177	LEU
21	o	216	GLU

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Mol	Chain	Res	Type
21	o	330	GLN
21	o	331	ILE
21	o	356	MET
21	o	418	LEU
21	o	451	ILE
23	y	162	ASN
23	y	168	LEU
26	e	25	THR
26	e	92	SER
28	g	66	ASN
29	h	16	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
6	A	155	ASN
6	A	310	ASN
6	A	326	ASN
6	A	344	ASN
6	A	508	GLN
6	A	509	HIS
6	A	542	HIS
6	A	617	ASN
6	A	636	HIS
6	A	643	ASN
6	A	760	ASN
6	A	828	HIS
6	A	830	ASN
6	A	848	ASN
6	A	976	GLN
6	A	1115	GLN
6	A	1140	ASN
6	A	1190	ASN
6	A	1472	ASN
6	A	1522	ASN
6	A	1532	HIS
6	A	1626	GLN
6	A	1856	ASN
6	A	1888	HIS
7	C	143	HIS
7	C	167	ASN
7	C	194	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	C	289	ASN
7	C	290	HIS
7	C	358	ASN
7	C	431	GLN
7	C	554	HIS
7	C	647	ASN
7	C	683	ASN
7	C	764	ASN
7	C	776	ASN
8	H	46	GLN
8	H	170	HIS
8	H	184	GLN
8	H	320	ASN
8	H	358	GLN
8	H	367	GLN
8	H	380	GLN
9	J	113	ASN
9	J	136	ASN
9	J	271	GLN
9	J	273	GLN
9	J	354	ASN
9	J	360	GLN
10	K	50	ASN
10	K	84	ASN
10	K	86	ASN
10	K	108	ASN
10	K	192	ASN
11	L	116	ASN
12	M	31	ASN
12	M	235	GLN
13	N	254	GLN
14	O	15	ASN
14	O	32	GLN
14	O	83	GLN
15	P	27	HIS
17	S	47	GLN
17	S	79	HIS
17	S	147	ASN
17	S	198	GLN
17	S	236	GLN
17	S	248	ASN
17	S	257	GLN

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Mol	Chain	Res	Type
19	a	177	ASN
21	o	183	ASN
21	o	259	ASN
21	o	261	HIS
21	o	287	GLN
21	o	330	GLN
21	o	337	HIS
21	o	413	ASN
23	y	99	GLN
23	y	185	ASN
24	b	40	HIS
26	e	34	GLN
26	e	86	ASN
27	f	54	ASN
27	f	65	HIS
28	g	66	ASN
29	h	86	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	32/95 (33%)	14 (43%)	4 (12%)
2	E	15/20 (75%)	5 (33%)	1 (6%)
3	2	48/1175 (4%)	19 (39%)	2 (4%)
4	6	98/112 (87%)	37 (37%)	3 (3%)
5	5	138/179 (77%)	61 (44%)	3 (2%)
All	All	331/1581 (20%)	136 (41%)	13 (3%)

All (136) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	2	U
1	I	3	A
1	I	4	U
1	I	10	A
1	I	11	A
1	I	13	U
1	I	14	U
1	I	15	A
1	I	16	U
1	I	61	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	70	A
1	I	71	C
1	I	72	A
1	I	73	A
2	E	-11	G
2	E	-10	A
2	E	-8	C
2	E	-4	A
2	E	-1	G
3	2	15	C
3	2	16	U
3	2	17	U
3	2	18	U
3	2	19	U
3	2	20	G
3	2	21	G
3	2	23	U
3	2	25	A
3	2	26	G
3	2	27	A
3	2	29	C
3	2	30	A
3	2	32	G
3	2	33	U
3	2	34	G
3	2	35	U
3	2	41	C
3	2	44	U
4	6	8	A
4	6	10	G
4	6	17	U
4	6	19	C
4	6	20	G
4	6	21	U
4	6	27	U
4	6	28	U
4	6	29	U
4	6	34	A
4	6	35	A
4	6	36	U
4	6	37	U
4	6	40	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	6	41	A
4	6	43	C
4	6	46	U
4	6	49	A
4	6	50	G
4	6	51	A
4	6	52	G
4	6	54	U
4	6	55	G
4	6	59	A
4	6	68	C
4	6	72	C
4	6	73	A
4	6	74	U
4	6	75	A
4	6	80	U
4	6	84	C
4	6	85	C
4	6	88	U
4	6	90	U
4	6	91	A
4	6	92	C
4	6	93	A
5	5	10	U
5	5	14	G
5	5	15	A
5	5	16	U
5	5	17	C
5	5	20	U
5	5	24	G
5	5	25	G
5	5	26	A
5	5	27	G
5	5	28	G
5	5	31	G
5	5	33	U
5	5	34	C
5	5	40	C
5	5	41	A
5	5	42	A
5	5	43	G
5	5	44	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	5	45	A
5	5	46	C
5	5	52	G
5	5	63	C
5	5	64	C
5	5	67	U
5	5	68	A
5	5	69	G
5	5	70	A
5	5	71	A
5	5	75	A
5	5	76	U
5	5	77	A
5	5	78	A
5	5	80	G
5	5	81	A
5	5	82	A
5	5	89	U
5	5	92	U
5	5	95	C
5	5	97	U
5	5	101	C
5	5	108	C
5	5	109	A
5	5	113	G
5	5	116	U
5	5	121	U
5	5	126	A
5	5	129	G
5	5	130	A
5	5	131	A
5	5	133	C
5	5	134	A
5	5	135	G
5	5	136	G
5	5	140	A
5	5	142	C
5	5	145	U
5	5	169	U
5	5	170	U
5	5	171	U
5	5	172	U

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	9	A
1	I	12	G
1	I	13	U
1	I	70	A
2	E	-7	U
3	2	15	C
3	2	17	U
4	6	16	C
4	6	45	A
4	6	92	C
5	5	27	G
5	5	39	U
5	5	45	A

