



## Full wwPDB EM Validation Report ⓘ

Oct 12, 2022 – 04:41 PM EDT

PDB ID : 7UND  
EMDB ID : EMD-26621  
Title : Pol II-DSIF-SPT6-PAF1c-TFIIS-nucleosome complex (stalled at +38)  
Authors : Filipovski, M.; Vos, S.M.; Farnung, L.  
Deposited on : 2022-04-10  
Resolution : 3.00 Å (reported)  
Based on initial models : 6TED, 3LZ0

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.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

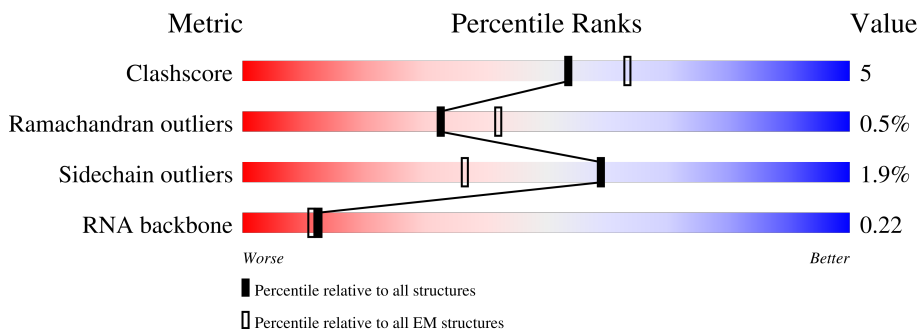
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	A	1984	
2	B	1251	
3	C	275	
4	D	184	
5	E	210	
6	F	127	
7	G	172	

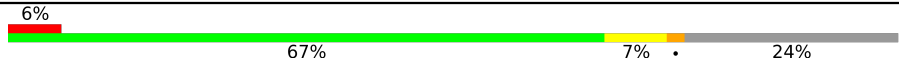
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Mol	Chain	Length	Quality of chain
8	H	150	82% 16% ...
9	I	125	59% 29% 7%
10	J	67	84% 10% ..
11	K	117	79% 15% ..
12	L	58	66% 14% 19%
13	M	1729	51% 53% 5% 42%
14	N	209	7% 30% 24% 43%
15	O	304	26% 45% 7% 47%
16	P	18	11% 22% 50% 28%
17	Q	1179	75% 59% 16% 25%
18	R	713	34% 26% 8% 66%
19	T	215	6% 33% 26% 39%
20	U	666	15% 15% 81%
21	V	531	42% 38% 6% 54%
22	W	305	98% 73% 25% ..
23	X	531	8% 6% 92%
24	Y	117	99% 70% 26% ..
25	Z	1087	40% 36% 10% 53%
26	a	136	23% 63% 7% 29%
26	e	136	9% 58% 12% 29%
27	b	103	18% 64% 17% 19%
27	f	103	9% 60% 16% 24%
28	c	130	57% 74% 5% 21%
28	g	130	69% 8% 19%
29	d	123	43% 67% 9% 23%

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Mol	Chain	Length	Quality of chain
29	h	123	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	ZN	C	301	-	-	X	-

## 2 Entry composition [i](#)

There are 31 unique types of molecules in this entry. The entry contains 129470 atoms, of which 61557 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P S		
1	A	1426	22640	7074	11385	2014	2095	2 70	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	1122	18004	5684	9024	1576	1656	64	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	258	4093	1300	2021	356	410	6	0	0

- Molecule 4 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	126	1985	630	981	170	200	4	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	209	3456	1089	1736	300	323	8	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	78	1284	401	658	106	114	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	G	171	2654	866	1321	214	245	8	0	0

- Molecule 8 is a protein called RPB8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	H	149	2354	759	1157	195	238	5	0	0

- Molecule 9 is a protein called RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	I	116	1816	582	874	168	181	11	0	0

- Molecule 10 is a protein called RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	J	66	1065	339	541	88	91	6	0	0

- Molecule 11 is a protein called RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	K	115	1862	593	942	152	173	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	L	47	804	246	407	77	68	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	M	1002	7565	2738	2638	1074	1108	7	0	0

There are 3 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
14	N	120	3815	1169	1355	433	738	120	0	0

- Molecule 15 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	161	1274	778	234	248	14	0	0

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
16	P	18	572	169	191	61	133	18	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	Q	890	14397	4579	7171	1264	1352	31	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	R	244	3537	1152	1701	340	337	7	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	SER	-	expression tag	UNP Q92541
R	-1	ASN	-	expression tag	UNP Q92541
R	0	ALA	-	expression tag	UNP Q92541

- Molecule 19 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
19	T	131	4138	1267	1458	518	764	131	0	0

- Molecule 20 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	U	125	1544	538	687	151	167	1	0	0

- Molecule 21 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	V	244	3161	1066	1450	306	335	4	0	0

- Molecule 22 is a protein called WDR61.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
22	W	300	4580	1483	2247	392	454	4	0	0

- Molecule 23 is a protein called Parafibromin.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
23	X	43	725	220	372	69	64	0	0

- Molecule 24 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	Y	116	1820	570	909	159	173	9	0	0

- Molecule 25 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms							AltConf	Trace
			Total	C	H	N	O	P	S		
25	Z	510	8071	2552	4046	709	745	1	18	0	0

- Molecule 26 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
26	a	97	1643	506	841	155	138	3	0	0
26	e	97	1640	504	839	155	139	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	102	ALA	GLY	engineered mutation	UNP P84233
e	102	ALA	GLY	engineered mutation	UNP P84233

- Molecule 27 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
27	b	83	1372	418	710	129	114	1	0	0
27	f	78	1279	391	660	120	107	1	0	0

- Molecule 28 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	H	N			O
28	c	103	1642	501	847	155	139	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
28	g	105	1674	510	865	158	141	0	0

- Molecule 29 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
29	d	95	1519	469	774	134	140	2	0	0
29	h	93	1475	457	749	130	137	2	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	0	MET	-	initiating methionine	UNP P02281
d	29	THR	SER	engineered mutation	UNP P02281
h	0	MET	-	initiating methionine	UNP P02281
h	29	THR	SER	engineered mutation	UNP P02281

- Molecule 30 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

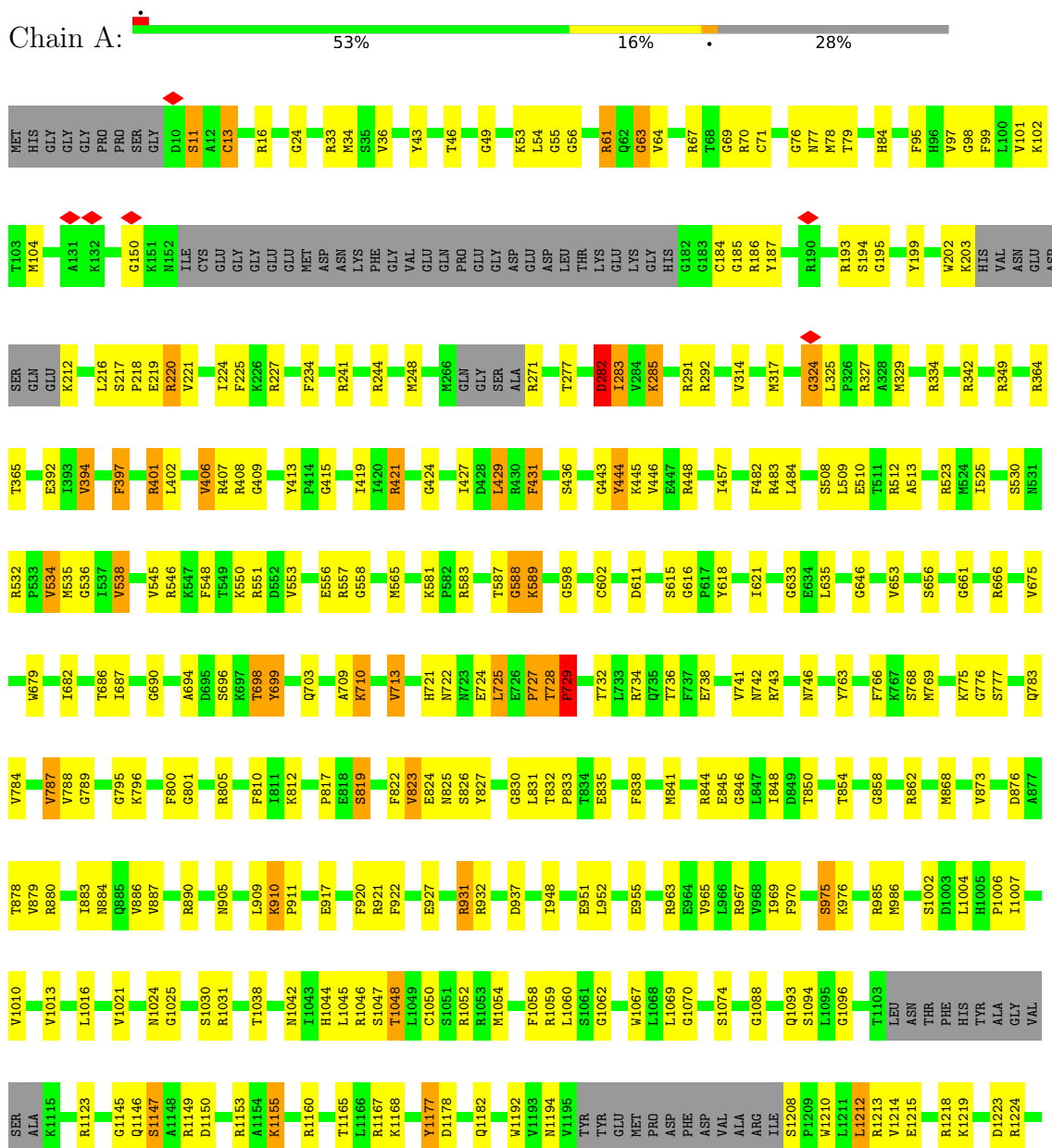
- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

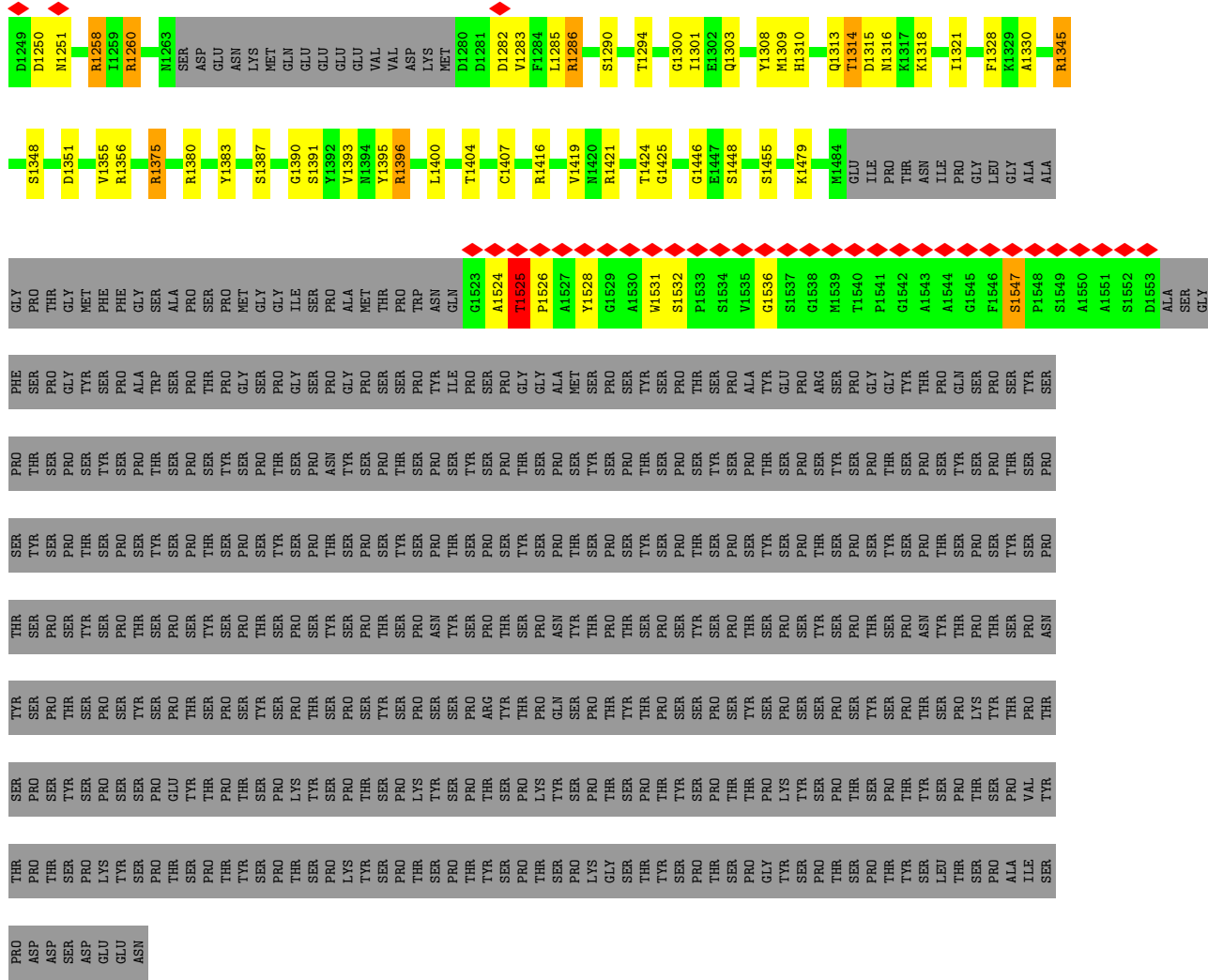
Mol	Chain	Residues	Atoms		AltConf
31	A	1	Total	Mg	0
			1	1	

### 3 Residue-property plots i

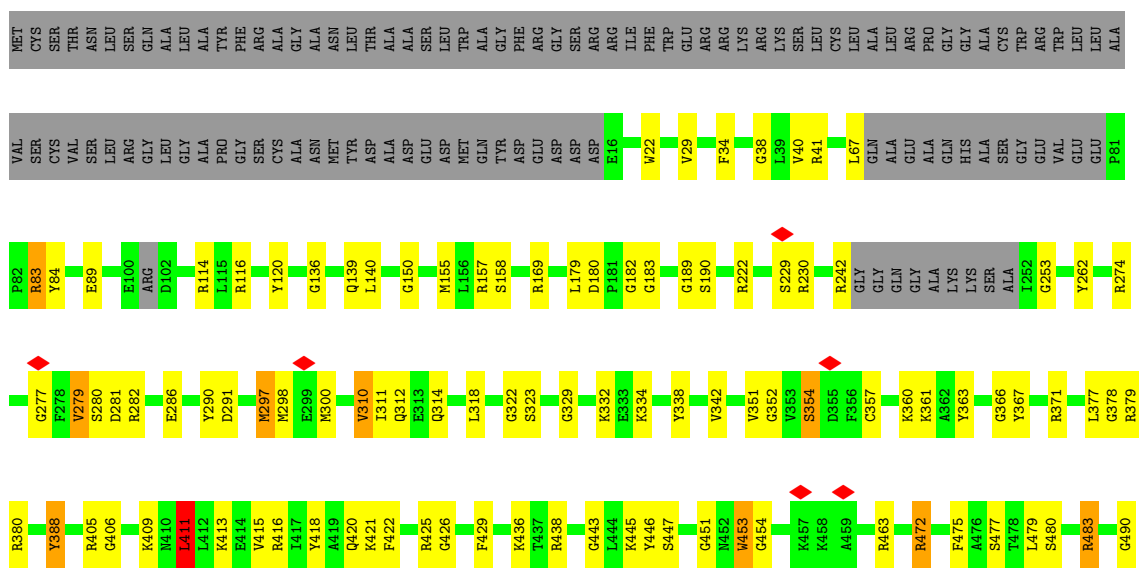
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

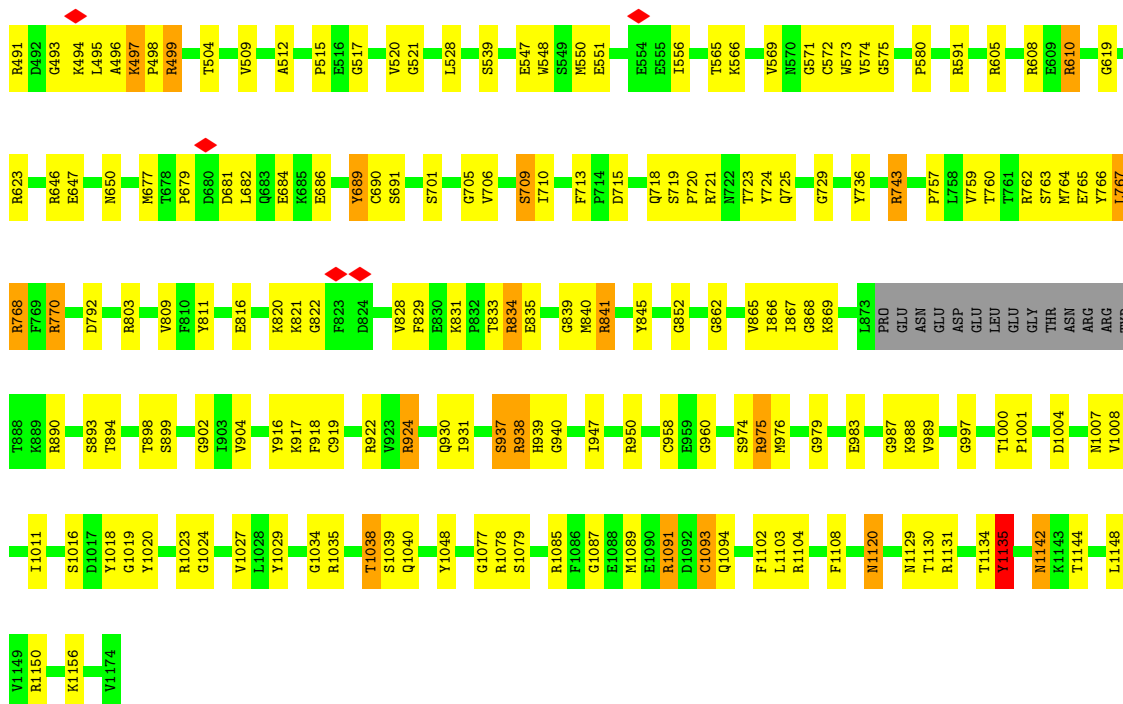
- Molecule 1: DNA-directed RNA polymerase subunit



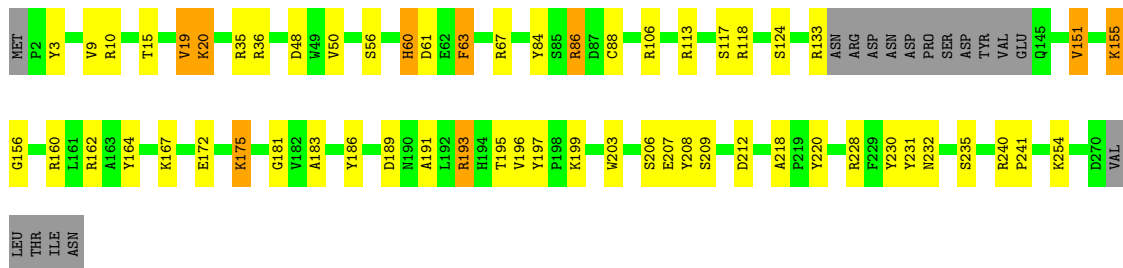


• Molecule 2: DNA-directed RNA polymerase subunit beta

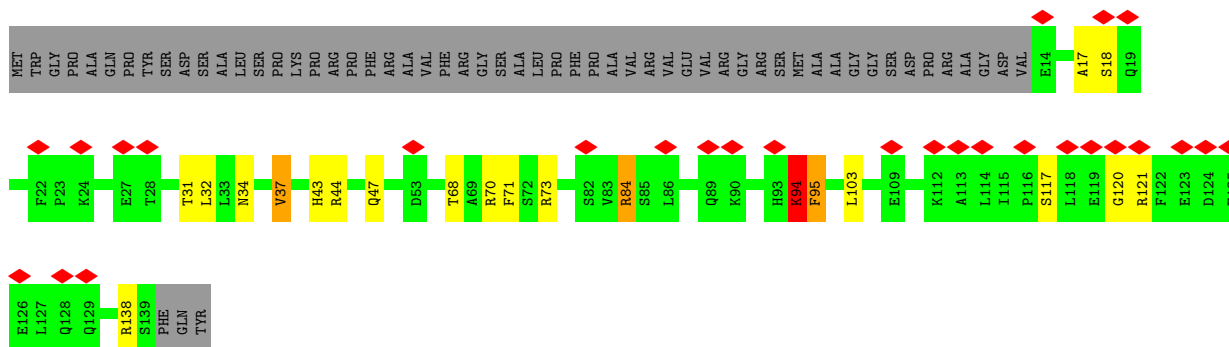




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

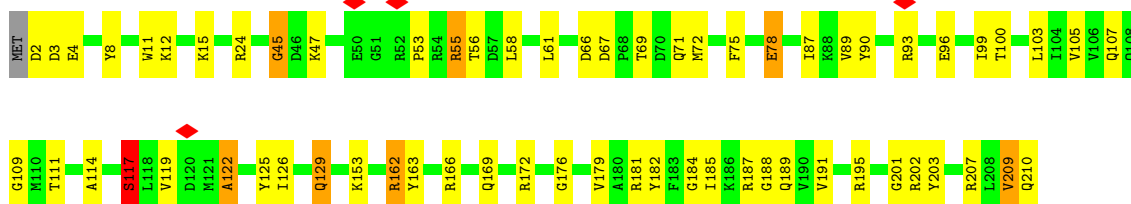


• Molecule 4: RPOL4c domain-containing protein



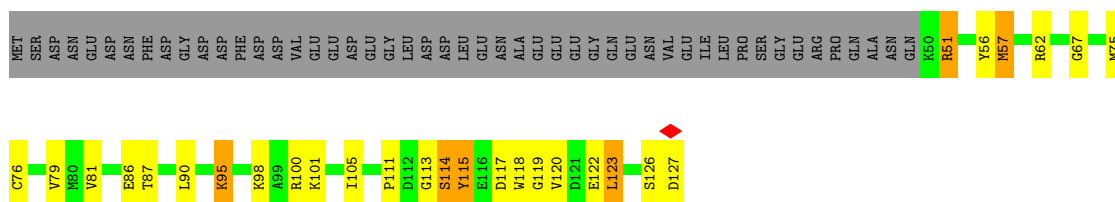
• Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E:  69% 27%




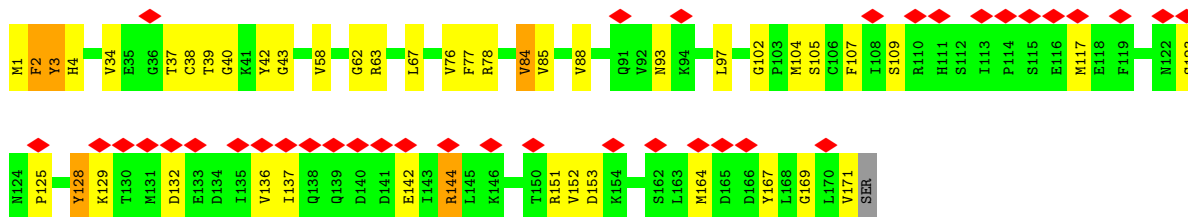
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:  39% 18% 5% 39%




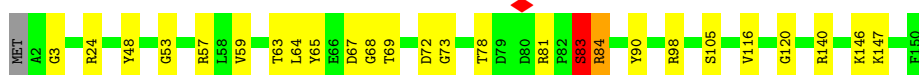
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:  22% 73% 23%



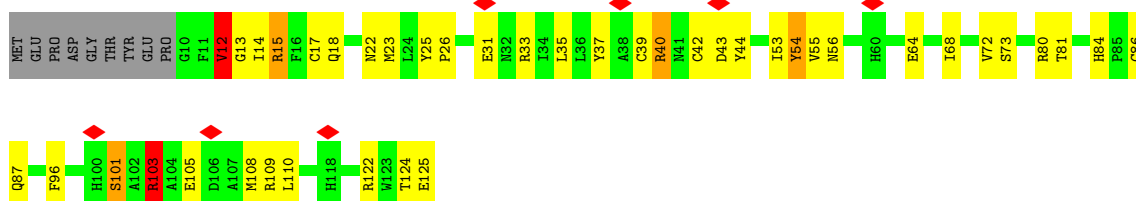
- Molecule 8: RPB8

Chain H:  82% 16%



- Molecule 9: RPB9

Chain I:  6% 59% 29% 7%

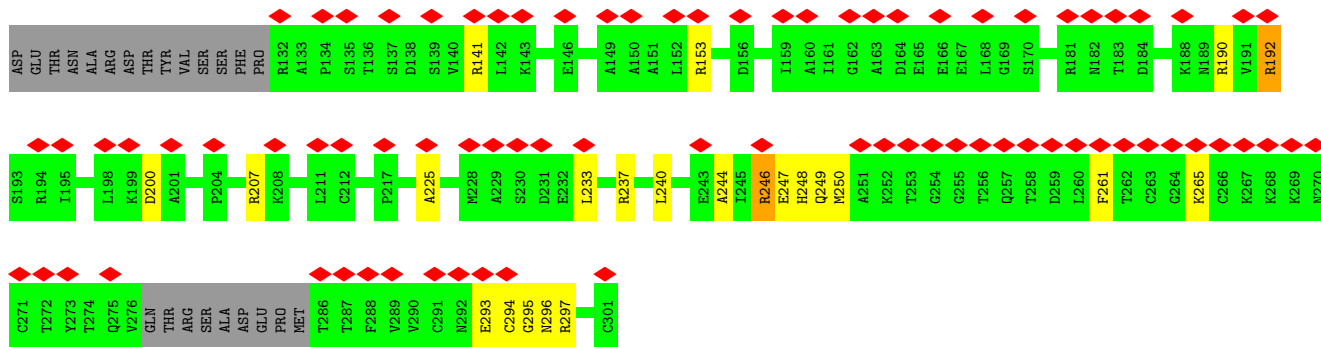




SER	Q546	E612	L673	C745	L609	G873	D936	K996	S1056	Y1116	GLN	I1240
ARG	F546	R613	K674	S746	R610	G874	I937	G997	R1057	G1117	GLY	P1241
LYS	G547	A614	G675	R747	L611	Q875	L938	T998	V1058	D1118	SER	T1242
LEU	E548	K615	VAL	K748	P612	Q876	C939	H999	H1059	K1119	ASP	K1243
LEU	N549	L616	GLU	L748	H613	L877	K940	L1000	P1060	H1120	THR	F1244
ARG	L550	N617	TYR	L749	H614	S878	K941	L1001	E1061	I1121	ALA	L1245
VAL	R551	I618	GLY	Y750	F614	S879	F942	K1002	T1062	T1122	ILE	S1246
ARG	R552	I619	ASN	V755	L615	S880	H943	I1003	Y1063	L1123	ARG	D1247
GLU	D553	T619	GLN	A756	ARG	I881	P944	I1004	E1064	Y1124	ASN	K1248
GLU	S553	P620	THR	F757	ARG	Q881	L945	K1005	W1065	D1125	ASP	V1250
GLY	Y554	T621	T684	Y758	THR	W882	Q946	Q1006	A1066	I1126	GLU	K1251
ASP	Q555	K622	Y685	Y759	ALA	E883	E947	N1007	R1067	R1127	GLY	L1252
GLU	Q556	K623	F686	F759	TRP	L884	H948	N1008	R1068	A1128	LEU	P1253
GLY	R556	K624	E687	P760	ARG	W885	H949	M1009	K1069	E1129	GLN	E1254
GLY	H557	G624	E688	D761	GLU	D886	H948	T1009	M1069	A1129	TRP	E1255
GLY	E558	R625	E689	Q762	E924	E887	H949	R1010	A1070	L1130	CYS	V1256
GLY	T559	K626	F692	Q763	E925	E888	H949	L1011	V1071	S1131	PHE	R1256
ASP	E560	D627	Y693	VAL	E926	R626	H949	E1012	D1072	C1132	CYS	R1257
GLU	E561	D628	Y694	GLU	E927	R627	H949	S1013	A1073	R1133	GLN	V1257
ALA	Q561	D629	Y695	GLU	E928	K628	H949	R1014	L1074	Y1134	GLN	K1258
ASP	F562	E630	D696	ASP	E929	K629	H949	T1015	E1075	K1135	ASP	G1260
GLU	P563	A631	R696	ASP	E930	A630	H949	Q1016	E1076	D1136	ASN	M1261
GLU	A564	A631	E697	PHE	E931	Q631	H949	L1017	Y1077	L1137	PHE	M1262
GLN	E565	H632	F698	ASP	E932	D632	H949	V1018	D1078	R1138	PRO	V1263
ARG	F566	Y633	S699	MET	E933	R633	H949	M1019	E1079	R1139	LEU	H1264
GLY	L567	A634	H700	GLU	E934	R634	H949	M1020	S1079	T1139	LEU	C1265
PRO	L567	A634	H700	GLU	E935	T635	H949	E961	E1080	A1140	GLY	R1266
GLU	E568	Y636	Q701	ASN	E936	T636	H949	F962	E1081	Y1141	VAL	R1267
LEU	L569	S637	V702	GLU	E937	R637	H949	H1022	D1082	R1142	TRP	M1268
LYS	A570	K638	Q703	ASP	E938	L638	H949	M1023	A1083	S1143	ASN	M1269
ALA	K571	Y639	E704	ASP	E939	K639	H949	G1024	M1084	I1149	PHE	K1269
SER	D572	H639	W705	GLU	E940	F639	H949	P1025	P1085	I1150	ASP	I1270
ARG		L640	R706	TYR	E941	R640	H949	K1026	A1086	F1150	SER	D1271
ARG		L641	R707	CYS	E942	L641	H949	V1027	A1087	M1151	GLY	M1272
ASP		L642	R708	GLN	E943	L642	H949	F1028	G1087	M1152	SER	E1273
MET		L643	Q708	THR	E944	H642	H949	E968	L1088	L1153	CYS	L1274
TYR		L644	R709	THR	E945	H643	H949	Y969	A1089	T1154	PRO	K1274
ILE		L645	R710	ILE	E946	K643	H949	G970	E1090	K1155	GLY	F1275
CYS		L646	M711	CYS	E947	K644	H949	Y971	E1091	E1156	GLN	S1276
GLN		L647	A712	PRO	E948	P645	H949	Y972	I1092	T1157	ALA	S1277
SER		L648	E646	PRO	E949	H646	H949	D972	L1093	Y1158	ALA	D1278
SER		L649	E647	PRO	E950	V647	H949	Y973	E1094	P1159	ALA	C1281
ALA		L650	E648	PRO	E951	W648	H949	Q912	E1095	E1159	ALA	R1282
GLY		L651	L652	PRO	E952	E852	H949	Q913	M1095	T1160	ALA	T1283
LEU		L652	L653	PRO	E953	E853	H949	Y914	P1096	F1161	ALA	S1284
ASP		L653	L654	PRO	E954	N654	H949	S915	P1097	Y1162	ALA	D1285
GLY		L654	L655	PRO	E955	N654	H949	L916	I1037	I1163	ALA	D1286
LEU		L655	L656	PRO	E956	N654	H949	E980	D1038	G1164	ALA	L1286
LEU		L656	L657	PRO	E957	N654	H949	P980	T1039	K1165	ALA	M1287
ALA		L657	L658	PRO	E958	N654	H949	Y981	ALA	L1166	ALA	ASP
ALA		L658	L659	PRO	E959	N654	H949	Y982	SER	D1101	ALA	ARG
LEU		L659	L660	PRO	E960	N654	H949	D922	LEU	L1102	ALA	ARG
LEU		L660	L661	PRO	E961	N654	H949	P923	GLY	L1103	ALA	ASN
LEU		L661	L662	PRO	E962	N654	H949	L924	ASP	D1104	ALA	ASN
LEU		L662	L663	PRO	E963	N654	H949	L925	SER	L1104	ALA	TRP
LEU		L663	L664	PRO	E964	N654	H949	E926	THR	D1105	ALA	LYS
LEU		L664	L665	PRO	E965	N654	H949	F927	ASP	A1106	ALA	LEU
LEU		L665	L666	PRO	E966	N654	H949	Q928	SER	F1107	ALA	PRO
LEU		L666	L667	PRO	E967	N654	H949	I929	TYR	I1108	ALA	PRO
LEU		L667	L668	PRO	E968	N654	H949	Y930	ILE	I1169	ALA	PRO
LEU		L668	L669	PRO	E969	N654	H949	E1051	ALA	A1108	ALA	LYS
LEU		L669	L670	PRO	E970	N654	H949	V1052	LEU	E1109	ALA	LYS
LEU		L670	L671	PRO	E971	N654	H949	L1053	LEU	E1110	ALA	ASP
LEU		L671	L672	PRO	E972	N654	H949	L1054	SER	L1111	ALA	THR
LEU		L672	L673	PRO	E973	N654	H949	G1055	ASP	E1112	ALA	TYR
LEU		L673	L674	PRO	E974	N654	H949	P994	SER	R1113	ALA	
LEU		L674	L675	PRO	E975	N654	H949	R995	ASP	Q1114	ALA	
LEU		L675	L676	PRO	E976	N654	H949			G1115	ALA	



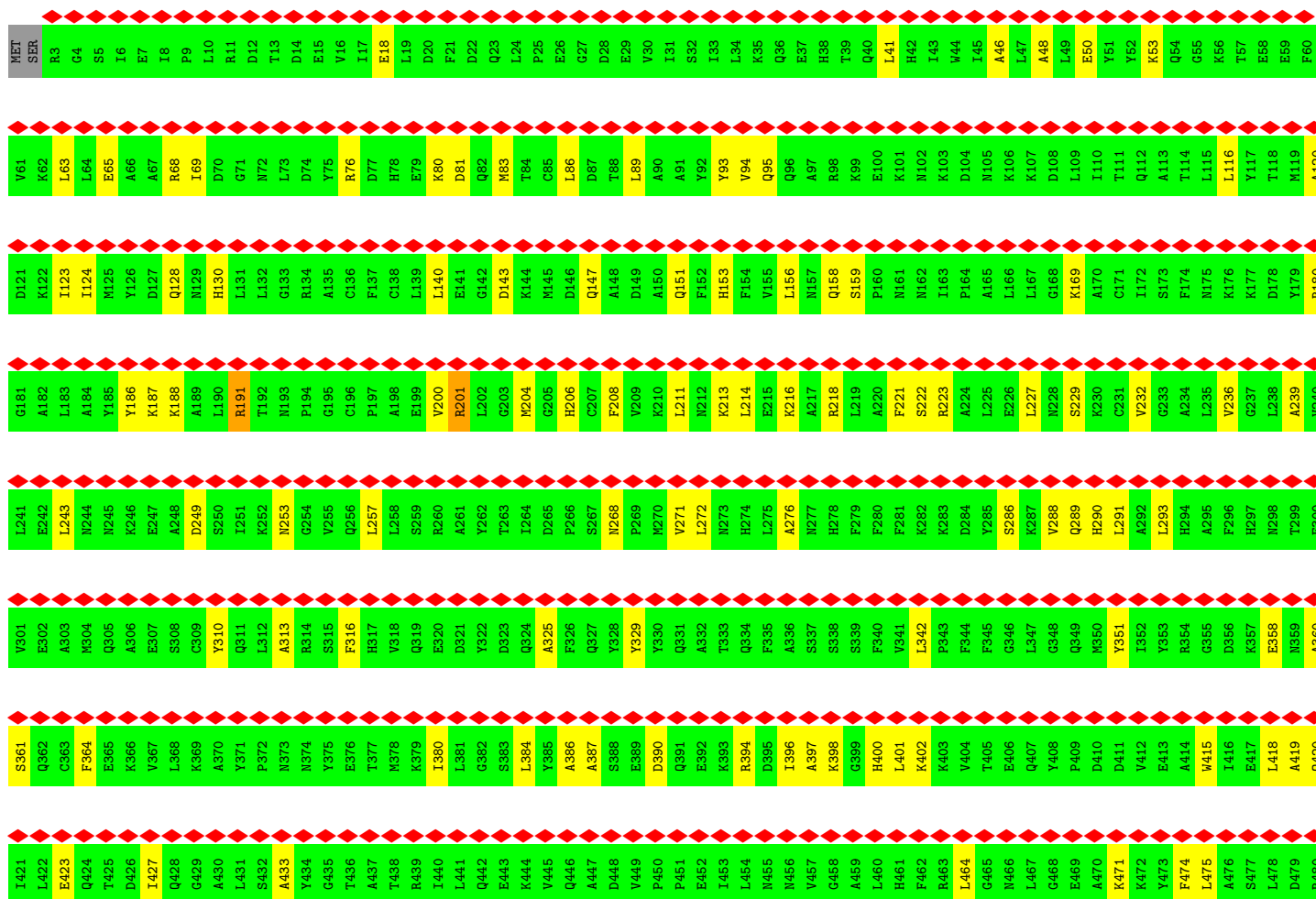
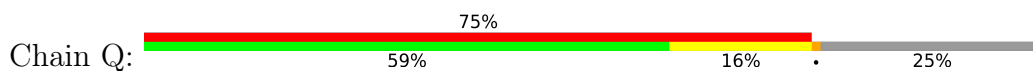




• Molecule 16: RNA

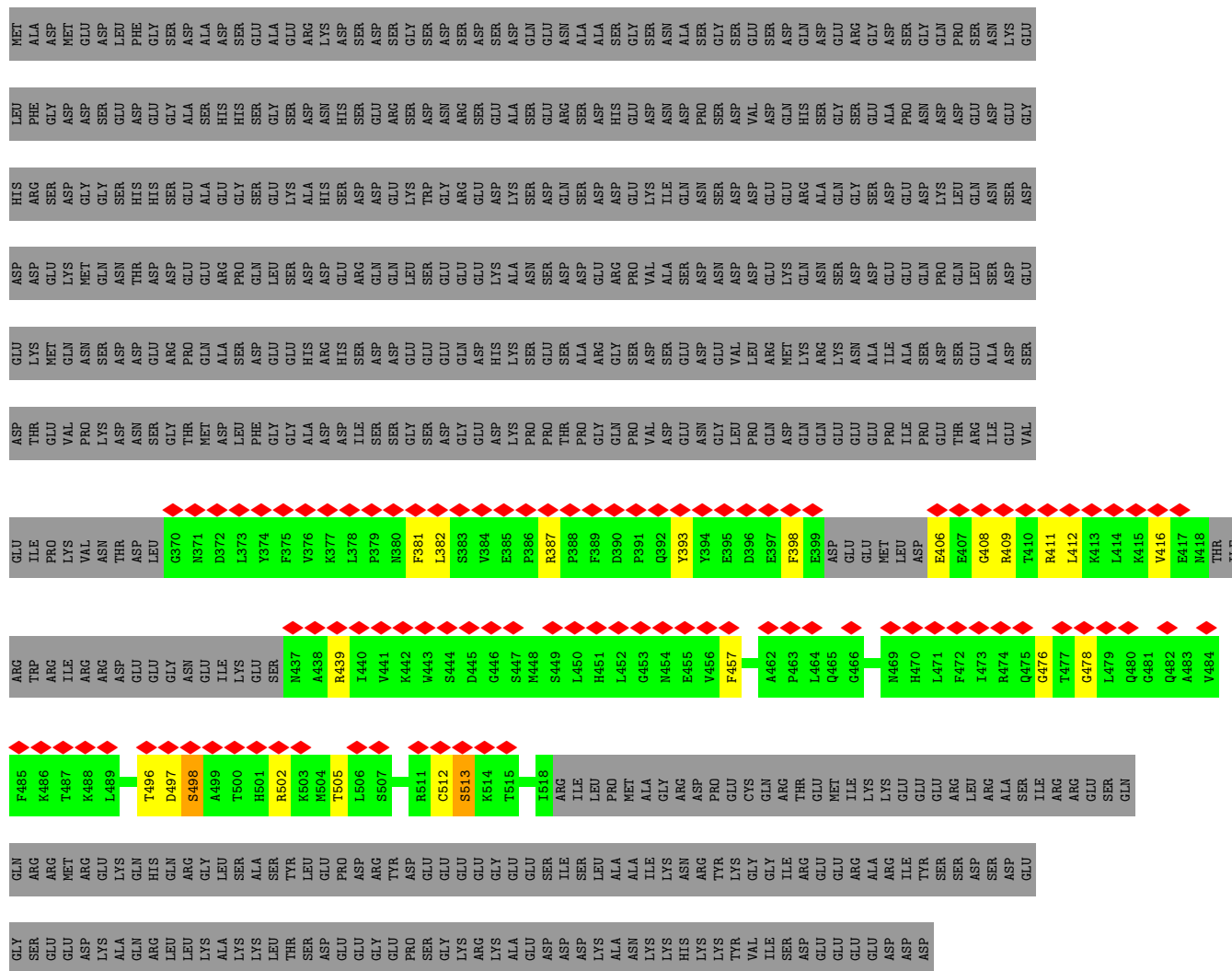


• Molecule 17: RNA polymerase-associated protein CTR9 homolog

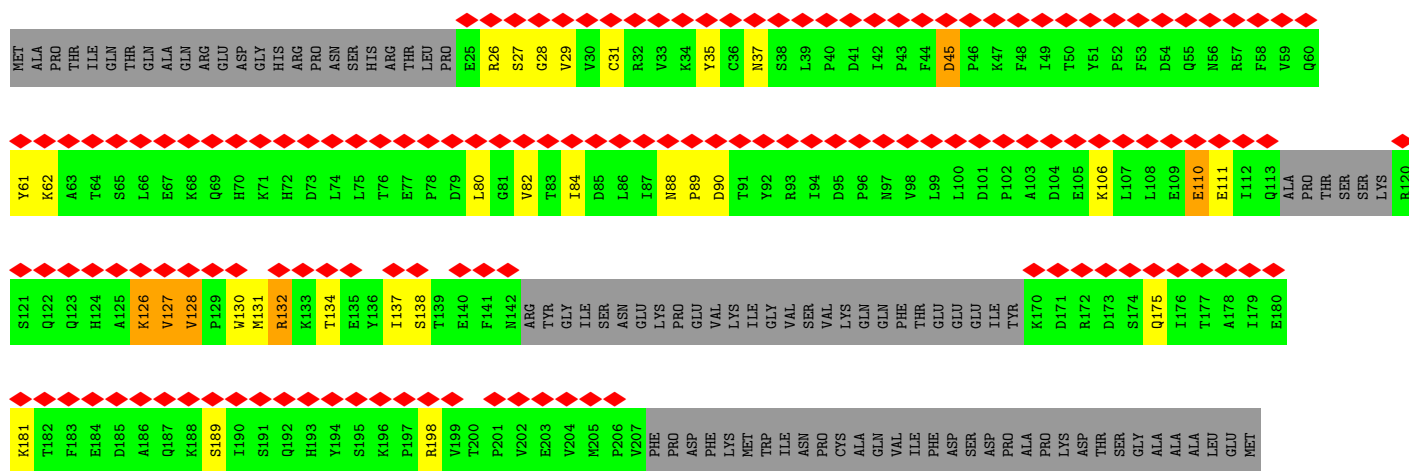
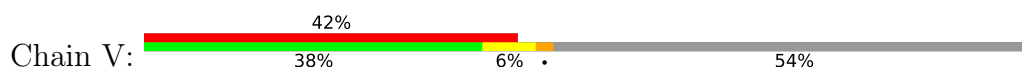


