



## Full wwPDB EM Validation Report ⓘ

Mar 15, 2025 – 06:23 am GMT

PDB ID : 9I8M  
EMDB ID : EMD-52729  
Title : NEDD1-bound native vertebrate gamma-tubulin ring complex from *Xenopus laevis*, focused reconstruction  
Authors : Vermeulen, B.J.A.; Pfeffer, S.  
Deposited on : 2025-02-05  
Resolution : 4.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

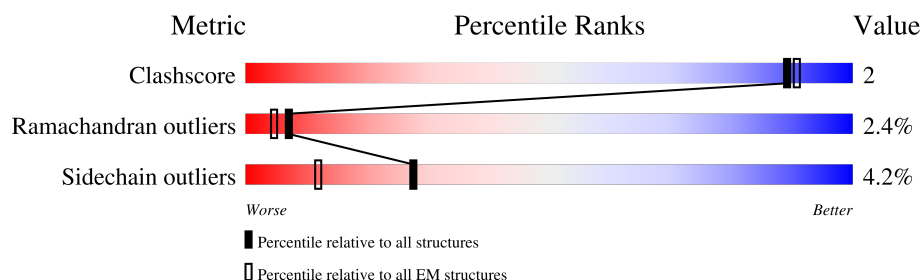
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*







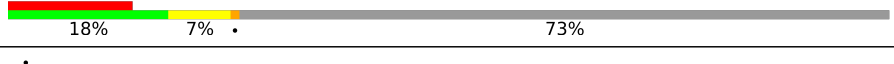

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	896	
1	C	896	
1	E	896	
1	G	896	
2	B	906	
2	D	906	
2	F	906	
2	H	906	

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Mol	Chain	Length	Quality of chain
2	O	906	
2	Q	906	
2	R	906	
2	S	906	
2	T	906	
3	I	666	
3	K	666	
4	J	1019	
5	L	1698	
6	U	671	
6	V	671	
6	W	671	
6	X	671	
7	o	72	
7	p	72	
7	q	72	
7	r	72	
7	s	72	
7	t	72	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 37358 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Gamma-tubulin complex component.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	275	Total	C	N	O	S	0	0
			2211	1412	369	421	9		
1	C	250	Total	C	N	O	S	0	0
			2014	1289	336	382	7		
1	E	253	Total	C	N	O	S	0	0
			2038	1306	340	385	7		
1	G	250	Total	C	N	O	S	0	0
			2014	1289	336	382	7		

- Molecule 2 is a protein called Gamma-tubulin complex component 3 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	294	Total	C	N	O	S	0	0
			2363	1517	401	434	11		
2	D	254	Total	C	N	O	S	0	0
			2059	1324	351	375	9		
2	F	242	Total	C	N	O	S	0	0
			1964	1263	337	355	9		
2	H	263	Total	C	N	O	S	0	0
			2135	1374	363	389	9		
2	O	93	Total	C	N	O	S	0	0
			753	480	137	134	2		
2	Q	109	Total	C	N	O	S	0	0
			878	557	160	159	2		
2	R	98	Total	C	N	O	S	0	0
			794	503	144	145	2		
2	S	109	Total	C	N	O	S	0	0
			878	557	160	159	2		
2	T	93	Total	C	N	O	S	0	0
			753	480	137	134	2		

- Molecule 3 is a protein called Gamma-tubulin complex component.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	287	Total	C	N	O	S	0	0
			2325	1500	394	418	13		
3	K	287	Total	C	N	O	S	0	0
			2325	1500	394	418	13		

- Molecule 4 is a protein called Gamma-tubulin complex component.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	352	Total	C	N	O	S	0	0
			2909	1881	493	522	13		

- Molecule 5 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	478	Total	C	N	O	S	0	0
			3794	2449	613	713	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	392	ASP	GLU	conflict	UNP A0A974HT83
L	394	VAL	ILE	conflict	UNP A0A974HT83

- Molecule 6 is a protein called NEDD1 gamma-tubulin ring complex targeting factor L homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	75	Total	C	N	O	S	0	0
			634	396	112	122	4		
6	V	75	Total	C	N	O	S	0	0
			634	396	112	122	4		
6	W	75	Total	C	N	O	S	0	0
			634	396	112	122	4		
6	X	75	Total	C	N	O	S	0	0
			634	396	112	122	4		

- Molecule 7 is a protein called Mitotic-spindle organizing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	o	52	Total	C	N	O	S	0	0
			403	248	71	79	5		
7	p	56	Total	C	N	O	S	0	0
			429	263	73	89	4		

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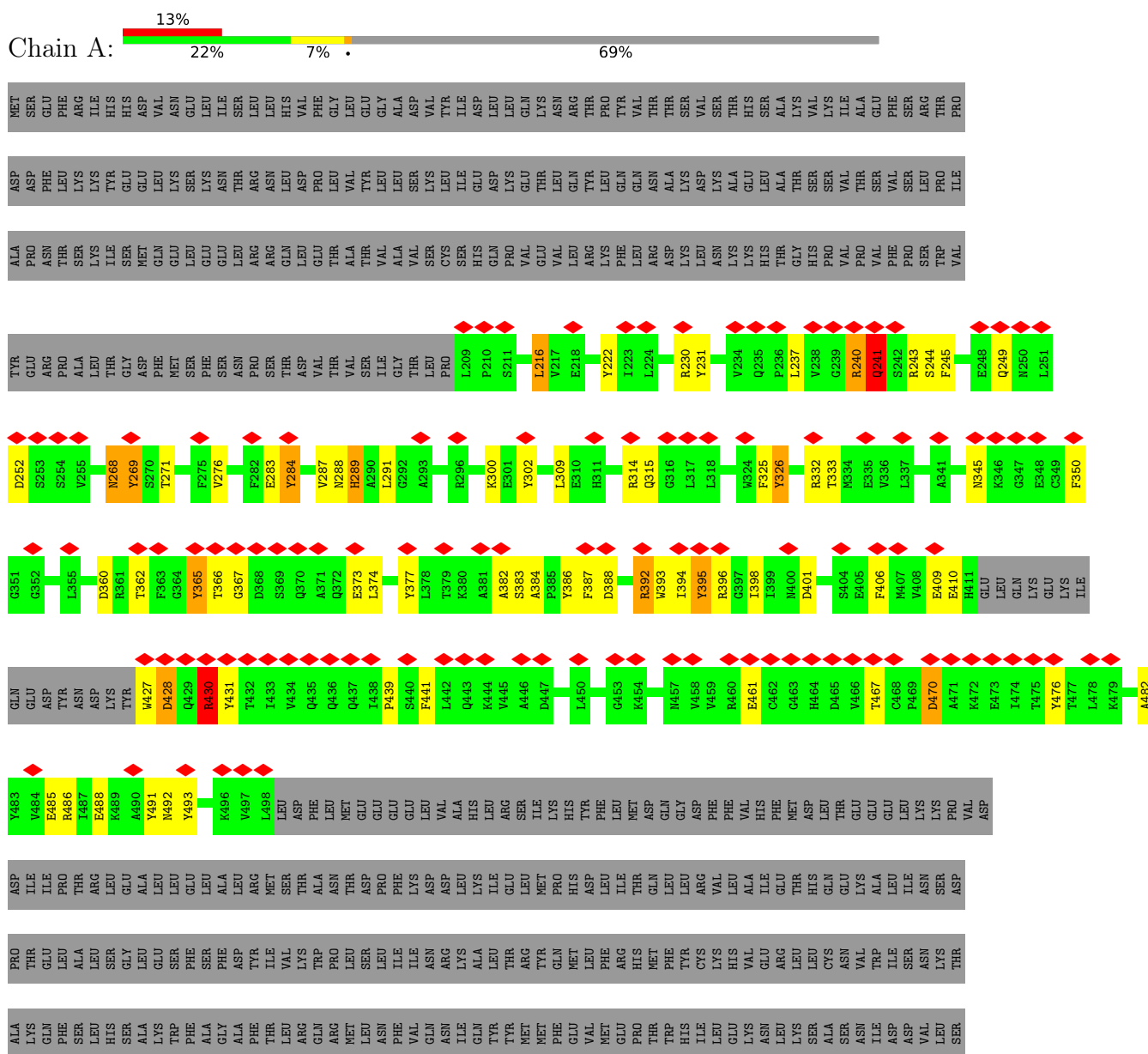
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Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	56	Total	C	N	O	S	0	0
			432	266	76	86	4		
7	r	59	Total	C	N	O	S	0	0
			454	278	80	91	5		
7	s	59	Total	C	N	O	S	0	0
			451	277	79	90	5		
7	t	58	Total	C	N	O	S	0	0
			446	274	78	89	5		

### 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: Gamma-tubulin complex component



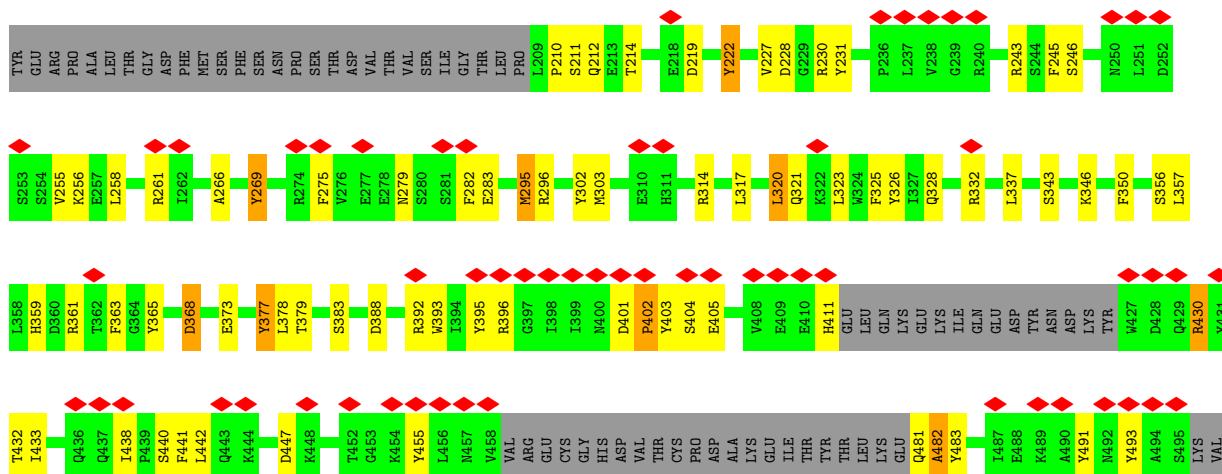
MET TYR SER THR THR SER ASP CYS GLU HIS TYR MET MET ILE ASN ILE ILE ARG TYR ARG LEU LEU ASP PHE PHE GLY ASN GLY PHE THR TYR THR TYR GLU ARG ARG LEU LYS GLN LEU LEU SER SER SER GLU ARG ASN GLN LYS ALA PRO LEU LEU GLY PRO ALA GLN HIS ALA VAL SER THR TYR

- Molecule 1: Gamma-tubulin complex component



ASP ASP PHE LEU LYS LYS TYR GLU GLU LEU LYS SER LYS ASN THR ARG ASN ASP PRO LEU VAL TYR LEU SER LYS LEU LEU ILE LEU GLU ASP LYS GLU THR LEU GLN TYR LEU GLN ALA ASP LYS ALA LYS GLU LEU ALA THR SER SER VAL THR SER VAL PRO TIF

ALA	PRO	ASN	THR	SER	LYS	ILE	SER	MET	GLN	GLU	LEU	GLU	GLU	GLU	THR	ALA	ALA	THR	THR	VAL	VAL	ALA	VAL	VAL	SER	SER	CYS	SER	SER	HIS	GLN	PRO	PRO	GLU	GLU	VAL	VAL	VAL	LEU	LEU	ARG	ASP	LYS	LYS	ASN	ASN	LYS	LYS	VAL	VAL	PRO	VAL	VAL	PHE	PRO	PRO	SER	SER	TRP	VAL	VAL	ALA
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LEU LEU LEU LEU ASP PHE MET MET GLU GLU GLU GLU VAL ALA HIS HIS HIS PHE TYR THR LEU MET ASP GLN GLY ASP ASP PHE PHE VAL HIS HIS PHE MET MET ASP THR LEU LEU LEU LYS LYS LYS PRO VAL ASP ASP ILE ILE ILE THR THR ARG LEU LEU GLU ALA LEU LEU LEU LEU

LEU ARG MET THR SER ALA ASN THR ASP ASP PHE LYS ASP ASP LYS LEU LEU ILE GLU LEU MET PRO HIS ASP LEU ILE THR GLN LEU ARG VAL LEU ILE ALA ILE GLU THR HIS GLN LEU LYS ALA LEU ILE ASN SER ASP THR PRO GLU THR LEU ALA LEU SER PHE SER PHE

ASP TYR ILE ILE VAL VAL LYS TRP PRO LEU LEU SER SER ILE ILE ASN ASN ARG ARG ALA ALA LEU LEU THR ARG TYR TYR GLN MET MET LEU LEU PHE PHE ARG ARG LYS LYS VAL VAL ARG ARG LEU LEU CYS CYS ASN ASN TRP TRP ILE ILE SER SER ASN ASN LYS LYS ALA ALA LYS GLN PHE PHE SER SER LEU LEU HIS HIS SER SER ALA ALA TYR TYR ASP

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CYC  
MET

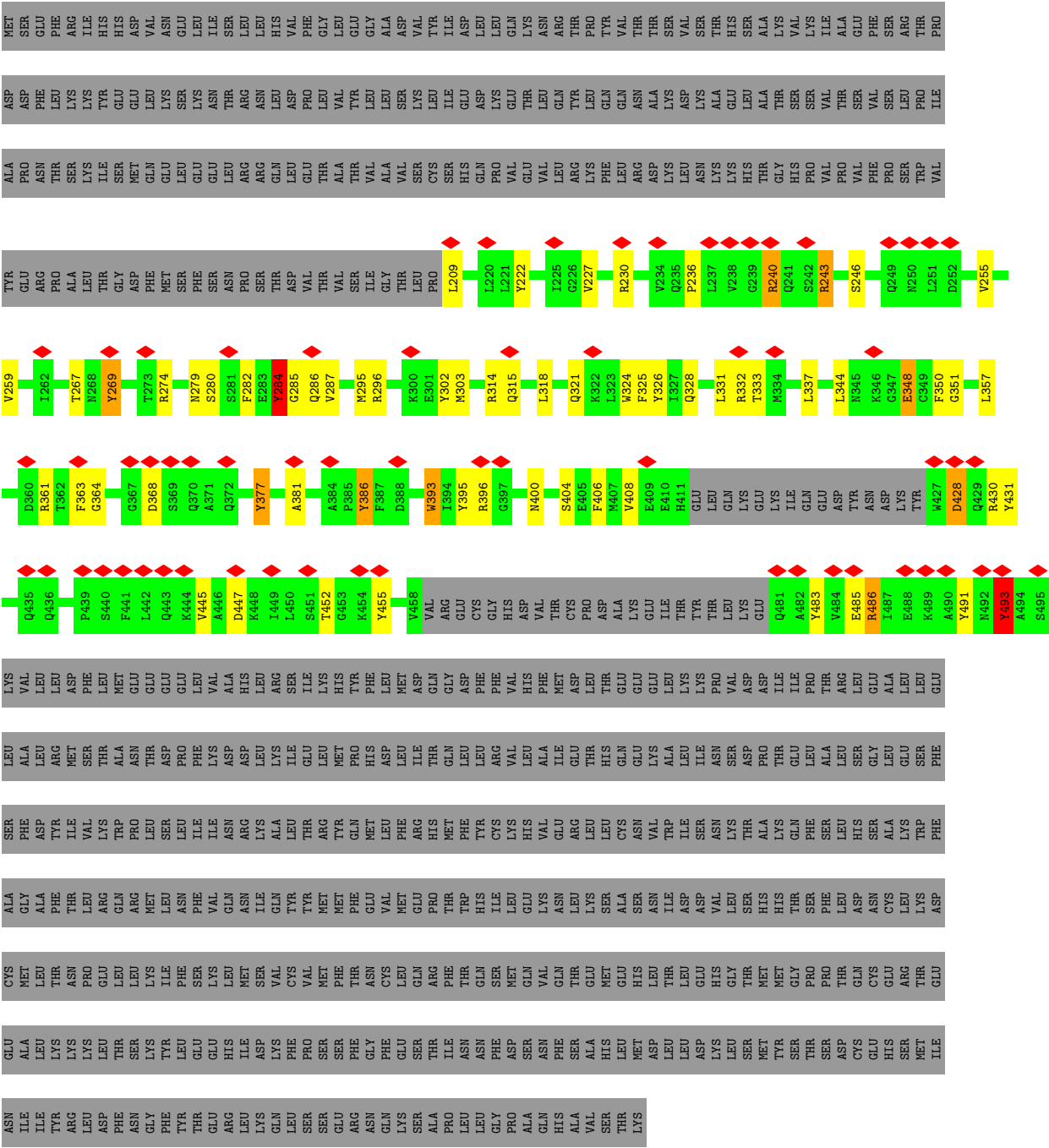
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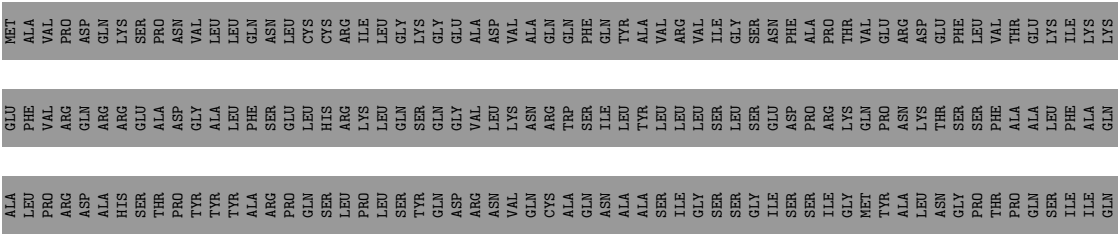
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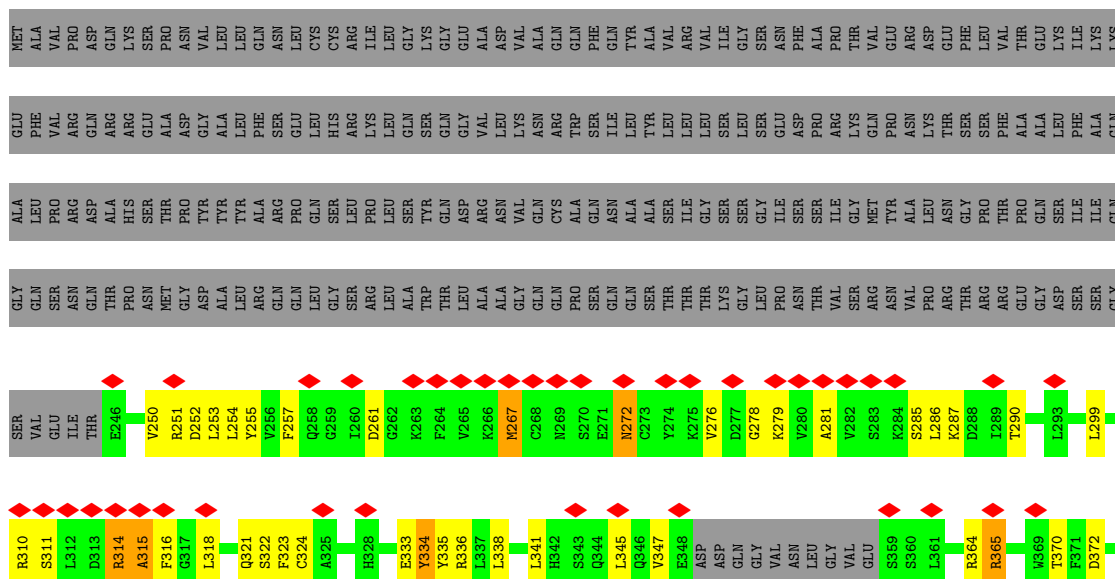
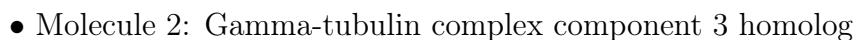


