



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:17 AM UTC

PDB ID : 7WB4 / pdb_00007wb4
EMDB ID : EMD-32394
Title : Cryo-EM structure of the NR subunit from *X. laevis* NPC
Authors : Huang, G.; Zhan, X.; Shi, Y.
Deposited on : 2021-12-15
Resolution : 5.60 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

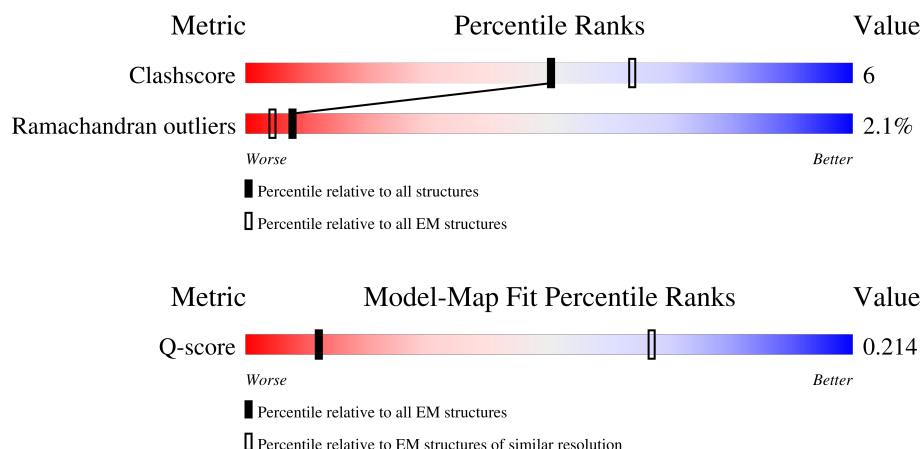
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	513 (5.10 - 6.10)

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

Mol	Chain	Length	Quality of chain
1	J	1140	
1	P	1140	
1	j	1140	
1	p	1140	
2	B	653	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	b	653	
3	C	375	
3	c	375	
4	F	326	
4	f	326	
5	D	360	
5	d	360	
6	E	1435	
6	e	1435	
7	K	1388	
8	H	320	
8	h	320	
9	G	923	
9	g	923	
10	I	916	
10	M	916	
10	i	916	
11	L	820	
11	O	820	
12	A	2011	
13	N	2408	
13	n	2408	

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 93534 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 outer Nup133.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	J	1021	Total	C	N	O	0	0
			5059	3017	1021	1021		
1	p	995	Total	C	N	O	0	0
			4934	2944	995	995		
1	j	995	Total	C	N	O	0	0
			4934	2944	995	995		
1	P	1021	Total	C	N	O	0	0
			5059	3017	1021	1021		

- Molecule 2 is a protein called Nuclear pore complex protein Nup85.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	628	Total	C	N	O	0	0
			3116	1860	628	628		
2	b	636	Total	C	N	O	0	0
			3156	1884	636	636		

- Molecule 3 is a protein called MGC154553 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	343	Total	C	N	O	0	0
			1694	1008	343	343		
3	c	346	Total	C	N	O	0	0
			1709	1017	346	346		

- Molecule 4 is a protein called MGC83926 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	318	Total	C	N	O	0	0
			1566	930	318	318		
4	f	321	Total	C	N	O	0	0
			1581	939	321	321		

- Molecule 5 is a protein called Nucleoporin SEH1-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	d	320	Total	C	N	O	0	0
			1581	941	320	320		
5	D	318	Total	C	N	O	0	0
			1571	935	318	318		

- Molecule 6 is a protein called outer Nup160.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	1363	Total	C	N	O	0	0
			6759	4033	1363	1363		
6	e	1310	Total	C	N	O	0	0
			6494	3874	1310	1310		

- Molecule 7 is a protein called Nup155-prov protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	K	330	Total	C	N	O	0	0
			1643	983	330	330		

- Molecule 8 is a protein called GATOR complex protein SEC13.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	306	Total	C	N	O	0	0
			1505	893	306	306		
8	h	307	Total	C	N	O	0	0
			1510	896	307	307		

- Molecule 9 is a protein called Nuclear pore complex protein Nup96.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	G	618	Total	C	N	O	0	0
			3062	1826	618	618		
9	g	672	Total	C	N	O	0	0
			3329	1985	672	672		

- Molecule 10 is a protein called Nuclear pore complex protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	I	796	Total	C	N	O	0	0
			3956	2364	796	796		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
10	i	796	Total	C	N	O	0	0
			3956	2364	796	796		
10	M	796	Total	C	N	O	0	0
			3956	2364	796	796		

- Molecule 11 is a protein called Nuclear pore complex protein Nup93.

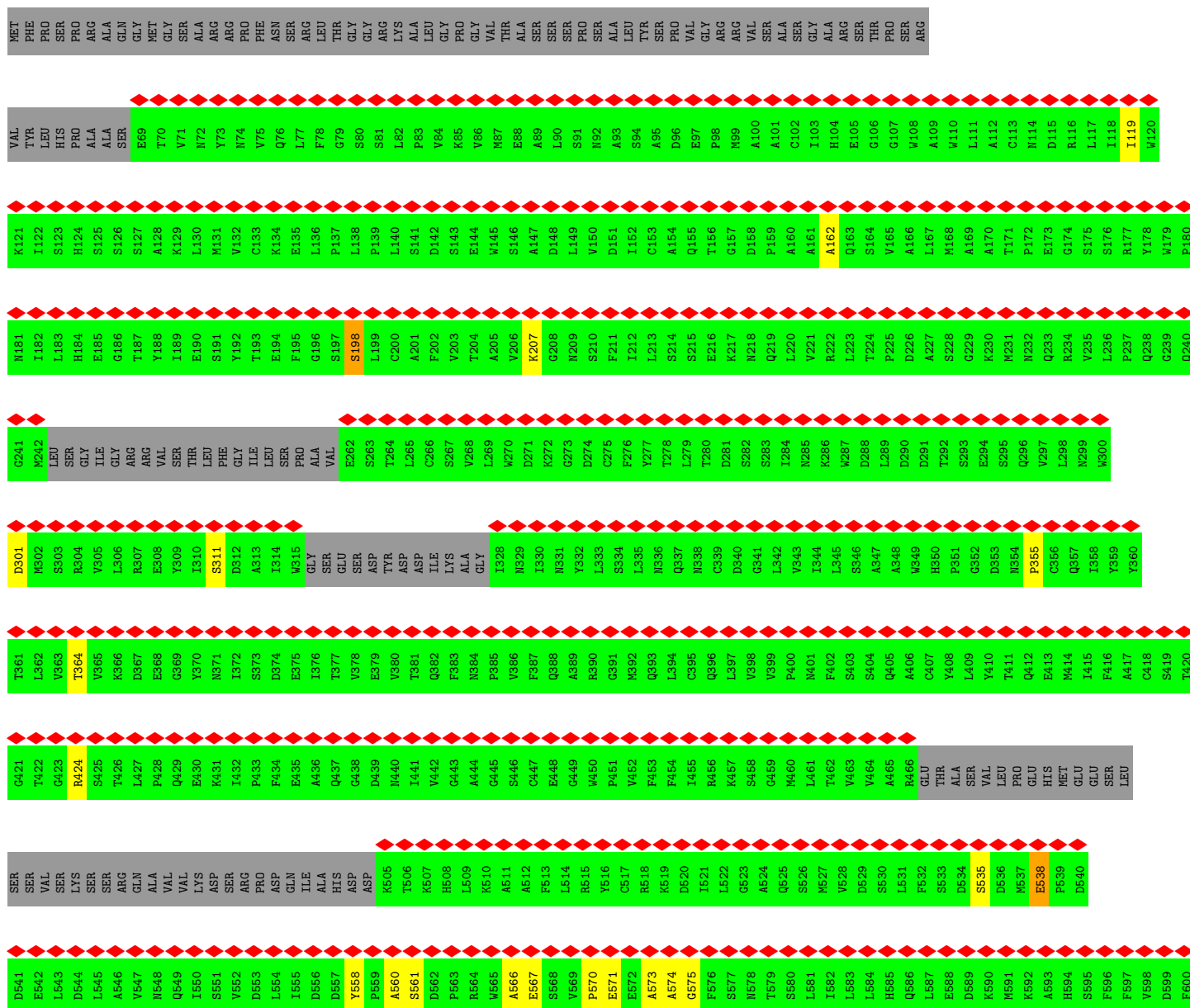
Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	641	Total	C	N	O	0	0
			3178	1896	641	641		
11	O	50	Total	C	N	O	0	0
			250	150	50	50		

- Molecule 12 is a protein called MGC83295 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	A	1796	Total	C	N	O	0	0
			8893	5301	1796	1796		

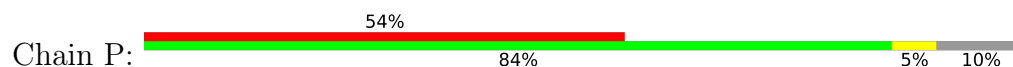
- Molecule 13 is a protein called Protein ELYS.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	n	910	Total	C	N	O	0	0
			4502	2682	910	910		
13	N	926	Total	C	N	O	0	0
			4581	2729	926	926		

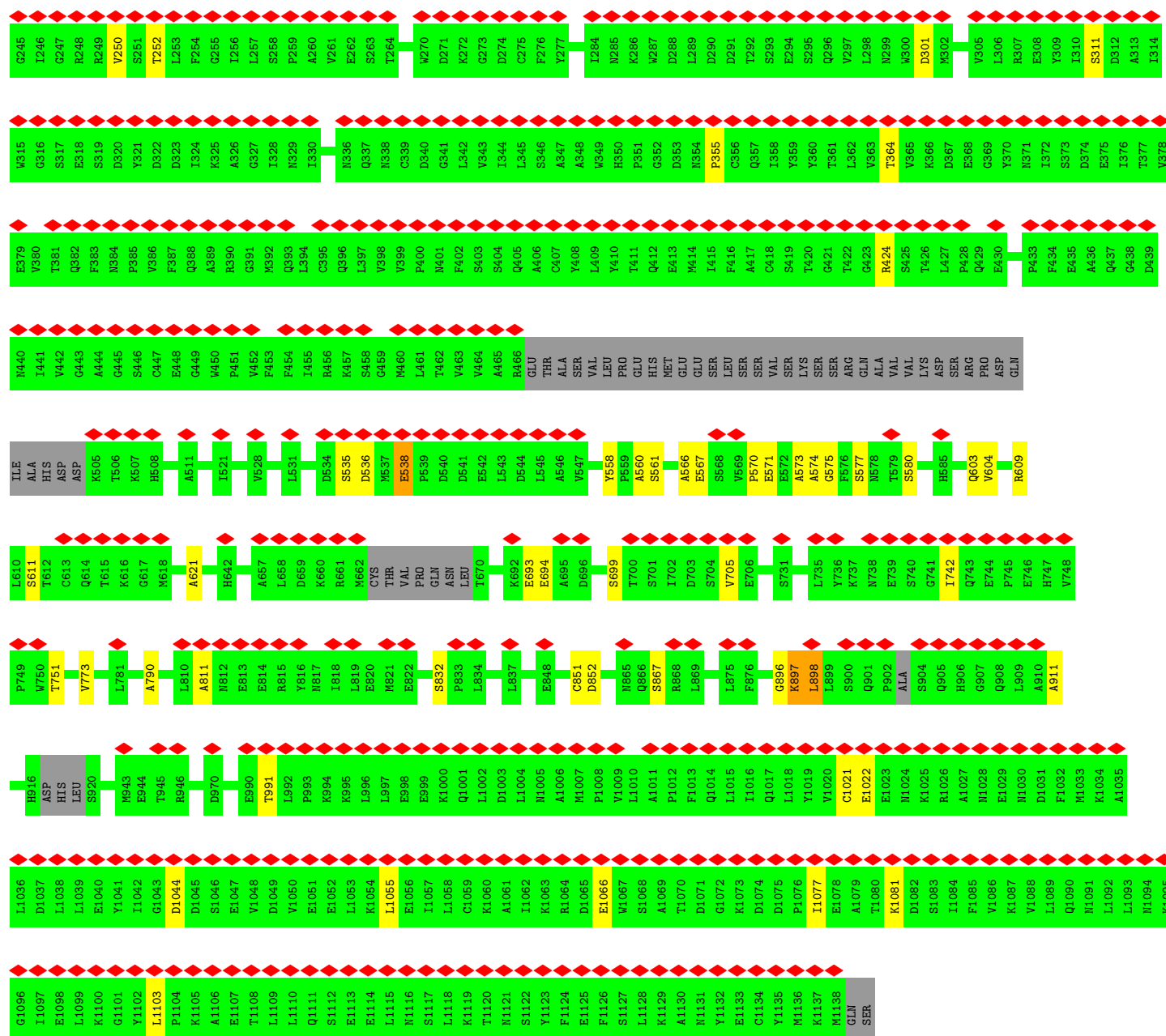


L601	H602	Q603	V604	G605	L606	F607	S608	R609	L610	S611	T612	C613	Q614	T615	K616	K617	M618	L619	V620	A621	T622	R623	L624	L625	L626	S627	E628	H629	A630	E631	K632	L633	S634	A635	A636	I637	V638	L639	K640	N641	H642	H643	A644	K645	K646	P647	V648	L649	V650	N651	S652	A653	I654	Q655	L656	A657	L658	D659	K660																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
						PRO	GLN	ASN	LEU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														</

• Molecule 1: outer Nup133

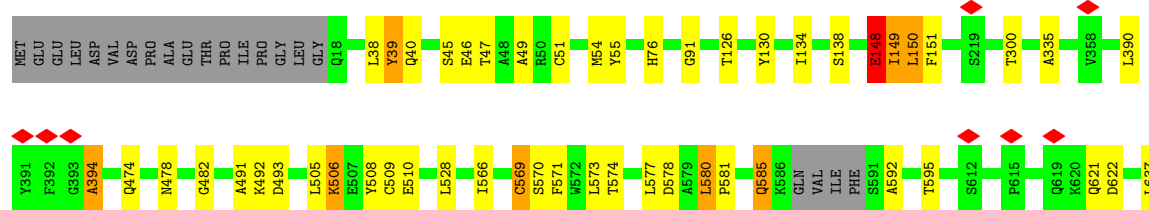


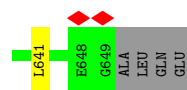
MET	PHE	PRO	SER	ARG	ALA	GLN	GLY	MET	GLY	SER	ALA	ARG	ARG	PRO	PHE	ASN	SER	ARG	LEU	THR	GLY	ARG	LYS	ALA	LEU	GLY	PRO	GLY	VAL	THR	ALA	SER	SER	SER	PRO	ALA	LEU	ALA	LEU	TYR	SER	PRO	VAL	GLY	ARG	ARG	VAL	SER	SER	ALA	GLY	ALA	ARG	SER	THR	PRO	THR	SER																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
VAL	TYR	HIS	PRO	ALA	ALA	SER	E69																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				



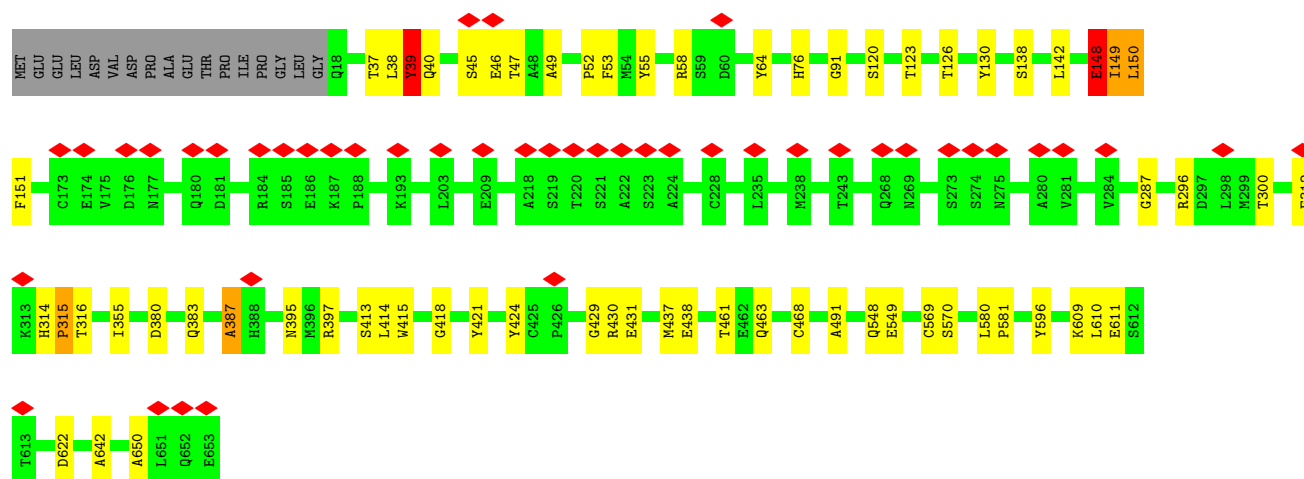
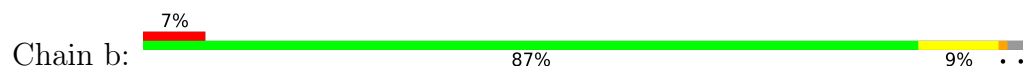
• Molecule 2: Nuclear pore complex protein Nup85

Chain B: 88% 7% . .

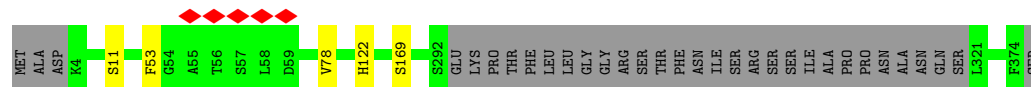
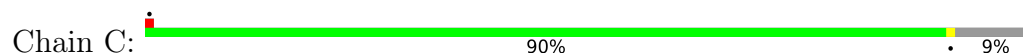




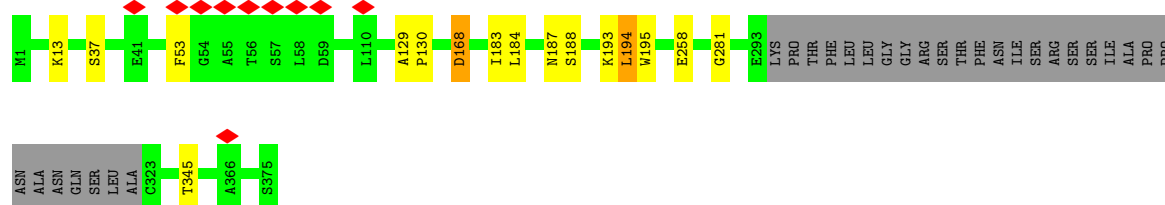
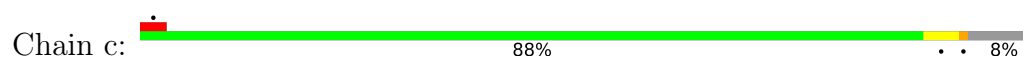
- Molecule 2: Nuclear pore complex protein Nup85



- Molecule 3: MGC154553 protein



- Molecule 3: MGC154553 protein



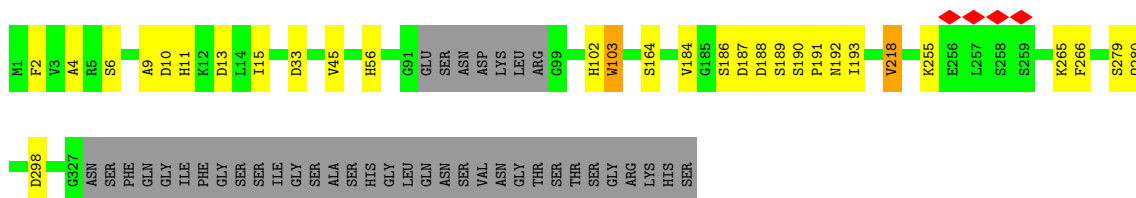
- Molecule 4: MGC83926 protein



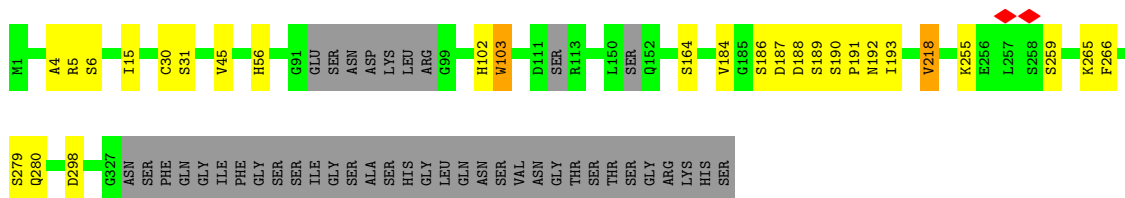
- Molecule 4: MGC83926 protein

Sequence logo for the 12th position. The y-axis represents information content in bits, ranging from 0 to 0.4. The x-axis lists amino acids: MET, LYS, GLN, ASP, SER, A6, S124, R253, Y272, P273, G274, K275, M276, K277, V298, and M326. The bar for A6 is the tallest, reaching approximately 0.38 bits. Other significant bars include S124, R253, Y272, P273, G274, K275, M276, K277, V298, and M326, all reaching between 0.1 and 0.2 bits. MET, LYS, GLN, and ASP have very low information content, near zero.

