



## Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 07:50 AM JST

PDB ID : 5YYS  
EMDB ID : EMD-6859  
Title : Cryo-EM structure of L-fucokinase, GDP-fucose pyrophosphorylase (FKP)in Bacteroides fragilis  
Authors : Wang, J.; Hu, H.; Liu, Y.; Zhou, Q.; Wu, P.; Yan, N.; Wang, H.W.; Wu, J.W.; Sun, L.  
Deposited on : 2017-12-11  
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

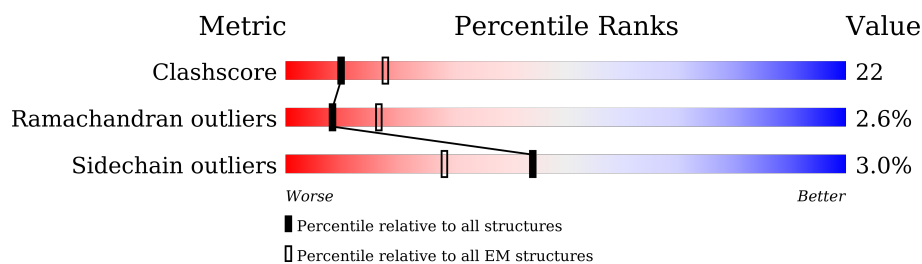
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	949	<div> <div>20%</div> <div> <div>44%</div> <div>33%</div> <div>6% •</div> <div>15%</div> </div> </div>
1	B	949	<div> <div>20%</div> <div> <div>44%</div> <div>33%</div> <div>6% •</div> <div>15%</div> </div> </div>
1	C	949	<div> <div>20%</div> <div> <div>44%</div> <div>33%</div> <div>6% •</div> <div>15%</div> </div> </div>
1	D	949	<div> <div>20%</div> <div> <div>44%</div> <div>34%</div> <div>6% •</div> <div>15%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24044 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.

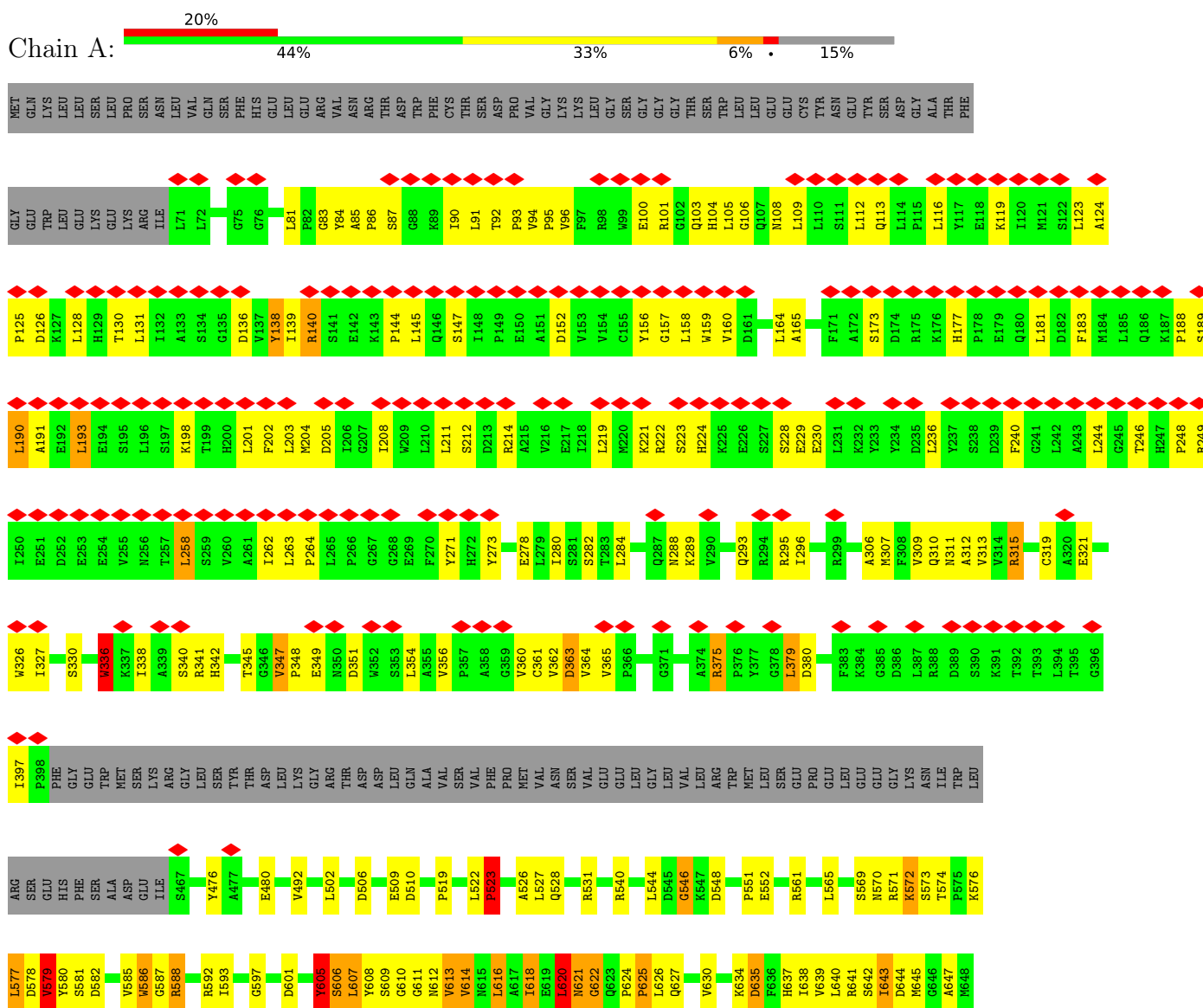
- Molecule 1 is a protein called L-fucokinase, L-fucose-1-P guanylyltransferase.

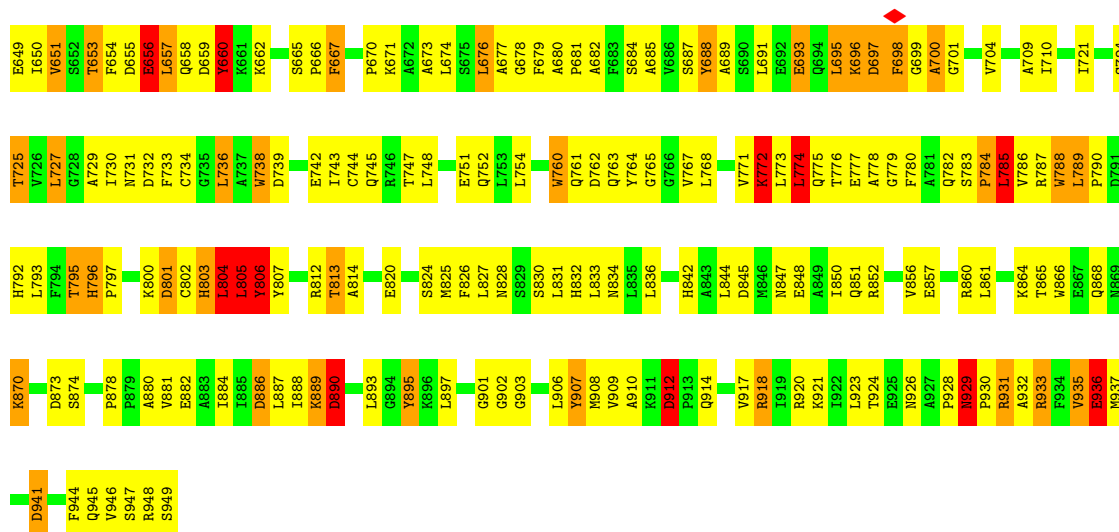
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	811	Total	C	N	O	S	0	0
			6011	3828	1037	1124	22		
1	B	811	Total	C	N	O	S	0	0
			6011	3828	1037	1124	22		
1	C	811	Total	C	N	O	S	0	0
			6011	3828	1037	1124	22		
1	D	811	Total	C	N	O	S	0	0
			6011	3828	1037	1124	22		

### 3 Residue-property plots

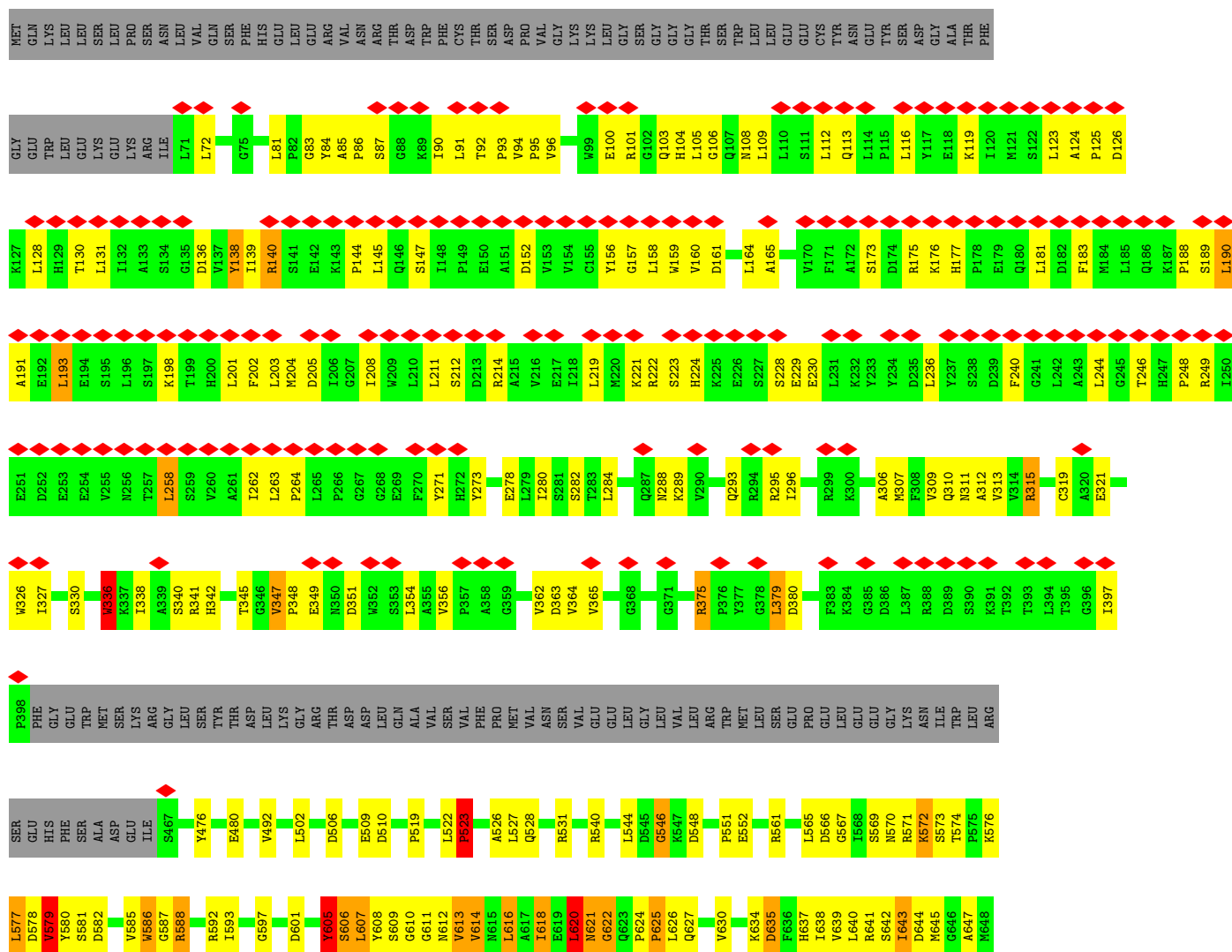
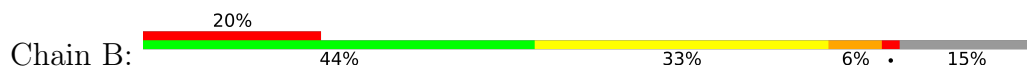
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: L-fucokinase, L-fucose-1-P guanylyltransferase

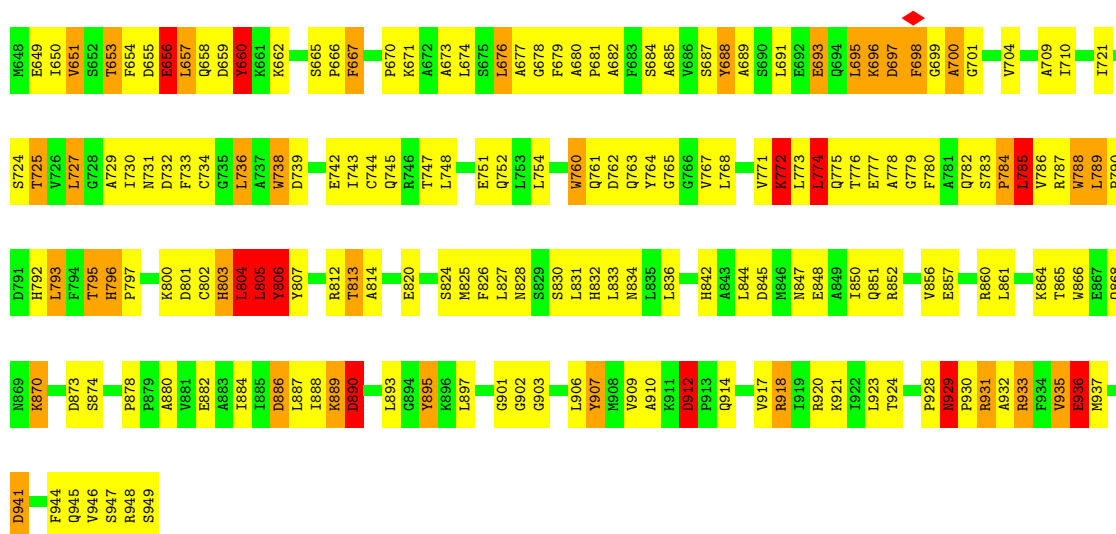




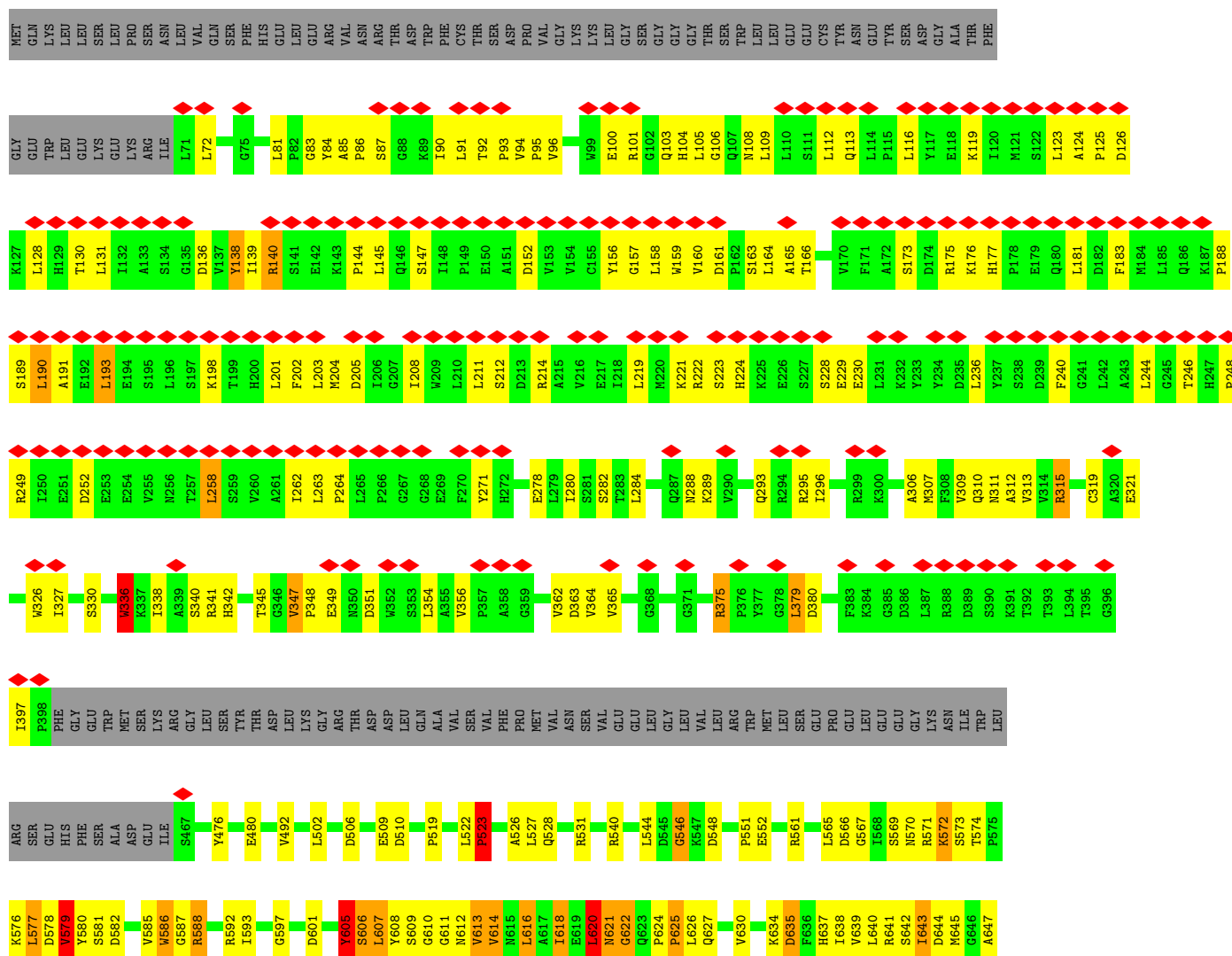
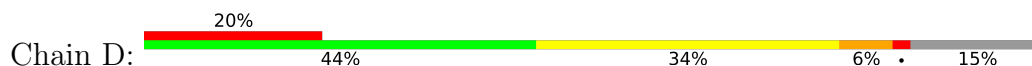
- Molecule 1: L-fucokinase, L-fucose-1-P guanylyltransferase







- Molecule 1: L-fucokinase, L-fucose-1-P guanylyltransferase







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96749	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.074	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.017	Depositor
Map size ( $\text{\AA}$ )	312.0, 312.0, 312.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.3, 1.3, 1.3	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.78	11/6143 (0.2%)	1.08	38/8362 (0.5%)
1	B	0.78	11/6143 (0.2%)	1.08	36/8362 (0.4%)
1	C	0.78	11/6143 (0.2%)	1.08	37/8362 (0.4%)
1	D	0.78	11/6143 (0.2%)	1.08	37/8362 (0.4%)
All	All	0.78	44/24572 (0.2%)	1.08	148/33448 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	72
1	B	0	73
1	C	0	73
1	D	0	72
All	All	0	290

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	760	TRP	CB-CG	-7.28	1.37	1.50
1	D	760	TRP	CB-CG	-7.27	1.37	1.50
1	B	760	TRP	CB-CG	-7.25	1.37	1.50
1	C	760	TRP	CB-CG	-7.25	1.37	1.50
1	C	688	TYR	CD1-CE1	-6.59	1.29	1.39
1	B	688	TYR	CD1-CE1	-6.54	1.29	1.39
1	A	688	TYR	CD1-CE1	-6.53	1.29	1.39
1	D	688	TYR	CD1-CE1	-6.52	1.29	1.39
1	A	660	TYR	CD2-CE2	-6.47	1.29	1.39
1	C	660	TYR	CD2-CE2	-6.45	1.29	1.39
1	D	660	TYR	CD2-CE2	-6.43	1.29	1.39
1	B	660	TYR	CD2-CE2	-6.40	1.29	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	HIS	C-N	6.20	1.46	1.34
1	D	177	HIS	C-N	6.20	1.46	1.34
1	B	177	HIS	C-N	6.18	1.46	1.34
1	C	177	HIS	C-N	6.16	1.46	1.34
1	D	586	TRP	CB-CG	-6.02	1.39	1.50
1	C	586	TRP	CB-CG	-6.02	1.39	1.50
1	B	586	TRP	CB-CG	-6.01	1.39	1.50
1	A	586	TRP	CB-CG	-6.01	1.39	1.50
1	C	738	TRP	CB-CG	-5.86	1.39	1.50
1	D	738	TRP	CB-CG	-5.82	1.39	1.50
1	A	738	TRP	CB-CG	-5.81	1.39	1.50
1	B	738	TRP	CB-CG	-5.81	1.39	1.50
1	B	336	TRP	CB-CG	-5.77	1.39	1.50
1	A	336	TRP	CB-CG	-5.75	1.40	1.50
1	C	336	TRP	CB-CG	-5.74	1.40	1.50
1	D	336	TRP	CB-CG	-5.74	1.40	1.50
1	B	907	TYR	CD2-CE2	-5.57	1.30	1.39
1	A	907	TYR	CD2-CE2	-5.54	1.31	1.39
1	D	907	TYR	CD2-CE2	-5.52	1.31	1.39
1	C	907	TYR	CD2-CE2	-5.51	1.31	1.39
1	C	788	TRP	CB-CG	-5.39	1.40	1.50
1	A	788	TRP	CB-CG	-5.37	1.40	1.50
1	D	788	TRP	CB-CG	-5.37	1.40	1.50
1	B	788	TRP	CB-CG	-5.34	1.40	1.50
1	C	895	TYR	CD1-CE1	-5.16	1.31	1.39
1	B	895	TYR	CD1-CE1	-5.15	1.31	1.39
1	D	895	TYR	CD1-CE1	-5.15	1.31	1.39
1	A	895	TYR	CD1-CE1	-5.12	1.31	1.39
1	B	895	TYR	CD2-CE2	-5.10	1.31	1.39
1	A	895	TYR	CD2-CE2	-5.07	1.31	1.39
1	C	895	TYR	CD2-CE2	-5.05	1.31	1.39
1	D	895	TYR	CD2-CE2	-5.01	1.31	1.39