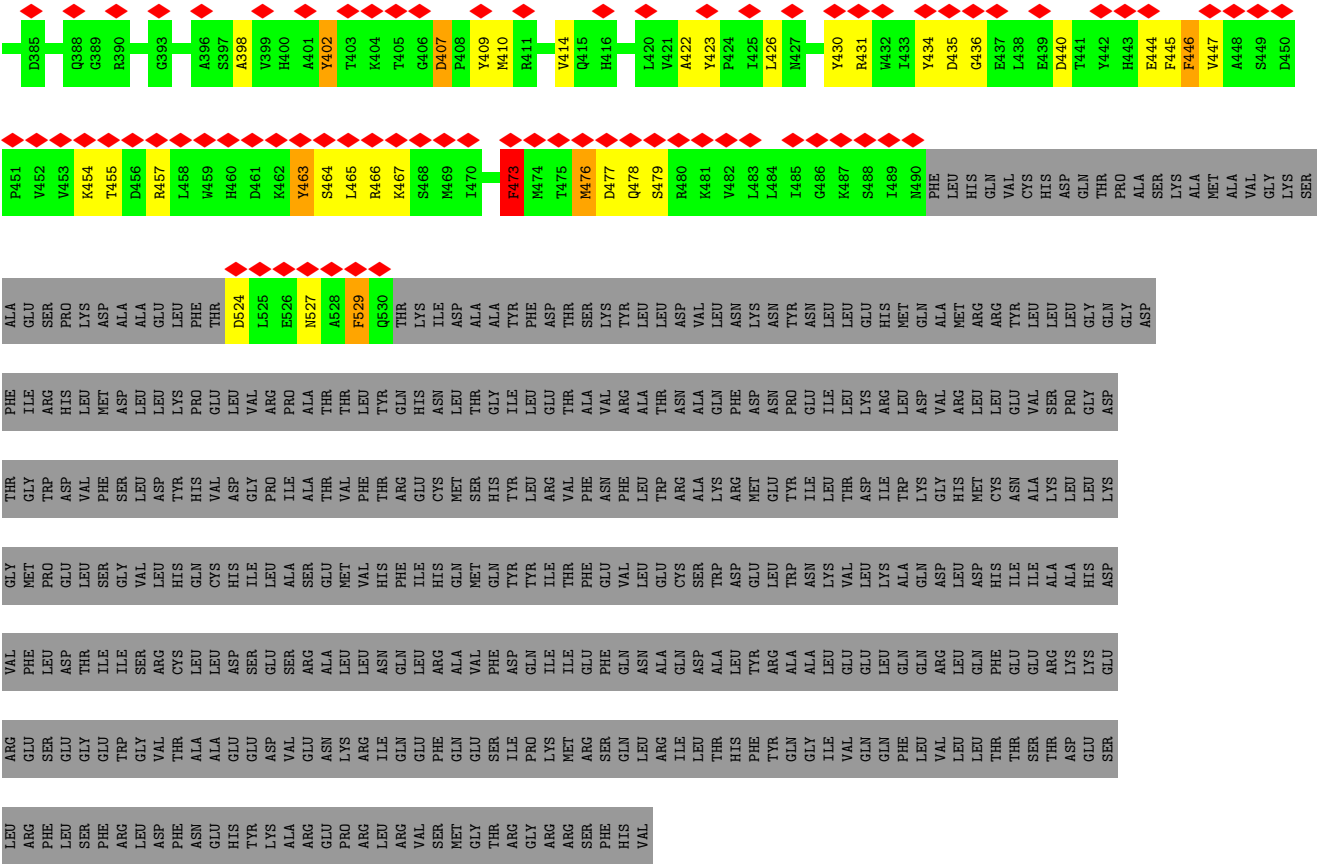


● Molecule 2: Gamma-tubulin complex component 3 homolog

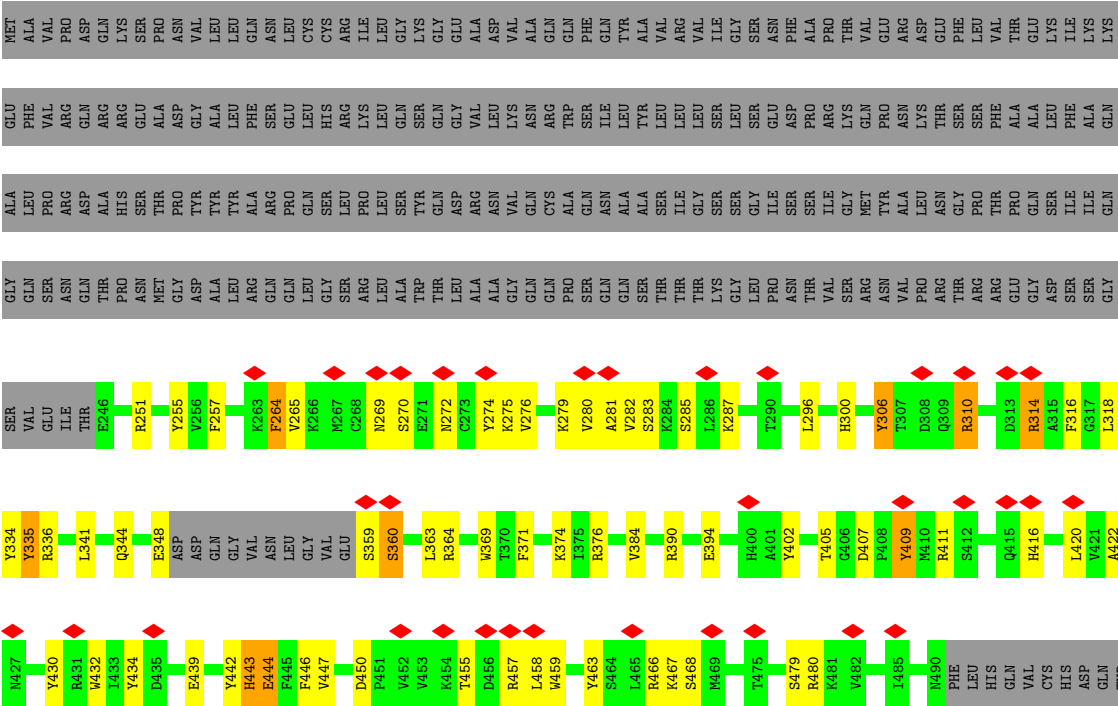


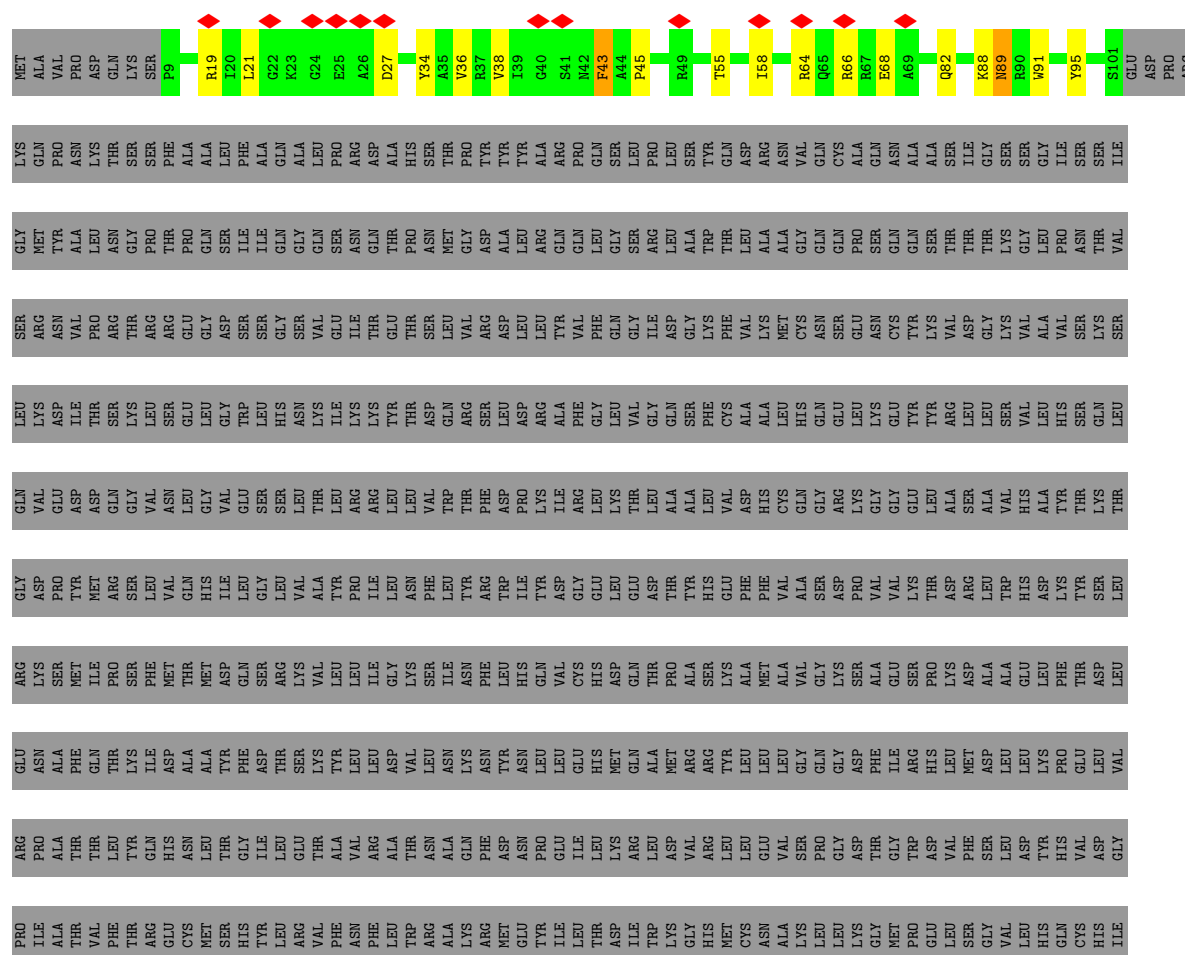






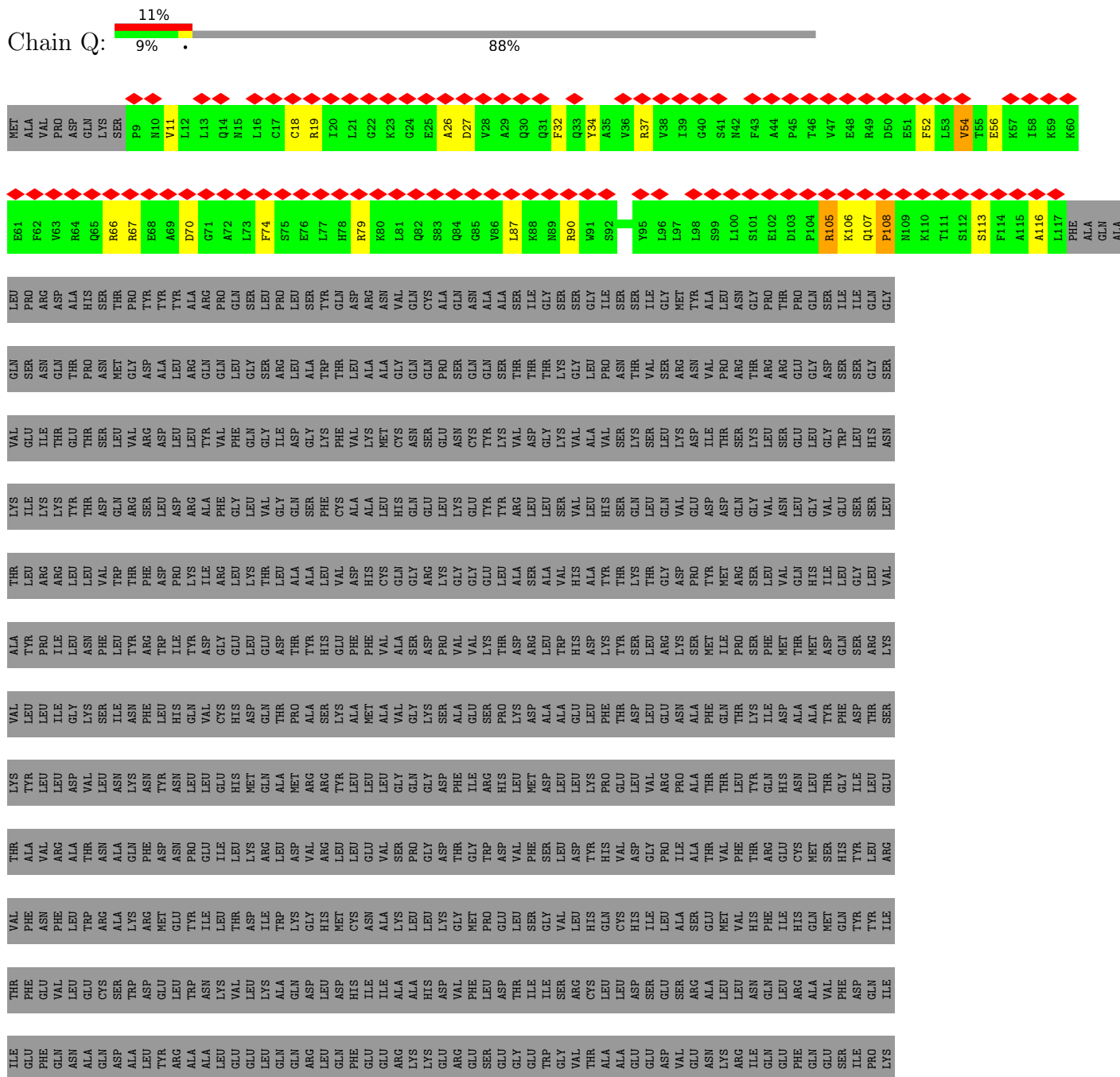
● Molecule 2: Gamma-tubulin complex component 3 homolog





[illegible]

- Molecule 2: Gamma-tubulin complex component 3 homolog



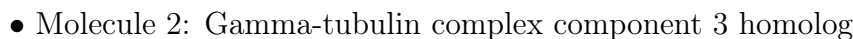
MET	ARG
SER	SER
GLN	PHE
LEU	HIS
ARG	VAL
ILE	
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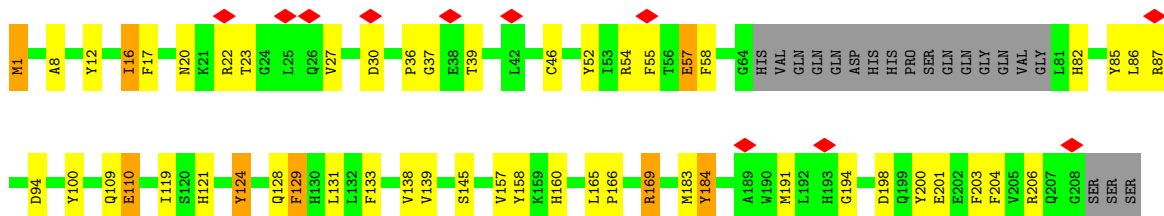
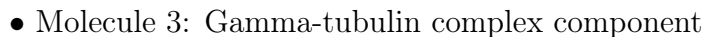
- Molecule 2: Gamma-tubulin complex component 3 homolog

[illegible]

- Molecule 2: Gamma-tubulin complex component 3 homolog









- Molecule 4: Gamma-tubulin complex component

[illegible]

GLN	VAL	ASP	ARG	THR	PRO	LEU	GLU	ASP	PRO	GLU	LYS	GLY	ALA	PRO	PRO	LEU	VAL	SER	TRP	LYS	VAL	GLY	GLU	PRO	D207	D208	A209	S210	W211	L212	Y220	W221	R224	A225	P226	P227	F228	S229	S232	W242	D243	Q244	H245	L246	D250	Y253	T254	P255	D256	D257	T260
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V261	T262	E263	T264	Q265	V266	S275	Q276	K279	L280	M286	D287	Q288	K289	V290	N291	V292	R293	L297	V298	T299	T302	Q303	N304	R307	S308	V309	L310	Y316	V319	R322	F326	E329	ILE	THR	GLY	HIS	GLY	SER	GLU	VAL	PRO	LEU	PRO	GLY	THR	LEU	PRO	THR
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	ALA	LYS	LYS	LHR	THR	GLU	ALA	PRO	R354	R359	M361	W362	Y365	K366	Y367	F371	E379	K385	D387	T388	V389	T390	I393	V394	L398	L408	H409	R410	G415	L416	A417	B418	V419	P420	P421	D422	T423	R424	R428	T435	L436	Y437	Y443	D444	N445	E448
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A449	A450	S451	S452	S453	S454	S455	S456	S457	S458	S459	S460	S461	S462	S463	S464	S465	S466	S467	S468	S469	S470	S471	S472	S473	S474	S475	S476	S477	S478	S479	S480	S481	S482	S483	S484	S485	S486	S487	S488	S489	S490	S491	S492	S493	S494	S495	S496	S497	S498	S499	S500	S501	S502	S503	S504	S505	S506	S507	S508	S509	S510	S511	S512	S513	S514	S515	S516	S517	S518	S519	S520	S521	S522	S523	S524	S525	S526	S527	S528	S529	S530	S531	S532	S533	S534	S535	S536	S537	S538	S539	S540	S541	S542	S543	S544	S545	S546	S547	S548	S549	S550	S551	S552	S553	S554	S555	S556	S557	S558	S559	S560	S561	S562	S563	S564	S565	S566	S567	S568	S569	S570	S571	S572	S573	S574	S575	S576	S577	S578	S579	S580	S581	S582	S583	S584	S585	S586	S587	S588	S589	S590	S591	S592	S593	S594	S595	S596	S597	S598	S599	S600	S601	S602	S603	S604	S605	S606	S607	S608	S609	S610	S611	S612	S613	S614	S615	S616	S617	S618	S619	S620	S621	S622	S623	S624	S625	S626	S627	S628	S629	S630	S631	S632	S633	S634	S635	S636	S637	S638	S639	S640	S641	S642	S643	S644	S645	S646	S647	S648	S649	S650	S651	S652	S653	S654	S655	S656	S657	S658	S659	S660	S661	S662	S663	S664	S665	S666	S667	S668	S669	S670	S671	S672	S673	S674	S675	S676	S677	S678	S679	S680	S681	S682	S683	S684	S685	S686	S687	S688	S689	S690	S691	S692	S693	S694	S695	S696	S697	S698	S699	S700	S701	S702	S703	S704	S705	S706	S707	S708	S709	S710	S711	S712	S713	S714	S715	S716	S717	S718	S719	S720	S721	S722	S723	S724	S725	S726	S727	S728	S729	S730	S731	S732	S733	S734	S735	S736	S737	S738	S739	S740	S741	S742	S743	S744	S745	S746	S747	S748	S749	S750	S751	S752	S753	S754	S755	S756	S757	S758	S759	S760	S761	S762	S763	S764	S765	S766	S767	S768	S769	S770	S771	S772	S773	S774	S775	S776	S777	S778	S779	S780	S781	S782	S783	S784	S785	S786	S787	S788	S789	S790	S791	S792	S793	S794	S795	S796	S797	S798	S799	S800	S801	S802	S803	S804	S805	S806	S807	S808	S809	S810	S811	S812	S813	S814	S815	S816	S817	S818	S819	S820	S821	S822	S823	S824	S825	S826	S827	S828	S829	S830	S831	S832	S833	S834	S835	S836	S837	S838	S839	S840	S841	S842	S843	S844	S845	S846	S847	S848	S849	S850	S851	S852	S853	S854	S855	S856	S857	S858	S859	S860	S861	S862	S863	S864	S865	S866	S867	S868	S869	S870	S871	S872	S873	S874	S875	S876	S877	S878	S879	S880	S881	S882	S883	S884	S885	S886	S887	S888	S889	S890	S891	S892	S893	S894	S895	S896	S897	S898	S899	S900	S901	S902	S903	S904	S905	S906	S907	S908	S909	S910	S911	S912	S913	S914	S915	S916	S917	S918	S919	S920	S921	S922	S923	S924	S925	S926	S927	S928	S929	S930	S931	S932	S933	S934	S935	S936	S937	S938	S939	S940	S941	S942	S943	S944	S945	S946	S947	S948	S949	S950	S951	S952	S953	S954	S955	S956	S957	S958	S959	S960	S961	S962	S963	S964	S965	S966	S967	S968	S969	S970	S971	S972	S973	S974	S975	S976	S977	S978	S979	S980	S981	S982	S983	S984	S985	S986	S987	S988	S989	S990	S991	S992	S993	S994	S995	S996	S997	S998	S999	S1000
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ASN	ALA	ALA	ALA	ALA	SER	SER	GLY	SER	SER	ASP	GLN	ALA	ALA	PRO	GLY	GLN	ARG	HIS	THR	MET	VAL	SER	PHE	L548	L555	L556	M557	M562	K566	C570	R571	R578	ALA	ALA	LEU	GLN	GLN	ASP	ASP	SER	SER	ARG	ASP	SER	SER	ASP	ARG	LYS	SER	L587	Y588	Q596	R597	R598	L599	Q600	H601	GLY	ASN
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[illegible]

VAL	CYS	VAL	ASP	ARG	SER	<b>\$670</b>	<b>\$671</b>	<b>\$672</b>	<b>\$673</b>	<b>\$674</b>	<b>\$675</b>	<b>\$676</b>	<b>\$677</b>	<b>\$678</b>	<b>\$679</b>	<b>\$680</b>	<b>\$681</b>	<b>\$682</b>	<b>\$683</b>	<b>\$687</b>	<b>\$688</b>	<b>\$689</b>	<b>\$692</b>	<b>\$701</b>	<b>\$702</b>	<b>\$703</b>	<b>\$704</b>	LEU	LYS	LYS	ASP	TYR	ARG	ARG	LEU	VAL	GLU	TYR	LEU	GLN	ALA	MET	ARG	ASN	PHE	PHE	LEU	LEU	GLU	ALA	GLY	ASP	THR	THR	TYR	TYR	ASP	PHE
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TYR	THR	PRO	THR	PRO	ILE	PHE	ASP	LYS	ILE	ARG	GLU	LYS	PRO	PRO	GLU	LEU	LEU	ASN	TYR	TYR	LEU	ASN	VAL	VAL	GLN	ILE	GLN	GLU	ALA	ALA	VAL	GLY	GLN	ARG	TYR	PRO	ASP	ASP	SER	SER	THR	ARG	LEU	SER	VAL	VAL	SER	GLU	PHE	THR	SER	VAL	VAL	LEU	ALA	LYS	LYS	LYS	LEU	PRO	VAL	HIS	THR	LEU	ASP	GLY
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LEU ILE LEU LEU SER TYR LYS VAL PRO PRO VAL ASP ILE VAL ILE SER SER SER ASN GLN GLN VAL PHE LEU LEU LEU ILE LYS TYR TRP ALA LYS SER SER SER LEU LEU ASP VAL LEU LEU PHE ASN ASN GLU LEU GLY ASN ALA SER SER THR LYS GLU GLY

ALA	THR	VAL	GLU	PRO	PHE	LEU	PRO	PRO	LEU	THR	SER	SER	PRO	GLY	PRO	PRO	LYS	GLY	GLN	ILE	HIS	ARG	MET	PHE	LEU	LEU	ARG	VAL	LYS	LEU	MET	HIS	HIS	ASN	TYR	LEU	MET	THR	ARG	ILE	LEU	HIS	SER	THR	GLY	GLY	GLU	PHE	GLN	HIS	GLN	VAL	THR
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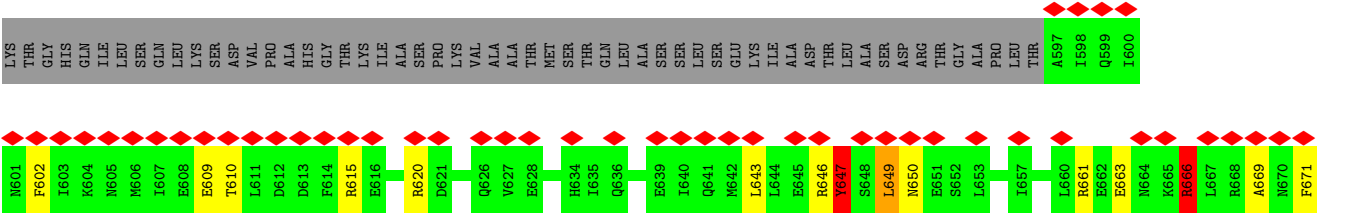
GLU ALA LYS LEU ASP GLN LEU LYS ILE ILE HIS TYR ARG TYR LEU SER THR ILE HIS ASP ARG CYS LEU LEU ARG GLU LYS VAL SER SER VAL LYS GLU ALA ILE MET MET VAL VAL LEU ASN VAL VAL LEU MET PHE LEU LEU VAL TRP TRP LYS LEU GLY GLY LEU GLY ALA ALA TRP LYS THR

Chain L:  12% 21% 6% 72%

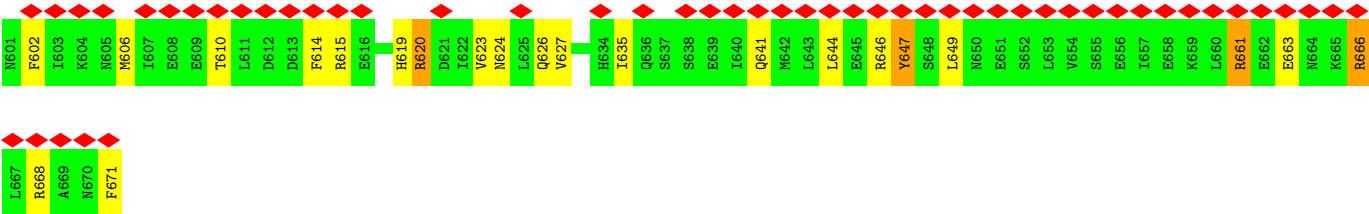
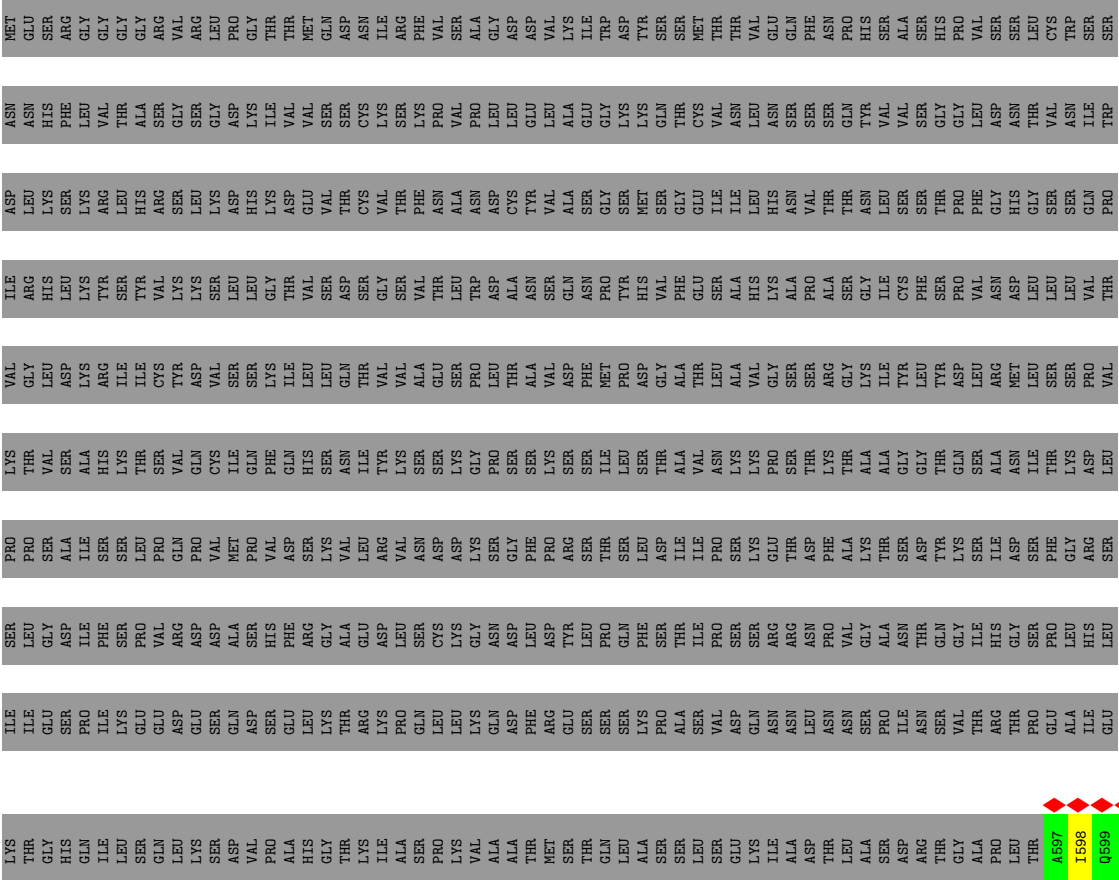




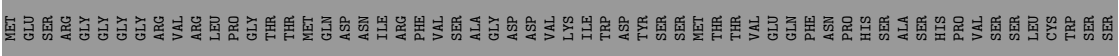




• Molecule 6: NEDD1 gamma-tubulin ring complex targeting factor L homeolog

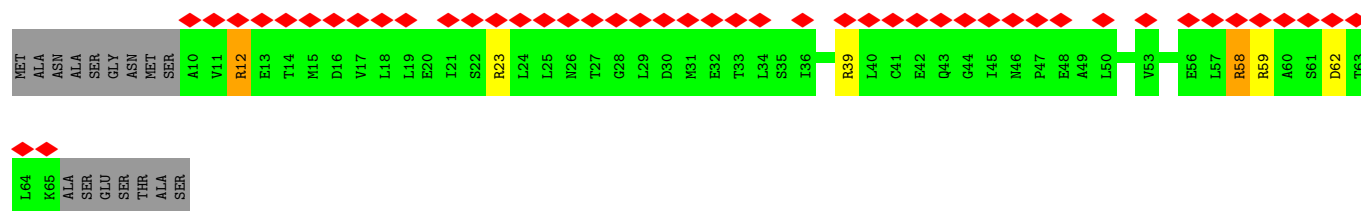


• Molecule 6: NEDD1 gamma-tubulin ring complex targeting factor L homeolog

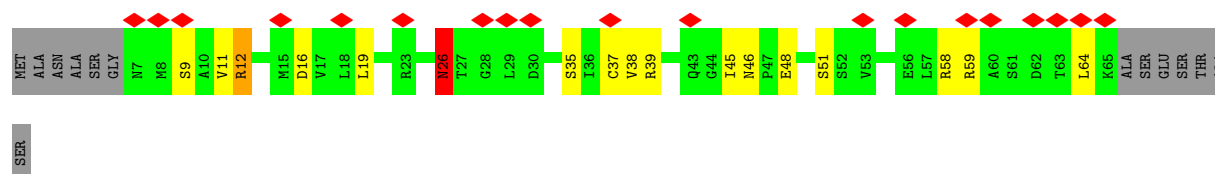




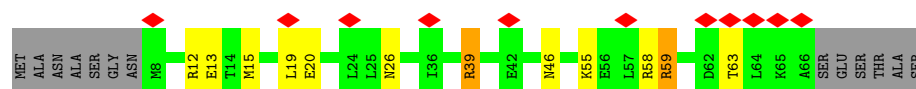




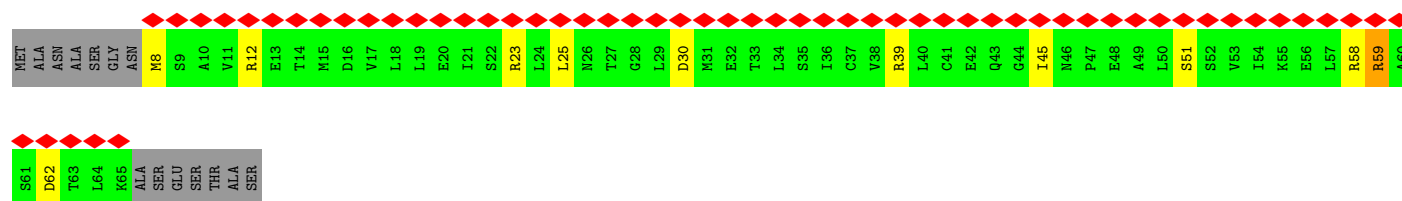
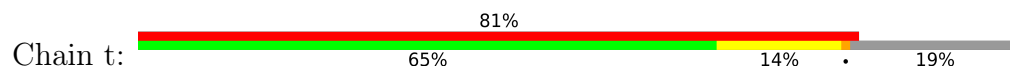
• Molecule 7: Mitotic-spindle organizing protein 1



• Molecule 7: Mitotic-spindle organizing protein 1



• Molecule 7: Mitotic-spindle organizing protein 1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	299022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	51	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.404	Depositor
Minimum map value	-0.286	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0421	Depositor
Map size (Å)	365.9392, 365.9392, 365.9392	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.42945, 1.42945, 1.42945	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	1.74	16/2254 (0.7%)	1.92	55/3055 (1.8%)
1	C	1.74	20/2053 (1.0%)	1.99	54/2781 (1.9%)
1	E	1.80	22/2077 (1.1%)	2.02	67/2813 (2.4%)
1	G	1.76	21/2053 (1.0%)	2.06	62/2781 (2.2%)
2	B	1.72	23/2413 (1.0%)	1.99	65/3257 (2.0%)
2	D	1.74	19/2101 (0.9%)	1.96	60/2831 (2.1%)
2	F	1.65	11/2004 (0.5%)	1.93	53/2700 (2.0%)
2	H	1.71	21/2178 (1.0%)	2.02	54/2936 (1.8%)
2	O	1.65	3/764 (0.4%)	1.82	13/1026 (1.3%)
2	Q	1.72	8/892 (0.9%)	1.90	16/1199 (1.3%)
2	R	1.73	8/805 (1.0%)	2.01	22/1081 (2.0%)
2	S	1.70	5/892 (0.6%)	1.92	18/1199 (1.5%)
2	T	1.75	6/764 (0.8%)	1.98	22/1026 (2.1%)
3	I	1.73	16/2377 (0.7%)	1.92	50/3212 (1.6%)
3	K	1.68	14/2377 (0.6%)	1.88	46/3212 (1.4%)
4	J	2.16	32/2976 (1.1%)	2.03	83/4037 (2.1%)
5	L	1.73	37/3862 (1.0%)	1.89	92/5228 (1.8%)
6	U	1.67	6/640 (0.9%)	2.00	17/854 (2.0%)
6	V	1.68	4/640 (0.6%)	2.12	14/854 (1.6%)
6	W	1.68	2/640 (0.3%)	1.82	18/854 (2.1%)
6	X	1.73	4/640 (0.6%)	2.01	17/854 (2.0%)
7	o	1.63	2/403 (0.5%)	1.97	8/541 (1.5%)
7	p	1.69	1/429 (0.2%)	1.96	9/577 (1.6%)
7	q	1.64	3/432 (0.7%)	1.96	10/581 (1.7%)
7	r	1.76	10/454 (2.2%)	1.91	12/610 (2.0%)
7	s	1.71	6/451 (1.3%)	1.72	9/606 (1.5%)
7	t	1.58	1/446 (0.2%)	2.11	14/599 (2.3%)
All	All	1.76	321/38017 (0.8%)	1.96	960/51304 (1.9%)