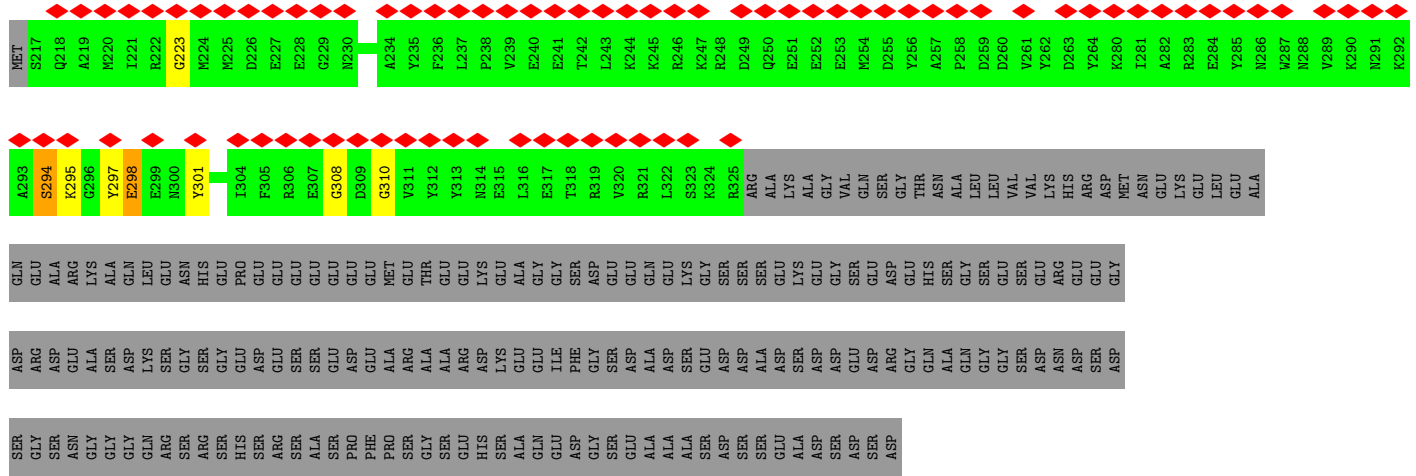




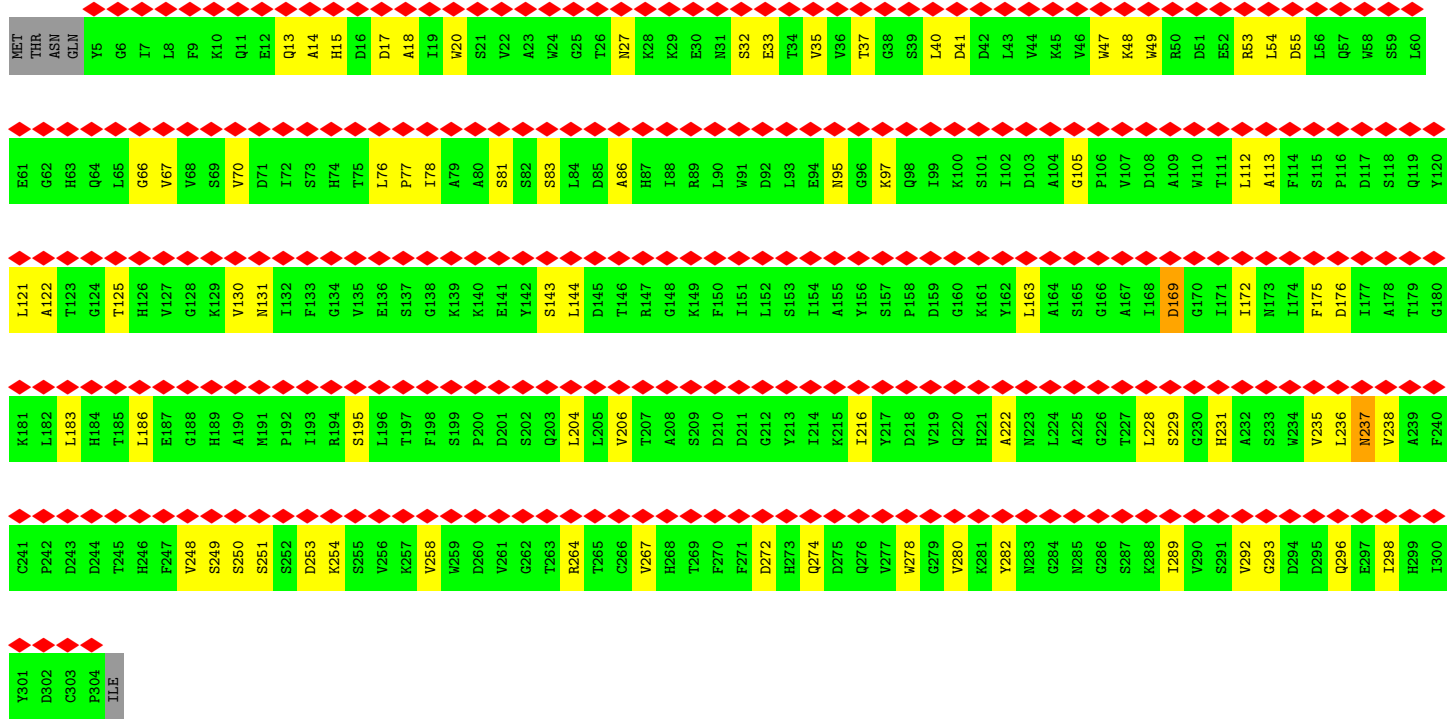
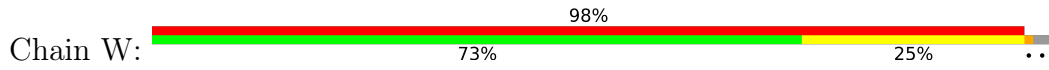


● Molecule 21: RNA polymerase II-associated factor 1 homolog

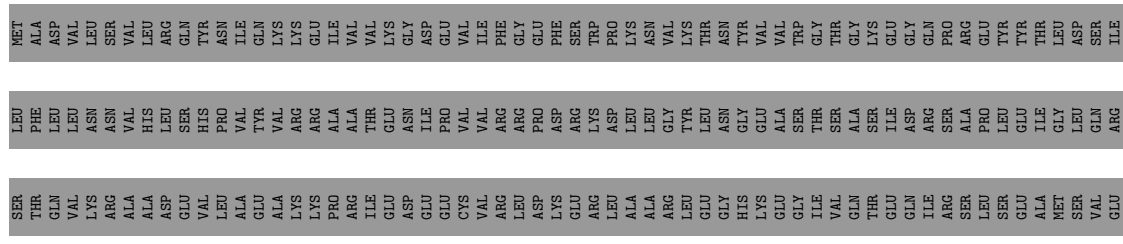


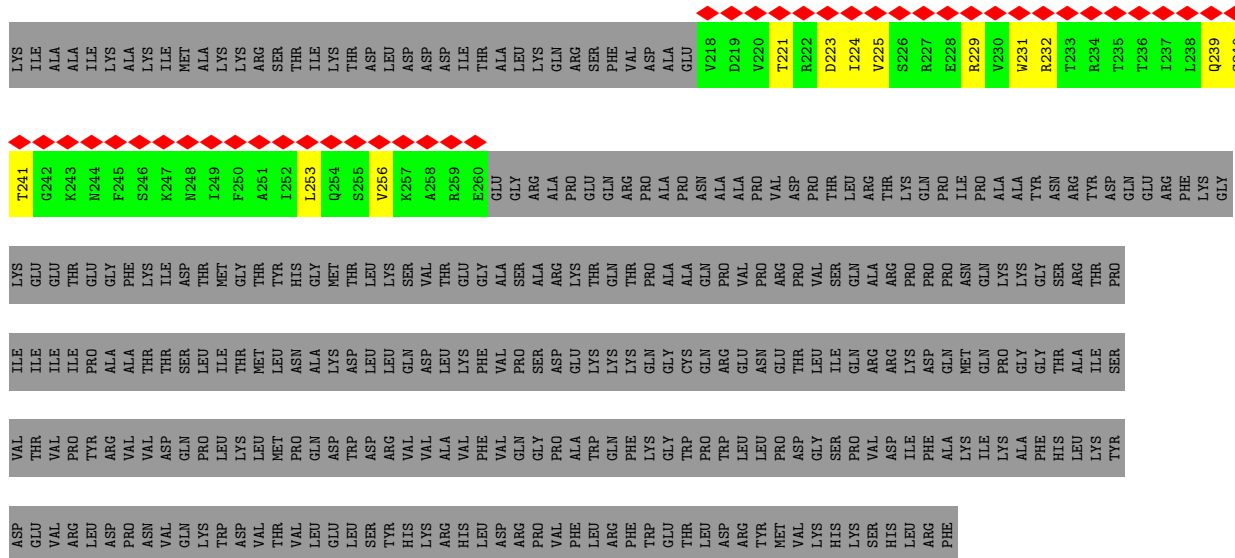


• Molecule 22: WDR61



• Molecule 23: Parafibromin

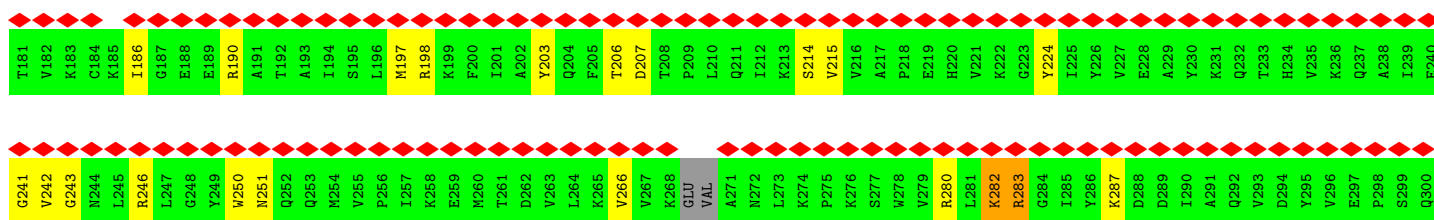
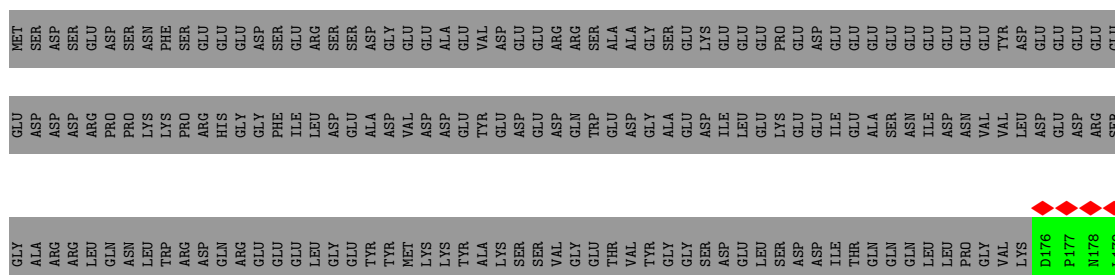
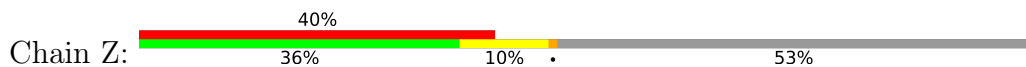




• Molecule 24: Transcription elongation factor SPT4

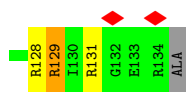


• Molecule 25: Transcription elongation factor SPT5

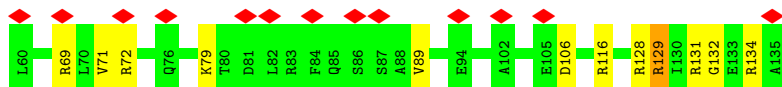
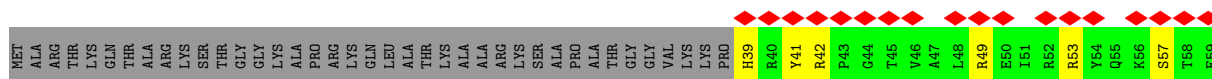




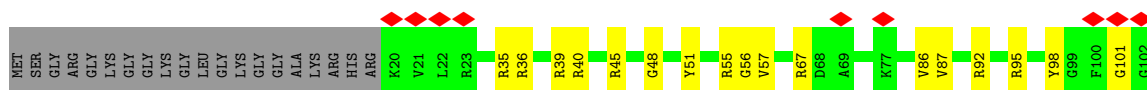




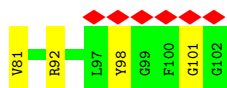
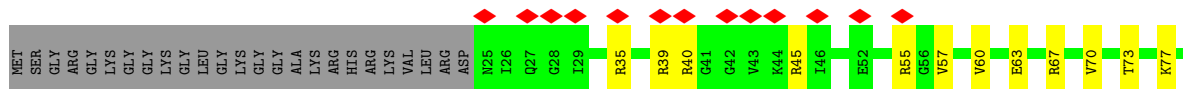
• Molecule 26: Histone H3.2



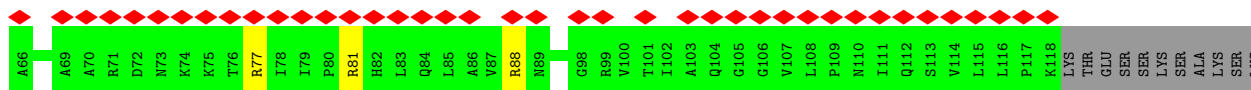
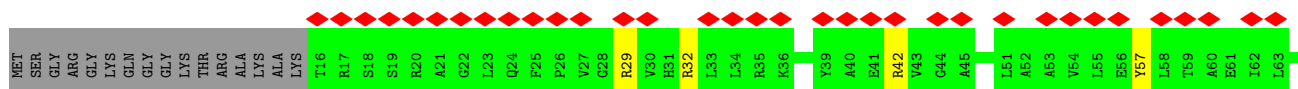
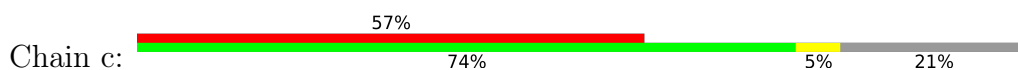
• Molecule 27: Histone H4



• Molecule 27: Histone H4

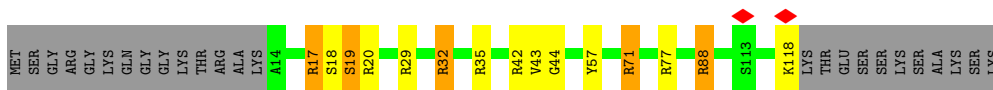


• Molecule 28: Histone H2A

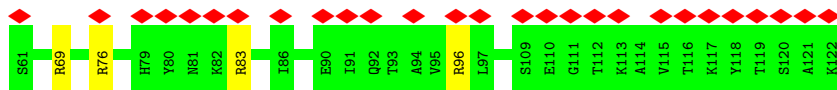
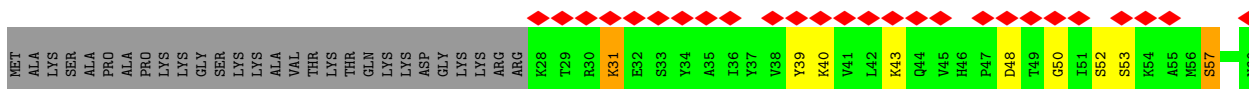
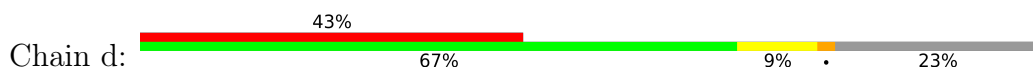


• Molecule 28: Histone H2A

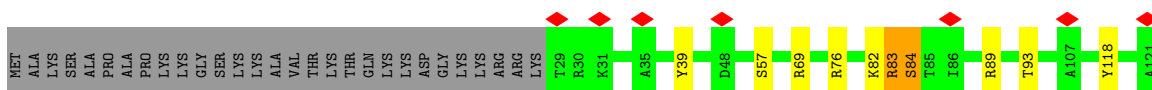




• Molecule 29: Histone H2B 1.1



• Molecule 29: Histone H2B 1.1



LYS

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105420	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 ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.935	Depositor
Minimum map value	-0.271	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.0832	Depositor
Map size (Å)	373.5, 373.5, 373.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, TPO, SEP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.72	230/11437 (2.0%)	1.50	109/15433 (0.7%)
2	B	1.78	203/9158 (2.2%)	1.55	90/12360 (0.7%)
3	C	1.91	53/2115 (2.5%)	1.62	18/2873 (0.6%)
4	D	1.55	14/1017 (1.4%)	1.36	6/1368 (0.4%)
5	E	1.86	47/1751 (2.7%)	1.50	23/2366 (1.0%)
6	F	2.18	25/636 (3.9%)	1.76	7/859 (0.8%)
7	G	1.79	38/1364 (2.8%)	1.52	14/1853 (0.8%)
8	H	1.49	19/1219 (1.6%)	1.41	8/1644 (0.5%)
9	I	1.89	25/964 (2.6%)	1.59	8/1305 (0.6%)
10	J	1.10	2/533 (0.4%)	1.20	2/719 (0.3%)
11	K	2.02	23/939 (2.4%)	1.65	6/1271 (0.5%)
12	L	1.45	6/403 (1.5%)	1.41	5/536 (0.9%)
13	M	0.93	24/4988 (0.5%)	1.18	29/6450 (0.4%)
14	N	1.68	41/2752 (1.5%)	2.95	218/4246 (5.1%)
15	O	0.63	0/1287	0.98	9/1721 (0.5%)
16	P	2.39	26/423 (6.1%)	4.27	98/657 (14.9%)
17	Q	1.08	63/7365 (0.9%)	0.98	24/9927 (0.2%)
18	R	1.45	27/1866 (1.4%)	1.33	8/2519 (0.3%)
19	T	1.73	51/3012 (1.7%)	2.66	279/4641 (6.0%)
20	U	1.52	13/872 (1.5%)	1.39	10/1187 (0.8%)
21	V	1.31	21/1739 (1.2%)	1.24	5/2375 (0.2%)
22	W	0.43	1/2392 (0.0%)	0.56	0/3257
23	X	0.58	1/356 (0.3%)	0.65	0/478
24	Y	1.78	21/927 (2.3%)	1.51	8/1250 (0.6%)
25	Z	1.34	46/4084 (1.1%)	1.24	16/5498 (0.3%)
26	a	1.35	7/814 (0.9%)	1.40	12/1092 (1.1%)
26	e	1.73	19/812 (2.3%)	1.58	10/1088 (0.9%)
27	b	1.57	12/669 (1.8%)	1.54	10/894 (1.1%)
27	f	1.39	10/626 (1.6%)	1.37	9/837 (1.1%)
28	c	1.11	4/805 (0.5%)	1.18	6/1088 (0.6%)
28	g	1.22	9/819 (1.1%)	1.30	10/1106 (0.9%)
29	d	1.09	7/756 (0.9%)	1.17	5/1015 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
29	h	1.31	7/737 (0.9%)	1.25	4/993 (0.4%)
All	All	1.52	1095/69637 (1.6%)	1.59	1066/94906 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
2	B	0	10
3	C	0	3
4	D	0	1
9	I	0	1
10	J	0	4
13	M	0	3
14	N	0	37
16	P	0	1
18	R	0	1
19	T	0	32
25	Z	0	1
26	a	0	1
28	c	0	1
28	g	0	4
29	h	0	1
All	All	0	111

