



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 11:52 AM UTC

PDB ID : 7UND / pdb_00007und
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 : 3LZ0, 6TED

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

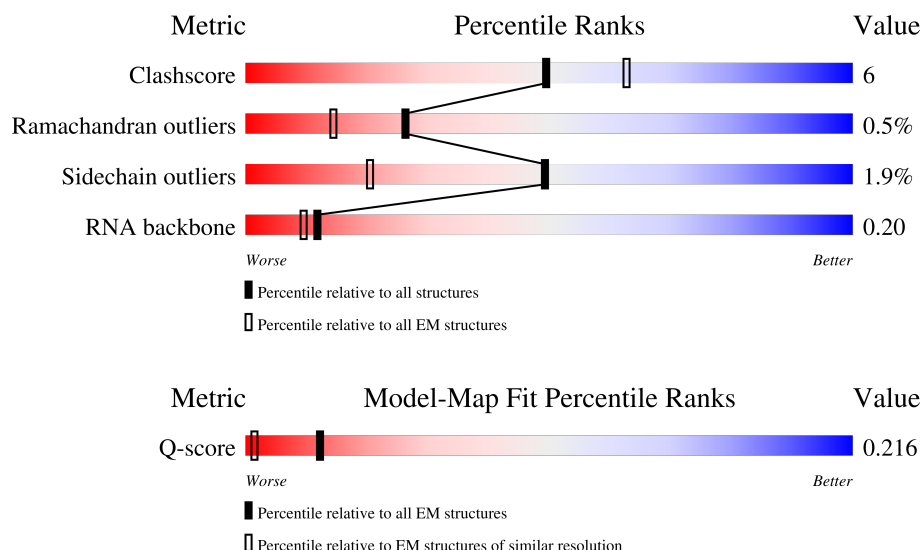
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	A	1984	
2	B	1251	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	184	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1729	
14	N	209	
15	O	304	
16	P	18	
17	Q	1179	
18	R	713	
19	T	215	
20	U	666	
21	V	531	
22	W	305	
23	X	531	
24	Y	117	
25	Z	1087	
26	a	136	
26	e	136	
27	b	103	

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Mol	Chain	Length	Quality of chain
27	f	103	
28	c	130	
28	g	130	
29	d	123	
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
1	A	1426	Total	C	H	N	O	P	S	0	0
			22640	7074	11385	2014	2095	2	70		

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 8 is a protein called RPB8.

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

- Molecule 9 is a protein called RPB9.

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

- Molecule 10 is a protein called RPB10.

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

- Molecule 11 is a protein called RPB11.

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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
16	P	18	Total	C	H	N	O	P	0	0
			572	169	191	61	133	18		

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

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

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
18	R	244	Total	C	H	N	O	S	0	0
			3537	1152	1701	340	337	7		

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
19	T	131	Total	C	H	N	O	P	0	0
			4138	1267	1458	518	764	131		

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

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

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

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

- Molecule 22 is a protein called WDR61.

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

- Molecule 23 is a protein called Parafibromin.

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

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

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

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

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

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

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

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
27	b	83	Total	C	H	N	O	S	0	0
			1372	418	710	129	114	1		
27	f	78	Total	C	H	N	O	S	0	0
			1279	391	660	120	107	1		

- Molecule 28 is a protein called Histone H2A.

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

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

- Molecule 29 is a protein called Histone H2B 1.1.

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

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 (CCD ID: 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	

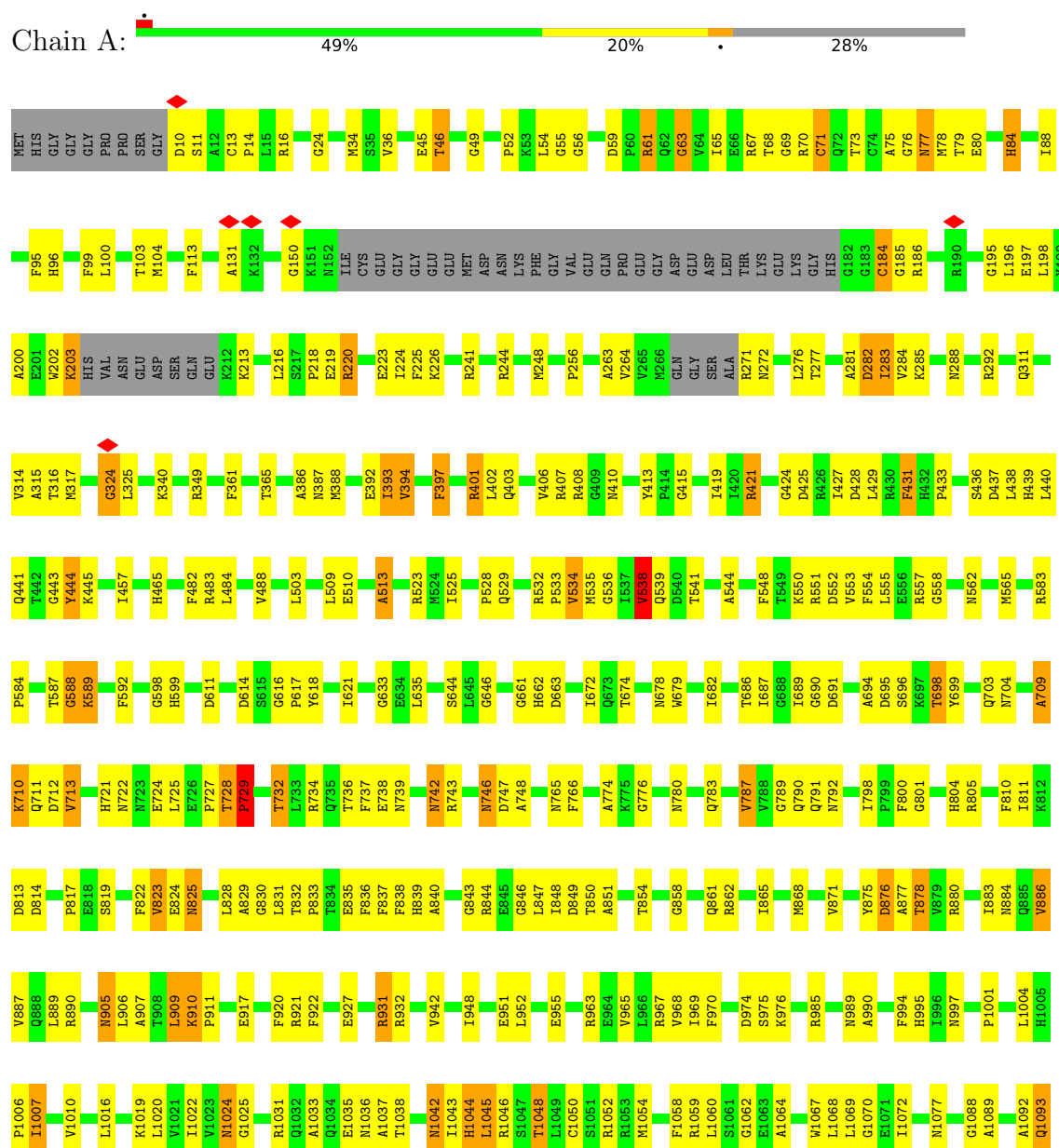
- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

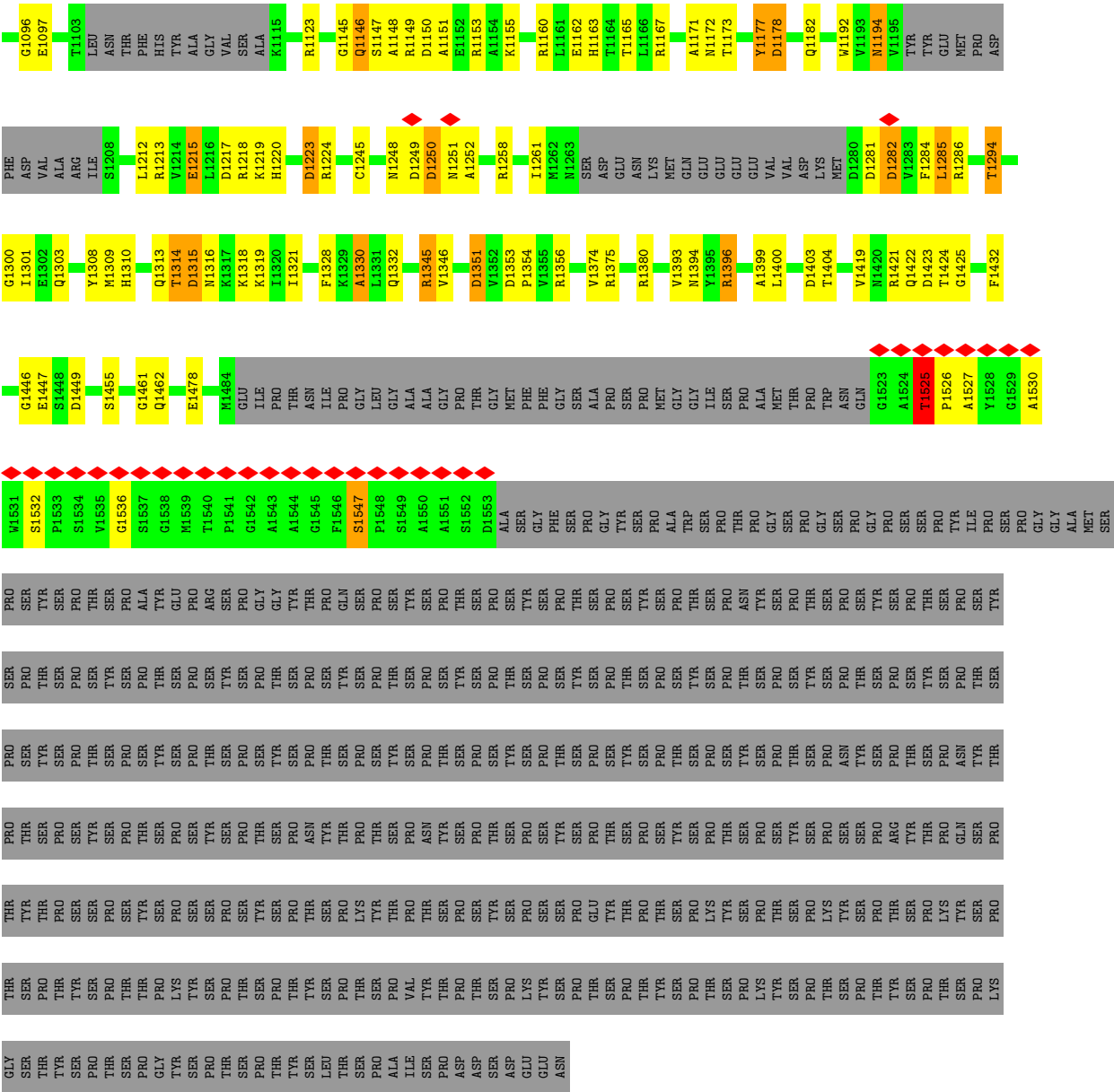
Mol	Chain	Residues	Atoms		AltConf
31	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

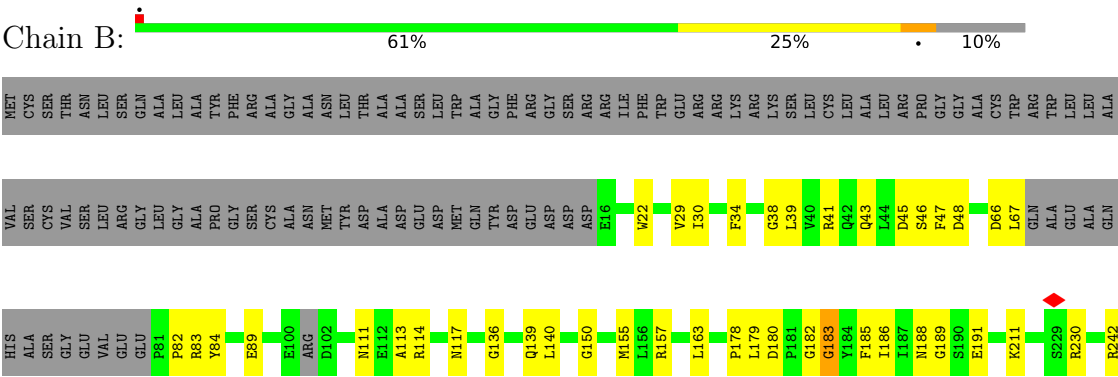
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

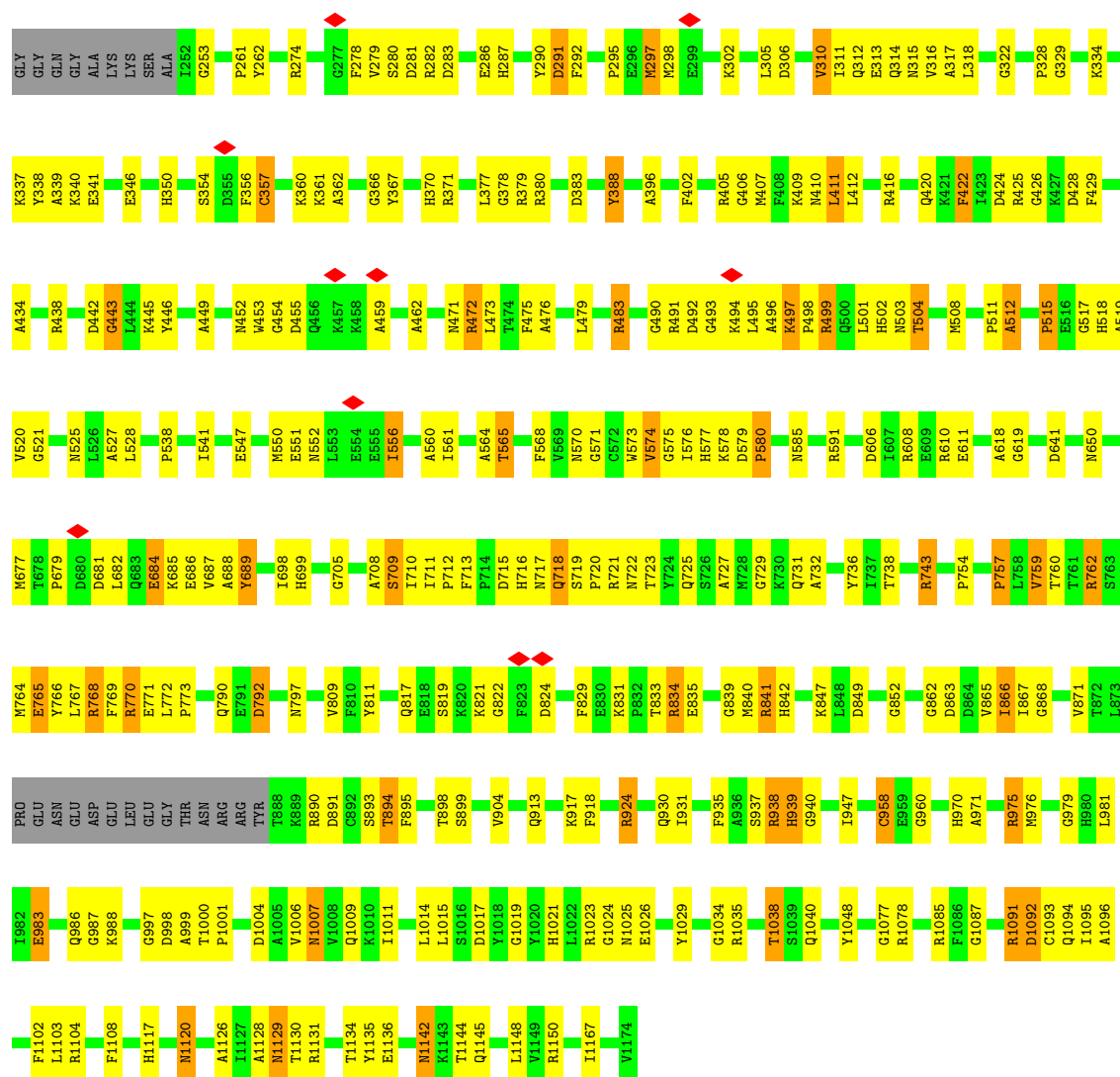
- Molecule 1: DNA-directed RNA polymerase subunit





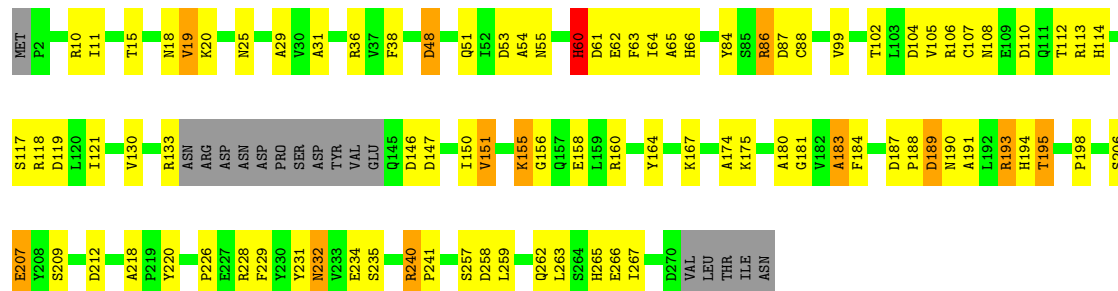
● Molecule 2: DNA-directed RNA polymerase subunit beta





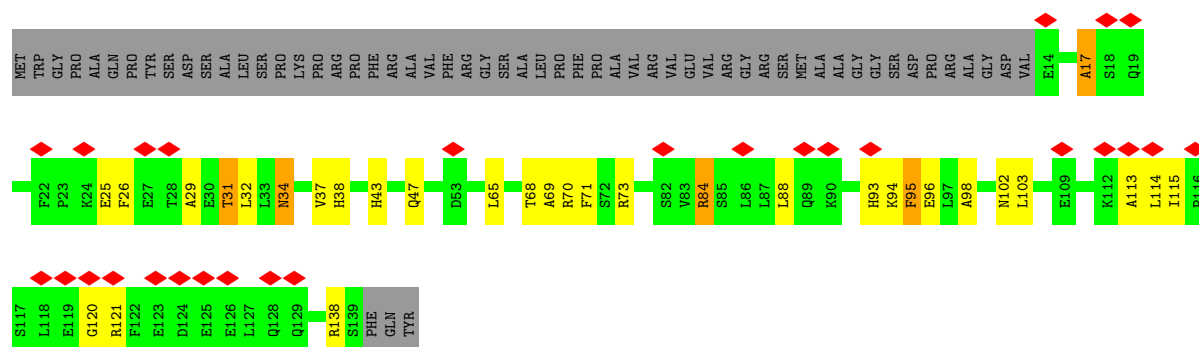
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 60% 29% 6%

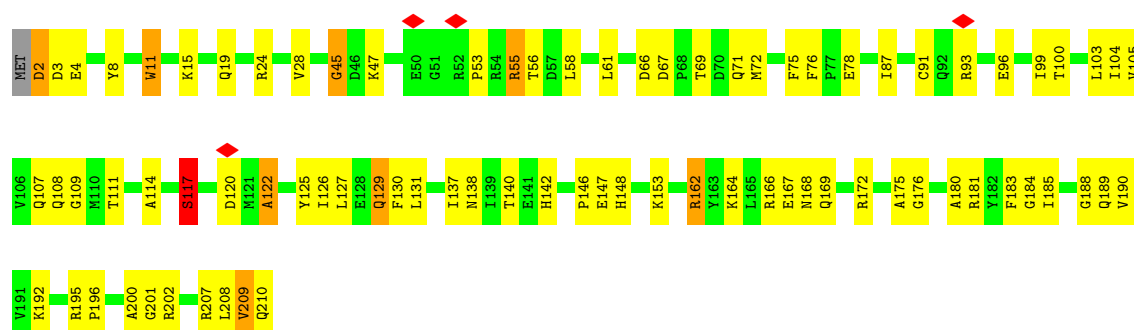


• Molecule 4: RPOL4c domain-containing protein

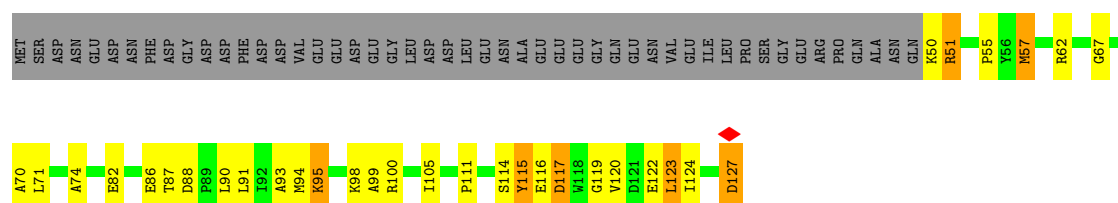
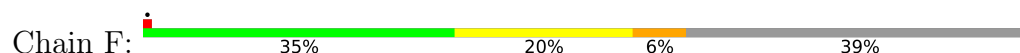
Chain D: 15% 51% 32%



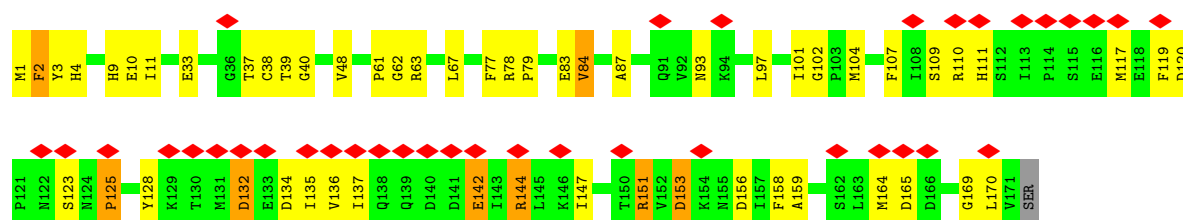
• Molecule 5: DNA-directed RNA polymerase II subunit E



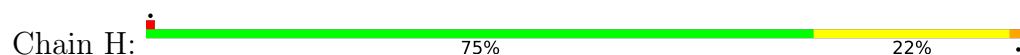
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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

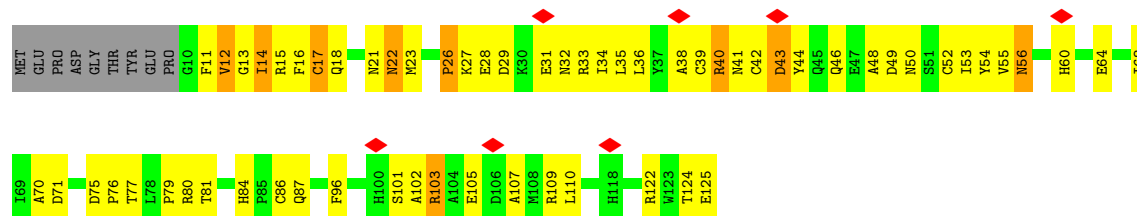


• Molecule 8: RPB8

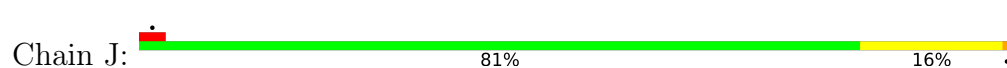




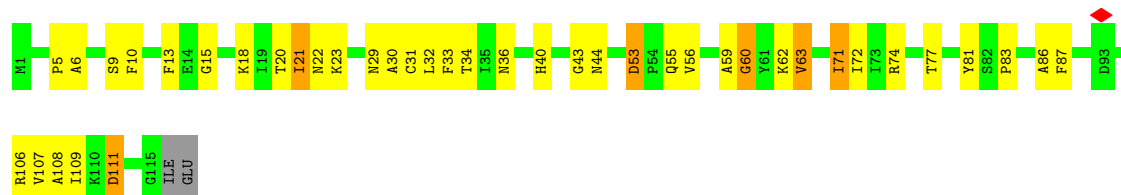
• Molecule 9: RPB9



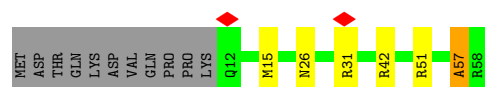
• Molecule 10: RPB10



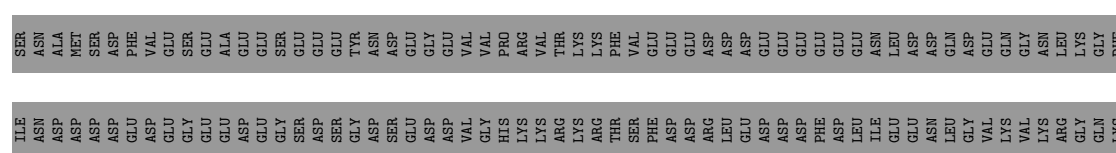
• Molecule 11: RPB11



• Molecule 12: RNA polymerase II subunit K

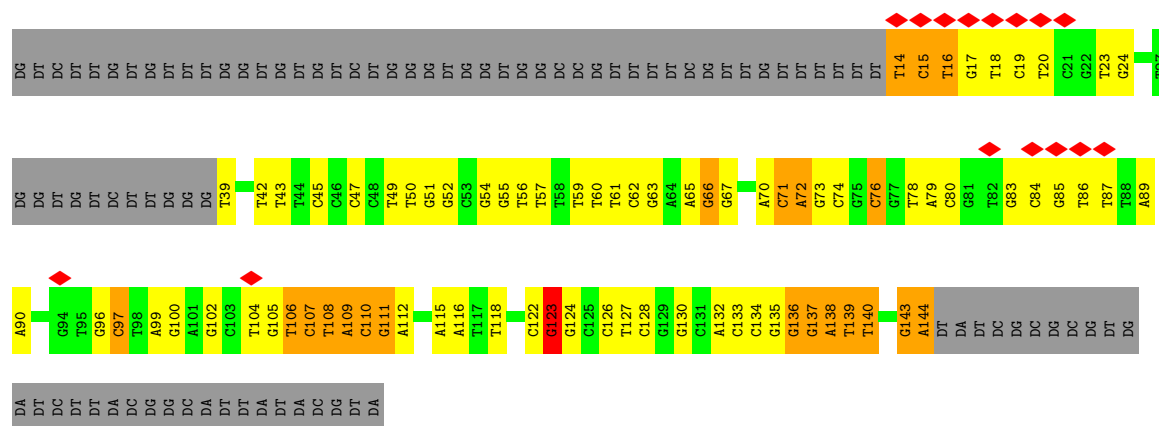


• Molecule 13: Transcription elongation factor SPT6

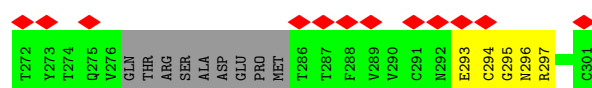
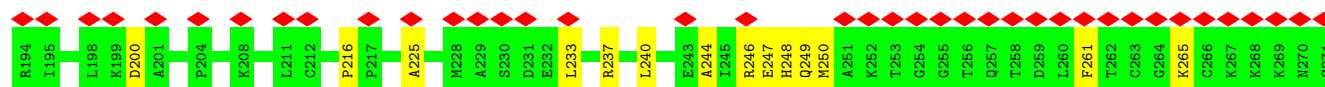
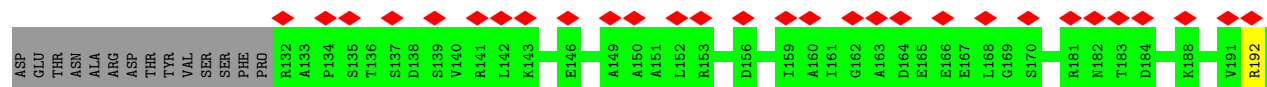




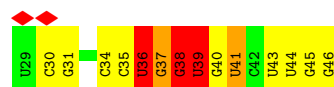
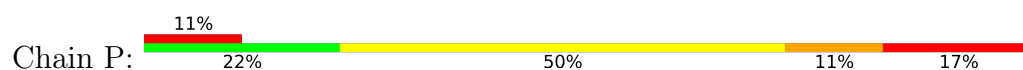




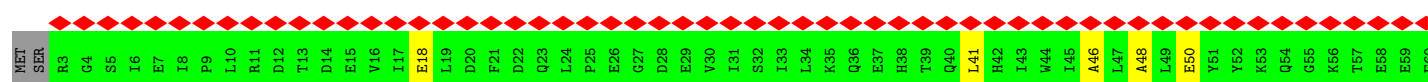
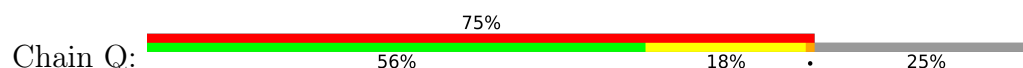
• Molecule 15: Transcription elongation factor A protein 1



• Molecule 16: RNA



• Molecule 17: RNA polymerase-associated protein CTR9 homolog





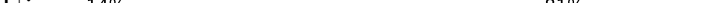
[illegible]

- Molecule 18: RNA polymerase-associated protein RTF1 homolog

[illegible]

- Molecule 19: Template DNA

[illegible]

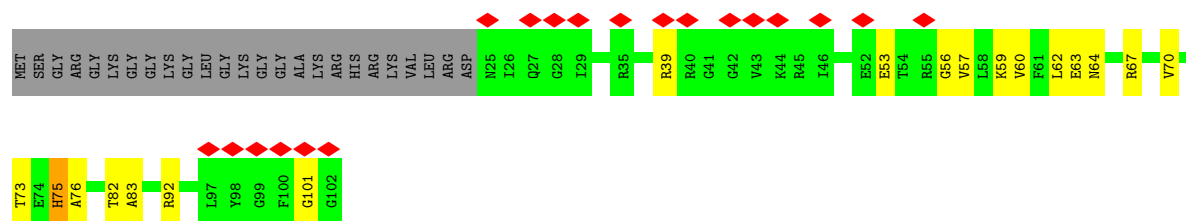
Chain U:  15% 14% 81%

F485	T486	T487	T488	T489	T490	T491	T492	T493	T494	T495	T496	T497	T498	T499	T500	T501	T502	T503	T504	T505	T506	T507	T508	T509	T510	T511	T512	T513	T514	T515	T516	T517	T518	T519	T520	T521	T522	T523	T524	T525	T526	T527	T528	T529	T530	T531	T532	T533	T534	T535	T536	T537	T538	T539	T540	T541	T542	T543	T544	T545	T546	T547	T548	T549	T550	T551	T552	T553	T554	T555	T556	T557	T558	T559	T560	T561	T562	T563	T564	T565	T566	T567	T568	T569	T570	T571	T572	T573	T574	T575	T576	T577	T578	T579	T580	T581	T582	T583	T584	T585	T586	T587	T588	T589	T590	T591	T592	T593	T594	T595	T596	T597	T598	T599	T600	T601	T602	T603	T604	T605	T606	T607	T608	T609	T610	T611	T612	T613	T614	T615	T616	T617	T618	T619	T620	T621	T622	T623	T624	T625	T626	T627	T628	T629	T630	T631	T632	T633	T634	T635	T636	T637	T638	T639	T640	T641	T642	T643	T644	T645	T646	T647	T648	T649	T650	T651	T652	T653	T654	T655	T656	T657	T658	T659	T660	T661	T662	T663	T664	T665	T666	T667	T668	T669	T670	T671	T672	T673	T674	T675	T676	T677	T678	T679	T680	T681	T682	T683	T684	T685	T686	T687	T688	T689	T690	T691	T692	T693	T694	T695	T696	T697	T698	T699	T700	T701	T702	T703	T704	T705	T706	T707	T708	T709	T710	T711	T712	T713	T714	T715	T716	T717	T718	T719	T720	T721	T722	T723	T724	T725	T726	T727	T728	T729	T730	T731	T732	T733	T734	T735	T736	T737	T738	T739	T740	T741	T742	T743	T744	T745	T746	T747	T748	T749	T750	T751	T752	T753	T754	T755	T756	T757	T758	T759	T760	T761	T762	T763	T764	T765	T766	T767	T768	T769	T770	T771	T772	T773	T774	T775	T776	T777	T778	T779	T780	T781	T782	T783	T784	T785	T786	T787	T788	T789	T790	T791	T792	T793	T794	T795	T796	T797	T798	T799	T800	T801	T802	T803	T804	T805	T806	T807	T808	T809	T810	T811	T812	T813	T814	T815	T816	T817	T818	T819	T820	T821	T822	T823	T824	T825	T826	T827	T828	T829	T830	T831	T832	T833	T834	T835	T836	T837	T838	T839	T840	T841	T842	T843	T844	T845	T846	T847	T848	T849	T850	T851	T852	T853	T854	T855	T856	T857	T858	T859	T860	T861	T862	T863	T864	T865	T866	T867	T868	T869	T870	T871	T872	T873	T874	T875	T876	T877	T878	T879	T880	T881	T882	T883	T884	T885	T886	T887	T888	T889	T890	T891	T892	T893	T894	T895	T896	T897	T898	T899	T900	T901	T902	T903	T904	T905	T906	T907	T908	T909	T910	T911	T912	T913	T914	T915	T916	T917	T918	T919	T920	T921	T922	T923	T924	T925	T926	T927	T928	T929	T930	T931	T932	T933	T934	T935	T936	T937	T938	T939	T940	T941	T942	T943	T944	T945	T946	T947	T948	T949	T950	T951	T952	T953	T954	T955	T956	T957	T958	T959	T960	T961	T962	T963	T964	T965	T966	T967	T968	T969	T970	T971	T972	T973	T974	T975	T976	T977	T978	T979	T980	T981	T982	T983	T984	T985	T986	T987	T988	T989	T990	T991	T992	T993	T994	T995	T99
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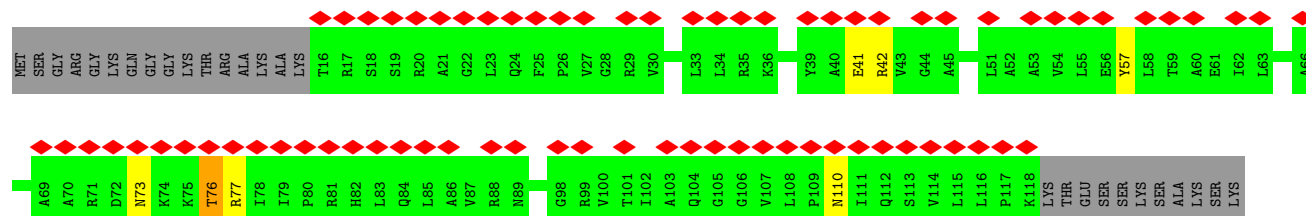
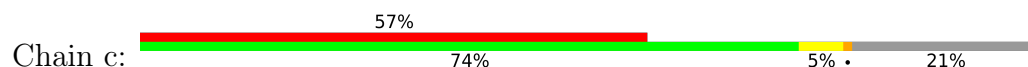


Chain Z: 40% 35% 11% 53%





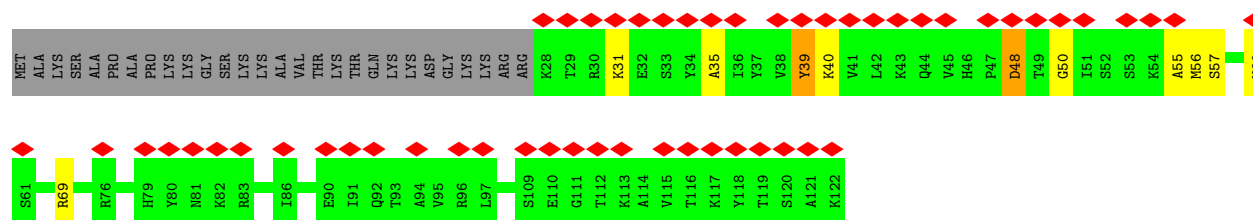
• Molecule 28: Histone H2A



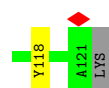
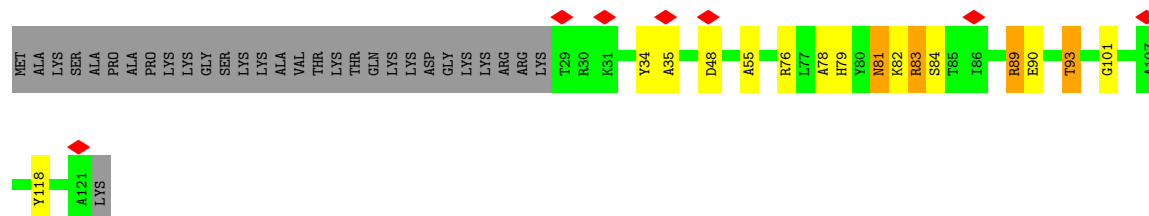
• Molecule 28: Histone H2A