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	6
1	C	0	6
1	E	0	8
1	G	0	10
2	B	0	5
2	D	0	6
2	F	0	10
2	H	0	11
2	O	0	2
2	Q	0	2
2	R	0	3
2	S	0	3
2	T	0	2
3	I	0	9
3	K	0	6
4	J	0	16
5	L	0	20
6	U	0	4
6	V	0	2
6	W	0	4
6	X	0	4
7	o	0	2
7	q	0	2
7	r	0	1
7	s	0	1
7	t	0	1
All	All	0	146

All (321) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	242	TRP	CD2-CE3	35.46	1.93	1.40
4	J	242	TRP	CD2-CE2	31.73	1.79	1.41
4	J	242	TRP	CE2-CZ2	30.77	1.92	1.39
4	J	242	TRP	CZ3-CH2	26.52	1.82	1.40
4	J	242	TRP	CE3-CZ3	26.23	1.83	1.38
4	J	242	TRP	CZ2-CH2	26.14	1.87	1.37
3	I	16	ILE	CG1-CD1	19.29	2.83	1.50
3	K	271	ARG	CZ-NH2	8.95	1.44	1.33
5	L	366	SER	CA-CB	8.85	1.66	1.52
1	E	483	TYR	CE1-CZ	8.56	1.49	1.38
3	I	295	ARG	NE-CZ	8.15	1.43	1.33
1	A	491	TYR	CG-CD2	7.88	1.49	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	466	ARG	CZ-NH2	7.84	1.43	1.33
7	q	59	ARG	NE-CZ	7.67	1.43	1.33
2	B	310	ARG	NE-CZ	7.59	1.43	1.33
2	H	479	SER	CA-CB	7.49	1.64	1.52
1	E	280	SER	CA-CB	-7.48	1.41	1.52
3	I	37	GLY	N-CA	-7.43	1.34	1.46
5	L	407	TYR	CB-CG	7.25	1.62	1.51
3	I	260	ARG	CZ-NH1	7.25	1.42	1.33
1	G	280	SER	CA-CB	7.22	1.63	1.52
5	L	159	GLU	CD-OE1	7.21	1.33	1.25
1	E	326	TYR	CE1-CZ	7.18	1.47	1.38
1	E	351	GLY	CA-C	-7.13	1.40	1.51
4	J	275	SER	CA-CB	7.12	1.63	1.52
1	C	314	ARG	NE-CZ	7.10	1.42	1.33
7	r	35	SER	CA-CB	7.09	1.63	1.52
3	K	124	TYR	CE1-CZ	7.04	1.47	1.38
5	L	213	ARG	CD-NE	7.01	1.58	1.46
2	D	271	GLU	CD-OE1	7.01	1.33	1.25
2	B	402	TYR	CE1-CZ	7.00	1.47	1.38
7	r	9	SER	CA-CB	6.99	1.63	1.52
2	D	464	SER	CA-CB	6.94	1.63	1.52
1	E	253	SER	CA-CB	6.87	1.63	1.52
1	G	377	TYR	CZ-OH	6.85	1.49	1.37
4	J	475	TRP	NE1-CE2	-6.82	1.28	1.37
1	C	210	PRO	N-CD	-6.81	1.38	1.47
2	D	248	SER	CB-OG	6.80	1.51	1.42
2	D	434	TYR	CB-CG	6.80	1.61	1.51
3	I	194	GLY	CA-C	6.80	1.62	1.51
1	G	274	ARG	CZ-NH2	6.77	1.41	1.33
2	F	479	SER	CA-CB	6.75	1.63	1.52
5	L	383	GLY	CA-C	-6.72	1.41	1.51
7	o	58	ARG	NE-CZ	6.69	1.41	1.33
6	X	646	ARG	NE-CZ	6.64	1.41	1.33
2	F	457	ARG	NE-CZ	6.58	1.41	1.33
4	J	365	TYR	CZ-OH	6.58	1.49	1.37
1	A	383	SER	CA-CB	6.53	1.62	1.52
1	E	302	TYR	CG-CD2	6.52	1.47	1.39
1	C	447	ASP	N-CA	-6.51	1.33	1.46
1	G	285	GLY	N-CA	-6.49	1.36	1.46
1	E	246	SER	CA-CB	6.48	1.62	1.52
2	F	255	TYR	CE2-CZ	6.45	1.47	1.38
2	B	364	ARG	CZ-NH1	6.45	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	322	PHE	CG-CD1	6.41	1.48	1.38
1	E	278	GLU	CG-CD	6.39	1.61	1.51
2	B	480	ARG	CD-NE	6.39	1.57	1.46
7	s	59	ARG	NE-CZ	6.37	1.41	1.33
2	H	457	ARG	CZ-NH1	6.36	1.41	1.33
4	J	482	PHE	CG-CD1	6.35	1.48	1.38
2	B	359	SER	CA-CB	6.34	1.62	1.52
1	A	461	GLU	CB-CG	6.33	1.64	1.52
2	Q	56	GLU	CD-OE2	6.32	1.32	1.25
5	L	535	PHE	CG-CD2	6.29	1.48	1.38
6	W	661	ARG	NE-CZ	6.29	1.41	1.33
2	D	402	TYR	CZ-OH	6.28	1.48	1.37
3	I	46	CYS	CB-SG	-6.25	1.71	1.82
1	E	493	TYR	CE1-CZ	6.25	1.46	1.38
2	D	324	CYS	CB-SG	6.22	1.92	1.82
1	C	296	ARG	CZ-NH2	6.22	1.41	1.33
5	L	472	ARG	CZ-NH2	6.22	1.41	1.33
3	I	145	SER	CA-CB	6.22	1.62	1.52
4	J	316	TYR	CE2-CZ	6.22	1.46	1.38
4	J	220	TYR	CG-CD2	6.21	1.47	1.39
2	D	442	TYR	CZ-OH	6.21	1.48	1.37
1	G	332	ARG	NE-CZ	6.20	1.41	1.33
2	O	68	GLU	CG-CD	6.19	1.61	1.51
2	T	67	ARG	NE-CZ	6.17	1.41	1.33
7	p	58	ARG	CZ-NH1	6.16	1.41	1.33
7	r	51	SER	CA-CB	6.16	1.62	1.52
2	S	79	ARG	CD-NE	6.13	1.56	1.46
3	K	341	TRP	NE1-CE2	-6.13	1.29	1.37
2	H	537	TYR	CG-CD2	6.13	1.47	1.39
2	B	431	ARG	NE-CZ	6.12	1.41	1.33
6	U	661	ARG	NE-CZ	6.10	1.41	1.33
5	L	1365	TYR	CE2-CZ	6.10	1.46	1.38
2	H	360	SER	CA-CB	6.09	1.62	1.52
7	r	38	VAL	CB-CG2	6.08	1.65	1.52
2	B	264	PHE	CG-CD1	6.04	1.47	1.38
5	L	407	TYR	CG-CD2	6.03	1.47	1.39
2	B	294	SER	CA-CB	6.03	1.61	1.52
6	U	647	TYR	CG-CD1	6.01	1.47	1.39
2	B	430	TYR	CG-CD2	6.00	1.47	1.39
7	t	58	ARG	NE-CZ	5.98	1.40	1.33
2	F	436	GLY	N-CA	-5.98	1.37	1.46
1	E	363	PHE	C-N	5.97	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	466	ARG	CZ-NH2	5.96	1.40	1.33
5	L	413	HIS	CB-CG	5.93	1.60	1.50
5	L	546	ARG	NE-CZ	5.93	1.40	1.33
4	J	309	VAL	CB-CG1	5.92	1.65	1.52
1	G	386	TYR	CE1-CZ	5.92	1.46	1.38
5	L	396	SER	CA-CB	5.89	1.61	1.52
7	s	59	ARG	CZ-NH1	5.88	1.40	1.33
4	J	443	TYR	CD1-CE1	5.88	1.48	1.39
1	G	396	ARG	CZ-NH2	5.87	1.40	1.33
1	A	387	PHE	CA-CB	5.87	1.66	1.53
1	G	491	TYR	CG-CD1	5.86	1.46	1.39
4	J	379	GLU	CD-OE2	5.86	1.32	1.25
2	Q	79	ARG	NE-CZ	5.86	1.40	1.33
2	D	402	TYR	CG-CD1	5.84	1.46	1.39
2	B	430	TYR	CE1-CZ	5.84	1.46	1.38
1	C	359	HIS	CB-CG	5.83	1.60	1.50
1	G	328	GLN	CG-CD	5.83	1.64	1.51
2	B	457	ARG	CZ-NH1	5.82	1.40	1.33
4	J	466	ARG	NE-CZ	5.82	1.40	1.33
2	H	316	PHE	CE2-CZ	5.82	1.48	1.37
3	I	54	ARG	CZ-NH2	5.81	1.40	1.33
5	L	168	TYR	CZ-OH	5.81	1.47	1.37
4	J	678	PHE	CG-CD1	5.80	1.47	1.38
1	E	387	PHE	CA-CB	5.80	1.66	1.53
7	r	12	ARG	CZ-NH1	5.79	1.40	1.33
2	B	457	ARG	CZ-NH2	5.79	1.40	1.33
2	H	257	PHE	CG-CD2	5.78	1.47	1.38
2	T	19	ARG	CZ-NH1	5.76	1.40	1.33
6	U	655	SER	CB-OG	5.76	1.49	1.42
2	D	434	TYR	CZ-OH	5.75	1.47	1.37
2	H	480	ARG	NE-CZ	5.75	1.40	1.33
5	L	532	TYR	CG-CD1	5.74	1.46	1.39
2	B	491	PHE	CG-CD2	5.74	1.47	1.38
3	I	124	TYR	CG-CD2	5.74	1.46	1.39
3	I	253	SER	CA-CB	5.73	1.61	1.52
3	I	278	PHE	CA-CB	5.73	1.66	1.53
5	L	179	ARG	CZ-NH1	5.72	1.40	1.33
2	F	333	GLU	CB-CG	5.72	1.63	1.52
1	G	269	TYR	CE1-CZ	5.72	1.46	1.38
6	X	656	GLU	CD-OE2	5.71	1.31	1.25
5	L	546	ARG	CZ-NH1	5.71	1.40	1.33
3	K	12	TYR	CE2-CZ	5.70	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	r	9	SER	CB-OG	5.70	1.49	1.42
1	E	486	ARG	NE-CZ	5.70	1.40	1.33
2	H	283	SER	CB-OG	5.70	1.49	1.42
1	E	482	ALA	CA-CB	5.69	1.64	1.52
3	I	307	PHE	CG-CD1	5.67	1.47	1.38
1	A	488	GLU	CD-OE1	5.67	1.31	1.25
2	B	447	VAL	CB-CG1	5.67	1.64	1.52
1	E	269	TYR	CE1-CZ	5.67	1.46	1.38
1	G	485	GLU	CG-CD	5.66	1.60	1.51
5	L	573	TYR	CE1-CZ	5.66	1.46	1.38
1	A	284	TYR	CD1-CE1	5.66	1.47	1.39
2	H	251	ARG	NE-CZ	5.66	1.40	1.33
5	L	1373	SER	CA-CB	5.66	1.61	1.52
5	L	410	ARG	NE-CZ	5.65	1.40	1.33
2	H	549	ASN	N-CA	-5.64	1.35	1.46
1	C	393	TRP	CA-CB	5.63	1.66	1.53
3	I	169	ARG	NE-CZ	5.62	1.40	1.33
2	D	335	TYR	CD1-CE1	5.61	1.47	1.39
2	O	34	TYR	CZ-OH	5.60	1.47	1.37
1	A	493	TYR	CG-CD1	5.59	1.46	1.39
2	H	265	VAL	CB-CG2	5.59	1.64	1.52
5	L	384	VAL	CB-CG1	5.59	1.64	1.52
2	H	255	TYR	CZ-OH	5.58	1.47	1.37
2	H	306	TYR	CG-CD1	5.58	1.46	1.39
2	H	376	ARG	CG-CD	5.57	1.65	1.51
6	V	620	ARG	CZ-NH2	5.57	1.40	1.33
1	E	405	GLU	CB-CG	5.57	1.62	1.52
1	C	211	SER	CA-CB	5.56	1.61	1.52
2	T	48	GLU	CG-CD	5.54	1.60	1.51
2	D	334	TYR	CG-CD1	-5.54	1.31	1.39
2	H	344	GLN	CA-CB	5.54	1.66	1.53
3	K	158	TYR	CB-CG	5.53	1.59	1.51
1	C	383	SER	CA-CB	5.53	1.61	1.52
4	J	437	TYR	CE1-CZ	5.51	1.45	1.38
4	J	253	TYR	CZ-OH	5.51	1.47	1.37
2	B	488	SER	CB-OG	5.51	1.49	1.42
2	B	547	VAL	CB-CG2	5.50	1.64	1.52
1	G	364	GLY	CA-C	-5.50	1.43	1.51
7	s	39	ARG	CZ-NH2	5.50	1.40	1.33
1	E	240	ARG	CZ-NH2	5.50	1.40	1.33
1	C	296	ARG	CD-NE	5.49	1.55	1.46
1	G	404	SER	CA-CB	5.49	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	591	VAL	CB-CG1	5.48	1.64	1.52
2	Q	67	ARG	CZ-NH2	5.47	1.40	1.33
4	J	367	TYR	CE2-CZ	5.47	1.45	1.38
2	F	477	ASP	CA-C	-5.46	1.38	1.52
7	r	48	GLU	CG-CD	5.46	1.60	1.51
2	B	522	PHE	CG-CD2	5.46	1.47	1.38
1	G	222	TYR	CG-CD2	5.46	1.46	1.39
6	X	647	TYR	CA-CB	5.46	1.66	1.53
2	F	409	TYR	CE1-CZ	5.45	1.45	1.38
2	H	439	GLU	CG-CD	5.45	1.60	1.51
2	D	274	TYR	CG-CD1	5.45	1.46	1.39
2	R	32	PHE	CA-CB	5.45	1.66	1.53
4	J	387	GLU	CG-CD	5.44	1.60	1.51
5	L	371	TYR	CZ-OH	5.44	1.47	1.37
5	L	523	SER	CB-OG	-5.44	1.35	1.42
2	Q	108	PRO	N-CD	-5.43	1.40	1.47
2	R	32	PHE	CG-CD2	5.43	1.46	1.38
5	L	541	TYR	CG-CD2	5.43	1.46	1.39
6	X	627	VAL	CB-CG2	5.42	1.64	1.52
1	G	246	SER	CA-CB	5.41	1.61	1.52
5	L	539	TRP	NE1-CE2	-5.40	1.30	1.37
7	q	12	ARG	NE-CZ	5.40	1.40	1.33
2	B	277	ASP	CB-CG	5.40	1.63	1.51
1	E	240	ARG	CZ-NH1	5.39	1.40	1.33
6	V	663	GLU	CG-CD	5.39	1.60	1.51
2	H	444	GLU	CD-OE1	5.38	1.31	1.25
1	A	222	TYR	CE1-CZ	5.37	1.45	1.38
2	T	76	GLU	CG-CD	5.37	1.60	1.51
2	Q	66	ARG	CZ-NH1	5.37	1.40	1.33
1	C	483	TYR	CE1-CZ	5.36	1.45	1.38
2	F	311	SER	CA-CB	5.35	1.60	1.52
4	J	326	PHE	CE2-CZ	5.35	1.47	1.37
1	A	410	GLU	CD-OE1	5.35	1.31	1.25
3	K	100	TYR	CG-CD1	5.34	1.46	1.39
4	J	410	ARG	NE-CZ	5.34	1.40	1.33
2	H	434	TYR	CB-CG	5.34	1.59	1.51
2	S	105	ARG	NE-CZ	5.34	1.40	1.33
5	L	1358	SER	CB-OG	-5.33	1.35	1.42
2	T	56	GLU	CB-CG	5.33	1.62	1.52
4	J	291	ASN	CA-C	-5.33	1.39	1.52
4	J	598	ARG	CZ-NH2	5.32	1.40	1.33
5	L	596	TYR	CE1-CZ	5.31	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	55	PHE	CG-CD1	5.31	1.46	1.38
2	R	43	PHE	CA-C	-5.31	1.39	1.52
5	L	158	PHE	CG-CD1	5.30	1.46	1.38
6	U	648	SER	CA-CB	5.30	1.60	1.52
7	s	20	GLU	CD-OE1	5.29	1.31	1.25
1	E	274	ARG	CZ-NH2	5.29	1.40	1.33
2	D	315	ALA	CA-CB	5.29	1.63	1.52
3	K	260	ARG	CZ-NH2	5.29	1.40	1.33
1	G	351	GLY	CA-C	-5.28	1.43	1.51
2	D	333	GLU	CD-OE2	5.28	1.31	1.25
1	E	288	ASN	CB-CG	5.28	1.63	1.51
2	Q	67	ARG	CD-NE	5.28	1.55	1.46
2	R	79	ARG	CZ-NH2	5.28	1.40	1.33
7	s	63	THR	N-CA	-5.27	1.35	1.46
1	G	455	TYR	CZ-OH	5.27	1.46	1.37
3	K	262	GLU	CD-OE1	5.27	1.31	1.25
4	J	242	TRP	CG-CD1	5.27	1.44	1.36
1	C	282	PHE	CG-CD1	5.25	1.46	1.38
5	L	343	PRO	CA-C	-5.25	1.42	1.52
2	O	95	TYR	CG-CD1	5.25	1.46	1.39
1	C	231	TYR	CG-CD1	5.25	1.46	1.39
2	F	464	SER	CA-CB	5.25	1.60	1.52
2	H	369	TRP	CZ2-CH2	5.25	1.47	1.37
1	C	231	TYR	CZ-OH	5.25	1.46	1.37
1	E	284	TYR	CE1-CZ	5.24	1.45	1.38
4	J	497	PRO	N-CD	5.24	1.55	1.47
6	U	666	ARG	NE-CZ	5.23	1.39	1.33
2	Q	11	VAL	CB-CG2	5.23	1.63	1.52
4	J	221	TRP	CG-CD2	5.23	1.52	1.43
5	L	158	PHE	CB-CG	5.23	1.60	1.51
2	S	92	SER	CB-OG	5.22	1.49	1.42
5	L	445	ARG	CZ-NH2	5.22	1.39	1.33
7	r	58	ARG	NE-CZ	5.19	1.39	1.33
3	I	110	GLU	CD-OE2	5.19	1.31	1.25
1	C	256	LYS	CA-CB	5.18	1.65	1.53
1	C	346	LYS	C-N	5.18	1.42	1.33
7	q	39	ARG	NE-CZ	5.18	1.39	1.33
1	A	314	ARG	NE-CZ	5.17	1.39	1.33
7	o	52	SER	CA-CB	-5.17	1.45	1.52
3	I	346	GLU	N-CA	-5.17	1.36	1.46
2	R	9	PRO	N-CD	-5.17	1.40	1.47
2	Q	18	CYS	CB-SG	5.17	1.91	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	r	11	VAL	CB-CG2	5.16	1.63	1.52
1	C	405	GLU	CA-CB	5.16	1.65	1.53
2	R	32	PHE	CE2-CZ	5.16	1.47	1.37
3	I	128	GLN	CG-CD	5.16	1.62	1.51
1	C	350	PHE	CG-CD1	5.15	1.46	1.38
2	B	491	PHE	CG-CD1	5.15	1.46	1.38
1	E	233	SER	CA-CB	5.15	1.60	1.52
5	L	573	TYR	CG-CD1	5.15	1.45	1.39
3	K	284	GLN	N-CA	-5.14	1.36	1.46
7	r	39	ARG	CZ-NH2	5.14	1.39	1.33
4	J	415	GLY	N-CA	-5.13	1.38	1.46
2	H	323	PHE	CG-CD1	5.13	1.46	1.38
2	B	463	TYR	CG-CD2	5.13	1.45	1.39
2	H	257	PHE	CD1-CE1	5.12	1.49	1.39
6	V	609	GLU	CD-OE1	5.12	1.31	1.25
1	C	402	PRO	N-CD	-5.12	1.40	1.47
1	G	230	ARG	NE-CZ	5.12	1.39	1.33
3	K	161	SER	CB-OG	-5.12	1.35	1.42
4	J	683	ARG	NE-CZ	5.12	1.39	1.33
2	R	92	SER	CA-CB	5.12	1.60	1.52
2	B	513	GLU	CB-CG	5.11	1.61	1.52
2	D	457	ARG	CZ-NH1	5.11	1.39	1.33
2	S	102	GLU	CG-CD	5.11	1.59	1.51
5	L	407	TYR	CE2-CZ	5.10	1.45	1.38
2	S	113	SER	CA-CB	5.10	1.60	1.52
3	K	22	ARG	NE-CZ	5.09	1.39	1.33
5	L	1365	TYR	CG-CD1	5.09	1.45	1.39
1	C	275	PHE	CG-CD1	5.09	1.46	1.38
2	B	330	GLU	CD-OE2	-5.08	1.20	1.25
2	T	56	GLU	CD-OE1	5.08	1.31	1.25
1	A	431	TYR	CG-CD1	5.07	1.45	1.39
5	L	568	TYR	CZ-OH	5.07	1.46	1.37
1	G	396	ARG	C-N	5.07	1.42	1.33
1	A	231	TYR	CG-CD1	5.07	1.45	1.39
1	A	245	PHE	CB-CG	5.07	1.59	1.51
1	E	361	ARG	CZ-NH2	5.07	1.39	1.33
1	G	348	GLU	CD-OE2	5.06	1.31	1.25
1	G	393	TRP	NE1-CE2	5.06	1.44	1.37
1	A	373	GLU	CB-CG	5.06	1.61	1.52
2	D	473	PHE	N-CA	-5.06	1.36	1.46
2	F	365	ARG	CZ-NH1	5.06	1.39	1.33
3	K	326	GLU	CD-OE2	5.05	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	365	ARG	CZ-NH1	5.05	1.39	1.33
3	K	101	ARG	CZ-NH2	5.04	1.39	1.33
5	L	462	PHE	CG-CD2	5.04	1.46	1.38
2	B	409	TYR	CZ-OH	5.03	1.46	1.37
7	s	13	GLU	CG-CD	5.03	1.59	1.51
6	V	650	ASN	CG-ND2	5.03	1.45	1.32
1	A	430	ARG	CZ-NH1	5.03	1.39	1.33
2	D	310	ARG	CD-NE	5.03	1.54	1.46
6	W	620	ARG	CZ-NH1	5.03	1.39	1.33
2	R	67	ARG	CZ-NH1	5.02	1.39	1.33
4	J	498	PHE	CG-CD1	5.02	1.46	1.38
1	A	269	TYR	CZ-OH	5.02	1.46	1.37
1	C	441	PHE	CE2-CZ	5.01	1.46	1.37
6	U	636	GLN	CG-CD	5.01	1.62	1.51
4	J	507	THR	N-CA	-5.00	1.36	1.46