All (1095) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	496	ALA	C-N	11.39	1.60	1.34
14	N	105	DG	C3'-O3'	11.07	1.58	1.44
19	T	-113	DG	C3'-O3'	11.07	1.58	1.44
16	P	42	C	C4-N4	-10.47	1.24	1.33
16	P	30	C	C5-C6	-9.40	1.26	1.34
16	P	42	C	C5-C6	-9.22	1.26	1.34
5	E	126	ILE	C-N	8.36	1.53	1.34
3	C	106	ARG	CZ-NH2	-8.10	1.22	1.33
5	E	55	ARG	CZ-NH2	-8.09	1.22	1.33
18	R	371	ARG	CZ-NH2	-8.08	1.22	1.33
2	B	491	ARG	CZ-NH2	-8.00	1.22	1.33
12	L	31	ARG	CZ-NH2	-7.98	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	128	ARG	CZ-NH2	-7.95	1.22	1.33
26	e	128	ARG	CZ-NH2	-7.95	1.22	1.33
26	a	129	ARG	CZ-NH2	-7.95	1.22	1.33
6	F	100	ARG	CZ-NH2	-7.93	1.22	1.33
2	B	380	ARG	CZ-NH2	-7.92	1.22	1.33
1	A	734	ARG	CZ-NH2	-7.92	1.22	1.33
1	A	1167	ARG	CZ-NH2	-7.91	1.22	1.33
26	e	129	ARG	CZ-NH2	-7.90	1.22	1.33
9	I	103	ARG	CZ-NH2	-7.89	1.22	1.33
2	B	379	ARG	CZ-NH2	-7.89	1.22	1.33
13	M	1355	ARG	CZ-NH2	-7.87	1.22	1.33
17	Q	191	ARG	CZ-NH2	-7.86	1.22	1.33
2	B	499	ARG	CZ-NH2	-7.85	1.22	1.33
27	f	67	ARG	CZ-NH2	-7.85	1.22	1.33
1	A	532	ARG	CZ-NH2	-7.84	1.22	1.33
7	G	63	ARG	CZ-NH2	-7.84	1.22	1.33
1	A	407	ARG	CZ-NH2	-7.83	1.22	1.33
27	b	55	ARG	CZ-NH2	-7.83	1.22	1.33
14	N	16	DT	P-OP1	7.82	1.62	1.49
29	h	89	ARG	CZ-NH2	-7.82	1.22	1.33
12	L	51	ARG	CZ-NH2	-7.82	1.22	1.33
2	B	1131	ARG	CZ-NH2	-7.82	1.22	1.33
3	C	160	ARG	CZ-NH2	-7.81	1.22	1.33
19	T	-70	DT	P-OP1	7.81	1.62	1.49
19	T	-112	DT	P-OP1	7.81	1.62	1.49
19	T	-109	DT	P-OP1	7.81	1.62	1.49
1	A	844	ARG	CZ-NH2	-7.81	1.22	1.33
20	U	411	ARG	CZ-NH2	-7.80	1.23	1.33
14	N	106	DT	P-OP1	7.80	1.62	1.49
25	Z	283	ARG	CZ-NH2	-7.80	1.23	1.33
1	A	292	ARG	CZ-NH2	-7.79	1.23	1.33
17	Q	218	ARG	CZ-NH2	-7.79	1.23	1.33
19	T	-144	DT	P-OP1	7.79	1.62	1.49
14	N	14	DT	P-OP1	7.79	1.62	1.49
14	N	139	DT	P-OP1	7.79	1.62	1.49
1	A	523	ARG	CZ-NH2	-7.79	1.23	1.33
14	N	140	DT	P-OP1	7.78	1.62	1.49
14	N	86	DT	P-OP1	7.78	1.62	1.49
19	T	-132	DT	P-OP1	7.78	1.62	1.49
1	A	557	ARG	CZ-NH2	-7.78	1.23	1.33
14	N	87	DT	P-OP1	7.78	1.62	1.49
14	N	108	DT	P-OP1	7.77	1.62	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	ARG	CZ-NH2	-7.77	1.23	1.33
1	A	408	ARG	CZ-NH2	-7.76	1.23	1.33
2	B	438	ARG	CZ-NH2	-7.76	1.23	1.33
17	Q	832	ARG	CZ-NH2	-7.76	1.23	1.33
2	B	841	ARG	CZ-NH2	-7.76	1.23	1.33
17	Q	830	ARG	CZ-NH2	-7.76	1.23	1.33
1	A	1380	ARG	CZ-NH2	-7.75	1.23	1.33
1	A	70	ARG	CZ-NH2	-7.75	1.23	1.33
4	D	73	ARG	CZ-NH2	-7.74	1.23	1.33
25	Z	610	ARG	CZ-NH2	-7.74	1.23	1.33
25	Z	246	ARG	CZ-NH2	-7.74	1.23	1.33
17	Q	791	ARG	CZ-NH2	-7.74	1.23	1.33
17	Q	667	ARG	CZ-NH2	-7.72	1.23	1.33
17	Q	725	ARG	CZ-NH2	-7.72	1.23	1.33
18	R	438	ARG	CZ-NH2	-7.72	1.23	1.33
5	E	103	LEU	C-N	7.72	1.51	1.34
19	T	-144	DT	P-OP2	7.71	1.62	1.49
1	A	1224	ARG	CZ-NH2	-7.71	1.23	1.33
5	E	162	ARG	CZ-NH2	-7.71	1.23	1.33
2	B	610	ARG	CZ-NH2	-7.70	1.23	1.33
28	g	35	ARG	CZ-NH2	-7.70	1.23	1.33
1	A	880	ARG	CZ-NH2	-7.70	1.23	1.33
21	V	26	ARG	CZ-NH2	-7.70	1.23	1.33
5	E	172	ARG	CZ-NH2	-7.70	1.23	1.33
26	e	53	ARG	CZ-NH2	-7.70	1.23	1.33
2	B	1104	ARG	CZ-NH2	-7.69	1.23	1.33
3	C	118	ARG	CZ-NH2	-7.69	1.23	1.33
4	D	70	ARG	CZ-NH2	-7.69	1.23	1.33
17	Q	763	ARG	CZ-NH2	-7.69	1.23	1.33
1	A	1149	ARG	CZ-NH2	-7.69	1.23	1.33
2	B	890	ARG	CZ-NH2	-7.69	1.23	1.33
20	U	439	ARG	CZ-NH2	-7.69	1.23	1.33
17	Q	201	ARG	CZ-NH2	-7.69	1.23	1.33
25	Z	494	ARG	CZ-NH2	-7.69	1.23	1.33
2	B	1091	ARG	CZ-NH2	-7.68	1.23	1.33
1	A	1218	ARG	CZ-NH2	-7.68	1.23	1.33
5	E	207	ARG	CZ-NH2	-7.68	1.23	1.33
1	A	551	ARG	CZ-NH2	-7.68	1.23	1.33
1	A	932	ARG	CZ-NH2	-7.68	1.23	1.33
14	N	39	DT	P-OP1	7.68	1.62	1.49
2	B	83	ARG	CZ-NH2	-7.68	1.23	1.33
7	G	144	ARG	CZ-NH2	-7.68	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	ARG	CZ-NH2	-7.67	1.23	1.33
20	U	409	ARG	CZ-NH2	-7.67	1.23	1.33
1	A	1375	ARG	CZ-NH2	-7.67	1.23	1.33
3	C	86	ARG	CZ-NH2	-7.67	1.23	1.33
9	I	33	ARG	CZ-NH2	-7.67	1.23	1.33
26	e	134	ARG	CZ-NH2	-7.67	1.23	1.33
8	H	84	ARG	CZ-NH2	-7.66	1.23	1.33
20	U	387	ARG	CZ-NH2	-7.66	1.23	1.33
1	A	1160	ARG	CZ-NH2	-7.66	1.23	1.33
1	A	1046	ARG	CZ-NH2	-7.66	1.23	1.33
2	B	938	ARG	CZ-NH2	-7.66	1.23	1.33
2	B	768	ARG	CZ-NH2	-7.65	1.23	1.33
2	B	1023	ARG	CZ-NH2	-7.65	1.23	1.33
1	A	421	ARG	CZ-NH2	-7.65	1.23	1.33
1	A	1345	ARG	CZ-NH2	-7.65	1.23	1.33
3	C	133	ARG	CZ-NH2	-7.65	1.23	1.33
5	E	202	ARG	CZ-NH2	-7.65	1.23	1.33
7	G	78	ARG	CZ-NH2	-7.65	1.23	1.33
5	E	24	ARG	CZ-NH2	-7.64	1.23	1.33
1	A	583	ARG	CZ-NH2	-7.64	1.23	1.33
2	B	1035	ARG	CZ-NH2	-7.64	1.23	1.33
5	E	195	ARG	CZ-NH2	-7.64	1.23	1.33
2	B	975	ARG	CZ-NH2	-7.64	1.23	1.33
6	F	51	ARG	CZ-NH2	-7.64	1.23	1.33
21	V	132	ARG	CZ-NH2	-7.63	1.23	1.33
1	A	1031	ARG	CZ-NH2	-7.63	1.23	1.33
2	B	834	ARG	CZ-NH2	-7.63	1.23	1.33
1	A	1153	ARG	CZ-NH2	-7.63	1.23	1.33
2	B	1150	ARG	CZ-NH2	-7.63	1.23	1.33
3	C	193	ARG	CZ-NH2	-7.63	1.23	1.33
1	A	805	ARG	CZ-NH2	-7.62	1.23	1.33
2	B	41	ARG	CZ-NH2	-7.62	1.23	1.33
1	A	890	ARG	CZ-NH2	-7.62	1.23	1.33
8	H	57	ARG	CZ-NH2	-7.62	1.23	1.33
1	A	1286	ARG	CZ-NH2	-7.62	1.23	1.33
24	Y	14	ARG	CZ-NH2	-7.61	1.23	1.33
2	B	483	ARG	CZ-NH2	-7.60	1.23	1.33
1	A	271	ARG	CZ-NH2	-7.60	1.23	1.33
5	E	181	ARG	CZ-NH2	-7.60	1.23	1.33
24	Y	111	ARG	CZ-NH2	-7.60	1.23	1.33
25	Z	749	ARG	CZ-NH2	-7.59	1.23	1.33
2	B	721	ARG	CZ-NH2	-7.59	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	121	ARG	CZ-NH2	-7.59	1.23	1.33
28	c	77	ARG	CZ-NH2	-7.59	1.23	1.33
28	g	42	ARG	CZ-NH2	-7.59	1.23	1.33
1	A	1059	ARG	CZ-NH2	-7.58	1.23	1.33
27	b	95	ARG	CZ-NH2	-7.58	1.23	1.33
2	B	425	ARG	CZ-NH2	-7.57	1.23	1.33
1	A	1356	ARG	CZ-NH2	-7.57	1.23	1.33
9	I	40	ARG	CZ-NH2	-7.57	1.23	1.33
26	e	49	ARG	CZ-NH2	-7.57	1.23	1.33
4	D	138	ARG	CZ-NH2	-7.56	1.23	1.33
3	C	228	ARG	CZ-NH2	-7.56	1.23	1.33
6	F	62	ARG	CZ-NH2	-7.56	1.23	1.33
24	Y	11	ARG	CZ-NH2	-7.56	1.23	1.33
2	B	230	ARG	CZ-NH2	-7.56	1.23	1.33
2	B	416	ARG	CZ-NH2	-7.56	1.23	1.33
2	B	371	ARG	CZ-NH2	-7.55	1.23	1.33
9	I	80	ARG	CZ-NH2	-7.55	1.23	1.33
2	B	242	ARG	CZ-NH2	-7.55	1.23	1.33
2	B	608	ARG	CZ-NH2	-7.55	1.23	1.33
3	C	10	ARG	CZ-NH2	-7.55	1.23	1.33
3	C	106	ARG	CZ-NH1	-7.55	1.23	1.33
2	B	770	ARG	CZ-NH2	-7.54	1.23	1.33
1	A	401	ARG	CZ-NH2	-7.54	1.23	1.33
5	E	55	ARG	CZ-NH1	-7.54	1.23	1.33
29	h	83	ARG	CZ-NH2	-7.54	1.23	1.33
5	E	166	ARG	CZ-NH2	-7.53	1.23	1.33
9	I	15	ARG	CZ-NH2	-7.53	1.23	1.33
12	L	31	ARG	CZ-NH1	-7.53	1.23	1.33
11	K	106	ARG	CZ-NH2	-7.53	1.23	1.33
18	R	597	ARG	CZ-NH2	-7.53	1.23	1.33
18	R	371	ARG	CZ-NH1	-7.52	1.23	1.33
18	R	596	ARG	CZ-NH2	-7.52	1.23	1.33
28	c	42	ARG	CZ-NH2	-7.51	1.23	1.33
8	H	84	ARG	CZ-NH1	-7.51	1.23	1.33
2	B	1078	ARG	CZ-NH2	-7.49	1.23	1.33
25	Z	198	ARG	CZ-NH2	-7.49	1.23	1.33
1	A	220	ARG	CZ-NH2	-7.48	1.23	1.33
2	B	282	ARG	CZ-NH2	-7.47	1.23	1.33
2	B	1131	ARG	CZ-NH1	-7.47	1.23	1.33
1	A	743	ARG	CZ-NH2	-7.44	1.23	1.33
2	B	491	ARG	CZ-NH1	-7.43	1.23	1.33
26	a	128	ARG	CZ-NH1	-7.42	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	T	-21	DG	P-OP1	7.42	1.61	1.49
14	N	83	DG	P-OP1	7.41	1.61	1.49
26	e	128	ARG	CZ-NH1	-7.41	1.23	1.33
26	a	129	ARG	CZ-NH1	-7.41	1.23	1.33
14	N	17	DG	P-OP1	7.41	1.61	1.49
2	B	380	ARG	CZ-NH1	-7.40	1.23	1.33
19	T	-71	DG	P-OP1	7.40	1.61	1.49
14	N	110	DC	P-OP1	7.40	1.61	1.49
19	T	-131	DG	P-OP1	7.40	1.61	1.49
19	T	-135	DC	P-OP1	7.40	1.61	1.49
19	T	-69	DC	P-OP1	7.39	1.61	1.49
14	N	135	DG	P-OP1	7.39	1.61	1.49
14	N	136	DG	P-OP1	7.39	1.61	1.49
14	N	67	DG	P-OP1	7.39	1.61	1.49
14	N	66	DG	P-OP1	7.39	1.61	1.49
19	T	-67	DC	P-OP1	7.39	1.61	1.49
3	C	113	ARG	CZ-NH2	-7.39	1.23	1.33
14	N	133	DC	P-OP1	7.39	1.61	1.49
2	B	379	ARG	CZ-NH1	-7.39	1.23	1.33
19	T	-110	DG	P-OP1	7.39	1.61	1.49
1	A	1167	ARG	CZ-NH1	-7.38	1.23	1.33
19	T	-111	DC	P-OP1	7.38	1.61	1.49
14	N	15	DC	P-OP1	7.38	1.61	1.49
19	T	-141	DG	P-OP1	7.38	1.61	1.49
19	T	-83	DC	P-OP1	7.38	1.61	1.49
14	N	137	DG	P-OP1	7.38	1.61	1.49
19	T	-142	DA	P-OP1	7.38	1.61	1.49
19	T	-68	DC	P-OP1	7.38	1.61	1.49
19	T	-20	DA	P-OP1	7.38	1.61	1.49
14	N	138	DA	P-OP1	7.38	1.61	1.49
19	T	-15	DG	P-OP1	7.38	1.61	1.49
19	T	-134	DG	P-OP1	7.37	1.61	1.49
19	T	-105	DC	P-OP1	7.37	1.61	1.49
19	T	-19	DG	P-OP1	7.37	1.61	1.49
14	N	84	DC	P-OP1	7.37	1.61	1.49
19	T	-133	DG	P-OP1	7.37	1.61	1.49
19	T	-107	DG	P-OP1	7.37	1.61	1.49
14	N	85	DG	P-OP1	7.37	1.61	1.49
14	N	112	DA	P-OP1	7.37	1.61	1.49
14	N	72	DA	P-OP1	7.37	1.61	1.49
19	T	-29	DC	P-OP1	7.37	1.61	1.49
14	N	143	DG	P-OP1	7.36	1.61	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1355	ARG	CZ-NH1	-7.36	1.23	1.33
19	T	-136	DC	P-OP1	7.36	1.61	1.49
19	T	-18	DA	P-OP1	7.36	1.61	1.49
14	N	111	DG	P-OP1	7.36	1.61	1.49
14	N	132	DA	P-OP1	7.36	1.61	1.49
7	G	63	ARG	CZ-NH1	-7.36	1.23	1.33
19	T	-14	DA	P-OP1	7.36	1.61	1.49
14	N	134	DC	P-OP1	7.36	1.61	1.49
19	T	-106	DA	P-OP1	7.36	1.61	1.49
19	T	-17	DC	P-OP1	7.36	1.61	1.49
2	B	499	ARG	CZ-NH1	-7.35	1.23	1.33
19	T	-130	DC	P-OP1	7.35	1.61	1.49
14	N	144	DA	P-OP1	7.35	1.61	1.49
19	T	-139	DA	P-OP1	7.35	1.61	1.49
14	N	65	DA	P-OP1	7.35	1.61	1.49
19	T	-143	DC	P-OP1	7.35	1.61	1.49
9	I	103	ARG	CZ-NH1	-7.34	1.23	1.33
14	N	71	DC	P-OP1	7.34	1.61	1.49
14	N	109	DA	P-OP1	7.34	1.61	1.49
14	N	107	DC	P-OP1	7.34	1.61	1.49
19	T	-66	DC	P-OP1	7.34	1.61	1.49
19	T	-108	DA	P-OP1	7.34	1.61	1.49
19	T	-140	DA	P-OP1	7.33	1.61	1.49
19	T	-30	DA	P-OP1	7.33	1.61	1.49
19	T	-16	DA	P-OP1	7.33	1.61	1.49
3	C	160	ARG	CZ-NH1	-7.32	1.23	1.33
19	T	-87	DA	P-OP1	7.32	1.61	1.49
4	D	70	ARG	CZ-NH1	-7.31	1.23	1.33
27	b	55	ARG	CZ-NH1	-7.31	1.23	1.33
2	B	438	ARG	CZ-NH1	-7.31	1.23	1.33
2	B	975	ARG	CZ-NH1	-7.31	1.23	1.33
5	E	162	ARG	CZ-NH1	-7.30	1.23	1.33
26	e	129	ARG	CZ-NH1	-7.30	1.23	1.33
1	A	734	ARG	CZ-NH1	-7.30	1.23	1.33
6	F	100	ARG	CZ-NH1	-7.29	1.23	1.33
1	A	1224	ARG	CZ-NH1	-7.28	1.23	1.33
1	A	1046	ARG	CZ-NH1	-7.28	1.23	1.33
1	A	408	ARG	CZ-NH1	-7.27	1.23	1.33
1	A	407	ARG	CZ-NH1	-7.27	1.23	1.33
1	A	1345	ARG	CZ-NH1	-7.27	1.23	1.33
5	E	172	ARG	CZ-NH1	-7.26	1.23	1.33
1	A	61	ARG	CZ-NH1	-7.26	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	532	ARG	CZ-NH1	-7.25	1.23	1.33
12	L	51	ARG	CZ-NH1	-7.25	1.23	1.33
1	A	70	ARG	CZ-NH1	-7.25	1.23	1.33
18	R	438	ARG	CZ-NH1	-7.25	1.23	1.33
25	Z	246	ARG	CZ-NH1	-7.25	1.23	1.33
25	Z	283	ARG	CZ-NH1	-7.24	1.23	1.33
1	A	844	ARG	CZ-NH1	-7.24	1.23	1.33
1	A	1380	ARG	CZ-NH1	-7.24	1.23	1.33
17	Q	725	ARG	CZ-NH1	-7.23	1.23	1.33
17	Q	201	ARG	CZ-NH1	-7.23	1.23	1.33
26	e	134	ARG	CZ-NH1	-7.22	1.23	1.33
2	B	416	ARG	CZ-NH1	-7.21	1.23	1.33
25	Z	610	ARG	CZ-NH1	-7.21	1.23	1.33
17	Q	763	ARG	CZ-NH1	-7.20	1.23	1.33
20	U	411	ARG	CZ-NH1	-7.20	1.23	1.33
21	V	26	ARG	CZ-NH1	-7.20	1.23	1.33
5	E	202	ARG	CZ-NH1	-7.19	1.23	1.33
1	A	186	ARG	CZ-NH1	-7.19	1.23	1.33
1	A	292	ARG	CZ-NH1	-7.19	1.23	1.33
29	h	89	ARG	CZ-NH1	-7.19	1.23	1.33
17	Q	191	ARG	CZ-NH1	-7.18	1.23	1.33
17	Q	830	ARG	CZ-NH1	-7.18	1.23	1.33
2	B	938	ARG	CZ-NH1	-7.18	1.23	1.33
17	Q	667	ARG	CZ-NH1	-7.18	1.23	1.33
17	Q	218	ARG	CZ-NH1	-7.18	1.23	1.33
1	A	1153	ARG	CZ-NH1	-7.17	1.23	1.33
29	h	83	ARG	CZ-NH1	-7.17	1.23	1.33
1	A	551	ARG	CZ-NH1	-7.17	1.23	1.33
4	D	73	ARG	CZ-NH1	-7.17	1.23	1.33
1	A	523	ARG	CZ-NH1	-7.17	1.23	1.33
17	Q	791	ARG	CZ-NH1	-7.17	1.23	1.33
1	A	880	ARG	CZ-NH1	-7.17	1.23	1.33
1	A	1059	ARG	CZ-NH1	-7.17	1.23	1.33
2	B	841	ARG	CZ-NH1	-7.17	1.23	1.33
2	B	1091	ARG	CZ-NH1	-7.16	1.23	1.33
2	B	768	ARG	CZ-NH1	-7.16	1.23	1.33
7	G	144	ARG	CZ-NH1	-7.16	1.23	1.33
5	E	207	ARG	CZ-NH1	-7.15	1.23	1.33
27	f	67	ARG	CZ-NH1	-7.15	1.23	1.33
2	B	1104	ARG	CZ-NH1	-7.15	1.23	1.33
7	G	78	ARG	CZ-NH1	-7.15	1.23	1.33
20	U	409	ARG	CZ-NH1	-7.15	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	832	ARG	CZ-NH1	-7.15	1.23	1.33
1	A	557	ARG	CZ-NH1	-7.15	1.23	1.33
2	B	1150	ARG	CZ-NH1	-7.14	1.23	1.33
1	A	271	ARG	CZ-NH1	-7.14	1.23	1.33
6	F	51	ARG	CZ-NH1	-7.14	1.23	1.33
1	A	932	ARG	CZ-NH1	-7.14	1.23	1.33
20	U	387	ARG	CZ-NH1	-7.14	1.23	1.33
21	V	132	ARG	CZ-NH1	-7.14	1.23	1.33
1	A	1356	ARG	CZ-NH1	-7.14	1.23	1.33
1	A	421	ARG	CZ-NH1	-7.13	1.23	1.33
1	A	1375	ARG	CZ-NH1	-7.13	1.23	1.33
1	A	401	ARG	CZ-NH1	-7.13	1.23	1.33
2	B	41	ARG	CZ-NH1	-7.13	1.23	1.33
2	B	890	ARG	CZ-NH1	-7.13	1.23	1.33
24	Y	14	ARG	CZ-NH1	-7.13	1.23	1.33
1	A	1149	ARG	CZ-NH1	-7.12	1.23	1.33
2	B	770	ARG	CZ-NH1	-7.12	1.23	1.33
1	A	890	ARG	CZ-NH1	-7.12	1.23	1.33
2	B	721	ARG	CZ-NH1	-7.12	1.23	1.33
1	A	1160	ARG	CZ-NH1	-7.12	1.23	1.33
28	g	35	ARG	CZ-NH1	-7.12	1.23	1.33
3	C	133	ARG	CZ-NH1	-7.10	1.23	1.33
25	Z	494	ARG	CZ-NH1	-7.10	1.23	1.33
28	c	77	ARG	CZ-NH1	-7.10	1.23	1.33
25	Z	749	ARG	CZ-NH1	-7.10	1.23	1.33
2	B	608	ARG	CZ-NH1	-7.10	1.23	1.33
5	E	181	ARG	CZ-NH1	-7.10	1.23	1.33
2	B	371	ARG	CZ-NH1	-7.10	1.23	1.33
5	E	195	ARG	CZ-NH1	-7.09	1.23	1.33
9	I	33	ARG	CZ-NH1	-7.08	1.23	1.33
3	C	118	ARG	CZ-NH1	-7.08	1.23	1.33
1	A	583	ARG	CZ-NH1	-7.08	1.23	1.33
2	B	230	ARG	CZ-NH1	-7.07	1.23	1.33
2	B	282	ARG	CZ-NH1	-7.07	1.23	1.33
2	B	834	ARG	CZ-NH1	-7.07	1.23	1.33
1	A	1031	ARG	CZ-NH1	-7.07	1.23	1.33
1	A	1286	ARG	CZ-NH1	-7.07	1.23	1.33
4	D	121	ARG	CZ-NH1	-7.07	1.23	1.33
5	E	24	ARG	CZ-NH1	-7.06	1.23	1.33
28	c	42	ARG	CZ-NH1	-7.06	1.23	1.33
1	A	1218	ARG	CZ-NH1	-7.05	1.23	1.33
26	e	53	ARG	CZ-NH1	-7.05	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	11	ARG	CZ-NH1	-7.05	1.23	1.33
4	D	138	ARG	CZ-NH1	-7.05	1.23	1.33
28	g	42	ARG	CZ-NH1	-7.05	1.23	1.33
8	H	57	ARG	CZ-NH1	-7.05	1.23	1.33
2	B	83	ARG	CZ-NH1	-7.04	1.23	1.33
2	B	1035	ARG	CZ-NH1	-7.04	1.23	1.33
5	E	166	ARG	CZ-NH1	-7.04	1.23	1.33
2	B	610	ARG	CZ-NH1	-7.04	1.24	1.33
24	Y	111	ARG	CZ-NH1	-7.03	1.24	1.33
3	C	86	ARG	CZ-NH1	-7.03	1.24	1.33
20	U	439	ARG	CZ-NH1	-7.03	1.24	1.33
1	A	805	ARG	CZ-NH1	-7.03	1.24	1.33
2	B	242	ARG	CZ-NH1	-7.03	1.24	1.33
27	b	95	ARG	CZ-NH1	-7.02	1.24	1.33
9	I	40	ARG	CZ-NH1	-7.01	1.24	1.33
26	e	49	ARG	CZ-NH1	-7.01	1.24	1.33
3	C	228	ARG	CZ-NH1	-7.00	1.24	1.33
2	B	1023	ARG	CZ-NH1	-6.99	1.24	1.33
9	I	80	ARG	CZ-NH1	-6.98	1.24	1.33
11	K	106	ARG	CZ-NH1	-6.97	1.24	1.33
2	B	483	ARG	CZ-NH1	-6.97	1.24	1.33
18	R	597	ARG	CZ-NH1	-6.97	1.24	1.33
18	R	596	ARG	CZ-NH1	-6.97	1.24	1.33
9	I	15	ARG	CZ-NH1	-6.96	1.24	1.33
3	C	10	ARG	CZ-NH1	-6.95	1.24	1.33
1	A	220	ARG	CZ-NH1	-6.94	1.24	1.33
6	F	62	ARG	CZ-NH1	-6.94	1.24	1.33
2	B	425	ARG	CZ-NH1	-6.93	1.24	1.33
3	C	193	ARG	CZ-NH1	-6.92	1.24	1.33
2	B	1078	ARG	CZ-NH1	-6.91	1.24	1.33
3	C	113	ARG	CZ-NH1	-6.91	1.24	1.33
1	A	743	ARG	CZ-NH1	-6.91	1.24	1.33
25	Z	198	ARG	CZ-NH1	-6.88	1.24	1.33
14	N	105	DG	O3'-P	6.83	1.69	1.61
16	P	31	G	C8-N7	-6.75	1.26	1.30
19	T	-113	DG	O3'-P	6.61	1.69	1.61
14	N	47	DC	C4-N4	-6.43	1.28	1.33
2	B	120	TYR	CD2-CE2	-6.38	1.29	1.39
2	B	1018	TYR	CD1-CE1	-6.35	1.29	1.39
16	P	42	C	N1-C6	-6.33	1.33	1.37
13	M	352	GLY	N-CA	-6.21	1.36	1.46
3	C	230	TYR	CD2-CE2	-6.12	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	120	TYR	CD1-CE1	-6.12	1.30	1.39
9	I	37	TYR	CD1-CE1	-6.09	1.30	1.39
1	A	598	GLY	N-CA	-6.05	1.36	1.46
1	A	1425	GLY	N-CA	-6.04	1.36	1.46
1	A	763	TYR	CD2-CE2	-6.02	1.30	1.39
2	B	960	GLY	N-CA	-6.02	1.37	1.46
7	G	102	GLY	N-CA	-6.00	1.37	1.46
2	B	84	TYR	CD2-CE2	-6.00	1.30	1.39
1	A	616	GLY	N-CA	-6.00	1.37	1.46
16	P	44	U	C5'-C4'	-6.00	1.44	1.51
25	Z	715	GLY	N-CA	-6.00	1.37	1.46
1	A	763	TYR	CD1-CE1	-5.99	1.30	1.39
1	A	1395	TYR	CD2-CE2	-5.98	1.30	1.39
2	B	367	TYR	CD2-CE2	-5.98	1.30	1.39
2	B	521	GLY	N-CA	-5.97	1.37	1.46
2	B	997	GLY	N-CA	-5.97	1.37	1.46
3	C	220	TYR	CD1-CE1	-5.97	1.30	1.39
2	B	367	TYR	CD1-CE1	-5.96	1.30	1.39
1	A	827	TYR	CD2-CE2	-5.96	1.30	1.39
5	E	182	TYR	CD2-CE2	-5.94	1.30	1.39
3	C	230	TYR	CD1-CE1	-5.93	1.30	1.39
8	H	90	TYR	CD2-CE2	-5.92	1.30	1.39
6	F	119	GLY	N-CA	-5.91	1.37	1.46
1	A	444	TYR	CD2-CE2	-5.90	1.30	1.39
1	A	199	TYR	CD2-CE2	-5.89	1.30	1.39
3	C	19	VAL	CB-CG2	-5.89	1.40	1.52
11	K	61	TYR	CD2-CE2	-5.89	1.30	1.39
2	B	852	GLY	N-CA	-5.89	1.37	1.46
1	A	199	TYR	CD1-CE1	-5.89	1.30	1.39
2	B	182	GLY	N-CA	-5.87	1.37	1.46
3	C	151	VAL	CB-CG1	-5.87	1.40	1.52
1	A	1395	TYR	CD1-CE1	-5.86	1.30	1.39
5	E	109	GLY	N-CA	-5.86	1.37	1.46
2	B	729	GLY	N-CA	-5.85	1.37	1.46
2	B	490	GLY	N-CA	-5.84	1.37	1.46
3	C	197	TYR	CD1-CE1	-5.84	1.30	1.39
1	A	827	TYR	CD1-CE1	-5.83	1.30	1.39
2	B	724	TYR	CD1-CE1	-5.83	1.30	1.39
2	B	1034	GLY	N-CA	-5.83	1.37	1.46
3	C	186	TYR	CD2-CE2	-5.83	1.30	1.39
16	P	43	U	C5'-C4'	-5.82	1.44	1.51
1	A	1383	TYR	CD2-CE2	-5.81	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	T	-137	DC	C4-N4	-5.80	1.28	1.33
2	B	378	GLY	N-CA	-5.79	1.37	1.46
6	F	115	TYR	CD1-CE1	-5.79	1.30	1.39
21	V	28	GLY	N-CA	-5.78	1.37	1.46
6	F	56	TYR	CD2-CE2	-5.78	1.30	1.39
2	B	290	TYR	CD1-CE1	-5.78	1.30	1.39
2	B	571	GLY	N-CA	-5.77	1.37	1.46
2	B	724	TYR	CD2-CE2	-5.77	1.30	1.39
3	C	208	TYR	CD2-CE2	-5.76	1.30	1.39
2	B	619	GLY	N-CA	-5.76	1.37	1.46
1	A	444	TYR	CD1-CE1	-5.75	1.30	1.39
24	Y	85	TYR	CD1-CE1	-5.75	1.30	1.39
11	K	61	TYR	CD1-CE1	-5.75	1.30	1.39
8	H	65	TYR	CD1-CE1	-5.74	1.30	1.39
9	I	54	TYR	CD1-CE1	-5.74	1.30	1.39
2	B	979	GLY	N-CA	-5.74	1.37	1.46
5	E	105	VAL	CB-CG1	-5.74	1.40	1.52
1	A	187	TYR	CD1-CE1	-5.74	1.30	1.39
2	B	451	GLY	N-CA	-5.74	1.37	1.46
8	H	48	TYR	CD1-CE1	-5.74	1.30	1.39
3	C	197	TYR	CD2-CE2	-5.74	1.30	1.39
7	G	3	TYR	CD2-CE2	-5.73	1.30	1.39
5	E	203	TYR	CD2-CE2	-5.73	1.30	1.39
2	B	1020	TYR	CD1-CE1	-5.72	1.30	1.39
5	E	163	TYR	CD2-CE2	-5.72	1.30	1.39
2	B	183	GLY	N-CA	-5.72	1.37	1.46
5	E	184	GLY	N-CA	-5.71	1.37	1.46
9	I	44	TYR	CD2-CE2	-5.71	1.30	1.39
2	B	418	TYR	CD2-CE2	-5.71	1.30	1.39
1	A	699	TYR	CD1-CE1	-5.71	1.30	1.39
2	B	845	TYR	CD2-CE2	-5.71	1.30	1.39
21	V	35	TYR	CD1-CE1	-5.70	1.30	1.39
3	C	220	TYR	CD2-CE2	-5.70	1.30	1.39
1	A	56	GLY	N-CA	-5.70	1.37	1.46
2	B	916	TYR	CD1-CE1	-5.70	1.30	1.39
3	C	208	TYR	CD1-CE1	-5.70	1.30	1.39
5	E	89	VAL	CB-CG1	-5.70	1.40	1.52
2	B	84	TYR	CD1-CE1	-5.69	1.30	1.39
9	I	13	GLY	N-CA	-5.69	1.37	1.46
3	C	3	TYR	CD2-CE2	-5.69	1.30	1.39
1	A	1383	TYR	CD1-CE1	-5.68	1.30	1.39
2	B	865	VAL	CB-CG1	-5.68	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	940	GLY	N-CA	-5.68	1.37	1.46
3	C	186	TYR	CD1-CE1	-5.68	1.30	1.39
2	B	1024	GLY	N-CA	-5.68	1.37	1.46
8	H	48	TYR	CD2-CE2	-5.68	1.30	1.39
18	R	425	GLY	N-CA	-5.67	1.37	1.46
1	A	558	GLY	N-CA	-5.67	1.37	1.46
11	K	81	TYR	CD2-CE2	-5.67	1.30	1.39
4	D	37	VAL	CB-CG1	-5.67	1.41	1.52
16	P	30	C	N1-C6	-5.66	1.33	1.37
20	U	476	GLY	N-CA	-5.66	1.37	1.46
1	A	553	VAL	CB-CG2	-5.66	1.41	1.52
17	Q	697	TYR	CD2-CE2	-5.66	1.30	1.39
25	Z	634	GLY	N-CA	-5.66	1.37	1.46
1	A	1088	GLY	N-CA	-5.66	1.37	1.46
16	P	46	G	C6-N1	-5.66	1.35	1.39
1	A	69	GLY	N-CA	-5.66	1.37	1.46
2	B	290	TYR	CD2-CE2	-5.66	1.30	1.39
1	A	1446	GLY	N-CA	-5.66	1.37	1.46
2	B	446	TYR	CD2-CE2	-5.66	1.30	1.39
5	E	163	TYR	CD1-CE1	-5.65	1.30	1.39
6	F	56	TYR	CD1-CE1	-5.65	1.30	1.39
1	A	43	TYR	CD1-CE1	-5.65	1.30	1.39
1	A	858	GLY	N-CA	-5.65	1.37	1.46
2	B	338	TYR	CD1-CE1	-5.65	1.30	1.39
5	E	8	TYR	CD2-CE2	-5.65	1.30	1.39
18	R	415	TYR	CD2-CE2	-5.65	1.30	1.39
16	P	45	G	C6-N1	-5.65	1.35	1.39
11	K	81	TYR	CD1-CE1	-5.65	1.30	1.39
26	a	99	TYR	CD1-CE1	-5.65	1.30	1.39
1	A	830	GLY	N-CA	-5.64	1.37	1.46
5	E	8	TYR	CD1-CE1	-5.64	1.30	1.39
2	B	705	GLY	N-CA	-5.64	1.37	1.46
2	B	987	GLY	N-CA	-5.64	1.37	1.46
2	B	136	GLY	N-CA	-5.64	1.37	1.46
2	B	363	TYR	CD2-CE2	-5.64	1.30	1.39
5	E	90	TYR	CD2-CE2	-5.64	1.30	1.39
18	R	485	TYR	CD2-CE2	-5.64	1.30	1.39
3	C	50	VAL	CB-CG1	-5.63	1.41	1.52
2	B	418	TYR	CD1-CE1	-5.63	1.30	1.39
25	Z	633	GLY	N-CA	-5.63	1.37	1.46
5	E	203	TYR	CD1-CE1	-5.63	1.30	1.39
16	P	31	G	N9-C8	-5.62	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	916	TYR	CD2-CE2	-5.62	1.30	1.39
2	B	1135	TYR	CD1-CE1	-5.62	1.30	1.39
5	E	176	GLY	N-CA	-5.62	1.37	1.46
2	B	1020	TYR	CD2-CE2	-5.62	1.30	1.39
8	H	65	TYR	CD2-CE2	-5.62	1.30	1.39
7	G	40	GLY	N-CA	-5.61	1.37	1.46
3	C	3	TYR	CD1-CE1	-5.61	1.30	1.39
6	F	115	TYR	CD2-CE2	-5.61	1.30	1.39
2	B	338	TYR	CD2-CE2	-5.61	1.30	1.39
2	B	366	GLY	N-CA	-5.61	1.37	1.46
1	A	49	GLY	N-CA	-5.61	1.37	1.46
1	A	406	VAL	CB-CG2	-5.61	1.41	1.52
1	A	536	GLY	N-CA	-5.61	1.37	1.46
9	I	37	TYR	CD2-CE2	-5.60	1.30	1.39
1	A	43	TYR	CD2-CE2	-5.60	1.30	1.39
9	I	25	TYR	CD2-CE2	-5.60	1.30	1.39
17	Q	722	TYR	CD1-CE1	-5.60	1.30	1.39
2	B	150	GLY	N-CA	-5.60	1.37	1.46
5	E	119	VAL	CB-CG2	-5.60	1.41	1.52
2	B	189	GLY	N-CA	-5.59	1.37	1.46
5	E	90	TYR	CD1-CE1	-5.59	1.30	1.39
16	P	33	G	C5'-C4'	-5.59	1.44	1.51
26	a	99	TYR	CD2-CE2	-5.59	1.30	1.39
2	B	689	TYR	CD1-CE1	-5.59	1.30	1.39
2	B	1087	GLY	N-CA	-5.59	1.37	1.46
16	P	33	G	C6-N1	-5.59	1.35	1.39
24	Y	85	TYR	CD2-CE2	-5.59	1.30	1.39
1	A	699	TYR	CD2-CE2	-5.58	1.30	1.39
1	A	661	GLY	N-CA	-5.58	1.37	1.46
1	A	406	VAL	CB-CG1	-5.58	1.41	1.52
2	B	446	TYR	CD1-CE1	-5.58	1.30	1.39
1	A	534	VAL	CB-CG1	-5.58	1.41	1.52
2	B	38	GLY	N-CA	-5.58	1.37	1.46
18	R	418	GLY	N-CA	-5.58	1.37	1.46
2	B	828	VAL	CB-CG2	-5.57	1.41	1.52
1	A	1448	SER	CB-OG	-5.56	1.35	1.42
16	P	40	G	C6-N1	-5.56	1.35	1.39
20	U	393	TYR	CD1-CE1	-5.56	1.31	1.39
5	E	78	GLU	CB-CG	-5.55	1.41	1.52
5	E	182	TYR	CD1-CE1	-5.55	1.31	1.39
17	Q	712	TYR	CD2-CE2	-5.55	1.31	1.39
25	Z	707	GLY	N-CA	-5.55	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	589	LYS	CE-NZ	-5.55	1.35	1.49
2	B	1018	TYR	CD2-CE2	-5.55	1.31	1.39
13	M	1033	GLY	N-CA	-5.55	1.37	1.46
13	M	1412	TYR	CD1-CE1	-5.55	1.31	1.39
16	P	45	G	N7-C5	-5.55	1.35	1.39
16	P	46	G	N7-C5	-5.55	1.35	1.39
1	A	1528	TYR	CD1-CE1	-5.54	1.31	1.39
21	V	35	TYR	CD2-CE2	-5.54	1.31	1.39
2	B	548	TRP	CD1-NE1	-5.54	1.28	1.38
2	B	1135	TYR	CD2-CE2	-5.54	1.31	1.39
7	G	3	TYR	CD1-CE1	-5.54	1.31	1.39
2	B	493	GLY	N-CA	-5.54	1.37	1.46
1	A	195	GLY	N-CA	-5.54	1.37	1.46
2	B	868	GLY	N-CA	-5.54	1.37	1.46
1	A	63	GLY	N-CA	-5.54	1.37	1.46
1	A	789	GLY	N-CA	-5.54	1.37	1.46
25	Z	754	GLY	N-CA	-5.53	1.37	1.46
2	B	689	TYR	CD2-CE2	-5.53	1.31	1.39
8	H	53	GLY	N-CA	-5.53	1.37	1.46
13	M	1235	GLY	N-CA	-5.53	1.37	1.46
2	B	839	GLY	N-CA	-5.53	1.37	1.46
18	R	415	TYR	CD1-CE1	-5.53	1.31	1.39
2	B	1008	VAL	CB-CG1	-5.53	1.41	1.52
18	R	419	GLY	N-CA	-5.52	1.37	1.46
1	A	776	GLY	N-CA	-5.52	1.37	1.46
1	A	424	GLY	N-CA	-5.52	1.37	1.46
1	A	1390	GLY	N-CA	-5.52	1.37	1.46
7	G	167	TYR	CD2-CE2	-5.52	1.31	1.39
16	P	40	G	N7-C5	-5.52	1.35	1.39
2	B	845	TYR	CD1-CE1	-5.51	1.31	1.39
2	B	763	SER	CB-OG	-5.51	1.35	1.42
17	Q	186	TYR	CD1-CE1	-5.51	1.31	1.39
5	E	201	GLY	N-CA	-5.50	1.37	1.46
16	P	38	G	C2-N2	-5.50	1.29	1.34
8	H	90	TYR	CD1-CE1	-5.50	1.31	1.39
1	A	846	GLY	N-CA	-5.50	1.37	1.46
1	A	646	GLY	N-CA	-5.50	1.37	1.46
2	B	190	SER	CB-OG	-5.50	1.35	1.42
11	K	63	VAL	CB-CG2	-5.50	1.41	1.52
2	B	822	GLY	N-CA	-5.49	1.37	1.46
2	B	862	GLY	N-CA	-5.49	1.37	1.46
25	Z	203	TYR	CD1-CE1	-5.49	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1300	GLY	N-CA	-5.49	1.37	1.46
17	Q	722	TYR	CD2-CE2	-5.49	1.31	1.39
1	A	690	GLY	N-CA	-5.49	1.37	1.46
7	G	128	TYR	CD1-CE1	-5.49	1.31	1.39
27	b	57	VAL	CB-CG2	-5.49	1.41	1.52
2	B	1077	GLY	N-CA	-5.49	1.37	1.46
9	I	44	TYR	CD1-CE1	-5.49	1.31	1.39
13	M	874	GLY	N-CA	-5.49	1.37	1.46
20	U	408	GLY	N-CA	-5.49	1.37	1.46
17	Q	795	TYR	CD2-CE2	-5.48	1.31	1.39
16	P	42	C	C5'-C4'	-5.48	1.44	1.51
2	B	322	GLY	N-CA	-5.48	1.37	1.46
4	D	120	GLY	N-CA	-5.48	1.37	1.46
5	E	119	VAL	CB-CG1	-5.48	1.41	1.52
8	H	120	GLY	N-CA	-5.48	1.37	1.46
20	U	478	GLY	N-CA	-5.48	1.37	1.46
1	A	713	VAL	CB-CG1	-5.48	1.41	1.52
2	B	988	LYS	CE-NZ	-5.47	1.35	1.49
9	I	25	TYR	CD1-CE1	-5.47	1.31	1.39
11	K	107	VAL	CB-CG1	-5.47	1.41	1.52
18	R	485	TYR	CD1-CE1	-5.47	1.31	1.39
9	I	54	TYR	CD2-CE2	-5.47	1.31	1.39
6	F	67	GLY	N-CA	-5.46	1.37	1.46
6	F	95	LYS	CE-NZ	-5.46	1.35	1.49
26	e	132	GLY	N-CA	-5.46	1.37	1.46
1	A	187	TYR	CD2-CE2	-5.46	1.31	1.39
28	g	44	GLY	N-CA	-5.46	1.37	1.46
1	A	203	LYS	CE-NZ	-5.46	1.35	1.49
13	M	1412	TYR	CD2-CE2	-5.46	1.31	1.39
21	V	128	VAL	CB-CG1	-5.46	1.41	1.52
2	B	517	GLY	N-CA	-5.46	1.37	1.46
2	B	709	SER	CB-OG	-5.46	1.35	1.42
7	G	42	TYR	CD1-CE1	-5.46	1.31	1.39
7	G	129	LYS	CE-NZ	-5.46	1.35	1.49
17	Q	704	TYR	CD1-CE1	-5.45	1.31	1.39
24	Y	50	TYR	CD2-CE2	-5.45	1.31	1.39
1	A	633	GLY	N-CA	-5.45	1.37	1.46
2	B	904	VAL	CB-CG1	-5.45	1.41	1.52
7	G	34	VAL	CB-CG1	-5.45	1.41	1.52
13	M	540	GLY	N-CA	-5.45	1.37	1.46
1	A	324	GLY	N-CA	-5.45	1.37	1.46
27	b	51	TYR	CD1-CE1	-5.45	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f	101	GLY	N-CA	-5.45	1.37	1.46
7	G	42	TYR	CD2-CE2	-5.44	1.31	1.39
12	L	50	LYS	CE-NZ	-5.44	1.35	1.49
18	R	424	LYS	CE-NZ	-5.44	1.35	1.49
1	A	1070	GLY	N-CA	-5.44	1.37	1.46
1	A	64	VAL	CB-CG1	-5.44	1.41	1.52
2	B	363	TYR	CD1-CE1	-5.44	1.31	1.39
17	Q	792	TYR	CD2-CE2	-5.44	1.31	1.39
16	P	33	G	N7-C5	-5.44	1.35	1.39
20	U	393	TYR	CD2-CE2	-5.44	1.31	1.39
1	A	1528	TYR	CD2-CE2	-5.43	1.31	1.39
2	B	494	LYS	CE-NZ	-5.43	1.35	1.49
3	C	50	VAL	CB-CG2	-5.43	1.41	1.52
16	P	41	U	C5'-C4'	-5.43	1.44	1.51
2	B	828	VAL	CB-CG1	-5.42	1.41	1.52
18	R	486	LYS	CE-NZ	-5.42	1.35	1.49
3	C	181	GLY	N-CA	-5.42	1.38	1.46
5	E	188	GLY	N-CA	-5.42	1.38	1.46
9	I	12	VAL	CB-CG1	-5.42	1.41	1.52
13	M	547	GLY	N-CA	-5.42	1.38	1.46
18	R	407	GLY	N-CA	-5.42	1.38	1.46
2	B	1019	GLY	N-CA	-5.42	1.38	1.46
7	G	128	TYR	CD2-CE2	-5.42	1.31	1.39
17	Q	187	LYS	CE-NZ	-5.42	1.35	1.49
1	A	409	GLY	N-CA	-5.41	1.38	1.46
17	Q	704	TYR	CD2-CE2	-5.41	1.31	1.39
1	A	150	GLY	N-CA	-5.41	1.38	1.46
1	A	588	GLY	N-CA	-5.41	1.38	1.46
8	H	3	GLY	N-CA	-5.41	1.38	1.46
1	A	795	GLY	N-CA	-5.41	1.38	1.46
17	Q	697	TYR	CD1-CE1	-5.41	1.31	1.39
2	B	40	VAL	CB-CG1	-5.41	1.41	1.52
17	Q	795	TYR	CD1-CE1	-5.41	1.31	1.39
2	B	406	GLY	N-CA	-5.40	1.38	1.46
6	F	79	VAL	CB-CG1	-5.40	1.41	1.52
6	F	120	VAL	CB-CG2	-5.40	1.41	1.52
7	G	136	VAL	CB-CG1	-5.40	1.41	1.52
17	Q	186	TYR	CD2-CE2	-5.40	1.31	1.39
21	V	138	SER	CB-OG	-5.40	1.35	1.42
24	Y	50	TYR	CD1-CE1	-5.40	1.31	1.39
3	C	235	SER	CB-OG	-5.40	1.35	1.42
27	b	51	TYR	CD2-CE2	-5.40	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	203	TYR	CD2-CE2	-5.40	1.31	1.39
1	A	656	SER	CB-OG	-5.39	1.35	1.42
26	e	41	TYR	CD2-CE2	-5.39	1.31	1.39
1	A	97	VAL	CB-CG2	-5.39	1.41	1.52
2	B	426	GLY	N-CA	-5.39	1.38	1.46
6	F	79	VAL	CB-CG2	-5.39	1.41	1.52
1	A	1096	GLY	N-CA	-5.39	1.38	1.46
2	B	917	LYS	CE-NZ	-5.38	1.35	1.49
17	Q	792	TYR	CD1-CE1	-5.38	1.31	1.39
27	b	101	GLY	N-CA	-5.38	1.38	1.46
1	A	394	VAL	CB-CG2	-5.38	1.41	1.52
11	K	48	SER	CB-OG	-5.38	1.35	1.42
5	E	105	VAL	CB-CG2	-5.38	1.41	1.52
26	e	71	VAL	CB-CG1	-5.38	1.41	1.52
2	B	253	GLY	N-CA	-5.38	1.38	1.46
2	B	575	GLY	N-CA	-5.38	1.38	1.46
1	A	185	GLY	N-CA	-5.37	1.38	1.46
17	Q	712	TYR	CD1-CE1	-5.37	1.31	1.39
1	A	101	VAL	CB-CG1	-5.37	1.41	1.52
2	B	904	VAL	CB-CG2	-5.37	1.41	1.52
1	A	202	TRP	CD1-NE1	-5.37	1.28	1.38
2	B	443	GLY	N-CA	-5.37	1.38	1.46
21	V	223	GLY	N-CA	-5.37	1.38	1.46
27	b	56	GLY	N-CA	-5.37	1.38	1.46
2	B	480	SER	CB-OG	-5.36	1.35	1.42
16	P	40	G	C5'-C4'	-5.36	1.45	1.51
1	A	97	VAL	CB-CG1	-5.36	1.41	1.52
2	B	539	SER	CB-OG	-5.36	1.35	1.42
1	A	24	GLY	N-CA	-5.36	1.38	1.46
7	G	167	TYR	CD1-CE1	-5.36	1.31	1.39
27	b	48	GLY	N-CA	-5.36	1.38	1.46
1	A	1145	GLY	N-CA	-5.35	1.38	1.46
11	K	56	VAL	CB-CG2	-5.35	1.41	1.52
1	A	1067	TRP	CD1-NE1	-5.35	1.28	1.38
13	M	1055	GLY	N-CA	-5.35	1.38	1.46
27	f	77	LYS	CE-NZ	-5.35	1.35	1.49
1	A	394	VAL	CB-CG1	-5.35	1.41	1.52
5	E	89	VAL	CB-CG2	-5.34	1.41	1.52
11	K	43	GLY	N-CA	-5.34	1.38	1.46
2	B	919	CYS	CB-SG	-5.34	1.73	1.81
2	B	454	GLY	N-CA	-5.34	1.38	1.46
9	I	12	VAL	CB-CG2	-5.34	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	869	LYS	CE-NZ	-5.33	1.35	1.49
6	F	118	TRP	CD1-NE1	-5.33	1.28	1.38
1	A	787	VAL	CB-CG2	-5.33	1.41	1.52
10	J	15	GLY	N-CA	-5.33	1.38	1.46
26	e	79	LYS	CE-NZ	-5.33	1.35	1.49
25	Z	243	GLY	N-CA	-5.33	1.38	1.46
1	A	675	VAL	CB-CG1	-5.33	1.41	1.52
1	A	1002	SER	CB-OG	-5.33	1.35	1.42
26	e	71	VAL	CB-CG2	-5.33	1.41	1.52
1	A	443	GLY	N-CA	-5.32	1.38	1.46
1	A	1455	SER	CB-OG	-5.32	1.35	1.42
17	Q	200	VAL	CB-CG2	-5.32	1.41	1.52
26	e	41	TYR	CD1-CE1	-5.32	1.31	1.39
1	A	679	TRP	CD1-NE1	-5.32	1.28	1.38
1	A	653	VAL	CB-CG1	-5.32	1.41	1.52
1	A	1393	VAL	CB-CG2	-5.32	1.41	1.52
25	Z	483	GLY	N-CA	-5.32	1.38	1.46
3	C	172	GLU	CB-CG	-5.32	1.42	1.52
27	f	81	VAL	CB-CG2	-5.32	1.41	1.52
1	A	826	SER	CB-OG	-5.31	1.35	1.42
28	g	118	LYS	CE-NZ	-5.31	1.35	1.49
2	B	453	TRP	CD1-NE1	-5.31	1.28	1.38
7	G	109	SER	CB-OG	-5.31	1.35	1.42
25	Z	609	GLY	N-CA	-5.31	1.38	1.46
1	A	675	VAL	CB-CG2	-5.30	1.41	1.52
14	N	21	DC	C4-N4	-5.30	1.29	1.33
2	B	509	VAL	CB-CG2	-5.30	1.41	1.52
6	F	81	VAL	CB-CG1	-5.30	1.41	1.52
13	M	1366	VAL	CB-CG1	-5.30	1.41	1.52
11	K	82	SER	CB-OG	-5.30	1.35	1.42
7	G	58	VAL	CB-CG2	-5.30	1.41	1.52
2	B	989	VAL	CB-CG1	-5.30	1.41	1.52
3	C	203	TRP	CD1-NE1	-5.30	1.28	1.38
7	G	58	VAL	CB-CG1	-5.30	1.41	1.52
9	I	101	SER	CB-OG	-5.30	1.35	1.42
7	G	136	VAL	CB-CG2	-5.29	1.41	1.52
2	B	1039	SER	CB-OG	-5.29	1.35	1.42
17	Q	681	SER	CB-OG	-5.29	1.35	1.42
1	A	768	SER	CB-OG	-5.29	1.35	1.42
6	F	81	VAL	CB-CG2	-5.29	1.41	1.52
2	B	497	LYS	CE-NZ	-5.29	1.35	1.49
6	F	101	LYS	CE-NZ	-5.29	1.35	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1238	GLY	N-CA	-5.29	1.38	1.46
1	A	415	GLY	N-CA	-5.29	1.38	1.46
1	A	819	SER	CB-OG	-5.29	1.35	1.42
3	C	9	VAL	CB-CG2	-5.29	1.41	1.52
3	C	19	VAL	CB-CG1	-5.29	1.41	1.52
1	A	1479	LYS	CE-NZ	-5.28	1.35	1.49
25	Z	612	GLY	N-CA	-5.28	1.38	1.46
26	e	89	VAL	CB-CG2	-5.28	1.41	1.52
21	V	310	GLY	N-CA	-5.27	1.38	1.46
1	A	1290	SER	CB-OG	-5.27	1.35	1.42
2	B	1027	VAL	CB-CG2	-5.27	1.41	1.52
6	F	113	GLY	N-CA	-5.27	1.38	1.46
7	G	171	VAL	CB-CG2	-5.27	1.41	1.52
11	K	60	GLY	N-CA	-5.27	1.38	1.46
6	F	76	CYS	CB-SG	-5.27	1.73	1.81
11	K	56	VAL	CB-CG1	-5.27	1.41	1.52
12	L	30	SER	CB-OG	-5.27	1.35	1.42
25	Z	385	GLY	N-CA	-5.27	1.38	1.46
1	A	741	VAL	CB-CG1	-5.27	1.41	1.52
1	A	530	SER	CB-OG	-5.26	1.35	1.42
1	A	545	VAL	CB-CG1	-5.26	1.41	1.52
1	A	788	VAL	CB-CG2	-5.26	1.41	1.52
1	A	1047	SER	CB-OG	-5.26	1.35	1.42
2	B	573	TRP	CD1-NE1	-5.26	1.28	1.38
9	I	55	VAL	CB-CG2	-5.26	1.41	1.52
25	Z	627	LYS	CE-NZ	-5.26	1.35	1.49
1	A	1532	SER	CB-OG	-5.26	1.35	1.42
11	K	9	SER	CB-OG	-5.26	1.35	1.42
1	A	801	GLY	N-CA	-5.26	1.38	1.46
1	A	55	GLY	N-CA	-5.26	1.38	1.46
1	A	1147	SER	CB-OG	-5.26	1.35	1.42
17	Q	802	LYS	CE-NZ	-5.25	1.35	1.49
24	Y	69	SER	CB-OG	-5.25	1.35	1.42
25	Z	438	GLY	N-CA	-5.25	1.38	1.46
7	G	43	GLY	N-CA	-5.25	1.38	1.46
1	A	1348	SER	CB-OG	-5.25	1.35	1.42
2	B	831	LYS	CE-NZ	-5.25	1.35	1.49
8	H	83	SER	CB-OG	-5.25	1.35	1.42
24	Y	91	GLY	N-CA	-5.25	1.38	1.46
7	G	62	GLY	N-CA	-5.24	1.38	1.46
25	Z	423	GLY	N-CA	-5.24	1.38	1.46
5	E	179	VAL	CB-CG2	-5.24	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	545	VAL	CB-CG2	-5.24	1.41	1.52
25	Z	442	SER	CB-OG	-5.24	1.35	1.42
1	A	101	VAL	CB-CG2	-5.23	1.41	1.52
1	A	1391	SER	CB-OG	-5.23	1.35	1.42
21	V	308	GLY	N-CA	-5.23	1.38	1.46
1	A	1074	SER	CB-OG	-5.23	1.35	1.42
19	T	-84	DG	C2-N2	-5.23	1.29	1.34
1	A	777	SER	CB-OG	-5.23	1.35	1.42
2	B	902	GLY	N-CA	-5.23	1.38	1.46
24	Y	55	SER	CB-OG	-5.23	1.35	1.42
25	Z	282	LYS	CE-NZ	-5.23	1.35	1.49
1	A	436	SER	CB-OG	-5.23	1.35	1.42
27	f	81	VAL	CB-CG1	-5.22	1.41	1.52
13	M	624	GLY	N-CA	-5.22	1.38	1.46
1	A	615	SER	CB-OG	-5.22	1.35	1.42
1	A	741	VAL	CB-CG2	-5.22	1.41	1.52
2	B	1027	VAL	CB-CG1	-5.22	1.41	1.52
16	P	40	G	C2'-C1'	-5.22	1.47	1.53
1	A	76	GLY	N-CA	-5.22	1.38	1.46
1	A	217	SER	CB-OG	-5.22	1.35	1.42
1	A	823	VAL	CB-CG1	-5.22	1.41	1.52
7	G	84	VAL	CB-CG1	-5.22	1.41	1.52
18	R	413	LYS	CE-NZ	-5.22	1.36	1.49
1	A	285	LYS	CE-NZ	-5.21	1.36	1.49
2	B	1093	CYS	CB-SG	-5.21	1.73	1.81
11	K	75	VAL	CB-CG2	-5.21	1.41	1.52
19	T	-45	DG	C2-N2	-5.21	1.29	1.34
29	d	57	SER	CB-OG	-5.21	1.35	1.42
1	A	784	VAL	CB-CG1	-5.21	1.42	1.52
29	h	57	SER	CB-OG	-5.21	1.35	1.42
2	B	477	SER	CB-OG	-5.21	1.35	1.42
21	V	130	TRP	CD1-NE1	-5.21	1.29	1.38
2	B	865	VAL	CB-CG2	-5.21	1.42	1.52
25	Z	242	VAL	CB-CG2	-5.21	1.42	1.52
1	A	975	SER	CB-OG	-5.21	1.35	1.42
19	T	-31	DC	C4-N4	-5.21	1.29	1.33
3	C	206	SER	CB-OG	-5.20	1.35	1.42
2	B	329	GLY	N-CA	-5.20	1.38	1.46
1	A	225	PHE	C-N	-5.20	1.22	1.34
3	C	151	VAL	CB-CG2	-5.20	1.42	1.52
25	Z	250	TRP	CD1-NE1	-5.20	1.29	1.38
1	A	1210	TRP	CD1-NE1	-5.20	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	713	LYS	CE-NZ	-5.20	1.36	1.49
24	Y	74	TRP	CD1-NE1	-5.20	1.29	1.38
10	J	53	VAL	CB-CG2	-5.20	1.42	1.52
1	A	1524	ALA	CA-CB	-5.20	1.41	1.52
7	G	85	VAL	CB-CG2	-5.19	1.42	1.52
19	T	-24	DC	C4-N4	-5.19	1.29	1.33
13	M	1380	VAL	CB-CG1	-5.19	1.42	1.52
14	N	19	DC	C4-N4	-5.19	1.29	1.33
1	A	796	LYS	CE-NZ	-5.19	1.36	1.49
16	P	34	C	N1-C2	-5.19	1.34	1.40
17	Q	833	LYS	CE-NZ	-5.19	1.36	1.49
18	R	368	LYS	CE-NZ	-5.19	1.36	1.49
1	A	1531	TRP	CD1-NE1	-5.19	1.29	1.38
3	C	124	SER	CB-OG	-5.19	1.35	1.42
3	C	155	LYS	CE-NZ	-5.19	1.36	1.49
2	B	354	SER	CB-OG	-5.19	1.35	1.42
2	B	821	LYS	CE-NZ	-5.19	1.36	1.49
1	A	98	GLY	N-CA	-5.18	1.38	1.46
1	A	508	SER	CB-OG	-5.18	1.35	1.42
1	A	1393	VAL	CB-CG1	-5.18	1.42	1.52
3	C	56	SER	CB-OG	-5.18	1.35	1.42
3	C	175	LYS	CE-NZ	-5.18	1.36	1.49
5	E	191	VAL	CB-CG2	-5.18	1.42	1.52
16	P	35	C	N1-C2	-5.18	1.34	1.40
17	Q	710	LYS	CE-NZ	-5.18	1.36	1.49
21	V	82	VAL	CB-CG2	-5.18	1.42	1.52
25	Z	443	VAL	CB-CG2	-5.18	1.42	1.52
2	B	342	VAL	CB-CG2	-5.18	1.42	1.52
2	B	436	LYS	CE-NZ	-5.18	1.36	1.49
2	B	509	VAL	CB-CG1	-5.18	1.42	1.52
17	Q	216	LYS	CE-NZ	-5.18	1.36	1.49
11	K	63	VAL	CB-CG1	-5.18	1.42	1.52
24	Y	56	SER	CB-OG	-5.18	1.35	1.42
2	B	974	SER	CB-OG	-5.17	1.35	1.42
18	R	372	TRP	CD1-NE1	-5.17	1.29	1.38
2	B	989	VAL	CB-CG2	-5.17	1.42	1.52
8	H	105	SER	CB-OG	-5.17	1.35	1.42
17	Q	731	GLY	N-CA	-5.17	1.38	1.46
17	Q	737	LYS	CE-NZ	-5.17	1.36	1.49
2	B	447	SER	CB-OG	-5.17	1.35	1.42
13	M	1360	GLY	N-CA	-5.17	1.38	1.46
27	f	60	VAL	CB-CG1	-5.17	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	229	SER	CB-OG	-5.16	1.35	1.42
7	G	152	VAL	CB-CG2	-5.16	1.42	1.52
1	A	1168	LYS	CE-NZ	-5.16	1.36	1.49
1	A	845	GLU	CB-CG	-5.16	1.42	1.52
2	B	310	VAL	CB-CG2	-5.16	1.42	1.52
2	B	820	LYS	CE-NZ	-5.16	1.36	1.49
13	M	1378	VAL	CB-CG2	-5.16	1.42	1.52
17	Q	222	SER	CB-OG	-5.16	1.35	1.42
29	h	82	LYS	CE-NZ	-5.16	1.36	1.49
2	B	421	LYS	CE-NZ	-5.16	1.36	1.49
7	G	84	VAL	CB-CG2	-5.16	1.42	1.52
2	B	1016	SER	CB-OG	-5.16	1.35	1.42
7	G	169	GLY	N-CA	-5.15	1.38	1.46
13	M	1380	VAL	CB-CG2	-5.15	1.42	1.52
18	R	558	SER	CB-OG	-5.15	1.35	1.42
2	B	1008	VAL	CB-CG2	-5.15	1.42	1.52
7	G	171	VAL	CB-CG1	-5.15	1.42	1.52
27	b	87	VAL	CB-CG2	-5.15	1.42	1.52
29	d	52	SER	CB-OG	-5.15	1.35	1.42
1	A	784	VAL	CB-CG2	-5.15	1.42	1.52
17	Q	777	LYS	CE-NZ	-5.15	1.36	1.49
17	Q	799	VAL	CB-CG1	-5.15	1.42	1.52
14	N	45	DC	C4-N4	-5.14	1.29	1.33
17	Q	229	SER	CB-OG	-5.14	1.35	1.42
9	I	73	SER	CB-OG	-5.14	1.35	1.42
17	Q	692	VAL	CB-CG2	-5.14	1.42	1.52
17	Q	729	LYS	CE-NZ	-5.14	1.36	1.49
17	Q	767	SER	CB-OG	-5.14	1.35	1.42
2	B	706	VAL	CB-CG2	-5.14	1.42	1.52
17	Q	695	LYS	CE-NZ	-5.14	1.36	1.49
24	Y	70	TRP	CD1-NE1	-5.14	1.29	1.38
1	A	221	VAL	CB-CG2	-5.14	1.42	1.52
2	B	415	VAL	CB-CG1	-5.14	1.42	1.52
2	B	1079	SER	CB-OG	-5.14	1.35	1.42
21	V	27	SER	CB-OG	-5.14	1.35	1.42
22	W	254	LYS	CE-NZ	-5.14	1.36	1.49
3	C	196	VAL	CB-CG1	-5.14	1.42	1.52
13	M	587	GLY	N-CA	-5.14	1.38	1.46
17	Q	53	LYS	CE-NZ	-5.14	1.36	1.49
2	B	277	GLY	N-CA	-5.14	1.38	1.46
9	I	72	VAL	CB-CG1	-5.14	1.42	1.52
25	Z	478	VAL	CB-CG1	-5.14	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	126	SER	CB-OG	-5.13	1.35	1.42
7	G	152	VAL	CB-CG1	-5.13	1.42	1.52
29	d	31	LYS	CE-NZ	-5.13	1.36	1.49
24	Y	84	VAL	CB-CG2	-5.13	1.42	1.52
1	A	11	SER	CB-OG	-5.13	1.35	1.42
17	Q	784	LYS	CE-NZ	-5.13	1.36	1.49
1	A	581	LYS	CE-NZ	-5.13	1.36	1.49
2	B	279	VAL	CB-CG2	-5.13	1.42	1.52
7	G	34	VAL	CB-CG2	-5.13	1.42	1.52
13	M	1393	ALA	CA-CB	-5.13	1.41	1.52
29	d	43	LYS	CE-NZ	-5.13	1.36	1.49
4	D	18	SER	CB-OG	-5.13	1.35	1.42
21	V	106	LYS	CE-NZ	-5.13	1.36	1.49
26	e	57	SER	CB-OG	-5.13	1.35	1.42
1	A	1208	SER	CB-OG	-5.12	1.35	1.42
2	B	351	VAL	CB-CG1	-5.12	1.42	1.52
2	B	893	SER	CB-OG	-5.12	1.35	1.42
13	M	1378	VAL	CB-CG1	-5.12	1.42	1.52
17	Q	773	LYS	CE-NZ	-5.12	1.36	1.49
1	A	446	VAL	CB-CG2	-5.12	1.42	1.52
1	A	1214	VAL	CB-CG2	-5.12	1.42	1.52
2	B	706	VAL	CB-CG1	-5.12	1.42	1.52
29	d	53	SER	CB-OG	-5.12	1.35	1.42
11	K	75	VAL	CB-CG1	-5.12	1.42	1.52
17	Q	692	VAL	CB-CG1	-5.12	1.42	1.52
21	V	189	SER	CB-OG	-5.12	1.35	1.42
29	d	40	LYS	CE-NZ	-5.12	1.36	1.49
1	A	823	VAL	CB-CG2	-5.11	1.42	1.52
2	B	323	SER	CB-OG	-5.11	1.35	1.42
17	Q	768	VAL	CB-CG1	-5.11	1.42	1.52
23	X	240	SER	CB-OG	-5.11	1.35	1.42
13	M	1366	VAL	CB-CG2	-5.11	1.42	1.52
1	A	550	LYS	CE-NZ	-5.11	1.36	1.49
2	B	445	LYS	CE-NZ	-5.11	1.36	1.49
7	G	85	VAL	CB-CG1	-5.11	1.42	1.52
25	Z	601	LYS	CE-NZ	-5.11	1.36	1.49
27	f	70	VAL	CB-CG2	-5.11	1.42	1.52
4	D	117	SER	CB-OG	-5.11	1.35	1.42
11	K	62	LYS	CE-NZ	-5.10	1.36	1.49
26	a	87	SER	CB-OG	-5.10	1.35	1.42
1	A	1155	LYS	CE-NZ	-5.10	1.36	1.49
2	B	816	GLU	CB-CG	-5.10	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	48	DC	C4-N4	-5.10	1.29	1.33
27	b	86	VAL	CB-CG1	-5.10	1.42	1.52
11	K	18	LYS	CE-NZ	-5.10	1.36	1.49
3	C	156	GLY	N-CA	-5.10	1.38	1.46
17	Q	188	LYS	CE-NZ	-5.10	1.36	1.49
24	Y	8	LYS	CE-NZ	-5.10	1.36	1.49
24	Y	54	SER	CB-OG	-5.10	1.35	1.42
25	Z	479	LYS	CE-NZ	-5.10	1.36	1.49
25	Z	630	VAL	CB-CG2	-5.10	1.42	1.52
25	Z	439	LYS	CE-NZ	-5.10	1.36	1.49
17	Q	732	LYS	CE-NZ	-5.09	1.36	1.49
1	A	446	VAL	CB-CG1	-5.09	1.42	1.52
1	A	194	SER	CB-OG	-5.09	1.35	1.42
1	A	553	VAL	CB-CG1	-5.09	1.42	1.52
2	B	342	VAL	CB-CG1	-5.09	1.42	1.52
17	Q	798	LYS	CE-NZ	-5.09	1.36	1.49
1	A	538	VAL	CB-CG2	-5.09	1.42	1.52
1	A	653	VAL	CB-CG2	-5.09	1.42	1.52
1	A	787	VAL	CB-CG1	-5.09	1.42	1.52
18	R	527	GLY	N-CA	-5.09	1.38	1.46
11	K	47	LYS	CE-NZ	-5.08	1.36	1.49
19	T	-26	DG	C2-N2	-5.08	1.29	1.34
25	Z	512	LYS	CE-NZ	-5.08	1.36	1.49
28	g	19	SER	CB-OG	-5.08	1.35	1.42
4	D	37	VAL	CB-CG2	-5.08	1.42	1.52
5	E	117	SER	CB-OG	-5.08	1.35	1.42
26	e	89	VAL	CB-CG1	-5.08	1.42	1.52
25	Z	473	LYS	CE-NZ	-5.08	1.36	1.49
27	f	60	VAL	CB-CG2	-5.08	1.42	1.52
29	h	84	SER	CB-OG	-5.08	1.35	1.42
1	A	445	LYS	CE-NZ	-5.08	1.36	1.49
2	B	361	LYS	CE-NZ	-5.08	1.36	1.49
5	E	12	LYS	CE-NZ	-5.08	1.36	1.49
17	Q	673	VAL	CB-CG2	-5.08	1.42	1.52
21	V	127	VAL	CB-CG1	-5.08	1.42	1.52
11	K	10	PHE	CD1-CE1	-5.07	1.29	1.39
7	G	88	VAL	CB-CG2	-5.07	1.42	1.52
8	H	146	LYS	CE-NZ	-5.07	1.36	1.49
1	A	1214	VAL	CB-CG1	-5.07	1.42	1.52
3	C	196	VAL	CB-CG2	-5.07	1.42	1.52
11	K	112	LYS	CE-NZ	-5.07	1.36	1.49
24	Y	83	GLY	N-CA	-5.07	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	873	VAL	CB-CG2	-5.07	1.42	1.52
8	H	59	VAL	CB-CG2	-5.07	1.42	1.52
25	Z	630	VAL	CB-CG1	-5.07	1.42	1.52
1	A	879	VAL	CB-CG2	-5.06	1.42	1.52
18	R	409	VAL	CB-CG1	-5.06	1.42	1.52
21	V	29	VAL	CB-CG1	-5.06	1.42	1.52
29	d	50	GLY	N-CA	-5.06	1.38	1.46
28	g	43	VAL	CB-CG2	-5.06	1.42	1.52
1	A	53	LYS	CE-NZ	-5.06	1.36	1.49
19	T	-51	DC	C4-N4	-5.06	1.29	1.33
17	Q	683	VAL	CB-CG2	-5.06	1.42	1.52
1	A	788	VAL	CB-CG1	-5.06	1.42	1.52
1	A	1025	GLY	N-CA	-5.06	1.38	1.46
1	A	1030	SER	CB-OG	-5.06	1.35	1.42
2	B	701	SER	CB-OG	-5.06	1.35	1.42
8	H	147	LYS	CE-NZ	-5.06	1.36	1.49
17	Q	673	VAL	CB-CG1	-5.06	1.42	1.52
1	A	212	LYS	CE-NZ	-5.05	1.36	1.49
2	B	352	GLY	N-CA	-5.05	1.38	1.46
13	M	1117	GLY	N-CA	-5.05	1.38	1.46
25	Z	453	LYS	CE-NZ	-5.05	1.36	1.49
2	B	690	CYS	CB-SG	-5.05	1.73	1.81
18	R	436	VAL	CB-CG2	-5.05	1.42	1.52
21	V	29	VAL	CB-CG2	-5.05	1.42	1.52
25	Z	214	SER	CB-OG	-5.05	1.35	1.42
2	B	569	VAL	CB-CG1	-5.05	1.42	1.52
18	R	436	VAL	CB-CG1	-5.05	1.42	1.52
1	A	1013	VAL	CB-CG2	-5.05	1.42	1.52
1	A	1094	SER	CB-OG	-5.05	1.35	1.42
1	A	713	VAL	CB-CG2	-5.04	1.42	1.52
3	C	20	LYS	CE-NZ	-5.04	1.36	1.49
2	B	937	SER	CB-OG	-5.04	1.35	1.42
19	T	-32	DA	C5-C4	-5.04	1.35	1.38
24	Y	23	LYS	CE-NZ	-5.04	1.36	1.49
19	T	-55	DC	C4-N4	-5.04	1.29	1.33
1	A	775	LYS	CE-NZ	-5.04	1.36	1.49
25	Z	646	ALA	CA-CB	-5.04	1.41	1.52
25	Z	241	GLY	N-CA	-5.04	1.38	1.46
3	C	9	VAL	CB-CG1	-5.03	1.42	1.52
14	N	46	DC	C4-N4	-5.03	1.29	1.33
2	B	310	VAL	CB-CG1	-5.03	1.42	1.52
1	A	534	VAL	CB-CG2	-5.03	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	199	LYS	CE-NZ	-5.03	1.36	1.49
1	A	1387	SER	CB-OG	-5.03	1.35	1.42
1	A	812	LYS	CE-NZ	-5.03	1.36	1.49
1	A	1283	VAL	CB-CG1	-5.03	1.42	1.52
6	F	120	VAL	CB-CG1	-5.03	1.42	1.52
17	Q	757	VAL	CB-CG2	-5.03	1.42	1.52
6	F	114	SER	CB-OG	-5.03	1.35	1.42
21	V	126	LYS	CE-NZ	-5.03	1.36	1.49
25	Z	266	VAL	CB-CG2	-5.03	1.42	1.52
2	B	413	LYS	CE-NZ	-5.02	1.36	1.49
7	G	105	SER	CB-OG	-5.02	1.35	1.42
16	P	34	C	C5'-C4'	-5.02	1.45	1.51
1	A	1021	VAL	CB-CG1	-5.02	1.42	1.52
5	E	209	VAL	CB-CG2	-5.02	1.42	1.52
13	M	997	GLY	N-CA	-5.02	1.38	1.46
1	A	887	VAL	CB-CG1	-5.02	1.42	1.52
2	B	415	VAL	CB-CG2	-5.02	1.42	1.52
4	D	94	LYS	CE-NZ	-5.01	1.36	1.49
7	G	76	VAL	CB-CG2	-5.01	1.42	1.52
3	C	254	LYS	CE-NZ	-5.01	1.36	1.49
8	H	59	VAL	CB-CG1	-5.01	1.42	1.52
1	A	1355	VAL	CB-CG1	-5.01	1.42	1.52
2	B	691	SER	CB-OG	-5.01	1.35	1.42
25	Z	215	VAL	CB-CG1	-5.01	1.42	1.52
27	f	57	VAL	CB-CG1	-5.01	1.42	1.52
2	B	409	LYS	CE-NZ	-5.00	1.36	1.49
17	Q	719	VAL	CB-CG1	-5.00	1.42	1.52
18	R	409	VAL	CB-CG2	-5.00	1.42	1.52
2	B	158	SER	CB-OG	-5.00	1.35	1.42
1	A	556	GLU	CB-CG	-5.00	1.42	1.52
1	A	1013	VAL	CB-CG1	-5.00	1.42	1.52
2	B	566	LYS	CE-NZ	-5.00	1.36	1.49
28	g	18	SER	CB-OG	-5.00	1.35	1.42