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

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

#### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 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	$\# Z  > 2$
34	GTP	C	1101	-	33,34,34	1.10	4 (12%)	50,54,54	1.79	8 (16%)
33	IHP	A	3001	-	36,36,36	0.71	0	60,60,60	1.07	4 (6%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	GTP	C	1101	-	-	7/22/38/38	0/3/3/3
33	IHP	A	3001	-	-	0/30/54/54	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	1101	GTP	C5-C4	2.87	1.46	1.38
34	C	1101	GTP	C5-N7	-2.61	1.33	1.39
34	C	1101	GTP	C6-N1	-2.16	1.34	1.38
34	C	1101	GTP	C4-N9	-2.15	1.32	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	1101	GTP	C5-C4-N3	-5.53	119.59	128.39
34	C	1101	GTP	C2-N3-C4	4.96	120.84	112.30
34	C	1101	GTP	N9-C4-N3	3.88	133.71	125.95
34	C	1101	GTP	C6-C5-N7	3.50	136.66	130.29
33	A	3001	IHP	C3-C2-C1	2.83	116.63	110.43
34	C	1101	GTP	O6-C6-C5	-2.67	119.49	126.53
34	C	1101	GTP	C4-C5-N7	-2.41	106.85	110.67
34	C	1101	GTP	O2B-PB-O1B	2.35	123.36	112.44
34	C	1101	GTP	C5-C6-N1	2.25	118.99	113.25
33	A	3001	IHP	C6-C1-C2	2.10	115.03	110.43
33	A	3001	IHP	O46-P6-O36	2.03	115.42	107.80
33	A	3001	IHP	O42-P2-O32	2.02	115.39	107.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

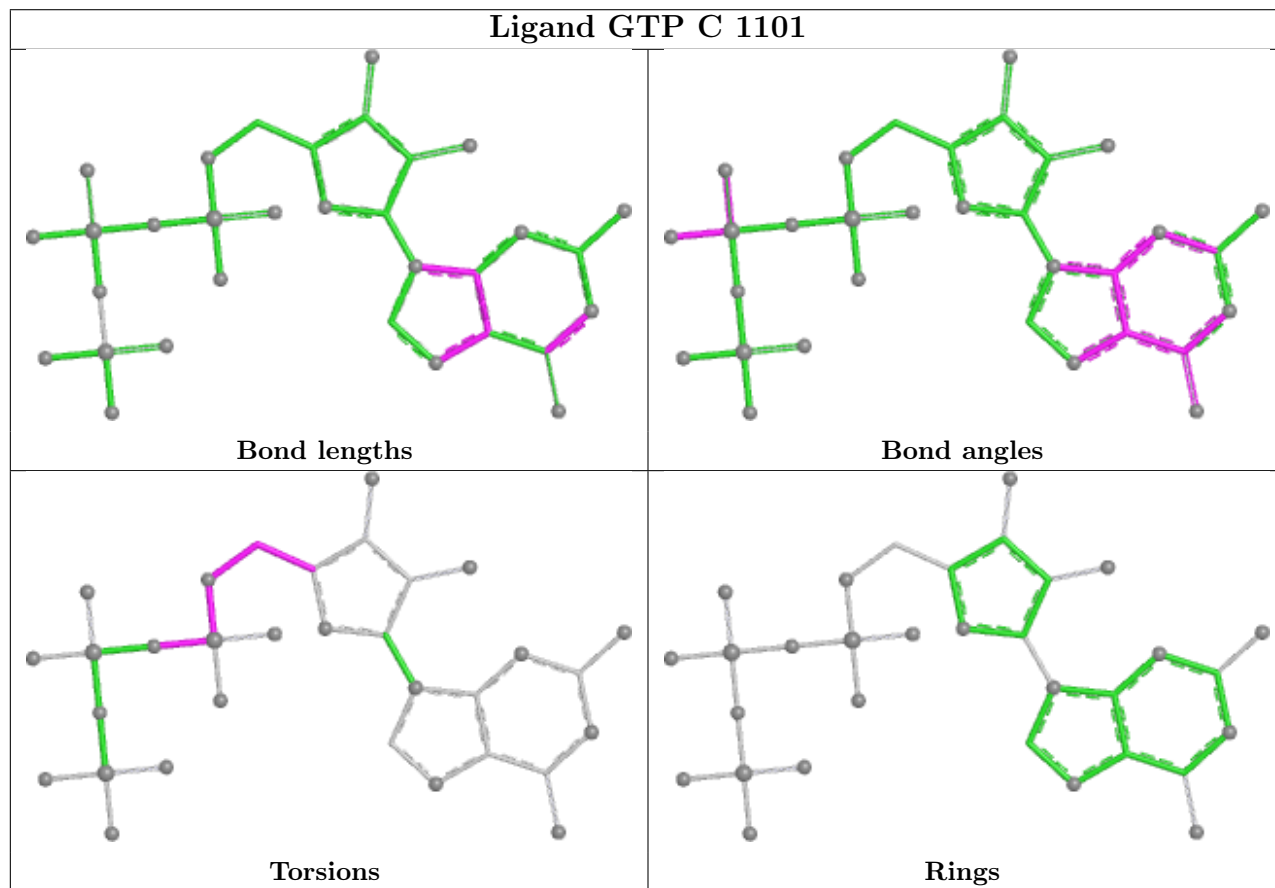
Mol	Chain	Res	Type	Atoms
34	C	1101	GTP	C5'-O5'-PA-O1A
34	C	1101	GTP	O4'-C4'-C5'-O5'
34	C	1101	GTP	C3'-C4'-C5'-O5'
34	C	1101	GTP	C4'-C5'-O5'-PA
34	C	1101	GTP	PB-O3A-PA-O2A
34	C	1101	GTP	C5'-O5'-PA-O3A
34	C	1101	GTP	PB-O3A-PA-O1A