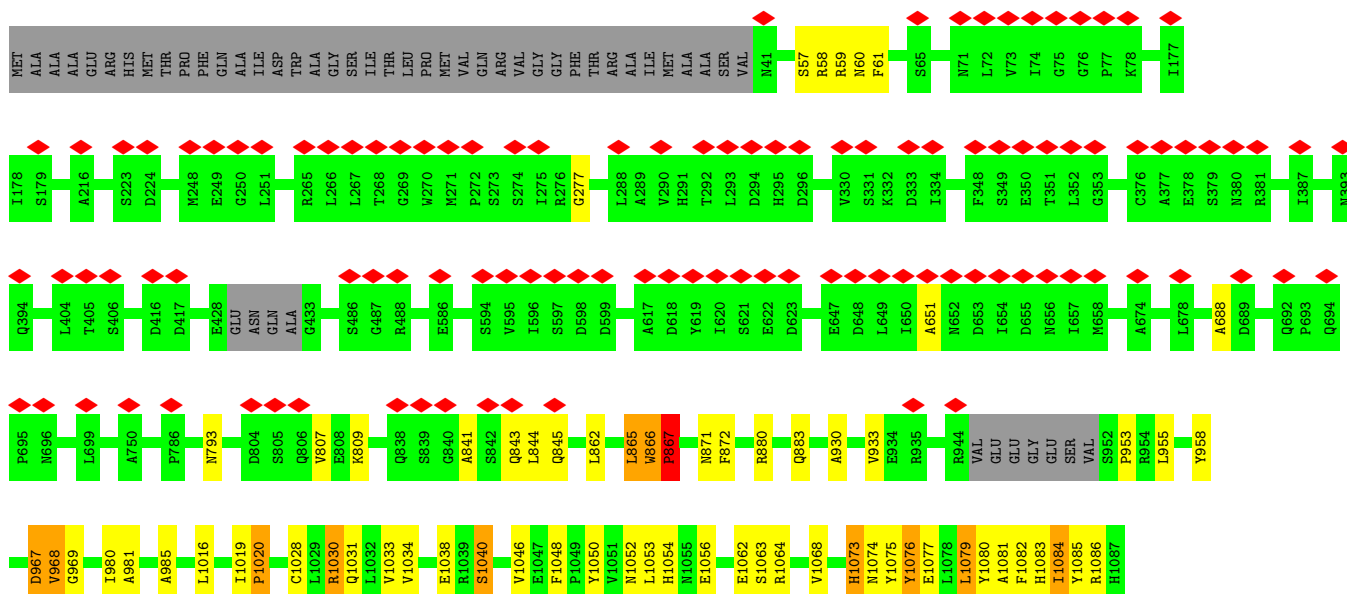
Chain d: 81% 8% 11%

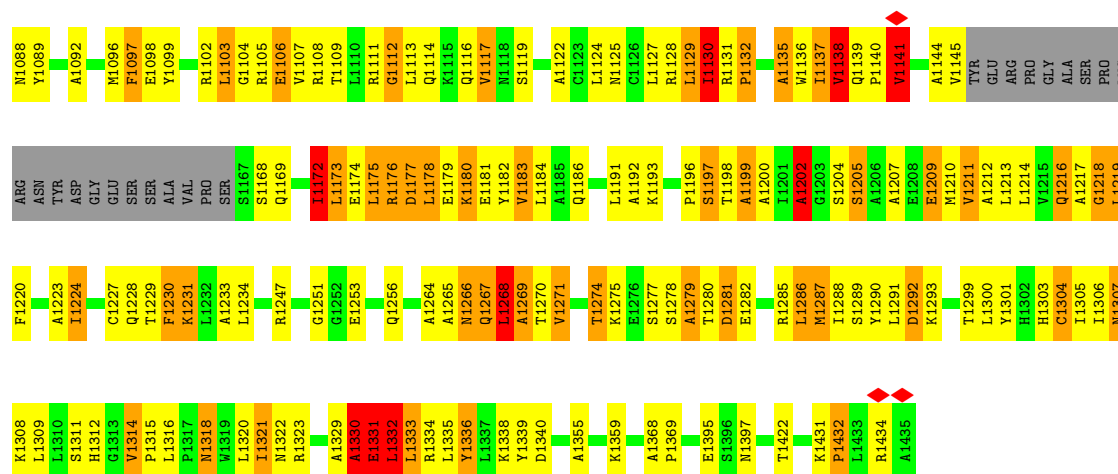


Chain D: 81% 7% 12%



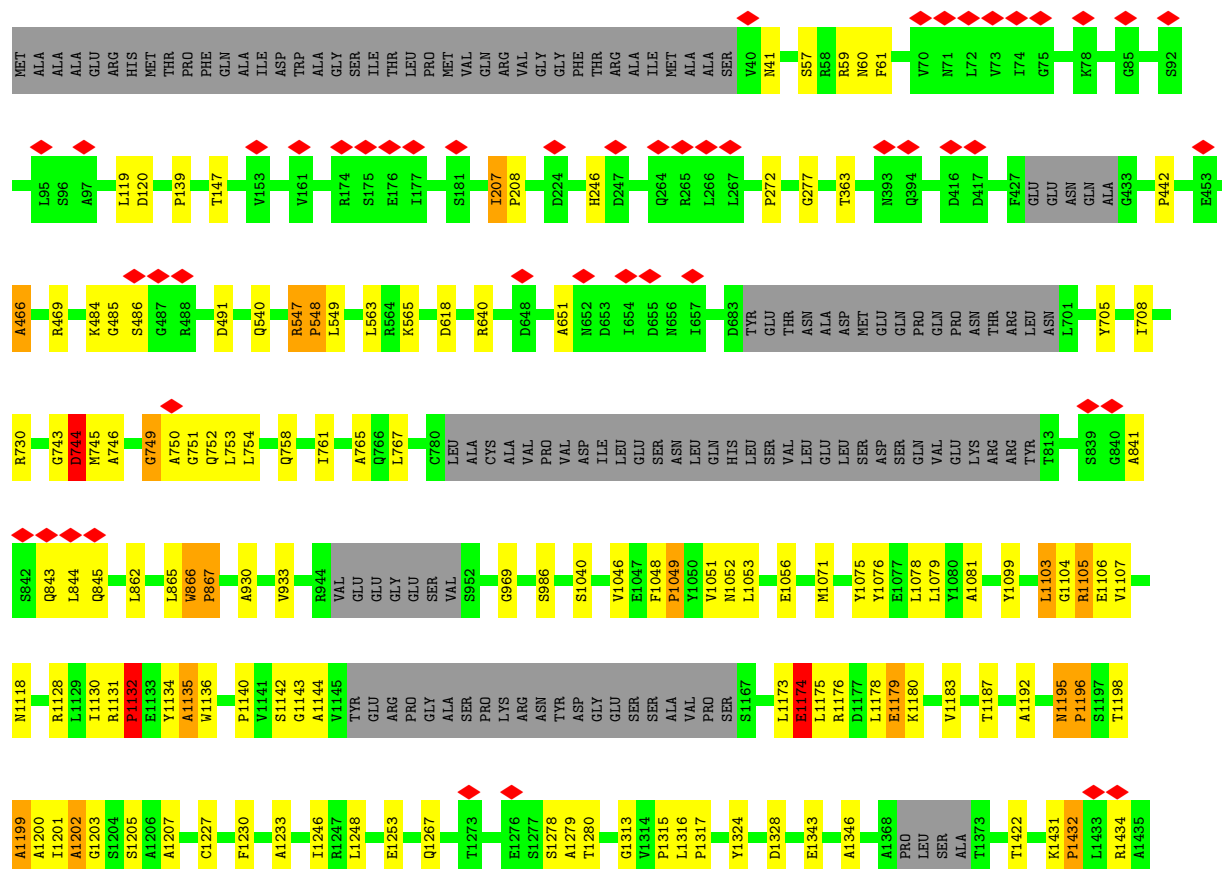
Chain E: 8% 79% 11% 5%





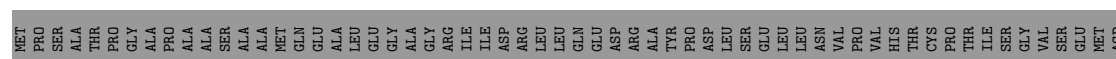
• Molecule 6: outer Nup160

Chain e: 82% 8% • 9%



• Molecule 7: Nup155-prov protein

Chain K: 17% 5% • 76%

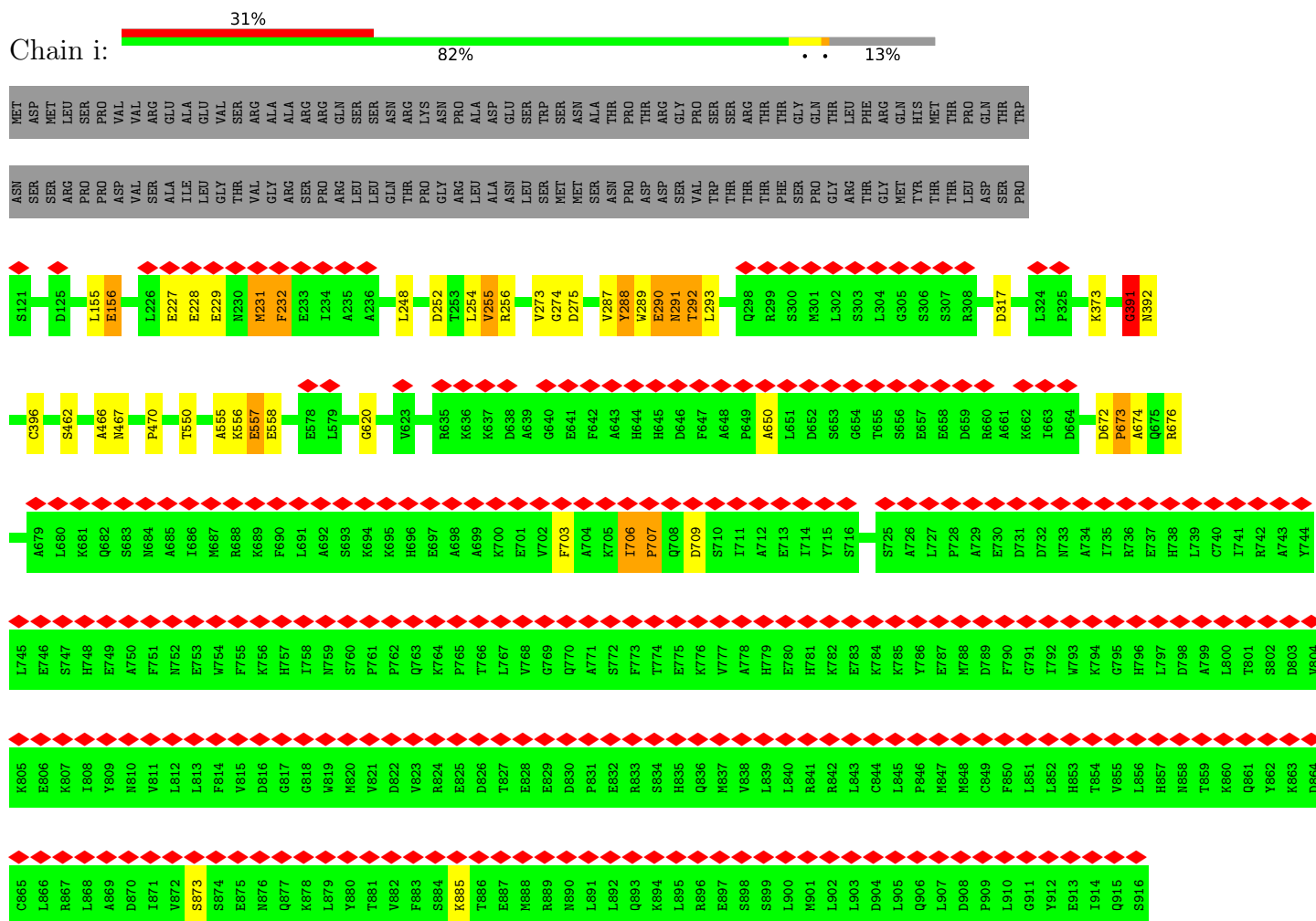






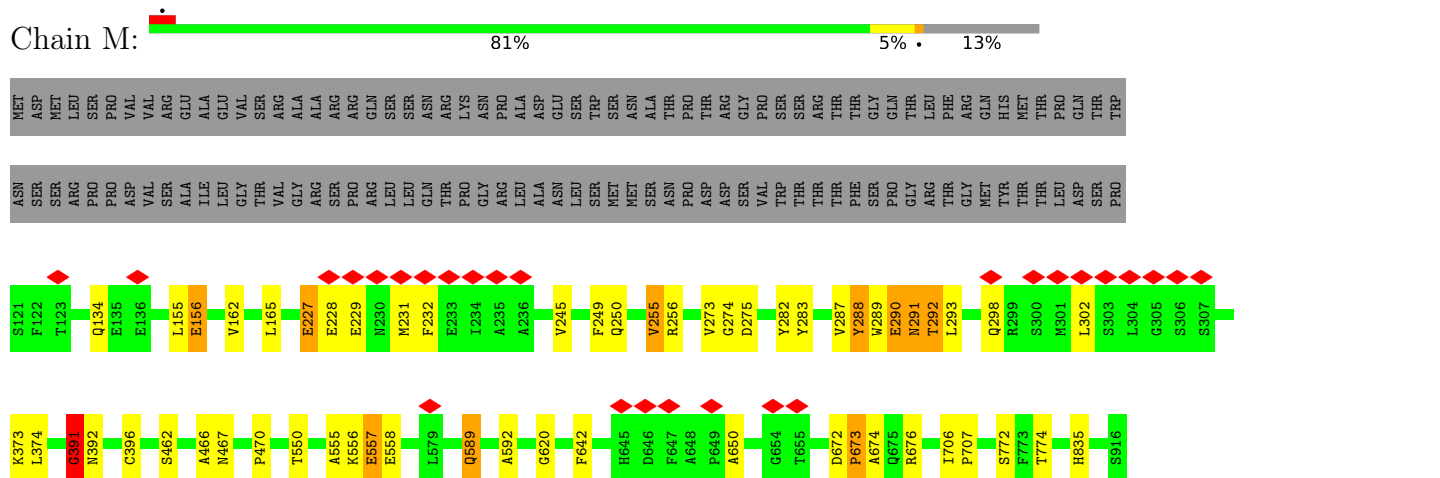
- Molecule 10: Nuclear pore complex protein

Chain i:



- Molecule 10: Nuclear pore complex protein

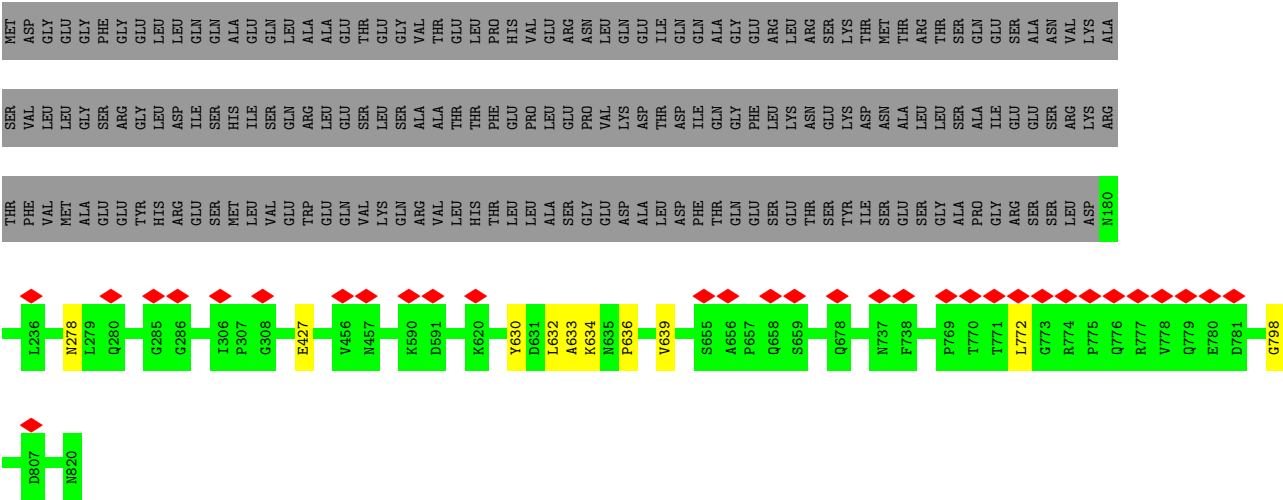
Chain M:



- Molecule 11: Nuclear pore complex protein Nup93

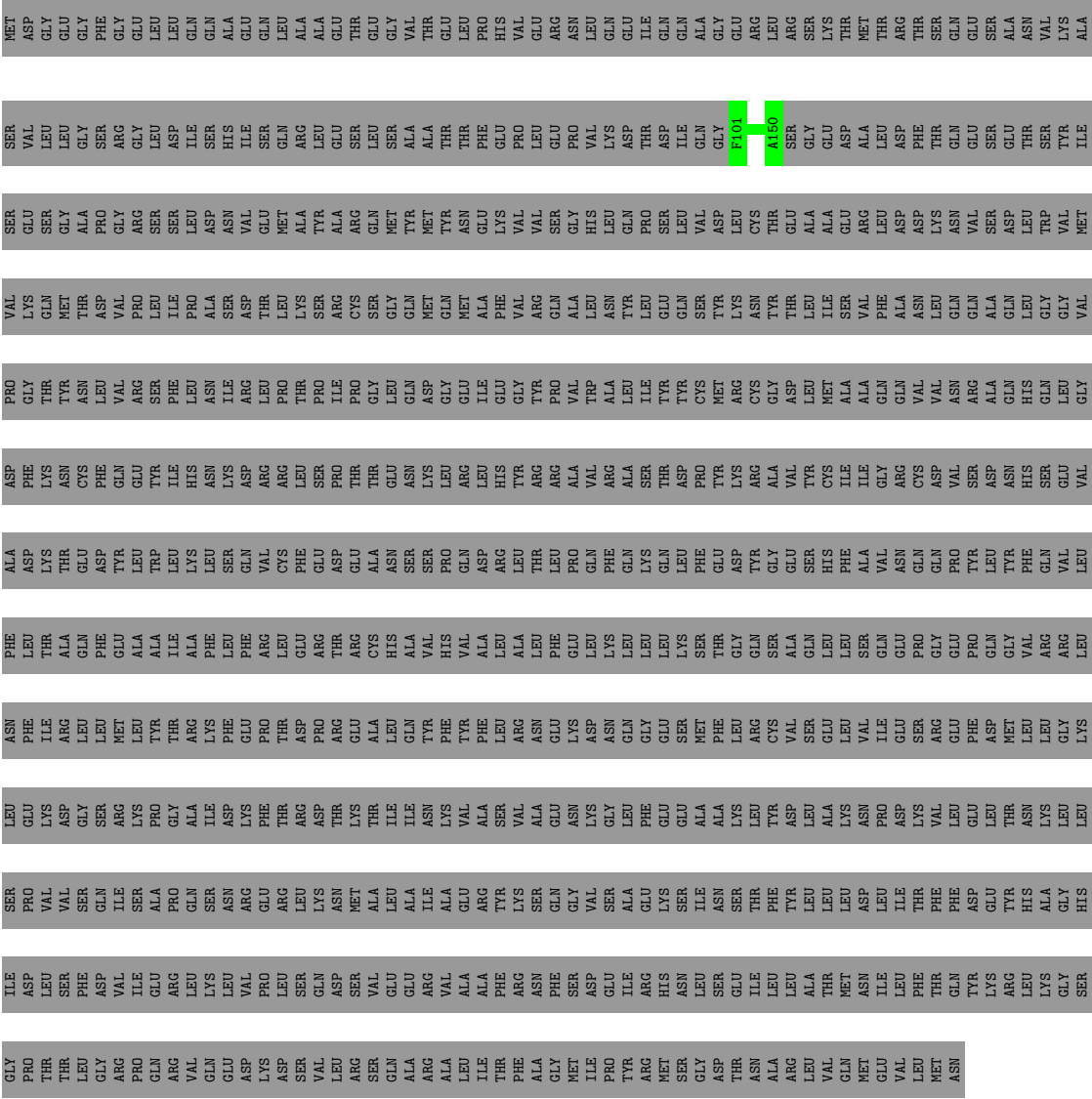
Chain L:



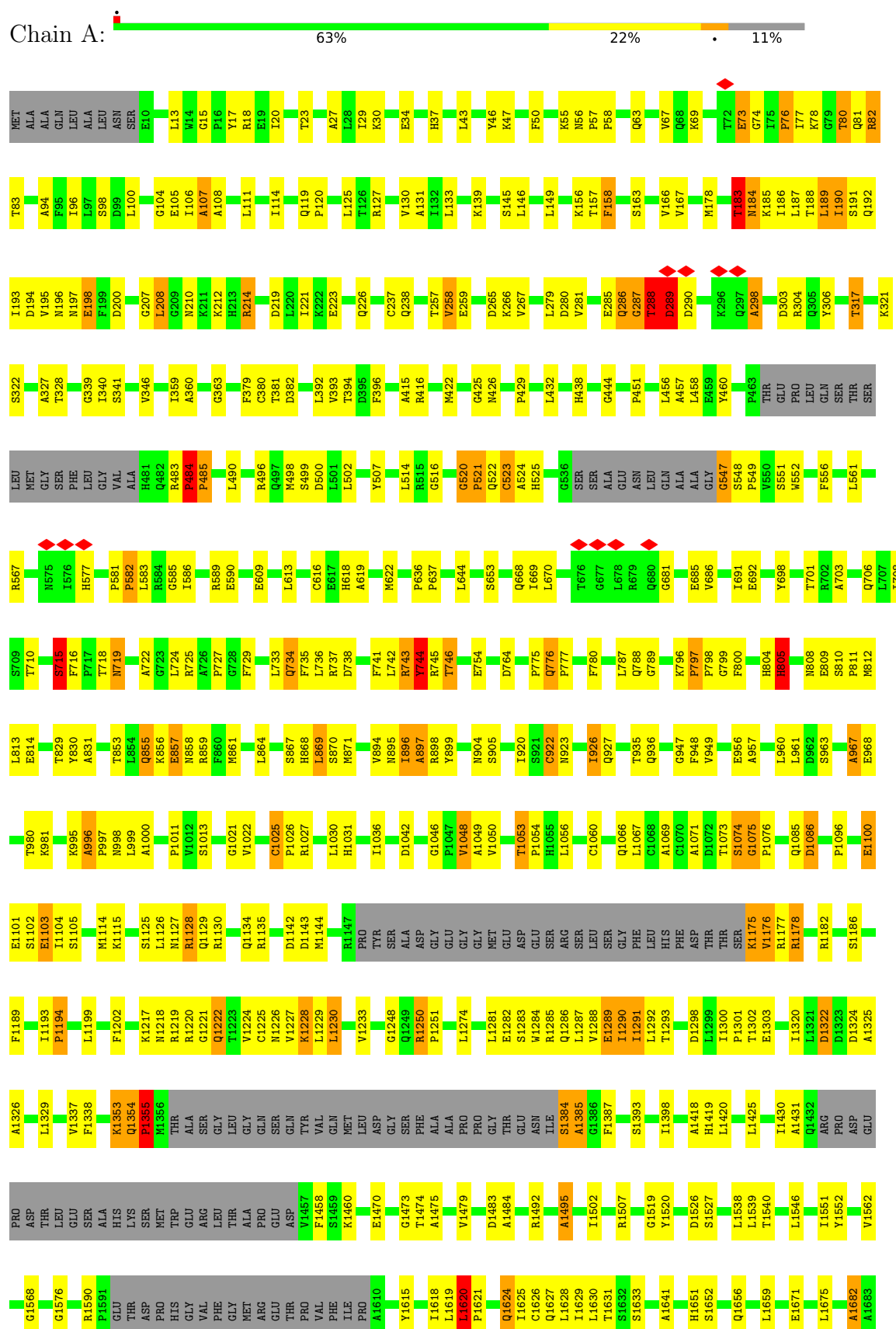


● Molecule 11: Nuclear pore complex protein Nup93

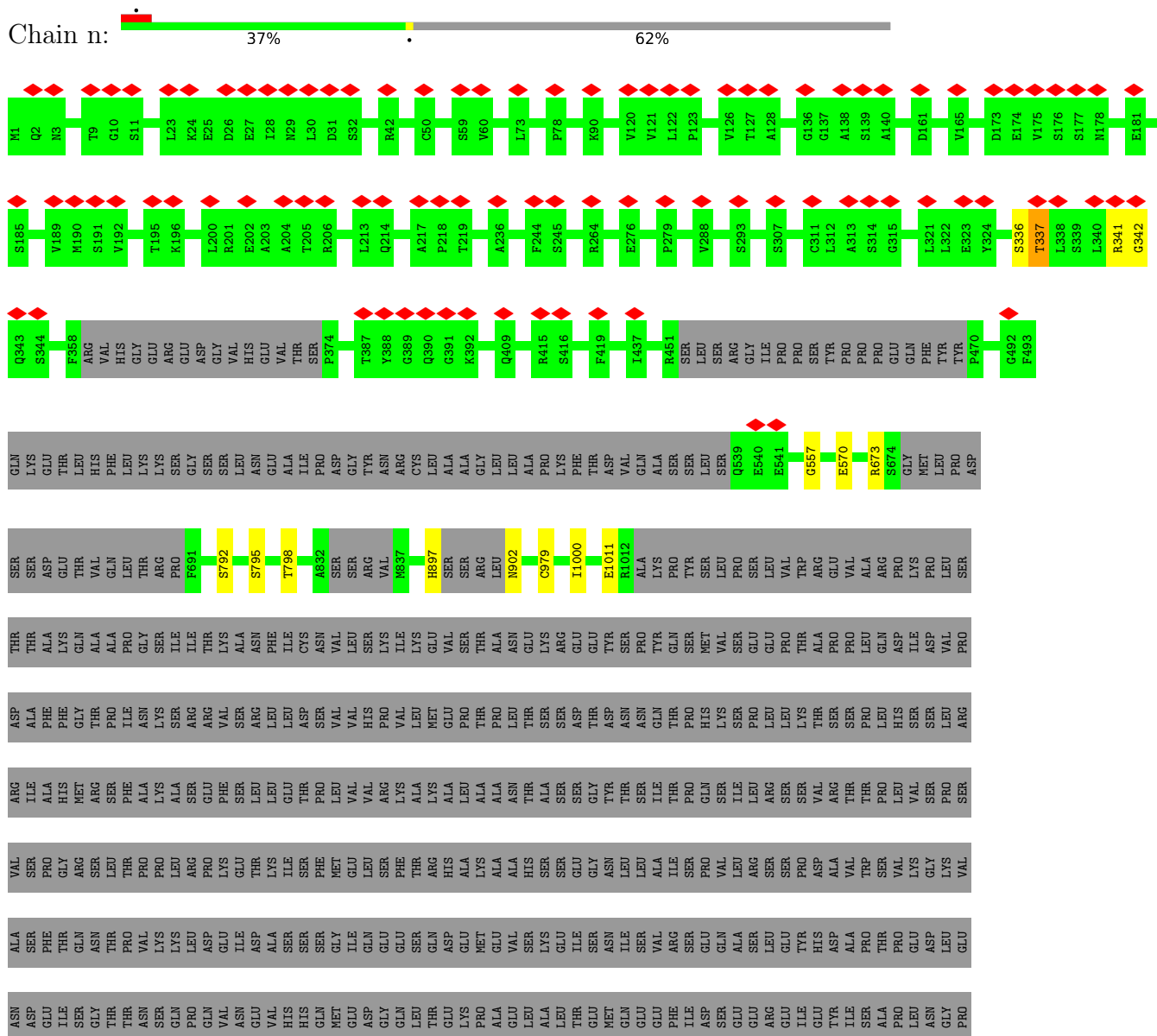
Chain O: 6% 94%



● Molecule 12: MGC83295 protein



- Molecule 13: Protein ELYS



- Molecule 13: Protein ELYS

Response	Percentage
Yes	34%
No	62%
No (Additional)	38%



T61	G62	E63	R64	I65	S66	A67	Y68	H69	F70	S71	G72	L73	T74	E75	R76	P77	P78	V79	V80	V81	A82	V83	K84	E85	F86	T87	W88	Q89	K90	K91	T92	G93	L94	L95	V96	G97	L98	V99	E100	A101	E102	G103	S104	V105	L106	C107	L108	V109	D110	I111	G112	I113	S114	K115	V116	V117	K118	A119	V120
V121	L122	P123	G124	S125	V126	T127	A128	V129	E130	P131	I132	I133	N134	H135	G136	G137	A138	S139	A140	T141	T142	Q143	H144	L145	H146	Q147	S148	L149	R150	W151	F152	F153	G154	V155	T156	A157	V158	V159	T160	D161	V162	G163	H164	V165	L166	L167	I168	D169	L170	C171	L172	D173	E174	V175	S176	S177	N178	Q179	D180
E181	L182	D183	A184	S185	D186	L187	E188	V189	M190	S191	V192	I193	P194	T195	K196	I197	P198	K199	L200	R201	E202	A203	A204	T205	R206	E207	R208	R209	H210	L211	C212	L213	Q214	L215	A216	A217	P218	T219	G220	T221	T222	V223	S224	C225	L226	S227	Y228	L229	S230	R231	T232	N233	Q234	L235	A236	V237	G238	Y239	S240
D241	G242	Y243	F244	S245	L246	W247	N248	M249	K250	T251	L252	R253	R254	D255	Y256	H257	V258	Q259	I260	E261	G262	G263	R264	V265	P266	V267	C268	A269	V270	A271	F272	Q273	E274	P275	E276	N277	D278	P279	R280	N281	C282	C283	Y284	L285	W286	A287	V288	Q289	S290	S291	E292	S293	G294	G295	D296	V297	S298	L299	H300
L301	L302	Q303	L304	A305	F306	S307	D308	R309	K310	C311	L312	A313	S314	G315	Q316	I317	M318	Y319	E320	L321	L322	E323	Y324	C325	E326	E327	R328	Y329	S330	L331	D332	L333	S334	G335	S336	T337	S338	S339	L340	R341	G342	Q343	S344	N345	N346	T347	K348	L349	L350	G351	C352	Q353	T354	I355	E356	K357	ARG	VAL	
HIS	GLY	ARG	GLU	ASP	GLY	VAL	HIS	GLU	THR	SER	P374	D375	T376	S377	V378	S379	V380	F381	S382	W383	Q384	N386	T387	D388	G389	Q390	G391	K392	P393	S394	V395	Y396	L397	G398	V399	F400	D401	I402	N403	R404	W405	Y406	Q407	A408	Q409	M410	P411	D412	S413	R415	S416	G417	F419	L420					
R421	N422	C423	S424	A425	F426	A427	F428	A429	W430	L431	E432	A433	V434	V435	N436	I437	T438	T439	Q440	D441	L442	I443	F444	D445	T446	L447	V448	H449	E450	R451	SER	LEU	SER	ARG	Y396	GLY	ILE	PRO	SER	TVR	PRO	PRO	PHE	GLN	ASP	THR	TTR	P470	S471	T472	Y473	N474	F475	D476	A477	C479	L480		
L481	N482	S483	G484	L485	L486	H487	F488	A489	C490	T491	G492	F493	GLN	LYS	GLU	THR	LEU	HIS	PHE	LEU	LYS	SER	GLY	SER	LEU	ASN	GLU	ILE	PRO	ASP	GLY	TTR	ASN	ARG	CYS	LEU	ALA	ALA	GLY	LEU	LEU	PRO	LYS	PHE	THR	ASP	VAL	GLN	ALA	SER	SER	LEU	SER	Q539	E540				
E541	Q542	L543	Q544	A545	I546	L547	A548	A549	A550	V551	E552	T553	S554	S555	L556	G557	L558	L559	T560	S561	C562	L563	K564	R565	V566	T567	A568	E569	E570	Q571	P572	R573	S574	A575	A576	N577	L578	R579	F580	V581	L582	E583	W584	T585	W586	K587	K588	V589	T590	L591	T592	K593	Q594	E595	F596	D597	R598	L599	C600
F601	R602	L603	F604	D605	G606	S607	C608	N609	F610	I611	D612	P613	H614	T615	L616	D617	S618	L619	Q620	C621	C622	H623	L624	Y625	F626	S627	N628	L629	T630	A631	V632	L633	N634	C635	F636	I637	A638	Q639	K641	E642	V643	T644	Q645	D646	G647	A648	V649	D650	L651	T652	N653	K654	Q655	S656	V657	T658	R659	L660	
L661	T662	L663	Y664	A665	S666	V667	V668	C672	R673	S674	G675	M676	L677	P678	D679	S680	S681	D682	E683	T684	V685	Q686	L687	T688	R689	F690	F691	Y692	N693	Y694	Q695	V696	L697	Q698	Q699	Y700	Y701	S702	D703	R704	K705	K706	K707	L708	E709	R710	L711	A712	R713	G714	K715	W716	D717	T718	S719	L720	L721	W722	
I723	D724	G725	L726	I727	W728	Q729	F730	G731	D732	R733	I734	Q735	Q736	L737	W738	S739	R740	D741	D742	W743	G744	T745	G746	K747	Y748	F749	P750	A751	W752	L753	H754	A755	L756	L757	D758	V759	Y760	L761	L762	E763	H764	A765	D766	E767	W768	S769	A772	I773	T774	I775	Y776	F777	L778	L779	D780	I781	W782	Y783	
S784	F785	P786	D787	K788	P789	D790	S791	S792	I793	E794	A799	I807	I810	Q811	W814	L815	L816	D817	H818	N819	D820	Y821	Q822	N823	S824	W825	D826	C827	L828	A829	A832	SER	SER	ARG	VAL	M837	S838	W839	S842	Q843	G844	I844	N847	L848	C850	H851	Q852	D853	S854	R855	Q862								
K872	K875	L876	H877	M878	T879	V880	A883	N884	R885	S886	I887	A890	L893	Q894	H897	SER	SER	ARG	LEU	N902	M910	Y911	E916	M917	G918	L919	I920	E921	E922	Q933	L936	H937	L940	Q941	T942	T943	G944	V945	Q946	N947	Q948	E949	L950	L951	L952	W953	L956												



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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	813020	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.018	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	554.8, 554.8, 554.8	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.774, 2.774, 2.774	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	J	0.99	2/5054 (0.0%)	1.70	46/7040 (0.7%)
1	P	0.99	2/5054 (0.0%)	1.70	46/7040 (0.7%)
1	j	1.01	5/4928 (0.1%)	1.71	50/6865 (0.7%)
1	p	1.02	5/4928 (0.1%)	1.70	46/6865 (0.7%)
2	B	1.18	15/3114 (0.5%)	1.57	23/4342 (0.5%)
2	b	1.01	7/3155 (0.2%)	1.33	17/4401 (0.4%)
3	C	0.61	0/1692	1.12	0/2353
3	c	0.79	2/1707 (0.1%)	1.37	8/2374 (0.3%)
4	F	0.57	0/1565	1.08	2/2175 (0.1%)
4	f	0.76	2/1580 (0.1%)	1.21	8/2196 (0.4%)
5	D	0.89	1/1567 (0.1%)	1.11	3/2176 (0.1%)
5	d	0.89	1/1579 (0.1%)	1.10	3/2196 (0.1%)
6	E	1.11	34/6755 (0.5%)	1.57	91/9417 (1.0%)
6	e	1.70	27/6487 (0.4%)	1.66	48/9037 (0.5%)
7	K	1.98	38/1640 (2.3%)	1.89	34/2287 (1.5%)
8	H	0.70	0/1504	1.08	0/2089
8	h	0.72	1/1509 (0.1%)	1.08	2/2096 (0.1%)
9	G	1.18	11/3060 (0.4%)	1.69	43/4264 (1.0%)
9	g	1.36	22/3326 (0.7%)	1.83	58/4633 (1.3%)
10	I	0.88	8/3955 (0.2%)	1.38	19/5521 (0.3%)
10	M	0.91	4/3955 (0.1%)	1.46	20/5521 (0.4%)
10	i	0.90	4/3955 (0.1%)	1.45	19/5521 (0.3%)
11	L	0.66	0/3177	1.24	0/4430
11	O	1.18	0/249	1.64	0/347
12	A	1.57	152/8883 (1.7%)	1.75	224/12368 (1.8%)
13	N	0.68	0/4575	1.21	3/6366 (0.0%)
13	n	0.68	0/4495	1.21	3/6253 (0.0%)
All	All	1.11	343/93448 (0.4%)	1.53	816/130173 (0.6%)

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
2	B	0	3
2	b	0	1
3	c	0	2
5	D	0	2
5	d	0	2
6	E	0	10
6	e	0	8
7	K	0	3
9	G	0	14
9	g	0	14
10	I	0	4
10	M	0	8
10	i	0	6
12	A	0	41
13	N	0	1
13	n	0	2
All	All	0	121