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	805	LEU	CA-CB-CG	11.96	142.80	115.30
1	A	805	LEU	CA-CB-CG	11.94	142.76	115.30
1	D	805	LEU	CA-CB-CG	11.94	142.76	115.30
1	B	805	LEU	CA-CB-CG	11.93	142.73	115.30
1	B	772	LYS	CD-CE-NZ	-8.84	91.36	111.70
1	C	772	LYS	CD-CE-NZ	-8.84	91.38	111.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	772	LYS	CD-CE-NZ	-8.83	91.39	111.70
1	D	772	LYS	CD-CE-NZ	-8.82	91.42	111.70
1	D	624	PRO	C-N-CD	-8.28	102.37	120.60
1	C	624	PRO	C-N-CD	-8.28	102.39	120.60
1	A	624	PRO	C-N-CD	-8.27	102.40	120.60
1	B	624	PRO	C-N-CD	-8.27	102.41	120.60
1	C	785	LEU	CA-CB-CG	8.13	134.00	115.30
1	B	785	LEU	CA-CB-CG	8.11	133.96	115.30
1	A	785	LEU	CA-CB-CG	8.11	133.94	115.30
1	D	785	LEU	CA-CB-CG	8.08	133.89	115.30
1	C	736	LEU	CA-CB-CG	7.81	133.26	115.30
1	D	736	LEU	CA-CB-CG	7.81	133.26	115.30
1	A	736	LEU	CA-CB-CG	7.80	133.25	115.30
1	B	736	LEU	CA-CB-CG	7.80	133.24	115.30
1	B	622	GLY	N-CA-C	-7.62	94.05	113.10
1	C	622	GLY	N-CA-C	-7.62	94.06	113.10
1	D	622	GLY	N-CA-C	-7.60	94.10	113.10
1	A	622	GLY	N-CA-C	-7.60	94.11	113.10
1	A	610	GLY	N-CA-C	-7.23	95.03	113.10
1	B	610	GLY	N-CA-C	-7.22	95.06	113.10
1	C	610	GLY	N-CA-C	-7.22	95.06	113.10
1	D	610	GLY	N-CA-C	-7.22	95.06	113.10
1	A	644	ASP	CB-CG-OD1	7.04	124.63	118.30
1	B	644	ASP	CB-CG-OD1	7.01	124.61	118.30
1	D	644	ASP	CB-CG-OD1	7.01	124.61	118.30
1	C	644	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	523	PRO	N-CA-CB	6.61	111.23	103.30
1	D	523	PRO	N-CA-CB	6.60	111.22	103.30
1	D	620	LEU	CA-CB-CG	-6.59	100.15	115.30
1	C	620	LEU	CA-CB-CG	-6.58	100.17	115.30
1	B	523	PRO	N-CA-CB	6.58	111.19	103.30
1	C	523	PRO	N-CA-CB	6.58	111.19	103.30
1	A	620	LEU	CA-CB-CG	-6.57	100.19	115.30
1	B	620	LEU	CA-CB-CG	-6.57	100.19	115.30
1	B	789	LEU	CA-CB-CG	6.51	130.28	115.30
1	B	193	LEU	CA-CB-CG	6.50	130.26	115.30
1	A	789	LEU	CA-CB-CG	6.50	130.25	115.30
1	C	789	LEU	CA-CB-CG	6.50	130.25	115.30
1	D	193	LEU	CA-CB-CG	6.50	130.24	115.30
1	D	789	LEU	CA-CB-CG	6.49	130.23	115.30
1	C	193	LEU	CA-CB-CG	6.49	130.22	115.30
1	A	193	LEU	CA-CB-CG	6.48	130.21	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	695	LEU	CA-CB-CG	6.43	130.09	115.30
1	D	695	LEU	CA-CB-CG	6.42	130.06	115.30
1	A	695	LEU	CA-CB-CG	6.41	130.03	115.30
1	B	695	LEU	CA-CB-CG	6.40	130.03	115.30
1	C	804	LEU	CB-CG-CD1	6.38	121.85	111.00
1	B	624	PRO	C-N-CA	6.37	148.74	122.00
1	D	624	PRO	C-N-CA	6.37	148.74	122.00
1	A	804	LEU	CB-CG-CD1	6.36	121.82	111.00
1	C	624	PRO	C-N-CA	6.36	148.71	122.00
1	A	579	VAL	CG1-CB-CG2	-6.35	100.74	110.90
1	A	624	PRO	C-N-CA	6.35	148.67	122.00
1	B	579	VAL	CG1-CB-CG2	-6.34	100.75	110.90
1	B	804	LEU	CB-CG-CD1	6.34	121.78	111.00
1	C	579	VAL	CG1-CB-CG2	-6.34	100.75	110.90
1	D	579	VAL	CG1-CB-CG2	-6.34	100.76	110.90
1	D	804	LEU	CB-CG-CD1	6.34	121.77	111.00
1	A	643	ILE	C-N-CA	6.22	137.24	121.70
1	C	643	ILE	C-N-CA	6.21	137.22	121.70
1	D	643	ILE	C-N-CA	6.21	137.21	121.70
1	B	643	ILE	C-N-CA	6.20	137.19	121.70
1	A	551	PRO	N-CA-CB	6.00	110.50	103.30
1	D	551	PRO	N-CA-CB	5.94	110.43	103.30
1	B	551	PRO	N-CA-CB	5.92	110.40	103.30
1	C	551	PRO	N-CA-CB	5.91	110.39	103.30
1	C	918	ARG	CG-CD-NE	5.90	124.19	111.80
1	D	918	ARG	CG-CD-NE	5.89	124.18	111.80
1	C	804	LEU	N-CA-C	5.89	126.90	111.00
1	B	918	ARG	CG-CD-NE	5.89	124.16	111.80
1	B	804	LEU	N-CA-C	5.87	126.84	111.00
1	A	918	ARG	CG-CD-NE	5.86	124.11	111.80
1	A	804	LEU	N-CA-C	5.86	126.82	111.00
1	D	804	LEU	N-CA-C	5.86	126.82	111.00
1	B	806	TYR	CB-CA-C	-5.85	98.70	110.40
1	C	806	TYR	CB-CA-C	-5.82	98.76	110.40
1	A	806	TYR	CB-CA-C	-5.82	98.76	110.40
1	D	806	TYR	CB-CA-C	-5.81	98.79	110.40
1	A	805	LEU	N-CA-C	5.69	126.37	111.00
1	C	696	LYS	C-N-CA	5.68	135.91	121.70
1	B	696	LYS	C-N-CA	5.67	135.87	121.70
1	D	805	LEU	N-CA-C	5.67	126.30	111.00
1	C	805	LEU	N-CA-C	5.66	126.29	111.00
1	A	696	LYS	C-N-CA	5.66	135.85	121.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	805	LEU	N-CA-C	5.66	126.28	111.00
1	D	696	LYS	C-N-CA	5.66	135.84	121.70
1	D	774	LEU	N-CA-C	5.55	125.99	111.00
1	C	774	LEU	N-CA-C	5.55	125.98	111.00
1	A	774	LEU	N-CA-C	5.54	125.96	111.00
1	B	727	LEU	CA-CB-CG	-5.54	102.55	115.30
1	B	774	LEU	N-CA-C	5.54	125.94	111.00
1	B	887	LEU	CA-CB-CG	5.53	128.03	115.30
1	D	887	LEU	CA-CB-CG	5.53	128.03	115.30
1	D	727	LEU	CA-CB-CG	-5.52	102.60	115.30
1	A	887	LEU	CA-CB-CG	5.52	128.00	115.30
1	C	887	LEU	CA-CB-CG	5.51	127.98	115.30
1	C	727	LEU	CA-CB-CG	-5.51	102.62	115.30
1	A	727	LEU	CA-CB-CG	-5.50	102.65	115.30
1	A	937	MET	C-N-CA	5.49	135.43	121.70
1	B	937	MET	C-N-CA	5.47	135.38	121.70
1	C	937	MET	C-N-CA	5.47	135.38	121.70
1	D	937	MET	C-N-CA	5.47	135.38	121.70
1	C	697	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	697	ASP	CB-CG-OD1	5.36	123.13	118.30
1	D	697	ASP	CB-CG-OD1	5.35	123.12	118.30
1	B	697	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	890	ASP	C-N-CA	-5.33	108.37	121.70
1	A	890	ASP	C-N-CA	-5.33	108.38	121.70
1	C	890	ASP	C-N-CA	-5.33	108.39	121.70
1	B	785	LEU	CB-CG-CD2	5.30	120.02	111.00
1	B	258	LEU	CA-CB-CG	5.30	127.49	115.30
1	C	258	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	258	LEU	CA-CB-CG	5.30	127.49	115.30
1	D	806	TYR	N-CA-C	5.30	125.31	111.00
1	D	890	ASP	C-N-CA	-5.30	108.45	121.70
1	D	258	LEU	CA-CB-CG	5.30	127.48	115.30
1	A	806	TYR	N-CA-C	5.29	125.29	111.00
1	B	806	TYR	N-CA-C	5.29	125.30	111.00
1	C	656	GLU	CA-CB-CG	5.29	125.03	113.40
1	C	785	LEU	CB-CG-CD2	5.29	119.99	111.00
1	B	656	GLU	CA-CB-CG	5.29	125.03	113.40
1	C	806	TYR	N-CA-C	5.28	125.27	111.00
1	D	785	LEU	CB-CG-CD2	5.28	119.98	111.00
1	D	656	GLU	CA-CB-CG	5.28	125.02	113.40
1	A	656	GLU	CA-CB-CG	5.28	125.01	113.40
1	A	785	LEU	CB-CG-CD2	5.27	119.96	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	912	ASP	N-CA-C	-5.26	96.79	111.00
1	C	912	ASP	N-CA-C	-5.26	96.78	111.00
1	D	912	ASP	N-CA-C	-5.26	96.79	111.00
1	A	912	ASP	N-CA-C	-5.26	96.80	111.00
1	D	519	PRO	N-CA-CB	5.11	109.43	103.30
1	A	519	PRO	N-CA-CB	5.10	109.42	103.30
1	C	519	PRO	N-CA-CB	5.09	109.41	103.30
1	B	792	HIS	C-N-CA	5.09	134.43	121.70
1	B	519	PRO	N-CA-CB	5.09	109.41	103.30
1	A	792	HIS	C-N-CA	5.08	134.41	121.70
1	C	792	HIS	C-N-CA	5.07	134.38	121.70
1	D	792	HIS	C-N-CA	5.05	134.33	121.70
1	A	336	TRP	CA-CB-CG	-5.03	104.14	113.70
1	D	336	TRP	CA-CB-CG	-5.01	104.18	113.70
1	A	801	ASP	C-N-CA	5.00	134.21	121.70
1	C	336	TRP	CA-CB-CG	-5.00	104.20	113.70

There are no chirality outliers.

All (290) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	THR	Peptide
1	A	136	ASP	Peptide
1	A	138	TYR	Peptide
1	A	147	SER	Peptide
1	A	189	SER	Peptide
1	A	288	ASN	Peptide
1	A	336	TRP	Peptide
1	A	347	VAL	Peptide
1	A	363	ASP	Peptide
1	A	375	ARG	Peptide
1	A	379	LEU	Peptide
1	A	523	PRO	Peptide
1	A	526	ALA	Peptide
1	A	528	GLN	Peptide
1	A	546	GLY	Peptide
1	A	577	LEU	Peptide
1	A	578	ASP	Peptide
1	A	592	ARG	Peptide
1	A	605	TYR	Peptide
1	A	606	SER	Peptide
1	A	607	LEU	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	608	TYR	Peptide
1	A	611	GLY	Peptide
1	A	613	VAL	Mainchain,Peptide
1	A	618	ILE	Peptide
1	A	620	LEU	Peptide
1	A	634	LYS	Peptide
1	A	635	ASP	Peptide
1	A	645	MET	Peptide
1	A	651	VAL	Peptide
1	A	653	THR	Peptide
1	A	657	LEU	Peptide
1	A	659	ASP	Peptide
1	A	660	TYR	Peptide
1	A	662	LYS	Peptide
1	A	666	PRO	Peptide
1	A	676	LEU	Peptide
1	A	680	ALA	Peptide
1	A	693	GLU	Peptide
1	A	697	ASP	Peptide
1	A	698	PHE	Peptide
1	A	700	ALA	Peptide
1	A	732	ASP	Peptide
1	A	772	LYS	Peptide
1	A	783	SER	Peptide
1	A	784	PRO	Peptide
1	A	785	LEU	Mainchain,Peptide
1	A	786	VAL	Peptide
1	A	787	ARG	Peptide
1	A	795	THR	Peptide
1	A	796	HIS	Peptide
1	A	797	PRO	Peptide
1	A	800	LYS	Peptide
1	A	801	ASP	Peptide
1	A	802	CYS	Peptide
1	A	803	HIS	Peptide
1	A	804	LEU	Peptide
1	A	805	LEU	Peptide
1	A	806	TYR	Peptide
1	A	813	THR	Peptide
1	A	886	ASP	Peptide
1	A	889	LYS	Peptide
1	A	890	ASP	Peptide

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	912	ASP	Peptide
1	A	929	ASN	Peptide
1	A	931	ARG	Peptide
1	A	933	ARG	Peptide
1	A	935	VAL	Peptide
1	A	936	GLU	Peptide
1	A	941	ASP	Peptide
1	B	130	THR	Peptide
1	B	136	ASP	Peptide
1	B	138	TYR	Peptide
1	B	147	SER	Peptide
1	B	189	SER	Peptide
1	B	288	ASN	Peptide
1	B	336	TRP	Peptide
1	B	347	VAL	Peptide
1	B	363	ASP	Peptide
1	B	375	ARG	Peptide
1	B	379	LEU	Peptide
1	B	523	PRO	Peptide
1	B	526	ALA	Peptide
1	B	528	GLN	Peptide
1	B	546	GLY	Peptide
1	B	577	LEU	Peptide
1	B	578	ASP	Peptide
1	B	592	ARG	Peptide
1	B	605	TYR	Peptide
1	B	606	SER	Peptide
1	B	607	LEU	Peptide
1	B	608	TYR	Peptide
1	B	611	GLY	Peptide
1	B	613	VAL	Mainchain,Peptide
1	B	618	ILE	Peptide
1	B	620	LEU	Peptide
1	B	634	LYS	Peptide
1	B	635	ASP	Peptide
1	B	645	MET	Peptide
1	B	651	VAL	Peptide
1	B	653	THR	Peptide
1	B	657	LEU	Peptide
1	B	659	ASP	Peptide
1	B	660	TYR	Peptide
1	B	662	LYS	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	666	PRO	Peptide
1	B	676	LEU	Peptide
1	B	680	ALA	Peptide
1	B	693	GLU	Peptide
1	B	697	ASP	Peptide
1	B	698	PHE	Peptide
1	B	700	ALA	Peptide
1	B	732	ASP	Peptide
1	B	772	LYS	Peptide
1	B	783	SER	Peptide
1	B	784	PRO	Peptide
1	B	785	LEU	Mainchain,Peptide
1	B	786	VAL	Peptide
1	B	787	ARG	Peptide
1	B	793	LEU	Peptide
1	B	795	THR	Peptide
1	B	796	HIS	Peptide
1	B	797	PRO	Peptide
1	B	800	LYS	Peptide
1	B	801	ASP	Peptide
1	B	802	CYS	Peptide
1	B	803	HIS	Peptide
1	B	804	LEU	Peptide
1	B	805	LEU	Peptide
1	B	806	TYR	Peptide
1	B	813	THR	Peptide
1	B	886	ASP	Peptide
1	B	889	LYS	Peptide
1	B	890	ASP	Peptide
1	B	912	ASP	Peptide
1	B	929	ASN	Peptide
1	B	931	ARG	Peptide
1	B	933	ARG	Peptide
1	B	935	VAL	Peptide
1	B	936	GLU	Peptide
1	B	941	ASP	Peptide
1	C	130	THR	Peptide
1	C	136	ASP	Peptide
1	C	138	TYR	Peptide
1	C	147	SER	Peptide
1	C	189	SER	Peptide
1	C	288	ASN	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	C	336	TRP	Peptide
1	C	347	VAL	Peptide
1	C	363	ASP	Peptide
1	C	375	ARG	Peptide
1	C	379	LEU	Peptide
1	C	523	PRO	Peptide
1	C	526	ALA	Peptide
1	C	528	GLN	Peptide
1	C	546	GLY	Peptide
1	C	577	LEU	Peptide
1	C	578	ASP	Peptide
1	C	592	ARG	Peptide
1	C	605	TYR	Peptide
1	C	606	SER	Peptide
1	C	607	LEU	Peptide
1	C	608	TYR	Peptide
1	C	611	GLY	Peptide
1	C	613	VAL	Mainchain,Peptide
1	C	618	ILE	Peptide
1	C	620	LEU	Peptide
1	C	634	LYS	Peptide
1	C	635	ASP	Peptide
1	C	645	MET	Peptide
1	C	651	VAL	Peptide
1	C	653	THR	Peptide
1	C	657	LEU	Peptide
1	C	659	ASP	Peptide
1	C	660	TYR	Peptide
1	C	662	LYS	Peptide
1	C	666	PRO	Peptide
1	C	676	LEU	Peptide
1	C	680	ALA	Peptide
1	C	693	GLU	Peptide
1	C	697	ASP	Peptide
1	C	698	PHE	Peptide
1	C	700	ALA	Peptide
1	C	732	ASP	Peptide
1	C	772	LYS	Peptide
1	C	783	SER	Peptide
1	C	784	PRO	Peptide
1	C	785	LEU	Mainchain,Peptide
1	C	786	VAL	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	C	787	ARG	Peptide
1	C	793	LEU	Peptide
1	C	795	THR	Peptide
1	C	796	HIS	Peptide
1	C	797	PRO	Peptide
1	C	800	LYS	Peptide
1	C	801	ASP	Peptide
1	C	802	CYS	Peptide
1	C	803	HIS	Peptide
1	C	804	LEU	Peptide
1	C	805	LEU	Peptide
1	C	806	TYR	Peptide
1	C	813	THR	Peptide
1	C	886	ASP	Peptide
1	C	889	LYS	Peptide
1	C	890	ASP	Peptide
1	C	912	ASP	Peptide
1	C	929	ASN	Peptide
1	C	931	ARG	Peptide
1	C	933	ARG	Peptide
1	C	935	VAL	Peptide
1	C	936	GLU	Peptide
1	C	941	ASP	Peptide
1	D	130	THR	Peptide
1	D	136	ASP	Peptide
1	D	138	TYR	Peptide
1	D	147	SER	Peptide
1	D	189	SER	Peptide
1	D	288	ASN	Peptide
1	D	336	TRP	Peptide
1	D	347	VAL	Peptide
1	D	363	ASP	Peptide
1	D	375	ARG	Peptide
1	D	379	LEU	Peptide
1	D	523	PRO	Peptide
1	D	526	ALA	Peptide
1	D	528	GLN	Peptide
1	D	546	GLY	Peptide
1	D	577	LEU	Peptide
1	D	578	ASP	Peptide
1	D	592	ARG	Peptide
1	D	605	TYR	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	D	606	SER	Peptide
1	D	607	LEU	Peptide
1	D	608	TYR	Peptide
1	D	611	GLY	Peptide
1	D	613	VAL	Mainchain,Peptide
1	D	618	ILE	Peptide
1	D	620	LEU	Peptide
1	D	634	LYS	Peptide
1	D	635	ASP	Peptide
1	D	645	MET	Peptide
1	D	651	VAL	Peptide
1	D	653	THR	Peptide
1	D	657	LEU	Peptide
1	D	659	ASP	Peptide
1	D	660	TYR	Peptide
1	D	662	LYS	Peptide
1	D	666	PRO	Peptide
1	D	676	LEU	Peptide
1	D	680	ALA	Peptide
1	D	693	GLU	Peptide
1	D	697	ASP	Peptide
1	D	698	PHE	Peptide
1	D	700	ALA	Peptide
1	D	732	ASP	Peptide
1	D	772	LYS	Peptide
1	D	783	SER	Peptide
1	D	784	PRO	Peptide
1	D	785	LEU	Mainchain,Peptide
1	D	786	VAL	Peptide
1	D	787	ARG	Peptide
1	D	795	THR	Peptide
1	D	796	HIS	Peptide
1	D	797	PRO	Peptide
1	D	800	LYS	Peptide
1	D	801	ASP	Peptide
1	D	802	CYS	Peptide
1	D	803	HIS	Peptide
1	D	804	LEU	Peptide
1	D	805	LEU	Peptide
1	D	806	TYR	Peptide
1	D	813	THR	Peptide
1	D	886	ASP	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	D	889	LYS	Peptide
1	D	890	ASP	Peptide
1	D	912	ASP	Peptide
1	D	929	ASN	Peptide
1	D	931	ARG	Peptide
1	D	933	ARG	Peptide
1	D	935	VAL	Peptide
1	D	936	GLU	Peptide
1	D	941	ASP	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6011	0	5773	257	0
1	B	6011	0	5773	265	0
1	C	6011	0	5773	259	0
1	D	6011	0	5773	268	0
All	All	24044	0	23092	1032	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 22.