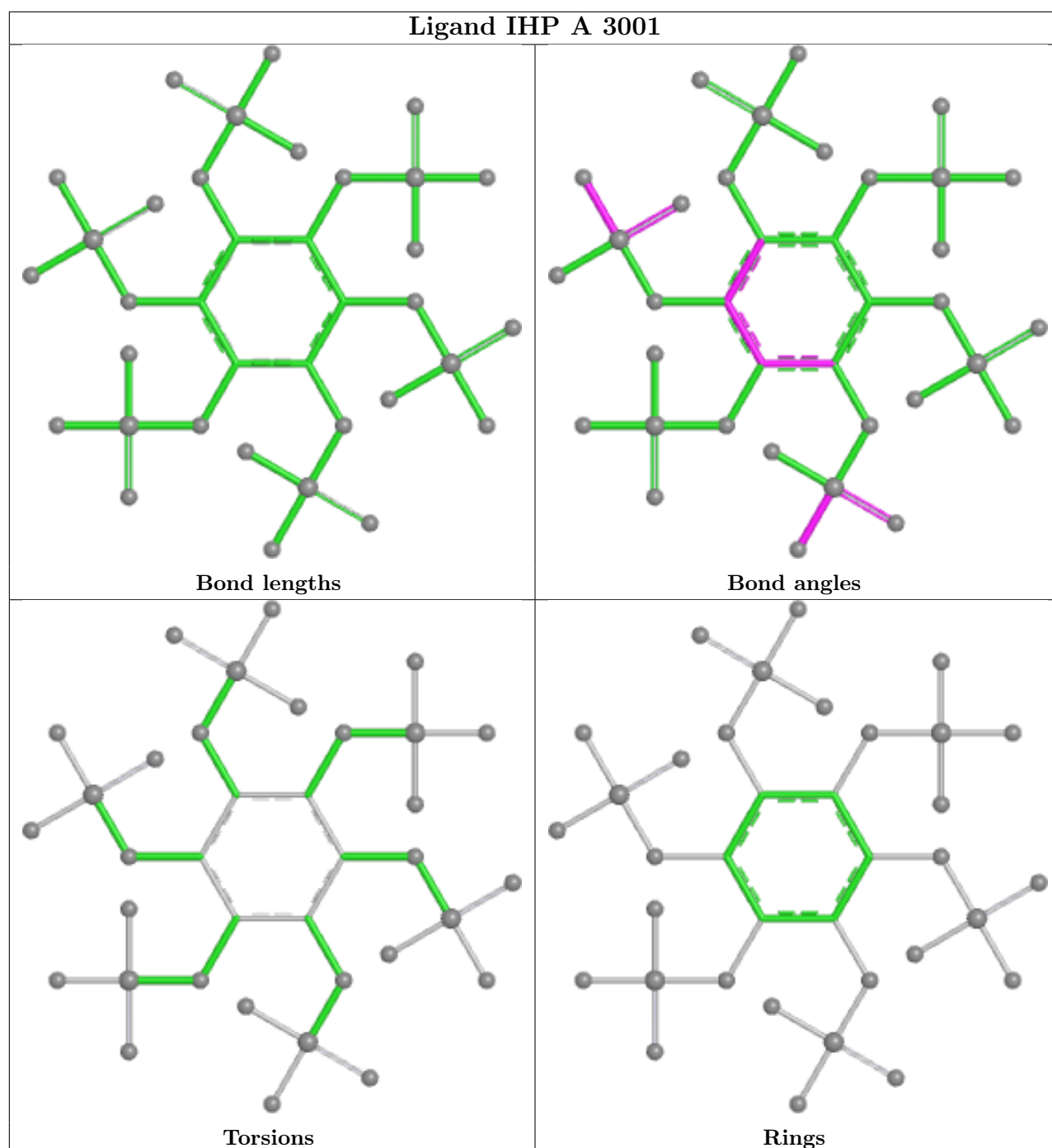
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	3001	IHP	1	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	o	1
22	X	1
7	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	423:LYS	C	428:PRO	N	10.32
1	X	27:UNK	C	86:UNK	N	8.48
1	C	770:VAL	C	774:LEU	N	6.52

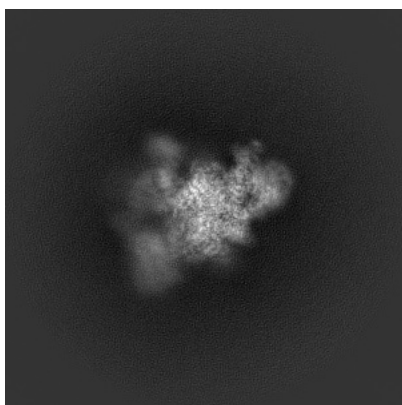
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3539. These allow visual inspection of the internal detail of the map and identification of artifacts.

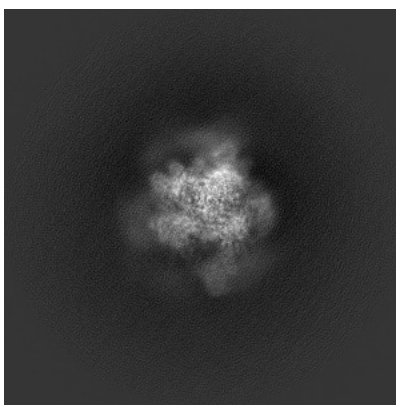
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

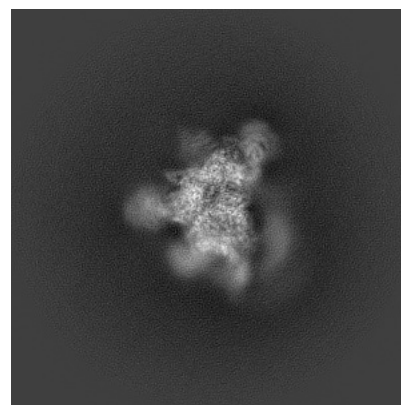
#### 6.1.1 Primary map



X



Y

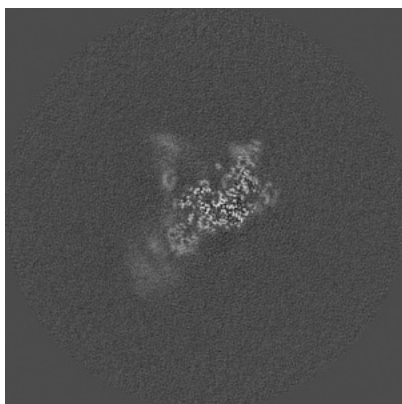


Z

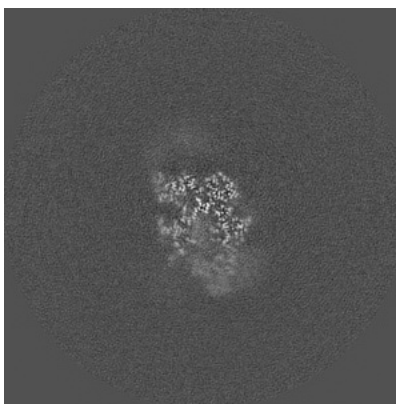
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