All (343) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	e	548	PRO	N-CA	19.58	1.70	1.47
12	A	1194	PRO	N-CA	19.33	1.69	1.47
9	g	577	TYR	C-N	18.91	1.60	1.33
4	f	273	PRO	N-CA	18.22	1.70	1.47
12	A	1722	GLY	C-N	17.85	1.50	1.33
7	K	1192	PRO	N-CA	17.59	1.69	1.47
6	e	1049	PRO	N-CA	17.39	1.69	1.47
12	A	904	ASN	C-N	17.24	1.58	1.33
10	i	673	PRO	N-CA	17.13	1.69	1.47
10	M	673	PRO	N-CA	17.10	1.69	1.47
2	b	315	PRO	N-CA	16.87	1.69	1.47
6	E	1020	PRO	N-CA	16.64	1.69	1.47
6	e	1174	GLU	C-O	15.66	1.43	1.24
5	D	218	VAL	C-N	15.37	1.55	1.33
5	d	218	VAL	C-N	15.31	1.55	1.33
12	A	285	GLU	C-N	14.45	1.53	1.33
9	g	219	THR	CA-C	-13.73	1.46	1.53
2	B	492	LYS	C-N	13.23	1.51	1.33
2	B	570	SER	C-O	12.92	1.41	1.24
9	g	739	ARG	C-N	12.65	1.51	1.33
12	A	1730	LEU	C-N	12.27	1.51	1.33
12	A	1685	PRO	C-N	11.42	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	396	PHE	C-N	11.02	1.47	1.34
12	A	1385	ALA	C-N	10.98	1.49	1.33
9	g	873	PRO	N-CA	10.97	1.69	1.46
12	A	287	GLY	C-N	10.97	1.49	1.33
12	A	552	TRP	C-N	10.92	1.48	1.33
7	K	1227	SER	C-O	10.91	1.36	1.24
6	E	1130	ILE	N-CA	10.89	1.59	1.46
2	B	585	GLN	N-CA	10.68	1.59	1.46
12	A	286	GLN	C-N	10.52	1.48	1.33
3	c	168	ASP	C-N	10.38	1.48	1.33
9	g	872	GLN	C-N	10.35	1.45	1.33
12	A	551	SER	C-N	10.31	1.47	1.34
6	e	1196	PRO	CA-C	10.31	1.66	1.52
6	e	547	ARG	C-N	10.28	1.45	1.33
12	A	1353	LYS	C-N	10.28	1.54	1.33
2	B	585	GLN	CA-C	10.16	1.66	1.52
12	A	1220	ARG	C-N	10.03	1.47	1.33
6	E	1266	ASN	CA-C	-9.77	1.40	1.52
12	A	1546	LEU	C-N	9.77	1.46	1.33
1	j	909	LEU	C-N	9.72	1.46	1.33
1	p	909	LEU	C-N	9.71	1.46	1.33
12	A	1420	LEU	C-N	9.70	1.46	1.33
12	A	304	ARG	C-N	-9.67	1.20	1.34
9	g	247	MET	N-CA	-9.66	1.33	1.46
9	G	682	PRO	C-N	9.55	1.49	1.33
12	A	1193	ILE	C-N	9.53	1.45	1.33
12	A	1659	LEU	C-N	9.53	1.47	1.33
9	g	682	PRO	C-N	9.52	1.49	1.33
12	A	29	ILE	C-N	9.50	1.48	1.33
2	b	570	SER	C-O	9.22	1.35	1.24
12	A	668	GLN	C-N	9.11	1.45	1.33
6	E	1019	ILE	C-N	8.99	1.45	1.34
12	A	787	LEU	C-N	8.91	1.46	1.33
6	e	1174	GLU	CA-C	8.74	1.64	1.52
2	B	570	SER	N-CA	8.68	1.57	1.46
12	A	1186	SER	C-N	8.63	1.43	1.33
9	G	856	MET	C-O	-8.63	1.14	1.24
12	A	1717	LEU	C-N	8.62	1.45	1.34
12	A	27	ALA	C-N	8.59	1.45	1.33
6	E	1287	MET	CA-C	-8.55	1.41	1.52
12	A	1562	VAL	C-N	8.53	1.46	1.33
12	A	460	TYR	C-N	8.49	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1355	PRO	C-N	8.46	1.45	1.33
2	b	314	HIS	C-N	8.30	1.45	1.33
12	A	1828	TYR	C-N	-8.30	1.23	1.33
6	e	1196	PRO	C-O	8.23	1.34	1.24
12	A	1495	ALA	C-N	8.17	1.45	1.33
12	A	1732	LEU	C-N	-8.17	1.21	1.33
12	A	1502	ILE	C-N	8.12	1.42	1.34
12	A	905	SER	C-N	8.09	1.44	1.33
12	A	50	PHE	C-N	8.08	1.44	1.33
12	A	23	THR	C-N	8.07	1.44	1.33
12	A	609	GLU	C-N	7.92	1.44	1.33
12	A	1431	ALA	C-N	7.91	1.44	1.33
12	A	864	LEU	C-N	7.91	1.44	1.34
12	A	613	LEU	C-N	7.81	1.44	1.33
12	A	547	GLY	C-N	7.76	1.49	1.33
12	A	701	THR	C-N	-7.75	1.23	1.33
12	A	1624	GLN	CA-C	-7.73	1.42	1.52
12	A	706	GLN	C-N	-7.70	1.24	1.33
6	e	1174	GLU	CA-CB	7.70	1.66	1.53
10	I	285	LYS	N-CA	7.67	1.56	1.45
12	A	1221	GLY	C-N	7.58	1.44	1.33
12	A	567	ARG	C-N	7.54	1.44	1.34
12	A	1527	SER	C-N	7.48	1.44	1.34
12	A	853	THR	C-O	-7.46	1.15	1.24
12	A	1219	ARG	C-N	-7.43	1.22	1.33
6	e	485	GLY	CA-C	7.41	1.58	1.52
9	g	322	LEU	CA-C	7.40	1.63	1.52
2	b	581	PRO	C-O	7.39	1.33	1.24
9	g	235	GLY	C-O	7.39	1.33	1.23
9	G	235	GLY	C-O	7.37	1.32	1.23
9	G	322	LEU	CA-C	7.36	1.63	1.52
12	A	869	LEU	C-N	7.27	1.43	1.33
6	E	1213	LEU	C-O	7.23	1.32	1.24
6	E	1314	VAL	CA-C	-7.21	1.45	1.52
12	A	1425	LEU	C-N	7.20	1.43	1.33
12	A	30	LYS	C-N	-7.18	1.23	1.33
6	E	1267	GLN	N-CA	-7.16	1.36	1.46
2	B	577	LEU	C-O	7.13	1.32	1.24
2	B	570	SER	CA-C	7.11	1.62	1.52
12	A	429	PRO	C-N	7.11	1.43	1.33
6	E	1178	LEU	N-CA	7.09	1.54	1.46
12	A	710	THR	C-N	-7.02	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1682	ALA	C-N	7.02	1.42	1.33
12	A	857	GLU	CA-C	-7.01	1.44	1.52
12	A	1710	PHE	C-N	7.01	1.42	1.33
12	A	438	HIS	C-N	7.00	1.43	1.33
7	K	1123	LYS	C-O	-6.97	1.16	1.24
7	K	1316	LYS	CA-C	6.95	1.61	1.52
2	B	574	THR	C-O	6.92	1.32	1.24
12	A	485	PRO	C-N	6.92	1.43	1.33
7	K	1110	GLN	CA-C	-6.88	1.43	1.52
7	K	1203	ILE	CA-CB	6.88	1.62	1.54
12	A	77	ILE	C-N	6.86	1.43	1.33
7	K	1226	LEU	C-O	-6.83	1.16	1.24
12	A	502	LEU	C-N	6.82	1.42	1.33
12	A	226	GLN	C-N	6.81	1.42	1.33
12	A	556	PHE	C-N	6.79	1.43	1.33
1	P	1077	ILE	CA-CB	-6.79	1.46	1.54
2	B	394	ALA	C-N	6.78	1.43	1.33
1	J	1077	ILE	CA-CB	-6.77	1.46	1.54
6	E	1333	LEU	CA-C	-6.77	1.43	1.52
12	A	1520	TYR	C-N	6.76	1.42	1.33
6	e	1316	LEU	C-N	6.74	1.49	1.33
12	A	636	PRO	C-N	6.73	1.49	1.33
6	E	1300	LEU	CA-C	-6.72	1.44	1.53
12	A	776	GLN	C-N	6.67	1.49	1.33
7	K	1151	GLN	CA-C	-6.67	1.43	1.52
3	c	129	ALA	C-N	6.67	1.49	1.33
9	g	239	LEU	CA-C	6.66	1.61	1.52
12	A	691	ILE	C-N	6.66	1.43	1.33
9	g	795	TRP	CA-C	-6.65	1.43	1.52
12	A	581	PRO	C-N	6.64	1.49	1.33
6	E	1198	THR	C-O	-6.63	1.15	1.24
12	A	149	LEU	C-N	6.63	1.41	1.33
6	e	1198	THR	C-O	-6.62	1.15	1.24
9	G	239	LEU	CA-C	6.60	1.61	1.52
6	e	1200	ALA	C-O	6.59	1.31	1.24
1	j	1077	ILE	CA-CB	-6.56	1.47	1.54
6	E	1137	ILE	N-CA	6.56	1.54	1.46
6	E	1200	ALA	C-O	6.53	1.31	1.24
12	A	871	MET	C-N	6.52	1.42	1.33
12	A	499	SER	C-N	6.45	1.42	1.33
1	p	1077	ILE	CA-CB	-6.44	1.47	1.54
9	g	321	TYR	C-O	-6.42	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	g	847	ALA	CA-C	-6.42	1.44	1.52
12	A	221	ILE	C-N	6.40	1.42	1.33
12	A	1458	PHE	C-N	6.38	1.42	1.33
7	K	1182	ILE	N-CA	6.37	1.53	1.46
6	E	1274	THR	N-CA	6.33	1.54	1.46
7	K	1145	LEU	C-O	-6.32	1.16	1.24
12	A	789	GLY	C-N	6.32	1.42	1.33
9	G	321	TYR	C-O	-6.32	1.16	1.24
12	A	394	THR	C-N	6.32	1.42	1.34
9	g	549	ILE	C-O	-6.31	1.17	1.24
12	A	1225	CYS	C-O	6.30	1.32	1.24
12	A	1652	SER	C-N	6.30	1.41	1.33
6	E	1076	TYR	C-O	6.29	1.32	1.24
8	h	5	ILE	C-N	6.29	1.42	1.33
6	E	1331	GLU	CA-C	-6.28	1.44	1.52
2	B	581	PRO	C-O	6.24	1.31	1.24
9	G	549	ILE	C-O	-6.24	1.17	1.24
6	e	363	THR	CA-C	6.24	1.58	1.52
12	A	1552	TYR	C-N	-6.23	1.25	1.33
12	A	619	ALA	C-N	6.23	1.43	1.33
6	e	147	THR	N-CA	6.22	1.50	1.45
7	K	1155	GLN	CA-C	-6.21	1.44	1.52
6	E	1179	GLU	CA-C	-6.21	1.45	1.52
12	A	764	ASP	C-N	-6.21	1.26	1.33
9	G	753	ASN	C-N	6.20	1.48	1.33
2	B	580	LEU	C-N	6.20	1.41	1.33
12	A	1096	PRO	C-N	6.19	1.42	1.33
12	A	82	ARG	C-N	6.18	1.42	1.33
7	K	1144	LYS	C-O	-6.18	1.16	1.24
12	A	1324	ASP	C-N	6.17	1.42	1.33
12	A	145	SER	C-N	6.16	1.41	1.33
1	j	909	LEU	N-CA	-6.16	1.38	1.46
12	A	744	TYR	CA-C	-6.15	1.44	1.52
6	E	1270	THR	CA-C	-6.14	1.45	1.52
12	A	1721	PHE	C-N	6.13	1.42	1.33
12	A	500	ASP	C-N	6.12	1.42	1.33
12	A	490	LEU	C-N	-6.11	1.25	1.33
12	A	47	LYS	C-N	6.10	1.41	1.33
12	A	868	HIS	C-N	6.10	1.41	1.33
1	p	909	LEU	N-CA	-6.10	1.38	1.46
2	b	570	SER	N-CA	6.09	1.54	1.46
12	A	214	ARG	C-N	-6.09	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	g	458	GLN	CA-C	-6.09	1.45	1.52
6	E	1175	LEU	CA-C	-6.08	1.44	1.52
12	A	1711	GLN	C-N	-6.08	1.25	1.33
12	A	1656	GLN	C-N	6.08	1.41	1.33
12	A	1479	VAL	C-N	6.07	1.41	1.33
9	g	807	ARG	C-O	-6.06	1.17	1.24
12	A	589	ARG	C-N	6.05	1.42	1.33
12	A	692	GLU	C-N	6.03	1.42	1.34
12	A	20	ILE	C-N	-6.02	1.26	1.33
12	A	1590	ARG	C-N	6.00	1.44	1.34
10	I	285	LYS	CA-C	6.00	1.61	1.53
12	A	306	TYR	C-N	6.00	1.41	1.33
12	A	1651	HIS	C-N	5.98	1.41	1.33
7	K	1155	GLN	C-O	-5.98	1.16	1.24
7	K	1154	ILE	CA-CB	-5.97	1.47	1.54
9	g	848	LYS	N-CA	-5.96	1.38	1.46
9	g	795	TRP	C-O	-5.96	1.16	1.24
12	A	178	MET	C-N	5.94	1.42	1.33
10	i	289	TRP	CA-C	5.94	1.60	1.52
12	A	78	LYS	C-N	5.94	1.42	1.33
12	A	590	GLU	C-N	-5.93	1.26	1.33
12	A	797	PRO	C-O	5.93	1.31	1.24
12	A	392	LEU	C-N	5.92	1.41	1.33
10	I	289	TRP	N-CA	5.91	1.53	1.46
12	A	1228	LYS	C-O	5.89	1.31	1.24
12	A	37	HIS	C-N	-5.89	1.25	1.34
10	M	289	TRP	CA-C	5.89	1.60	1.52
12	A	34	GLU	C-N	-5.84	1.25	1.33
6	E	1286	LEU	C-O	-5.81	1.16	1.24
12	A	561	LEU	C-N	5.81	1.41	1.33
12	A	754	GLU	C-N	-5.77	1.26	1.33
12	A	788	GLN	C-N	5.76	1.42	1.33
6	e	1107	VAL	N-CA	5.76	1.53	1.46
7	K	1147	VAL	CA-C	-5.74	1.45	1.52
6	E	1330	ALA	CA-C	-5.72	1.45	1.52
6	E	1079	LEU	CA-C	-5.71	1.45	1.52
12	A	1568	GLY	C-N	5.71	1.41	1.33
12	A	616	CYS	C-N	5.71	1.42	1.33
12	A	799	GLY	C-O	-5.69	1.17	1.24
7	K	1107	SER	N-CA	-5.68	1.38	1.46
12	A	1025	CYS	C-N	5.68	1.41	1.33
7	K	1224	LYS	C-O	5.66	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	e	1076	TYR	C-O	5.65	1.30	1.24
12	A	1430	ILE	C-N	5.65	1.41	1.33
9	G	239	LEU	N-CA	5.65	1.53	1.46
12	A	1733	GLN	C-N	5.64	1.42	1.33
7	K	1134	ASP	CA-C	5.64	1.60	1.52
12	A	1483	ASP	C-N	5.64	1.41	1.34
9	G	322	LEU	CA-CB	5.63	1.62	1.53
9	G	736	ASP	CA-C	5.63	1.55	1.52
9	g	322	LEU	CA-CB	5.62	1.62	1.53
12	A	896	ILE	CA-C	-5.62	1.45	1.52
12	A	1819	LYS	C-N	-5.61	1.26	1.33
7	K	1138	LEU	CA-C	5.60	1.60	1.52
7	K	1200	LEU	C-O	-5.60	1.17	1.24
12	A	1675	LEU	C-N	5.59	1.41	1.34
12	A	18	ARG	C-N	-5.59	1.26	1.33
9	g	239	LEU	N-CA	5.59	1.53	1.46
12	A	1821	SER	C-N	5.58	1.41	1.33
2	B	578	ASP	C-O	5.58	1.30	1.24
6	E	1320	LEU	CA-C	-5.57	1.45	1.52
12	A	523	CYS	CA-C	-5.57	1.45	1.52
12	A	1289	GLU	CA-C	-5.56	1.46	1.52
6	E	1268	LEU	N-CA	-5.55	1.39	1.46
12	A	1576	GLY	C-N	5.55	1.41	1.33
9	g	847	ALA	N-CA	-5.54	1.39	1.46
12	A	281	VAL	C-N	5.53	1.40	1.33
12	A	670	LEU	C-N	-5.52	1.25	1.33
7	K	1181	ASP	CA-C	5.52	1.60	1.52
12	A	708	ILE	C-N	-5.51	1.27	1.33
6	E	1062	GLU	CA-C	-5.50	1.45	1.52
7	K	1112	LEU	N-CA	5.48	1.53	1.46
12	A	393	VAL	C-N	5.48	1.41	1.33
7	K	1316	LYS	N-CA	5.48	1.53	1.46
12	A	1182	ARG	C-N	5.46	1.40	1.33
12	A	496	ARG	C-N	5.45	1.41	1.34
6	e	1196	PRO	N-CA	5.43	1.54	1.47
10	M	288	TYR	CA-CB	5.43	1.62	1.53
6	E	1321	ILE	N-CA	-5.42	1.40	1.46
10	i	288	TYR	CA-CB	5.42	1.62	1.53
12	A	897	ALA	CA-C	-5.41	1.45	1.52
6	e	207	ILE	CA-C	5.41	1.58	1.52
6	E	1304	CYS	C-O	5.39	1.30	1.24
7	K	1115	ILE	CA-CB	5.39	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	219	ASP	C-N	5.38	1.41	1.33
1	j	909	LEU	C-O	-5.38	1.17	1.24
1	P	119	ILE	CA-C	-5.38	1.46	1.52
10	I	163	PHE	C-O	-5.38	1.17	1.23
7	K	1111	ARG	C-O	-5.36	1.17	1.24
1	p	119	ILE	CA-C	-5.34	1.46	1.52
12	A	1000	ALA	C-N	5.33	1.41	1.33
1	p	909	LEU	C-O	-5.32	1.17	1.24
12	A	1419	HIS	C-N	-5.32	1.26	1.33
12	A	743	ARG	CA-C	-5.31	1.46	1.52
12	A	1222	GLN	C-N	-5.31	1.26	1.33
12	A	1526	ASP	C-N	-5.31	1.26	1.33
1	j	119	ILE	CA-C	-5.30	1.46	1.52
7	K	1196	SER	CA-CB	5.29	1.61	1.53
12	A	734	GLN	CA-C	-5.28	1.46	1.52
7	K	1173	SER	N-CA	5.28	1.52	1.46
12	A	107	ALA	C-N	5.27	1.40	1.33
7	K	1135	GLY	N-CA	5.26	1.52	1.45
10	I	241	GLU	C-O	-5.26	1.18	1.24
12	A	198	GLU	C-O	5.25	1.30	1.24
12	A	498	MET	C-N	5.25	1.41	1.33
7	K	1188	GLN	CA-CB	5.24	1.61	1.53
12	A	1128	ARG	N-CA	5.24	1.52	1.46
7	K	1139	HIS	N-CA	5.24	1.52	1.46
12	A	1816	HIS	C-N	-5.24	1.27	1.33
1	J	119	ILE	CA-C	-5.23	1.46	1.52
10	i	288	TYR	CA-C	5.23	1.59	1.52
7	K	1137	PHE	CA-CB	5.21	1.61	1.53
12	A	1290	ILE	CA-C	-5.21	1.46	1.52
7	K	1129	SER	CA-CB	5.21	1.61	1.53
12	A	223	GLU	C-N	-5.20	1.27	1.33
12	A	1060	CYS	C-N	5.20	1.41	1.34
6	E	1173	LEU	N-CA	-5.18	1.39	1.46
10	M	288	TYR	CA-C	5.18	1.59	1.52
7	K	1196	SER	C-O	-5.17	1.18	1.24
2	B	585	GLN	C-N	5.17	1.40	1.33
6	E	1184	LEU	CA-C	-5.17	1.46	1.52
10	I	288	TYR	CA-C	5.16	1.60	1.52
6	e	640	ARG	N-CA	5.15	1.52	1.46
2	B	509	CYS	N-CA	5.15	1.52	1.46
6	E	1103	LEU	CA-C	-5.15	1.45	1.52
6	e	730	ARG	N-CA	5.14	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1982	GLU	C-N	5.12	1.41	1.33
7	K	1141	LEU	C-O	-5.12	1.17	1.24
6	e	486	SER	N-CA	5.12	1.52	1.46
6	e	618	ASP	CA-C	5.11	1.59	1.52
6	e	466	ALA	CA-C	5.11	1.58	1.53
6	e	1099	TYR	C-O	-5.10	1.18	1.24
2	b	148	GLU	CA-C	-5.10	1.46	1.52
12	A	43	LEU	C-N	5.10	1.41	1.33
4	f	272	TYR	C-N	5.09	1.45	1.33
7	K	1111	ARG	N-CA	-5.09	1.39	1.46
6	E	1180	LYS	N-CA	-5.09	1.40	1.46
6	E	1316	LEU	N-CA	5.08	1.51	1.45
12	A	1813	VAL	C-N	5.05	1.40	1.33
10	I	286	SER	N-CA	5.05	1.52	1.45
7	K	1227	SER	N-CA	5.04	1.52	1.46
12	A	146	LEU	C-N	-5.04	1.27	1.33
2	B	148	GLU	CA-C	-5.04	1.46	1.52
7	K	1191	ASP	C-N	5.04	1.45	1.33
12	A	1418	ALA	C-N	5.04	1.40	1.33
9	g	848	LYS	CA-C	-5.03	1.45	1.52
6	e	139	PRO	N-CA	-5.03	1.41	1.47
10	I	556	LYS	N-CA	5.03	1.52	1.46
6	E	1139	GLN	N-CA	5.01	1.50	1.45
6	e	1048	PHE	C-N	5.01	1.45	1.33
2	b	39	TYR	CA-C	5.01	1.59	1.52
6	e	708	ILE	N-CA	5.01	1.52	1.46
7	K	1159	THR	CA-C	-5.01	1.46	1.52