All (1032) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:ASN:HD22	1:B:572:LYS:HB3	1.46	0.81
1:D:570:ASN:HD22	1:D:572:LYS:HB3	1.46	0.80
1:B:729:ALA:O	1:B:733:PHE:HB2	1.82	0.80
1:D:729:ALA:O	1:D:733:PHE:HB2	1.82	0.80
1:A:729:ALA:O	1:A:733:PHE:HB2	1.82	0.79
1:A:825:MET:SD	1:A:828:ASN:ND2	2.55	0.79
1:C:729:ALA:O	1:C:733:PHE:HB2	1.82	0.79
1:C:825:MET:SD	1:C:828:ASN:ND2	2.55	0.79
1:A:847:ASN:O	1:A:851:GLN:HB2	1.83	0.78
1:C:847:ASN:O	1:C:851:GLN:HB2	1.83	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ASN:HD22	1:A:572:LYS:HB3	1.46	0.78
1:C:570:ASN:HD22	1:C:572:LYS:HB3	1.46	0.78
1:B:825:MET:SD	1:B:828:ASN:ND2	2.55	0.78
1:D:825:MET:SD	1:D:828:ASN:ND2	2.55	0.78
1:B:847:ASN:O	1:B:851:GLN:HB2	1.83	0.77
1:D:847:ASN:O	1:D:851:GLN:HB2	1.83	0.77
1:C:803:HIS:HB3	1:C:804:LEU:HG	1.67	0.75
1:B:803:HIS:HB3	1:B:804:LEU:HG	1.67	0.75
1:A:803:HIS:HB3	1:A:804:LEU:HG	1.67	0.75
1:D:803:HIS:HB3	1:D:804:LEU:HG	1.67	0.75
1:B:587:GLY:HA2	1:B:945:GLN:HA	1.70	0.73
1:D:587:GLY:HA2	1:D:945:GLN:HA	1.70	0.72
1:C:587:GLY:HA2	1:C:945:GLN:HA	1.70	0.71
1:A:587:GLY:HA2	1:A:945:GLN:HA	1.70	0.71
1:C:689:ALA:O	1:C:693:GLU:HB2	1.91	0.71
1:A:689:ALA:O	1:A:693:GLU:HB2	1.91	0.71
1:B:689:ALA:O	1:B:693:GLU:HB2	1.91	0.70
1:D:689:ALA:O	1:D:693:GLU:HB2	1.91	0.70
1:A:586:TRP:HE1	1:A:627:GLN:HB2	1.57	0.69
1:C:586:TRP:HE1	1:C:627:GLN:HB2	1.57	0.69
1:A:929:ASN:OD1	1:A:929:ASN:N	2.26	0.68
1:C:929:ASN:OD1	1:C:929:ASN:N	2.26	0.68
1:A:607:LEU:HD21	1:A:827:LEU:H	1.59	0.68
1:A:576:LYS:HD2	1:A:736:LEU:HD23	1.75	0.68
1:B:586:TRP:HE1	1:B:627:GLN:HB2	1.57	0.68
1:C:607:LEU:HD21	1:C:827:LEU:H	1.59	0.68
1:D:586:TRP:HE1	1:D:627:GLN:HB2	1.57	0.68
1:C:576:LYS:HD2	1:C:736:LEU:HD23	1.75	0.67
1:D:93:PRO:HA	1:D:104:HIS:HB2	1.76	0.67
1:D:576:LYS:HD2	1:D:736:LEU:HD23	1.75	0.67
1:B:93:PRO:HA	1:B:104:HIS:HB2	1.76	0.67
1:B:576:LYS:HD2	1:B:736:LEU:HD23	1.75	0.67
1:D:929:ASN:OD1	1:D:929:ASN:N	2.26	0.67
1:B:221:LYS:HG2	1:B:230:GLU:HG2	1.76	0.67
1:B:929:ASN:N	1:B:929:ASN:OD1	2.26	0.67
1:D:221:LYS:HG2	1:D:230:GLU:HG2	1.77	0.67
1:C:221:LYS:HG2	1:C:230:GLU:HG2	1.76	0.67
1:A:221:LYS:HG2	1:A:230:GLU:HG2	1.76	0.67
1:B:96:VAL:HG22	1:B:100:GLU:H	1.58	0.66
1:D:156:TYR:HB2	1:D:205:ASP:HA	1.77	0.66
1:D:223:SER:HA	1:D:228:SER:HA	1.76	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:LEU:HD21	1:B:827:LEU:H	1.59	0.66
1:D:607:LEU:HD21	1:D:827:LEU:H	1.59	0.66
1:B:223:SER:HA	1:B:228:SER:HA	1.76	0.66
1:B:156:TYR:HB2	1:B:205:ASP:HA	1.78	0.66
1:B:771:VAL:HG11	1:B:788:TRP:HA	1.78	0.66
1:D:96:VAL:HG22	1:D:100:GLU:H	1.59	0.66
1:D:771:VAL:HG11	1:D:788:TRP:HA	1.78	0.66
1:A:223:SER:HA	1:A:228:SER:HA	1.76	0.66
1:C:156:TYR:HB2	1:C:205:ASP:HA	1.77	0.66
1:A:93:PRO:HA	1:A:104:HIS:HB2	1.76	0.66
1:A:771:VAL:HG11	1:A:788:TRP:HA	1.78	0.66
1:C:93:PRO:HA	1:C:104:HIS:HB2	1.76	0.66
1:A:156:TYR:HB2	1:A:205:ASP:HA	1.78	0.66
1:C:96:VAL:HG22	1:C:100:GLU:H	1.59	0.66
1:C:223:SER:HA	1:C:228:SER:HA	1.76	0.66
1:C:577:LEU:N	1:C:734:CYS:O	2.27	0.66
1:C:771:VAL:HG11	1:C:788:TRP:HA	1.78	0.66
1:D:577:LEU:N	1:D:734:CYS:O	2.27	0.65
1:A:96:VAL:HG22	1:A:100:GLU:H	1.58	0.65
1:B:577:LEU:N	1:B:734:CYS:O	2.27	0.65
1:A:577:LEU:N	1:A:734:CYS:O	2.26	0.65
1:C:640:LEU:HB2	1:C:649:GLU:HB2	1.79	0.65
1:A:640:LEU:HB2	1:A:649:GLU:HB2	1.79	0.65
1:B:642:SER:OG	1:B:643:ILE:N	2.29	0.65
1:D:654:PHE:N	1:D:688:TYR:OH	2.29	0.65
1:D:642:SER:OG	1:D:643:ILE:N	2.29	0.65
1:B:654:PHE:N	1:B:688:TYR:OH	2.29	0.65
1:B:640:LEU:HB2	1:B:649:GLU:HB2	1.79	0.64
1:B:946:VAL:HB	1:B:948:ARG:HG2	1.78	0.64
1:C:946:VAL:HB	1:C:948:ARG:HG2	1.78	0.64
1:D:640:LEU:HB2	1:D:649:GLU:HB2	1.79	0.64
1:D:946:VAL:HB	1:D:948:ARG:HG2	1.78	0.64
1:B:81:LEU:HG	1:B:83:GLY:H	1.63	0.64
1:D:81:LEU:HG	1:D:83:GLY:H	1.63	0.64
1:A:106:GLY:H	1:A:109:LEU:H	1.46	0.64
1:A:641:ARG:HD3	1:C:641:ARG:HD3	1.79	0.64
1:A:946:VAL:HB	1:A:948:ARG:HG2	1.79	0.64
1:C:106:GLY:H	1:C:109:LEU:H	1.46	0.64
1:A:654:PHE:N	1:A:688:TYR:OH	2.30	0.64
1:B:106:GLY:H	1:B:109:LEU:H	1.46	0.64
1:C:654:PHE:N	1:C:688:TYR:OH	2.29	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:GLY:H	1:D:109:LEU:H	1.46	0.64
1:A:81:LEU:HG	1:A:83:GLY:H	1.63	0.63
1:C:81:LEU:HG	1:C:83:GLY:H	1.63	0.63
1:B:581:SER:OG	1:B:582:ASP:N	2.32	0.63
1:C:364:VAL:HG11	1:C:379:LEU:HD21	1.81	0.63
1:C:616:LEU:HD13	1:C:618:ILE:HG23	1.81	0.63
1:C:772:LYS:HZ3	1:C:775:GLN:HG3	1.64	0.63
1:A:364:VAL:HG11	1:A:379:LEU:HD21	1.81	0.63
1:A:616:LEU:HD13	1:A:618:ILE:HG23	1.81	0.63
1:D:581:SER:OG	1:D:582:ASP:N	2.32	0.63
1:B:654:PHE:O	1:B:658:GLN:NE2	2.31	0.62
1:D:654:PHE:O	1:D:658:GLN:NE2	2.31	0.62
1:C:581:SER:OG	1:C:582:ASP:N	2.32	0.62
1:A:581:SER:OG	1:A:582:ASP:N	2.32	0.62
1:C:654:PHE:O	1:C:658:GLN:NE2	2.31	0.62
1:D:576:LYS:HB3	1:D:734:CYS:HB3	1.82	0.62
1:B:576:LYS:HB3	1:B:734:CYS:HB3	1.82	0.62
1:B:948:ARG:HH22	1:D:933:ARG:HD3	1.64	0.62
1:B:933:ARG:HD3	1:D:948:ARG:HH22	1.64	0.62
1:A:654:PHE:O	1:A:658:GLN:NE2	2.31	0.62
1:C:582:ASP:N	1:C:582:ASP:OD1	2.30	0.62
1:A:582:ASP:N	1:A:582:ASP:OD1	2.30	0.62
1:B:641:ARG:HD3	1:D:641:ARG:HD3	1.80	0.61
1:B:364:VAL:HG11	1:B:379:LEU:HD21	1.81	0.61
1:B:616:LEU:HD13	1:B:618:ILE:HG23	1.81	0.61
1:D:364:VAL:HG11	1:D:379:LEU:HD21	1.81	0.61
1:A:647:ALA:O	1:C:641:ARG:NH1	2.33	0.61
1:D:616:LEU:HD13	1:D:618:ILE:HG23	1.81	0.61
1:A:897:LEU:HD13	1:A:901:GLY:HA2	1.83	0.61
1:A:576:LYS:HB3	1:A:734:CYS:HB3	1.82	0.61
1:C:642:SER:OG	1:C:643:ILE:N	2.29	0.61
1:C:897:LEU:HD13	1:C:901:GLY:HA2	1.83	0.61
1:D:582:ASP:N	1:D:582:ASP:OD1	2.30	0.61
1:A:630:VAL:HG23	1:A:704:VAL:HG22	1.83	0.61
1:A:772:LYS:HZ3	1:A:775:GLN:HG3	1.65	0.61
1:C:576:LYS:HB3	1:C:734:CYS:HB3	1.82	0.61
1:C:630:VAL:HG23	1:C:704:VAL:HG22	1.83	0.61
1:A:642:SER:OG	1:A:643:ILE:N	2.29	0.60
1:B:582:ASP:N	1:B:582:ASP:OD1	2.30	0.60
1:C:870:LYS:NZ	1:C:882:GLU:OE2	2.35	0.60
1:C:941:ASP:OD1	1:C:941:ASP:N	2.34	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:820:GLU:O	1:C:824:SER:N	2.32	0.60
1:A:870:LYS:NZ	1:A:882:GLU:OE2	2.35	0.60
1:A:941:ASP:OD1	1:A:941:ASP:N	2.34	0.60
1:A:820:GLU:O	1:A:824:SER:N	2.32	0.60
1:B:630:VAL:HG23	1:B:704:VAL:HG22	1.83	0.60
1:D:684:SER:N	1:D:687:SER:OG	2.31	0.60
1:D:870:LYS:NZ	1:D:882:GLU:OE2	2.35	0.60
1:A:580:TYR:OH	1:C:929:ASN:O	2.20	0.60
1:B:606:SER:OG	1:B:609:SER:N	2.35	0.60
1:B:870:LYS:NZ	1:B:882:GLU:OE2	2.35	0.60
1:D:630:VAL:HG23	1:D:704:VAL:HG22	1.83	0.60
1:B:691:LEU:O	1:B:695:LEU:CB	2.50	0.60
1:D:606:SER:OG	1:D:609:SER:N	2.35	0.60
1:B:684:SER:N	1:B:687:SER:OG	2.31	0.59
1:C:224:HIS:HD2	1:C:229:GLU:HB2	1.67	0.59
1:D:691:LEU:O	1:D:695:LEU:CB	2.50	0.59
1:D:897:LEU:HD13	1:D:901:GLY:HA2	1.83	0.59
1:A:224:HIS:HD2	1:A:229:GLU:HB2	1.68	0.59
1:A:606:SER:OG	1:A:609:SER:N	2.35	0.59
1:B:897:LEU:HD13	1:B:901:GLY:HA2	1.83	0.59
1:B:941:ASP:N	1:B:941:ASP:OD1	2.34	0.59
1:A:540:ARG:O	1:A:544:LEU:CB	2.50	0.59
1:D:941:ASP:N	1:D:941:ASP:OD1	2.34	0.59
1:B:609:SER:HA	1:B:778:ALA:HB3	1.85	0.59
1:C:606:SER:OG	1:C:609:SER:N	2.35	0.59
1:D:609:SER:HA	1:D:778:ALA:HB3	1.85	0.59
1:B:782:GLN:HE21	1:B:784:PRO:HD3	1.67	0.59
1:C:691:LEU:O	1:C:695:LEU:CB	2.50	0.59
1:D:540:ARG:O	1:D:544:LEU:CB	2.50	0.59
1:A:684:SER:N	1:A:687:SER:OG	2.31	0.59
1:A:782:GLN:HE21	1:A:784:PRO:HD3	1.67	0.59
1:B:103:GLN:NE2	1:B:108:ASN:OD1	2.35	0.59
1:B:540:ARG:O	1:B:544:LEU:CB	2.50	0.59
1:C:540:ARG:O	1:C:544:LEU:CB	2.50	0.59
1:C:782:GLN:HE21	1:C:784:PRO:HD3	1.67	0.59
1:A:691:LEU:O	1:A:695:LEU:CB	2.50	0.59
1:C:103:GLN:NE2	1:C:108:ASN:OD1	2.35	0.59
1:D:782:GLN:HE21	1:D:784:PRO:HD3	1.67	0.59
1:B:912:ASP:O	1:B:914:GLN:N	2.36	0.59
1:D:103:GLN:NE2	1:D:108:ASN:OD1	2.35	0.59
1:A:103:GLN:NE2	1:A:108:ASN:OD1	2.35	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:912:ASP:O	1:A:914:GLN:N	2.36	0.59
1:C:912:ASP:O	1:C:914:GLN:N	2.36	0.59
1:D:912:ASP:O	1:D:914:GLN:N	2.36	0.59
1:B:321:GLU:HG3	1:B:338:ILE:HG13	1.85	0.59
1:D:224:HIS:HD2	1:D:229:GLU:HB2	1.67	0.59
1:D:321:GLU:HG3	1:D:338:ILE:HG13	1.85	0.59
1:C:173:SER:HB3	1:C:181:LEU:HD12	1.85	0.58
1:C:609:SER:HA	1:C:778:ALA:HB3	1.85	0.58
1:C:684:SER:N	1:C:687:SER:OG	2.31	0.58
1:B:224:HIS:HD2	1:B:229:GLU:HB2	1.67	0.58
1:A:173:SER:HB3	1:A:181:LEU:HD12	1.85	0.58
1:A:609:SER:HA	1:A:778:ALA:HB3	1.85	0.58
1:A:614:VAL:HG22	1:A:773:LEU:HB2	1.85	0.58
1:C:614:VAL:HG22	1:C:773:LEU:HB2	1.85	0.58
1:C:910:ALA:HB2	1:C:918:ARG:HE	1.69	0.58
1:A:910:ALA:HB2	1:A:918:ARG:HE	1.69	0.58
1:B:221:LYS:HA	1:B:230:GLU:HA	1.85	0.58
1:A:321:GLU:HG3	1:A:338:ILE:HG13	1.85	0.58
1:A:933:ARG:HD3	1:C:948:ARG:HH22	1.66	0.58
1:B:295:ARG:HB2	1:B:312:ALA:HA	1.86	0.58
1:D:221:LYS:HA	1:D:230:GLU:HA	1.85	0.58
1:D:295:ARG:HB2	1:D:312:ALA:HA	1.86	0.58
1:A:830:SER:HB3	1:A:832:HIS:HD2	1.67	0.58
1:B:173:SER:HB3	1:B:181:LEU:HD12	1.85	0.58
1:C:321:GLU:HG3	1:C:338:ILE:HG13	1.85	0.58
1:C:830:SER:HB3	1:C:832:HIS:HD2	1.67	0.58
1:C:380:ASP:OD1	1:C:380:ASP:N	2.36	0.58
1:D:173:SER:HB3	1:D:181:LEU:HD12	1.85	0.58
1:A:380:ASP:OD1	1:A:380:ASP:N	2.36	0.58
1:B:830:SER:HB3	1:B:832:HIS:HD2	1.67	0.58
1:C:696:LYS:HZ3	1:C:700:ALA:HB3	1.67	0.58
1:D:830:SER:HB3	1:D:832:HIS:HD2	1.67	0.58
1:A:691:LEU:O	1:A:695:LEU:HB3	2.05	0.57
1:B:805:LEU:HD12	1:B:936:GLU:HB3	1.86	0.57
1:C:221:LYS:HA	1:C:230:GLU:HA	1.85	0.57
1:C:691:LEU:O	1:C:695:LEU:HB3	2.04	0.57
1:D:805:LEU:HD12	1:D:936:GLU:HB3	1.86	0.57
1:D:635:ASP:OD1	1:D:635:ASP:N	2.34	0.57
1:A:221:LYS:HA	1:A:230:GLU:HA	1.85	0.57
1:B:635:ASP:N	1:B:635:ASP:OD1	2.34	0.57
1:D:910:ALA:HB2	1:D:918:ARG:HE	1.69	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ASP:OD1	1:A:635:ASP:N	2.34	0.57
1:D:691:LEU:O	1:D:695:LEU:HB3	2.04	0.57
1:B:691:LEU:O	1:B:695:LEU:HB3	2.04	0.57
1:B:910:ALA:HB2	1:B:918:ARG:HE	1.69	0.57
1:A:805:LEU:HD12	1:A:936:GLU:HB3	1.86	0.57
1:B:614:VAL:HG22	1:B:773:LEU:HB2	1.85	0.57
1:C:635:ASP:OD1	1:C:635:ASP:N	2.34	0.57
1:D:614:VAL:HG22	1:D:773:LEU:HB2	1.85	0.57
1:A:878:PRO:HD3	1:A:902:GLY:HA2	1.87	0.56
1:B:601:ASP:OD1	1:B:775:GLN:NE2	2.38	0.56
1:C:805:LEU:HD12	1:C:936:GLU:HB3	1.86	0.56
1:C:878:PRO:HD3	1:C:902:GLY:HA2	1.87	0.56
1:D:601:ASP:OD1	1:D:775:GLN:NE2	2.39	0.56
1:A:295:ARG:HB2	1:A:312:ALA:HA	1.86	0.56
1:B:548:ASP:O	1:B:552:GLU:N	2.34	0.56
1:C:295:ARG:HB2	1:C:312:ALA:HA	1.86	0.56
1:A:342:HIS:NE2	1:A:349:GLU:OE2	2.38	0.56
1:C:342:HIS:NE2	1:C:349:GLU:OE2	2.38	0.56
1:A:762:ASP:OD1	1:A:762:ASP:N	2.34	0.56
1:B:641:ARG:HH11	1:D:641:ARG:HH11	1.53	0.56
1:B:848:GLU:OE2	1:B:852:ARG:NH2	2.38	0.56
1:C:762:ASP:N	1:C:762:ASP:OD1	2.34	0.56
1:D:848:GLU:OE2	1:D:852:ARG:NH2	2.38	0.56
1:A:795:THR:O	1:A:796:HIS:ND1	2.39	0.56
1:C:548:ASP:O	1:C:552:GLU:N	2.34	0.56
1:A:601:ASP:OD1	1:A:775:GLN:NE2	2.38	0.56
1:B:613:VAL:HG21	1:B:761:GLN:HB3	1.88	0.56
1:D:613:VAL:HG21	1:D:761:GLN:HB3	1.88	0.56
1:C:795:THR:O	1:C:796:HIS:ND1	2.39	0.56
1:D:548:ASP:O	1:D:552:GLU:N	2.34	0.56
1:D:820:GLU:O	1:D:824:SER:N	2.32	0.56
1:A:696:LYS:HZ3	1:A:700:ALA:HB3	1.69	0.56
1:C:601:ASP:OD1	1:C:775:GLN:NE2	2.38	0.56
1:A:548:ASP:O	1:A:552:GLU:N	2.34	0.55
1:B:609:SER:OG	1:B:777:GLU:O	2.22	0.55
1:B:762:ASP:OD1	1:B:762:ASP:N	2.34	0.55
1:C:848:GLU:OE2	1:C:852:ARG:NH2	2.38	0.55
1:A:848:GLU:OE2	1:A:852:ARG:NH2	2.38	0.55
1:B:158:LEU:HB3	1:B:204:MET:HB2	1.89	0.55
1:B:655:ASP:OD1	1:B:660:TYR:OH	2.24	0.55
1:B:878:PRO:HD3	1:B:902:GLY:HA2	1.87	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:LEU:HB3	1:D:204:MET:HB2	1.89	0.55
1:D:762:ASP:OD1	1:D:762:ASP:N	2.34	0.55
1:A:739:ASP:HB3	1:A:742:GLU:HG2	1.89	0.55
1:B:593:ILE:HG13	1:B:616:LEU:HD11	1.89	0.55
1:C:739:ASP:HB3	1:C:742:GLU:HG2	1.89	0.55
1:D:289:LYS:HB2	1:D:306:ALA:HA	1.88	0.55
1:D:609:SER:OG	1:D:777:GLU:O	2.22	0.55
1:D:655:ASP:OD1	1:D:660:TYR:OH	2.24	0.55
1:D:739:ASP:HB3	1:D:742:GLU:HG2	1.89	0.55
1:B:638:ILE:N	1:B:651:VAL:O	2.39	0.55
1:B:739:ASP:HB3	1:B:742:GLU:HG2	1.89	0.55
1:D:593:ILE:HG13	1:D:616:LEU:HD11	1.89	0.55
1:D:638:ILE:N	1:D:651:VAL:O	2.39	0.55
1:D:878:PRO:HD3	1:D:902:GLY:HA2	1.87	0.55
1:A:138:TYR:N	1:A:271:TYR:O	2.38	0.55
1:B:289:LYS:HB2	1:B:306:ALA:HA	1.88	0.55
1:B:380:ASP:OD1	1:B:380:ASP:N	2.36	0.55
1:C:138:TYR:N	1:C:271:TYR:O	2.38	0.55
1:D:380:ASP:N	1:D:380:ASP:OD1	2.36	0.55
1:A:576:LYS:HE2	1:A:695:LEU:HD11	1.89	0.55
1:A:948:ARG:HH22	1:C:933:ARG:HD3	1.71	0.55
1:B:820:GLU:O	1:B:824:SER:N	2.33	0.55
1:C:289:LYS:HB2	1:C:306:ALA:HA	1.88	0.55
1:D:795:THR:O	1:D:796:HIS:ND1	2.39	0.55
1:C:613:VAL:HG21	1:C:761:GLN:HB3	1.88	0.55
1:A:289:LYS:HB2	1:A:306:ALA:HA	1.88	0.55
1:B:795:THR:O	1:B:796:HIS:ND1	2.39	0.55
1:C:203:LEU:HD11	1:C:262:ILE:HG21	1.89	0.55
1:C:576:LYS:HE2	1:C:695:LEU:HD11	1.89	0.55
1:C:621:ASN:ND2	1:C:935:VAL:O	2.36	0.55
1:C:721:ILE:O	1:C:724:SER:OG	2.23	0.55
1:A:203:LEU:HD11	1:A:262:ILE:HG21	1.89	0.55
1:A:655:ASP:OD1	1:A:660:TYR:OH	2.24	0.55
1:B:375:ARG:HB2	1:B:397:ILE:HB	1.89	0.55
1:C:609:SER:OG	1:C:777:GLU:O	2.22	0.55
1:A:635:ASP:O	1:A:637:HIS:N	2.39	0.54
1:A:638:ILE:N	1:A:651:VAL:O	2.39	0.54
1:C:86:PRO:HB3	1:C:375:ARG:HH11	1.72	0.54
1:C:635:ASP:O	1:C:637:HIS:N	2.39	0.54
1:D:375:ARG:HB2	1:D:397:ILE:HB	1.89	0.54
1:A:609:SER:OG	1:A:777:GLU:O	2.22	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:VAL:HG21	1:A:761:GLN:HB3	1.88	0.54
1:B:588:ARG:HE	1:B:944:PHE:H	1.55	0.54
1:C:638:ILE:N	1:C:651:VAL:O	2.39	0.54
1:C:655:ASP:OD1	1:C:660:TYR:OH	2.24	0.54
1:A:375:ARG:HB2	1:A:397:ILE:HB	1.89	0.54
1:A:86:PRO:HB3	1:A:375:ARG:HH11	1.72	0.54
1:A:621:ASN:ND2	1:A:935:VAL:O	2.36	0.54
1:A:657:LEU:HB2	1:A:658:GLN:HB2	1.89	0.54
1:D:588:ARG:HE	1:D:944:PHE:H	1.55	0.54
1:A:574:THR:O	1:A:576:LYS:NZ	2.41	0.54
1:C:375:ARG:HB2	1:C:397:ILE:HB	1.89	0.54
1:D:86:PRO:HB3	1:D:375:ARG:HH11	1.72	0.54
1:B:86:PRO:HB3	1:B:375:ARG:HH11	1.72	0.54
1:B:576:LYS:HE2	1:B:695:LEU:HD11	1.89	0.54
1:C:657:LEU:HB2	1:C:658:GLN:HB2	1.89	0.54
1:D:203:LEU:HD11	1:D:262:ILE:HG21	1.89	0.54
1:D:576:LYS:HE2	1:D:695:LEU:HD11	1.89	0.54
1:B:203:LEU:HD11	1:B:262:ILE:HG21	1.89	0.54
1:A:313:VAL:HG22	1:A:330:SER:H	1.73	0.54
1:D:657:LEU:HB2	1:D:658:GLN:HB2	1.89	0.54
1:B:657:LEU:HB2	1:B:658:GLN:HB2	1.89	0.54
1:C:158:LEU:HB3	1:C:204:MET:HB2	1.89	0.54
1:C:593:ILE:HG13	1:C:616:LEU:HD11	1.89	0.54
1:A:588:ARG:HE	1:A:944:PHE:H	1.55	0.54
1:A:593:ILE:HG13	1:A:616:LEU:HD11	1.89	0.54
1:C:313:VAL:HG22	1:C:330:SER:H	1.73	0.54
1:C:561:ARG:O	1:C:752:GLN:NE2	2.41	0.54
1:D:342:HIS:NE2	1:D:349:GLU:OE2	2.38	0.54
1:A:158:LEU:HB3	1:A:204:MET:HB2	1.89	0.53
1:A:183:PHE:HA	1:A:246:THR:HA	1.90	0.53
1:A:561:ARG:O	1:A:752:GLN:NE2	2.41	0.53
1:B:342:HIS:NE2	1:B:349:GLU:OE2	2.38	0.53
1:A:527:LEU:O	1:A:531:ARG:N	2.33	0.53
1:A:641:ARG:HH11	1:C:641:ARG:HH11	1.56	0.53
1:B:637:HIS:O	1:B:637:HIS:ND1	2.41	0.53
1:C:183:PHE:HA	1:C:246:THR:HA	1.90	0.53
1:C:588:ARG:HE	1:C:944:PHE:H	1.55	0.53
1:D:637:HIS:O	1:D:637:HIS:ND1	2.41	0.53
1:B:621:ASN:ND2	1:B:935:VAL:O	2.36	0.53
1:A:637:HIS:ND1	1:A:637:HIS:O	2.41	0.53
1:A:641:ARG:NH1	1:C:647:ALA:O	2.41	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:ILE:O	1:A:724:SER:OG	2.23	0.53
1:B:502:LEU:O	1:B:506:ASP:N	2.35	0.53
1:B:635:ASP:O	1:B:637:HIS:N	2.39	0.53
1:D:561:ARG:O	1:D:565:LEU:N	2.42	0.53
1:A:774:LEU:O	1:A:776:THR:OG1	2.24	0.53
1:B:310:GLN:OE1	1:B:315:ARG:NH1	2.36	0.53
1:B:561:ARG:O	1:B:565:LEU:N	2.42	0.53
1:B:721:ILE:O	1:B:725:THR:OG1	2.27	0.53
1:C:637:HIS:O	1:C:637:HIS:ND1	2.41	0.53
1:D:635:ASP:O	1:D:637:HIS:N	2.39	0.53
1:D:721:ILE:O	1:D:725:THR:OG1	2.27	0.53
1:A:101:ARG:HH22	1:A:480:GLU:HA	1.74	0.53
1:B:601:ASP:OD1	1:B:761:GLN:N	2.37	0.53
1:B:606:SER:OG	1:B:607:LEU:N	2.41	0.53
1:D:502:LEU:O	1:D:506:ASP:N	2.35	0.53
1:D:574:THR:O	1:D:576:LYS:NZ	2.41	0.53
1:D:621:ASN:ND2	1:D:935:VAL:O	2.36	0.53
1:D:606:SER:OG	1:D:607:LEU:N	2.41	0.53
1:B:561:ARG:O	1:B:752:GLN:NE2	2.41	0.53
1:B:574:THR:O	1:B:576:LYS:NZ	2.41	0.53
1:C:101:ARG:HH22	1:C:480:GLU:HA	1.74	0.53
1:C:774:LEU:O	1:C:776:THR:OG1	2.24	0.53
1:C:827:LEU:HA	1:C:833:LEU:HD21	1.91	0.53
1:D:561:ARG:O	1:D:752:GLN:NE2	2.41	0.53
1:D:601:ASP:OD1	1:D:761:GLN:N	2.37	0.53
1:A:606:SER:OG	1:A:607:LEU:N	2.41	0.53
1:C:606:SER:OG	1:C:607:LEU:N	2.41	0.53
1:A:827:LEU:HA	1:A:833:LEU:HD21	1.91	0.52
1:B:246:THR:HB	1:B:248:PRO:HD2	1.91	0.52
1:A:105:LEU:HA	1:A:108:ASN:HB2	1.91	0.52
1:D:105:LEU:HA	1:D:108:ASN:HB2	1.91	0.52
1:D:313:VAL:HG22	1:D:330:SER:H	1.73	0.52
1:D:774:LEU:O	1:D:776:THR:OG1	2.24	0.52
1:B:105:LEU:HA	1:B:108:ASN:HB2	1.92	0.52
1:D:246:THR:HB	1:D:248:PRO:HD2	1.92	0.52
1:A:561:ARG:O	1:A:565:LEU:N	2.42	0.52
1:B:340:SER:OG	1:B:341:ARG:N	2.40	0.52
1:B:774:LEU:O	1:B:776:THR:OG1	2.24	0.52
1:C:105:LEU:HA	1:C:108:ASN:HB2	1.91	0.52
1:A:310:GLN:OE1	1:A:315:ARG:NH1	2.36	0.52
1:B:313:VAL:HG22	1:B:330:SER:H	1.73	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:ASP:OD1	1:C:212:SER:OG	2.28	0.52
1:C:561:ARG:O	1:C:565:LEU:N	2.42	0.52
1:C:246:THR:HB	1:C:248:PRO:HD2	1.91	0.52
1:D:340:SER:OG	1:D:341:ARG:N	2.40	0.52
1:A:152:ASP:OD1	1:A:212:SER:OG	2.28	0.52
1:B:86:PRO:HB3	1:B:375:ARG:HD2	1.92	0.52
1:D:86:PRO:HB3	1:D:375:ARG:HD2	1.92	0.52
1:A:246:THR:HB	1:A:248:PRO:HD2	1.92	0.52
1:B:152:ASP:OD1	1:B:212:SER:OG	2.28	0.52
1:B:827:LEU:HA	1:B:833:LEU:HD21	1.91	0.52
1:D:827:LEU:HA	1:D:833:LEU:HD21	1.91	0.52
1:B:138:TYR:N	1:B:271:TYR:O	2.38	0.52
1:B:236:LEU:O	1:B:240:PHE:CB	2.58	0.52
1:B:772:LYS:HZ1	1:B:775:GLN:N	2.08	0.52
1:D:236:LEU:O	1:D:240:PHE:CB	2.58	0.52
1:A:847:ASN:O	1:A:851:GLN:CB	2.57	0.51
1:C:310:GLN:OE1	1:C:315:ARG:NH1	2.36	0.51
1:D:152:ASP:OD1	1:D:212:SER:OG	2.28	0.51
1:A:721:ILE:O	1:A:725:THR:OG1	2.27	0.51
1:B:572:LYS:HD3	1:B:574:THR:HG23	1.92	0.51
1:C:86:PRO:HB3	1:C:375:ARG:HD2	1.92	0.51
1:C:721:ILE:O	1:C:725:THR:OG1	2.27	0.51
1:D:138:TYR:N	1:D:271:TYR:O	2.38	0.51
1:D:572:LYS:HD3	1:D:574:THR:HG23	1.92	0.51
1:B:183:PHE:HA	1:B:246:THR:HA	1.90	0.51
1:D:183:PHE:HA	1:D:246:THR:HA	1.90	0.51
1:A:86:PRO:HB3	1:A:375:ARG:HD2	1.92	0.51
1:C:847:ASN:O	1:C:851:GLN:CB	2.57	0.51
1:D:721:ILE:O	1:D:724:SER:OG	2.23	0.51
1:A:236:LEU:O	1:A:240:PHE:CB	2.58	0.51
1:C:90:ILE:HG13	1:C:106:GLY:HA3	1.92	0.51
1:B:573:SER:O	1:B:573:SER:OG	2.26	0.51
1:C:502:LEU:O	1:C:506:ASP:N	2.35	0.51
1:D:573:SER:O	1:D:573:SER:OG	2.26	0.51
1:D:748:LEU:HB2	1:D:763:GLN:HE22	1.76	0.51
1:A:90:ILE:HG13	1:A:106:GLY:HA3	1.92	0.51
1:C:236:LEU:O	1:C:240:PHE:CB	2.58	0.51
1:D:696:LYS:HZ3	1:D:700:ALA:HB3	1.76	0.51
1:B:721:ILE:O	1:B:724:SER:OG	2.23	0.51
1:B:748:LEU:HB2	1:B:763:GLN:HE22	1.76	0.51
1:A:502:LEU:O	1:A:506:ASP:N	2.35	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:GLN:NE2	1:A:764:TYR:OH	2.44	0.51
1:C:745:GLN:NE2	1:C:764:TYR:OH	2.44	0.51
1:A:572:LYS:HD3	1:A:574:THR:HG23	1.93	0.50
1:B:527:LEU:O	1:B:531:ARG:N	2.33	0.50
1:B:731:ASN:HD22	1:B:743:ILE:HD11	1.76	0.50
1:B:745:GLN:NE2	1:B:764:TYR:OH	2.44	0.50
1:C:572:LYS:HD3	1:C:574:THR:HG23	1.92	0.50
1:D:527:LEU:O	1:D:531:ARG:N	2.33	0.50
1:D:731:ASN:HD22	1:D:743:ILE:HD11	1.76	0.50
1:D:745:GLN:NE2	1:D:764:TYR:OH	2.44	0.50
1:B:647:ALA:O	1:D:641:ARG:NH1	2.45	0.50
1:A:789:LEU:HD12	1:A:790:PRO:HD2	1.94	0.50
1:B:101:ARG:HH22	1:B:480:GLU:HA	1.74	0.50
1:B:641:ARG:NH1	1:D:647:ALA:O	2.45	0.50
1:B:688:TYR:HA	1:B:691:LEU:HB2	1.94	0.50
1:C:789:LEU:HD12	1:C:790:PRO:HD2	1.94	0.50
1:D:101:ARG:HH22	1:D:480:GLU:HA	1.74	0.50
1:B:789:LEU:HD12	1:B:790:PRO:HD2	1.94	0.50
1:C:688:TYR:HA	1:C:691:LEU:HB2	1.94	0.50
1:A:340:SER:OG	1:A:341:ARG:N	2.40	0.50
1:B:90:ILE:HG13	1:B:106:GLY:HA3	1.92	0.50
1:C:340:SER:OG	1:C:341:ARG:N	2.40	0.50
1:D:688:TYR:HA	1:D:691:LEU:HB2	1.94	0.50
1:D:789:LEU:HD12	1:D:790:PRO:HD2	1.94	0.50
1:A:85:ALA:O	1:A:87:SER:N	2.43	0.50
1:A:688:TYR:HA	1:A:691:LEU:HB2	1.94	0.50
1:D:90:ILE:HG13	1:D:106:GLY:HA3	1.92	0.50
1:D:743:ILE:O	1:D:747:THR:OG1	2.24	0.50
1:A:637:HIS:N	1:A:701:GLY:HA3	2.27	0.50
1:B:190:LEU:O	1:B:193:LEU:N	2.45	0.50
1:C:85:ALA:O	1:C:87:SER:N	2.43	0.50
1:C:637:HIS:N	1:C:701:GLY:HA3	2.27	0.50
1:D:190:LEU:O	1:D:193:LEU:N	2.45	0.50
1:B:612:ASN:HD21	1:B:844:LEU:HD11	1.77	0.49
1:B:672:ALA:O	1:B:675:SER:OG	2.22	0.49
1:B:696:LYS:HZ3	1:B:700:ALA:HB3	1.77	0.49
1:B:743:ILE:O	1:B:747:THR:OG1	2.24	0.49
1:D:124:ALA:HB3	1:D:128:LEU:HA	1.94	0.49
1:A:748:LEU:HB2	1:A:763:GLN:HE22	1.76	0.49
1:B:124:ALA:HB3	1:B:128:LEU:HA	1.94	0.49
1:D:156:TYR:HE2	1:D:208:ILE:H	1.61	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:612:ASN:HD21	1:D:844:LEU:HD11	1.78	0.49
1:A:116:LEU:HD11	1:A:131:LEU:HD23	1.94	0.49
1:A:319:CYS:HB2	1:A:336:TRP:HB2	1.94	0.49
1:A:640:LEU:HD13	1:A:670:PRO:HB2	1.94	0.49
1:B:156:TYR:HE2	1:B:208:ILE:H	1.61	0.49
1:B:236:LEU:O	1:B:240:PHE:HB3	2.12	0.49
1:C:116:LEU:HD11	1:C:131:LEU:HD23	1.94	0.49
1:D:236:LEU:O	1:D:240:PHE:HB3	2.13	0.49
1:A:124:ALA:HB3	1:A:128:LEU:HA	1.94	0.49
1:A:573:SER:O	1:A:573:SER:OG	2.26	0.49
1:C:319:CYS:HB2	1:C:336:TRP:HB2	1.94	0.49
1:C:190:LEU:O	1:C:193:LEU:N	2.45	0.49
1:C:640:LEU:HD13	1:C:670:PRO:HB2	1.94	0.49
1:C:748:LEU:HB2	1:C:763:GLN:HE22	1.76	0.49
1:D:847:ASN:O	1:D:851:GLN:CB	2.57	0.49
1:A:156:TYR:HE2	1:A:208:ILE:H	1.61	0.49
1:B:691:LEU:O	1:B:695:LEU:HB2	2.13	0.49
1:B:847:ASN:O	1:B:851:GLN:CB	2.57	0.49
1:D:672:ALA:O	1:D:675:SER:OG	2.22	0.49
1:A:612:ASN:HD21	1:A:844:LEU:HD11	1.78	0.49
1:B:640:LEU:HD13	1:B:670:PRO:HB2	1.94	0.49
1:B:920:ARG:O	1:B:924:THR:OG1	2.27	0.49
1:D:86:PRO:O	1:D:341:ARG:NH2	2.45	0.49
1:C:124:ALA:HB3	1:C:128:LEU:HA	1.94	0.49
1:C:156:TYR:HE2	1:C:208:ILE:H	1.61	0.49
1:D:85:ALA:O	1:D:87:SER:N	2.43	0.49
1:D:640:LEU:HD13	1:D:670:PRO:HB2	1.94	0.49
1:D:691:LEU:O	1:D:695:LEU:HB2	2.13	0.49
1:A:190:LEU:O	1:A:193:LEU:N	2.45	0.49
1:B:571:ARG:HH22	1:B:679:PHE:HB2	1.78	0.49
1:C:92:THR:O	1:C:104:HIS:ND1	2.46	0.49
1:C:236:LEU:O	1:C:240:PHE:HB3	2.13	0.49
1:C:573:SER:O	1:C:573:SER:OG	2.26	0.49
1:D:571:ARG:HH22	1:D:679:PHE:HB2	1.78	0.49
1:A:92:THR:O	1:A:104:HIS:ND1	2.46	0.49
1:A:236:LEU:O	1:A:240:PHE:HB3	2.13	0.49
1:A:920:ARG:O	1:A:924:THR:OG1	2.27	0.49
1:B:85:ALA:O	1:B:87:SER:N	2.43	0.49
1:B:86:PRO:O	1:B:341:ARG:NH2	2.45	0.49
1:B:92:THR:O	1:B:104:HIS:ND1	2.46	0.49
1:B:637:HIS:N	1:B:701:GLY:HA3	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:ASN:HD21	1:C:844:LEU:HD11	1.78	0.49
1:C:731:ASN:HD22	1:C:743:ILE:HD11	1.77	0.49
1:C:920:ARG:O	1:C:924:THR:OG1	2.27	0.49
1:D:92:THR:O	1:D:104:HIS:ND1	2.46	0.49
1:A:113:GLN:HA	1:A:116:LEU:HB3	1.95	0.48
1:A:345:THR:HB	1:A:347:VAL:H	1.78	0.48
1:C:113:GLN:HA	1:C:116:LEU:HB3	1.95	0.48
1:D:116:LEU:HD11	1:D:131:LEU:HD23	1.94	0.48
1:D:637:HIS:N	1:D:701:GLY:HA3	2.27	0.48
1:D:920:ARG:O	1:D:924:THR:OG1	2.27	0.48
1:A:731:ASN:HD22	1:A:743:ILE:HD11	1.77	0.48
1:B:113:GLN:HA	1:B:116:LEU:HB3	1.95	0.48
1:C:345:THR:HB	1:C:347:VAL:H	1.79	0.48
1:D:345:THR:HB	1:D:347:VAL:H	1.78	0.48
1:A:86:PRO:O	1:A:341:ARG:NH2	2.45	0.48
1:A:698:PHE:O	1:A:700:ALA:N	2.46	0.48
1:B:116:LEU:HD11	1:B:131:LEU:HD23	1.94	0.48
