



Full wwPDB EM Validation Report ⓘ

Dec 31, 2024 – 06:32 AM EST

PDB ID : 8HLZ
EMDB ID : EMD-34886
Title : F8-A22-E4 complex of MPXV in hexameric form
Authors : Li, Y.N.; Shen, Y.P.; Hu, Z.W.; Yan, R.H.
Deposited on : 2022-12-02
Resolution : 3.50 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

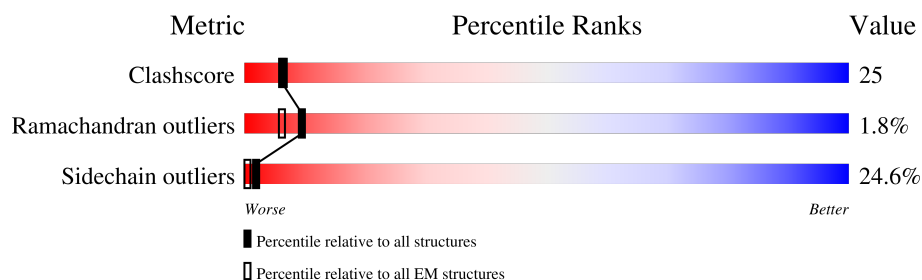
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	C	426	<div> <div>14%</div> <div>41% 38% 8% 13%</div> </div>
1	F	426	<div> <div>17%</div> <div>41% 38% 8% 13%</div> </div>
2	B	218	<div> <div>77%</div> <div>41% 44% 15%</div> </div>
2	E	218	<div> <div>41% 42% 17%</div> </div>
3	A	1006	<div> <div>45%</div> <div>45% 35% 12% 8%</div> </div>
3	D	1006	<div> <div>45%</div> <div>45% 35% 12% 8%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24718 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 DNA polymerase processivity factor component A20.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	370	Total	C	N	O	S	0	0
			3020	1937	495	578	10		
1	C	370	Total	C	N	O	S	0	0
			3020	1937	495	578	10		

- Molecule 2 is a protein called E4R.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	218	Total	C	N	O	S	0	0
			1772	1149	292	325	6		
2	B	218	Total	C	N	O	S	0	0
			1772	1149	292	325	6		

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	929	Total	C	N	O	S	0	0
			7567	4835	1262	1420	50		
3	A	929	Total	C	N	O	S	0	0
			7567	4835	1262	1420	50		

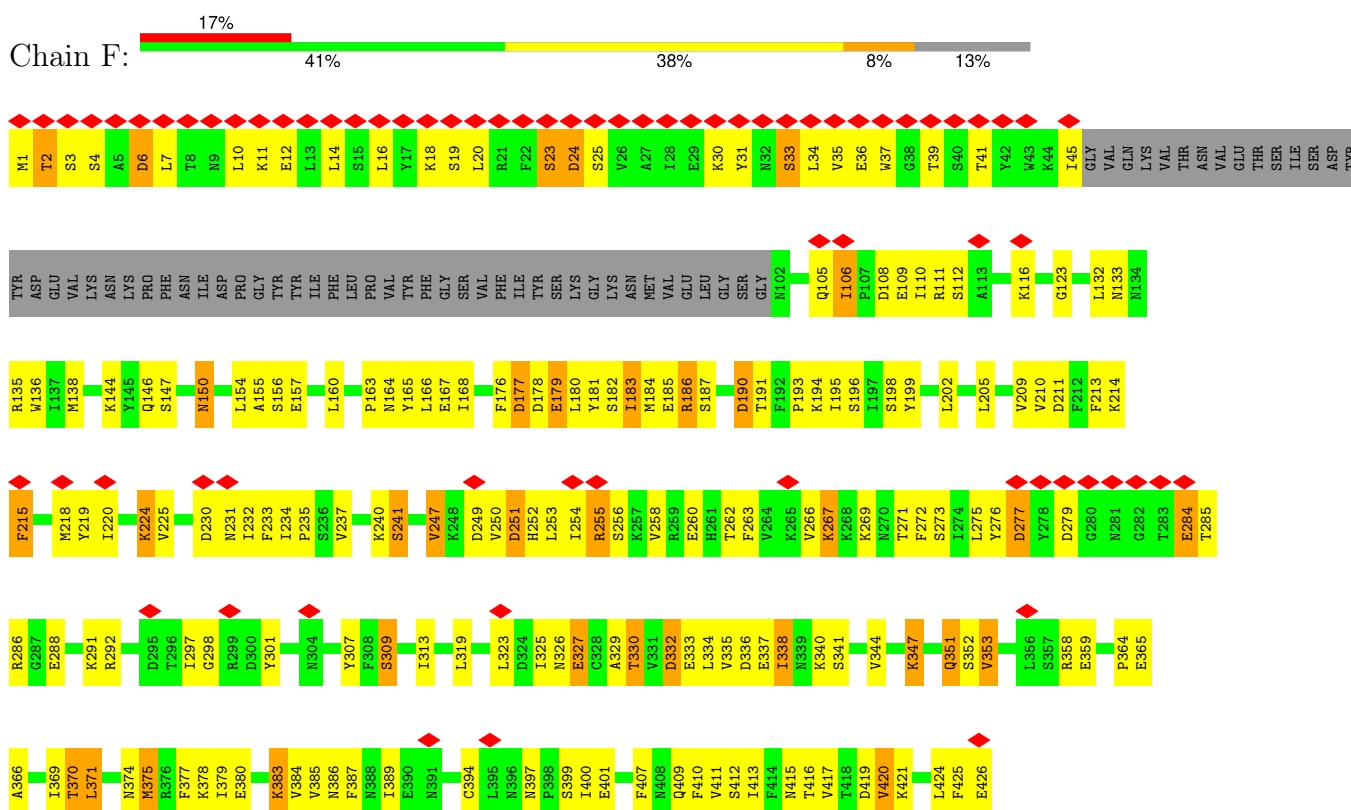
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	108	PHE	LEU	conflict	UNP A0A2L0AR76
A	108	PHE	LEU	conflict	UNP A0A2L0AR76

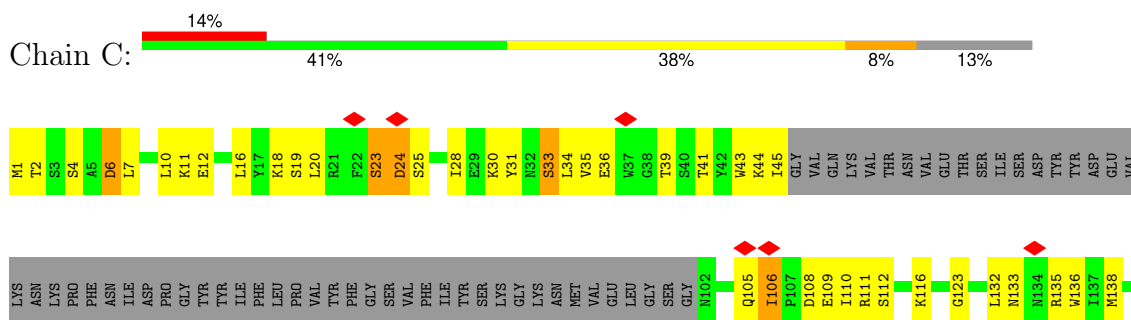
3 Residue-property plots

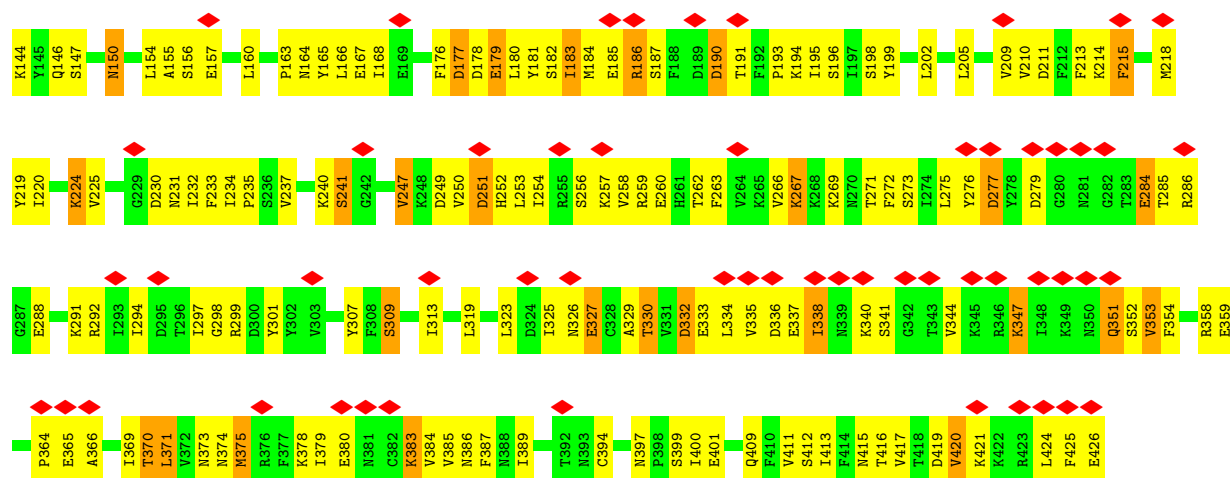
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: DNA polymerase processivity factor component A20



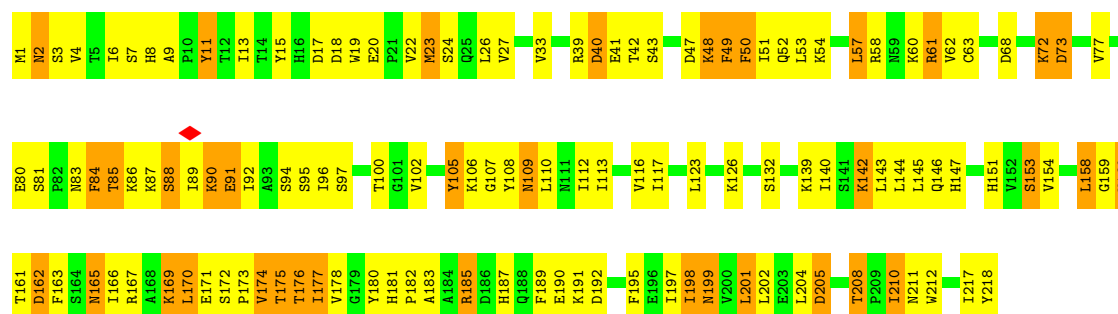
- Molecule 1: DNA polymerase processivity factor component A20





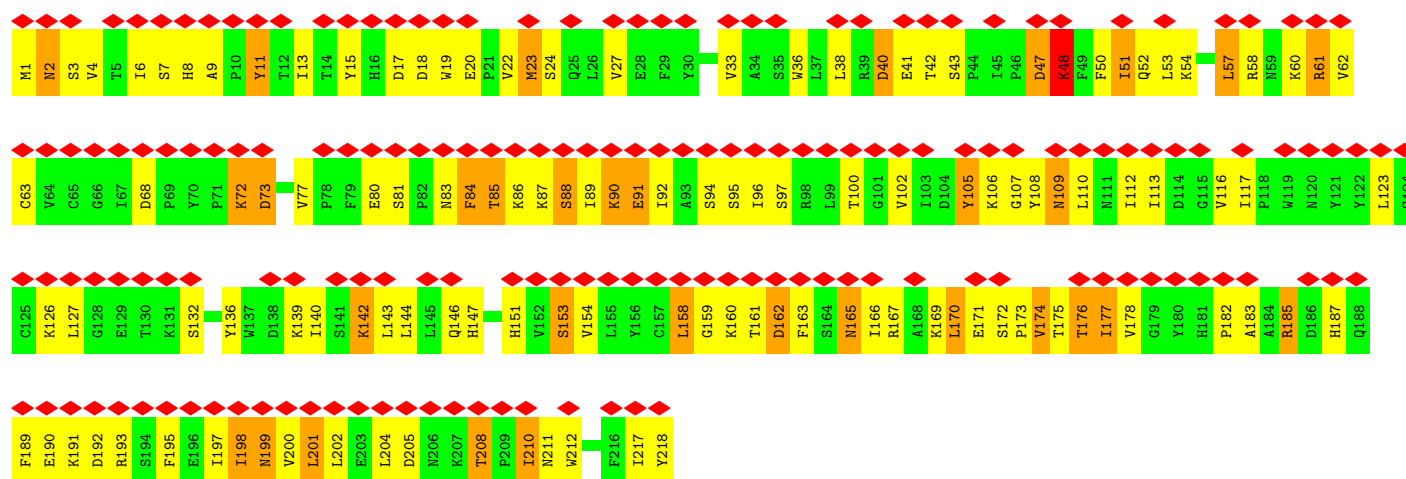
• Molecule 2: E4R

Chain E: 41% 42% 17%



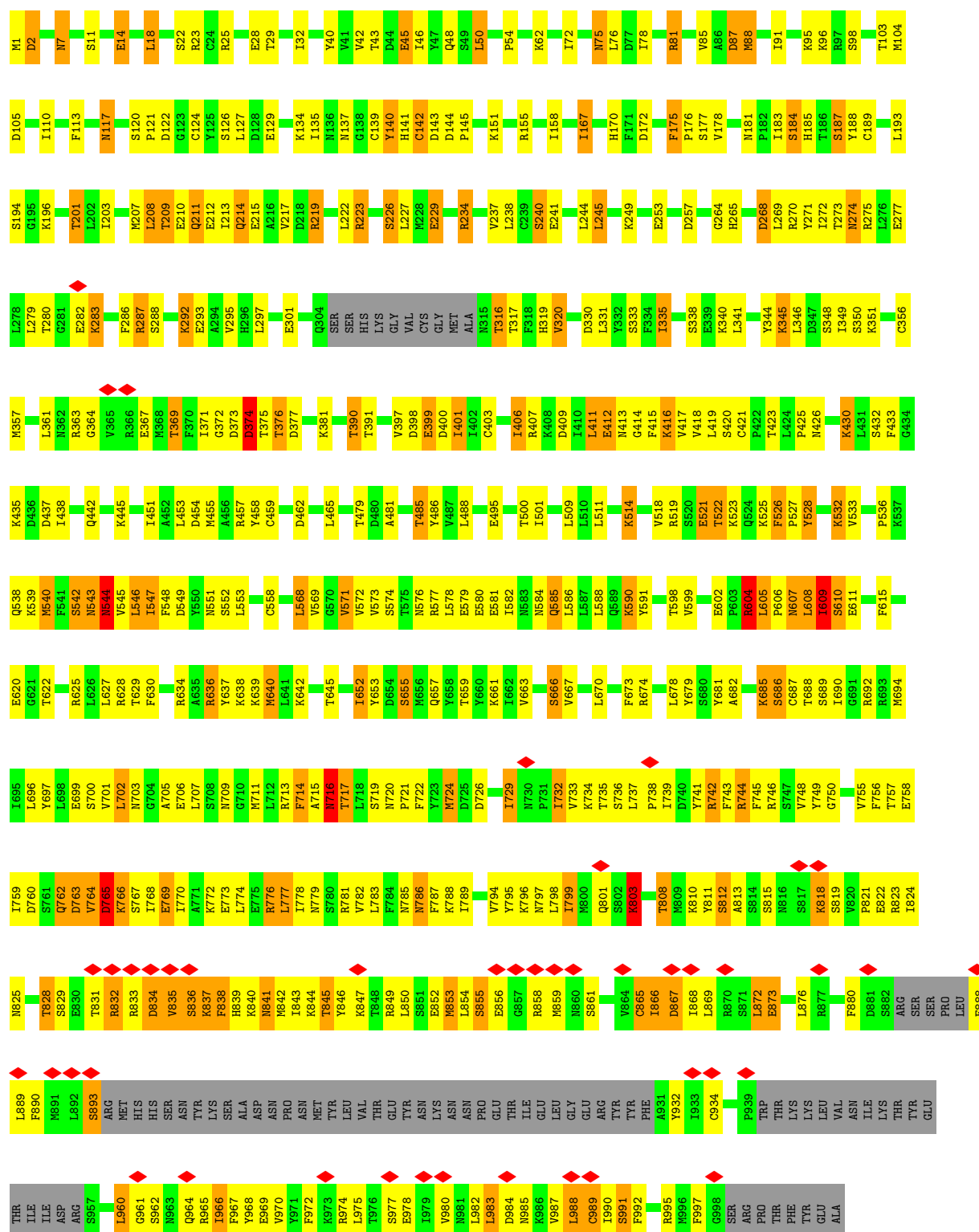
• Molecule 2: E4R

Chain B: 41% 44% 15%



• Molecule 3: DNA polymerase

Chain D: 45% 35% 12% 8%



L889	F890	M891	L892	S893	ARG	MET	HIS	HIS	SER	ASN	TYR	LYS	SER	ALA	ASP	ASN	PRO	ASN	MET	TYR	VAL	THR	GLU	TYR	ASN	LYS	ASN	ASN	PRO	GLU	THR	ILE	GLU	LEU	GLY	ARG	TYR	PHE	A931	Y932	I933	C934	P935	A936	N937	V938	P939	TRP	THR	LYS	LYS	LEU	VAL	ASN	ILE	LYS								
S829	E830	T831	R832	R833	R834	V835	K836	K837	F838	H839	K840	N841	M842	I843	K844	T845	T846	K847	T848	R849	L850	S851	M852	M853	L854	S855	E856	G857	R858	L859	M860	S861	M862	Q863	V864	C865	I866	D867	I868	L869	R870	S871	L872	E873	T874	D875	L876	R877	S878	S879	F880	D881	S882	ARG	SER	SER	PRO	LEU	E888					
G704	A705	E706	L707	S708	N709	G710	M711	L712	R713	F714	A715	N716	T717	L718	S719	N720	F721	F722	Y723	M724	D725	T726	R727	I728	I729	N730	F731	T732	V733	K734	T735	S736	L737	F738	I739	D740	Y741	T808	M809	F743	R744	F745	R746	S747	Y749	G750	V755	F756	T757	E758	I759	D760	S761	Q762	I763	V764	D765	K766						
S767	I768	E769	I770	A771	K772	E773	L774	E775	R776	I777	N778	S779	R780	R781	V782	L783	F784	N785	N786	F787	T788	I789	A793	V794	K795	N796	L797	L798	I799	M800	Q801	S802	K803	K804	K805	Y806	T807	T808	M809	F743	R744	F745	R746	S747	Y749	G750	V755	F756	T757	E758	I759	D760	S761	Q762	I763	V764	D765	K766						
R636	Y637	K638	K639	M640	L641	K642	Q643	A644	T645	S646	A651	I652	Y653	D654	S655	M656	Q657	T658	T659	T660	K661	V662	V663	S666	V667	L670	F673	B674	N675	L678	V679	S680	L681	L682	F683	K684	C685	I686	D687	I688	L689	R690	R691	R692	R693	M694	T695	L696	V697	L698	E699	S700	W701	L702	N703									
G704	A705	E706	L707	S708	N709	G710	M711	L712	R713	F714	A715	N716	T717	L718	S719	N720	F721	F722	Y723	M724	D725	T726	R727	I728	I729	N730	F731	T732	V733	K734	T735	S736	L737	F738	I739	D740	Y741	T808	M809	F743	R744	F745	R746	S747	Y749	G750	V755	F756	T757	E758	I759	D760	S761	Q762	I763	V764	D765	K766						
S767	I768	E769	I770	A771	K772	E773	L774	E775	R776	I777	N778	S779	R780	R781	V782	L783	F784	N785	N786	F787	T788	I789	A793	V794	K795	N796	L797	L798	I799	M800	Q801	S802	K803	K804	K805	Y806	T807	T808	M809	F743	R744	F745	R746	S747	Y749	G750	V755	F756	T757	E758	I759	D760	S761	Q762	I763	V764	D765	K766						
S829	E830	T831	R832	R833	R834	V835	K836	K837	F838	H839	K840	N841	M842	I843	K844	T845	T846	K847	T848	R849	L850	S851	M852	M853	L854	S855	E856	G857	R858	L859	M860	S861	M862	Q863	V864	C865	I866	D867	I868	L869	R870	S871	L872	E873	T874	D875	L876	R877	S878	S879	F880	D881	S882	ARG	SER	SER	PRO	LEU	E888					
K79	D80	R81	S84	V85	A86	D87	M88	V89	L90	I91	E92	K95	K96	R97	S98	I99	Q100	N101	A102	M104	D105	I110	F113	N117	G118	D122	G123	I125	S126	L127	D128	E129	Q130	Y131	L132	T133	K134	I135	N136	M137	G138	C139	Y140	H141	C142	D143	D144	P145	R146	N147	C148													
F149	A150	K151	E152	I153	P154	F155	F156	D157	I158	P159	R160	S161	Y162	I167	E168	C169	H170	F171	D172	K173	K174	F175	P176	S177	V178	F179	I180	N181	P182	I183	S184	H185	R186	S187	Y188	L189	C189	Y190	I191	D192	L193	S194	G195	K196	F200	T201	L202	T203	N204	E205	L206	M207	L208	Y209	P145	R146	N147	C148						
Q214	E215	A216	V217	D218	R219	G220	C221	L222	R223	I224	Q225	S226	L227	M228	E229	M230	D231	Y232	E233	R234	E235	L236	V237	C238	C239	S240	E241	I242	V243	L244	L245	R246	I247	A248	K249	Q250	E253	L254	T255	F256	D257	N263	G264	H265	N266	F267	D268	L269	R270	Y271	L272	T273	N274	R275	L276	E277	L278							
L279	T280	G281	E282	K283	L284	I285	F286	R287	S288	P289	D290	K291	K292	E293	A294	V295	H296	L297	C298	E301	R302	N303	Q304	SER	SER	HIS	LYS	GLY	VAL	GLY	CYS	GLY	MET	ALA	N315	T316	T317	F318	H319	V320	N324	G325	D330	L331	S333	F334	L335	S338	E339	D400	I401	L402	C403	I406	R407	K408	D409	I410	L411	E412	N413	G414	F415	V417
V418	L419	S420	C421	P422	T423	L424	P425	N426	D427	L428	Y429	K430	L431	S432	F433	G434	K435	D436	D437	L438	D439	Q442	N443	Y444	K445	D446	Y447	N448	L449	N450	L451	A452	L453	D454	M455	A456	R457	Y458	C459	D462	W470	E476	T479	D480	A481	T485	V486	Y487	L488	P489	Q490	S491	M492											
V493	F494	E495	Y496	R497	T500	I501	G504	P505	L506	L507	K508	L509	L510	L511	E512	T513	K514	T515	I516	L517	V518	R519	E520	E521	T522	K523	E524	K525	F526	P527	Y528	E529	D454	M455	A456	R457	Y458	C459	D462	W470	E476	T479	D480	A481	T485	V486	Y487	L488	P489	Q490	S491	M492												
C558	L558	V559	G570	V571	V572	V573	S574	T575	N576	R577	L578	E579	E580	E581	I582	N583	N584	O585	L586	L587	L588	O589	K590	Y591	T598	V599	H600	C601	E602	P603	R604	L605	P606	N607	L608	L609	S610	E611	F614	F615	S618	L619	E620	G621	T622	R625	L626	L627	R628	L546	T547	F548	D549	Y550	N551	S552	L553							
R636	Y637	K638	K639	M640	L641	K642	Q643	A644	T645	S646	A651	I652	Y653	D654	S655	M656	Q657	T658	T659	T660	K661	V662	V663	S666	V667	L670	F673	B674	N675	L678	V679	S680	L681	L682	F683	K684	C685	I686	D687	I688	L689	R690	R691	R692	R693	M694	T695	L696	V697	L698	E699	S700	W701	L702	N703									
G704	A705	E706	L707	S708	N709	G710	M711	L712	R713	F714	A715	N716	T717	L718	S719	N720	F721	F722	Y723	M724	D725	T726	R727	I728	I729	N730	F731	T732	V733	K734	T735	S736	L737	F738	I739	D740	Y741	T808	M809	F743	R744	F745	R746	S747	Y749	G750	V755	F756	T757	E758	I759	D760	S761	Q762	I763	V764	D765	K766						
S767	I768	E769	I770	A771	K772	E773	L774	E775	R776	I777	N778	S779	R780	R781	V782	L783	F784	N785	N786	F787	T788	I789	A793	V794	K795	N796	L797	L798	I799	M800	Q801	S802	K803	K804	K805	Y806	T807	T808	M809	F743	R744	F745	R746	S747	Y749	G750	V755	F756	T757	E758	I759	D760	S761	Q762	I763	V764	D765	K766						
S829	E830	T831	R832	R833	R834	V835	K836	K837	F838	H839	K840	N841	M842	I843	K844	T845	T846	K847	T848	R849	L850	S851	M852	M853	L854	S855	E856	G857	R858	L859	M860	S861	M862	Q863	V864	C865	I866	D867	I868	L869	R870	S871	L872	E873	T874	D875	L876	R877	S878	S879	F880	D881	S882	ARG	SER	SER	PRO	LEU	E888					

THR	TTR	GLU	THR	IIE	ASP	ARG	S967	F958	K959	L960	G961	S962	N963	Q964	R965	I966	F967	Y968	E969	V970	Y971	F972	K973	R974	L975	T976	S977	E978	I979	V980	N981	L982	L983	D984	N985	K986	V987	L988	C989	I990	S991	F992	F993	Q994	R995	M996	F997	G998	SER	ARG	PRO	THR	PHE	TYR	GLU	ALA
-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	391085	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	315.36002, 315.36002, 315.36002	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	C	0.41	0/3073	0.57	0/4142
1	F	0.41	0/3073	0.57	0/4142
2	B	0.42	0/1822	0.63	0/2479
2	E	0.42	0/1822	0.63	0/2479
3	A	0.53	0/7720	0.63	0/10418
3	D	0.53	0/7720	0.63	0/10418
All	All	0.49	0/25230	0.61	0/34078

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	C	3020	0	3035	138	0
1	F	3020	0	3035	142	0
2	B	1772	0	1764	95	0
2	E	1772	0	1764	98	0
3	A	7567	0	7528	407	0
3	D	7567	0	7528	392	0
All	All	24718	0	24654	1253	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 25.