All (816) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	394	ALA	O-C-N	-32.08	86.68	123.25
9	g	577	TYR	O-C-N	-24.14	90.49	122.59
9	G	753	ASN	CA-C-N	24.04	149.89	119.84
9	G	753	ASN	C-N-CA	24.04	149.89	119.84
9	g	739	ARG	CA-C-N	-22.83	77.93	121.54
9	g	739	ARG	C-N-CA	-22.83	77.93	121.54
6	E	1019	ILE	CA-C-N	21.62	141.45	118.97
6	E	1019	ILE	C-N-CA	21.62	141.45	118.97
2	B	492	LYS	CA-C-N	-21.27	87.72	122.17
2	B	492	LYS	C-N-CA	-21.27	87.72	122.17
12	A	1193	ILE	CA-C-N	21.27	141.59	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1193	ILE	C-N-CA	21.27	141.59	119.90
9	g	872	GLN	CA-C-N	21.00	142.01	120.38
9	g	872	GLN	C-N-CA	21.00	142.01	120.38
12	A	581	PRO	CA-C-N	20.84	145.90	119.84
12	A	581	PRO	C-N-CA	20.84	145.90	119.84
3	c	129	ALA	CA-C-N	20.68	145.69	119.84
3	c	129	ALA	C-N-CA	20.68	145.69	119.84
12	A	776	GLN	CA-C-N	20.63	145.62	119.84
12	A	776	GLN	C-N-CA	20.63	145.62	119.84
6	e	1316	LEU	CA-C-N	20.39	145.33	119.84
6	e	1316	LEU	C-N-CA	20.39	145.33	119.84
9	g	219	THR	N-CA-C	-20.26	92.17	108.78
12	A	636	PRO	CA-C-N	20.14	145.02	119.84
12	A	636	PRO	C-N-CA	20.14	145.02	119.84
6	e	547	ARG	CA-C-N	19.97	141.30	119.93
6	e	547	ARG	C-N-CA	19.97	141.30	119.93
12	A	805	HIS	O-C-N	-19.80	99.06	122.22
2	B	492	LYS	O-C-N	19.79	156.44	122.21
6	E	1179	GLU	N-CA-C	-19.56	90.02	111.14
12	A	1354	GLN	O-C-N	-19.08	99.38	121.32
2	b	314	HIS	CA-C-N	18.47	140.90	119.47
2	b	314	HIS	C-N-CA	18.47	140.90	119.47
6	e	1048	PHE	CA-C-N	17.70	141.96	119.84
6	e	1048	PHE	C-N-CA	17.70	141.96	119.84
12	A	1053	THR	CA-C-N	17.51	137.02	120.21
12	A	1053	THR	C-N-CA	17.51	137.02	120.21
10	M	391	GLY	CA-C-N	-17.40	98.78	121.74
10	M	391	GLY	C-N-CA	-17.40	98.78	121.74
10	i	391	GLY	CA-C-N	-17.39	98.79	121.74
10	i	391	GLY	C-N-CA	-17.39	98.79	121.74
7	K	1191	ASP	CA-C-N	17.32	141.49	119.84
7	K	1191	ASP	C-N-CA	17.32	141.49	119.84
9	G	682	PRO	O-C-N	-17.24	97.72	122.37
9	g	682	PRO	O-C-N	-17.22	97.74	122.37
6	E	1136	TRP	N-CA-C	16.97	135.05	108.07
10	M	672	ASP	CA-C-N	16.47	140.43	119.84
10	M	672	ASP	C-N-CA	16.47	140.43	119.84
10	i	672	ASP	CA-C-N	16.46	140.42	119.84
10	i	672	ASP	C-N-CA	16.46	140.42	119.84
12	A	1385	ALA	O-C-N	-16.38	102.75	122.25
12	A	1355	PRO	CA-C-N	16.36	151.15	121.70
12	A	1355	PRO	C-N-CA	16.36	151.15	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1268	LEU	N-CA-C	-15.54	77.70	110.80
1	p	1007	MET	CA-C-N	14.60	134.49	120.03
1	p	1007	MET	C-N-CA	14.60	134.49	120.03
1	j	1007	MET	CA-C-N	14.59	134.47	120.03
1	j	1007	MET	C-N-CA	14.59	134.47	120.03
2	B	394	ALA	CA-C-N	14.39	150.37	123.32
2	B	394	ALA	C-N-CA	14.39	150.37	123.32
12	A	1175	LYS	O-C-N	-14.20	100.29	123.00
4	f	272	TYR	CA-C-N	14.19	137.58	119.84
4	f	272	TYR	C-N-CA	14.19	137.58	119.84
7	K	1341	TYR	CA-C-N	13.53	142.79	122.08
7	K	1341	TYR	C-N-CA	13.53	142.79	122.08
2	B	580	LEU	CA-C-N	-13.36	104.58	119.28
2	B	580	LEU	C-N-CA	-13.36	104.58	119.28
12	A	904	ASN	O-C-N	12.94	139.05	122.23
12	A	800	PHE	N-CA-C	-12.86	97.31	111.07
6	E	1300	LEU	N-CA-C	-12.62	81.92	107.41
10	i	287	VAL	N-CA-C	12.46	122.90	107.70
10	M	287	VAL	N-CA-C	12.42	122.85	107.70
10	i	254	LEU	N-CA-C	-12.30	96.39	111.40
3	c	187	ASN	O-C-N	-12.12	108.51	123.17
6	e	1195	ASN	O-C-N	-11.97	110.74	121.39
12	A	1355	PRO	O-C-N	-11.88	106.61	122.64
12	A	286	GLN	O-C-N	-11.70	107.22	122.43
10	I	285	LYS	N-CA-C	11.66	126.73	109.95
12	A	56	ASN	N-CA-C	11.61	118.67	108.22
3	c	168	ASP	O-C-N	-10.93	110.48	123.27
6	E	1332	LEU	N-CA-C	-10.91	87.56	110.80
9	g	247	MET	N-CA-CB	-10.73	92.35	110.49
2	B	569	CYS	O-C-N	-10.42	108.74	122.59
12	A	1354	GLN	CA-C-N	10.17	132.55	119.84
12	A	1354	GLN	C-N-CA	10.17	132.55	119.84
12	A	1384	SER	O-C-N	-10.16	106.75	123.00
12	A	805	HIS	CA-C-N	10.07	137.81	120.68
12	A	805	HIS	C-N-CA	10.07	137.81	120.68
6	E	1234	LEU	N-CA-C	10.03	126.39	108.24
7	K	1110	GLN	N-CA-C	-9.94	100.29	111.82
6	E	1275	LYS	N-CA-C	9.90	125.44	113.16
10	M	292	THR	N-CA-C	-9.87	99.12	111.75
10	I	292	THR	N-CA-C	-9.85	99.14	111.75
10	i	292	THR	N-CA-C	-9.83	99.17	111.75
6	e	1174	GLU	N-CA-C	-9.73	90.07	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	729	PHE	N-CA-C	-9.73	101.62	112.72
9	g	682	PRO	CA-C-N	9.63	138.52	121.76
9	g	682	PRO	C-N-CA	9.63	138.52	121.76
9	G	682	PRO	CA-C-N	9.63	138.51	121.76
9	G	682	PRO	C-N-CA	9.63	138.51	121.76
1	J	897	LYS	CA-C-N	9.57	133.88	120.29
1	J	897	LYS	C-N-CA	9.57	133.88	120.29
1	P	897	LYS	CA-C-N	9.51	133.79	120.29
1	P	897	LYS	C-N-CA	9.51	133.79	120.29
12	A	1103	GLU	N-CA-C	-9.47	99.62	111.75
9	G	855	GLU	N-CA-C	-9.45	100.95	111.07
6	e	752	GLN	N-CA-C	-9.43	101.08	111.36
9	G	608	TYR	N-CA-C	-9.38	99.14	111.24
6	E	1112	GLY	N-CA-C	-9.35	101.32	112.64
9	g	608	TYR	N-CA-C	-9.35	99.18	111.24
9	G	623	SER	N-CA-C	-9.32	99.21	111.24
9	g	623	SER	N-CA-C	-9.28	99.28	111.24
6	E	1129	LEU	N-CA-C	9.24	121.04	110.97
3	c	187	ASN	CA-C-N	9.22	139.15	121.54
3	c	187	ASN	C-N-CA	9.22	139.15	121.54
6	E	1316	LEU	N-CA-C	9.21	120.90	109.57
6	e	1183	VAL	N-CA-C	-9.15	101.63	110.42
1	J	611	SER	CB-CA-C	-9.12	98.46	111.14
1	P	611	SER	CB-CA-C	-9.05	98.56	111.14
12	A	288	THR	O-C-N	-9.01	112.77	123.13
6	E	1172	ILE	N-CA-C	9.01	128.08	109.34
6	e	1196	PRO	N-CA-C	9.01	125.47	113.40
6	e	1174	GLU	O-C-N	-9.01	110.61	122.59
9	G	560	PHE	N-CA-C	-8.91	101.23	112.90
1	j	611	SER	CB-CA-C	-8.91	98.75	111.14
9	g	560	PHE	N-CA-C	-8.91	101.23	112.90
1	p	611	SER	CB-CA-C	-8.88	98.80	111.14
12	A	77	ILE	O-C-N	-8.85	112.14	122.94
12	A	1990	SER	N-CA-C	-8.80	103.38	114.56
6	E	1076	TYR	CA-C-N	-8.78	108.69	120.54
6	E	1076	TYR	C-N-CA	-8.78	108.69	120.54
12	A	80	THR	O-C-N	-8.76	113.02	123.27
12	A	1723	GLY	O-C-N	-8.71	116.01	123.59
2	B	570	SER	CA-C-O	8.69	129.76	119.60
12	A	1302	THR	N-CA-C	-8.67	101.80	112.38
9	G	512	THR	CA-C-N	8.66	130.67	119.84
9	G	512	THR	C-N-CA	8.66	130.67	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	g	512	THR	CA-C-N	8.63	130.63	119.84
9	g	512	THR	C-N-CA	8.63	130.63	119.84
7	K	1144	LYS	N-CA-C	-8.54	101.47	112.23
12	A	1812	GLY	N-CA-C	-8.50	102.11	113.24
12	A	267	VAL	N-CA-C	8.48	118.50	110.53
7	K	1119	ILE	N-CA-C	-8.44	102.32	110.42
9	g	478	MET	N-CA-C	-8.42	102.10	111.28
9	G	321	TYR	N-CA-CB	8.41	122.27	110.07
10	i	707	PRO	N-CA-C	8.38	122.95	111.22
12	A	74	GLY	CA-C-N	8.35	130.72	123.04
12	A	74	GLY	C-N-CA	8.35	130.72	123.04
9	g	321	TYR	N-CA-CB	8.34	122.16	110.07
12	A	1972	GLU	N-CA-C	-8.33	103.28	113.19
6	E	1312	HIS	N-CA-C	8.32	123.24	112.26
9	G	225	LEU	N-CA-C	-8.28	93.99	108.23
6	E	1097	PHE	CB-CA-C	-8.22	97.20	110.84
6	e	1174	GLU	N-CA-CB	8.19	124.33	110.49
6	e	750	ALA	CA-C-N	8.18	129.00	120.00
6	e	750	ALA	C-N-CA	8.18	129.00	120.00
10	I	556	LYS	CA-C-N	-8.18	105.93	121.54
10	I	556	LYS	C-N-CA	-8.18	105.93	121.54
9	G	860	VAL	N-CA-C	-8.10	102.65	110.42
6	E	1030	ARG	CB-CA-C	8.08	126.50	110.42
10	i	287	VAL	CB-CA-C	-8.06	104.17	111.74
12	A	861	MET	N-CA-C	-8.04	102.47	111.07
10	M	287	VAL	CB-CA-C	-8.02	104.20	111.74
12	A	73	GLU	O-C-N	-7.98	110.86	122.99
12	A	1046	GLY	CA-C-N	-7.96	109.89	119.84
12	A	1046	GLY	C-N-CA	-7.96	109.89	119.84
12	A	1870	LYS	N-CA-C	-7.94	102.62	111.28
12	A	1781	PHE	O-C-N	-7.91	113.62	123.27
9	G	321	TYR	N-CA-C	-7.89	102.62	111.14
6	E	1030	ARG	CA-C-O	-7.83	109.31	120.51
10	i	391	GLY	O-C-N	7.82	132.87	122.70
6	E	1217	ALA	N-CA-C	7.80	121.80	109.39
9	g	321	TYR	N-CA-C	-7.79	102.72	111.14
12	A	1748	MET	N-CA-C	-7.79	102.87	111.36
9	G	464	ARG	N-CA-C	-7.77	101.93	111.33
10	M	391	GLY	O-C-N	7.76	132.79	122.70
1	P	898	LEU	N-CA-CB	-7.75	98.69	110.16
12	A	796	LYS	CA-C-N	-7.73	112.42	120.38
12	A	796	LYS	C-N-CA	-7.73	112.42	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	898	LEU	N-CA-CB	-7.72	98.73	110.16
9	g	225	LEU	N-CA-C	-7.71	93.92	108.17
12	A	298	ALA	O-C-N	-7.70	112.91	122.68
6	e	1174	GLU	CA-C-O	7.70	131.51	120.51
1	j	1022	GLU	CA-C-N	7.64	130.85	120.38
1	j	1022	GLU	C-N-CA	7.64	130.85	120.38
1	p	1022	GLU	CA-C-N	7.63	130.84	120.38
1	p	1022	GLU	C-N-CA	7.63	130.84	120.38
6	e	750	ALA	N-CA-C	7.61	119.21	111.07
7	K	1159	THR	N-CA-C	-7.60	94.62	110.80
2	B	138	SER	N-CA-C	-7.59	102.95	111.14
2	b	580	LEU	CA-C-N	-7.57	110.69	119.32
2	b	580	LEU	C-N-CA	-7.57	110.69	119.32
6	E	1274	THR	N-CA-C	7.57	126.92	110.80
9	G	526	CYS	N-CA-C	7.57	122.27	112.89
10	I	230	ASN	N-CA-C	7.55	120.27	110.53
12	A	500	ASP	O-C-N	-7.54	113.75	123.02
12	A	77	ILE	CA-C-N	7.53	133.24	121.26
12	A	77	ILE	C-N-CA	7.53	133.24	121.26
6	E	1202	ALA	N-CA-C	-7.52	103.36	112.54
12	A	286	GLN	CA-C-N	7.52	136.15	121.41
12	A	286	GLN	C-N-CA	7.52	136.15	121.41
12	A	904	ASN	CA-C-N	-7.51	107.73	120.58
12	A	904	ASN	C-N-CA	-7.51	107.73	120.58
10	I	289	TRP	N-CA-C	7.51	126.80	110.80
1	j	909	LEU	N-CA-CB	7.51	121.27	110.16
9	g	322	LEU	CB-CA-C	7.50	123.29	110.84
9	G	322	LEU	CB-CA-C	7.49	123.27	110.84
1	P	1022	GLU	CA-C-N	7.48	130.63	120.38
1	P	1022	GLU	C-N-CA	7.48	130.63	120.38
9	g	526	CYS	N-CA-C	7.47	122.16	112.89
1	J	1022	GLU	CA-C-N	7.47	130.61	120.38
1	J	1022	GLU	C-N-CA	7.47	130.61	120.38
6	E	1138	VAL	CB-CA-C	-7.47	99.05	111.29
1	p	909	LEU	N-CA-CB	7.47	121.21	110.16
6	E	1209	GLU	N-CA-C	-7.40	103.29	111.36
6	E	1267	GLN	N-CA-C	-7.40	95.05	110.80
12	A	949	VAL	N-CA-C	7.39	117.52	110.42
7	K	1113	GLU	N-CA-C	-7.38	103.24	111.28
2	b	569	CYS	O-C-N	-7.34	112.78	122.33
12	A	746	THR	N-CA-C	7.33	121.07	108.02
9	G	482	ILE	N-CA-C	-7.33	103.15	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1761	GLU	O-C-N	7.33	129.62	122.07
6	E	1216	GLN	CA-C-N	-7.32	110.95	122.23
6	E	1216	GLN	C-N-CA	-7.32	110.95	122.23
12	A	208	LEU	N-CA-C	-7.32	99.19	110.10
4	f	273	PRO	N-CA-C	-7.31	97.41	112.47
9	g	482	ILE	N-CA-C	-7.27	103.20	110.62
2	b	596	TYR	N-CA-C	-7.26	102.76	111.69
6	E	1287	MET	CB-CA-C	-7.26	95.97	110.42
9	G	865	ARG	N-CA-C	-7.26	103.31	111.07
7	K	1154	ILE	N-CA-C	-7.25	103.20	113.07
9	G	514	VAL	N-CA-C	-7.24	98.35	108.27
7	K	1341	TYR	O-C-N	-7.24	98.62	122.06
9	g	514	VAL	N-CA-C	-7.23	98.36	108.27
6	E	1266	ASN	N-CA-C	-7.22	98.20	108.96
1	j	852	ASP	N-CA-C	-7.22	102.37	111.90
1	j	1007	MET	N-CA-C	7.22	116.44	108.14
7	K	1155	GLN	N-CA-C	-7.21	95.43	110.80
12	A	1129	GLN	CA-C-N	7.21	130.25	120.44
12	A	1129	GLN	C-N-CA	7.21	130.25	120.44
1	p	852	ASP	N-CA-C	-7.21	102.38	111.90
6	e	1202	ALA	N-CA-C	-7.17	103.39	111.14
3	c	194	LEU	O-C-N	-7.17	114.85	123.10
1	p	1007	MET	N-CA-C	7.17	116.39	108.14
12	A	1629	ILE	CB-CA-C	-7.15	99.56	111.29
10	I	287	VAL	N-CA-C	7.13	120.73	108.90
6	E	1136	TRP	CB-CA-C	-7.12	97.78	110.03
12	A	1288	VAL	CB-CA-C	-7.06	102.85	111.88
2	B	134	ILE	N-CA-C	-7.03	103.62	110.72
2	b	76	HIS	N-CA-C	-7.01	103.57	111.14
2	B	76	HIS	N-CA-C	-7.01	103.57	111.14
12	A	500	ASP	CA-C-N	7.01	132.08	122.34
12	A	500	ASP	C-N-CA	7.01	132.08	122.34
6	e	1178	LEU	N-CA-C	-7.00	104.21	112.89
6	E	1315	PRO	N-CA-C	-6.97	98.10	112.47
6	E	1076	TYR	N-CA-C	-6.96	103.75	111.82
6	E	1073	HIS	N-CA-C	6.96	120.87	107.44
12	A	1393	SER	N-CA-C	-6.92	103.74	111.28
12	A	897	ALA	N-CA-CB	-6.90	98.83	110.49
12	A	1731	SER	O-C-N	-6.90	113.09	122.33
1	P	558	TYR	CA-C-N	6.87	126.50	119.56
1	P	558	TYR	C-N-CA	6.87	126.50	119.56
1	J	558	TYR	CA-C-N	6.87	126.50	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	558	TYR	C-N-CA	6.87	126.50	119.56
2	B	571	PHE	N-CA-C	-6.85	104.19	112.54
7	K	1145	LEU	N-CA-C	-6.84	103.90	111.36
9	g	848	LYS	CA-C-N	-6.83	111.29	120.79
9	g	848	LYS	C-N-CA	-6.83	111.29	120.79
6	E	1117	VAL	N-CA-CB	-6.80	102.96	110.51
12	A	1725	ASP	CA-C-N	6.79	129.38	120.28
12	A	1725	ASP	C-N-CA	6.79	129.38	120.28
9	G	501	GLU	CB-CA-C	6.79	121.64	110.17
9	g	848	LYS	N-CA-C	-6.79	103.06	111.75
1	j	558	TYR	CA-C-N	6.78	126.41	119.56
1	j	558	TYR	C-N-CA	6.78	126.41	119.56
1	J	538	GLU	O-C-N	-6.77	113.53	121.32
1	p	558	TYR	CA-C-N	6.77	126.40	119.56
1	p	558	TYR	C-N-CA	6.77	126.40	119.56
1	P	538	GLU	O-C-N	-6.76	113.55	121.32
12	A	82	ARG	O-C-N	-6.75	115.26	123.30
12	A	1298	ASP	N-CA-C	-6.72	102.28	111.56
5	d	255	LYS	N-CA-C	6.71	119.06	108.79
5	D	255	LYS	N-CA-C	6.70	119.05	108.79
6	E	1056	GLU	N-CA-C	-6.70	103.22	111.40
6	E	1234	LEU	N-CA-CB	-6.70	100.65	110.49
12	A	1551	ILE	O-C-N	6.66	128.69	121.83
12	A	1723	GLY	CA-C-N	6.66	134.25	121.54
12	A	1723	GLY	C-N-CA	6.66	134.25	121.54
2	b	570	SER	CA-C-O	6.60	127.58	119.79
1	J	867	SER	CA-C-N	6.60	129.66	120.29
1	J	867	SER	C-N-CA	6.60	129.66	120.29
1	J	243	LEU	CA-C-N	6.60	132.48	123.11
1	J	243	LEU	C-N-CA	6.60	132.48	123.11
1	P	243	LEU	CA-C-N	6.59	132.46	123.11
1	P	243	LEU	C-N-CA	6.59	132.46	123.11
12	A	130	VAL	O-C-N	6.58	128.60	121.83
1	P	867	SER	CA-C-N	6.58	129.63	120.29
1	P	867	SER	C-N-CA	6.58	129.63	120.29
1	p	538	GLU	O-C-N	-6.57	113.77	121.32
6	E	1286	LEU	N-CA-CB	6.57	120.51	110.14
1	j	1008	PRO	N-CA-C	6.55	121.24	111.41
6	E	1183	VAL	N-CA-C	-6.55	103.16	110.62
1	j	538	GLU	O-C-N	-6.55	113.79	121.32
12	A	715	SER	N-CA-C	-6.54	96.86	110.80
1	p	1008	PRO	N-CA-C	6.54	121.23	111.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	g	247	MET	CB-CA-C	6.54	123.43	110.42
9	g	501	GLU	CB-CA-C	6.51	121.74	110.01
6	e	1198	THR	N-CA-C	-6.50	105.21	113.01
10	I	240	SER	N-CA-C	-6.49	100.42	110.10
9	G	819	GLU	N-CA-C	-6.49	105.75	113.21
12	A	183	THR	CA-C-N	6.48	133.92	121.54
12	A	183	THR	C-N-CA	6.48	133.92	121.54
7	K	1330	GLY	N-CA-C	-6.48	104.80	112.64
12	A	1739	LEU	N-CA-C	-6.47	104.22	111.28
12	A	1880	LYS	N-CA-C	-6.47	104.30	111.36
12	A	1519	GLY	O-C-N	-6.47	114.32	122.41
9	g	387	TRP	N-CA-C	-6.46	97.04	110.80
12	A	1074	SER	N-CA-C	6.46	118.12	108.31
9	G	387	TRP	N-CA-C	-6.45	97.07	110.80
10	I	228	GLU	N-CA-C	-6.44	99.15	109.39
12	A	1684	LEU	O-C-N	-6.44	113.91	121.32
6	E	1336	TYR	N-CA-C	6.44	117.96	111.07
6	E	1321	ILE	CB-CA-C	-6.44	103.56	111.87
1	p	867	SER	CA-C-N	6.43	129.42	120.29
1	p	867	SER	C-N-CA	6.43	129.42	120.29
6	e	1106	GLU	N-CA-C	6.43	120.96	113.18
6	E	1224	ILE	N-CA-CB	6.42	118.49	110.47
2	B	585	GLN	N-CA-C	6.42	124.47	110.80
12	A	669	ILE	O-C-N	6.42	128.36	121.94
9	g	600	VAL	N-CA-C	6.41	122.67	109.34
7	K	1150	ILE	CA-C-O	-6.39	114.40	121.17
1	j	867	SER	CA-C-N	6.38	129.35	120.29
1	j	867	SER	C-N-CA	6.38	129.35	120.29
9	G	600	VAL	N-CA-C	6.37	122.59	109.34
12	A	1872	GLY	N-CA-C	-6.37	105.11	112.50
10	i	288	TYR	N-CA-C	6.37	124.36	110.80
2	B	566	ILE	N-CA-C	-6.36	104.29	110.72
10	M	288	TYR	N-CA-C	6.36	124.35	110.80
12	A	1218	ASN	O-C-N	-6.35	114.90	122.65
6	E	1136	TRP	N-CA-CB	-6.35	100.96	111.69
12	A	1329	LEU	CA-C-N	6.35	127.65	119.78
12	A	1329	LEU	C-N-CA	6.35	127.65	119.78
12	A	867	SER	CA-C-N	6.34	132.51	122.61
12	A	867	SER	C-N-CA	6.34	132.51	122.61
6	E	1339	TYR	CB-CA-C	6.33	119.07	111.22
7	K	1125	SER	CA-C-O	-6.33	114.18	120.82
12	A	382	ASP	N-CA-C	6.32	118.25	109.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1387	PHE	N-CA-C	-6.32	105.21	113.17
12	A	1177	ARG	O-C-N	-6.31	115.13	122.95
6	E	1318	ASN	N-CA-C	6.30	124.23	110.80
6	E	1141	VAL	CB-CA-C	-6.29	100.97	111.29
12	A	522	GLN	N-CA-C	-6.29	104.34	111.07
12	A	1620	LEU	CA-C-N	-6.29	111.98	119.84
12	A	1620	LEU	C-N-CA	-6.29	111.98	119.84
12	A	867	SER	O-C-N	-6.26	113.28	122.43
6	E	1286	LEU	N-CA-C	-6.26	103.74	111.75
6	E	1107	VAL	CA-C-N	6.24	133.47	121.54
6	E	1107	VAL	C-N-CA	6.24	133.47	121.54
12	A	1470	GLU	CA-C-N	6.24	128.92	120.38
12	A	1470	GLU	C-N-CA	6.24	128.92	120.38
6	E	1106	GLU	N-CA-C	6.23	120.90	113.12
12	A	926	ILE	N-CA-C	6.22	120.66	112.76
12	A	1322	ASP	O-C-N	-6.22	116.13	123.22
7	K	1146	GLU	N-CA-C	-6.21	104.42	111.07
6	E	1186	GLN	CA-C-N	-6.19	111.37	120.28
6	E	1186	GLN	C-N-CA	-6.19	111.37	120.28
9	g	463	HIS	N-CA-C	-6.18	104.62	111.36
4	f	276	MET	N-CA-C	-6.17	99.81	109.25
5	D	266	PHE	N-CA-C	6.16	119.58	109.72
9	G	229	GLU	N-CA-C	-6.15	105.49	112.87
6	E	1299	THR	N-CA-C	6.14	119.39	107.71
5	d	266	PHE	N-CA-C	6.14	119.54	109.72
2	b	387	ALA	N-CA-C	-6.14	106.43	114.04
1	P	773	VAL	N-CA-C	-6.13	106.76	112.83
7	K	1228	ASP	N-CA-C	-6.13	104.60	111.28
1	j	773	VAL	N-CA-C	-6.12	106.77	112.83
12	A	381	THR	N-CA-C	6.12	119.13	111.24
9	g	500	GLU	CA-C-N	-6.12	111.31	122.38
9	g	500	GLU	C-N-CA	-6.12	111.31	122.38
12	A	1074	SER	CB-CA-C	-6.12	109.51	116.54
12	A	63	GLN	O-C-N	6.11	129.12	122.15
12	A	1722	GLY	CA-C-N	6.11	129.39	122.67
12	A	1722	GLY	C-N-CA	6.11	129.39	122.67
12	A	1458	PHE	O-C-N	6.11	129.11	122.15
6	E	1207	ALA	N-CA-C	6.10	120.19	112.87
12	A	1218	ASN	CA-C-N	6.10	130.46	120.63
12	A	1218	ASN	C-N-CA	6.10	130.46	120.63
1	J	773	VAL	N-CA-C	-6.10	106.79	112.83
1	p	773	VAL	N-CA-C	-6.10	106.79	112.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	438	GLU	CA-C-N	-6.09	112.66	122.23
2	b	438	GLU	C-N-CA	-6.09	112.66	122.23
12	A	1086	ASP	CA-C-N	6.06	128.69	120.44
12	A	1086	ASP	C-N-CA	6.06	128.69	120.44
9	g	809	ILE	CB-CA-C	-6.05	103.96	111.70
6	E	1314	VAL	CA-C-N	-6.04	112.28	119.84
6	E	1314	VAL	C-N-CA	-6.04	112.28	119.84
7	K	1225	GLU	N-CA-C	-6.04	104.69	111.28
10	I	241	GLU	N-CA-C	-6.04	104.62	111.14
6	e	1176	ARG	N-CA-C	6.03	123.65	110.80
9	g	248	GLY	N-CA-C	-6.03	98.89	113.18
12	A	797	PRO	N-CA-C	6.03	118.05	110.70
2	b	461	THR	N-CA-C	6.00	117.90	111.36
9	g	739	ARG	O-C-N	-6.00	114.61	122.59
10	I	288	TYR	CB-CA-C	5.99	123.32	110.21
7	K	1116	SER	N-CA-C	-5.98	104.77	111.28
12	A	1615	TYR	N-CA-C	-5.97	104.77	111.28
7	K	1119	ILE	N-CA-CB	5.96	117.53	110.55
6	E	1175	LEU	N-CA-C	-5.95	98.12	110.80
7	K	1203	ILE	N-CA-C	-5.95	104.71	110.42
12	A	287	GLY	CA-C-N	-5.94	114.28	122.30
12	A	287	GLY	C-N-CA	-5.94	114.28	122.30
6	e	1118	ASN	N-CA-C	-5.92	104.83	111.28
9	g	803	LEU	N-CA-C	-5.91	104.74	111.07
6	e	484	LYS	CA-C-N	5.91	126.64	122.33
6	e	484	LYS	C-N-CA	5.91	126.64	122.33
1	p	311	SER	CA-C-N	5.90	128.18	120.28
1	p	311	SER	C-N-CA	5.90	128.18	120.28
6	E	1274	THR	CB-CA-C	-5.89	98.70	110.42
2	b	315	PRO	N-CA-C	-5.89	105.27	113.81
12	A	1991	ARG	CA-C-N	5.89	128.76	120.28
12	A	1991	ARG	C-N-CA	5.89	128.76	120.28
12	A	114	ILE	O-C-N	5.88	127.89	121.83
6	e	1179	GLU	N-CA-CB	5.88	118.54	110.01
12	A	1290	ILE	N-CA-C	-5.88	104.12	110.23
9	g	323	MET	CA-C-N	-5.88	112.50	119.84
9	g	323	MET	C-N-CA	-5.88	112.50	119.84
1	j	311	SER	CA-C-N	5.87	128.14	120.28
1	j	311	SER	C-N-CA	5.87	128.14	120.28
9	G	323	MET	CA-C-N	-5.86	112.51	119.84
9	G	323	MET	C-N-CA	-5.86	112.51	119.84
12	A	363	GLY	N-CA-C	-5.85	105.57	115.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1460	LYS	CA-C-N	5.85	128.12	120.28
12	A	1460	LYS	C-N-CA	5.85	128.12	120.28
1	j	850	TYR	CA-C-N	5.85	131.47	121.29
1	j	850	TYR	C-N-CA	5.85	131.47	121.29
1	p	850	TYR	CA-C-N	5.85	131.46	121.29
1	p	850	TYR	C-N-CA	5.85	131.46	121.29
4	F	124	SER	CA-C-N	5.84	127.67	122.47
4	F	124	SER	C-N-CA	5.84	127.67	122.47
4	f	124	SER	CA-C-N	5.83	127.66	122.47
4	f	124	SER	C-N-CA	5.83	127.66	122.47
7	K	1316	LYS	N-CA-C	5.83	122.70	109.81
12	A	76	PRO	O-C-N	-5.83	114.77	122.64
12	A	808	ASN	N-CA-C	-5.83	100.65	108.86
12	A	1224	VAL	O-C-N	-5.83	116.78	123.07
12	A	74	GLY	O-C-N	-5.82	115.13	122.70
12	A	800	PHE	CA-C-N	-5.82	112.48	120.28
12	A	800	PHE	C-N-CA	-5.82	112.48	120.28
10	I	285	LYS	CB-CA-C	-5.82	100.37	111.48
12	A	207	GLY	N-CA-C	-5.82	105.75	112.73
12	A	485	PRO	O-C-N	-5.81	115.76	122.85
9	G	868	LEU	N-CA-C	-5.81	105.03	111.36
12	A	996	ALA	CA-C-N	5.79	127.08	119.84
12	A	996	ALA	C-N-CA	5.79	127.08	119.84
12	A	1398	ILE	N-CA-C	-5.77	104.89	110.72
12	A	484	PRO	N-CA-C	5.76	117.73	110.70
2	b	418	GLY	N-CA-C	-5.75	105.83	112.50
12	A	1100	GLU	N-CA-C	-5.75	105.02	111.28
6	e	1187	THR	N-CA-C	-5.74	104.93	111.07
2	B	573	LEU	CA-C-N	-5.73	112.81	120.54
2	B	573	LEU	C-N-CA	-5.73	112.81	120.54
12	A	622	MET	CA-C-N	5.72	125.40	119.05
12	A	622	MET	C-N-CA	5.72	125.40	119.05
6	E	1122	ALA	N-CA-C	5.71	117.18	111.07
6	e	749	GLY	CA-C-N	-5.71	113.02	120.44
6	e	749	GLY	C-N-CA	-5.71	113.02	120.44
12	A	1293	THR	N-CA-C	5.71	117.50	111.28
12	A	855	GLN	CA-C-N	-5.70	111.19	120.72
12	A	855	GLN	C-N-CA	-5.70	111.19	120.72
9	g	226	VAL	N-CA-C	5.70	121.19	108.88
12	A	200	ASP	N-CA-C	5.70	120.39	113.38
6	E	1323	ARG	N-CA-C	5.69	119.96	113.19
9	g	389	GLN	N-CA-C	-5.69	98.69	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	923	ASN	CA-C-N	5.68	127.83	120.44
12	A	923	ASN	C-N-CA	5.68	127.83	120.44
1	j	198	SER	N-CA-CB	5.67	120.08	110.49
6	e	1128	ARG	CB-CA-C	5.67	120.60	109.72
1	P	1021	CYS	CA-C-N	5.67	127.88	120.28
1	P	1021	CYS	C-N-CA	5.67	127.88	120.28
1	p	198	SER	N-CA-CB	5.67	120.07	110.49
12	A	547	GLY	O-C-N	-5.67	113.94	123.00
12	A	1989	ARG	N-CA-C	-5.66	106.97	112.97
1	J	311	SER	CA-C-N	5.65	127.85	120.28
1	J	311	SER	C-N-CA	5.65	127.85	120.28
1	J	603	GLN	N-CA-C	5.65	117.24	111.14
2	B	573	LEU	CB-CA-C	-5.65	101.46	110.84
12	A	716	PHE	N-CA-C	-5.65	97.33	109.81
9	G	389	GLN	N-CA-C	-5.64	98.78	110.80
12	A	317	THR	N-CA-C	-5.64	106.29	112.72
12	A	328	THR	N-CA-C	5.64	117.23	111.14
1	P	603	GLN	N-CA-C	5.64	117.23	111.14
1	j	1081	LYS	CA-C-N	5.64	128.63	120.79
1	j	1081	LYS	C-N-CA	5.64	128.63	120.79
12	A	359	ILE	O-C-N	5.64	127.64	121.83
1	J	790	ALA	N-CA-C	5.63	117.10	111.07
12	A	869	LEU	O-C-N	-5.63	116.01	122.93
1	P	790	ALA	N-CA-C	5.62	117.08	111.07
1	J	198	SER	N-CA-CB	5.62	119.98	110.49
1	p	700	THR	N-CA-C	-5.62	105.21	112.68
1	p	1081	LYS	CA-C-N	5.62	128.60	120.79
1	p	1081	LYS	C-N-CA	5.62	128.60	120.79
6	E	1199	ALA	N-CA-C	-5.61	104.85	110.97
1	J	1021	CYS	CA-C-N	5.61	127.79	120.28
1	J	1021	CYS	C-N-CA	5.61	127.79	120.28
1	P	198	SER	N-CA-CB	5.61	119.97	110.49
1	P	311	SER	CA-C-N	5.60	127.78	120.28
1	P	311	SER	C-N-CA	5.60	127.78	120.28
1	p	922	LEU	O-C-N	5.59	128.04	122.12
12	A	158	PHE	O-C-N	-5.58	116.46	123.27
6	e	1075	TYR	N-CA-C	-5.58	104.89	110.97
12	A	258	VAL	N-CA-C	-5.58	101.99	109.30
12	A	1684	LEU	CA-C-N	5.58	126.81	119.84
12	A	1684	LEU	C-N-CA	5.58	126.81	119.84
1	j	922	LEU	O-C-N	5.58	128.03	122.12
6	E	1212	ALA	N-CA-C	5.57	117.05	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	424	ARG	N-CA-C	5.57	117.35	111.28
6	e	1199	ALA	N-CA-C	-5.57	104.90	110.97
6	E	1333	LEU	CA-C-N	-5.57	111.41	120.71
6	E	1333	LEU	C-N-CA	-5.57	111.41	120.71
1	P	424	ARG	N-CA-C	5.57	117.34	111.28
10	i	275	ASP	N-CA-C	5.56	119.23	111.56
6	e	752	GLN	CA-C-O	-5.55	114.53	120.42
7	K	1334	GLU	CA-C-N	5.55	126.78	119.84
7	K	1334	GLU	C-N-CA	5.55	126.78	119.84
12	A	789	GLY	O-C-N	-5.55	115.38	122.43
1	p	693	GLU	CA-C-O	-5.55	114.98	120.70
1	J	991	THR	N-CA-CB	5.54	118.51	110.47
1	j	693	GLU	CA-C-O	-5.54	114.99	120.70
10	i	290	GLU	CA-C-N	5.54	132.11	121.54
10	i	290	GLU	C-N-CA	5.54	132.11	121.54
12	A	288	THR	CA-C-N	5.53	132.11	121.54
12	A	288	THR	C-N-CA	5.53	132.11	121.54
1	J	1081	LYS	CA-C-N	5.53	128.48	120.79
1	J	1081	LYS	C-N-CA	5.53	128.48	120.79
10	M	290	GLU	CA-C-N	5.53	132.10	121.54
10	M	290	GLU	C-N-CA	5.53	132.10	121.54
9	G	236	ARG	N-CA-C	-5.52	105.26	111.28
1	p	424	ARG	N-CA-C	5.52	117.30	111.28
1	j	424	ARG	N-CA-C	5.52	117.30	111.28
1	P	1081	LYS	CA-C-N	5.52	128.47	120.79
1	P	1081	LYS	C-N-CA	5.52	128.47	120.79
9	g	822	GLY	N-CA-C	5.52	119.35	112.73
10	M	275	ASP	N-CA-C	5.51	119.17	111.56
1	P	991	THR	N-CA-CB	5.51	118.47	110.47
12	A	125	LEU	N-CA-C	5.51	117.77	109.23
6	e	1132	PRO	N-CA-C	5.51	123.82	112.47
1	p	790	ALA	N-CA-C	5.51	116.96	111.07
9	g	236	ARG	N-CA-C	-5.50	105.28	111.28
6	E	1205	SER	N-CA-C	5.50	122.51	110.80
10	M	227	GLU	CA-C-N	-5.49	111.05	121.54
10	M	227	GLU	C-N-CA	-5.49	111.05	121.54
12	A	549	PRO	O-C-N	-5.49	115.23	122.64
12	A	432	LEU	N-CA-C	5.49	117.81	110.35
10	I	467	ASN	N-CA-C	5.48	117.73	109.23
7	K	1203	ILE	N-CA-CB	5.48	116.96	110.55
10	M	467	ASN	N-CA-C	5.48	117.72	109.23
1	J	1044	ASP	CA-C-N	5.48	127.89	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	1044	ASP	C-N-CA	5.48	127.89	120.38
10	I	555	ALA	CA-C-N	5.47	132.00	121.54
10	I	555	ALA	C-N-CA	5.47	132.00	121.54
1	J	693	GLU	CA-C-O	-5.47	115.07	120.70
1	P	693	GLU	CA-C-O	-5.47	115.07	120.70
1	j	790	ALA	N-CA-C	5.47	116.92	111.07
12	A	1893	SER	N-CA-C	-5.46	105.22	111.07
6	e	1046	VAL	N-CA-C	-5.46	105.53	110.82
8	h	5	ILE	CA-C-N	5.46	128.84	120.82
8	h	5	ILE	C-N-CA	5.46	128.84	120.82
6	E	1307	ASN	CA-C-N	-5.46	112.41	120.38
6	E	1307	ASN	C-N-CA	-5.46	112.41	120.38
10	i	467	ASN	N-CA-C	5.46	117.69	109.23
6	E	1074	ASN	N-CA-C	-5.45	99.18	110.80
6	E	872	PHE	CB-CA-C	5.45	121.26	110.42
10	I	201	LEU	N-CA-C	-5.44	105.43	111.36
6	E	1046	VAL	N-CA-C	-5.43	105.55	110.82
12	A	1762	TYR	CA-C-N	5.43	127.56	120.28
12	A	1762	TYR	C-N-CA	5.43	127.56	120.28
1	P	1044	ASP	CA-C-N	5.43	127.82	120.38
1	P	1044	ASP	C-N-CA	5.43	127.82	120.38
7	K	1189	TYR	CB-CA-C	5.43	120.09	110.85
2	B	621	GLN	CA-C-N	5.43	131.91	121.54
2	B	621	GLN	C-N-CA	5.43	131.91	121.54
6	E	1338	LYS	CB-CA-C	-5.42	99.86	110.11
1	j	162	ALA	O-C-N	-5.42	116.37	122.12
1	P	832	SER	CA-C-O	-5.42	112.73	120.16
12	A	618	HIS	CA-C-N	5.42	128.55	120.31
12	A	618	HIS	C-N-CA	5.42	128.55	120.31
10	M	282	TYR	CA-C-N	5.42	127.54	120.28
10	M	282	TYR	C-N-CA	5.42	127.54	120.28
1	p	832	SER	CA-C-O	-5.42	112.74	120.16
1	J	694	GLU	N-CA-C	5.42	117.88	111.33
12	A	507	TYR	CA-C-N	5.42	126.50	119.78
12	A	507	TYR	C-N-CA	5.42	126.50	119.78
1	j	535	SER	N-CA-C	-5.42	107.23	112.97
9	G	235	GLY	N-CA-C	-5.42	106.11	113.37
1	p	1044	ASP	CA-C-N	5.42	127.80	120.38
1	p	1044	ASP	C-N-CA	5.42	127.80	120.38
9	g	235	GLY	N-CA-C	-5.41	106.12	113.37
1	J	832	SER	CA-C-O	-5.41	112.75	120.16
7	K	1143	GLU	N-CA-C	-5.41	105.41	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1136	TRP	CA-C-O	-5.40	115.07	121.06
10	i	706	ILE	N-CA-C	-5.40	97.22	108.88
12	A	1874	ALA	N-CA-C	-5.40	105.48	111.36
6	e	485	GLY	O-C-N	-5.40	118.41	123.48
12	A	1722	GLY	O-C-N	-5.39	115.49	122.29
1	j	1044	ASP	CA-C-N	5.39	127.76	120.38
1	j	1044	ASP	C-N-CA	5.39	127.76	120.38
12	A	1042	ASP	N-CA-C	-5.38	106.69	113.20
1	J	162	ALA	O-C-N	-5.38	116.42	122.12
10	i	255	VAL	CB-CA-C	-5.38	104.81	111.70
1	p	535	SER	N-CA-C	-5.37	107.28	112.97
1	p	162	ALA	O-C-N	-5.37	116.43	122.12
12	A	133	LEU	O-C-N	5.37	127.60	122.07
1	j	832	SER	CA-C-O	-5.37	112.81	120.16
12	A	1300	ILE	CA-C-N	-5.36	113.14	119.84
12	A	1300	ILE	C-N-CA	-5.36	113.14	119.84
1	J	364	THR	N-CA-CB	5.36	118.99	110.57
12	A	20	ILE	O-C-N	5.36	127.16	121.91
12	A	698	TYR	CA-C-N	5.36	124.69	118.85
12	A	698	TYR	C-N-CA	5.36	124.69	118.85
12	A	746	THR	CB-CA-C	-5.36	102.53	110.62
12	A	139	LYS	O-C-N	5.35	128.25	122.15
6	e	1173	LEU	CA-C-N	5.35	131.76	121.54
6	e	1173	LEU	C-N-CA	5.35	131.76	121.54
12	A	1816	HIS	O-C-N	5.35	127.58	122.07
1	P	694	GLU	N-CA-C	5.35	117.80	111.33
1	p	364	THR	N-CA-CB	5.35	118.96	110.57
12	A	289	ASP	O-C-N	-5.34	115.48	122.59
10	M	255	VAL	CB-CA-C	-5.34	104.86	111.70
1	P	535	SER	N-CA-C	-5.34	107.31	112.97
7	K	1200	LEU	N-CA-C	-5.33	105.36	111.07
1	P	364	THR	N-CA-CB	5.33	118.94	110.57
1	j	364	THR	N-CA-CB	5.33	118.94	110.57
6	E	1268	LEU	CB-CA-C	-5.33	99.81	110.42
6	E	867	PRO	N-CA-CB	5.33	108.84	103.25
2	B	474	GLN	N-CA-C	-5.32	105.48	111.28
1	j	1021	CYS	CA-C-N	5.32	127.41	120.28
1	j	1021	CYS	C-N-CA	5.32	127.41	120.28
6	e	442	PRO	N-CA-CB	5.32	108.97	103.38
9	g	841	LEU	N-CA-C	5.32	119.74	112.88
6	E	1119	SER	CA-C-N	-5.32	112.23	120.31
6	E	1119	SER	C-N-CA	-5.32	112.23	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	991	THR	N-CA-CB	5.31	118.18	110.47
12	A	1908	GLU	N-CA-C	-5.31	105.18	110.97
6	E	1304	CYS	CA-C-N	-5.31	114.24	120.72
6	E	1304	CYS	C-N-CA	-5.31	114.24	120.72
12	A	1671	GLU	O-C-N	5.30	127.74	122.12
10	I	556	LYS	CA-C-O	-5.30	112.93	120.51
1	p	1021	CYS	CA-C-N	5.30	127.38	120.28
1	p	1021	CYS	C-N-CA	5.30	127.38	120.28
1	P	162	ALA	O-C-N	-5.30	116.50	122.12
9	G	390	LEU	N-CA-C	5.30	117.92	109.65
12	A	1492	ARG	O-C-N	5.30	128.19	122.15
1	p	991	THR	N-CA-CB	5.30	118.15	110.47
6	E	1292	ASP	CA-C-N	-5.30	112.95	120.89
6	E	1292	ASP	C-N-CA	-5.30	112.95	120.89
9	g	390	LEU	N-CA-C	5.30	117.91	109.65
1	p	621	ALA	N-CA-C	5.29	117.05	111.28
3	c	258	GLU	O-C-N	5.28	129.69	122.46
12	A	685	GLU	CA-C-N	5.28	127.92	120.42
12	A	685	GLU	C-N-CA	5.28	127.92	120.42
5	D	56	HIS	N-CA-C	5.28	116.02	108.74
1	j	699	SER	CA-C-N	5.27	127.35	120.28
1	j	699	SER	C-N-CA	5.27	127.35	120.28
1	J	535	SER	N-CA-C	-5.27	107.39	112.97
6	E	1079	LEU	CA-C-N	-5.27	113.16	120.38
6	E	1079	LEU	C-N-CA	-5.27	113.16	120.38
1	j	621	ALA	N-CA-C	5.26	117.02	111.28
1	J	705	VAL	CA-C-N	5.26	127.85	120.28
1	J	705	VAL	C-N-CA	5.26	127.85	120.28
6	E	1211	VAL	N-CA-CB	5.25	116.34	110.51
2	B	506	LYS	N-CA-C	-5.25	104.81	111.11
6	e	272	PRO	CA-C-N	5.25	128.04	120.38
6	e	272	PRO	C-N-CA	5.25	128.04	120.38
9	g	239	LEU	O-C-N	-5.24	115.62	122.59
1	J	898	LEU	CB-CA-C	-5.24	101.94	110.85
12	A	1274	LEU	N-CA-C	5.24	116.68	111.07
7	K	1071	LYS	CA-C-N	5.24	127.16	120.56
7	K	1071	LYS	C-N-CA	5.24	127.16	120.56
1	P	611	SER	N-CA-CB	5.24	118.54	110.79
13	n	337	THR	N-CA-C	5.24	121.95	110.80
12	A	589	ARG	O-C-N	5.23	128.11	122.15
12	A	1651	HIS	CA-C-N	5.23	127.29	120.28
12	A	1651	HIS	C-N-CA	5.23	127.29	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	705	VAL	CA-C-N	5.23	127.81	120.28
1	P	705	VAL	C-N-CA	5.23	127.81	120.28
9	G	489	TRP	N-CA-C	-5.22	105.58	111.28
1	P	898	LEU	CB-CA-C	-5.22	101.97	110.85
5	d	56	HIS	N-CA-C	5.22	115.95	108.74
12	A	1178	ARG	CA-C-N	5.22	127.28	120.28
12	A	1178	ARG	C-N-CA	5.22	127.28	120.28
9	G	600	VAL	CB-CA-C	-5.22	102.73	111.29
1	p	1055	LEU	N-CA-C	5.22	116.78	111.14
9	G	479	ARG	N-CA-C	-5.22	106.87	113.18
12	A	30	LYS	CA-C-N	5.22	129.53	122.07
12	A	30	LYS	C-N-CA	5.22	129.53	122.07
1	J	699	SER	CA-C-N	5.21	127.27	120.28
1	J	699	SER	C-N-CA	5.21	127.27	120.28
1	J	611	SER	N-CA-CB	5.21	118.50	110.79
9	G	239	LEU	O-C-N	-5.21	115.66	122.59
9	g	219	THR	CA-C-N	-5.21	111.59	121.54
9	g	219	THR	C-N-CA	-5.21	111.59	121.54
9	G	600	VAL	CA-C-N	5.21	127.51	120.38
9	G	600	VAL	C-N-CA	5.21	127.51	120.38
13	N	337	THR	N-CA-C	5.21	121.89	110.80
6	e	867	PRO	N-CA-CB	5.20	108.71	103.25
9	g	489	TRP	N-CA-C	-5.20	105.61	111.28
7	K	1150	ILE	N-CA-C	-5.20	105.43	110.42
1	p	855	ILE	N-CA-C	5.19	115.92	110.62
12	A	1075	GLY	CA-C-N	-5.19	113.36	119.84
12	A	1075	GLY	C-N-CA	-5.19	113.36	119.84
6	e	1179	GLU	N-CA-C	-5.19	105.52	111.07
10	M	274	GLY	N-CA-C	-5.19	100.89	113.18
6	e	1313	GLY	CA-C-O	-5.18	118.09	122.29
4	f	272	TYR	O-C-N	-5.18	116.10	121.28
10	i	274	GLY	N-CA-C	-5.18	100.90	113.18
6	E	1117	VAL	N-CA-C	-5.18	104.92	110.36
7	K	1140	GLU	N-CA-C	-5.18	105.63	111.28
1	p	811	ALA	N-CA-C	5.18	116.92	111.28
1	j	1055	LEU	N-CA-C	5.17	116.73	111.14
1	P	699	SER	CA-C-N	5.17	127.21	120.28
1	P	699	SER	C-N-CA	5.17	127.21	120.28
1	P	898	LEU	O-C-N	5.17	128.05	122.15
12	A	780	PHE	N-CA-C	-5.17	106.75	113.16
12	A	922	CYS	N-CA-C	5.17	121.82	110.80
12	A	744	TYR	N-CA-CB	-5.17	101.75	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1177	ARG	CA-C-N	5.17	128.19	120.90
12	A	1177	ARG	C-N-CA	5.17	128.19	120.90
12	A	920	ILE	N-CA-C	-5.17	105.29	110.30
12	A	346	VAL	N-CA-C	5.16	111.73	106.21
1	P	811	ALA	N-CA-C	5.16	116.90	111.28
1	p	850	TYR	O-C-N	5.16	129.16	122.71
1	j	919	LEU	CA-C-N	5.16	128.85	120.60
1	j	919	LEU	C-N-CA	5.16	128.85	120.60
9	g	479	ARG	N-CA-C	-5.15	106.95	113.18
10	I	234	ILE	N-CA-C	5.15	115.27	107.75
1	p	919	LEU	CA-C-N	5.15	128.84	120.60
1	p	919	LEU	C-N-CA	5.15	128.84	120.60
1	j	850	TYR	O-C-N	5.15	129.15	122.71
1	j	811	ALA	N-CA-C	5.15	116.89	111.28
1	J	898	LEU	O-C-N	5.14	128.01	122.15
1	j	855	ILE	N-CA-C	5.14	115.87	110.62
12	A	106	ILE	CA-C-N	5.14	127.59	120.29
12	A	106	ILE	C-N-CA	5.14	127.59	120.29
12	A	787	LEU	O-C-N	-5.14	117.20	123.27
1	P	250	VAL	CB-CA-C	-5.14	105.19	111.92
9	g	600	VAL	CA-C-N	5.14	127.42	120.38
9	g	600	VAL	C-N-CA	5.14	127.42	120.38
1	j	705	VAL	CA-C-N	5.13	127.67	120.28
1	j	705	VAL	C-N-CA	5.13	127.67	120.28
12	A	1763	CYS	O-C-N	5.13	127.56	122.12
12	A	521	PRO	N-CA-C	5.13	123.03	112.47
1	p	603	GLN	N-CA-C	5.13	116.95	111.36
1	J	250	VAL	CB-CA-C	-5.12	105.21	111.92
12	A	1326	ALA	CA-C-N	5.12	128.80	120.60
12	A	1326	ALA	C-N-CA	5.12	128.80	120.60
9	g	600	VAL	CB-CA-C	-5.12	102.89	111.29
13	n	336	SER	CA-C-N	5.12	131.32	121.54
13	n	336	SER	C-N-CA	5.12	131.32	121.54
6	E	1202	ALA	O-C-N	-5.12	115.57	122.43
6	E	1368	ALA	N-CA-C	5.12	122.38	107.84
1	P	1055	LEU	N-CA-C	5.12	116.67	111.14
6	e	246	HIS	CA-C-N	5.12	130.98	122.54
6	e	246	HIS	C-N-CA	5.12	130.98	122.54
9	G	346	ASN	N-CA-C	-5.11	102.72	110.24
1	j	603	GLN	N-CA-C	5.11	116.93	111.36
1	j	719	LYS	N-CA-C	5.11	116.66	111.14
13	N	336	SER	CA-C-N	5.11	131.30	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	336	SER	C-N-CA	5.11	131.30	121.54
1	J	621	ALA	N-CA-C	5.11	116.84	111.28
12	A	379	PHE	N-CA-C	-5.11	105.84	111.71
1	P	621	ALA	N-CA-C	5.10	116.84	111.28
1	p	719	LYS	N-CA-C	5.09	116.64	111.14
7	K	1199	LYS	N-CA-C	-5.09	105.63	111.07
9	g	475	SER	CB-CA-C	-5.09	105.18	113.37
9	g	842	ILE	O-C-N	5.09	127.72	122.79
12	A	716	PHE	CA-C-N	-5.08	113.49	119.84
12	A	716	PHE	C-N-CA	-5.08	113.49	119.84
1	J	1055	LEU	N-CA-C	5.08	116.62	111.14
12	A	514	LEU	O-C-N	5.08	127.50	122.12
1	J	811	ALA	N-CA-C	5.07	116.81	111.28
10	i	156	GLU	N-CA-C	5.07	121.61	110.80
12	A	1519	GLY	CA-C-N	5.07	127.49	120.29
12	A	1519	GLY	C-N-CA	5.07	127.49	120.29
2	b	52	PRO	CA-C-N	-5.07	114.52	122.73
2	b	52	PRO	C-N-CA	-5.07	114.52	122.73
6	e	1075	TYR	O-C-N	-5.07	116.76	122.03
9	G	752	TRP	N-CA-C	5.07	116.81	111.28
10	M	156	GLU	N-CA-C	5.07	121.60	110.80
12	A	1460	LYS	O-C-N	-5.06	116.86	122.07
4	f	277	LYS	CA-C-O	-5.06	116.13	120.88
9	g	330	LYS	N-CA-C	-5.06	105.89	111.71
10	I	156	GLU	N-CA-C	5.05	121.56	110.80
6	E	1279	ALA	N-CA-C	-5.05	100.04	110.80
6	e	1056	GLU	N-CA-C	-5.05	105.85	111.36
6	E	1307	ASN	N-CA-CB	5.05	117.30	109.98
6	E	1081	ALA	N-CA-C	5.05	117.18	111.02
6	E	1209	GLU	CA-C-N	-5.05	113.78	120.79
6	E	1209	GLU	C-N-CA	-5.05	113.78	120.79
2	b	380	ASP	N-CA-C	-5.04	105.86	111.36
1	P	207	LYS	N-CA-C	5.04	117.20	110.35
12	A	1022	VAL	O-C-N	-5.04	117.19	122.83
9	G	561	GLN	N-CA-C	-5.03	103.41	110.50
1	j	611	SER	N-CA-CB	5.03	118.24	110.79
6	E	1129	LEU	CA-C-O	-5.03	115.72	121.00
1	j	207	LYS	N-CA-C	5.03	117.19	110.35
1	J	243	LEU	CB-CA-C	5.02	118.04	109.80
12	A	1353	LYS	O-C-N	-5.02	116.06	122.34
12	A	1250	ARG	CA-C-N	-5.02	113.65	119.47
12	A	1250	ARG	C-N-CA	-5.02	113.65	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	243	LEU	CB-CA-C	5.02	118.03	109.80
12	A	799	GLY	N-CA-C	5.02	120.88	114.66
9	g	479	ARG	CB-CA-C	5.01	119.93	109.95
1	p	611	SER	N-CA-CB	5.01	118.21	110.79
12	A	859	ARG	N-CA-C	5.01	116.43	111.07
1	J	719	LYS	N-CA-C	5.01	116.55	111.14
9	G	330	LYS	N-CA-C	-5.01	105.95	111.71