1:C:86:PRO:O	1:C:341:ARG:NH2	2.45	0.48
1:A:605:TYR:CD2	1:A:778:ALA:HB1	2.49	0.48
1:A:691:LEU:O	1:A:695:LEU:HB2	2.13	0.48
1:B:157:GLY:H	1:B:264:PRO:HA	1.78	0.48
1:B:345:THR:HB	1:B:347:VAL:H	1.79	0.48
1:B:673:ALA:HA	1:B:727:LEU:HD21	1.95	0.48
1:D:113:GLN:HA	1:D:116:LEU:HB3	1.95	0.48
1:D:157:GLY:H	1:D:264:PRO:HA	1.78	0.48
1:D:319:CYS:HB2	1:D:336:TRP:HB2	1.94	0.48
1:D:605:TYR:CD2	1:D:778:ALA:HB1	2.49	0.48
1:D:673:ALA:HA	1:D:727:LEU:HD21	1.95	0.48
1:A:157:GLY:H	1:A:264:PRO:HA	1.78	0.48
1:B:605:TYR:CD2	1:B:778:ALA:HB1	2.49	0.48
1:C:605:TYR:CD2	1:C:778:ALA:HB1	2.49	0.48
1:B:319:CYS:HB2	1:B:336:TRP:HB2	1.94	0.48
1:C:157:GLY:H	1:C:264:PRO:HA	1.79	0.48
1:C:698:PHE:O	1:C:700:ALA:N	2.47	0.48
1:D:812:ARG:HB3	1:D:814:ALA:HA	1.96	0.48
1:A:826:PHE:O	1:A:828:ASN:N	2.45	0.48
1:B:585:VAL:HA	1:B:947:SER:HA	1.96	0.48
1:B:730:ILE:O	1:B:733:PHE:N	2.46	0.48
1:B:812:ARG:HB3	1:B:814:ALA:HA	1.96	0.48
1:C:691:LEU:O	1:C:695:LEU:HB2	2.13	0.48
1:C:812:ARG:HB3	1:C:814:ALA:HA	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:585:VAL:HA	1:D:947:SER:HA	1.96	0.48
1:D:888:ILE:HG22	1:D:890:ASP:HB3	1.95	0.48
1:A:571:ARG:HH22	1:A:679:PHE:HB2	1.78	0.48
1:A:812:ARG:HB3	1:A:814:ALA:HA	1.96	0.48
1:C:571:ARG:HH22	1:C:679:PHE:HB2	1.78	0.48
1:C:826:PHE:O	1:C:828:ASN:N	2.45	0.48
1:C:866:TRP:HZ3	1:C:897:LEU:HB2	1.79	0.48
1:D:772:LYS:HZ1	1:D:775:GLN:N	2.11	0.48
1:B:744:CYS:O	1:B:763:GLN:NE2	2.47	0.48
1:B:888:ILE:HG22	1:B:890:ASP:HB3	1.95	0.48
1:C:585:VAL:HA	1:C:947:SER:HA	1.96	0.48
1:D:730:ILE:O	1:D:733:PHE:N	2.46	0.48
1:D:744:CYS:O	1:D:763:GLN:NE2	2.47	0.48
1:A:188:PRO:HB2	1:A:193:LEU:HB2	1.96	0.48
1:A:866:TRP:HZ3	1:A:897:LEU:HB2	1.79	0.48
1:A:888:ILE:HG22	1:A:890:ASP:HB3	1.95	0.48
1:C:188:PRO:HB2	1:C:193:LEU:HB2	1.96	0.48
1:A:313:VAL:O	1:A:315:ARG:NH1	2.47	0.47
1:A:585:VAL:HA	1:A:947:SER:HA	1.96	0.47
1:A:744:CYS:O	1:A:763:GLN:NE2	2.47	0.47
1:C:313:VAL:O	1:C:315:ARG:NH1	2.47	0.47
1:C:744:CYS:O	1:C:763:GLN:NE2	2.47	0.47
1:C:888:ILE:HG22	1:C:890:ASP:HB3	1.95	0.47
1:A:673:ALA:HA	1:A:727:LEU:HD21	1.95	0.47
1:A:929:ASN:O	1:C:580:TYR:OH	2.31	0.47
1:C:889:LYS:HD2	1:C:889:LYS:HA	1.70	0.47
1:B:698:PHE:O	1:B:700:ALA:N	2.47	0.47
1:D:698:PHE:O	1:D:700:ALA:N	2.47	0.47
1:D:772:LYS:HZ3	1:D:775:GLN:HG3	1.79	0.47
1:A:614:VAL:HA	1:A:772:LYS:HG3	1.96	0.47
1:C:574:THR:O	1:C:576:LYS:NZ	2.41	0.47
1:C:673:ALA:HA	1:C:727:LEU:HD21	1.95	0.47
1:B:620:LEU:HA	1:B:620:LEU:HD23	1.65	0.47
1:B:768:LEU:HD12	1:B:768:LEU:HA	1.75	0.47
1:B:866:TRP:HZ3	1:B:897:LEU:HB2	1.79	0.47
1:C:614:VAL:HA	1:C:772:LYS:HG3	1.96	0.47
1:A:119:LYS:HD2	1:A:145:LEU:HD23	1.97	0.47
1:A:601:ASP:OD1	1:A:761:GLN:N	2.37	0.47
1:B:165:ALA:HB1	1:B:188:PRO:HG2	1.97	0.47
1:B:188:PRO:HB2	1:B:193:LEU:HB2	1.96	0.47
1:B:293:GLN:HB2	1:B:311:ASN:HA	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:SER:HB2	1:B:667:PHE:HD2	1.79	0.47
1:C:119:LYS:HD2	1:C:145:LEU:HD23	1.97	0.47
1:C:159:TRP:NE1	1:C:202:PHE:O	2.41	0.47
1:D:165:ALA:HB1	1:D:188:PRO:HG2	1.97	0.47
1:D:263:LEU:HD12	1:D:264:PRO:HD2	1.97	0.47
1:D:293:GLN:HB2	1:D:311:ASN:HA	1.97	0.47
1:D:665:SER:HB2	1:D:667:PHE:HD2	1.79	0.47
1:D:768:LEU:HD12	1:D:768:LEU:HA	1.75	0.47
1:A:665:SER:HB2	1:A:667:PHE:HD2	1.79	0.47
1:C:165:ALA:HB1	1:C:188:PRO:HG2	1.97	0.47
1:C:665:SER:HB2	1:C:667:PHE:HD2	1.79	0.47
1:D:866:TRP:HZ3	1:D:897:LEU:HB2	1.79	0.47
1:B:263:LEU:HD12	1:B:264:PRO:HD2	1.97	0.47
1:C:601:ASP:OD1	1:C:761:GLN:N	2.37	0.47
1:D:188:PRO:HB2	1:D:193:LEU:HB2	1.96	0.47
1:D:729:ALA:O	1:D:733:PHE:CB	2.60	0.47
1:A:159:TRP:NE1	1:A:202:PHE:O	2.41	0.47
1:A:263:LEU:HD12	1:A:264:PRO:HD2	1.97	0.47
1:A:165:ALA:HB1	1:A:188:PRO:HG2	1.97	0.46
1:B:119:LYS:HD2	1:B:145:LEU:HD23	1.97	0.46
1:B:313:VAL:O	1:B:315:ARG:NH1	2.47	0.46
1:B:614:VAL:HA	1:B:772:LYS:HG3	1.96	0.46
1:B:729:ALA:O	1:B:733:PHE:CB	2.60	0.46
1:C:263:LEU:HD12	1:C:264:PRO:HD2	1.97	0.46
1:D:119:LYS:HD2	1:D:145:LEU:HD23	1.97	0.46
1:D:614:VAL:HA	1:D:772:LYS:HG3	1.96	0.46
1:C:307:MET:HG3	1:C:476:TYR:HA	1.97	0.46
1:D:313:VAL:O	1:D:315:ARG:NH1	2.47	0.46
1:A:606:SER:HA	1:A:836:LEU:HD21	1.97	0.46
1:B:280:ILE:O	1:B:284:LEU:N	2.49	0.46
1:A:244:LEU:HD13	1:A:249:ARG:HE	1.80	0.46
1:A:307:MET:HG3	1:A:476:TYR:HA	1.98	0.46
1:C:620:LEU:HD23	1:C:620:LEU:HA	1.65	0.46
1:D:222:ARG:N	1:D:229:GLU:O	2.49	0.46
1:A:90:ILE:HG23	1:A:91:LEU:HG	1.97	0.46
1:A:825:MET:HG2	1:A:826:PHE:CD1	2.51	0.46
1:B:222:ARG:N	1:B:229:GLU:O	2.49	0.46
1:B:244:LEU:HD13	1:B:249:ARG:HE	1.80	0.46
1:B:779:GLY:HA2	1:B:780:PHE:HA	1.61	0.46
1:B:917:VAL:O	1:B:921:LYS:HG2	2.15	0.46
1:C:90:ILE:HG23	1:C:91:LEU:HG	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:LEU:HD11	1:C:219:LEU:HD12	1.98	0.46
1:C:244:LEU:HD13	1:C:249:ARG:HE	1.80	0.46
1:C:280:ILE:O	1:C:284:LEU:N	2.49	0.46
1:D:310:GLN:OE1	1:D:315:ARG:NH1	2.37	0.46
1:D:327:ILE:HD11	1:D:338:ILE:HG21	1.97	0.46
1:A:211:LEU:HD11	1:A:219:LEU:HD12	1.98	0.46
1:A:280:ILE:O	1:A:284:LEU:N	2.49	0.46
1:A:620:LEU:O	1:A:622:GLY:N	2.49	0.46
1:A:647:ALA:HA	1:C:641:ARG:HH22	1.81	0.46
1:B:327:ILE:HD11	1:B:338:ILE:HG21	1.97	0.46
1:C:222:ARG:N	1:C:229:GLU:O	2.49	0.46
1:C:606:SER:HA	1:C:836:LEU:HD21	1.97	0.46
1:C:620:LEU:O	1:C:622:GLY:N	2.49	0.46
1:C:731:ASN:OD1	1:C:738:TRP:N	2.42	0.46
1:C:825:MET:HG2	1:C:826:PHE:CD1	2.51	0.46
1:D:244:LEU:HD13	1:D:249:ARG:HE	1.80	0.46
1:D:280:ILE:O	1:D:284:LEU:N	2.49	0.46
1:D:917:VAL:O	1:D:921:LYS:HG2	2.16	0.46
1:B:278:GLU:O	1:B:282:SER:OG	2.33	0.46
1:B:825:MET:HG2	1:B:826:PHE:CD1	2.51	0.46
1:D:826:PHE:O	1:D:828:ASN:N	2.45	0.46
1:B:696:LYS:NZ	1:B:700:ALA:HB3	2.30	0.46
1:C:873:ASP:HA	1:C:874:SER:HA	1.55	0.46
1:D:278:GLU:O	1:D:282:SER:OG	2.33	0.46
1:D:696:LYS:NZ	1:D:700:ALA:HB3	2.30	0.46
1:D:825:MET:HG2	1:D:826:PHE:CD1	2.51	0.46
1:A:222:ARG:N	1:A:229:GLU:O	2.49	0.46
1:B:826:PHE:O	1:B:828:ASN:N	2.45	0.46
1:C:865:THR:HA	1:C:868:GLN:HB2	1.98	0.46
1:A:278:GLU:O	1:A:282:SER:OG	2.33	0.45
1:A:696:LYS:NZ	1:A:700:ALA:HB3	2.30	0.45
1:A:917:VAL:O	1:A:921:LYS:HG2	2.16	0.45
1:B:842:HIS:CD2	1:B:864:LYS:HD2	2.51	0.45
1:C:278:GLU:O	1:C:282:SER:OG	2.33	0.45
1:C:696:LYS:NZ	1:C:700:ALA:HB3	2.30	0.45
1:C:760:TRP:HE1	1:C:764:TYR:HE2	1.65	0.45
1:D:842:HIS:CD2	1:D:864:LYS:HD2	2.51	0.45
1:A:760:TRP:HE1	1:A:764:TYR:HE2	1.65	0.45
1:A:842:HIS:CD2	1:A:864:LYS:HD2	2.51	0.45
1:A:873:ASP:HA	1:A:874:SER:HA	1.55	0.45
1:B:125:PRO:O	1:B:128:LEU:N	2.49	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:842:HIS:CD2	1:C:864:LYS:HD2	2.51	0.45
1:A:351:ASP:HB3	1:A:354:LEU:HD11	1.99	0.45
1:A:729:ALA:O	1:A:733:PHE:CB	2.59	0.45
1:B:620:LEU:O	1:B:622:GLY:N	2.49	0.45
1:B:878:PRO:HA	1:B:879:PRO:HD3	1.86	0.45
1:C:293:GLN:HB2	1:C:311:ASN:HA	1.97	0.45
1:D:125:PRO:O	1:D:128:LEU:N	2.49	0.45
1:D:211:LEU:HD11	1:D:219:LEU:HD12	1.98	0.45
1:D:779:GLY:HA2	1:D:780:PHE:HA	1.61	0.45
1:A:293:GLN:HB2	1:A:311:ASN:HA	1.97	0.45
1:A:865:THR:HA	1:A:868:GLN:HB2	1.98	0.45
1:B:640:LEU:O	1:B:649:GLU:N	2.44	0.45
1:B:760:TRP:HE1	1:B:764:TYR:HE2	1.65	0.45
1:C:917:VAL:O	1:C:921:LYS:HG2	2.16	0.45
1:A:731:ASN:OD1	1:A:738:TRP:N	2.42	0.45
1:B:90:ILE:HG23	1:B:91:LEU:HG	1.97	0.45
1:B:211:LEU:HD11	1:B:219:LEU:HD12	1.98	0.45
1:B:307:MET:HG3	1:B:476:TYR:HA	1.98	0.45
1:C:351:ASP:HB3	1:C:354:LEU:HD11	1.99	0.45
1:D:90:ILE:HG23	1:D:91:LEU:HG	1.97	0.45
1:D:620:LEU:O	1:D:622:GLY:N	2.49	0.45
1:D:760:TRP:HE1	1:D:764:TYR:HE2	1.65	0.45
1:D:307:MET:HG3	1:D:476:TYR:HA	1.98	0.45
1:D:736:LEU:HD13	1:D:738:TRP:CE2	2.52	0.45
1:D:824:SER:HA	1:D:825:MET:HG3	1.99	0.45
1:D:878:PRO:HA	1:D:879:PRO:HD3	1.86	0.45
1:A:327:ILE:HD11	1:A:338:ILE:HG21	1.97	0.45
1:A:929:ASN:HA	1:A:931:ARG:NE	2.32	0.45
1:C:929:ASN:HA	1:C:931:ARG:NE	2.32	0.45
1:D:606:SER:HA	1:D:836:LEU:HD21	1.97	0.45
1:D:640:LEU:O	1:D:649:GLU:N	2.44	0.45
1:A:764:TYR:CE2	1:A:785:LEU:HD21	2.52	0.45
1:B:606:SER:HA	1:B:836:LEU:HD21	1.97	0.45
1:B:736:LEU:HD13	1:B:738:TRP:CE2	2.52	0.45
1:B:824:SER:HA	1:B:825:MET:HG3	1.99	0.45
1:B:929:ASN:HA	1:B:931:ARG:NE	2.32	0.45
1:C:736:LEU:HD13	1:C:738:TRP:CE2	2.52	0.45
1:C:751:GLU:HA	1:C:754:LEU:HD12	1.99	0.45
1:D:929:ASN:HA	1:D:931:ARG:NE	2.32	0.45
1:A:736:LEU:HD13	1:A:738:TRP:CE2	2.52	0.45
1:A:751:GLU:HA	1:A:754:LEU:HD12	1.99	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:GLU:O	1:A:861:LEU:HG	2.17	0.45
1:B:865:THR:HA	1:B:868:GLN:HB2	1.98	0.45
1:C:309:VAL:HB	1:C:326:TRP:CD1	2.52	0.45
1:C:729:ALA:O	1:C:733:PHE:CB	2.60	0.45
1:C:764:TYR:CE2	1:C:785:LEU:HD21	2.52	0.45
1:A:125:PRO:O	1:A:128:LEU:N	2.49	0.45
1:A:309:VAL:HB	1:A:326:TRP:CD1	2.52	0.45
1:A:779:GLY:HA2	1:A:780:PHE:HA	1.61	0.45
1:B:94:VAL:HG22	1:B:104:HIS:HA	1.99	0.45
1:B:764:TYR:CE2	1:B:785:LEU:HD21	2.52	0.45
1:C:125:PRO:O	1:C:128:LEU:N	2.49	0.45
1:C:857:GLU:O	1:C:861:LEU:HG	2.17	0.45
1:C:327:ILE:HD11	1:C:338:ILE:HG21	1.97	0.44
1:D:94:VAL:HG22	1:D:104:HIS:HA	1.99	0.44
1:D:764:TYR:CE2	1:D:785:LEU:HD21	2.52	0.44
1:A:635:ASP:HB2	1:A:637:HIS:NE2	2.32	0.44
1:B:635:ASP:HB2	1:B:637:HIS:NE2	2.32	0.44
1:D:635:ASP:HB2	1:D:637:HIS:NE2	2.32	0.44
1:D:865:THR:HA	1:D:868:GLN:HB2	1.98	0.44
1:D:889:LYS:HA	1:D:889:LYS:HD2	1.69	0.44
1:B:309:VAL:HB	1:B:326:TRP:CD1	2.52	0.44
1:C:635:ASP:HB2	1:C:637:HIS:NE2	2.32	0.44
1:C:762:ASP:O	1:C:765:GLY:N	2.50	0.44
1:D:309:VAL:HB	1:D:326:TRP:CD1	2.52	0.44
1:A:762:ASP:O	1:A:765:GLY:N	2.50	0.44
1:A:948:ARG:HA	1:A:949:SER:HA	1.72	0.44
1:B:571:ARG:NE	1:B:677:ALA:O	2.50	0.44
1:B:751:GLU:HA	1:B:754:LEU:HD12	1.99	0.44
1:B:762:ASP:O	1:B:765:GLY:N	2.50	0.44
1:B:889:LYS:HA	1:B:889:LYS:HD2	1.70	0.44
1:C:527:LEU:O	1:C:531:ARG:N	2.33	0.44
1:D:351:ASP:HB3	1:D:354:LEU:HD11	1.99	0.44
1:A:730:ILE:O	1:A:733:PHE:N	2.46	0.44
1:B:351:ASP:HB3	1:B:354:LEU:HD11	1.99	0.44
1:C:730:ILE:O	1:C:733:PHE:N	2.46	0.44
1:D:762:ASP:O	1:D:765:GLY:N	2.50	0.44
1:B:160:VAL:HG21	1:B:164:LEU:HD12	1.99	0.44
1:C:948:ARG:HA	1:C:949:SER:HA	1.72	0.44
1:D:160:VAL:HG21	1:D:164:LEU:HD12	1.99	0.44
1:D:509:GLU:HA	1:D:510:ASP:HA	1.59	0.44
1:A:830:SER:OG	1:A:831:LEU:N	2.51	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:HIS:CD2	1:B:229:GLU:HB2	2.50	0.44
1:D:751:GLU:HA	1:D:754:LEU:HD12	1.99	0.44
1:D:857:GLU:O	1:D:861:LEU:HG	2.17	0.44
1:A:807:TYR:OH	1:A:926:ASN:O	2.27	0.44
1:B:857:GLU:O	1:B:861:LEU:HG	2.17	0.44
1:B:580:TYR:OH	1:D:929:ASN:O	2.36	0.44
1:B:830:SER:OG	1:B:831:LEU:N	2.50	0.44
1:B:929:ASN:O	1:D:580:TYR:OH	2.36	0.44
1:C:640:LEU:O	1:C:649:GLU:N	2.44	0.44
1:C:928:PRO:HB2	1:C:930:PRO:HD2	2.00	0.44
1:D:687:SER:O	1:D:690:SER:OG	2.24	0.44
1:A:928:PRO:HB2	1:A:930:PRO:HD2	2.00	0.43
1:D:224:HIS:CD2	1:D:229:GLU:HB2	2.50	0.43
1:D:767:VAL:HG23	1:D:768:LEU:HD13	2.00	0.43
1:A:772:LYS:NZ	1:A:785:LEU:HB2	2.33	0.43
1:A:824:SER:HA	1:A:825:MET:HG3	1.99	0.43
1:B:767:VAL:HG23	1:B:768:LEU:HD13	2.00	0.43
1:B:928:PRO:HB2	1:B:930:PRO:HD2	2.00	0.43
1:C:824:SER:HA	1:C:825:MET:HG3	1.99	0.43
1:D:163:SER:O	1:D:166:THR:OG1	2.29	0.43
1:D:830:SER:OG	1:D:831:LEU:N	2.51	0.43
1:B:509:GLU:HA	1:B:510:ASP:HA	1.59	0.43
1:C:772:LYS:NZ	1:C:785:LEU:HB2	2.33	0.43
1:A:160:VAL:HG21	1:A:164:LEU:HD12	1.99	0.43
1:B:772:LYS:NZ	1:B:785:LEU:HB2	2.33	0.43
1:D:928:PRO:HB2	1:D:930:PRO:HD2	2.00	0.43
1:A:94:VAL:HG22	1:A:104:HIS:HA	1.99	0.43
1:C:94:VAL:HG22	1:C:104:HIS:HA	1.99	0.43
1:D:772:LYS:NZ	1:D:785:LEU:HB2	2.33	0.43
1:A:138:TYR:CE1	1:A:271:TYR:HB2	2.53	0.43
1:C:160:VAL:HG21	1:C:164:LEU:HD12	1.99	0.43
1:C:658:GLN:HG3	1:C:671:LYS:HD2	2.01	0.43
1:C:779:GLY:HA2	1:C:780:PHE:HA	1.61	0.43
1:A:658:GLN:HG3	1:A:671:LYS:HD2	2.01	0.43
1:A:743:ILE:O	1:A:747:THR:OG1	2.24	0.43
1:B:569:SER:HA	1:B:570:ASN:HA	1.57	0.43
1:B:658:GLN:HG3	1:B:671:LYS:HD2	2.01	0.43
1:C:138:TYR:CE1	1:C:271:TYR:HB2	2.53	0.43
1:C:296:ILE:HB	1:C:310:GLN:HE22	1.84	0.43
1:C:625:PRO:HB2	1:C:626:LEU:H	1.68	0.43
1:D:658:GLN:HG3	1:D:671:LYS:HD2	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:LEU:O	1:A:649:GLU:N	2.44	0.43
1:A:948:ARG:NH1	1:A:949:SER:O	2.50	0.43
1:B:579:VAL:HG23	1:B:580:TYR:HA	2.00	0.43
1:B:613:VAL:HG11	1:B:761:GLN:HB2	2.01	0.43
1:B:630:VAL:HB	1:B:704:VAL:HG13	2.01	0.43
1:B:762:ASP:OD1	1:B:763:GLN:N	2.52	0.43
1:B:948:ARG:NH1	1:B:949:SER:O	2.50	0.43
1:C:743:ILE:O	1:C:747:THR:OG1	2.24	0.43
1:C:767:VAL:HG23	1:C:768:LEU:HD13	2.00	0.43
1:C:948:ARG:NH1	1:C:949:SER:O	2.50	0.43
1:D:569:SER:HA	1:D:570:ASN:HA	1.57	0.43
1:D:812:ARG:HG2	1:D:903:GLY:HA3	2.01	0.43
1:A:571:ARG:NE	1:A:677:ALA:O	2.50	0.43
1:A:656:GLU:H	1:A:657:LEU:HA	1.84	0.43
1:A:767:VAL:HG23	1:A:768:LEU:HD13	2.00	0.43
1:B:138:TYR:CE1	1:B:271:TYR:HB2	2.53	0.43
1:B:812:ARG:HG2	1:B:903:GLY:HA3	2.01	0.43
1:B:812:ARG:HA	1:B:903:GLY:HA3	2.01	0.43
1:C:571:ARG:NE	1:C:677:ALA:O	2.50	0.43
1:D:579:VAL:HG23	1:D:580:TYR:HA	2.00	0.43
1:D:620:LEU:HA	1:D:620:LEU:HD23	1.64	0.43
1:D:762:ASP:OD1	1:D:763:GLN:N	2.52	0.43
1:A:296:ILE:HB	1:A:310:GLN:HE22	1.84	0.43
1:A:812:ARG:HA	1:A:903:GLY:HA3	2.01	0.43
1:B:685:ALA:HA	1:B:688:TYR:CE1	2.54	0.43
1:C:656:GLU:H	1:C:657:LEU:HA	1.84	0.43
1:C:812:ARG:HA	1:C:903:GLY:HA3	2.01	0.43
1:C:842:HIS:O	1:C:845:ASP:HB3	2.19	0.43
1:D:613:VAL:HG11	1:D:761:GLN:HB2	2.01	0.43
1:D:630:VAL:HB	1:D:704:VAL:HG13	2.01	0.43
1:D:771:VAL:HG21	1:D:788:TRP:HA	2.01	0.43
1:D:812:ARG:HA	1:D:903:GLY:HA3	2.01	0.43
1:D:948:ARG:NH1	1:D:949:SER:O	2.50	0.43
1:A:572:LYS:H	1:A:572:LYS:HG3	1.60	0.42
1:A:882:GLU:O	1:A:886:ASP:HB2	2.19	0.42
1:B:175:ARG:HA	1:B:176:LYS:HA	1.79	0.42
1:B:771:VAL:HG21	1:B:788:TRP:HA	2.01	0.42
1:D:138:TYR:CE1	1:D:271:TYR:HB2	2.53	0.42
1:D:685:ALA:HA	1:D:688:TYR:CE1	2.54	0.42
1:A:812:ARG:HG2	1:A:903:GLY:HA3	2.01	0.42
1:A:842:HIS:O	1:A:845:ASP:HB3	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:882:GLU:O	1:C:886:ASP:HB2	2.19	0.42
1:A:889:LYS:HD2	1:A:889:LYS:HA	1.69	0.42
1:B:296:ILE:HB	1:B:310:GLN:HE22	1.84	0.42
1:C:569:SER:HA	1:C:570:ASN:HA	1.57	0.42
1:C:812:ARG:HG2	1:C:903:GLY:HA3	2.01	0.42
1:A:569:SER:HA	1:A:570:ASN:HA	1.57	0.42
1:A:685:ALA:HA	1:A:688:TYR:CE1	2.54	0.42
1:B:576:LYS:HE2	1:B:576:LYS:HB2	1.87	0.42
1:B:709:ALA:HB3	1:B:710:ILE:HD12	2.02	0.42
1:B:731:ASN:OD1	1:B:738:TRP:N	2.42	0.42
1:C:509:GLU:HA	1:C:510:ASP:HA	1.59	0.42
1:C:685:ALA:HA	1:C:688:TYR:CE1	2.55	0.42
1:D:296:ILE:HB	1:D:310:GLN:HE22	1.84	0.42
1:D:566:ASP:HA	1:D:567:GLY:HA3	1.88	0.42
1:B:842:HIS:O	1:B:845:ASP:HB3	2.19	0.42
1:B:882:GLU:O	1:B:886:ASP:HB2	2.19	0.42
1:D:175:ARG:HA	1:D:176:LYS:HA	1.79	0.42
1:D:709:ALA:HB3	1:D:710:ILE:HD12	2.02	0.42
1:D:842:HIS:O	1:D:845:ASP:HB3	2.19	0.42
1:D:887:LEU:HA	1:D:888:ILE:HA	1.73	0.42
1:B:654:PHE:H	1:B:688:TYR:HH	1.63	0.42
1:C:681:PRO:HA	1:C:682:ALA:HA	1.76	0.42
1:C:813:THR:N	1:C:814:ALA:HA	2.35	0.42
1:D:882:GLU:O	1:D:886:ASP:HB2	2.19	0.42
1:A:613:VAL:HG11	1:A:761:GLN:HB2	2.01	0.42
1:A:813:THR:N	1:A:814:ALA:HA	2.35	0.42
1:B:347:VAL:O	1:B:349:GLU:N	2.51	0.42
1:B:656:GLU:H	1:B:657:LEU:HA	1.84	0.42
1:C:210:LEU:HD23	1:C:210:LEU:HA	1.91	0.42
1:C:576:LYS:HE2	1:C:576:LYS:HB2	1.87	0.42
1:C:613:VAL:HG11	1:C:761:GLN:HB2	2.01	0.42
1:C:630:VAL:HB	1:C:704:VAL:HG13	2.01	0.42
1:D:656:GLU:H	1:D:657:LEU:HA	1.84	0.42
1:D:880:ALA:O	1:D:884:ILE:HG12	2.20	0.42
1:D:948:ARG:HD2	1:D:948:ARG:HA	1.80	0.42
1:A:579:VAL:HG23	1:A:580:TYR:HA	2.01	0.42
1:A:739:ASP:O	1:A:743:ILE:N	2.31	0.42
1:A:895:TYR:HB2	1:A:906:LEU:HD23	2.01	0.42
1:B:667:PHE:O	1:B:671:LYS:HG2	2.20	0.42
1:B:880:ALA:O	1:B:884:ILE:HG12	2.19	0.42
1:C:597:GLY:HA3	1:C:613:VAL:HA	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:VAL:O	1:D:349:GLU:N	2.51	0.42
1:D:576:LYS:HE2	1:D:576:LYS:HB2	1.87	0.42
1:D:895:TYR:HB2	1:D:906:LEU:HD23	2.01	0.42
1:A:630:VAL:HB	1:A:704:VAL:HG13	2.01	0.42
1:A:880:ALA:O	1:A:884:ILE:HG12	2.19	0.42
1:B:576:LYS:HE3	1:B:676:LEU:HD13	2.02	0.42
1:B:895:TYR:HB2	1:B:906:LEU:HD23	2.01	0.42
1:C:338:ILE:HD13	1:C:362:VAL:HB	2.02	0.42
1:C:572:LYS:H	1:C:572:LYS:HG3	1.60	0.42
1:C:579:VAL:HG23	1:C:580:TYR:HA	2.00	0.42
1:C:601:ASP:OD2	1:C:760:TRP:N	2.46	0.42
1:C:667:PHE:O	1:C:671:LYS:HG2	2.20	0.42
1:C:880:ALA:O	1:C:884:ILE:HG12	2.19	0.42
1:C:895:TYR:HB2	1:C:906:LEU:HD23	2.01	0.42
1:D:667:PHE:O	1:D:671:LYS:HG2	2.20	0.42
1:D:731:ASN:OD1	1:D:738:TRP:N	2.42	0.42
1:A:597:GLY:HA3	1:A:613:VAL:HA	2.02	0.42
1:A:667:PHE:O	1:A:671:LYS:HG2	2.20	0.42
1:B:813:THR:N	1:B:814:ALA:HA	2.35	0.42
1:C:762:ASP:OD1	1:C:763:GLN:N	2.52	0.42
1:D:576:LYS:HE3	1:D:676:LEU:HD13	2.02	0.42
1:D:813:THR:N	1:D:814:ALA:HA	2.35	0.42
1:A:90:ILE:HA	1:A:105:LEU:O	2.20	0.41
1:A:338:ILE:HD13	1:A:362:VAL:HB	2.02	0.41
1:A:601:ASP:OD2	1:A:760:TRP:N	2.46	0.41
1:A:771:VAL:HG21	1:A:788:TRP:HA	2.01	0.41
1:B:566:ASP:HA	1:B:567:GLY:HA3	1.88	0.41
1:B:656:GLU:OE1	1:B:658:GLN:N	2.42	0.41
1:B:772:LYS:HZ3	1:B:775:GLN:HG3	1.85	0.41
1:C:566:ASP:HA	1:C:567:GLY:HA3	1.88	0.41
1:C:771:VAL:HG21	1:C:788:TRP:HA	2.01	0.41
1:D:625:PRO:HG2	1:D:626:LEU:HD12	2.02	0.41
1:D:804:LEU:HG	1:D:804:LEU:H	1.30	0.41
1:D:948:ARG:HA	1:D:949:SER:HA	1.73	0.41
1:A:198:LYS:H	1:A:201:LEU:HD12	1.85	0.41
1:A:762:ASP:OD1	1:A:763:GLN:N	2.52	0.41
1:B:90:ILE:HA	1:B:105:LEU:O	2.20	0.41
1:B:625:PRO:HG2	1:B:626:LEU:HD12	2.02	0.41
1:C:90:ILE:HA	1:C:105:LEU:O	2.20	0.41
1:D:354:LEU:HB3	1:D:356:VAL:HG23	2.01	0.41
1:D:754:LEU:HA	1:D:754:LEU:HD23	1.82	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:GLU:HA	1:A:510:ASP:HA	1.59	0.41
1:A:576:LYS:HE3	1:A:676:LEU:HD13	2.01	0.41
1:B:354:LEU:HB3	1:B:356:VAL:HG23	2.02	0.41
1:B:597:GLY:HA3	1:B:613:VAL:HA	2.02	0.41
1:B:948:ARG:HD2	1:B:948:ARG:HA	1.80	0.41
1:C:576:LYS:HE3	1:C:676:LEU:HD13	2.02	0.41
1:D:90:ILE:HA	1:D:105:LEU:O	2.20	0.41
1:A:354:LEU:HB3	1:A:356:VAL:HG23	2.02	0.41
1:A:639:VAL:HG22	1:A:650:ILE:HD12	2.03	0.41
1:A:677:ALA:H	1:A:678:GLY:HA2	1.86	0.41
1:A:893:LEU:HD11	1:A:909:VAL:HB	2.03	0.41
1:B:338:ILE:HD13	1:B:362:VAL:HB	2.02	0.41
1:B:804:LEU:HG	1:B:804:LEU:H	1.30	0.41
1:C:677:ALA:H	1:C:678:GLY:HA2	1.86	0.41
1:D:72:LEU:HD23	1:D:72:LEU:HA	1.92	0.41
1:D:597:GLY:HA3	1:D:613:VAL:HA	2.02	0.41
1:D:804:LEU:HB2	1:D:907:TYR:HB2	2.02	0.41
1:D:895:TYR:HB3	1:D:908:MET:HB3	2.02	0.41
1:B:72:LEU:HD23	1:B:72:LEU:HA	1.92	0.41
1:C:198:LYS:H	1:C:201:LEU:HD12	1.85	0.41
1:C:354:LEU:HB3	1:C:356:VAL:HG23	2.02	0.41
1:C:639:VAL:HG22	1:C:650:ILE:HD12	2.03	0.41
1:C:893:LEU:HD11	1:C:909:VAL:HB	2.03	0.41
1:D:338:ILE:HD13	1:D:362:VAL:HB	2.02	0.41
1:D:607:LEU:HD23	1:D:607:LEU:HA	1.87	0.41
1:D:656:GLU:OE1	1:D:658:GLN:N	2.42	0.41
1:A:576:LYS:HE2	1:A:576:LYS:HB2	1.87	0.41
1:A:804:LEU:HB2	1:A:907:TYR:HB2	2.02	0.41
1:B:639:VAL:HG22	1:B:650:ILE:HD12	2.03	0.41
1:B:677:ALA:H	1:B:678:GLY:HA2	1.86	0.41
1:B:754:LEU:HA	1:B:754:LEU:HD23	1.82	0.41
1:B:804:LEU:HB2	1:B:907:TYR:HB2	2.02	0.41
1:B:877:ASN:HA	1:B:878:PRO:HD3	1.90	0.41
1:B:895:TYR:HB3	1:B:908:MET:HB3	2.02	0.41
1:B:948:ARG:HA	1:B:949:SER:HA	1.72	0.41
1:C:224:HIS:CD2	1:C:229:GLU:HB2	2.50	0.41
1:D:104:HIS:O	1:D:108:ASN:N	2.34	0.41
1:D:639:VAL:HG22	1:D:650:ILE:HD12	2.03	0.41
1:D:654:PHE:H	1:D:688:TYR:HH	1.64	0.41
1:D:677:ALA:H	1:D:678:GLY:HA2	1.86	0.41
1:D:681:PRO:HA	1:D:682:ALA:HA	1.76	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:920:ARG:HA	1:A:923:LEU:HB3	2.03	0.41
1:D:198:LYS:H	1:D:201:LEU:HD12	1.84	0.41
1:A:81:LEU:HB3	1:A:84:TYR:CE2	2.56	0.41
1:A:360:VAL:HG12	1:A:361:CYS:H	1.86	0.41
1:A:681:PRO:HA	1:A:682:ALA:HA	1.76	0.41
1:B:81:LEU:HB3	1:B:84:TYR:CE2	2.56	0.41
1:B:198:LYS:H	1:B:201:LEU:HD12	1.84	0.41
1:B:920:ARG:HA	1:B:923:LEU:HB3	2.03	0.41
1:C:360:VAL:HG12	1:C:361:CYS:H	1.86	0.41
1:C:739:ASP:O	1:C:743:ILE:N	2.31	0.41
1:D:81:LEU:HB3	1:D:84:TYR:CE2	2.56	0.41
1:D:920:ARG:HA	1:D:923:LEU:HB3	2.03	0.41
1:A:92:THR:H	1:A:104:HIS:CD2	2.39	0.41
1:A:139:ILE:HG13	1:A:140:ARG:H	1.85	0.41
1:A:224:HIS:CD2	1:A:229:GLU:HB2	2.51	0.41
1:A:620:LEU:HD22	1:A:935:VAL:HG12	2.03	0.41
1:A:625:PRO:HG2	1:A:626:LEU:HD12	2.02	0.41
1:A:807:TYR:CD1	1:A:932:ALA:HA	2.56	0.41
1:A:893:LEU:O	1:A:918:ARG:NH2	2.54	0.41
1:B:95:PRO:HA	1:B:101:ARG:HA	2.03	0.41
1:B:607:LEU:HD23	1:B:607:LEU:HA	1.87	0.41
1:C:81:LEU:HB3	1:C:84:TYR:CE2	2.56	0.41
1:C:92:THR:H	1:C:104:HIS:CD2	2.39	0.41
1:C:620:LEU:HD22	1:C:935:VAL:HG12	2.03	0.41
1:C:804:LEU:HB2	1:C:907:TYR:HB2	2.02	0.41
1:C:807:TYR:CD1	1:C:932:ALA:HA	2.56	0.41
1:C:893:LEU:O	1:C:918:ARG:NH2	2.54	0.41
1:C:920:ARG:HA	1:C:923:LEU:HB3	2.03	0.41
1:D:807:TYR:OH	1:D:926:ASN:O	2.27	0.41
1:A:709:ALA:HB3	1:A:710:ILE:HD12	2.02	0.41
1:A:856:VAL:O	1:A:860:ARG:HG2	2.21	0.41
1:B:104:HIS:O	1:B:108:ASN:N	2.34	0.41
1:B:662:LYS:HG2	1:B:663:ILE:H	1.86	0.41
1:C:625:PRO:HG2	1:C:626:LEU:HD12	2.02	0.41
1:C:709:ALA:HB3	1:C:710:ILE:HD12	2.02	0.41
1:C:830:SER:OG	1:C:831:LEU:N	2.51	0.41
1:C:856:VAL:O	1:C:860:ARG:HG2	2.21	0.41
1:D:95:PRO:HA	1:D:101:ARG:HA	2.03	0.41
1:D:572:LYS:H	1:D:572:LYS:HG3	1.60	0.41
1:D:893:LEU:HD11	1:D:909:VAL:HB	2.03	0.41
1:A:112:LEU:HD11	1:A:139:ILE:HG21	2.02	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:LEU:O	1:A:834:ASN:HB3	2.21	0.40
1:B:681:PRO:HA	1:B:682:ALA:HA	1.76	0.40
1:C:803:HIS:HB3	1:C:804:LEU:H	1.56	0.40
1:D:662:LYS:HG2	1:D:663:ILE:H	1.86	0.40
1:D:877:ASN:HA	1:D:878:PRO:HD3	1.90	0.40
1:A:95:PRO:HA	1:A:101:ARG:HA	2.03	0.40
1:A:363:ASP:OD1	1:A:363:ASP:N	2.49	0.40
1:B:893:LEU:HD11	1:B:909:VAL:HB	2.03	0.40
1:B:893:LEU:O	1:B:918:ARG:NH2	2.54	0.40
1:C:95:PRO:HA	1:C:101:ARG:HA	2.03	0.40
1:C:123:LEU:HB3	1:C:128:LEU:HG	2.03	0.40
1:C:139:ILE:HG13	1:C:140:ARG:H	1.85	0.40
1:D:123:LEU:HB3	1:D:128:LEU:HG	2.03	0.40
1:D:807:TYR:CD1	1:D:932:ALA:HA	2.56	0.40
1:A:123:LEU:HB3	1:A:128:LEU:HG	2.03	0.40
1:A:895:TYR:HB3	1:A:908:MET:HB3	2.02	0.40
1:B:159:TRP:NE1	1:B:202:PHE:O	2.41	0.40
1:B:161:ASP:OD1	1:B:161:ASP:N	2.55	0.40
1:C:831:LEU:O	1:C:834:ASN:HB3	2.21	0.40
1:D:161:ASP:OD1	1:D:161:ASP:N	2.55	0.40
1:D:893:LEU:O	1:D:918:ARG:NH2	2.54	0.40
1:B:112:LEU:HD11	1:B:139:ILE:HG21	2.02	0.40
1:B:123:LEU:HB3	1:B:128:LEU:HG	2.03	0.40
1:C:112:LEU:HD11	1:C:139:ILE:HG21	2.02	0.40
1:C:138:TYR:HB3	1:C:273:TYR:CZ	2.57	0.40
1:C:572:LYS:HB2	1:C:573:SER:H	1.67	0.40
1:D:112:LEU:HD11	1:D:139:ILE:HG21	2.02	0.40
1:D:159:TRP:NE1	1:D:202:PHE:O	2.41	0.40
1:D:831:LEU:O	1:D:834:ASN:HB3	2.21	0.40
1:A:138:TYR:HB3	1:A:273:TYR:CZ	2.57	0.40
1:A:878:PRO:O	1:A:881:VAL:N	2.52	0.40
1:B:138:TYR:HB3	1:B:273:TYR:CZ	2.57	0.40
1:B:139:ILE:HG13	1:B:140:ARG:H	1.85	0.40
1:B:313:VAL:HG21	1:B:327:ILE:HG22	2.04	0.40
1:B:807:TYR:CD1	1:B:932:ALA:HA	2.56	0.40
1:B:831:LEU:O	1:B:834:ASN:HB3	2.21	0.40
1:D:139:ILE:HG13	1:D:140:ARG:H	1.85	0.40
1:D:244:LEU:HD21	1:D:252:ASP:HB3	2.03	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	807/949 (85%)	565 (70%)	221 (27%)	21 (3%)	5	35
1	B	807/949 (85%)	565 (70%)	221 (27%)	21 (3%)	5	35
1	C	807/949 (85%)	566 (70%)	220 (27%)	21 (3%)	5	35
1	D	807/949 (85%)	566 (70%)	220 (27%)	21 (3%)	5	35
All	All	3228/3796 (85%)	2262 (70%)	882 (27%)	84 (3%)	8	35