All (960) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	364	ARG	NE-CZ-NH2	-21.14	109.73	120.30
6	V	661	ARG	NE-CZ-NH1	20.07	130.33	120.30
4	J	571	ARG	NE-CZ-NH1	20.02	130.31	120.30
5	L	410	ARG	NE-CZ-NH1	19.87	130.23	120.30
4	J	501	ARG	NE-CZ-NH1	18.54	129.57	120.30
2	B	402	TYR	CB-CG-CD2	-17.97	110.22	121.00
6	U	666	ARG	NE-CZ-NH2	-16.56	112.02	120.30
1	G	284	TYR	CB-CG-CD2	-16.16	111.30	121.00
1	G	230	ARG	NE-CZ-NH2	-16.02	112.29	120.30
1	G	431	TYR	CB-CG-CD2	15.99	130.60	121.00
3	K	271	ARG	NE-CZ-NH1	15.77	128.18	120.30
2	H	411	ARG	NE-CZ-NH2	-15.64	112.48	120.30
2	B	314	ARG	NE-CZ-NH2	15.52	128.06	120.30
2	H	314	ARG	NE-CZ-NH2	15.37	127.98	120.30
1	C	403	TYR	CB-CG-CD2	-15.03	111.98	121.00
3	I	133	PHE	CB-CG-CD1	14.99	131.30	120.80
5	L	34	ARG	NE-CZ-NH1	14.70	127.65	120.30
2	T	90	ARG	NE-CZ-NH2	-14.69	112.95	120.30
6	V	661	ARG	NE-CZ-NH2	-14.52	113.04	120.30
4	J	571	ARG	NE-CZ-NH2	-14.51	113.05	120.30
7	t	12	ARG	NE-CZ-NH1	14.45	127.53	120.30
2	R	79	ARG	NE-CZ-NH2	-14.36	113.12	120.30
1	A	326	TYR	CB-CG-CD1	14.18	129.51	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	ARG	NE-CZ-NH1	14.12	127.36	120.30
7	o	59	ARG	NE-CZ-NH2	14.12	127.36	120.30
2	H	466	ARG	NE-CZ-NH1	14.01	127.30	120.30
7	q	23	ARG	NE-CZ-NH1	13.86	127.23	120.30
7	t	39	ARG	NE-CZ-NH2	13.78	127.19	120.30
7	r	58	ARG	NE-CZ-NH1	13.69	127.14	120.30
1	G	274	ARG	NE-CZ-NH1	13.62	127.11	120.30
1	G	431	TYR	CB-CG-CD1	-13.29	113.03	121.00
2	S	34	TYR	CB-CG-CD2	-13.23	113.06	121.00
5	L	407	TYR	CB-CG-CD2	-13.21	113.08	121.00
2	H	314	ARG	NE-CZ-NH1	-13.08	113.76	120.30
7	p	39	ARG	NE-CZ-NH2	-13.06	113.77	120.30
5	L	445	ARG	NE-CZ-NH1	12.96	126.78	120.30
5	L	465	ARG	NE-CZ-NH2	12.95	126.77	120.30
4	J	424	ARG	NE-CZ-NH1	-12.77	113.92	120.30
1	E	361	ARG	NE-CZ-NH2	-12.75	113.92	120.30
1	E	430	ARG	NE-CZ-NH2	12.73	126.67	120.30
6	X	646	ARG	NE-CZ-NH1	12.69	126.65	120.30
2	O	43	PHE	CB-CG-CD1	-12.69	111.92	120.80
2	B	431	ARG	NE-CZ-NH2	-12.60	114.00	120.30
2	Q	90	ARG	NE-CZ-NH2	12.52	126.56	120.30
1	A	326	TYR	CB-CG-CD2	-12.51	113.49	121.00
1	C	430	ARG	NE-CZ-NH2	12.39	126.50	120.30
2	S	37	ARG	NE-CZ-NH2	12.36	126.48	120.30
1	G	240	ARG	NE-CZ-NH2	-12.30	114.15	120.30
2	B	390	ARG	NE-CZ-NH2	-12.30	114.15	120.30
3	K	169	ARG	NE-CZ-NH2	-12.21	114.20	120.30
3	K	91	ARG	NE-CZ-NH2	-12.08	114.26	120.30
3	K	271	ARG	NE-CZ-NH2	-12.04	114.28	120.30
2	R	64	ARG	NE-CZ-NH1	11.99	126.30	120.30
2	R	52	PHE	CB-CG-CD2	-11.98	112.42	120.80
3	K	169	ARG	NE-CZ-NH1	11.93	126.27	120.30
2	D	442	TYR	CB-CG-CD1	-11.77	113.94	121.00
3	I	260	ARG	NE-CZ-NH2	-11.73	114.44	120.30
1	G	274	ARG	NE-CZ-NH2	-11.72	114.44	120.30
7	t	12	ARG	NE-CZ-NH2	-11.67	114.46	120.30
6	X	647	TYR	CB-CG-CD1	-11.65	114.01	121.00
3	I	333	ARG	NE-CZ-NH1	11.63	126.12	120.30
4	J	503	PHE	CB-CG-CD2	11.63	128.94	120.80
1	C	303	MET	CG-SD-CE	-11.62	81.60	100.20
2	D	390	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	C	275	PHE	CB-CG-CD1	-11.57	112.70	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	615	ARG	NE-CZ-NH2	-11.57	114.52	120.30
1	G	332	ARG	NE-CZ-NH2	-11.56	114.52	120.30
2	Q	32	PHE	CB-CG-CD1	11.53	128.87	120.80
2	R	49	ARG	NE-CZ-NH1	11.52	126.06	120.30
7	o	58	ARG	NE-CZ-NH2	-11.52	114.54	120.30
2	H	310	ARG	NE-CZ-NH1	11.51	126.05	120.30
2	H	274	TYR	CB-CG-CD2	11.46	127.87	121.00
4	J	598	ARG	NE-CZ-NH2	-11.36	114.62	120.30
5	L	44	TYR	CB-CG-CD2	-11.35	114.19	121.00
6	V	646	ARG	NE-CZ-NH1	11.30	125.95	120.30
2	T	90	ARG	NE-CZ-NH1	11.23	125.91	120.30
2	R	49	ARG	NE-CZ-NH2	-11.17	114.72	120.30
7	q	23	ARG	NE-CZ-NH2	-11.14	114.73	120.30
2	F	255	TYR	CB-CG-CD2	-11.09	114.35	121.00
4	J	365	TYR	CB-CG-CD2	-11.07	114.36	121.00
2	D	335	TYR	CB-CG-CD1	-11.06	114.36	121.00
1	A	396	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	E	455	TYR	CB-CG-CD1	11.01	127.61	121.00
6	V	647	TYR	CB-CG-CD1	10.97	127.58	121.00
1	E	361	ARG	NE-CZ-NH1	10.91	125.75	120.30
4	J	428	ARG	NE-CZ-NH1	10.86	125.73	120.30
3	K	91	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	E	240	ARG	NE-CZ-NH1	10.80	125.70	120.30
7	q	58	ARG	NE-CZ-NH1	10.78	125.69	120.30
2	B	255	TYR	CB-CG-CD2	-10.73	114.56	121.00
2	Q	32	PHE	CB-CG-CD2	-10.73	113.29	120.80
6	W	668	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	G	430	ARG	NE-CZ-NH2	-10.63	114.98	120.30
1	E	430	ARG	NE-CZ-NH1	-10.61	115.00	120.30
6	V	602	PHE	CB-CG-CD2	-10.59	113.39	120.80
5	L	313	TYR	CB-CG-CD1	-10.49	114.71	121.00
5	L	537	TYR	CB-CG-CD2	-10.40	114.76	121.00
2	F	365	ARG	NE-CZ-NH2	-10.39	115.10	120.30
5	L	573	TYR	CB-CG-CD1	-10.39	114.77	121.00
3	I	158	TYR	CB-CG-CD1	-10.38	114.77	121.00
5	L	438	ARG	NE-CZ-NH1	10.37	125.49	120.30
1	C	441	PHE	CB-CG-CD1	-10.37	113.55	120.80
1	G	314	ARG	NE-CZ-NH2	10.33	125.46	120.30
2	H	457	ARG	NE-CZ-NH2	10.31	125.46	120.30
1	A	365	TYR	CB-CG-CD2	-10.31	114.81	121.00
7	t	58	ARG	NE-CZ-NH2	-10.31	115.15	120.30
1	G	406	PHE	CB-CG-CD1	-10.30	113.59	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	274	TYR	CB-CG-CD1	-10.29	114.82	121.00
1	C	363	PHE	CB-CG-CD1	10.28	128.00	120.80
1	E	243	ARG	NE-CZ-NH2	-10.28	115.16	120.30
4	J	503	PHE	CB-CG-CD1	-10.28	113.61	120.80
6	V	615	ARG	NE-CZ-NH1	10.27	125.44	120.30
3	I	191	MET	CG-SD-CE	-10.27	83.78	100.20
1	E	392	ARG	NE-CZ-NH2	-10.26	115.17	120.30
2	Q	66	ARG	NE-CZ-NH2	10.25	125.43	120.30
1	E	261	ARG	NE-CZ-NH1	-10.23	115.19	120.30
4	J	224	ARG	NE-CZ-NH2	-10.19	115.20	120.30
1	G	377	TYR	CB-CG-CD2	-10.10	114.94	121.00
2	B	457	ARG	NE-CZ-NH1	10.00	125.30	120.30
7	o	39	ARG	NE-CZ-NH2	-9.99	115.30	120.30
6	U	615	ARG	NE-CZ-NH1	9.99	125.29	120.30
2	B	402	TYR	CB-CG-CD1	9.98	126.99	121.00
2	Q	90	ARG	NE-CZ-NH1	-9.97	115.31	120.30
2	T	34	TYR	CB-CG-CD1	9.97	126.98	121.00
2	F	473	PHE	CB-CG-CD1	9.95	127.77	120.80
7	q	12	ARG	NE-CZ-NH2	-9.94	115.33	120.30
6	W	668	ARG	NE-CZ-NH1	9.88	125.24	120.30
4	J	365	TYR	CB-CG-CD1	9.87	126.92	121.00
2	D	430	TYR	CB-CG-CD1	9.84	126.91	121.00
1	E	363	PHE	CB-CG-CD2	-9.83	113.92	120.80
4	J	468	TYR	CB-CG-CD1	-9.78	115.13	121.00
1	E	493	TYR	CB-CG-CD2	-9.78	115.14	121.00
2	D	251	ARG	NE-CZ-NH1	9.77	125.19	120.30
6	X	666	ARG	NE-CZ-NH1	9.76	125.18	120.30
2	H	423	TYR	CB-CG-CD2	-9.75	115.15	121.00
7	p	59	ARG	NE-CZ-NH2	-9.75	115.43	120.30
7	o	23	ARG	NE-CZ-NH1	-9.74	115.43	120.30
1	E	428	ASP	CB-CG-OD2	-9.74	109.54	118.30
4	J	687	TYR	CB-CG-CD2	-9.73	115.16	121.00
5	L	385	TYR	CB-CG-CD1	-9.73	115.16	121.00
7	p	23	ARG	NE-CZ-NH1	9.73	125.16	120.30
1	G	493	TYR	CB-CG-CD2	-9.72	115.17	121.00
4	J	687	TYR	CB-CG-CD1	9.68	126.81	121.00
6	U	668	ARG	NE-CZ-NH1	9.68	125.14	120.30
2	F	477	ASP	CB-CG-OD2	9.66	126.99	118.30
3	I	200	TYR	CB-CG-CD1	-9.64	115.21	121.00
3	I	200	TYR	CB-CG-CD2	9.64	126.78	121.00
2	F	323	PHE	CB-CG-CD1	-9.63	114.06	120.80
4	J	468	TYR	CG-CD1-CE1	-9.63	113.60	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	409	TYR	CB-CG-CD2	9.60	126.76	121.00
3	I	169	ARG	NE-CZ-NH1	-9.51	115.55	120.30
1	C	403	TYR	CB-CG-CD1	9.45	126.67	121.00
6	U	620	ARG	NE-CZ-NH1	-9.45	115.58	120.30
1	E	269	TYR	CB-CG-CD1	-9.44	115.33	121.00
2	B	376	ARG	NE-CZ-NH1	9.39	125.00	120.30
3	K	101	ARG	NE-CZ-NH1	9.39	125.00	120.30
2	O	66	ARG	NE-CZ-NH1	-9.37	115.61	120.30
1	C	455	TYR	CB-CG-CD2	-9.37	115.38	121.00
6	U	646	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	C	396	ARG	NE-CZ-NH2	-9.36	115.62	120.30
3	I	133	PHE	CB-CG-CD2	-9.30	114.29	120.80
5	L	404	TYR	CB-CG-CD1	9.29	126.58	121.00
1	E	325	PHE	CB-CG-CD2	-9.29	114.30	120.80
2	H	251	ARG	NE-CZ-NH2	-9.28	115.66	120.30
2	D	274	TYR	CB-CG-CD2	9.26	126.56	121.00
2	H	264	PHE	CB-CG-CD2	-9.24	114.33	120.80
4	J	703	TYR	CB-CG-CD2	9.23	126.54	121.00
1	G	377	TYR	CB-CG-CD1	9.22	126.53	121.00
5	L	407	TYR	CB-CG-CD1	9.21	126.53	121.00
7	q	59	ARG	NE-CZ-NH1	-9.20	115.70	120.30
1	G	296	ARG	NE-CZ-NH1	9.20	124.90	120.30
2	D	365	ARG	NE-CZ-NH1	-9.19	115.70	120.30
6	W	614	PHE	CB-CG-CD2	-9.17	114.38	120.80
1	A	230	ARG	NE-CZ-NH1	9.14	124.87	120.30
3	I	58	PHE	CB-CG-CD1	-9.10	114.43	120.80
2	D	316	PHE	CB-CG-CD1	9.09	127.16	120.80
5	L	537	TYR	CB-CG-CD1	9.09	126.45	121.00
1	G	455	TYR	CB-CG-CD1	9.07	126.44	121.00
2	B	529	PHE	CB-CG-CD2	-9.05	114.46	120.80
1	E	222	TYR	CB-CG-CD2	-9.00	115.60	121.00
2	T	66	ARG	NE-CZ-NH1	-8.97	115.81	120.30
3	I	333	ARG	NE-CZ-NH2	-8.94	115.83	120.30
2	Q	79	ARG	NE-CZ-NH2	8.94	124.77	120.30
2	F	402	TYR	CB-CG-CD2	-8.93	115.64	121.00
4	J	598	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	E	274	ARG	NE-CZ-NH2	-8.92	115.84	120.30
2	B	466	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	A	396	ARG	NE-CZ-NH2	-8.88	115.86	120.30
2	D	274	TYR	CB-CG-CD1	-8.86	115.68	121.00
2	S	95	TYR	CB-CG-CD1	-8.85	115.69	121.00
3	K	100	TYR	CB-CG-CD2	8.85	126.31	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	ARG	NE-CZ-NH1	8.84	124.72	120.30
6	V	620	ARG	NE-CZ-NH1	8.82	124.71	120.30
5	L	560	TYR	CB-CG-CD2	-8.82	115.71	121.00
2	F	435	ASP	CB-CG-OD2	-8.80	110.38	118.30
2	D	314	ARG	NE-CZ-NH2	-8.79	115.91	120.30
2	H	364	ARG	NE-CZ-NH1	8.78	124.69	120.30
2	S	49	ARG	NE-CZ-NH1	8.76	124.68	120.30
2	F	435	ASP	CB-CG-OD1	8.75	126.18	118.30
1	G	363	PHE	CB-CG-CD2	-8.75	114.67	120.80
1	E	314	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	G	483	TYR	CB-CG-CD1	-8.72	115.77	121.00
2	F	336	ARG	NE-CZ-NH2	-8.71	115.95	120.30
4	J	394	VAL	CG1-CB-CG2	8.66	124.76	110.90
6	U	661	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	C	243	ARG	NE-CZ-NH1	-8.65	115.97	120.30
3	I	12	TYR	CB-CG-CD1	8.62	126.17	121.00
4	J	501	ARG	NE-CZ-NH2	-8.61	115.99	120.30
2	H	423	TYR	CB-CG-CD1	8.58	126.15	121.00
2	D	251	ARG	NE-CZ-NH2	-8.57	116.01	120.30
2	D	463	TYR	CB-CG-CD2	-8.57	115.86	121.00
2	F	466	ARG	NE-CZ-NH2	-8.53	116.03	120.30
2	B	365	ARG	NE-CZ-NH1	8.53	124.56	120.30
3	I	55	PHE	CB-CG-CD2	-8.53	114.83	120.80
4	J	209	ARG	NE-CZ-NH1	8.52	124.56	120.30
2	B	480	ARG	NE-CZ-NH1	8.51	124.56	120.30
2	R	67	ARG	NE-CZ-NH2	8.51	124.56	120.30
1	E	377	TYR	CB-CG-CD2	8.50	126.10	121.00
2	H	446	PHE	CB-CG-CD2	8.49	126.74	120.80
1	E	377	TYR	CB-CG-CD1	-8.48	115.91	121.00
5	L	77	PHE	CB-CG-CD1	-8.48	114.86	120.80
2	H	432	TRP	CB-CG-CD1	8.47	138.01	127.00
1	G	303	MET	CG-SD-CE	-8.45	86.69	100.20
4	J	703	TYR	CB-CG-CD1	-8.44	115.94	121.00
2	B	335	TYR	CB-CG-CD2	-8.43	115.94	121.00
4	J	428	ARG	NE-CZ-NH2	-8.41	116.09	120.30
2	F	251	ARG	NE-CZ-NH2	-8.41	116.09	120.30
2	R	74	PHE	CB-CG-CD2	8.39	126.67	120.80
2	T	32	PHE	CB-CG-CD2	8.39	126.67	120.80
2	D	435	ASP	CB-CG-OD1	-8.38	110.76	118.30
4	J	262	THR	N-CA-CB	8.31	126.09	110.30
1	E	332	ARG	NE-CZ-NH1	-8.29	116.16	120.30
1	C	373	GLU	OE1-CD-OE2	8.28	133.24	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	615	ARG	NE-CZ-NH1	8.25	124.43	120.30
2	R	52	PHE	CB-CG-CD1	8.23	126.56	120.80
2	O	64	ARG	NE-CZ-NH1	8.20	124.40	120.30
3	I	206	ARG	NE-CZ-NH2	-8.16	116.22	120.30
5	L	445	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	C	441	PHE	CB-CG-CD2	8.11	126.47	120.80
2	B	364	ARG	NE-CZ-NH2	8.06	124.33	120.30
2	R	34	TYR	CB-CG-CD1	-8.03	116.19	121.00
3	I	313	ARG	NE-CZ-NH1	8.01	124.31	120.30
5	L	546	ARG	NE-CZ-NH1	8.01	124.31	120.30
2	Q	74	PHE	CB-CG-CD1	-7.99	115.21	120.80
4	J	355	ARG	NE-CZ-NH1	7.99	124.29	120.30
7	q	59	ARG	NE-CZ-NH2	-7.97	116.31	120.30
2	D	316	PHE	CB-CG-CD2	-7.96	115.23	120.80
1	A	360	ASP	CB-CG-OD1	7.95	125.46	118.30
3	I	52	TYR	CB-CG-CD2	-7.95	116.23	121.00
7	r	12	ARG	NE-CZ-NH2	7.95	124.27	120.30
3	I	55	PHE	CB-CG-CD1	7.91	126.34	120.80
1	A	365	TYR	CB-CG-CD1	7.90	125.74	121.00
2	B	335	TYR	CB-CG-CD1	7.90	125.74	121.00
6	X	646	ARG	NE-CZ-NH2	-7.89	116.35	120.30
2	F	255	TYR	CB-CG-CD1	7.89	125.73	121.00
2	F	365	ARG	NE-CZ-NH1	7.88	124.24	120.30
6	V	620	ARG	NE-CZ-NH2	-7.87	116.36	120.30
4	J	209	ARG	NE-CZ-NH2	-7.87	116.37	120.30
4	J	224	ARG	NE-CZ-NH1	-7.85	116.37	120.30
2	S	34	TYR	CG-CD2-CE2	-7.85	115.02	121.30
5	L	568	TYR	CD1-CE1-CZ	-7.81	112.78	119.80
7	q	59	ARG	NH1-CZ-NH2	7.78	127.96	119.40
6	X	620	ARG	NE-CZ-NH1	7.78	124.19	120.30
4	J	307	ARG	NE-CZ-NH2	-7.78	116.41	120.30
2	B	411	ARG	NE-CZ-NH2	7.77	124.19	120.30
2	F	434	TYR	CB-CG-CD2	7.77	125.66	121.00
2	O	91	TRP	CA-CB-CG	7.76	128.44	113.70
6	W	647	TYR	CB-CG-CD1	7.73	125.64	121.00
3	K	341	TRP	NE1-CE2-CD2	7.73	115.03	107.30
1	C	483	TYR	CB-CG-CD2	-7.72	116.37	121.00
2	B	480	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	C	395	TYR	CB-CG-CD1	-7.70	116.38	121.00
2	D	457	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	A	441	PHE	CB-CG-CD1	-7.69	115.42	120.80
1	G	455	TYR	CB-CG-CD2	-7.68	116.39	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	307	PHE	CB-CG-CD2	-7.66	115.44	120.80
2	B	434	TYR	CB-CG-CD2	7.66	125.60	121.00
3	K	100	TYR	CD1-CE1-CZ	7.66	126.69	119.80
2	F	402	TYR	CB-CG-CD1	7.64	125.58	121.00
4	J	367	TYR	CB-CG-CD1	-7.64	116.42	121.00
2	F	477	ASP	CB-CG-OD1	-7.63	111.43	118.30
1	E	428	ASP	CB-CG-OD1	7.62	125.15	118.30
5	L	541	TYR	CB-CG-CD2	-7.62	116.43	121.00
7	o	39	ARG	NE-CZ-NH1	7.61	124.10	120.30
6	V	602	PHE	CB-CG-CD1	7.61	126.12	120.80
5	L	547	ASP	CB-CG-OD1	-7.60	111.46	118.30
5	L	546	ARG	NE-CZ-NH2	-7.59	116.50	120.30
3	K	328	VAL	CG1-CB-CG2	7.59	123.04	110.90
1	G	230	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	C	432	THR	CA-CB-CG2	-7.57	101.80	112.40
5	L	560	TYR	CB-CG-CD1	7.57	125.54	121.00
6	X	614	PHE	CB-CG-CD2	-7.54	115.52	120.80
1	G	269	TYR	CB-CG-CD1	-7.54	116.48	121.00
3	I	16	ILE	CB-CG1-CD1	7.54	135.00	113.90
5	L	410	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	E	231	TYR	CB-CG-CD2	7.52	125.51	121.00
2	B	334	TYR	CB-CG-CD2	-7.51	116.50	121.00
1	E	491	TYR	CG-CD2-CE2	-7.50	115.30	121.30
1	A	243	ARG	NE-CZ-NH2	7.50	124.05	120.30
4	J	224	ARG	NH1-CZ-NH2	7.50	127.65	119.40
2	H	264	PHE	CB-CG-CD1	7.49	126.04	120.80
2	F	457	ARG	NE-CZ-NH1	7.48	124.04	120.30
2	H	537	TYR	CB-CG-CD2	-7.46	116.52	121.00
5	L	532	TYR	CB-CG-CD2	-7.45	116.53	121.00
3	K	341	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	G	284	TYR	CG-CD2-CE2	-7.44	115.35	121.30
6	X	633	PHE	CB-CG-CD2	-7.43	115.59	120.80
3	I	129	PHE	CB-CG-CD1	-7.42	115.61	120.80
1	G	325	PHE	CB-CG-CD2	7.42	125.99	120.80
2	Q	105	ARG	NE-CZ-NH2	-7.41	116.59	120.30
2	B	531	THR	CA-CB-CG2	-7.41	102.03	112.40
1	A	486	ARG	NE-CZ-NH2	-7.40	116.60	120.30
4	J	557	MET	CG-SD-CE	-7.40	88.35	100.20
7	r	64	LEU	CB-CG-CD2	7.40	123.58	111.00
2	D	334	TYR	CB-CG-CD1	7.40	125.44	121.00
6	W	614	PHE	CB-CG-CD1	7.40	125.98	120.80
1	G	428	ASP	CB-CG-OD2	7.40	124.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	305	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	G	284	TYR	CB-CG-CD1	7.38	125.43	121.00
2	D	480	ARG	NE-CZ-NH1	-7.36	116.62	120.30
2	B	336	ARG	CD-NE-CZ	7.35	133.89	123.60
4	J	362	TRP	CZ3-CH2-CZ2	7.35	130.42	121.60
7	o	59	ARG	NH1-CZ-NH2	-7.34	111.33	119.40
2	D	273	CYS	CA-CB-SG	-7.33	100.81	114.00
1	G	428	ASP	CB-CG-OD1	-7.33	111.70	118.30
3	I	87	ARG	NE-CZ-NH1	7.32	123.96	120.30
2	S	67	ARG	NE-CZ-NH2	-7.32	116.64	120.30
6	V	649	LEU	N-CA-CB	7.31	125.02	110.40
2	D	482	VAL	CA-CB-CG1	-7.31	99.94	110.90
1	C	325	PHE	CB-CG-CD2	-7.30	115.69	120.80
2	H	543	TYR	CB-CG-CD2	-7.29	116.62	121.00
1	G	350	PHE	CB-CG-CD2	-7.29	115.70	120.80
7	r	58	ARG	NE-CZ-NH2	-7.29	116.66	120.30
3	K	182	VAL	CA-CB-CG2	-7.28	99.98	110.90
7	t	62	ASP	CB-CG-OD1	-7.28	111.75	118.30
2	F	364	ARG	NE-CZ-NH2	-7.27	116.67	120.30
3	I	8	ALA	N-CA-CB	7.26	120.27	110.10
2	F	334	TYR	CB-CG-CD2	-7.25	116.65	121.00
6	V	666	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	C	377	TYR	CB-CG-CD1	7.24	125.34	121.00
2	B	409	TYR	CB-CG-CD1	7.23	125.34	121.00
2	B	325	ALA	CB-CA-C	-7.22	99.27	110.10
6	W	602	PHE	CB-CG-CD1	-7.22	115.75	120.80
1	E	455	TYR	CB-CG-CD2	-7.22	116.67	121.00
5	L	90	ARG	NE-CZ-NH2	-7.21	116.70	120.30
3	I	16	ILE	CA-CB-CG1	7.20	124.69	111.00
2	F	310	ARG	NE-CZ-NH1	7.20	123.90	120.30
2	D	335	TYR	CG-CD1-CE1	-7.17	115.56	121.30
1	C	392	ARG	NE-CZ-NH1	7.15	123.88	120.30
4	J	253	TYR	CB-CG-CD2	-7.15	116.71	121.00
5	L	504	TYR	CG-CD1-CE1	7.13	127.01	121.30
5	L	227	ASP	CB-CG-OD2	7.13	124.72	118.30
4	J	227	ARG	NE-CZ-NH2	7.11	123.85	120.30
4	J	256	ASP	CB-CG-OD2	-7.11	111.90	118.30
4	J	488	PHE	CG-CD2-CE2	-7.11	112.98	120.80
7	t	51	SER	CB-CA-C	-7.10	96.61	110.10
2	B	395	LEU	CB-CG-CD1	7.09	123.05	111.00
5	L	44	TYR	CB-CG-CD1	7.09	125.25	121.00
2	B	290	THR	CA-CB-CG2	-7.08	102.48	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	307	PHE	CB-CG-CD1	7.06	125.74	120.80
1	A	406	PHE	CB-CG-CD2	-7.05	115.87	120.80
2	D	431	ARG	NE-CZ-NH1	7.03	123.81	120.30
7	p	39	ARG	NH1-CZ-NH2	7.03	127.13	119.40
3	K	307	PHE	CB-CG-CD1	7.02	125.71	120.80
3	I	52	TYR	CB-CG-CD1	7.01	125.21	121.00
4	J	488	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	C	411	HIS	N-CA-CB	7.00	123.20	110.60
6	X	648	SER	N-CA-CB	7.00	120.99	110.50
1	G	486	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	C	343	SER	O-C-N	-6.98	111.53	122.70
2	S	41	SER	N-CA-CB	6.97	120.96	110.50
1	G	325	PHE	CB-CG-CD1	-6.97	115.92	120.80
7	s	58	ARG	NE-CZ-NH2	-6.97	116.82	120.30
2	S	43	PHE	CB-CG-CD2	-6.96	115.93	120.80
2	H	336	ARG	NE-CZ-NH2	-6.95	116.82	120.30
2	D	446	PHE	CB-CG-CD2	-6.95	115.94	120.80
3	K	307	PHE	CB-CG-CD2	-6.94	115.94	120.80
2	H	336	ARG	NE-CZ-NH1	6.93	123.77	120.30
3	I	271	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	E	491	TYR	CB-CG-CD1	-6.92	116.85	121.00
2	H	255	TYR	CB-CG-CD2	-6.91	116.86	121.00
5	L	473	TYR	CG-CD1-CE1	-6.91	115.77	121.30
2	H	394	GLU	O-C-N	6.91	133.75	122.70
5	L	44	TYR	CG-CD1-CE1	-6.89	115.79	121.30
2	T	67	ARG	NE-CZ-NH1	-6.86	116.87	120.30
2	T	89	ASN	N-CA-CB	6.86	122.95	110.60
1	E	491	TYR	CD1-CG-CD2	6.85	125.44	117.90
5	L	504	TYR	CB-CG-CD2	6.82	125.09	121.00
2	F	407	ASP	N-CA-CB	6.82	122.87	110.60
1	C	282	PHE	CB-CG-CD1	-6.81	116.03	120.80
1	C	326	TYR	CB-CG-CD1	-6.81	116.91	121.00
2	F	446	PHE	CB-CG-CD2	-6.81	116.03	120.80
2	D	423	TYR	CZ-CE2-CD2	6.81	125.93	119.80
5	L	326	TYR	CB-CG-CD2	-6.81	116.92	121.00
1	C	493	TYR	CB-CG-CD1	-6.79	116.93	121.00
2	B	514	SER	N-CA-CB	6.78	120.67	110.50
5	L	564	ARG	NE-CZ-NH1	-6.77	116.92	120.30
6	X	652	SER	N-CA-CB	6.77	120.65	110.50
4	J	250	ASP	CB-CG-OD1	6.77	124.39	118.30
4	J	562	MET	CG-SD-CE	-6.77	89.38	100.20
1	C	261	ARG	CB-CA-C	6.76	123.92	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	334	TYR	CB-CG-CD2	-6.76	116.94	121.00
2	H	341	LEU	CB-CG-CD2	6.75	122.48	111.00
2	F	445	PHE	CB-CG-CD2	-6.75	116.07	120.80
1	E	274	ARG	CD-NE-CZ	6.75	133.05	123.60
5	L	206	ASP	CB-CA-C	6.74	123.88	110.40
4	J	362	TRP	CE3-CZ3-CH2	-6.74	113.79	121.20
1	G	493	TYR	CB-CG-CD1	6.73	125.04	121.00
6	X	614	PHE	CG-CD2-CE2	-6.71	113.42	120.80
2	F	440	ASP	N-CA-CB	6.70	122.66	110.60
2	H	430	TYR	N-CA-CB	6.69	122.64	110.60
2	S	34	TYR	CD1-CG-CD2	6.69	125.26	117.90
3	K	200	TYR	CG-CD2-CE2	-6.68	115.95	121.30
5	L	532	TYR	CG-CD1-CE1	-6.68	115.95	121.30
3	I	157	VAL	CA-CB-CG2	-6.68	100.88	110.90
2	D	407	ASP	CB-CG-OD1	6.67	124.30	118.30
2	O	36	VAL	CG1-CB-CG2	6.67	121.57	110.90
7	t	23	ARG	NE-CZ-NH2	6.66	123.63	120.30
7	t	62	ASP	CB-CG-OD2	6.66	124.29	118.30
1	C	231	TYR	CB-CG-CD2	-6.65	117.01	121.00
3	K	133	PHE	CB-CG-CD2	6.65	125.46	120.80
2	D	423	TYR	CG-CD2-CE2	-6.65	115.98	121.30
2	H	306	TYR	CB-CG-CD1	-6.62	117.03	121.00
7	t	8	MET	CG-SD-CE	-6.62	89.61	100.20
2	B	299	LEU	CB-CG-CD1	6.62	122.25	111.00
1	E	325	PHE	CG-CD2-CE2	-6.60	113.54	120.80
2	T	95	TYR	CB-CG-CD2	-6.59	117.05	121.00
7	s	12	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	G	483	TYR	CG-CD1-CE1	-6.58	116.03	121.30
6	V	647	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	A	302	TYR	CG-CD1-CE1	-6.57	116.05	121.30
2	B	442	TYR	CG-CD2-CE2	-6.57	116.05	121.30
2	B	281	ALA	N-CA-C	-6.55	93.30	111.00
2	H	543	TYR	CB-CG-CD1	6.55	124.93	121.00
4	J	466	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	E	403	TYR	CB-CG-CD1	-6.52	117.09	121.00
3	I	204	PHE	CB-CG-CD2	6.52	125.36	120.80
3	I	305	ASP	CB-CG-OD2	6.52	124.17	118.30
2	R	79	ARG	NH1-CZ-NH2	6.52	126.57	119.40
2	F	315	ALA	N-CA-CB	6.51	119.22	110.10
2	H	430	TYR	CG-CD2-CE2	6.50	126.50	121.30
2	S	114	PHE	CB-CG-CD1	6.50	125.35	120.80
2	Q	52	PHE	CB-CG-CD1	-6.49	116.25	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	615	ARG	NE-CZ-NH2	6.49	123.55	120.30
2	D	452	VAL	N-CA-C	-6.48	93.50	111.00
4	J	498	PHE	CB-CG-CD2	-6.48	116.26	120.80
2	H	480	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	G	361	ARG	NE-CZ-NH1	6.46	123.53	120.30
6	W	615	ARG	NE-CZ-NH1	6.46	123.53	120.30
2	R	103	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	268	ASN	N-CA-CB	6.45	122.22	110.60
4	J	588	TYR	CG-CD2-CE2	-6.45	116.14	121.30
2	O	38	VAL	CA-CB-CG1	6.45	120.57	110.90
1	E	441	PHE	CB-CG-CD2	-6.45	116.29	120.80
2	F	434	TYR	CB-CG-CD1	-6.44	117.14	121.00
6	W	671	PHE	CB-CG-CD1	-6.43	116.30	120.80
3	K	267	TYR	CG-CD2-CE2	-6.42	116.16	121.30
7	o	23	ARG	NH1-CZ-NH2	6.42	126.47	119.40
1	G	395	TYR	CB-CG-CD2	-6.42	117.15	121.00
1	E	403	TYR	CB-CG-CD2	6.41	124.84	121.00
6	W	646	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	401	ASP	CB-CG-OD1	-6.40	112.54	118.30
2	F	336	ARG	NE-CZ-NH1	6.40	123.50	120.30
5	L	469	ARG	NE-CZ-NH2	-6.39	117.10	120.30
4	J	310	LEU	CB-CG-CD2	6.39	121.86	111.00
2	B	316	PHE	CB-CG-CD1	-6.38	116.33	120.80
6	X	615	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	B	491	PHE	CB-CG-CD1	6.38	125.26	120.80
5	L	539	TRP	CA-CB-CG	6.33	125.73	113.70
6	W	615	ARG	NH1-CZ-NH2	-6.32	112.44	119.40
2	F	529	PHE	CB-CG-CD1	-6.32	116.38	120.80
6	U	647	TYR	CB-CG-CD2	6.31	124.78	121.00
7	q	62	ASP	CB-CG-OD1	6.30	123.97	118.30
1	E	486	ARG	O-C-N	-6.30	112.61	122.70
2	B	407	ASP	CB-CG-OD2	-6.29	112.64	118.30
6	U	668	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	E	350	PHE	CG-CD2-CE2	6.28	127.70	120.80