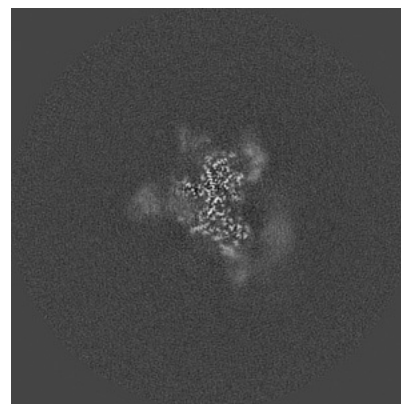
#### 6.2.1 Primary map



X Index: 206



Y Index: 206

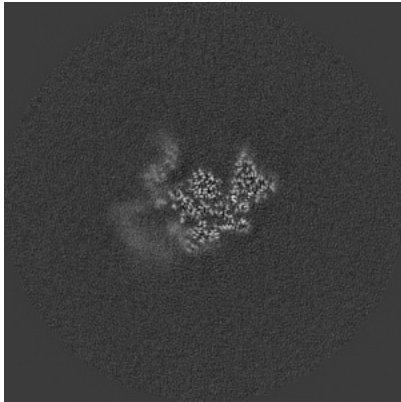


Z Index: 206

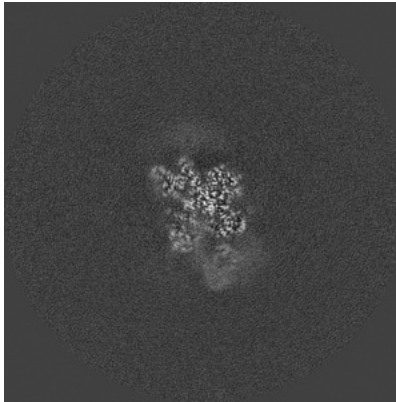
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

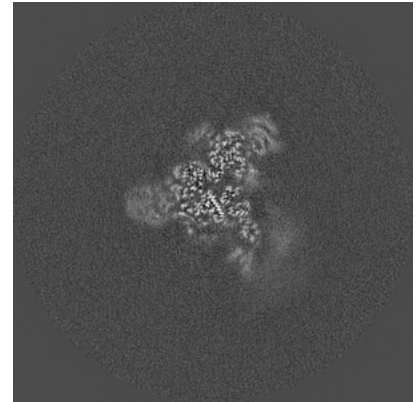
### 6.3.1 Primary map



X Index: 225



Y Index: 201

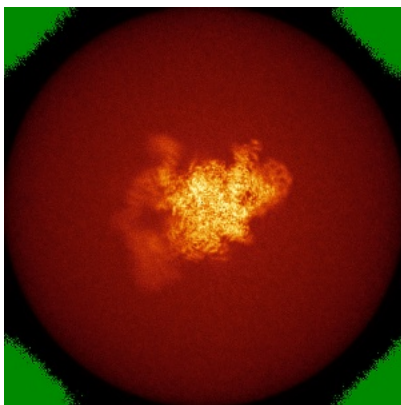


Z Index: 224

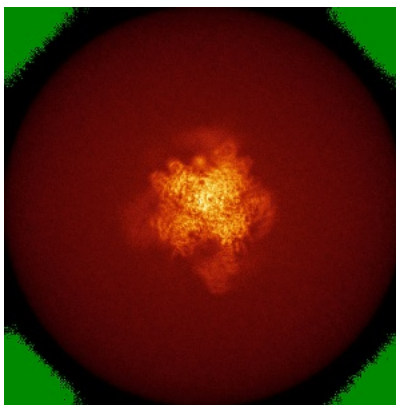
The images above show the largest variance slices of the map in three orthogonal directions.