• Molecule 29: Histone H2B 1.1



• Molecule 29: Histone H2B 1.1



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 ($\text{\AA}$)	373.5, 373.5, 373.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: ZN, TPO, MG, 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	1.98	207/11437 (1.8%)	2.01	435/15433 (2.8%)
2	B	2.01	191/9158 (2.1%)	2.00	329/12360 (2.7%)
3	C	2.14	42/2115 (2.0%)	2.13	107/2873 (3.7%)
4	D	1.83	22/1017 (2.2%)	1.86	33/1368 (2.4%)
5	E	2.08	48/1751 (2.7%)	1.97	72/2366 (3.0%)
6	F	2.52	17/636 (2.7%)	2.31	38/859 (4.4%)
7	G	1.98	21/1364 (1.5%)	2.02	56/1853 (3.0%)
8	H	1.65	16/1219 (1.3%)	1.72	32/1644 (1.9%)
9	I	2.14	25/964 (2.6%)	2.07	59/1305 (4.5%)
10	J	1.26	2/533 (0.4%)	1.49	5/719 (0.7%)
11	K	2.29	14/939 (1.5%)	2.29	50/1271 (3.9%)
12	L	1.56	7/403 (1.7%)	1.58	4/536 (0.7%)
13	M	1.24	13/4988 (0.3%)	1.78	61/6450 (0.9%)
14	N	0.97	35/2752 (1.3%)	1.96	36/4246 (0.8%)
15	O	0.72	0/1287	1.19	1/1721 (0.1%)
16	P	1.42	0/423	1.51	4/657 (0.6%)
17	Q	1.21	55/7365 (0.7%)	1.22	125/9927 (1.3%)
18	R	1.66	21/1866 (1.1%)	1.87	84/2519 (3.3%)
19	T	1.00	42/3012 (1.4%)	1.69	26/4641 (0.6%)
20	U	1.68	15/872 (1.7%)	1.89	34/1187 (2.9%)
21	V	1.55	14/1739 (0.8%)	1.88	62/2375 (2.6%)
22	W	0.49	1/2392 (0.0%)	0.56	9/3257 (0.3%)
23	X	0.64	0/356	0.79	0/478
24	Y	1.95	17/927 (1.8%)	2.00	46/1250 (3.7%)
25	Z	1.50	35/4084 (0.9%)	1.64	105/5498 (1.9%)
26	a	1.55	11/814 (1.4%)	1.84	26/1092 (2.4%)
26	e	1.96	21/812 (2.6%)	2.09	33/1088 (3.0%)
27	b	1.71	10/669 (1.5%)	1.92	22/894 (2.5%)
27	f	1.57	8/626 (1.3%)	1.82	18/837 (2.2%)
28	c	1.29	6/805 (0.7%)	1.62	8/1088 (0.7%)
28	g	1.40	12/819 (1.5%)	1.68	12/1106 (1.1%)
29	d	1.27	3/756 (0.4%)	1.68	6/1015 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	h	1.61	12/737 (1.6%)	1.76	13/993 (1.3%)
All	All	1.66	943/69637 (1.4%)	1.80	1951/94906 (2.1%)

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 (943) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	103	LEU	C-N	14.30	1.51	1.33
5	E	126	ILE	C-N	13.06	1.53	1.33
2	B	496	ALA	C-N	12.90	1.60	1.33
1	A	225	PHE	C-N	-9.12	1.22	1.33
1	A	96	HIS	ND1-CE1	-9.06	1.23	1.32
2	B	939	HIS	CE1-NE2	-8.98	1.23	1.32
3	C	194	HIS	CE1-NE2	-8.91	1.23	1.32
1	A	1220	HIS	CE1-NE2	-8.90	1.23	1.32
17	Q	689	HIS	CE1-NE2	-8.88	1.23	1.32
26	e	39	HIS	CE1-NE2	-8.88	1.23	1.32
5	E	142	HIS	CE1-NE2	-8.86	1.23	1.32
25	Z	625	HIS	CE1-NE2	-8.86	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	114	HIS	CE1-NE2	-8.86	1.23	1.32
1	A	599	HIS	CE1-NE2	-8.83	1.23	1.32
2	B	716	HIS	CE1-NE2	-8.83	1.23	1.32
25	Z	234	HIS	CE1-NE2	-8.83	1.23	1.32
22	W	87	HIS	ND1-CE1	-8.83	1.23	1.32
28	g	31	HIS	CE1-NE2	-8.82	1.23	1.32
2	B	370	HIS	CE1-NE2	-8.80	1.23	1.32
4	D	93	HIS	CE1-NE2	-8.80	1.23	1.32
29	h	79	HIS	CE1-NE2	-8.80	1.23	1.32
4	D	38	HIS	CE1-NE2	-8.78	1.23	1.32
1	A	1163	HIS	CE1-NE2	-8.78	1.23	1.32
11	K	40	HIS	CE1-NE2	-8.78	1.23	1.32
24	Y	12	HIS	CE1-NE2	-8.77	1.23	1.32
5	E	148	HIS	CE1-NE2	-8.76	1.23	1.32
2	B	1021	HIS	CE1-NE2	-8.76	1.23	1.32
1	A	804	HIS	CE1-NE2	-8.75	1.23	1.32
2	B	502	HIS	CE1-NE2	-8.75	1.23	1.32
29	h	79	HIS	ND1-CE1	-8.75	1.23	1.32
2	B	518	HIS	CE1-NE2	-8.75	1.23	1.32
2	B	577	HIS	CE1-NE2	-8.75	1.23	1.32
2	B	842	HIS	CE1-NE2	-8.74	1.23	1.32
7	G	111	HIS	CE1-NE2	-8.74	1.23	1.32
1	A	662	HIS	CE1-NE2	-8.74	1.23	1.32
1	A	1044	HIS	CE1-NE2	-8.74	1.23	1.32
17	Q	714	HIS	CE1-NE2	-8.74	1.23	1.32
1	A	439	HIS	CE1-NE2	-8.73	1.23	1.32
9	I	60	HIS	CE1-NE2	-8.72	1.23	1.32
7	G	9	HIS	CE1-NE2	-8.71	1.23	1.32
3	C	265	HIS	CE1-NE2	-8.71	1.23	1.32
1	A	995	HIS	CE1-NE2	-8.69	1.23	1.32
1	A	465	HIS	ND1-CE1	-8.69	1.23	1.32
2	B	1117	HIS	ND1-CE1	-8.68	1.23	1.32
2	B	287	HIS	CE1-NE2	-8.67	1.23	1.32
1	A	839	HIS	ND1-CE1	-8.65	1.23	1.32
27	f	75	HIS	CE1-NE2	-8.65	1.23	1.32
1	A	218	PRO	CA-CB	-8.61	1.47	1.53
1	A	56	GLY	N-CA	-8.44	1.37	1.44
3	C	106	ARG	CZ-NH2	-8.41	1.22	1.33
5	E	55	ARG	CZ-NH2	-8.40	1.22	1.33
18	R	425	GLY	N-CA	-8.40	1.37	1.44
18	R	371	ARG	CZ-NH2	-8.39	1.22	1.33
2	B	491	ARG	CZ-NH2	-8.31	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	575	GLY	N-CA	-8.29	1.38	1.45
12	L	31	ARG	CZ-NH2	-8.29	1.22	1.33
26	a	128	ARG	CZ-NH2	-8.26	1.22	1.33
26	e	128	ARG	CZ-NH2	-8.26	1.22	1.33
2	B	939	HIS	CD2-NE2	-8.26	1.28	1.37
26	a	129	ARG	CZ-NH2	-8.25	1.22	1.33
6	F	100	ARG	CZ-NH2	-8.23	1.22	1.33
2	B	380	ARG	CZ-NH2	-8.23	1.22	1.33
1	A	734	ARG	CZ-NH2	-8.22	1.22	1.33
1	A	1167	ARG	CZ-NH2	-8.22	1.22	1.33
26	e	129	ARG	CZ-NH2	-8.21	1.22	1.33
2	B	379	ARG	CZ-NH2	-8.20	1.22	1.33
9	I	103	ARG	CZ-NH2	-8.20	1.22	1.33
13	M	1355	ARG	CZ-NH2	-8.18	1.22	1.33
17	Q	191	ARG	CZ-NH2	-8.16	1.22	1.33
2	B	499	ARG	CZ-NH2	-8.16	1.22	1.33
3	C	114	HIS	CD2-NE2	-8.16	1.28	1.37
2	B	287	HIS	CD2-NE2	-8.16	1.28	1.37
27	f	67	ARG	CZ-NH2	-8.16	1.22	1.33
1	A	532	ARG	CZ-NH2	-8.15	1.22	1.33
2	B	370	HIS	CD2-NE2	-8.15	1.28	1.37
7	G	63	ARG	CZ-NH2	-8.15	1.22	1.33
4	D	93	HIS	CD2-NE2	-8.14	1.28	1.37
1	A	407	ARG	CZ-NH2	-8.14	1.22	1.33
1	A	995	HIS	CD2-NE2	-8.14	1.28	1.37
1	A	1163	HIS	CD2-NE2	-8.14	1.28	1.37
27	b	55	ARG	CZ-NH2	-8.13	1.22	1.33
29	h	89	ARG	CZ-NH2	-8.13	1.22	1.33
12	L	51	ARG	CZ-NH2	-8.12	1.22	1.33
2	B	1131	ARG	CZ-NH2	-8.12	1.22	1.33
3	C	160	ARG	CZ-NH2	-8.12	1.22	1.33
1	A	844	ARG	CZ-NH2	-8.12	1.22	1.33
1	A	599	HIS	CD2-NE2	-8.11	1.28	1.37
7	G	9	HIS	CD2-NE2	-8.12	1.28	1.37
5	E	148	HIS	CD2-NE2	-8.11	1.28	1.37
20	U	411	ARG	CZ-NH2	-8.11	1.23	1.33
3	C	194	HIS	CD2-NE2	-8.11	1.28	1.37
25	Z	283	ARG	CZ-NH2	-8.11	1.23	1.33
27	f	75	HIS	CD2-NE2	-8.11	1.28	1.37
1	A	292	ARG	CZ-NH2	-8.10	1.23	1.33
17	Q	218	ARG	CZ-NH2	-8.10	1.23	1.33
1	A	523	ARG	CZ-NH2	-8.10	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	38	HIS	CD2-NE2	-8.10	1.28	1.37
1	A	1044	HIS	CD2-NE2	-8.09	1.28	1.37
2	B	842	HIS	CD2-NE2	-8.09	1.28	1.37
1	A	557	ARG	CZ-NH2	-8.09	1.23	1.33
2	B	1021	HIS	CD2-NE2	-8.09	1.28	1.37
3	C	265	HIS	CD2-NE2	-8.09	1.28	1.37
1	A	61	ARG	CZ-NH2	-8.08	1.23	1.33
29	h	79	HIS	CD2-NE2	-8.07	1.28	1.37
1	A	408	ARG	CZ-NH2	-8.07	1.23	1.33
1	A	662	HIS	CD2-NE2	-8.07	1.28	1.37
2	B	438	ARG	CZ-NH2	-8.07	1.23	1.33
17	Q	832	ARG	CZ-NH2	-8.07	1.23	1.33
17	Q	830	ARG	CZ-NH2	-8.06	1.23	1.33
2	B	841	ARG	CZ-NH2	-8.06	1.23	1.33
2	B	577	HIS	CD2-NE2	-8.06	1.28	1.37
2	B	716	HIS	CD2-NE2	-8.06	1.28	1.37
1	A	1380	ARG	CZ-NH2	-8.06	1.23	1.33
25	Z	625	HIS	CD2-NE2	-8.06	1.28	1.37
1	A	70	ARG	CZ-NH2	-8.05	1.23	1.33
25	Z	234	HIS	CD2-NE2	-8.05	1.28	1.37
4	D	73	ARG	CZ-NH2	-8.05	1.23	1.33
9	I	60	HIS	CD2-NE2	-8.05	1.28	1.37
11	K	40	HIS	CD2-NE2	-8.05	1.28	1.37
25	Z	246	ARG	CZ-NH2	-8.05	1.23	1.33
25	Z	610	ARG	CZ-NH2	-8.05	1.23	1.33
7	G	111	HIS	CD2-NE2	-8.04	1.29	1.37
17	Q	791	ARG	CZ-NH2	-8.04	1.23	1.33
17	Q	667	ARG	CZ-NH2	-8.03	1.23	1.33
17	Q	725	ARG	CZ-NH2	-8.03	1.23	1.33
18	R	438	ARG	CZ-NH2	-8.03	1.23	1.33
24	Y	12	HIS	CD2-NE2	-8.03	1.29	1.37
2	B	518	HIS	CD2-NE2	-8.02	1.29	1.37
1	A	536	GLY	N-CA	-8.02	1.37	1.45
1	A	1224	ARG	CZ-NH2	-8.02	1.23	1.33
5	E	162	ARG	CZ-NH2	-8.02	1.23	1.33
2	B	610	ARG	CZ-NH2	-8.01	1.23	1.33
5	E	109	GLY	N-CA	-8.01	1.37	1.45
28	g	35	ARG	CZ-NH2	-8.01	1.23	1.33
1	A	880	ARG	CZ-NH2	-8.01	1.23	1.33
17	Q	714	HIS	CD2-NE2	-8.01	1.29	1.37
21	V	26	ARG	CZ-NH2	-8.01	1.23	1.33
5	E	172	ARG	CZ-NH2	-8.01	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	e	53	ARG	CZ-NH2	-8.00	1.23	1.33
1	A	1220	HIS	CD2-NE2	-8.00	1.29	1.37
2	B	1104	ARG	CZ-NH2	-8.00	1.23	1.33
3	C	118	ARG	CZ-NH2	-8.00	1.23	1.33
4	D	70	ARG	CZ-NH2	-8.00	1.23	1.33
17	Q	689	HIS	CD2-NE2	-8.00	1.29	1.37
17	Q	763	ARG	CZ-NH2	-8.00	1.23	1.33
20	U	439	ARG	CZ-NH2	-8.00	1.23	1.33
1	A	1149	ARG	CZ-NH2	-8.00	1.23	1.33
2	B	890	ARG	CZ-NH2	-8.00	1.23	1.33
17	Q	201	ARG	CZ-NH2	-8.00	1.23	1.33
25	Z	494	ARG	CZ-NH2	-8.00	1.23	1.33
2	B	1091	ARG	CZ-NH2	-7.99	1.23	1.33
1	A	1218	ARG	CZ-NH2	-7.99	1.23	1.33
5	E	207	ARG	CZ-NH2	-7.99	1.23	1.33
1	A	551	ARG	CZ-NH2	-7.99	1.23	1.33
28	g	31	HIS	CD2-NE2	-7.99	1.29	1.37
1	A	932	ARG	CZ-NH2	-7.99	1.23	1.33
2	B	83	ARG	CZ-NH2	-7.98	1.23	1.33
7	G	144	ARG	CZ-NH2	-7.98	1.23	1.33
1	A	186	ARG	CZ-NH2	-7.98	1.23	1.33
1	A	439	HIS	CD2-NE2	-7.98	1.29	1.37
20	U	409	ARG	CZ-NH2	-7.98	1.23	1.33
1	A	1375	ARG	CZ-NH2	-7.98	1.23	1.33
9	I	33	ARG	CZ-NH2	-7.97	1.23	1.33
26	e	134	ARG	CZ-NH2	-7.97	1.23	1.33
3	C	86	ARG	CZ-NH2	-7.97	1.23	1.33
20	U	387	ARG	CZ-NH2	-7.97	1.23	1.33
8	H	84	ARG	CZ-NH2	-7.97	1.23	1.33
1	A	1160	ARG	CZ-NH2	-7.97	1.23	1.33
1	A	1046	ARG	CZ-NH2	-7.96	1.23	1.33
2	B	938	ARG	CZ-NH2	-7.96	1.23	1.33
2	B	768	ARG	CZ-NH2	-7.96	1.23	1.33
1	A	421	ARG	CZ-NH2	-7.96	1.23	1.33
1	A	1345	ARG	CZ-NH2	-7.96	1.23	1.33
2	B	1023	ARG	CZ-NH2	-7.96	1.23	1.33
5	E	142	HIS	CD2-NE2	-7.96	1.29	1.37
21	V	223	GLY	N-CA	-7.96	1.38	1.45
3	C	133	ARG	CZ-NH2	-7.96	1.23	1.33
5	E	202	ARG	CZ-NH2	-7.96	1.23	1.33
7	G	78	ARG	CZ-NH2	-7.96	1.23	1.33
1	A	804	HIS	CD2-NE2	-7.95	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	24	ARG	CZ-NH2	-7.95	1.23	1.33
1	A	583	ARG	CZ-NH2	-7.95	1.23	1.33
2	B	1035	ARG	CZ-NH2	-7.95	1.23	1.33
2	B	975	ARG	CZ-NH2	-7.95	1.23	1.33
5	E	195	ARG	CZ-NH2	-7.95	1.23	1.33
6	F	51	ARG	CZ-NH2	-7.95	1.23	1.33
21	V	132	ARG	CZ-NH2	-7.94	1.23	1.33
2	B	834	ARG	CZ-NH2	-7.94	1.23	1.33
1	A	1031	ARG	CZ-NH2	-7.94	1.23	1.33
1	A	1153	ARG	CZ-NH2	-7.94	1.23	1.33
2	B	1150	ARG	CZ-NH2	-7.94	1.23	1.33
3	C	193	ARG	CZ-NH2	-7.93	1.23	1.33
1	A	805	ARG	CZ-NH2	-7.93	1.23	1.33
2	B	41	ARG	CZ-NH2	-7.93	1.23	1.33
1	A	890	ARG	CZ-NH2	-7.93	1.23	1.33
1	A	1286	ARG	CZ-NH2	-7.92	1.23	1.33
2	B	502	HIS	CD2-NE2	-7.92	1.29	1.37
8	H	57	ARG	CZ-NH2	-7.92	1.23	1.33
26	e	39	HIS	CD2-NE2	-7.92	1.29	1.37
24	Y	14	ARG	CZ-NH2	-7.91	1.23	1.33
2	B	483	ARG	CZ-NH2	-7.91	1.23	1.33
1	A	271	ARG	CZ-NH2	-7.91	1.23	1.33
5	E	181	ARG	CZ-NH2	-7.90	1.23	1.33
24	Y	111	ARG	CZ-NH2	-7.90	1.23	1.33
25	Z	749	ARG	CZ-NH2	-7.90	1.23	1.33
2	B	721	ARG	CZ-NH2	-7.90	1.23	1.33
4	D	121	ARG	CZ-NH2	-7.90	1.23	1.33
28	c	77	ARG	CZ-NH2	-7.89	1.23	1.33
28	g	42	ARG	CZ-NH2	-7.89	1.23	1.33
1	A	1059	ARG	CZ-NH2	-7.88	1.23	1.33
27	b	95	ARG	CZ-NH2	-7.88	1.23	1.33
2	B	425	ARG	CZ-NH2	-7.88	1.23	1.33
1	A	1356	ARG	CZ-NH2	-7.88	1.23	1.33
9	I	40	ARG	CZ-NH2	-7.88	1.23	1.33
26	e	49	ARG	CZ-NH2	-7.87	1.23	1.33
4	D	138	ARG	CZ-NH2	-7.87	1.23	1.33
3	C	228	ARG	CZ-NH2	-7.87	1.23	1.33
6	F	62	ARG	CZ-NH2	-7.87	1.23	1.33
24	Y	11	ARG	CZ-NH2	-7.87	1.23	1.33
2	B	230	ARG	CZ-NH2	-7.87	1.23	1.33
2	B	416	ARG	CZ-NH2	-7.87	1.23	1.33
2	B	371	ARG	CZ-NH2	-7.86	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	80	ARG	CZ-NH2	-7.86	1.23	1.33
2	B	608	ARG	CZ-NH2	-7.86	1.23	1.33
3	C	10	ARG	CZ-NH2	-7.86	1.23	1.33
2	B	242	ARG	CZ-NH2	-7.86	1.23	1.33
2	B	770	ARG	CZ-NH2	-7.85	1.23	1.33
1	A	401	ARG	CZ-NH2	-7.85	1.23	1.33
29	h	83	ARG	CZ-NH2	-7.84	1.23	1.33
9	I	15	ARG	CZ-NH2	-7.84	1.23	1.33
5	E	166	ARG	CZ-NH2	-7.84	1.23	1.33
11	K	106	ARG	CZ-NH2	-7.84	1.23	1.33
18	R	597	ARG	CZ-NH2	-7.83	1.23	1.33
18	R	596	ARG	CZ-NH2	-7.83	1.23	1.33
1	A	69	GLY	N-CA	-7.82	1.37	1.44
28	c	42	ARG	CZ-NH2	-7.82	1.23	1.33
2	B	1078	ARG	CZ-NH2	-7.80	1.23	1.33
25	Z	198	ARG	CZ-NH2	-7.80	1.23	1.33
1	A	220	ARG	CZ-NH2	-7.79	1.23	1.33
1	A	1025	GLY	N-CA	-7.79	1.38	1.45
2	B	282	ARG	CZ-NH2	-7.78	1.23	1.33
1	A	743	ARG	CZ-NH2	-7.75	1.23	1.33
3	C	113	ARG	CZ-NH2	-7.70	1.23	1.33
2	B	999	ALA	CA-CB	-7.67	1.43	1.53
1	A	263	ALA	CA-CB	-7.65	1.43	1.52
25	Z	380	ALA	CA-CB	-7.57	1.42	1.53
17	Q	726	ALA	CA-CB	-7.52	1.42	1.53
1	A	776	GLY	N-CA	-7.49	1.37	1.45
25	Z	483	GLY	N-CA	-7.45	1.38	1.45
1	A	1527	ALA	CA-CB	-7.42	1.42	1.53
7	G	159	ALA	CA-CB	-7.34	1.42	1.53
1	A	63	GLY	N-CA	-7.14	1.37	1.45
8	H	108	ALA	CA-CB	-7.13	1.42	1.53
18	R	407	GLY	N-CA	-7.06	1.38	1.44
29	d	50	GLY	N-CA	-7.01	1.38	1.44
26	a	127	ALA	CA-CB	-7.00	1.42	1.53
5	E	122	ALA	CA-CB	-6.96	1.42	1.53
26	a	102	ALA	CA-CB	-6.95	1.42	1.53
18	R	592	ASP	N-CA	-6.93	1.42	1.46
26	e	88	ALA	CA-CB	-6.92	1.42	1.53
1	A	830	GLY	N-CA	-6.91	1.37	1.45
14	N	16	DT	P-OP1	6.90	1.62	1.48
19	T	-70	DT	P-OP1	6.89	1.62	1.48
19	T	-112	DT	P-OP1	6.89	1.62	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	T	-109	DT	P-OP1	6.89	1.62	1.48
14	N	106	DT	P-OP1	6.88	1.62	1.48
27	f	83	ALA	CA-CB	-6.87	1.42	1.53
14	N	14	DT	P-OP1	6.87	1.62	1.48
19	T	-144	DT	P-OP1	6.87	1.62	1.48
14	N	139	DT	P-OP1	6.87	1.62	1.48
14	N	86	DT	P-OP1	6.86	1.62	1.48
14	N	140	DT	P-OP1	6.86	1.62	1.48
19	T	-132	DT	P-OP1	6.86	1.62	1.48
26	e	75	ALA	CA-CB	-6.86	1.42	1.53
14	N	87	DT	P-OP1	6.86	1.62	1.48
14	N	108	DT	P-OP1	6.86	1.62	1.48
24	Y	62	ALA	CA-CB	-6.85	1.42	1.53
2	B	113	ALA	CA-CB	-6.84	1.42	1.53
19	T	-144	DT	P-OP2	6.81	1.62	1.48
3	C	106	ARG	CZ-NH1	-6.79	1.23	1.32
17	Q	224	ALA	CA-CB	-6.79	1.42	1.53
1	A	76	GLY	N-CA	-6.79	1.38	1.45
5	E	55	ARG	CZ-NH1	-6.79	1.23	1.32
12	L	31	ARG	CZ-NH1	-6.78	1.23	1.32
14	N	39	DT	P-OP1	6.78	1.62	1.48
18	R	371	ARG	CZ-NH1	-6.77	1.23	1.32
1	A	774	ALA	CA-CB	-6.77	1.42	1.53
17	Q	811	ALA	CA-CB	-6.76	1.42	1.53
25	Z	612	GLY	N-CA	-6.76	1.38	1.45
8	H	84	ARG	CZ-NH1	-6.76	1.23	1.32
26	a	95	ALA	CA-CB	-6.74	1.42	1.53
17	Q	789	ALA	CA-CB	-6.73	1.42	1.53
2	B	1131	ARG	CZ-NH1	-6.72	1.23	1.32
29	h	78	ALA	CA-CB	-6.72	1.43	1.53
18	R	548	ALA	CA-CB	-6.72	1.42	1.53
1	A	1064	ALA	CA-CB	-6.71	1.42	1.53
17	Q	671	ALA	CA-CB	-6.69	1.43	1.53
2	B	1077	GLY	N-CA	-6.69	1.37	1.45
17	Q	831	ALA	CA-CB	-6.69	1.43	1.53
2	B	491	ARG	CZ-NH1	-6.68	1.23	1.32
1	A	748	ALA	CA-CB	-6.68	1.43	1.53
17	Q	782	ALA	CA-CB	-6.68	1.42	1.53
26	a	128	ARG	CZ-NH1	-6.67	1.23	1.32
3	C	29	ALA	CA-CB	-6.67	1.42	1.53
26	a	129	ARG	CZ-NH1	-6.67	1.23	1.32
26	e	128	ARG	CZ-NH1	-6.67	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	380	ARG	CZ-NH1	-6.66	1.23	1.32
2	B	1126	ALA	CA-CB	-6.66	1.43	1.53
1	A	1089	ALA	CA-CB	-6.66	1.43	1.53
18	R	521	ALA	CA-CB	-6.66	1.42	1.53
2	B	379	ARG	CZ-NH1	-6.64	1.23	1.32
1	A	1167	ARG	CZ-NH1	-6.64	1.23	1.32
26	a	91	ALA	CA-CB	-6.63	1.43	1.53
2	B	868	GLY	N-CA	-6.63	1.37	1.45
13	M	1355	ARG	CZ-NH1	-6.62	1.23	1.32
7	G	63	ARG	CZ-NH1	-6.62	1.23	1.32
11	K	86	ALA	CA-CB	-6.62	1.43	1.53
6	F	119	GLY	N-CA	-6.62	1.37	1.45
2	B	499	ARG	CZ-NH1	-6.61	1.23	1.32
9	I	103	ARG	CZ-NH1	-6.61	1.23	1.32
12	L	57	ALA	CA-CB	-6.59	1.42	1.53
5	E	104	ILE	C-N	-6.59	1.27	1.33
24	Y	114	ALA	CA-CB	-6.59	1.43	1.53
3	C	160	ARG	CZ-NH1	-6.58	1.23	1.32
2	B	1096	ALA	CA-CB	-6.58	1.43	1.53
4	D	70	ARG	CZ-NH1	-6.57	1.23	1.32
27	b	55	ARG	CZ-NH1	-6.57	1.23	1.32
2	B	438	ARG	CZ-NH1	-6.57	1.23	1.32
2	B	975	ARG	CZ-NH1	-6.57	1.23	1.32
5	E	162	ARG	CZ-NH1	-6.57	1.23	1.32
17	Q	217	ALA	CA-CB	-6.57	1.42	1.53
26	e	129	ARG	CZ-NH1	-6.57	1.23	1.32
1	A	281	ALA	CA-CB	-6.56	1.43	1.53
1	A	734	ARG	CZ-NH1	-6.56	1.23	1.32
1	A	840	ALA	CA-CB	-6.56	1.43	1.53
19	T	-21	DG	P-OP1	6.56	1.61	1.48
6	F	100	ARG	CZ-NH1	-6.55	1.23	1.32
14	N	83	DG	P-OP1	6.55	1.61	1.48
1	A	1224	ARG	CZ-NH1	-6.55	1.23	1.32
14	N	17	DG	P-OP1	6.55	1.61	1.48
1	A	1046	ARG	CZ-NH1	-6.54	1.23	1.32
2	B	302	LYS	CA-CB	-6.54	1.48	1.54
19	T	-71	DG	P-OP1	6.54	1.61	1.48
1	A	408	ARG	CZ-NH1	-6.54	1.23	1.32
14	N	110	DC	P-OP1	6.54	1.61	1.48
19	T	-131	DG	P-OP1	6.54	1.61	1.48
19	T	-135	DC	P-OP1	6.54	1.61	1.48
19	T	-69	DC	P-OP1	6.54	1.61	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	407	ARG	CZ-NH1	-6.53	1.23	1.32
1	A	1345	ARG	CZ-NH1	-6.53	1.23	1.32
14	N	135	DG	P-OP1	6.53	1.61	1.48
14	N	136	DG	P-OP1	6.53	1.61	1.48
14	N	67	DG	P-OP1	6.53	1.61	1.48
14	N	66	DG	P-OP1	6.53	1.61	1.48
14	N	133	DC	P-OP1	6.53	1.61	1.48
19	T	-67	DC	P-OP1	6.53	1.61	1.48
5	E	172	ARG	CZ-NH1	-6.53	1.23	1.32
19	T	-111	DC	P-OP1	6.53	1.61	1.48
19	T	-110	DG	P-OP1	6.53	1.61	1.48
1	A	61	ARG	CZ-NH1	-6.53	1.23	1.32
14	N	15	DC	P-OP1	6.53	1.61	1.48
27	b	83	ALA	CA-CB	-6.53	1.43	1.53
4	D	69	ALA	CA-CB	-6.52	1.43	1.53
19	T	-141	DG	P-OP1	6.52	1.61	1.48
19	T	-83	DC	P-OP1	6.52	1.61	1.48
1	A	532	ARG	CZ-NH1	-6.52	1.23	1.32
9	I	13	GLY	N-CA	-6.52	1.37	1.45
12	L	51	ARG	CZ-NH1	-6.52	1.23	1.32
14	N	137	DG	P-OP1	6.52	1.61	1.48
1	A	70	ARG	CZ-NH1	-6.52	1.23	1.32
2	B	362	ALA	CA-CB	-6.52	1.43	1.53
14	N	138	DA	P-OP1	6.52	1.61	1.48
18	R	438	ARG	CZ-NH1	-6.52	1.23	1.32
19	T	-142	DA	P-OP1	6.52	1.61	1.48
19	T	-68	DC	P-OP1	6.52	1.61	1.48
19	T	-20	DA	P-OP1	6.52	1.61	1.48
19	T	-15	DG	P-OP1	6.52	1.61	1.48
19	T	-134	DG	P-OP1	6.52	1.61	1.48
19	T	-105	DC	P-OP1	6.52	1.61	1.48
19	T	-19	DG	P-OP1	6.52	1.61	1.48
14	N	84	DC	P-OP1	6.52	1.61	1.48
19	T	-133	DG	P-OP1	6.52	1.61	1.48
19	T	-107	DG	P-OP1	6.52	1.61	1.48
14	N	85	DG	P-OP1	6.51	1.61	1.48
14	N	112	DA	P-OP1	6.51	1.61	1.48
25	Z	246	ARG	CZ-NH1	-6.51	1.23	1.32
6	F	93	ALA	CA-CB	-6.51	1.43	1.53
14	N	72	DA	P-OP1	6.51	1.61	1.48
19	T	-29	DC	P-OP1	6.51	1.61	1.48
1	A	844	ARG	CZ-NH1	-6.51	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	143	DG	P-OP1	6.51	1.61	1.48
17	Q	829	ALA	CA-CB	-6.51	1.43	1.53
25	Z	283	ARG	CZ-NH1	-6.51	1.23	1.32
19	T	-18	DA	P-OP1	6.51	1.61	1.48
1	A	990	ALA	CA-CB	-6.51	1.43	1.53
1	A	1380	ARG	CZ-NH1	-6.51	1.23	1.32
14	N	111	DG	P-OP1	6.51	1.61	1.48
14	N	132	DA	P-OP1	6.51	1.61	1.48
19	T	-136	DC	P-OP1	6.51	1.61	1.48
19	T	-14	DA	P-OP1	6.50	1.61	1.48
14	N	134	DC	P-OP1	6.50	1.61	1.48
19	T	-106	DA	P-OP1	6.50	1.61	1.48
19	T	-17	DC	P-OP1	6.50	1.61	1.48
14	N	144	DA	P-OP1	6.50	1.61	1.48
17	Q	201	ARG	CZ-NH1	-6.50	1.23	1.32
17	Q	725	ARG	CZ-NH1	-6.50	1.23	1.32
19	T	-139	DA	P-OP1	6.50	1.61	1.48
19	T	-130	DC	P-OP1	6.50	1.61	1.48
14	N	65	DA	P-OP1	6.50	1.61	1.48
18	R	412	ALA	CA-CB	-6.50	1.43	1.53
19	T	-143	DC	P-OP1	6.50	1.61	1.48
1	A	513	ALA	CA-CB	-6.50	1.43	1.53
14	N	71	DC	P-OP1	6.49	1.61	1.48
11	K	108	ALA	CA-CB	-6.49	1.43	1.53
14	N	109	DA	P-OP1	6.49	1.61	1.48
1	A	1092	ALA	CA-CB	-6.49	1.43	1.53
14	N	107	DC	P-OP1	6.49	1.61	1.48
19	T	-66	DC	P-OP1	6.49	1.61	1.48
26	e	134	ARG	CZ-NH1	-6.49	1.23	1.32
19	T	-108	DA	P-OP1	6.49	1.61	1.48
2	B	416	ARG	CZ-NH1	-6.49	1.23	1.32
25	Z	610	ARG	CZ-NH1	-6.49	1.23	1.32
19	T	-140	DA	P-OP1	6.48	1.61	1.48
1	A	315	ALA	CA-CB	-6.48	1.43	1.53
19	T	-30	DA	P-OP1	6.48	1.61	1.48
19	T	-16	DA	P-OP1	6.48	1.61	1.48
17	Q	763	ARG	CZ-NH1	-6.47	1.23	1.32
27	b	56	GLY	N-CA	-6.47	1.38	1.45
19	T	-87	DA	P-OP1	6.47	1.61	1.48
20	U	411	ARG	CZ-NH1	-6.47	1.23	1.32
21	V	26	ARG	CZ-NH1	-6.47	1.23	1.32
5	E	202	ARG	CZ-NH1	-6.47	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	GLY	N-CA	-6.46	1.38	1.45
1	A	75	ALA	CA-CB	-6.46	1.42	1.53
1	A	186	ARG	CZ-NH1	-6.46	1.23	1.32
2	B	618	ALA	CA-CB	-6.46	1.43	1.53
9	I	48	ALA	CA-CB	-6.46	1.43	1.53
1	A	292	ARG	CZ-NH1	-6.46	1.23	1.32
29	h	89	ARG	CZ-NH1	-6.46	1.23	1.32
6	F	70	ALA	CA-CB	-6.46	1.43	1.53