All (1253) 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)
3:D:701:VAL:HA	3:D:715:ALA:CB	1.45	1.45
3:A:701:VAL:HA	3:A:715:ALA:CB	1.45	1.45
3:D:701:VAL:CA	3:D:715:ALA:HB2	1.55	1.35
3:A:701:VAL:CA	3:A:715:ALA:HB2	1.55	1.35
3:D:547:ILE:HD12	3:D:756:PHE:CE1	1.72	1.24
3:A:763:ASP:HB2	3:A:767:SER:HB3	1.22	1.20
3:D:604:ARG:HG3	3:D:611:GLU:OE1	1.40	1.19
3:A:701:VAL:CG1	3:A:715:ALA:HB3	1.74	1.16
3:D:701:VAL:CG1	3:D:715:ALA:HB3	1.74	1.16
3:A:45:GLU:OE1	3:A:46:ILE:HG12	1.44	1.15
3:D:45:GLU:OE1	3:D:46:ILE:HG12	1.46	1.14
3:D:547:ILE:CD1	3:D:756:PHE:CD1	2.33	1.12
3:D:799:ILE:HG23	3:D:982:LEU:HD13	1.12	1.11
3:D:540:MET:HA	3:D:797:ASN:HB2	1.22	1.10
3:A:540:MET:HA	3:A:797:ASN:HB3	1.20	1.07
3:A:799:ILE:HG23	3:A:982:LEU:HD13	1.12	1.06
3:A:608:LEU:O	3:A:609:ILE:HG23	1.55	1.06
3:D:608:LEU:O	3:D:609:ILE:HG23	1.55	1.05
3:A:701:VAL:HG12	3:A:715:ALA:HB3	1.06	1.04
3:A:547:ILE:HG12	3:A:794:VAL:H	1.21	1.04
3:A:799:ILE:HG23	3:A:982:LEU:CD1	1.88	1.03
3:D:546:LEU:HD23	3:D:548:PHE:CE2	1.94	1.02
3:D:701:VAL:HG12	3:D:715:ALA:HB3	1.06	1.02
3:D:799:ILE:HG23	3:D:982:LEU:CD1	1.88	1.02
3:A:763:ASP:CB	3:A:767:SER:HB3	1.90	1.01
1:C:256:SER:HB2	1:C:258:VAL:HG23	1.39	1.01
3:A:539:LYS:O	3:A:982:LEU:HG	1.63	0.99
3:D:547:ILE:CD1	3:D:756:PHE:HD1	1.75	0.98
3:D:533:VAL:HG13	3:D:803:LYS:HD2	1.46	0.98
3:A:533:VAL:HG13	3:A:803:LYS:HD2	1.45	0.97
3:D:539:LYS:O	3:D:982:LEU:HG	1.63	0.97
3:D:547:ILE:CD1	3:D:756:PHE:CE1	2.46	0.96
3:D:773:GLU:O	3:D:776:ARG:HB2	1.65	0.96
3:A:773:GLU:O	3:A:776:ARG:HB2	1.65	0.96
3:D:547:ILE:HD12	3:D:756:PHE:CD1	1.95	0.96
3:A:796:LYS:HG3	3:A:823:ARG:HH12	1.31	0.94
3:A:547:ILE:CG1	3:A:794:VAL:H	1.81	0.94
3:A:540:MET:CA	3:A:797:ASN:HB3	1.98	0.93
3:D:796:LYS:HG3	3:D:823:ARG:HH12	1.31	0.93
3:D:605:LEU:HD12	3:D:605:LEU:H	1.33	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:GLU:N	1:F:109:GLU:OE2	2.03	0.91
3:D:701:VAL:CA	3:D:715:ALA:CB	2.29	0.90
3:D:547:ILE:HD12	3:D:756:PHE:HE1	1.32	0.90
1:C:109:GLU:N	1:C:109:GLU:OE2	2.02	0.90
3:A:605:LEU:HD12	3:A:605:LEU:H	1.34	0.90
3:A:608:LEU:O	3:A:609:ILE:CG2	2.21	0.88
3:D:608:LEU:O	3:D:609:ILE:CG2	2.21	0.88
3:A:701:VAL:HG12	3:A:715:ALA:CB	2.00	0.88
3:D:840:LYS:O	3:D:841:ASN:HB2	1.73	0.87
3:A:840:LYS:O	3:A:841:ASN:HB2	1.72	0.87
3:D:540:MET:HA	3:D:797:ASN:CB	2.04	0.87
3:A:540:MET:HA	3:A:797:ASN:CB	2.03	0.87
3:A:701:VAL:CA	3:A:715:ALA:CB	2.29	0.85
2:E:50:PHE:HB3	2:E:53:LEU:HD13	1.56	0.85
3:D:542:SER:CB	3:D:758:GLU:HG3	2.06	0.85
3:A:542:SER:CB	3:A:758:GLU:HG3	2.06	0.84
3:A:542:SER:HB2	3:A:758:GLU:HG3	1.59	0.84
3:A:547:ILE:CG1	3:A:794:VAL:N	2.40	0.84
3:D:701:VAL:HG12	3:D:715:ALA:CB	2.00	0.84
3:D:542:SER:HB2	3:D:758:GLU:HG3	1.59	0.84
3:A:836:SER:HA	3:A:837:LYS:HE3	1.60	0.84
3:A:544:ASN:O	3:A:544:ASN:ND2	2.12	0.83
3:A:716:ASN:O	3:A:717:THR:OG1	1.96	0.83
2:E:48:LYS:HD2	2:E:48:LYS:N	1.93	0.82
3:D:544:ASN:O	3:D:544:ASN:ND2	2.12	0.82
3:D:838:PHE:HB2	3:D:960:LEU:HD22	1.62	0.82
3:D:836:SER:HA	3:D:837:LYS:HE3	1.59	0.81
3:A:45:GLU:HG3	3:A:46:ILE:H	1.44	0.81
3:D:45:GLU:HG3	3:D:46:ILE:H	1.45	0.81
1:C:256:SER:HB2	1:C:258:VAL:CG2	2.09	0.81
3:A:838:PHE:HB2	3:A:960:LEU:HD22	1.62	0.81
3:D:539:LYS:O	3:D:540:MET:CB	2.28	0.81
3:A:545:VAL:HG11	3:A:756:PHE:HB3	1.63	0.81
3:A:547:ILE:HD12	3:A:756:PHE:HE1	1.47	0.80
1:C:6:ASP:N	1:C:6:ASP:OD1	2.15	0.80
3:A:796:LYS:HG3	3:A:823:ARG:NH1	1.96	0.80
3:D:545:VAL:HG11	3:D:756:PHE:HB3	1.63	0.80
1:C:218:MET:HG2	1:C:266:VAL:HG11	1.63	0.80
3:A:688:THR:O	3:A:692:ARG:HB2	1.82	0.80
1:F:332:ASP:N	1:F:332:ASP:OD1	2.13	0.80
3:A:539:LYS:O	3:A:540:MET:CB	2.28	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:547:ILE:HG13	3:D:794:VAL:HB	1.63	0.79
3:D:688:THR:O	3:D:692:ARG:HB2	1.82	0.79
1:C:335:VAL:HG12	1:C:420:VAL:HG12	1.63	0.79
3:A:832:ARG:HD3	3:A:893:SER:HB2	1.64	0.79
3:D:832:ARG:HD3	3:D:893:SER:HB2	1.64	0.79
1:C:332:ASP:OD1	1:C:332:ASP:N	2.13	0.79
3:A:547:ILE:HG13	3:A:794:VAL:N	1.97	0.79
1:F:218:MET:HG2	1:F:266:VAL:HG11	1.63	0.79
1:F:135:ARG:HE	1:F:136:TRP:H	1.29	0.79
1:F:335:VAL:HG12	1:F:420:VAL:HG12	1.63	0.79
3:D:724:MET:N	3:D:724:MET:HE2	1.98	0.78
3:D:796:LYS:HG3	3:D:823:ARG:NH1	1.96	0.78
1:F:6:ASP:OD1	1:F:6:ASP:N	2.15	0.78
3:D:546:LEU:HD23	3:D:548:PHE:CZ	2.19	0.78
3:D:540:MET:CA	3:D:797:ASN:HB2	2.09	0.78
3:D:167:ILE:HD11	3:D:268:ASP:HA	1.66	0.77
3:D:796:LYS:CG	3:D:823:ARG:HH22	1.97	0.77
1:C:135:ARG:HE	1:C:136:TRP:H	1.29	0.77
1:F:190:ASP:N	1:F:190:ASP:OD1	2.16	0.77
3:A:406:ILE:O	3:A:407:ARG:NH1	2.16	0.77
3:A:167:ILE:HD11	3:A:268:ASP:HA	1.66	0.77
1:F:182:SER:HB2	1:F:186:ARG:HH12	1.50	0.77
1:F:179:GLU:HA	1:F:182:SER:OG	1.85	0.76
1:C:190:ASP:N	1:C:190:ASP:OD1	2.16	0.76
2:E:84:PHE:HE1	2:E:90:LYS:HA	1.50	0.76
3:D:799:ILE:CG2	3:D:982:LEU:HD13	2.06	0.76
2:E:84:PHE:HD2	2:E:107:GLY:HA2	1.50	0.76
3:D:701:VAL:CG1	3:D:715:ALA:CB	2.61	0.76
3:A:701:VAL:HA	3:A:715:ALA:HB2	0.78	0.76
3:D:406:ILE:O	3:D:407:ARG:NH1	2.16	0.76
2:B:84:PHE:HE1	2:B:90:LYS:HA	1.50	0.76
3:A:796:LYS:CG	3:A:823:ARG:HH22	1.97	0.76
3:D:972:PHE:HA	3:D:975:LEU:HD12	1.68	0.76
3:A:972:PHE:HA	3:A:975:LEU:HD12	1.68	0.76
3:D:876:LEU:HD11	3:D:968:TYR:HB3	1.68	0.76
2:B:84:PHE:HD2	2:B:107:GLY:HA2	1.50	0.76
3:D:989:CYS:SG	3:D:990:ILE:N	2.58	0.75
3:A:876:LEU:HD11	3:A:968:TYR:HB3	1.68	0.75
3:A:989:CYS:SG	3:A:990:ILE:N	2.58	0.75
3:A:539:LYS:O	3:A:982:LEU:CG	2.34	0.75
3:D:779:ASN:HB2	3:D:789:ILE:HG22	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:701:VAL:HA	3:D:715:ALA:HB2	0.78	0.75
1:C:33:SER:O	1:C:36:GLU:HB3	1.86	0.75
3:A:808:THR:HG21	3:A:810:LYS:HE3	1.69	0.74
3:D:486:TYR:CE2	3:D:501:ILE:HD12	2.22	0.74
3:D:605:LEU:HD12	3:D:605:LEU:N	2.03	0.74
2:B:72:LYS:HB2	2:B:72:LYS:NZ	2.02	0.74
1:F:33:SER:O	1:F:36:GLU:HB3	1.86	0.74
3:A:840:LYS:HE2	3:A:843:ILE:HB	1.68	0.74
1:F:182:SER:HB2	1:F:186:ARG:NH1	2.03	0.74
3:D:361:LEU:HD11	3:D:371:ILE:HB	1.69	0.74
2:E:72:LYS:HB2	2:E:72:LYS:NZ	2.03	0.74
3:D:627:LEU:HD21	3:D:667:VAL:HG11	1.69	0.74
2:E:72:LYS:HB2	2:E:72:LYS:HZ2	1.52	0.74
3:D:539:LYS:O	3:D:982:LEU:CG	2.34	0.74
3:A:547:ILE:HD12	3:A:756:PHE:CE1	2.23	0.73
3:A:701:VAL:CG1	3:A:715:ALA:CB	2.61	0.73
3:A:779:ASN:HB2	3:A:789:ILE:HG22	1.68	0.73
3:D:45:GLU:HG3	3:D:46:ILE:N	2.04	0.73
3:D:796:LYS:HG3	3:D:823:ARG:HH22	1.52	0.73
1:C:351:GLN:O	1:C:421:LYS:NZ	2.21	0.73
3:A:486:TYR:CE2	3:A:501:ILE:HD12	2.22	0.73
2:E:6:ILE:HG22	2:E:27:VAL:HG13	1.69	0.73
3:D:546:LEU:CD2	3:D:548:PHE:CE2	2.72	0.73
3:D:840:LYS:O	3:D:841:ASN:CB	2.36	0.73
3:A:605:LEU:HD12	3:A:605:LEU:N	2.03	0.73
3:A:627:LEU:HD21	3:A:667:VAL:HG11	1.69	0.73
3:A:796:LYS:HG3	3:A:823:ARG:HH22	1.51	0.73
3:A:361:LEU:HD11	3:A:371:ILE:HB	1.69	0.73
3:A:840:LYS:O	3:A:841:ASN:CB	2.36	0.73
1:F:351:GLN:O	1:F:421:LYS:NZ	2.21	0.73
2:E:50:PHE:HB3	2:E:53:LEU:CD1	2.18	0.73
1:C:182:SER:HB2	1:C:186:ARG:HH12	1.53	0.73
3:D:701:VAL:N	3:D:715:ALA:HB2	2.04	0.73
3:D:808:THR:HG21	3:D:810:LYS:HE3	1.69	0.73
2:B:6:ILE:HG22	2:B:27:VAL:HG13	1.69	0.73
3:A:964:GLN:HB3	3:A:968:TYR:HE2	1.53	0.73
3:D:519:ARG:NH2	3:D:679:TYR:O	2.21	0.73
3:A:45:GLU:HG3	3:A:46:ILE:N	2.03	0.72
3:A:742:ARG:NH1	3:A:742:ARG:HG3	2.04	0.72
3:A:846:TYR:HE1	3:A:868:ILE:HB	1.54	0.72
1:C:177:ASP:H	1:C:180:LEU:HB2	1.52	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:604:ARG:HB2	3:D:605:LEU:HD12	1.71	0.72
3:D:840:LYS:HE2	3:D:843:ILE:HB	1.68	0.72
1:F:177:ASP:H	1:F:180:LEU:HB2	1.52	0.72
3:D:964:GLN:HB3	3:D:968:TYR:HE2	1.53	0.72
2:E:47:ASP:C	2:E:48:LYS:HD2	2.10	0.72
2:B:72:LYS:HB2	2:B:72:LYS:HZ2	1.51	0.72
3:A:701:VAL:N	3:A:715:ALA:HB2	2.04	0.72
3:D:609:ILE:N	3:D:609:ILE:HD13	2.05	0.71
3:D:249:LYS:NZ	3:D:283:LYS:O	2.21	0.71
1:C:179:GLU:HA	1:C:182:SER:OG	1.90	0.71
3:A:249:LYS:NZ	3:A:283:LYS:O	2.21	0.71
3:D:523:LYS:O	3:D:674:ARG:NH2	2.23	0.71
3:D:846:TYR:HE1	3:D:868:ILE:HB	1.54	0.71
3:A:519:ARG:NH2	3:A:679:TYR:O	2.21	0.71
3:A:523:LYS:O	3:A:674:ARG:NH2	2.23	0.71
3:D:700:SER:O	3:D:715:ALA:HB2	1.91	0.71
1:C:182:SER:HB2	1:C:186:ARG:NH1	2.06	0.71
1:F:330:THR:N	1:F:333:GLU:OE2	2.20	0.71
1:C:330:THR:N	1:C:333:GLU:OE2	2.20	0.71
3:A:609:ILE:N	3:A:609:ILE:HD13	2.05	0.71
3:A:701:VAL:HA	3:A:715:ALA:CA	2.21	0.71
3:D:23:ARG:NH1	3:D:29:THR:OG1	2.24	0.70
3:D:742:ARG:HG3	3:D:742:ARG:NH1	2.05	0.70
3:A:23:ARG:NH1	3:A:29:THR:OG1	2.24	0.70
3:A:700:SER:O	3:A:715:ALA:HB2	1.91	0.70
3:A:742:ARG:HG3	3:A:742:ARG:HH11	1.55	0.70
3:A:605:LEU:H	3:A:605:LEU:CD1	2.04	0.70
3:D:742:ARG:HG3	3:D:742:ARG:HH11	1.55	0.70
3:D:988:LEU:HA	3:D:991:SER:HB2	1.74	0.69
3:A:187:SER:O	3:A:188:TYR:CD1	2.45	0.69
3:A:821:PRO:HG2	3:A:823:ARG:HE	1.57	0.69
3:A:580:GLU:O	3:A:584:ASN:HB2	1.93	0.69
3:A:799:ILE:CG2	3:A:982:LEU:HD13	2.06	0.69
3:D:187:SER:O	3:D:188:TYR:CD1	2.46	0.69
1:C:334:LEU:O	1:C:338:ILE:HG12	1.93	0.69
3:A:547:ILE:HG12	3:A:794:VAL:N	2.00	0.69
1:F:334:LEU:O	1:F:338:ILE:HG12	1.93	0.69
3:D:605:LEU:H	3:D:605:LEU:CD1	2.03	0.69
3:D:821:PRO:HG2	3:D:823:ARG:HE	1.57	0.69
2:B:18:ASP:OD1	2:B:58:ARG:NH2	2.20	0.69
2:B:47:ASP:O	2:B:48:LYS:HD2	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:580:GLU:O	3:D:584:ASN:HB2	1.93	0.69
3:D:574:SER:N	3:D:610:SER:OG	2.25	0.68
3:D:701:VAL:HA	3:D:715:ALA:CA	2.21	0.68
3:A:574:SER:N	3:A:610:SER:OG	2.25	0.68
3:A:988:LEU:HA	3:A:991:SER:HB2	1.74	0.68
3:D:840:LYS:HB3	3:D:889:LEU:O	1.94	0.68
3:A:81:ARG:HG2	3:A:81:ARG:HH11	1.59	0.68
3:D:872:LEU:HD21	3:D:972:PHE:HB3	1.75	0.67
3:A:411:LEU:HB2	3:A:414:GLY:H	1.60	0.67
3:D:700:SER:C	3:D:715:ALA:HB2	2.15	0.67
3:A:872:LEU:HD21	3:A:972:PHE:HB3	1.75	0.67
3:A:18:LEU:HD21	3:A:110:ILE:HD11	1.75	0.67
2:B:62:VAL:HG23	2:B:154:VAL:HB	1.77	0.67
2:E:18:ASP:OD1	2:E:58:ARG:NH2	2.20	0.67
2:E:62:VAL:HG23	2:E:154:VAL:HB	1.77	0.67
3:A:546:LEU:HD23	3:A:771:ALA:HB2	1.76	0.67
3:D:547:ILE:HD13	3:D:756:PHE:HD1	1.57	0.67
3:A:796:LYS:HG3	3:A:823:ARG:NH2	2.10	0.67
3:D:18:LEU:HD21	3:D:110:ILE:HD11	1.75	0.67
1:C:183:ILE:HG13	1:C:184:MET:N	2.10	0.67
3:A:687:CYS:O	3:A:688:THR:OG1	2.13	0.67
3:D:411:LEU:HB2	3:D:414:GLY:H	1.60	0.67
2:B:36:TRP:NE1	3:A:179:PHE:HB3	2.09	0.67
3:A:700:SER:C	3:A:715:ALA:HB2	2.15	0.67
2:E:40:ASP:N	2:E:40:ASP:OD1	2.28	0.66
3:D:546:LEU:CD2	3:D:548:PHE:HE2	2.09	0.66
3:D:634:ARG:HE	3:D:661:LYS:HB2	1.60	0.66
3:D:539:LYS:H	3:D:982:LEU:HA	1.59	0.66
3:A:840:LYS:HB3	3:A:889:LEU:O	1.94	0.66
1:F:194:LYS:NZ	1:F:196:SER:O	2.21	0.66
3:A:573:VAL:HA	3:A:610:SER:OG	1.95	0.66
1:C:194:LYS:NZ	1:C:196:SER:OG	2.29	0.66
3:A:81:ARG:HG2	3:A:81:ARG:NH1	2.10	0.66
3:A:724:MET:HE2	3:A:724:MET:N	2.11	0.66
3:A:777:LEU:HD23	3:A:781:ARG:HB3	1.77	0.66
3:D:81:ARG:HG2	3:D:81:ARG:HH11	1.59	0.66
3:D:796:LYS:HG3	3:D:823:ARG:NH2	2.10	0.66
1:F:183:ILE:HG13	1:F:184:MET:N	2.10	0.66
1:F:194:LYS:NZ	1:F:196:SER:OG	2.29	0.66
3:A:659:THR:O	3:A:663:VAL:HG13	1.96	0.66
3:D:608:LEU:C	3:D:609:ILE:HG23	2.17	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:81:ARG:HG2	3:D:81:ARG:NH1	2.10	0.65
3:D:573:VAL:HA	3:D:610:SER:OG	1.95	0.65
3:D:777:LEU:HD23	3:D:781:ARG:HB3	1.77	0.65
3:A:539:LYS:H	3:A:982:LEU:HA	1.59	0.65
3:A:701:VAL:HB	3:A:714:PHE:HB3	1.78	0.65
3:A:608:LEU:C	3:A:609:ILE:HG23	2.16	0.65
3:D:687:CYS:O	3:D:688:THR:OG1	2.13	0.65
3:D:797:ASN:ND2	3:D:854:LEU:O	2.30	0.65
3:D:659:THR:O	3:D:663:VAL:HG13	1.96	0.65
3:D:765:ASP:O	3:D:768:ILE:HG13	1.97	0.65
3:A:547:ILE:HD11	3:A:794:VAL:HB	1.77	0.65
3:A:763:ASP:CG	3:A:767:SER:CA	2.65	0.65
2:E:26:LEU:HD21	2:E:50:PHE:HE2	1.62	0.65
3:A:833:ARG:O	3:A:835:VAL:HG13	1.97	0.65
3:D:486:TYR:CZ	3:D:663:VAL:HG12	2.31	0.64
2:B:40:ASP:OD1	2:B:40:ASP:N	2.28	0.64
1:C:288:GLU:OE2	1:C:288:GLU:N	2.24	0.64
3:A:486:TYR:CZ	3:A:663:VAL:HG12	2.31	0.64
3:A:634:ARG:HE	3:A:661:LYS:HB2	1.60	0.64
2:E:7:SER:OG	2:E:8:HIS:ND1	2.31	0.64
3:D:836:SER:CA	3:D:837:LYS:HE3	2.27	0.64
1:C:109:GLU:HG2	1:C:110:ILE:HG12	1.80	0.64
3:A:761:SER:O	3:A:762:GLN:HB3	1.98	0.64
3:D:701:VAL:HB	3:D:714:PHE:HB3	1.78	0.64
3:D:779:ASN:HD22	3:D:789:ILE:HA	1.63	0.64
1:F:255:ARG:O	1:F:255:ARG:HG2	1.98	0.64
3:D:833:ARG:O	3:D:835:VAL:HG13	1.97	0.64
1:C:386:ASN:OD1	1:C:387:PHE:N	2.31	0.64
2:B:7:SER:OG	2:B:8:HIS:ND1	2.31	0.64
3:A:211:GLN:OE1	3:A:212:GLU:N	2.31	0.64
3:A:547:ILE:CD1	3:A:794:VAL:HB	2.27	0.64
1:F:109:GLU:HG2	1:F:110:ILE:HG12	1.80	0.64
3:A:521:GLU:OE1	3:A:522:THR:N	2.31	0.64
3:A:546:LEU:HD12	3:A:546:LEU:N	2.13	0.64
3:D:211:GLN:OE1	3:D:212:GLU:N	2.31	0.64
3:D:374:ASP:O	3:D:376:THR:N	2.31	0.64
3:D:521:GLU:OE1	3:D:522:THR:N	2.31	0.64
3:A:175:PHE:HD1	3:A:176:PRO:HD2	1.63	0.64
1:F:288:GLU:OE2	1:F:288:GLU:N	2.24	0.63
3:D:175:PHE:HD1	3:D:176:PRO:HD2	1.63	0.63
3:A:509:LEU:HD11	3:A:625:ARG:HE	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ALA:HB1	1:C:160:LEU:HB2	1.80	0.63
3:A:551:ASN:HD21	3:A:788:LYS:HB2	1.63	0.63
1:F:155:ALA:HB1	1:F:160:LEU:HB2	1.80	0.63
3:D:551:ASN:HD21	3:D:788:LYS:HB2	1.63	0.63
1:F:386:ASN:OD1	1:F:387:PHE:N	2.31	0.63
3:D:184:SER:OG	3:D:185:HIS:ND1	2.23	0.63
3:A:763:ASP:CG	3:A:767:SER:HB3	2.19	0.63
3:A:538:GLN:NE2	3:A:984:ASP:OD2	2.31	0.63
1:F:353:VAL:HG12	1:F:417:VAL:HG13	1.80	0.63
2:E:199:ASN:HA	2:E:202:LEU:HB2	1.80	0.63
1:C:354:PHE:HE2	3:A:578:LEU:HD23	1.64	0.63
2:B:199:ASN:HA	2:B:202:LEU:HB2	1.80	0.63
3:A:836:SER:CA	3:A:837:LYS:HE3	2.28	0.63
3:D:538:GLN:NE2	3:D:984:ASP:OD2	2.31	0.62
3:A:779:ASN:HD22	3:A:789:ILE:HA	1.63	0.62
1:F:182:SER:O	1:F:185:GLU:HB3	1.99	0.62
3:A:762:GLN:O	3:A:762:GLN:HG3	1.99	0.62
1:F:251:ASP:OD1	1:F:251:ASP:N	2.20	0.62
3:A:801:GLN:O	3:A:801:GLN:HG2	1.99	0.62
1:C:182:SER:O	1:C:185:GLU:HB3	2.00	0.62
3:D:371:ILE:HD11	3:D:411:LEU:HD11	1.81	0.62
3:D:547:ILE:HG22	3:D:547:ILE:O	1.99	0.62
3:D:509:LEU:HD11	3:D:625:ARG:HE	1.63	0.62
3:A:209:THR:OG1	3:A:211:GLN:NE2	2.32	0.62
3:A:374:ASP:O	3:A:376:THR:N	2.31	0.62
3:A:609:ILE:HG12	3:A:609:ILE:O	2.00	0.62
3:A:78:ILE:HG21	3:A:569:VAL:HG12	1.81	0.62
3:D:209:THR:OG1	3:D:211:GLN:NE2	2.32	0.62
3:D:605:LEU:O	3:D:607:ASN:N	2.33	0.62
3:D:801:GLN:HG2	3:D:801:GLN:O	1.99	0.62
3:D:78:ILE:HG21	3:D:569:VAL:HG12	1.81	0.61
3:D:773:GLU:HA	3:D:776:ARG:HG3	1.82	0.61
3:A:797:ASN:OD1	3:A:797:ASN:N	2.32	0.61
1:F:14:LEU:HD11	2:B:200:VAL:HG13	1.82	0.61
3:A:371:ILE:HD11	3:A:411:LEU:HD11	1.81	0.61
3:D:540:MET:CB	3:D:982:LEU:HG	2.30	0.61
3:A:773:GLU:HA	3:A:776:ARG:HG3	1.82	0.61
3:A:605:LEU:O	3:A:607:ASN:N	2.33	0.61
2:E:48:LYS:O	2:E:49:PHE:HB2	2.01	0.61
3:D:609:ILE:HG12	3:D:609:ILE:O	2.00	0.61
3:A:540:MET:CB	3:A:982:LEU:HG	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:345:LYS:HD3	3:D:346:LEU:N	2.16	0.61
1:C:353:VAL:HG12	1:C:417:VAL:HG13	1.81	0.61
3:D:454:ASP:OD1	3:D:457:ARG:NH2	2.34	0.60
3:A:720:ASN:ND2	3:A:721:PRO:O	2.35	0.60
3:A:742:ARG:HH11	3:A:742:ARG:CG	2.14	0.60
2:E:102:VAL:HG21	2:E:218:TYR:OH	2.02	0.60
3:D:363:ARG:NH2	3:D:426:ASN:O	2.35	0.60
3:D:620:GLU:OE2	3:D:628:ARG:NH1	2.34	0.60
2:B:84:PHE:CD2	2:B:107:GLY:HA2	2.35	0.60
3:A:45:GLU:CG	3:A:46:ILE:N	2.64	0.60
3:A:620:GLU:OE2	3:A:628:ARG:NH1	2.35	0.60
2:B:62:VAL:HG21	2:B:198:ILE:HD11	1.84	0.60
3:A:345:LYS:HD3	3:A:346:LEU:N	2.16	0.60
3:A:363:ARG:NH2	3:A:426:ASN:O	2.35	0.60
3:A:763:ASP:CG	3:A:767:SER:CB	2.70	0.60
1:C:341:SER:OG	1:C:344:VAL:HG23	2.01	0.60
2:B:165:ASN:OD1	2:B:165:ASN:N	2.35	0.60
3:A:454:ASP:OD1	3:A:457:ARG:NH2	2.35	0.60
2:E:62:VAL:HG21	2:E:198:ILE:HD11	1.84	0.60
2:E:165:ASN:OD1	2:E:165:ASN:N	2.35	0.60
2:B:102:VAL:HG21	2:B:218:TYR:OH	2.02	0.60
3:D:546:LEU:O	3:D:547:ILE:HG12	2.00	0.60
3:A:372:GLY:O	3:A:414:GLY:HA3	2.02	0.60
3:D:45:GLU:CG	3:D:46:ILE:N	2.65	0.60
3:D:720:ASN:ND2	3:D:721:PRO:O	2.35	0.59
3:A:526:PHE:HD1	3:A:526:PHE:N	2.00	0.59
3:A:763:ASP:O	3:A:764:VAL:HB	2.02	0.59
3:D:742:ARG:HH11	3:D:742:ARG:CG	2.14	0.59
3:A:526:PHE:N	3:A:526:PHE:CD1	2.70	0.59
3:D:331:LEU:O	3:D:335:ILE:HG13	2.03	0.59
1:C:291:LYS:HE2	1:C:389:ILE:HG23	1.84	0.59
3:A:547:ILE:HG13	3:A:794:VAL:HG23	1.84	0.59
3:D:372:GLY:HA3	3:D:415:PHE:CE1	2.38	0.59
3:A:135:ILE:HD11	3:A:141:HIS:HB2	1.85	0.59
3:D:372:GLY:O	3:D:414:GLY:HA3	2.02	0.59
3:D:23:ARG:NH2	3:D:257:ASP:OD2	2.36	0.59
3:D:135:ILE:HD11	3:D:141:HIS:HB2	1.85	0.59
3:D:526:PHE:N	3:D:526:PHE:CD1	2.70	0.59
3:D:533:VAL:CG1	3:D:803:LYS:HD2	2.25	0.59
3:D:713:ARG:O	3:D:714:PHE:HB2	2.03	0.59
3:D:997:PHE:CZ	1:C:183:ILE:HD13	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:175:PHE:CD1	3:D:176:PRO:HD2	2.37	0.59
2:E:84:PHE:CD2	2:E:107:GLY:HA2	2.35	0.58
3:D:526:PHE:N	3:D:526:PHE:HD1	2.00	0.58
3:D:547:ILE:HD11	3:D:756:PHE:CD1	2.32	0.58
3:A:533:VAL:CG1	3:A:803:LYS:HD2	2.25	0.58
1:F:24:ASP:OD1	1:F:24:ASP:N	2.36	0.58
3:D:846:TYR:CE1	3:D:868:ILE:HB	2.36	0.58
1:C:194:LYS:NZ	1:C:196:SER:O	2.22	0.58
3:A:14:GLU:N	3:A:14:GLU:OE2	2.35	0.58
3:A:331:LEU:O	3:A:335:ILE:HG13	2.03	0.58
3:A:372:GLY:HA3	3:A:415:PHE:CE1	2.38	0.58
1:F:123:GLY:O	1:F:144:LYS:NZ	2.29	0.58
1:F:291:LYS:HE2	1:F:389:ILE:HG23	1.84	0.58
3:A:544:ASN:OD1	3:A:762:GLN:OE1	2.21	0.58
2:E:166:ILE:O	2:E:170:LEU:HD12	2.02	0.58
3:D:113:PHE:O	3:D:117:ASN:HB2	2.03	0.58
3:D:542:SER:HB3	3:D:758:GLU:HG3	1.85	0.58
3:D:547:ILE:HG12	3:D:794:VAL:H	1.69	0.58
3:D:796:LYS:HG3	3:D:823:ARG:CZ	2.33	0.58
3:A:184:SER:OG	3:A:185:HIS:ND1	2.23	0.58
3:A:713:ARG:O	3:A:714:PHE:HB2	2.03	0.58
3:A:796:LYS:HG3	3:A:823:ARG:CZ	2.33	0.58
3:D:14:GLU:N	3:D:14:GLU:OE2	2.36	0.58
3:D:547:ILE:HD13	3:D:756:PHE:CD1	2.35	0.58
1:C:179:GLU:O	1:C:183:ILE:HG23	2.04	0.58
2:B:166:ILE:O	2:B:170:LEU:HD12	2.02	0.58
3:A:175:PHE:CD1	3:A:176:PRO:HD2	2.37	0.58
3:D:409:ASP:HB3	3:D:416:LYS:HB3	1.86	0.58
3:D:961:GLY:O	3:D:964:GLN:NE2	2.37	0.58
3:A:573:VAL:CA	3:A:610:SER:OG	2.52	0.58
1:C:219:TYR:HB3	1:C:240:LYS:HG2	1.86	0.58
1:F:179:GLU:O	1:F:183:ILE:HG23	2.04	0.58
3:D:287:ARG:HD3	3:D:287:ARG:N	2.19	0.58
3:A:113:PHE:O	3:A:117:ASN:HB2	2.03	0.58
3:A:187:SER:HB2	3:A:201:THR:HG23	1.86	0.57
3:D:533:VAL:HG13	3:D:803:LYS:CD	2.28	0.57
1:C:24:ASP:OD1	1:C:24:ASP:N	2.36	0.57
3:A:763:ASP:CG	3:A:767:SER:N	2.58	0.57
1:F:2:THR:HG1	2:B:192:ASP:CG	2.08	0.57
2:E:183:ALA:O	2:E:185:ARG:NH1	2.38	0.57
3:D:779:ASN:ND2	3:D:788:LYS:O	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:768:ILE:HD12	3:A:816:ASN:HB2	1.87	0.57
1:F:7:LEU:O	1:F:11:LYS:HG2	2.04	0.57
1:F:284:GLU:OE1	1:F:292:ARG:NH2	2.35	0.57
3:D:76:LEU:HD22	3:D:586:LEU:HB3	1.86	0.57
1:C:7:LEU:O	1:C:11:LYS:HG2	2.04	0.57
3:A:23:ARG:NH2	3:A:257:ASP:OD2	2.36	0.57
3:A:717:THR:HG22	3:A:719:SER:H	1.69	0.57
3:A:779:ASN:ND2	3:A:788:LYS:O	2.37	0.57
1:F:351:GLN:OE1	1:F:351:GLN:HA	2.05	0.57