All (1066) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	107	DC	OP1-P-O3'	-45.63	4.81	105.20
14	N	85	DG	OP1-P-O3'	-45.29	5.57	105.20
19	T	-71	DG	OP1-P-O3'	-45.29	5.57	105.20
14	N	86	DT	OP1-P-O3'	-45.28	5.58	105.20
19	T	-133	DG	OP1-P-O3'	-45.26	5.63	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	15	DC	OP1-P-O3'	-44.98	6.25	105.20
14	N	139	DT	OP1-P-O3'	-44.76	6.73	105.20
19	T	-110	DG	OP1-P-O3'	-44.41	7.49	105.20
14	N	138	DA	OP1-P-O3'	-43.85	8.72	105.20
13	M	1329	HIS	C-N-CD	-24.38	66.96	120.60
14	N	57	DT	O5'-P-OP2	-24.05	81.84	110.70
19	T	-113	DG	O3'-P-O5'	23.67	148.98	104.00
14	N	105	DG	OP1-P-O3'	-23.42	53.68	105.20
14	N	57	DT	O5'-P-OP1	-22.75	83.40	110.70
19	T	-113	DG	OP1-P-O3'	-22.70	55.27	105.20
14	N	105	DG	O3'-P-O5'	20.59	143.11	104.00
14	N	105	DG	OP2-P-O3'	-20.20	60.75	105.20
19	T	-113	DG	OP2-P-O3'	-18.73	63.99	105.20
16	P	40	G	C2-N3-C4	18.52	121.16	111.90
16	P	33	G	C2-N3-C4	18.48	121.14	111.90
16	P	45	G	C2-N3-C4	18.47	121.13	111.90
16	P	46	G	C2-N3-C4	18.46	121.13	111.90
16	P	33	G	N3-C4-C5	-17.91	119.65	128.60
16	P	46	G	N3-C4-C5	-17.88	119.66	128.60
16	P	40	G	N3-C4-C5	-17.86	119.67	128.60
16	P	45	G	N3-C4-C5	-17.84	119.68	128.60
14	N	56	DT	O3'-P-O5'	15.33	133.12	104.00
16	P	45	G	C5-C6-N1	13.74	118.37	111.50
16	P	46	G	C5-C6-N1	13.73	118.36	111.50
16	P	40	G	C5-C6-N1	13.72	118.36	111.50
16	P	45	G	N3-C4-N9	13.71	134.23	126.00
16	P	40	G	N3-C4-N9	13.69	134.21	126.00
16	P	33	G	C5-C6-N1	13.67	118.34	111.50
16	P	33	G	N3-C4-N9	13.67	134.20	126.00
16	P	46	G	N3-C4-N9	13.67	134.20	126.00
16	P	45	G	C5-C6-O6	-12.95	120.83	128.60
16	P	46	G	C5-C6-O6	-12.90	120.86	128.60
16	P	33	G	C5-C6-O6	-12.87	120.88	128.60
16	P	40	G	C5-C6-O6	-12.85	120.89	128.60
13	M	327	THR	C-N-CD	-12.26	93.62	120.60
14	N	56	DT	OP1-P-O3'	-12.15	78.47	105.20
14	N	105	DG	P-O3'-C3'	11.92	134.01	119.70
19	T	-103	DG	O4'-C1'-N9	11.75	116.22	108.00
19	T	-113	DG	P-O3'-C3'	11.62	133.64	119.70
16	P	36	U	C2-N3-C4	-11.35	120.19	127.00
16	P	39	U	C2-N3-C4	-11.32	120.21	127.00
16	P	41	U	C2-N3-C4	-11.30	120.22	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	44	U	C2-N3-C4	-11.29	120.23	127.00
16	P	29	U	C2-N3-C4	-11.27	120.24	127.00
16	P	32	U	C2-N3-C4	-11.26	120.24	127.00
16	P	43	U	C2-N3-C4	-11.22	120.27	127.00
16	P	31	G	N7-C8-N9	11.12	118.66	113.10
14	N	57	DT	OP1-P-OP2	11.04	136.16	119.60
19	T	-132	DT	OP1-P-OP2	-10.87	103.29	119.60
14	N	14	DT	OP1-P-OP2	-10.87	103.30	119.60
14	N	16	DT	OP1-P-OP2	-10.87	103.30	119.60
14	N	139	DT	OP1-P-OP2	-10.87	103.30	119.60
19	T	-144	DT	OP1-P-OP2	-10.87	103.30	119.60
14	N	86	DT	OP1-P-OP2	-10.87	103.30	119.60
14	N	106	DT	OP1-P-OP2	-10.87	103.30	119.60
19	T	-112	DT	OP1-P-OP2	-10.87	103.30	119.60
19	T	-109	DT	OP1-P-OP2	-10.87	103.30	119.60
14	N	108	DT	OP1-P-OP2	-10.86	103.30	119.60
14	N	87	DT	OP1-P-OP2	-10.85	103.32	119.60
14	N	140	DT	OP1-P-OP2	-10.85	103.32	119.60
19	T	-70	DT	OP1-P-OP2	-10.85	103.33	119.60
14	N	39	DT	OP1-P-OP2	-10.85	103.33	119.60
1	A	220	ARG	N-CA-CB	10.77	129.99	110.60
13	M	1360	GLY	N-CA-C	10.58	139.54	113.10
14	N	56	DT	OP2-P-O3'	-10.47	82.17	105.20
25	Z	757	ARG	C-N-CD	-10.40	97.71	120.60
2	B	591	ARG	NE-CZ-NH2	10.31	125.46	120.30
16	P	46	G	C5-N7-C8	10.18	109.39	104.30
1	A	985	ARG	NE-CZ-NH2	10.15	125.38	120.30
16	P	41	U	N1-C2-N3	10.13	120.98	114.90
16	P	36	U	N1-C2-N3	10.13	120.98	114.90
16	P	32	U	N1-C2-N3	10.12	120.97	114.90
16	P	29	U	N1-C2-N3	10.11	120.97	114.90
3	C	36	ARG	NE-CZ-NH2	10.10	125.35	120.30
16	P	33	G	C5-N7-C8	10.10	109.35	104.30
16	P	44	U	N1-C2-N3	10.09	120.95	114.90
16	P	39	U	N1-C2-N3	10.08	120.95	114.90
16	P	40	G	C5-N7-C8	10.05	109.33	104.30
16	P	45	G	C5-N7-C8	10.05	109.32	104.30
16	P	43	U	N1-C2-N3	10.01	120.90	114.90
14	N	99	DA	N1-C6-N6	-9.98	112.61	118.60
19	T	-78	DA	N1-C6-N6	-9.94	112.63	118.60
13	M	1358	SER	N-CA-C	9.86	137.62	111.00
19	T	-23	DA	N1-C6-N6	-9.71	112.77	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	PRO	N-CA-CB	-9.66	91.71	103.30
19	T	-35	DA	N1-C6-N6	-9.61	112.83	118.60
19	T	-88	DA	N1-C6-N6	-9.58	112.85	118.60
16	P	29	U	C5-C4-O4	-9.45	120.23	125.90
16	P	43	U	C5-C4-O4	-9.43	120.24	125.90
16	P	32	U	C5-C4-O4	-9.43	120.25	125.90
16	P	31	G	C6-N1-C2	9.41	130.75	125.10
16	P	41	U	C5-C4-O4	-9.39	120.27	125.90
16	P	44	U	C5-C4-O4	-9.37	120.28	125.90
16	P	39	U	C5-C4-O4	-9.31	120.32	125.90
16	P	36	U	C5-C4-O4	-9.29	120.33	125.90
14	N	64	DA	N1-C6-N6	-9.15	113.11	118.60
19	T	-43	DA	N1-C6-N6	-9.06	113.16	118.60
14	N	120	DA	N1-C6-N6	-9.03	113.18	118.60
1	A	225	PHE	O-C-N	-8.99	108.32	122.70
16	P	33	G	C4-C5-N7	-8.98	107.21	110.80
16	P	46	G	C4-C5-N7	-8.95	107.22	110.80
19	T	-44	DA	N1-C6-N6	-8.95	113.23	118.60
14	N	101	DA	N1-C6-N6	-8.90	113.26	118.60
16	P	40	G	C4-C5-N7	-8.89	107.24	110.80
1	A	218	PRO	CB-CA-C	-8.88	89.80	112.00
19	T	-118	DA	N1-C6-N6	-8.85	113.29	118.60
16	P	45	G	C4-C5-N7	-8.84	107.26	110.80
14	N	113	DC	O4'-C1'-N1	8.79	114.15	108.00
28	g	32	ARG	NE-CZ-NH2	8.69	124.64	120.30
19	T	-49	DA	N1-C6-N6	-8.65	113.41	118.60
4	D	84	ARG	NE-CZ-NH2	8.64	124.62	120.30
1	A	1396	ARG	NE-CZ-NH2	8.63	124.62	120.30
19	T	-49	DA	C5-C6-N1	8.63	122.02	117.70
13	M	1358	SER	O-C-N	8.62	136.50	122.70
19	T	-56	DA	N1-C6-N6	-8.62	113.43	118.60
2	B	724	TYR	CB-CG-CD2	8.52	126.11	121.00
19	T	-105	DC	P-O3'-C3'	8.46	129.86	119.70
1	A	282	ASP	CB-CA-C	8.44	127.27	110.40
19	T	-119	DC	N3-C2-O2	-8.43	116.00	121.90
7	G	128	TYR	CB-CG-CD2	8.43	126.06	121.00
19	T	-27	DA	N1-C6-N6	-8.42	113.55	118.60
14	N	116	DA	N1-C6-N6	-8.40	113.56	118.60
2	B	114	ARG	NE-CZ-NH2	8.38	124.49	120.30
2	B	743	ARG	NE-CZ-NH2	8.37	124.48	120.30
14	N	122	DC	N3-C2-O2	-8.37	116.04	121.90
19	T	-86	DA	N1-C6-N6	-8.33	113.60	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ARG	O-C-N	-8.27	109.46	122.70
1	A	444	TYR	CB-CG-CD2	8.27	125.96	121.00
14	N	79	DA	O4'-C1'-N9	8.24	113.77	108.00
19	T	-39	DA	N1-C6-N6	-8.23	113.66	118.60
19	T	-58	DA	N1-C6-N6	-8.22	113.67	118.60
16	P	36	U	O4'-C1'-N1	8.21	114.77	108.20
19	T	-35	DA	C4-C5-C6	-8.20	112.90	117.00
14	N	142	DT	O4'-C1'-N1	8.20	113.74	108.00
19	T	-117	DA	C5-C6-N1	8.16	121.78	117.70
19	T	-32	DA	N1-C6-N6	-8.14	113.72	118.60
14	N	70	DA	O4'-C1'-N9	8.13	113.69	108.00
19	T	-39	DA	C5-C6-N1	8.13	121.76	117.70
19	T	-60	DA	O4'-C1'-N9	8.12	113.69	108.00
5	E	129	GLN	O-C-N	-8.12	109.71	122.70
14	N	53	DC	N3-C2-O2	-8.08	116.25	121.90
28	g	88	ARG	NE-CZ-NH2	8.08	124.34	120.30
2	B	495	LEU	O-C-N	-8.05	109.82	122.70
19	T	-113	DG	C4'-C3'-C2'	-8.05	95.86	103.10
16	P	39	U	N3-C4-C5	8.04	119.43	114.60
26	a	131	ARG	NE-CZ-NH2	8.04	124.32	120.30
16	P	41	U	N3-C4-C5	8.04	119.42	114.60
14	N	19	DC	N3-C2-O2	-8.03	116.28	121.90
16	P	29	U	N3-C4-C5	8.03	119.42	114.60
16	P	32	U	N3-C4-C5	8.03	119.42	114.60
11	K	74	ARG	NE-CZ-NH2	8.02	124.31	120.30
19	T	-96	DC	N3-C2-O2	-8.01	116.30	121.90
16	P	43	U	N3-C4-C5	8.00	119.40	114.60
16	P	44	U	N3-C4-C5	8.00	119.40	114.60
16	P	36	U	N3-C4-C5	8.00	119.40	114.60
19	T	-86	DA	C5-C6-N1	8.00	121.70	117.70
16	P	40	G	C6-N1-C2	-8.00	120.30	125.10
16	P	46	G	C6-N1-C2	-7.97	120.32	125.10
14	N	97	DC	N3-C2-O2	-7.96	116.33	121.90
1	A	699	TYR	CB-CG-CD2	7.96	125.77	121.00
16	P	45	G	C6-N1-C2	-7.95	120.33	125.10
16	P	33	G	C6-N1-C2	-7.93	120.34	125.10
19	T	-41	DA	N1-C6-N6	-7.92	113.85	118.60
19	T	-82	DA	N1-C6-N6	-7.92	113.85	118.60
19	T	-60	DA	C5-C6-N1	7.92	121.66	117.70
19	T	-32	DA	C5-C6-N1	7.92	121.66	117.70
19	T	-95	DA	C5-C6-N1	7.91	121.66	117.70
14	N	115	DA	N1-C6-N6	-7.90	113.86	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	79	DA	C5-C6-N1	7.90	121.65	117.70
19	T	-36	DC	O4'-C4'-C3'	-7.87	101.28	106.00
26	e	116	ARG	NE-CZ-NH2	7.87	124.24	120.30
13	M	1359	LYS	C-N-CA	7.85	138.78	122.30
1	A	241	ARG	NE-CZ-NH2	7.84	124.22	120.30
19	T	-95	DA	N1-C6-N6	-7.83	113.90	118.60
19	T	-59	DA	C5-C6-N1	7.83	121.61	117.70
2	B	924	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	A	1528	TYR	CB-CG-CD2	7.82	125.69	121.00
19	T	-104	DA	N1-C6-N6	-7.82	113.91	118.60
19	T	-60	DA	N1-C6-N6	-7.81	113.91	118.60
19	T	-113	DG	O4'-C4'-C3'	7.81	110.69	106.00
14	N	70	DA	C5-C6-N1	7.78	121.59	117.70
5	E	129	GLN	C-N-CA	7.78	141.15	121.70
19	T	-28	DC	N3-C2-O2	-7.78	116.45	121.90
19	T	-32	DA	C4-C5-C6	-7.77	113.12	117.00
19	T	-113	DG	O4'-C1'-N9	7.76	113.43	108.00
17	Q	704	TYR	CB-CG-CD2	7.76	125.65	121.00
19	T	-58	DA	C5-C6-N1	7.75	121.57	117.70
1	A	216	LEU	O-C-N	-7.73	110.33	122.70
19	T	-88	DA	P-O3'-C3'	7.71	128.96	119.70
19	T	-50	DA	N1-C6-N6	-7.70	113.98	118.60
19	T	-42	DA	N1-C6-N6	-7.70	113.98	118.60
17	Q	792	TYR	CB-CG-CD2	7.68	125.61	121.00
16	P	30	C	C6-N1-C2	-7.68	117.23	120.30
19	T	-62	DG	O4'-C1'-N9	7.67	113.37	108.00
19	T	-57	DA	N1-C6-N6	-7.67	114.00	118.60
19	T	-74	DG	O4'-C1'-N9	7.64	113.35	108.00
1	A	349	ARG	NE-CZ-NH2	7.64	124.12	120.30
24	Y	85	TYR	CB-CG-CD2	7.64	125.58	121.00
27	b	35	ARG	NE-CZ-NH2	7.63	124.12	120.30
13	M	663	GLY	O-C-N	-7.60	110.54	122.70
19	T	-98	DA	N1-C6-N6	-7.60	114.04	118.60
2	B	472	ARG	NE-CZ-NH2	7.58	124.09	120.30
19	T	-43	DA	C4-C5-C6	-7.58	113.21	117.00
1	A	1258	ARG	NE-CZ-NH2	7.57	124.08	120.30
14	N	70	DA	N1-C6-N6	-7.55	114.07	118.60
14	N	74	DC	N3-C2-O2	-7.55	116.62	121.90
1	A	244	ARG	NE-CZ-NH2	7.55	124.07	120.30
26	a	83	ARG	NE-CZ-NH2	7.54	124.07	120.30
14	N	21	DC	N3-C2-O2	-7.54	116.62	121.90
16	P	42	C	C6-N1-C2	-7.53	117.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	T	-88	DA	C5-C6-N1	7.51	121.46	117.70
19	T	-34	DA	N1-C6-N6	-7.50	114.10	118.60
19	T	-42	DA	C5-C6-N1	7.49	121.44	117.70
19	T	-44	DA	C4-C5-C6	-7.48	113.26	117.00
14	N	76	DC	N3-C2-O2	-7.47	116.67	121.90
14	N	91	DG	O4'-C1'-N9	7.47	113.23	108.00
19	T	-55	DC	N3-C2-O2	-7.44	116.69	121.90
19	T	-123	DC	O4'-C1'-N1	7.44	113.21	108.00
19	T	-50	DA	C5-C6-N1	7.43	121.42	117.70
19	T	-29	DC	P-O3'-C3'	7.40	128.57	119.70
19	T	-61	DA	C5-C6-N1	7.38	121.39	117.70
14	N	101	DA	C4-C5-C6	-7.38	113.31	117.00
13	M	1176	HIS	N-CA-C	7.37	130.90	111.00
19	T	-98	DA	C5-C6-N1	7.36	121.38	117.70
14	N	99	DA	C4-C5-C6	-7.35	113.32	117.00
19	T	-124	DC	N3-C2-O2	-7.35	116.76	121.90
19	T	-78	DA	C4-C5-C6	-7.34	113.33	117.00
14	N	128	DC	N3-C2-O2	-7.32	116.78	121.90
14	N	62	DC	N3-C2-O2	-7.32	116.78	121.90
19	T	-82	DA	C5-C6-N1	7.32	121.36	117.70
18	R	503	ARG	NE-CZ-NH2	7.31	123.96	120.30
2	B	274	ARG	NE-CZ-NH2	7.31	123.95	120.30
19	T	-40	DC	N3-C2-O2	-7.30	116.79	121.90
25	Z	469	ARG	NE-CZ-NH2	7.29	123.95	120.30
2	B	1085	ARG	NE-CZ-NH2	7.28	123.94	120.30
19	T	-78	DA	C5-C6-N1	7.28	121.34	117.70
14	N	25	DC	N3-C2-O2	-7.27	116.81	121.90
14	N	90	DA	C5-C6-N1	7.27	121.33	117.70
8	H	24	ARG	NE-CZ-NH2	7.26	123.93	120.30
14	N	92	DC	N3-C2-O2	-7.26	116.82	121.90
19	T	-81	DC	O4'-C1'-N1	7.26	113.08	108.00
27	f	39	ARG	NE-CZ-NH2	7.25	123.92	120.30
14	N	90	DA	N1-C6-N6	-7.24	114.25	118.60
19	T	-127	DA	C5-C6-N1	7.24	121.32	117.70
14	N	105	DG	O4'-C4'-C3'	7.20	110.32	106.00
14	N	48	DC	N3-C2-O2	-7.19	116.87	121.90
29	d	69	ARG	NE-CZ-NH2	7.19	123.89	120.30
19	T	-121	DC	N3-C2-O2	-7.19	116.87	121.90
19	T	-43	DA	C5-C6-N1	7.19	121.29	117.70
1	A	827	TYR	CB-CG-CD2	7.18	125.31	121.00
17	Q	722	TYR	CB-CG-CD2	7.18	125.31	121.00
1	A	1421	ARG	NE-CZ-NH2	7.17	123.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	153	ARG	NE-CZ-NH2	-7.17	116.72	120.30
19	T	-56	DA	C4-C5-C6	-7.16	113.42	117.00
19	T	-41	DA	C5-C6-N1	7.16	121.28	117.70
26	e	69	ARG	NE-CZ-NH2	7.16	123.88	120.30
19	T	-100	DC	N3-C2-O2	-7.16	116.89	121.90
2	B	767	LEU	CA-CB-CG	7.15	131.75	115.30
19	T	-94	DC	N3-C2-O2	-7.14	116.90	121.90
19	T	-22	DC	N3-C2-O2	-7.14	116.90	121.90
14	N	101	DA	C5-C6-N1	7.13	121.27	117.70
2	B	290	TYR	CB-CG-CD2	7.12	125.27	121.00
14	N	79	DA	N1-C6-N6	-7.12	114.33	118.60
19	T	-75	DC	N3-C2-O2	-7.12	116.92	121.90
19	T	-34	DA	C5-C6-N1	7.11	121.25	117.70
1	A	187	TYR	CB-CG-CD2	7.10	125.26	121.00
14	N	125	DC	N3-C2-O2	-7.08	116.94	121.90
19	T	-102	DC	O4'-C1'-N1	7.08	112.96	108.00
1	A	16	ARG	NE-CZ-NH2	7.08	123.84	120.30
19	T	-49	DA	C4-C5-C6	-7.07	113.47	117.00
19	T	-77	DC	N3-C2-O2	-7.07	116.95	121.90
19	T	-79	DT	O4'-C1'-N1	7.07	112.94	108.00
14	N	115	DA	C5-C6-N1	7.06	121.23	117.70
14	N	20	DT	O4'-C1'-N1	7.06	112.94	108.00
2	B	975	ARG	CD-NE-CZ	7.06	133.48	123.60
19	T	-85	DC	N3-C2-O2	-7.05	116.96	121.90
19	T	-57	DA	C4-C5-C6	-7.05	113.47	117.00
14	N	103	DC	N3-C2-O2	-7.05	116.97	121.90
14	N	114	DC	N3-C2-O2	-7.05	116.97	121.90
16	P	31	G	C8-N9-C4	-7.05	103.58	106.40
2	B	762	ARG	NE-CZ-NH2	7.04	123.82	120.30
14	N	46	DC	N3-C2-O2	-7.02	116.99	121.90
20	U	393	TYR	CB-CG-CD2	7.02	125.21	121.00
14	N	113	DC	N3-C2-O2	-6.99	117.01	121.90
16	P	42	C	N3-C4-C5	-6.99	119.11	121.90
19	T	-65	DT	N3-C2-O2	-6.99	118.11	122.30
19	T	-44	DA	C5-C6-N1	6.99	121.19	117.70
27	b	36	ARG	NE-CZ-NH2	6.98	123.79	120.30
15	O	141	ARG	NE-CZ-NH2	-6.97	116.81	120.30
14	N	120	DA	C4-C5-C6	-6.97	113.52	117.00
26	e	72	ARG	NE-CZ-NH2	6.97	123.78	120.30
19	T	-50	DA	C4-C5-C6	-6.97	113.52	117.00
26	e	131	ARG	NE-CZ-NH2	6.96	123.78	120.30
19	T	-102	DC	N3-C2-O2	-6.96	117.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	153	ARG	NE-CZ-NH1	6.96	123.78	120.30
11	K	13	PHE	CB-CG-CD2	6.95	125.67	120.80
19	T	-123	DC	N3-C2-O2	-6.95	117.03	121.90
19	T	-27	DA	C4-C5-C6	-6.95	113.52	117.00
27	f	92	ARG	NE-CZ-NH2	6.95	123.78	120.30
1	A	1123	ARG	NE-CZ-NH2	6.94	123.77	120.30
7	G	2	PHE	CB-CG-CD2	6.94	125.66	120.80
3	C	3	TYR	CB-CG-CD2	6.94	125.16	121.00
28	g	29	ARG	NE-CZ-NH2	6.92	123.76	120.30
19	T	-76	DG	O4'-C1'-N9	6.92	112.84	108.00
2	B	916	TYR	CB-CG-CD2	6.91	125.15	121.00
3	C	193	ARG	CD-NE-CZ	6.91	133.27	123.60
1	A	104	MET	CA-CB-CG	6.90	125.03	113.30
14	N	64	DA	C4-C5-C6	-6.89	113.55	117.00
19	T	-119	DC	N1-C2-O2	6.89	123.03	118.90
17	Q	218	ARG	CD-NE-CZ	6.89	133.24	123.60
25	Z	474	MET	CA-CB-CG	6.88	125.00	113.30
14	N	89	DA	N1-C6-N6	-6.88	114.47	118.60
2	B	157	ARG	NE-CZ-NH2	6.87	123.74	120.30
17	Q	674	ARG	NE-CZ-NH2	6.86	123.73	120.30
2	B	338	TYR	CB-CG-CD2	6.86	125.12	121.00
1	A	431	PHE	CB-CG-CD2	6.85	125.59	120.80
19	T	-51	DC	N3-C2-O2	-6.84	117.11	121.90
14	N	45	DC	N3-C2-O2	-6.84	117.11	121.90
2	B	405	ARG	NE-CZ-NH2	6.83	123.72	120.30
11	K	81	TYR	CB-CG-CD2	6.83	125.10	121.00
19	T	-91	DC	N3-C2-O2	-6.82	117.12	121.90
14	N	19	DC	N1-C2-O2	6.82	122.99	118.90
13	M	906	TYR	C-N-CD	-6.81	105.62	120.60
28	g	20	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	A	225	PHE	CB-CG-CD2	6.81	125.57	120.80
2	B	689	TYR	CB-CG-CD2	6.80	125.08	121.00
19	T	-23	DA	C4-C5-C6	-6.80	113.60	117.00
9	I	44	TYR	CB-CG-CD2	6.80	125.08	121.00
14	N	109	DA	OP1-P-OP2	-6.80	109.40	119.60
14	N	144	DA	OP1-P-OP2	-6.80	109.41	119.60
19	T	-137	DC	N1-C2-O2	6.79	122.97	118.90
19	T	-87	DA	OP1-P-OP2	-6.79	109.42	119.60
19	T	-16	DA	OP1-P-OP2	-6.79	109.42	119.60
14	N	138	DA	OP1-P-OP2	-6.79	109.42	119.60
19	T	-140	DA	OP1-P-OP2	-6.79	109.42	119.60
19	T	-106	DA	OP1-P-OP2	-6.79	109.42	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	T	-30	DA	OP1-P-OP2	-6.79	109.42	119.60
14	N	136	DG	OP1-P-OP2	-6.78	109.42	119.60
14	N	67	DG	OP1-P-OP2	-6.78	109.43	119.60
19	T	-139	DA	OP1-P-OP2	-6.78	109.43	119.60
14	N	66	DG	OP1-P-OP2	-6.78	109.43	119.60
14	N	135	DG	OP1-P-OP2	-6.78	109.43	119.60
19	T	-142	DA	OP1-P-OP2	-6.78	109.43	119.60
19	T	-131	DG	OP1-P-OP2	-6.78	109.43	119.60
19	T	-108	DA	OP1-P-OP2	-6.78	109.43	119.60
14	N	132	DA	OP1-P-OP2	-6.78	109.43	119.60
14	N	143	DG	OP1-P-OP2	-6.78	109.43	119.60
19	T	-19	DG	OP1-P-OP2	-6.78	109.43	119.60
19	T	-18	DA	OP1-P-OP2	-6.78	109.43	119.60
19	T	-14	DA	OP1-P-OP2	-6.78	109.43	119.60
14	N	65	DA	OP1-P-OP2	-6.78	109.43	119.60
14	N	72	DA	OP1-P-OP2	-6.78	109.43	119.60
14	N	105	DG	C4'-C3'-C2'	-6.78	97.00	103.10
14	N	112	DA	OP1-P-OP2	-6.78	109.44	119.60
19	T	-110	DG	OP1-P-OP2	-6.78	109.43	119.60
19	T	-20	DA	OP1-P-OP2	-6.78	109.44	119.60
14	N	17	DG	OP1-P-OP2	-6.78	109.44	119.60
14	N	111	DG	OP1-P-OP2	-6.78	109.44	119.60
19	T	-107	DG	OP1-P-OP2	-6.78	109.44	119.60
19	T	-133	DG	OP1-P-OP2	-6.77	109.44	119.60
19	T	-71	DG	OP1-P-OP2	-6.77	109.44	119.60
19	T	-134	DG	OP1-P-OP2	-6.77	109.44	119.60
14	N	85	DG	OP1-P-OP2	-6.77	109.45	119.60
19	T	-21	DG	OP1-P-OP2	-6.77	109.44	119.60
14	N	83	DG	OP1-P-OP2	-6.77	109.45	119.60
19	T	-15	DG	OP1-P-OP2	-6.77	109.45	119.60
14	N	15	DC	OP1-P-OP2	-6.76	109.46	119.60
19	T	-68	DC	OP1-P-OP2	-6.76	109.46	119.60
19	T	-56	DA	C5-C6-N1	6.76	121.08	117.70
14	N	110	DC	OP1-P-OP2	-6.76	109.46	119.60
19	T	-143	DC	OP1-P-OP2	-6.76	109.46	119.60
19	T	-141	DG	OP1-P-OP2	-6.76	109.46	119.60
20	U	387	ARG	CD-NE-CZ	6.76	133.06	123.60
14	N	84	DC	OP1-P-OP2	-6.76	109.47	119.60
14	N	107	DC	OP1-P-OP2	-6.76	109.47	119.60
14	N	137	DG	OP1-P-OP2	-6.76	109.47	119.60
19	T	-105	DC	OP1-P-OP2	-6.75	109.47	119.60
19	T	-17	DC	OP1-P-OP2	-6.75	109.47	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	134	DC	OP1-P-OP2	-6.75	109.47	119.60
15	O	192	ARG	NE-CZ-NH1	6.75	123.68	120.30
19	T	-29	DC	OP1-P-OP2	-6.75	109.47	119.60
19	T	-135	DC	OP1-P-OP2	-6.75	109.47	119.60
19	T	-67	DC	OP1-P-OP2	-6.75	109.47	119.60
14	N	71	DC	OP1-P-OP2	-6.75	109.48	119.60
19	T	-136	DC	OP1-P-OP2	-6.75	109.48	119.60
19	T	-111	DC	OP1-P-OP2	-6.75	109.48	119.60
19	T	-66	DC	OP1-P-OP2	-6.75	109.48	119.60
14	N	133	DC	OP1-P-OP2	-6.74	109.49	119.60
19	T	-83	DC	OP1-P-OP2	-6.74	109.49	119.60
19	T	-69	DC	OP1-P-OP2	-6.74	109.49	119.60
14	N	115	DA	C4-C5-C6	-6.74	113.63	117.00
19	T	-130	DC	OP1-P-OP2	-6.74	109.50	119.60
2	B	721	ARG	CD-NE-CZ	6.73	133.03	123.60
14	N	116	DA	C4-C5-C6	-6.73	113.64	117.00
2	B	379	ARG	CD-NE-CZ	6.72	133.01	123.60
8	H	84	ARG	CD-NE-CZ	6.72	133.00	123.60
25	Z	203	TYR	CB-CG-CD2	6.72	125.03	121.00
9	I	40	ARG	CD-NE-CZ	6.71	133.00	123.60
1	A	186	ARG	C-N-CA	6.71	138.47	121.70
5	E	207	ARG	CD-NE-CZ	6.70	132.99	123.60
1	A	61	ARG	CD-NE-CZ	6.70	132.97	123.60
8	H	140	ARG	NE-CZ-NH2	6.70	123.65	120.30
19	T	-72	DT	O4'-C1'-N1	6.69	112.69	108.00
1	A	218	PRO	O-C-N	6.68	133.40	122.70
5	E	90	TYR	CB-CG-CD2	6.68	125.01	121.00
19	T	-86	DA	C4-C5-C6	-6.68	113.66	117.00
1	A	1123	ARG	NE-CZ-NH1	-6.68	116.96	120.30
19	T	-118	DA	C5-C6-N1	6.68	121.04	117.70
19	T	-63	DC	N3-C2-O2	-6.68	117.23	121.90
20	U	409	ARG	CD-NE-CZ	6.67	132.94	123.60
2	B	841	ARG	CD-NE-CZ	6.66	132.93	123.60
7	G	144	ARG	CD-NE-CZ	6.66	132.93	123.60
17	Q	830	ARG	CD-NE-CZ	6.66	132.92	123.60
19	T	-93	DC	N3-C2-O2	-6.66	117.24	121.90
14	N	116	DA	C5-C6-N1	6.66	121.03	117.70
2	B	829	PHE	CB-CG-CD2	6.65	125.46	120.80
1	A	890	ARG	CD-NE-CZ	6.65	132.91	123.60
1	A	800	PHE	CB-CG-CD2	6.65	125.45	120.80
19	T	-88	DA	C4-C5-C6	-6.65	113.68	117.00
5	E	24	ARG	CD-NE-CZ	6.65	132.90	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	e	53	ARG	CD-NE-CZ	6.65	132.90	123.60
19	T	-129	DC	N3-C2-O2	-6.64	117.25	121.90
20	U	398	PHE	CB-CG-CD2	6.64	125.45	120.80
24	Y	11	ARG	CD-NE-CZ	6.64	132.89	123.60
2	B	768	ARG	CD-NE-CZ	6.64	132.89	123.60
26	a	129	ARG	CD-NE-CZ	6.64	132.89	123.60
17	Q	763	ARG	CD-NE-CZ	6.63	132.88	123.60
19	T	-104	DA	C5-C6-N1	6.63	121.01	117.70
21	V	26	ARG	CD-NE-CZ	6.63	132.88	123.60
1	A	1167	ARG	CD-NE-CZ	6.63	132.88	123.60
12	L	31	ARG	CD-NE-CZ	6.63	132.88	123.60
19	T	-137	DC	N3-C2-O2	-6.63	117.26	121.90
19	T	-24	DC	N3-C2-O2	-6.63	117.26	121.90
24	Y	111	ARG	CD-NE-CZ	6.62	132.87	123.60
16	P	46	G	N7-C8-N9	-6.62	109.79	113.10
1	A	248	MET	CA-CB-CG	6.61	124.54	113.30
19	T	-86	DA	O4'-C1'-N9	6.61	112.63	108.00
2	B	646	ARG	NE-CZ-NH2	6.61	123.61	120.30
3	C	106	ARG	CD-NE-CZ	6.61	132.85	123.60
26	e	128	ARG	CD-NE-CZ	6.61	132.85	123.60
1	A	1396	ARG	NE-CZ-NH1	-6.60	117.00	120.30
2	B	803	ARG	NE-CZ-NH2	6.60	123.60	120.30
17	Q	186	TYR	CB-CG-CD2	6.60	124.96	121.00
17	Q	697	TYR	CB-CG-CD2	6.60	124.96	121.00
17	Q	791	ARG	CD-NE-CZ	6.60	132.84	123.60
19	T	-127	DA	C4-C5-C6	-6.59	113.70	117.00
1	A	805	ARG	CD-NE-CZ	6.58	132.81	123.60
2	B	938	ARG	CD-NE-CZ	6.58	132.81	123.60
2	B	890	ARG	CD-NE-CZ	6.57	132.80	123.60
17	Q	815	ARG	NE-CZ-NH2	6.57	123.58	120.30
1	A	70	ARG	CD-NE-CZ	6.57	132.79	123.60
2	B	550	MET	CA-CB-CG	6.56	124.46	113.30
7	G	78	ARG	CD-NE-CZ	6.55	132.78	123.60
15	O	207	ARG	NE-CZ-NH1	6.55	123.58	120.30
16	P	33	G	N7-C8-N9	-6.55	109.82	113.10
17	Q	832	ARG	CD-NE-CZ	6.55	132.78	123.60
17	Q	221	PHE	CB-CG-CD2	6.55	125.39	120.80
5	E	203	TYR	CB-CG-CD2	6.55	124.93	121.00
29	h	76	ARG	NE-CZ-NH2	6.55	123.57	120.30
5	E	181	ARG	CD-NE-CZ	6.54	132.76	123.60
16	P	30	C	N3-C4-C5	-6.54	119.28	121.90
1	A	551	ARG	CD-NE-CZ	6.54	132.76	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	77	ARG	CD-NE-CZ	6.54	132.75	123.60
18	R	501	ARG	NE-CZ-NH2	6.53	123.57	120.30
3	C	220	TYR	CB-CG-CD2	6.53	124.92	121.00
27	b	92	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	880	ARG	CD-NE-CZ	6.52	132.73	123.60
16	P	45	G	N7-C8-N9	-6.52	109.84	113.10
2	B	1104	ARG	CD-NE-CZ	6.52	132.72	123.60
1	A	1380	ARG	CD-NE-CZ	6.51	132.72	123.60
19	T	-52	DC	N3-C2-O2	-6.51	117.34	121.90
26	e	134	ARG	CD-NE-CZ	6.51	132.72	123.60
18	R	596	ARG	CD-NE-CZ	6.51	132.71	123.60
19	T	-42	DA	C4-C5-C6	-6.50	113.75	117.00
1	A	838	PHE	CB-CG-CD2	6.50	125.35	120.80
19	T	-65	DT	C6-C5-C7	-6.50	119.00	122.90
16	P	40	G	N7-C8-N9	-6.50	109.85	113.10
2	B	363	TYR	CB-CG-CD2	6.49	124.89	121.00
2	B	834	ARG	CD-NE-CZ	6.48	132.67	123.60
1	A	1218	ARG	CD-NE-CZ	6.48	132.67	123.60
14	N	60	DT	C6-C5-C7	-6.48	119.01	122.90
25	Z	517	ASP	N-CA-CB	6.48	122.26	110.60
14	N	98	DT	C6-C5-C7	-6.47	119.02	122.90
1	A	99	PHE	CB-CG-CD2	6.47	125.33	120.80
2	B	380	ARG	CD-NE-CZ	6.47	132.65	123.60
14	N	18	DT	O4'-C1'-N1	6.46	112.53	108.00
5	E	162	ARG	CD-NE-CZ	6.46	132.64	123.60
2	B	1023	ARG	CD-NE-CZ	6.45	132.63	123.60
19	T	-117	DA	C4-C5-C6	-6.45	113.78	117.00
14	N	74	DC	N1-C2-O2	6.44	122.76	118.90
18	R	377	PHE	CB-CG-CD2	6.44	125.31	120.80
14	N	56	DT	O4'-C1'-N1	6.44	112.51	108.00
2	B	483	ARG	CD-NE-CZ	6.43	132.60	123.60
14	N	128	DC	N1-C2-O2	6.43	122.76	118.90
14	N	97	DC	N1-C2-O2	6.43	122.76	118.90
2	B	495	LEU	C-N-CA	6.42	137.76	121.70
18	R	485	TYR	CB-CG-CD2	6.42	124.86	121.00
1	A	1058	PHE	CB-CG-CD2	6.42	125.29	120.80
28	g	77	ARG	NE-CZ-NH1	-6.41	117.09	120.30
8	H	57	ARG	CD-NE-CZ	6.41	132.57	123.60
1	A	583	ARG	CD-NE-CZ	6.41	132.57	123.60
2	B	840	MET	CA-CB-CG	6.41	124.19	113.30
19	T	-127	DA	N1-C6-N6	-6.41	114.76	118.60
19	T	-59	DA	C4-C5-C6	-6.40	113.80	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	80	DC	N3-C2-O2	-6.40	117.42	121.90
1	A	1153	ARG	CD-NE-CZ	6.40	132.56	123.60
4	D	70	ARG	CD-NE-CZ	6.39	132.55	123.60
26	e	41	TYR	CB-CG-CD2	6.39	124.84	121.00
5	E	103	LEU	C-N-CA	6.39	137.68	121.70
2	B	41	ARG	CD-NE-CZ	6.38	132.53	123.60
14	N	89	DA	C5-C6-N1	6.38	120.89	117.70
14	N	20	DT	C6-C5-C7	-6.38	119.08	122.90
16	P	30	C	C5-C6-N1	6.37	124.19	121.00
29	d	76	ARG	NE-CZ-NH2	6.37	123.49	120.30
14	N	64	DA	C5-C6-N1	6.37	120.88	117.70
16	P	36	U	P-O3'-C3'	6.37	127.34	119.70
19	T	-117	DA	N1-C6-N6	-6.37	114.78	118.60
1	A	1356	ARG	CD-NE-CZ	6.37	132.51	123.60
7	G	3	TYR	CB-CG-CD2	6.37	124.82	121.00
27	f	55	ARG	NE-CZ-NH2	6.37	123.48	120.30
19	T	-54	DC	N3-C2-O2	-6.36	117.45	121.90
19	T	-104	DA	C4-C5-C6	-6.36	113.82	117.00
19	T	-82	DA	C4-C5-C6	-6.36	113.82	117.00
28	g	77	ARG	NE-CZ-NH2	6.36	123.48	120.30
2	B	371	ARG	CD-NE-CZ	6.36	132.50	123.60
27	f	40	ARG	NE-CZ-NH2	6.35	123.48	120.30
19	T	-118	DA	C4-C5-C6	-6.34	113.83	117.00
1	A	1224	ARG	CD-NE-CZ	6.34	132.48	123.60
19	T	-27	DA	C5-C6-N1	6.34	120.87	117.70
1	A	408	ARG	CD-NE-CZ	6.32	132.45	123.60
14	N	73	DG	O4'-C1'-N9	6.32	112.42	108.00
25	Z	516	ARG	NE-CZ-NH2	6.32	123.46	120.30
2	B	1108	PHE	CB-CG-CD2	6.31	125.22	120.80
14	N	122	DC	N1-C2-O2	6.31	122.68	118.90
1	A	216	LEU	C-N-CA	6.31	137.46	121.70
14	N	70	DA	C4-C5-C6	-6.31	113.85	117.00
26	a	116	ARG	NE-CZ-NH2	6.31	123.45	120.30
8	H	90	TYR	CB-CG-CD2	6.30	124.78	121.00
24	Y	28	PHE	CB-CG-CD2	6.29	125.21	120.80
2	B	282	ARG	CD-NE-CZ	6.27	132.38	123.60
1	A	985	ARG	NE-CZ-NH1	-6.27	117.17	120.30
19	T	-115	DT	C6-C5-C7	-6.27	119.14	122.90
6	F	51	ARG	CD-NE-CZ	6.27	132.37	123.60
16	P	37	G	O4'-C1'-N9	6.27	113.21	108.20
19	T	-37	DC	N3-C2-O2	-6.27	117.51	121.90
19	T	-57	DA	C5-C6-N1	6.27	120.83	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	T	-95	DA	C4-C5-C6	-6.26	113.87	117.00
19	T	-81	DC	N3-C2-O2	-6.26	117.52	121.90
14	N	47	DC	N3-C2-O2	-6.26	117.52	121.90
15	O	141	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	B	425	ARG	CD-NE-CZ	6.25	132.36	123.60
13	M	1358	SER	CA-C-N	-6.25	103.44	117.20
3	C	10	ARG	CD-NE-CZ	6.25	132.35	123.60
5	E	103	LEU	O-C-N	-6.25	112.70	122.70
16	P	45	G	C6-C5-N7	6.25	134.15	130.40
19	T	-60	DA	C4-C5-C6	-6.24	113.88	117.00
14	N	95	DT	N3-C2-O2	-6.24	118.56	122.30
14	N	99	DA	C5-C6-N1	6.24	120.82	117.70