17	Q	191	ARG	CZ-NH1	-6.46	1.23	1.32
17	Q	830	ARG	CZ-NH1	-6.46	1.23	1.32
2	B	938	ARG	CZ-NH1	-6.46	1.23	1.32
17	Q	667	ARG	CZ-NH1	-6.46	1.23	1.32
4	D	98	ALA	CA-CB	-6.45	1.43	1.53
7	G	87	ALA	CA-CB	-6.45	1.42	1.53
17	Q	218	ARG	CZ-NH1	-6.45	1.23	1.32
1	A	1153	ARG	CZ-NH1	-6.45	1.23	1.32
29	h	83	ARG	CZ-NH1	-6.45	1.23	1.32
1	A	551	ARG	CZ-NH1	-6.45	1.23	1.32
4	D	73	ARG	CZ-NH1	-6.45	1.23	1.32
17	Q	791	ARG	CZ-NH1	-6.44	1.23	1.32
1	A	523	ARG	CZ-NH1	-6.44	1.23	1.32
1	A	558	GLY	N-CA	-6.44	1.37	1.45
1	A	880	ARG	CZ-NH1	-6.44	1.23	1.32
1	A	1059	ARG	CZ-NH1	-6.44	1.23	1.32
1	A	1330	ALA	CA-CB	-6.44	1.43	1.53
2	B	317	ALA	CA-CB	-6.44	1.43	1.53
2	B	841	ARG	CZ-NH1	-6.44	1.23	1.32
2	B	1091	ARG	CZ-NH1	-6.44	1.23	1.32
2	B	768	ARG	CZ-NH1	-6.43	1.23	1.32
7	G	144	ARG	CZ-NH1	-6.43	1.23	1.32
1	A	1088	GLY	N-CA	-6.43	1.37	1.45
1	A	1300	GLY	N-CA	-6.43	1.37	1.45
5	E	207	ARG	CZ-NH1	-6.43	1.23	1.32
7	G	78	ARG	CZ-NH1	-6.43	1.23	1.32
27	f	67	ARG	CZ-NH1	-6.43	1.23	1.32
2	B	1104	ARG	CZ-NH1	-6.42	1.23	1.32
17	Q	832	ARG	CZ-NH1	-6.42	1.23	1.32
20	U	409	ARG	CZ-NH1	-6.42	1.23	1.32
1	A	557	ARG	CZ-NH1	-6.42	1.23	1.32
2	B	519	ALA	CA-CB	-6.42	1.43	1.53
2	B	527	ALA	CA-CB	-6.42	1.43	1.53
2	B	1150	ARG	CZ-NH1	-6.42	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	ARG	CZ-NH1	-6.42	1.23	1.32
1	A	709	ALA	CA-CB	-6.42	1.43	1.53
6	F	51	ARG	CZ-NH1	-6.42	1.23	1.32
1	A	1252	ALA	CA-CB	-6.42	1.43	1.53
1	A	932	ARG	CZ-NH1	-6.41	1.23	1.32
20	U	387	ARG	CZ-NH1	-6.41	1.23	1.32
21	V	132	ARG	CZ-NH1	-6.41	1.23	1.32
1	A	1356	ARG	CZ-NH1	-6.41	1.23	1.32
1	A	421	ARG	CZ-NH1	-6.41	1.23	1.32
1	A	1375	ARG	CZ-NH1	-6.41	1.23	1.32
24	Y	83	GLY	N-CA	-6.41	1.38	1.45
1	A	401	ARG	CZ-NH1	-6.41	1.23	1.32
2	B	688	ALA	CA-CB	-6.41	1.43	1.53
2	B	41	ARG	CZ-NH1	-6.41	1.23	1.32
2	B	890	ARG	CZ-NH1	-6.41	1.23	1.32
24	Y	14	ARG	CZ-NH1	-6.41	1.23	1.32
17	Q	165	ALA	CA-CB	-6.40	1.42	1.53
17	Q	758	ALA	CA-CB	-6.40	1.43	1.53
1	A	588	GLY	N-CA	-6.40	1.38	1.45
1	A	1149	ARG	CZ-NH1	-6.40	1.23	1.32
2	B	443	GLY	N-CA	-6.40	1.38	1.45
6	F	67	GLY	N-CA	-6.40	1.37	1.45
2	B	770	ARG	CZ-NH1	-6.40	1.23	1.32
1	A	890	ARG	CZ-NH1	-6.39	1.23	1.32
2	B	721	ARG	CZ-NH1	-6.39	1.23	1.32
1	A	1160	ARG	CZ-NH1	-6.39	1.23	1.32
28	g	35	ARG	CZ-NH1	-6.39	1.23	1.32
3	C	133	ARG	CZ-NH1	-6.38	1.23	1.32
25	Z	494	ARG	CZ-NH1	-6.38	1.23	1.32
28	c	77	ARG	CZ-NH1	-6.38	1.23	1.32
25	Z	749	ARG	CZ-NH1	-6.38	1.23	1.32
1	A	200	ALA	CA-CB	-6.38	1.42	1.53
2	B	608	ARG	CZ-NH1	-6.38	1.23	1.32
5	E	181	ARG	CZ-NH1	-6.38	1.23	1.32
2	B	371	ARG	CZ-NH1	-6.38	1.23	1.32
21	V	103	ALA	CA-CB	-6.38	1.42	1.53
5	E	195	ARG	CZ-NH1	-6.37	1.23	1.32
28	g	40	ALA	CA-CB	-6.37	1.43	1.53
5	E	196	PRO	CA-CB	-6.37	1.47	1.54
26	e	127	ALA	CA-CB	-6.37	1.42	1.53
9	I	33	ARG	CZ-NH1	-6.36	1.23	1.32
17	Q	220	ALA	CA-CB	-6.36	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	118	ARG	CZ-NH1	-6.36	1.23	1.32
1	A	583	ARG	CZ-NH1	-6.36	1.23	1.32
2	B	230	ARG	CZ-NH1	-6.35	1.23	1.32
2	B	282	ARG	CZ-NH1	-6.35	1.23	1.32
1	A	1031	ARG	CZ-NH1	-6.35	1.23	1.32
2	B	834	ARG	CZ-NH1	-6.35	1.23	1.32
11	K	60	GLY	N-CA	-6.35	1.38	1.45
13	M	547	GLY	N-CA	-6.35	1.38	1.45
4	D	121	ARG	CZ-NH1	-6.35	1.23	1.32
1	A	1286	ARG	CZ-NH1	-6.35	1.23	1.32
5	E	24	ARG	CZ-NH1	-6.34	1.23	1.32
1	A	1218	ARG	CZ-NH1	-6.34	1.23	1.32
28	c	42	ARG	CZ-NH1	-6.34	1.23	1.32
24	Y	11	ARG	CZ-NH1	-6.33	1.23	1.32
26	e	53	ARG	CZ-NH1	-6.33	1.23	1.32
4	D	138	ARG	CZ-NH1	-6.33	1.23	1.32
21	V	310	GLY	N-CA	-6.33	1.38	1.45
28	g	42	ARG	CZ-NH1	-6.33	1.23	1.32
8	H	57	ARG	CZ-NH1	-6.33	1.23	1.32
29	d	35	ALA	CA-CB	-6.33	1.43	1.53
2	B	83	ARG	CZ-NH1	-6.33	1.23	1.32
2	B	406	GLY	N-CA	-6.33	1.38	1.45
2	B	727	ALA	CA-CB	-6.33	1.43	1.53
2	B	1035	ARG	CZ-NH1	-6.33	1.23	1.32
5	E	166	ARG	CZ-NH1	-6.32	1.23	1.32
2	B	732	ALA	CA-CB	-6.32	1.43	1.53
2	B	610	ARG	CZ-NH1	-6.32	1.24	1.32
3	C	86	ARG	CZ-NH1	-6.32	1.24	1.32
24	Y	111	ARG	CZ-NH1	-6.32	1.24	1.32
20	U	439	ARG	CZ-NH1	-6.31	1.24	1.32
1	A	805	ARG	CZ-NH1	-6.31	1.24	1.32
2	B	242	ARG	CZ-NH1	-6.31	1.24	1.32
27	b	95	ARG	CZ-NH1	-6.31	1.24	1.32
9	I	40	ARG	CZ-NH1	-6.30	1.24	1.32
26	e	49	ARG	CZ-NH1	-6.30	1.24	1.32
29	h	55	ALA	CA-CB	-6.30	1.43	1.53
17	Q	184	ALA	CA-CB	-6.29	1.42	1.53
27	b	101	GLY	N-CA	-6.29	1.38	1.45
3	C	228	ARG	CZ-NH1	-6.29	1.24	1.32
1	A	877	ALA	CA-CB	-6.28	1.44	1.53
2	B	1023	ARG	CZ-NH1	-6.28	1.24	1.32
9	I	80	ARG	CZ-NH1	-6.26	1.24	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	106	ARG	CZ-NH1	-6.26	1.24	1.32
2	B	483	ARG	CZ-NH1	-6.26	1.24	1.32
18	R	597	ARG	CZ-NH1	-6.26	1.24	1.32
1	A	1530	ALA	CA-CB	-6.26	1.42	1.53
4	D	29	ALA	CA-CB	-6.26	1.43	1.53
18	R	596	ARG	CZ-NH1	-6.25	1.24	1.32
1	A	1399	ALA	CA-CB	-6.25	1.43	1.53
6	F	74	ALA	CA-CB	-6.25	1.43	1.53
9	I	15	ARG	CZ-NH1	-6.25	1.24	1.32
3	C	10	ARG	CZ-NH1	-6.24	1.24	1.32
11	K	59	ALA	CA-CB	-6.24	1.43	1.53
1	A	220	ARG	CZ-NH1	-6.23	1.24	1.32
6	F	62	ARG	CZ-NH1	-6.23	1.24	1.32
27	f	76	ALA	CA-CB	-6.23	1.42	1.53
2	B	425	ARG	CZ-NH1	-6.22	1.24	1.32
9	I	38	ALA	CA-CB	-6.21	1.43	1.53
17	Q	189	ALA	CA-CB	-6.21	1.43	1.53
3	C	193	ARG	CZ-NH1	-6.21	1.24	1.32
29	h	35	ALA	CA-CB	-6.21	1.43	1.53
1	A	846	GLY	N-CA	-6.21	1.37	1.45
1	A	743	ARG	CZ-NH1	-6.20	1.24	1.32
2	B	1078	ARG	CZ-NH1	-6.20	1.24	1.32
3	C	113	ARG	CZ-NH1	-6.20	1.24	1.32
17	Q	666	ALA	CA-CB	-6.20	1.43	1.53
25	Z	238	ALA	CA-CB	-6.20	1.44	1.53
17	Q	234	ALA	CA-CB	-6.20	1.43	1.53
2	B	1129	ASN	CA-CB	-6.19	1.46	1.53
3	C	65	ALA	CA-CB	-6.19	1.43	1.53
26	a	88	ALA	CA-CB	-6.18	1.43	1.53
17	Q	700	ALA	CA-CB	-6.18	1.43	1.53
25	Z	198	ARG	CZ-NH1	-6.18	1.24	1.32
1	A	544	ALA	CA-CB	-6.17	1.43	1.53
2	B	434	ALA	CA-CB	-6.17	1.43	1.53
3	C	31	ALA	CA-CB	-6.17	1.43	1.53
1	A	907	ALA	CA-CB	-6.16	1.43	1.53
1	A	1033	ALA	CA-CB	-6.16	1.43	1.53
2	B	979	GLY	N-CA	-6.16	1.37	1.45
3	C	183	ALA	CA-CB	-6.16	1.42	1.53
1	A	801	GLY	N-CA	-6.15	1.38	1.45
21	V	219	ALA	CA-CB	-6.15	1.43	1.52
1	A	1070	GLY	N-CA	-6.14	1.37	1.45
2	B	971	ALA	CA-CB	-6.13	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	30	ALA	CA-CB	-6.13	1.43	1.53
1	A	1096	GLY	N-CA	-6.12	1.38	1.45
3	C	180	ALA	CA-CB	-6.12	1.43	1.53
8	H	76	ASN	CA-CB	-6.08	1.46	1.53
2	B	708	ALA	CA-CB	-6.07	1.43	1.53
17	Q	676	ALA	CA-CB	-6.07	1.43	1.53
9	I	107	ALA	CA-CB	-6.05	1.43	1.53
2	B	987	GLY	N-CA	-6.05	1.37	1.45
2	B	449	ALA	CA-CB	-6.04	1.44	1.54
10	J	15	GLY	N-CA	-6.03	1.38	1.45
1	A	829	ALA	CA-CB	-6.03	1.43	1.53
24	Y	15	ALA	CA-CB	-6.03	1.43	1.53
2	B	490	GLY	N-CA	-6.02	1.37	1.45
5	E	180	ALA	CA-CB	-6.01	1.43	1.53
2	B	366	GLY	N-CA	-6.01	1.37	1.45
13	M	587	GLY	N-CA	-6.00	1.38	1.45
17	Q	198	ALA	CA-CB	-5.99	1.43	1.53
1	A	646	GLY	N-CA	-5.99	1.37	1.45
3	C	54	ALA	CA-CB	-5.95	1.42	1.53
17	Q	688	ALA	CA-CB	-5.95	1.43	1.53
6	F	99	ALA	CA-CB	-5.93	1.42	1.53
11	K	6	ALA	CA-CB	-5.93	1.43	1.53
4	D	115	ILE	N-CA	-5.92	1.42	1.46
13	M	624	GLY	N-CA	-5.92	1.38	1.45
1	A	386	ALA	CA-CB	-5.92	1.43	1.53
1	A	1148	ALA	CA-CB	-5.92	1.43	1.53
1	A	223	GLU	C-N	5.91	1.41	1.33
1	A	131	ALA	CA-CB	-5.90	1.43	1.53
29	d	55	ALA	CA-CB	-5.88	1.43	1.53
2	B	1128	ALA	CA-CB	-5.88	1.43	1.53
2	B	512	ALA	CA-CB	-5.87	1.43	1.53
8	H	76	ASN	N-CA	-5.87	1.41	1.46
8	H	85	ALA	CA-CB	-5.87	1.43	1.53
5	E	175	ALA	CA-CB	-5.86	1.43	1.53
13	M	997	GLY	N-CA	-5.86	1.38	1.45
1	A	1171	ALA	CA-CB	-5.84	1.43	1.54
28	g	103	ALA	CA-CB	-5.83	1.43	1.53
8	H	149	ALA	CA-CB	-5.83	1.43	1.53
17	Q	808	ALA	CA-CB	-5.82	1.43	1.53
13	M	352	GLY	N-CA	-5.82	1.36	1.44
17	Q	810	ALA	CA-CB	-5.81	1.43	1.53
2	B	960	GLY	N-CA	-5.76	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	184	GLY	N-CA	-5.76	1.37	1.45
25	Z	202	ALA	CA-CB	-5.74	1.43	1.53
1	A	1446	GLY	N-CA	-5.73	1.37	1.45
2	B	579	ASP	CA-CB	-5.71	1.47	1.53
25	Z	633	GLY	N-CA	-5.70	1.37	1.45
1	A	1151	ALA	CA-CB	-5.68	1.43	1.53
3	C	174	ALA	CA-CB	-5.68	1.43	1.53
1	A	52	PRO	CA-CB	-5.67	1.46	1.53
1	A	858	GLY	N-CA	-5.67	1.37	1.45
1	A	1037	ALA	CA-CB	-5.66	1.43	1.53
2	B	189	GLY	N-CA	-5.66	1.37	1.45
2	B	997	GLY	N-CA	-5.66	1.37	1.45
2	B	496	ALA	CA-CB	-5.66	1.44	1.53
1	A	532	ARG	CD-NE	-5.65	1.38	1.46
5	E	172	ARG	CD-NE	-5.65	1.38	1.46
1	A	1425	GLY	N-CA	-5.64	1.36	1.44
2	B	852	GLY	N-CA	-5.63	1.37	1.45
9	I	26	PRO	CA-CB	-5.62	1.46	1.53
7	G	63	ARG	CD-NE	-5.61	1.38	1.46
2	B	975	ARG	CD-NE	-5.61	1.38	1.46
2	B	182	GLY	N-CA	-5.60	1.37	1.45
7	G	102	GLY	N-CA	-5.59	1.37	1.44
1	A	1375	ARG	CD-NE	-5.59	1.38	1.46
1	A	616	GLY	N-CA	-5.59	1.37	1.44
25	Z	715	GLY	N-CA	-5.59	1.37	1.44
2	B	1019	GLY	N-CA	-5.58	1.38	1.45
2	B	476	ALA	CA-CB	-5.58	1.43	1.53
2	B	322	GLY	N-CA	-5.58	1.37	1.45
5	E	200	ALA	CA-CB	-5.58	1.44	1.53
2	B	150	GLY	N-CA	-5.57	1.37	1.45
2	B	462	ALA	CA-CB	-5.57	1.44	1.53
17	Q	725	ARG	CD-NE	-5.55	1.38	1.46
25	Z	482	ALA	CA-CB	-5.55	1.44	1.53
1	A	1001	PRO	CA-CB	-5.55	1.46	1.53
1	A	932	ARG	CD-NE	-5.54	1.38	1.46
2	B	1035	ARG	CD-NE	-5.53	1.38	1.46
2	B	339	ALA	CA-CB	-5.53	1.43	1.53
26	e	132	GLY	N-CA	-5.52	1.37	1.45
2	B	1091	ARG	CD-NE	-5.51	1.38	1.46
27	b	55	ARG	CD-NE	-5.51	1.38	1.46
2	B	499	ARG	CD-NE	-5.50	1.38	1.46
21	V	28	GLY	N-CA	-5.50	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	GLY	N-CA	-5.50	1.37	1.45
6	F	62	ARG	CD-NE	-5.49	1.38	1.46
2	B	491	ARG	CD-NE	-5.48	1.38	1.46
1	A	292	ARG	CD-NE	-5.48	1.38	1.46
9	I	70	ALA	CA-CB	-5.48	1.44	1.53
25	Z	246	ARG	CD-NE	-5.48	1.38	1.46
2	B	705	GLY	N-CA	-5.47	1.37	1.45
3	C	118	ARG	CD-NE	-5.47	1.38	1.46
3	C	133	ARG	CD-NE	-5.47	1.38	1.46
14	N	105	DG	O3'-P	5.46	1.69	1.61
21	V	308	GLY	N-CA	-5.46	1.38	1.46
6	F	100	ARG	CD-NE	-5.46	1.38	1.46
8	H	61	ALA	CA-CB	-5.46	1.43	1.53
2	B	438	ARG	CD-NE	-5.46	1.38	1.46
25	Z	610	ARG	CD-NE	-5.45	1.38	1.46
2	B	822	GLY	N-CA	-5.45	1.37	1.45
9	I	15	ARG	CD-NE	-5.45	1.38	1.46
13	M	1355	ARG	CD-NE	-5.45	1.38	1.46
1	A	186	ARG	CD-NE	-5.45	1.38	1.46
1	A	523	ARG	CD-NE	-5.44	1.38	1.46
3	C	86	ARG	CD-NE	-5.43	1.38	1.46
5	E	55	ARG	CD-NE	-5.43	1.38	1.46
1	A	1046	ARG	CD-NE	-5.43	1.38	1.46
1	A	844	ARG	CD-NE	-5.43	1.38	1.46
21	V	282	ALA	CA-CB	-5.43	1.44	1.53
17	Q	679	ASP	CA-CB	-5.43	1.46	1.53
25	Z	283	ARG	CD-NE	-5.42	1.38	1.46
2	B	610	ARG	CD-NE	-5.42	1.38	1.46
8	H	84	ARG	CD-NE	-5.42	1.38	1.46
1	A	851	ALA	CA-CB	-5.42	1.44	1.53
17	Q	191	ARG	CD-NE	-5.41	1.38	1.46
1	A	1097	GLU	N-CA	-5.41	1.42	1.46
1	A	421	ARG	CD-NE	-5.41	1.38	1.46
5	E	176	GLY	N-CA	-5.41	1.37	1.45
28	g	45	ALA	CA-CB	-5.41	1.45	1.53
25	Z	634	GLY	N-CA	-5.41	1.37	1.45
1	A	407	ARG	CD-NE	-5.40	1.38	1.46
9	I	33	ARG	CD-NE	-5.39	1.38	1.46
2	B	1087	GLY	N-CA	-5.39	1.37	1.44
2	B	1131	ARG	CD-NE	-5.39	1.38	1.46
20	U	476	GLY	N-CA	-5.39	1.37	1.45
18	R	438	ARG	CD-NE	-5.38	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	608	ARG	CD-NE	-5.38	1.38	1.46
26	e	129	ARG	CD-NE	-5.38	1.38	1.46
29	h	89	ARG	CD-NE	-5.38	1.38	1.46
2	B	230	ARG	CD-NE	-5.38	1.38	1.46
2	B	1150	ARG	CD-NE	-5.38	1.38	1.46
2	B	416	ARG	CD-NE	-5.38	1.38	1.46
1	A	690	GLY	N-CA	-5.38	1.37	1.45
5	E	76	PHE	CA-CB	-5.38	1.47	1.53
1	A	1031	ARG	CD-NE	-5.38	1.38	1.46
2	B	329	GLY	N-CA	-5.37	1.38	1.45
7	G	61	PRO	CA-CB	-5.37	1.46	1.53
6	F	51	ARG	CD-NE	-5.37	1.38	1.46
8	H	3	GLY	N-CA	-5.37	1.38	1.45
11	K	63	VAL	N-CA	-5.36	1.41	1.46
24	Y	14	ARG	CD-NE	-5.36	1.38	1.46
2	B	454	GLY	N-CA	-5.36	1.38	1.45
11	K	5	PRO	CA-CB	-5.36	1.46	1.53
1	A	271	ARG	CD-NE	-5.36	1.38	1.46
1	A	1059	ARG	CD-NE	-5.36	1.38	1.46
2	B	1078	ARG	CD-NE	-5.36	1.38	1.46
1	A	401	ARG	CD-NE	-5.35	1.38	1.46
2	B	83	ARG	CD-NE	-5.35	1.38	1.46
1	A	1286	ARG	CD-NE	-5.35	1.38	1.46
8	H	49	PRO	CA-CB	-5.35	1.47	1.53
1	A	1356	ARG	CD-NE	-5.35	1.38	1.46
26	e	49	ARG	CD-NE	-5.35	1.38	1.46
2	B	938	ARG	CD-NE	-5.34	1.38	1.46
1	A	220	ARG	CD-NE	-5.34	1.38	1.46
1	A	408	ARG	CD-NE	-5.34	1.38	1.46
18	R	371	ARG	CD-NE	-5.33	1.38	1.46
4	D	121	ARG	CD-NE	-5.33	1.38	1.46
1	A	49	GLY	N-CA	-5.33	1.37	1.45
18	R	597	ARG	CD-NE	-5.33	1.38	1.46
2	B	768	ARG	CD-NE	-5.33	1.38	1.46
13	M	1033	GLY	N-CA	-5.33	1.37	1.45
4	D	73	ARG	CD-NE	-5.33	1.38	1.46
17	Q	201	ARG	CD-NE	-5.33	1.38	1.46
21	V	132	ARG	CD-NE	-5.32	1.38	1.46
26	a	128	ARG	CD-NE	-5.32	1.38	1.46
3	C	160	ARG	CD-NE	-5.32	1.38	1.46
17	Q	667	ARG	CD-NE	-5.32	1.38	1.46
5	E	166	ARG	CD-NE	-5.31	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	51	ARG	CD-NE	-5.31	1.38	1.46
27	f	67	ARG	CD-NE	-5.31	1.38	1.46
1	A	661	GLY	N-CA	-5.31	1.37	1.45
3	C	106	ARG	CD-NE	-5.30	1.38	1.46
1	A	1160	ARG	CD-NE	-5.30	1.38	1.46
2	B	38	GLY	N-CA	-5.30	1.37	1.45
2	B	459	ALA	CA-CB	-5.30	1.44	1.53
18	R	418	GLY	N-CA	-5.30	1.37	1.45
1	A	734	ARG	CD-NE	-5.30	1.38	1.46
25	Z	494	ARG	CD-NE	-5.30	1.38	1.46
29	h	83	ARG	CD-NE	-5.30	1.38	1.46
25	Z	198	ARG	CD-NE	-5.29	1.38	1.46
1	A	1449	ASP	CA-CB	-5.29	1.47	1.53
19	T	-113	DG	O3'-P	5.29	1.69	1.61
20	U	439	ARG	CD-NE	-5.29	1.38	1.46
1	A	551	ARG	CD-NE	-5.28	1.38	1.46
1	A	1423	ASP	CA-CB	-5.28	1.46	1.52
9	I	80	ARG	CD-NE	-5.28	1.38	1.46
5	E	162	ARG	CD-NE	-5.28	1.38	1.46
7	G	78	ARG	CD-NE	-5.28	1.38	1.46
5	E	195	ARG	CD-NE	-5.28	1.38	1.46
1	A	1380	ARG	CD-NE	-5.27	1.38	1.46
5	E	202	ARG	CD-NE	-5.26	1.38	1.46
2	B	493	GLY	N-CA	-5.26	1.37	1.45
5	E	24	ARG	CD-NE	-5.26	1.38	1.46
2	B	379	ARG	CD-NE	-5.26	1.38	1.46
1	A	70	ARG	CD-NE	-5.26	1.38	1.46
1	A	195	GLY	N-CA	-5.26	1.37	1.45
1	A	789	GLY	N-CA	-5.26	1.37	1.45
2	B	712	PRO	CA-CB	-5.26	1.46	1.53
26	e	128	ARG	CD-NE	-5.26	1.38	1.46
1	A	1167	ARG	CD-NE	-5.25	1.38	1.46
25	Z	754	GLY	N-CA	-5.25	1.37	1.45
2	B	770	ARG	CD-NE	-5.25	1.38	1.46
26	a	129	ARG	CD-NE	-5.25	1.38	1.46
2	B	839	GLY	N-CA	-5.25	1.37	1.45
2	B	721	ARG	CD-NE	-5.25	1.39	1.46
3	C	113	ARG	CD-NE	-5.25	1.39	1.46
8	H	57	ARG	CD-NE	-5.25	1.39	1.46
18	R	419	GLY	N-CA	-5.24	1.37	1.45
18	R	407	GLY	CA-C	-5.24	1.47	1.52
27	b	48	GLY	N-CA	-5.24	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	832	ARG	CD-NE	-5.24	1.39	1.46
1	A	805	ARG	CD-NE	-5.23	1.39	1.46
2	B	483	ARG	CD-NE	-5.23	1.39	1.46
21	V	112	ILE	N-CA	-5.23	1.42	1.46
4	D	70	ARG	CD-NE	-5.23	1.39	1.46
14	N	105	DG	C3'-O3'	5.23	1.58	1.42
1	A	743	ARG	CD-NE	-5.23	1.39	1.46
2	B	380	ARG	CD-NE	-5.23	1.39	1.46
19	T	-113	DG	C3'-O3'	5.23	1.58	1.42
2	B	396	ALA	CA-CB	-5.23	1.43	1.53
1	A	633	GLY	N-CA	-5.22	1.37	1.45
2	B	578	LYS	C-N	-5.22	1.29	1.33
5	E	201	GLY	N-CA	-5.22	1.37	1.45
20	U	411	ARG	CD-NE	-5.22	1.39	1.46
6	F	55	PRO	CA-CB	-5.22	1.46	1.53
5	E	207	ARG	CD-NE	-5.22	1.39	1.46
20	U	383	SER	CA-CB	-5.21	1.46	1.52
2	B	862	GLY	N-CA	-5.21	1.37	1.45
20	U	387	ARG	CD-NE	-5.21	1.39	1.46
1	A	1149	ARG	CD-NE	-5.21	1.39	1.46
1	A	1462	GLN	CD-NE2	-5.21	1.22	1.33
2	B	1023	ARG	CD-NE	-5.21	1.39	1.46
2	B	371	ARG	CD-NE	-5.21	1.39	1.46
13	M	874	GLY	N-CA	-5.21	1.37	1.45
28	g	35	ARG	CD-NE	-5.21	1.39	1.46
2	B	242	ARG	CD-NE	-5.20	1.39	1.46
18	R	596	ARG	CD-NE	-5.20	1.39	1.46
2	B	841	ARG	CD-NE	-5.20	1.39	1.46
8	H	120	GLY	N-CA	-5.20	1.37	1.45
20	U	409	ARG	CD-NE	-5.20	1.39	1.46
20	U	478	GLY	N-CA	-5.20	1.37	1.45
2	B	834	ARG	CD-NE	-5.20	1.39	1.46
1	A	533	PRO	CA-CB	-5.20	1.47	1.53
2	B	328	PRO	CA-CB	-5.19	1.47	1.53
17	Q	218	ARG	CD-NE	-5.19	1.39	1.46
25	Z	749	ARG	CD-NE	-5.19	1.39	1.46
5	E	181	ARG	CD-NE	-5.19	1.39	1.46
9	I	103	ARG	CD-NE	-5.19	1.39	1.46
1	A	890	ARG	CD-NE	-5.19	1.39	1.46
4	D	113	ALA	CA-CB	-5.19	1.45	1.53
7	G	79	PRO	CA-CB	-5.19	1.46	1.53
1	A	1153	ARG	CD-NE	-5.18	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	378	GLY	N-CA	-5.18	1.37	1.45
3	C	193	ARG	CD-NE	-5.18	1.39	1.46
5	E	108	GLN	C-N	-5.18	1.28	1.33
17	Q	791	ARG	CD-NE	-5.18	1.39	1.46
7	G	144	ARG	CD-NE	-5.18	1.39	1.46
28	g	44	GLY	N-CA	-5.18	1.37	1.45
1	A	1224	ARG	CD-NE	-5.18	1.39	1.46
2	B	1034	GLY	N-CA	-5.18	1.37	1.45
2	B	517	GLY	N-CA	-5.18	1.37	1.45
24	Y	91	GLY	N-CA	-5.18	1.38	1.45
24	Y	111	ARG	CD-NE	-5.18	1.39	1.46
1	A	583	ARG	CD-NE	-5.17	1.39	1.46
2	B	773	PRO	CA-CB	-5.17	1.47	1.54
2	B	754	PRO	CA-CB	-5.17	1.46	1.53
12	L	31	ARG	CD-NE	-5.17	1.39	1.46
2	B	521	GLY	N-CA	-5.17	1.37	1.45
21	V	26	ARG	CD-NE	-5.17	1.39	1.46
28	c	42	ARG	CD-NE	-5.17	1.39	1.46
27	f	101	GLY	N-CA	-5.17	1.37	1.45
2	B	538	PRO	CA-CB	-5.16	1.46	1.53
17	Q	763	ARG	CD-NE	-5.16	1.39	1.46
26	e	53	ARG	CD-NE	-5.16	1.39	1.46
27	b	95	ARG	CD-NE	-5.16	1.39	1.46
24	Y	11	ARG	CD-NE	-5.15	1.39	1.46
1	A	1093	GLN	CD-NE2	-5.15	1.22	1.33
28	g	42	ARG	CD-NE	-5.15	1.39	1.46
2	B	82	PRO	CA-CB	-5.15	1.46	1.53
3	C	10	ARG	CD-NE	-5.15	1.39	1.46
26	e	134	ARG	CD-NE	-5.14	1.39	1.46
3	C	181	GLY	N-CA	-5.14	1.38	1.45
5	E	188	GLY	N-CA	-5.14	1.38	1.45
11	K	106	ARG	CD-NE	-5.14	1.39	1.46
2	B	41	ARG	CD-NE	-5.14	1.39	1.46
1	A	433	PRO	CA-CB	-5.13	1.46	1.53
1	A	822	PHE	CA-CB	-5.13	1.46	1.52
2	B	183	GLY	N-CA	-5.13	1.37	1.45
13	M	1135	LYS	N-CA	-5.13	1.39	1.46
1	A	150	GLY	N-CA	-5.13	1.38	1.45
2	B	757	PRO	CA-CB	-5.13	1.46	1.53
5	E	109	GLY	CA-C	-5.12	1.47	1.52
1	A	880	ARG	CD-NE	-5.12	1.39	1.46
10	J	64	PRO	CA-CB	-5.11	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	619	GLY	N-CA	-5.11	1.37	1.45
7	G	120	ASP	CA-CB	-5.11	1.47	1.53
2	B	729	GLY	N-CA	-5.10	1.37	1.45
1	A	184	CYS	CA-CB	-5.10	1.46	1.52
1	A	1345	ARG	CD-NE	-5.10	1.39	1.46
2	B	253	GLY	N-CA	-5.09	1.38	1.45
7	G	1	MET	N-CA	-5.09	1.38	1.49
1	A	185	GLY	N-CA	-5.09	1.38	1.45
9	I	76	PRO	CA-CB	-5.09	1.46	1.53
17	Q	830	ARG	CD-NE	-5.09	1.39	1.46
2	B	1007	ASN	CA-CB	-5.09	1.47	1.53
1	A	532	ARG	CA-CB	-5.09	1.47	1.54
2	B	282	ARG	CD-NE	-5.09	1.39	1.46
2	B	1104	ARG	CD-NE	-5.09	1.39	1.46
6	F	57	MET	CA-CB	-5.08	1.46	1.53
25	Z	241	GLY	N-CA	-5.08	1.38	1.45
5	E	146	PRO	CA-CB	-5.08	1.46	1.53
9	I	40	ARG	CD-NE	-5.08	1.39	1.46
2	B	425	ARG	CD-NE	-5.07	1.39	1.46
3	C	228	ARG	CD-NE	-5.07	1.39	1.46
1	A	1145	GLY	N-CA	-5.07	1.38	1.45
28	c	77	ARG	CD-NE	-5.07	1.39	1.46
13	M	1055	GLY	N-CA	-5.06	1.38	1.45
11	K	43	GLY	N-CA	-5.06	1.38	1.45
1	A	61	ARG	CD-NE	-5.06	1.39	1.46
4	D	114	LEU	C-N	-5.05	1.29	1.33
9	I	102	ALA	CA-CB	-5.05	1.45	1.53
2	B	515	PRO	CA-CB	-5.05	1.47	1.53
2	B	452	ASN	CA-CB	-5.04	1.46	1.53
1	A	443	GLY	N-CA	-5.04	1.38	1.45
4	D	138	ARG	CD-NE	-5.04	1.39	1.46
2	B	1024	GLY	N-CA	-5.04	1.37	1.45
8	H	77	PRO	CA-CB	-5.04	1.46	1.53
17	Q	711	PHE	CA-CB	-5.04	1.46	1.52
2	B	511	PRO	CA-CB	-5.03	1.46	1.53
7	G	125	PRO	CA-CB	-5.03	1.47	1.54
2	B	136	GLY	N-CA	-5.03	1.37	1.45
2	B	772	LEU	CA-CB	-5.03	1.47	1.53
1	A	1218	ARG	CD-NE	-5.03	1.39	1.46
3	C	156	GLY	N-CA	-5.03	1.38	1.45
24	Y	86	ALA	CA-CB	-5.03	1.44	1.53
1	A	617	PRO	CA-CB	-5.02	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	609	GLY	N-CA	-5.02	1.38	1.45
2	B	261	PRO	CA-CB	-5.02	1.47	1.53
2	B	717	ASN	CG-ND2	-5.01	1.22	1.33
1	A	186	ARG	C-N	-5.01	1.25	1.33
2	B	571	GLY	N-CA	-5.00	1.37	1.45
13	M	1238	GLY	N-CA	-5.00	1.38	1.45
25	Z	423	GLY	N-CA	-5.00	1.38	1.45