3:D:547:ILE:HG13	3:D:794:VAL:CB	2.34	0.57
3:D:573:VAL:CA	3:D:610:SER:OG	2.52	0.57
3:D:763:ASP:O	3:D:764:VAL:HB	2.03	0.57
1:C:123:GLY:O	1:C:144:LYS:NZ	2.29	0.57
1:C:330:THR:OG1	1:C:333:GLU:HG3	2.05	0.57
3:D:964:GLN:HB3	3:D:968:TYR:CE2	2.39	0.57
1:C:284:GLU:OE1	1:C:292:ARG:NH2	2.35	0.57
3:A:409:ASP:HB3	3:A:416:LYS:HB3	1.86	0.57
2:E:57:LEU:HB3	2:E:151:HIS:CD2	2.39	0.57
3:D:532:LYS:HG3	3:D:533:VAL:N	2.19	0.57
2:B:57:LEU:HB3	2:B:151:HIS:CD2	2.39	0.57
2:B:183:ALA:O	2:B:185:ARG:NH1	2.37	0.57
3:A:961:GLY:O	3:A:964:GLN:NE2	2.37	0.57
3:A:983:LEU:HD22	3:A:983:LEU:H	1.70	0.57
2:E:89:ILE:HD11	2:E:108:TYR:HD2	1.69	0.56
3:D:187:SER:HB2	3:D:201:THR:HG23	1.86	0.56
3:D:983:LEU:H	3:D:983:LEU:HD22	1.70	0.56
3:A:45:GLU:OE1	3:A:46:ILE:CG1	2.35	0.56
1:F:219:TYR:HB3	1:F:240:LYS:HG2	1.86	0.56
2:E:50:PHE:CD1	2:E:50:PHE:N	2.73	0.56
2:E:205:ASP:OD1	1:C:44:LYS:HD3	2.05	0.56
3:D:117:ASN:OD1	3:D:145:PRO:HB2	2.05	0.56
1:C:351:GLN:OE1	1:C:351:GLN:HA	2.05	0.56
2:B:84:PHE:CE1	2:B:90:LYS:HA	2.37	0.56
2:B:89:ILE:HD11	2:B:108:TYR:HD2	1.69	0.56
3:A:763:ASP:OD1	3:A:770:ILE:HD12	2.05	0.56
3:A:846:TYR:CE1	3:A:868:ILE:HB	2.36	0.56
1:F:167:GLU:HB3	1:F:199:TYR:CE1	2.40	0.56
3:D:363:ARG:NH2	3:D:425:PRO:O	2.38	0.56
3:D:837:LYS:O	3:D:888:GLU:N	2.39	0.56
2:B:167:ARG:HH22	2:B:173:PRO:HA	1.70	0.56
3:A:76:LEU:HD22	3:A:586:LEU:HB3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:363:ARG:NH2	3:A:425:PRO:O	2.38	0.56
3:A:532:LYS:HG3	3:A:533:VAL:N	2.19	0.56
3:A:837:LYS:O	3:A:888:GLU:N	2.39	0.56
1:F:167:GLU:HB3	1:F:199:TYR:HE1	1.71	0.56
3:D:45:GLU:OE1	3:D:46:ILE:CG1	2.37	0.56
3:D:551:ASN:OD1	3:D:551:ASN:N	2.35	0.56
2:B:88:SER:O	2:B:92:ILE:HG12	2.06	0.56
3:A:390:THR:HG22	3:A:391:THR:HG23	1.88	0.56
1:F:330:THR:OG1	1:F:333:GLU:HG3	2.04	0.56
2:E:167:ARG:HH22	2:E:173:PRO:HA	1.70	0.56
3:D:637:TYR:HA	3:D:640:MET:HG3	1.87	0.56
3:A:117:ASN:OD1	3:A:145:PRO:HB2	2.05	0.56
3:A:745:PHE:HE2	3:A:774:LEU:HD22	1.70	0.56
1:C:167:GLU:HB3	1:C:199:TYR:CE1	2.40	0.56
1:C:219:TYR:HD1	1:C:240:LYS:HB3	1.71	0.56
3:A:825:ASN:OD1	3:A:828:THR:N	2.39	0.56
2:E:88:SER:O	2:E:92:ILE:HG12	2.06	0.56
3:D:319:HIS:CE1	3:D:495:GLU:HG2	2.41	0.56
1:C:108:ASP:OD1	1:C:111:ARG:NH2	2.39	0.56
2:B:72:LYS:O	2:B:73:ASP:HB2	2.04	0.56
3:A:287:ARG:N	3:A:287:ARG:HD3	2.19	0.56
3:A:369:THR:OG1	3:A:418:VAL:HG22	2.05	0.56
2:E:26:LEU:HD21	2:E:50:PHE:CE2	2.40	0.56
2:E:72:LYS:O	2:E:73:ASP:HB2	2.04	0.56
3:A:170:HIS:O	3:A:181:ASN:ND2	2.30	0.56
3:A:746:ARG:HD2	3:A:760:ASP:OD2	2.06	0.56
2:E:3:SER:HA	2:E:13:ILE:O	2.06	0.55
3:D:369:THR:OG1	3:D:418:VAL:HG22	2.05	0.55
3:D:745:PHE:HE2	3:D:774:LEU:HD22	1.70	0.55
1:C:135:ARG:HE	1:C:136:TRP:N	2.02	0.55
1:C:167:GLU:HB3	1:C:199:TYR:HE1	1.71	0.55
1:C:257:LYS:O	1:C:259:ARG:HG3	2.06	0.55
3:A:865:CYS:O	3:A:869:LEU:HD12	2.06	0.55
3:D:707:LEU:HD13	3:D:742:ARG:HE	1.71	0.55
1:C:220:ILE:HD12	1:C:237:VAL:HG13	1.88	0.55
3:A:699:GLU:OE2	3:A:755:VAL:HG22	2.06	0.55
1:F:108:ASP:OD1	1:F:111:ARG:NH2	2.39	0.55
3:D:183:ILE:HD12	3:D:245:LEU:HD21	1.89	0.55
3:D:514:LYS:N	3:D:514:LYS:HD2	2.21	0.55
2:B:18:ASP:OD2	2:B:57:LEU:N	2.27	0.55
3:A:286:PHE:HB2	3:A:295:VAL:HG23	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:699:GLU:OE2	3:D:755:VAL:HG22	2.06	0.55
3:A:43:THR:HA	3:A:88:MET:HE3	1.88	0.55
3:A:707:LEU:HD13	3:A:742:ARG:HE	1.71	0.55
1:F:219:TYR:HD1	1:F:240:LYS:HB3	1.71	0.55
3:D:286:PHE:HB2	3:D:295:VAL:HG23	1.88	0.55
1:C:336:ASP:O	1:C:340:LYS:HG2	2.06	0.55
2:B:3:SER:HA	2:B:13:ILE:O	2.07	0.55
3:A:637:TYR:HA	3:A:640:MET:HG3	1.87	0.55
3:D:746:ARG:HD2	3:D:760:ASP:OD2	2.06	0.55
3:D:821:PRO:HG3	3:D:823:ARG:HH21	1.72	0.55
1:C:416:THR:O	1:C:420:VAL:HG22	2.07	0.55
3:A:319:HIS:CE1	3:A:495:GLU:HG2	2.41	0.55
3:D:43:THR:HA	3:D:88:MET:HE3	1.89	0.55
2:B:187:HIS:HB3	2:B:190:GLU:HG3	1.89	0.55
1:F:16:LEU:HD21	1:F:30:LYS:HD2	1.89	0.55
3:D:390:THR:HG22	3:D:391:THR:HG23	1.88	0.55
1:C:16:LEU:HD21	1:C:30:LYS:HD2	1.89	0.55
3:A:778:ILE:HG23	3:A:779:ASN:H	1.72	0.55
1:F:336:ASP:O	1:F:340:LYS:HG2	2.06	0.54
3:A:774:LEU:O	3:A:778:ILE:HG22	2.07	0.54
3:D:825:ASN:OD1	3:D:828:THR:N	2.39	0.54
3:A:183:ILE:HD12	3:A:245:LEU:HD21	1.89	0.54
1:F:334:LEU:HD23	1:F:420:VAL:HG11	1.89	0.54
3:D:778:ILE:HG23	3:D:779:ASN:H	1.72	0.54
3:D:865:CYS:O	3:D:869:LEU:HD12	2.06	0.54
3:A:514:LYS:HD2	3:A:514:LYS:N	2.21	0.54
3:A:821:PRO:HG3	3:A:823:ARG:HH21	1.72	0.54
1:F:220:ILE:HD12	1:F:237:VAL:HG13	1.88	0.54
3:A:547:ILE:HG13	3:A:794:VAL:CB	2.38	0.54
1:F:135:ARG:HE	1:F:136:TRP:N	2.02	0.54
3:D:774:LEU:O	3:D:778:ILE:HG22	2.07	0.54
1:C:247:VAL:HG12	1:C:252:HIS:CE1	2.43	0.54
1:F:178:ASP:HA	1:F:181:TYR:CZ	2.43	0.54
2:B:153:SER:O	2:B:153:SER:OG	2.26	0.54
1:F:2:THR:OG1	2:B:192:ASP:CG	2.46	0.54
3:D:700:SER:OG	3:D:701:VAL:N	2.41	0.54
1:F:247:VAL:HG12	1:F:252:HIS:CE1	2.42	0.54
2:E:153:SER:O	2:E:153:SER:OG	2.26	0.54
1:C:329:ALA:N	1:C:333:GLU:OE2	2.41	0.54
3:A:964:GLN:HB3	3:A:968:TYR:CE2	2.39	0.54
3:A:974:ARG:O	3:A:977:SER:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:416:THR:O	1:F:420:VAL:HG22	2.07	0.54
1:C:267:LYS:HG3	1:C:276:TYR:CD1	2.43	0.54
1:C:334:LEU:HD23	1:C:420:VAL:HG11	1.89	0.54
1:C:178:ASP:HA	1:C:181:TYR:CZ	2.43	0.54
1:C:193:PRO:HA	1:C:272:PHE:CZ	2.43	0.53
1:F:2:THR:OG1	2:B:192:ASP:OD2	2.26	0.53
1:F:193:PRO:HA	1:F:272:PHE:CZ	2.43	0.53
2:E:84:PHE:CE1	2:E:90:LYS:HA	2.37	0.53
2:E:187:HIS:HB3	2:E:190:GLU:HG3	1.89	0.53
3:D:742:ARG:HG3	3:D:742:ARG:O	2.09	0.53
3:A:542:SER:HB3	3:A:758:GLU:HG3	1.85	0.53
1:F:254:ILE:C	1:F:256:SER:H	2.12	0.53
3:D:767:SER:O	3:D:770:ILE:HB	2.09	0.53
1:C:16:LEU:HD11	1:C:31:TYR:HB2	1.91	0.53
1:F:16:LEU:HD11	1:F:31:TYR:HB2	1.91	0.53
1:F:329:ALA:N	1:F:333:GLU:OE2	2.41	0.53
3:A:187:SER:HB3	3:A:459:CYS:SG	2.49	0.53
3:D:187:SER:HB3	3:D:459:CYS:SG	2.49	0.53
3:D:208:LEU:HB2	3:D:213:ILE:HD11	1.91	0.53
3:D:974:ARG:O	3:D:977:SER:N	2.41	0.53
3:A:700:SER:OG	3:A:701:VAL:N	2.41	0.53
1:F:267:LYS:HG3	1:F:276:TYR:CD1	2.43	0.53
2:E:18:ASP:OD2	2:E:57:LEU:N	2.28	0.53
3:D:840:LYS:HG2	3:D:841:ASN:H	1.74	0.52
1:C:193:PRO:HA	1:C:272:PHE:CE2	2.43	0.52
3:D:14:GLU:CD	3:D:14:GLU:H	2.13	0.52
2:B:172:SER:O	2:B:174:VAL:N	2.41	0.52
3:A:551:ASN:OD1	3:A:551:ASN:N	2.35	0.52
3:D:547:ILE:CG1	3:D:794:VAL:H	2.21	0.52
3:D:716:ASN:N	3:D:716:ASN:OD1	2.42	0.52
3:D:842:MET:O	3:D:845:THR:N	2.43	0.52
3:A:604:ARG:HB3	3:A:605:LEU:HD12	1.90	0.52
3:A:715:ALA:O	3:A:716:ASN:HB3	2.08	0.52
1:F:193:PRO:HA	1:F:272:PHE:CE2	2.43	0.52
1:C:373:ASN:OD1	3:A:577:ARG:HG3	2.10	0.52
3:A:240:SER:OG	3:A:241:GLU:N	2.42	0.52
3:A:717:THR:HG22	3:A:718:LEU:N	2.23	0.52
3:A:742:ARG:HG3	3:A:742:ARG:O	2.09	0.52
3:A:842:MET:O	3:A:845:THR:N	2.42	0.52
1:F:215:PHE:CD1	1:F:215:PHE:C	2.83	0.52
2:B:57:LEU:HG	2:B:151:HIS:CG	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:442:GLN:HA	3:A:445:LYS:HG3	1.91	0.52
1:F:30:LYS:HE2	1:F:34:LEU:HG	1.91	0.52
2:E:57:LEU:HG	2:E:151:HIS:CG	2.45	0.52
3:A:703:ASN:N	3:A:714:PHE:O	2.43	0.52
2:E:23:MET:HG3	2:E:24:SER:N	2.25	0.52
3:A:208:LEU:HB2	3:A:213:ILE:HD11	1.91	0.52
2:B:41:GLU:OE1	2:B:127:LEU:HB3	2.10	0.52
3:A:724:MET:N	3:A:724:MET:CE	2.73	0.52
1:F:375:MET:HB3	1:F:389:ILE:HA	1.92	0.52
3:D:703:ASN:N	3:D:714:PHE:O	2.43	0.52
1:C:215:PHE:CD1	1:C:215:PHE:C	2.83	0.52
1:F:132:LEU:HD22	1:F:193:PRO:HD2	1.92	0.51
1:C:375:MET:HB3	1:C:389:ILE:HA	1.92	0.51
3:A:666:SER:O	3:A:666:SER:OG	2.27	0.51
3:D:876:LEU:CD1	3:D:968:TYR:HB3	2.40	0.51
1:C:251:ASP:OD1	1:C:251:ASP:N	2.20	0.51
3:A:609:ILE:N	3:A:609:ILE:CD1	2.73	0.51
1:F:37:TRP:HZ3	3:A:674:ARG:HH22	1.58	0.51
1:C:370:THR:O	1:C:374:ASN:ND2	2.43	0.51
3:A:540:MET:C	3:A:797:ASN:HB3	2.31	0.51
1:F:253:LEU:HD12	1:F:258:VAL:HG21	1.92	0.51
3:D:442:GLN:HA	3:D:445:LYS:HG3	1.91	0.51
2:E:18:ASP:HB3	2:E:57:LEU:HB2	1.93	0.51
3:D:525:LYS:HE3	3:D:527:PRO:HA	1.93	0.51
1:C:30:LYS:HE2	1:C:34:LEU:HG	1.92	0.51
3:A:546:LEU:N	3:A:546:LEU:CD1	2.73	0.51
3:A:840:LYS:HG2	3:A:841:ASN:H	1.74	0.51
2:E:172:SER:O	2:E:174:VAL:N	2.41	0.51
3:D:1:MET:N	3:D:129:GLU:OE2	2.35	0.51
1:F:230:ASP:O	1:F:232:ILE:HG13	2.11	0.51
3:D:399:GLU:O	3:D:401:ILE:N	2.44	0.51
3:D:604:ARG:HG3	3:D:611:GLU:CD	2.25	0.51
3:A:14:GLU:CD	3:A:14:GLU:H	2.13	0.51
3:D:724:MET:N	3:D:724:MET:CE	2.73	0.51
1:C:132:LEU:HD22	1:C:193:PRO:HD2	1.92	0.51
3:D:568:LEU:HB2	3:D:615:PHE:CE1	2.46	0.50
1:C:230:ASP:O	1:C:232:ILE:HG13	2.11	0.50
1:F:3:SER:C	2:B:193:ARG:HH12	2.14	0.50
3:D:717:THR:HG22	3:D:729:ILE:CG2	2.41	0.50
1:F:12:GLU:HB3	1:F:30:LYS:HE3	1.94	0.50
1:F:377:PHE:CE2	3:D:578:LEU:HD22	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:240:SER:OG	3:D:241:GLU:N	2.42	0.50
3:D:810:LYS:N	3:D:822:GLU:O	2.44	0.50
1:C:253:LEU:HD12	1:C:258:VAL:HG21	1.92	0.50
3:A:525:LYS:HE3	3:A:527:PRO:HA	1.93	0.50
2:B:18:ASP:HB3	2:B:57:LEU:HB2	1.93	0.50
3:A:810:LYS:N	3:A:822:GLU:O	2.44	0.50
3:D:609:ILE:N	3:D:609:ILE:CD1	2.73	0.50
2:B:23:MET:HG3	2:B:24:SER:N	2.25	0.50
3:A:568:LEU:HB2	3:A:615:PHE:CE1	2.46	0.50
2:E:40:ASP:OD2	2:E:126:LYS:HE3	2.12	0.50
3:A:533:VAL:HG13	3:A:803:LYS:CD	2.28	0.50
1:F:370:THR:O	1:F:374:ASN:ND2	2.43	0.50
1:C:12:GLU:HB3	1:C:30:LYS:HE3	1.93	0.50
3:A:701:VAL:HG11	3:A:717:THR:O	2.12	0.50
2:E:110:LEU:HD12	2:E:113:ILE:HD12	1.94	0.50
3:A:43:THR:OG1	3:A:46:ILE:HG13	2.12	0.50
3:A:526:PHE:CE2	3:A:604:ARG:HD2	2.46	0.50
3:A:538:GLN:OE1	3:A:746:ARG:NH2	2.41	0.50
3:A:777:LEU:O	3:A:781:ARG:N	2.23	0.50
3:D:170:HIS:HB2	3:D:207:MET:CE	2.42	0.50
3:D:849:ARG:O	3:D:853:MET:HE2	2.12	0.50
2:B:40:ASP:OD2	2:B:126:LYS:HE3	2.12	0.50
2:B:110:LEU:HD12	2:B:113:ILE:HD12	1.94	0.50
3:A:763:ASP:OD2	3:A:767:SER:N	2.45	0.50
1:F:319:LEU:O	1:F:323:LEU:HD12	2.12	0.49
3:D:876:LEU:HD13	3:D:972:PHE:CD2	2.47	0.49
2:B:15:TYR:CZ	2:B:53:LEU:HD22	2.47	0.49
3:D:170:HIS:O	3:D:181:ASN:ND2	2.30	0.49
3:D:714:PHE:CZ	3:D:782:VAL:HG21	2.47	0.49
1:C:319:LEU:O	1:C:323:LEU:HD12	2.12	0.49
3:A:399:GLU:O	3:A:401:ILE:N	2.44	0.49
3:D:547:ILE:CD1	3:D:756:PHE:HE1	2.04	0.49
3:A:714:PHE:CZ	3:A:782:VAL:HG21	2.47	0.49
1:F:256:SER:HB3	1:F:258:VAL:CG2	2.43	0.49
3:D:666:SER:O	3:D:666:SER:OG	2.27	0.49
3:A:763:ASP:OD1	3:A:767:SER:CB	2.59	0.49
3:A:590:LYS:HG3	3:A:591:TYR:N	2.28	0.49
1:F:225:VAL:HB	1:F:233:PHE:HB3	1.95	0.49
1:F:424:LEU:HD22	1:F:425:PHE:CE1	2.48	0.49
2:E:15:TYR:CZ	2:E:53:LEU:HD22	2.47	0.49
3:D:526:PHE:HD2	3:D:604:ARG:HB3	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:604:ARG:N	3:D:611:GLU:OE1	2.46	0.49
1:C:225:VAL:HB	1:C:233:PHE:HB3	1.95	0.49
2:B:36:TRP:HE1	3:A:179:PHE:HB3	1.77	0.49
3:A:876:LEU:HD13	3:A:972:PHE:CD2	2.47	0.49
2:E:87:LYS:HZ1	2:E:185:ARG:HH12	1.61	0.49
2:E:182:PRO:HB3	2:E:189:PHE:HB3	1.94	0.49
3:D:223:ARG:CG	3:D:223:ARG:HH11	2.26	0.49
2:B:107:GLY:H	2:B:217:ILE:HB	1.77	0.49
3:A:412:GLU:OE1	3:A:413:ASN:HB2	2.12	0.49
3:A:836:SER:C	3:A:837:LYS:HG3	2.33	0.49
2:E:15:TYR:HD2	2:E:23:MET:HB3	1.77	0.49
3:D:209:THR:HG23	3:D:212:GLU:OE2	2.13	0.49
1:C:219:TYR:HB2	1:C:263:PHE:CE2	2.48	0.49
1:C:424:LEU:HD22	1:C:425:PHE:CE1	2.48	0.49
3:A:170:HIS:HB2	3:A:207:MET:CE	2.42	0.49
1:F:183:ILE:HD13	3:A:997:PHE:CZ	2.48	0.48
1:F:219:TYR:CD1	1:F:240:LYS:HB3	2.47	0.48
3:D:412:GLU:OE1	3:D:413:ASN:HB2	2.12	0.48
1:C:378:LYS:HB3	1:C:386:ASN:HB3	1.95	0.48
2:B:15:TYR:HD2	2:B:23:MET:HB3	1.77	0.48
3:A:604:ARG:N	3:A:611:GLU:OE1	2.46	0.48
3:D:542:SER:O	3:D:758:GLU:CD	2.52	0.48
3:D:682:ALA:O	3:D:686:SER:OG	2.29	0.48
2:E:62:VAL:O	2:E:116:VAL:HA	2.14	0.48
2:E:169:LYS:HB2	2:E:169:LYS:HE3	1.56	0.48
2:E:187:HIS:O	2:E:190:GLU:HB2	2.13	0.48
3:D:2:ASP:OD1	3:D:2:ASP:N	2.46	0.48
3:D:625:ARG:O	3:D:629:THR:HG23	2.13	0.48
3:D:777:LEU:O	3:D:781:ARG:N	2.23	0.48
3:A:542:SER:O	3:A:758:GLU:CD	2.52	0.48
1:F:219:TYR:HB2	1:F:263:PHE:CE2	2.48	0.48
3:D:43:THR:OG1	3:D:46:ILE:HG13	2.12	0.48
3:D:590:LYS:HG3	3:D:591:TYR:N	2.28	0.48
1:C:219:TYR:CD1	1:C:240:LYS:HB3	2.47	0.48
2:B:182:PRO:HB3	2:B:189:PHE:HB3	1.94	0.48
3:A:577:ARG:C	3:A:579:GLU:H	2.17	0.48
1:F:417:VAL:HA	1:F:420:VAL:CG2	2.43	0.48
3:D:72:ILE:HA	3:D:571:VAL:HG22	1.96	0.48
3:A:209:THR:HG23	3:A:212:GLU:OE2	2.13	0.48
3:A:625:ARG:O	3:A:629:THR:HG23	2.13	0.48
2:E:107:GLY:H	2:E:217:ILE:HB	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:158:LEU:HD23	2:E:182:PRO:HD3	1.96	0.48
3:D:538:GLN:OE1	3:D:746:ARG:NH2	2.41	0.48
3:A:750:GLY:HA2	3:A:755:VAL:HA	1.96	0.48
3:D:706:GLU:HA	3:D:711:MET:HB3	1.96	0.48
1:C:383:LYS:HE2	1:C:415:ASN:HB3	1.96	0.48
3:A:124:CYS:SG	3:A:155:ARG:HA	2.54	0.48
3:A:223:ARG:CG	3:A:223:ARG:HH11	2.26	0.48
3:A:766:LYS:O	3:A:769:GLU:HG3	2.14	0.48
1:F:178:ASP:HA	1:F:181:TYR:CE1	2.49	0.48
3:D:836:SER:C	3:D:837:LYS:HG3	2.33	0.48
3:A:364:GLY:O	3:A:423:THR:OG1	2.31	0.48
1:F:271:THR:HG23	1:F:272:PHE:CD2	2.49	0.48
1:F:366:ALA:O	1:F:369:ILE:N	2.33	0.48
1:F:383:LYS:HE2	1:F:415:ASN:HB3	1.96	0.48
3:D:700:SER:O	3:D:715:ALA:CB	2.61	0.48
3:D:750:GLY:HA2	3:D:755:VAL:HA	1.96	0.48
1:C:178:ASP:HA	1:C:181:TYR:CE1	2.49	0.48
2:B:62:VAL:O	2:B:116:VAL:HA	2.14	0.48
2:B:174:VAL:HG12	2:B:176:THR:HG22	1.96	0.48
3:A:142:CYS:SG	3:A:143:ASP:N	2.87	0.48
3:A:706:GLU:HA	3:A:711:MET:HB3	1.95	0.48
2:E:142:LYS:O	2:E:146:GLN:HG2	2.13	0.47
3:D:54:PRO:HB3	3:D:91:ILE:HD11	1.96	0.47
3:D:652:ILE:HG22	3:D:653:TYR:CD1	2.49	0.47
3:D:748:VAL:HG12	3:D:757:THR:HA	1.96	0.47
1:C:417:VAL:HA	1:C:420:VAL:CG2	2.44	0.47
2:B:83:ASN:OD1	2:B:85:THR:HB	2.14	0.47
2:B:158:LEU:HD23	2:B:182:PRO:HD3	1.96	0.47
3:A:630:PHE:CD2	3:A:663:VAL:HG23	2.49	0.47
3:A:779:ASN:ND2	3:A:789:ILE:HA	2.29	0.47
1:F:177:ASP:N	1:F:180:LEU:HB2	2.24	0.47
1:F:378:LYS:HB3	1:F:386:ASN:HB3	1.95	0.47
3:D:124:CYS:SG	3:D:155:ARG:HA	2.54	0.47
3:D:630:PHE:CD2	3:D:663:VAL:HG23	2.49	0.47
2:B:202:LEU:HD23	2:B:202:LEU:HA	1.66	0.47
3:A:229:GLU:HA	3:A:229:GLU:OE1	2.14	0.47
3:D:229:GLU:OE1	3:D:229:GLU:HA	2.14	0.47
3:D:345:LYS:HD3	3:D:346:LEU:H	1.78	0.47
1:C:176:PHE:HD1	1:C:210:VAL:HG11	1.79	0.47
1:C:177:ASP:N	1:C:180:LEU:HB2	2.24	0.47
2:B:187:HIS:O	2:B:190:GLU:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:546:LEU:HD13	3:A:757:THR:O	2.15	0.47
1:F:110:ILE:HD11	1:F:135:ARG:NH2	2.30	0.47
1:F:176:PHE:HD1	1:F:210:VAL:HG11	1.79	0.47
3:D:351:LYS:HG3	3:D:432:SER:OG	2.14	0.47
1:C:285:THR:HG22	1:C:286:ARG:H	1.80	0.47
1:C:366:ALA:O	1:C:369:ILE:N	2.33	0.47
3:A:547:ILE:HG13	3:A:794:VAL:CG2	2.44	0.47
3:A:652:ILE:HG22	3:A:653:TYR:CD1	2.49	0.47
3:D:364:GLY:O	3:D:423:THR:OG1	2.31	0.47
3:D:873:GLU:HB2	3:D:992:PHE:HE2	1.79	0.47
2:B:142:LYS:O	2:B:146:GLN:HG2	2.14	0.47
3:A:748:VAL:HG12	3:A:757:THR:HA	1.96	0.47
3:D:577:ARG:C	3:D:579:GLU:H	2.17	0.47
3:D:763:ASP:HB2	3:D:767:SER:HB3	1.95	0.47
3:D:768:ILE:HG12	3:D:795:TYR:OH	2.15	0.47
1:C:332:ASP:O	1:C:335:VAL:HG22	2.14	0.47
2:B:61:ARG:NE	2:B:208:THR:HG23	2.29	0.47
3:A:54:PRO:HB3	3:A:91:ILE:HD11	1.96	0.47
3:A:525:LYS:HG3	3:A:527:PRO:HD3	1.97	0.47
3:A:808:THR:HB	3:A:810:LYS:HG3	1.95	0.47
2:E:61:ARG:NE	2:E:208:THR:HG23	2.29	0.47
2:E:83:ASN:OD1	2:E:85:THR:HB	2.14	0.47
3:D:81:ARG:HH11	3:D:81:ARG:CG	2.23	0.47
3:D:316:THR:OG1	3:D:317:THR:N	2.48	0.47
3:D:702:LEU:HD23	3:D:702:LEU:HA	1.54	0.47
3:D:779:ASN:ND2	3:D:789:ILE:HA	2.29	0.47
3:D:808:THR:HB	3:D:810:LYS:HG3	1.95	0.47
3:D:835:VAL:HG23	3:D:836:SER:N	2.29	0.47
1:C:110:ILE:HD11	1:C:135:ARG:NH2	2.30	0.47
1:C:271:THR:HG23	1:C:272:PHE:CD2	2.49	0.47
2:B:60:LYS:HA	2:B:60:LYS:HD3	1.68	0.47
2:B:87:LYS:HZ1	2:B:185:ARG:HH12	1.61	0.47
3:A:72:ILE:HA	3:A:571:VAL:HG22	1.96	0.47
3:A:81:ARG:HH11	3:A:81:ARG:CG	2.23	0.47
3:A:835:VAL:HG23	3:A:836:SER:N	2.29	0.47
3:A:873:GLU:HB2	3:A:992:PHE:HE2	1.80	0.47
3:A:876:LEU:CD1	3:A:968:TYR:HB3	2.40	0.47
1:F:409:GLN:O	1:F:413:ILE:HG22	2.15	0.47
3:D:226:SER:OG	3:D:227:LEU:N	2.47	0.47
3:D:542:SER:O	3:D:758:GLU:OE2	2.33	0.47
3:A:711:MET:SD	3:A:732:ILE:HD11	2.55	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:837:LYS:HA	3:A:890:PHE:CD1	2.50	0.47
3:A:839:HIS:CE1	3:A:967:PHE:HB2	2.50	0.47
3:D:525:LYS:HG3	3:D:527:PRO:HD3	1.97	0.47
3:D:711:MET:SD	3:D:732:ILE:HD11	2.55	0.47
3:D:836:SER:C	3:D:837:LYS:HE3	2.35	0.47
3:A:849:ARG:O	3:A:853:MET:HE2	2.14	0.47
2:E:9:ALA:HA	2:E:11:TYR:CD1	2.49	0.47
2:E:174:VAL:HG12	2:E:176:THR:HG22	1.96	0.47
3:A:46:ILE:O	3:A:50:LEU:HB2	2.15	0.47
3:D:839:HIS:CE1	3:D:967:PHE:HB2	2.50	0.46
3:A:542:SER:O	3:A:758:GLU:OE2	2.33	0.46
1:F:335:VAL:CG1	1:F:420:VAL:HG12	2.39	0.46
3:A:351:LYS:HG3	3:A:432:SER:OG	2.14	0.46
1:F:35:VAL:HA	1:F:45:ILE:HG12	1.98	0.46
2:E:175:THR:HA	1:C:43:TRP:CD1	2.51	0.46
3:D:701:VAL:CB	3:D:715:ALA:CB	2.92	0.46
3:D:837:LYS:HA	3:D:890:PHE:CD1	2.50	0.46
1:C:35:VAL:HA	1:C:45:ILE:HG12	1.98	0.46
2:B:9:ALA:HA	2:B:11:TYR:CD1	2.49	0.46
3:A:2:ASP:OD1	3:A:2:ASP:N	2.46	0.46
3:A:134:LYS:HD3	3:A:134:LYS:HA	1.54	0.46
1:F:176:PHE:H	1:F:210:VAL:HG11	1.80	0.46
1:F:379:ILE:HG23	1:F:383:LYS:H	1.81	0.46
3:A:219:ARG:HH21	3:A:453:LEU:HD12	1.81	0.46
3:A:345:LYS:HD3	3:A:346:LEU:H	1.78	0.46
3:A:446:ASP:OD1	3:A:446:ASP:N	2.40	0.46
3:A:700:SER:O	3:A:715:ALA:CB	2.61	0.46
1:F:218:MET:O	1:F:263:PHE:HA	2.15	0.46
3:D:46:ILE:O	3:D:50:LEU:HB2	2.15	0.46
3:D:142:CYS:SG	3:D:143:ASP:N	2.87	0.46
3:D:407:ARG:HB2	3:D:418:VAL:HB	1.98	0.46
1:C:176:PHE:H	1:C:210:VAL:HG11	1.80	0.46
2:B:9:ALA:HA	2:B:11:TYR:HD1	1.81	0.46
2:B:105:TYR:N	2:B:105:TYR:CD1	2.84	0.46
3:A:407:ARG:HB2	3:A:418:VAL:HB	1.98	0.46
3:D:270:ARG:O	3:D:274:ASN:HB2	2.15	0.46
1:C:409:GLN:O	1:C:413:ILE:HG22	2.15	0.46
1:C:397:ASN:OD1	1:C:399:SER:N	2.49	0.46
2:B:177:ILE:HD12	2:B:177:ILE:HA	1.73	0.46
3:A:270:ARG:O	3:A:274:ASN:HB2	2.15	0.46
2:E:9:ALA:HA	2:E:11:TYR:HD1	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:19:TRP:CE3	2:E:147:HIS:HD2	2.33	0.46
3:D:539:LYS:O	3:D:982:LEU:HA	2.16	0.46
3:A:297:LEU:HD11	3:A:320:VAL:HG22	1.98	0.46
3:A:701:VAL:CB	3:A:715:ALA:CB	2.92	0.46
3:A:759:ILE:HG22	3:A:762:GLN:H	1.81	0.46
1:F:332:ASP:O	1:F:335:VAL:HG22	2.14	0.46
3:D:397:VAL:HG23	3:D:401:ILE:O	2.16	0.46
3:D:744:ARG:NH1	3:D:744:ARG:HG3	2.31	0.46
3:D:852:GLU:O	3:D:855:SER:OG	2.34	0.46
3:A:1:MET:N	3:A:129:GLU:OE2	2.35	0.46
3:A:536:PRO:HA	3:A:749:TYR:CD1	2.51	0.46
1:F:285:THR:HG22	1:F:286:ARG:H	1.80	0.46
1:C:241:SER:O	1:C:241:SER:OG	2.34	0.46
2:B:163:PHE:HD1	2:B:166:ILE:HG21	1.81	0.46
3:A:316:THR:OG1	3:A:317:THR:N	2.48	0.46
3:A:699:GLU:OE1	3:A:748:VAL:HG23	2.16	0.46
3:D:219:ARG:HH21	3:D:453:LEU:HD12	1.81	0.45
3:D:292:LYS:HB2	3:D:292:LYS:HE2	1.44	0.45
3:D:717:THR:HG22	3:D:729:ILE:HG21	1.96	0.45
3:A:539:LYS:O	3:A:982:LEU:HA	2.16	0.45
3:A:685:LYS:O	3:A:689:SER:OG	2.29	0.45