2	H	432	TRP	CB-CG-CD2	-6.28	118.44	126.60
2	R	34	TYR	CB-CG-CD2	6.27	124.76	121.00
2	F	476	MET	CG-SD-CE	-6.27	90.16	100.20
2	B	466	ARG	N-CA-CB	6.26	121.88	110.60
2	T	62	PHE	CB-CG-CD1	-6.26	116.42	120.80
2	B	277	ASP	CB-CG-OD1	6.25	123.93	118.30
1	C	222	TYR	CB-CG-CD1	-6.25	117.25	121.00
3	K	205	VAL	CA-CB-CG2	-6.24	101.54	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	610	THR	CA-CB-CG2	-6.24	103.67	112.40
2	Q	37	ARG	NE-CZ-NH2	6.23	123.41	120.30
2	R	43	PHE	CB-CG-CD1	-6.21	116.45	120.80
1	G	381	ALA	N-CA-CB	6.21	118.79	110.10
2	D	314	ARG	N-CA-CB	6.20	121.77	110.60
3	I	1	MET	CG-SD-CE	-6.20	90.29	100.20
3	I	94	ASP	CB-CG-OD1	6.19	123.87	118.30
6	U	620	ARG	NH1-CZ-NH2	6.19	126.21	119.40
5	L	586	VAL	CB-CA-C	6.19	123.16	111.40
2	D	528	ALA	N-CA-CB	6.17	118.75	110.10
2	D	390	ARG	NE-CZ-NH2	-6.17	117.22	120.30
2	R	62	PHE	CB-CG-CD2	6.17	125.12	120.80
2	B	461	ASP	CB-CG-OD1	6.17	123.85	118.30
2	S	27	ASP	CB-CG-OD2	6.17	123.85	118.30
3	K	295	ARG	NE-CZ-NH2	-6.15	117.22	120.30
4	J	319	VAL	CA-CB-CG1	6.14	120.11	110.90
2	F	250	VAL	CG1-CB-CG2	-6.13	101.09	110.90
1	A	332	ARG	NH1-CZ-NH2	-6.13	112.66	119.40
6	X	661	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	E	314	ARG	NE-CZ-NH2	-6.13	117.24	120.30
5	L	421	ASP	CB-CG-OD2	-6.13	112.79	118.30
2	B	534	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	G	447	ASP	CB-CG-OD2	-6.12	112.79	118.30
2	D	376	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	276	VAL	CA-CB-CG2	6.12	120.08	110.90
2	S	66	ARG	NE-CZ-NH1	6.12	123.36	120.30
7	s	58	ARG	CD-NE-CZ	-6.12	115.03	123.60
5	L	315	THR	CA-CB-CG2	-6.12	103.84	112.40
4	J	454	VAL	O-C-N	-6.11	112.92	122.70
2	T	19	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	E	261	ARG	NH1-CZ-NH2	6.11	126.12	119.40
6	U	671	PHE	CB-CG-CD1	-6.11	116.53	120.80
3	K	164	GLY	O-C-N	6.10	132.47	122.70
2	R	34	TYR	CG-CD1-CE1	-6.10	116.42	121.30
1	G	447	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	222	TYR	CB-CG-CD1	6.10	124.66	121.00
1	A	384	ALA	N-CA-CB	6.09	118.63	110.10
2	D	442	TYR	CB-CG-CD2	6.08	124.65	121.00
1	E	441	PHE	CB-CG-CD1	6.08	125.05	120.80
1	A	222	TYR	CB-CG-CD2	-6.07	117.36	121.00
3	K	298	SER	N-CA-CB	6.04	119.56	110.50
2	F	322	SER	N-CA-CB	6.03	119.55	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	592	ALA	N-CA-CB	6.03	118.55	110.10
4	J	246	LEU	CB-CG-CD2	6.03	121.25	111.00
2	D	457	ARG	NE-CZ-NH2	-6.02	117.29	120.30
4	J	244	GLN	N-CA-CB	6.02	121.43	110.60
6	W	647	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	A	345	ASN	CB-CA-C	-6.01	98.37	110.40
3	K	111	PHE	CB-CG-CD2	-6.01	116.59	120.80
1	G	236	PRO	N-CA-CB	6.01	110.52	103.30
1	E	324	TRP	CB-CG-CD1	-6.00	119.21	127.00
1	A	365	TYR	CG-CD2-CE2	-5.99	116.51	121.30
5	L	467	LEU	CB-CG-CD2	5.99	121.18	111.00
2	F	398	ALA	N-CA-CB	5.99	118.48	110.10
3	I	310	GLU	OE1-CD-OE2	5.98	130.47	123.30
2	T	63	VAL	CA-CB-CG2	-5.97	101.94	110.90
2	H	280	VAL	CA-CB-CG2	-5.95	101.97	110.90
2	B	427	ASN	N-CA-CB	5.95	121.30	110.60
2	H	457	ARG	NH1-CZ-NH2	-5.95	112.86	119.40
2	H	537	TYR	CB-CG-CD1	5.94	124.57	121.00
2	Q	54	VAL	CA-CB-CG1	-5.94	101.98	110.90
2	F	267	MET	N-CA-CB	5.93	121.28	110.60
7	t	59	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	395	TYR	CB-CG-CD1	5.93	124.56	121.00
2	F	382	ALA	N-CA-CB	5.92	118.39	110.10
4	J	502	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	428	ASP	N-CA-CB	5.92	121.25	110.60
1	G	282	PHE	CB-CG-CD1	5.92	124.94	120.80
3	K	277	LEU	CB-CG-CD1	-5.92	100.94	111.00
1	C	230	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	E	296	ARG	NE-CZ-NH1	-5.91	117.34	120.30
3	I	100	TYR	CB-CG-CD1	-5.91	117.45	121.00
2	B	529	PHE	CB-CG-CD1	5.91	124.94	120.80
4	J	263	GLU	CG-CD-OE2	-5.91	106.48	118.30
4	J	242	TRP	NE1-CE2-CZ2	5.91	136.90	130.40
6	U	666	ARG	NH1-CZ-NH2	5.91	125.90	119.40
7	p	59	ARG	CD-NE-CZ	5.91	131.87	123.60
2	D	364	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	392	ARG	NH1-CZ-NH2	-5.90	112.91	119.40
2	H	531	THR	CA-CB-CG2	-5.90	104.14	112.40
6	X	620	ARG	NE-CZ-NH2	-5.90	117.35	120.30
7	p	59	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	D	284	LYS	N-CA-CB	5.89	121.21	110.60
5	L	159	GLU	OE1-CD-OE2	-5.89	116.23	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	433	ILE	N-CA-C	-5.89	95.09	111.00
2	O	88	LYS	CA-CB-CG	5.89	126.36	113.40
2	F	323	PHE	CB-CG-CD2	5.89	124.92	120.80
5	L	393	ASN	CB-CA-C	-5.89	98.62	110.40
2	S	19	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	258	LEU	CB-CG-CD2	5.88	121.00	111.00
2	B	461	ASP	CB-CG-OD2	-5.88	113.01	118.30
4	J	322	ARG	NE-CZ-NH2	5.87	123.23	120.30
2	B	431	ARG	NE-CZ-NH1	5.86	123.23	120.30
5	L	518	TYR	CG-CD1-CE1	5.86	125.99	121.30
1	C	269	TYR	CB-CG-CD2	5.86	124.51	121.00
2	T	95	TYR	CG-CD2-CE2	-5.85	116.62	121.30
1	C	323	LEU	CB-CG-CD1	5.85	120.95	111.00
1	E	491	TYR	CB-CG-CD2	-5.85	117.49	121.00
3	K	296	THR	C-N-CA	5.83	134.55	122.30
6	U	639	GLU	CB-CA-C	-5.83	98.73	110.40
1	A	470	ASP	CB-CG-OD1	-5.83	113.05	118.30
5	L	465	ARG	NE-CZ-NH1	-5.83	117.38	120.30
2	R	37	ARG	NE-CZ-NH2	-5.83	117.38	120.30
2	R	75	SER	N-CA-CB	-5.83	101.75	110.50
1	A	241	GLN	N-CA-CB	5.83	121.09	110.60
6	X	666	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	485	GLU	OE1-CD-OE2	5.82	130.28	123.30
2	D	407	ASP	CB-CG-OD2	-5.81	113.07	118.30
2	D	402	TYR	CB-CG-CD1	5.81	124.49	121.00
2	B	431	ARG	CD-NE-CZ	-5.81	115.47	123.60
1	G	406	PHE	CB-CG-CD2	5.81	124.87	120.80
3	K	62	TYR	CB-CG-CD2	5.81	124.49	121.00
2	Q	27	ASP	N-CA-CB	5.80	121.05	110.60
2	F	372	ASP	CB-CG-OD2	-5.79	113.09	118.30
2	B	376	ARG	NE-CZ-NH2	-5.79	117.41	120.30
3	I	325	PHE	N-CA-CB	-5.79	100.18	110.60
3	K	124	TYR	CD1-CE1-CZ	-5.79	114.59	119.80
1	A	486	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	G	318	LEU	CB-CG-CD2	5.78	120.83	111.00
2	F	345	LEU	CB-CG-CD1	5.78	120.82	111.00
1	G	486	ARG	CG-CD-NE	-5.78	99.67	111.80
6	X	633	PHE	CB-CG-CD1	5.78	124.84	120.80
2	R	89	ASN	N-CA-C	-5.77	95.41	111.00
1	E	245	PHE	CB-CG-CD1	-5.77	116.76	120.80
3	K	33	PHE	CZ-CE2-CD2	-5.77	113.17	120.10
1	C	482	ALA	N-CA-CB	5.77	118.18	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	606	LYS	N-CA-CB	5.77	120.98	110.60
3	I	257	PHE	CB-CG-CD1	-5.76	116.77	120.80
5	L	426	ASN	CB-CG-OD1	5.76	133.12	121.60
2	D	420	LEU	CB-CG-CD2	5.76	120.80	111.00
1	A	482	ALA	N-CA-CB	5.76	118.16	110.10
2	D	376	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	H	359	SER	C-N-CA	5.76	136.09	121.70
1	E	363	PHE	CB-CG-CD1	5.75	124.83	120.80
2	F	311	SER	C-N-CA	5.75	136.08	121.70
5	L	585	PRO	N-CA-C	5.75	127.04	112.10
2	D	405	THR	C-N-CA	5.74	134.36	122.30
1	G	269	TYR	CG-CD2-CE2	-5.74	116.71	121.30
7	s	63	THR	O-C-N	5.74	131.88	122.70
4	J	502	ASP	CB-CA-C	-5.74	98.93	110.40
2	F	409	TYR	CB-CG-CD2	-5.74	117.56	121.00
2	D	265	VAL	CA-CB-CG1	-5.73	102.30	110.90
3	K	286	PHE	CB-CG-CD2	-5.73	116.79	120.80
5	L	1365	TYR	CB-CG-CD2	5.73	124.44	121.00
1	A	287	VAL	CA-CB-CG1	-5.73	102.31	110.90
5	L	568	TYR	CB-CG-CD1	-5.72	117.56	121.00
2	T	19	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	431	TYR	CD1-CE1-CZ	5.72	124.95	119.80
5	L	573	TYR	CG-CD2-CE2	-5.71	116.73	121.30
1	E	350	PHE	CZ-CE2-CD2	-5.71	113.24	120.10
2	B	463	TYR	CG-CD1-CE1	-5.71	116.73	121.30
1	G	445	VAL	CA-CB-CG1	-5.71	102.33	110.90
4	J	398	LEU	CB-CG-CD1	5.71	120.71	111.00
7	r	16	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	A	401	ASP	CB-CG-OD2	-5.70	113.17	118.30
2	B	538	PHE	CB-CG-CD2	-5.70	116.81	120.80
3	I	157	VAL	O-C-N	-5.70	113.59	122.70
3	K	100	TYR	CG-CD2-CE2	5.70	125.86	121.30
2	O	27	ASP	CB-CG-OD2	5.70	123.42	118.30
1	A	284	TYR	CB-CG-CD1	-5.69	117.58	121.00
1	C	368	ASP	N-CA-CB	5.69	120.85	110.60
2	H	283	SER	N-CA-CB	-5.69	101.97	110.50
3	I	37	GLY	O-C-N	-5.68	113.60	122.70
4	J	483	ASP	CB-CG-OD1	-5.68	113.18	118.30
6	X	668	ARG	NE-CZ-NH2	5.68	123.14	120.30
2	S	103	ASP	CB-CG-OD2	5.68	123.41	118.30
2	T	77	LEU	O-C-N	-5.67	113.62	122.70
1	G	491	TYR	CZ-CE2-CD2	-5.67	114.70	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	310	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	G	296	ARG	NH1-CZ-NH2	-5.65	113.18	119.40
4	J	450	SER	N-CA-CB	5.65	118.98	110.50
5	L	410	ARG	NH1-CZ-NH2	-5.65	113.19	119.40
1	E	243	ARG	CG-CD-NE	-5.64	99.95	111.80
1	E	392	ARG	N-CA-CB	5.64	120.75	110.60
5	L	408	TYR	CB-CG-CD2	5.64	124.38	121.00
1	G	227	VAL	CA-CB-CG2	-5.64	102.44	110.90
2	B	432	TRP	CA-CB-CG	5.63	124.40	113.70
3	K	204	PHE	CB-CG-CD2	-5.63	116.86	120.80
6	U	646	ARG	NH1-CZ-NH2	-5.62	113.21	119.40
1	C	332	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	G	287	VAL	CA-CB-CG1	-5.62	102.47	110.90
2	Q	116	ALA	CB-CA-C	-5.62	101.67	110.10
2	O	95	TYR	CB-CG-CD1	5.61	124.37	121.00
7	p	34	LEU	CB-CG-CD1	5.61	120.54	111.00
7	t	45	ILE	C-N-CA	5.61	135.73	121.70
2	H	459	TRP	CB-CG-CD1	-5.61	119.71	127.00
2	H	251	ARG	CD-NE-CZ	5.60	131.44	123.60
2	O	89	ASN	N-CA-CB	5.60	120.68	110.60
2	S	109	ASN	N-CA-CB	5.60	120.67	110.60
2	F	422	ALA	CB-CA-C	-5.60	101.71	110.10
2	B	390	ARG	NH1-CZ-NH2	5.59	125.55	119.40
2	B	479	SER	N-CA-CB	5.59	118.88	110.50
4	J	266	VAL	CG1-CB-CG2	-5.59	101.96	110.90
6	U	613	ASP	CB-CG-OD2	-5.59	113.27	118.30
2	S	32	PHE	CB-CG-CD1	5.58	124.71	120.80
5	L	592	ALA	CB-CA-C	-5.57	101.75	110.10
7	r	37	CYS	O-C-N	5.57	131.61	122.70
2	D	334	TYR	CG-CD1-CE1	5.57	125.75	121.30
5	L	447	CYS	CA-CB-SG	-5.57	103.98	114.00
3	K	278	PHE	CB-CG-CD2	5.56	124.69	120.80
2	Q	70	ASP	N-CA-CB	5.56	120.61	110.60
1	C	266	ALA	N-CA-CB	5.55	117.88	110.10
5	L	596	TYR	CB-CG-CD2	5.55	124.33	121.00
2	R	62	PHE	CB-CG-CD1	-5.55	116.92	120.80
2	D	438	LEU	CB-CG-CD2	5.54	120.43	111.00
2	T	95	TYR	CZ-CE2-CD2	5.54	124.79	119.80
7	s	59	ARG	NE-CZ-NH1	5.54	123.07	120.30
5	L	95	VAL	CA-CB-CG1	5.54	119.21	110.90
2	T	49	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	F	431	ARG	NE-CZ-NH2	-5.54	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	264	THR	CA-CB-CG2	-5.52	104.67	112.40
1	A	386	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	C	302	TYR	CG-CD1-CE1	-5.51	116.89	121.30
2	D	432	TRP	CA-CB-CG	5.51	124.16	113.70
1	E	431	TYR	CB-CG-CD1	-5.50	117.70	121.00
4	J	475	TRP	CB-CG-CD1	5.50	134.16	127.00
2	B	286	LEU	CB-CG-CD2	5.50	120.35	111.00
2	H	384	VAL	CA-CB-CG2	-5.50	102.65	110.90
4	J	326	PHE	CB-CG-CD1	5.50	124.65	120.80
5	L	102	ASN	N-CA-C	-5.50	96.16	111.00
5	L	34	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	350	PHE	CB-CG-CD2	5.49	124.64	120.80
2	D	435	ASP	CB-CG-OD2	5.49	123.24	118.30
1	G	331	LEU	CB-CG-CD1	5.49	120.33	111.00
3	I	85	TYR	CZ-CE2-CD2	-5.48	114.87	119.80
1	C	219	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	C	361	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	295	MET	CA-CB-CG	5.48	122.61	113.30
3	K	295	ARG	NE-CZ-NH1	5.47	123.04	120.30
3	K	272	VAL	CA-CB-CG2	-5.47	102.69	110.90
1	A	243	ARG	NH1-CZ-NH2	-5.47	113.38	119.40
3	I	158	TYR	CB-CG-CD2	5.47	124.28	121.00
3	K	263	MET	CG-SD-CE	-5.47	91.45	100.20
1	E	234	VAL	CG1-CB-CG2	5.47	119.65	110.90
2	H	272	ASN	N-CA-C	-5.46	96.25	111.00
3	I	200	TYR	C-N-CA	5.46	135.35	121.70
1	G	408	VAL	CA-CB-CG1	-5.46	102.71	110.90
4	J	410	ARG	N-CA-CB	5.46	120.42	110.60
5	L	212	THR	CA-CB-CG2	-5.46	104.76	112.40
5	L	329	HIS	CA-CB-CG	5.46	122.88	113.60
2	D	306	TYR	O-C-N	5.45	131.43	122.70
1	G	491	TYR	CB-CG-CD1	5.45	124.27	121.00
2	F	372	ASP	CB-CG-OD1	5.45	123.21	118.30
1	E	262	ILE	CA-CB-CG2	-5.45	100.00	110.90
4	J	443	TYR	CB-CG-CD1	-5.45	117.73	121.00
4	J	326	PHE	CB-CG-CD2	-5.44	116.99	120.80
1	A	325	PHE	CB-CG-CD1	5.44	124.61	120.80
1	G	243	ARG	NE-CZ-NH2	-5.44	117.58	120.30
5	L	414	PHE	CB-CG-CD1	5.44	124.61	120.80
6	W	627	VAL	CA-CB-CG1	5.44	119.06	110.90
2	B	334	TYR	CB-CG-CD1	5.43	124.26	121.00
1	A	216	LEU	CB-CG-CD1	5.43	120.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	s	15	MET	CG-SD-CE	5.43	108.89	100.20
1	C	231	TYR	CG-CD1-CE1	-5.43	116.96	121.30
3	I	201	GLU	N-CA-CB	5.42	120.36	110.60
5	L	527	THR	N-CA-CB	5.42	120.59	110.30
7	t	30	ASP	CB-CG-OD2	5.42	123.17	118.30
6	W	606	MET	N-CA-CB	5.41	120.34	110.60
2	B	401	ALA	CB-CA-C	-5.41	101.99	110.10
1	E	337	LEU	O-C-N	-5.41	114.05	122.70
4	J	468	TYR	CD1-CG-CD2	5.41	123.85	117.90
5	L	351	THR	CA-CB-CG2	-5.41	104.83	112.40
2	D	340	VAL	CA-CB-CG2	5.41	119.01	110.90
2	B	252	ASP	CB-CG-OD2	5.40	123.16	118.30
3	K	341	TRP	CD2-CE2-CZ2	-5.40	115.82	122.30
1	E	317	LEU	O-C-N	-5.40	114.07	122.70
2	B	522	PHE	CB-CG-CD2	-5.39	117.03	120.80
2	F	347	VAL	CA-CB-CG2	-5.39	102.81	110.90
1	A	393	TRP	CA-CB-CG	5.39	123.94	113.70
3	K	58	PHE	CB-CG-CD1	5.39	124.57	120.80
2	D	251	ARG	CD-NE-CZ	-5.39	116.06	123.60
5	L	566	LYS	N-CA-CB	5.39	120.30	110.60
5	L	392	ASP	CB-CG-OD1	5.38	123.14	118.30
7	s	58	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	D	261	ASP	CB-CG-OD2	5.38	123.14	118.30
3	I	94	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	E	402	PRO	N-CD-CG	5.37	111.26	103.20
1	E	493	TYR	CB-CG-CD1	5.37	124.22	121.00
2	F	463	TYR	CB-CA-C	-5.37	99.66	110.40
1	E	365	TYR	CB-CG-CD2	-5.37	117.78	121.00
2	B	291	SER	N-CA-CB	5.37	118.55	110.50
1	G	350	PHE	CB-CG-CD1	5.37	124.56	120.80
5	L	104	ILE	CA-CB-CG2	-5.36	100.17	110.90
5	L	8	PHE	CB-CG-CD1	-5.36	117.05	120.80
4	J	299	THR	CA-CB-CG2	-5.35	104.91	112.40
4	J	354	PHE	CB-CG-CD1	-5.35	117.05	120.80
2	O	95	TYR	CG-CD2-CE2	5.35	125.58	121.30
1	G	222	TYR	CD1-CE1-CZ	5.35	124.62	119.80
1	C	388	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	302	TYR	CB-CG-CD2	-5.34	117.79	121.00
4	J	449	ALA	C-N-CA	5.34	135.05	121.70
4	J	227	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	388	ASP	CB-CG-OD2	-5.33	113.50	118.30
5	L	518	TYR	CB-CG-CD1	5.33	124.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	348	GLU	N-CA-CB	5.33	120.19	110.60
6	U	621	ASP	CB-CG-OD2	5.33	123.10	118.30
3	K	198	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	C	440	SER	O-C-N	5.33	131.23	122.70
1	G	267	THR	CA-CB-CG2	-5.33	104.94	112.40
6	V	669	ALA	CB-CA-C	-5.33	102.11	110.10
2	S	43	PHE	CB-CG-CD1	5.33	124.53	120.80
1	C	245	PHE	CB-CG-CD1	5.33	124.53	120.80
1	C	222	TYR	CB-CG-CD2	5.32	124.19	121.00
3	K	333	ARG	NE-CZ-NH2	5.32	122.96	120.30
2	F	524	ASP	C-N-CA	5.32	135.00	121.70
5	L	217	PHE	CB-CG-CD1	5.32	124.52	120.80
2	B	430	TYR	CB-CG-CD1	5.32	124.19	121.00
2	B	310	ARG	NE-CZ-NH2	5.31	122.95	120.30
3	K	98	GLN	N-CA-CB	5.31	120.16	110.60
2	H	416	HIS	CA-CB-CG	5.31	122.62	113.60
5	L	531	PRO	N-CA-CB	5.31	109.67	103.30
7	s	19	LEU	CB-CG-CD1	-5.30	101.98	111.00
1	G	314	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
4	J	211	TRP	CB-CG-CD2	5.30	133.49	126.60
5	L	326	TYR	CG-CD1-CE1	-5.30	117.06	121.30
1	C	214	THR	CA-CB-CG2	-5.30	104.98	112.40
3	I	183	MET	CA-CB-CG	5.29	122.30	113.30
2	B	497	HIS	N-CA-CB	5.29	120.12	110.60
6	W	620	ARG	NE-CZ-NH1	-5.29	117.66	120.30
7	q	62	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	G	318	LEU	CB-CA-C	5.28	120.24	110.20
2	H	420	LEU	O-C-N	-5.28	114.25	122.70
3	K	91	ARG	C-N-CA	5.28	133.39	122.30
7	r	19	LEU	CB-CG-CD1	5.28	119.97	111.00
2	Q	52	PHE	CB-CG-CD2	5.28	124.49	120.80
3	I	321	SER	N-CA-CB	5.27	118.41	110.50
2	O	82	GLN	CG-CD-OE1	-5.27	111.06	121.60
2	H	443	HIS	N-CA-CB	5.27	120.09	110.60
2	D	362	THR	CA-CB-CG2	-5.27	105.02	112.40
2	H	430	TYR	CB-CG-CD2	5.26	124.16	121.00
2	D	335	TYR	CD1-CG-CD2	5.26	123.69	117.90
3	I	100	TYR	CB-CG-CD2	5.26	124.16	121.00
7	r	39	ARG	NE-CZ-NH1	5.26	122.93	120.30
3	K	33	PHE	CG-CD2-CE2	5.26	126.58	120.80
2	B	459	TRP	CE2-CD2-CG	-5.26	103.09	107.30
4	J	361	MET	CG-SD-CE	-5.25	91.79	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	79	ARG	CA-CB-CG	5.25	124.96	113.40
2	H	276	VAL	N-CA-C	-5.25	96.82	111.00
2	D	529	PHE	CB-CG-CD1	5.25	124.48	120.80
1	A	427	TRP	CE3-CZ3-CH2	-5.25	115.43	121.20
4	J	362	TRP	NE1-CE2-CZ2	-5.25	124.63	130.40
1	E	244	SER	N-CA-CB	-5.25	102.63	110.50
2	T	95	TYR	N-CA-CB	5.25	120.04	110.60
2	F	272	ASN	N-CA-CB	5.24	120.04	110.60
1	E	293	ALA	N-CA-CB	5.24	117.44	110.10
2	H	335	TYR	CD1-CE1-CZ	5.24	124.51	119.80
2	H	274	TYR	CG-CD2-CE2	5.24	125.49	121.30
4	J	261	VAL	C-N-CA	5.24	134.79	121.70
2	F	529	PHE	CG-CD1-CE1	-5.23	115.05	120.80
2	D	448	ALA	CB-CA-C	-5.23	102.25	110.10
5	L	541	TYR	CB-CG-CD1	5.23	124.14	121.00
6	W	663	GLU	N-CA-CB	5.23	120.01	110.60
2	B	477	ASP	CB-CG-OD1	-5.23	113.60	118.30
7	r	59	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	C	483	TYR	CG-CD2-CE2	-5.22	117.12	121.30
2	R	63	VAL	CA-CB-CG1	-5.22	103.07	110.90
7	q	58	ARG	NE-CZ-NH2	-5.22	117.69	120.30
5	L	567	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	430	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
4	J	466	ARG	CA-C-N	5.21	131.68	117.10
4	J	293	ARG	NE-CZ-NH2	-5.21	117.70	120.30
2	O	21	LEU	N-CA-CB	5.21	120.81	110.40
1	E	395	TYR	CD1-CE1-CZ	-5.20	115.12	119.80
2	F	261	ASP	CB-CG-OD1	5.20	122.98	118.30
2	B	253	LEU	CB-CG-CD1	5.20	119.83	111.00
2	T	54	VAL	CA-CB-CG1	5.20	118.69	110.90
1	E	326	TYR	CZ-CE2-CD2	-5.19	115.13	119.80
1	E	222	TYR	CB-CG-CD1	5.19	124.11	121.00
5	L	561	LEU	CB-CG-CD2	5.19	119.82	111.00
7	t	25	LEU	CB-CA-C	-5.19	100.34	110.20
2	F	364	ARG	NH1-CZ-NH2	5.19	125.11	119.40
3	I	30	ASP	CB-CG-OD2	-5.19	113.63	118.30
4	J	362	TRP	CH2-CZ2-CE2	-5.19	112.21	117.40
2	D	466	ARG	CD-NE-CZ	-5.18	116.35	123.60
5	L	175	THR	CA-CB-CG2	-5.18	105.15	112.40
5	L	420	LEU	CB-CG-CD2	5.18	119.81	111.00
1	A	392	ARG	CD-NE-CZ	-5.18	116.35	123.60
1	A	377	TYR	CG-CD1-CE1	-5.17	117.16	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	252	ASP	CB-CG-OD2	5.17	122.96	118.30
2	H	364	ARG	NH1-CZ-NH2	5.17	125.09	119.40
7	t	23	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	C	246	SER	C-N-CA	5.17	134.62	121.70
5	L	564	ARG	CB-CG-CD	5.17	125.04	111.60
7	s	26	ASN	N-CA-CB	5.17	119.90	110.60
1	A	315	GLN	N-CA-C	-5.17	97.05	111.00
5	L	542	SER	CB-CA-C	-5.17	100.28	110.10
5	L	229	ASP	CB-CG-OD2	-5.16	113.66	118.30
5	L	107	SER	N-CA-CB	5.16	118.24	110.50
6	V	671	PHE	N-CA-CB	5.16	119.89	110.60
2	H	287	LYS	CB-CA-C	-5.16	100.09	110.40
2	T	56	GLU	OE1-CD-OE2	-5.16	117.11	123.30
2	D	418	LEU	CB-CG-CD2	5.16	119.76	111.00
2	R	34	TYR	CD1-CE1-CZ	5.16	124.44	119.80
2	R	50	ASP	CB-CG-OD1	-5.16	113.66	118.30
2	H	422	ALA	N-CA-CB	5.15	117.31	110.10
6	W	666	ARG	NE-CZ-NH1	5.14	122.87	120.30
5	L	438	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	379	THR	CA-CB-CG2	5.14	119.60	112.40
1	C	255	VAL	CA-CB-CG1	-5.14	103.19	110.90
2	T	96	LEU	O-C-N	-5.13	114.48	122.70
2	B	463	TYR	CB-CG-CD1	-5.13	117.92	121.00
2	Q	74	PHE	CB-CG-CD2	5.13	124.39	120.80
1	E	431	TYR	CB-CG-CD2	5.13	124.08	121.00
4	J	228	PHE	CB-CG-CD1	-5.13	117.21	120.80
4	J	250	ASP	N-CA-CB	5.13	119.83	110.60
2	D	534	ASP	CB-CG-OD2	5.12	122.91	118.30
4	J	466	ARG	NE-CZ-NH1	5.12	122.86	120.30
4	J	435	THR	CA-CB-CG2	-5.12	105.24	112.40
1	A	409	GLU	O-C-N	-5.12	114.51	122.70
1	E	245	PHE	CB-CG-CD2	5.11	124.38	120.80
2	H	459	TRP	CB-CG-CD2	5.11	133.24	126.60
1	G	400	ASN	CB-CG-OD1	-5.10	111.39	121.60
1	A	395	TYR	N-CA-CB	5.10	119.78	110.60
5	L	553	MET	N-CA-CB	5.10	119.78	110.60
5	L	42	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	E	429	GLN	N-CA-CB	5.10	119.78	110.60
2	T	44	ALA	CB-CA-C	-5.10	102.46	110.10
2	F	341	LEU	CB-CG-CD1	5.09	119.66	111.00
1	E	495	SER	O-C-N	-5.09	114.55	122.70
1	G	302	TYR	CA-CB-CG	5.09	123.07	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	131	LEU	CB-CG-CD2	5.09	119.65	111.00
2	H	529	PHE	CB-CG-CD2	-5.09	117.24	120.80
2	D	449	SER	N-CA-CB	5.09	118.13	110.50
1	A	269	TYR	CB-CG-CD2	5.08	124.05	121.00
2	H	348	GLU	OE1-CD-OE2	-5.08	117.20	123.30
1	A	240	ARG	NE-CZ-NH1	5.08	122.84	120.30
6	U	633	PHE	CB-CG-CD1	-5.08	117.24	120.80
1	E	279	ASN	CB-CA-C	-5.08	100.24	110.40
5	L	583	CYS	CB-CA-C	5.08	120.56	110.40
3	K	331	ARG	NE-CZ-NH1	5.08	122.84	120.30
5	L	569	TRP	CB-CG-CD1	5.08	133.60	127.00
7	r	35	SER	N-CA-CB	5.07	118.11	110.50
3	I	57	GLU	O-C-N	-5.07	114.59	122.70
2	B	466	ARG	NH1-CZ-NH2	5.07	124.97	119.40
3	I	157	VAL	CA-C-O	5.07	130.74	120.10
1	E	362	THR	CA-CB-OG1	5.06	119.64	109.00
7	o	10	ALA	N-CA-CB	5.06	117.19	110.10
5	L	224	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	476	TYR	CG-CD1-CE1	-5.06	117.25	121.30
1	C	326	TYR	CG-CD2-CE2	-5.06	117.25	121.30
3	K	319	LEU	N-CA-C	-5.06	97.34	111.00
7	p	30	ASP	CB-CG-OD1	5.05	122.85	118.30
2	B	492	LEU	CB-CG-CD1	-5.05	102.42	111.00
4	J	279	LYS	N-CA-C	-5.05	97.37	111.00
2	B	420	LEU	CB-CG-CD1	5.05	119.58	111.00
1	G	209	LEU	CA-C-N	5.05	131.24	117.10
2	B	491	PHE	CB-CG-CD2	-5.05	117.27	120.80
5	L	313	TYR	CB-CG-CD2	5.04	124.03	121.00
2	D	250	VAL	CA-CB-CG1	-5.04	103.34	110.90
7	r	64	LEU	CB-CG-CD1	-5.04	102.43	111.00
1	C	356	SER	N-CA-CB	5.04	118.06	110.50
2	D	465	LEU	CB-CG-CD1	-5.04	102.43	111.00
2	B	336	ARG	NE-CZ-NH1	-5.04	117.78	120.30
5	L	1365	TYR	CB-CG-CD1	-5.04	117.98	121.00
2	F	318	LEU	CB-CG-CD1	5.03	119.55	111.00
4	J	242	TRP	CG-CD1-NE1	5.03	115.13	110.10
5	L	422	SER	CB-CA-C	-5.03	100.55	110.10
2	T	64	ARG	N-CA-CB	5.03	119.64	110.60
4	J	571	ARG	N-CA-CB	5.02	119.64	110.60
1	A	284	TYR	CG-CD1-CE1	-5.02	117.28	121.30
1	G	285	GLY	N-CA-C	-5.02	100.55	113.10
1	E	275	PHE	CB-CG-CD1	5.02	124.31	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	447	VAL	CA-CB-CG1	-5.02	103.37	110.90
3	K	44	ARG	NE-CZ-NH1	5.02	122.81	120.30
4	J	371	PHE	CB-CG-CD1	-5.02	117.29	120.80
3	K	133	PHE	CB-CG-CD1	-5.02	117.29	120.80
1	C	482	ALA	CB-CA-C	5.01	117.62	110.10
7	p	17	VAL	CA-CB-CG1	-5.01	103.38	110.90
1	E	303	MET	CG-SD-CE	-5.01	92.18	100.20
1	G	393	TRP	CD1-CG-CD2	5.01	110.31	106.30
4	J	362	TRP	CG-CD2-CE3	5.01	138.41	133.90
1	A	300	LYS	N-CA-CB	5.01	119.61	110.60
1	A	491	TYR	O-C-N	-5.01	114.69	122.70
1	E	402	PRO	N-CA-CB	5.01	109.31	103.30
7	r	26	ASN	N-CA-CB	5.01	119.61	110.60