All (1951) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	107	DC	OP1-P-O3'	-34.40	4.81	108.00
14	N	85	DG	OP1-P-O3'	-34.14	5.57	108.00
19	T	-71	DG	OP1-P-O3'	-34.14	5.57	108.00
14	N	86	DT	OP1-P-O3'	-34.14	5.58	108.00
19	T	-133	DG	OP1-P-O3'	-34.12	5.63	108.00
14	N	15	DC	OP1-P-O3'	-33.92	6.25	108.00
14	N	139	DT	OP1-P-O3'	-33.76	6.73	108.00
19	T	-110	DG	OP1-P-O3'	-33.50	7.49	108.00
14	N	138	DA	OP1-P-O3'	-33.09	8.72	108.00
19	T	-113	DG	O3'-P-O5'	29.98	148.98	104.00
14	N	105	DG	O3'-P-O5'	26.07	143.11	104.00
14	N	56	DT	O3'-P-O5'	19.41	133.12	104.00
13	M	1358	SER	N-CA-C	19.01	137.62	114.04
14	N	105	DG	OP1-P-O3'	-18.11	53.68	108.00
19	T	-113	DG	OP1-P-O3'	-17.58	55.27	108.00
14	N	105	DG	OP2-P-O3'	-15.75	60.75	108.00
1	A	218	PRO	CB-CA-C	-15.55	89.80	112.04
19	T	-113	DG	OP2-P-O3'	-14.67	63.99	108.00
13	M	1329	HIS	C-N-CD	-14.16	66.96	125.00
1	A	220	ARG	N-CA-C	-13.38	94.70	111.02
1	A	220	ARG	N-CA-CB	13.27	129.99	109.82
1	A	225	PHE	O-C-N	-13.02	108.32	122.12
5	E	129	GLN	CA-C-N	12.14	141.15	122.94
5	E	129	GLN	C-N-CA	12.14	141.15	122.94
5	E	103	LEU	CA-C-N	11.88	137.68	122.95
5	E	103	LEU	C-N-CA	11.88	137.68	122.95
13	M	1358	SER	O-C-N	11.87	136.50	122.25
1	A	225	PHE	CA-C-N	11.52	136.16	120.38
1	A	225	PHE	C-N-CA	11.52	136.16	120.38
13	M	1360	GLY	N-CA-C	11.12	139.54	113.18
1	A	729	PRO	N-CA-CB	-10.99	91.71	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	222	ARG	CA-C-N	10.84	129.02	121.65
21	V	222	ARG	C-N-CA	10.84	129.02	121.65
2	B	495	LEU	O-C-N	-10.66	109.82	122.93
5	E	129	GLN	O-C-N	-10.63	109.71	123.21
1	A	219	GLU	CA-C-N	10.56	135.47	120.79
1	A	219	GLU	C-N-CA	10.56	135.47	120.79
1	A	216	LEU	O-C-N	-10.02	110.33	122.96
1	A	186	ARG	O-C-N	-9.87	109.46	122.59
14	N	56	DT	OP1-P-O3'	-9.84	78.47	108.00
18	R	591	MET	CA-C-N	9.68	130.58	119.83
18	R	591	MET	C-N-CA	9.68	130.58	119.83
1	A	186	ARG	CA-C-N	9.64	138.47	122.76
1	A	186	ARG	C-N-CA	9.64	138.47	122.76
13	M	663	GLY	O-C-N	-9.36	110.54	122.70
1	A	75	ALA	CA-C-N	9.24	128.73	121.61
1	A	75	ALA	C-N-CA	9.24	128.73	121.61
14	N	105	DG	P-O3'-C3'	9.20	134.01	120.20
21	V	25	GLU	CA-C-N	9.14	132.88	120.54
21	V	25	GLU	C-N-CA	9.14	132.88	120.54
21	V	309	ASP	CA-C-N	9.14	128.49	122.18
21	V	309	ASP	C-N-CA	9.14	128.49	122.18
1	A	1192	TRP	CA-C-N	9.05	135.86	120.29
1	A	1192	TRP	C-N-CA	9.05	135.86	120.29
19	T	-113	DG	P-O3'-C3'	8.96	133.64	120.20
13	M	1359	LYS	CA-C-N	8.86	138.78	121.41
13	M	1359	LYS	C-N-CA	8.86	138.78	121.41
2	B	495	LEU	CA-C-N	8.83	137.76	121.52
2	B	495	LEU	C-N-CA	8.83	137.76	121.52
14	N	57	DT	O5'-P-OP2	-8.72	81.84	108.00
1	A	216	LEU	CA-C-N	8.70	137.46	120.94
1	A	216	LEU	C-N-CA	8.70	137.46	120.94
21	V	87	ILE	CA-C-N	8.66	130.37	120.06
21	V	87	ILE	C-N-CA	8.66	130.37	120.06
5	E	122	ALA	O-C-N	-8.62	111.41	121.32
14	N	56	DT	OP2-P-O3'	-8.61	82.17	108.00
18	R	406	THR	CA-C-N	8.60	129.04	121.82
18	R	406	THR	C-N-CA	8.60	129.04	121.82
3	C	63	PHE	CA-CB-CG	8.58	122.38	113.80
1	A	218	PRO	O-C-N	8.56	133.40	122.44
1	A	535	MET	CA-C-N	8.55	129.78	122.17
1	A	535	MET	C-N-CA	8.55	129.78	122.17
14	N	57	DT	O5'-P-OP1	-8.53	83.40	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	103	LEU	O-C-N	-8.52	112.70	123.26
1	A	282	ASP	CB-CA-C	8.47	127.27	110.42
5	E	104	ILE	CA-C-N	8.44	129.59	121.65
5	E	104	ILE	C-N-CA	8.44	129.59	121.65
2	B	568	PHE	CA-CB-CG	8.09	121.89	113.80
5	E	122	ALA	CA-C-N	8.05	129.91	119.84
5	E	122	ALA	C-N-CA	8.05	129.91	119.84
1	A	113	PHE	CA-CB-CG	7.96	121.76	113.80
2	B	575	GLY	N-CA-C	7.94	120.10	112.08
1	A	1354	PRO	CA-C-N	7.87	130.30	122.66
1	A	1354	PRO	C-N-CA	7.87	130.30	122.66
3	C	61	ASP	CA-CB-CG	7.81	120.41	112.60
1	A	218	PRO	N-CA-C	7.81	127.44	113.70
7	G	132	ASP	CA-CB-CG	7.78	120.38	112.60
2	B	829	PHE	CA-CB-CG	7.75	121.56	113.80
1	A	1351	ASP	CA-CB-CG	7.73	120.33	112.60
1	A	99	PHE	CA-CB-CG	7.68	121.48	113.80
26	e	123	ASP	CA-C-N	7.67	130.50	120.60
26	e	123	ASP	C-N-CA	7.67	130.50	120.60
2	B	292	PHE	CA-CB-CG	7.66	121.46	113.80
13	M	327	THR	C-N-CD	-7.65	93.62	125.00
2	B	1142	ASN	CA-CB-CG	7.59	120.19	112.60
1	A	800	PHE	CA-CB-CG	7.58	121.38	113.80
13	M	1406	ASP	CA-CB-CG	7.58	120.17	112.60
17	Q	772	GLU	CA-C-N	7.56	135.31	121.70
17	Q	772	GLU	C-N-CA	7.56	135.31	121.70
6	F	127	ASP	CA-CB-CG	7.56	120.16	112.60
9	I	11	PHE	CA-CB-CG	7.55	121.35	113.80
3	C	190	ASN	CA-CB-CG	7.53	120.13	112.60
21	V	85	ASP	CA-CB-CG	7.53	120.13	112.60
17	Q	714	HIS	CA-CB-CG	7.53	121.33	113.80
11	K	53	ASP	CA-CB-CG	7.52	120.12	112.60
20	U	398	PHE	CA-CB-CG	7.50	121.30	113.80
1	A	95	PHE	CA-CB-CG	7.50	121.30	113.80
1	A	1461	GLY	CA-C-N	7.50	132.71	120.94
1	A	1461	GLY	C-N-CA	7.50	132.71	120.94
26	e	52	ARG	CA-C-N	7.49	130.18	120.44
26	e	52	ARG	C-N-CA	7.49	130.18	120.44
18	R	377	PHE	CA-CB-CG	7.47	121.27	113.80
1	A	1194	ASN	CA-CB-CG	7.42	120.02	112.60
2	B	422	PHE	CA-CB-CG	7.42	121.22	113.80
25	Z	494	ARG	CA-C-N	7.41	130.74	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	494	ARG	C-N-CA	7.41	130.74	122.59
25	Z	517	ASP	N-CA-C	-7.39	104.24	113.18
20	U	380	ASN	CA-CB-CG	7.38	119.98	112.60
24	Y	28	PHE	CA-CB-CG	7.37	121.17	113.80
29	d	48	ASP	CA-CB-CG	7.35	119.95	112.60
7	G	158	PHE	CA-CB-CG	7.33	121.13	113.80
2	B	525	ASN	CA-CB-CG	7.31	119.91	112.60
2	B	842	HIS	CA-CB-CG	7.29	121.09	113.80
1	A	225	PHE	CA-CB-CG	7.29	121.09	113.80
1	A	905	ASN	CA-CB-CG	7.29	119.89	112.60
17	Q	208	PHE	CA-CB-CG	7.28	121.08	113.80
2	B	797	ASN	CA-CB-CG	7.27	119.87	112.60
13	M	786	PHE	N-CA-C	7.26	114.73	108.78
9	I	52	CYS	CA-C-N	7.26	130.09	122.97
9	I	52	CYS	C-N-CA	7.26	130.09	122.97
25	Z	492	ILE	CA-C-N	7.25	130.03	121.84
25	Z	492	ILE	C-N-CA	7.25	130.03	121.84
5	E	142	HIS	CA-CB-CG	7.25	121.05	113.80
1	A	974	ASP	CA-CB-CG	7.24	119.84	112.60
1	A	1042	ASN	CA-CB-CG	7.24	119.84	112.60
25	Z	503	PHE	CA-CB-CG	7.23	121.03	113.80
18	R	564	ASN	CA-CB-CG	7.22	119.83	112.60
2	B	606	ASP	CA-CB-CG	7.22	119.82	112.60
1	A	428	ASP	CA-CB-CG	7.20	119.80	112.60
17	Q	670	PHE	CA-CB-CG	7.19	120.99	113.80
11	K	87	PHE	CA-CB-CG	7.18	120.98	113.80
29	h	79	HIS	CA-CB-CG	7.17	120.97	113.80
22	W	87	HIS	CA-CB-CG	7.17	120.97	113.80
10	J	54	ASP	CA-CB-CG	7.17	119.77	112.60
17	Q	835	ASP	CA-CB-CG	7.16	119.76	112.60
1	A	1178	ASP	CA-CB-CG	7.15	119.75	112.60
7	G	9	HIS	CA-CB-CG	7.15	120.95	113.80
4	D	93	HIS	CA-CB-CG	7.15	120.95	113.80
2	B	442	ASP	CA-CB-CG	7.15	119.75	112.60
26	a	104	PHE	CA-CB-CG	7.12	120.92	113.80
2	B	570	ASN	CA-CB-CG	7.12	119.72	112.60
5	E	130	PHE	CA-CB-CG	7.12	120.92	113.80
25	Z	444	ASP	CA-CB-CG	7.11	119.71	112.60
9	I	60	HIS	CA-CB-CG	7.11	120.91	113.80
13	M	1176	HIS	N-CA-C	7.11	130.90	111.00
17	Q	728	PHE	CA-CB-CG	7.11	120.91	113.80
1	A	272	ASN	CA-CB-CG	7.09	119.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	13	PHE	CA-CB-CG	7.08	120.88	113.80
17	Q	221	PHE	CA-CB-CG	7.08	120.88	113.80
28	g	31	HIS	CA-CB-CG	7.07	120.87	113.80
1	A	77	ASN	CA-CB-CG	7.07	119.67	112.60
1	A	256	PRO	N-CA-CB	7.07	107.15	103.19
13	M	1379	ASP	CA-CB-CG	7.07	119.67	112.60
2	B	45	ASP	CA-CB-CG	7.05	119.65	112.60
25	Z	517	ASP	N-CA-CB	7.05	122.26	110.41
3	C	184	PHE	CA-CB-CG	7.04	120.84	113.80
2	B	502	HIS	CA-CB-CG	7.04	120.83	113.80
2	B	863	ASP	CA-CB-CG	7.04	119.64	112.60
25	Z	456	ASP	CA-CB-CG	7.03	119.63	112.60
1	A	1250	ASP	CA-CB-CG	7.02	119.62	112.60
1	A	1177	TYR	CB-CA-C	7.02	121.35	111.74
2	B	792	ASP	CA-CB-CG	7.02	119.62	112.60
25	Z	502	LEU	CA-C-N	7.02	131.96	122.84
25	Z	502	LEU	C-N-CA	7.02	131.96	122.84
2	B	895	PHE	CA-CB-CG	7.02	120.82	113.80
26	e	81	ASP	CA-CB-CG	7.01	119.61	112.60
3	C	147	ASP	CA-CB-CG	7.00	119.60	112.60
3	C	110	ASP	CA-CB-CG	7.00	119.60	112.60
25	Z	499	PHE	CA-CB-CG	7.00	120.80	113.80
1	A	1248	ASN	CA-CB-CG	6.98	119.58	112.60
2	B	769	PHE	CA-CB-CG	6.97	120.77	113.80
17	Q	756	ASN	CA-CB-CG	6.96	119.56	112.60
2	B	591	ARG	NE-CZ-NH2	6.95	125.46	119.20
2	B	471	ASN	CA-CB-CG	6.95	119.55	112.60
2	B	383	ASP	CA-CB-CG	6.95	119.55	112.60
26	a	63	ARG	N-CA-C	6.94	120.44	110.10
1	A	437	ASP	CA-CB-CG	6.94	119.54	112.60
4	D	114	LEU	CA-C-N	6.93	130.75	122.85
4	D	114	LEU	C-N-CA	6.93	130.75	122.85
9	I	71	ASP	CA-CB-CG	6.93	119.53	112.60
7	G	119	PHE	CA-C-N	6.93	130.47	122.85
7	G	119	PHE	C-N-CA	6.93	130.47	122.85
24	Y	86	ALA	CA-C-N	6.93	130.09	121.85
24	Y	86	ALA	C-N-CA	6.93	130.09	121.85
25	Z	517	ASP	CA-CB-CG	6.93	119.53	112.60
26	a	101	VAL	CA-C-N	6.93	129.89	120.54
26	a	101	VAL	C-N-CA	6.93	129.89	120.54
3	C	99	VAL	CA-C-N	6.92	131.95	122.19
3	C	99	VAL	C-N-CA	6.92	131.95	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	378	PHE	CA-CB-CG	6.92	120.72	113.80
18	R	484	ASN	CA-CB-CG	6.92	119.52	112.60
24	Y	9	ASP	CA-CB-CG	6.92	119.52	112.60
9	I	29	ASP	CA-CB-CG	6.90	119.50	112.60
13	M	1402	PHE	CA-CB-CG	6.90	120.70	113.80
1	A	678	ASN	CA-CB-CG	6.89	119.50	112.60
2	B	717	ASN	CA-CB-CG	6.89	119.49	112.60
6	F	51	ARG	CA-C-N	6.89	130.84	122.16
6	F	51	ARG	C-N-CA	6.89	130.84	122.16
29	d	60	ASN	CA-CB-CG	6.88	119.48	112.60
1	A	765	ASN	CA-CB-CG	6.88	119.48	112.60
2	B	117	ASN	CA-CB-CG	6.88	119.48	112.60
1	A	1036	ASN	CA-CB-CG	6.88	119.47	112.60
3	C	194	HIS	CA-CB-CG	6.87	120.67	113.80
16	P	36	U	C2'-C3'-O3'	6.87	119.81	109.50
5	E	148	HIS	CA-CB-CG	6.87	120.67	113.80
2	B	492	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	1353	ASP	CA-CB-CG	6.87	119.47	112.60
9	I	75	ASP	CA-CB-CG	6.87	119.47	112.60
2	B	34	PHE	CA-CB-CG	6.86	120.66	113.80
1	A	985	ARG	NE-CZ-NH2	6.86	125.38	119.20
1	A	1403	ASP	CA-CB-CG	6.86	119.46	112.60
7	G	136	VAL	CA-C-N	6.86	131.23	122.93
7	G	136	VAL	C-N-CA	6.86	131.23	122.93
9	I	22	ASN	CA-CB-CG	6.86	119.46	112.60
7	G	2	PHE	CA-CB-CG	6.85	120.65	113.80
3	C	146	ASP	CA-CB-CG	6.85	119.45	112.60
1	A	1223	ASP	CA-CB-CG	6.85	119.45	112.60
1	A	739	ASN	CA-CB-CG	6.84	119.44	112.60
2	B	453	TRP	CA-C-N	6.84	128.85	120.51
2	B	453	TRP	C-N-CA	6.84	128.85	120.51
3	C	36	ARG	NE-CZ-NH2	6.83	125.35	119.20
24	Y	68	ASP	CA-CB-CG	6.83	119.43	112.60
2	B	508	MET	CA-C-N	6.83	132.09	123.14
2	B	508	MET	C-N-CA	6.83	132.09	123.14
8	H	79	ASP	CA-CB-CG	6.83	119.43	112.60
13	M	1362	ASN	CA-CB-CG	6.82	119.42	112.60
4	D	26	PHE	CA-CB-CG	6.82	120.62	113.80
3	C	114	HIS	CA-CB-CG	6.82	120.62	113.80
9	I	56	ASN	CA-CB-CG	6.82	119.42	112.60
2	B	410	ASN	CA-CB-CG	6.82	119.42	112.60
7	G	111	HIS	CA-CB-CG	6.81	120.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1358	SER	CA-C-N	6.81	133.50	122.81
13	M	1358	SER	C-N-CA	6.81	133.50	122.81
17	Q	162	ASN	CA-CB-CG	6.81	119.41	112.60
1	A	288	ASN	CA-CB-CG	6.80	119.40	112.60
9	I	50	ASN	CA-CB-CG	6.80	119.40	112.60
29	h	81	ASN	CA-CB-CG	6.79	119.39	112.60
3	C	104	ASP	CA-CB-CG	6.78	119.38	112.60
21	V	90	ASP	CA-CB-CG	6.78	119.38	112.60
22	W	103	ASP	CA-CB-CG	6.78	119.38	112.60
24	Y	12	HIS	CA-CB-CG	6.77	120.57	113.80
24	Y	112	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	814	ASP	CA-CB-CG	6.76	119.36	112.60
7	G	165	ASP	CA-CB-CG	6.76	119.36	112.60
2	B	428	ASP	CA-CB-CG	6.75	119.35	112.60
3	C	112	THR	CA-C-N	6.75	131.75	122.77
3	C	112	THR	C-N-CA	6.75	131.75	122.77
19	T	-84	DG	O3'-P-O5'	6.75	114.13	104.00
1	A	1077	ASN	CA-CB-CG	6.75	119.35	112.60
1	A	1172	ASN	CA-CB-CG	6.75	119.34	112.60
1	A	387	ASN	CA-CB-CG	6.74	119.34	112.60
17	Q	711	PHE	CA-CB-CG	6.74	120.54	113.80
5	E	75	PHE	CA-CB-CG	6.74	120.54	113.80
8	H	47	ILE	CA-C-N	6.74	129.88	122.74
8	H	47	ILE	C-N-CA	6.74	129.88	122.74
5	E	2	ASP	CA-CB-CG	6.72	119.32	112.60
20	U	498	SER	N-CA-C	6.72	119.37	109.69
5	E	138	ASN	CA-CB-CG	6.72	119.32	112.60
2	B	310	VAL	CA-C-N	6.71	131.72	122.93
2	B	310	VAL	C-N-CA	6.71	131.72	122.93
26	e	77	ASP	CA-CB-CG	6.71	119.31	112.60
2	B	188	ASN	CA-CB-CG	6.71	119.31	112.60
27	f	64	ASN	CA-CB-CG	6.71	119.31	112.60
1	A	997	ASN	CA-CB-CG	6.71	119.31	112.60
1	A	876	ASP	CA-CB-CG	6.71	119.31	112.60
1	A	1163	HIS	CA-CB-CG	6.71	120.51	113.80
5	E	120	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	1220	HIS	CA-CB-CG	6.69	120.49	113.80
2	B	287	HIS	CA-CB-CG	6.69	120.49	113.80
3	C	232	ASN	CA-CB-CG	6.69	119.29	112.60
2	B	552	ASN	CA-CB-CG	6.69	119.29	112.60
21	V	86	LEU	CA-C-N	6.68	130.23	122.35
21	V	86	LEU	C-N-CA	6.68	130.23	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	44	ASN	CA-CB-CG	6.68	119.28	112.60
1	A	663	ASP	CA-CB-CG	6.68	119.28	112.60
1	A	1249	ASP	CA-CB-CG	6.67	119.28	112.60
2	B	178	PRO	CA-C-N	6.67	132.82	121.14
2	B	178	PRO	C-N-CA	6.67	132.82	121.14
1	A	410	ASN	CA-CB-CG	6.66	119.26	112.60
2	B	585	ASN	CA-CB-CG	6.66	119.26	112.60
25	Z	757	ARG	C-N-CD	-6.66	97.71	125.00
11	K	22	ASN	CA-CB-CG	6.65	119.25	112.60
17	Q	228	ASN	CA-CB-CG	6.64	119.25	112.60
1	A	970	PHE	CA-CB-CG	6.64	120.44	113.80
2	B	1021	HIS	CA-CB-CG	6.64	120.44	113.80
17	Q	775	ASN	CA-CB-CG	6.64	119.24	112.60
2	B	1025	ASN	CA-CB-CG	6.64	119.24	112.60
26	e	78	PHE	CA-CB-CG	6.63	120.43	113.80
17	Q	651	ASN	CA-CB-CG	6.63	119.23	112.60
1	A	397	PHE	CA-CB-CG	6.63	120.43	113.80
18	R	437	PHE	CA-CB-CG	6.62	120.42	113.80
25	Z	424	ASP	CA-CB-CG	6.62	119.22	112.60
3	C	108	ASN	CA-CB-CG	6.62	119.22	112.60
20	U	390	ASP	CA-CB-CG	6.62	119.22	112.60
8	H	54	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	1024	ASN	CA-CB-CG	6.61	119.21	112.60
1	A	813	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	1281	ASP	CA-CB-CG	6.60	119.20	112.60
2	B	577	HIS	CA-CB-CG	6.59	120.39	113.80
20	U	396	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	1284	PHE	CA-CB-CG	6.59	120.39	113.80
2	B	541	ILE	CA-C-N	6.59	129.11	120.28
2	B	541	ILE	C-N-CA	6.59	129.11	120.28
2	B	847	LYS	CA-C-N	6.59	132.46	122.65
2	B	847	LYS	C-N-CA	6.59	132.46	122.65
11	K	44	ASN	CA-CB-CG	6.58	119.19	112.60
2	B	824	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	989	ASN	CA-CB-CG	6.58	119.18	112.60
11	K	62	LYS	CA-C-N	6.57	130.48	123.25
11	K	62	LYS	C-N-CA	6.57	130.48	123.25
9	I	77	THR	CA-C-N	6.57	131.36	122.56
9	I	77	THR	C-N-CA	6.57	131.36	122.56
28	c	110	ASN	CA-CB-CG	6.56	119.16	112.60
27	b	64	ASN	CA-CB-CG	6.56	119.16	112.60
2	B	47	PHE	CA-CB-CG	6.56	120.36	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	866	ILE	CA-C-N	6.56	132.02	123.10
2	B	866	ILE	C-N-CA	6.56	132.02	123.10
2	B	1129	ASN	CA-CB-CG	6.55	119.15	112.60
2	B	1026	GLU	CA-C-N	6.55	131.07	122.95
2	B	1026	GLU	C-N-CA	6.55	131.07	122.95
1	A	1217	ASP	CA-CB-CG	6.54	119.14	112.60
25	Z	459	ASP	CA-C-N	6.54	131.34	122.84
25	Z	459	ASP	C-N-CA	6.54	131.34	122.84
4	D	34	ASN	CA-CB-CG	6.54	119.14	112.60
6	F	88	ASP	CA-CB-CG	6.53	119.13	112.60
27	b	100	PHE	CA-CB-CG	6.53	120.33	113.80
3	C	48	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	592	PHE	CA-CB-CG	6.52	120.32	113.80
28	c	73	ASN	CA-CB-CG	6.51	119.11	112.60
2	B	455	ASP	CA-CB-CG	6.50	119.10	112.60
11	K	29	ASN	CA-CB-CG	6.50	119.10	112.60
11	K	36	ASN	CA-CB-CG	6.50	119.10	112.60
5	E	183	PHE	CA-CB-CG	6.50	120.30	113.80
1	A	704	ASN	CA-CB-CG	6.49	119.09	112.60
17	Q	686	ASN	CA-CB-CG	6.49	119.09	112.60
2	B	1077	GLY	CA-C-N	6.49	129.50	120.29
2	B	1077	GLY	C-N-CA	6.49	129.50	120.29
2	B	975	ARG	CD-NE-CZ	6.49	133.48	124.40
1	A	59	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	875	TYR	CA-C-N	6.47	131.06	120.63
1	A	875	TYR	C-N-CA	6.47	131.06	120.63
9	I	41	ASN	CA-CB-CG	6.47	119.07	112.60
5	E	168	ASN	CA-CB-CG	6.47	119.07	112.60
1	A	742	ASN	CA-CB-CG	6.47	119.07	112.60
1	A	562	ASN	CA-CB-CG	6.46	119.06	112.60
1	A	1315	ASP	CA-CB-CG	6.46	119.06	112.60
3	C	62	GLU	CA-C-N	6.46	128.94	120.28
3	C	62	GLU	C-N-CA	6.46	128.94	120.28
1	A	747	ASP	CA-CB-CG	6.46	119.06	112.60
2	B	575	GLY	CA-C-N	6.46	132.01	122.71
2	B	575	GLY	C-N-CA	6.46	132.01	122.71
6	F	117	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	837	PHE	CA-CB-CG	6.46	120.25	113.80
3	C	198	PRO	CA-C-N	6.45	130.35	122.42
3	C	198	PRO	C-N-CA	6.45	130.35	122.42
17	Q	161	ASN	CA-CB-CG	6.44	119.04	112.60
1	A	1044	HIS	CA-CB-CG	6.44	120.24	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	T	-105	DC	P-O3'-C3'	6.44	129.86	120.20
2	B	48	ASP	CA-CB-CG	6.43	119.03	112.60
2	B	578	LYS	CA-C-N	6.43	129.98	122.52
2	B	578	LYS	C-N-CA	6.43	129.98	122.52
17	Q	731	GLY	N-CA-C	6.43	121.74	114.67
1	A	554	PHE	CA-CB-CG	6.42	120.22	113.80
8	H	88	PHE	CA-CB-CG	6.42	120.22	113.80
1	A	425	ASP	CA-CB-CG	6.41	119.01	112.60
3	C	265	HIS	CA-CB-CG	6.41	120.21	113.80
1	A	548	PHE	CA-CB-CG	6.41	120.20	113.80
2	B	350	HIS	CA-CB-CG	6.40	120.20	113.80
8	H	86	ASP	CA-CB-CG	6.40	119.00	112.60
18	R	407	GLY	CA-C-N	6.40	130.89	122.95
18	R	407	GLY	C-N-CA	6.40	130.89	122.95
25	Z	625	HIS	CA-CB-CG	6.39	120.19	113.80
25	Z	472	PHE	CA-CB-CG	6.39	120.19	113.80
2	B	1108	PHE	CA-CB-CG	6.39	120.19	113.80
9	I	16	PHE	CA-CB-CG	6.39	120.19	113.80
17	Q	679	ASP	CA-CB-CG	6.39	118.99	112.60
2	B	771	GLU	CA-C-N	6.39	130.88	123.15
2	B	771	GLU	C-N-CA	6.39	130.88	123.15
5	E	76	PHE	CA-CB-CG	6.39	120.19	113.80
17	Q	755	PHE	CA-CB-CG	6.39	120.19	113.80
2	B	713	PHE	CA-CB-CG	6.38	120.18	113.80
17	Q	689	HIS	CA-CB-CG	6.38	120.19	113.80
1	A	96	HIS	CA-CB-CG	6.38	120.18	113.80
3	C	258	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	746	ASN	CA-CB-CG	6.37	118.97	112.60
1	A	1449	ASP	CA-CB-CG	6.37	118.97	112.60
2	B	1017	ASP	CA-CB-CG	6.37	118.97	112.60
2	B	891	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	712	ASP	CA-CB-CG	6.35	118.95	112.60
2	B	424	ASP	CA-CB-CG	6.35	118.95	112.60
2	B	278	PHE	CA-CB-CG	6.35	120.15	113.80
2	B	1117	HIS	CA-CB-CG	6.34	120.14	113.80
9	I	32	ASN	CA-CB-CG	6.34	118.94	112.60
2	B	475	PHE	CA-CB-CG	6.34	120.14	113.80
3	C	193	ARG	CD-NE-CZ	6.34	133.27	124.40
1	A	68	THR	CA-C-N	6.33	129.53	122.69
1	A	68	THR	C-N-CA	6.33	129.53	122.69
1	A	63	GLY	CA-C-N	6.33	129.99	120.75
1	A	63	GLY	C-N-CA	6.33	129.99	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	f	56	GLY	CA-C-N	6.33	129.06	120.77
27	f	56	GLY	C-N-CA	6.33	129.06	120.77
2	B	939	HIS	CA-CB-CG	6.32	120.12	113.80
3	C	187	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	282	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	825	ASN	CA-CB-CG	6.32	118.92	112.60
17	Q	218	ARG	CD-NE-CZ	6.32	133.24	124.40
1	A	1058	PHE	CA-CB-CG	6.31	120.11	113.80
24	Y	83	GLY	N-CA-C	6.31	119.38	110.74
2	B	940	GLY	CA-C-N	6.30	131.24	122.79
2	B	940	GLY	C-N-CA	6.30	131.24	122.79
1	A	838	PHE	CA-CB-CG	6.29	120.09	113.80
1	A	804	HIS	CA-CB-CG	6.28	120.08	113.80
3	C	130	VAL	CA-C-N	6.28	131.59	121.98
3	C	130	VAL	C-N-CA	6.28	131.59	121.98
25	Z	381	VAL	CA-C-N	6.28	130.33	122.48
25	Z	381	VAL	C-N-CA	6.28	130.33	122.48
1	A	849	ASP	CA-CB-CG	6.28	118.88	112.60
24	Y	82	PRO	CA-C-N	6.28	129.07	120.72
24	Y	82	PRO	C-N-CA	6.28	129.07	120.72
1	A	276	LEU	CA-C-N	6.27	128.69	120.28
1	A	276	LEU	C-N-CA	6.27	128.69	120.28
20	U	483	ALA	CA-C-N	6.27	130.32	121.66
20	U	483	ALA	C-N-CA	6.27	130.32	121.66
1	A	218	PRO	CA-C-N	6.27	132.43	121.52
1	A	218	PRO	C-N-CA	6.27	132.43	121.52
2	B	189	GLY	CA-C-N	6.27	131.83	122.99
2	B	189	GLY	C-N-CA	6.27	131.83	122.99
25	Z	234	HIS	CA-CB-CG	6.26	120.06	113.80
18	R	488	ASN	CA-CB-CG	6.26	118.86	112.60
2	B	283	ASP	CA-CB-CG	6.25	118.85	112.60
5	E	105	VAL	N-CA-C	6.25	112.89	106.21
19	T	-113	DG	C2'-C3'-O3'	6.25	120.87	111.50
2	B	641	ASP	CA-CB-CG	6.24	118.84	112.60
11	K	71	ILE	CA-C-N	6.24	131.32	123.14
11	K	71	ILE	C-N-CA	6.24	131.32	123.14
29	h	48	ASP	CA-CB-CG	6.24	118.84	112.60
27	b	56	GLY	CA-C-N	6.24	128.42	120.56
27	b	56	GLY	C-N-CA	6.24	128.42	120.56
1	A	284	VAL	CA-C-N	6.24	128.64	120.28
1	A	284	VAL	C-N-CA	6.24	128.64	120.28
1	A	790	GLN	CA-C-N	6.23	130.71	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	790	GLN	C-N-CA	6.23	130.71	122.42
6	F	123	LEU	CA-C-N	6.23	130.28	122.43
6	F	123	LEU	C-N-CA	6.23	130.28	122.43
7	G	151	ARG	CA-C-N	6.23	130.78	122.93
7	G	151	ARG	C-N-CA	6.23	130.78	122.93
2	B	722	ASN	CA-CB-CG	6.23	118.83	112.60
2	B	711	ILE	N-CA-CB	6.22	115.87	110.08
27	b	61	PHE	CA-CB-CG	6.22	120.02	113.80
8	H	147	LYS	CA-C-N	6.22	130.70	122.42
8	H	147	LYS	C-N-CA	6.22	130.70	122.42
3	C	151	VAL	CA-C-N	6.22	131.77	123.00
3	C	151	VAL	C-N-CA	6.22	131.77	123.00
3	C	229	PHE	CA-C-N	6.22	130.70	122.30
3	C	229	PHE	C-N-CA	6.22	130.70	122.30
2	B	998	ASP	CA-CB-CG	6.22	118.82	112.60
9	I	21	ASN	CA-CB-CG	6.21	118.81	112.60
2	B	1145	GLN	CA-C-N	6.20	131.56	122.94
2	B	1145	GLN	C-N-CA	6.20	131.56	122.94
25	Z	272	ASN	CA-CB-CG	6.20	118.80	112.60
1	A	1421	ARG	CA-C-N	6.19	129.63	120.90
1	A	1421	ARG	C-N-CA	6.19	129.63	120.90
20	U	387	ARG	CD-NE-CZ	6.19	133.06	124.40
5	E	167	GLU	CA-C-N	6.18	131.05	120.72
5	E	167	GLU	C-N-CA	6.18	131.05	120.72
2	B	306	ASP	CA-CB-CG	6.18	118.78	112.60
13	M	786	PHE	CA-C-O	6.18	121.52	117.94
3	C	55	ASN	CA-CB-CG	6.18	118.78	112.60
7	G	120	ASP	CA-CB-CG	6.18	118.78	112.60
27	b	47	SER	CA-C-N	6.17	127.91	120.13
27	b	47	SER	C-N-CA	6.17	127.91	120.13
2	B	315	ASN	CA-CB-CG	6.17	118.77	112.60
2	B	721	ARG	CD-NE-CZ	6.16	133.03	124.40
4	D	38	HIS	CA-CB-CG	6.16	119.96	113.80
1	A	65	ILE	CA-C-N	6.16	130.96	122.77
1	A	65	ILE	C-N-CA	6.16	130.96	122.77
7	G	142	GLU	CA-C-N	6.16	130.78	122.90
7	G	142	GLU	C-N-CA	6.16	130.78	122.90
3	C	53	ASP	CA-CB-CG	6.15	118.75	112.60
2	B	379	ARG	CD-NE-CZ	6.15	133.01	124.40
5	E	75	PHE	CA-C-N	6.15	129.98	122.42
5	E	75	PHE	C-N-CA	6.15	129.98	122.42
8	H	84	ARG	CD-NE-CZ	6.14	133.00	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	40	ARG	CD-NE-CZ	6.14	133.00	124.40
24	Y	21	LEU	CA-C-N	6.14	130.17	122.43
24	Y	21	LEU	C-N-CA	6.14	130.17	122.43
9	I	34	ILE	CA-C-N	6.14	130.94	122.77
9	I	34	ILE	C-N-CA	6.14	130.94	122.77
19	T	-137	DC	O3'-P-O5'	6.14	113.21	104.00
17	Q	771	ASP	CA-CB-CG	6.14	118.74	112.60
3	C	87	ASP	CA-CB-CG	6.14	118.74	112.60
2	B	370	HIS	CA-CB-CG	6.13	119.93	113.80
5	E	207	ARG	CD-NE-CZ	6.13	132.99	124.40
2	B	83	ARG	CA-C-N	6.13	133.49	122.64
2	B	83	ARG	C-N-CA	6.13	133.49	122.64
11	K	86	ALA	CA-C-N	6.13	128.49	120.28
11	K	86	ALA	C-N-CA	6.13	128.49	120.28
25	Z	251	ASN	CA-CB-CG	6.13	118.73	112.60
1	A	61	ARG	CD-NE-CZ	6.12	132.97	124.40
2	B	571	GLY	CA-C-N	6.12	130.92	122.77
2	B	571	GLY	C-N-CA	6.12	130.92	122.77
1	A	780	ASN	CA-CB-CG	6.12	118.72	112.60
11	K	32	LEU	CA-C-N	6.12	130.57	122.30
11	K	32	LEU	C-N-CA	6.12	130.57	122.30
2	B	918	PHE	CA-CB-CG	6.12	119.92	113.80
1	A	737	PHE	CA-CB-CG	6.11	119.91	113.80
2	B	821	LYS	CA-C-N	6.11	129.07	120.57
2	B	821	LYS	C-N-CA	6.11	129.07	120.57
25	Z	459	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	1319	LYS	CA-C-N	6.10	130.62	122.93
1	A	1319	LYS	C-N-CA	6.10	130.62	122.93
20	U	409	ARG	CD-NE-CZ	6.10	132.94	124.40
2	B	503	ASN	CA-CB-CG	6.10	118.70	112.60
5	E	188	GLY	CA-C-N	6.10	131.42	122.39
5	E	188	GLY	C-N-CA	6.10	131.42	122.39
25	Z	435	ASN	CA-CB-CG	6.10	118.70	112.60
26	a	124	ILE	N-CA-CB	6.10	117.28	110.51
29	d	39	TYR	CA-C-N	6.09	128.76	120.54
29	d	39	TYR	C-N-CA	6.09	128.76	120.54
2	B	841	ARG	CD-NE-CZ	6.09	132.93	124.40
7	G	144	ARG	CD-NE-CZ	6.09	132.93	124.40
1	A	528	PRO	CA-C-N	6.09	128.72	120.44
1	A	528	PRO	C-N-CA	6.09	128.72	120.44
13	M	1365	THR	CA-C-N	6.09	130.50	122.95
13	M	1365	THR	C-N-CA	6.09	130.50	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	134	THR	CA-C-N	6.09	132.56	122.33
21	V	134	THR	C-N-CA	6.09	132.56	122.33
4	D	102	ASN	CA-CB-CG	6.09	118.69	112.60
17	Q	830	ARG	CD-NE-CZ	6.09	132.92	124.40
3	C	158	GLU	CA-C-N	6.08	130.65	121.40
3	C	158	GLU	C-N-CA	6.08	130.65	121.40
11	K	40	HIS	CA-CB-CG	6.08	119.88	113.80
1	A	995	HIS	CA-CB-CG	6.08	119.88	113.80
1	A	890	ARG	CD-NE-CZ	6.08	132.91	124.40
11	K	111	ASP	CA-CB-CG	6.08	118.68	112.60
5	E	24	ARG	CD-NE-CZ	6.07	132.90	124.40
26	e	53	ARG	CD-NE-CZ	6.07	132.90	124.40
2	B	564	ALA	CA-C-N	6.07	130.10	121.42
2	B	564	ALA	C-N-CA	6.07	130.10	121.42
17	Q	679	ASP	CA-C-N	6.07	131.09	123.14
17	Q	679	ASP	C-N-CA	6.07	131.09	123.14
7	G	156	ASP	CA-CB-CG	6.07	118.67	112.60
24	Y	11	ARG	CD-NE-CZ	6.07	132.89	124.40
2	B	768	ARG	CD-NE-CZ	6.06	132.89	124.40
26	a	129	ARG	CD-NE-CZ	6.06	132.89	124.40
17	Q	763	ARG	CD-NE-CZ	6.06	132.88	124.40
1	A	73	THR	CA-C-N	6.06	130.73	122.19
1	A	73	THR	C-N-CA	6.06	130.73	122.19
2	B	452	ASN	CA-CB-CG	6.06	118.66	112.60
11	K	33	PHE	CA-CB-CG	6.06	119.86	113.80
21	V	26	ARG	CD-NE-CZ	6.06	132.88	124.40
1	A	1167	ARG	CD-NE-CZ	6.05	132.88	124.40
12	L	31	ARG	CD-NE-CZ	6.05	132.88	124.40
1	A	836	PHE	CA-CB-CG	6.05	119.85	113.80
1	A	614	ASP	CA-CB-CG	6.05	118.65	112.60
2	B	1034	GLY	CA-C-N	6.05	130.07	121.42
2	B	1034	GLY	C-N-CA	6.05	130.07	121.42
24	Y	111	ARG	CD-NE-CZ	6.05	132.87	124.40
28	g	32	ARG	NE-CZ-NH2	6.05	124.64	119.20
14	N	116	DA	C4'-C3'-O3'	6.05	119.07	110.00
20	U	395	GLU	CA-C-N	6.05	130.46	122.42
20	U	395	GLU	C-N-CA	6.05	130.46	122.42
7	G	135	ILE	CA-C-N	6.04	130.85	122.93
7	G	135	ILE	C-N-CA	6.04	130.85	122.93
11	K	34	THR	CA-C-N	6.04	130.16	122.37
11	K	34	THR	C-N-CA	6.04	130.16	122.37
25	Z	610	ARG	CA-C-N	6.04	131.50	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	610	ARG	C-N-CA	6.04	131.50	122.99
3	C	106	ARG	CD-NE-CZ	6.04	132.85	124.40
26	e	128	ARG	CD-NE-CZ	6.04	132.85	124.40
1	A	431	PHE	CA-CB-CG	6.03	119.83	113.80
17	Q	791	ARG	CD-NE-CZ	6.03	132.84	124.40
26	a	90	MET	CA-C-N	6.03	128.60	120.65
26	a	90	MET	C-N-CA	6.03	128.60	120.65
9	I	11	PHE	CA-C-N	6.02	131.37	123.06
9	I	11	PHE	C-N-CA	6.02	131.37	123.06
17	Q	771	ASP	CA-C-N	6.02	131.26	122.77
17	Q	771	ASP	C-N-CA	6.02	131.26	122.77
13	M	844	LYS	O-C-N	-6.02	114.39	121.32
4	D	84	ARG	NE-CZ-NH2	6.02	124.62	119.20
14	N	74	DC	O5'-C5'-C4'	6.02	119.83	110.80
1	A	1396	ARG	NE-CZ-NH2	6.02	124.62	119.20
26	a	106	ASP	CA-CB-CG	6.02	118.62	112.60
5	E	190	VAL	CA-C-N	6.02	131.10	123.10
5	E	190	VAL	C-N-CA	6.02	131.10	123.10
2	B	1095	ILE	CA-C-N	6.01	128.34	120.28
2	B	1095	ILE	C-N-CA	6.01	128.34	120.28
29	h	76	ARG	CA-C-N	6.01	128.26	120.44
29	h	76	ARG	C-N-CA	6.01	128.26	120.44
1	A	805	ARG	CD-NE-CZ	6.01	132.81	124.40
2	B	39	LEU	CA-C-N	6.01	129.71	122.26
2	B	39	LEU	C-N-CA	6.01	129.71	122.26
2	B	938	ARG	CD-NE-CZ	6.01	132.81	124.40
4	D	71	PHE	CA-CB-CG	6.00	119.80	113.80
5	E	172	ARG	CA-C-N	6.00	131.88	122.70
5	E	172	ARG	C-N-CA	6.00	131.88	122.70
19	T	-97	DG	C4'-C3'-O3'	6.00	119.00	110.00
2	B	890	ARG	CD-NE-CZ	6.00	132.80	124.40
18	R	487	PHE	CA-CB-CG	6.00	119.80	113.80
1	A	70	ARG	CD-NE-CZ	5.99	132.79	124.40
3	C	119	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	599	HIS	CA-CB-CG	5.99	119.79	113.80
8	H	62	SER	CA-C-N	5.99	131.94	122.36
8	H	62	SER	C-N-CA	5.99	131.94	122.36
5	E	147	GLU	CA-C-N	5.99	131.43	123.05
5	E	147	GLU	C-N-CA	5.99	131.43	123.05
7	G	78	ARG	CD-NE-CZ	5.98	132.78	124.40
17	Q	832	ARG	CD-NE-CZ	5.98	132.78	124.40
9	I	44	TYR	CA-C-N	5.98	131.60	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	44	TYR	C-N-CA	5.98	131.60	123.11
21	V	126	LYS	CA-C-N	5.98	128.01	120.72
21	V	126	LYS	C-N-CA	5.98	128.01	120.72
1	A	839	HIS	CA-CB-CG	5.97	119.77	113.80
5	E	181	ARG	CD-NE-CZ	5.97	132.76	124.40
26	e	124	ILE	N-CA-CB	5.97	117.14	110.51
1	A	551	ARG	CD-NE-CZ	5.97	132.76	124.40
2	B	1092	ASP	CA-CB-CG	5.97	118.57	112.60
3	C	189	ASP	CA-CB-CG	5.97	118.57	112.60
2	B	579	ASP	CA-CB-CG	5.97	118.57	112.60
13	M	1256	ARG	CA-C-O	5.97	121.40	117.94
28	c	77	ARG	CD-NE-CZ	5.96	132.75	124.40
1	A	674	THR	CA-C-N	5.96	128.19	120.56
1	A	674	THR	C-N-CA	5.96	128.19	120.56
1	A	1285	LEU	CA-C-N	5.96	128.75	120.29
1	A	1285	LEU	C-N-CA	5.96	128.75	120.29
7	G	119	PHE	CA-CB-CG	5.95	119.75	113.80
1	A	84	HIS	CB-CG-CD2	-5.95	123.46	131.20
1	A	880	ARG	CD-NE-CZ	5.95	132.73	124.40
2	B	1104	ARG	CD-NE-CZ	5.95	132.72	124.40
7	G	77	PHE	CA-CB-CG	5.95	119.75	113.80
13	M	1337	PHE	CA-CB-CG	5.95	119.75	113.80