There are no chirality outliers.

All (121) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A	1048	VAL	Mainchain
12	A	1053	THR	Peptide
12	A	1071	ALA	Peptide
12	A	1175	LYS	Mainchain
12	A	1176	VAL	Mainchain
12	A	1353	LYS	Mainchain
12	A	1354	GLN	Mainchain
12	A	1355	PRO	Peptide,Mainchain
12	A	1384	SER	Mainchain
12	A	1385	ALA	Mainchain
12	A	158	PHE	Mainchain
12	A	163	SER	Peptide
12	A	1684	LEU	Mainchain
12	A	1695	LEU	Peptide
12	A	1732	LEU	Mainchain
12	A	1973	SER	Peptide
12	A	1975	GLN	Peptide
12	A	257	THR	Peptide
12	A	286	GLN	Mainchain
12	A	288	THR	Mainchain
12	A	289	ASP	Mainchain
12	A	298	ALA	Mainchain
12	A	303	ASP	Mainchain
12	A	317	THR	Peptide
12	A	321	LYS	Peptide
12	A	485	PRO	Mainchain
12	A	547	GLY	Mainchain
12	A	548	SER	Mainchain
12	A	55	LYS	Peptide
12	A	653	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
12	A	715	SER	Peptide
12	A	73	GLU	Mainchain
12	A	76	PRO	Mainchain
12	A	80	THR	Mainchain
12	A	805	HIS	Mainchain
12	A	81	GLN	Mainchain
12	A	82	ARG	Mainchain
12	A	83	THR	Mainchain
12	A	869	LEU	Mainchain
12	A	996	ALA	Peptide
2	B	39	TYR	Peptide
2	B	394	ALA	Mainchain
2	B	569	CYS	Mainchain
5	D	184	VAL	Mainchain
5	D	218	VAL	Mainchain
6	E	1132	PRO	Peptide
6	E	1202	ALA	Mainchain
6	E	1265	ALA	Mainchain
6	E	1271	VAL	Peptide
6	E	1431	LYS	Peptide
6	E	1432	PRO	Peptide
6	E	1434	ARG	Peptide
6	E	57	SER	Peptide
6	E	865	LEU	Mainchain
6	E	871	ASN	Mainchain
9	G	347	ALA	Peptide
9	G	386	LEU	Mainchain
9	G	388	GLY	Peptide
9	G	395	ALA	Peptide
9	G	434	PRO	Peptide
9	G	512	THR	Peptide
9	G	577	TYR	Mainchain
9	G	607	LEU	Mainchain
9	G	609	SER	Peptide
9	G	644	LEU	Mainchain
9	G	682	PRO	Mainchain
9	G	701	VAL	Peptide
9	G	737	GLY	Peptide
9	G	818	ASP	Mainchain
10	I	155	LEU	Mainchain
10	I	231	MET	Peptide
10	I	290	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
10	I	550	THR	Mainchain
7	K	1106	ILE	Peptide
7	K	1163	SER	Peptide
7	K	1341	TYR	Mainchain
10	M	155	LEU	Mainchain
10	M	231	MET	Peptide
10	M	250	GLN	Peptide
10	M	273	VAL	Peptide
10	M	290	GLU	Peptide
10	M	391	GLY	Mainchain
10	M	550	THR	Mainchain
10	M	706	ILE	Peptide
13	N	1011	GLU	Peptide
2	b	39	TYR	Peptide
3	c	168	ASP	Mainchain
3	c	194	LEU	Mainchain
5	d	184	VAL	Mainchain
5	d	218	VAL	Mainchain
6	e	1195	ASN	Mainchain
6	e	1431	LYS	Peptide
6	e	1432	PRO	Peptide
6	e	1434	ARG	Peptide
6	e	57	SER	Peptide
6	e	744	ASP	Mainchain
6	e	751	GLY	Mainchain
6	e	865	LEU	Mainchain
9	g	246	PHE	Mainchain
9	g	386	LEU	Mainchain
9	g	388	GLY	Peptide
9	g	395	ALA	Peptide
9	g	434	PRO	Peptide
9	g	457	ALA	Mainchain
9	g	512	THR	Peptide
9	g	577	TYR	Mainchain
9	g	607	LEU	Mainchain
9	g	609	SER	Peptide
9	g	682	PRO	Mainchain
9	g	701	VAL	Peptide
9	g	737	GLY	Peptide
9	g	739	ARG	Mainchain
10	i	155	LEU	Mainchain
10	i	231	MET	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
10	i	273	VAL	Peptide
10	i	290	GLU	Peptide
10	i	391	GLY	Mainchain
10	i	550	THR	Mainchain
13	n	1011	GLU	Peptide
13	n	979	CYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	5059	0	2291	12	0
1	P	5059	0	2291	8	0
1	j	4934	0	2231	14	0
1	p	4934	0	2231	18	0
2	B	3116	0	1397	22	0
2	b	3156	0	1417	37	0
3	C	1694	0	751	2	0
3	c	1709	0	760	4	0
4	F	1566	0	722	1	0
4	f	1581	0	731	5	0
5	D	1571	0	716	17	0
5	d	1581	0	722	19	0
6	E	6759	0	3045	117	0
6	e	6494	0	2928	59	0
7	K	1643	0	709	35	0
8	H	1505	0	688	15	0
8	h	1510	0	693	15	0
9	G	3062	0	1356	53	0
9	g	3329	0	1466	90	0
10	I	3956	0	1777	27	0
10	M	3956	0	1777	29	0
10	i	3956	0	1777	26	0
11	L	3178	0	1424	7	0
11	O	250	0	111	0	0
12	A	8893	0	3941	206	0
13	N	4581	0	2042	9	0
13	n	4502	0	2010	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	93534	0	42004	764	0