1:F:110:ILE:HG13	1:F:136:TRP:CD1	2.51	0.45
3:D:687:CYS:C	3:D:689:SER:H	2.20	0.45
3:D:823:ARG:HA	3:D:823:ARG:HD3	1.58	0.45
1:C:214:LYS:HA	1:C:214:LYS:HD3	1.68	0.45
1:C:218:MET:O	1:C:263:PHE:HA	2.15	0.45
3:A:702:LEU:HD23	3:A:702:LEU:HA	1.54	0.45
1:F:20:LEU:HA	1:F:23:SER:OG	2.17	0.45
2:E:163:PHE:HD1	2:E:166:ILE:HG21	1.81	0.45
3:D:95:LYS:HD3	3:D:95:LYS:HA	1.63	0.45
3:D:785:ASN:O	3:D:787:PHE:N	2.49	0.45
2:B:210:ILE:HD12	2:B:210:ILE:HA	1.72	0.45
3:A:226:SER:OG	3:A:227:LEU:N	2.47	0.45
3:A:552:SER:O	3:A:552:SER:OG	2.34	0.45
3:A:743:PHE:CD1	3:A:743:PHE:N	2.84	0.45
1:F:397:ASN:OD1	1:F:399:SER:N	2.49	0.45
2:E:105:TYR:CD1	2:E:105:TYR:N	2.84	0.45
2:E:201:LEU:N	2:E:201:LEU:HD13	2.32	0.45
3:D:576:ASN:HD21	3:D:579:GLU:HG3	1.82	0.45
3:D:743:PHE:N	3:D:743:PHE:CD1	2.84	0.45
2:B:19:TRP:CE3	2:B:147:HIS:HD2	2.33	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:ILE:HG21	2:B:212:TRP:CE2	2.51	0.45
3:A:576:ASN:HD21	3:A:579:GLU:HG3	1.82	0.45
3:D:374:ASP:O	3:D:376:THR:HG23	2.17	0.45
3:D:759:ILE:HG22	3:D:762:GLN:H	1.81	0.45
3:A:717:THR:HG22	3:A:719:SER:N	2.32	0.45
3:A:836:SER:C	3:A:837:LYS:HE3	2.36	0.45
3:A:876:LEU:HD13	3:A:972:PHE:CE2	2.52	0.45
1:F:256:SER:CB	1:F:258:VAL:HG23	2.46	0.45
3:D:685:LYS:O	3:D:689:SER:OG	2.29	0.45
3:D:699:GLU:OE1	3:D:748:VAL:HG23	2.16	0.45
3:D:739:ILE:HG13	3:D:741:TYR:CE1	2.52	0.45
3:D:997:PHE:CE1	1:C:183:ILE:HD13	2.52	0.45
1:C:224:LYS:O	1:C:235:PRO:HA	2.17	0.45
1:C:225:VAL:HA	1:C:234:ILE:O	2.17	0.45
3:A:213:ILE:HG21	3:A:223:ARG:HH12	1.82	0.45
3:A:244:LEU:HD23	3:A:245:LEU:HD23	1.99	0.45
3:A:397:VAL:HG23	3:A:401:ILE:O	2.16	0.45
3:A:687:CYS:C	3:A:689:SER:H	2.20	0.45
1:F:195:ILE:HD12	1:F:211:ASP:OD2	2.17	0.45
2:E:105:TYR:N	2:E:105:TYR:HD1	2.15	0.45
3:D:223:ARG:HH11	3:D:223:ARG:HG3	1.82	0.45
3:D:842:MET:O	3:D:843:ILE:C	2.54	0.45
1:C:335:VAL:CG1	1:C:420:VAL:HG12	2.39	0.45
3:A:223:ARG:HH11	3:A:223:ARG:HG3	1.82	0.45
3:A:696:LEU:O	3:A:700:SER:HB3	2.17	0.45
2:E:22:VAL:HB	2:E:143:LEU:HD21	1.98	0.45
2:E:210:ILE:HG21	2:E:212:TRP:CE2	2.51	0.45
3:D:398:ASP:OD1	3:D:430:LYS:HB2	2.17	0.45
3:D:526:PHE:CD2	3:D:604:ARG:HB3	2.51	0.45
3:D:692:ARG:O	3:D:696:LEU:HG	2.17	0.45
1:C:110:ILE:HG13	1:C:136:TRP:CD1	2.51	0.45
3:A:95:LYS:HA	3:A:95:LYS:HD3	1.63	0.45
3:A:763:ASP:CB	3:A:767:SER:H	2.28	0.45
2:E:18:ASP:CB	2:E:57:LEU:HB2	2.47	0.45
1:C:20:LEU:HA	1:C:23:SER:OG	2.17	0.45
1:C:195:ILE:HD12	1:C:211:ASP:OD2	2.17	0.45
1:C:358:ARG:NH1	1:C:359:GLU:OE1	2.50	0.45
3:A:773:GLU:C	3:A:776:ARG:HB2	2.35	0.45
3:A:785:ASN:O	3:A:787:PHE:N	2.49	0.45
3:D:785:ASN:HB3	3:D:786:ASN:H	1.62	0.45
1:C:379:ILE:HG23	1:C:383:LYS:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:SER:HG	2:B:8:HIS:CE1	2.33	0.45
2:B:22:VAL:HB	2:B:143:LEU:HD21	1.98	0.45
2:B:105:TYR:N	2:B:105:TYR:HD1	2.15	0.45
1:F:224:LYS:O	1:F:235:PRO:HA	2.17	0.44
3:D:709:ASN:HB3	3:D:737:LEU:HD13	1.99	0.44
3:D:766:LYS:CD	3:D:766:LYS:C	2.86	0.44
3:D:876:LEU:HD13	3:D:972:PHE:CE2	2.52	0.44
3:A:269:LEU:O	3:A:273:THR:HG22	2.16	0.44
3:A:374:ASP:HB3	3:A:375:THR:H	1.56	0.44
3:A:533:VAL:CG1	3:A:803:LYS:CD	2.93	0.44
3:D:222:LEU:HD22	3:D:234:ARG:HG2	2.00	0.44
3:D:223:ARG:HG3	3:D:223:ARG:NH1	2.33	0.44
3:D:269:LEU:O	3:D:273:THR:HG22	2.17	0.44
3:D:403:CYS:SG	3:D:419:LEU:HB3	2.58	0.44
3:D:696:LEU:O	3:D:700:SER:HB3	2.17	0.44
3:D:767:SER:O	3:D:770:ILE:HG13	2.17	0.44
3:A:398:ASP:OD1	3:A:430:LYS:HB2	2.17	0.44
3:A:717:THR:CG2	3:A:718:LEU:N	2.80	0.44
3:A:744:ARG:NH1	3:A:744:ARG:HG3	2.31	0.44
1:F:232:ILE:HG23	1:F:307:TYR:HB3	1.99	0.44
3:D:103:THR:OG1	3:D:104:MET:N	2.50	0.44
3:D:213:ILE:HG21	3:D:223:ARG:HH12	1.82	0.44
3:D:275:ARG:O	3:D:279:LEU:HG	2.17	0.44
3:D:297:LEU:HD11	3:D:320:VAL:HG22	1.98	0.44
3:D:701:VAL:HA	3:D:715:ALA:N	2.32	0.44
2:B:113:ILE:O	2:B:116:VAL:HG22	2.17	0.44
2:B:201:LEU:HD13	2:B:201:LEU:N	2.32	0.44
3:A:438:ILE:HD12	3:A:458:TYR:CE2	2.53	0.44
3:A:542:SER:O	3:A:758:GLU:CG	2.65	0.44
3:A:692:ARG:O	3:A:696:LEU:HG	2.17	0.44
1:F:379:ILE:HG21	3:D:582:ILE:HD13	2.00	0.44
1:F:383:LYS:CE	1:F:415:ASN:HB3	2.48	0.44
3:D:407:ARG:HA	3:D:407:ARG:HD3	1.81	0.44
3:A:213:ILE:O	3:A:217:VAL:HG23	2.18	0.44
3:A:763:ASP:HB3	3:A:767:SER:H	1.82	0.44
3:D:542:SER:O	3:D:758:GLU:CG	2.65	0.44
3:A:514:LYS:HD2	3:A:514:LYS:H	1.82	0.44
3:A:934:CYS:O	3:A:966:ILE:HD13	2.18	0.44
1:F:358:ARG:NH1	1:F:359:GLU:OE1	2.50	0.44
2:E:72:LYS:O	2:E:86:LYS:NZ	2.50	0.44
3:D:485:THR:OG1	3:D:659:THR:HG21	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:ILE:HG23	1:C:307:TYR:HB3	1.99	0.44
2:B:50:PHE:HB3	2:B:53:LEU:HD13	2.00	0.44
3:A:682:ALA:O	3:A:686:SER:OG	2.29	0.44
3:A:823:ARG:HA	3:A:823:ARG:HD3	1.58	0.44
3:A:842:MET:O	3:A:843:ILE:C	2.54	0.44
3:A:852:GLU:O	3:A:855:SER:OG	2.34	0.44
1:F:241:SER:O	1:F:241:SER:OG	2.34	0.44
2:E:15:TYR:CE1	2:E:53:LEU:HD13	2.53	0.44
3:D:536:PRO:HA	3:D:749:TYR:CD1	2.51	0.44
3:A:76:LEU:HD12	3:A:76:LEU:HA	1.79	0.44
3:A:701:VAL:HA	3:A:715:ALA:N	2.32	0.44
2:E:113:ILE:O	2:E:116:VAL:HG22	2.17	0.44
3:D:934:CYS:O	3:D:966:ILE:HD13	2.17	0.44
1:C:383:LYS:CE	1:C:415:ASN:HB3	2.48	0.44
3:A:103:THR:OG1	3:A:104:MET:N	2.50	0.44
3:A:698:LEU:HD12	3:A:698:LEU:HA	1.64	0.44
3:A:763:ASP:CG	3:A:767:SER:HA	2.38	0.44
3:A:811:TYR:CE1	3:A:813:ALA:HB2	2.53	0.44
3:A:866:ILE:HG22	3:A:867:ASP:N	2.32	0.44
2:E:72:LYS:NZ	2:E:72:LYS:CB	2.74	0.44
3:D:773:GLU:C	3:D:776:ARG:HB2	2.35	0.44
3:A:275:ARG:O	3:A:279:LEU:HG	2.17	0.44
3:A:292:LYS:HB2	3:A:292:LYS:HE2	1.44	0.44
3:A:485:THR:OG1	3:A:659:THR:HG21	2.17	0.44
1:F:179:GLU:HA	1:F:179:GLU:OE1	2.18	0.43
3:A:374:ASP:O	3:A:376:THR:HG23	2.17	0.43
3:A:639:LYS:O	3:A:642:LYS:N	2.51	0.43
3:A:724:MET:HE3	3:A:724:MET:HB2	1.80	0.43
1:F:144:LYS:O	1:F:205:LEU:HD11	2.18	0.43
1:F:154:LEU:O	1:F:157:GLU:N	2.51	0.43
1:F:225:VAL:HA	1:F:234:ILE:O	2.17	0.43
2:E:210:ILE:HD12	2:E:210:ILE:HA	1.72	0.43
3:D:533:VAL:CG1	3:D:803:LYS:CD	2.93	0.43
3:D:880:PHE:CE1	3:D:965:ARG:HB3	2.53	0.43
3:A:268:ASP:O	3:A:272:ILE:HG13	2.18	0.43
3:D:187:SER:O	3:D:188:TYR:CG	2.71	0.43
3:D:636:ARG:HG2	3:D:637:TYR:N	2.31	0.43
1:C:378:LYS:HD2	1:C:378:LYS:HA	1.87	0.43
2:B:15:TYR:CE1	2:B:53:LEU:HD13	2.53	0.43
3:A:403:CYS:SG	3:A:419:LEU:HB3	2.58	0.43
3:A:486:TYR:CZ	3:A:501:ILE:HD12	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:709:ASN:HB3	3:A:737:LEU:HD13	1.99	0.43
3:A:762:GLN:O	3:A:763:ASP:C	2.55	0.43
1:F:387:PHE:CE1	1:F:411:VAL:HG21	2.53	0.43
2:E:109:ASN:OD1	2:E:109:ASN:C	2.57	0.43
3:D:438:ILE:HD12	3:D:458:TYR:CE2	2.53	0.43
3:D:639:LYS:O	3:D:642:LYS:N	2.51	0.43
3:D:811:TYR:CE1	3:D:813:ALA:HB2	2.53	0.43
3:D:876:LEU:HD12	3:D:876:LEU:HA	1.63	0.43
1:C:266:VAL:HA	1:C:276:TYR:H	1.83	0.43
1:C:387:PHE:CE1	1:C:411:VAL:HG21	2.53	0.43
3:A:739:ILE:HG13	3:A:741:TYR:CE1	2.52	0.43
1:F:214:LYS:HA	1:F:214:LYS:HD3	1.68	0.43
1:F:297:ILE:HG13	1:F:298:GLY:N	2.32	0.43
2:B:18:ASP:CB	2:B:57:LEU:HB2	2.47	0.43
3:A:222:LEU:HD22	3:A:234:ARG:HG2	2.00	0.43
3:A:223:ARG:HG3	3:A:223:ARG:NH1	2.33	0.43
3:A:407:ARG:HA	3:A:407:ARG:HD3	1.81	0.43
3:A:768:ILE:CD1	3:A:816:ASN:HB2	2.49	0.43
2:E:145:LEU:HD12	2:E:145:LEU:HA	1.78	0.43
3:D:265:HIS:CE1	3:D:330:ASP:HB2	2.53	0.43
3:D:407:ARG:HB2	3:D:418:VAL:CG2	2.48	0.43
3:D:811:TYR:HE1	3:D:813:ALA:HB2	1.84	0.43
3:D:866:ILE:HG22	3:D:867:ASP:N	2.32	0.43
1:C:250:VAL:O	1:C:254:ILE:HG13	2.19	0.43
2:B:48:LYS:HG3	2:B:51:ILE:HG12	1.99	0.43
3:A:227:LEU:HD12	3:A:227:LEU:HA	1.78	0.43
3:A:265:HIS:CE1	3:A:330:ASP:HB2	2.53	0.43
3:A:636:ARG:HG2	3:A:637:TYR:N	2.31	0.43
1:F:266:VAL:HA	1:F:276:TYR:H	1.83	0.43
3:D:268:ASP:O	3:D:272:ILE:HG13	2.18	0.43
3:D:481:ALA:O	3:D:485:THR:OG1	2.37	0.43
3:D:766:LYS:O	3:D:766:LYS:HD3	2.19	0.43
1:C:154:LEU:O	1:C:157:GLU:N	2.51	0.43
3:D:244:LEU:HD23	3:D:245:LEU:HD23	1.99	0.43
3:D:341:LEU:HB2	3:D:344:TYR:CE1	2.54	0.43
3:D:779:ASN:HA	3:D:783:LEU:HD12	2.00	0.43
1:C:144:LYS:O	1:C:205:LEU:HD11	2.18	0.43
2:B:167:ARG:NH2	2:B:173:PRO:HA	2.34	0.43
3:D:170:HIS:HB2	3:D:207:MET:HE1	2.00	0.43
3:D:213:ILE:O	3:D:217:VAL:HG23	2.18	0.43
3:D:514:LYS:HD2	3:D:514:LYS:H	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:697:TYR:O	3:D:701:VAL:HG22	2.19	0.43
3:A:526:PHE:CE2	3:A:604:ARG:CD	3.01	0.43
3:A:705:ALA:CB	3:A:744:ARG:HB2	2.49	0.43
3:A:779:ASN:HA	3:A:783:LEU:HD12	2.00	0.43
3:A:991:SER:O	3:A:995:ARG:HG3	2.19	0.43
3:D:215:GLU:O	3:D:219:ARG:HB2	2.19	0.43
3:D:768:ILE:C	3:D:770:ILE:N	2.73	0.43
3:D:991:SER:O	3:D:995:ARG:HG3	2.19	0.43
1:C:231:ASN:O	1:C:309:SER:HA	2.19	0.43
1:C:297:ILE:HG13	1:C:298:GLY:N	2.33	0.43
2:B:109:ASN:OD1	2:B:109:ASN:C	2.56	0.43
3:A:187:SER:O	3:A:188:TYR:CG	2.71	0.43
3:A:744:ARG:HG3	3:A:744:ARG:HH11	1.84	0.43
1:F:337:GLU:HA	1:F:340:LYS:HE3	2.01	0.42
2:B:72:LYS:O	2:B:86:LYS:NZ	2.51	0.42
3:A:407:ARG:HB2	3:A:418:VAL:CG2	2.48	0.42
3:A:547:ILE:HG13	3:A:794:VAL:HB	2.01	0.42
3:A:724:MET:CE	3:A:724:MET:H	2.32	0.42
1:C:164:ASN:O	1:C:166:LEU:HG	2.20	0.42
3:A:341:LEU:HB2	3:A:344:TYR:CE1	2.54	0.42
3:A:880:PHE:CE1	3:A:965:ARG:HB3	2.53	0.42
1:F:106:ILE:HG23	1:F:136:TRP:CE2	2.55	0.42
1:F:231:ASN:O	1:F:309:SER:HA	2.19	0.42
1:F:286:ARG:NH2	1:F:401:GLU:OE2	2.52	0.42
1:F:371:LEU:CD1	1:F:400:ILE:HG23	2.49	0.42
3:D:227:LEU:HD12	3:D:227:LEU:HA	1.78	0.42
3:D:705:ALA:CB	3:D:744:ARG:HB2	2.49	0.42
3:D:738:PRO:HG2	3:D:769:GLU:OE2	2.20	0.42
1:C:337:GLU:HA	1:C:340:LYS:HE3	2.01	0.42
2:E:39:ARG:HE	2:E:39:ARG:HB2	1.63	0.42
2:E:202:LEU:HD23	2:E:202:LEU:HA	1.66	0.42
3:D:7:ASN:C	3:D:7:ASN:OD1	2.57	0.42
3:D:486:TYR:CZ	3:D:501:ILE:HD12	2.53	0.42
3:D:734:LYS:HA	3:D:734:LYS:HD3	1.81	0.42
3:D:840:LYS:HB2	3:D:890:PHE:CZ	2.54	0.42
1:C:106:ILE:HG23	1:C:136:TRP:CE2	2.55	0.42
2:B:41:GLU:OE1	2:B:127:LEU:CB	2.68	0.42
3:A:215:GLU:O	3:A:219:ARG:HB2	2.19	0.42
3:A:697:TYR:O	3:A:701:VAL:HG22	2.19	0.42
3:A:729:ILE:H	3:A:729:ILE:HG13	1.59	0.42
1:F:413:ILE:O	1:F:417:VAL:HG12	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ILE:O	1:C:417:VAL:HG12	2.20	0.42
3:A:7:ASN:OD1	3:A:7:ASN:C	2.57	0.42
3:A:481:ALA:O	3:A:485:THR:OG1	2.37	0.42
3:A:812:SER:O	3:A:812:SER:OG	2.37	0.42
3:A:832:ARG:HH21	3:A:834:ASP:HB2	1.84	0.42
3:A:837:LYS:HA	3:A:890:PHE:HD1	1.85	0.42
2:E:47:ASP:O	2:E:48:LYS:HE2	2.20	0.42
3:D:741:TYR:HE2	3:D:766:LYS:NZ	2.17	0.42
3:D:837:LYS:HA	3:D:890:PHE:HD1	1.85	0.42
3:D:865:CYS:SG	3:D:985:ASN:ND2	2.93	0.42
3:A:87:ASP:OD1	3:A:87:ASP:N	2.52	0.42
1:F:3:SER:O	2:B:193:ARG:NH1	2.52	0.42
1:F:250:VAL:O	1:F:254:ILE:HG13	2.19	0.42
2:B:2:ASN:OD1	2:B:2:ASN:N	2.51	0.42
3:A:170:HIS:HB2	3:A:207:MET:HE1	2.01	0.42
3:A:865:CYS:SG	3:A:985:ASN:ND2	2.93	0.42
1:F:326:ASN:OD1	1:F:327:GLU:N	2.53	0.42
2:E:48:LYS:O	2:E:49:PHE:CB	2.67	0.42
2:E:159:GLY:HA3	2:E:162:ASP:OD1	2.20	0.42
2:E:177:ILE:HD12	2:E:177:ILE:HA	1.72	0.42
2:E:195:PHE:CD2	2:E:212:TRP:CZ2	3.08	0.42
3:D:87:ASP:N	3:D:87:ASP:OD1	2.52	0.42
3:D:552:SER:OG	3:D:552:SER:O	2.34	0.42
3:A:553:LEU:HD12	3:A:553:LEU:HA	1.89	0.42
3:A:681:TYR:HE1	3:A:685:LYS:HZ2	1.64	0.42
3:A:759:ILE:CG2	3:A:762:GLN:H	2.33	0.42
3:A:811:TYR:HE1	3:A:813:ALA:HB2	1.84	0.42
1:F:12:GLU:HB3	1:F:30:LYS:NZ	2.35	0.42
1:F:347:LYS:HE3	1:F:347:LYS:HB3	1.71	0.42
1:F:378:LYS:CB	1:F:386:ASN:HB3	2.50	0.42
2:E:60:LYS:HA	2:E:60:LYS:HD3	1.68	0.42
3:D:540:MET:C	3:D:542:SER:N	2.73	0.42
3:D:681:TYR:HE1	3:D:685:LYS:HZ2	1.64	0.42
3:D:876:LEU:HD22	3:D:972:PHE:CB	2.50	0.42
1:C:286:ARG:NH2	1:C:401:GLU:OE2	2.52	0.42
1:C:326:ASN:OD1	1:C:327:GLU:N	2.53	0.42
2:B:11:TYR:HD1	2:B:11:TYR:N	2.17	0.42
2:B:87:LYS:O	2:B:91:GLU:HG2	2.20	0.42
3:A:437:ASP:C	3:A:438:ILE:HG12	2.40	0.42
3:A:540:MET:C	3:A:542:SER:N	2.73	0.42
3:A:546:LEU:HD23	3:A:771:ALA:CB	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:840:LYS:HB2	3:A:890:PHE:CZ	2.54	0.42
2:E:11:TYR:HD1	2:E:11:TYR:N	2.17	0.42
2:E:167:ARG:NH2	2:E:173:PRO:HA	2.34	0.42
3:D:818:LYS:N	3:D:818:LYS:HD3	2.34	0.42
1:C:184:MET:HA	1:C:187:SER:OG	2.20	0.42
1:C:371:LEU:CD1	1:C:400:ILE:HG23	2.49	0.42
1:C:378:LYS:CB	1:C:386:ASN:HB3	2.50	0.42
3:A:602:GLU:HA	3:A:603:PRO:HD3	1.93	0.42
1:F:164:ASN:O	1:F:166:LEU:HG	2.20	0.41
1:F:256:SER:HB3	1:F:258:VAL:HG23	2.01	0.41
2:E:2:ASN:N	2:E:2:ASN:OD1	2.51	0.41
2:E:52:GLN:NE2	2:E:77:VAL:HG13	2.35	0.41
3:D:288:SER:OG	3:D:293:GLU:HB3	2.20	0.41
3:D:528:TYR:CD1	3:D:528:TYR:N	2.88	0.41
1:C:146:GLN:HG2	1:C:150:ASN:OD1	2.20	0.41
1:C:179:GLU:HA	1:C:179:GLU:OE1	2.18	0.41
2:B:92:ILE:HD11	2:B:182:PRO:HG2	2.02	0.41
2:B:195:PHE:CD2	2:B:212:TRP:CZ2	3.08	0.41
3:D:317:THR:HG22	3:D:319:HIS:NE2	2.35	0.41
3:D:744:ARG:HG3	3:D:744:ARG:HH11	1.84	0.41
3:D:832:ARG:HH21	3:D:834:ASP:HB2	1.84	0.41
1:C:179:GLU:HA	1:C:182:SER:HG	1.83	0.41
2:B:48:LYS:HG3	2:B:51:ILE:CG1	2.50	0.41
1:F:146:GLN:HG2	1:F:150:ASN:OD1	2.20	0.41
1:F:163:PRO:HD2	1:F:165:TYR:CE2	2.55	0.41
3:D:547:ILE:HD11	3:D:756:PHE:CE1	2.48	0.41
2:B:52:GLN:HE22	2:B:77:VAL:HA	1.85	0.41
3:A:528:TYR:CD1	3:A:528:TYR:N	2.88	0.41
3:A:574:SER:H	3:A:610:SER:HG	1.66	0.41
2:E:19:TRP:CD1	2:E:53:LEU:O	2.73	0.41
2:E:87:LYS:O	2:E:91:GLU:HG2	2.20	0.41
3:D:437:ASP:C	3:D:438:ILE:HG12	2.41	0.41
3:D:453:LEU:HD23	3:D:453:LEU:HA	1.85	0.41
3:D:839:HIS:CE1	3:D:890:PHE:HZ	2.39	0.41
1:C:28:ILE:H	1:C:28:ILE:HG13	1.75	0.41
2:B:19:TRP:CD1	2:B:53:LEU:O	2.73	0.41
3:A:140:TYR:N	3:A:140:TYR:CD1	2.88	0.41
3:A:288:SER:OG	3:A:293:GLU:HB3	2.20	0.41
3:A:876:LEU:HD22	3:A:972:PHE:CB	2.50	0.41
2:E:52:GLN:HE22	2:E:77:VAL:HA	1.85	0.41
3:D:140:TYR:CD1	3:D:140:TYR:N	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:767:SER:O	3:D:770:ILE:CB	2.68	0.41
1:C:12:GLU:HB3	1:C:30:LYS:NZ	2.35	0.41
1:C:163:PRO:HD2	1:C:165:TYR:CE2	2.55	0.41
1:C:294:ILE:HD13	1:C:294:ILE:HA	1.82	0.41
1:C:344:VAL:HA	1:C:347:LYS:NZ	2.36	0.41
2:B:195:PHE:HD2	2:B:212:TRP:CZ2	2.38	0.41
3:A:543:ASN:O	3:A:544:ASN:CG	2.59	0.41
3:A:839:HIS:CE1	3:A:890:PHE:HZ	2.39	0.41
1:F:184:MET:HA	1:F:187:SER:OG	2.20	0.41
3:D:465:LEU:HD23	3:D:465:LEU:HA	1.83	0.41
3:D:553:LEU:HD12	3:D:553:LEU:HA	1.90	0.41
2:B:11:TYR:CD1	2:B:11:TYR:N	2.88	0.41
3:A:317:THR:HG22	3:A:319:HIS:NE2	2.35	0.41
1:F:325:ILE:HB	1:F:337:GLU:CD	2.41	0.41
2:E:7:SER:HG	2:E:8:HIS:CE1	2.37	0.41
3:D:275:ARG:HH21	3:D:279:LEU:HD11	1.85	0.41
3:D:411:LEU:HB2	3:D:414:GLY:C	2.41	0.41
3:D:543:ASN:O	3:D:544:ASN:CG	2.59	0.41
3:D:812:SER:O	3:D:812:SER:OG	2.37	0.41
1:C:299:ARG:HA	1:C:299:ARG:HD3	1.85	0.41
2:B:159:GLY:HA3	2:B:162:ASP:OD1	2.20	0.41
3:A:411:LEU:HB2	3:A:414:GLY:C	2.41	0.41
3:A:690:ILE:HG23	3:A:722:PHE:CZ	2.56	0.41
2:E:11:TYR:CD1	2:E:11:TYR:N	2.88	0.41
2:E:17:ASP:HA	2:E:20:GLU:HG2	2.03	0.41
2:E:96:ILE:O	2:E:100:THR:HG23	2.20	0.41
3:D:581:GLU:O	3:D:585:GLN:HG3	2.20	0.41
1:C:154:LEU:HA	1:C:157:GLU:OE1	2.21	0.41
3:A:547:ILE:CG1	3:A:794:VAL:HB	2.50	0.41
3:A:581:GLU:O	3:A:585:GLN:HG3	2.20	0.41
3:A:818:LYS:N	3:A:818:LYS:HD3	2.35	0.41
2:E:13:ILE:HG23	2:E:15:TYR:CE1	2.56	0.41
2:E:181:HIS:HA	2:E:182:PRO:HD3	1.97	0.41
3:D:75:ASN:HB2	3:D:76:LEU:H	1.69	0.41
3:D:398:ASP:O	3:D:399:GLU:HB2	2.21	0.41
3:D:724:MET:CE	3:D:724:MET:H	2.33	0.41
3:D:839:HIS:ND1	3:D:890:PHE:HZ	2.19	0.41
1:C:276:TYR:O	1:C:277:ASP:O	2.38	0.41
1:C:285:THR:HG22	1:C:286:ARG:N	2.35	0.41
1:C:325:ILE:HB	1:C:337:GLU:CD	2.41	0.41
2:B:38:LEU:H	2:B:38:LEU:HG	1.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:GLN:NE2	2:B:77:VAL:HG13	2.35	0.41
3:A:763:ASP:CB	3:A:767:SER:CB	2.79	0.41
3:A:763:ASP:O	3:A:764:VAL:CB	2.65	0.41
1:F:177:ASP:HB3	1:F:178:ASP:H	1.74	0.41
2:E:147:HIS:CE1	2:E:151:HIS:HE1	2.39	0.41
2:E:195:PHE:HD2	2:E:212:TRP:CZ2	2.38	0.41
3:D:759:ILE:CG2	3:D:762:GLN:H	2.33	0.41
1:C:251:ASP:HA	1:C:254:ILE:HD12	2.03	0.41
2:B:17:ASP:HA	2:B:20:GLU:HG2	2.03	0.41
3:A:214:GLN:OE1	3:A:214:GLN:HA	2.20	0.41
1:F:215:PHE:C	1:F:215:PHE:HD1	2.24	0.40
1:F:251:ASP:HA	1:F:254:ILE:HD12	2.03	0.40
1:F:269:LYS:HB3	1:F:272:PHE:O	2.22	0.40
1:F:276:TYR:O	1:F:277:ASP:O	2.38	0.40
1:F:407:PHE:O	1:F:410:PHE:N	2.55	0.40
2:E:107:GLY:N	2:E:217:ILE:HB	2.37	0.40
3:D:126:SER:HB3	3:D:151:LYS:HD3	2.02	0.40
3:D:214:GLN:OE1	3:D:214:GLN:HA	2.21	0.40
3:D:745:PHE:N	3:D:745:PHE:CD1	2.89	0.40
3:D:872:LEU:HG	3:D:972:PHE:CD2	2.56	0.40
3:A:734:LYS:HD3	3:A:734:LYS:HA	1.80	0.40
3:A:783:LEU:HD23	3:A:783:LEU:HA	1.96	0.40
1:F:154:LEU:HA	1:F:157:GLU:OE1	2.21	0.40
1:F:297:ILE:HD12	1:F:301:TYR:HB2	2.03	0.40
1:F:344:VAL:HA	1:F:347:LYS:NZ	2.36	0.40
3:D:542:SER:CB	3:D:758:GLU:CG	2.90	0.40
3:D:724:MET:HE2	3:D:724:MET:H	1.79	0.40
1:C:108:ASP:N	1:C:109:GLU:OE2	2.54	0.40
1:C:276:TYR:C	1:C:277:ASP:O	2.56	0.40
2:B:107:GLY:N	2:B:217:ILE:HB	2.36	0.40
3:A:40:TYR:HB2	3:A:91:ILE:HG23	2.02	0.40
3:A:110:ILE:HD12	3:A:110:ILE:HA	1.84	0.40
3:A:275:ARG:HH21	3:A:279:LEU:HD11	1.85	0.40
3:A:367:GLU:HA	3:A:419:LEU:O	2.22	0.40
3:A:398:ASP:O	3:A:399:GLU:HB2	2.21	0.40
1:F:7:LEU:O	1:F:10:LEU:HG	2.22	0.40
1:F:123:GLY:O	1:F:144:LYS:HG3	2.22	0.40
3:D:346:LEU:HA	3:D:349:ILE:HD11	2.03	0.40
3:D:540:MET:O	3:D:542:SER:N	2.54	0.40
1:C:7:LEU:O	1:C:10:LEU:HG	2.22	0.40
1:C:297:ILE:HD12	1:C:301:TYR:HB2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:TYR:CE1	3:A:179:PHE:CE1	3.09	0.40
3:A:960:LEU:H	3:A:960:LEU:HG	1.69	0.40
2:E:92:ILE:HD11	2:E:182:PRO:HG2	2.02	0.40
3:D:40:TYR:HB2	3:D:91:ILE:HG23	2.02	0.40
3:D:120:SER:HA	3:D:121:PRO:HD3	1.94	0.40
3:D:397:VAL:C	3:D:399:GLU:H	2.25	0.40
3:D:577:ARG:O	3:D:578:LEU:HB3	2.22	0.40
3:A:126:SER:HB3	3:A:151:LYS:HD3	2.02	0.40
3:A:346:LEU:HA	3:A:349:ILE:HD11	2.03	0.40
3:A:762:GLN:HG2	3:A:858:ARG:HH21	1.86	0.40
3:A:796:LYS:HD3	3:A:796:LYS:HA	1.60	0.40
3:A:839:HIS:ND1	3:A:890:PHE:HZ	2.19	0.40
1:F:12:GLU:HB3	1:F:30:LYS:CE	2.52	0.40
1:F:285:THR:HG22	1:F:286:ARG:N	2.36	0.40
2:E:160:LYS:HB2	2:E:180:TYR:CE1	2.57	0.40
3:D:40:TYR:HB2	3:D:91:ILE:CG2	2.52	0.40
3:D:264:GLY:HA2	3:D:268:ASP:HB2	2.04	0.40
3:D:481:ALA:HB2	3:D:655:SER:OG	2.22	0.40
3:D:690:ILE:HG23	3:D:722:PHE:CZ	2.56	0.40
1:C:269:LYS:HB3	1:C:272:PHE:O	2.22	0.40
2:B:15:TYR:HD2	2:B:23:MET:CB	2.34	0.40
2:B:96:ILE:O	2:B:100:THR:HG23	2.20	0.40
3:A:215:GLU:OE1	3:A:449:LEU:HD23	2.21	0.40
3:A:493:VAL:HG12	3:A:494:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	366/426 (86%)	333 (91%)	31 (8%)	2 (0%)	25 59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	366/426 (86%)	332 (91%)	31 (8%)	3 (1%)	16	51
2	B	216/218 (99%)	199 (92%)	15 (7%)	2 (1%)	14	49
2	E	216/218 (99%)	198 (92%)	16 (7%)	2 (1%)	14	49
3	A	919/1006 (91%)	769 (84%)	128 (14%)	22 (2%)	5	30
3	D	919/1006 (91%)	768 (84%)	129 (14%)	22 (2%)	5	30
All	All	3002/3300 (91%)	2599 (87%)	350 (12%)	53 (2%)	9	35