1	A	994	PHE	CA-CB-CG	5.94	119.74	113.80
2	B	681	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	1380	ARG	CD-NE-CZ	5.94	132.72	124.40
26	e	134	ARG	CD-NE-CZ	5.94	132.72	124.40
27	f	75	HIS	CA-CB-CG	5.94	119.74	113.80
13	M	353	PRO	CA-N-CD	-5.94	103.69	112.00
3	C	51	GLN	CA-C-N	5.94	129.91	122.43
3	C	51	GLN	C-N-CA	5.94	129.91	122.43
24	Y	61	ILE	CA-C-N	5.94	130.31	122.06
24	Y	61	ILE	C-N-CA	5.94	130.31	122.06
25	Z	752	THR	CA-C-N	5.94	129.36	122.35
25	Z	752	THR	C-N-CA	5.94	129.36	122.35
18	R	596	ARG	CD-NE-CZ	5.94	132.71	124.40
25	Z	612	GLY	CA-C-N	5.93	131.36	123.00
25	Z	612	GLY	C-N-CA	5.93	131.36	123.00
2	B	687	VAL	CA-C-N	5.92	129.25	120.95
2	B	687	VAL	C-N-CA	5.92	129.25	120.95
1	A	822	PHE	N-CA-CB	5.92	119.24	109.88
7	G	153	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	534	VAL	CA-C-N	5.92	130.64	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	VAL	C-N-CA	5.92	130.64	122.77
1	A	1070	GLY	CA-C-N	5.91	128.13	120.44
1	A	1070	GLY	C-N-CA	5.91	128.13	120.44
21	V	219	ALA	CA-C-N	5.91	130.63	122.77
21	V	219	ALA	C-N-CA	5.91	130.63	122.77
2	B	834	ARG	CD-NE-CZ	5.91	132.67	124.40
1	A	1218	ARG	CD-NE-CZ	5.91	132.67	124.40
1	A	968	VAL	CA-C-N	5.91	128.09	120.88
1	A	968	VAL	C-N-CA	5.91	128.09	120.88
3	C	25	ASN	CA-CB-CG	5.90	118.50	112.60
17	Q	781	ASN	CA-CB-CG	5.90	118.50	112.60
3	C	18	ASN	CA-C-N	5.90	130.87	123.14
3	C	18	ASN	C-N-CA	5.90	130.87	123.14
2	B	380	ARG	CD-NE-CZ	5.89	132.65	124.40
5	E	162	ARG	CD-NE-CZ	5.88	132.64	124.40
11	K	20	THR	CA-C-N	5.88	129.96	122.37
11	K	20	THR	C-N-CA	5.88	129.96	122.37
2	B	790	GLN	N-CA-C	5.88	119.28	111.75
2	B	114	ARG	NE-CZ-NH2	5.88	124.49	119.20
2	B	1023	ARG	CD-NE-CZ	5.88	132.63	124.40
17	Q	188	LYS	CA-C-N	5.88	129.25	120.31
17	Q	188	LYS	C-N-CA	5.88	129.25	120.31
20	U	437	ASN	CA-C-N	5.88	131.76	122.94
20	U	437	ASN	C-N-CA	5.88	131.76	122.94
3	C	183	ALA	CA-C-N	5.88	129.82	121.42
3	C	183	ALA	C-N-CA	5.88	129.82	121.42
1	A	672	ILE	N-CA-CB	5.87	116.78	110.62
25	Z	442	SER	CA-C-N	5.87	130.75	123.12
25	Z	442	SER	C-N-CA	5.87	130.75	123.12
2	B	743	ARG	NE-CZ-NH2	5.87	124.48	119.20
2	B	282	ARG	CA-CB-CG	5.87	125.83	114.10
7	G	83	GLU	CA-C-N	5.87	131.31	123.10
7	G	83	GLU	C-N-CA	5.87	131.31	123.10
2	B	483	ARG	CD-NE-CZ	5.86	132.60	124.40
1	A	584	PRO	CA-C-N	5.86	131.26	123.00
1	A	584	PRO	C-N-CA	5.86	131.26	123.00
7	G	147	ILE	N-CA-CB	5.86	117.73	111.46
29	h	101	GLY	N-CA-C	5.86	119.29	112.50
2	B	186	ILE	CA-C-N	5.85	131.06	123.10
2	B	186	ILE	C-N-CA	5.85	131.06	123.10
9	I	23	MET	CA-C-N	5.85	129.86	121.50
9	I	23	MET	C-N-CA	5.85	129.86	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	36	LEU	CA-C-N	5.85	131.37	122.95
9	I	36	LEU	C-N-CA	5.85	131.37	122.95
13	M	1333	HIS	N-CA-C	5.85	116.12	107.88
1	A	436	SER	CA-C-N	5.84	129.19	120.31
1	A	436	SER	C-N-CA	5.84	129.19	120.31
8	H	57	ARG	CD-NE-CZ	5.84	132.57	124.40
19	T	-88	DA	P-O3'-C3'	5.84	128.96	120.20
1	A	583	ARG	CD-NE-CZ	5.83	132.57	124.40
12	L	26	ASN	CA-CB-CG	5.83	118.43	112.60
28	c	76	THR	CA-C-N	5.83	130.77	122.72
28	c	76	THR	C-N-CA	5.83	130.77	122.72
2	B	1126	ALA	CA-C-N	5.83	130.56	122.93
2	B	1126	ALA	C-N-CA	5.83	130.56	122.93
1	A	1153	ARG	CD-NE-CZ	5.83	132.56	124.40
2	B	611	GLU	CA-C-N	5.83	130.69	123.12
2	B	611	GLU	C-N-CA	5.83	130.69	123.12
26	e	106	ASP	CA-CB-CG	5.83	118.43	112.60
2	B	66	ASP	CA-CB-CG	5.82	118.42	112.60
8	H	89	GLU	CA-C-N	5.82	131.13	122.86
8	H	89	GLU	C-N-CA	5.82	131.13	122.86
4	D	70	ARG	CD-NE-CZ	5.82	132.55	124.40
2	B	975	ARG	CB-CG-CD	5.82	124.68	111.30
2	B	41	ARG	CD-NE-CZ	5.81	132.53	124.40
2	B	402	PHE	CA-CB-CG	5.81	119.61	113.80
19	T	-98	DA	C4'-C3'-O3'	5.81	118.71	110.00
1	A	439	HIS	N-CA-CB	5.80	118.65	109.71
24	Y	66	PRO	CA-C-N	5.80	129.13	120.31
24	Y	66	PRO	C-N-CA	5.80	129.13	120.31
2	B	185	PHE	CA-CB-CG	5.80	119.60	113.80
25	Z	241	GLY	CA-C-N	5.80	129.85	122.37
25	Z	241	GLY	C-N-CA	5.80	129.85	122.37
1	A	1356	ARG	CD-NE-CZ	5.79	132.51	124.40
9	I	43	ASP	CA-CB-CG	5.79	118.39	112.60
2	B	371	ARG	CD-NE-CZ	5.79	132.50	124.40
24	Y	64	MET	CA-C-N	5.79	130.28	123.16
24	Y	64	MET	C-N-CA	5.79	130.28	123.16
1	A	282	ASP	N-CA-C	-5.78	98.48	110.80
21	V	303	PHE	CA-C-N	5.78	130.89	123.03
21	V	303	PHE	C-N-CA	5.78	130.89	123.03
7	G	62	GLY	CA-C-N	5.78	131.88	122.81
7	G	62	GLY	C-N-CA	5.78	131.88	122.81
1	A	1035	GLU	CA-C-N	5.77	128.29	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1035	GLU	C-N-CA	5.77	128.29	120.44
2	B	716	HIS	CA-C-N	5.77	131.87	122.81
2	B	716	HIS	C-N-CA	5.77	131.87	122.81
2	B	849	ASP	CA-C-N	5.77	129.84	120.60
2	B	849	ASP	C-N-CA	5.77	129.84	120.60
24	Y	52	CYS	CA-C-N	5.77	129.03	120.95
24	Y	52	CYS	C-N-CA	5.77	129.03	120.95
1	A	792	ASN	CA-CB-CG	5.77	118.37	112.60
1	A	1224	ARG	CD-NE-CZ	5.77	132.48	124.40
17	Q	672	GLN	CA-C-N	5.77	127.94	120.56
17	Q	672	GLN	C-N-CA	5.77	127.94	120.56
2	B	560	ALA	CA-C-N	5.76	129.72	121.02
2	B	560	ALA	C-N-CA	5.76	129.72	121.02
1	A	1245	CYS	CA-C-N	5.76	132.34	121.97
1	A	1245	CYS	C-N-CA	5.76	132.34	121.97
21	V	111	GLU	CA-C-N	5.76	129.59	121.53
21	V	111	GLU	C-N-CA	5.76	129.59	121.53
9	I	46	GLN	CA-C-N	5.76	130.07	121.72
9	I	46	GLN	C-N-CA	5.76	130.07	121.72
2	B	402	PHE	CA-C-N	5.76	128.46	120.63
2	B	402	PHE	C-N-CA	5.76	128.46	120.63
19	T	-116	DT	O5'-C5'-C4'	5.75	119.43	110.80
1	A	408	ARG	CD-NE-CZ	5.75	132.45	124.40
1	A	197	GLU	CA-C-N	5.75	130.60	122.09
1	A	197	GLU	C-N-CA	5.75	130.60	122.09
28	g	42	ARG	CA-C-N	5.75	130.32	123.19
28	g	42	ARG	C-N-CA	5.75	130.32	123.19
2	B	185	PHE	CA-C-N	5.74	130.45	122.93
2	B	185	PHE	C-N-CA	5.74	130.45	122.93
17	Q	663	PHE	CA-CB-CG	5.74	119.54	113.80
17	Q	688	ALA	CA-C-N	5.74	128.44	120.29
17	Q	688	ALA	C-N-CA	5.74	128.44	120.29
17	Q	203	GLY	CA-C-N	5.74	128.24	120.44
17	Q	203	GLY	C-N-CA	5.74	128.24	120.44
3	C	105	VAL	CA-C-N	5.73	130.85	122.77
3	C	105	VAL	C-N-CA	5.73	130.85	122.77
26	e	88	ALA	CA-C-N	5.73	127.90	120.56
26	e	88	ALA	C-N-CA	5.73	127.90	120.56
5	E	117	SER	CA-C-N	5.73	128.43	120.29
5	E	117	SER	C-N-CA	5.73	128.43	120.29
14	N	105	DG	C2'-C3'-O3'	5.73	120.10	111.50
11	K	55	GLN	CA-C-N	5.73	130.90	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	55	GLN	C-N-CA	5.73	130.90	123.11
2	B	716	HIS	CA-CB-CG	5.73	119.53	113.80
25	Z	519	GLN	CA-C-N	5.73	130.29	122.84
25	Z	519	GLN	C-N-CA	5.73	130.29	122.84
1	A	1215	GLU	CA-C-N	5.73	132.65	121.66
1	A	1215	GLU	C-N-CA	5.73	132.65	121.66
2	B	764	MET	CA-C-N	5.73	128.23	120.44
2	B	764	MET	C-N-CA	5.73	128.23	120.44
25	Z	383	THR	CA-C-N	5.72	130.26	122.19
25	Z	383	THR	C-N-CA	5.72	130.26	122.19
18	R	482	ALA	CA-C-N	5.72	128.22	120.44
18	R	482	ALA	C-N-CA	5.72	128.22	120.44
25	Z	209	PRO	CA-C-N	5.72	130.89	123.00
25	Z	209	PRO	C-N-CA	5.72	130.89	123.00
9	I	17	CYS	N-CA-CB	5.72	118.44	110.26
1	A	931	ARG	CA-C-N	5.71	128.21	120.44
1	A	931	ARG	C-N-CA	5.71	128.21	120.44
21	V	302	PHE	CA-C-N	5.71	131.21	122.93
21	V	302	PHE	C-N-CA	5.71	131.21	122.93
28	g	88	ARG	NE-CZ-NH2	5.71	124.34	119.20
25	Z	477	HIS	CA-C-N	5.70	130.69	123.10
25	Z	477	HIS	C-N-CA	5.70	130.69	123.10
1	A	644	SER	CA-C-N	5.70	131.18	122.29
1	A	644	SER	C-N-CA	5.70	131.18	122.29
2	B	282	ARG	CD-NE-CZ	5.70	132.38	124.40
6	F	51	ARG	CD-NE-CZ	5.70	132.37	124.40
9	I	21	ASN	CA-C-N	5.70	133.22	123.03
9	I	21	ASN	C-N-CA	5.70	133.22	123.03
18	R	485	TYR	CA-C-N	5.70	129.44	121.24
18	R	485	TYR	C-N-CA	5.70	129.44	121.24
6	F	57	MET	N-CA-CB	5.69	119.05	109.94
2	B	282	ARG	CA-C-N	5.69	128.96	120.31
2	B	282	ARG	C-N-CA	5.69	128.96	120.31
1	A	445	LYS	CA-C-N	5.69	130.51	123.12
1	A	445	LYS	C-N-CA	5.69	130.51	123.12
2	B	865	VAL	N-CA-CB	5.69	116.92	110.72
25	Z	200	PHE	CA-CB-CG	5.69	119.49	113.80
26	a	131	ARG	NE-CZ-NH2	5.69	124.32	119.20
2	B	425	ARG	CD-NE-CZ	5.68	132.36	124.40
24	Y	88	SER	CA-C-N	5.68	131.05	123.10
24	Y	88	SER	C-N-CA	5.68	131.05	123.10
1	A	787	VAL	CA-C-N	5.68	128.86	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	787	VAL	C-N-CA	5.68	128.86	120.74
3	C	10	ARG	CD-NE-CZ	5.68	132.35	124.40
25	Z	483	GLY	N-CA-C	5.68	118.28	110.56
1	A	1097	GLU	N-CA-CB	5.68	117.12	110.42
4	D	95	PHE	N-CA-CB	5.68	118.47	110.12
11	K	74	ARG	NE-CZ-NH2	5.68	124.31	119.20
25	Z	761	MET	CA-C-N	5.68	129.95	122.06
25	Z	761	MET	C-N-CA	5.68	129.95	122.06
2	B	334	LYS	CA-CB-CG	5.67	125.44	114.10
3	C	229	PHE	CA-CB-CG	5.67	119.47	113.80
1	A	1088	GLY	CA-C-N	5.67	127.87	120.28
1	A	1088	GLY	C-N-CA	5.67	127.87	120.28
3	C	54	ALA	CA-C-N	5.67	130.90	122.86
3	C	54	ALA	C-N-CA	5.67	130.90	122.86
1	A	316	THR	CA-C-N	5.66	127.80	120.44
1	A	316	THR	C-N-CA	5.66	127.80	120.44
1	A	1020	LEU	CA-C-N	5.66	130.15	122.90
1	A	1020	LEU	C-N-CA	5.66	130.15	122.90
21	V	283	ARG	CA-C-N	5.66	128.90	120.87
21	V	283	ARG	C-N-CA	5.66	128.90	120.87
1	A	847	LEU	CA-C-N	5.66	127.80	120.56
1	A	847	LEU	C-N-CA	5.66	127.80	120.56
1	A	810	PHE	CA-CB-CG	5.65	119.45	113.80
1	A	1319	LYS	N-CA-CB	5.65	118.27	109.85
5	E	8	TYR	N-CA-CB	5.65	118.21	110.01
7	G	110	ARG	CA-C-N	5.65	127.79	120.44
7	G	110	ARG	C-N-CA	5.65	127.79	120.44
25	Z	490	GLY	CA-C-N	5.65	131.45	122.74
25	Z	490	GLY	C-N-CA	5.65	131.45	122.74
1	A	887	VAL	CA-C-N	5.65	131.88	122.73
1	A	887	VAL	C-N-CA	5.65	131.88	122.73
21	V	218	GLN	CA-C-N	5.64	129.23	121.33
21	V	218	GLN	C-N-CA	5.64	129.23	121.33
1	A	877	ALA	CA-C-N	5.64	131.67	122.81
1	A	877	ALA	C-N-CA	5.64	131.67	122.81
2	B	290	TYR	CA-C-N	5.64	130.17	122.84
2	B	290	TYR	C-N-CA	5.64	130.17	122.84
21	V	110	GLU	CA-C-N	5.64	130.28	121.76
21	V	110	GLU	C-N-CA	5.64	130.28	121.76
2	B	904	VAL	N-CA-CB	5.64	116.97	110.49
17	Q	775	ASN	CA-C-N	5.64	130.12	120.71
17	Q	775	ASN	C-N-CA	5.64	130.12	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	893	SER	CA-C-N	5.63	130.43	122.09
2	B	893	SER	C-N-CA	5.63	130.43	122.09
1	A	198	LEU	CA-C-N	5.63	130.93	122.99
1	A	198	LEU	C-N-CA	5.63	130.93	122.99
1	A	822	PHE	CA-CB-CG	5.62	119.42	113.80
2	B	913	GLN	CA-C-N	5.62	132.31	121.18
2	B	913	GLN	C-N-CA	5.62	132.31	121.18
18	R	412	ALA	CA-C-N	5.62	131.46	123.14
18	R	412	ALA	C-N-CA	5.62	131.46	123.14
4	D	113	ALA	CA-C-N	5.62	128.08	120.44
4	D	113	ALA	C-N-CA	5.62	128.08	120.44
1	A	557	ARG	CD-NE-CZ	5.61	132.26	124.40
11	K	106	ARG	CD-NE-CZ	5.61	132.26	124.40
1	A	878	THR	CA-C-N	5.61	129.91	122.95
1	A	878	THR	C-N-CA	5.61	129.91	122.95
1	A	1282	ASP	CA-CB-CG	5.61	118.21	112.60
18	R	377	PHE	CA-C-N	5.61	127.80	120.28
18	R	377	PHE	C-N-CA	5.61	127.80	120.28
19	T	-36	DC	C5'-C4'-C3'	-5.61	106.48	114.90
25	Z	480	VAL	N-CA-CB	5.61	116.64	110.53
11	K	30	ALA	CA-C-N	5.61	131.40	122.59
11	K	30	ALA	C-N-CA	5.61	131.40	122.59
9	I	79	PRO	CA-C-N	5.61	130.90	122.99
9	I	79	PRO	C-N-CA	5.61	130.90	122.99
1	A	1067	TRP	CA-C-N	5.60	127.72	120.44
1	A	1067	TRP	C-N-CA	5.60	127.72	120.44
27	b	53	GLU	CA-C-N	5.60	127.72	120.44
27	b	53	GLU	C-N-CA	5.60	127.72	120.44
13	M	328	PRO	CA-N-CD	-5.60	104.17	112.00
26	e	116	ARG	NE-CZ-NH2	5.60	124.24	119.20
13	M	1060	PRO	CA-N-CD	-5.59	104.17	112.00
1	A	798	ILE	N-CA-CB	5.59	116.38	110.17
9	I	28	GLU	N-CA-CB	5.59	118.62	109.95
2	B	565	THR	CA-C-N	5.59	130.43	122.72
2	B	565	THR	C-N-CA	5.59	130.43	122.72
5	E	195	ARG	CD-NE-CZ	5.59	132.23	124.40
1	A	551	ARG	CA-C-N	5.59	131.43	122.83
1	A	551	ARG	C-N-CA	5.59	131.43	122.83
3	C	262	GLN	CA-C-N	5.59	127.70	120.44
3	C	262	GLN	C-N-CA	5.59	127.70	120.44
13	M	543	PRO	CA-N-CD	-5.59	104.18	112.00
25	Z	511	LEU	CA-C-N	5.59	131.04	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	511	LEU	C-N-CA	5.59	131.04	123.11
25	Z	628	LYS	CA-C-N	5.59	128.80	120.87
25	Z	628	LYS	C-N-CA	5.59	128.80	120.87
20	U	379	PRO	CA-C-N	5.58	127.76	120.28
20	U	379	PRO	C-N-CA	5.58	127.76	120.28
19	T	-29	DC	P-O3'-C3'	5.58	128.57	120.20
1	A	241	ARG	NE-CZ-NH2	5.58	124.22	119.20
8	H	46	GLN	CA-C-N	5.58	129.45	121.02
8	H	46	GLN	C-N-CA	5.58	129.45	121.02
11	K	109	ILE	N-CA-CB	5.58	116.70	110.62
13	M	1158	PRO	CA-N-CD	-5.58	104.19	112.00
26	a	99	TYR	N-CA-CB	5.58	118.10	110.01
13	M	1025	PRO	CA-N-CD	-5.58	104.19	112.00
3	C	11	ILE	N-CA-CB	5.58	117.01	110.82
5	E	140	THR	CA-C-N	5.57	130.03	120.72
5	E	140	THR	C-N-CA	5.57	130.03	120.72
25	Z	758	PRO	CA-N-CD	-5.57	104.20	112.00
13	M	944	PRO	CA-N-CD	-5.57	104.20	112.00
17	Q	798	LYS	CA-C-N	5.57	128.55	120.98
17	Q	798	LYS	C-N-CA	5.57	128.55	120.98
19	T	-132	DT	OP1-P-OP2	-5.57	103.29	120.00
2	B	924	ARG	NE-CZ-NH2	5.57	124.21	119.20
7	G	134	ASP	CA-C-N	5.57	129.44	122.48
7	G	134	ASP	C-N-CA	5.57	129.44	122.48
14	N	14	DT	OP1-P-OP2	-5.57	103.30	120.00
14	N	16	DT	OP1-P-OP2	-5.57	103.30	120.00
14	N	86	DT	OP1-P-OP2	-5.57	103.30	120.00
14	N	106	DT	OP1-P-OP2	-5.57	103.30	120.00
14	N	139	DT	OP1-P-OP2	-5.57	103.30	120.00
19	T	-144	DT	OP1-P-OP2	-5.57	103.30	120.00
19	T	-112	DT	OP1-P-OP2	-5.57	103.30	120.00
19	T	-109	DT	OP1-P-OP2	-5.57	103.30	120.00
27	f	59	LYS	CA-C-N	5.57	127.78	120.60
27	f	59	LYS	C-N-CA	5.57	127.78	120.60
27	f	63	GLU	CA-CB-CG	5.57	125.23	114.10
4	D	120	GLY	CA-C-N	5.57	128.19	120.29
4	D	120	GLY	C-N-CA	5.57	128.19	120.29
14	N	108	DT	OP1-P-OP2	-5.57	103.30	120.00
13	M	907	PRO	CA-N-CD	-5.56	104.21	112.00
13	M	994	PRO	CA-N-CD	-5.56	104.21	112.00
2	B	280	SER	N-CA-CB	5.56	118.18	110.17
13	M	908	PRO	CA-N-CD	-5.56	104.21	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	563	PRO	CA-N-CD	-5.56	104.21	112.00
1	A	976	LYS	CA-CB-CG	5.56	125.22	114.10
14	N	87	DT	OP1-P-OP2	-5.56	103.32	120.00
14	N	140	DT	OP1-P-OP2	-5.56	103.32	120.00
14	N	39	DT	OP1-P-OP2	-5.56	103.33	120.00
19	T	-70	DT	OP1-P-OP2	-5.56	103.33	120.00
25	Z	519	GLN	CB-CG-CD	5.56	122.05	112.60
1	A	552	ASP	CA-C-N	5.55	130.21	122.93
1	A	552	ASP	C-N-CA	5.55	130.21	122.93
2	B	685	LYS	CA-C-N	5.55	130.45	122.23
2	B	685	LYS	C-N-CA	5.55	130.45	122.23
13	M	980	PRO	CA-N-CD	-5.55	104.23	112.00
13	M	1330	PRO	CA-N-CD	-5.55	104.23	112.00
14	N	97	DC	N1-C1'-C2'	5.55	121.83	113.50
21	V	187	GLN	CA-C-N	5.55	130.94	121.29
21	V	187	GLN	C-N-CA	5.55	130.94	121.29
27	f	57	VAL	N-CA-CB	5.55	116.44	110.62
18	R	550	ASP	CA-C-N	5.55	127.98	120.44
18	R	550	ASP	C-N-CA	5.55	127.98	120.44
21	V	188	LYS	CA-C-N	5.54	129.43	121.50
21	V	188	LYS	C-N-CA	5.54	129.43	121.50
2	B	608	ARG	N-CA-CB	5.54	118.11	110.07
13	M	1227	GLY	N-CA-C	5.54	119.64	112.54
13	M	1360	GLY	CA-C-N	5.54	130.97	122.93
13	M	1360	GLY	C-N-CA	5.54	130.97	122.93
18	R	557	ILE	CA-C-N	5.54	127.97	120.38
18	R	557	ILE	C-N-CA	5.54	127.97	120.38
16	P	38	G	C4'-C3'-C2'	-5.54	97.06	102.60
2	B	424	ASP	CA-C-N	5.54	129.46	120.60
2	B	424	ASP	C-N-CA	5.54	129.46	120.60
3	C	220	TYR	N-CA-CB	5.54	118.16	109.69
1	A	1163	HIS	CA-C-N	5.53	130.97	123.11
1	A	1163	HIS	C-N-CA	5.53	130.97	123.11
4	D	138	ARG	CD-NE-CZ	5.53	132.15	124.40
6	F	117	ASP	CA-C-N	5.53	130.57	122.77
6	F	117	ASP	C-N-CA	5.53	130.57	122.77
2	B	426	GLY	CA-C-N	5.53	130.99	121.86
2	B	426	GLY	C-N-CA	5.53	130.99	121.86
2	B	475	PHE	N-CA-CB	5.53	118.25	110.12
4	D	65	LEU	CA-C-N	5.53	127.95	120.38
4	D	65	LEU	C-N-CA	5.53	127.95	120.38
21	V	223	GLY	CA-C-N	5.53	129.41	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	223	GLY	C-N-CA	5.53	129.41	121.50
1	A	96	HIS	CE1-NE2-CD2	-5.53	103.47	109.00
1	A	1422	GLN	N-CA-CB	5.53	118.48	109.69
24	Y	91	GLY	N-CA-C	5.53	118.76	111.52
2	B	445	LYS	CA-CB-CG	5.52	125.14	114.10
11	K	23	LYS	N-CA-CB	5.52	118.23	109.51
9	I	14	ILE	CA-C-N	5.52	130.11	122.77
9	I	14	ILE	C-N-CA	5.52	130.11	122.77
1	A	791	GLN	CA-C-N	5.52	130.87	122.65
1	A	791	GLN	C-N-CA	5.52	130.87	122.65
28	g	30	VAL	CA-C-N	5.52	127.94	120.44
28	g	30	VAL	C-N-CA	5.52	127.94	120.44
26	a	129	ARG	CA-C-N	5.51	127.62	120.56
26	a	129	ARG	C-N-CA	5.51	127.62	120.56
5	E	184	GLY	CA-C-N	5.51	128.80	120.75
5	E	184	GLY	C-N-CA	5.51	128.80	120.75
25	Z	482	ALA	CA-C-N	5.51	129.39	121.56
25	Z	482	ALA	C-N-CA	5.51	129.39	121.56
2	B	988	LYS	CA-CB-CG	5.51	125.12	114.10
25	Z	265	LYS	CA-C-N	5.51	130.81	122.98
25	Z	265	LYS	C-N-CA	5.51	130.81	122.98
26	e	75	ALA	CA-C-N	5.51	127.93	120.38
26	e	75	ALA	C-N-CA	5.51	127.93	120.38
4	D	25	GLU	CA-C-N	5.51	131.14	122.11
4	D	25	GLU	C-N-CA	5.51	131.14	122.11
4	D	29	ALA	CA-C-N	5.51	130.00	122.84
4	D	29	ALA	C-N-CA	5.51	130.00	122.84
27	b	96	THR	CA-C-N	5.51	130.77	123.00
27	b	96	THR	C-N-CA	5.51	130.77	123.00
1	A	46	THR	CA-C-N	5.50	130.76	123.00
1	A	46	THR	C-N-CA	5.50	130.76	123.00
24	Y	8	LYS	CA-C-N	5.50	130.91	122.93
24	Y	8	LYS	C-N-CA	5.50	130.91	122.93
1	A	439	HIS	CA-CB-CG	5.50	119.30	113.80
1	A	679	TRP	N-CA-CB	5.50	118.21	110.12
9	I	55	VAL	CA-C-N	5.50	130.07	121.76
9	I	55	VAL	C-N-CA	5.50	130.07	121.76
18	R	370	GLU	CA-C-N	5.50	128.68	120.31
18	R	370	GLU	C-N-CA	5.50	128.68	120.31
1	A	510	GLU	CA-CB-CG	5.50	125.10	114.10
1	A	589	LYS	CG-CD-CE	5.50	123.95	111.30
2	B	981	LEU	CA-C-N	5.50	128.00	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	981	LEU	C-N-CA	5.50	128.00	120.46
9	I	40	ARG	CA-C-N	5.50	127.65	120.28
9	I	40	ARG	C-N-CA	5.50	127.65	120.28
18	R	424	LYS	CA-C-N	5.50	129.42	122.77
18	R	424	LYS	C-N-CA	5.50	129.42	122.77
1	A	196	LEU	CA-C-N	5.49	130.74	122.99
1	A	196	LEU	C-N-CA	5.49	130.74	122.99
11	K	83	PRO	CA-C-N	5.49	127.58	120.44
11	K	83	PRO	C-N-CA	5.49	127.58	120.44
24	Y	69	SER	CA-C-N	5.49	128.09	120.29
24	Y	69	SER	C-N-CA	5.49	128.09	120.29
25	Z	264	LEU	CA-C-N	5.49	128.64	120.95
25	Z	264	LEU	C-N-CA	5.49	128.64	120.95
24	Y	60	ILE	CA-C-N	5.49	130.61	122.71
24	Y	60	ILE	C-N-CA	5.49	130.61	122.71
7	G	9	HIS	CA-C-N	5.49	130.74	123.00
7	G	9	HIS	C-N-CA	5.49	130.74	123.00
17	Q	676	ALA	CA-C-N	5.48	130.65	122.86
17	Q	676	ALA	C-N-CA	5.48	130.65	122.86
25	Z	634	GLY	CA-C-N	5.48	131.16	122.94
25	Z	634	GLY	C-N-CA	5.48	131.16	122.94
27	f	70	VAL	N-CA-CB	5.48	116.60	110.51
2	B	211	LYS	CA-C-N	5.48	132.01	121.54
2	B	211	LYS	C-N-CA	5.48	132.01	121.54
11	K	108	ALA	CA-C-N	5.48	127.55	120.70
11	K	108	ALA	C-N-CA	5.48	127.55	120.70
7	G	10	GLU	CA-C-N	5.48	130.62	123.06
7	G	10	GLU	C-N-CA	5.48	130.62	123.06
14	N	123	DG	O5'-C5'-C4'	5.48	119.02	110.80
2	B	371	ARG	N-CA-CB	5.48	118.77	110.28
8	H	53	GLY	CA-C-N	5.48	128.65	120.87
8	H	53	GLY	C-N-CA	5.48	128.65	120.87
17	Q	695	LYS	CA-C-N	5.48	130.13	122.79
17	Q	695	LYS	C-N-CA	5.48	130.13	122.79
2	B	580	PRO	CA-C-N	5.47	131.29	121.66
2	B	580	PRO	C-N-CA	5.47	131.29	121.66
17	Q	710	LYS	CA-C-N	5.47	130.31	122.21
17	Q	710	LYS	C-N-CA	5.47	130.31	122.21
2	B	30	ILE	N-CA-CB	5.47	116.95	110.55
2	B	770	ARG	CD-NE-CZ	5.47	132.06	124.40
5	E	207	ARG	CA-C-N	5.47	129.91	122.19
5	E	207	ARG	C-N-CA	5.47	129.91	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	MET	CA-CB-CG	5.47	125.03	114.10
1	A	349	ARG	NE-CZ-NH2	5.47	124.12	119.20
2	B	824	ASP	CA-C-N	5.47	130.54	123.00
2	B	824	ASP	C-N-CA	5.47	130.54	123.00
6	F	55	PRO	CA-C-N	5.47	130.86	122.93
6	F	55	PRO	C-N-CA	5.47	130.86	122.93
1	A	839	HIS	CE1-NE2-CD2	-5.46	103.53	109.00
4	D	38	HIS	N-CA-CB	5.46	118.15	110.12
27	b	35	ARG	NE-CZ-NH2	5.46	124.12	119.20
13	M	380	ARG	N-CA-C	5.46	116.57	108.60
18	R	415	TYR	CA-C-N	5.46	129.89	122.19
18	R	415	TYR	C-N-CA	5.46	129.89	122.19
1	A	55	GLY	CA-C-N	5.46	129.38	122.77
1	A	55	GLY	C-N-CA	5.46	129.38	122.77
4	D	17	ALA	CA-C-N	5.46	127.59	120.28
4	D	17	ALA	C-N-CA	5.46	127.59	120.28
9	I	107	ALA	CA-C-N	5.46	131.21	122.86
9	I	107	ALA	C-N-CA	5.46	131.21	122.86
1	A	71	CYS	N-CA-CB	5.46	118.07	109.83
7	G	87	ALA	CA-C-N	5.46	130.14	123.10
7	G	87	ALA	C-N-CA	5.46	130.14	123.10
18	R	553	ARG	CA-C-N	5.46	127.59	120.28
18	R	553	ARG	C-N-CA	5.46	127.59	120.28
19	T	-79	DT	O5'-C5'-C4'	5.46	118.98	110.80
5	E	207	ARG	CB-CG-CD	5.45	123.84	111.30
29	h	89	ARG	CA-C-N	5.45	128.37	120.79
29	h	89	ARG	C-N-CA	5.45	128.37	120.79
25	Z	474	MET	CA-CB-CG	5.45	125.00	114.10
3	C	207	GLU	CA-C-N	5.45	131.53	122.54
3	C	207	GLU	C-N-CA	5.45	131.53	122.54
3	C	226	PRO	CA-C-N	5.45	131.31	122.53
3	C	226	PRO	C-N-CA	5.45	131.31	122.53
2	B	501	LEU	N-CA-CB	5.45	118.14	110.24
2	B	379	ARG	CA-CB-CG	5.45	124.99	114.10
5	E	208	LEU	CA-C-N	5.45	128.39	120.98
5	E	208	LEU	C-N-CA	5.45	128.39	120.98
2	B	291	ASP	CA-CB-CG	5.44	118.04	112.60
6	F	82	GLU	CA-C-N	5.44	129.66	122.42
6	F	82	GLU	C-N-CA	5.44	129.66	122.42
2	B	1117	HIS	CE1-NE2-CD2	-5.44	103.56	109.00
7	G	109	SER	N-CA-CB	5.44	118.13	110.36
1	A	836	PHE	N-CA-CB	5.43	117.89	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	472	ARG	NE-CZ-NH2	5.43	124.09	119.20
11	K	87	PHE	CA-C-N	5.43	127.50	120.44
11	K	87	PHE	C-N-CA	5.43	127.50	120.44
1	A	1148	ALA	CA-C-N	5.43	129.26	121.71
1	A	1148	ALA	C-N-CA	5.43	129.26	121.71
2	B	380	ARG	CG-CD-NE	5.43	123.95	112.00
1	A	1258	ARG	NE-CZ-NH2	5.43	124.08	119.20
3	C	206	SER	N-CA-CB	5.43	118.02	110.26
11	K	31	CYS	CA-C-N	5.43	130.57	122.86
11	K	31	CYS	C-N-CA	5.43	130.57	122.86
17	Q	201	ARG	CA-C-N	5.42	127.81	120.44
17	Q	201	ARG	C-N-CA	5.42	127.81	120.44
17	Q	686	ASN	CA-C-N	5.42	127.55	120.28
17	Q	686	ASN	C-N-CA	5.42	127.55	120.28
25	Z	272	ASN	CA-C-N	5.42	130.76	122.95
25	Z	272	ASN	C-N-CA	5.42	130.76	122.95
3	C	228	ARG	CD-NE-CZ	5.42	131.99	124.40
1	A	1022	ILE	CA-C-N	5.42	129.25	122.48
1	A	1022	ILE	C-N-CA	5.42	129.25	122.48
8	H	75	TYR	CA-C-N	5.42	128.81	122.52
8	H	75	TYR	C-N-CA	5.42	128.81	122.52
1	A	244	ARG	NE-CZ-NH2	5.42	124.07	119.20
2	B	295	PRO	CA-C-N	5.42	127.48	120.44
2	B	295	PRO	C-N-CA	5.42	127.48	120.44
3	C	38	PHE	CA-CB-CG	5.42	119.22	113.80
27	f	82	THR	CA-C-N	5.42	127.98	120.29
27	f	82	THR	C-N-CA	5.42	127.98	120.29
1	A	393	ILE	CA-C-N	5.42	129.13	121.66
1	A	393	ILE	C-N-CA	5.42	129.13	121.66
1	A	1096	GLY	CA-C-N	5.42	126.49	119.78
1	A	1096	GLY	C-N-CA	5.42	126.49	119.78
3	C	235	SER	N-CA-CB	5.42	117.97	110.17
26	a	83	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	A	830	GLY	CA-C-N	5.41	130.18	122.72
1	A	830	GLY	C-N-CA	5.41	130.18	122.72
25	Z	627	LYS	CA-C-N	5.41	127.53	120.28
25	Z	627	LYS	C-N-CA	5.41	127.53	120.28
2	B	305	LEU	CA-C-N	5.41	127.52	120.28
2	B	305	LEU	C-N-CA	5.41	127.52	120.28
4	D	96	GLU	CA-C-N	5.41	127.97	120.29
4	D	96	GLU	C-N-CA	5.41	127.97	120.29
17	Q	220	ALA	CA-C-N	5.41	127.97	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	220	ALA	C-N-CA	5.41	127.97	120.29
2	B	797	ASN	O-C-N	-5.40	116.37	123.02
1	A	465	HIS	CE1-NE2-CD2	-5.40	103.60	109.00
1	A	403	GLN	N-CA-CB	5.40	117.84	110.01
20	U	408	GLY	CA-C-N	5.40	127.96	120.29
20	U	408	GLY	C-N-CA	5.40	127.96	120.29
3	C	19	VAL	CA-C-N	5.40	130.61	123.05
3	C	19	VAL	C-N-CA	5.40	130.61	123.05
1	A	836	PHE	CA-C-N	5.40	127.46	120.44
1	A	836	PHE	C-N-CA	5.40	127.46	120.44
5	E	202	ARG	CD-NE-CZ	5.40	131.96	124.40
20	U	387	ARG	CA-CB-CG	5.40	124.89	114.10
25	Z	707	GLY	CA-C-N	5.40	131.56	122.87
25	Z	707	GLY	C-N-CA	5.40	131.56	122.87
3	C	66	HIS	CB-CG-CD2	-5.39	124.19	131.20
7	G	169	GLY	CA-C-N	5.39	128.53	120.87
7	G	169	GLY	C-N-CA	5.39	128.53	120.87
11	K	10	PHE	CA-C-N	5.39	129.79	122.19
11	K	10	PHE	C-N-CA	5.39	129.79	122.19
26	a	128	ARG	CD-NE-CZ	5.39	131.95	124.40
2	B	356	PHE	CA-C-N	5.39	130.65	122.08
2	B	356	PHE	C-N-CA	5.39	130.65	122.08
9	I	14	ILE	N-CA-CB	5.39	116.80	110.82
14	N	57	DT	OP1-P-OP2	5.39	136.16	120.00
9	I	103	ARG	CA-CB-CG	5.38	124.87	114.10
3	C	156	GLY	CA-C-N	5.38	131.27	122.07
3	C	156	GLY	C-N-CA	5.38	131.27	122.07
13	M	1256	ARG	N-CA-C	5.38	113.19	108.78
2	B	699	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	A	789	GLY	CA-C-N	5.38	129.56	122.30
1	A	789	GLY	C-N-CA	5.38	129.56	122.30
2	B	983	GLU	N-CA-CB	5.38	117.81	110.01
3	C	228	ARG	CA-C-N	5.38	129.56	122.30
3	C	228	ARG	C-N-CA	5.38	129.56	122.30
3	C	266	GLU	CA-C-N	5.38	127.28	120.72
3	C	266	GLU	C-N-CA	5.38	127.28	120.72
1	A	96	HIS	ND1-CG-CD2	-5.37	100.73	106.10
1	A	421	ARG	CA-CB-CG	5.37	124.84	114.10
1	A	691	ASP	CA-C-N	5.37	130.80	122.26
1	A	691	ASP	C-N-CA	5.37	130.80	122.26
17	Q	732	LYS	CA-C-N	5.37	130.62	122.56
17	Q	732	LYS	C-N-CA	5.37	130.62	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	425	GLY	CA-C-N	5.37	130.35	122.77
18	R	425	GLY	C-N-CA	5.37	130.35	122.77
18	R	516	LEU	CA-C-N	5.37	127.48	120.28
18	R	516	LEU	C-N-CA	5.37	127.48	120.28
1	A	523	ARG	CA-C-N	5.37	130.97	122.60
1	A	523	ARG	C-N-CA	5.37	130.97	122.60
9	I	22	ASN	CA-C-N	5.37	129.50	121.72
9	I	22	ASN	C-N-CA	5.37	129.50	121.72
11	K	21	ILE	CA-C-N	5.36	130.33	122.77
11	K	21	ILE	C-N-CA	5.36	130.33	122.77
13	M	1394	THR	CA-C-N	5.36	130.71	122.77
13	M	1394	THR	C-N-CA	5.36	130.71	122.77
1	A	828	LEU	CA-C-N	5.36	128.46	120.31
1	A	828	LEU	C-N-CA	5.36	128.46	120.31
8	H	64	LEU	CA-C-N	5.36	129.16	121.50
8	H	64	LEU	C-N-CA	5.36	129.16	121.50
2	B	286	GLU	CA-CB-CG	5.36	124.82	114.10
1	A	1031	ARG	CA-CB-CG	5.36	124.81	114.10
3	C	257	SER	CA-C-N	5.36	127.41	120.44
3	C	257	SER	C-N-CA	5.36	127.41	120.44
22	W	87	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
6	F	91	LEU	CA-C-N	5.36	127.31	120.56
6	F	91	LEU	C-N-CA	5.36	127.31	120.56
20	U	498	SER	N-CA-CB	5.36	118.96	110.87
1	A	1375	ARG	N-CA-CB	5.35	117.83	110.07
2	B	406	GLY	CA-C-N	5.35	128.45	120.31
2	B	406	GLY	C-N-CA	5.35	128.45	120.31
1	A	710	LYS	CA-CB-CG	5.35	124.80	114.10
25	Z	214	SER	CA-C-N	5.35	130.22	123.10
25	Z	214	SER	C-N-CA	5.35	130.22	123.10
18	R	529	GLN	CA-C-N	5.35	127.44	120.28
18	R	529	GLN	C-N-CA	5.35	127.44	120.28
11	K	18	LYS	N-CA-CB	5.35	117.72	109.91
1	A	886	VAL	N-CA-CB	5.34	116.94	110.95
25	Z	513	VAL	CA-C-N	5.34	127.92	120.65
25	Z	513	VAL	C-N-CA	5.34	127.92	120.65
1	A	823	VAL	N-CA-CB	5.34	116.75	110.82
1	A	1250	ASP	CA-C-N	5.34	131.88	122.42
1	A	1250	ASP	C-N-CA	5.34	131.88	122.42
15	O	216	PRO	N-CA-CB	5.34	106.00	103.22
17	Q	810	ALA	CA-C-N	5.34	127.44	120.28
17	Q	810	ALA	C-N-CA	5.34	127.44	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	554	PHE	CA-C-N	5.34	130.95	122.94
1	A	554	PHE	C-N-CA	5.34	130.95	122.94
1	A	909	LEU	N-CA-CB	5.34	117.81	109.85
13	M	1364	LEU	CA-C-N	5.34	130.53	123.05
13	M	1364	LEU	C-N-CA	5.34	130.53	123.05
28	c	41	GLU	CA-C-N	5.34	131.47	122.87
28	c	41	GLU	C-N-CA	5.34	131.47	122.87
17	Q	127	ASP	CA-C-N	5.34	127.97	120.28
17	Q	127	ASP	C-N-CA	5.34	127.97	120.28
17	Q	216	LYS	CA-C-N	5.34	127.87	120.29
17	Q	216	LYS	C-N-CA	5.34	127.87	120.29
3	C	107	CYS	N-CA-CB	5.34	117.98	110.24
24	Y	21	LEU	N-CA-CB	5.34	118.35	109.60
26	e	106	ASP	CA-C-N	5.33	127.69	120.65
26	e	106	ASP	C-N-CA	5.33	127.69	120.65
2	B	684	GLU	CA-C-N	5.33	130.43	122.86
2	B	684	GLU	C-N-CA	5.33	130.43	122.86
2	B	894	THR	CA-C-N	5.33	131.18	122.81
2	B	894	THR	C-N-CA	5.33	131.18	122.81
20	U	411	ARG	CD-NE-CZ	5.33	131.86	124.40
25	Z	433	LEU	CA-C-N	5.33	128.76	120.34
25	Z	433	LEU	C-N-CA	5.33	128.76	120.34
1	A	96	HIS	CG-CD2-NE2	5.33	112.53	107.20
12	L	31	ARG	CG-CD-NE	5.33	123.72	112.00
27	b	86	VAL	CA-C-N	5.33	127.98	120.42
27	b	86	VAL	C-N-CA	5.33	127.98	120.42
1	A	695	ASP	CA-C-N	5.32	131.71	121.54
1	A	695	ASP	C-N-CA	5.32	131.71	121.54
1	A	1224	ARG	CG-CD-NE	5.32	123.71	112.00
18	R	408	VAL	CA-C-N	5.32	130.11	122.45
18	R	408	VAL	C-N-CA	5.32	130.11	122.45
26	e	55	GLN	CA-C-N	5.32	129.73	120.68
26	e	55	GLN	C-N-CA	5.32	129.73	120.68
6	F	100	ARG	CA-C-N	5.32	130.56	122.37
6	F	100	ARG	C-N-CA	5.32	130.56	122.37
11	K	18	LYS	CA-C-N	5.32	130.36	122.71
11	K	18	LYS	C-N-CA	5.32	130.36	122.71
27	f	60	VAL	N-CA-CB	5.31	116.41	110.51
1	A	195	GLY	CA-C-N	5.31	130.28	121.99
1	A	195	GLY	C-N-CA	5.31	130.28	121.99
1	A	1024	ASN	N-CA-CB	5.31	117.78	109.97
1	A	538	VAL	N-CA-C	5.31	120.38	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	155	LYS	CA-C-N	5.31	130.74	122.30
3	C	155	LYS	C-N-CA	5.31	130.74	122.30
13	M	1404	ASP	CA-C-N	5.31	131.46	122.65
13	M	1404	ASP	C-N-CA	5.31	131.46	122.65
2	B	917	LYS	CA-C-N	5.31	130.25	121.86
2	B	917	LYS	C-N-CA	5.31	130.25	121.86