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

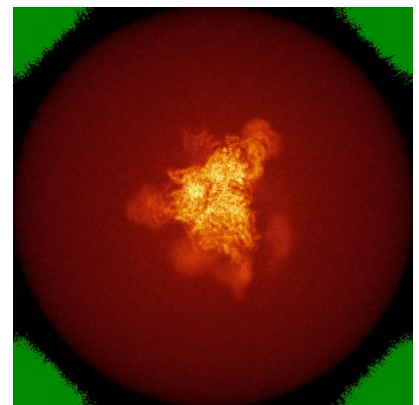
### 6.4.1 Primary map



X



Y

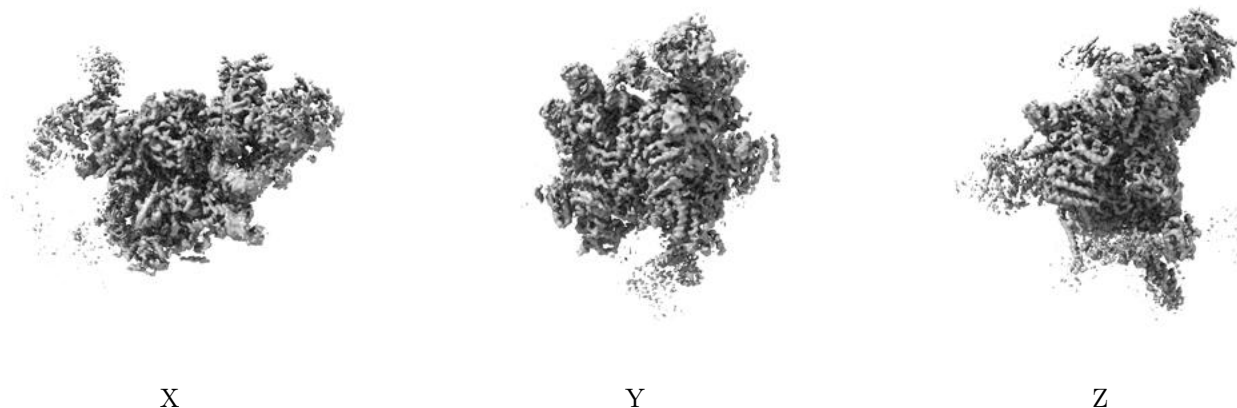


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

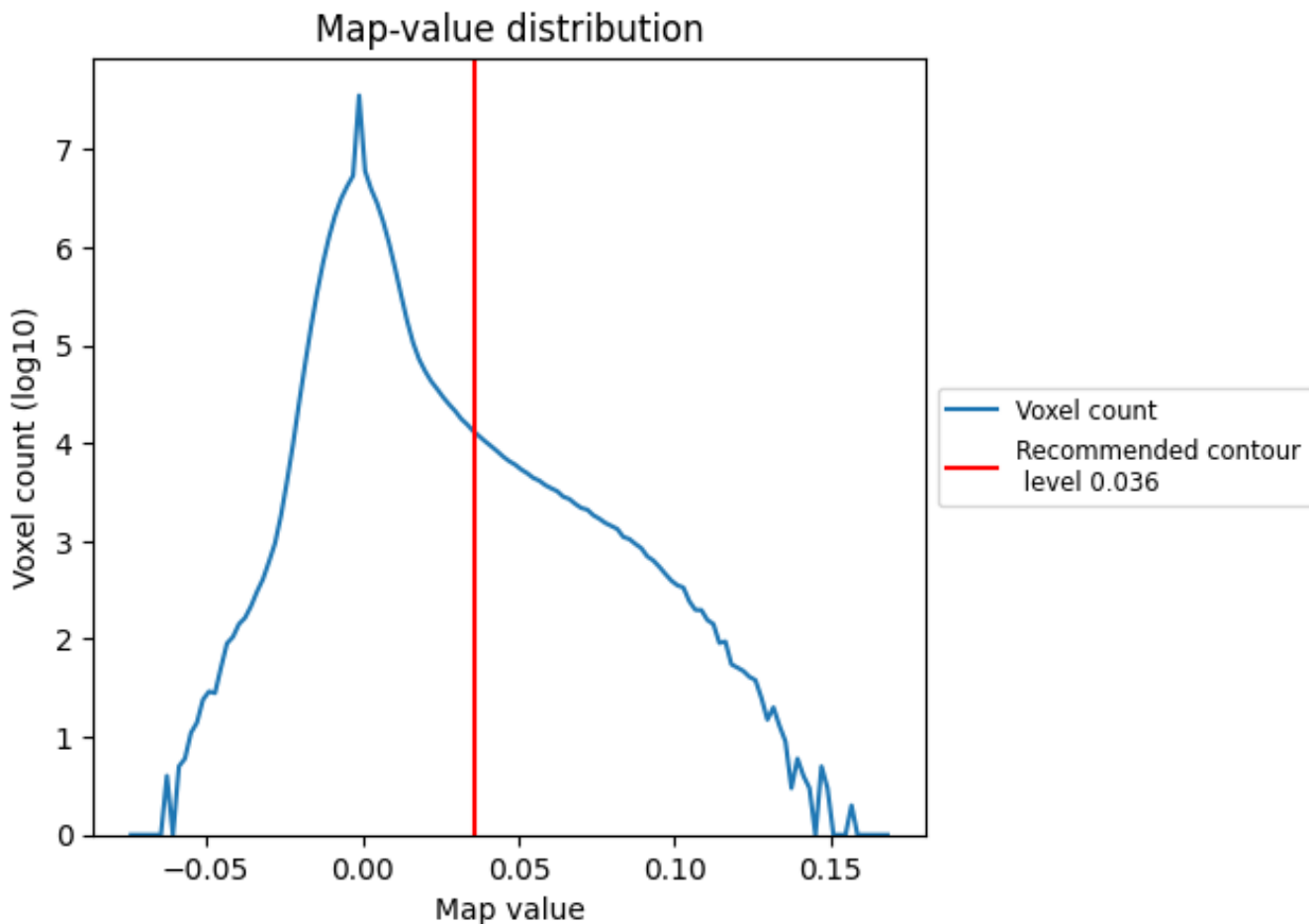
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

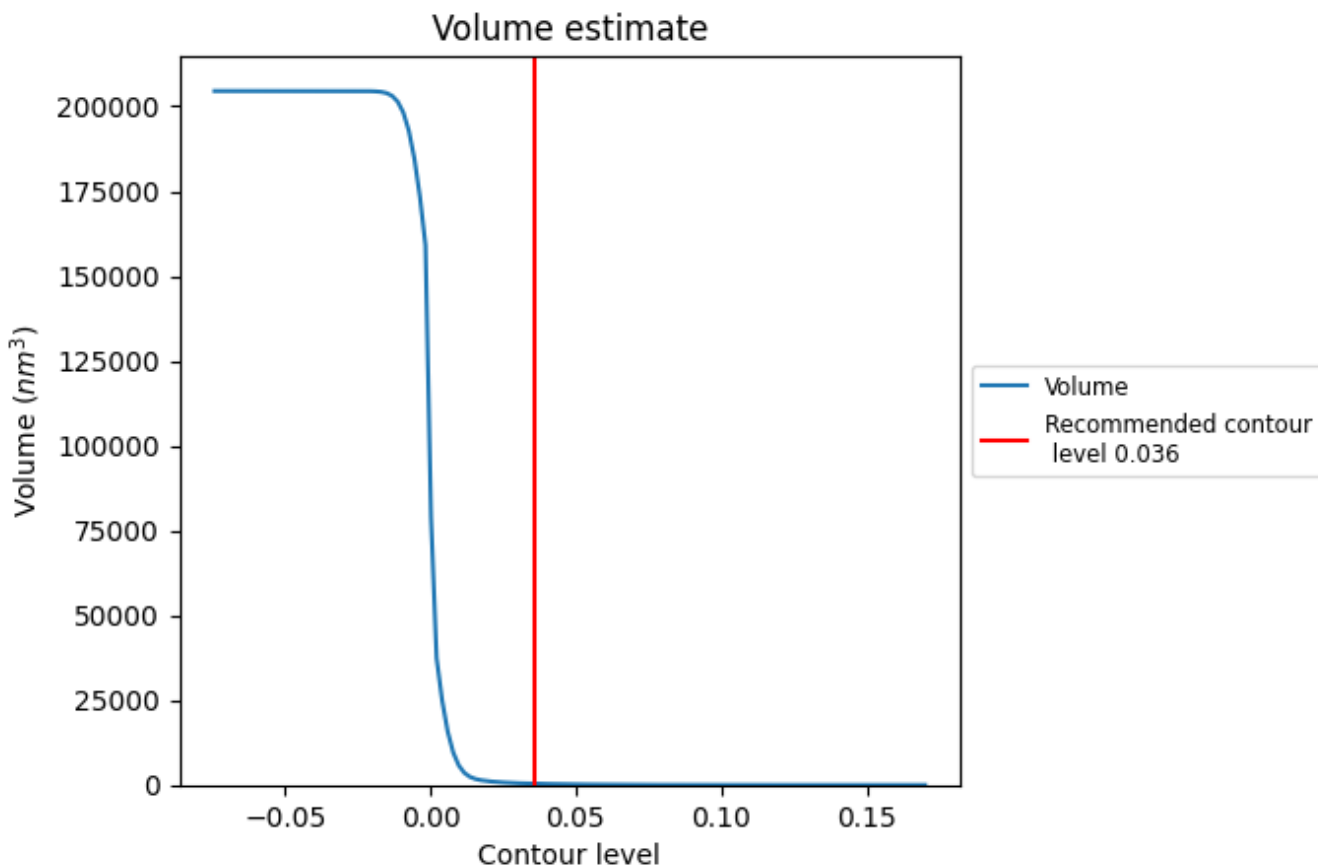
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