19	T	-58	DA	C4-C5-C6	-6.23	113.88	117.00
16	P	46	G	C6-C5-N7	6.23	134.14	130.40
16	P	38	G	C8-N9-C4	-6.22	103.91	106.40
14	N	131	DC	O4'-C1'-N1	6.22	112.36	108.00
19	T	-38	DC	N3-C2-O2	-6.22	117.55	121.90
25	Z	190	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	A	364	ARG	NE-CZ-NH2	6.21	123.41	120.30
14	N	101	DA	O4'-C1'-N9	6.21	112.35	108.00
16	P	33	G	C6-C5-N7	6.20	134.12	130.40
16	P	40	G	C6-C5-N7	6.20	134.12	130.40
14	N	22	DG	O4'-C1'-N9	6.20	112.34	108.00
1	A	43	TYR	CB-CG-CD2	6.19	124.72	121.00
1	A	397	PHE	CB-CG-CD2	6.19	125.14	120.80
1	A	557	ARG	CD-NE-CZ	6.18	132.26	123.60
11	K	106	ARG	CD-NE-CZ	6.18	132.26	123.60
14	N	115	DA	P-O3'-C3'	6.18	127.12	119.70
14	N	131	DC	N3-C2-O2	-6.17	117.58	121.90
5	E	195	ARG	CD-NE-CZ	6.16	132.23	123.60
17	Q	795	TYR	CB-CG-CD2	6.16	124.70	121.00
14	N	53	DC	N1-C2-O2	6.16	122.60	118.90
25	Z	747	ARG	NE-CZ-NH2	6.16	123.38	120.30
14	N	61	DT	C6-C5-C7	-6.15	119.21	122.90
17	Q	204	MET	CA-CB-CG	6.15	123.75	113.30
27	b	45	ARG	NE-CZ-NH2	6.14	123.37	120.30
19	T	-55	DC	C1'-O4'-C4'	-6.14	103.96	110.10
2	B	475	PHE	CB-CG-CD2	6.14	125.10	120.80
14	N	127	DT	N3-C2-O2	-6.13	118.62	122.30
2	B	169	ARG	NE-CZ-NH2	6.12	123.36	120.30
14	N	23	DT	O4'-C1'-N1	6.12	112.28	108.00
28	c	81	ARG	NE-CZ-NH2	6.12	123.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	922	ARG	NE-CZ-NH2	6.12	123.36	120.30
2	B	34	PHE	CB-CG-CD2	6.11	125.08	120.80
4	D	138	ARG	CD-NE-CZ	6.10	132.15	123.60
19	T	-31	DC	N3-C2-O2	-6.10	117.63	121.90
2	B	120	TYR	CB-CG-CD2	6.09	124.66	121.00
14	N	74	DC	O4'-C1'-N1	6.09	112.27	108.00
19	T	-143	DC	OP1-P-O3'	6.09	118.59	105.20
9	I	25	TYR	CB-CG-CD2	6.09	124.65	121.00
14	N	120	DA	C5-C6-N1	6.09	120.74	117.70
19	T	-36	DC	N3-C2-O2	-6.08	117.64	121.90
19	T	-64	DT	N3-C2-O2	-6.08	118.65	122.30
4	D	44	ARG	NE-CZ-NH2	6.08	123.34	120.30
25	Z	416	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	A	448	ARG	NE-CZ-NH2	6.08	123.34	120.30
5	E	163	TYR	CB-CG-CD2	6.07	124.64	121.00
9	I	37	TYR	CB-CG-CD2	6.07	124.64	121.00
14	N	93	DG	N1-C6-O6	-6.06	116.27	119.90
14	N	27	DT	C6-C5-C7	-6.05	119.27	122.90
14	N	126	DC	N3-C2-O2	-6.05	117.66	121.90
2	B	623	ARG	NE-CZ-NH2	6.05	123.32	120.30
16	P	43	U	C5-C6-N1	-6.04	119.68	122.70
2	B	770	ARG	CD-NE-CZ	6.04	132.06	123.60
9	I	54	TYR	CB-CG-CD2	6.04	124.62	121.00
1	A	220	ARG	N-CA-C	-6.04	94.70	111.00
19	T	-138	DT	C6-C5-C7	-6.02	119.29	122.90
2	B	1018	TYR	CB-CG-CD2	6.01	124.61	121.00
7	G	104	MET	CA-CB-CG	6.01	123.53	113.30
15	O	246	ARG	NE-CZ-NH1	6.01	123.30	120.30
19	T	-130	DC	P-O3'-C3'	6.01	126.91	119.70
14	N	18	DT	C6-C5-C7	-6.00	119.30	122.90
19	T	-55	DC	N1-C2-O2	6.00	122.50	118.90
19	T	-17	DC	OP1-P-O3'	6.00	118.40	105.20
19	T	-23	DA	C5-C6-N1	6.00	120.70	117.70
27	b	98	TYR	CB-CG-CD2	-6.00	117.40	121.00
25	Z	197	MET	CA-CB-CG	5.99	123.49	113.30
26	a	104	PHE	CB-CG-CD2	5.99	125.00	120.80
3	C	228	ARG	CD-NE-CZ	5.99	131.99	123.60
16	P	39	U	C5-C6-N1	-5.98	119.71	122.70
16	P	36	U	C5-C6-N1	-5.97	119.71	122.70
16	P	41	U	C5-C6-N1	-5.97	119.71	122.70
5	E	202	ARG	CD-NE-CZ	5.97	131.96	123.60
19	T	-124	DC	O4'-C1'-N1	5.97	112.18	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	T	-80	DG	O4'-C1'-N9	5.97	112.18	108.00
6	F	75	MET	CA-CB-CG	5.96	123.44	113.30
26	a	128	ARG	CD-NE-CZ	5.96	131.95	123.60
16	P	44	U	C5-C6-N1	-5.96	119.72	122.70
14	N	106	DT	OP1-P-O3'	5.96	118.31	105.20
19	T	-89	DT	C6-C5-C7	-5.96	119.32	122.90
16	P	29	U	C5-C6-N1	-5.96	119.72	122.70
19	T	-140	DA	OP1-P-O3'	5.96	118.31	105.20
14	N	82	DT	C6-C5-C7	-5.95	119.33	122.90
14	N	76	DC	N1-C2-O2	5.95	122.47	118.90
14	N	88	DT	C6-C5-C7	-5.95	119.33	122.90
16	P	32	U	C5-C6-N1	-5.95	119.73	122.70
26	a	42	ARG	NE-CZ-NH2	5.94	123.27	120.30
24	Y	64	MET	CA-CB-CG	5.93	123.39	113.30
19	T	-92	DG	N1-C6-O6	-5.93	116.34	119.90
14	N	58	DT	N3-C2-O2	-5.93	118.74	122.30
19	T	-39	DA	C4-C5-C6	-5.92	114.04	117.00
14	N	142	DT	N3-C2-O2	-5.92	118.75	122.30
24	Y	50	TYR	CB-CG-CD2	5.91	124.55	121.00
9	I	23	MET	CA-CB-CG	5.91	123.35	113.30
5	E	75	PHE	CB-CG-CD2	5.91	124.94	120.80
14	N	66	DG	OP1-P-O3'	5.91	118.20	105.20
29	h	69	ARG	NE-CZ-NH2	5.91	123.25	120.30
19	T	-122	DG	O4'-C1'-N9	5.91	112.13	108.00
1	A	218	PRO	N-CA-C	5.90	127.44	112.10
20	U	411	ARG	CD-NE-CZ	5.90	131.86	123.60
26	a	69	ARG	NE-CZ-NH2	5.90	123.25	120.30
2	B	155	MET	CA-CB-CG	5.90	123.33	113.30
2	B	1089	MET	CA-CB-CG	5.89	123.32	113.30
13	M	1412	TYR	CB-CG-CD2	5.88	124.53	121.00
16	P	42	C	C4-C5-C6	5.88	120.34	117.40
14	N	42	DT	N3-C2-O2	-5.88	118.77	122.30
1	A	1059	ARG	CD-NE-CZ	5.88	131.83	123.60
8	H	98	ARG	NE-CZ-NH2	5.87	123.24	120.30
14	N	92	DC	N1-C2-O2	5.87	122.42	118.90
17	Q	208	PHE	CB-CG-CD2	5.87	124.91	120.80
19	T	-55	DC	N3-C4-N4	-5.87	113.89	118.00
19	T	-135	DC	OP1-P-O3'	5.86	118.09	105.20
19	T	-113	DG	O4'-C1'-C2'	-5.86	101.21	105.90
28	c	88	ARG	NE-CZ-NH2	5.86	123.23	120.30
3	C	160	ARG	CD-NE-CZ	5.86	131.80	123.60
27	b	67	ARG	NE-CZ-NH2	5.86	123.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	83	DG	OP1-P-O3'	5.84	118.06	105.20
14	N	117	DT	C6-C5-C7	-5.84	119.39	122.90
19	T	-96	DC	N1-C2-O2	5.84	122.41	118.90
1	A	666	ARG	NE-CZ-NH2	5.84	123.22	120.30
14	N	127	DT	C6-C5-C7	-5.84	119.39	122.90
14	N	118	DT	C6-C5-C7	-5.84	119.40	122.90
19	T	-108	DA	OP1-P-O3'	5.84	118.05	105.20
19	T	-70	DT	OP1-P-O3'	5.84	118.04	105.20
14	N	56	DT	C6-C5-C7	-5.83	119.40	122.90
1	A	216	LEU	CA-C-N	5.83	130.03	117.20
2	B	1020	TYR	CB-CG-CD2	5.83	124.50	121.00
19	T	-69	DC	OP1-P-O3'	5.83	118.02	105.20
14	N	41	DT	C6-C5-C7	-5.83	119.40	122.90
29	h	89	ARG	CD-NE-CZ	5.83	131.76	123.60
17	Q	712	TYR	CB-CG-CD2	5.82	124.49	121.00
19	T	-18	DA	OP1-P-O3'	5.82	118.01	105.20
2	B	495	LEU	CA-C-N	5.82	130.00	117.20
19	T	-124	DC	N1-C2-O2	5.81	122.39	118.90
19	T	-61	DA	N1-C6-N6	-5.81	115.11	118.60
19	T	-79	DT	C6-C5-C7	-5.81	119.41	122.90
1	A	1395	TYR	CB-CG-CD2	5.80	124.48	121.00
17	Q	667	ARG	CD-NE-CZ	5.80	131.73	123.60
14	N	91	DG	N1-C6-O6	-5.80	116.42	119.90
14	N	109	DA	OP1-P-O3'	5.80	117.95	105.20
19	T	-99	DT	N3-C2-O2	-5.80	118.82	122.30
13	M	1157	THR	C-N-CD	-5.79	107.86	120.60
8	H	48	TYR	CB-CG-CD2	5.79	124.47	121.00
2	B	380	ARG	CG-CD-NE	5.79	123.95	111.80
14	N	93	DG	O4'-C1'-N9	5.79	112.05	108.00
1	A	225	PHE	C-N-CA	5.79	136.16	121.70
28	c	42	ARG	CD-NE-CZ	5.79	131.70	123.60
9	I	108	MET	CA-CB-CG	5.78	123.13	113.30
14	N	42	DT	C6-C5-C7	-5.78	119.43	122.90
28	g	17	ARG	NE-CZ-NH2	5.78	123.19	120.30
14	N	90	DA	C4-C5-C6	-5.78	114.11	117.00
16	P	38	G	N7-C8-N9	5.77	115.99	113.10
7	G	1	MET	CA-CB-CG	5.77	123.10	113.30
19	T	-19	DG	OP1-P-O3'	5.76	117.88	105.20
1	A	1416	ARG	NE-CZ-NH2	5.76	123.18	120.30
2	B	116	ARG	NE-CZ-NH2	5.76	123.18	120.30
19	T	-106	DA	OP1-P-O3'	5.76	117.87	105.20
19	T	-98	DA	C4-C5-C6	-5.75	114.12	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	T	-37	DC	C4'-C3'-C2'	-5.75	97.92	103.10
14	N	132	DA	OP1-P-O3'	5.75	117.85	105.20
14	N	16	DT	OP1-P-O3'	5.74	117.84	105.20
1	A	193	ARG	NE-CZ-NH2	5.74	123.17	120.30
14	N	56	DT	N3-C2-O2	-5.74	118.86	122.30
19	T	-128	DG	N1-C6-O6	-5.74	116.45	119.90
1	A	1160	ARG	CD-NE-CZ	5.74	131.63	123.60
3	C	35	ARG	NE-CZ-NH2	5.73	123.17	120.30
14	N	65	DA	OP1-P-O3'	5.73	117.81	105.20
17	Q	754	MET	CA-CB-CG	5.73	123.04	113.30
19	T	-51	DC	N1-C2-O2	5.73	122.34	118.90
14	N	84	DC	OP1-P-O3'	5.73	117.80	105.20
1	A	95	PHE	CB-CG-CD2	5.71	124.80	120.80
14	N	134	DC	OP1-P-O3'	5.71	117.77	105.20
19	T	-73	DC	N3-C2-O2	-5.70	117.91	121.90
3	C	67	ARG	NE-CZ-NH2	5.70	123.15	120.30
19	T	-72	DT	C4'-C3'-C2'	-5.69	97.98	103.10
1	A	512	ARG	NE-CZ-NH2	5.68	123.14	120.30
14	N	89	DA	C4-C5-C6	-5.68	114.16	117.00
12	L	31	ARG	CG-CD-NE	5.67	123.72	111.80
14	N	58	DT	O4'-C1'-N1	5.67	111.97	108.00
19	T	-89	DT	P-O3'-C3'	5.67	126.51	119.70
1	A	1224	ARG	CG-CD-NE	5.67	123.71	111.80
1	A	727	PRO	CA-C-N	-5.67	104.72	117.20
19	T	-109	DT	OP1-P-O3'	5.66	117.66	105.20
1	A	1192	TRP	C-N-CA	5.66	135.86	121.70
19	T	-134	DG	OP1-P-O3'	5.66	117.65	105.20
14	N	57	DT	N3-C2-O2	-5.66	118.91	122.30
4	D	71	PHE	CB-CG-CD2	5.65	124.76	120.80
1	A	317	MET	CA-CB-CG	5.65	122.91	113.30
2	B	1135	TYR	CB-CG-CD2	5.65	124.39	121.00
28	c	29	ARG	NE-CZ-NH2	5.65	123.13	120.30
2	B	282	ARG	CA-CB-CG	5.65	125.83	113.40
17	Q	223	ARG	NE-CZ-NH2	5.65	123.13	120.30
18	R	371	ARG	CD-NE-CZ	5.65	131.51	123.60
1	A	291	ARG	NE-CZ-NH2	5.64	123.12	120.30
2	B	297	MET	CA-CB-CG	5.64	122.89	113.30
19	T	-27	DA	O4'-C4'-C3'	5.64	109.38	106.00
20	U	498	SER	N-CA-CB	5.64	118.96	110.50
19	T	-99	DT	C6-C5-C7	-5.64	119.52	122.90
1	A	33	ARG	NE-CZ-NH2	5.63	123.12	120.30
7	G	164	MET	CA-CB-CG	5.63	122.87	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	T	-41	DA	C4-C5-C6	-5.63	114.18	117.00
3	C	113	ARG	CD-NE-CZ	5.62	131.47	123.60
14	N	82	DT	N3-C2-O2	-5.62	118.93	122.30
14	N	62	DC	N1-C2-O2	5.62	122.27	118.90
14	N	98	DT	N3-C2-O2	-5.62	118.93	122.30
2	B	713	PHE	CB-CG-CD2	5.62	124.73	120.80
19	T	-101	DT	C6-C5-C7	-5.62	119.53	122.90
14	N	105	DG	C5-C6-N1	5.61	114.31	111.50
2	B	300	MET	CA-CB-CG	5.61	122.84	113.30
19	T	-30	DA	OP1-P-O3'	5.61	117.54	105.20
19	T	-90	DT	N3-C2-O2	-5.61	118.93	122.30
1	A	1383	TYR	CB-CG-CD2	5.61	124.36	121.00
19	T	-20	DA	OP1-P-O3'	5.61	117.53	105.20
19	T	-141	DG	OP1-P-O3'	5.61	117.53	105.20
7	G	77	PHE	CB-CG-CD2	5.60	124.72	120.80
14	N	117	DT	O4'-C1'-N1	5.60	111.92	108.00
14	N	111	DG	OP1-P-O3'	5.60	117.52	105.20
19	T	-100	DC	N1-C2-O2	5.60	122.26	118.90
14	N	105	DG	O4'-C1'-N9	5.60	111.92	108.00
14	N	25	DC	N1-C2-O2	5.60	122.26	118.90
19	T	-65	DT	N1-C2-N3	5.60	117.96	114.60
2	B	950	ARG	NE-CZ-NH2	5.59	123.10	120.30
16	P	35	C	N3-C4-C5	-5.59	119.66	121.90
19	T	-137	DC	O4'-C4'-C3'	5.59	109.36	106.00
19	T	-26	DG	O4'-C1'-N9	5.59	111.92	108.00
19	T	-115	DT	N3-C2-O2	-5.59	118.95	122.30
14	N	142	DT	C6-C5-C7	-5.59	119.55	122.90
3	C	36	ARG	NE-CZ-NH1	-5.59	117.51	120.30
11	K	74	ARG	NE-CZ-NH1	-5.58	117.51	120.30
13	M	353	PRO	CA-N-CD	-5.58	103.69	111.50
27	b	51	TYR	CB-CG-CD2	5.57	124.34	121.00
2	B	422	PHE	CB-CG-CD2	5.57	124.70	120.80
2	B	446	TYR	CB-CG-CD2	5.57	124.34	121.00
1	A	725	LEU	CA-CB-CG	5.57	128.10	115.30
19	T	-64	DT	C6-C5-C7	-5.57	119.56	122.90
19	T	-97	DG	N1-C6-O6	-5.56	116.56	119.90
2	B	976	MET	CA-CB-CG	5.56	122.75	113.30
26	a	99	TYR	CB-CG-CD2	5.56	124.33	121.00
25	Z	635	MET	CA-CB-CG	5.55	122.74	113.30
18	R	566	ARG	NE-CZ-NH2	5.55	123.07	120.30
28	g	77	ARG	CD-NE-CZ	5.55	131.37	123.60
1	A	822	PHE	CB-CG-CD2	5.55	124.68	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	39	ARG	NE-CZ-NH2	5.55	123.07	120.30
14	N	47	DC	C4'-C3'-C2'	-5.54	98.11	103.10
2	B	1091	ARG	CD-NE-CZ	5.54	131.35	123.60
14	N	103	DC	N1-C2-O2	5.54	122.22	118.90
16	P	38	G	C4'-C3'-C2'	-5.54	97.06	102.60
15	O	190	ARG	NE-CZ-NH1	5.54	123.07	120.30
19	T	-90	DT	C6-C5-C7	-5.54	119.58	122.90
19	T	-112	DT	OP1-P-O3'	5.53	117.37	105.20
19	T	-131	DG	OP1-P-O3'	5.53	117.36	105.20
14	N	50	DT	C6-C5-C7	-5.52	119.59	122.90
14	N	77	DG	O4'-C1'-N9	5.52	111.86	108.00
19	T	-116	DT	C6-C5-C7	-5.52	119.59	122.90
1	A	407	ARG	CD-NE-CZ	5.52	131.33	123.60
1	A	810	PHE	CB-CG-CD2	5.52	124.66	120.80
14	N	117	DT	N3-C2-O2	-5.52	118.99	122.30
19	T	-103	DG	C1'-O4'-C4'	-5.52	104.58	110.10
19	T	-33	DG	N1-C6-O6	-5.51	116.59	119.90
1	A	219	GLU	C-N-CA	5.51	135.47	121.70
1	A	334	ARG	NE-CZ-NH2	5.51	123.05	120.30
16	P	31	G	C5-N7-C8	-5.51	101.55	104.30
16	P	34	C	N3-C4-C5	-5.51	119.70	121.90
1	A	841	MET	CA-CB-CG	5.50	122.65	113.30
19	T	-57	DA	C4'-C3'-C2'	-5.50	98.15	103.10
19	T	-38	DC	N3-C4-C5	5.50	124.10	121.90
19	T	-123	DC	N1-C2-O2	5.49	122.19	118.90
19	T	-57	DA	O4'-C1'-N9	5.49	111.84	108.00
19	T	-28	DC	P-O3'-C3'	5.49	126.29	119.70
19	T	-144	DT	OP1-P-O3'	5.49	117.27	105.20
19	T	-72	DT	N3-C2-O2	-5.49	119.01	122.30
19	T	-21	DG	OP1-P-O3'	5.49	117.27	105.20
1	A	1260	ARG	NE-CZ-NH2	5.49	123.04	120.30
5	E	162	ARG	CG-CD-NE	5.49	123.32	111.80
14	N	45	DC	N1-C2-O2	5.49	122.19	118.90
1	A	546	ARG	NE-CZ-NH2	5.48	123.04	120.30
7	G	167	TYR	CB-CG-CD2	5.48	124.29	121.00
21	V	26	ARG	CG-CD-NE	5.48	123.32	111.80
19	T	-31	DC	N3-C4-C5	5.48	124.09	121.90
27	f	98	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	A	1177	TYR	CB-CA-C	5.48	121.35	110.40
14	N	93	DG	C1'-O4'-C4'	-5.48	104.62	110.10
2	B	334	LYS	CA-CB-CG	5.47	125.44	113.40
14	N	27	DT	N3-C2-O2	-5.47	119.02	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1031	ARG	CD-NE-CZ	5.47	131.25	123.60
7	G	144	ARG	CG-CD-NE	5.47	123.28	111.80
27	b	95	ARG	CD-NE-CZ	5.46	131.25	123.60
1	A	225	PHE	CA-C-N	5.45	129.19	117.20
25	Z	733	ARG	NE-CZ-NH2	5.45	123.03	120.30
2	B	918	PHE	CB-CG-CD2	5.45	124.61	120.80
1	A	769	MET	CA-CB-CG	5.45	122.56	113.30
2	B	605	ARG	NE-CZ-NH2	5.45	123.02	120.30
17	Q	772	GLU	C-N-CA	5.44	135.31	121.70
2	B	379	ARG	CG-CD-NE	5.44	123.23	111.80
11	K	61	TYR	CB-CG-CD2	5.44	124.26	121.00
14	N	43	DT	C6-C5-C7	-5.44	119.64	122.90
2	B	463	ARG	NE-CZ-NH2	5.44	123.02	120.30
10	J	42	ARG	NE-CZ-NH2	5.44	123.02	120.30
14	N	105	DG	N1-C6-O6	-5.44	116.64	119.90
19	T	-136	DC	OP1-P-O3'	5.43	117.16	105.20
19	T	-107	DG	OP1-P-O3'	5.43	117.16	105.20
16	P	42	C	C5-C6-N1	5.43	123.72	121.00
17	Q	832	ARG	CG-CD-NE	5.43	123.19	111.80
2	B	230	ARG	CD-NE-CZ	5.42	131.19	123.60
14	N	71	DC	OP1-P-O3'	5.42	117.12	105.20
12	L	48	ARG	NE-CZ-NH2	5.42	123.01	120.30
2	B	605	ARG	NE-CZ-NH1	5.42	123.01	120.30
19	T	-81	DC	N3-C4-N4	-5.42	114.21	118.00
8	H	65	TYR	CB-CG-CD2	5.41	124.25	121.00
28	g	42	ARG	CD-NE-CZ	5.41	131.18	123.60
19	T	-67	DC	OP1-P-O3'	5.40	117.09	105.20
10	J	47	ARG	NE-CZ-NH2	5.39	123.00	120.30
3	C	197	TYR	CB-CG-CD2	5.39	124.24	121.00
19	T	-111	DC	OP1-P-O3'	5.39	117.06	105.20
1	A	1212	LEU	CA-CB-CG	5.39	127.70	115.30
5	E	129	GLN	CA-C-N	5.39	129.05	117.20
14	N	113	DC	N1-C2-O2	5.39	122.13	118.90
2	B	367	TYR	CB-CG-CD2	5.39	124.23	121.00
16	P	31	G	C5-C6-N1	-5.38	108.81	111.50
19	T	-15	DG	OP1-P-O3'	5.38	117.05	105.20
19	T	-59	DA	N1-C6-N6	-5.38	115.37	118.60
20	U	409	ARG	CG-CD-NE	5.38	123.10	111.80
27	f	63	GLU	CA-CB-CG	5.38	125.23	113.40
1	A	976	LYS	CA-CB-CG	5.37	125.22	113.40
19	T	-138	DT	O4'-C4'-C3'	5.37	109.22	106.00
14	N	114	DC	N1-C2-O2	5.37	122.12	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	49	ARG	NE-CZ-NH2	5.36	122.98	120.30
14	N	133	DC	OP1-P-O3'	5.36	116.98	105.20
14	N	136	DG	OP1-P-O3'	5.36	116.98	105.20
13	M	1359	LYS	CA-C-N	-5.35	105.49	116.20
5	E	166	ARG	CD-NE-CZ	5.35	131.09	123.60
12	L	42	ARG	NE-CZ-NH2	5.35	122.97	120.30
14	N	82	DT	O4'-C4'-C3'	5.35	109.21	106.00
14	N	135	DG	OP1-P-O3'	5.35	116.96	105.20
7	G	78	ARG	CG-CD-NE	5.34	123.02	111.80
2	B	445	LYS	CA-CB-CG	5.34	125.14	113.40
29	d	83	ARG	NE-CZ-NH2	5.34	122.97	120.30
14	N	77	DG	N1-C6-O6	-5.34	116.70	119.90
19	T	-84	DG	O3'-P-O5'	5.33	114.13	104.00
2	B	988	LYS	CA-CB-CG	5.33	125.12	113.40
19	T	-103	DG	O4'-C1'-C2'	-5.33	101.64	105.90
24	Y	111	ARG	CG-CD-NE	5.32	122.98	111.80
14	N	143	DG	OP1-P-O3'	5.32	116.91	105.20
19	T	-113	DG	N3-C4-C5	-5.32	125.94	128.60
19	T	-16	DA	OP1-P-O3'	5.32	116.91	105.20
24	Y	11	ARG	CG-CD-NE	5.32	122.97	111.80
1	A	510	GLU	CA-CB-CG	5.32	125.10	113.40
2	B	491	ARG	CD-NE-CZ	5.32	131.04	123.60
14	N	22	DG	N1-C6-O6	-5.31	116.72	119.90
1	A	970	PHE	CB-CG-CD2	5.30	124.51	120.80
14	N	108	DT	OP1-P-O3'	5.30	116.87	105.20
19	T	-126	DG	N1-C6-O6	-5.30	116.72	119.90
14	N	26	DC	N3-C2-O2	-5.30	118.19	121.90
14	N	95	DT	C6-C5-C7	-5.30	119.72	122.90
19	T	-102	DC	N1-C2-O2	5.29	122.08	118.90
19	T	-54	DC	O4'-C1'-N1	5.29	111.71	108.00
3	C	106	ARG	CG-CD-NE	5.28	122.90	111.80
19	T	-61	DA	C4-C5-C6	-5.28	114.36	117.00
19	T	-138	DT	N3-C2-O2	-5.28	119.13	122.30
2	B	572	CYS	CA-CB-SG	5.28	123.50	114.00
14	N	45	DC	P-O3'-C3'	5.28	126.03	119.70
21	V	198	ARG	NE-CZ-NH1	5.28	122.94	120.30
14	N	102	DG	O4'-C1'-N9	5.27	111.69	108.00
2	B	379	ARG	CA-CB-CG	5.27	124.99	113.40
19	T	-36	DC	O4'-C1'-N1	5.27	111.69	108.00
14	N	75	DG	N1-C6-O6	-5.26	116.74	119.90
1	A	13	CYS	CA-CB-SG	5.26	123.47	114.00
15	O	207	ARG	NE-CZ-NH2	-5.25	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	TYR	CB-CG-CD2	5.25	124.15	121.00
2	B	222	ARG	NE-CZ-NH2	5.25	122.92	120.30
29	d	96	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	227	ARG	NE-CZ-NH2	5.24	122.92	120.30
13	M	328	PRO	CA-N-CD	-5.24	104.17	111.50
13	M	1060	PRO	CA-N-CD	-5.24	104.17	111.50
14	N	104	DT	N3-C2-O2	-5.24	119.16	122.30
19	T	-113	DG	N1-C6-O6	-5.24	116.76	119.90
27	f	35	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	743	ARG	CD-NE-CZ	5.23	130.93	123.60
14	N	92	DC	O4'-C1'-N1	5.23	111.66	108.00
13	M	543	PRO	CA-N-CD	-5.23	104.18	111.50
20	U	412	LEU	CA-CB-CG	5.23	127.33	115.30
19	T	-94	DC	O4'-C1'-N1	5.23	111.66	108.00
19	T	-72	DT	C6-C5-C7	-5.23	119.76	122.90
13	M	1158	PRO	CA-N-CD	-5.22	104.19	111.50
20	U	387	ARG	CA-CB-CG	5.22	124.89	113.40
26	e	53	ARG	CG-CD-NE	5.22	122.77	111.80
13	M	1025	PRO	CA-N-CD	-5.22	104.19	111.50
14	N	79	DA	C4-C5-C6	-5.22	114.39	117.00
5	E	187	ARG	NE-CZ-NH2	5.22	122.91	120.30
25	Z	758	PRO	CA-N-CD	-5.22	104.20	111.50
28	g	71	ARG	NE-CZ-NH2	5.22	122.91	120.30
9	I	103	ARG	CA-CB-CG	5.21	124.87	113.40
27	f	67	ARG	CD-NE-CZ	5.21	130.90	123.60
13	M	944	PRO	CA-N-CD	-5.21	104.20	111.50
19	T	-28	DC	N1-C2-O2	5.21	122.03	118.90
4	D	95	PHE	CB-CG-CD2	5.21	124.45	120.80
14	N	59	DT	C5-C6-N1	-5.21	120.58	123.70
25	Z	749	ARG	CD-NE-CZ	5.21	130.89	123.60
13	M	907	PRO	CA-N-CD	-5.21	104.21	111.50
13	M	994	PRO	CA-N-CD	-5.21	104.21	111.50
13	M	908	PRO	CA-N-CD	-5.21	104.21	111.50
1	A	618	TYR	CB-CG-CD2	-5.20	117.88	121.00
13	M	563	PRO	CA-N-CD	-5.20	104.21	111.50
1	A	421	ARG	CA-CB-CG	5.20	124.84	113.40
28	c	32	ARG	NE-CZ-NH2	5.20	122.90	120.30
13	M	980	PRO	CA-N-CD	-5.20	104.23	111.50
27	b	40	ARG	NE-CZ-NH2	5.20	122.90	120.30
13	M	1330	PRO	CA-N-CD	-5.19	104.23	111.50
14	N	48	DC	N1-C2-O2	5.19	122.02	118.90
14	N	104	DT	C6-C5-C7	-5.19	119.78	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	242	ARG	CD-NE-CZ	5.19	130.87	123.60
14	N	96	DG	N1-C6-O6	-5.19	116.78	119.90
2	B	286	GLU	CA-CB-CG	5.19	124.82	113.40
1	A	1031	ARG	CA-CB-CG	5.19	124.81	113.40
1	A	548	PHE	CB-CG-CD2	5.18	124.43	120.80
2	B	834	ARG	CG-CD-NE	5.18	122.69	111.80
14	N	18	DT	N3-C2-O2	-5.18	119.19	122.30
1	A	710	LYS	CA-CB-CG	5.18	124.80	113.40
19	T	-79	DT	N3-C2-O2	-5.18	119.19	122.30
18	R	562	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	A	342	ARG	NE-CZ-NH2	5.18	122.89	120.30
5	E	8	TYR	CB-CG-CD2	5.17	124.10	121.00
14	N	14	DT	OP1-P-O3'	5.17	116.58	105.20
19	T	-84	DG	N1-C6-O6	-5.17	116.80	119.90
5	E	24	ARG	CG-CD-NE	5.17	122.66	111.80
19	T	-34	DA	C4-C5-C6	-5.17	114.42	117.00
13	M	943	HIS	C-N-CD	-5.17	109.23	120.60
19	T	-33	DG	C5-C6-N1	5.16	114.08	111.50
14	N	50	DT	C5-C6-N1	-5.16	120.60	123.70
14	N	61	DT	N3-C2-O2	-5.16	119.20	122.30
26	a	131	ARG	NE-CZ-NH1	-5.16	117.72	120.30
14	N	74	DC	C1'-O4'-C4'	-5.16	104.94	110.10
3	C	63	PHE	CB-CG-CD2	5.15	124.41	120.80
2	B	845	TYR	CB-CG-CD2	5.15	124.09	121.00
14	N	55	DG	O4'-C1'-N9	5.15	111.61	108.00
2	B	411	LEU	CA-CB-CG	5.14	127.13	115.30
17	Q	663	PHE	CB-CG-CD2	5.14	124.40	120.80
17	Q	713	LYS	CA-CB-CG	5.14	124.71	113.40
20	U	498	SER	CB-CA-C	5.14	119.86	110.10
14	N	95	DT	O4'-C1'-N1	5.14	111.60	108.00
1	A	218	PRO	CA-C-N	-5.13	105.91	117.20
5	E	55	ARG	CD-NE-CZ	5.13	130.78	123.60
19	T	-91	DC	O4'-C1'-N1	5.13	111.59	108.00
6	F	115	TYR	CB-CG-CD2	5.13	124.08	121.00
16	P	30	C	C4-C5-C6	5.13	119.96	117.40
19	T	-124	DC	C1'-O4'-C4'	-5.12	104.98	110.10
2	B	280	SER	N-CA-CB	5.12	118.18	110.50
19	T	-120	DT	C6-C5-C7	-5.12	119.83	122.90
14	N	104	DT	O4'-C1'-N1	5.12	111.58	108.00
19	T	-129	DC	N1-C2-O2	5.12	121.97	118.90
29	h	83	ARG	CD-NE-CZ	5.12	130.76	123.60
14	N	58	DT	O4'-C1'-C2'	-5.11	101.81	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	T	-79	DT	C1'-O4'-C4'	-5.11	104.99	110.10
16	P	36	U	O4'-C1'-C2'	-5.11	100.69	105.80
2	B	764	MET	CA-CB-CG	5.10	121.97	113.30
2	B	831	LYS	CA-CB-CG	5.10	124.63	113.40
5	E	122	ALA	O-C-N	-5.10	111.41	121.10
1	A	535	MET	CA-CB-CG	5.10	121.97	113.30
13	M	1337	PHE	CB-CG-CD2	5.10	124.37	120.80
25	Z	499	PHE	CB-CG-CD2	5.10	124.37	120.80
14	N	49	DT	C5-C6-N1	-5.10	120.64	123.70
19	T	-94	DC	N1-C2-O2	5.10	121.96	118.90
12	L	51	ARG	CD-NE-CZ	5.09	130.73	123.60
1	A	271	ARG	CA-CB-CG	5.09	124.60	113.40
14	N	20	DT	N3-C2-O2	-5.09	119.25	122.30
19	T	-92	DG	O4'-C1'-N9	5.09	111.56	108.00
2	B	917	LYS	CA-CB-CG	5.09	124.60	113.40
7	G	109	SER	N-CA-CB	5.09	118.13	110.50
3	C	10	ARG	CA-CB-CG	5.09	124.59	113.40
3	C	162	ARG	NE-CZ-NH2	5.08	122.84	120.30
14	N	81	DG	N1-C6-O6	-5.08	116.85	119.90
19	T	-77	DC	O4'-C1'-N1	5.08	111.55	108.00
1	A	1167	ARG	CG-CD-NE	5.07	122.45	111.80
6	F	62	ARG	CD-NE-CZ	5.07	130.70	123.60
21	V	110	GLU	CA-CB-CG	5.07	124.54	113.40
1	A	429	LEU	CA-CB-CG	5.06	126.95	115.30
16	P	29	U	O4'-C1'-N1	5.06	112.25	108.20
14	N	48	DC	O4'-C1'-N1	5.06	111.54	108.00
5	E	153	LYS	CA-CB-CG	5.05	124.51	113.40
6	F	56	TYR	CB-CG-CD2	5.05	124.03	121.00
26	a	105	GLU	CA-CB-CG	5.05	124.51	113.40
14	N	113	DC	N3-C4-C5	5.05	123.92	121.90
29	d	40	LYS	CA-CB-CG	5.05	124.50	113.40
1	A	1345	ARG	CD-NE-CZ	5.04	130.66	123.60
14	N	63	DG	N1-C6-O6	-5.04	116.88	119.90
19	T	-68	DC	OP1-P-O3'	5.04	116.28	105.20
19	T	-40	DC	N1-C2-O2	5.04	121.92	118.90
1	A	327	ARG	NE-CZ-NH2	5.03	122.82	120.30
7	G	128	TYR	CD1-CG-CD2	-5.03	112.36	117.90
19	T	-125	DG	N1-C6-O6	-5.03	116.88	119.90
2	B	975	ARG	CB-CG-CD	5.03	124.68	111.60
1	A	203	LYS	CA-CB-CG	5.03	124.46	113.40
14	N	47	DC	N1-C2-O2	5.03	121.92	118.90
14	N	40	DG	N3-C2-N2	-5.02	116.38	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	f	45	ARG	NE-CZ-NH2	5.02	122.81	120.30
6	F	57	MET	CA-CB-CG	5.02	121.83	113.30
21	V	131	MET	CA-CB-CG	5.02	121.83	113.30
13	M	1381	ARG	NE-CZ-NH2	5.01	122.81	120.30
3	C	206	SER	N-CA-CB	5.01	118.02	110.50
2	B	380	ARG	CA-CB-CG	5.01	124.43	113.40
19	T	-35	DA	C6-C5-N7	5.01	135.81	132.30
26	e	42	ARG	NE-CZ-NH2	5.01	122.80	120.30
1	A	986	MET	CA-CB-CG	5.00	121.81	113.30
6	F	115	TYR	CD1-CG-CD2	-5.00	112.40	117.90
25	Z	453	LYS	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (111) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1177	TYR	Sidechain
1	A	1213	ARG	Sidechain
1	A	1396	ARG	Sidechain
1	A	1525	TPO	Mainchain
1	A	1547	SEP	Mainchain
1	A	413	TYR	Sidechain
1	A	727	PRO	Mainchain
1	A	84	HIS	Sidechain
1	A	862	ARG	Sidechain
1	A	910	LYS	Peptide
2	B	1029	TYR	Sidechain
2	B	1048	TYR	Sidechain
2	B	472	ARG	Sidechain
2	B	547	GLU	Peptide
2	B	686	GLU	Peptide
2	B	736	TYR	Sidechain
2	B	743	ARG	Sidechain
2	B	766	TYR	Sidechain
2	B	811	TYR	Sidechain
2	B	924	ARG	Sidechain
3	C	164	TYR	Sidechain
3	C	231	TYR	Sidechain
3	C	240	ARG	Sidechain
4	D	84	ARG	Sidechain
9	I	31	GLU	Peptide
10	J	42	ARG	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
10	J	43	TYR	Sidechain
10	J	47	ARG	Sidechain
10	J	6	ARG	Sidechain
13	M	1334	ASN	Peptide
13	M	1359	LYS	Peptide
13	M	663	GLY	Mainchain
14	N	100	DG	Sidechain
14	N	102	DG	Sidechain
14	N	104	DT	Sidechain
14	N	118	DT	Sidechain
14	N	123	DG	Sidechain
14	N	124	DG	Sidechain
14	N	127	DT	Sidechain
14	N	128	DC	Sidechain
14	N	130	DG	Sidechain
14	N	18	DT	Sidechain
14	N	19	DC	Sidechain
14	N	20	DT	Sidechain
14	N	23	DT	Sidechain
14	N	24	DG	Sidechain
14	N	43	DT	Sidechain
14	N	45	DC	Sidechain
14	N	47	DC	Sidechain
14	N	49	DT	Sidechain
14	N	50	DT	Sidechain
14	N	51	DG	Sidechain
14	N	52	DG	Sidechain
14	N	54	DG	Sidechain
14	N	55	DG	Sidechain
14	N	59	DT	Sidechain
14	N	61	DT	Sidechain
14	N	63	DG	Sidechain
14	N	70	DA	Sidechain
14	N	73	DG	Sidechain
14	N	76	DC	Sidechain
14	N	78	DT	Sidechain
14	N	79	DA	Sidechain
14	N	80	DC	Sidechain
14	N	89	DA	Sidechain
14	N	90	DA	Sidechain
14	N	96	DG	Sidechain
14	N	97	DC	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
14	N	99	DA	Sidechain
16	P	37	G	Sidechain
18	R	592	ASP	Peptide
19	T	-101	DT	Sidechain
19	T	-117	DA	Sidechain
19	T	-120	DT	Sidechain
19	T	-121	DC	Sidechain
19	T	-122	DG	Sidechain
19	T	-127	DA	Sidechain
19	T	-128	DG	Sidechain
19	T	-32	DA	Sidechain
19	T	-40	DC	Sidechain
19	T	-41	DA	Sidechain
19	T	-46	DG	Sidechain
19	T	-48	DG	Sidechain
19	T	-52	DC	Sidechain
19	T	-54	DC	Sidechain
19	T	-55	DC	Sidechain
19	T	-56	DA	Sidechain
19	T	-57	DA	Sidechain
19	T	-60	DA	Sidechain
19	T	-61	DA	Sidechain
19	T	-62	DG	Sidechain
19	T	-72	DT	Sidechain
19	T	-73	DC	Sidechain
19	T	-76	DG	Sidechain
19	T	-77	DC	Sidechain
19	T	-78	DA	Sidechain
19	T	-81	DC	Sidechain
19	T	-84	DG	Sidechain
19	T	-85	DC	Sidechain
19	T	-86	DA	Sidechain
19	T	-90	DT	Sidechain
19	T	-91	DC	Sidechain
19	T	-92	DG	Sidechain
25	Z	775	TPO	Mainchain
26	a	69	ARG	Sidechain
28	c	57	TYR	Sidechain
28	g	17	ARG	Sidechain
28	g	32	ARG	Sidechain
28	g	57	TYR	Sidechain
28	g	88	ARG	Sidechain