17	Q	713	LYS	CA-CB-CG	5.31	124.71	114.10
1	A	529	GLN	CA-C-N	5.30	129.88	121.18
1	A	529	GLN	C-N-CA	5.30	129.88	121.18
1	A	1059	ARG	CD-NE-CZ	5.30	131.83	124.40
6	F	67	GLY	CA-C-N	5.30	127.65	120.44
6	F	67	GLY	C-N-CA	5.30	127.65	120.44
24	Y	25	ILE	CA-C-N	5.30	127.82	120.29
24	Y	25	ILE	C-N-CA	5.30	127.82	120.29
28	g	118	LYS	CB-CG-CD	5.30	123.49	111.30
3	C	195	THR	CA-C-N	5.30	130.30	123.10
3	C	195	THR	C-N-CA	5.30	130.30	123.10
9	I	33	ARG	CA-C-N	5.30	130.23	123.03
9	I	33	ARG	C-N-CA	5.30	130.23	123.03
2	B	1009	GLN	CA-C-N	5.29	127.64	120.44
2	B	1009	GLN	C-N-CA	5.29	127.64	120.44
2	B	1167	ILE	O-C-N	-5.29	117.62	123.18
3	C	60	HIS	CA-C-N	5.29	132.92	121.64
3	C	60	HIS	C-N-CA	5.29	132.92	121.64
5	E	11	TRP	CA-C-N	5.29	127.32	120.44
5	E	11	TRP	C-N-CA	5.29	127.32	120.44
18	R	369	LEU	CA-C-N	5.29	127.37	120.28
18	R	369	LEU	C-N-CA	5.29	127.37	120.28
2	B	313	GLU	CA-C-N	5.29	127.36	120.28
2	B	313	GLU	C-N-CA	5.29	127.36	120.28
3	C	160	ARG	CD-NE-CZ	5.29	131.80	124.40
18	R	407	GLY	N-CA-C	5.29	118.86	111.14
18	R	503	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	1356	ARG	CA-C-N	5.28	130.79	122.34
1	A	1356	ARG	C-N-CA	5.28	130.79	122.34
2	B	274	ARG	NE-CZ-NH2	5.28	123.95	119.20
4	D	88	LEU	CA-C-N	5.28	127.89	120.28
4	D	88	LEU	C-N-CA	5.28	127.89	120.28
22	W	87	HIS	ND1-CG-CD2	-5.28	100.82	106.10
25	Z	440	ILE	CA-C-N	5.28	128.73	122.44
25	Z	440	ILE	C-N-CA	5.28	128.73	122.44
5	E	104	ILE	O-C-N	-5.28	115.25	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	33	GLU	CA-C-N	5.28	130.56	122.69
7	G	33	GLU	C-N-CA	5.28	130.56	122.69
2	B	494	LYS	CA-C-N	5.28	128.34	120.95
2	B	494	LYS	C-N-CA	5.28	128.34	120.95
7	G	170	LEU	N-CA-CB	5.27	117.72	109.97
25	Z	469	ARG	NE-CZ-NH2	5.27	123.95	119.20
27	b	53	GLU	N-CA-CB	5.27	117.87	110.12
25	Z	600	VAL	CA-C-N	5.27	130.85	122.74
25	Z	600	VAL	C-N-CA	5.27	130.85	122.74
1	A	415	GLY	CA-C-N	5.27	130.86	122.59
1	A	415	GLY	C-N-CA	5.27	130.86	122.59
1	A	1393	VAL	CA-C-N	5.27	128.35	120.87
1	A	1393	VAL	C-N-CA	5.27	128.35	120.87
2	B	1085	ARG	NE-CZ-NH2	5.27	123.94	119.20
17	Q	775	ASN	N-CA-CB	5.27	117.78	110.04
2	B	341	GLU	CA-C-N	5.27	127.90	120.42
2	B	341	GLU	C-N-CA	5.27	127.90	120.42
1	A	1284	PHE	N-CA-CB	5.26	117.95	110.16
3	C	188	PRO	CA-C-N	5.26	128.95	121.42
3	C	188	PRO	C-N-CA	5.26	128.95	121.42
1	A	1455	SER	CA-C-N	5.26	127.28	120.44
1	A	1455	SER	C-N-CA	5.26	127.28	120.44
2	B	831	LYS	CA-CB-CG	5.26	124.63	114.10
1	A	1294	THR	CA-C-N	5.26	130.33	122.86
1	A	1294	THR	C-N-CA	5.26	130.33	122.86
2	B	46	SER	CA-C-N	5.26	127.28	120.44
2	B	46	SER	C-N-CA	5.26	127.28	120.44
2	B	987	GLY	CA-C-N	5.26	127.76	120.29
2	B	987	GLY	C-N-CA	5.26	127.76	120.29
5	E	192	LYS	CA-C-N	5.26	130.45	122.98
5	E	192	LYS	C-N-CA	5.26	130.45	122.98
26	e	103	LEU	N-CA-CB	5.26	117.64	110.01
2	B	361	LYS	CA-C-N	5.26	127.59	120.44
2	B	361	LYS	C-N-CA	5.26	127.59	120.44
21	V	82	VAL	CA-C-N	5.26	128.81	121.24
21	V	82	VAL	C-N-CA	5.26	128.81	121.24
26	a	105	GLU	CA-C-N	5.26	127.85	120.28
26	a	105	GLU	C-N-CA	5.26	127.85	120.28
8	H	24	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	A	813	ASP	CA-C-N	5.26	131.07	123.13
1	A	813	ASP	C-N-CA	5.26	131.07	123.13
1	A	839	HIS	CG-CD2-NE2	5.25	112.45	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	77	PHE	CA-C-N	5.25	130.17	122.66
7	G	77	PHE	C-N-CA	5.25	130.17	122.66
13	M	1379	ASP	CA-C-N	5.25	128.64	120.34
13	M	1379	ASP	C-N-CA	5.25	128.64	120.34
20	U	383	SER	CA-C-N	5.25	128.42	120.75
20	U	383	SER	C-N-CA	5.25	128.42	120.75
29	h	89	ARG	CD-NE-CZ	5.25	131.76	124.40
1	A	271	ARG	CA-CB-CG	5.25	124.60	114.10
6	F	115	TYR	CA-C-N	5.25	130.83	122.74
6	F	115	TYR	C-N-CA	5.25	130.83	122.74
1	A	1067	TRP	N-CA-CB	5.25	117.76	109.94
1	A	1173	THR	CA-C-N	5.25	131.94	123.33
1	A	1173	THR	C-N-CA	5.25	131.94	123.33
2	B	917	LYS	CA-CB-CG	5.25	124.60	114.10
17	Q	224	ALA	CA-C-N	5.25	128.29	120.31
17	Q	224	ALA	C-N-CA	5.25	128.29	120.31
27	f	39	ARG	NE-CZ-NH2	5.25	123.92	119.20
2	B	1117	HIS	CG-CD2-NE2	5.25	112.45	107.20
13	M	475	ILE	CA-C-N	5.25	124.86	119.56
13	M	475	ILE	C-N-CA	5.25	124.86	119.56
18	R	560	ILE	CA-C-N	5.25	127.31	120.28
18	R	560	ILE	C-N-CA	5.25	127.31	120.28
21	V	105	GLU	CA-C-N	5.25	127.84	120.28
21	V	105	GLU	C-N-CA	5.25	127.84	120.28
21	V	131	MET	CA-C-N	5.25	131.35	122.12
21	V	131	MET	C-N-CA	5.25	131.35	122.12
17	Q	781	ASN	CA-C-N	5.25	127.31	120.28
17	Q	781	ASN	C-N-CA	5.25	127.31	120.28
3	C	10	ARG	CA-CB-CG	5.24	124.59	114.10
1	A	861	GLN	N-CA-CB	5.24	117.82	110.12
13	M	976	ALA	CA-C-N	5.24	128.37	123.08
13	M	976	ALA	C-N-CA	5.24	128.37	123.08
14	N	76	DC	O5'-C5'-C4'	5.24	118.66	110.80
1	A	465	HIS	CG-CD2-NE2	5.24	112.44	107.20
1	A	465	HIS	ND1-CG-CD2	-5.24	100.86	106.10
9	I	43	ASP	CA-C-N	5.24	130.55	123.11
9	I	43	ASP	C-N-CA	5.24	130.55	123.11
19	T	-86	DA	O5'-C5'-C4'	5.24	118.65	110.80
1	A	76	GLY	N-CA-C	5.23	119.91	111.38
2	B	1117	HIS	ND1-CG-CD2	-5.23	100.87	106.10
13	M	1353	ILE	CA-C-N	5.23	130.06	123.10
13	M	1353	ILE	C-N-CA	5.23	130.06	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	39	U	C5'-C4'-C3'	-5.23	108.15	116.00
17	Q	667	ARG	CD-NE-CZ	5.23	131.73	124.40
1	A	264	VAL	CA-C-N	5.23	131.06	122.64
1	A	264	VAL	C-N-CA	5.23	131.06	122.64
1	A	618	TYR	CA-C-N	5.23	127.24	120.44
1	A	618	TYR	C-N-CA	5.23	127.24	120.44
1	A	1346	VAL	CA-C-N	5.23	127.55	120.38
1	A	1346	VAL	C-N-CA	5.23	127.55	120.38
20	U	438	ALA	CA-C-N	5.23	130.48	122.95
20	U	438	ALA	C-N-CA	5.23	130.48	122.95
24	Y	10	LEU	CA-C-N	5.23	129.56	122.19
24	Y	10	LEU	C-N-CA	5.23	129.56	122.19
1	A	63	GLY	N-CA-C	5.23	118.14	112.29
2	B	297	MET	CA-C-N	5.23	127.74	120.63
2	B	297	MET	C-N-CA	5.23	127.74	120.63
1	A	822	PHE	CA-C-N	5.23	129.02	121.18
1	A	822	PHE	C-N-CA	5.23	129.02	121.18
1	A	1281	ASP	CA-C-N	5.23	127.74	120.63
1	A	1281	ASP	C-N-CA	5.23	127.74	120.63
1	A	598	GLY	CA-C-N	5.22	130.41	123.20
1	A	598	GLY	C-N-CA	5.22	130.41	123.20
1	A	837	PHE	N-CA-CB	5.22	117.59	110.01
2	B	552	ASN	N-CA-CB	5.22	118.23	110.29
3	C	174	ALA	CA-C-N	5.22	127.80	120.28
3	C	174	ALA	C-N-CA	5.22	127.80	120.28
11	K	72	ILE	CA-C-N	5.22	130.13	123.13
11	K	72	ILE	C-N-CA	5.22	130.13	123.13
1	A	248	MET	CA-CB-CG	5.22	124.54	114.10
1	A	541	THR	N-CA-CB	5.22	117.89	110.16
21	V	110	GLU	CA-CB-CG	5.22	124.54	114.10
2	B	1014	LEU	CA-C-N	5.22	127.28	120.28
2	B	1014	LEU	C-N-CA	5.22	127.28	120.28
3	C	194	HIS	CA-C-N	5.22	130.77	122.94
3	C	194	HIS	C-N-CA	5.22	130.77	122.94
28	g	41	GLU	CA-C-N	5.22	130.50	122.93
28	g	41	GLU	C-N-CA	5.22	130.50	122.93
1	A	1374	VAL	CB-CA-C	-5.22	105.21	112.04
1	A	1432	PHE	CA-C-N	5.22	130.72	121.80
1	A	1432	PHE	C-N-CA	5.22	130.72	121.80
11	K	15	GLY	CA-C-N	5.22	128.25	120.95
11	K	15	GLY	C-N-CA	5.22	128.25	120.95
19	T	-103	DG	O4'-C1'-N9	5.22	116.22	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	69	ARG	NE-CZ-NH2	5.22	123.89	119.20
1	A	810	PHE	CA-C-N	5.21	130.98	122.69
1	A	810	PHE	C-N-CA	5.21	130.98	122.69
4	D	70	ARG	CA-C-N	5.21	130.67	122.49
4	D	70	ARG	C-N-CA	5.21	130.67	122.49
17	Q	182	ALA	CA-C-N	5.21	127.27	120.28
17	Q	182	ALA	C-N-CA	5.21	127.27	120.28
18	R	506	PRO	N-CA-C	5.21	117.06	110.70
28	c	42	ARG	CD-NE-CZ	5.21	131.70	124.40
1	A	438	LEU	CA-C-N	5.21	128.75	121.24
1	A	438	LEU	C-N-CA	5.21	128.75	121.24
2	B	1015	LEU	N-CA-CB	5.21	117.78	110.12
17	Q	217	ALA	CA-C-N	5.21	127.22	120.44
17	Q	217	ALA	C-N-CA	5.21	127.22	120.44
20	U	415	LYS	CB-CA-C	5.21	117.78	109.02
26	e	93	GLN	N-CA-CB	5.21	117.52	109.91
29	h	79	HIS	ND1-CG-CD2	-5.21	100.89	106.10
14	N	57	DT	O5'-C5'-C4'	5.21	118.61	110.80
18	R	534	GLN	CA-C-N	5.21	127.12	120.56
18	R	534	GLN	C-N-CA	5.21	127.12	120.56
1	A	1068	LEU	N-CA-CB	5.21	117.56	110.01
2	B	1077	GLY	N-CA-C	5.21	119.24	112.68
5	E	153	LYS	CA-CB-CG	5.21	124.51	114.10
1	A	1421	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	1162	GLU	N-CA-CB	5.20	117.62	109.97
18	R	544	GLU	CA-C-N	5.20	127.68	120.29
18	R	544	GLU	C-N-CA	5.20	127.68	120.29
26	a	105	GLU	CA-CB-CG	5.20	124.51	114.10
1	A	394	VAL	N-CA-CB	5.20	116.20	110.53
1	A	839	HIS	ND1-CG-CD2	-5.20	100.90	106.10
2	B	997	GLY	CA-C-N	5.20	130.33	123.05
2	B	997	GLY	C-N-CA	5.20	130.33	123.05
8	H	84	ARG	CB-CG-CD	5.20	123.26	111.30
14	N	62	DC	O5'-C5'-C4'	5.20	118.60	110.80
17	Q	692	VAL	CA-C-N	5.20	127.68	120.29
17	Q	692	VAL	C-N-CA	5.20	127.68	120.29
1	A	843	GLY	CA-C-N	5.20	128.22	120.31
1	A	843	GLY	C-N-CA	5.20	128.22	120.31
7	G	40	GLY	CA-C-N	5.20	130.36	122.56
7	G	40	GLY	C-N-CA	5.20	130.36	122.56
29	d	40	LYS	CA-CB-CG	5.20	124.50	114.10
5	E	137	ILE	CA-C-N	5.20	130.05	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	137	ILE	C-N-CA	5.20	130.05	122.41
26	e	69	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A	444	TYR	CA-C-N	5.20	130.32	122.99
1	A	444	TYR	C-N-CA	5.20	130.32	122.99
3	C	102	THR	CA-C-N	5.20	130.33	123.00
3	C	102	THR	C-N-CA	5.20	130.33	123.00
2	B	357	CYS	CA-C-N	5.20	127.76	120.28
2	B	357	CYS	C-N-CA	5.20	127.76	120.28
1	A	553	VAL	CA-C-N	5.19	130.31	122.99
1	A	553	VAL	C-N-CA	5.19	130.31	122.99
1	A	710	LYS	CA-C-N	5.19	127.67	120.29
1	A	710	LYS	C-N-CA	5.19	127.67	120.29
2	B	871	VAL	CA-C-N	5.19	128.85	121.42
2	B	871	VAL	C-N-CA	5.19	128.85	121.42
26	a	124	ILE	CA-C-N	5.19	127.24	120.28
26	a	124	ILE	C-N-CA	5.19	127.24	120.28
1	A	1149	ARG	CA-C-N	5.19	128.22	120.95
1	A	1149	ARG	C-N-CA	5.19	128.22	120.95
2	B	958	CYS	CA-C-N	5.19	132.32	123.03
2	B	958	CYS	C-N-CA	5.19	132.32	123.03
11	K	63	VAL	CA-C-O	-5.19	117.35	120.88
22	W	87	HIS	CG-CD2-NE2	5.19	112.39	107.20
2	B	45	ASP	CA-C-N	5.19	127.19	120.44
2	B	45	ASP	C-N-CA	5.19	127.19	120.44
1	A	737	PHE	N-CA-CB	5.19	117.48	109.91
25	Z	300	GLN	CB-CG-CD	5.19	121.42	112.60
3	C	259	LEU	N-CA-CB	5.18	117.67	109.94
18	R	536	GLN	CA-C-N	5.18	127.23	120.28
18	R	536	GLN	C-N-CA	5.18	127.23	120.28
13	M	584	VAL	N-CA-C	5.18	115.77	108.36
13	M	1400	GLU	CA-C-N	5.18	130.78	121.66
13	M	1400	GLU	C-N-CA	5.18	130.78	121.66
18	R	368	LYS	CA-C-N	5.18	127.65	120.29
18	R	368	LYS	C-N-CA	5.18	127.65	120.29
1	A	203	LYS	CA-CB-CG	5.18	124.46	114.10
2	B	473	LEU	CA-C-N	5.18	130.71	121.75
2	B	473	LEU	C-N-CA	5.18	130.71	121.75
2	B	550	MET	CA-CB-CG	5.18	124.46	114.10
5	E	91	CYS	CA-C-N	5.18	127.64	120.29
5	E	91	CYS	C-N-CA	5.18	127.64	120.29
1	A	1394	ASN	CA-C-N	5.18	127.73	120.28
1	A	1394	ASN	C-N-CA	5.18	127.73	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	539	GLN	OE1-CD-NE2	-5.17	117.42	122.60
1	A	1163	HIS	N-CA-CB	5.17	118.06	109.88
27	b	99	GLY	CA-C-N	5.17	130.31	122.08
27	b	99	GLY	C-N-CA	5.17	130.31	122.08
1	A	441	GLN	CA-C-N	5.17	127.21	120.28
1	A	441	GLN	C-N-CA	5.17	127.21	120.28
1	A	932	ARG	CA-C-N	5.17	129.26	120.88
1	A	932	ARG	C-N-CA	5.17	129.26	120.88
4	D	102	ASN	CA-C-N	5.17	127.63	120.29
4	D	102	ASN	C-N-CA	5.17	127.63	120.29
5	E	209	VAL	N-CA-CB	5.17	116.67	110.31
13	M	619	THR	CA-C-N	5.17	125.07	119.85
13	M	619	THR	C-N-CA	5.17	125.07	119.85
1	A	1001	PRO	CA-C-N	5.17	129.97	121.39
1	A	1001	PRO	C-N-CA	5.17	129.97	121.39
1	A	732	THR	CA-C-N	5.17	127.47	120.44
1	A	732	THR	C-N-CA	5.17	127.47	120.44
1	A	1160	ARG	CD-NE-CZ	5.17	131.63	124.40
2	B	338	TYR	N-CA-CB	5.17	117.47	109.98
2	B	1136	GLU	CA-C-N	5.17	130.93	123.13
2	B	1136	GLU	C-N-CA	5.17	130.93	123.13
5	E	164	LYS	CA-C-N	5.17	130.05	122.77
5	E	164	LYS	C-N-CA	5.17	130.05	122.77
2	B	380	ARG	CA-CB-CG	5.16	124.43	114.10
5	E	19	GLN	CA-C-N	5.16	127.65	120.63
5	E	19	GLN	C-N-CA	5.16	127.65	120.63
1	A	889	LEU	CA-C-N	5.16	131.09	122.73
1	A	889	LEU	C-N-CA	5.16	131.09	122.73
2	B	709	SER	CA-C-N	5.16	129.20	121.77
2	B	709	SER	C-N-CA	5.16	129.20	121.77
1	A	440	LEU	CA-C-N	5.16	133.10	123.09
1	A	440	LEU	C-N-CA	5.16	133.10	123.09
1	A	1146	GLN	CA-C-N	5.16	127.91	120.38
1	A	1146	GLN	C-N-CA	5.16	127.91	120.38
18	R	598	GLN	CA-C-N	5.16	129.72	122.09
18	R	598	GLN	C-N-CA	5.16	129.72	122.09
22	W	275	ASP	CA-C-N	5.16	128.17	120.95
22	W	275	ASP	C-N-CA	5.16	128.17	120.95
26	a	129	ARG	N-CA-CB	5.16	117.63	109.94
2	B	790	GLN	OE1-CD-NE2	-5.16	117.44	122.60
5	E	127	LEU	CA-C-N	5.16	130.80	122.29
5	E	127	LEU	C-N-CA	5.16	130.80	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	441	LEU	CA-C-N	5.16	129.26	122.30
25	Z	441	LEU	C-N-CA	5.16	129.26	122.30
24	Y	53	THR	CA-C-N	5.15	131.47	122.81
24	Y	53	THR	C-N-CA	5.15	131.47	122.81
1	A	16	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	A	1532	SER	CB-CA-C	5.15	115.08	110.44
18	R	371	ARG	CA-C-N	5.15	130.58	122.49
18	R	371	ARG	C-N-CA	5.15	130.58	122.49
18	R	487	PHE	CA-C-N	5.15	129.44	120.68
18	R	487	PHE	C-N-CA	5.15	129.44	120.68
25	Z	453	LYS	CA-CB-CG	5.15	124.41	114.10
25	Z	481	ILE	CA-C-N	5.15	130.40	122.93
25	Z	481	ILE	C-N-CA	5.15	130.40	122.93
2	B	316	VAL	CA-C-N	5.15	127.44	120.44
2	B	316	VAL	C-N-CA	5.15	127.44	120.44
2	B	446	TYR	N-CA-CB	5.15	117.64	110.07
2	B	608	ARG	CB-CG-CD	5.15	123.14	111.30
5	E	55	ARG	CA-CB-CG	5.15	124.40	114.10
1	A	689	ILE	N-CA-CB	5.15	116.22	110.51
3	C	155	LYS	CB-CG-CD	5.15	123.14	111.30
21	V	188	LYS	CA-CB-CG	5.15	124.40	114.10
17	Q	760	VAL	CA-C-N	5.15	127.13	120.44
17	Q	760	VAL	C-N-CA	5.15	127.13	120.44
25	Z	478	VAL	CA-C-N	5.15	130.58	123.07
25	Z	478	VAL	C-N-CA	5.15	130.58	123.07
5	E	162	ARG	CG-CD-NE	5.14	123.32	112.00
21	V	26	ARG	CG-CD-NE	5.14	123.32	112.00
26	e	79	LYS	CA-C-N	5.14	129.93	121.39
26	e	79	LYS	C-N-CA	5.14	129.93	121.39
26	e	93	GLN	CA-C-N	5.14	127.13	120.44
26	e	93	GLN	C-N-CA	5.14	127.13	120.44
1	A	550	LYS	CA-CB-CG	5.14	124.39	114.10
17	Q	667	ARG	CA-CB-CG	5.14	124.39	114.10
29	h	34	TYR	CA-C-N	5.14	127.17	120.28
29	h	34	TYR	C-N-CA	5.14	127.17	120.28
2	B	689	TYR	N-CA-CB	5.14	117.63	110.07
6	F	50	LYS	CA-C-N	5.14	129.18	121.72
6	F	50	LYS	C-N-CA	5.14	129.18	121.72
2	B	346	GLU	CA-C-N	5.14	128.77	121.42
2	B	346	GLU	C-N-CA	5.14	128.77	121.42
13	M	1379	ASP	N-CA-CB	5.14	117.76	110.46
1	A	839	HIS	N-CA-CB	5.14	117.67	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	89	PRO	CA-C-N	5.14	127.58	120.29
21	V	89	PRO	C-N-CA	5.14	127.58	120.29
27	b	89	ALA	CA-C-N	5.14	127.47	120.54
27	b	89	ALA	C-N-CA	5.14	127.47	120.54
2	B	762	ARG	NE-CZ-NH2	5.13	123.82	119.20
2	B	1021	HIS	N-CA-CB	5.13	117.55	109.69
17	Q	722	TYR	CA-C-N	5.13	127.42	120.44
17	Q	722	TYR	C-N-CA	5.13	127.42	120.44
21	V	314	ASN	CA-C-N	5.13	128.50	120.75
21	V	314	ASN	C-N-CA	5.13	128.50	120.75
1	A	906	LEU	CA-C-N	5.13	127.58	120.29
1	A	906	LEU	C-N-CA	5.13	127.58	120.29
2	B	988	LYS	CA-C-N	5.13	127.49	120.46
2	B	988	LYS	C-N-CA	5.13	127.49	120.46
21	V	226	ASP	CA-C-N	5.13	127.41	120.38
21	V	226	ASP	C-N-CA	5.13	127.41	120.38
1	A	1151	ALA	CA-C-N	5.13	127.42	120.44
1	A	1151	ALA	C-N-CA	5.13	127.42	120.44
2	B	1024	GLY	CA-C-N	5.13	129.00	120.94
2	B	1024	GLY	C-N-CA	5.13	129.00	120.94
2	B	865	VAL	CA-C-N	5.13	131.20	121.97
2	B	865	VAL	C-N-CA	5.13	131.20	121.97
7	G	144	ARG	CG-CD-NE	5.13	123.28	112.00
18	R	533	LYS	CA-C-N	5.13	127.57	120.29
18	R	533	LYS	C-N-CA	5.13	127.57	120.29
24	Y	113	THR	CA-C-N	5.13	128.75	121.42
24	Y	113	THR	C-N-CA	5.13	128.75	121.42
24	Y	27	GLN	CA-CB-CG	5.12	124.35	114.10
25	Z	630	VAL	CA-C-N	5.12	128.60	121.02
25	Z	630	VAL	C-N-CA	5.12	128.60	121.02
1	A	871	VAL	N-CA-CB	5.12	116.38	110.49
8	H	83	SER	CA-C-N	5.12	129.28	120.72
8	H	83	SER	C-N-CA	5.12	129.28	120.72
8	H	120	GLY	CA-C-N	5.12	129.94	122.41
8	H	120	GLY	C-N-CA	5.12	129.94	122.41
25	Z	438	GLY	CA-C-N	5.12	128.75	121.42
25	Z	438	GLY	C-N-CA	5.12	128.75	121.42
1	A	401	ARG	N-CA-CB	5.12	117.44	110.01
2	B	499	ARG	CA-CB-CG	5.12	124.34	114.10
25	Z	200	PHE	N-CA-CB	5.12	117.44	110.01
6	F	116	GLU	CA-C-N	5.12	129.41	122.19
6	F	116	GLU	C-N-CA	5.12	129.41	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	998	ASP	CA-C-N	5.12	131.13	122.79
2	B	998	ASP	C-N-CA	5.12	131.13	122.79
14	N	115	DA	C2'-C3'-O3'	5.12	119.17	111.50
1	A	284	VAL	N-CA-C	5.12	115.84	110.62
2	B	890	ARG	CA-CB-CG	5.12	124.33	114.10
2	B	935	PHE	CA-CB-CG	-5.12	108.69	113.80
6	F	94	MET	CA-C-N	5.12	127.09	120.44
6	F	94	MET	C-N-CA	5.12	127.09	120.44
1	A	213	LYS	CA-C-N	5.11	129.47	121.85
1	A	213	LYS	C-N-CA	5.11	129.47	121.85
17	Q	774	SER	CA-C-N	5.11	128.47	120.75
17	Q	774	SER	C-N-CA	5.11	128.47	120.75
26	a	87	SER	CA-C-N	5.11	127.55	120.29
26	a	87	SER	C-N-CA	5.11	127.55	120.29
17	Q	650	ALA	CA-C-N	5.11	127.08	120.44
17	Q	650	ALA	C-N-CA	5.11	127.08	120.44
18	R	537	ASP	CA-C-N	5.11	127.55	120.29
18	R	537	ASP	C-N-CA	5.11	127.55	120.29
16	P	36	U	O4'-C1'-C2'	-5.11	100.69	105.80
18	R	530	ASP	CA-C-N	5.11	127.08	120.44
18	R	530	ASP	C-N-CA	5.11	127.08	120.44
2	B	379	ARG	CG-CD-NE	5.10	123.23	112.00
9	I	27	LYS	CA-C-N	5.10	128.80	121.50
9	I	27	LYS	C-N-CA	5.10	128.80	121.50
6	F	124	ILE	CA-C-N	5.10	128.00	120.91
6	F	124	ILE	C-N-CA	5.10	128.00	120.91
2	B	191	GLU	CA-C-N	5.10	130.04	123.00
2	B	191	GLU	C-N-CA	5.10	130.04	123.00
3	C	234	GLU	CA-C-N	5.10	128.95	120.94
3	C	234	GLU	C-N-CA	5.10	128.95	120.94
17	Q	776	LEU	CA-C-N	5.10	127.11	120.28
17	Q	776	LEU	C-N-CA	5.10	127.11	120.28
1	A	99	PHE	CA-C-N	5.10	127.38	120.44
1	A	99	PHE	C-N-CA	5.10	127.38	120.44
25	Z	708	GLN	CA-C-N	5.10	129.12	121.72
25	Z	708	GLN	C-N-CA	5.10	129.12	121.72
27	b	36	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A	1167	ARG	CB-CG-CD	5.10	123.03	111.30
17	Q	646	ASN	CA-C-N	5.10	127.53	120.29
17	Q	646	ASN	C-N-CA	5.10	127.53	120.29
1	A	14	PRO	CA-C-N	5.09	129.18	122.30
1	A	14	PRO	C-N-CA	5.09	129.18	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1042	ASN	CA-C-N	5.09	126.98	120.56
1	A	1042	ASN	C-N-CA	5.09	126.98	120.56
14	N	126	DC	O5'-C5'-C4'	5.09	118.44	110.80
18	R	419	GLY	CA-C-N	5.09	129.85	121.39
18	R	419	GLY	C-N-CA	5.09	129.85	121.39
26	e	72	ARG	NE-CZ-NH2	5.09	123.78	119.20
17	Q	681	SER	CA-C-N	5.09	127.52	120.29
17	Q	681	SER	C-N-CA	5.09	127.52	120.29
17	Q	794	SER	CA-C-N	5.09	127.52	120.29
17	Q	794	SER	C-N-CA	5.09	127.52	120.29
27	b	57	VAL	N-CA-CB	5.09	116.51	110.55
2	B	970	HIS	CB-CG-CD2	-5.09	124.58	131.20
20	U	473	ILE	CA-C-N	5.09	131.28	122.32
20	U	473	ILE	C-N-CA	5.09	131.28	122.32
26	e	131	ARG	NE-CZ-NH2	5.09	123.78	119.20
17	Q	832	ARG	CG-CD-NE	5.09	123.19	112.00
2	B	768	ARG	CA-C-N	5.09	129.33	120.68
2	B	768	ARG	C-N-CA	5.09	129.33	120.68
7	G	11	ILE	CA-C-N	5.09	130.23	122.65
7	G	11	ILE	C-N-CA	5.09	130.23	122.65
7	G	104	MET	CA-C-N	5.09	131.29	122.64
7	G	104	MET	C-N-CA	5.09	131.29	122.64
14	N	42	DT	C4'-C3'-O3'	5.09	117.63	110.00
17	Q	675	GLU	CA-CB-CG	5.08	124.27	114.10
1	A	1045	LEU	N-CA-CB	5.08	117.59	110.12
9	I	29	ASP	N-CA-CB	5.08	118.07	109.94
18	R	424	LYS	CA-CB-CG	5.08	124.27	114.10
25	Z	240	GLU	N-CA-CB	5.08	118.16	109.87
27	f	92	ARG	NE-CZ-NH2	5.08	123.78	119.20
1	A	711	GLN	CA-C-N	5.08	127.05	120.44
1	A	711	GLN	C-N-CA	5.08	127.05	120.44
1	A	1072	ILE	N-CA-CB	5.08	116.50	110.55
2	B	1017	ASP	CA-C-N	5.08	130.93	122.54
2	B	1017	ASP	C-N-CA	5.08	130.93	122.54
3	C	150	ILE	CA-C-N	5.08	130.42	123.46
3	C	150	ILE	C-N-CA	5.08	130.42	123.46
17	Q	834	GLN	CA-C-N	5.08	127.05	120.44
17	Q	834	GLN	C-N-CA	5.08	127.05	120.44
18	R	547	GLU	CA-C-N	5.08	127.09	120.28
18	R	547	GLU	C-N-CA	5.08	127.09	120.28
1	A	1123	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	A	1375	ARG	CA-C-N	5.08	127.04	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1375	ARG	C-N-CA	5.08	127.04	120.44
18	R	484	ASN	CA-C-N	5.08	129.08	121.72
18	R	484	ASN	C-N-CA	5.08	129.08	121.72
2	B	84	TYR	CA-C-N	5.08	130.18	122.56
2	B	84	TYR	C-N-CA	5.08	130.18	122.56
2	B	976	MET	CA-C-N	5.08	129.56	122.05
2	B	976	MET	C-N-CA	5.08	129.56	122.05
2	B	1035	ARG	CA-CB-CG	5.08	124.25	114.10
18	R	371	ARG	CD-NE-CZ	5.08	131.51	124.40
1	A	10	ASP	CA-C-N	5.08	129.84	122.08
1	A	10	ASP	C-N-CA	5.08	129.84	122.08
1	A	588	GLY	CA-C-N	5.08	127.08	120.28
1	A	588	GLY	C-N-CA	5.08	127.08	120.28
2	B	1091	ARG	CA-C-N	5.08	127.08	120.28
2	B	1091	ARG	C-N-CA	5.08	127.08	120.28
18	R	486	LYS	CA-C-N	5.08	129.69	122.08
18	R	486	LYS	C-N-CA	5.08	129.69	122.08
20	U	474	ARG	CA-C-N	5.08	130.21	122.65
20	U	474	ARG	C-N-CA	5.08	130.21	122.65
26	a	127	ALA	CA-C-N	5.08	127.34	120.44
26	a	127	ALA	C-N-CA	5.08	127.34	120.44
2	B	821	LYS	N-CA-CB	5.07	117.43	110.07
9	I	76	PRO	CA-C-N	5.07	130.90	122.73
9	I	76	PRO	C-N-CA	5.07	130.90	122.73
17	Q	725	ARG	CA-C-N	5.07	131.73	122.50
17	Q	725	ARG	C-N-CA	5.07	131.73	122.50
24	Y	26	ASP	CA-C-N	5.07	127.49	120.29
24	Y	26	ASP	C-N-CA	5.07	127.49	120.29
1	A	317	MET	N-CA-CB	5.07	117.36	110.01
1	A	1092	ALA	CA-C-N	5.07	127.49	120.29
1	A	1092	ALA	C-N-CA	5.07	127.49	120.29
3	C	240	ARG	CA-C-N	5.07	124.73	119.56
3	C	240	ARG	C-N-CA	5.07	124.73	119.56
1	A	1019	LYS	CA-C-N	5.07	129.55	122.05
1	A	1019	LYS	C-N-CA	5.07	129.55	122.05
28	g	29	ARG	NE-CZ-NH2	5.07	123.76	119.20
6	F	95	LYS	N-CA-CB	5.07	117.36	110.01
21	V	306	ARG	CA-C-N	5.07	129.71	122.21
21	V	306	ARG	C-N-CA	5.07	129.71	122.21
6	F	82	GLU	N-CA-CB	5.07	117.44	109.69
17	Q	666	ALA	CA-C-N	5.07	127.07	120.28
17	Q	666	ALA	C-N-CA	5.07	127.07	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1006	VAL	CA-C-N	5.06	130.91	122.20
2	B	1006	VAL	C-N-CA	5.06	130.91	122.20
2	B	573	TRP	N-CA-CB	5.06	117.65	110.46
6	F	95	LYS	CA-C-N	5.06	127.06	120.28
6	F	95	LYS	C-N-CA	5.06	127.06	120.28
17	Q	221	PHE	CA-C-N	5.06	127.02	120.44
17	Q	221	PHE	C-N-CA	5.06	127.02	120.44
17	Q	764	LEU	N-CA-CB	5.06	117.65	110.16
17	Q	727	LEU	CA-C-N	5.06	129.72	121.98
17	Q	727	LEU	C-N-CA	5.06	129.72	121.98
21	V	310	GLY	N-CA-C	5.06	120.05	111.19
2	B	340	LYS	CA-CB-CG	5.06	124.22	114.10
2	B	718	GLN	N-CA-CB	5.06	117.39	109.85
20	U	411	ARG	CA-C-N	5.06	128.00	120.31
20	U	411	ARG	C-N-CA	5.06	128.00	120.31
25	Z	439	LYS	N-CA-CB	5.06	117.70	110.06
10	J	64	PRO	CA-C-N	5.06	130.53	122.94
10	J	64	PRO	C-N-CA	5.06	130.53	122.94
17	Q	806	ASP	CA-C-N	5.06	130.90	122.66
17	Q	806	ASP	C-N-CA	5.06	130.90	122.66
3	C	267	ILE	N-CA-CB	5.05	116.36	110.65
5	E	138	ASN	N-CA-CB	5.05	117.88	110.35
8	H	71	ASP	CA-C-N	5.05	129.22	120.58
8	H	71	ASP	C-N-CA	5.05	129.22	120.58
1	A	529	GLN	CA-CB-CG	5.05	124.20	114.10
3	C	113	ARG	CD-NE-CZ	5.05	131.47	124.40
29	h	89	ARG	N-CA-CB	5.05	117.33	110.01
1	A	1462	GLN	CA-CB-CG	5.05	124.20	114.10
2	B	819	SER	CA-C-N	5.05	130.25	122.77
2	B	819	SER	C-N-CA	5.05	130.25	122.77
17	Q	784	LYS	CA-C-N	5.05	127.00	120.44
17	Q	784	LYS	C-N-CA	5.05	127.00	120.44
22	W	63	HIS	CA-C-N	5.05	127.00	120.44
22	W	63	HIS	C-N-CA	5.05	127.00	120.44
12	L	51	ARG	CA-CB-CG	5.05	124.20	114.10
1	A	1162	GLU	CA-CB-CG	5.05	124.19	114.10
2	B	497	LYS	CB-CG-CD	5.05	122.91	111.30
3	C	64	ILE	CA-C-N	5.05	127.04	120.28
3	C	64	ILE	C-N-CA	5.05	127.04	120.28
18	R	416	GLN	CA-C-N	5.05	130.79	123.12
18	R	416	GLN	C-N-CA	5.05	130.79	123.12
18	R	427	GLN	N-CA-CB	5.05	117.63	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	86	VAL	N-CA-CB	5.05	116.11	110.51
1	A	226	LYS	N-CA-CB	5.04	117.63	110.06
20	U	409	ARG	CG-CD-NE	5.04	123.10	112.00
2	B	840	MET	CA-CB-CG	5.04	124.19	114.10
6	F	71	LEU	N-CA-CB	5.04	117.32	110.01
7	G	84	VAL	CA-C-N	5.04	130.89	122.57
7	G	84	VAL	C-N-CA	5.04	130.89	122.57
17	Q	795	TYR	N-CA-CB	5.04	117.62	110.16
1	A	95	PHE	CA-C-N	5.04	130.02	122.86
1	A	95	PHE	C-N-CA	5.04	130.02	122.86
25	Z	448	ILE	N-CA-C	5.04	115.26	110.42
25	Z	512	LYS	CA-C-N	5.04	130.68	123.27
25	Z	512	LYS	C-N-CA	5.04	130.68	123.27
2	B	157	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	A	80	GLU	CA-CB-CG	5.04	124.18	114.10
2	B	452	ASN	CA-C-N	5.04	129.51	122.05
2	B	452	ASN	C-N-CA	5.04	129.51	122.05
1	A	103	THR	CA-C-N	5.04	127.03	120.28
1	A	103	THR	C-N-CA	5.04	127.03	120.28
3	C	263	LEU	N-CA-CB	5.04	117.31	110.01
17	Q	218	ARG	N-CA-CB	5.04	117.31	110.01
1	A	45	GLU	CA-C-N	5.04	130.22	122.42
1	A	45	GLU	C-N-CA	5.04	130.22	122.42
1	A	424	GLY	CA-C-N	5.04	130.33	122.17
1	A	424	GLY	C-N-CA	5.04	130.33	122.17
17	Q	674	ARG	NE-CZ-NH2	5.04	123.73	119.20
21	V	28	GLY	CA-C-N	5.04	127.83	120.98
21	V	28	GLY	C-N-CA	5.04	127.83	120.98
21	V	173	ASP	CA-CB-CG	5.04	117.64	112.60
2	B	111	ASN	CA-CB-CG	-5.03	107.57	112.60
9	I	49	ASP	CA-C-N	5.03	127.96	120.31
9	I	49	ASP	C-N-CA	5.03	127.96	120.31
24	Y	72	SER	CA-C-N	5.03	127.44	120.29
24	Y	72	SER	C-N-CA	5.03	127.44	120.29
2	B	890	ARG	N-CA-CB	5.03	117.66	110.06
2	B	986	GLN	N-CA-CB	5.03	118.05	110.30
17	Q	667	ARG	CA-C-N	5.03	127.43	120.29
17	Q	667	ARG	C-N-CA	5.03	127.43	120.29
17	Q	753	LEU	CA-C-N	5.03	127.52	120.28
17	Q	753	LEU	C-N-CA	5.03	127.52	120.28
19	T	-120	DT	O5'-C5'-C4'	5.03	118.34	110.80
21	V	109	GLU	CA-C-N	5.03	128.44	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	109	GLU	C-N-CA	5.03	128.44	120.89
1	A	1332	GLN	CB-CG-CD	5.03	121.15	112.60
2	B	328	PRO	CA-C-N	5.03	125.44	120.31
2	B	328	PRO	C-N-CA	5.03	125.44	120.31
2	B	47	PHE	N-CA-CB	5.03	117.30	110.01
10	J	1	MET	CA-C-N	5.03	130.14	122.25
10	J	1	MET	C-N-CA	5.03	130.14	122.25
18	R	424	LYS	CG-CD-CE	5.03	122.86	111.30
8	H	57	ARG	N-CA-CB	5.02	117.98	109.94
1	A	76	GLY	CA-C-N	5.02	129.68	121.74
1	A	76	GLY	C-N-CA	5.02	129.68	121.74
1	A	1043	ILE	N-CA-CB	5.02	116.43	110.55
1	A	433	PRO	CA-C-N	5.02	127.40	120.67
1	A	433	PRO	C-N-CA	5.02	127.40	120.67
2	B	765	GLU	N-CA-CB	5.02	117.35	110.07
17	Q	651	ASN	N-CA-CB	5.02	117.29	110.01
2	B	405	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	A	100	LEU	N-CA-CB	5.02	117.34	110.07
2	B	337	LYS	CA-CB-CG	5.02	124.13	114.10
17	Q	731	GLY	CA-C-N	5.02	130.24	122.26
17	Q	731	GLY	C-N-CA	5.02	130.24	122.26
2	B	409	LYS	CA-CB-CG	5.01	124.13	114.10
2	B	699	HIS	CA-CB-CG	-5.01	108.78	113.80
17	Q	231	CYS	N-CA-CB	5.01	117.43	109.71
18	R	483	LEU	N-CA-CB	5.01	117.34	110.07
24	Y	70	TRP	N-CA-CB	5.01	117.58	110.16
2	B	334	LYS	CG-CD-CE	5.01	122.83	111.30
2	B	367	TYR	N-CA-CB	5.01	117.28	110.01
1	A	1447	GLU	CA-C-N	5.01	130.06	122.99
1	A	1447	GLU	C-N-CA	5.01	130.06	122.99
20	U	406	GLU	CA-C-N	5.01	127.25	120.44
20	U	406	GLU	C-N-CA	5.01	127.25	120.44
26	a	103	LEU	N-CA-CB	5.01	117.44	109.82
26	e	127	ALA	CA-C-N	5.01	127.31	120.54
26	e	127	ALA	C-N-CA	5.01	127.31	120.54
1	A	1045	LEU	CA-C-N	5.01	129.91	121.14
1	A	1045	LEU	C-N-CA	5.01	129.91	121.14
1	A	1286	ARG	CA-C-N	5.01	127.40	120.29
1	A	1286	ARG	C-N-CA	5.01	127.40	120.29
7	G	78	ARG	CG-CD-NE	5.01	123.02	112.00
21	V	85	ASP	CA-C-N	5.01	130.04	122.08
21	V	85	ASP	C-N-CA	5.01	130.04	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	479	LYS	CA-C-N	5.01	128.57	121.66
25	Z	479	LYS	C-N-CA	5.01	128.57	121.66
1	A	311	GLN	N-CA-CB	5.01	117.48	110.12
26	e	56	LYS	CA-CB-CG	5.01	124.11	114.10
27	f	70	VAL	CA-C-N	5.01	128.33	120.82
27	f	70	VAL	C-N-CA	5.01	128.33	120.82
1	A	407	ARG	CA-C-N	5.01	127.92	120.31
1	A	407	ARG	C-N-CA	5.01	127.92	120.31
1	A	1478	GLU	CA-C-N	5.01	127.49	120.28
1	A	1478	GLU	C-N-CA	5.01	127.49	120.28
2	B	817	GLN	CA-C-N	5.01	131.15	122.64
2	B	817	GLN	C-N-CA	5.01	131.15	122.64
17	Q	788	LEU	CA-C-N	5.01	126.99	120.28
17	Q	788	LEU	C-N-CA	5.01	126.99	120.28
1	A	1223	ASP	CA-C-N	5.00	130.22	122.26
1	A	1223	ASP	C-N-CA	5.00	130.22	122.26
2	B	550	MET	N-CA-CB	5.00	117.10	110.29
28	g	20	ARG	NE-CZ-NH2	5.00	123.70	119.20
2	B	412	LEU	CA-C-N	5.00	127.91	120.31
2	B	412	LEU	C-N-CA	5.00	127.91	120.31
1	A	541	THR	CA-C-N	5.00	127.39	120.29
1	A	541	THR	C-N-CA	5.00	127.39	120.29
1	A	1043	ILE	CA-C-N	5.00	127.29	120.54
1	A	1043	ILE	C-N-CA	5.00	127.29	120.54
3	C	60	HIS	CB-CG-CD2	-5.00	124.70	131.20
6	F	70	ALA	CA-C-N	5.00	126.94	120.44
6	F	70	ALA	C-N-CA	5.00	126.94	120.44
17	Q	759	LEU	N-CA-CB	5.00	117.47	110.12
27	f	62	LEU	CA-C-N	5.00	127.74	120.79
27	f	62	LEU	C-N-CA	5.00	127.74	120.79