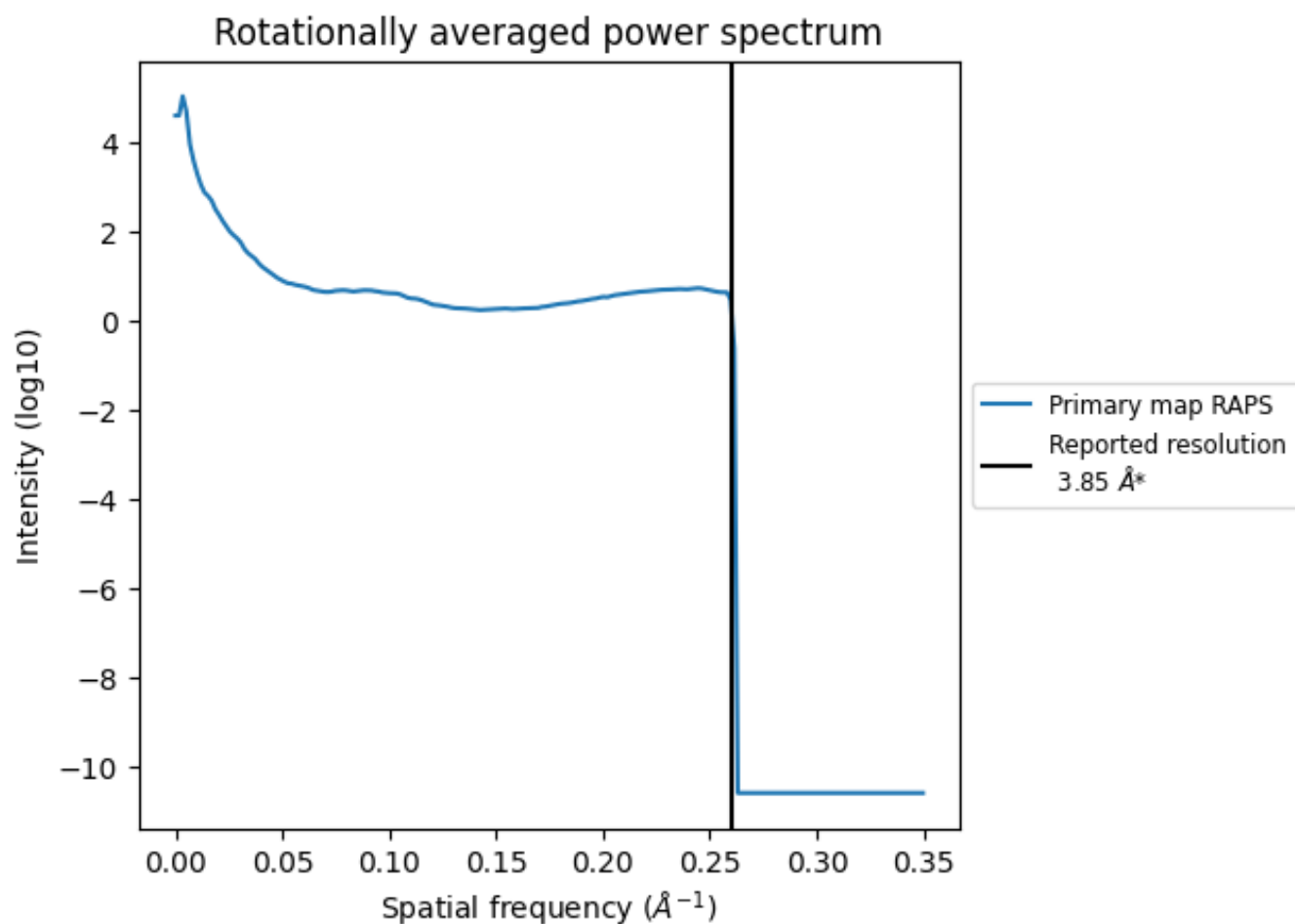
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 372  $\text{nm}^3$ ; this corresponds to an approximate mass of 336 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 [\(i\)](#)