There are no chirality outliers.

All (146) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	TYR	Sidechain
1	A	284	TYR	Sidechain
1	A	326	TYR	Sidechain
1	A	365	TYR	Sidechain
1	A	395	TYR	Sidechain
1	A	430	ARG	Sidechain
2	B	274	TYR	Sidechain
2	B	306	TYR	Sidechain
2	B	409	TYR	Sidechain
2	B	423	TYR	Sidechain
2	B	460	HIS	Sidechain
1	C	222	TYR	Sidechain
1	C	269	TYR	Sidechain
1	C	365	TYR	Sidechain
1	C	368	ASP	Sidechain
1	C	377	TYR	Sidechain
1	C	491	TYR	Sidechain
2	D	266	LYS	Peptide
2	D	306	TYR	Sidechain
2	D	313	ASP	Peptide
2	D	376	ARG	Sidechain
2	D	423	TYR	Sidechain
2	D	466	ARG	Sidechain
1	E	222	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	E	282	PHE	Peptide
1	E	363	PHE	Sidechain
1	E	365	TYR	Sidechain
1	E	395	TYR	Sidechain
1	E	431	TYR	Sidechain
1	E	433	ILE	Mainchain
1	E	483	TYR	Sidechain
2	F	257	PHE	Sidechain
2	F	306	TYR	Sidechain
2	F	335	TYR	Sidechain
2	F	402	TYR	Sidechain
2	F	423	TYR	Sidechain
2	F	430	TYR	Sidechain
2	F	446	PHE	Sidechain
2	F	463	TYR	Sidechain
2	F	473	PHE	Sidechain
2	F	529	PHE	Sidechain
1	G	240	ARG	Sidechain
1	G	243	ARG	Sidechain
1	G	269	TYR	Sidechain
1	G	284	TYR	Sidechain
1	G	326	TYR	Sidechain
1	G	348	GLU	Peptide
1	G	377	TYR	Sidechain
1	G	386	TYR	Sidechain
1	G	486	ARG	Sidechain
1	G	493	TYR	Sidechain
2	H	264	PHE	Sidechain
2	H	310	ARG	Sidechain
2	H	323	PHE	Sidechain
2	H	334	TYR	Sidechain
2	H	335	TYR	Sidechain
2	H	390	ARG	Sidechain
2	H	402	TYR	Sidechain
2	H	409	TYR	Sidechain
2	H	423	TYR	Sidechain
2	H	442	TYR	Sidechain
2	H	543	TYR	Sidechain
3	I	124	TYR	Sidechain
3	I	129	PHE	Sidechain
3	I	169	ARG	Sidechain
3	I	17	PHE	Sidechain

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Mol	Chain	Res	Type	Group
3	I	184	TYR	Sidechain
3	I	203	PHE	Sidechain
3	I	22	ARG	Sidechain
3	I	278	PHE	Sidechain
3	I	312	HIS	Sidechain
4	J	209	ARG	Sidechain
4	J	224	ARG	Sidechain
4	J	226	PRO	Peptide
4	J	261	VAL	Peptide
4	J	276	GLY	Peptide
4	J	291	ASN	Peptide
4	J	307	ARG	Peptide,Mainchain
4	J	354	PHE	Sidechain
4	J	424	ARG	Sidechain,Peptide
4	J	466	ARG	Sidechain
4	J	482	PHE	Sidechain
4	J	508	TYR	Sidechain
4	J	677	SER	Peptide
4	J	687	TYR	Sidechain
3	K	129	PHE	Sidechain
3	K	257	PHE	Sidechain
3	K	267	TYR	Sidechain
3	K	295	ARG	Sidechain
3	K	33	PHE	Sidechain
3	K	54	ARG	Sidechain
5	L	110	HIS	Sidechain
5	L	224	ARG	Sidechain
5	L	313	TYR	Sidechain
5	L	326	TYR	Sidechain
5	L	347	LEU	Peptide
5	L	385	TYR	Peptide,Mainchain
5	L	413	HIS	Sidechain
5	L	443	TYR	Sidechain
5	L	444	TYR	Sidechain
5	L	504	TYR	Sidechain
5	L	506	TYR	Sidechain
5	L	541	TYR	Sidechain
5	L	552	PHE	Sidechain
5	L	573	TYR	Sidechain
5	L	580	VAL	Mainchain
5	L	585	PRO	Peptide
5	L	596	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	L	77	PHE	Sidechain
5	L	97	TYR	Sidechain
2	O	19	ARG	Sidechain
2	O	43	PHE	Sidechain
2	Q	19	ARG	Sidechain
2	Q	34	TYR	Sidechain
2	R	19	ARG	Sidechain
2	R	34	TYR	Sidechain
2	R	74	PHE	Sidechain
2	S	34	TYR	Sidechain
2	S	64	ARG	Sidechain
2	S	66	ARG	Sidechain
2	T	52	PHE	Sidechain
2	T	62	PHE	Sidechain
6	U	620	ARG	Sidechain
6	U	647	TYR	Sidechain
6	U	666	ARG	Sidechain
6	U	668	ARG	Sidechain
6	V	647	TYR	Sidechain
6	V	666	ARG	Sidechain
6	W	619	HIS	Sidechain
6	W	647	TYR	Sidechain
6	W	661	ARG	Sidechain
6	W	666	ARG	Sidechain
6	X	602	PHE	Sidechain
6	X	615	ARG	Sidechain
6	X	620	ARG	Sidechain
6	X	634	HIS	Sidechain
7	o	12	ARG	Sidechain
7	o	23	ARG	Sidechain
7	q	12	ARG	Sidechain
7	q	58	ARG	Sidechain
7	r	12	ARG	Sidechain
7	s	59	ARG	Sidechain
7	t	59	ARG	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	2211	0	2199	6	0
1	C	2014	0	1998	5	0
1	E	2038	0	2031	5	0
1	G	2014	0	1998	6	0
2	B	2363	0	2379	6	0
2	D	2059	0	2080	8	0
2	F	1964	0	1988	8	0
2	H	2135	0	2160	4	0
2	O	753	0	779	1	0
2	Q	878	0	903	1	0
2	R	794	0	814	1	0
2	S	878	0	903	4	0
2	T	753	0	779	3	0
3	I	2325	0	2335	34	0
3	K	2325	0	2335	9	0
4	J	2909	0	2916	42	0
5	L	3794	0	3844	6	0
6	U	634	0	635	2	0
6	V	634	0	635	1	0
6	W	634	0	635	4	0
6	X	634	0	635	0	0
7	o	403	0	426	0	0
7	p	429	0	446	0	0
7	q	432	0	457	0	0
7	r	454	0	477	0	0
7	s	451	0	476	0	0
7	t	446	0	471	0	0
All	All	37358	0	37734	120	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 2.

All (120) 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)
4:J:242:TRP:CZ3	4:J:242:TRP:CE3	1.83	1.66
4:J:242:TRP:CZ2	4:J:242:TRP:CH2	1.87	1.61
4:J:242:TRP:CZ3	4:J:242:TRP:CH2	1.82	1.59
4:J:242:TRP:CZ2	4:J:242:TRP:CE2	1.92	1.57
4:J:242:TRP:CE3	4:J:242:TRP:CD2	1.93	1.56
4:J:242:TRP:CE2	4:J:242:TRP:CD2	1.79	1.53
3:I:16:ILE:CG1	4:J:242:TRP:CZ2	2.27	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:16:ILE:CG1	4:J:242:TRP:CE2	2.29	1.15
3:I:16:ILE:CG1	4:J:242:TRP:CD2	2.31	1.14
3:I:16:ILE:CD1	4:J:242:TRP:CE2	2.30	1.12
3:I:16:ILE:HG12	4:J:242:TRP:CE2	1.84	1.12
3:I:16:ILE:CG1	4:J:242:TRP:CH2	2.33	1.11
3:I:16:ILE:CD1	4:J:242:TRP:CD2	2.33	1.10
3:I:16:ILE:CG1	4:J:242:TRP:CE3	2.33	1.10
3:I:16:ILE:CD1	4:J:242:TRP:CZ2	2.35	1.10
3:I:16:ILE:CG1	4:J:242:TRP:CZ3	2.35	1.09
3:I:16:ILE:CD1	4:J:242:TRP:CE3	2.38	1.07
3:I:16:ILE:HG13	4:J:242:TRP:CE3	1.89	1.06
3:I:16:ILE:CD1	4:J:242:TRP:CH2	2.40	1.05
3:I:16:ILE:CD1	4:J:242:TRP:CZ3	2.40	1.04
3:I:16:ILE:HD11	4:J:242:TRP:CD2	2.00	0.95
3:I:16:ILE:HD13	4:J:242:TRP:CZ2	2.03	0.93
3:I:16:ILE:HD12	4:J:242:TRP:CZ3	2.05	0.92
3:I:16:ILE:HG13	4:J:242:TRP:CD2	2.11	0.84
3:I:16:ILE:CB	4:J:242:TRP:CH2	2.64	0.80
3:I:16:ILE:HG12	4:J:242:TRP:CZ2	2.20	0.76
3:I:16:ILE:HD11	4:J:242:TRP:CE2	2.24	0.72
3:I:16:ILE:HD12	4:J:242:TRP:CE3	2.29	0.68
1:C:320:LEU:HD22	1:C:320:LEU:H	1.63	0.63
3:I:16:ILE:HG12	4:J:242:TRP:CD2	2.33	0.62
2:D:364:ARG:HA	2:D:364:ARG:HE	1.65	0.62
2:R:58:ILE:HG12	2:R:98:LEU:HD13	1.84	0.60
1:G:284:TYR:HB3	1:G:286:GLN:H	1.65	0.60
3:I:16:ILE:HD13	4:J:242:TRP:CH2	2.36	0.59
3:K:193:HIS:CE1	3:K:294:SER:HB3	2.39	0.57
1:E:269:TYR:CE1	1:E:273:THR:HG21	2.39	0.57
3:I:16:ILE:CG2	4:J:242:TRP:CZ3	2.88	0.56
3:K:119:ILE:H	3:K:119:ILE:HD13	1.70	0.56
3:I:16:ILE:CG1	3:I:16:ILE:CD1	2.83	0.56
3:I:300:LEU:HD11	3:I:339:HIS:CE1	2.43	0.54
1:E:303:MET:HA	1:E:306:ILE:HD12	1.90	0.54
2:H:296:LEU:HD13	2:H:374:LYS:HD3	1.90	0.53
5:L:427:GLY:HA2	5:L:551:GLU:H	1.73	0.52
3:K:295:ARG:HH12	3:K:340:LEU:HB3	1.74	0.52
2:S:96:LEU:C	2:S:96:LEU:HD13	2.30	0.51
2:D:323:PHE:CG	2:D:395:LEU:HD22	2.46	0.51
3:I:16:ILE:CB	4:J:242:TRP:CZ3	2.94	0.50
4:J:492:ARG:HE	4:J:492:ARG:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:598:ILE:HD12	6:U:598:ILE:H	1.77	0.50
2:B:340:VAL:HG11	5:L:216:LEU:HD13	1.94	0.49
2:F:253:LEU:HD22	2:F:290:THR:HG22	1.94	0.49
2:F:321:GLN:HA	2:F:324:CYS:SG	2.53	0.49
3:I:16:ILE:HA	4:J:242:TRP:CH2	2.48	0.49
2:S:90:ARG:HD2	2:S:91:TRP:H	1.78	0.49
2:B:465:LEU:HD23	2:B:465:LEU:H	1.78	0.48
1:E:311:HIS:CE1	2:F:365:ARG:HD2	2.48	0.48
2:H:306:TYR:HD2	2:H:324:CYS:HG	1.57	0.48
4:J:419:VAL:HB	4:J:420:PRO:HD3	1.95	0.48
5:L:377:SER:HA	5:L:406:THR:HG23	1.95	0.48
1:E:396:ARG:HA	1:E:396:ARG:HE	1.79	0.48
1:G:295:MET:SD	1:G:337:LEU:HD22	2.55	0.47
2:T:37:ARG:HH12	6:W:635:ILE:HG21	1.79	0.47
2:D:475:THR:HG22	2:D:476:MET:H	1.79	0.47
3:I:138:VAL:HG12	3:I:160:HIS:CE1	2.50	0.47
2:F:276:VAL:HG12	2:F:278:GLY:H	1.80	0.46
3:K:86:LEU:HD21	3:K:149:HIS:HA	1.97	0.46
1:A:333:THR:HG23	1:A:374:LEU:HD22	1.96	0.46
2:F:334:TYR:CZ	2:F:338:LEU:HD11	2.51	0.46
1:G:255:VAL:O	1:G:259:VAL:HG23	2.16	0.46
2:H:447:VAL:HG13	2:H:463:TYR:HB3	1.97	0.45
5:L:586:VAL:HG13	5:L:588:LEU:HD21	1.99	0.45
2:D:372:ASP:HB3	2:D:373:PRO:HD3	1.98	0.45
4:J:209:ARG:CD	2:S:19:ARG:HH11	2.30	0.45
3:I:295:ARG:HA	3:I:339:HIS:CD2	2.53	0.44
4:J:302:THR:HG22	4:J:304:ASN:H	1.82	0.44
6:W:623:VAL:HA	6:W:626:GLN:HE21	1.81	0.44
3:I:139:VAL:HG22	3:I:160:HIS:CD2	2.52	0.44
3:K:38:GLU:O	3:K:42:LEU:HG	2.18	0.44
2:T:48:GLU:HA	2:T:91:TRP:CZ2	2.52	0.44
6:U:643:LEU:HD13	6:W:641:GLN:HE21	1.82	0.44
2:B:490:ASN:HA	2:B:493:HIS:CD2	2.53	0.44
1:C:212:GLN:H	1:C:212:GLN:HG2	1.58	0.44
2:D:428:PHE:HA	2:D:431:ARG:HE	1.83	0.44
2:T:43:PHE:HA	6:W:624:ASN:HD21	1.83	0.44
1:A:283:GLU:HB2	1:A:289:HIS:HB2	2.00	0.44
2:B:465:LEU:H	2:B:465:LEU:CD2	2.30	0.44
1:C:430:ARG:HA	1:C:430:ARG:HE	1.83	0.43
2:F:314:ARG:HH22	1:G:368:ASP:HB2	1.82	0.43
1:A:392:ARG:HE	1:A:398:ILE:HD11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:363:LEU:HD12	2:H:363:LEU:H	1.83	0.43
2:D:418:LEU:HD22	2:D:524:ASP:N	2.34	0.43
3:K:180:HIS:CE1	3:K:320:PHE:CG	3.07	0.43
2:O:55:THR:HA	2:O:58:ILE:HD12	2.01	0.43
2:Q:108:PRO:HA	2:S:49:ARG:HE	1.83	0.43
1:E:261:ARG:H	1:E:261:ARG:HG2	1.66	0.42
4:J:475:TRP:CE2	4:J:492:ARG:HD3	2.54	0.42
1:A:291:LEU:HD13	1:A:382:ALA:HB2	2.02	0.42
4:J:390:THR:H	4:J:393:ILE:HG22	1.83	0.42
2:D:293:LEU:C	2:D:293:LEU:HD23	2.38	0.42
6:V:643:LEU:O	6:V:647:TYR:CD2	2.73	0.42
1:G:344:LEU:HD21	1:G:357:LEU:HD22	2.02	0.41
3:K:17:PHE:HB3	3:K:25:LEU:HD21	2.01	0.41
5:L:71:LYS:HE2	5:L:117:VAL:HG11	2.02	0.41
4:J:437:TYR:CG	4:J:548:LEU:HD11	2.55	0.41
3:I:110:GLU:HG2	3:I:121:HIS:CE1	2.56	0.41
2:B:299:LEU:HA	2:B:302:LYS:HG2	2.02	0.41
1:C:227:VAL:HG13	1:C:228:ASP:O	2.20	0.41
2:B:293:LEU:O	2:B:293:LEU:HD13	2.21	0.41
2:F:334:TYR:CE2	2:F:338:LEU:HD11	2.56	0.41
5:L:452:PRO:HA	5:L:453:ALA:HA	1.85	0.41
2:D:296:LEU:HA	2:D:299:LEU:HD23	2.03	0.41
4:J:365:TYR:CD1	3:K:131:LEU:HD23	2.55	0.41
1:C:337:LEU:HD13	1:C:378:LEU:HD11	2.04	0.40
2:F:410:MET:O	2:F:414:VAL:HG22	2.21	0.40
4:J:297:ILE:HG22	4:J:303:GLN:HB2	2.03	0.40
1:A:240:ARG:O	1:A:241:GLN:HG2	2.21	0.40
1:A:237:LEU:HD12	1:A:244:SER:H	1.86	0.40
1:G:321:GLN:HA	1:G:324:TRP:HB3	2.02	0.40
3:I:184:TYR:HB3	3:I:315:LYS:HE2	2.03	0.40
3:K:329:LEU:HA	3:K:332:ILE:HG22	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/896 (30%)	250 (92%)	14 (5%)	7 (3%)	4	26
1	C	244/896 (27%)	217 (89%)	21 (9%)	6 (2%)	4	27
1	E	247/896 (28%)	229 (93%)	12 (5%)	6 (2%)	5	28
1	G	244/896 (27%)	232 (95%)	11 (4%)	1 (0%)	30	67
2	B	290/906 (32%)	261 (90%)	20 (7%)	9 (3%)	3	23
2	D	248/906 (27%)	224 (90%)	17 (7%)	7 (3%)	4	25
2	F	236/906 (26%)	214 (91%)	13 (6%)	9 (4%)	2	20
2	H	257/906 (28%)	227 (88%)	20 (8%)	10 (4%)	2	19
2	O	91/906 (10%)	85 (93%)	5 (6%)	1 (1%)	12	46
2	Q	107/906 (12%)	97 (91%)	6 (6%)	4 (4%)	2	21
2	R	96/906 (11%)	90 (94%)	4 (4%)	2 (2%)	5	31
2	S	107/906 (12%)	96 (90%)	8 (8%)	3 (3%)	4	25
2	T	91/906 (10%)	85 (93%)	4 (4%)	2 (2%)	5	30
3	I	281/666 (42%)	255 (91%)	20 (7%)	6 (2%)	5	31
3	K	281/666 (42%)	259 (92%)	13 (5%)	9 (3%)	3	22
4	J	342/1019 (34%)	317 (93%)	15 (4%)	10 (3%)	3	24
5	L	462/1698 (27%)	422 (91%)	26 (6%)	14 (3%)	3	23
6	U	73/671 (11%)	73 (100%)	0	0	100	100
6	V	73/671 (11%)	72 (99%)	0	1 (1%)	9	40
6	W	73/671 (11%)	71 (97%)	1 (1%)	1 (1%)	9	40
6	X	73/671 (11%)	72 (99%)	1 (1%)	0	100	100
7	o	50/72 (69%)	50 (100%)	0	0	100	100
7	p	54/72 (75%)	54 (100%)	0	0	100	100
7	q	54/72 (75%)	53 (98%)	1 (2%)	0	100	100
7	r	57/72 (79%)	54 (95%)	1 (2%)	2 (4%)	3	21
7	s	57/72 (79%)	54 (95%)	3 (5%)	0	100	100
7	t	56/72 (78%)	55 (98%)	1 (2%)	0	100	100
All	All	4515/18903 (24%)	4168 (92%)	237 (5%)	110 (2%)	7	28