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	LEU
1	A	492	VAL
1	B	190	LEU
1	B	492	VAL
1	C	190	LEU
1	C	492	VAL
1	D	190	LEU
1	D	492	VAL
1	A	191	ALA
1	A	614	VAL
1	A	616	LEU
1	A	621	ASN
1	A	785	LEU
1	A	936	GLU
1	B	191	ALA
1	B	614	VAL
1	B	616	LEU
1	B	621	ASN
1	B	785	LEU
1	B	936	GLU
1	C	191	ALA
1	C	614	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	616	LEU
1	C	621	ASN
1	C	785	LEU
1	C	936	GLU
1	D	191	ALA
1	D	614	VAL
1	D	616	LEU
1	D	621	ASN
1	D	785	LEU
1	D	936	GLU
1	A	126	ASP
1	A	348	PRO
1	A	605	TYR
1	B	126	ASP
1	B	348	PRO
1	B	605	TYR
1	C	126	ASP
1	C	348	PRO
1	C	605	TYR
1	D	126	ASP
1	D	348	PRO
1	D	605	TYR
1	A	522	LEU
1	A	699	GLY
1	A	912	ASP
1	B	522	LEU
1	B	699	GLY
1	B	912	ASP
1	C	522	LEU
1	C	699	GLY
1	C	912	ASP
1	D	522	LEU
1	D	699	GLY
1	D	912	ASP
1	A	523	PRO
1	A	806	TYR
1	B	523	PRO
1	B	806	TYR
1	C	523	PRO
1	C	806	TYR
1	D	258	LEU
1	D	523	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	806	TYR
1	A	258	LEU
1	A	667	PHE
1	B	258	LEU
1	B	667	PHE
1	C	258	LEU
1	C	667	PHE
1	D	667	PHE
1	A	546	GLY
1	B	546	GLY
1	C	546	GLY
1	D	546	GLY
1	A	144	PRO
1	B	144	PRO
1	C	144	PRO
1	D	144	PRO
1	A	625	PRO
1	C	625	PRO
1	B	625	PRO
1	D	625	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	599/805 (74%)	581 (97%)	18 (3%)	41	63
1	B	599/805 (74%)	581 (97%)	18 (3%)	41	63
1	C	599/805 (74%)	581 (97%)	18 (3%)	41	63
1	D	599/805 (74%)	581 (97%)	18 (3%)	41	63
All	All	2396/3220 (74%)	2324 (97%)	72 (3%)	44	63