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
29	h	118	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11255	11385	11373	213	0
2	B	8980	9024	9022	65	0
3	C	2072	2021	2022	18	0
4	D	1004	981	980	8	0
5	E	1720	1736	1737	22	0
6	F	626	658	657	10	0
7	G	1333	1321	1321	13	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	6	0
12	L	397	407	405	3	0
13	M	4927	2638	2622	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	97	0
18	R	1836	1701	1699	28	0
19	T	2680	1458	1441	39	0
20	U	857	687	684	17	0
21	V	1711	1450	1446	18	0
22	W	2333	2247	2246	47	0
23	X	353	372	371	8	0
24	Y	911	909	907	10	0
25	Z	4025	4046	4041	48	0
26	a	802	841	841	1	0
26	e	801	839	838	2	0
27	b	662	710	709	0	0
27	f	619	660	659	3	0
28	c	795	847	846	0	0
28	g	809	865	864	0	0
29	d	745	774	773	2	0
29	h	726	749	747	4	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	62740	714	0

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

All (714) 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	1.50
1:A:1314:THR:C	15:O:295:GLY:CA	1.91	1.40
1:A:1223:ASP:CG	15:O:244:ALA:HB2	1.45	1.39
1:A:1314:THR:HG22	15:O:297:ARG:NE	1.31	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1314:THR:CG2	15:O:297:ARG:NE	1.79	1.35
1:A:1223:ASP:CG	15:O:244:ALA:CB	2.01	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: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
1:A:1308:TYR:HB3	15:O:250:MET:HE2	1.24	1.08
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:1309:MET:N	15:O:250:MET:HE3	1.75	1.00
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
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
1:A:1315:ASP:N	15:O:295:GLY:C	2.24	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
1:A:1314:THR:HA	15:O:295:GLY:C	1.93	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
1:A:1223:ASP:CG	15:O:244:ALA:HB1	1.97	0.90
20:U:381:PHE:HZ	20:U:497:ASP:O	1.53	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1314:THR:CG2	15:O:297:ARG:CZ	2.55	0.85
1:A:1314:THR:C	15:O:295:GLY:C	2.43	0.84
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:1318:LYS:NZ	15:O:293:GLU:C	2.37	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
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:1318:LYS:HZ2	15:O:294:CYS:N	1.83	0.77
1:A:11:SER:O	2:B:1135:TYR:OH	2.03	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:CA	15:O:295:GLY:C	2.54	0.76
1:A:1318:LYS:HZ2	15:O:293:GLU:C	1.94	0.75
17:Q:65:GLU:OE2	17:Q:93:TYR:OH	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1315:ASP:H	15:O:295:GLY:C	1.94	0.72
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:910:LYS:HZ1	15:O:265:LYS:HA	1.53	0.71
2:B:1040:GLN:OE1	3:C:195:THR:OG1	2.08	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
18:R:455:TRP:CD1	18:R:459:MET:HE3	2.27	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
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
1:A:1308:TYR:C	15:O:250:MET:HE3	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1318:LYS:HZ3	15:O:293:GLU:C	2.06	0.63
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
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
25:Z:307:MET:HE3	25:Z:308:ILE:H	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1308:TYR:CB	15:O:250:MET:HE2	2.13	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:911:PRO:O	1:A:963:ARG:NH1	2.34	0.59
2:B:155:MET:HE3	2:B:183:GLY:HA2	1.82	0.59
1:A:1315:ASP:N	15:O:295:GLY:O	2.33	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
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
2:B:298:MET:HE3	9:I:14:ILE:HD12	1.86	0.58
9:I:42:CYS:SG	9:I:43:ASP:N	2.75	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
25:Z:554:GLU:OE2	25:Z:559:GLN:NE2	2.36	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:1315:ASP:CG	15:O:294:CYS:CB	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1315:ASP:CG	15:O:296:ASN:N	2.63	0.56
5:E:67:ASP:OD1	5:E:69:THR:OG1	2.22	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:1318:LYS:HD2	15:O:294:CYS:C	2.31	0.56
1:A:1212:LEU:HD12	1:A:1285:LEU:HD13	1.88	0.56
1:A:1314:THR:C	15:O:295:GLY:O	2.47	0.55
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
25:Z:474:MET:HE2	25:Z:494:ARG:HA	1.87	0.55
1:A:868:MET:HG3	1:A:1404:THR:HG21	1.88	0.55
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
27:f:75:HIS:CD2	29:h:93:THR:HG21	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:f:75:HIS:NE2	29:h:90:GLU:OE2	2.40	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
1:A:1318:LYS:HZ2	15:O:294:CYS:CA	2.20	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
5:E:55:ARG:O	5:E:56:THR:OG1	2.25	0.53
17:Q:737:LYS:HZ3	17:Q:761:LEU:HD23	1.73	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
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
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
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
26:e:67:PHE:O	26:e:71:VAL:HG23	2.09	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
1:A:1315:ASP:CG	15:O:294:CYS:SG	2.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:565:MET:HE3	11:K:60:GLY:C	2.35	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:803:MET:HE1	17:Q:807:LEU:HD11	1.93	0.51
21:V:294:SER:O	21:V:295:LYS:C	2.54	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
13:M:1341:GLU:HG2	13:M:1344:MET:HE2	1.94	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
17:Q:849:LYS:O	17:Q:852:LEU:HG	2.12	0.50
2:B:411:LEU:HD12	2:B:411:LEU:C	2.37	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
13:M:1459:ILE:HD11	13:M:1469:PHE:HB3	1.94	0.50
21:V:297:TYR:O	21:V:298:GLU:C	2.55	0.50
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.77	0.50
7:G:164:MET:HE1	25:Z:474:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
3:C:189:ASP:OD1	3:C:209:SER:OG	2.24	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
1:A:282:ASP:O	1:A:283:ILE:C	2.56	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
29:d:56:MET:O	29:d:56:MET:HE3	2.13	0.49
2:B:1094:GLN:HB2	2:B:1103:LEU:HD13	1.94	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
1:A:361:PHE:C	1:A:388:MET:HE3	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
29:h:89:ARG:O	29:h:93:THR:HG22	2.14	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
24:Y:48:MET:HE3	24:Y:48:MET:HA	1.96	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
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
1:A:728:THR:O	1:A:729:PRO:C	2.57	0.47
6:F:114:SER:OG	6:F:115:TYR:N	2.44	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
25:Z:546:THR:HG23	25:Z:563:MET:HE2	1.97	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:281:ASP:CG	9:I:22:ASN:HD22	2.22	0.46
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
17:Q:386:ALA:HB1	17:Q:394:ARG:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:128:ARG:NE	26:a:133:GLU:OE1	2.42	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
17:Q:83:MET:HE3	17:Q:124:ILE:HB	1.97	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
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
2:B:898:THR:O	2:B:899:SER:OG	2.26	0.46
9:I:86:CYS:SG	9:I:87:GLN:N	2.89	0.45
20:U:381:PHE:CZ	20:U:497:ASP:C	2.94	0.45
1:A:713:VAL:HG21	1:A:817:PRO:HD3	1.98	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:1309:MET:C	15:O:250:MET:HE3	2.41	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
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:483:ARG:C	1:A:484:LEU:HD12	2.42	0.45
1:A:1038:THR:O	1:A:1042:ASN:ND2	2.48	0.45
2:B:833:THR:C	2:B:835:GLU:H	2.25	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
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
20:U:406:GLU:CD	20:U:502:ARG:CB	2.89	0.45
25:Z:603:ILE:HG23	25:Z:604:ASP:N	2.31	0.45
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:240:VAL:HG21	17:Q:270:MET:HE3	1.99	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:565:MET:HE3	11:K:60:GLY:HA3	1.99	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
1:A:283:ILE:HD11	1:A:314:VAL:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:865:ILE:HG21	2:B:1092:ASP:CG	2.43	0.43
2:B:792:ASP:CG	2:B:975:ARG:HH12	2.26	0.43
19:T:-21:DG:H4'	25:Z:283:ARG:HE	1.84	0.43
1:A:388:MET:HE1	1:A:503:LEU:CD2	2.49	0.43
1:A:823:VAL:HG22	1:A:835:GLU:HB2	2.00	0.43
1:A:1308:TYR:C	15:O:250:MET:CE	2.88	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
17:Q:764:LEU:C	17:Q:764:LEU:HD23	2.44	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:407:MET:HE1	2:B:443:GLY:C	2.43	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
7:G:38:CYS:SG	7:G:39:THR:N	2.91	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
29:h:81:ASN:O	29:h:82:LYS:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
18:R:458:ALA:HB3	18:R:459:MET:HE2	2.01	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
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
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
21:V:295:LYS:O	21:V:296:GLY:C	2.61	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
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: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
29:d:31:LYS:HD2	29:d:31:LYS:O	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:358:GLU:O	17:Q:361:SER:OG	2.38	0.42
25:Z:759:GLY:O	25:Z:760:GLY:C	2.63	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
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:211:LEU:HD12	17:Q:213:LYS:HZ1	1.85	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:931:CYS:C	13:M:932:SER:HG	2.09	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
1:A:1309:MET:C	15:O:250:MET:SD	3.04	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
1:A:1315:ASP:CG	15:O:296:ASN:H	2.27	0.41
9:I:64:GLU:O	9:I:68:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:211:LEU:HB2	17:Q:213:LYS:HZ2	1.85	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
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
26:e:121:PRO:HB3	27:f:53:GLU:HG3	2.02	0.41
1:A:920:PHE:HD1	1:A:1050:CYS:SG	2.44	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
1:A:1313:GLN:C	15:O:295:GLY:HA2	2.44	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
20:U:457:PHE:CE1	20:U:496:THR:C	2.99	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
13:M:843:LYS:C	13:M:845:PRO:HD3	2.46	0.40
17:Q:386:ALA:HB1	17:Q:394:ARG:CG	2.51	0.40
17:Q:592:LEU:O	17:Q:597:THR:OG1	2.31	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
2:B:420:GLN:C	2:B:422:PHE:H	2.29	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
2:B:43:GLN:C	2:B:155:MET:HE1	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:202:TRP:O	1:A:203:LYS:C	2.65	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: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
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: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%)	24	60
2	B	1112/1251 (89%)	1024 (92%)	85 (8%)	3 (0%)	36	70
3	C	254/275 (92%)	239 (94%)	13 (5%)	2 (1%)	16	50
4	D	124/184 (67%)	122 (98%)	2 (2%)	0	100	100
5	E	207/210 (99%)	197 (95%)	8 (4%)	2 (1%)	12	45
6	F	76/127 (60%)	71 (93%)	5 (7%)	0	100	100
7	G	169/172 (98%)	155 (92%)	13 (8%)	1 (1%)	21	56
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%)	7	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
12	L	45/58 (78%)	40 (89%)	4 (9%)	1 (2%)	5	26
13	M	976/1729 (56%)	860 (88%)	98 (10%)	18 (2%)	6	31
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%)	7	32
21	V	236/531 (44%)	200 (85%)	33 (14%)	3 (1%)	9	38
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%)	30	65
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
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%)	26	60

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	1217 (98%)	28 (2%)	45	74
2	B	986/1084 (91%)	956 (97%)	30 (3%)	36	69
3	C	235/252 (93%)	231 (98%)	4 (2%)	53	78
4	D	109/160 (68%)	108 (99%)	1 (1%)	70	85
5	E	191/192 (100%)	186 (97%)	5 (3%)	40	72
6	F	68/111 (61%)	67 (98%)	1 (2%)	57	80
7	G	146/153 (95%)	141 (97%)	5 (3%)	32	66
8	H	130/131 (99%)	127 (98%)	3 (2%)	44	74
9	I	104/112 (93%)	102 (98%)	2 (2%)	50	76
10	J	55/56 (98%)	54 (98%)	1 (2%)	51	77
11	K	104/106 (98%)	100 (96%)	4 (4%)	29	63
12	L	44/55 (80%)	43 (98%)	1 (2%)	44	74
13	M	207/1524 (14%)	206 (100%)	1 (0%)	81	89
15	O	140/268 (52%)	140 (100%)	0	100	100
17	Q	761/1011 (75%)	756 (99%)	5 (1%)	76	86
18	R	170/625 (27%)	168 (99%)	2 (1%)	63	82
20	U	66/590 (11%)	65 (98%)	1 (2%)	57	80
21	V	148/462 (32%)	145 (98%)	3 (2%)	48	76
22	W	255/260 (98%)	252 (99%)	3 (1%)	63	82
23	X	40/467 (9%)	39 (98%)	1 (2%)	42	72
24	Y	102/103 (99%)	101 (99%)	1 (1%)	68	84
25	Z	435/939 (46%)	431 (99%)	4 (1%)	70	85
26	a	85/111 (77%)	83 (98%)	2 (2%)	43	73
26	e	84/111 (76%)	81 (96%)	3 (4%)	31	65
27	b	68/79 (86%)	67 (98%)	1 (2%)	57	80
27	f	63/79 (80%)	62 (98%)	1 (2%)	55	79
28	c	82/102 (80%)	81 (99%)	1 (1%)	63	82
28	g	83/102 (81%)	82 (99%)	1 (1%)	63	82
29	d	81/103 (79%)	78 (96%)	3 (4%)	30	64
29	h	79/103 (77%)	76 (96%)	3 (4%)	29	63
All	All	6366/11212 (57%)	6245 (98%)	121 (2%)	49	76

All (121) 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	88	ILE
1	A	184	CYS
1	A	277	THR
1	A	340	LYS
1	A	393	ILE
1	A	488	VAL
1	A	538	VAL
1	A	555	LEU
1	A	698	THR
1	A	713	VAL
1	A	728	THR
1	A	729	PRO
1	A	732	THR
1	A	811	ILE
1	A	942	VAL
1	A	1007	ILE
1	A	1048	THR
1	A	1182	GLN
1	A	1261	ILE
1	A	1282	ASP
1	A	1314	THR
1	A	1419	VAL
2	B	29	VAL
2	B	89	GLU
2	B	139	GLN
2	B	140	LEU
2	B	163	LEU
2	B	180	ASP
2	B	291	ASP
2	B	354	SER
2	B	388	TYR
2	B	411	LEU
2	B	429	PHE
2	B	504	THR
2	B	556	ILE
2	B	561	ILE
2	B	574	VAL

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Mol	Chain	Res	Type
2	B	576	ILE
2	B	698	ILE
2	B	710	ILE
2	B	731	GLN
2	B	738	THR
2	B	759	VAL
2	B	762	ARG
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	1148	LEU
3	C	15	THR
3	C	117	SER
3	C	121	ILE
3	C	151	VAL
4	D	31	THR
5	E	28	VAL
5	E	107	GLN
5	E	117	SER
5	E	129	GLN
5	E	131	LEU
6	F	120	VAL
7	G	4	HIS
7	G	48	VAL
7	G	67	LEU
7	G	101	ILE
7	G	132	ASP
8	H	67	ASP
8	H	78	THR
8	H	116	VAL
9	I	12	VAL
9	I	101	SER
10	J	30	THR
11	K	9	SER
11	K	21	ILE
11	K	107	VAL
11	K	111	ASP
12	L	42	ARG

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Mol	Chain	Res	Type
13	M	1365	THR
17	Q	552	ASP
17	Q	690	ILE
17	Q	697	TYR
17	Q	714	HIS
17	Q	779	VAL
18	R	411	THR
18	R	572	ILE
20	U	498	SER
21	V	37	ASN
21	V	45	ASP
21	V	134	THR
22	W	43	LEU
22	W	169	ASP
22	W	237	ASN
23	X	241	THR
24	Y	113	THR
25	Z	190	ARG
25	Z	224	TYR
25	Z	251	ASN
25	Z	614	ILE
26	a	105	GLU
26	a	129	ARG
27	b	95	ARG
28	c	76	THR
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
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 (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	72	GLN

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Mol	Chain	Res	Type
1	A	278	HIS
1	A	330	GLN
1	A	539	GLN
1	A	562	ASN
1	A	599	HIS
1	A	620	HIS
1	A	790	GLN
1	A	791	GLN
1	A	792	ASN
1	A	804	HIS
1	A	861	GLN
1	A	884	ASN
1	A	1032	GLN
1	A	1093	GLN
1	A	1417	HIS
1	A	1420	ASN
2	B	143	GLN
2	B	175	ASN
2	B	314	GLN
2	B	461	GLN
2	B	471	ASN
2	B	525	ASN
2	B	585	ASN
2	B	725	GLN
2	B	1021	HIS
2	B	1049	GLN
2	B	1068	GLN
2	B	1071	ASN
2	B	1120	ASN
3	C	111	GLN
3	C	123	ASN
3	C	217	GLN
4	D	43	HIS
4	D	47	GLN
4	D	48	ASN
8	H	126	GLN
8	H	130	ASN
8	H	131	ASN
9	I	56	ASN
9	I	100	HIS
9	I	121	HIS
11	K	69	HIS

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Mol	Chain	Res	Type
12	L	26	ASN
15	O	214	ASN
17	Q	40	GLN
17	Q	128	GLN
17	Q	147	GLN
17	Q	151	GLN
17	Q	153	HIS
17	Q	278	HIS
17	Q	289	GLN
17	Q	359	ASN
17	Q	424	GLN
17	Q	559	GLN
17	Q	585	GLN
17	Q	860	GLN
17	Q	871	GLN
17	Q	887	ASN
18	R	588	ASN
20	U	418	ASN
21	V	70	HIS
21	V	124	HIS
21	V	175	GLN
21	V	300	ASN
22	W	57	GLN
22	W	98	GLN
22	W	246	HIS
22	W	268	HIS
22	W	296	GLN
25	Z	234	HIS
25	Z	418	HIS
25	Z	559	GLN
27	b	27	GLN
28	c	112	GLN
29	d	44	GLN
26	e	108	ASN
29	h	81	ASN

5.3.3 RNA ⓘ

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 ⓘ

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	2.12	2 (25%)	10,14,16	2.05	2 (20%)
1	SEP	A	1547	1	8,9,10	2.09	2 (25%)	7,12,14	1.42	1 (14%)
25	TPO	Z	775	25	8,10,11	1.73	1 (12%)	10,14,16	2.13	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	-	0/6/8/10	-
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	3.90	1.34	1.20
25	Z	775	TPO	O-C	3.88	1.34	1.20
1	A	1547	SEP	O-C	3.87	1.34	1.20
1	A	1547	SEP	P-O1P	3.54	1.61	1.50
1	A	1525	TPO	P-O1P	3.52	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	775	TPO	P-OG1-CB	-5.99	107.06	123.33
1	A	1525	TPO	P-OG1-CB	-5.62	108.06	123.33
1	A	1547	SEP	OG-CB-CA	3.20	111.26	108.14
1	A	1525	TPO	CG2-CB-CA	-2.17	109.03	113.26

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
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

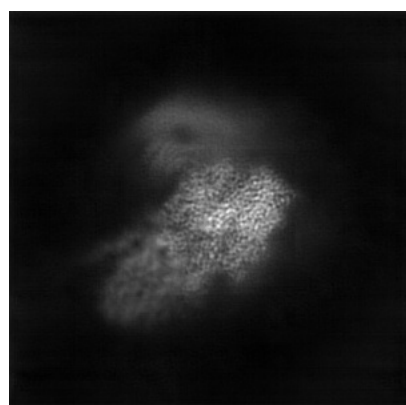
6 Map visualisation [i](#)

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.