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

All (764) 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)
9:g:873:PRO:N	9:g:873:PRO:CA	1.69	1.54
4:f:273:PRO:CA	4:f:273:PRO:N	1.70	1.54
6:e:1049:PRO:N	6:e:1049:PRO:CA	1.69	1.53
6:e:548:PRO:N	6:e:548:PRO:CA	1.70	1.52
8:h:2:VAL:CB	9:g:309:LEU:HA	1.34	1.52
10:i:673:PRO:N	10:i:673:PRO:CA	1.69	1.52
6:E:1020:PRO:N	6:E:1020:PRO:CA	1.69	1.51
7:K:1192:PRO:N	7:K:1192:PRO:CA	1.69	1.50
10:M:673:PRO:N	10:M:673:PRO:CA	1.69	1.50
12:A:1194:PRO:N	12:A:1194:PRO:CA	1.69	1.50
2:b:315:PRO:N	2:b:315:PRO:CA	1.69	1.50
12:A:94:ALA:HA	12:A:105:GLU:CB	1.57	1.32
9:g:348:GLY:HA2	9:g:643:ALA:HB1	1.25	1.19
12:A:120:PRO:O	12:A:1026:PRO:HA	1.40	1.18
6:e:1422:THR:CB	9:g:241:ILE:CB	2.20	1.17
8:h:68:PRO:CB	9:g:735:ARG:CB	2.21	1.16
8:H:216:ASP:CB	8:H:266:HIS:CB	2.23	1.14
6:E:933:VAL:CB	6:E:953:PRO:CB	2.27	1.12
8:h:2:VAL:CB	9:g:309:LEU:CA	2.27	1.12
6:E:1145:VAL:CB	6:E:1168:SER:CB	2.28	1.11
5:d:2:PHE:CB	2:b:58:ARG:H	1.64	1.10
12:A:98:SER:HA	12:A:104:GLY:HA2	1.33	1.08
8:H:68:PRO:CB	9:G:735:ARG:CB	2.34	1.05
8:h:166:SER:CB	9:g:685:HIS:CB	2.35	1.04
12:A:1767:MET:O	12:A:1771:SER:HA	1.60	1.02
6:E:1138:VAL:HA	6:E:1172:ILE:HA	1.40	1.00
8:H:166:SER:CB	9:G:685:HIS:CB	2.40	1.00
5:d:279:SER:CB	5:d:298:ASP:CB	2.41	0.98
9:g:751:GLN:CB	9:g:755:CYS:CB	2.41	0.98
6:e:761:ILE:CB	13:n:798:THR:CB	2.44	0.96
5:D:279:SER:CB	5:D:298:ASP:CB	2.43	0.95
12:A:94:ALA:CA	12:A:105:GLU:CB	2.45	0.95
12:A:1641:ALA:HB1	12:A:1682:ALA:HA	1.46	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:i:373:LYS:CB	10:i:391:GLY:HA2	1.97	0.94
6:E:1340:ASP:CB	12:A:722:ALA:HB1	2.00	0.92
7:K:1197:GLU:CB	7:K:1252:TYR:CB	2.48	0.91
6:E:1145:VAL:CA	6:E:1168:SER:CB	2.50	0.90
5:d:4:ALA:HB1	2:b:55:TYR:HA	1.52	0.89
12:A:120:PRO:CB	12:A:1021:GLY:HA2	2.02	0.89
12:A:1143:ASP:CB	12:A:1178:ARG:N	2.36	0.88
12:A:98:SER:HA	12:A:104:GLY:CA	2.01	0.88
1:j:989:GLN:CB	1:j:1009:VAL:CB	2.53	0.87
1:p:989:GLN:CB	1:p:1009:VAL:CB	2.53	0.86
9:g:791:HIS:O	10:I:489:ALA:HA	1.75	0.86
10:I:642:PHE:CB	10:I:836:GLN:CA	2.52	0.86
12:A:120:PRO:CB	12:A:1025:CYS:O	2.23	0.85
10:I:642:PHE:CB	10:I:836:GLN:N	2.40	0.85
10:M:373:LYS:CB	10:M:391:GLY:HA2	2.07	0.85
12:A:120:PRO:O	12:A:1026:PRO:CA	2.24	0.85
9:G:392:GLU:CB	9:G:395:ALA:HB2	2.07	0.84
6:E:1073:HIS:C	6:E:1075:TYR:H	1.82	0.83
9:g:392:GLU:CB	9:g:395:ALA:HB2	2.07	0.83
12:A:98:SER:CA	12:A:104:GLY:HA2	2.08	0.82
2:B:592:ALA:HB2	2:B:641:LEU:HA	1.61	0.82
9:G:463:HIS:CB	9:G:466:SER:CB	2.57	0.82
2:B:528:LEU:CB	10:M:774:THR:CB	2.57	0.82
9:G:461:GLY:O	10:I:317:ASP:CB	2.27	0.82
12:A:776:GLN:CB	5:D:259:SER:CB	2.58	0.81
12:A:1767:MET:O	12:A:1771:SER:CA	2.27	0.81
6:e:749:GLY:O	6:e:753:LEU:CB	2.28	0.81
1:J:922:LEU:CB	10:I:909:PRO:CB	2.58	0.81
10:I:642:PHE:CB	10:I:836:GLN:CB	2.59	0.80
7:K:1079:TRP:CB	7:K:1091:ALA:HB1	2.13	0.79
1:p:1130:ALA:HB1	1:P:580:SER:HA	1.65	0.79
9:g:751:GLN:CB	9:g:755:CYS:H	1.96	0.79
12:A:1766:LEU:O	12:A:1770:ASN:CB	2.31	0.78
7:K:1105:GLU:O	7:K:1107:SER:CB	2.31	0.78
2:b:287:GLY:HA3	2:b:312:PHE:O	1.84	0.78
12:A:1066:GLN:HA	12:A:1069:ALA:HB3	1.65	0.78
6:e:969:GLY:HA3	4:f:275:LYS:HA	1.66	0.77
12:A:156:LYS:H	12:A:238:GLN:HA	1.47	0.77
6:E:1132:PRO:HA	6:E:1135:ALA:H	1.49	0.77
10:I:653:SER:O	10:I:695:LYS:CB	2.33	0.77
12:A:957:ALA:HB3	12:A:963:SER:HA	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:651:ALA:CB	13:N:557:GLY:HA3	2.15	0.76
8:h:211:SER:CB	11:L:278:ASN:CB	2.63	0.76
2:b:355:ILE:H	2:b:387:ALA:HB1	1.50	0.76
4:f:273:PRO:N	4:f:273:PRO:C	2.44	0.76
6:e:862:LEU:O	6:e:866:TRP:CB	2.34	0.75
12:A:1066:GLN:O	12:A:1067:LEU:C	2.28	0.75
5:d:2:PHE:CB	2:b:58:ARG:N	2.46	0.75
9:g:751:GLN:CB	9:g:755:CYS:N	2.49	0.75
1:j:920:SER:HA	1:j:923:HIS:CB	2.16	0.75
9:G:254:GLY:HA2	9:G:262:VAL:O	1.85	0.75
9:G:767:ALA:O	9:G:771:GLU:N	2.20	0.75
1:p:920:SER:HA	1:p:923:HIS:CB	2.16	0.74
9:G:767:ALA:O	9:G:771:GLU:CA	2.36	0.74
9:g:348:GLY:HA2	9:g:643:ALA:CB	2.12	0.74
10:I:644:HIS:HA	10:I:839:LEU:CB	2.18	0.74
10:I:669:LEU:O	10:I:675:GLN:CB	2.36	0.74
10:I:231:MET:CB	10:I:232:PHE:CB	2.66	0.74
9:g:767:ALA:O	9:g:771:GLU:N	2.20	0.73
12:A:1630:LEU:O	12:A:1633:SER:CB	2.36	0.73
9:g:767:ALA:O	9:g:771:GLU:CA	2.36	0.73
12:A:210:ASN:C	12:A:212:LYS:H	1.94	0.73
10:i:231:MET:CB	10:i:232:PHE:CB	2.66	0.73
6:E:1268:LEU:O	6:E:1269:ALA:C	2.32	0.72
12:A:1971:GLY:C	12:A:1973:SER:H	1.97	0.72
6:e:540:GLN:CB	1:p:308:GLU:CB	2.68	0.72
12:A:105:GLU:O	12:A:108:ALA:N	2.23	0.72
9:g:348:GLY:HA3	9:g:643:ALA:O	1.90	0.71
1:J:580:SER:HA	1:j:1130:ALA:HB1	1.71	0.71
2:b:650:ALA:HB2	6:e:1040:SER:CB	2.21	0.70
10:i:885:LYS:HA	1:j:964:ALA:HB1	1.71	0.70
8:h:268:SER:CB	9:g:254:GLY:HA3	2.22	0.70
2:B:54:MET:H	5:D:6:SER:HA	1.56	0.70
7:K:1159:THR:O	7:K:1164:HIS:HA	1.90	0.70
1:J:896:GLY:O	1:J:911:ALA:HB1	1.91	0.70
9:G:767:ALA:O	9:G:772:ASN:N	2.25	0.70
7:K:1099:ALA:HB2	7:K:1118:ALA:HB1	1.74	0.70
8:h:305:GLY:N	9:g:266:ASP:O	2.25	0.70
9:g:817:GLN:O	9:g:818:ASP:C	2.35	0.70
10:i:673:PRO:N	10:i:673:PRO:CB	2.54	0.70
1:P:896:GLY:O	1:P:911:ALA:HB1	1.91	0.70
5:D:15:ILE:HA	5:D:31:SER:HA	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:1287:MET:O	6:E:1288:ILE:C	2.34	0.69
5:d:6:SER:CB	2:b:53:PHE:CB	2.70	0.69
10:I:548:PHE:CB	10:I:553:LEU:O	2.40	0.69
12:A:1194:PRO:N	12:A:1194:PRO:CB	2.55	0.69
10:M:673:PRO:N	10:M:673:PRO:CB	2.54	0.69
9:g:873:PRO:N	9:g:873:PRO:CB	2.55	0.69
12:A:13:LEU:HA	12:A:46:TYR:CB	2.22	0.69
6:e:547:ARG:O	6:e:565:LYS:CB	2.40	0.69
6:e:1049:PRO:N	6:e:1049:PRO:CB	2.55	0.69
12:A:1248:GLY:O	10:M:772:SER:CB	2.41	0.68
6:e:119:LEU:O	6:e:705:TYR:HA	1.94	0.68
12:A:380:CYS:O	12:A:451:PRO:CB	2.41	0.68
5:d:13:ASP:CB	5:d:33:ASP:N	2.57	0.68
8:H:224:GLY:CA	9:G:686:ILE:CB	2.71	0.68
2:b:287:GLY:HA2	2:b:312:PHE:CB	2.24	0.68
2:B:482:GLY:HA3	3:C:169:SER:O	1.93	0.68
6:E:862:LEU:O	6:E:866:TRP:CB	2.41	0.68
6:E:1138:VAL:HA	6:E:1172:ILE:CA	2.21	0.68
7:K:1192:PRO:N	7:K:1192:PRO:CB	2.56	0.68
12:A:1767:MET:O	12:A:1771:SER:N	2.27	0.68
9:g:791:HIS:C	10:I:489:ALA:HA	2.18	0.68
9:g:767:ALA:O	9:g:772:ASN:N	2.26	0.68
12:A:444:GLY:HA2	12:A:516:GLY:HA3	1.76	0.68
12:A:1484:ALA:HA	12:A:1495:ALA:HB3	1.74	0.68
4:f:273:PRO:N	4:f:273:PRO:CB	2.57	0.68
6:E:1020:PRO:N	6:E:1020:PRO:CB	2.56	0.67
12:A:288:THR:C	12:A:290:ASP:H	2.01	0.67
9:g:868:LEU:O	9:g:869:SER:C	2.38	0.67
6:E:1145:VAL:HA	6:E:1168:SER:CB	2.25	0.67
6:E:1422:THR:CB	9:G:241:ILE:CB	2.73	0.67
8:h:211:SER:CB	11:L:278:ASN:HA	2.25	0.67
10:M:642:PHE:CB	10:M:835:HIS:CB	2.73	0.67
8:h:272:THR:O	9:g:663:ALA:HB2	1.93	0.67
10:M:374:LEU:O	10:M:391:GLY:HA3	1.95	0.67
12:A:105:GLU:C	12:A:107:ALA:H	2.02	0.66
9:g:840:GLU:HA	9:g:897:LEU:HA	1.77	0.66
12:A:210:ASN:C	12:A:212:LYS:N	2.46	0.66
6:e:548:PRO:N	6:e:548:PRO:CB	2.56	0.66
12:A:105:GLU:C	12:A:107:ALA:N	2.52	0.66
12:A:1143:ASP:CB	12:A:1178:ARG:CA	2.73	0.66
2:b:315:PRO:N	2:b:315:PRO:CB	2.56	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1973:SER:HA	12:A:1975:GLN:N	2.11	0.65
6:E:1073:HIS:C	6:E:1075:TYR:N	2.52	0.65
12:A:13:LEU:CB	12:A:46:TYR:HA	2.27	0.65
12:A:1484:ALA:HB2	12:A:1495:ALA:HB1	1.78	0.65
2:b:429:GLY:C	2:b:431:GLU:H	2.04	0.65
6:E:958:TYR:CB	6:E:981:ALA:HB1	2.26	0.65
6:E:651:ALA:HB2	13:N:557:GLY:HA3	1.79	0.65
9:g:343:PHE:N	9:g:679:LEU:O	2.24	0.65
2:B:491:ALA:C	2:B:493:ASP:N	2.47	0.64
12:A:1641:ALA:HB1	12:A:1682:ALA:CA	2.24	0.64
10:M:227:GLU:O	10:M:229:GLU:N	2.29	0.64
6:e:1174:GLU:O	6:e:1175:LEU:C	2.39	0.64
7:K:1099:ALA:HB2	7:K:1118:ALA:CB	2.27	0.64
6:E:980:ILE:CB	13:N:862:GLN:CB	2.76	0.64
2:B:148:GLU:O	2:B:149:ILE:C	2.41	0.64
9:G:492:LEU:C	9:G:494:VAL:H	2.06	0.64
12:A:1971:GLY:C	12:A:1973:SER:N	2.53	0.64
6:e:1202:ALA:HA	6:e:1205:SER:CB	2.28	0.64
1:p:885:LEU:O	1:p:889:TYR:CB	2.46	0.64
1:P:898:LEU:N	1:P:911:ALA:CB	2.61	0.63
2:b:148:GLU:O	2:b:149:ILE:C	2.41	0.63
3:c:281:GLY:HA3	3:c:345:THR:O	1.99	0.63
6:E:1104:GLY:O	6:E:1105:ARG:C	2.41	0.63
12:A:681:GLY:HA2	12:A:686:VAL:CB	2.29	0.63
5:D:15:ILE:HA	5:D:30:CYS:O	1.97	0.63
2:B:595:THR:CB	2:B:637:LEU:CB	2.77	0.63
2:B:528:LEU:CB	10:M:774:THR:HA	2.29	0.63
6:E:1083:HIS:O	6:E:1088:ASN:CB	2.47	0.63
12:A:1538:LEU:C	12:A:1540:THR:H	2.05	0.63
12:A:1973:SER:HA	12:A:1974:LEU:C	2.24	0.63
9:g:751:GLN:C	9:g:753:ASN:H	2.07	0.63
12:A:894:VAL:O	12:A:897:ALA:HB3	1.99	0.63
6:e:651:ALA:HA	13:n:557:GLY:HA2	1.81	0.63
9:g:795:TRP:O	9:g:796:GLU:C	2.42	0.63
12:A:1974:LEU:C	12:A:1976:LYS:H	2.06	0.63
1:p:884:PHE:O	1:p:888:TRP:CB	2.46	0.63
9:g:476:GLN:C	9:g:478:MET:H	2.08	0.62
1:J:898:LEU:N	1:J:911:ALA:CB	2.61	0.62
6:e:549:LEU:CB	6:e:563:LEU:O	2.47	0.62
9:G:631:TYR:O	9:G:632:ARG:C	2.39	0.62
2:b:126:THR:O	2:b:130:TYR:N	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:15:ILE:CA	5:D:30:CYS:O	2.47	0.62
10:M:673:PRO:N	10:M:673:PRO:C	2.56	0.62
6:e:120:ASP:HA	6:e:705:TYR:H	1.63	0.62
12:A:1102:SER:C	12:A:1104:ILE:N	2.53	0.62
2:b:355:ILE:N	2:b:387:ALA:HB1	2.15	0.62
9:G:463:HIS:C	9:G:466:SER:H	2.06	0.61
8:h:68:PRO:O	9:g:735:ARG:HA	2.00	0.61
12:A:1990:SER:O	12:A:1994:PHE:CB	2.48	0.61
2:B:54:MET:CB	5:D:5:ARG:O	2.48	0.61
6:e:749:GLY:O	6:e:753:LEU:N	2.33	0.61
10:i:248:LEU:O	10:i:252:ASP:N	2.32	0.61
2:b:437:MET:CB	2:b:463:GLN:CB	2.78	0.61
6:E:980:ILE:HA	13:N:862:GLN:CB	2.31	0.61
12:A:1973:SER:HA	12:A:1975:GLN:CB	2.31	0.61
6:E:980:ILE:CA	13:N:862:GLN:CB	2.79	0.61
12:A:681:GLY:CA	12:A:686:VAL:CB	2.79	0.61
2:b:421:TYR:O	2:b:424:TYR:CB	2.49	0.61
6:e:1227:CYS:CB	6:e:1233:ALA:O	2.49	0.60
12:A:1473:GLY:C	12:A:1475:ALA:H	2.09	0.60
2:b:315:PRO:N	2:b:315:PRO:C	2.57	0.60
6:E:1141:VAL:O	6:E:1169:GLN:HA	2.01	0.60
6:E:1332:LEU:O	6:E:1333:LEU:C	2.44	0.60
9:g:868:LEU:HA	9:g:871:GLN:CB	2.31	0.60
12:A:1631:THR:C	12:A:1633:SER:H	2.10	0.60
6:E:1332:LEU:C	6:E:1334:ARG:N	2.56	0.60
10:i:396:CYS:C	10:i:466:ALA:CB	2.75	0.60
10:M:396:CYS:C	10:M:466:ALA:CB	2.75	0.60
6:E:1307:ASN:O	6:E:1308:LYS:C	2.45	0.59
10:I:396:CYS:C	10:I:466:ALA:CB	2.75	0.59
10:M:674:ALA:C	10:M:676:ARG:H	2.10	0.59
12:A:1226:ASN:O	12:A:1227:VAL:C	2.45	0.59
10:i:674:ALA:C	10:i:676:ARG:H	2.10	0.59
6:e:753:LEU:CB	13:n:673:ARG:CB	2.80	0.59
2:b:126:THR:O	2:b:130:TYR:CB	2.50	0.59
12:A:98:SER:CB	12:A:104:GLY:HA2	2.32	0.59
12:A:111:LEU:CB	12:A:131:ALA:HB1	2.33	0.58
9:G:392:GLU:CB	9:G:395:ALA:CB	2.81	0.58
6:E:930:ALA:O	6:E:933:VAL:CB	2.51	0.58
12:A:120:PRO:CB	12:A:1021:GLY:CA	2.79	0.58
12:A:1067:LEU:HA	12:A:1073:THR:CB	2.34	0.58
12:A:1912:LEU:O	12:A:1913:HIS:C	2.46	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:1173:LEU:HA	6:E:1177:ASP:CB	2.33	0.58
6:e:1196:PRO:O	6:e:1199:ALA:HB3	2.03	0.58
8:H:224:GLY:HA3	9:G:686:ILE:CB	2.34	0.58
9:g:751:GLN:CB	9:g:755:CYS:CA	2.81	0.58
9:g:392:GLU:CB	9:g:395:ALA:CB	2.81	0.58
10:I:642:PHE:CB	10:I:836:GLN:HA	2.33	0.58
12:A:98:SER:CA	12:A:104:GLY:CA	2.76	0.58
10:M:162:VAL:O	10:M:165:LEU:CB	2.51	0.58
9:g:847:ALA:O	9:g:848:LYS:C	2.45	0.58
5:d:4:ALA:HB1	2:b:55:TYR:CA	2.30	0.57
9:g:848:LYS:O	9:g:849:ASP:C	2.43	0.57
12:A:829:THR:C	12:A:831:ALA:H	2.11	0.57
10:i:673:PRO:N	10:i:673:PRO:C	2.56	0.57
8:H:216:ASP:CB	8:H:266:HIS:CA	2.83	0.57
12:A:585:GLY:O	12:A:586:ILE:C	2.48	0.57
12:A:1751:ALA:O	12:A:1752:MET:C	2.47	0.57
12:A:1756:CYS:O	12:A:1757:SER:C	2.45	0.57
2:B:528:LEU:CB	10:M:774:THR:CA	2.83	0.57
6:E:1218:GLY:O	6:E:1219:LEU:C	2.47	0.57
2:B:55:TYR:HA	5:D:4:ALA:HB1	1.86	0.57
6:E:1079:LEU:O	6:E:1080:TYR:C	2.46	0.57
6:e:1132:PRO:HA	6:e:1135:ALA:HB2	1.87	0.57
9:g:462:ASP:CB	10:i:317:ASP:CB	2.83	0.57
9:g:815:ILE:O	9:g:816:GLN:C	2.48	0.57
7:K:1155:GLN:O	7:K:1156:GLU:C	2.46	0.57
12:A:1011:PRO:C	12:A:1013:SER:H	2.12	0.57
12:A:1229:LEU:O	12:A:1233:VAL:CB	2.53	0.57
6:e:1201:ILE:O	6:e:1205:SER:CB	2.53	0.56
5:D:15:ILE:CB	5:D:30:CYS:O	2.52	0.56
9:G:321:TYR:O	9:G:322:LEU:C	2.48	0.56
12:A:189:LEU:O	12:A:190:ILE:C	2.48	0.56
6:e:1227:CYS:O	6:e:1230:PHE:O	2.22	0.56
9:g:343:PHE:O	9:g:680:HIS:HA	2.04	0.56
12:A:743:ARG:O	12:A:744:TYR:C	2.48	0.56
2:b:150:LEU:O	2:b:151:PHE:C	2.49	0.56
12:A:1910:TYR:O	12:A:1911:LEU:C	2.48	0.56
9:g:321:TYR:O	9:g:322:LEU:C	2.48	0.56
12:A:743:ARG:O	12:A:745:ARG:N	2.39	0.56
10:I:589:GLN:O	10:I:592:ALA:HB3	2.05	0.56
12:A:120:PRO:O	12:A:1027:ARG:N	2.39	0.56
10:i:227:GLU:C	10:i:229:GLU:H	2.14	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1538:LEU:C	12:A:1540:THR:N	2.64	0.56
6:E:967:ASP:O	6:E:969:GLY:N	2.39	0.56
6:E:1210:MET:O	6:E:1211:VAL:C	2.47	0.56
6:E:1279:ALA:O	6:E:1280:THR:C	2.48	0.56
6:e:1103:LEU:O	6:e:1104:GLY:C	2.47	0.56
8:H:224:GLY:HA2	9:G:686:ILE:CB	2.35	0.56
12:A:743:ARG:C	12:A:745:ARG:N	2.62	0.56
7:K:1140:GLU:O	7:K:1144:LYS:N	2.37	0.55
8:H:2:VAL:CB	9:G:310:SER:O	2.54	0.55
12:A:1624:GLN:O	12:A:1625:ILE:C	2.50	0.55
12:A:1289:GLU:O	12:A:1290:ILE:C	2.50	0.55
6:E:1176:ARG:O	6:E:1178:LEU:N	2.40	0.55
12:A:265:ASP:O	12:A:266:LYS:C	2.50	0.55
10:i:707:PRO:C	10:i:709:ASP:H	2.13	0.55
2:B:150:LEU:O	2:B:151:PHE:C	2.49	0.54
5:d:13:ASP:CB	5:d:33:ASP:H	2.20	0.54
10:i:707:PRO:C	10:i:709:ASP:N	2.65	0.54
12:A:1291:ILE:O	12:A:1292:LEU:C	2.50	0.54
1:p:566:ALA:HB2	1:p:573:ALA:HB1	1.90	0.54
6:E:1102:ARG:O	6:E:1103:LEU:C	2.50	0.54
8:h:211:SER:CB	11:L:278:ASN:CA	2.86	0.54
1:j:566:ALA:HB2	1:j:573:ALA:HB1	1.89	0.54
9:g:463:HIS:H	10:i:317:ASP:CB	2.20	0.54
9:g:577:TYR:C	9:g:579:GLU:H	2.16	0.54
6:E:1264:ALA:C	6:E:1266:ASN:H	2.14	0.54
6:E:1330:ALA:O	6:E:1331:GLU:C	2.51	0.54
6:E:1330:ALA:O	6:E:1332:LEU:N	2.41	0.54
12:A:1075:GLY:O	12:A:1076:PRO:C	2.51	0.54
1:P:566:ALA:HB2	1:P:573:ALA:HB1	1.89	0.54
2:b:642:ALA:HB2	6:e:1081:ALA:HB1	1.90	0.53
6:E:1305:ILE:O	6:E:1306:ILE:C	2.48	0.53
12:A:192:GLN:O	12:A:193:ILE:C	2.51	0.53
12:A:718:THR:O	12:A:719:ASN:C	2.51	0.53
1:J:566:ALA:HB2	1:J:573:ALA:HB1	1.89	0.53
12:A:67:VAL:C	12:A:69:LYS:H	2.15	0.53
6:E:1178:LEU:HA	6:E:1181:GLU:H	1.73	0.53
6:E:1247:ARG:O	6:E:1251:GLY:N	2.41	0.53
6:E:1355:ALA:HA	6:E:1359:LYS:O	2.09	0.53
9:G:237:GLY:O	9:G:238:SER:C	2.52	0.53
9:g:799:GLY:O	9:g:800:LYS:C	2.50	0.53
9:g:901:GLU:O	13:n:1000:ILE:HA	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:1099:ALA:CB	7:K:1118:ALA:HB1	2.38	0.53
12:A:157:THR:CB	12:A:237:CYS:CB	2.86	0.53
8:H:17:HIS:O	9:G:251:PHE:HA	2.09	0.53
9:g:237:GLY:O	9:g:238:SER:C	2.51	0.53
9:g:641:LEU:O	9:g:645:ASN:O	2.26	0.53
10:i:255:VAL:O	10:i:256:ARG:C	2.51	0.53
5:d:15:ILE:O	2:b:37:THR:O	2.27	0.53
9:g:237:GLY:C	9:g:239:LEU:N	2.65	0.53
5:D:102:HIS:O	5:D:103:TRP:C	2.52	0.53
10:M:255:VAL:O	10:M:256:ARG:C	2.51	0.53
5:d:9:ALA:C	5:d:11:HIS:H	2.17	0.53
6:E:980:ILE:CB	13:N:862:GLN:CA	2.87	0.53
9:G:229:GLU:O	9:G:230:LYS:C	2.52	0.53
5:d:102:HIS:O	5:d:103:TRP:C	2.52	0.52
6:E:1016:LEU:CB	6:E:1028:CYS:CB	2.87	0.52
12:A:1999:VAL:O	12:A:2003:ARG:CB	2.57	0.52
3:c:184:LEU:HA	3:c:193:LYS:O	2.09	0.52
9:g:808:VAL:O	9:g:809:ILE:C	2.49	0.52
12:A:1067:LEU:O	12:A:1074:SER:N	2.43	0.52
9:g:747:LEU:C	9:g:749:GLY:H	2.17	0.52
7:K:1123:LYS:O	7:K:1126:THR:O	2.27	0.52
10:M:555:ALA:C	10:M:557:GLU:H	2.17	0.52
2:B:46:GLU:O	2:B:47:THR:C	2.53	0.52
2:b:120:SER:O	2:b:123:THR:O	2.28	0.52
6:E:1321:ILE:O	6:E:1322:ASN:C	2.49	0.52
2:b:46:GLU:O	2:b:47:THR:C	2.53	0.52
6:E:1291:LEU:O	6:E:1292:ASP:C	2.52	0.52
10:i:555:ALA:C	10:i:557:GLU:H	2.18	0.52
2:B:508:TYR:C	2:B:510:GLU:H	2.18	0.52
6:E:1285:ARG:O	6:E:1286:LEU:C	2.52	0.52
9:g:816:GLN:O	9:g:817:GLN:O	2.28	0.52
12:A:741:PHE:O	12:A:742:LEU:C	2.51	0.52
12:A:857:GLU:O	12:A:858:ASN:C	2.53	0.52
7:K:1095:VAL:CB	7:K:1121:SER:CB	2.88	0.51
8:h:1:MET:O	9:g:312:GLU:CB	2.58	0.51
12:A:1301:PRO:C	12:A:1303:GLU:N	2.63	0.51
12:A:1048:VAL:O	12:A:1050:VAL:N	2.43	0.51
9:G:818:ASP:C	9:G:820:SER:H	2.16	0.51
12:A:1189:PHE:O	12:A:1325:ALA:HA	2.10	0.51
2:B:592:ALA:HB2	2:B:641:LEU:CA	2.35	0.51
6:e:1278:SER:C	6:e:1280:THR:H	2.18	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1142:ASP:O	12:A:1143:ASP:C	2.53	0.51
12:A:1754:GLN:O	12:A:1755:ILE:C	2.53	0.51
6:E:1280:THR:O	6:E:1282:GLU:N	2.44	0.51
10:M:589:GLN:O	10:M:592:ALA:HB3	2.11	0.51
1:J:898:LEU:CA	1:J:911:ALA:HB3	2.41	0.51
5:d:13:ASP:CB	5:d:33:ASP:CB	2.89	0.51
6:E:1141:VAL:O	6:E:1169:GLN:CB	2.59	0.51
6:e:744:ASP:C	6:e:746:ALA:H	2.17	0.51
9:g:476:GLN:C	9:g:478:MET:N	2.69	0.51
9:g:767:ALA:O	9:g:771:GLU:HA	2.10	0.51
12:A:208:LEU:CB	12:A:214:ARG:HA	2.40	0.51
12:A:735:PHE:O	12:A:736:LEU:C	2.52	0.51
10:M:373:LYS:CB	10:M:392:ASN:H	2.23	0.51
6:e:1278:SER:C	6:e:1280:THR:N	2.69	0.50
9:g:751:GLN:C	9:g:753:ASN:N	2.68	0.50
6:E:1098:GLU:O	6:E:1099:TYR:C	2.51	0.50
12:A:895:ASN:O	12:A:896:ILE:C	2.53	0.50
1:P:898:LEU:CA	1:P:911:ALA:HB3	2.41	0.50
7:K:1186:PHE:O	7:K:1187:GLY:C	2.52	0.50
9:G:666:GLU:O	9:G:667:ASN:C	2.54	0.50
9:g:477:GLU:C	9:g:480:GLU:H	2.20	0.50
12:A:187:LEU:O	12:A:188:THR:C	2.55	0.50
12:A:1974:LEU:C	12:A:1976:LYS:N	2.67	0.50
6:E:1334:ARG:O	6:E:1335:LEU:C	2.53	0.50
6:e:1104:GLY:O	6:e:1105:ARG:C	2.54	0.50
8:H:216:ASP:CB	8:H:266:HIS:HA	2.42	0.50
12:A:737:ARG:O	12:A:738:ASP:C	2.53	0.50
12:A:1473:GLY:C	12:A:1475:ALA:N	2.69	0.50
1:j:851:CYS:C	1:j:853:PHE:N	2.67	0.50
10:M:556:LYS:O	10:M:558:GLU:N	2.38	0.50
6:E:793:ASN:CB	6:E:880:ARG:O	2.60	0.50
9:G:237:GLY:C	9:G:239:LEU:N	2.65	0.50
9:g:666:GLU:O	9:g:667:ASN:C	2.54	0.50
10:i:885:LYS:HA	1:j:964:ALA:CB	2.38	0.50
12:A:1484:ALA:HA	12:A:1495:ALA:CB	2.41	0.50
6:e:466:ALA:O	6:e:469:ARG:CB	2.60	0.50
9:g:811:MET:O	9:g:812:LEU:C	2.55	0.50
12:A:193:ILE:O	12:A:194:ASP:C	2.55	0.50
12:A:1049:ALA:HB2	12:A:1054:PRO:C	2.37	0.50
12:A:1538:LEU:O	12:A:1540:THR:N	2.45	0.50
10:M:298:GLN:O	10:M:302:LEU:O	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:1303:HIS:O	6:E:1304:CYS:C	2.54	0.49
10:M:291:ASN:C	10:M:293:LEU:N	2.65	0.49
1:p:851:CYS:C	1:p:853:PHE:N	2.67	0.49
12:A:183:THR:O	12:A:186:ILE:N	2.45	0.49
12:A:327:ALA:HB1	12:A:360:ALA:HA	1.93	0.49
10:M:245:VAL:O	10:M:249:PHE:N	2.46	0.49
3:c:183:ILE:O	3:c:195:TRP:N	2.46	0.49
10:I:241:GLU:O	10:I:242:LYS:C	2.55	0.49
9:G:461:GLY:C	10:I:317:ASP:CB	2.85	0.49
12:A:1290:ILE:O	12:A:1291:ILE:C	2.56	0.49
6:E:865:LEU:C	6:E:867:PRO:N	2.70	0.49
9:G:853:GLN:O	9:G:857:ALA:N	2.43	0.49
12:A:897:ALA:O	12:A:899:TYR:N	2.46	0.49
6:E:1278:SER:O	6:E:1279:ALA:C	2.56	0.49
9:g:817:GLN:O	9:g:819:GLU:N	2.46	0.49
6:E:1145:VAL:N	6:E:1168:SER:CB	2.75	0.49
7:K:1111:ARG:HA	7:K:1114:TYR:CB	2.43	0.49
7:K:1229:SER:CB	7:K:1237:ARG:CB	2.90	0.49
9:G:499:GLN:CB	9:G:502:ARG:CB	2.90	0.49
9:G:767:ALA:O	9:G:771:GLU:HA	2.09	0.49
10:I:291:ASN:C	10:I:293:LEU:N	2.66	0.49
10:i:556:LYS:O	10:i:558:GLU:N	2.38	0.49
9:g:765:ALA:HB2	9:g:852:ALA:CB	2.43	0.49
10:i:291:ASN:C	10:i:293:LEU:N	2.65	0.49
12:A:15:GLY:C	12:A:17:TYR:H	2.20	0.49
12:A:279:LEU:O	12:A:280:ASP:C	2.55	0.49
12:A:1102:SER:O	12:A:1105:SER:N	2.46	0.49
6:E:1130:ILE:O	6:E:1131:ARG:C	2.55	0.49
2:b:149:ILE:O	2:b:150:LEU:C	2.56	0.48
9:g:450:ILE:O	9:g:451:SER:C	2.56	0.48
10:i:291:ASN:O	10:i:292:THR:C	2.56	0.48
12:A:1125:SER:C	12:A:1127:ASN:N	2.70	0.48
1:p:697:LEU:C	1:p:699:SER:N	2.70	0.48
6:e:930:ALA:O	6:e:933:VAL:CB	2.61	0.48
6:E:1082:PHE:O	6:E:1083:HIS:C	2.56	0.48
6:e:1134:TYR:C	6:e:1136:TRP:N	2.70	0.48
6:e:1192:ALA:HB1	6:e:1199:ALA:HB1	1.94	0.48
12:A:1631:THR:C	12:A:1633:SER:N	2.70	0.48
6:E:980:ILE:CB	13:N:862:GLN:HA	2.43	0.48
6:E:1050:TYR:CB	6:E:1054:HIS:HA	2.44	0.48
12:A:120:PRO:O	12:A:1026:PRO:C	2.56	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:288:THR:C	12:A:290:ASP:N	2.67	0.48
12:A:339:GLY:O	12:A:341:SER:N	2.46	0.48
12:A:1143:ASP:CB	12:A:1178:ARG:HA	2.43	0.48
5:d:164:SER:O	5:d:186:SER:HA	2.14	0.48
6:e:758:GLN:HA	13:n:795:SER:CB	2.44	0.48
12:A:1283:SER:O	12:A:1284:TRP:C	2.56	0.48
5:d:187:ASP:O	5:d:188:ASP:C	2.56	0.48
6:E:1111:ARG:O	6:E:1112:GLY:C	2.55	0.48
10:i:373:LYS:CB	10:i:392:ASN:H	2.26	0.48
12:A:897:ALA:C	12:A:899:TYR:N	2.70	0.48
6:e:1343:GLU:O	6:e:1346:ALA:N	2.45	0.48
8:H:267:VAL:HA	8:H:277:ALA:O	2.14	0.48
12:A:1250:ARG:O	12:A:1251:PRO:C	2.55	0.48
1:p:854:ASP:O	1:p:858:GLN:CB	2.62	0.48
1:j:867:SER:CB	1:j:910:ALA:HA	2.44	0.48
13:N:897:HIS:O	13:N:902:ASN:CB	2.62	0.48
2:B:478:ASN:O	3:C:122:HIS:CB	2.62	0.48
6:E:651:ALA:HB1	13:N:557:GLY:HA3	1.93	0.48
6:E:967:ASP:C	6:E:969:GLY:N	2.71	0.48
6:E:1030:ARG:CB	1:p:701:SER:CB	2.92	0.48
9:g:223:GLN:O	9:g:302:PHE:CB	2.62	0.48
12:A:67:VAL:C	12:A:69:LYS:N	2.70	0.48
12:A:1620:LEU:O	12:A:1621:PRO:C	2.54	0.48
5:D:189:SER:O	5:D:190:SER:C	2.57	0.48
2:B:149:ILE:O	2:B:150:LEU:C	2.56	0.48
6:e:1179:GLU:O	6:e:1180:LYS:C	2.56	0.48
12:A:483:ARG:O	12:A:484:PRO:C	2.57	0.48
5:D:164:SER:O	5:D:186:SER:HA	2.14	0.48
12:A:197:ASN:O	12:A:198:GLU:C	2.57	0.47
12:A:1641:ALA:O	12:A:1682:ALA:HB1	2.14	0.47
12:A:1734:ASP:O	12:A:1735:ASP:C	2.53	0.47
9:g:318:LEU:O	9:g:319:GLN:C	2.58	0.47
9:g:868:LEU:O	9:g:871:GLN:N	2.47	0.47
12:A:1142:ASP:C	12:A:1144:MET:N	2.69	0.47
5:d:189:SER:O	5:d:190:SER:C	2.57	0.47
9:G:492:LEU:C	9:G:494:VAL:N	2.69	0.47
12:A:1102:SER:O	12:A:1103:GLU:C	2.53	0.47
6:E:1180:LYS:O	6:E:1181:GLU:C	2.55	0.47
12:A:736:LEU:O	12:A:737:ARG:C	2.56	0.47
5:D:192:ASN:O	5:D:193:ILE:C	2.56	0.47
12:A:813:LEU:O	12:A:814:GLU:C	2.56	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:829:THR:C	12:A:831:ALA:N	2.71	0.47
5:D:187:ASP:O	5:D:188:ASP:C	2.56	0.47
1:p:867:SER:CB	1:p:910:ALA:HA	2.44	0.47
6:E:1089:TYR:O	6:E:1092:ALA:HB3	2.14	0.47
12:A:947:GLY:O	12:A:948:PHE:C	2.58	0.47
10:M:162:VAL:O	10:M:165:LEU:N	2.47	0.47
6:E:1202:ALA:O	6:E:1204:SER:N	2.47	0.47
9:g:463:HIS:O	9:g:464:ARG:C	2.58	0.47
9:g:800:LYS:O	9:g:801:VAL:C	2.57	0.47
1:j:854:ASP:O	1:j:858:GLN:CB	2.62	0.47
6:e:207:ILE:HA	6:e:208:PRO:C	2.39	0.47
12:A:94:ALA:CB	12:A:105:GLU:CB	2.93	0.47
6:e:59:ARG:O	6:e:61:PHE:N	2.48	0.47
1:p:1130:ALA:HA	1:P:577:SER:CB	2.45	0.47
4:F:274:GLY:HA2	6:E:968:VAL:HA	1.96	0.47
5:d:190:SER:O	5:d:191:PRO:C	2.58	0.47
6:e:744:ASP:C	6:e:746:ALA:N	2.73	0.47
9:G:318:LEU:O	9:G:319:GLN:C	2.58	0.47
12:A:734:GLN:O	12:A:735:PHE:C	2.57	0.47
12:A:960:LEU:O	12:A:961:LEU:C	2.58	0.47
12:A:1692:ASP:HA	12:A:1696:ASN:HA	1.97	0.47
12:A:1898:THR:O	12:A:1899:CYS:C	2.56	0.47
10:i:703:PHE:O	10:i:706:ILE:O	2.32	0.46
9:G:856:MET:O	9:G:857:ALA:C	2.56	0.46
6:E:1229:THR:C	6:E:1231:LYS:H	2.24	0.46
6:E:1289:SER:C	6:E:1291:LEU:N	2.73	0.46
6:E:1182:TYR:O	6:E:1183:VAL:C	2.54	0.46
6:E:1197:SER:C	6:E:1199:ALA:N	2.69	0.46
8:h:5:ILE:CB	9:g:308:LYS:H	2.28	0.46
12:A:1100:GLU:O	12:A:1101:GLU:C	2.59	0.46
2:B:126:THR:O	2:B:130:TYR:N	2.47	0.46
6:E:1127:LEU:O	6:E:1128:ARG:C	2.55	0.46
2:b:138:SER:O	2:b:142:LEU:CB	2.63	0.46
6:e:1132:PRO:CA	6:e:1135:ALA:HB2	2.46	0.46
8:H:17:HIS:HA	9:G:248:GLY:O	2.16	0.46
9:g:866:VAL:O	9:g:869:SER:CB	2.63	0.46
12:A:1048:VAL:C	12:A:1050:VAL:N	2.72	0.46
6:E:1020:PRO:N	6:E:1020:PRO:C	2.63	0.46
7:K:1099:ALA:CB	7:K:1118:ALA:CB	2.94	0.46
12:A:1229:LEU:O	12:A:1230:LEU:C	2.59	0.46
6:e:1051:VAL:C	6:e:1053:LEU:H	2.24	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:1078:LEU:O	6:e:1079:LEU:C	2.58	0.46
12:A:1320:ILE:C	12:A:1322:ASP:H	2.24	0.46
12:A:1618:ILE:O	12:A:1619:LEU:C	2.59	0.46
1:j:915:ALA:O	1:j:916:HIS:C	2.59	0.46
6:E:967:ASP:C	6:E:969:GLY:H	2.22	0.46
5:D:190:SER:O	5:D:191:PRO:C	2.57	0.46
10:M:291:ASN:O	10:M:292:THR:C	2.56	0.46
5:d:9:ALA:C	5:d:11:HIS:N	2.74	0.46
6:e:765:ALA:C	6:e:767:LEU:H	2.23	0.46
9:g:847:ALA:C	9:g:849:ASP:N	2.65	0.46
9:g:868:LEU:O	9:g:871:GLN:CB	2.64	0.46
11:L:632:LEU:C	11:L:634:LYS:H	2.23	0.46
6:E:1230:PHE:O	6:E:1231:LYS:C	2.58	0.45
6:E:1332:LEU:H	6:E:1334:ARG:H	1.64	0.45
7:K:1159:THR:C	7:K:1164:HIS:HA	2.40	0.45
7:K:1164:HIS:O	7:K:1165:HIS:C	2.59	0.45
9:G:313:GLN:O	9:G:314:LYS:C	2.59	0.45
9:G:606:LYS:O	9:G:609:SER:N	2.49	0.45
9:g:243:MET:O	9:g:247:MET:CB	2.64	0.45
10:I:291:ASN:O	10:I:292:THR:C	2.56	0.45
12:A:809:GLU:O	12:A:810:SER:C	2.58	0.45
6:E:1280:THR:O	6:E:1281:ASP:C	2.59	0.45
7:K:1331:TYR:O	7:K:1332:VAL:C	2.57	0.45
9:g:606:LYS:O	9:g:609:SER:N	2.49	0.45
12:A:184:ASN:O	12:A:185:LYS:C	2.56	0.45
12:A:582:PRO:O	12:A:583:LEU:C	2.58	0.45
12:A:1143:ASP:CB	12:A:1178:ARG:H	2.23	0.45
6:E:1332:LEU:O	6:E:1335:LEU:N	2.50	0.45
9:G:752:TRP:HA	9:G:755:CYS:CB	2.46	0.45
12:A:811:PRO:O	12:A:812:MET:C	2.58	0.45
12:A:1130:ARG:O	12:A:1134:GLN:N	2.43	0.45
10:I:139:GLY:N	10:I:197:THR:HA	2.31	0.45
12:A:956:GLU:O	12:A:957:ALA:C	2.59	0.45
12:A:1900:LEU:O	12:A:1901:TYR:C	2.59	0.45
6:E:955:LEU:HA	6:E:985:ALA:HB2	1.99	0.45
9:G:450:ILE:O	9:G:451:SER:C	2.56	0.45
9:g:447:GLY:O	9:g:448:GLY:C	2.58	0.45
9:g:804:ASP:O	9:g:805:TYR:C	2.56	0.45
5:d:192:ASN:O	5:d:193:ILE:C	2.56	0.45
6:E:1218:GLY:O	6:E:1220:PHE:N	2.49	0.45
8:H:2:VAL:CB	9:G:309:LEU:C	2.90	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:447:GLY:O	9:G:448:GLY:C	2.58	0.45
12:A:1134:GLN:O	12:A:1135:ARG:C	2.58	0.45
6:e:754:LEU:CB	13:n:792:SER:CB	2.95	0.45
9:G:235:GLY:O	9:G:236:ARG:C	2.60	0.45
9:G:312:GLU:O	9:G:313:GLN:C	2.59	0.45
12:A:1011:PRO:C	12:A:1013:SER:N	2.73	0.45
2:b:296:ARG:O	2:b:300:THR:N	2.43	0.45
6:e:1202:ALA:O	6:e:1203:GLY:C	2.60	0.45
12:A:188:THR:O	12:A:189:LEU:C	2.58	0.45
12:A:804:HIS:O	12:A:805:HIS:C	2.58	0.45
12:A:1217:LYS:HA	12:A:1222:GLN:O	2.17	0.45
1:p:897:LYS:C	1:p:899:LEU:H	2.24	0.45
2:b:468:CYS:CB	2:b:491:ALA:HB2	2.47	0.45
6:E:1278:SER:O	6:E:1280:THR:N	2.50	0.45
1:P:896:GLY:O	1:P:911:ALA:CB	2.63	0.45
1:J:896:GLY:O	1:J:911:ALA:CB	2.63	0.45
6:E:1116:GLN:O	6:E:1117:VAL:C	2.59	0.45
7:K:1184:LYS:O	7:K:1185:MET:C	2.60	0.45
1:J:922:LEU:N	10:I:909:PRO:CB	2.79	0.44
7:K:1110:GLN:O	7:K:1114:TYR:N	2.49	0.44
12:A:797:PRO:O	12:A:798:PRO:C	2.59	0.44
12:A:456:LEU:C	12:A:458:LEU:N	2.74	0.44
12:A:1286:GLN:O	12:A:1287:LEU:C	2.59	0.44
6:E:1063:SER:O	6:E:1064:ARG:C	2.59	0.44
12:A:980:THR:O	12:A:981:LYS:C	2.59	0.44
5:D:15:ILE:HA	5:D:31:SER:CA	2.45	0.44
6:E:1129:LEU:O	6:E:1131:ARG:N	2.50	0.44
9:g:235:GLY:O	9:g:236:ARG:C	2.60	0.44
9:g:812:LEU:O	9:g:813:ASN:C	2.60	0.44
12:A:1199:LEU:CB	12:A:1202:PHE:O	2.65	0.44
2:B:149:ILE:O	2:B:150:LEU:O	2.35	0.44
6:E:1289:SER:C	6:E:1291:LEU:H	2.24	0.44
8:h:2:VAL:CB	9:g:309:LEU:CB	2.92	0.44
12:A:415:ALA:O	12:A:416:ARG:C	2.61	0.44
12:A:520:GLY:O	12:A:523:CYS:N	2.50	0.44
12:A:1625:ILE:O	12:A:1626:CYS:C	2.57	0.44
2:b:413:SER:O	2:b:415:TRP:N	2.51	0.44
9:G:460:SER:O	10:I:317:ASP:CB	2.65	0.44
1:p:697:LEU:C	1:p:699:SER:H	2.24	0.44
6:E:1113:LEU:O	6:E:1114:GLN:C	2.60	0.44
6:E:1191:LEU:C	6:E:1193:LYS:N	2.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:1223:ALA:O	6:E:1224:ILE:C	2.55	0.44
7:K:1108:LEU:O	7:K:1112:LEU:N	2.51	0.44
7:K:1111:ARG:O	7:K:1115:ILE:N	2.49	0.44
12:A:1996:GLN:CB	10:M:283:TYR:HA	2.48	0.44
13:n:897:HIS:O	13:n:902:ASN:CB	2.65	0.44
2:b:149:ILE:O	2:b:150:LEU:O	2.35	0.43
6:E:58:ARG:O	6:E:59:ARG:C	2.60	0.43
6:e:1142:SER:C	6:e:1144:ALA:H	2.26	0.43
7:K:1159:THR:O	7:K:1160:ARG:C	2.57	0.43
9:G:491:LYS:C	9:G:493:GLN:N	2.74	0.43
10:I:158:PRO:C	10:I:160:SER:N	2.75	0.43
10:i:873:SER:CB	1:j:956:GLY:HA3	2.48	0.43
12:A:98:SER:HA	12:A:104:GLY:N	2.32	0.43
12:A:196:ASN:O	12:A:197:ASN:C	2.61	0.43
12:A:998:ASN:O	12:A:999:LEU:C	2.61	0.43
6:e:1324:TYR:O	6:e:1328:ASP:N	2.39	0.43
12:A:98:SER:CB	12:A:104:GLY:C	2.91	0.43
12:A:967:ALA:O	12:A:968:GLU:C	2.59	0.43
6:E:1332:LEU:O	6:E:1336:TYR:N	2.36	0.43
6:e:1051:VAL:C	6:e:1053:LEU:N	2.76	0.43
12:A:1054:PRO:C	12:A:1056:LEU:H	2.25	0.43
12:A:1970:PHE:C	12:A:1972:GLU:H	2.26	0.43
1:p:884:PHE:O	1:p:888:TRP:N	2.42	0.43
1:p:915:ALA:O	1:p:916:HIS:C	2.59	0.43
6:E:862:LEU:O	6:E:866:TRP:N	2.47	0.43
8:H:68:PRO:O	9:G:735:ARG:HA	2.17	0.43
9:g:384:GLU:O	9:g:388:GLY:CA	2.66	0.43
12:A:1048:VAL:C	12:A:1050:VAL:H	2.25	0.43
2:b:395:ASN:C	2:b:397:ARG:N	2.74	0.43
6:E:1104:GLY:O	6:E:1106:GLU:N	2.52	0.43
12:A:96:ILE:O	12:A:100:LEU:N	2.52	0.43
12:A:258:VAL:O	12:A:259:GLU:C	2.60	0.43
12:A:1627:GLN:O	12:A:1628:LEU:C	2.60	0.43
10:M:373:LYS:O	10:M:392:ASN:N	2.50	0.43
6:E:1289:SER:O	6:E:1291:LEU:N	2.51	0.43
6:E:1279:ALA:C	6:E:1282:GLU:H	2.26	0.43
12:A:681:GLY:HA3	12:A:686:VAL:CB	2.49	0.43
9:G:384:GLU:O	9:G:388:GLY:CA	2.66	0.43
12:A:1285:ARG:O	12:A:1286:GLN:C	2.60	0.43
6:E:1124:LEU:O	6:E:1125:ASN:C	2.62	0.43
7:K:1227:SER:O	7:K:1228:ASP:C	2.60	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:2:VAL:CB	9:G:309:LEU:HA	2.49	0.43
6:E:1214:LEU:C	6:E:1216:GLN:N	2.74	0.42
6:e:862:LEU:O	6:e:866:TRP:N	2.48	0.42
6:E:1192:ALA:HB2	6:E:1199:ALA:HA	2.01	0.42
7:K:1158:LEU:HA	7:K:1161:GLN:CB	2.49	0.42
9:g:802:TYR:O	9:g:803:LEU:C	2.62	0.42
12:A:743:ARG:O	12:A:746:THR:N	2.52	0.42
12:A:1337:VAL:O	12:A:1338:PHE:C	2.62	0.42
2:B:55:TYR:HA	5:D:4:ALA:CB	2.49	0.42
6:E:1209:GLU:O	6:E:1210:MET:C	2.62	0.42
6:E:1279:ALA:HA	6:E:1282:GLU:CB	2.48	0.42
9:g:746:LEU:O	9:g:749:GLY:O	2.37	0.42
12:A:935:THR:O	12:A:936:GLN:C	2.62	0.42
6:E:1227:CYS:O	6:E:1228:GLN:C	2.60	0.42
6:e:743:GLY:C	6:e:745:MET:H	2.27	0.42
12:A:210:ASN:O	12:A:212:LYS:N	2.52	0.42
2:b:609:LYS:C	2:b:611:GLU:N	2.77	0.42
6:e:1246:ILE:C	6:e:1248:LEU:N	2.77	0.42
11:L:636:PRO:O	11:L:639:VAL:N	2.53	0.42
12:A:185:LYS:O	12:A:186:ILE:C	2.63	0.42
12:A:1766:LEU:O	12:A:1770:ASN:N	2.50	0.42
2:B:505:LEU:O	2:B:506:LYS:C	2.58	0.42
5:d:279:SER:CB	5:d:298:ASP:CA	2.97	0.42
6:e:969:GLY:HA3	4:f:275:LYS:CA	2.44	0.42
7:K:1272:VAL:O	7:K:1276:SER:N	2.52	0.42
11:L:630:TYR:O	11:L:633:ALA:HB3	2.19	0.42
10:M:674:ALA:C	10:M:676:ARG:N	2.75	0.42
6:E:1141:VAL:O	6:E:1169:GLN:CA	2.67	0.42
6:E:1253:GLU:O	6:E:1256:GLN:N	2.53	0.42
7:K:1092:ALA:O	7:K:1096:ALA:CB	2.68	0.42
12:A:896:ILE:O	12:A:897:ALA:C	2.61	0.42
12:A:1988:VAL:C	12:A:1990:SER:H	2.27	0.42
2:b:413:SER:C	2:b:415:TRP:N	2.77	0.42
6:E:1033:VAL:O	6:E:1034:VAL:C	2.62	0.42
6:e:1192:ALA:HA	6:e:1199:ALA:HA	2.02	0.42
9:g:457:ALA:HA	9:g:461:GLY:HA3	2.02	0.42
12:A:1911:LEU:O	12:A:1912:LEU:C	2.63	0.42
2:b:609:LYS:O	2:b:611:GLU:N	2.53	0.42
9:G:232:VAL:O	9:G:233:THR:C	2.63	0.42
9:G:345:PRO:O	9:G:346:ASN:C	2.62	0.42
9:g:224:GLU:O	9:g:226:VAL:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:1291:LEU:O	6:E:1293:LYS:N	2.52	0.41
9:g:873:PRO:N	9:g:873:PRO:C	2.63	0.41
6:E:59:ARG:O	6:E:61:PHE:N	2.53	0.41
6:E:1076:TYR:O	6:E:1077:GLU:C	2.63	0.41
8:h:266:HIS:CB	9:g:252:ARG:HA	2.50	0.41
9:g:433:GLY:O	9:g:434:PRO:C	2.64	0.41
12:A:926:ILE:O	12:A:927:GLN:C	2.63	0.41
12:A:1226:ASN:C	12:A:1228:LYS:N	2.77	0.41
6:E:1038:GLU:C	6:E:1040:SER:H	2.27	0.41
9:g:854:SER:O	9:g:855:GLU:C	2.62	0.41
12:A:1507:ARG:O	10:M:134:GLN:CB	2.67	0.41
1:J:897:LYS:C	1:J:911:ALA:CB	2.93	0.41
2:b:315:PRO:N	2:b:316:THR:N	2.68	0.41
9:G:349:VAL:O	9:G:350:ALA:CB	2.68	0.41
9:G:433:GLY:O	9:G:434:PRO:C	2.64	0.41
9:g:794:ASP:O	9:g:795:TRP:C	2.61	0.41
10:I:396:CYS:CB	10:I:466:ALA:HB3	2.51	0.41
10:i:396:CYS:CB	10:i:466:ALA:HB3	2.51	0.41
12:A:733:LEU:O	12:A:734:GLN:C	2.64	0.41
2:B:148:GLU:O	2:B:149:ILE:O	2.39	0.41
7:K:1159:THR:C	7:K:1161:GLN:N	2.77	0.41
7:K:1189:TYR:O	7:K:1190:ALA:C	2.63	0.41
9:g:499:GLN:CB	9:g:502:ARG:CB	2.99	0.41
9:g:879:ASP:O	9:g:880:SER:C	2.63	0.41
12:A:105:GLU:O	12:A:107:ALA:N	2.53	0.41
1:J:580:SER:CA	1:j:1130:ALA:HB1	2.45	0.41
12:A:1114:MET:O	12:A:1115:LYS:C	2.62	0.41
6:e:651:ALA:HA	13:n:557:GLY:CA	2.50	0.41
7:K:1185:MET:O	7:K:1186:PHE:C	2.62	0.41
9:G:457:ALA:O	9:G:458:GLN:C	2.62	0.41
12:A:1125:SER:O	12:A:1126:LEU:C	2.63	0.41
10:M:396:CYS:CB	10:M:466:ALA:HB3	2.51	0.41
1:P:897:LYS:C	1:P:911:ALA:CB	2.93	0.41
9:G:392:GLU:O	9:G:393:LEU:C	2.64	0.41
2:b:429:GLY:C	2:b:431:GLU:N	2.69	0.41
6:E:843:GLN:C	6:E:845:GLN:H	2.29	0.41
7:K:1109:LYS:C	7:K:1112:LEU:H	2.29	0.41
9:g:392:GLU:O	9:g:393:LEU:C	2.64	0.41
10:I:139:GLY:CA	10:I:197:THR:HA	2.51	0.41
10:i:674:ALA:C	10:i:676:ARG:N	2.75	0.41
12:A:166:VAL:O	12:A:167:VAL:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:194:ASP:O	12:A:195:VAL:C	2.63	0.41
12:A:422:MET:O	12:A:426:ASN:N	2.54	0.41
12:A:523:CYS:O	12:A:524:ALA:C	2.64	0.41
12:A:855:GLN:O	12:A:856:LYS:C	2.61	0.41
12:A:1048:VAL:O	12:A:1049:ALA:C	2.63	0.41
12:A:1085:GLN:O	12:A:1086:ASP:C	2.63	0.41
12:A:1281:LEU:O	12:A:1282:GLU:C	2.63	0.41
6:E:1264:ALA:C	6:E:1266:ASN:N	2.79	0.41
9:G:767:ALA:O	9:G:771:GLU:C	2.64	0.41
10:i:885:LYS:CB	1:j:964:ALA:O	2.69	0.41
12:A:524:ALA:O	12:A:525:HIS:C	2.62	0.41
6:E:1084:ILE:O	6:E:1086:ARG:N	2.54	0.40
6:E:1096:MET:O	6:E:1097:PHE:C	2.60	0.40
9:g:245:LEU:C	9:g:247:MET:N	2.77	0.40
3:c:13:LYS:O	3:c:37:SER:HA	2.21	0.40
6:E:1280:THR:C	6:E:1282:GLU:N	2.78	0.40
12:A:191:SER:O	12:A:192:GLN:C	2.63	0.40
12:A:1284:TRP:O	12:A:1285:ARG:C	2.64	0.40
1:J:577:SER:CB	1:j:1130:ALA:HA	2.51	0.40
2:b:413:SER:C	2:b:415:TRP:H	2.29	0.40
6:E:1064:ARG:CB	1:p:703:ASP:N	2.84	0.40
6:E:1309:LEU:C	6:E:1311:SER:N	2.78	0.40
6:e:843:GLN:C	6:e:845:GLN:H	2.29	0.40
6:e:1134:TYR:C	6:e:1136:TRP:H	2.29	0.40
12:A:810:SER:O	12:A:811:PRO:C	2.63	0.40
12:A:1970:PHE:C	12:A:1972:GLU:N	2.78	0.40
7:K:1334:GLU:O	7:K:1336:SER:N	2.55	0.40
12:A:644:LEU:CB	12:A:703:ALA:HB1	2.52	0.40
12:A:1030:LEU:O	12:A:1031:HIS:C	2.64	0.40
1:J:898:LEU:CA	1:J:911:ALA:CB	3.00	0.40
6:e:744:ASP:O	6:e:746:ALA:N	2.54	0.40
7:K:1203:ILE:O	7:K:1204:HIS:C	2.64	0.40
9:g:793:GLN:N	10:I:489:ALA:HB1	2.36	0.40
10:I:759:ASN:CB	11:L:798:GLY:HA3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	1011/1140 (89%)	920 (91%)	70 (7%)	21 (2%)	5	29
1	P	1011/1140 (89%)	920 (91%)	70 (7%)	21 (2%)	5	29
1	j	983/1140 (86%)	896 (91%)	68 (7%)	19 (2%)	6	31
1	p	983/1140 (86%)	899 (92%)	65 (7%)	19 (2%)	6	31
2	B	624/653 (96%)	585 (94%)	23 (4%)	16 (3%)	4	25
2	b	634/653 (97%)	584 (92%)	33 (5%)	17 (3%)	4	24
3	C	339/375 (90%)	322 (95%)	14 (4%)	3 (1%)	14	50
3	c	342/375 (91%)	327 (96%)	12 (4%)	3 (1%)	14	50
4	F	316/326 (97%)	307 (97%)	7 (2%)	2 (1%)	21	59
4	f	319/326 (98%)	308 (97%)	8 (2%)	3 (1%)	14	50
5	D	310/360 (86%)	286 (92%)	20 (6%)	4 (1%)	9	41
5	d	316/360 (88%)	291 (92%)	20 (6%)	5 (2%)	7	36
6	E	1355/1435 (94%)	1184 (87%)	110 (8%)	61 (4%)	2	16
6	e	1296/1435 (90%)	1197 (92%)	71 (6%)	28 (2%)	5	28
7	K	324/1388 (23%)	287 (89%)	27 (8%)	10 (3%)	3	21
8	H	304/320 (95%)	290 (95%)	10 (3%)	4 (1%)	9	41
8	h	305/320 (95%)	293 (96%)	10 (3%)	2 (1%)	18	55
9	G	614/923 (66%)	511 (83%)	79 (13%)	24 (4%)	2	18
9	g	666/923 (72%)	536 (80%)	92 (14%)	38 (6%)	1	13
10	I	794/916 (87%)	751 (95%)	32 (4%)	11 (1%)	9	39
10	M	794/916 (87%)	749 (94%)	33 (4%)	12 (2%)	8	38
10	i	794/916 (87%)	750 (94%)	34 (4%)	10 (1%)	9	41
11	L	639/820 (78%)	623 (98%)	14 (2%)	2 (0%)	36	72
11	O	48/820 (6%)	48 (100%)	0	0	100	100
12	A	1776/2011 (88%)	1558 (88%)	167 (9%)	51 (3%)	3	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	N	914/2408 (38%)	886 (97%)	24 (3%)	4 (0%)	30	67
13	n	896/2408 (37%)	867 (97%)	25 (3%)	4 (0%)	30	67
All	All	18707/25947 (72%)	17175 (92%)	1138 (6%)	394 (2%)	8	29