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	214	ARG
1	A	315	ARG
1	A	365	VAL
1	A	572	LYS
1	A	579	VAL
1	A	588	ARG
1	A	653	THR
1	A	656	GLU
1	A	674	LEU
1	A	725	THR
1	A	772	LYS
1	A	774	LEU
1	A	793	LEU
1	A	804	LEU
1	A	850	ILE
1	A	870	LYS
1	A	929	ASN
1	B	140	ARG
1	B	214	ARG
1	B	315	ARG
1	B	365	VAL
1	B	572	LYS
1	B	579	VAL
1	B	588	ARG
1	B	653	THR
1	B	656	GLU
1	B	674	LEU
1	B	725	THR
1	B	772	LYS
1	B	774	LEU
1	B	793	LEU
1	B	804	LEU
1	B	850	ILE
1	B	870	LYS
1	B	929	ASN
1	C	140	ARG
1	C	214	ARG
1	C	315	ARG
1	C	365	VAL
1	C	572	LYS
1	C	579	VAL
1	C	588	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	653	THR
1	C	656	GLU
1	C	674	LEU
1	C	725	THR
1	C	772	LYS
1	C	774	LEU
1	C	793	LEU
1	C	804	LEU
1	C	850	ILE
1	C	870	LYS
1	C	929	ASN
1	D	140	ARG
1	D	214	ARG
1	D	315	ARG
1	D	365	VAL
1	D	572	LYS
1	D	579	VAL
1	D	588	ARG
1	D	653	THR
1	D	656	GLU
1	D	674	LEU
1	D	725	THR
1	D	772	LYS
1	D	774	LEU
1	D	793	LEU
1	D	804	LEU
1	D	850	ILE
1	D	870	LYS
1	D	929	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	104	HIS
1	A	108	ASN
1	A	146	GLN
1	A	167	HIS
1	A	224	HIS
1	A	570	ASN
1	A	745	GLN
1	A	763	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	782	GLN
1	A	803	HIS
1	A	832	HIS
1	A	877	ASN
1	B	103	GLN
1	B	104	HIS
1	B	108	ASN
1	B	146	GLN
1	B	167	HIS
1	B	224	HIS
1	B	570	ASN
1	B	745	GLN
1	B	763	GLN
1	B	782	GLN
1	B	803	HIS
1	B	832	HIS
1	B	877	ASN
1	C	103	GLN
1	C	104	HIS
1	C	108	ASN
1	C	146	GLN
1	C	167	HIS
1	C	224	HIS
1	C	570	ASN
1	C	745	GLN
1	C	763	GLN
1	C	782	GLN
1	C	803	HIS
1	C	832	HIS
1	C	877	ASN
1	D	103	GLN
1	D	104	HIS
1	D	108	ASN
1	D	146	GLN
1	D	167	HIS
1	D	224	HIS
1	D	570	ASN
1	D	745	GLN
1	D	763	GLN
1	D	782	GLN
1	D	803	HIS
1	D	832	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	877	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 monosaccharides 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.