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	374	ASP
3	D	375	THR
3	D	540	MET
3	D	544	ASN
3	D	547	ILE
3	D	604	ARG
3	D	609	ILE
3	D	764	VAL
3	D	765	ASP
2	B	48	LYS
3	A	374	ASP
3	A	375	THR
3	A	540	MET
3	A	544	ASN
3	A	609	ILE
3	A	716	ASN
3	A	763	ASP
3	A	764	VAL
3	A	765	ASP
3	D	75	ASN
3	D	786	ASN
3	D	798	LEU
3	D	841	ASN
3	A	75	ASN
3	A	604	ARG
3	A	786	ASN
3	A	798	LEU
3	A	841	ASN
1	F	277	ASP
1	F	364	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	543	ASN
3	D	607	ASN
3	D	714	PHE
3	D	716	ASN
1	C	277	ASP
1	C	364	PRO
3	A	543	ASN
3	A	607	ASN
3	A	714	PHE
3	A	717	THR
1	F	255	ARG
2	E	49	PHE
2	E	73	ASP
3	D	803	LYS
2	B	73	ASP
3	A	803	LYS
3	D	546	LEU
3	D	606	PRO
3	D	610	SER
3	A	606	PRO
3	A	610	SER
3	D	400	ASP
3	A	400	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	346/396 (87%)	278 (80%)	68 (20%)	1	6
1	F	346/396 (87%)	277 (80%)	69 (20%)	1	6
2	B	200/200 (100%)	136 (68%)	64 (32%)	0	2
2	E	200/200 (100%)	134 (67%)	66 (33%)	0	2
3	A	853/928 (92%)	645 (76%)	208 (24%)	0	3
3	D	853/928 (92%)	639 (75%)	214 (25%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2798/3048 (92%)	2109 (75%)	689 (25%)	2 3