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Mol	Chain	Res	Type	Group
29	h	118	TYR	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11255	11385	11372	207	0
2	B	8980	9024	9022	59	0
3	C	2072	2021	2022	18	0
4	D	1004	981	980	8	0
5	E	1720	1736	1736	22	0
6	F	626	658	657	10	0
7	G	1333	1321	1321	12	0
8	H	1197	1157	1156	5	0
9	I	942	874	872	17	0
10	J	524	541	542	2	0
11	K	920	942	942	4	0
12	L	397	407	405	3	0
13	M	4927	2638	2622	21	0
14	N	2460	1355	1345	23	0
15	O	1274	0	1277	107	0
16	P	381	191	186	34	0
17	Q	7226	7171	7169	92	0
18	R	1836	1701	1699	26	0
19	T	2680	1458	1441	39	0
20	U	857	687	684	14	0
21	V	1711	1450	1446	17	0
22	W	2333	2247	2246	49	0
23	X	353	372	371	8	0
24	Y	911	909	907	10	0
25	Z	4025	4046	4041	43	0
26	a	802	841	841	0	0
26	e	801	839	838	0	0
27	b	662	710	709	0	0
27	f	619	660	659	0	0
28	c	795	847	846	0	0
28	g	809	865	864	0	0
29	d	745	774	773	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	h	726	749	747	0	0
30	A	2	0	0	0	0
30	B	1	0	0	0	0
30	C	1	0	0	2	0
30	I	2	0	0	0	0
30	J	1	0	0	0	0
30	R	1	0	0	0	0
30	Y	1	0	0	0	0
31	A	1	0	0	0	0
All	All	67913	61557	62738	677	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 5.