All (394) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	252	THR
1	J	538	GLU
1	J	561	SER
1	J	567	GLU
1	J	574	ALA
1	J	609	ARG
1	J	851	CYS
1	J	1066	GLU
2	B	39	TYR
2	B	40	GLN
2	B	51	CYS
2	B	585	GLN
2	B	622	ASP
4	F	253	ARG
2	b	39	TYR
2	b	40	GLN
2	b	610	LEU
3	c	130	PRO
6	E	866	TRP
6	E	867	PRO
6	E	883	GLN
6	E	968	VAL
6	E	1052	ASN
6	E	1053	LEU
6	E	1068	VAL
6	E	1108	ARG
6	E	1130	ILE
6	E	1137	ILE
6	E	1138	VAL
6	E	1140	PRO
6	E	1141	VAL
6	E	1174	GLU
6	E	1176	ARG
6	E	1177	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	E	1219	LEU
6	E	1233	ALA
6	E	1268	LEU
6	E	1269	ALA
6	E	1271	VAL
6	E	1281	ASP
6	E	1331	GLU
6	E	1369	PRO
6	E	1432	PRO
6	e	866	TRP
6	e	867	PRO
6	e	986	SER
6	e	1131	ARG
6	e	1132	PRO
6	e	1174	GLU
6	e	1315	PRO
6	e	1432	PRO
4	f	253	ARG
4	f	273	PRO
7	K	1107	SER
7	K	1335	PRO
9	G	350	ALA
9	G	372	VAL
9	G	473	VAL
9	G	476	GLN
9	G	626	PRO
9	g	226	VAL
9	g	348	GLY
9	g	500	GLU
9	g	578	LEU
9	g	626	PRO
9	g	739	ARG
9	g	817	GLN
9	g	818	ASP
9	g	873	PRO
9	g	880	SER
9	g	881	SER
10	I	156	GLU
10	I	160	SER
10	I	232	PHE
10	I	289	TRP
10	I	589	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	I	650	ALA
10	i	232	PHE
10	i	288	TYR
10	i	650	ALA
12	A	183	THR
12	A	184	ASN
12	A	287	GLY
12	A	289	ASP
12	A	322	SER
12	A	484	PRO
12	A	582	PRO
12	A	637	PRO
12	A	715	SER
12	A	727	PRO
12	A	777	PRO
12	A	898	ARG
12	A	1128	ARG
12	A	1176	VAL
12	A	1291	ILE
12	A	1355	PRO
12	A	1696	ASN
12	A	1772	PRO
12	A	1991	ARG
10	M	232	PHE
10	M	288	TYR
10	M	589	GLN
10	M	650	ALA
10	M	707	PRO
1	p	538	GLU
1	p	561	SER
1	p	567	GLU
1	p	574	ALA
1	p	606	LEU
1	p	609	ARG
1	p	1066	GLU
1	j	538	GLU
1	j	561	SER
1	j	567	GLU
1	j	574	ALA
1	j	606	LEU
1	j	609	ARG
1	j	1066	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	252	THR
1	P	538	GLU
1	P	561	SER
1	P	567	GLU
1	P	575	GLY
1	P	609	ARG
1	P	851	CYS
1	P	1066	GLU
13	n	337	THR
13	N	337	THR
1	J	575	GLY
2	B	38	LEU
2	B	91	GLY
2	B	149	ILE
2	B	150	LEU
2	B	335	ALA
2	B	390	LEU
3	C	53	PHE
5	d	103	TRP
5	d	265	LYS
2	b	38	LEU
2	b	91	GLY
2	b	149	ILE
2	b	150	LEU
2	b	414	LEU
2	b	548	GLN
3	c	53	PHE
6	E	688	ALA
6	E	967	ASP
6	E	1031	GLN
6	E	1040	SER
6	E	1084	ILE
6	E	1205	SER
6	E	1231	LYS
6	E	1274	THR
6	E	1277	SER
6	E	1332	LEU
6	e	1143	GLY
7	K	1164	HIS
9	G	227	PRO
9	G	460	SER
9	G	511	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	G	625	THR
9	G	671	TRP
9	G	739	ARG
9	g	511	GLY
9	g	625	THR
9	g	671	TRP
9	g	886	PRO
10	i	156	GLU
10	i	557	GLU
11	L	772	LEU
12	A	724	LEU
12	A	744	TYR
12	A	870	SER
12	A	922	CYS
12	A	995	LYS
12	A	1620	LEU
12	A	1911	LEU
5	D	103	TRP
5	D	265	LYS
10	M	156	GLU
10	M	228	GLU
10	M	557	GLU
1	p	575	GLY
1	p	904	SER
1	j	575	GLY
1	j	904	SER
1	P	574	ALA
1	J	198	SER
1	J	560	ALA
1	J	571	GLU
1	J	742	ILE
1	J	751	THR
1	J	852	ASP
2	B	49	ALA
2	b	49	ALA
2	b	64	TYR
2	b	549	GLU
6	E	60	ASN
6	E	844	LEU
6	E	1085	TYR
6	E	1109	THR
6	E	1135	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	E	1144	ALA
6	E	1196	PRO
6	E	1197	SER
6	E	1290	TYR
6	E	1318	ASN
6	E	1395	GLU
6	e	41	ASN
6	e	277	GLY
6	e	844	LEU
6	e	1052	ASN
6	e	1105	ARG
6	e	1140	PRO
6	e	1253	GLU
7	K	1151	GLN
7	K	1157	THR
8	H	55	GLY
9	G	303	LYS
9	G	594	SER
9	G	719	CYS
8	h	55	GLY
9	g	227	PRO
9	g	303	LYS
9	g	317	GLU
9	g	594	SER
9	g	632	ARG
9	g	752	TRP
9	g	753	ASN
9	g	819	GLU
9	g	869	SER
10	i	228	GLU
12	A	119	GLN
12	A	127	ARG
12	A	425	GLY
12	A	457	ALA
12	A	577	HIS
12	A	725	ARG
12	A	830	TYR
12	A	1036	ILE
12	A	1474	THR
12	A	1539	LEU
12	A	1975	GLN
1	p	198	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	p	560	ALA
1	p	571	GLU
1	p	608	SER
1	p	742	ILE
1	p	751	THR
1	j	198	SER
1	j	560	ALA
1	j	571	GLU
1	j	608	SER
1	j	742	ILE
1	j	751	THR
1	P	198	SER
1	P	560	ALA
1	P	571	GLU
1	P	742	ILE
1	P	751	THR
1	P	852	ASP
13	n	342	GLY
13	n	570	GLU
13	N	342	GLY
13	N	570	GLU
2	B	148	GLU
2	B	300	THR
3	C	11	SER
3	C	78	VAL
2	b	148	GLU
2	b	622	ASP
3	c	188	SER
6	E	807	VAL
6	E	809	LYS
6	E	1175	LEU
6	E	1330	ALA
6	E	1397	ASN
6	e	60	ASN
6	e	1071	MET
6	e	1135	ALA
6	e	1207	ALA
6	e	1267	GLN
7	K	1108	LEU
7	K	1128	MET
9	G	645	ASN
9	g	646	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	g	797	THR
9	g	898	PRO
9	g	902	ASP
10	I	470	PRO
10	I	620	GLY
10	i	470	PRO
10	i	620	GLY
11	L	427	GLU
12	A	719	ASN
12	A	775	PRO
12	A	997	PRO
12	A	1230	LEU
12	A	1685	PRO
5	D	280	GLN
10	M	470	PRO
10	M	620	GLY
1	J	355	PRO
1	J	570	PRO
2	B	45	SER
5	d	10	ASP
5	d	280	GLN
2	b	45	SER
2	b	383	GLN
2	b	430	ARG
6	E	1048	PHE
6	E	1172	ILE
6	E	1230	PHE
6	E	1267	GLN
6	E	1329	ALA
6	e	491	ASP
6	e	744	ASP
6	e	1103	LEU
6	e	1279	ALA
7	K	1192	PRO
8	H	46	GLY
8	H	172	SER
9	G	230	LYS
9	G	310	SER
9	G	589	PRO
9	G	646	TYR
8	h	46	GLY
9	g	310	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	g	350	ALA
9	g	589	PRO
10	I	556	LYS
10	I	590	GLU
10	i	462	SER
12	A	58	PRO
12	A	189	LEU
12	A	521	PRO
12	A	967	ALA
12	A	1846	PRO
10	M	462	SER
1	p	301	ASP
1	p	355	PRO
1	p	570	PRO
1	j	301	ASP
1	j	355	PRO
1	j	570	PRO
1	P	355	PRO
1	P	570	PRO
1	J	301	ASP
1	J	536	ASP
1	J	1103	LEU
2	B	580	LEU
6	E	277	GLY
6	E	841	ALA
6	E	1301	TYR
6	e	841	ALA
7	K	1260	PRO
8	H	5	ILE
9	G	448	GLY
9	G	600	VAL
9	G	754	PRO
9	g	221	ARG
9	g	448	GLY
9	g	600	VAL
9	g	845	TYR
10	I	462	SER
10	i	291	ASN
12	A	190	ILE
10	M	291	ASN
1	p	1103	LEU
1	j	1103	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	301	ASP
1	P	536	ASP
1	P	1103	LEU
13	n	341	ARG
13	N	341	ARG
1	J	604	VAL
7	K	1106	ILE
1	P	604	VAL
6	E	1218	GLY
6	e	1130	ILE
9	G	512	THR
9	G	872	GLN
9	g	512	THR
4	F	298	VAL
6	e	1317	PRO
4	f	298	VAL
9	g	801	VAL
12	A	57	PRO
12	A	340	ILE
5	d	45	VAL
6	E	1314	VAL
9	g	373	VAL
12	A	520	GLY
5	D	45	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