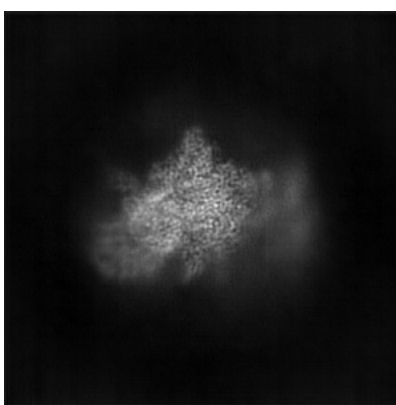
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

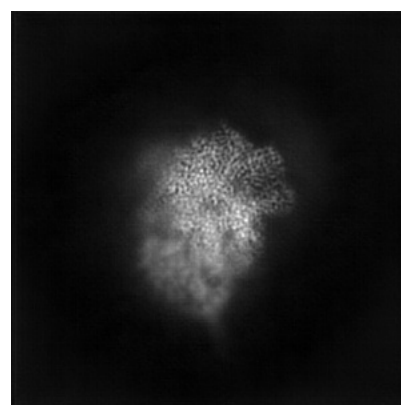
6.1.1 Primary map



X



Y

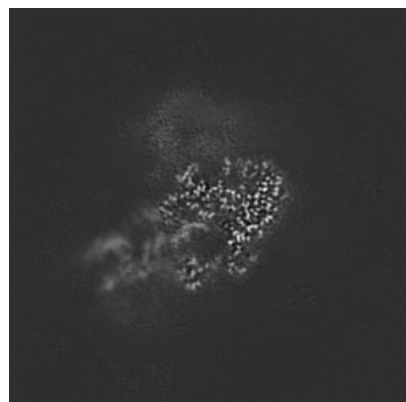


Z

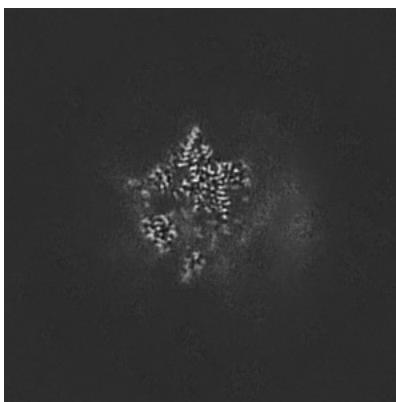
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

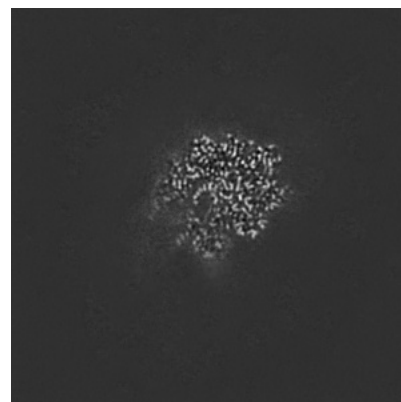
6.2.1 Primary map



X Index: 225



Y Index: 225

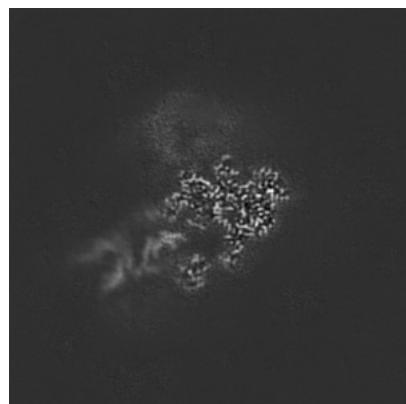


Z Index: 225

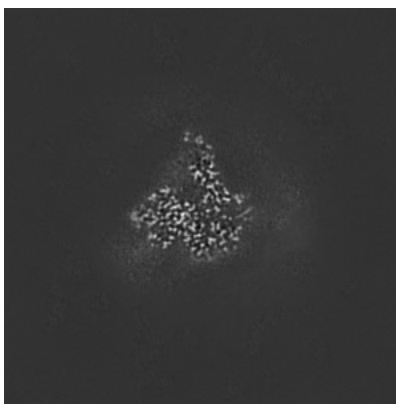
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

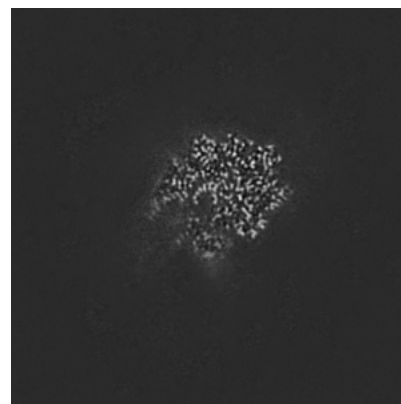
6.3.1 Primary map



X Index: 230



Y Index: 257

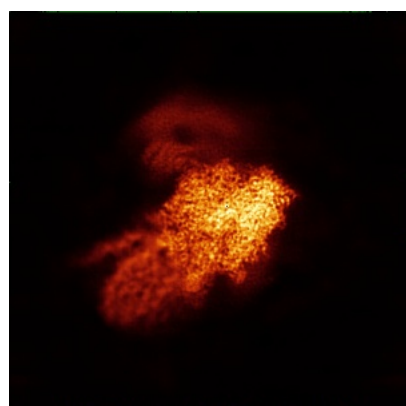


Z Index: 224

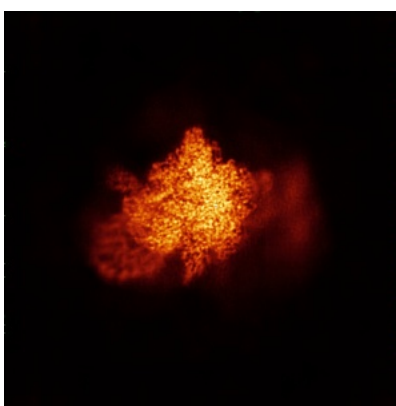
The images above show the largest variance slices of the map in three orthogonal directions.

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

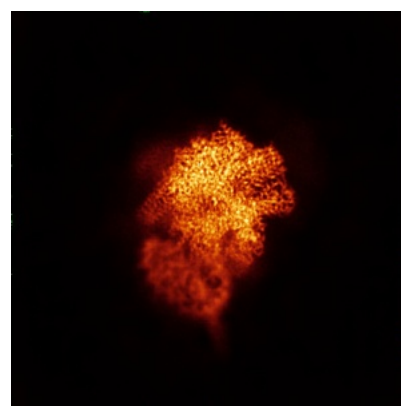
6.4.1 Primary map



X



Y

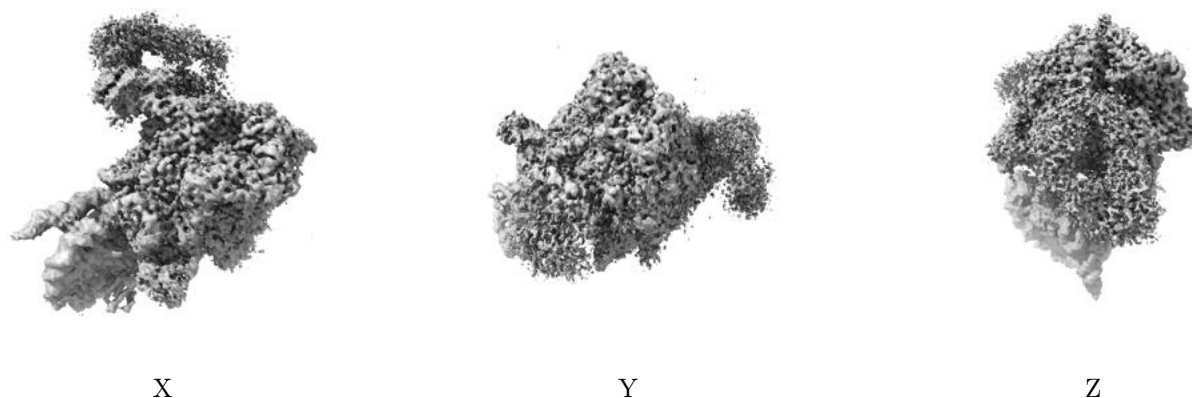


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

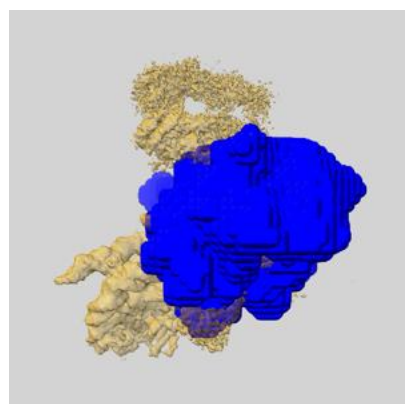
6.6 Mask visualisation [i](#)

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

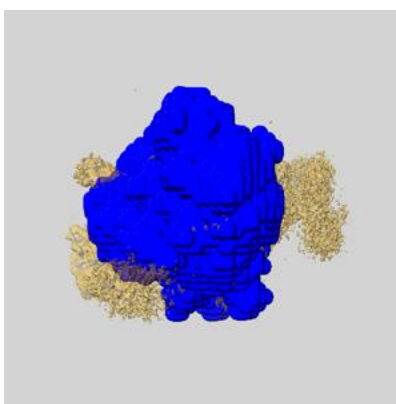
A mask typically either:

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

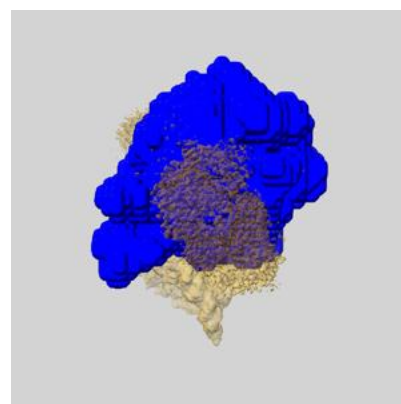
6.6.1 emd_26621_msk_1.map [i](#)



X

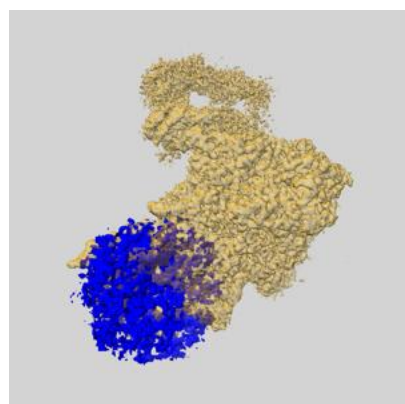


Y

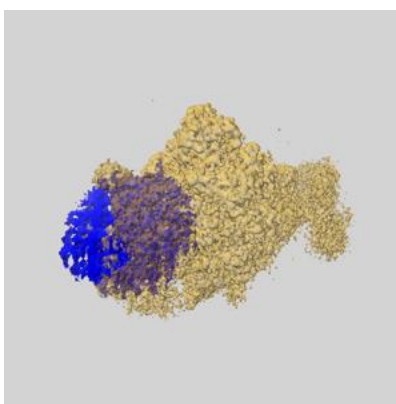


Z

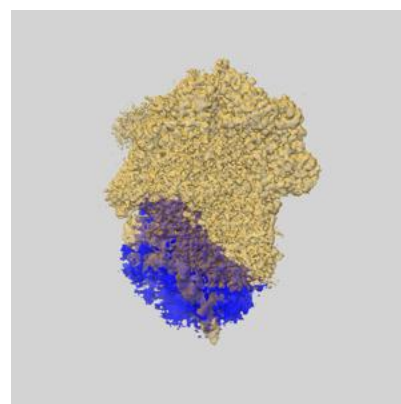
6.6.2 emd_26621_msk_2.map [i](#)



X

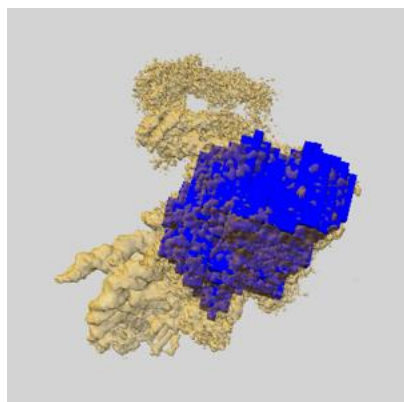


Y

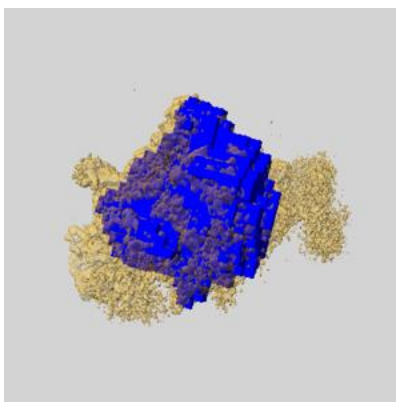


Z

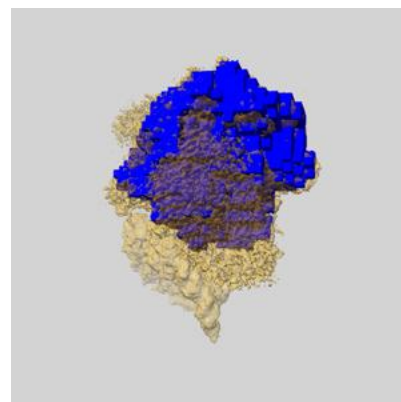
6.6.3 emd_26621_msk_3.map [i](#)



X



Y

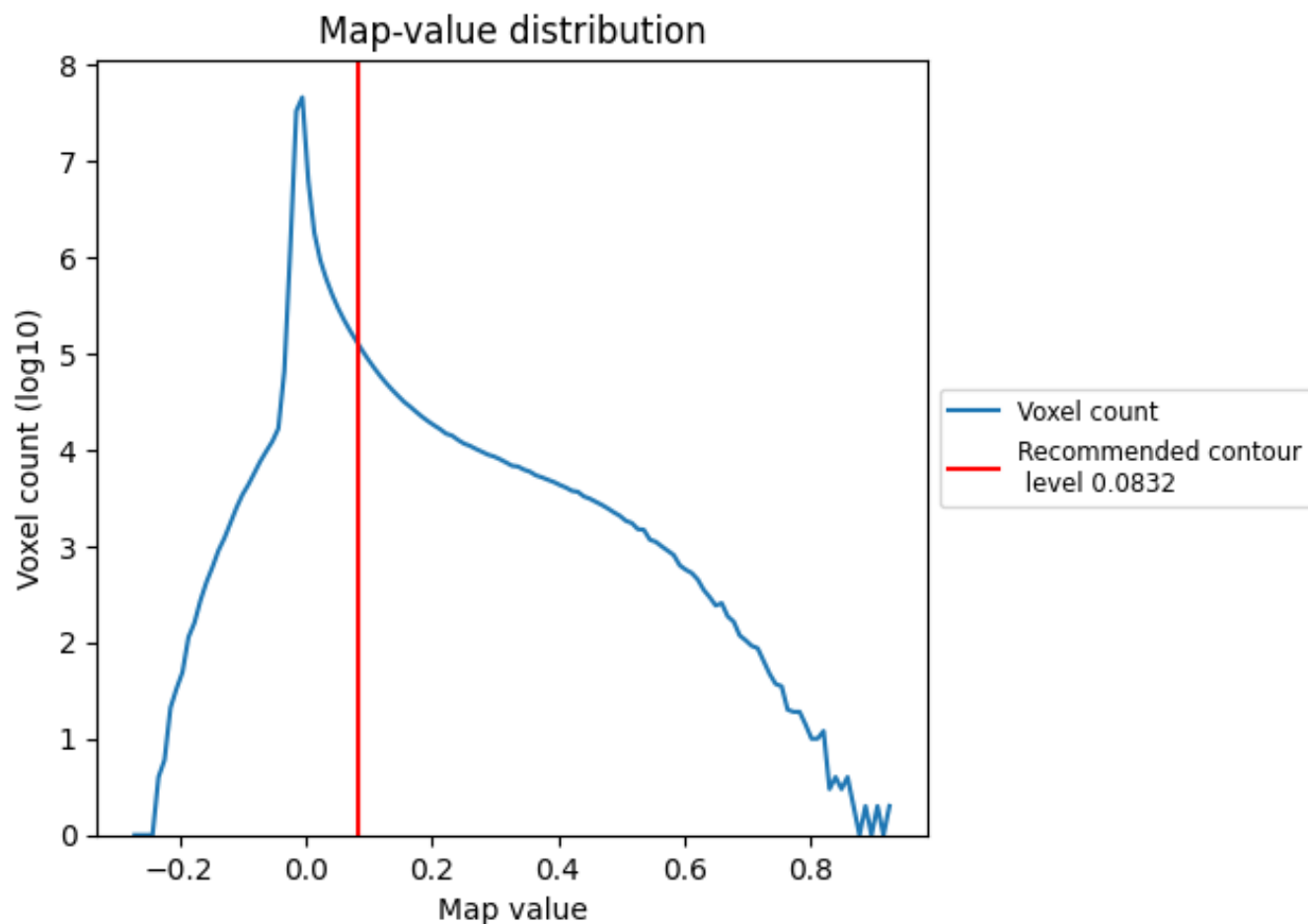


Z

7 Map analysis [i](#)

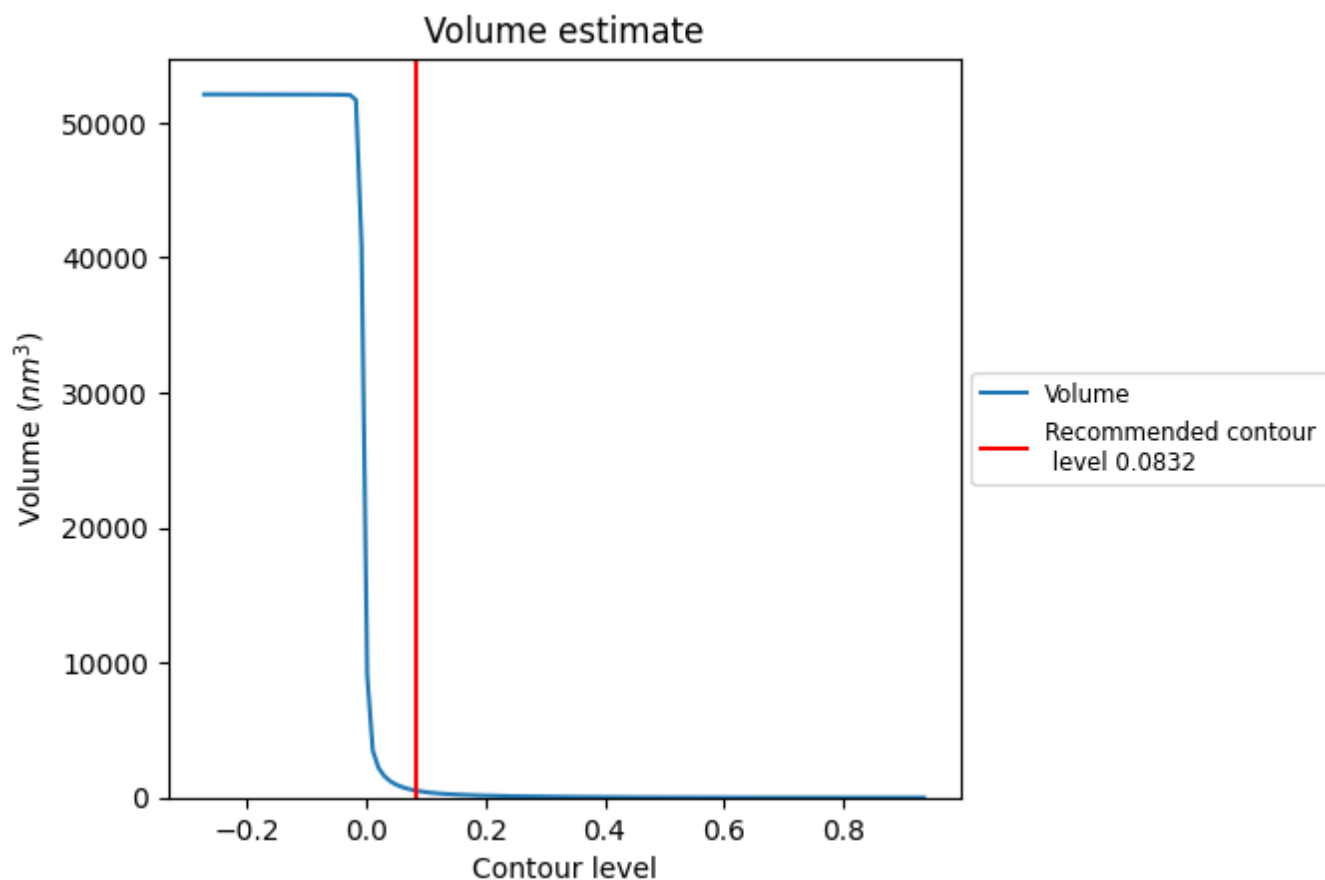
This section contains the results of statistical analysis of the map.

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.

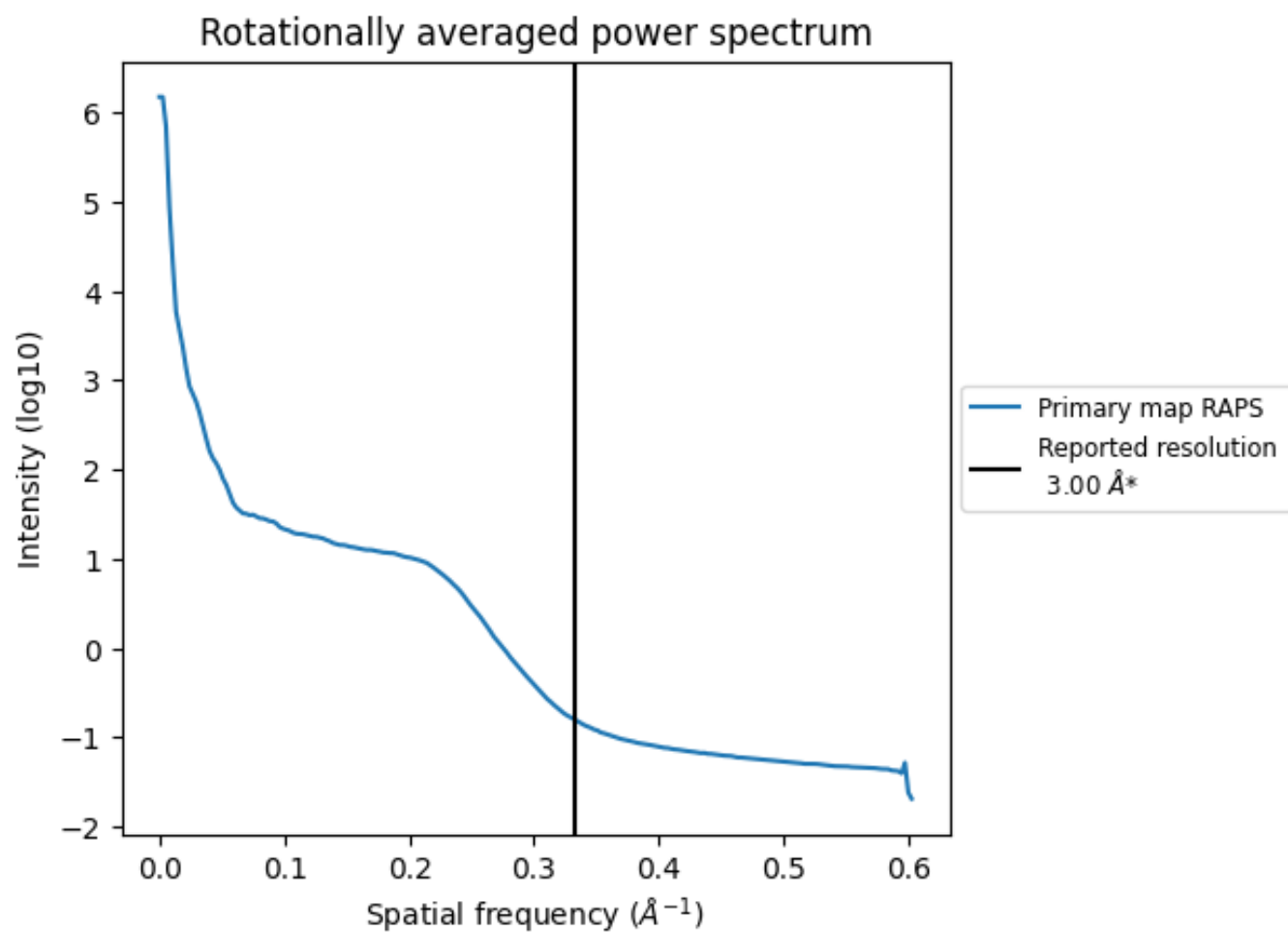
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 522 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

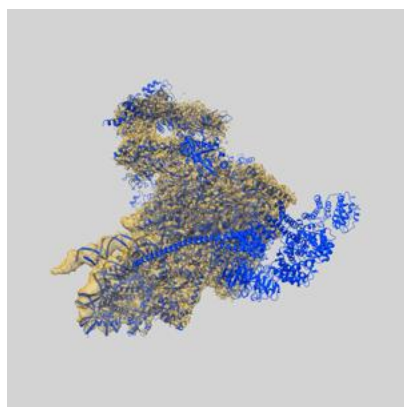
8 Fourier-Shell correlation

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

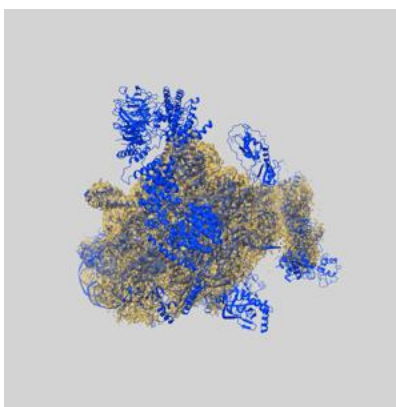
9 Map-model fit [i](#)

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](#).

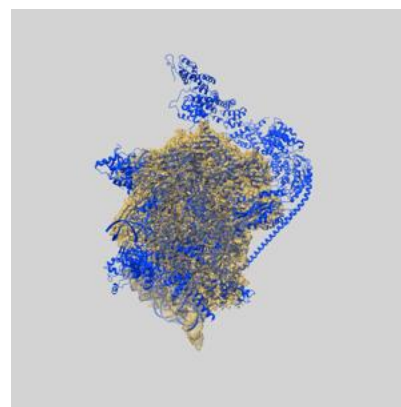
9.1 Map-model overlay [i](#)



X



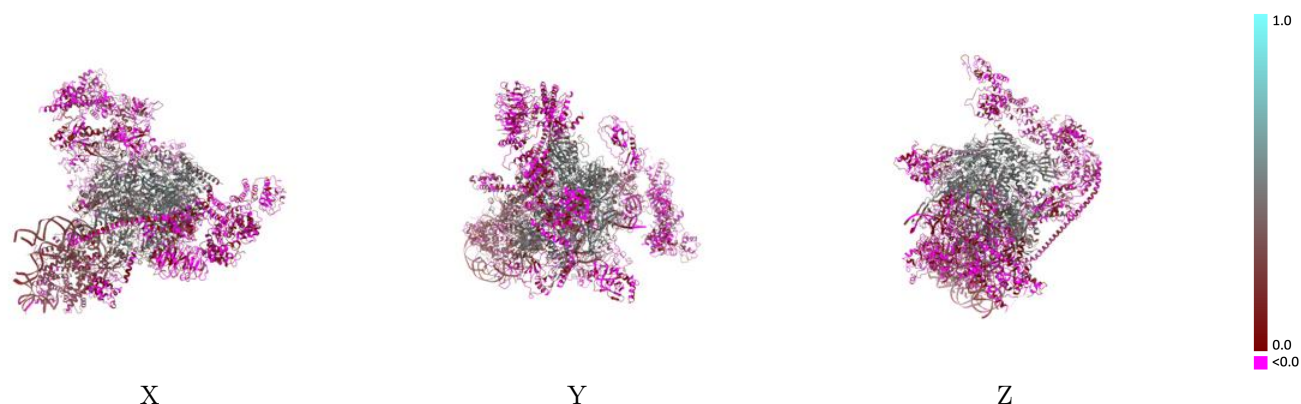
Y



Z

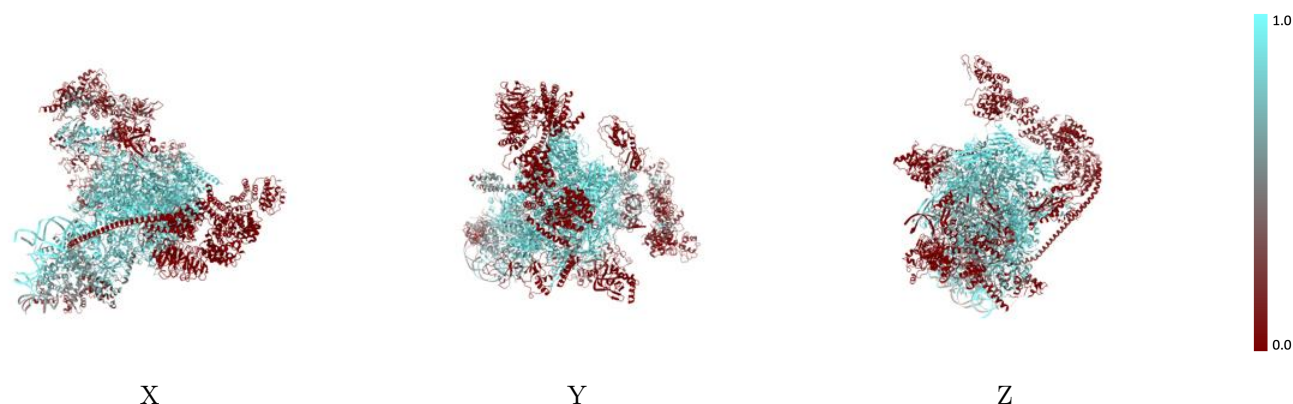
The images above show the 3D surface view of the map at the recommended contour level 0.0832 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



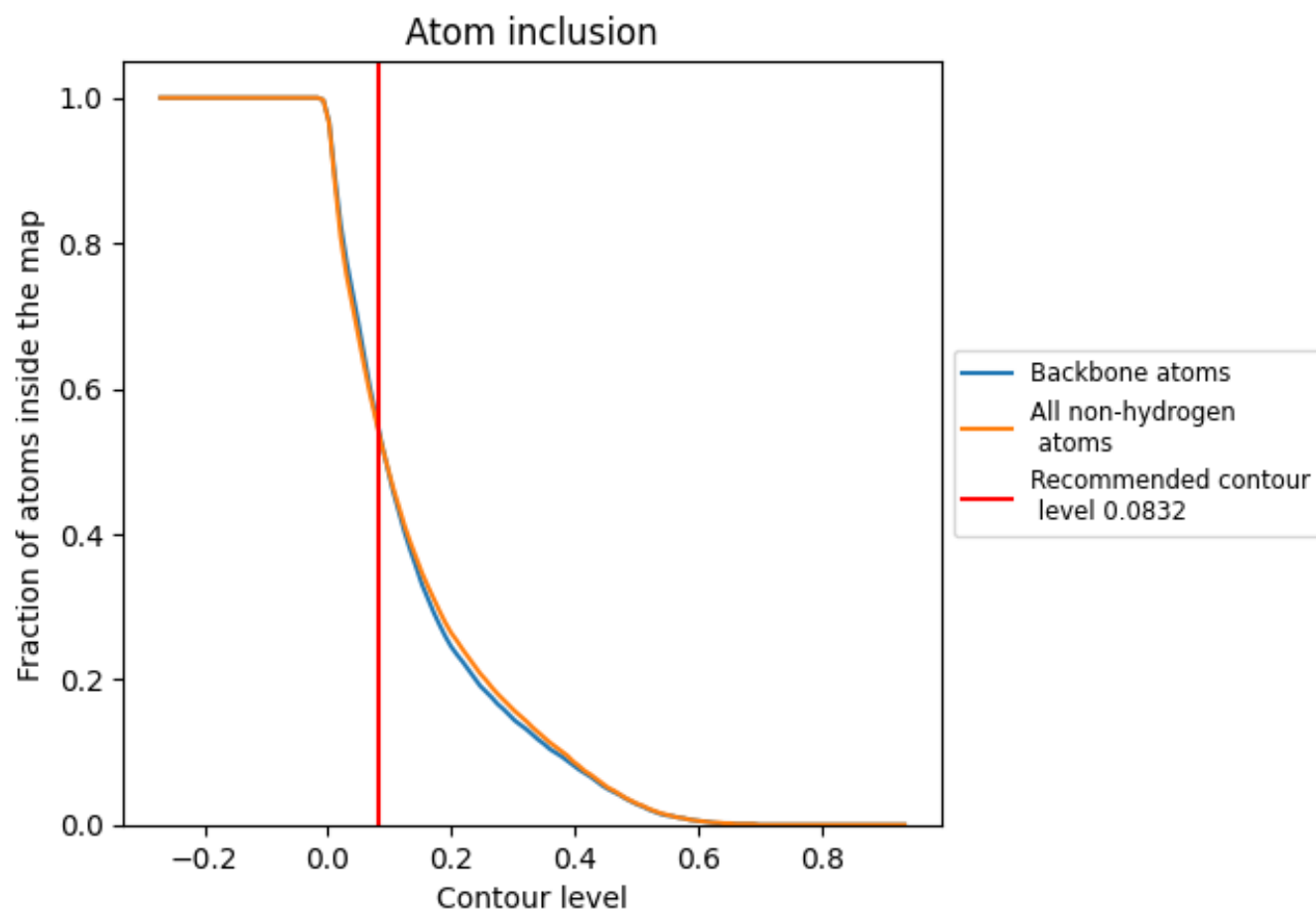
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.5370	 0.2160
A	 0.8900	 0.4080
B	 0.9010	 0.4260
C	 0.9340	 0.4660
D	 0.6280	 0.0950
E	 0.8750	 0.3370
F	 0.9130	 0.4550
G	 0.6570	 0.1730
H	 0.9020	 0.4280
I	 0.8040	 0.2330
J	 0.9060	 0.4630
K	 0.9260	 0.4680
L	 0.8530	 0.3870
M	 0.0870	 0.0240
N	 0.7610	 0.1640
O	 0.4130	 0.0160
P	 0.7660	 0.2450
Q	 0.0010	 0.0130
R	 0.0160	 0.0010
T	 0.8040	 0.2060
U	 0.2170	 0.0850
V	 0.0900	 0.0480
W	 0.0000	 -0.0010
X	 0.0000	 0.0470
Y	 0.0000	 0.0160
Z	 0.1410	 0.0610
a	 0.7450	 0.1410
b	 0.6760	 0.1640
c	 0.2520	 0.1160
d	 0.3350	 0.1300
e	 0.5610	 0.0830
f	 0.6350	 0.1020
g	 0.7810	 0.1820
h	 0.7240	 0.1610