All (677) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1314:THR:CG2	15:O:297:ARG:HE	0.95	1.59
1:A:1314:THR:C	15:O:295:GLY:HA3	1.09	1.45
1:A:1314:THR:HG22	15:O:297:ARG:NE	1.31	1.38
1:A:1314:THR:C	15:O:295:GLY:CA	1.91	1.35
1:A:1314:THR:CG2	15:O:297:ARG:NE	1.79	1.35
1:A:1223:ASP:CG	15:O:244:ALA:HB2	1.45	1.34
16:P:45:G:C6	19:T:-36:DC:N4	1.96	1.32
16:P:45:G:N1	19:T:-36:DC:N4	1.77	1.31
1:A:1223:ASP:OD1	15:O:244:ALA:CB	1.78	1.31
1:A:1223:ASP:CG	15:O:244:ALA:CB	2.01	1.29
1:A:1315:ASP:OD2	15:O:294:CYS:SG	2.02	1.17
1:A:1314:THR:O	15:O:295:GLY:HA3	1.44	1.15
16:P:35:C:C4	16:P:36:U:C5	2.32	1.15
1:A:1223:ASP:OD1	15:O:244:ALA:HB2	1.31	1.14
1:A:1314:THR:HG21	15:O:297:ARG:HE	0.99	1.12
16:P:45:G:N1	16:P:46:G:C6	2.19	1.11
16:P:45:G:N1	19:T:-36:DC:N3	2.02	1.07
1:A:1314:THR:HA	15:O:295:GLY:O	1.55	1.06
16:P:45:G:O6	19:T:-36:DC:N4	1.88	1.04
1:A:1314:THR:CA	15:O:295:GLY:CA	2.34	1.03
1:A:1314:THR:CA	15:O:295:GLY:O	2.08	1.01
1:A:1318:LYS:HZ3	15:O:293:GLU:C	1.64	1.01
16:P:35:C:C4	16:P:36:U:H5	1.74	0.99
16:P:35:C:N4	16:P:36:U:H5	1.59	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:45:G:H1	19:T:-36:DC:N4	1.45	0.99
1:A:1315:ASP:N	15:O:295:GLY:HA3	1.77	0.98
1:A:1308:TYR:HB3	15:O:250:MET:CE	1.92	0.98
1:A:1309:MET:O	15:O:250:MET:HG3	1.65	0.95
16:P:45:G:N2	19:T:-36:DC:N3	2.16	0.94
16:P:45:G:N1	16:P:46:G:O6	2.00	0.94
1:A:611:ASP:OD2	15:O:261:PHE:CE1	2.22	0.93
16:P:45:G:N1	19:T:-36:DC:C4	2.24	0.92
1:A:1314:THR:HA	15:O:295:GLY:CA	1.98	0.92
16:P:45:G:C2	19:T:-36:DC:N3	2.37	0.92
20:U:381:PHE:HZ	20:U:497:ASP:O	1.53	0.90
1:A:1315:ASP:N	15:O:295:GLY:C	2.24	0.90
1:A:1223:ASP:OD2	15:O:244:ALA:HB2	1.72	0.89
1:A:1315:ASP:OD2	15:O:294:CYS:CB	2.20	0.89
1:A:1223:ASP:OD1	15:O:244:ALA:HB3	1.70	0.89
1:A:1313:GLN:O	15:O:295:GLY:HA2	1.73	0.89
1:A:1314:THR:HG21	15:O:297:ARG:NE	1.66	0.88
1:A:1314:THR:HA	15:O:295:GLY:C	1.93	0.88
1:A:1315:ASP:N	15:O:295:GLY:CA	2.34	0.88
1:A:1525:TPO:O	1:A:1526:PRO:O	1.84	0.88
1:A:1314:THR:CA	15:O:295:GLY:HA3	2.01	0.88
1:A:1314:THR:HG22	15:O:297:ARG:HE	0.78	0.88
1:A:1314:THR:HB	15:O:295:GLY:O	1.72	0.88
1:A:1308:TYR:HB3	15:O:250:MET:HE1	1.54	0.87
1:A:910:LYS:NZ	15:O:265:LYS:HA	1.90	0.86
1:A:1314:THR:HG22	15:O:297:ARG:CZ	2.04	0.86
16:P:35:C:N3	16:P:36:U:C5	2.43	0.86
1:A:431:PHE:HZ	16:P:34:C:N4	1.72	0.86
18:R:387:VAL:HG13	18:R:405:ILE:HD11	1.57	0.86
1:A:1223:ASP:CG	15:O:244:ALA:HB1	1.97	0.86
1:A:1314:THR:CG2	15:O:297:ARG:CZ	2.55	0.85
13:M:931:CYS:O	13:M:932:SER:OG	1.96	0.83
11:K:77:THR:OG1	11:K:81:TYR:O	1.97	0.82
1:A:1024:ASN:O	5:E:162:ARG:NH1	2.13	0.81
1:A:1314:THR:CB	15:O:295:GLY:O	2.28	0.81
14:N:15:DC:C6	14:N:16:DT:H72	2.15	0.81
1:A:1309:MET:O	15:O:250:MET:CG	2.29	0.80
1:A:1308:TYR:CB	15:O:250:MET:CE	2.60	0.79
18:R:388:ARG:NH2	18:R:446:GLU:O	2.15	0.79
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.65	0.79
16:P:45:G:C2	16:P:46:G:C6	2.70	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:381:PHE:CZ	20:U:497:ASP:O	2.36	0.79
22:W:40:LEU:HD12	22:W:66:GLY:HA3	1.63	0.78
14:N:138:DA:H2"	14:N:139:DT:OP2	1.82	0.78
20:U:406:GLU:OE1	20:U:502:ARG:CB	2.31	0.78
2:B:357:CYS:SG	2:B:360:LYS:NZ	2.56	0.78
22:W:206:VAL:HG11	22:W:238:VAL:HG21	1.65	0.78
1:A:1310:HIS:CD2	15:O:250:MET:SD	2.76	0.78
1:A:917:GLU:OE2	1:A:921:ARG:NH2	2.17	0.78
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.17	0.78
1:A:11:SER:O	2:B:1135:TYR:OH	2.03	0.77
1:A:1318:LYS:NZ	15:O:293:GLU:C	2.37	0.77
1:A:1314:THR:HG23	15:O:297:ARG:HH21	1.49	0.76
20:U:457:PHE:CE1	20:U:497:ASP:CB	2.68	0.76
16:P:45:G:C2	16:P:46:G:C5	2.74	0.76
17:Q:276:ALA:HB1	17:Q:288:VAL:HG23	1.67	0.76
1:A:1314:THR:C	15:O:295:GLY:C	2.43	0.75
17:Q:65:GLU:OE2	17:Q:93:TYR:OH	2.02	0.75
1:A:1308:TYR:HB3	15:O:250:MET:HE2	1.68	0.75
18:R:366:ARG:NH2	25:Z:775:TPO:OG1	2.20	0.75
1:A:729:PRO:HG3	15:O:247:GLU:HA	1.68	0.74
5:E:71:GLN:HB2	5:E:99:ILE:HG22	1.69	0.74
16:P:35:C:C4	16:P:36:U:C6	2.76	0.74
4:D:34:ASN:O	4:D:68:THR:OG1	2.06	0.73
9:I:109:ARG:HD3	9:I:124:THR:HG21	1.70	0.73
16:P:45:G:C6	16:P:46:G:O6	2.40	0.73
1:A:1315:ASP:OD2	15:O:294:CYS:HB2	1.89	0.73
1:A:1250:ASP:HB3	15:O:237:ARG:HH22	1.53	0.73
1:A:729:PRO:HA	15:O:247:GLU:O	1.89	0.72
22:W:66:GLY:O	22:W:83:SER:OG	2.07	0.72
1:A:1314:THR:CA	15:O:295:GLY:C	2.54	0.71
1:A:910:LYS:HZ1	15:O:265:LYS:HA	1.53	0.71
1:A:1315:ASP:H	15:O:295:GLY:C	1.94	0.70
1:A:1318:LYS:HZ3	15:O:294:CYS:N	1.88	0.70
2:B:1040:GLN:OE1	3:C:195:THR:OG1	2.08	0.70
1:A:1308:TYR:CB	15:O:250:MET:HE1	2.20	0.70
1:A:1309:MET:O	15:O:250:MET:SD	2.48	0.70
1:A:611:ASP:OD2	15:O:261:PHE:HE1	1.73	0.70
1:A:1250:ASP:HB2	15:O:225:ALA:HB1	1.73	0.70
25:Z:539:LEU:HD22	25:Z:616:HIS:HB3	1.74	0.70
20:U:382:LEU:HD11	20:U:497:ASP:CB	2.22	0.70
16:P:45:G:N2	19:T:-36:DC:C2	2.58	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:54:TYR:OH	9:I:56:ASN:ND2	2.25	0.69
1:A:729:PRO:CG	15:O:246:ARG:O	2.40	0.69
19:T:-68:DC:H2"	19:T:-67:DC:OP2	1.92	0.69
16:P:35:C:N4	16:P:36:U:C5	2.48	0.69
1:A:1314:THR:CA	15:O:295:GLY:HA2	2.22	0.69
14:N:137:DG:H2"	14:N:138:DA:OP2	1.91	0.69
19:T:-110:DG:H2"	19:T:-109:DT:OP2	1.93	0.68
1:A:1314:THR:HA	15:O:295:GLY:HA2	1.74	0.68
19:T:-67:DC:H2"	19:T:-66:DC:C5	2.29	0.68
25:Z:504:SER:OG	25:Z:507:THR:O	2.10	0.68
8:H:69:THR:OG1	8:H:81:ARG:NH1	2.27	0.68
25:Z:558:PHE:N	25:Z:570:VAL:O	2.27	0.68
1:A:1536:GLY:O	13:M:1480:ARG:NH1	2.26	0.68
17:Q:799:VAL:O	17:Q:802:LYS:NZ	2.28	0.67
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	1.77	0.67
25:Z:759:GLY:O	25:Z:761:MET:N	2.27	0.67
17:Q:41:LEU:HD23	17:Q:81:ASP:HB3	1.76	0.67
9:I:103:ARG:NH1	9:I:105:GLU:OE2	2.28	0.67
1:A:825:ASN:ND2	1:A:835:GLU:OE2	2.29	0.66
22:W:169:ASP:N	22:W:169:ASP:OD1	2.29	0.66
1:A:729:PRO:CA	15:O:247:GLU:O	2.44	0.65
22:W:228:LEU:HD13	22:W:264:ARG:HB3	1.77	0.65
18:R:405:ILE:HG23	18:R:426:LEU:HD11	1.78	0.65
22:W:13:GLN:NE2	22:W:15:HIS:O	2.29	0.65
24:Y:3:LEU:O	24:Y:8:LYS:NZ	2.29	0.65
19:T:-69:DC:H2"	19:T:-68:DC:C6	2.32	0.65
25:Z:563:MET:HA	25:Z:637:VAL:HG11	1.78	0.65
1:A:729:PRO:HB2	15:O:249:GLN:O	1.97	0.64
1:A:910:LYS:HZ3	15:O:265:LYS:HA	1.60	0.64
1:A:513:ALA:HB2	6:F:90:LEU:HD21	1.78	0.64
3:C:193:ARG:NH1	3:C:218:ALA:O	2.31	0.64
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.79	0.64
19:T:-132:DT:H2"	19:T:-131:DG:OP2	1.98	0.64
1:A:1314:THR:CG2	15:O:297:ARG:NH2	2.62	0.64
1:A:431:PHE:CZ	16:P:34:C:N4	2.63	0.63
1:A:1310:HIS:CG	15:O:250:MET:SD	2.92	0.63
25:Z:478:VAL:HB	25:Z:518:LEU:HD11	1.81	0.62
1:A:54:LEU:O	1:A:61:ARG:NH1	2.32	0.62
2:B:650:ASN:ND2	20:U:496:THR:CB	2.62	0.62
2:B:866:ILE:HG22	2:B:867:ILE:HG13	1.81	0.62
17:Q:605:LEU:O	17:Q:609:ASN:ND2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:206:VAL:HG22	22:W:216:ILE:HG12	1.82	0.62
2:B:792:ASP:OD1	2:B:975:ARG:NH2	2.29	0.62
19:T:-142:DA:H2"	19:T:-141:DG:OP2	1.98	0.62
1:A:910:LYS:HZ1	15:O:265:LYS:CA	2.13	0.62
5:E:2:ASP:OD1	5:E:4:GLU:N	2.32	0.62
17:Q:94:VAL:HG23	17:Q:140:LEU:HD11	1.81	0.62
22:W:195:SER:OG	22:W:236:LEU:O	2.16	0.62
1:A:1330:ALA:HB3	15:O:294:CYS:HA	1.82	0.61
21:V:45:ASP:OD1	21:V:45:ASP:N	2.33	0.61
25:Z:478:VAL:HG21	25:Z:502:LEU:HD22	1.81	0.61
1:A:1250:ASP:CB	15:O:237:ARG:HH22	2.12	0.61
1:A:1314:THR:CG2	15:O:297:ARG:HH21	2.13	0.61
1:A:955:GLU:OE1	1:A:1010:VAL:HG22	2.00	0.61
22:W:272:ASP:O	22:W:274:GLN:NE2	2.33	0.61
3:C:88:CYS:SG	30:C:301:ZN:ZN	1.88	0.61
17:Q:95:GLN:NE2	21:V:84:ILE:O	2.34	0.61
5:E:66:ASP:OD1	5:E:67:ASP:N	2.33	0.61
24:Y:35:ASN:ND2	24:Y:85:TYR:OH	2.33	0.61
20:U:457:PHE:HE1	20:U:497:ASP:CB	2.13	0.60
7:G:93:ASN:O	7:G:128:TYR:OH	2.18	0.60
13:M:1335:ILE:HD12	13:M:1340:ALA:HB2	1.83	0.60
14:N:139:DT:H2"	14:N:140:DT:OP2	2.00	0.60
17:Q:423:GLU:OE1	23:X:231:TRP:NE1	2.31	0.60
22:W:27:ASN:O	22:W:32:SER:OG	2.16	0.60
3:C:86:ARG:NH2	25:Z:716:PRO:O	2.33	0.60
2:B:834:ARG:NH1	2:B:841:ARG:O	2.34	0.60
1:A:1301:ILE:HG22	1:A:1345:ARG:HH11	1.66	0.60
1:A:729:PRO:CB	15:O:249:GLN:O	2.50	0.60
24:Y:75:GLN:O	24:Y:111:ARG:NH2	2.35	0.60
1:A:1315:ASP:N	15:O:295:GLY:O	2.33	0.60
1:A:911:PRO:O	1:A:963:ARG:NH1	2.34	0.59
9:I:42:CYS:SG	9:I:43:ASP:N	2.75	0.59
13:M:1371:SER:HB2	13:M:1374:ILE:HD13	1.84	0.59
17:Q:401:LEU:HD22	17:Q:418:LEU:HG	1.84	0.59
22:W:48:LYS:N	22:W:55:ASP:O	2.30	0.59
1:A:1016:LEU:HD22	1:A:1069:LEU:HD22	1.84	0.59
9:I:39:CYS:SG	9:I:40:ARG:N	2.75	0.59
1:A:742:ASN:O	1:A:746:ASN:ND2	2.36	0.59
16:P:46:G:C6	19:T:-36:DC:N3	2.71	0.59
1:A:282:ASP:O	1:A:285:LYS:N	2.36	0.58
17:Q:620:ARG:NH2	17:Q:659:HIS:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:364:PHE:HB3	17:Q:380:ILE:HD11	1.85	0.58
22:W:176:ASP:HB2	22:W:183:LEU:HD11	1.85	0.58
25:Z:554:GLU:OE1	25:Z:557:THR:OG1	2.21	0.58
24:Y:93:LEU:HD22	24:Y:97:ILE:HD11	1.84	0.58
17:Q:286:SER:O	17:Q:290:HIS:ND1	2.36	0.58
17:Q:856:LEU:HD23	17:Q:857:LEU:HD22	1.86	0.58
19:T:-133:DG:H2'	19:T:-132:DT:C6	2.39	0.58
22:W:95:ASN:O	22:W:97:LYS:NZ	2.36	0.58
1:A:1309:MET:N	15:O:250:MET:HE2	2.19	0.58
25:Z:554:GLU:OE2	25:Z:559:GLN:NE2	2.36	0.58
2:B:298:MET:HE3	9:I:14:ILE:HD12	1.86	0.58
9:I:35:LEU:HD21	9:I:53:ILE:HD11	1.85	0.58
17:Q:68:ARG:HE	17:Q:89:LEU:HD12	1.68	0.58
18:R:406:THR:OG1	18:R:427:GLN:O	2.21	0.57
1:A:927:GLU:O	1:A:931:ARG:NE	2.36	0.57
14:N:15:DC:N1	14:N:16:DT:H72	2.18	0.57
1:A:710:LYS:NZ	1:A:824:GLU:OE1	2.37	0.57
16:P:40:G:H1	19:T:-31:DC:N4	2.03	0.57
17:Q:776:LEU:O	17:Q:779:VAL:HG22	2.03	0.57
1:A:848:ILE:HD11	2:B:499:ARG:O	2.04	0.57
2:B:551:GLU:HB3	2:B:556:ILE:HD13	1.85	0.57
22:W:112:LEU:HD22	22:W:121:LEU:HD21	1.87	0.57
1:A:876:ASP:HB3	1:A:878:THR:HG22	1.85	0.57
22:W:14:ALA:N	22:W:296:GLN:O	2.32	0.57
17:Q:387:ALA:N	17:Q:390:ASP:OD2	2.31	0.56
25:Z:478:VAL:HG11	25:Z:492:ILE:HG23	1.87	0.56
25:Z:529:ASP:HB3	25:Z:553:LEU:HD23	1.87	0.56
2:B:279:VAL:HG23	2:B:312:GLN:O	2.06	0.56
16:P:46:G:N1	19:T:-36:DC:C2	2.73	0.56
22:W:236:LEU:N	22:W:250:SER:O	2.37	0.56
2:B:179:LEU:HD22	2:B:768:ARG:HD3	1.87	0.56
23:X:221:THR:O	23:X:225:VAL:HG22	2.06	0.56
1:A:687:ILE:HD11	1:A:766:PHE:CE1	2.40	0.56
1:A:1155:LYS:HE2	15:O:248:HIS:CB	2.36	0.56
1:A:1194:ASN:OD1	15:O:192:ARG:NH1	2.39	0.56
1:A:1212:LEU:HD12	1:A:1285:LEU:HD13	1.88	0.56
4:D:103:LEU:O	7:G:144:ARG:NH1	2.39	0.55
17:Q:384:LEU:HD13	17:Q:397:ALA:HB2	1.89	0.55
17:Q:568:TRP:HE1	17:Q:591:ILE:HD12	1.71	0.55
2:B:809:VAL:HG21	3:C:60:HIS:CD2	2.42	0.55
1:A:868:MET:HG3	1:A:1404:THR:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:494:ALA:HB1	23:X:224:ILE:HG12	1.89	0.55
17:Q:474:PHE:HB2	17:Q:503:LEU:HD13	1.89	0.55
16:P:45:G:N1	16:P:46:G:C5	2.69	0.55
17:Q:620:ARG:NH1	17:Q:629:GLN:OE1	2.40	0.55
1:A:421:ARG:NE	1:A:427:ILE:HD11	2.22	0.54
1:A:1309:MET:N	15:O:250:MET:CE	2.70	0.54
5:E:111:THR:HG23	5:E:114:ALA:H	1.71	0.54
1:A:729:PRO:HG2	15:O:246:ARG:O	2.07	0.54
22:W:131:ASN:ND2	22:W:143:SER:OG	2.37	0.54
1:A:1310:HIS:CB	15:O:250:MET:SD	2.95	0.54
3:C:175:LYS:NZ	12:L:57:ALA:O	2.37	0.54
1:A:738:GLU:O	1:A:742:ASN:ND2	2.36	0.54
14:N:138:DA:H1'	14:N:139:DT:H5'	1.90	0.54
20:U:512:CYS:O	20:U:513:SER:CB	2.54	0.54
19:T:-68:DC:H2''	19:T:-67:DC:C6	2.43	0.54
25:Z:588:ASP:OD1	25:Z:592:ASN:N	2.35	0.54
1:A:324:GLY:O	1:A:325:LEU:HD22	2.07	0.54
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.36	0.54
19:T:-68:DC:H2''	19:T:-67:DC:H6	1.72	0.54
1:A:421:ARG:HE	1:A:427:ILE:HD11	1.71	0.54
1:A:832:THR:HG23	1:A:833:PRO:HD2	1.90	0.54
14:N:106:DT:H2''	14:N:107:DC:C6	2.43	0.54
19:T:-111:DC:H2''	19:T:-110:DG:C8	2.42	0.54
22:W:251:SER:OG	22:W:253:ASP:OD1	2.23	0.54
16:P:35:C:C5	16:P:36:U:C6	2.95	0.53
25:Z:525:ALA:HB1	25:Z:552:ARG:HH12	1.74	0.53
2:B:297:MET:HG2	2:B:377:LEU:HD11	1.89	0.53
17:Q:768:VAL:HG21	17:Q:778:GLU:HG3	1.91	0.53
3:C:189:ASP:OD1	3:C:209:SER:OG	2.24	0.53
20:U:382:LEU:CD1	20:U:497:ASP:CB	2.86	0.53
24:Y:40:LEU:HD22	24:Y:42:MET:HB3	1.91	0.53
1:A:1315:ASP:CG	15:O:294:CYS:CB	2.77	0.53
17:Q:420:GLN:O	23:X:229:ARG:NH2	2.42	0.53
7:G:37:THR:OG1	7:G:38:CYS:N	2.40	0.53
17:Q:643:ASP:OD2	23:X:239:GLN:NE2	2.35	0.53
22:W:113:ALA:HB3	22:W:122:ALA:HB3	1.89	0.53
19:T:-109:DT:H2''	19:T:-108:DA:C8	2.44	0.52
1:A:1314:THR:OG1	1:A:1316:ASN:OD1	2.28	0.52
5:E:67:ASP:OD1	5:E:69:THR:OG1	2.22	0.52
21:V:61:TYR:N	21:V:62:LYS:HA	2.24	0.52
17:Q:753:LEU:O	17:Q:757:VAL:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:PHE:CD2	1:A:952:LEU:HD23	2.45	0.52
3:C:20:LYS:NZ	3:C:207:GLU:OE2	2.42	0.52
22:W:163:LEU:O	22:W:175:PHE:N	2.37	0.52
2:B:938:ARG:NH1	2:B:983:GLU:OE2	2.41	0.52
17:Q:143:ASP:N	17:Q:143:ASP:OD1	2.43	0.52
17:Q:380:ILE:HG21	17:Q:396:ILE:HD12	1.90	0.52
1:A:886:VAL:HG12	5:E:169:GLN:O	2.10	0.52
19:T:-67:DC:H2''	19:T:-66:DC:C6	2.45	0.52
22:W:248:VAL:HG12	22:W:258:VAL:HG22	1.90	0.52
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.92	0.51
5:E:185:ILE:HD12	5:E:209:VAL:HG21	1.92	0.51
22:W:130:VAL:HB	22:W:144:LEU:HD12	1.90	0.51
1:A:1314:THR:HG23	15:O:297:ARG:NH2	2.20	0.51
1:A:1315:ASP:CG	15:O:296:ASN:N	2.63	0.51
2:B:898:THR:O	2:B:899:SER:OG	2.26	0.51
18:R:355:LEU:HD12	18:R:356:PRO:HD2	1.93	0.51
1:A:431:PHE:HZ	16:P:34:C:H41	1.57	0.51
17:Q:86:LEU:HD11	17:Q:116:LEU:HB3	1.91	0.51
17:Q:211:LEU:HD12	17:Q:213:LYS:HZ1	1.75	0.51
22:W:125:THR:OG1	22:W:131:ASN:OD1	2.25	0.51
6:F:51:ARG:NH2	6:F:122:GLU:OE1	2.37	0.51
1:A:77:ASN:OD1	1:A:78:MET:N	2.43	0.51
25:Z:506:LEU:HD11	25:Z:552:ARG:HH11	1.75	0.51
25:Z:610:ARG:HD2	25:Z:629:LEU:HD21	1.92	0.51
4:D:37:VAL:HG21	7:G:2:PHE:CD2	2.46	0.51
21:V:88:ASN:OD1	21:V:89:PRO:HD3	2.10	0.51
1:A:909:LEU:O	1:A:911:PRO:HD3	2.11	0.51
3:C:88:CYS:HG	30:C:301:ZN:ZN	1.25	0.51
22:W:76:LEU:HD12	22:W:77:PRO:HD2	1.92	0.51
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.93	0.51
14:N:14:DT:H2''	14:N:15:DC:C6	2.46	0.51
17:Q:772:GLU:HA	17:Q:773:LYS:HB2	1.92	0.51
17:Q:156:LEU:HD11	17:Q:169:LYS:HE2	1.92	0.51
25:Z:492:ILE:HG22	25:Z:502:LEU:HB3	1.92	0.50
1:A:1223:ASP:CB	15:O:244:ALA:HB1	2.41	0.50
18:R:359:LEU:HD11	18:R:386:PHE:CE2	2.46	0.50
6:F:105:ILE:HD12	6:F:117:ASP:HB3	1.94	0.50
6:F:114:SER:OG	6:F:115:TYR:N	2.44	0.50
13:M:1370:VAL:HG21	13:M:1376:GLN:HG3	1.92	0.50
22:W:292:VAL:HG12	22:W:298:ILE:HG12	1.91	0.50
14:N:71:DC:H2''	14:N:72:DA:OP2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:849:LYS:O	17:Q:852:LEU:HG	2.12	0.50
17:Q:86:LEU:HG	17:Q:120:ALA:HB2	1.93	0.50
18:R:485:TYR:OH	18:R:489:ASP:OD2	2.30	0.50
1:A:686:THR:HG21	2:B:1040:GLN:O	2.12	0.50
1:A:1318:LYS:HZ2	15:O:295:GLY:N	2.10	0.50
13:M:1459:ILE:HD11	13:M:1469:PHE:HB3	1.94	0.50
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.77	0.50
1:A:1251:ASN:ND2	15:O:200:ASP:OD2	2.45	0.50
17:Q:201:ARG:HH22	17:Q:227:LEU:HD13	1.77	0.50
25:Z:542:LEU:CD2	25:Z:560:VAL:HG11	2.42	0.50
1:A:850:THR:O	1:A:854:THR:HG23	2.12	0.49
1:A:1318:LYS:HD2	15:O:294:CYS:C	2.31	0.49
1:A:513:ALA:CB	6:F:90:LEU:HD21	2.41	0.49
1:A:1054:MET:SD	1:A:1060:LEU:HD12	2.52	0.49
17:Q:803:MET:HE1	17:Q:807:LEU:HD11	1.94	0.49
1:A:1315:ASP:OD1	15:O:296:ASN:N	2.46	0.49
17:Q:524:LEU:HD11	17:Q:537:LEU:HD12	1.95	0.49
1:A:951:GLU:HG2	1:A:1007:ILE:HD11	1.95	0.49
2:B:835:GLU:N	2:B:835:GLU:OE1	2.46	0.49
2:B:310:VAL:HG23	2:B:311:ILE:HD12	1.95	0.49
13:M:1470:LEU:HD11	13:M:1481:ILE:HD12	1.93	0.49
13:M:1376:GLN:HG2	13:M:1466:PRO:HB2	1.93	0.49
1:A:587:THR:HG22	1:A:588:GLY:N	2.28	0.49
17:Q:708:LEU:HD21	17:Q:719:VAL:HG21	1.95	0.49
18:R:353:VAL:HG11	18:R:472:ILE:HD12	1.94	0.49
21:V:127:VAL:HG23	21:V:128:VAL:H	1.77	0.49
5:E:47:LYS:O	5:E:53:PRO:HD2	2.12	0.49
17:Q:232:VAL:O	17:Q:236:VAL:HG22	2.11	0.49
2:B:1094:GLN:HB2	2:B:1103:LEU:HD13	1.94	0.48
1:A:1318:LYS:NZ	15:O:294:CYS:N	2.59	0.48
5:E:61:LEU:HD12	5:E:72:MET:O	2.13	0.48
16:P:46:G:O6	19:T:-36:DC:C4	2.66	0.48
19:T:-133:DG:H2'	19:T:-132:DT:O4'	2.13	0.48
20:U:457:PHE:CD1	20:U:497:ASP:CB	2.96	0.48
1:A:525:ILE:O	1:A:534:VAL:HG22	2.12	0.48
13:M:1460:CYS:SG	13:M:1461:ALA:N	2.86	0.48
18:R:405:ILE:HG12	18:R:426:LEU:HD21	1.96	0.48
6:F:98:LYS:NZ	6:F:127:ASP:O	2.46	0.48
16:P:38:G:H3'	16:P:39:U:C5	2.49	0.48
1:A:1006:PRO:O	1:A:1010:VAL:HG23	2.14	0.48
14:N:109:DA:N6	19:T:-110:DG:O6	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:86:LEU:HD12	17:Q:89:LEU:HB2	1.95	0.48
25:Z:282:LYS:O	25:Z:287:LYS:NZ	2.44	0.48
1:A:725:LEU:HD21	1:A:736:THR:HG23	1.95	0.48
13:M:717:LEU:O	13:M:722:TYR:N	2.43	0.48
14:N:107:DC:H2''	14:N:108:DT:H71	1.95	0.48
17:Q:65:GLU:HA	17:Q:89:LEU:HD11	1.96	0.48
18:R:353:VAL:HG23	18:R:456:LYS:NZ	2.29	0.48
25:Z:505:ASP:OD2	25:Z:525:ALA:HB2	2.13	0.48
17:Q:419:ALA:HB2	17:Q:433:ALA:HB3	1.96	0.48
13:M:1509:LYS:O	13:M:1513:GLN:NE2	2.42	0.48
1:A:394:VAL:HG23	1:A:444:TYR:O	2.13	0.47
25:Z:542:LEU:HD21	25:Z:560:VAL:HG11	1.94	0.47
17:Q:69:ILE:H	17:Q:69:ILE:HD12	1.79	0.47
1:A:963:ARG:O	1:A:967:ARG:HG3	2.13	0.47
17:Q:415:TRP:HA	17:Q:418:LEU:HD12	1.97	0.47
18:R:359:LEU:HD11	18:R:386:PHE:CD2	2.48	0.47
18:R:592:ASP:O	18:R:594:PHE:N	2.43	0.47
2:B:677:MET:H	2:B:682:LEU:HD22	1.79	0.47
1:A:1250:ASP:HB3	15:O:237:ARG:NH2	2.26	0.47
7:G:123:SER:OG	7:G:125:PRO:O	2.31	0.47
17:Q:239:ALA:HB2	17:Q:257:LEU:HB3	1.95	0.47
1:A:392:GLU:OE2	1:A:401:ARG:NH1	2.48	0.47
1:A:1038:THR:HG22	1:A:1038:THR:O	2.15	0.47
1:A:1315:ASP:CG	15:O:294:CYS:SG	2.89	0.47
17:Q:214:LEU:HD23	17:Q:214:LEU:O	2.14	0.47
17:Q:351:TYR:HB2	17:Q:360:ALA:HB2	1.97	0.47
17:Q:682:ASP:O	17:Q:686:ASN:ND2	2.45	0.47
18:R:359:LEU:HD22	18:R:452:PHE:HE1	1.78	0.47
1:A:948:ILE:HG23	1:A:1007:ILE:HD13	1.97	0.47
1:A:1146:GLN:NE2	1:A:1150:ASP:OD2	2.47	0.47
21:V:110:GLU:HG3	21:V:111:GLU:H	1.80	0.47
7:G:117:MET:SD	7:G:117:MET:N	2.87	0.47
14:N:108:DT:H2''	14:N:109:DA:OP2	2.15	0.47
17:Q:120:ALA:HB1	17:Q:130:HIS:HE1	1.80	0.47
21:V:45:ASP:HB3	23:X:232:ARG:HE	1.80	0.47
22:W:41:ASP:OD1	22:W:41:ASP:N	2.47	0.47
14:N:136:DG:H2''	14:N:137:DG:H8	1.79	0.47
17:Q:651:ASN:ND2	17:Q:682:ASP:OD2	2.48	0.47
25:Z:424:ASP:HB2	25:Z:440:ILE:HD12	1.97	0.47
2:B:1129:ASN:HB3	2:B:1134:THR:HG22	1.97	0.46
17:Q:123:ILE:HG13	17:Q:124:ILE:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:386:ALA:HB1	17:Q:394:ARG:HG3	1.96	0.46
1:A:419:ILE:HG23	1:A:427:ILE:HB	1.97	0.46
1:A:1155:LYS:HE2	15:O:248:HIS:HB2	1.97	0.46
13:M:1440:LEU:HD13	13:M:1470:LEU:HD22	1.96	0.46
17:Q:18:GLU:N	17:Q:18:GLU:OE1	2.49	0.46
21:V:294:SER:O	21:V:295:LYS:C	2.54	0.46
1:A:1310:HIS:CA	15:O:250:MET:SD	3.04	0.46
2:B:1142:ASN:O	2:B:1144:THR:HG22	2.16	0.46
17:Q:80:LYS:O	17:Q:83:MET:HG3	2.15	0.46
17:Q:249:ASP:O	17:Q:253:ASN:ND2	2.49	0.46
25:Z:542:LEU:HD22	25:Z:570:VAL:HG11	1.97	0.46
14:N:110:DC:H2''	14:N:111:DG:OP2	2.14	0.46
18:R:359:LEU:HD22	18:R:452:PHE:CE1	2.51	0.46
19:T:-71:DG:H2''	19:T:-70:DT:C6	2.49	0.46
25:Z:280:ARG:HG3	25:Z:386:VAL:HG13	1.98	0.46
1:A:729:PRO:HG3	15:O:246:ARG:O	2.16	0.46
5:E:55:ARG:HB2	5:E:78:GLU:HG3	1.97	0.46
10:J:10:CYS:SG	10:J:45:CYS:SG	3.14	0.46
19:T:-30:DA:H2''	19:T:-29:DC:H6	1.79	0.46
1:A:1212:LEU:HD11	1:A:1285:LEU:HB3	1.98	0.46
1:A:1250:ASP:CA	15:O:237:ARG:HH22	2.27	0.46
5:E:45:GLY:HA3	5:E:53:PRO:HD3	1.96	0.46
25:Z:610:ARG:HD2	25:Z:629:LEU:HD11	1.98	0.46
1:A:710:LYS:CE	1:A:824:GLU:OE1	2.64	0.46
1:A:1251:ASN:HA	15:O:233:LEU:CD2	2.46	0.46
1:A:1318:LYS:HZ2	15:O:295:GLY:H	1.63	0.46
17:Q:494:ALA:HB2	23:X:223:ASP:OD2	2.16	0.46
18:R:403:ALA:HB3	18:R:428:LEU:HD13	1.97	0.46
19:T:-15:DG:H2''	19:T:-14:DA:H5'	1.98	0.46
22:W:278:TRP:HB2	22:W:293:GLY:HA2	1.97	0.46
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.96	0.46
2:B:759:VAL:O	2:B:759:VAL:HG22	2.16	0.46
9:I:12:VAL:HG21	9:I:53:ILE:O	2.16	0.46
13:M:843:LYS:O	13:M:845:PRO:HD3	2.16	0.46
18:R:355:LEU:HG	18:R:357:GLU:H	1.81	0.46
1:A:920:PHE:HD1	1:A:1050:CYS:HG	1.63	0.46
9:I:86:CYS:SG	9:I:87:GLN:N	2.89	0.45
2:B:411:LEU:HD12	2:B:411:LEU:C	2.37	0.45
24:Y:16:CYS:SG	24:Y:53:THR:OG1	2.71	0.45
1:A:713:VAL:HG21	1:A:817:PRO:HD3	1.98	0.45
1:A:1314:THR:C	15:O:295:GLY:O	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:759:VAL:O	2:B:759:VAL:CG2	2.64	0.45
17:Q:504:ALA:HB2	17:Q:519:LEU:HB3	1.99	0.45
22:W:37:THR:HA	22:W:70:VAL:HG21	1.99	0.45
22:W:237:ASN:HD22	22:W:238:VAL:H	1.65	0.45
25:Z:546:THR:HG22	25:Z:547:VAL:N	2.31	0.45
2:B:22:TRP:CG	2:B:679:PRO:HG3	2.51	0.45
2:B:757:PRO:HB2	2:B:760:THR:HG22	1.98	0.45
2:B:833:THR:HG22	2:B:835:GLU:OE1	2.16	0.45
16:P:43:U:H2'	16:P:44:U:O4'	2.15	0.45
17:Q:316:PHE:HB2	17:Q:325:ALA:HB2	1.98	0.45
21:V:297:TYR:O	21:V:298:GLU:C	2.55	0.45
25:Z:280:ARG:HB2	25:Z:382:ILE:HG23	1.98	0.45
1:A:1147:SER:OG	1:A:1351:ASP:OD2	2.34	0.45
2:B:1007:ASN:O	2:B:1011:ILE:HG13	2.17	0.45
18:R:404:GLU:OE2	18:R:455:TRP:NE1	2.43	0.45
1:A:457:ILE:HG21	2:B:1102:PHE:CZ	2.52	0.45
2:B:689:TYR:CE1	18:R:599:CYS:CB	3.00	0.45
17:Q:158:GLN:HG3	17:Q:159:SER:H	1.79	0.45
1:A:1044:HIS:O	1:A:1048:THR:HG23	2.17	0.45
17:Q:737:LYS:HZ2	17:Q:764:LEU:HD13	1.82	0.45
22:W:67:VAL:HG13	22:W:81:SER:OG	2.17	0.45
22:W:86:ALA:HB1	22:W:105:GLY:HA2	1.99	0.45
1:A:1038:THR:O	1:A:1042:ASN:ND2	2.48	0.45
2:B:1120:ASN:HD22	2:B:1120:ASN:N	2.15	0.45
22:W:237:ASN:HB3	22:W:280:VAL:HG22	1.97	0.45
17:Q:380:ILE:HD12	17:Q:400:HIS:HE1	1.82	0.45
19:T:-109:DT:H2''	19:T:-108:DA:N7	2.32	0.45
22:W:231:HIS:CE1	22:W:249:SER:HG	2.34	0.45
1:A:392:GLU:HG2	1:A:402:LEU:HD11	1.98	0.45
1:A:565:MET:CE	11:K:60:GLY:HA3	2.47	0.45
1:A:611:ASP:OD2	15:O:261:PHE:CD1	2.67	0.45
2:B:709:SER:OG	2:B:767:LEU:HD11	2.18	0.45
3:C:48:ASP:OD1	3:C:175:LYS:NZ	2.47	0.45
9:I:84:HIS:ND1	9:I:125:GLU:OE1	2.50	0.45
19:T:-66:DC:OP2	19:T:-66:DC:H6	1.99	0.45
25:Z:603:ILE:HG23	25:Z:604:ASP:N	2.31	0.45
1:A:282:ASP:O	1:A:283:ILE:C	2.56	0.44
1:A:819:SER:O	1:A:819:SER:OG	2.34	0.44
1:A:1212:LEU:CD1	1:A:1285:LEU:HD13	2.46	0.44
24:Y:4:GLU:O	24:Y:27:GLN:NE2	2.50	0.44
1:A:709:ALA:O	1:A:713:VAL:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:931:ILE:HD12	2:B:947:ILE:HA	1.99	0.44
5:E:2:ASP:OD1	5:E:3:ASP:N	2.50	0.44
16:P:40:G:H2'	16:P:41:U:C6	2.53	0.44
20:U:416:VAL:HG23	21:V:175:GLN:HA	1.99	0.44
25:Z:568:VAL:HG13	25:Z:570:VAL:HG13	2.00	0.44
2:B:479:LEU:O	2:B:483:ARG:HG3	2.17	0.44
5:E:100:THR:HA	5:E:125:TYR:HD1	1.82	0.44
5:E:189:GLN:O	5:E:209:VAL:HG23	2.17	0.44
18:R:560:ILE:HD13	21:V:137:ILE:O	2.17	0.44
25:Z:353:ALA:HB3	25:Z:360:ILE:HB	1.99	0.44
13:M:1230:THR:O	13:M:1238:GLY:N	2.50	0.44
17:Q:313:ALA:HB3	17:Q:329:TYR:CE1	2.52	0.44
17:Q:591:ILE:HG22	17:Q:592:LEU:HD12	1.99	0.44
25:Z:501:ILE:HD11	25:Z:510:GLU:HB3	1.99	0.44
1:A:682:ILE:O	2:B:1038:THR:HG23	2.17	0.44
1:A:722:ASN:HB2	1:A:724:GLU:OE1	2.18	0.44
14:N:107:DC:H2''	14:N:108:DT:C7	2.48	0.44
1:A:1165:THR:HG21	1:A:1294:THR:O	2.17	0.44
19:T:-30:DA:H2''	19:T:-29:DC:C6	2.53	0.44
21:V:126:LYS:HE3	21:V:126:LYS:HA	1.99	0.44
22:W:248:VAL:HG13	22:W:282:TYR:OH	2.18	0.44
1:A:397:PHE:HB3	6:F:87:THR:HG22	2.00	0.44
1:A:1310:HIS:HA	15:O:250:MET:SD	2.58	0.44
1:A:1330:ALA:CB	15:O:294:CYS:HA	2.46	0.44
17:Q:719:VAL:HG23	17:Q:720:VAL:N	2.33	0.44
1:A:883:ILE:HD11	1:A:1424:THR:HG22	2.00	0.44
1:A:1251:ASN:HA	15:O:233:LEU:HD23	1.99	0.44
21:V:88:ASN:O	21:V:90:ASP:N	2.50	0.44
25:Z:473:LYS:O	25:Z:492:ILE:HD11	2.17	0.44
1:A:721:HIS:CD2	9:I:110:LEU:HD21	2.52	0.43
3:C:84:TYR:CZ	3:C:167:LYS:HE3	2.53	0.43
3:C:175:LYS:CE	12:L:57:ALA:O	2.66	0.43
7:G:137:ILE:HG23	7:G:137:ILE:O	2.18	0.43
13:M:1471:LEU:HD21	13:M:1508:PHE:CE2	2.53	0.43
1:A:831:LEU:HG	2:B:715:ASP:O	2.18	0.43
5:E:87:ILE:HD11	5:E:117:SER:OG	2.17	0.43
17:Q:427:ILE:HG21	17:Q:464:LEU:HD21	2.00	0.43
17:Q:471:LYS:O	17:Q:475:LEU:HD23	2.18	0.43
17:Q:886:LYS:O	17:Q:890:MET:HG2	2.18	0.43
22:W:33:GLU:O	22:W:49:TRP:N	2.50	0.43
25:Z:312:ASP:O	25:Z:315:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ILE:HD11	1:A:314:VAL:HA	1.99	0.43
1:A:783:GLN:HA	1:A:787:VAL:O	2.17	0.43
2:B:497:LYS:N	2:B:498:PRO:CD	2.81	0.43
17:Q:288:VAL:HG13	17:Q:289:GLN:HG3	2.00	0.43
13:M:1395:LEU:HD23	13:M:1397:ILE:HG23	2.00	0.43
17:Q:48:ALA:HB2	17:Q:63:LEU:HD11	1.99	0.43
7:G:38:CYS:SG	7:G:39:THR:N	2.91	0.43
24:Y:40:LEU:HD21	24:Y:52:CYS:SG	2.59	0.43
1:A:699:TYR:O	1:A:703:GLN:HG2	2.19	0.43
19:T:-21:DG:H4'	25:Z:283:ARG:HE	1.84	0.43
1:A:823:VAL:HG22	1:A:835:GLU:HB2	2.00	0.43
2:B:388:TYR:H	2:B:504:THR:CG2	2.31	0.43
6:F:86:GLU:OE2	6:F:95:LYS:NZ	2.30	0.43
17:Q:268:ASN:HB3	17:Q:271:VAL:HG12	2.00	0.43
18:R:403:ALA:HB1	18:R:428:LEU:HB3	2.01	0.43
22:W:236:LEU:HD13	22:W:278:TRP:CE3	2.54	0.43
1:A:538:VAL:HG12	1:A:538:VAL:O	2.19	0.43
2:B:497:LYS:N	2:B:498:PRO:HD2	2.34	0.43
17:Q:147:GLN:O	17:Q:151:GLN:HG2	2.19	0.43
17:Q:153:HIS:HA	17:Q:169:LYS:HE3	2.01	0.43
17:Q:272:LEU:HD22	17:Q:291:LEU:HD22	1.99	0.43
20:U:457:PHE:HE1	20:U:497:ASP:N	2.17	0.43
22:W:17:ASP:OD1	22:W:18:ALA:N	2.45	0.43
1:A:1219:LYS:HB3	15:O:240:LEU:HD22	2.01	0.43
5:E:185:ILE:HD12	5:E:209:VAL:CG2	2.49	0.43
9:I:81:THR:HG23	9:I:96:PHE:CE1	2.54	0.43
20:U:381:PHE:CE1	20:U:497:ASP:CB	3.02	0.43
24:Y:33:CYS:SG	24:Y:36:CYS:N	2.92	0.43
17:Q:239:ALA:HA	17:Q:257:LEU:HD13	2.00	0.42
18:R:353:VAL:HG12	18:R:469:LEU:HD13	2.01	0.42
22:W:172:ILE:HB	22:W:186:LEU:HB2	1.99	0.42
1:A:724:GLU:OE1	1:A:724:GLU:N	2.52	0.42
1:A:1321:ILE:O	1:A:1328:PHE:O	2.37	0.42
3:C:84:TYR:CE1	3:C:167:LYS:HE3	2.54	0.42
4:D:43:HIS:CD2	4:D:47:GLN:HE21	2.37	0.42
9:I:68:ILE:HB	9:I:122:ARG:HD3	2.01	0.42
14:N:139:DT:H1'	14:N:140:DT:O5'	2.19	0.42
17:Q:721:LEU:HD11	21:V:31:CYS:HA	2.01	0.42
18:R:397:LYS:HB3	18:R:398:PRO:HD3	2.01	0.42
22:W:76:LEU:HD23	22:W:78:ILE:HG12	2.00	0.42
22:W:186:LEU:HD11	22:W:222:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:ASN:HD21	6:F:111:PRO:HB3	1.84	0.42
2:B:1091:ARG:HG3	2:B:1103:LEU:HD11	2.01	0.42
7:G:84:VAL:HG23	7:G:84:VAL:O	2.19	0.42
22:W:258:VAL:O	22:W:267:VAL:HG22	2.18	0.42
25:Z:479:LYS:NZ	25:Z:521:CYS:O	2.35	0.42
25:Z:524:THR:HG22	25:Z:525:ALA:N	2.34	0.42
2:B:682:LEU:HD21	18:R:597:ARG:NH1	2.35	0.42
4:D:32:LEU:HD13	4:D:37:VAL:HG12	2.00	0.42
13:M:1502:ASN:O	13:M:1506:ARG:HG2	2.19	0.42
1:A:1223:ASP:CB	15:O:244:ALA:CB	2.91	0.42
3:C:175:LYS:HE2	12:L:57:ALA:O	2.19	0.42
5:E:93:ARG:HA	5:E:96:GLU:OE1	2.20	0.42
17:Q:310:TYR:CE2	17:Q:342:LEU:HD13	2.54	0.42
1:A:589:LYS:HG2	1:A:635:LEU:HD23	2.01	0.42
1:A:1525:TPO:O3P	13:M:1355:ARG:NH1	2.52	0.42
5:E:55:ARG:O	5:E:56:THR:OG1	2.25	0.42
17:Q:398:LYS:O	17:Q:402:LYS:HD3	2.19	0.42
21:V:84:ILE:O	21:V:84:ILE:HG23	2.20	0.42
23:X:253:LEU:O	23:X:256:VAL:HG12	2.20	0.42
25:Z:339:LEU:HD23	25:Z:339:LEU:H	1.85	0.42
25:Z:489:THR:HG22	25:Z:490:GLY:N	2.34	0.42
1:A:728:THR:O	1:A:729:PRO:C	2.57	0.42
8:H:64:LEU:O	8:H:84:ARG:N	2.44	0.42
18:R:470:ASP:OD1	18:R:471:GLU:N	2.53	0.42
22:W:53:ARG:NH2	22:W:54:LEU:O	2.53	0.42
25:Z:613:GLU:O	25:Z:625:HIS:N	2.50	0.42
1:A:1308:TYR:C	15:O:250:MET:CE	2.88	0.42
2:B:515:PRO:O	2:B:520:VAL:HA	2.19	0.42
13:M:1487:THR:OG1	13:M:1490:GLY:N	2.53	0.42
17:Q:511:CYS:O	22:W:229:SER:OG	2.38	0.42
22:W:204:LEU:HD22	22:W:216:ILE:HG22	2.02	0.42
2:B:281:ASP:CG	9:I:22:ASN:HD22	2.22	0.42
2:B:528:LEU:HD21	2:B:767:LEU:HD21	2.01	0.42
6:F:57:MET:HB2	6:F:123:LEU:HD13	2.02	0.42
17:Q:239:ALA:O	17:Q:243:LEU:HG	2.20	0.42
1:A:406:VAL:HG13	1:A:429:LEU:HD11	2.01	0.42
14:N:122:DC:H1'	14:N:123:DG:C8	2.55	0.42
17:Q:358:GLU:O	17:Q:361:SER:OG	2.38	0.42
2:B:718:GLN:HG2	2:B:720:PRO:HD2	2.02	0.41
5:E:209:VAL:O	5:E:210:GLN:HB2	2.20	0.41
8:H:72:ASP:OD1	8:H:73:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:17:CYS:SG	9:I:18:GLN:N	2.93	0.41
14:N:143:DG:H2''	14:N:144:DA:OP2	2.20	0.41
17:Q:206:HIS:HB3	21:V:80:LEU:HD11	2.02	0.41
17:Q:745:HIS:HB2	22:W:20:TRP:CH2	2.55	0.41
1:A:917:GLU:O	1:A:921:ARG:HB2	2.19	0.41
1:A:1400:LEU:O	1:A:1404:THR:HG23	2.20	0.41
7:G:151:ARG:NE	7:G:153:ASP:OD1	2.53	0.41
13:M:1335:ILE:HD11	13:M:1355:ARG:HB3	2.02	0.41
17:Q:761:LEU:HD22	17:Q:785:GLU:HB3	2.02	0.41
17:Q:835:ASP:O	17:Q:839:ARG:HG3	2.20	0.41
19:T:-71:DG:H2''	19:T:-70:DT:OP2	2.20	0.41
21:V:127:VAL:HG23	21:V:128:VAL:N	2.33	0.41
22:W:144:LEU:HD13	22:W:175:PHE:CG	2.55	0.41
1:A:729:PRO:HB3	15:O:249:GLN:O	2.19	0.41
17:Q:833:LYS:O	17:Q:836:GLU:HG3	2.20	0.41
1:A:729:PRO:HB3	15:O:247:GLU:O	2.20	0.41
1:A:1093:GLN:HE22	2:B:1093:CYS:HA	1.85	0.41
2:B:67:LEU:HD22	2:B:420:GLN:OE1	2.20	0.41
13:M:1366:VAL:HG11	13:M:1413:VAL:HG21	2.02	0.41
17:Q:76:ARG:HH21	17:Q:76:ARG:HG3	1.85	0.41
1:A:509:LEU:HD23	1:A:509:LEU:HA	1.96	0.41
4:D:17:ALA:HB1	4:D:95:PHE:CZ	2.55	0.41
1:A:729:PRO:CB	15:O:247:GLU:O	2.68	0.41
2:B:725:GLN:NE2	2:B:937:SER:O	2.54	0.41
25:Z:206:THR:OG1	25:Z:207:ASP:N	2.51	0.41
1:A:694:ALA:HB1	1:A:698:THR:HB	2.02	0.41
4:D:31:THR:HG21	4:D:94:LYS:O	2.20	0.41
5:E:11:TRP:CZ2	5:E:15:LYS:HE2	2.55	0.41
14:N:66:DG:H1	19:T:-66:DC:H42	1.67	0.41
14:N:140:DT:O2	19:T:-139:DA:H2	2.03	0.41
17:Q:635:ILE:O	17:Q:639:VAL:HG22	2.21	0.41
9:I:64:GLU:O	9:I:68:ILE:HG12	2.21	0.41
14:N:60:DT:H5'	14:N:60:DT:C6	2.56	0.41
14:N:71:DC:H6	14:N:71:DC:H2'	1.75	0.41
14:N:137:DG:H1'	14:N:138:DA:O5'	2.21	0.41
17:Q:46:ALA:O	17:Q:50:GLU:HG2	2.21	0.41
17:Q:879:ALA:O	17:Q:882:VAL:HG12	2.20	0.41
22:W:35:VAL:HB	22:W:47:TRP:HB2	2.01	0.41
1:A:365:THR:HG22	1:A:482:PHE:CD2	2.56	0.41
1:A:905:ASN:OD1	1:A:975:SER:OG	2.08	0.41
1:A:965:VAL:O	1:A:969:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1308:TYR:C	15:O:250:MET:HE3	2.41	0.41
2:B:512:ALA:O	2:B:723:THR:HA	2.21	0.41
2:B:574:VAL:O	2:B:574:VAL:HG22	2.20	0.41
2:B:684:GLU:HA	2:B:684:GLU:OE1	2.20	0.41
8:H:83:SER:OG	8:H:84:ARG:N	2.51	0.41
11:K:53:ASP:HB3	11:K:56:VAL:HG23	2.03	0.41
17:Q:772:GLU:HA	17:Q:773:LYS:CB	2.51	0.41
18:R:363:ARG:NH1	18:R:365:SER:OG	2.53	0.41
19:T:-107:DG:H2''	19:T:-106:DA:C8	2.56	0.41
19:T:-67:DC:OP2	19:T:-67:DC:H6	2.04	0.41
2:B:314:GLN:O	2:B:318:LEU:HD23	2.21	0.41
20:U:381:PHE:HE1	20:U:497:ASP:CB	2.34	0.41
1:A:1215:GLU:N	1:A:1215:GLU:OE1	2.55	0.40
3:C:189:ASP:O	3:C:191:ALA:N	2.51	0.40
17:Q:289:GLN:O	17:Q:293:LEU:HD23	2.20	0.40
1:A:611:ASP:N	1:A:611:ASP:OD1	2.49	0.40
7:G:97:LEU:O	7:G:107:PHE:HA	2.22	0.40
10:J:53:VAL:O	10:J:53:VAL:HG13	2.20	0.40
17:Q:386:ALA:HB1	17:Q:394:ARG:CG	2.51	0.40
17:Q:837:GLU:O	17:Q:840:GLU:HG3	2.20	0.40
25:Z:186:ILE:H	25:Z:186:ILE:HD12	1.86	0.40
3:C:212:ASP:OD1	3:C:212:ASP:N	2.41	0.40
5:E:58:LEU:HD23	5:E:58:LEU:H	1.86	0.40
25:Z:426:VAL:HG13	25:Z:440:ILE:HD11	2.03	0.40
4:D:31:THR:HG22	7:G:3:TYR:CZ	2.57	0.40
16:P:34:C:H6	16:P:34:C:H2'	1.66	0.40
1:A:63:GLY:HA2	1:A:71:CYS:SG	2.62	0.40
1:A:220:ARG:HD2	1:A:220:ARG:HA	2.01	0.40
1:A:431:PHE:HZ	16:P:34:C:H42	1.63	0.40
1:A:483:ARG:C	1:A:484:LEU:HD12	2.42	0.40
1:A:1223:ASP:OD2	15:O:244:ALA:CB	2.48	0.40
2:B:719:SER:OG	2:B:720:PRO:HD3	2.22	0.40
2:B:833:THR:C	2:B:835:GLU:H	2.25	0.40
8:H:63:THR:HG21	8:H:68:GLY:HA2	2.03	0.40
9:I:26:PRO:CB	9:I:53:ILE:HD12	2.51	0.40
22:W:231:HIS:HD1	22:W:235:VAL:HG22	1.85	0.40
22:W:248:VAL:HG11	22:W:289:ILE:HD13	2.02	0.40
24:Y:22:VAL:HB	24:Y:84:VAL:HG12	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1408/1984 (71%)	1296 (92%)	105 (8%)	7 (0%)	29	68
2	B	1112/1251 (89%)	1024 (92%)	85 (8%)	3 (0%)	41	76
3	C	254/275 (92%)	239 (94%)	13 (5%)	2 (1%)	19	57
4	D	124/184 (67%)	122 (98%)	2 (2%)	0	100	100
5	E	207/210 (99%)	197 (95%)	8 (4%)	2 (1%)	15	53
6	F	76/127 (60%)	71 (93%)	5 (7%)	0	100	100
7	G	169/172 (98%)	155 (92%)	13 (8%)	1 (1%)	25	64
8	H	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
9	I	114/125 (91%)	104 (91%)	10 (9%)	0	100	100
10	J	64/67 (96%)	61 (95%)	2 (3%)	1 (2%)	9	40
11	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
12	L	45/58 (78%)	40 (89%)	4 (9%)	1 (2%)	6	31
13	M	976/1729 (56%)	860 (88%)	98 (10%)	18 (2%)	8	37
15	O	157/304 (52%)	154 (98%)	3 (2%)	0	100	100
17	Q	888/1179 (75%)	838 (94%)	50 (6%)	0	100	100
18	R	240/713 (34%)	224 (93%)	16 (7%)	0	100	100
20	U	119/666 (18%)	93 (78%)	24 (20%)	2 (2%)	9	39
21	V	236/531 (44%)	200 (85%)	33 (14%)	3 (1%)	12	45
22	W	298/305 (98%)	269 (90%)	29 (10%)	0	100	100
23	X	41/531 (8%)	40 (98%)	1 (2%)	0	100	100
24	Y	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
25	Z	497/1087 (46%)	452 (91%)	43 (9%)	2 (0%)	34	72
26	a	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
26	e	95/136 (70%)	90 (95%)	5 (5%)	0	100	100
27	b	81/103 (79%)	79 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	f	76/103 (74%)	70 (92%)	6 (8%)	0	100	100
28	c	101/130 (78%)	99 (98%)	2 (2%)	0	100	100
28	g	103/130 (79%)	93 (90%)	10 (10%)	0	100	100
29	d	93/123 (76%)	89 (96%)	4 (4%)	0	100	100
29	h	91/123 (74%)	83 (91%)	8 (9%)	0	100	100
All	All	8134/12866 (63%)	7488 (92%)	604 (7%)	42 (0%)	32	68