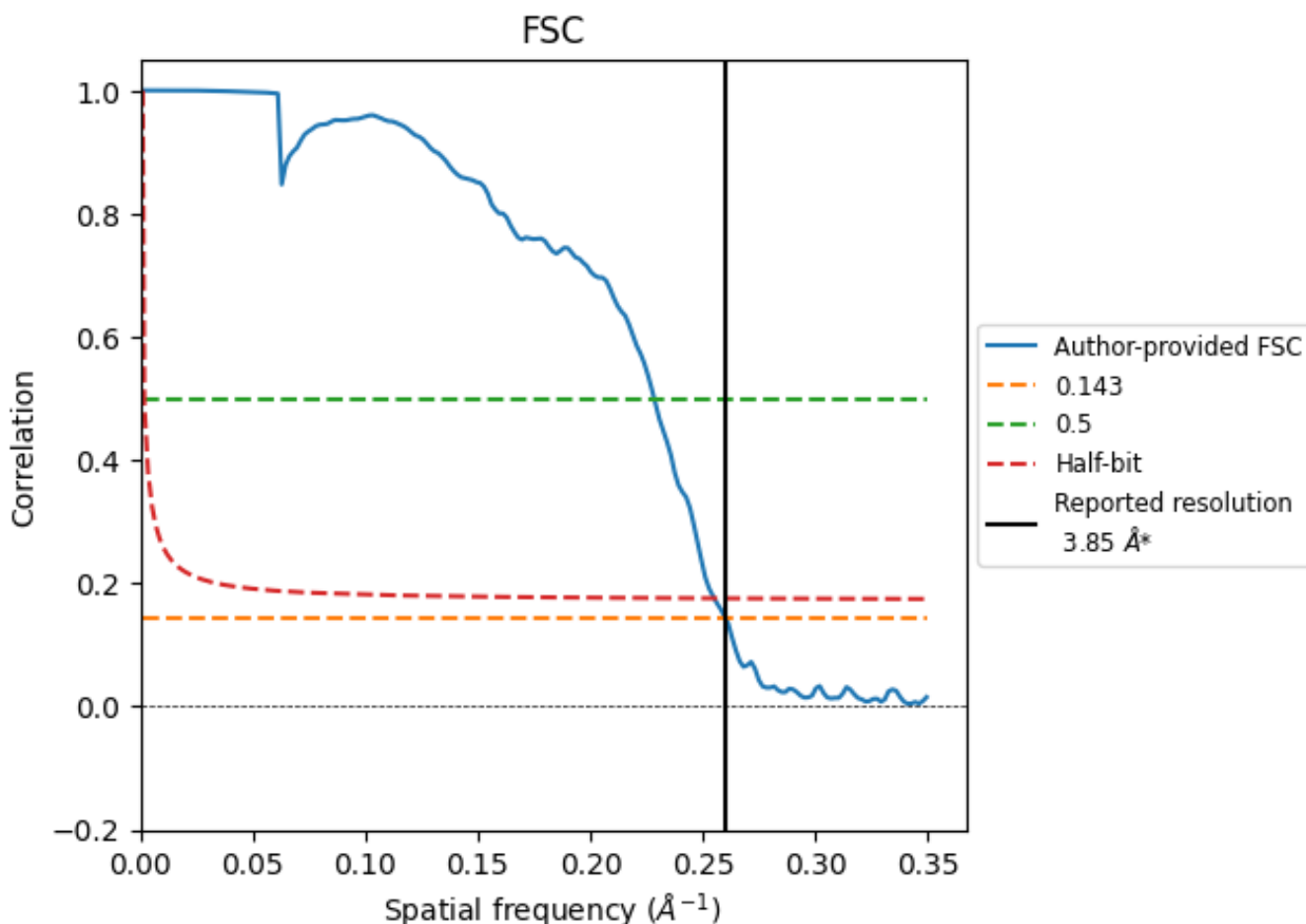


\*Reported resolution corresponds to spatial frequency of 0.260 Å<sup>-1</sup>

## 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 0.260 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

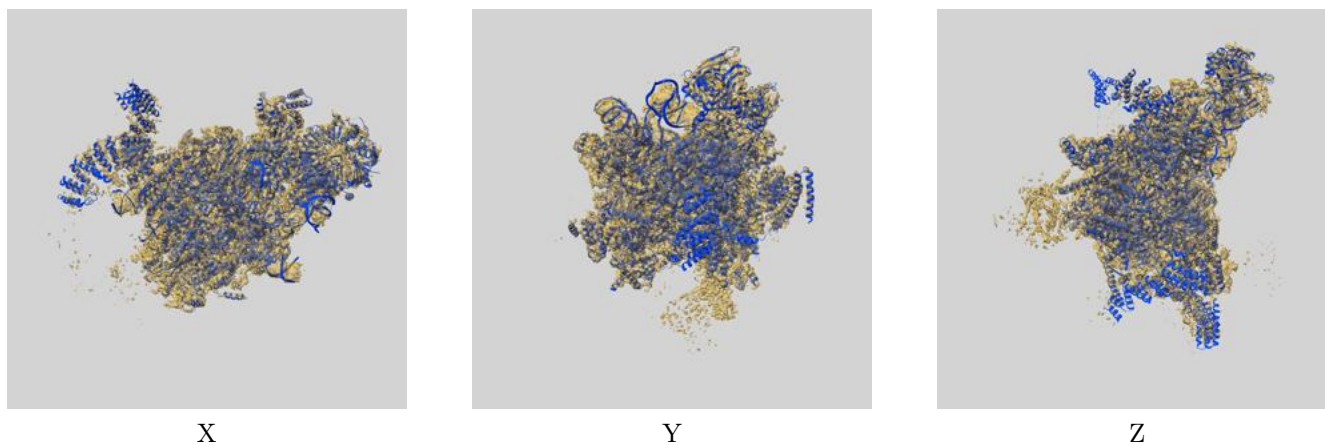
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.85	-	-
Author-provided FSC curve	3.84	4.38	3.92
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

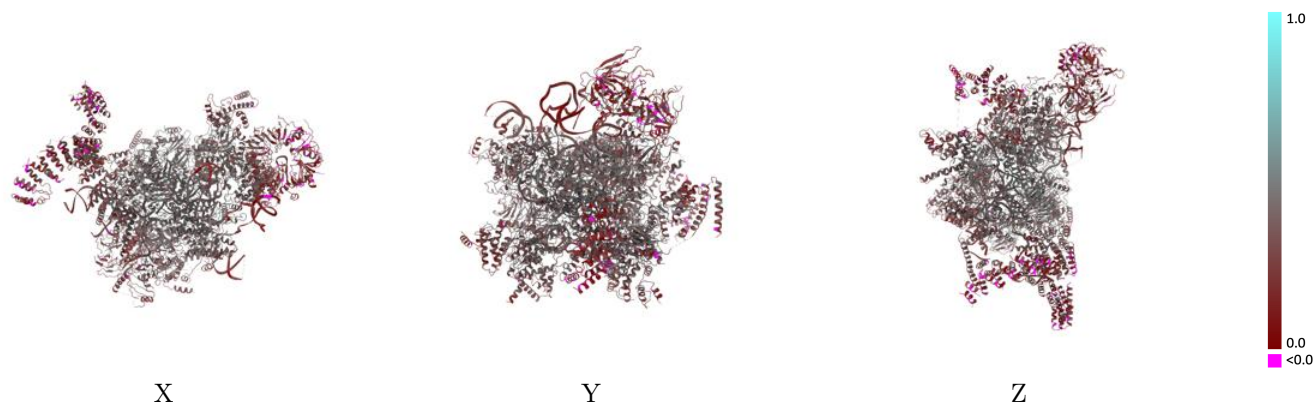
This section contains information regarding the fit between EMDB map EMD-3539 and PDB model 5MPS. Per-residue inclusion information can be found in section 3 on page 12.