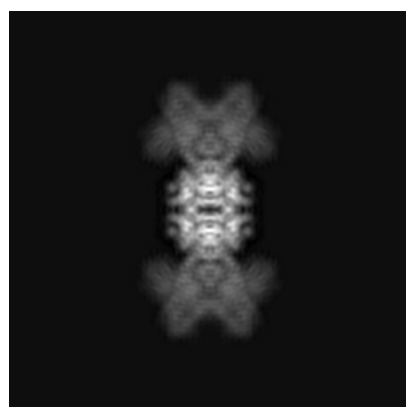
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6859. These allow visual inspection of the internal detail of the map and identification of artifacts.

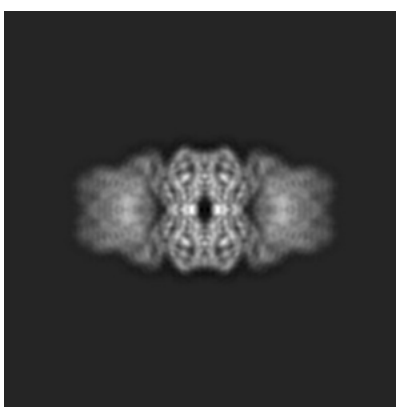
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

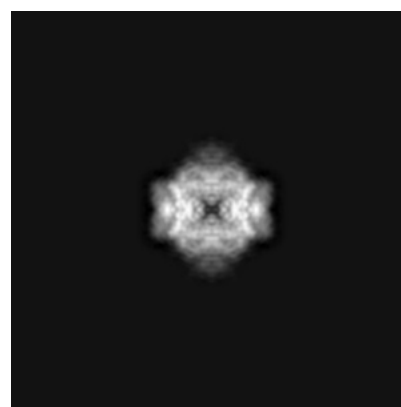
#### 6.1.1 Primary map



X



Y

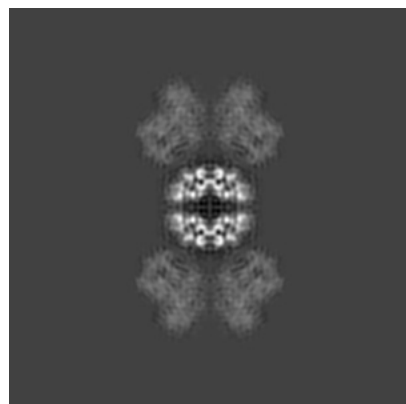


Z

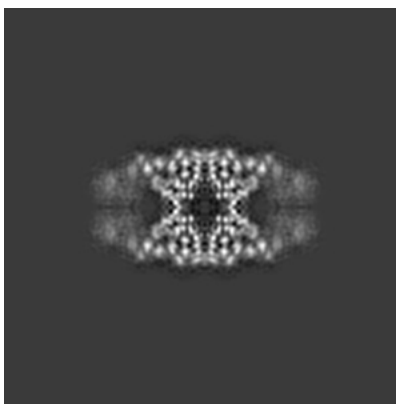
The images above show the map projected in three orthogonal directions.

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

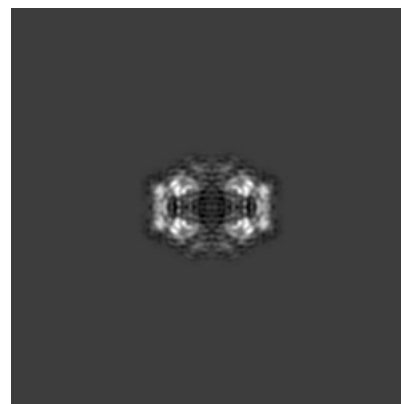
#### 6.2.1 Primary map



X Index: 120



Y Index: 120

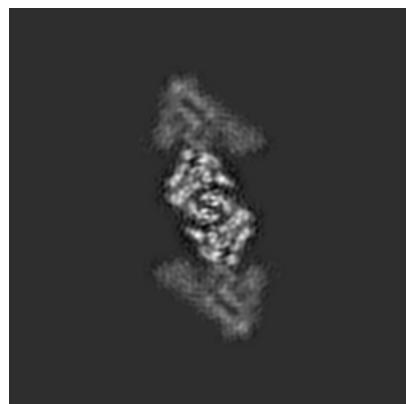


Z Index: 120

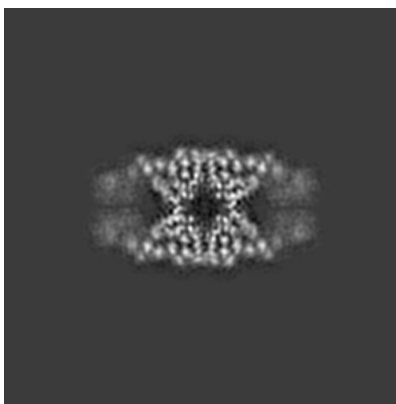
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 104



Y Index: 121



Z Index: 125

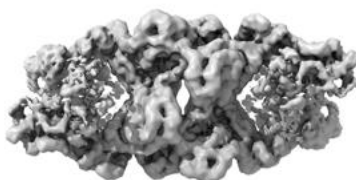
The images above show the largest variance slices of the map in three orthogonal directions.

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

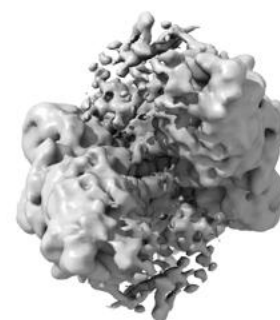
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



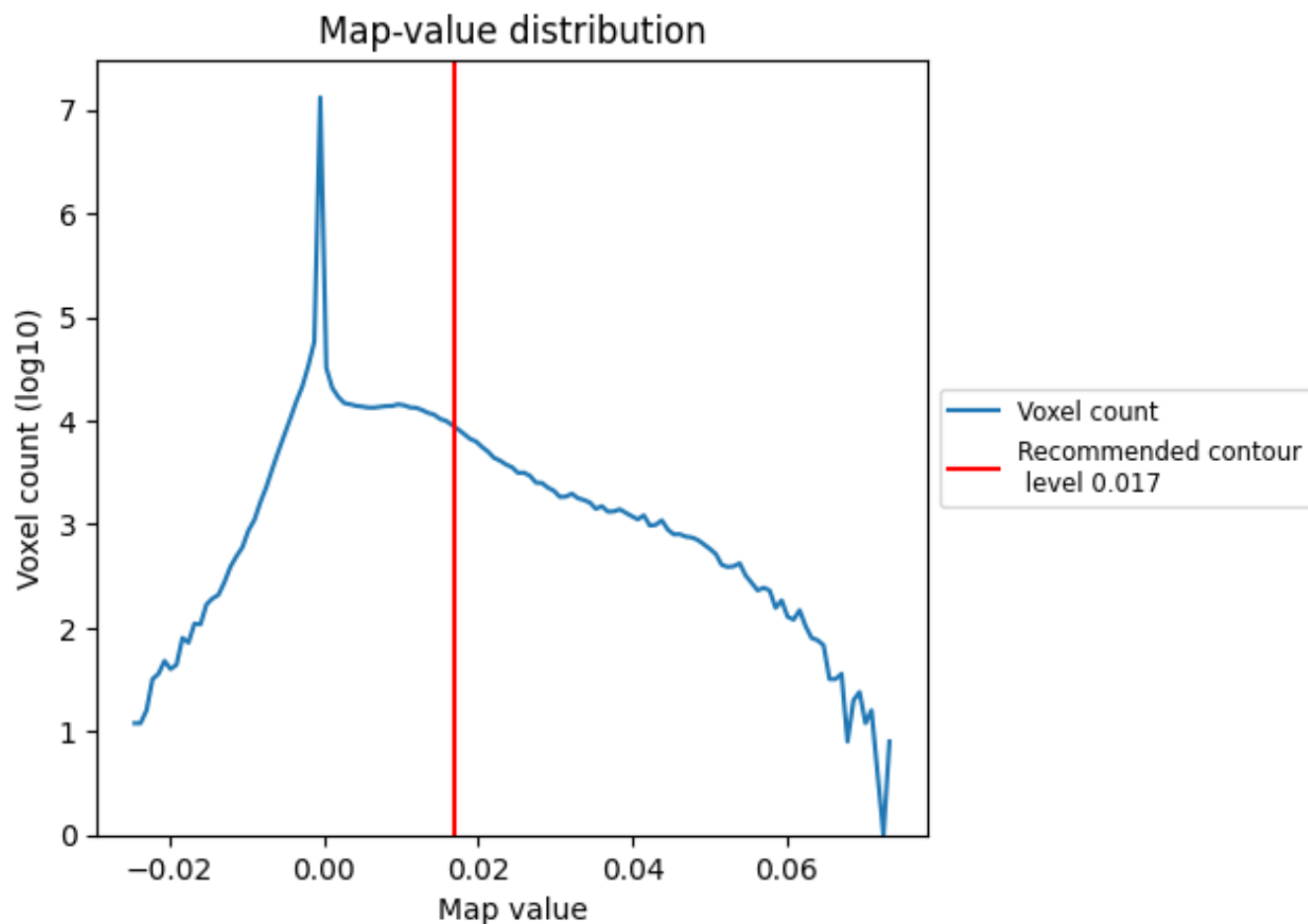
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