All (110) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ASP
1	A	428	ASP
2	B	312	LEU
2	D	314	ARG
2	F	281	ALA
2	F	285	SER
2	F	314	ARG
2	F	476	MET
2	F	527	ASN
2	H	314	ARG
2	H	468	SER
3	I	82	HIS
3	I	254	LEU
3	I	298	SER
4	J	224	ARG
4	J	229	SER
4	J	417	ALA
4	J	449	ALA
3	K	128	GLN
3	K	203	PHE
5	L	571	HIS
5	L	580	VAL
2	Q	26	ALA
2	S	26	ALA
6	V	649	LEU
1	A	241	GLN
1	C	482	ALA
2	D	311	SER
2	D	315	ALA
2	D	406	GLY
2	D	459	TRP
1	E	231	TYR
1	E	432	THR
2	F	272	ASN
2	F	315	ALA
2	H	281	ALA
4	J	262	THR
4	J	388	THR
4	J	490	ILE
3	K	264	LEU
3	K	297	GLY
5	L	107	SER
5	L	547	ASP

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Mol	Chain	Res	Type
5	L	566	LYS
5	L	586	VAL
2	O	89	ASN
2	Q	105	ARG
2	S	23	LYS
2	S	47	VAL
2	T	88	LYS
1	A	439	PRO
2	B	263	LYS
2	B	462	LYS
1	C	402	PRO
2	D	407	ASP
1	E	317	LEU
2	F	316	PHE
1	G	428	ASP
2	H	269	ASN
2	H	285	SER
2	H	443	HIS
3	I	165	LEU
3	I	335	THR
4	J	448	GLU
4	J	499	ASN
3	K	193	HIS
5	L	375	LEU
5	L	564	ARG
2	R	7	LYS
2	B	407	ASP
1	C	283	GLU
2	D	261	ASP
2	F	407	ASP
2	H	270	SER
2	H	360	SER
2	H	407	ASP
4	J	423	THR
3	K	290	ASN
5	L	105	GLN
5	L	422	SER
5	L	607	LEU
2	Q	87	LEU
2	Q	113	SER
2	T	89	ASN
6	W	649	LEU

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Mol	Chain	Res	Type
7	r	26	ASN
7	r	45	ILE
1	A	249	GLN
1	A	470	ASP
2	B	443	HIS
2	B	469	MET
2	B	527	ASN
1	C	404	SER
1	C	442	LEU
1	E	429	GLN
3	K	165	LEU
3	K	195	LEU
5	L	222	HIS
5	L	340	THR
2	B	439	GLU
1	C	317	LEU
2	R	50	ASP
2	H	450	ASP
2	B	319	VAL
1	E	439	PRO
3	K	115	PRO
3	I	265	PRO
1	E	227	VAL
5	L	362	ILE
1	A	367	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	244/824 (30%)	232 (95%)	12 (5%)	21	43
1	C	221/824 (27%)	213 (96%)	8 (4%)	30	52
1	E	224/824 (27%)	213 (95%)	11 (5%)	21	43
1	G	221/824 (27%)	215 (97%)	6 (3%)	40	60
2	B	260/798 (33%)	246 (95%)	14 (5%)	18	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	227/798 (28%)	219 (96%)	8 (4%)	31	53
2	F	217/798 (27%)	202 (93%)	15 (7%)	13	34
2	H	236/798 (30%)	224 (95%)	12 (5%)	20	43
2	O	82/798 (10%)	81 (99%)	1 (1%)	67	79
2	Q	96/798 (12%)	93 (97%)	3 (3%)	35	56
2	R	87/798 (11%)	86 (99%)	1 (1%)	70	80
2	S	96/798 (12%)	89 (93%)	7 (7%)	11	32
2	T	82/798 (10%)	79 (96%)	3 (4%)	29	51
3	I	259/595 (44%)	241 (93%)	18 (7%)	13	34
3	K	259/595 (44%)	247 (95%)	12 (5%)	23	46
4	J	326/933 (35%)	313 (96%)	13 (4%)	27	49
5	L	431/1539 (28%)	417 (97%)	14 (3%)	34	55
6	U	72/598 (12%)	69 (96%)	3 (4%)	25	48
6	V	72/598 (12%)	70 (97%)	2 (3%)	38	59
6	W	72/598 (12%)	69 (96%)	3 (4%)	25	48
6	X	72/598 (12%)	70 (97%)	2 (3%)	38	59
7	o	48/62 (77%)	46 (96%)	2 (4%)	25	48
7	p	51/62 (82%)	51 (100%)	0	100	100
7	q	51/62 (82%)	51 (100%)	0	100	100
7	r	54/62 (87%)	52 (96%)	2 (4%)	29	51
7	s	53/62 (86%)	50 (94%)	3 (6%)	17	40
7	t	53/62 (86%)	53 (100%)	0	100	100
All	All	4166/16904 (25%)	3991 (96%)	175 (4%)	27	48

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LEU
1	A	268	ASN
1	A	271	THR
1	A	288	ASN
1	A	289	HIS
1	A	309	LEU
1	A	362	THR

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Mol	Chain	Res	Type
1	A	366	THR
1	A	394	ILE
1	A	430	ARG
1	A	467	THR
1	A	492	ASN
2	B	265	VAL
2	B	288	ASP
2	B	314	ARG
2	B	337	LEU
2	B	402	TYR
2	B	426	LEU
2	B	430	TYR
2	B	441	THR
2	B	458	LEU
2	B	460	HIS
2	B	465	LEU
2	B	477	ASP
2	B	514	SER
2	B	532	LYS
1	C	279	ASN
1	C	295	MET
1	C	320	LEU
1	C	321	GLN
1	C	328	GLN
1	C	357	LEU
1	C	438	ILE
1	C	481	GLN
2	D	279	LYS
2	D	293	LEU
2	D	299	LEU
2	D	301	ASN
2	D	363	LEU
2	D	364	ARG
2	D	475	THR
2	D	532	LYS
1	E	215	CYS
1	E	237	LEU
1	E	240	ARG
1	E	249	GLN
1	E	264	PRO
1	E	296	ARG
1	E	358	LEU

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Mol	Chain	Res	Type
1	E	427	TRP
1	E	443	GLN
1	E	444	LYS
1	E	493	TYR
2	F	254	LEU
2	F	267	MET
2	F	279	LYS
2	F	286	LEU
2	F	287	LYS
2	F	299	LEU
2	F	370	THR
2	F	426	LEU
2	F	444	GLU
2	F	454	LYS
2	F	455	THR
2	F	465	LEU
2	F	467	LYS
2	F	473	PHE
2	F	478	GLN
1	G	279	ASN
1	G	315	GLN
1	G	333	THR
1	G	393	TRP
1	G	452	THR
1	G	493	TYR
2	H	275	LYS
2	H	279	LYS
2	H	282	VAL
2	H	300	HIS
2	H	318	LEU
2	H	371	PHE
2	H	405	THR
2	H	444	GLU
2	H	455	THR
2	H	458	LEU
2	H	467	LYS
2	H	540	THR
3	I	1	MET
3	I	20	ASN
3	I	23	THR
3	I	27	VAL
3	I	36	PRO

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Mol	Chain	Res	Type
3	I	39	THR
3	I	57	GLU
3	I	86	LEU
3	I	109	GLN
3	I	119	ILE
3	I	166	PRO
3	I	198	ASP
3	I	284	GLN
3	I	285	MET
3	I	287	GLU
3	I	300	LEU
3	I	302	ASN
3	I	331	ARG
4	J	299	THR
4	J	354	PHE
4	J	361	MET
4	J	408	LEU
4	J	421	PRO
4	J	499	ASN
4	J	501	ARG
4	J	598	ARG
4	J	674	THR
4	J	679	GLU
4	J	680	LEU
4	J	681	THR
4	J	692	LYS
3	K	2	ILE
3	K	109	GLN
3	K	117	LEU
3	K	119	ILE
3	K	134	PRO
3	K	147	LYS
3	K	149	HIS
3	K	265	PRO
3	K	271	ARG
3	K	296	THR
3	K	322	LEU
3	K	340	LEU
5	L	224	ARG
5	L	240	ASN
5	L	340	THR
5	L	346	VAL

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Mol	Chain	Res	Type
5	L	355	LYS
5	L	368	THR
5	L	382	GLN
5	L	452	PRO
5	L	471	LEU
5	L	474	LEU
5	L	519	PRO
5	L	537	TYR
5	L	573	TYR
5	L	606	LYS
2	O	45	PRO
2	Q	54	VAL
2	Q	106	LYS
2	Q	107	GLN
2	R	16	LEU
2	S	16	LEU
2	S	23	LYS
2	S	66	ARG
2	S	88	LYS
2	S	90	ARG
2	S	110	LYS
2	S	113	SER
2	T	23	LYS
2	T	79	ARG
2	T	93	ILE
6	U	600	ILE
6	U	625	LEU
6	U	643	LEU
6	V	610	THR
6	V	666	ARG
6	W	598	ILE
6	W	620	ARG
6	W	644	LEU
6	X	609	GLU
6	X	666	ARG
7	o	8	MET
7	o	33	THR
7	r	26	ASN
7	r	46	ASN
7	s	39	ARG
7	s	46	ASN
7	s	55	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	372	GLN
2	B	300	HIS
2	B	493	HIS
1	C	311	HIS
1	C	345	ASN
2	D	300	HIS
2	D	301	ASN
1	E	311	HIS
1	E	481	GLN
2	F	300	HIS
1	G	260	ASN
1	G	279	ASN
1	G	289	HIS
1	G	311	HIS
1	G	328	GLN
1	G	481	GLN
2	H	415	GLN
3	I	35	HIS
3	I	121	HIS
3	I	180	HIS
3	I	193	HIS
3	I	207	GLN
3	I	339	HIS
4	J	294	ASN
4	J	480	ASN
3	K	146	GLN
3	K	149	HIS
3	K	180	HIS
3	K	193	HIS
3	K	290	ASN
3	K	312	HIS
5	L	105	GLN
5	L	240	ASN
5	L	359	ASN
5	L	413	HIS
5	L	590	HIS
2	Q	82	GLN
2	S	15	ASN
6	U	619	HIS
6	U	626	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	V	599	GLN
6	V	626	GLN
6	V	634	HIS
6	V	636	GLN
6	W	624	ASN
6	W	626	GLN
6	W	632	GLN
6	W	641	GLN
7	r	46	ASN
7	t	46	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

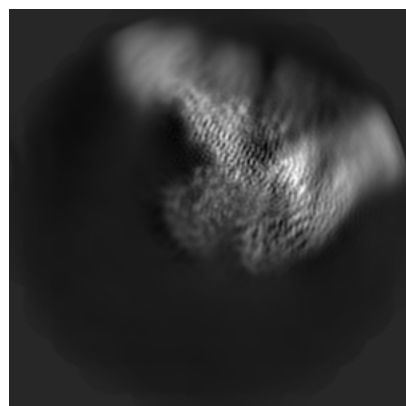
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52729. These allow visual inspection of the internal detail of the map and identification of artifacts.

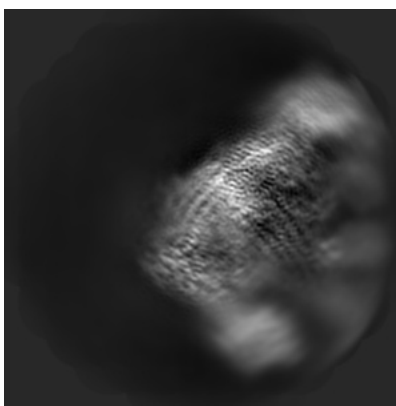
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

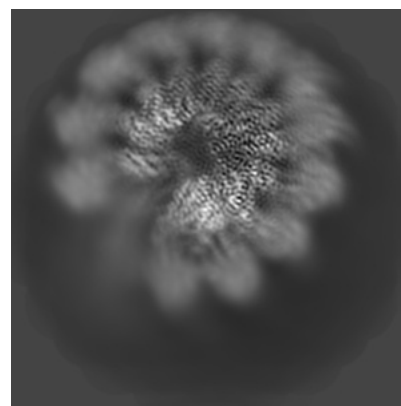
#### 6.1.1 Primary map



X

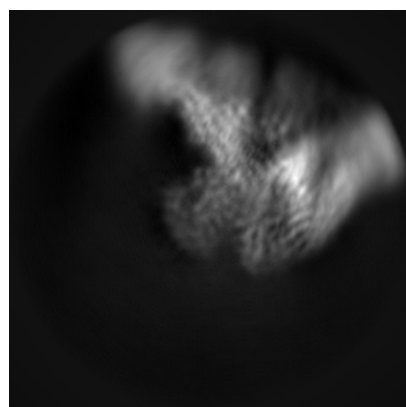


Y

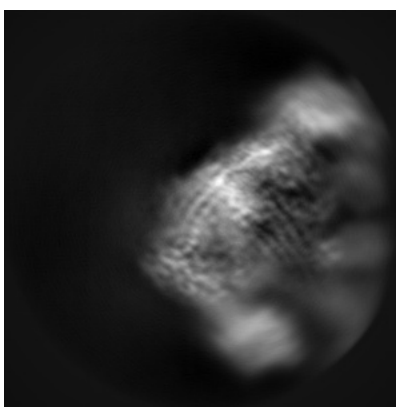


Z

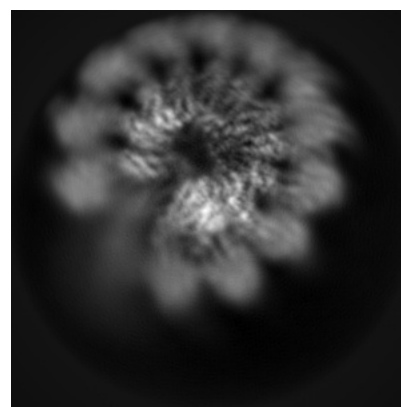
#### 6.1.2 Raw map



X



Y

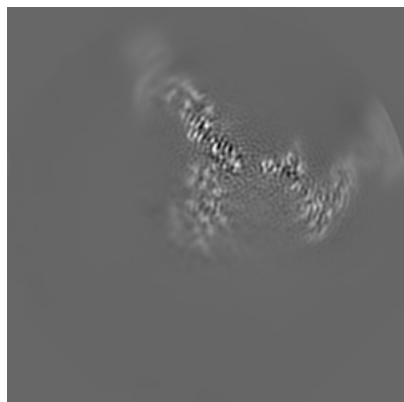


Z

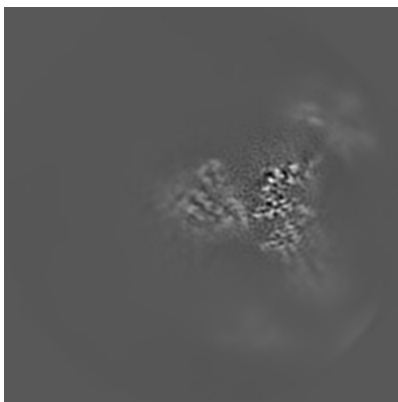
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

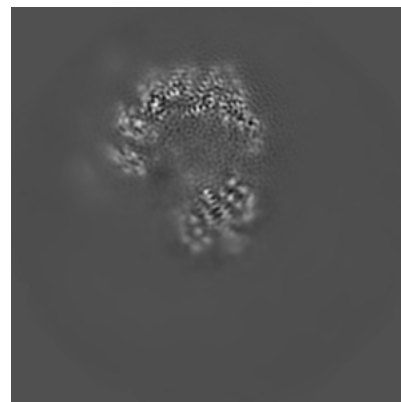
### 6.2.1 Primary map



X Index: 128

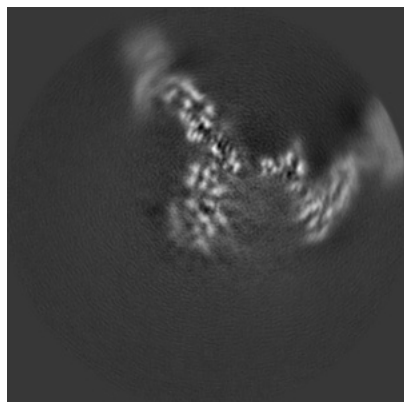


Y Index: 128

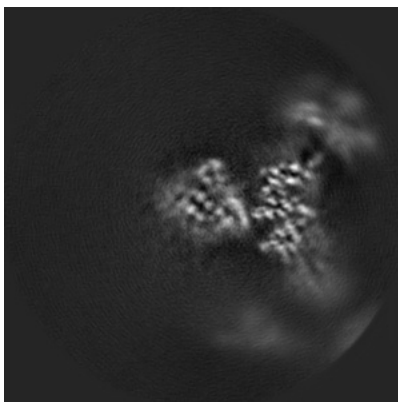


Z Index: 128

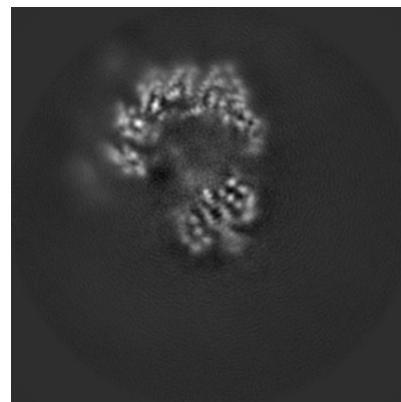
### 6.2.2 Raw map



X Index: 128



Y Index: 128



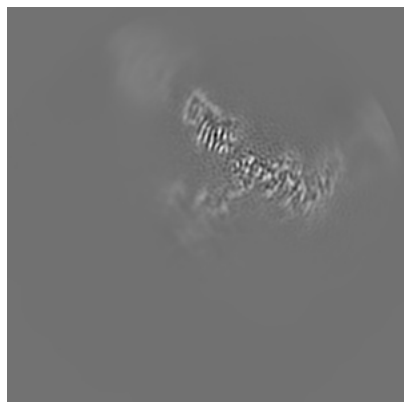
Z Index: 128

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

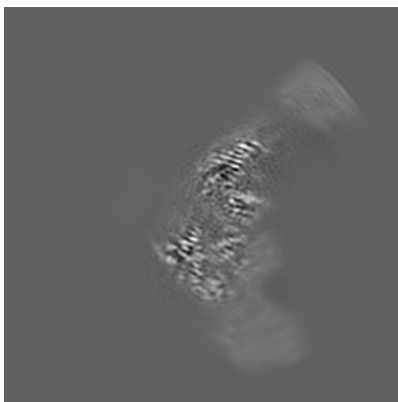


## 6.3 Largest variance slices [i](#)

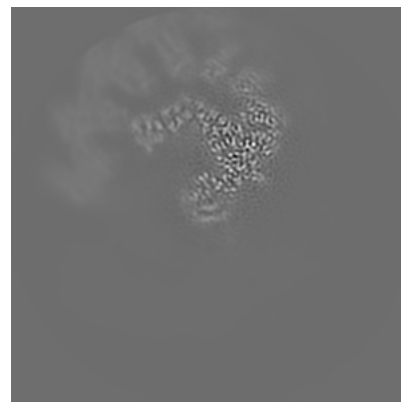
### 6.3.1 Primary map



X Index: 148

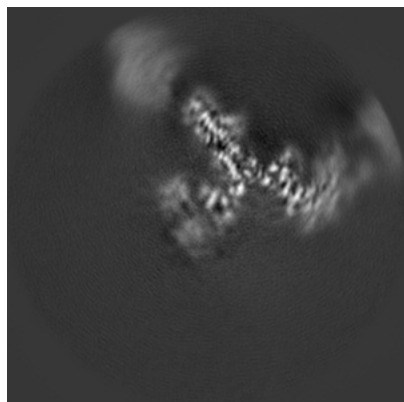


Y Index: 184

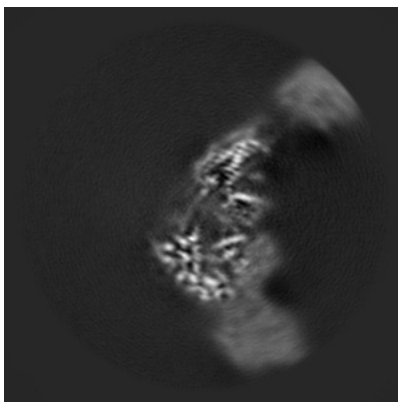


Z Index: 150

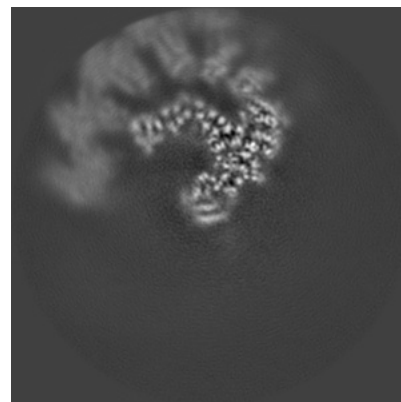
### 6.3.2 Raw map



X Index: 145



Y Index: 183

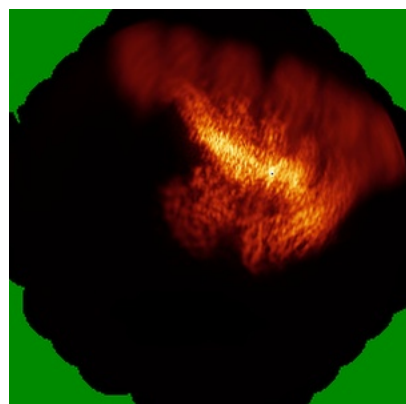


Z Index: 151

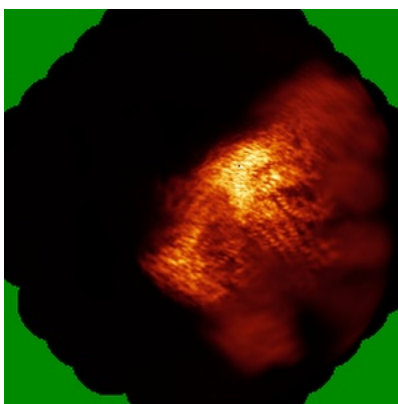
The images above show the largest variance slices of the map in three orthogonal directions.