All (689) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1	MET
1	F	2	THR
1	F	4	SER
1	F	6	ASP
1	F	18	LYS
1	F	19	SER
1	F	23	SER
1	F	24	ASP
1	F	25	SER
1	F	33	SER
1	F	39	THR
1	F	41	THR
1	F	105	GLN
1	F	106	ILE
1	F	112	SER
1	F	116	LYS
1	F	133	ASN
1	F	138	MET
1	F	147	SER
1	F	150	ASN
1	F	156	SER
1	F	168	ILE
1	F	177	ASP
1	F	179	GLU
1	F	183	ILE
1	F	186	ARG
1	F	190	ASP
1	F	191	THR
1	F	198	SER
1	F	202	LEU
1	F	209	VAL
1	F	213	PHE
1	F	215	PHE
1	F	224	LYS
1	F	241	SER
1	F	247	VAL
1	F	249	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	251	ASP
1	F	260	GLU
1	F	262	THR
1	F	267	LYS
1	F	273	SER
1	F	275	LEU
1	F	279	ASP
1	F	284	GLU
1	F	309	SER
1	F	313	ILE
1	F	327	GLU
1	F	330	THR
1	F	332	ASP
1	F	338	ILE
1	F	341	SER
1	F	347	LYS
1	F	351	GLN
1	F	352	SER
1	F	353	VAL
1	F	365	GLU
1	F	370	THR
1	F	371	LEU
1	F	375	MET
1	F	380	GLU
1	F	383	LYS
1	F	384	VAL
1	F	385	VAL
1	F	394	CYS
1	F	412	SER
1	F	419	ASP
1	F	420	VAL
1	F	426	GLU
2	E	1	MET
2	E	2	ASN
2	E	4	VAL
2	E	11	TYR
2	E	23	MET
2	E	33	VAL
2	E	40	ASP
2	E	41	GLU
2	E	42	THR
2	E	43	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	48	LYS
2	E	50	PHE
2	E	51	ILE
2	E	54	LYS
2	E	57	LEU
2	E	61	ARG
2	E	63	CYS
2	E	68	ASP
2	E	72	LYS
2	E	80	GLU
2	E	81	SER
2	E	84	PHE
2	E	85	THR
2	E	88	SER
2	E	90	LYS
2	E	91	GLU
2	E	94	SER
2	E	95	SER
2	E	97	SER
2	E	105	TYR
2	E	106	LYS
2	E	109	ASN
2	E	112	ILE
2	E	117	ILE
2	E	123	LEU
2	E	132	SER
2	E	139	LYS
2	E	140	ILE
2	E	142	LYS
2	E	144	LEU
2	E	153	SER
2	E	158	LEU
2	E	160	LYS
2	E	161	THR
2	E	162	ASP
2	E	165	ASN
2	E	169	LYS
2	E	170	LEU
2	E	171	GLU
2	E	174	VAL
2	E	175	THR
2	E	176	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	177	ILE
2	E	178	VAL
2	E	185	ARG
2	E	191	LYS
2	E	192	ASP
2	E	197	ILE
2	E	198	ILE
2	E	199	ASN
2	E	201	LEU
2	E	204	LEU
2	E	205	ASP
2	E	208	THR
2	E	210	ILE
2	E	211	ASN
3	D	2	ASP
3	D	7	ASN
3	D	11	SER
3	D	14	GLU
3	D	18	LEU
3	D	22	SER
3	D	25	ARG
3	D	28	GLU
3	D	32	ILE
3	D	42	VAL
3	D	45	GLU
3	D	48	GLN
3	D	50	LEU
3	D	62	LYS
3	D	81	ARG
3	D	85	VAL
3	D	87	ASP
3	D	88	MET
3	D	96	LYS
3	D	98	SER
3	D	105	ASP
3	D	117	ASN
3	D	122	ASP
3	D	127	LEU
3	D	134	LYS
3	D	137	ASN
3	D	139	CYS
3	D	140	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	142	CYS
3	D	144	ASP
3	D	158	ILE
3	D	167	ILE
3	D	172	ASP
3	D	175	PHE
3	D	177	SER
3	D	178	VAL
3	D	184	SER
3	D	187	SER
3	D	189	CYS
3	D	193	LEU
3	D	194	SER
3	D	196	LYS
3	D	201	THR
3	D	203	ILE
3	D	208	LEU
3	D	209	THR
3	D	210	GLU
3	D	211	GLN
3	D	214	GLN
3	D	219	ARG
3	D	223	ARG
3	D	226	SER
3	D	229	GLU
3	D	234	ARG
3	D	237	VAL
3	D	238	LEU
3	D	240	SER
3	D	245	LEU
3	D	253	GLU
3	D	268	ASP
3	D	271	TYR
3	D	274	ASN
3	D	277	GLU
3	D	280	THR
3	D	282	GLU
3	D	283	LYS
3	D	287	ARG
3	D	292	LYS
3	D	301	GLU
3	D	316	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	320	VAL
3	D	333	SER
3	D	335	ILE
3	D	338	SER
3	D	340	LYS
3	D	345	LYS
3	D	348	SER
3	D	350	SER
3	D	356	CYS
3	D	357	MET
3	D	367	GLU
3	D	369	THR
3	D	373	ASP
3	D	374	ASP
3	D	376	THR
3	D	377	ASP
3	D	381	LYS
3	D	390	THR
3	D	399	GLU
3	D	401	ILE
3	D	406	ILE
3	D	411	LEU
3	D	412	GLU
3	D	416	LYS
3	D	417	VAL
3	D	420	SER
3	D	421	CYS
3	D	430	LYS
3	D	433	PHE
3	D	435	LYS
3	D	451	ILE
3	D	455	MET
3	D	462	ASP
3	D	479	THR
3	D	485	THR
3	D	488	LEU
3	D	500	THR
3	D	511	LEU
3	D	514	LYS
3	D	518	VAL
3	D	521	GLU
3	D	522	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	526	PHE
3	D	528	TYR
3	D	532	LYS
3	D	542	SER
3	D	544	ASN
3	D	549	ASP
3	D	558	CYS
3	D	568	LEU
3	D	571	VAL
3	D	572	VAL
3	D	585	GLN
3	D	588	LEU
3	D	590	LYS
3	D	598	THR
3	D	599	VAL
3	D	602	GLU
3	D	604	ARG
3	D	605	LEU
3	D	608	LEU
3	D	609	ILE
3	D	622	THR
3	D	636	ARG
3	D	638	LYS
3	D	640	MET
3	D	645	THR
3	D	652	ILE
3	D	655	SER
3	D	657	GLN
3	D	666	SER
3	D	670	LEU
3	D	673	PHE
3	D	678	LEU
3	D	685	LYS
3	D	686	SER
3	D	694	MET
3	D	702	LEU
3	D	716	ASN
3	D	717	THR
3	D	719	SER
3	D	724	MET
3	D	726	ASP
3	D	729	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	732	ILE
3	D	733	VAL
3	D	735	THR
3	D	736	SER
3	D	742	ARG
3	D	744	ARG
3	D	762	GLN
3	D	763	ASP
3	D	765	ASP
3	D	766	LYS
3	D	769	GLU
3	D	772	LYS
3	D	776	ARG
3	D	777	LEU
3	D	799	ILE
3	D	803	LYS
3	D	808	THR
3	D	812	SER
3	D	815	SER
3	D	818	LYS
3	D	819	SER
3	D	824	ILE
3	D	828	THR
3	D	829	SER
3	D	831	THR
3	D	832	ARG
3	D	834	ASP
3	D	835	VAL
3	D	836	SER
3	D	837	LYS
3	D	838	PHE
3	D	844	LYS
3	D	845	THR
3	D	847	LYS
3	D	850	LEU
3	D	853	MET
3	D	855	SER
3	D	856	GLU
3	D	858	ARG
3	D	859	MET
3	D	861	SER
3	D	865	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	866	ILE
3	D	867	ASP
3	D	872	LEU
3	D	873	GLU
3	D	893	SER
3	D	932	TYR
3	D	960	LEU
3	D	962	SER
3	D	966	ILE
3	D	969	GLU
3	D	970	VAL
3	D	978	GLU
3	D	980	VAL
3	D	983	LEU
3	D	987	VAL
3	D	988	LEU
3	D	989	CYS
3	D	991	SER
1	C	1	MET
1	C	2	THR
1	C	4	SER
1	C	6	ASP
1	C	18	LYS
1	C	19	SER
1	C	23	SER
1	C	24	ASP
1	C	25	SER
1	C	33	SER
1	C	39	THR
1	C	41	THR
1	C	105	GLN
1	C	106	ILE
1	C	112	SER
1	C	116	LYS
1	C	133	ASN
1	C	138	MET
1	C	147	SER
1	C	150	ASN
1	C	156	SER
1	C	168	ILE
1	C	177	ASP
1	C	179	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	183	ILE
1	C	186	ARG
1	C	190	ASP
1	C	191	THR
1	C	198	SER
1	C	202	LEU
1	C	209	VAL
1	C	213	PHE
1	C	215	PHE
1	C	224	LYS
1	C	241	SER
1	C	247	VAL
1	C	249	ASP
1	C	251	ASP
1	C	260	GLU
1	C	262	THR
1	C	267	LYS
1	C	273	SER
1	C	275	LEU
1	C	279	ASP
1	C	284	GLU
1	C	309	SER
1	C	313	ILE
1	C	327	GLU
1	C	330	THR
1	C	332	ASP
1	C	338	ILE
1	C	347	LYS
1	C	351	GLN
1	C	352	SER
1	C	353	VAL
1	C	365	GLU
1	C	370	THR
1	C	371	LEU
1	C	375	MET
1	C	380	GLU
1	C	383	LYS
1	C	384	VAL
1	C	385	VAL
1	C	394	CYS
1	C	412	SER
1	C	419	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	420	VAL
1	C	426	GLU
2	B	1	MET
2	B	2	ASN
2	B	4	VAL
2	B	11	TYR
2	B	23	MET
2	B	33	VAL
2	B	40	ASP
2	B	42	THR
2	B	43	SER
2	B	47	ASP
2	B	48	LYS
2	B	51	ILE
2	B	54	LYS
2	B	57	LEU
2	B	61	ARG
2	B	63	CYS
2	B	68	ASP
2	B	72	LYS
2	B	80	GLU
2	B	81	SER
2	B	84	PHE
2	B	85	THR
2	B	88	SER
2	B	90	LYS
2	B	91	GLU
2	B	94	SER
2	B	95	SER
2	B	97	SER
2	B	105	TYR
2	B	106	LYS
2	B	109	ASN
2	B	112	ILE
2	B	117	ILE
2	B	123	LEU
2	B	132	SER
2	B	139	LYS
2	B	140	ILE
2	B	142	LYS
2	B	144	LEU
2	B	153	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	158	LEU
2	B	160	LYS
2	B	161	THR
2	B	162	ASP
2	B	165	ASN
2	B	169	LYS
2	B	170	LEU
2	B	171	GLU
2	B	174	VAL
2	B	175	THR
2	B	176	THR
2	B	177	ILE
2	B	178	VAL
2	B	185	ARG
2	B	191	LYS
2	B	197	ILE
2	B	198	ILE
2	B	199	ASN
2	B	201	LEU
2	B	204	LEU
2	B	205	ASP
2	B	208	THR
2	B	210	ILE
2	B	211	ASN
3	A	2	ASP
3	A	7	ASN
3	A	11	SER
3	A	14	GLU
3	A	18	LEU
3	A	22	SER
3	A	25	ARG
3	A	28	GLU
3	A	32	ILE
3	A	42	VAL
3	A	45	GLU
3	A	48	GLN
3	A	50	LEU
3	A	62	LYS
3	A	81	ARG
3	A	85	VAL
3	A	87	ASP
3	A	88	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	96	LYS
3	A	98	SER
3	A	105	ASP
3	A	117	ASN
3	A	122	ASP
3	A	127	LEU
3	A	134	LYS
3	A	137	ASN
3	A	139	CYS
3	A	140	TYR
3	A	142	CYS
3	A	144	ASP
3	A	158	ILE
3	A	167	ILE
3	A	172	ASP
3	A	175	PHE
3	A	177	SER
3	A	178	VAL
3	A	184	SER
3	A	187	SER
3	A	189	CYS
3	A	193	LEU
3	A	194	SER
3	A	196	LYS
3	A	201	THR
3	A	203	ILE
3	A	208	LEU
3	A	209	THR
3	A	210	GLU
3	A	211	GLN
3	A	214	GLN
3	A	219	ARG
3	A	223	ARG
3	A	226	SER
3	A	229	GLU
3	A	234	ARG
3	A	237	VAL
3	A	238	LEU
3	A	240	SER
3	A	245	LEU
3	A	253	GLU
3	A	268	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	271	TYR
3	A	274	ASN
3	A	277	GLU
3	A	280	THR
3	A	282	GLU
3	A	283	LYS
3	A	287	ARG
3	A	292	LYS
3	A	301	GLU
3	A	316	THR
3	A	320	VAL
3	A	333	SER
3	A	335	ILE
3	A	338	SER
3	A	340	LYS
3	A	345	LYS
3	A	348	SER
3	A	350	SER
3	A	356	CYS
3	A	357	MET
3	A	367	GLU
3	A	369	THR
3	A	373	ASP
3	A	374	ASP
3	A	376	THR
3	A	377	ASP
3	A	381	LYS
3	A	390	THR
3	A	399	GLU
3	A	401	ILE
3	A	406	ILE
3	A	411	LEU
3	A	412	GLU
3	A	416	LYS
3	A	417	VAL
3	A	420	SER
3	A	421	CYS
3	A	430	LYS
3	A	433	PHE
3	A	435	LYS
3	A	451	ILE
3	A	455	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	462	ASP
3	A	479	THR
3	A	485	THR
3	A	488	LEU
3	A	500	THR
3	A	511	LEU
3	A	514	LYS
3	A	518	VAL
3	A	521	GLU
3	A	522	THR
3	A	526	PHE
3	A	528	TYR
3	A	532	LYS
3	A	542	SER
3	A	544	ASN
3	A	549	ASP
3	A	558	CYS
3	A	568	LEU
3	A	571	VAL
3	A	572	VAL
3	A	585	GLN
3	A	588	LEU
3	A	590	LYS
3	A	598	THR
3	A	599	VAL
3	A	602	GLU
3	A	605	LEU
3	A	608	LEU
3	A	609	ILE
3	A	622	THR
3	A	636	ARG
3	A	638	LYS
3	A	640	MET
3	A	645	THR
3	A	652	ILE
3	A	655	SER
3	A	657	GLN
3	A	666	SER
3	A	670	LEU
3	A	673	PHE
3	A	678	LEU
3	A	685	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	686	SER
3	A	694	MET
3	A	702	LEU
3	A	719	SER
3	A	724	MET
3	A	726	ASP
3	A	729	ILE
3	A	732	ILE
3	A	733	VAL
3	A	735	THR
3	A	736	SER
3	A	742	ARG
3	A	744	ARG
3	A	763	ASP
3	A	772	LYS
3	A	776	ARG
3	A	777	LEU
3	A	797	ASN
3	A	799	ILE
3	A	803	LYS
3	A	808	THR
3	A	812	SER
3	A	815	SER
3	A	818	LYS
3	A	819	SER
3	A	824	ILE
3	A	828	THR
3	A	829	SER
3	A	831	THR
3	A	832	ARG
3	A	834	ASP
3	A	835	VAL
3	A	836	SER
3	A	837	LYS
3	A	838	PHE
3	A	844	LYS
3	A	845	THR
3	A	847	LYS
3	A	850	LEU
3	A	853	MET
3	A	855	SER
3	A	856	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	858	ARG
3	A	859	MET
3	A	861	SER
3	A	865	CYS
3	A	866	ILE
3	A	867	ASP
3	A	872	LEU
3	A	873	GLU
3	A	893	SER
3	A	932	TYR
3	A	960	LEU
3	A	962	SER
3	A	966	ILE
3	A	969	GLU
3	A	970	VAL
3	A	978	GLU
3	A	980	VAL
3	A	983	LEU
3	A	987	VAL
3	A	988	LEU
3	A	989	CYS
3	A	991	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	270	ASN
1	F	388	ASN
2	E	52	GLN
2	E	151	HIS
2	E	181	HIS
3	D	562	ASN
3	D	585	GLN
3	D	720	ASN
3	D	762	GLN
3	D	937	ASN
3	D	985	ASN
1	C	388	ASN
2	B	52	GLN
2	B	151	HIS
2	B	181	HIS
3	A	562	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	576	ASN
3	A	585	GLN
3	A	720	ASN
3	A	816	ASN
3	A	937	ASN
3	A	985	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