### 9.1 Map-model overlay [i](#)



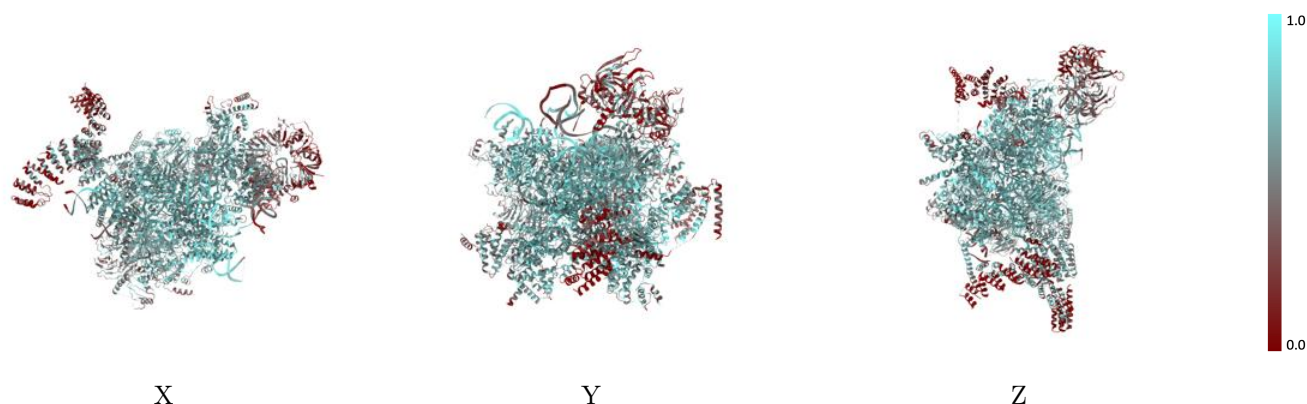
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



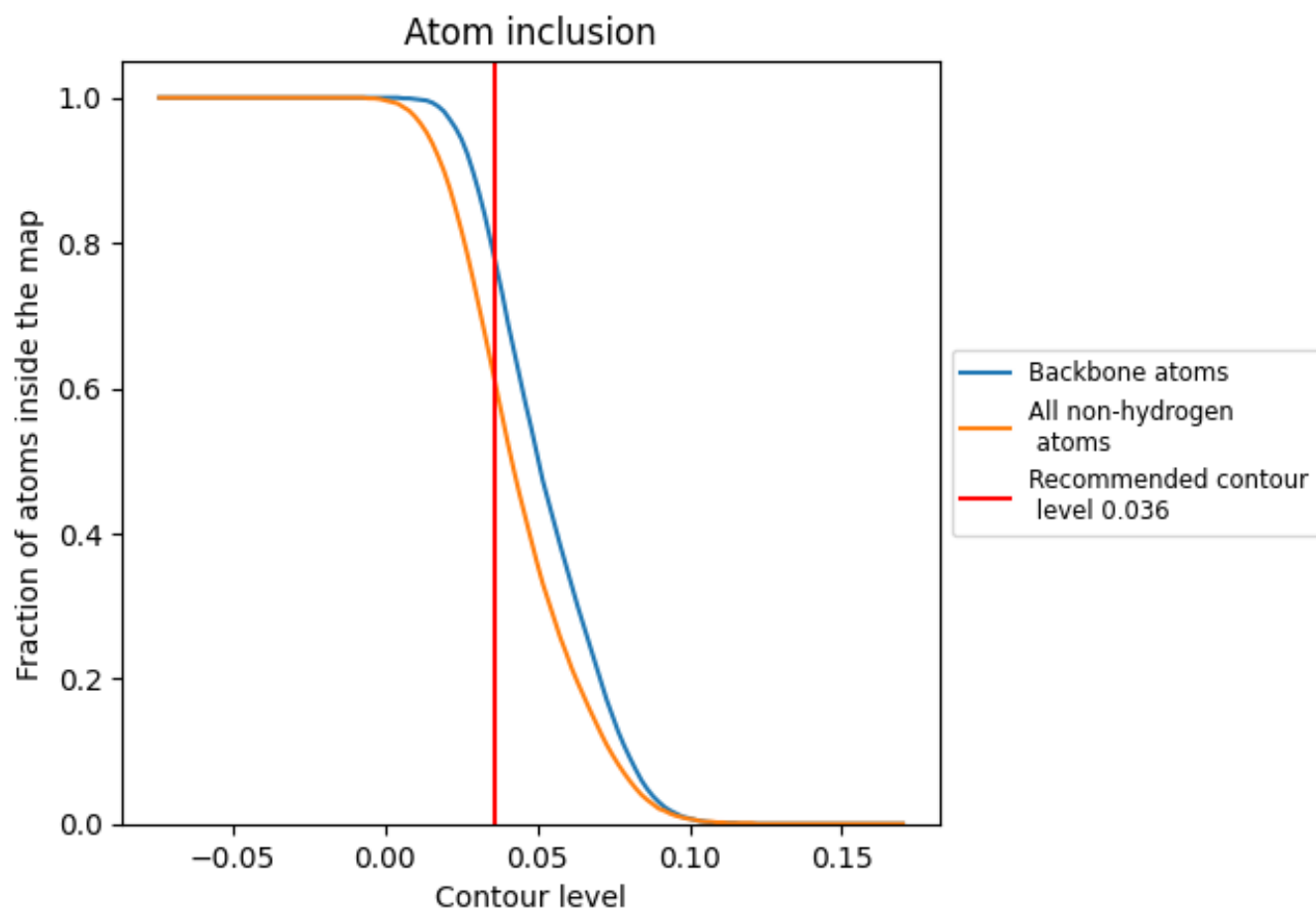
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.036).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 61% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6100	 0.3560
2	 0.6470	 0.3100
5	 0.7210	 0.3090
6	 0.8350	 0.3890
A	 0.7020	 0.4130
C	 0.6740	 0.3940
E	 0.6940	 0.4080
H	 0.3800	 0.2640
I	 0.6220	 0.3090
J	 0.7020	 0.4300
K	 0.5730	 0.3780
L	 0.7680	 0.4020
M	 0.6650	 0.3780
N	 0.6020	 0.3560
O	 0.6170	 0.3700
P	 0.6410	 0.4360
R	 0.4280	 0.3020
S	 0.4930	 0.3020
T	 0.3990	 0.2400
X	 0.5500	 0.3240
a	 0.5260	 0.2870
b	 0.4280	 0.2850
c	 0.5480	 0.3150
d	 0.4870	 0.3460
e	 0.2060	 0.1840
f	 0.2400	 0.1840
g	 0.3450	 0.2640
h	 0.3490	 0.2450
j	 0.2060	 0.1900
o	 0.5180	 0.3300
y	 0.6110	 0.3410