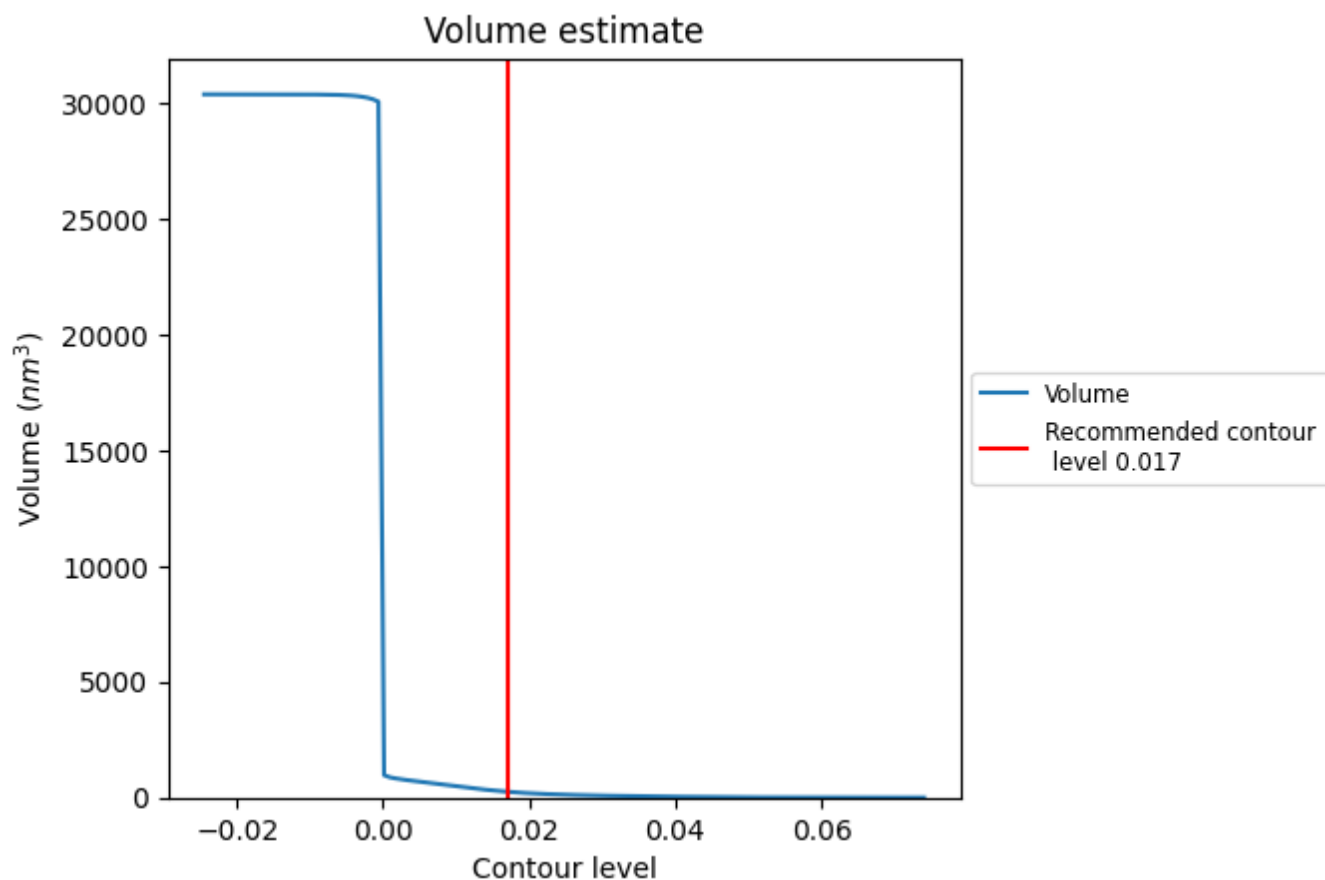
This section contains the results of statistical analysis of the map.

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



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

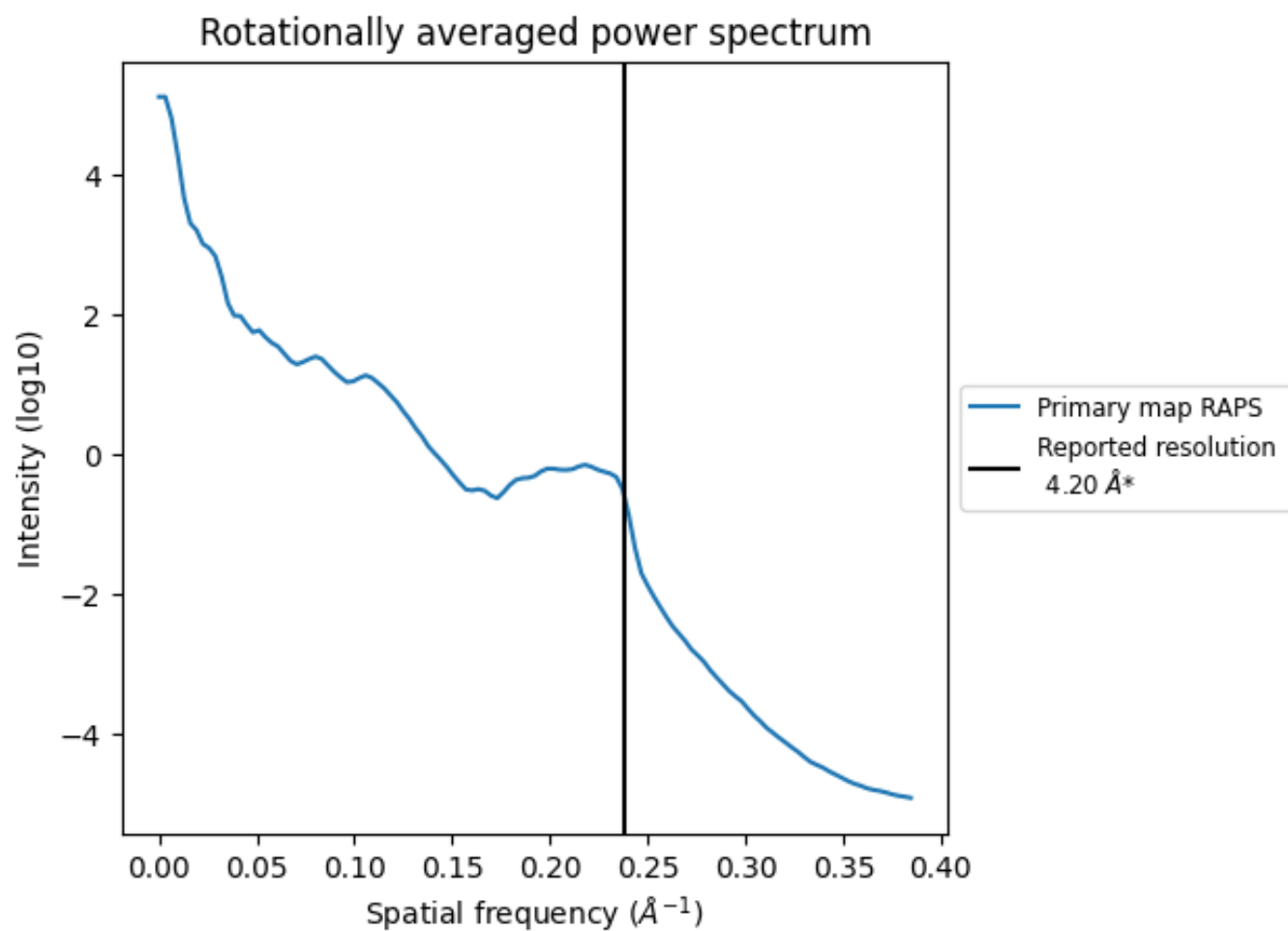
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm<sup>3</sup>; this corresponds to an approximate mass of 228 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

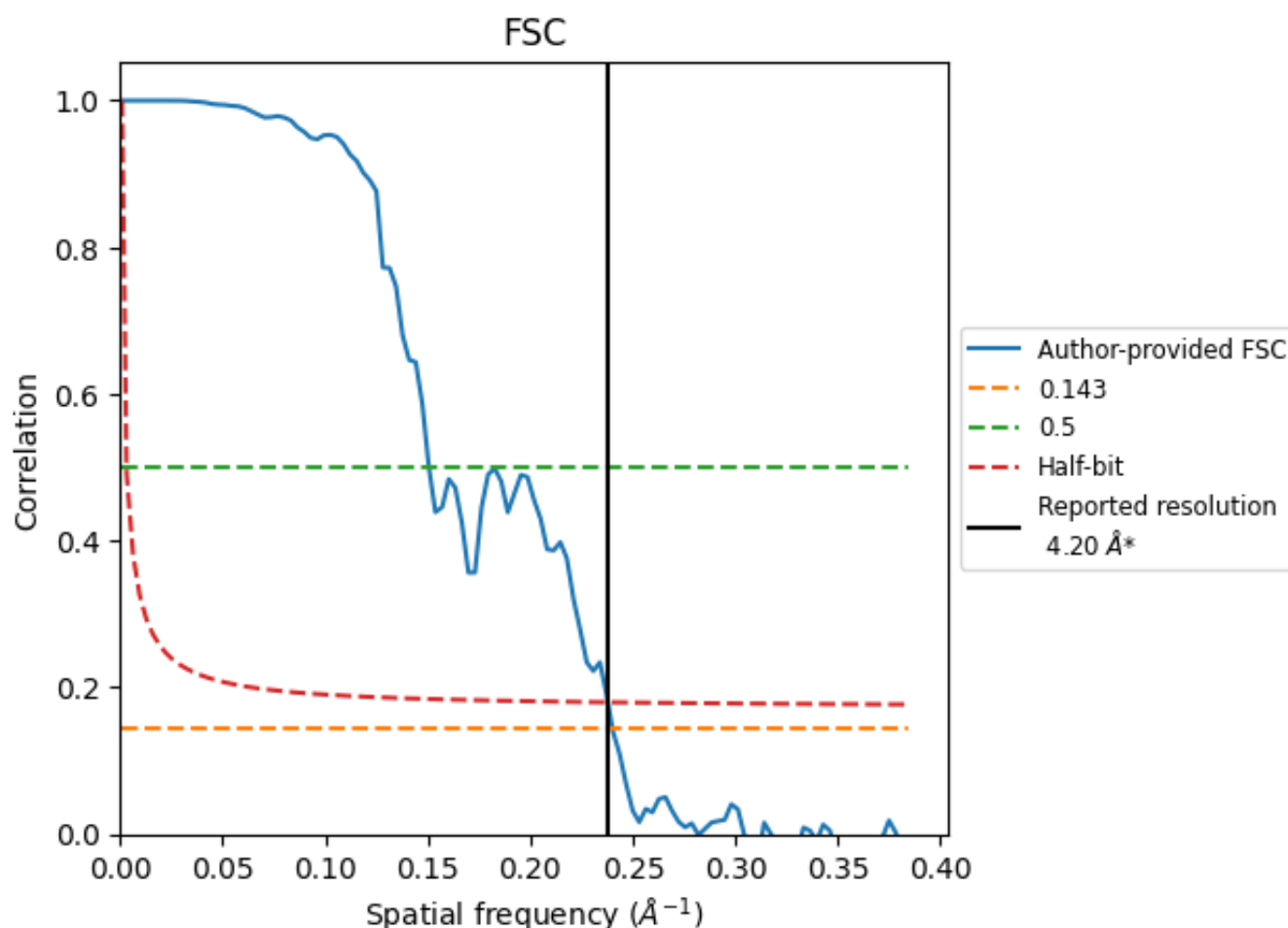


\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.238 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

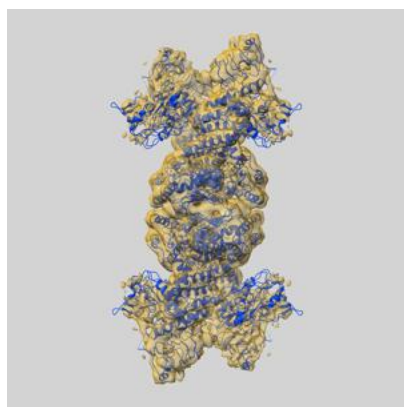
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.16	6.64	4.20
Unmasked-calculated*	-	-	-

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

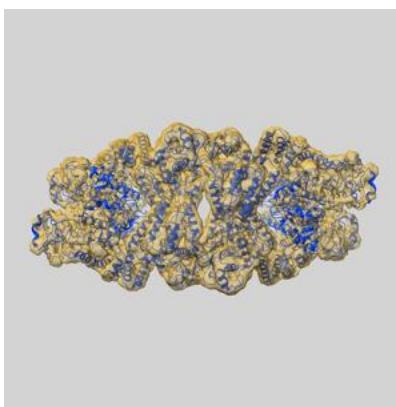
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6859 and PDB model 5YYS. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

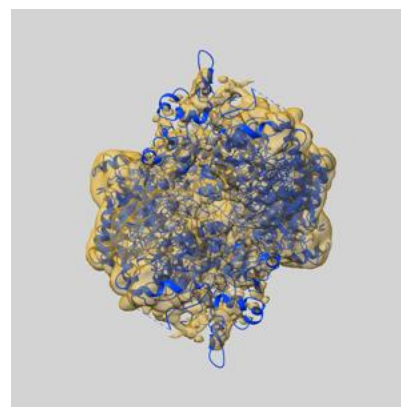
### 9.1 Map-model overlay [i](#)



X



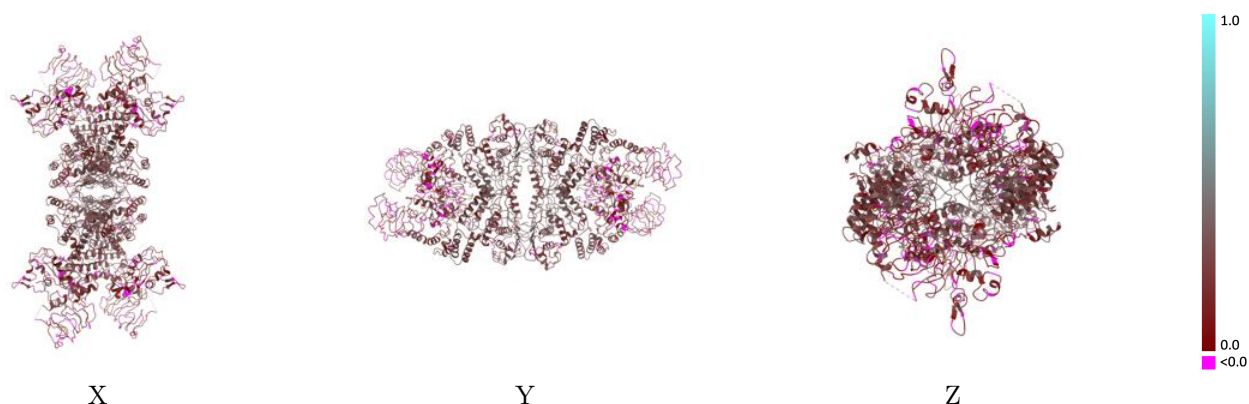
Y



Z

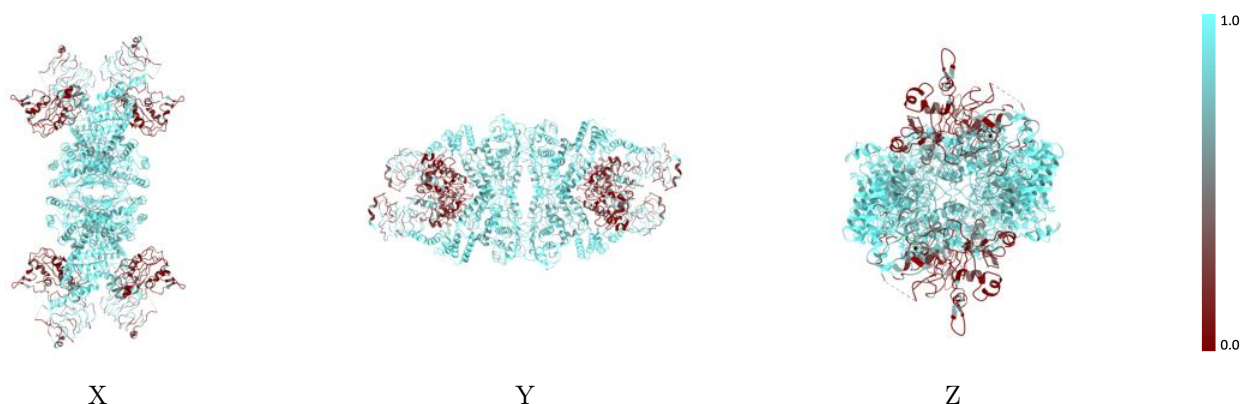
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

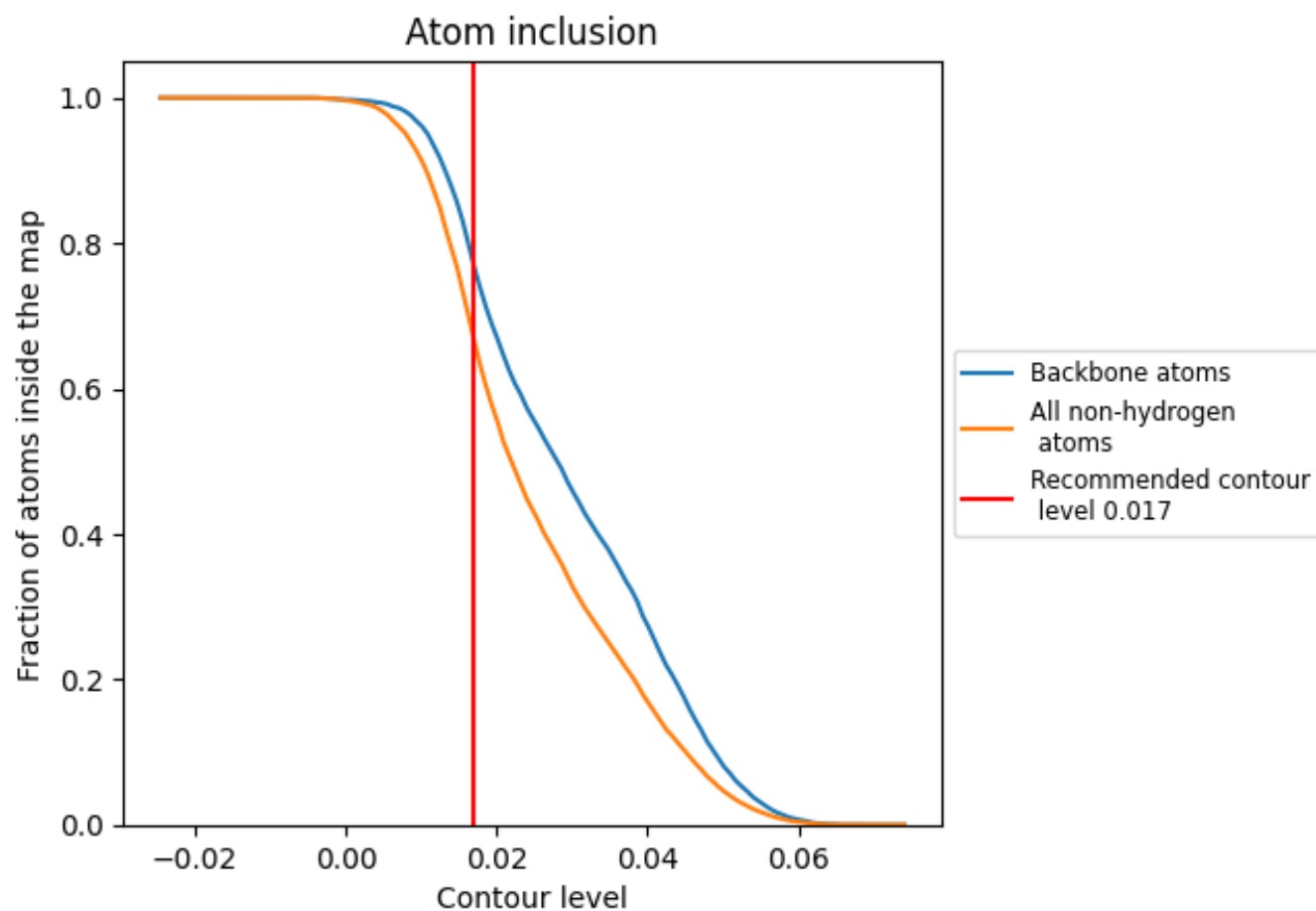
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.017).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 67% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6682	<div></div> 0.2240
A	<div></div> 0.6677	<div></div> 0.2240
B	<div></div> 0.6686	<div></div> 0.2230
C	<div></div> 0.6681	<div></div> 0.2240
D	<div></div> 0.6684	<div></div> 0.2240