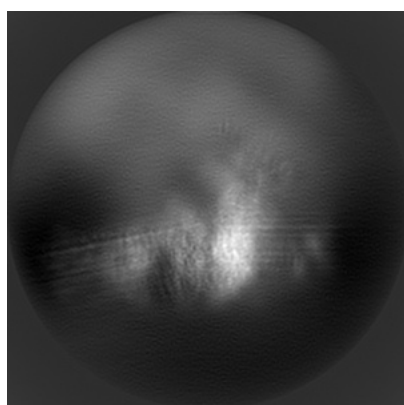
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32394. These allow visual inspection of the internal detail of the map and identification of artifacts.

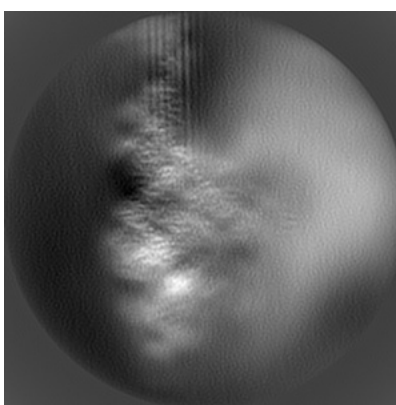
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

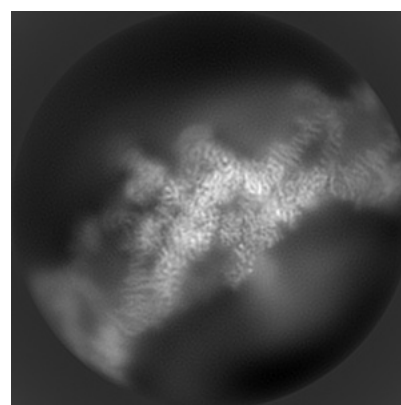
6.1.1 Primary map



X



Y

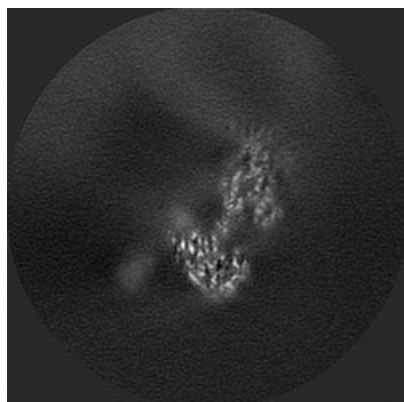


Z

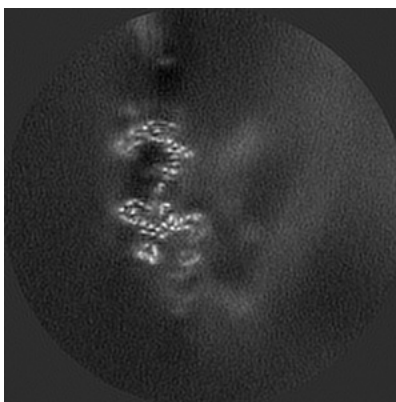
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

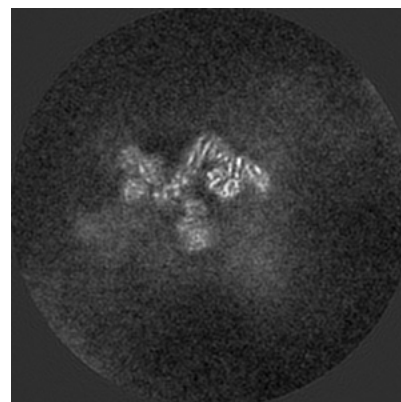
6.2.1 Primary map



X Index: 100



Y Index: 100

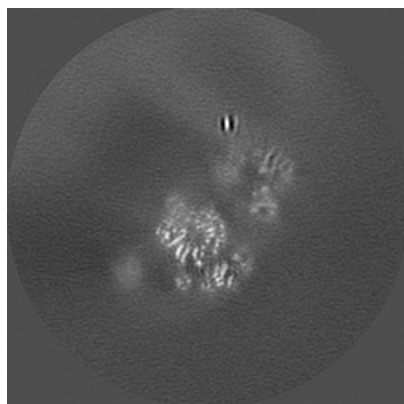


Z Index: 100

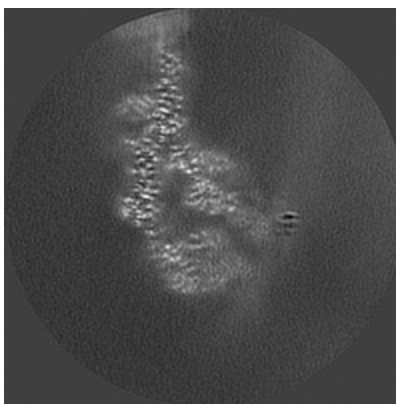
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

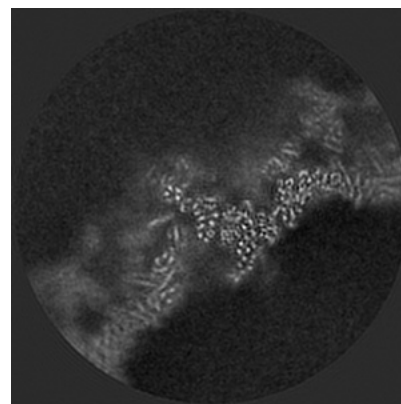
6.3.1 Primary map



X Index: 94



Y Index: 113

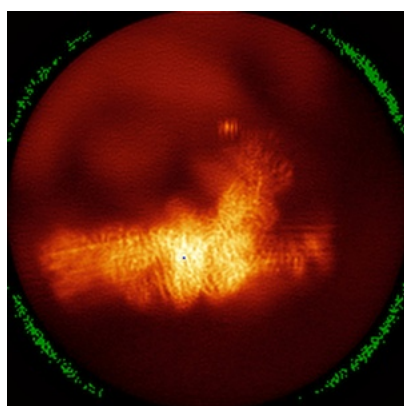


Z Index: 79

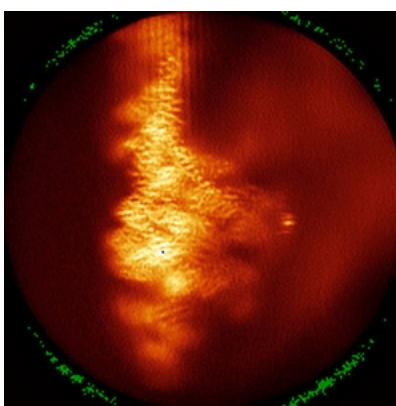
The images above show the largest variance slices of the map in three orthogonal directions.

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

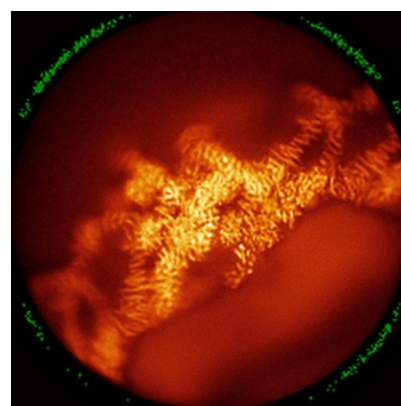
6.4.1 Primary map



X



Y

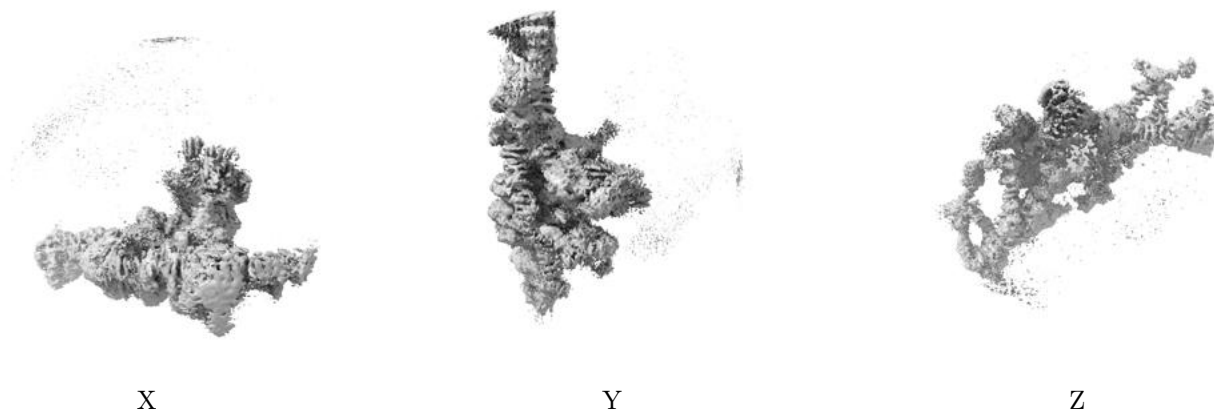


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

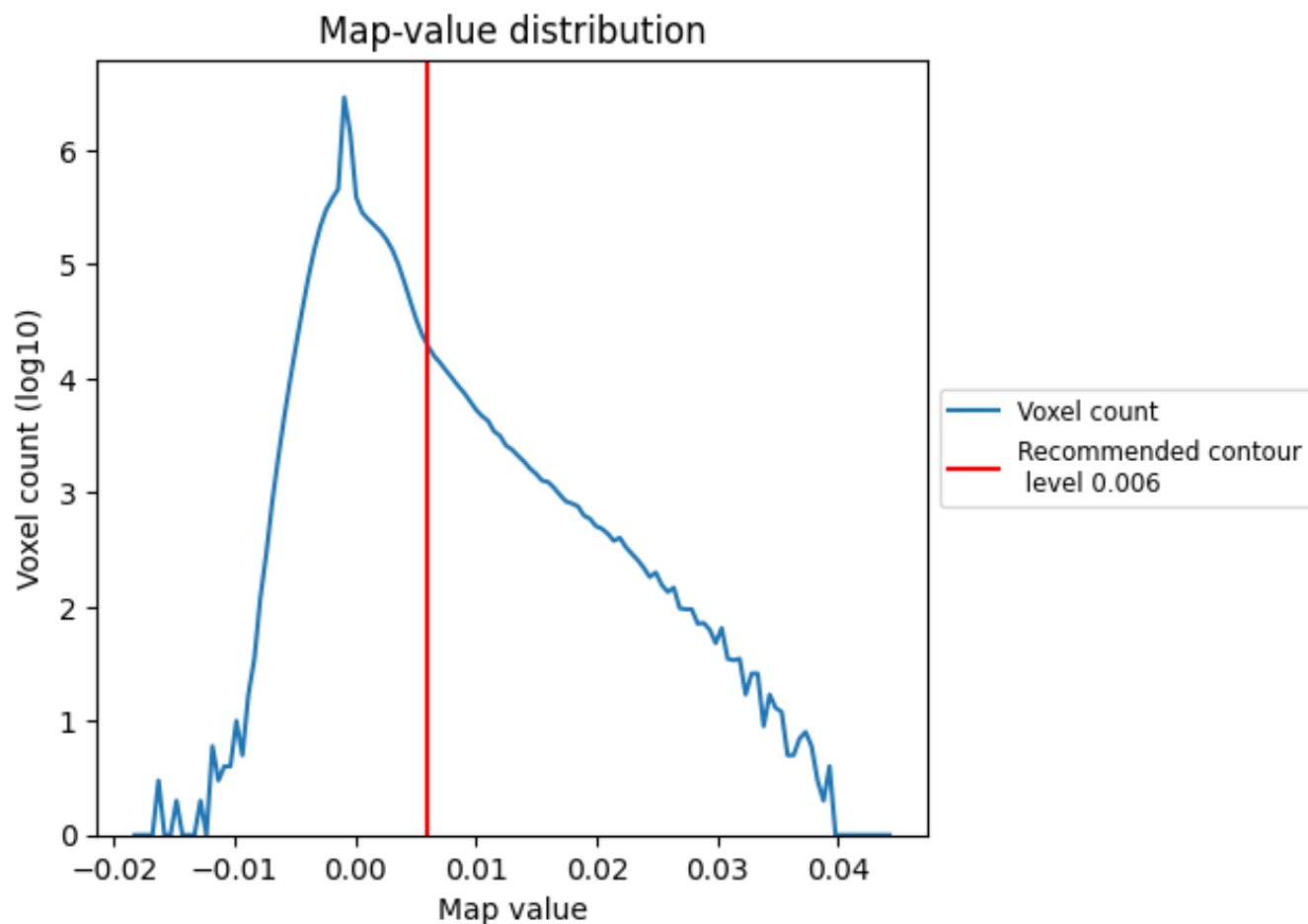
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

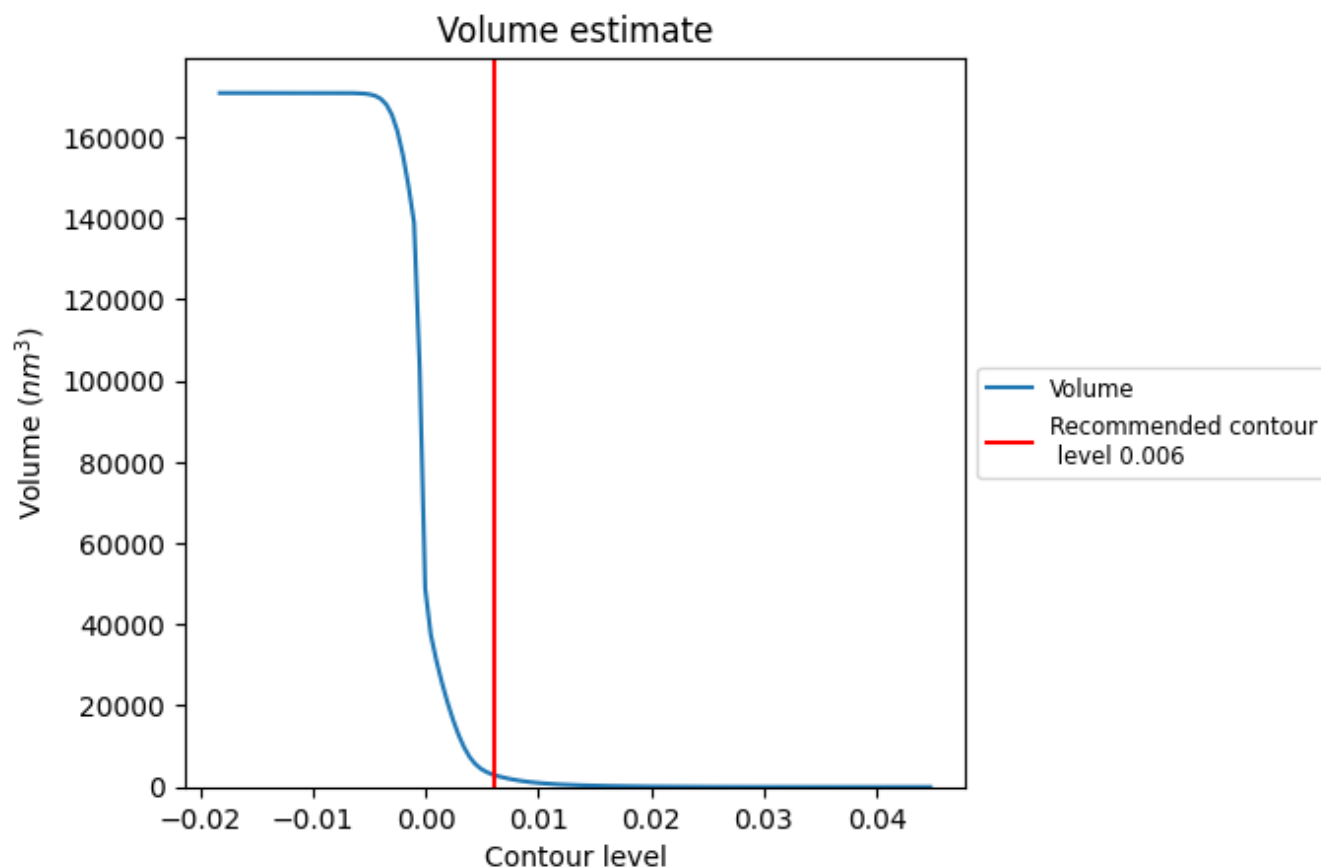
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

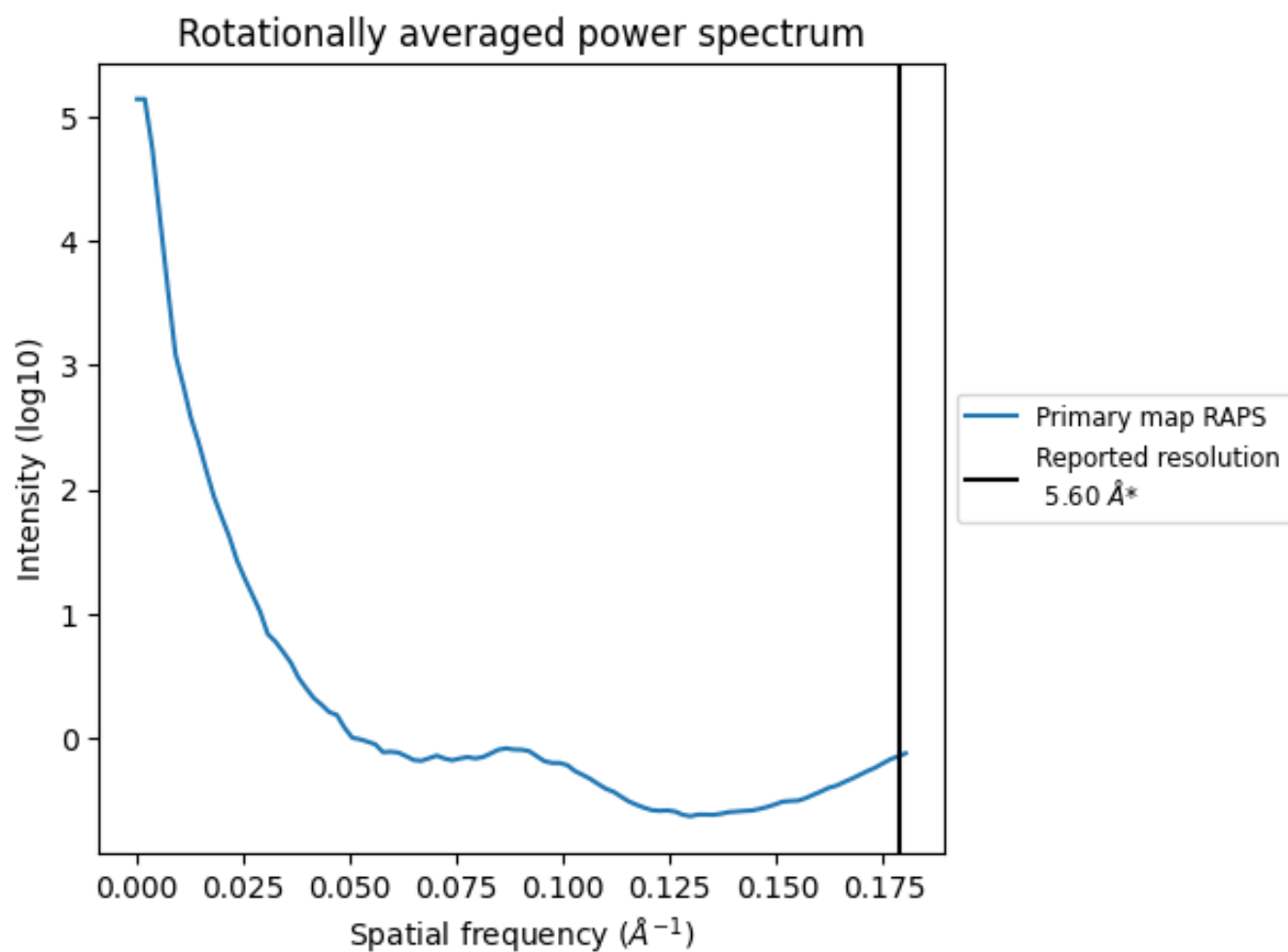
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3013 nm³; this corresponds to an approximate mass of 2722 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 0.179 Å⁻¹

8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32394 and PDB model 7WB4. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

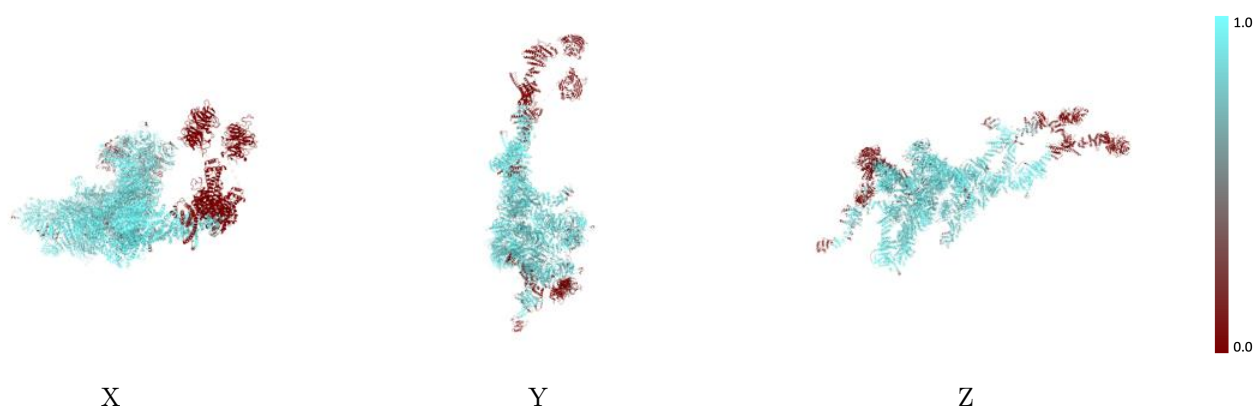
This section was not generated.

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



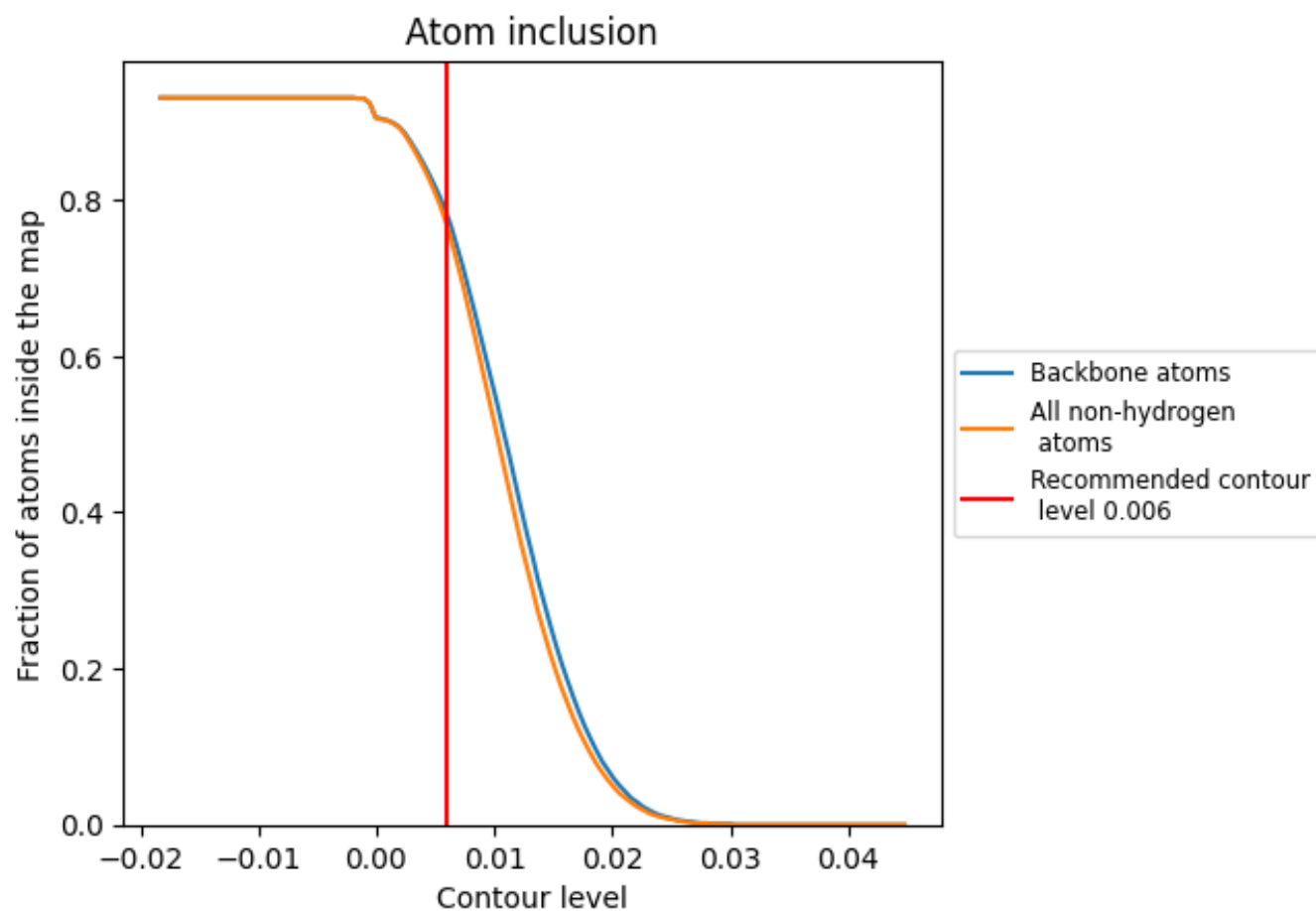
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7670	 0.2140
A	 0.9890	 0.2680
B	 0.9770	 0.2570
C	 0.9810	 0.2870
D	 0.9860	 0.2990
E	 0.8980	 0.2630
F	 0.9940	 0.2890
G	 0.9620	 0.2710
H	 0.9700	 0.2820
I	 0.9110	 0.2350
J	 0.2330	 0.0770
K	 0.8820	 0.2440
L	 0.9320	 0.2370
M	 0.9480	 0.2380
N	 0.1220	 0.0990
O	 1.0000	 0.2640
P	 0.4010	 0.1390
b	 0.9010	 0.2240
c	 0.9570	 0.2740
d	 0.9750	 0.2970
e	 0.9360	 0.2520
f	 0.9990	 0.2810
g	 0.9640	 0.2650
h	 0.9760	 0.2660
i	 0.6230	 0.1640
j	 0.0000	 -0.0030
n	 0.8760	 0.2050
p	 0.8320	 0.2360