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

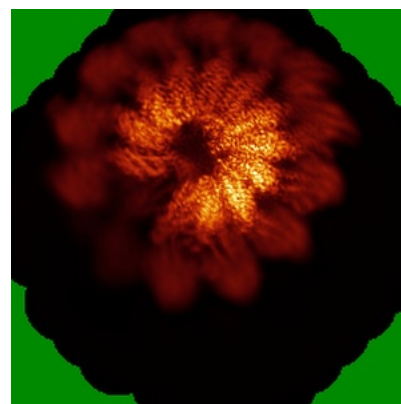
### 6.4.1 Primary map



X

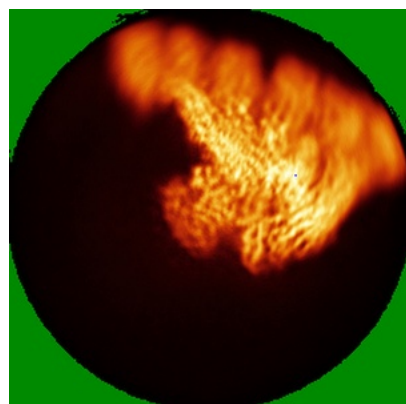


Y

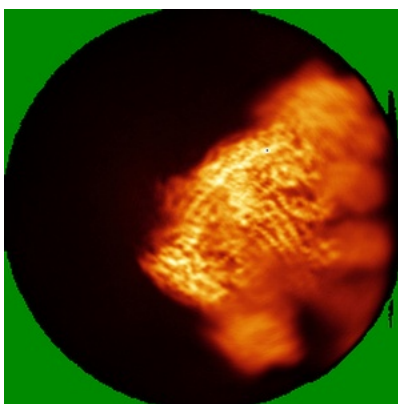


Z

### 6.4.2 Raw map



X



Y

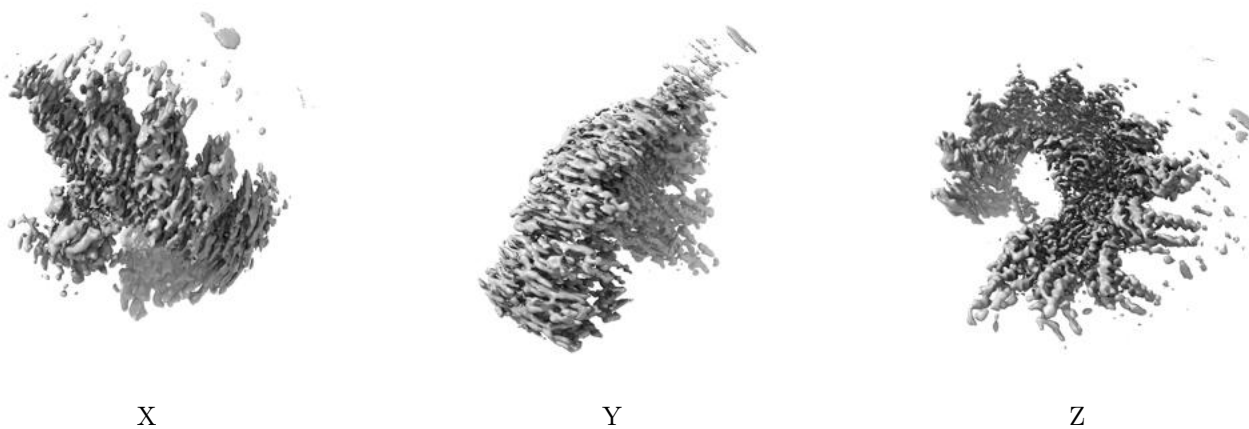


Z

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

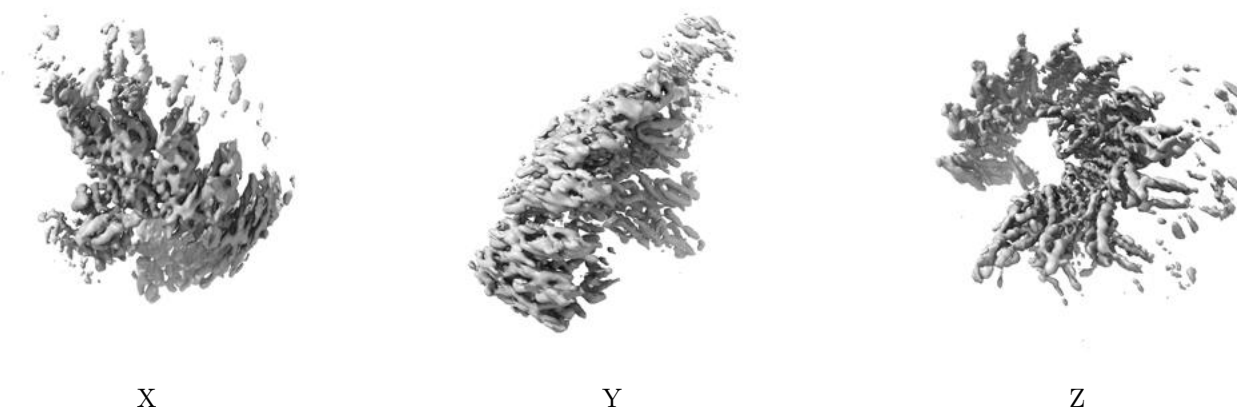
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0421. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

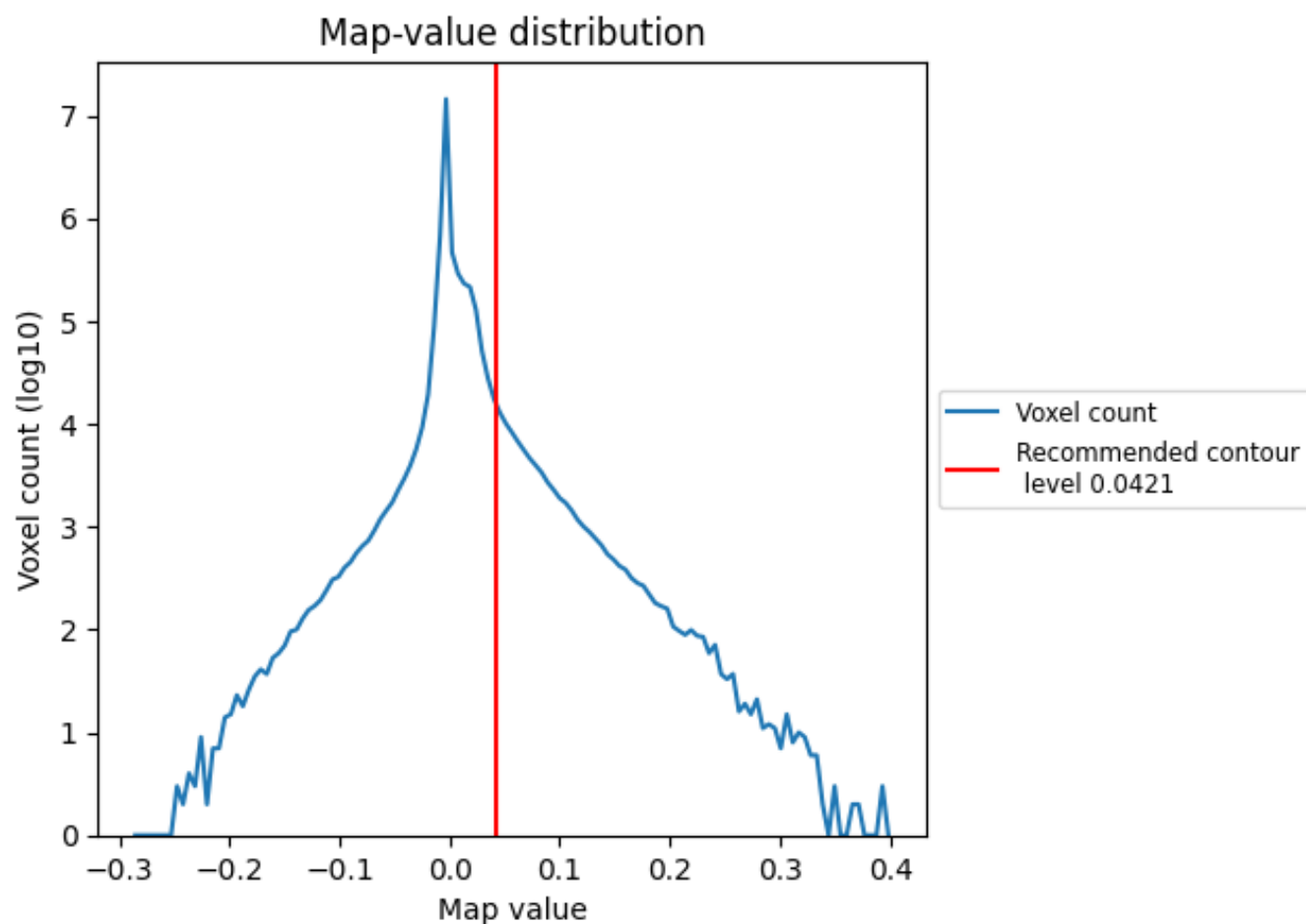
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

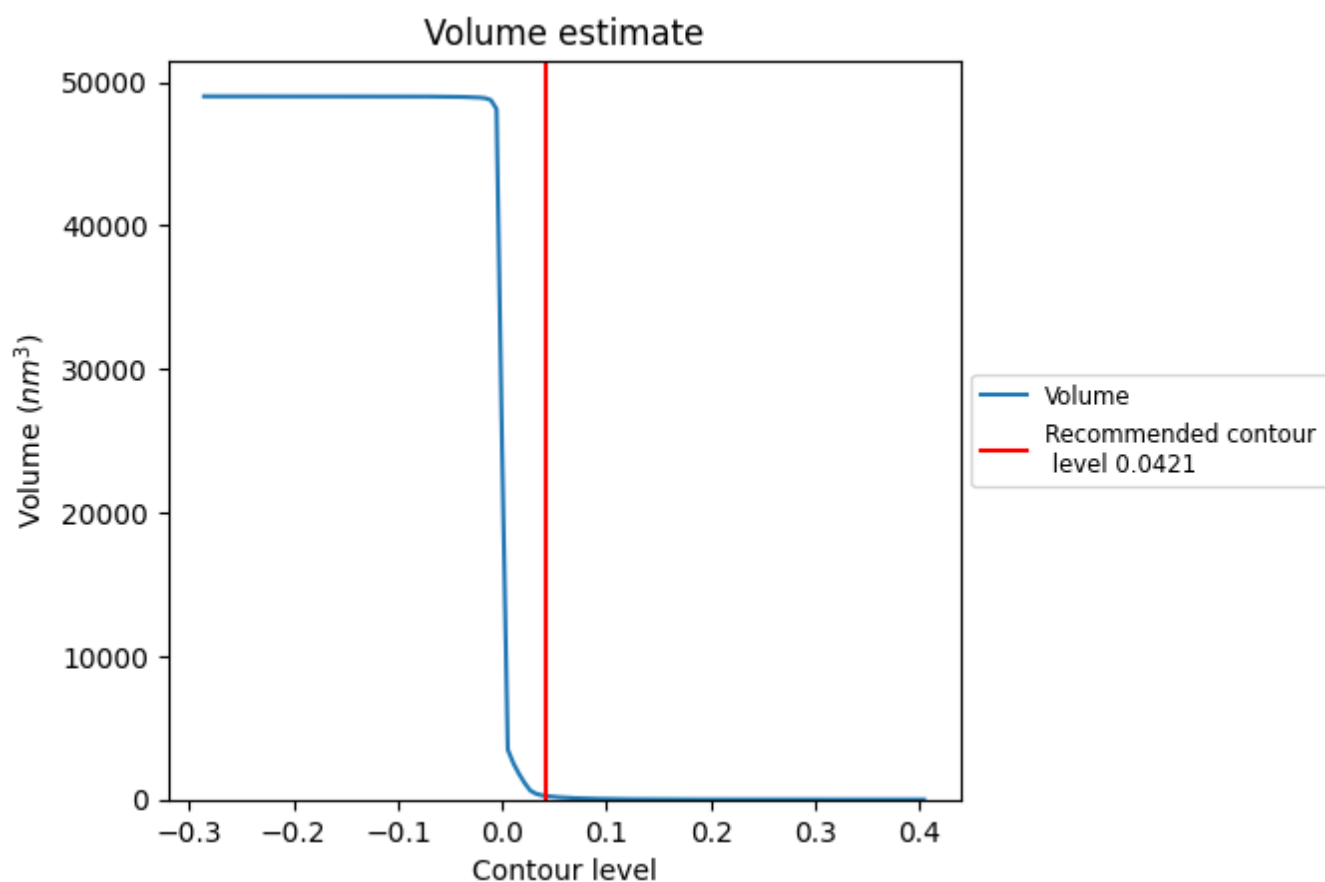
This section contains the results of statistical analysis of the map.

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



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

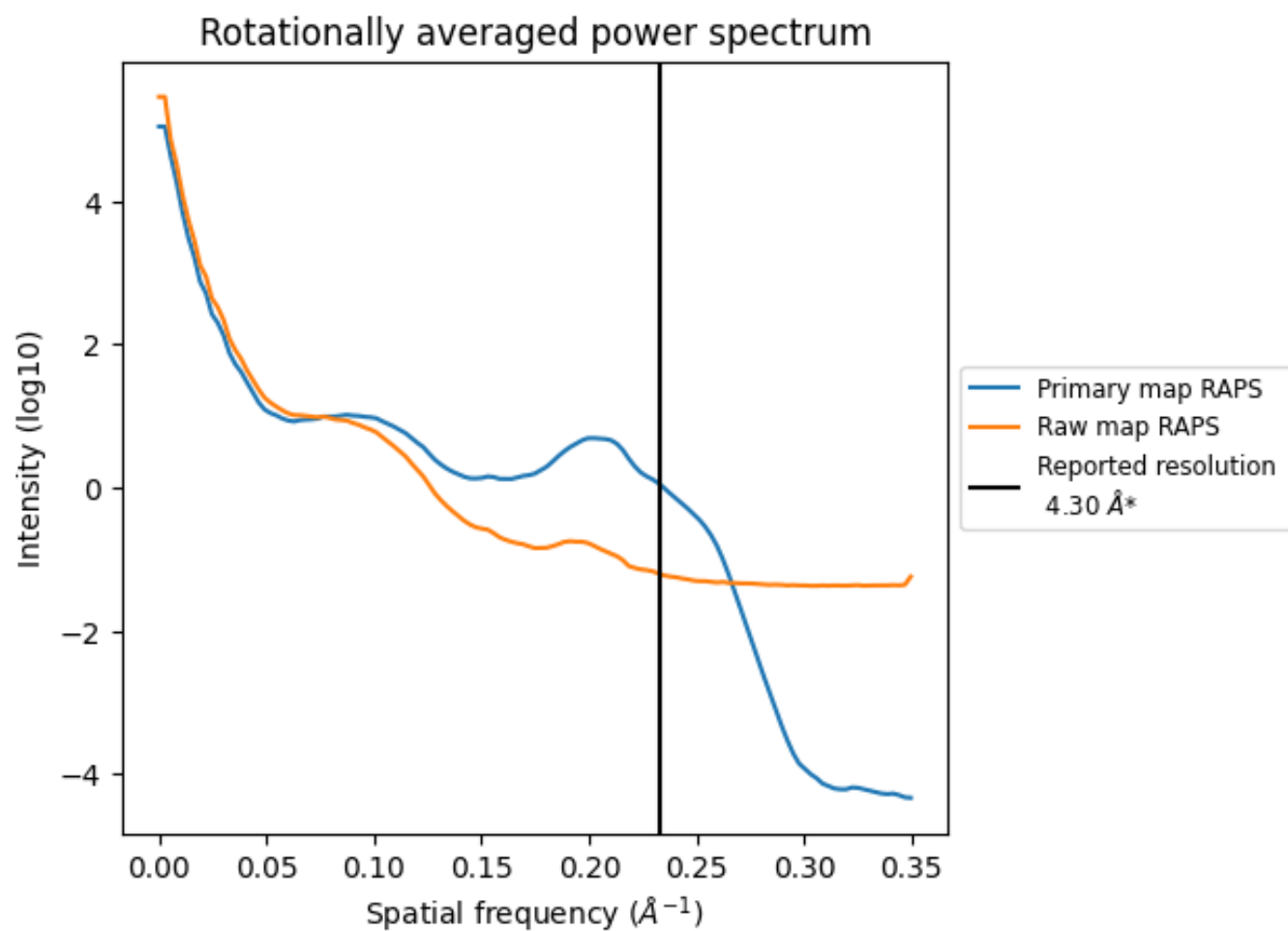
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252  $\text{nm}^3$ ; this corresponds to an approximate mass of 227 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 ⓘ

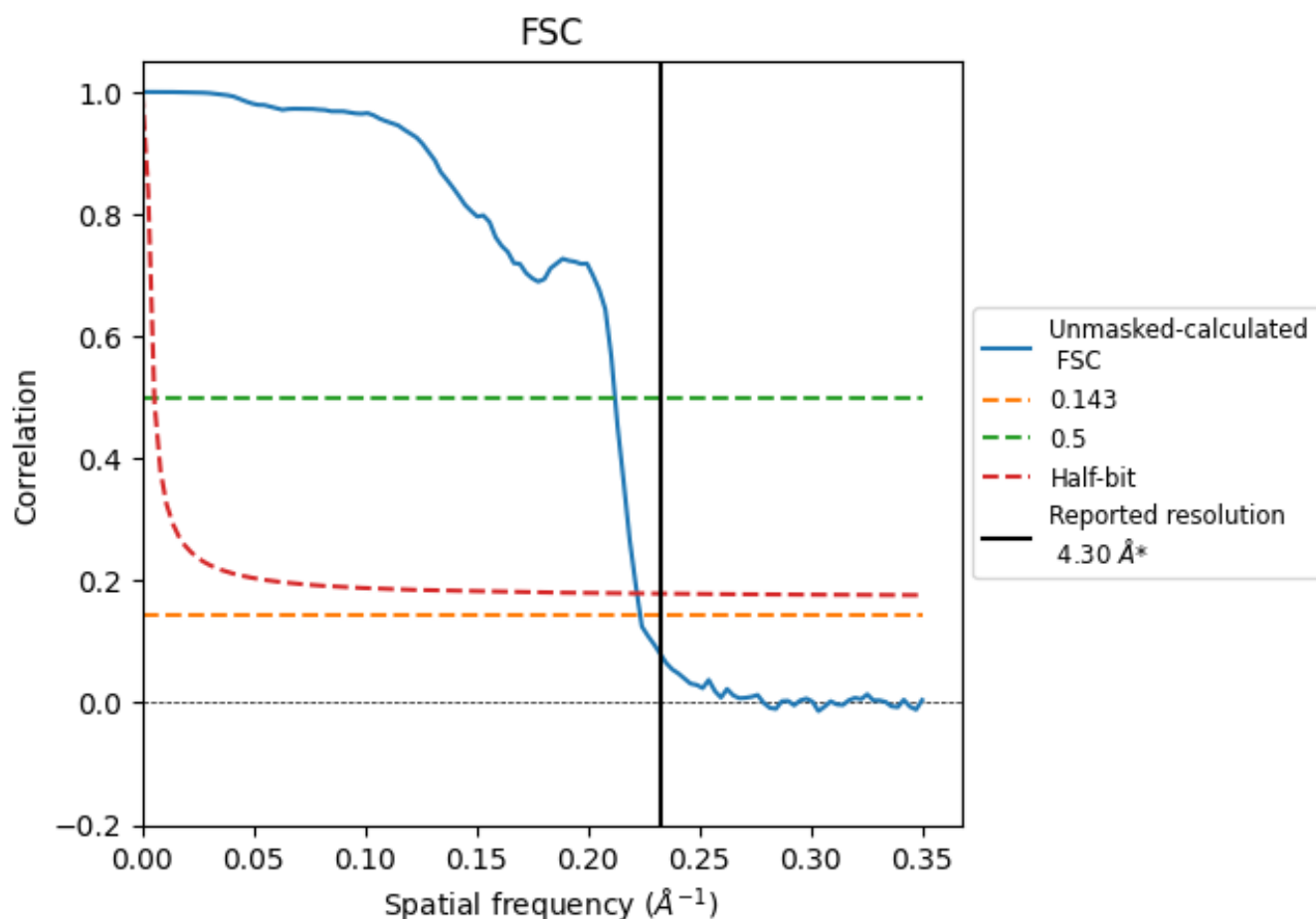


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.233  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.48	4.72	4.50

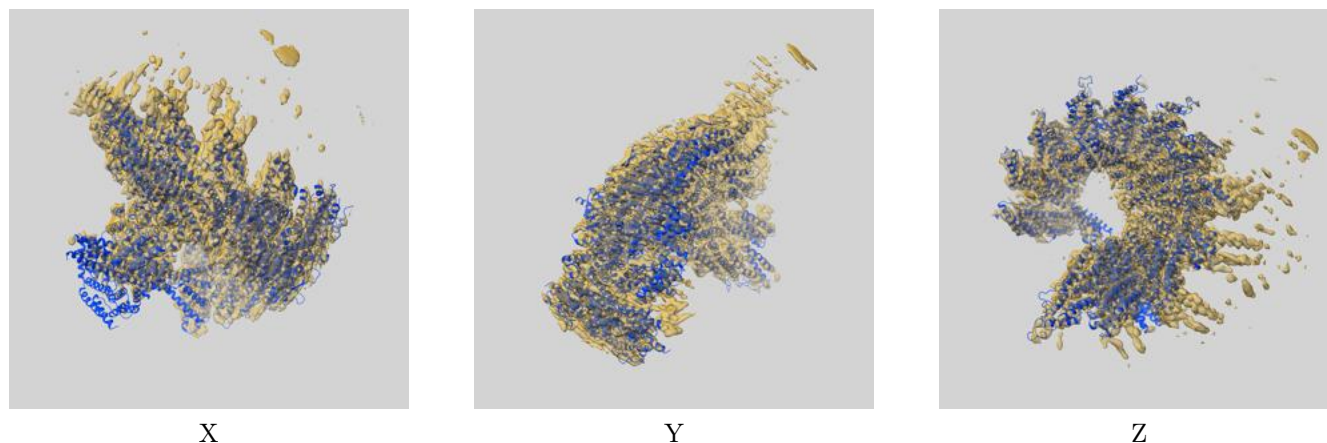
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



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

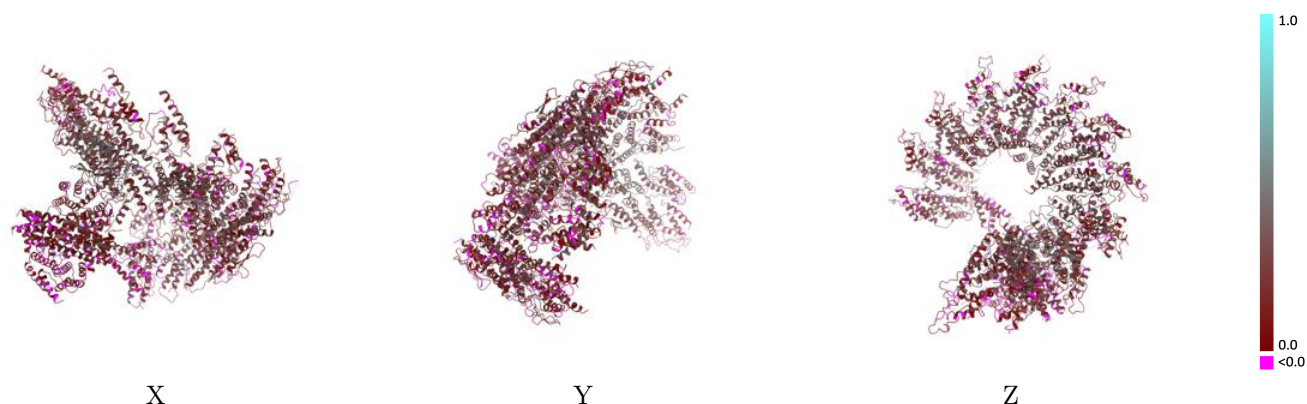
This section contains information regarding the fit between EMDB map EMD-52729 and PDB model 9I8M. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



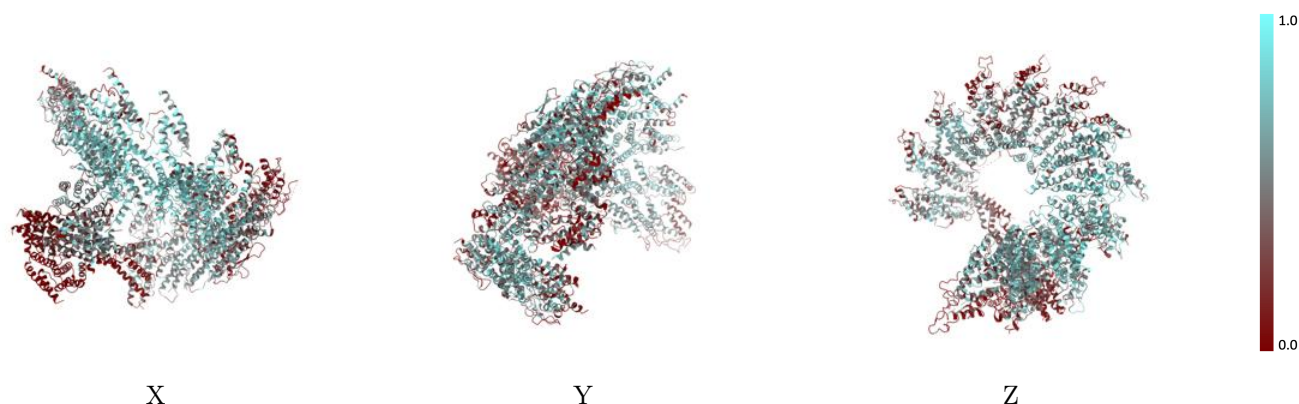
The images above show the 3D surface view of the map at the recommended contour level 0.0421 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



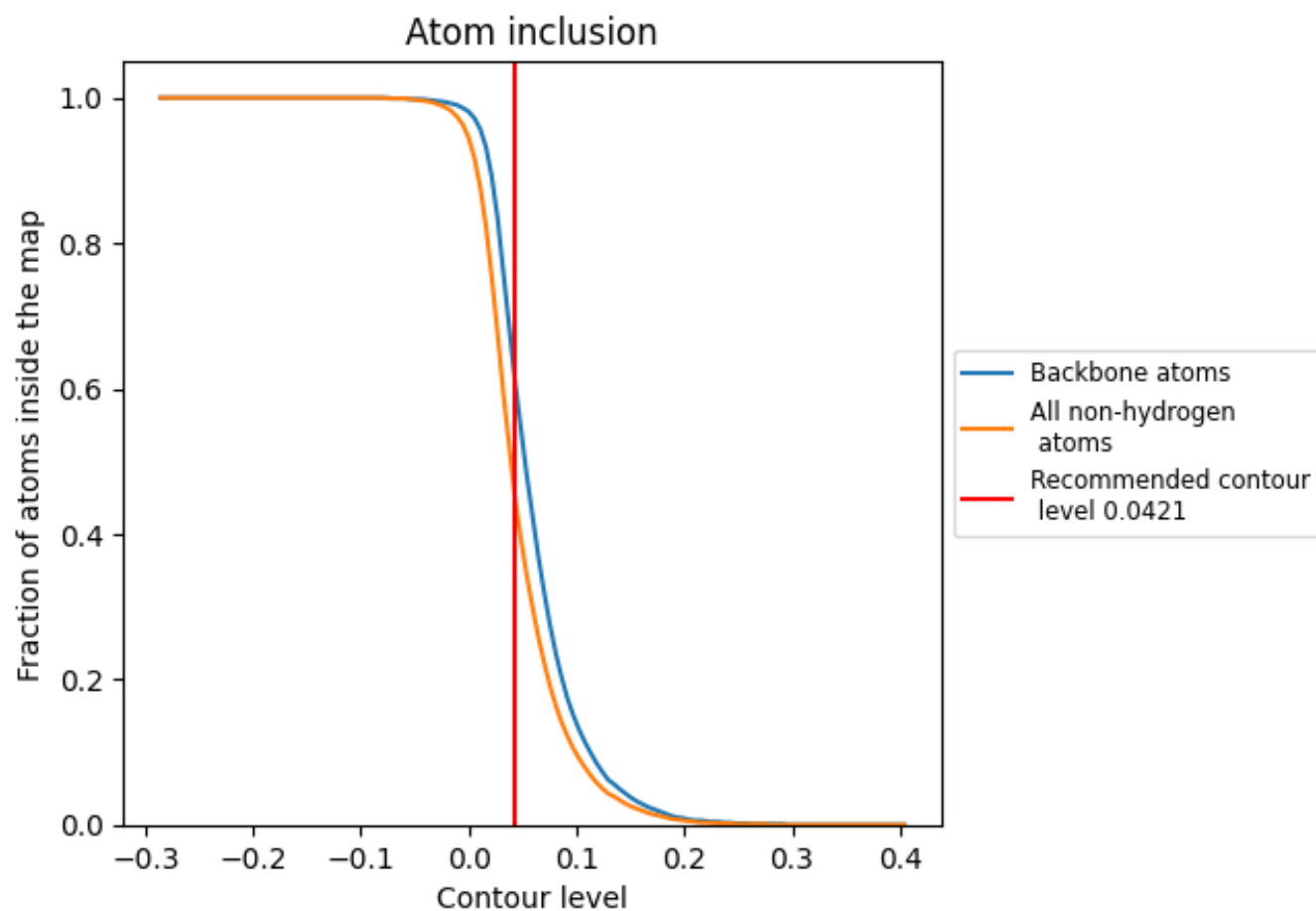
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0421).

























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 46% 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 (0.0421) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4610	 0.1990
A	 0.4370	 0.1340
B	 0.4790	 0.1530
C	 0.5550	 0.1810
D	 0.3590	 0.1690
E	 0.3630	 0.1960
F	 0.3810	 0.2020
G	 0.5550	 0.2200
H	 0.6540	 0.2460
I	 0.6440	 0.2650
J	 0.6320	 0.2690
K	 0.5640	 0.2530
L	 0.4320	 0.2020
O	 0.6400	 0.2920
Q	 0.1310	 0.1250
R	 0.3820	 0.1750
S	 0.4280	 0.1670
T	 0.0490	 0.0990
U	 0.3300	 0.1960
V	 0.2790	 0.1550
W	 0.2160	 0.1210
X	 0.1970	 0.1160
o	 0.6900	 0.3130
p	 0.4750	 0.2310
q	 0.1470	 0.0950
r	 0.4640	 0.1750
s	 0.5460	 0.1970
t	 0.0230	 0.1270