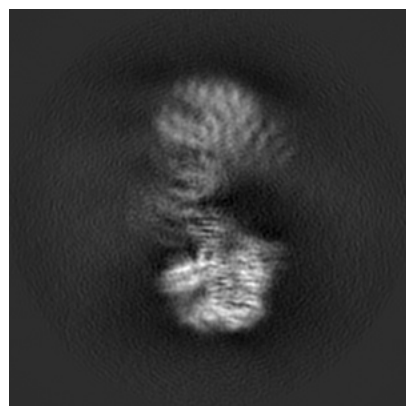
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34886. These allow visual inspection of the internal detail of the map and identification of artifacts.

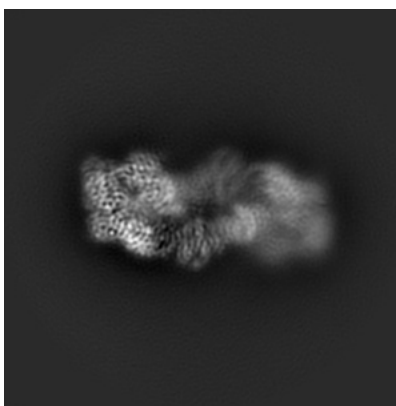
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

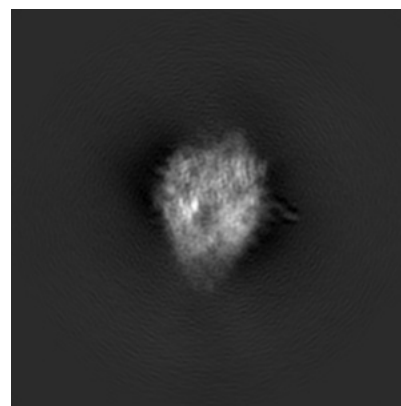
6.1.1 Primary map



X

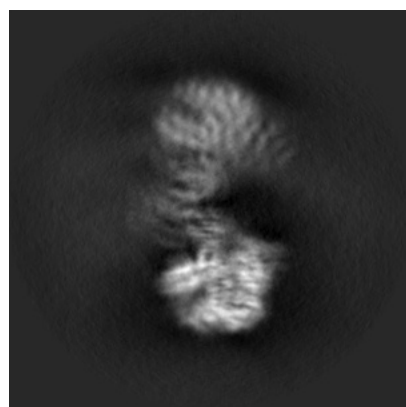


Y

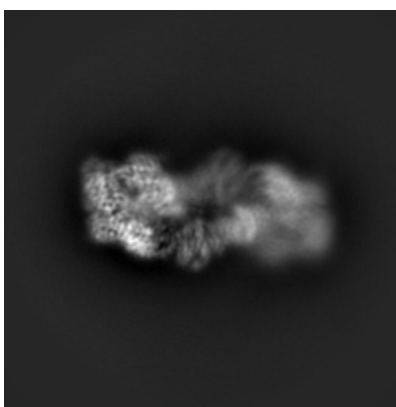


Z

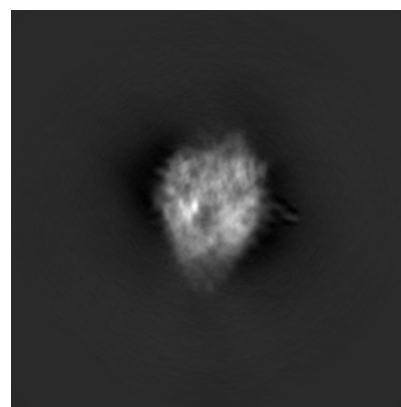
6.1.2 Raw map



X



Y

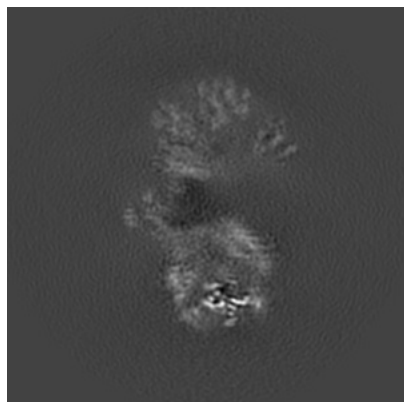


Z

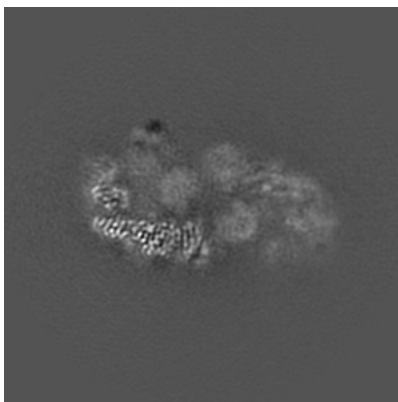
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

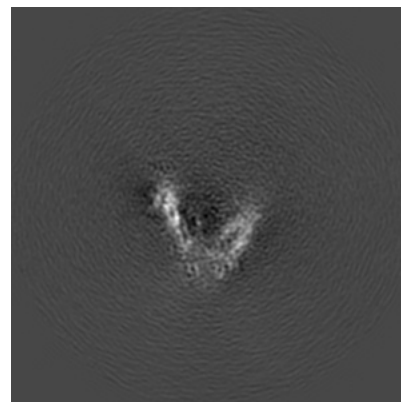
6.2.1 Primary map



X Index: 144

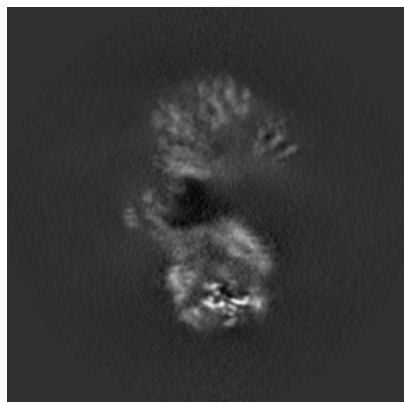


Y Index: 144

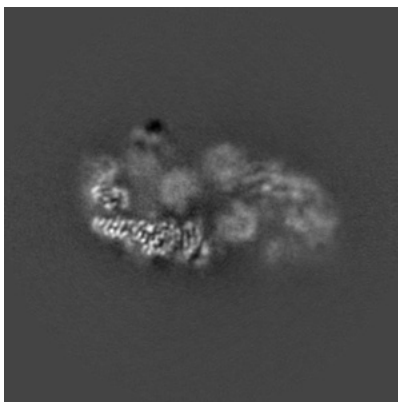


Z Index: 144

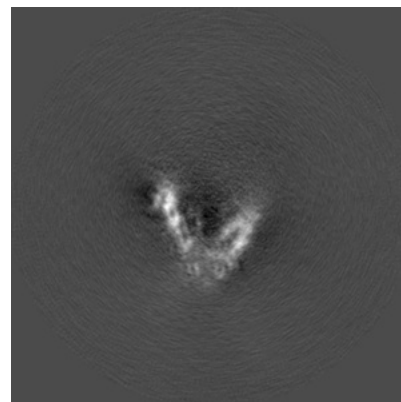
6.2.2 Raw map



X Index: 144



Y Index: 144

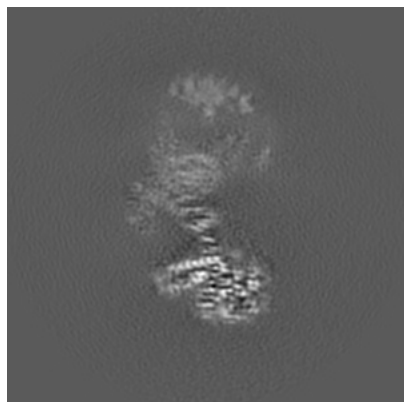


Z Index: 144

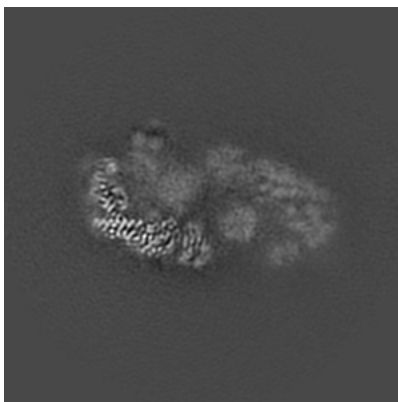
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

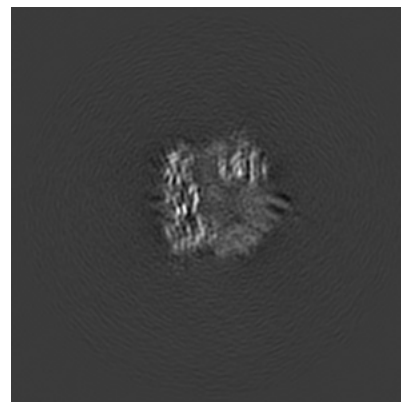
6.3.1 Primary map



X Index: 129

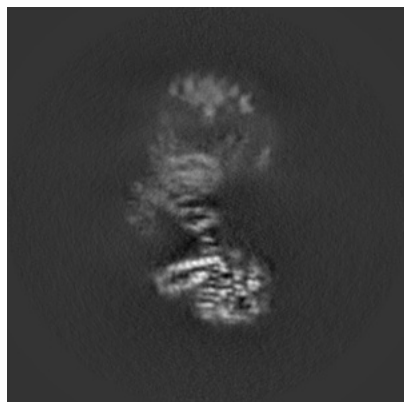


Y Index: 147

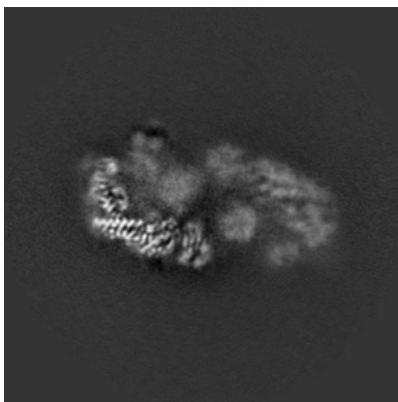


Z Index: 98

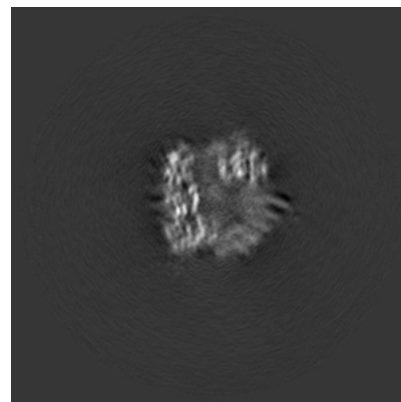
6.3.2 Raw map



X Index: 129



Y Index: 147

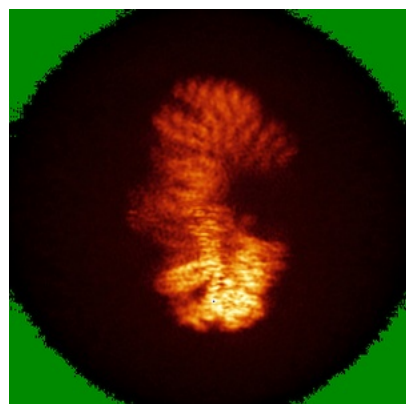


Z Index: 98

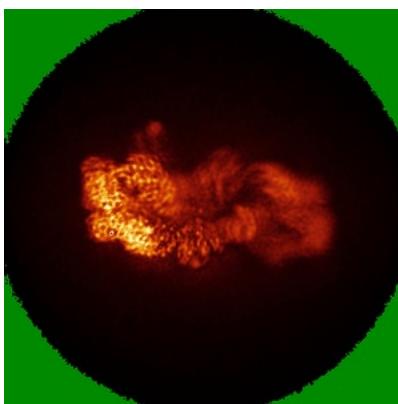
The images above show the largest variance slices of the map in three orthogonal directions.

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

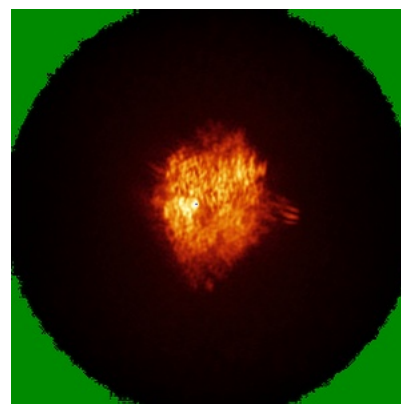
6.4.1 Primary map



X



Y

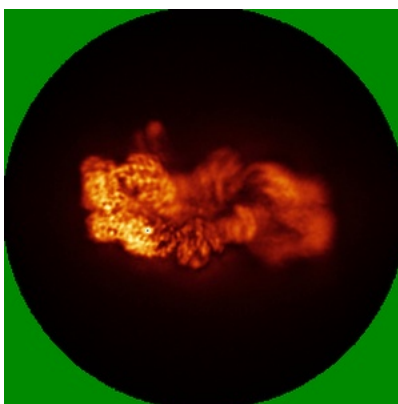


Z

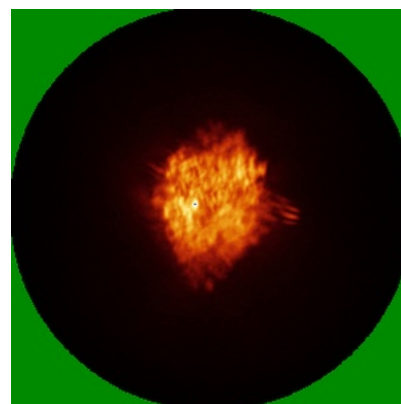
6.4.2 Raw map



X



Y

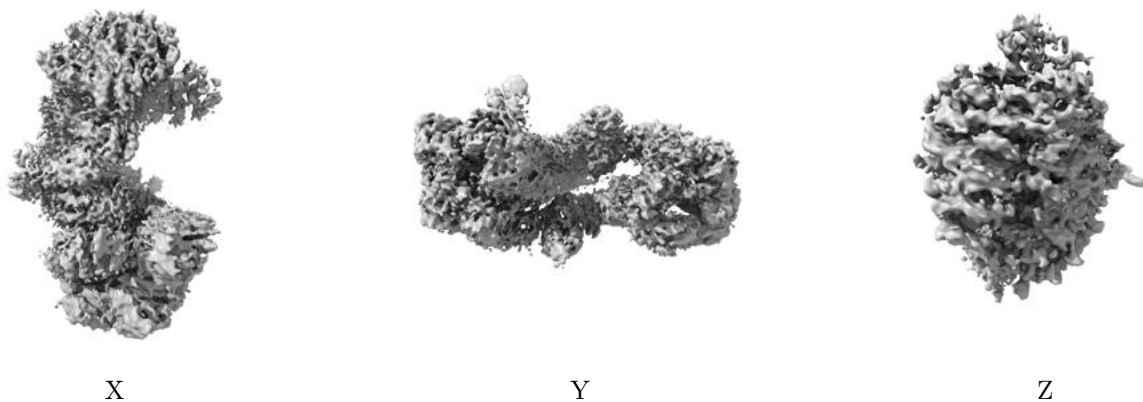


Z

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

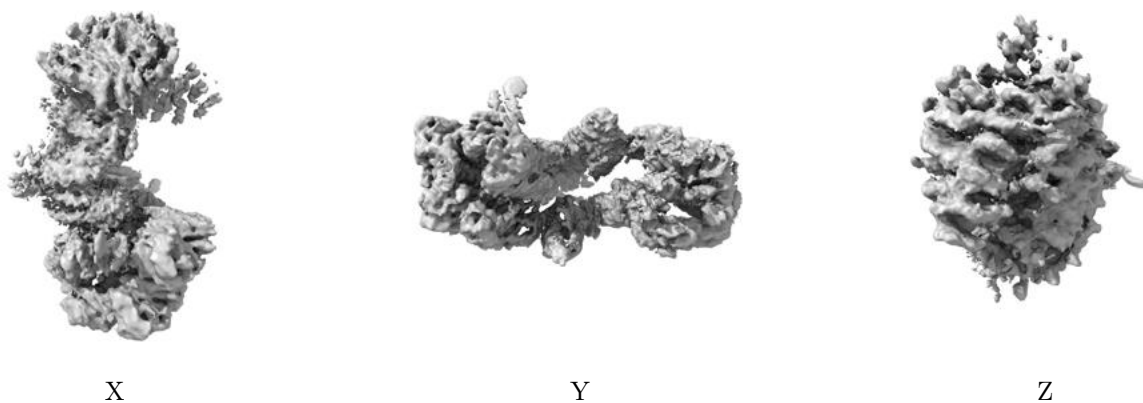
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