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	M	294	LEU
13	M	373	VAL
13	M	376	ILE
13	M	385	GLU
13	M	779	ILE
13	M	1141	TYR
13	M	1249	VAL
13	M	1263	VAL
13	M	1330	PRO
13	M	1360	GLY
20	U	513	SER
25	Z	760	GLY
13	M	1262	THR
1	A	283	ILE
2	B	262	TYR
13	M	378	PHE
13	M	1091	GLU
20	U	505	THR
1	A	696	SER
1	A	729	PRO
1	A	1303	GLN
3	C	155	LYS
5	E	122	ALA
7	G	142	GLU
13	M	1334	ASN
21	V	301	TYR
2	B	1004	ASP
3	C	60	HIS
10	J	64	PRO
13	M	854	ASN

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Mol	Chain	Res	Type
13	M	1142	ARG
13	M	1171	VAL
21	V	294	SER
21	V	298	GLU
1	A	1178	ASP
12	L	15	MET
1	A	224	ILE
5	E	45	GLY
13	M	880	ILE
2	B	1001	PRO
1	A	621	ILE
25	Z	445	GLY

### 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	
1	A	1245/1761 (71%)	1216 (98%)	29 (2%)	50	80
2	B	986/1084 (91%)	958 (97%)	28 (3%)	43	77
3	C	235/252 (93%)	230 (98%)	5 (2%)	53	82
4	D	109/160 (68%)	108 (99%)	1 (1%)	78	92
5	E	191/192 (100%)	188 (98%)	3 (2%)	62	86
6	F	68/111 (61%)	67 (98%)	1 (2%)	65	87
7	G	146/153 (95%)	143 (98%)	3 (2%)	53	82
8	H	130/131 (99%)	126 (97%)	4 (3%)	40	75
9	I	104/112 (93%)	100 (96%)	4 (4%)	33	69
10	J	55/56 (98%)	54 (98%)	1 (2%)	59	85
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	44/55 (80%)	42 (96%)	2 (4%)	27	64
13	M	207/1524 (14%)	205 (99%)	2 (1%)	76	91
15	O	140/268 (52%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	761/1011 (75%)	753 (99%)	8 (1%)	73	90
18	R	170/625 (27%)	167 (98%)	3 (2%)	59	85
20	U	66/590 (11%)	65 (98%)	1 (2%)	65	87
21	V	148/462 (32%)	143 (97%)	5 (3%)	37	72
22	W	255/260 (98%)	253 (99%)	2 (1%)	81	93
23	X	40/467 (9%)	39 (98%)	1 (2%)	47	79
24	Y	102/103 (99%)	101 (99%)	1 (1%)	76	91
25	Z	435/939 (46%)	431 (99%)	4 (1%)	78	92
26	a	85/111 (77%)	83 (98%)	2 (2%)	49	79
26	e	84/111 (76%)	81 (96%)	3 (4%)	35	70
27	b	68/79 (86%)	68 (100%)	0	100	100
27	f	63/79 (80%)	62 (98%)	1 (2%)	62	86
28	c	82/102 (80%)	82 (100%)	0	100	100
28	g	83/102 (81%)	81 (98%)	2 (2%)	49	79
29	d	81/103 (79%)	77 (95%)	4 (5%)	25	61
29	h	79/103 (77%)	75 (95%)	4 (5%)	24	60
All	All	6366/11212 (57%)	6242 (98%)	124 (2%)	59	84

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	CYS
1	A	34	MET
1	A	36	VAL
1	A	46	THR
1	A	67	ARG
1	A	79	THR
1	A	102	LYS
1	A	184	CYS
1	A	234	PHE
1	A	277	THR
1	A	282	ASP
1	A	329	MET
1	A	602	CYS
1	A	698	THR
1	A	728	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	729	PRO
1	A	732	THR
1	A	931	ARG
1	A	937	ASP
1	A	1048	THR
1	A	1182	GLN
1	A	1258	ARG
1	A	1260	ARG
1	A	1282	ASP
1	A	1286	ARG
1	A	1314	THR
1	A	1375	ARG
1	A	1407	CYS
1	A	1419	VAL
2	B	29	VAL
2	B	83	ARG
2	B	89	GLU
2	B	139	GLN
2	B	140	LEU
2	B	180	ASP
2	B	291	ASP
2	B	332	LYS
2	B	354	SER
2	B	388	TYR
2	B	411	LEU
2	B	429	PHE
2	B	453	TRP
2	B	610	ARG
2	B	647	GLU
2	B	681	ASP
2	B	710	ILE
2	B	894	THR
2	B	930	GLN
2	B	958	CYS
2	B	1000	THR
2	B	1038	THR
2	B	1120	ASN
2	B	1130	THR
2	B	1135	TYR
2	B	1142	ASN
2	B	1148	LEU
2	B	1156	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	15	THR
3	C	61	ASP
3	C	63	PHE
3	C	117	SER
3	C	151	VAL
4	D	94	LYS
5	E	107	GLN
5	E	117	SER
5	E	129	GLN
6	F	123	LEU
7	G	4	HIS
7	G	67	LEU
7	G	132	ASP
8	H	67	ASP
8	H	78	THR
8	H	83	SER
8	H	116	VAL
9	I	12	VAL
9	I	15	ARG
9	I	101	SER
9	I	103	ARG
10	J	30	THR
12	L	37	ARG
12	L	42	ARG
13	M	1359	LYS
13	M	1365	THR
17	Q	128	GLN
17	Q	180	ARG
17	Q	191	ARG
17	Q	697	TYR
17	Q	707	CYS
17	Q	714	HIS
17	Q	858	LYS
17	Q	887	ASN
18	R	411	THR
18	R	474	LYS
18	R	567	ASN
20	U	498	SER
21	V	37	ASN
21	V	45	ASP
21	V	132	ARG
21	V	134	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	V	181	LYS
22	W	169	ASP
22	W	237	ASN
23	X	241	THR
24	Y	113	THR
25	Z	224	TYR
25	Z	251	ASN
25	Z	467	GLU
25	Z	705	LEU
26	a	105	GLU
26	a	129	ARG
29	d	31	LYS
29	d	39	TYR
29	d	48	ASP
29	d	57	SER
26	e	39	HIS
26	e	106	ASP
26	e	129	ARG
27	f	73	THR
28	g	19	SER
28	g	71	ARG
29	h	39	TYR
29	h	83	ARG
29	h	84	SER
29	h	93	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	562	ASN
1	A	731	ASN
1	A	884	ASN
1	A	1093	GLN
1	A	1417	HIS
2	B	143	GLN
2	B	1120	ASN
4	D	47	GLN
9	I	56	ASN
9	I	121	HIS
17	Q	151	GLN
17	Q	289	GLN
17	Q	373	ASN

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Mol	Chain	Res	Type
17	Q	887	ASN
21	V	300	ASN
22	W	98	GLN
24	Y	41	GLN
25	Z	234	HIS
29	d	44	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	17/18 (94%)	6 (35%)	2 (11%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	30	C
16	P	31	G
16	P	36	U
16	P	37	G
16	P	39	U
16	P	41	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	36	U
16	P	38	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPO	A	1525	1	8,10,11	2.04	2 (25%)	10,14,16	1.86	2 (20%)
1	SEP	A	1547	1	8,9,10	2.01	2 (25%)	8,12,14	1.72	2 (25%)
25	TPO	Z	775	25	8,10,11	1.66	1 (12%)	10,14,16	1.93	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	1525	1	-	4/9/11/13	-
1	SEP	A	1547	1	-	0/5/8/10	-
25	TPO	Z	775	25	-	2/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1525	TPO	O-C	3.72	1.34	1.19
25	Z	775	TPO	O-C	3.71	1.34	1.19
1	A	1547	SEP	O-C	3.70	1.34	1.19
1	A	1547	SEP	P-O1P	3.39	1.61	1.50
1	A	1525	TPO	P-O1P	3.37	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	775	TPO	P-OG1-CB	-5.34	107.06	123.21
1	A	1525	TPO	P-OG1-CB	-5.02	108.06	123.21
1	A	1547	SEP	OG-CB-CA	3.20	111.26	108.14
1	A	1547	SEP	P-OG-CB	-3.14	109.64	118.30
1	A	1525	TPO	CG2-CB-CA	-2.09	109.03	113.16

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1525	TPO	N-CA-CB-CG2
1	A	1525	TPO	N-CA-CB-OG1
1	A	1525	TPO	C-CA-CB-CG2
1	A	1525	TPO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
25	Z	775	TPO	O-C-CA-CB
25	Z	775	TPO	C-CA-CB-CG2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1525	TPO	2	0
25	Z	775	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

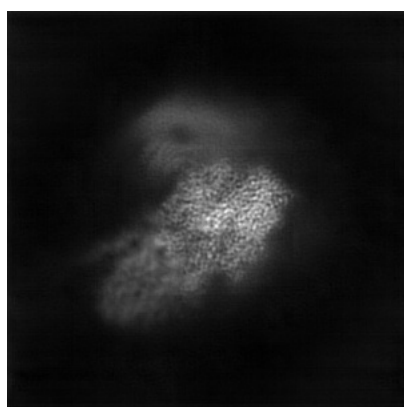
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26621. These allow visual inspection of the internal detail of the map and identification of artifacts.

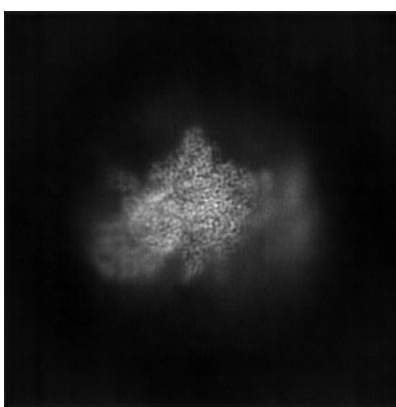
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

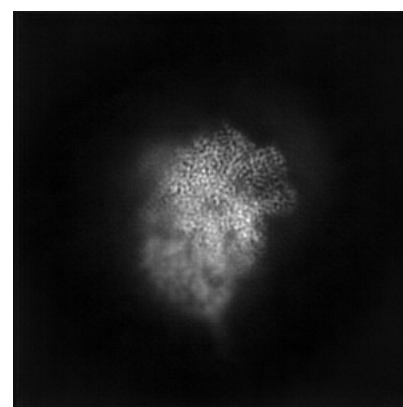
#### 6.1.1 Primary map



X



Y

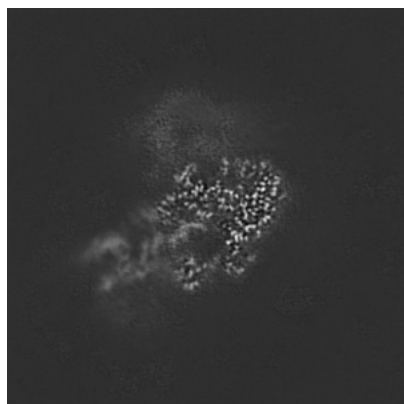


Z

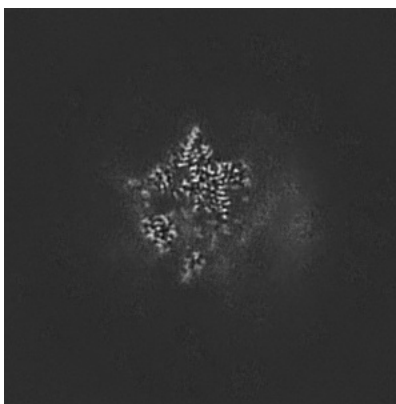
The images above show the map projected in three orthogonal directions.

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

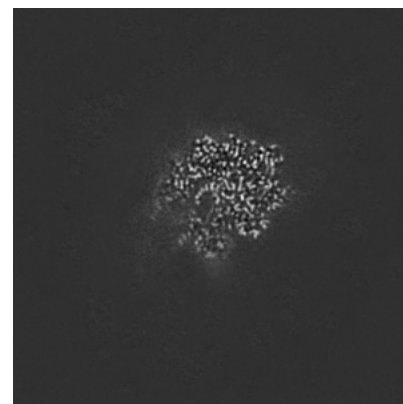
#### 6.2.1 Primary map



X Index: 225



Y Index: 225



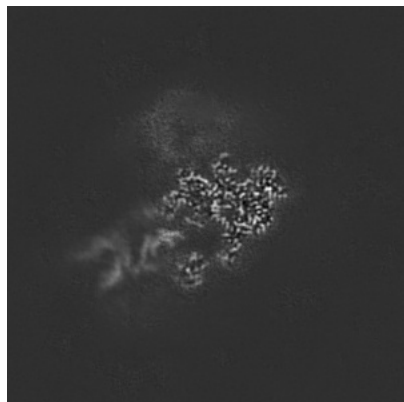
Z Index: 225



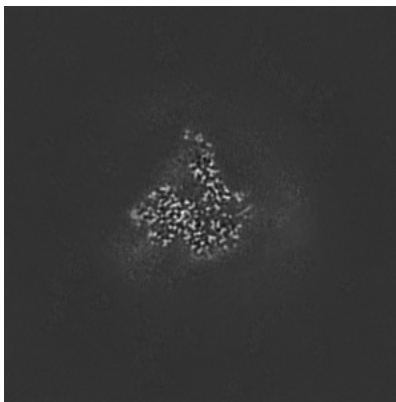
The images above show central slices of the map in three orthogonal directions.

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

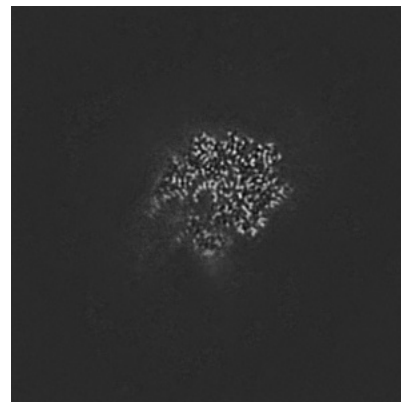
### 6.3.1 Primary map



X Index: 230



Y Index: 257



Z Index: 224

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0832. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

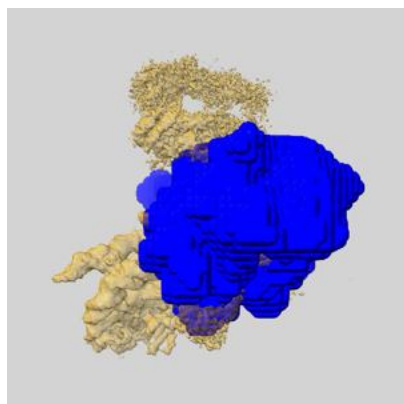
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

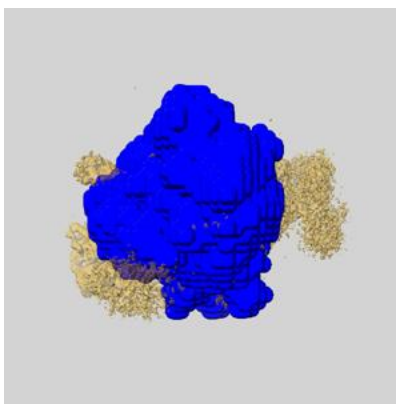
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

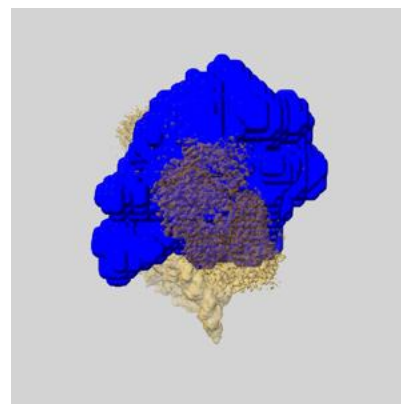
### 6.5.1 emd\_26621\_msk\_1.map [i](#)



X

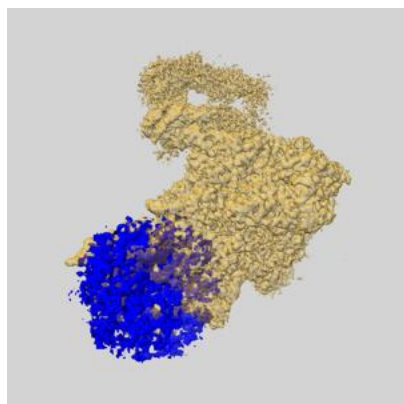


Y

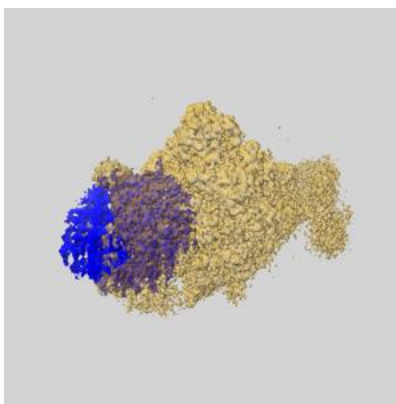


Z

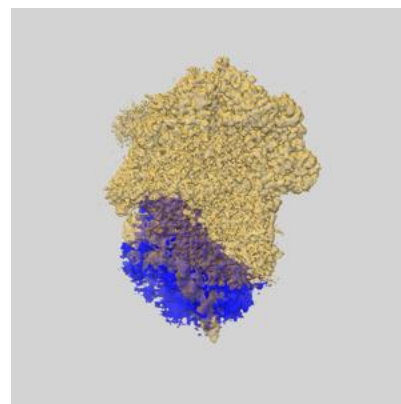
### 6.5.2 emd\_26621\_msk\_2.map [i](#)



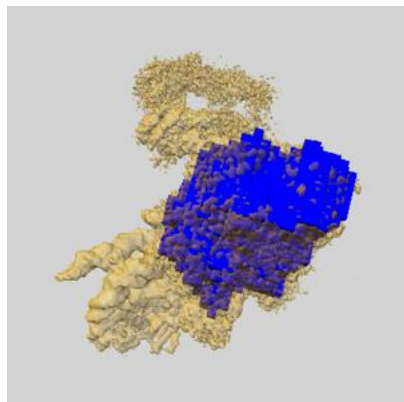
X



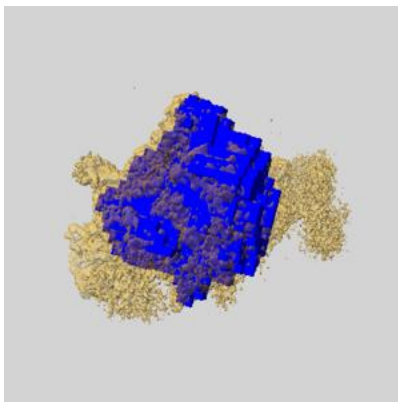
Y



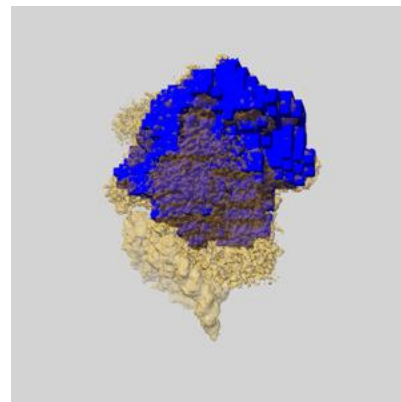
Z

6.5.3 emd\_26621\_msk\_3.map [i](#)

X



Y

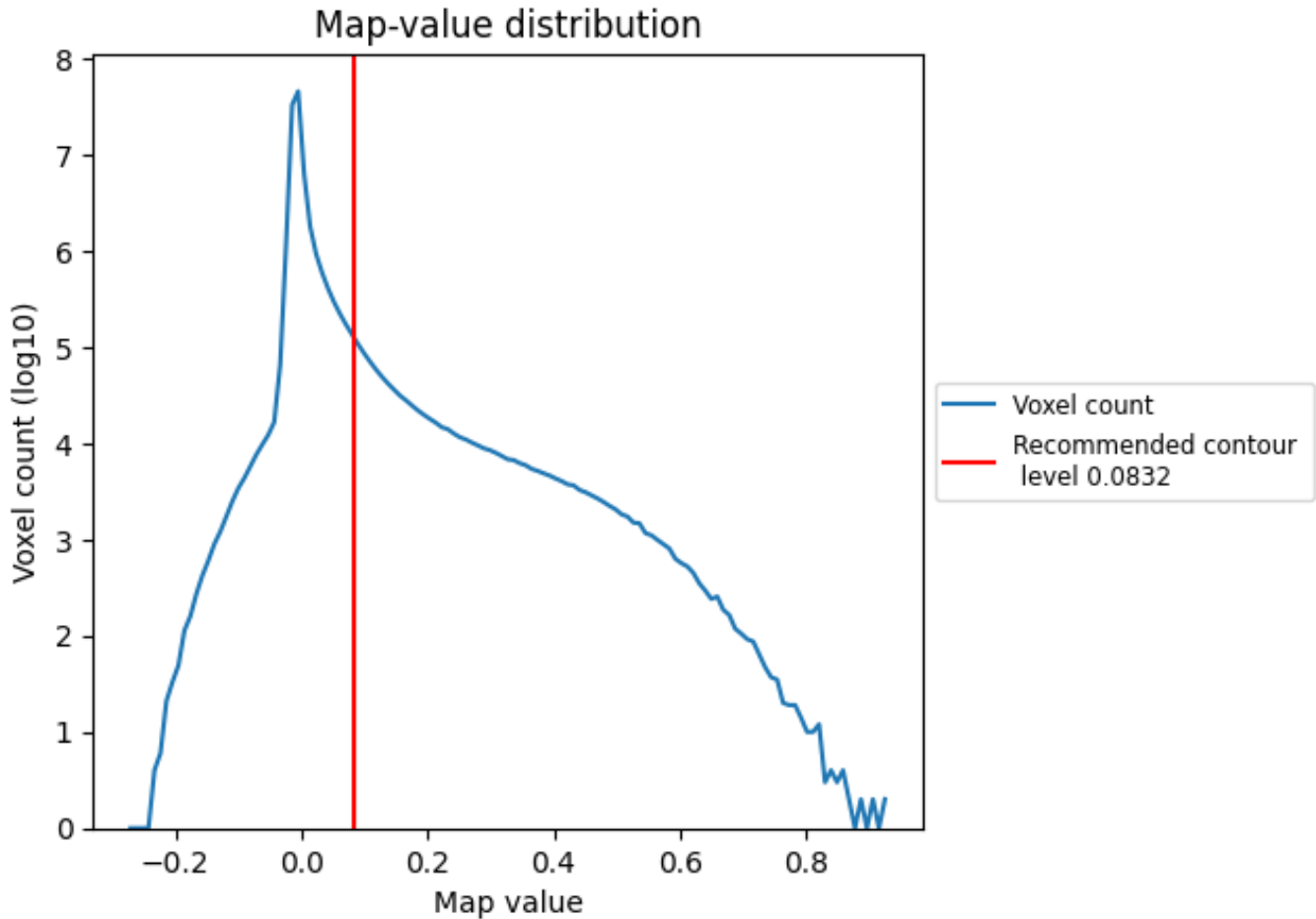


Z

## 7 Map analysis [i](#)

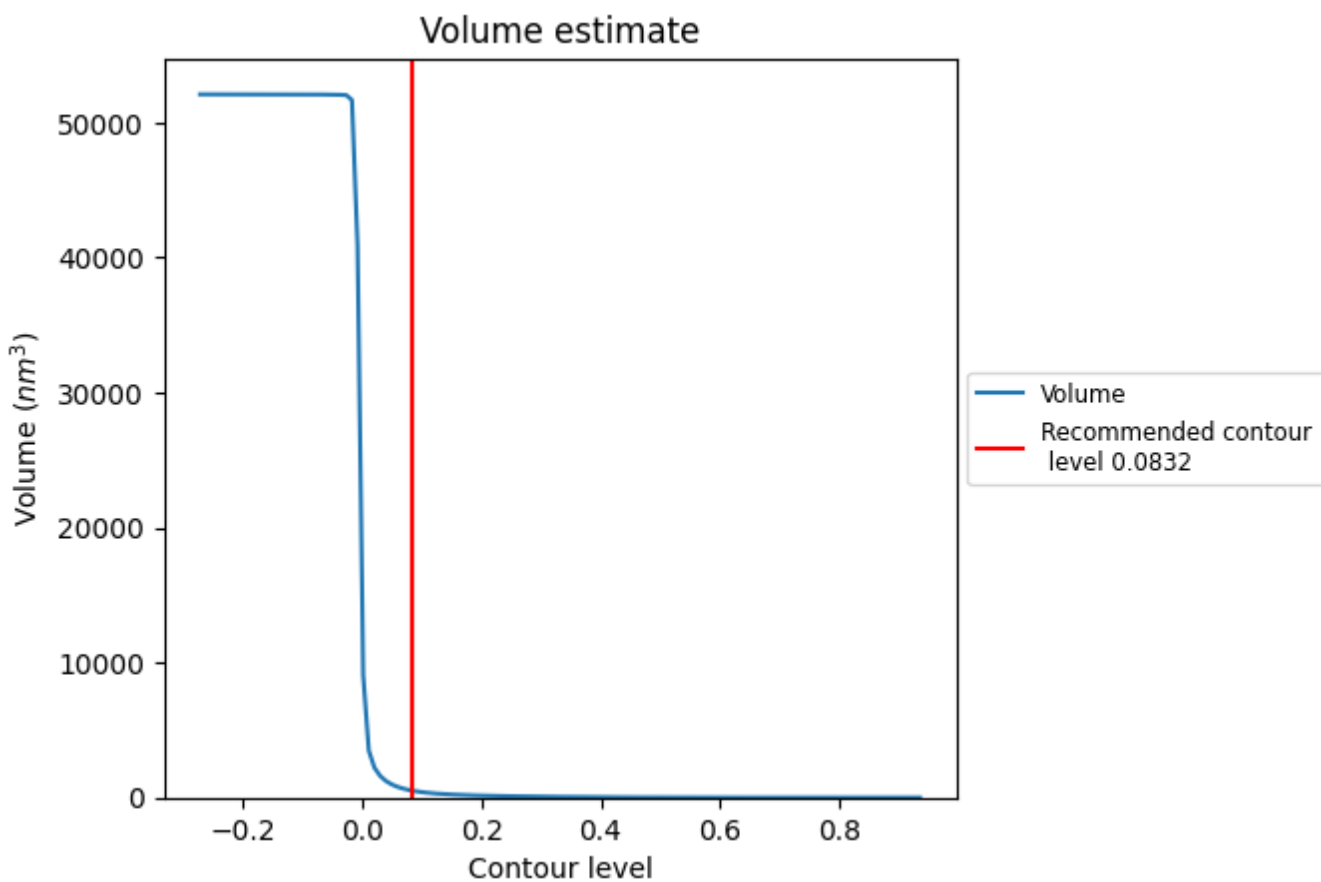
This section contains the results of statistical analysis of the map.

### 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.

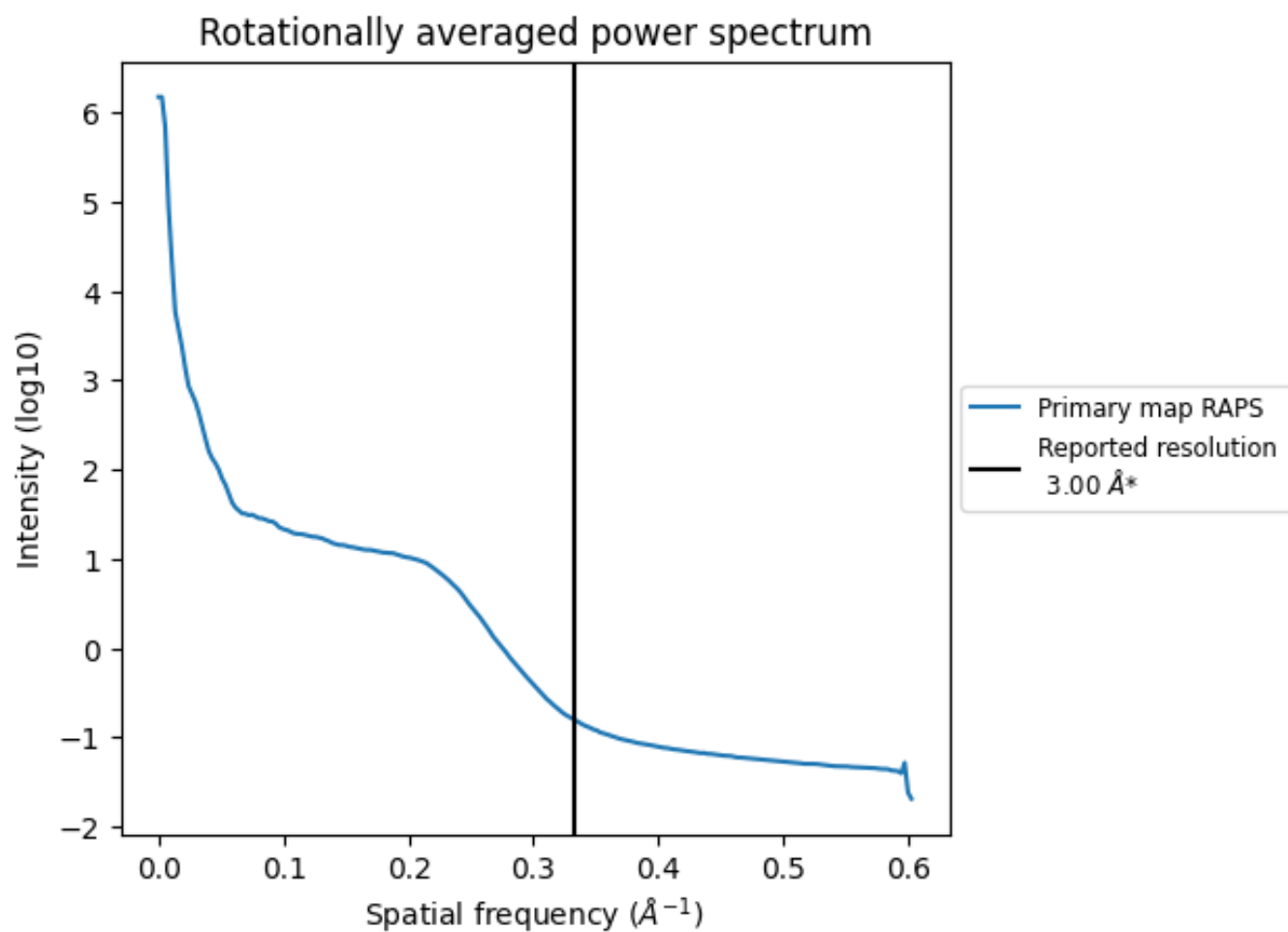
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 522 nm<sup>3</sup>; this corresponds to an approximate mass of 472 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 0.333 Å<sup>-1</sup>

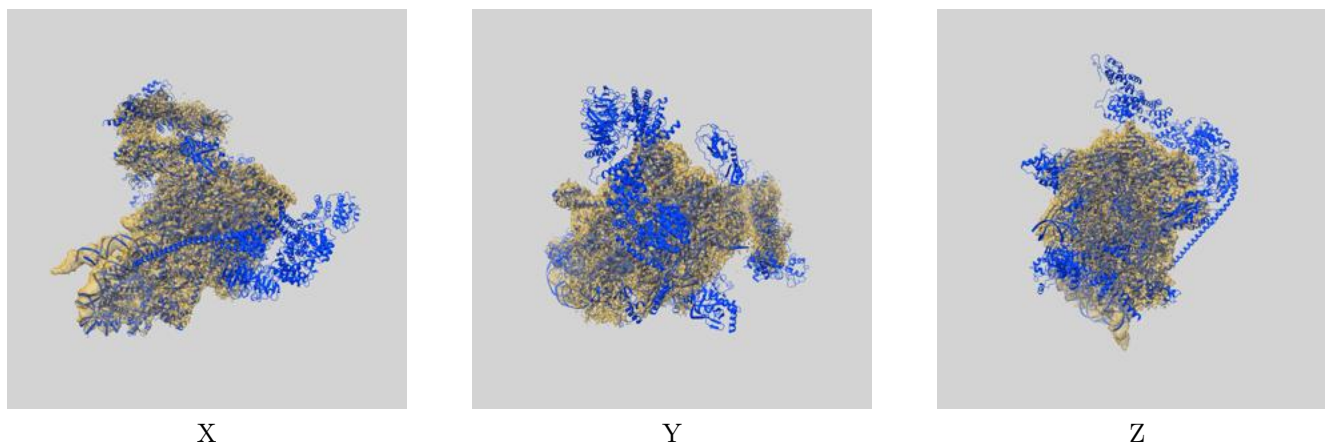
## 8 Fourier-Shell correlation

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

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

This section contains information regarding the fit between EMDB map EMD-26621 and PDB model 7UND. Per-residue inclusion information can be found in section 3 on page 11.

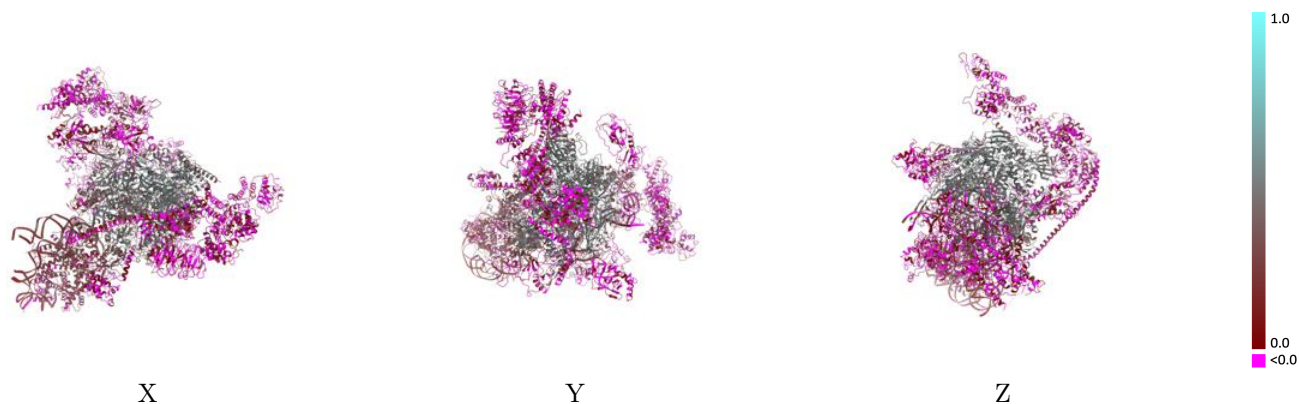
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0832 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.

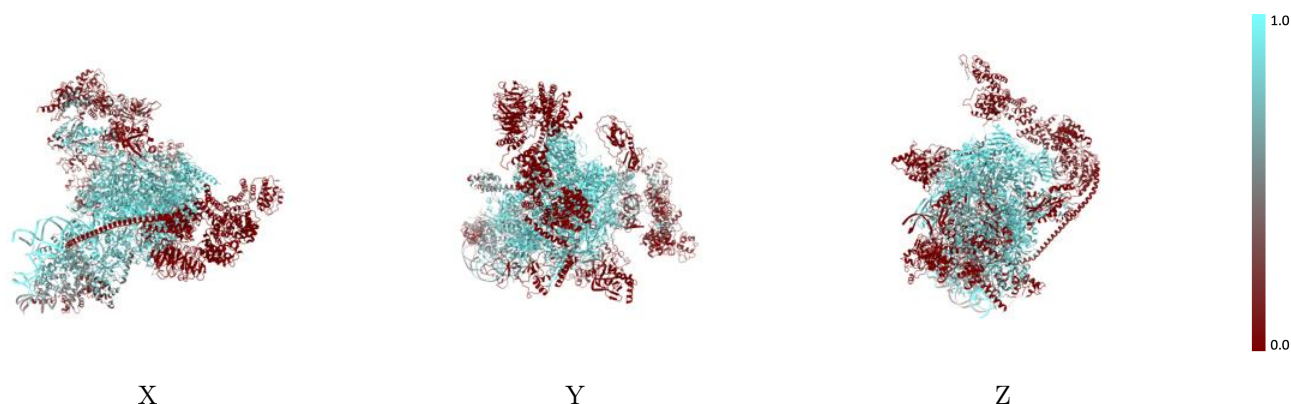


## 9.2 Q-score mapped to coordinate model [i](#)



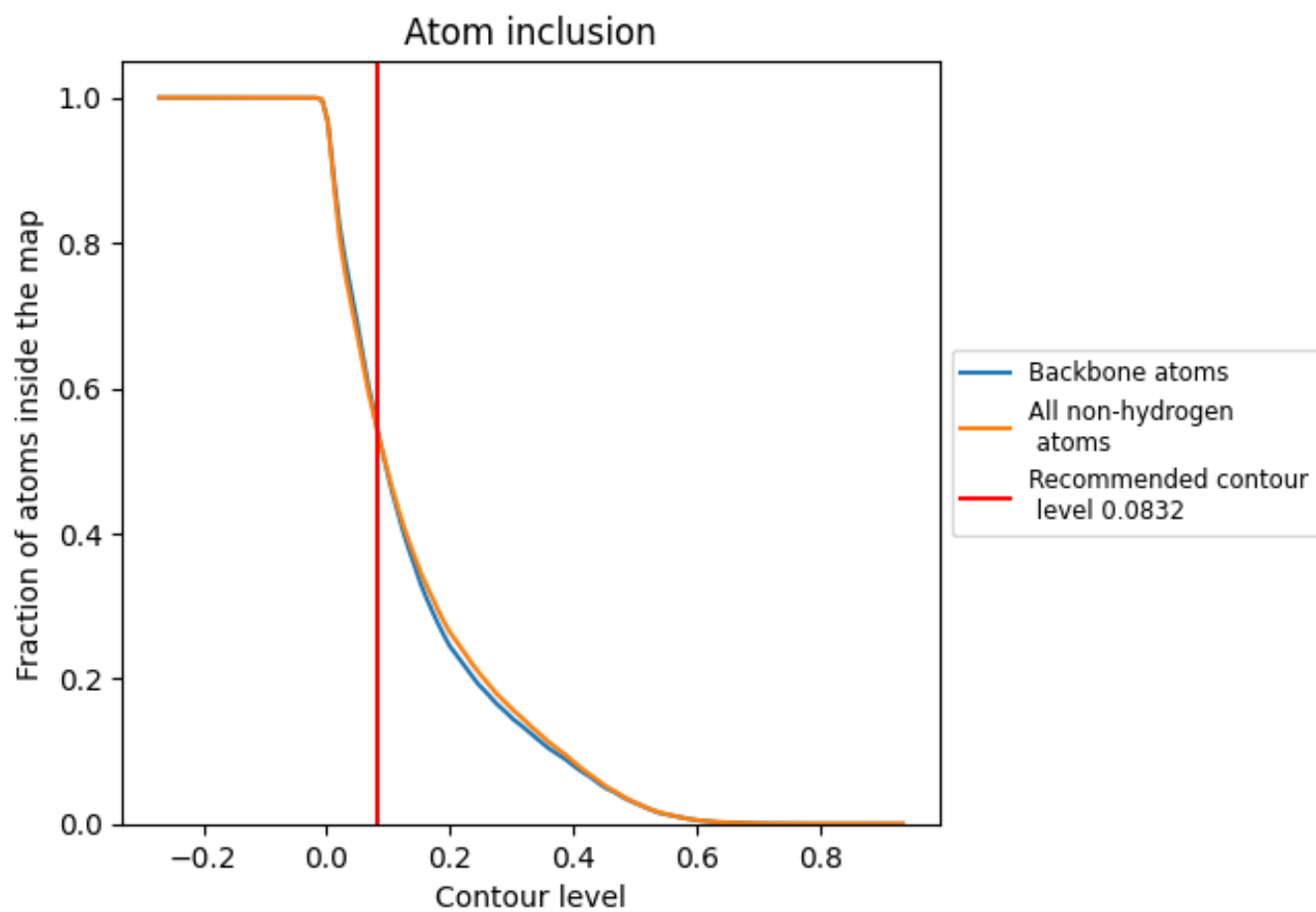
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0832).





































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 54% 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 (0.0832) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5372	 0.2160
A	 0.8900	 0.4080
B	 0.9014	 0.4260
C	 0.9345	 0.4660
D	 0.6276	 0.0950
E	 0.8755	 0.3370
F	 0.9127	 0.4550
G	 0.6575	 0.1730
H	 0.9017	 0.4280
I	 0.8039	 0.2330
J	 0.9062	 0.4630
K	 0.9265	 0.4680
L	 0.8526	 0.3870
M	 0.0875	 0.0240
N	 0.7614	 0.1640
O	 0.4135	 0.0160
P	 0.7664	 0.2450
Q	 0.0013	 0.0130
R	 0.0156	 0.0010
T	 0.8045	 0.2060
U	 0.2168	 0.0850
V	 0.0902	 0.0480
W	 0.0000	 -0.0010
X	 0.0000	 0.0470
Y	 0.0000	 0.0160
Z	 0.1408	 0.0610
a	 0.7445	 0.1410
b	 0.6761	 0.1640
c	 0.2519	 0.1160
d	 0.3352	 0.1300
e	 0.5610	 0.0830
f	 0.6353	 0.1020
g	 0.7806	 0.1820
h	 0.7236	 0.1610