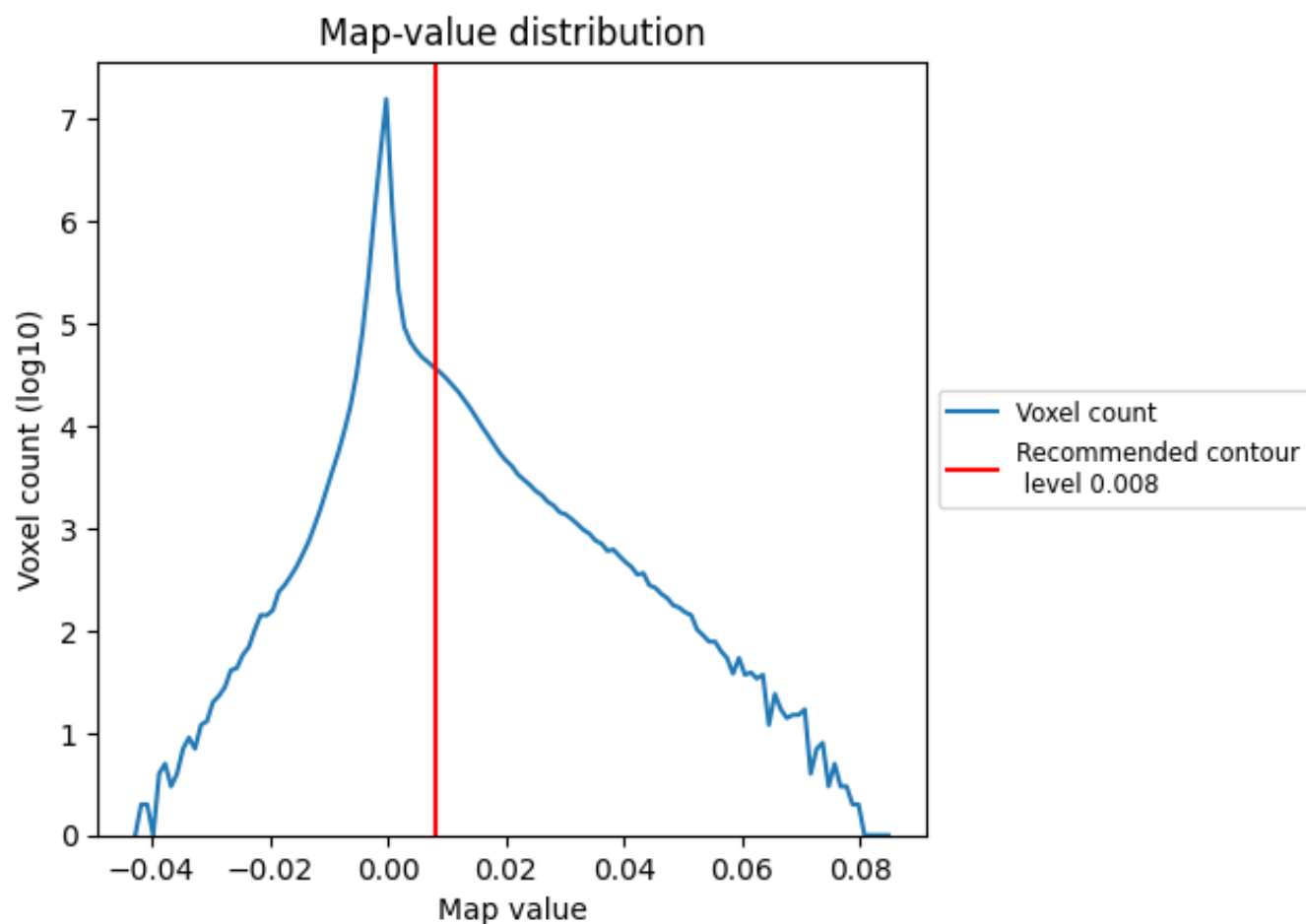
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

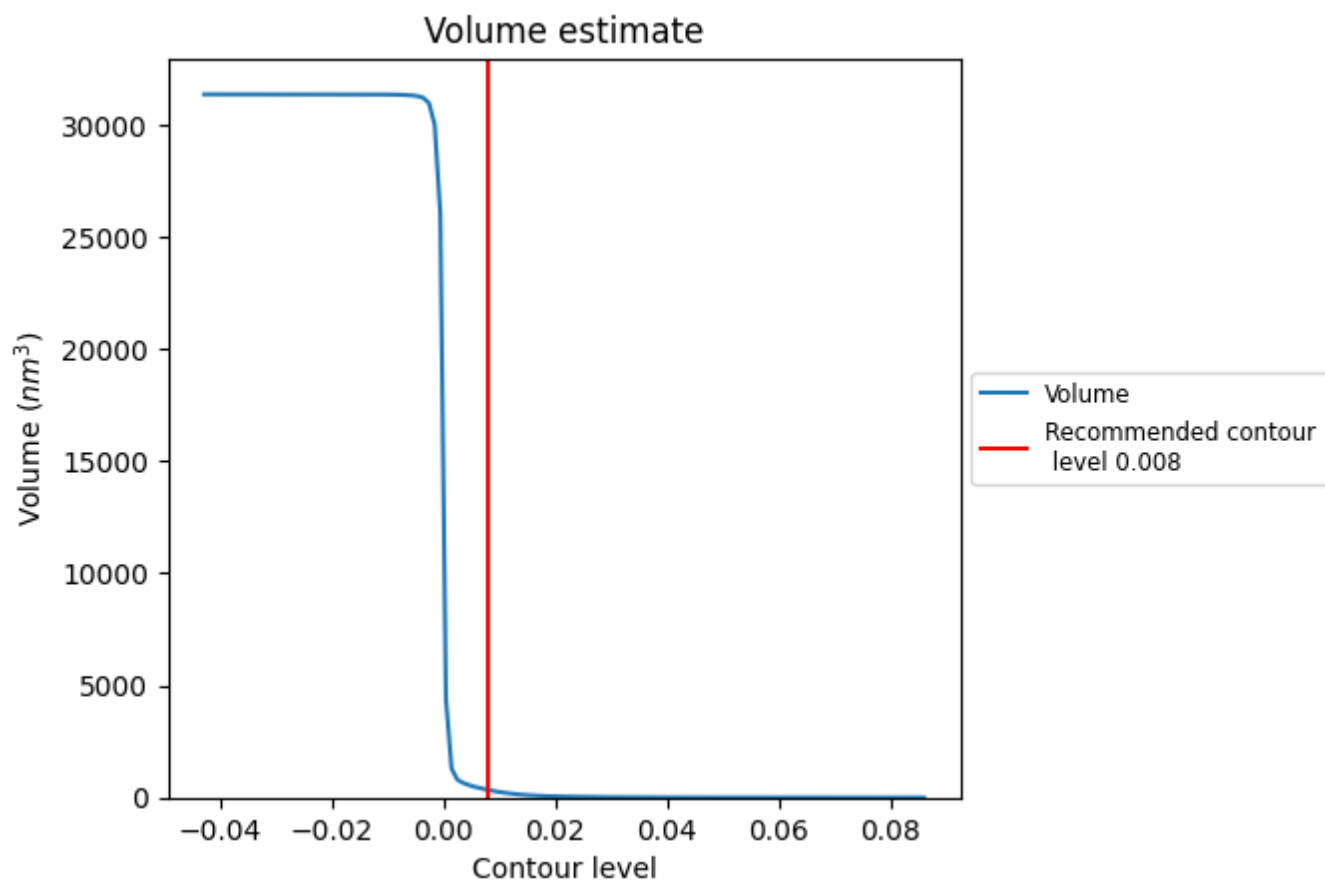
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

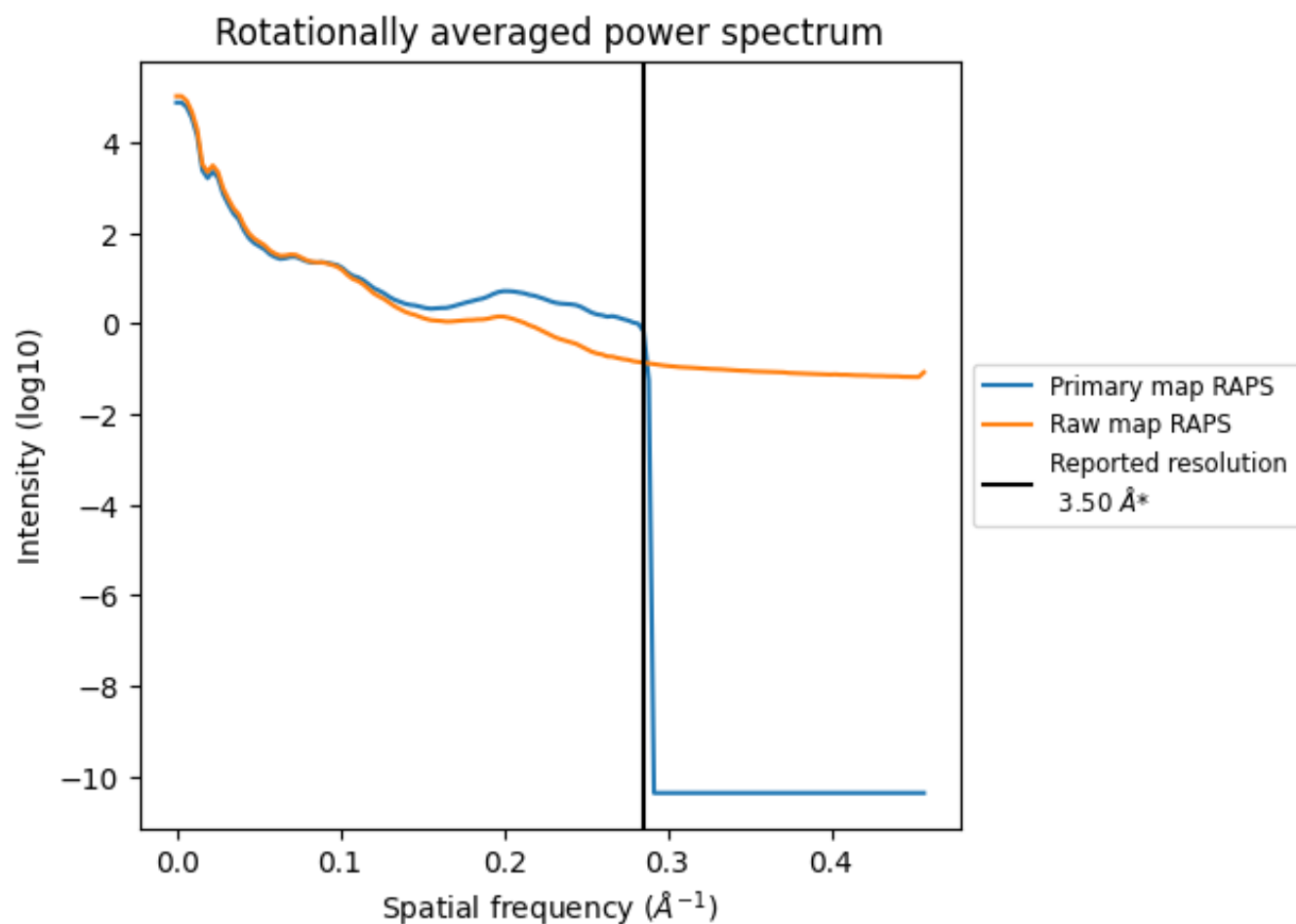
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339 nm³; this corresponds to an approximate mass of 306 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 ⓘ

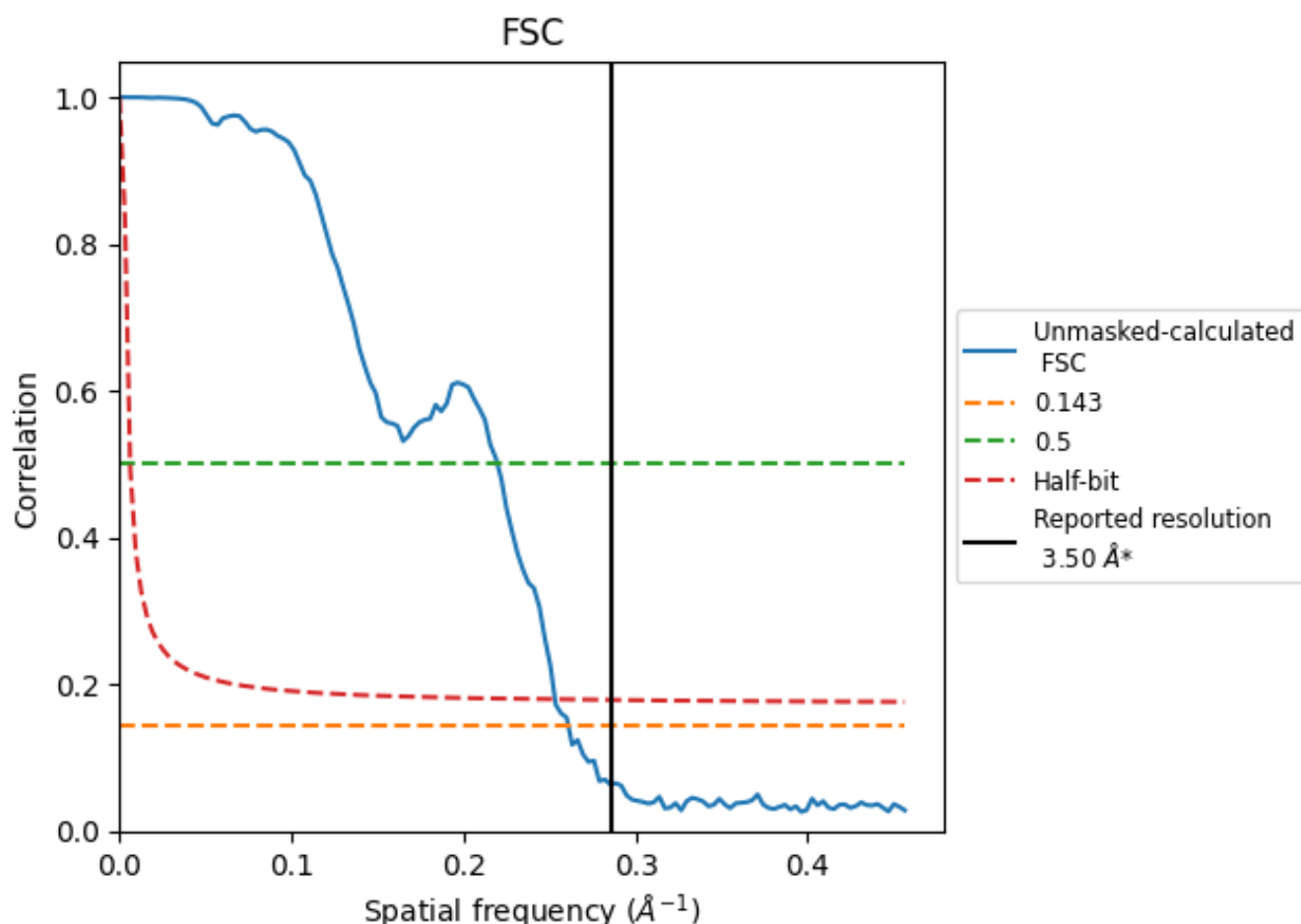


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

8.2 Resolution estimates [i](#)

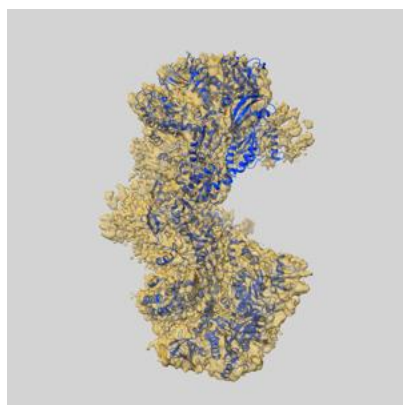
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	4.55	3.95

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

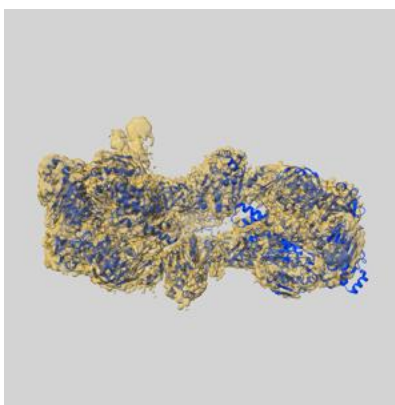
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34886 and PDB model 8HLZ. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

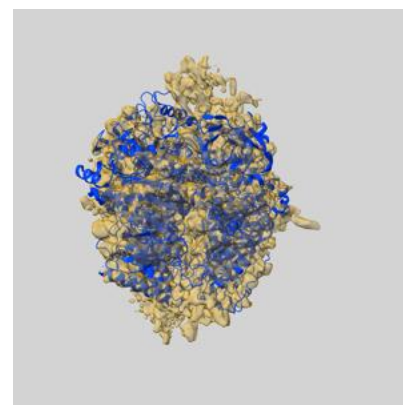
9.1 Map-model overlay [i](#)



X



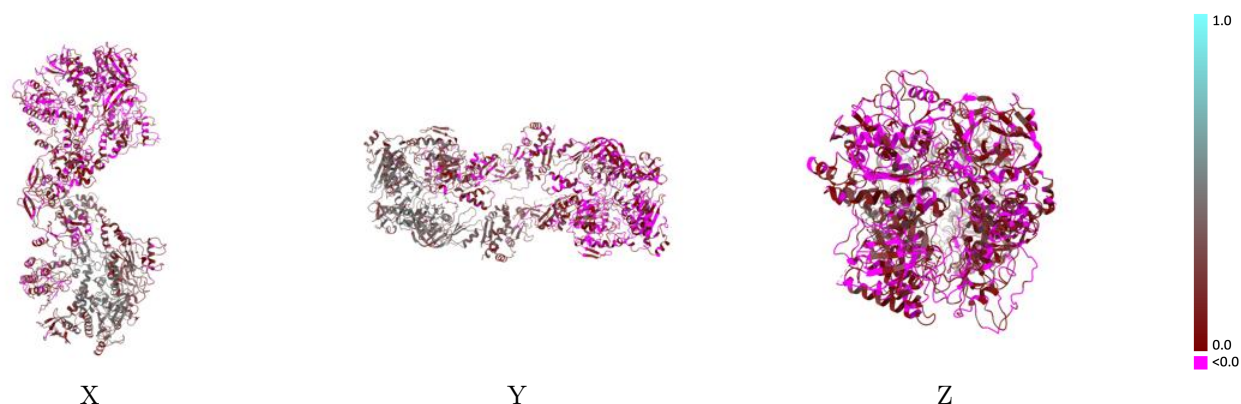
Y



Z

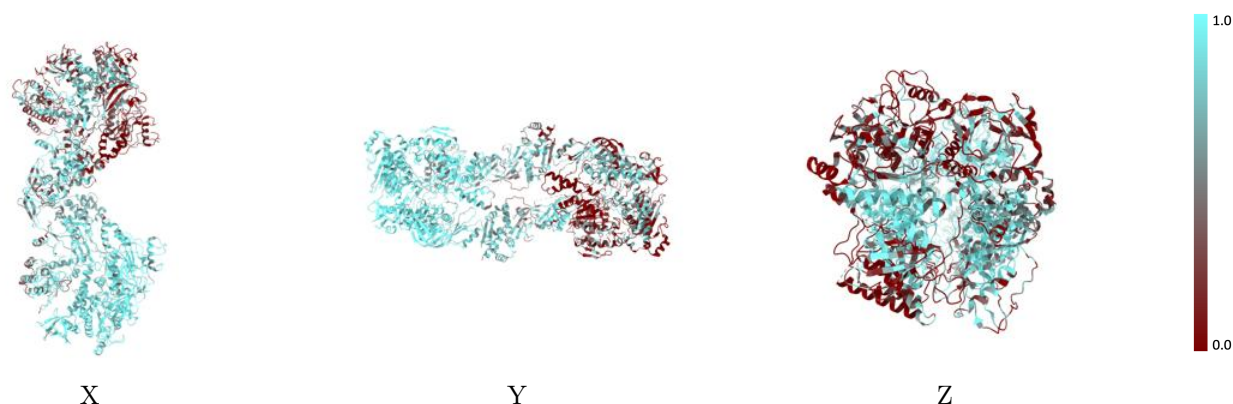
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



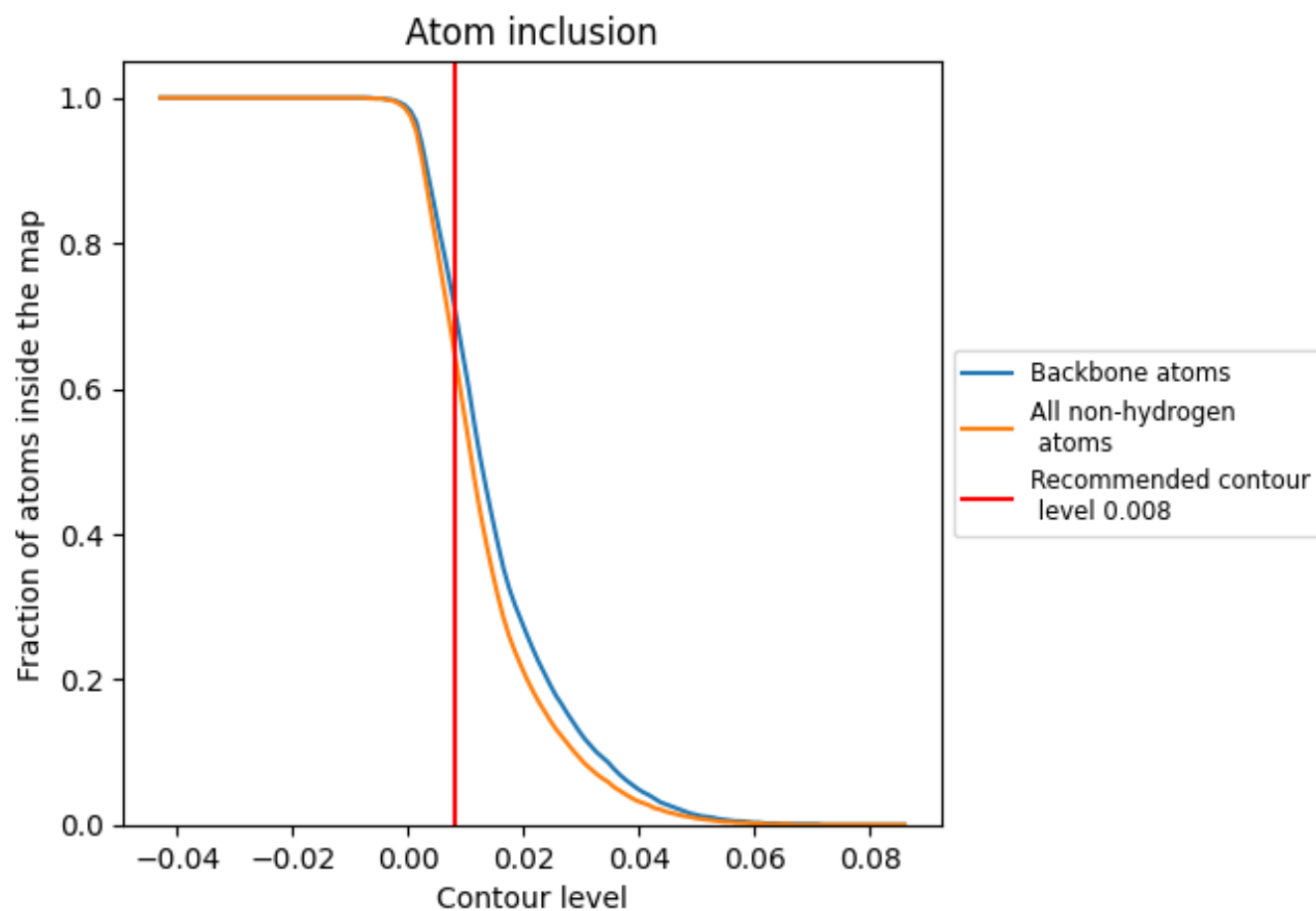
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 65% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6530	<div></div> 0.1650
A	<div></div> 0.4480	<div></div> 0.0340
B	<div></div> 0.2230	<div></div> 0.0160
C	<div></div> 0.7080	<div></div> 0.1090
D	<div></div> 0.8710	<div></div> 0.3220
E	<div></div> 0.9050	<div></div> 0.2750
F	<div></div> 0.6750	<div></div> 0.1810

1.0

0.0

<0.0